Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 02:25 PM EDT

PDB ID	:	6I0D
Title	:	Respiratory complex I from Thermus thermophilus with bound Decyl-Ubiquinone
Authors	:	Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on	:	2018-10-25
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

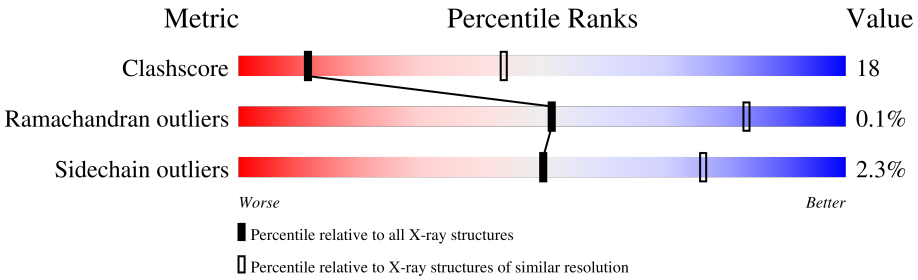
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	61% 39%
1	B	438	53% 47%
2	2	181	67% 30%
2	C	181	58% 39%
3	3	783	62% 34%
3	D	783	62% 34%
4	4	409	48% 44% 6%
4	E	409	54% 40% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	5	207	63% 30% • 5%
5	F	207	61% 33% • 5%
6	6	181	51% 38% • 8%
6	G	181	43% 46% • 8%
7	9	182	58% 39% ••
7	O	182	64% 35% ••
8	7	129	64% 34% ••
8	I	129	68% 30% •
9	W	131	78% 18% ••
9	X	131	72% 24% ••
10	A	119	55% 41% ••
10	P	119	59% 37% ••
11	J	176	60% 30% • 9%
11	R	176	60% 30% • 9%
12	K	95	72% 27% •
12	S	95	77% 22% •
13	L	606	66% 34%
13	T	606	62% 37% •
14	M	469	60% 38% •
14	U	469	63% 36% •
15	N	427	62% 37%
15	V	427	63% 37%
16	H	365	52% 39% 5% •
16	Q	365	51% 43% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	3	803	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	B	501	-	-	X	-
17	SF4	D	803	-	-	X	-
17	SF4	O	201	-	-	X	-
18	FMN	1	502	-	-	X	-
18	FMN	B	502	-	-	X	-
19	FES	D	804	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 74132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	B	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	C	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	756	Total	C	N	O	S	0	0	0
			5895	3754	1057	1053	31			
3	D	756	Total	C	N	O	S	0	0	0
			5895	3754	1057	1053	31			

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	384	Total	C	N	O	S	0	0	0
			3067	1975	522	559	11			
4	E	384	Total	C	N	O	S	0	0	0
			3067	1975	522	559	11			

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	F	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	166	Total	C	N	O	S	0	0	0
			1289	815	235	226	13			
6	G	166	Total	C	N	O	S	0	0	0
			1289	815	235	226	13			

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	180	Total	C	N	O	S	0	0	0
			1388	890	232	255	11			
7	O	180	Total	C	N	O	S	0	0	0
			1388	890	232	255	11			

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	I	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	W	127	Total	C	N	O	S	0	0	0
			967	623	165	175	4			
9	X	127	Total	C	N	O	S	0	0	0
			967	623	165	175	4			

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A	117	Total	C	N	O	S	0	0	0
			910	624	138	144	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	P	117	Total	C	N	O	S	0	0	0
			910	624	138	144	4			

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	160	Total	C	N	O	S	0	0	0
			1183	806	183	191	3			
11	R	160	Total	C	N	O	S	0	0	0
			1183	806	183	191	3			

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	95	Total	C	N	O	S	0	0	0
			703	456	118	126	3			
12	S	95	Total	C	N	O	S	0	0	0
			703	456	118	126	3			

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	605	Total	C	N	O	S	0	0	0
			4604	3089	740	756	19			
13	T	605	Total	C	N	O	S	0	0	0
			4604	3089	740	756	19			

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	467	Total	C	N	O	S	0	0	0
			3489	2363	546	572	8			
14	U	467	Total	C	N	O	S	0	0	0
			3489	2363	546	572	8			

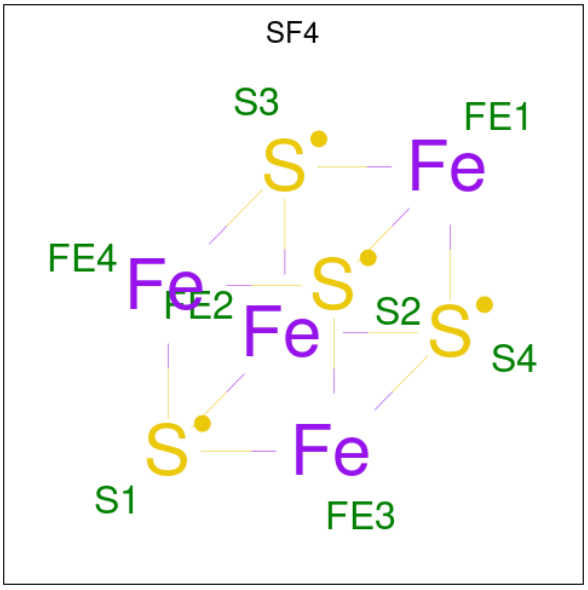
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	427	Total	C	N	O	S	0	0	0
			3154	2125	505	518	6			
15	V	427	Total	C	N	O	S	0	0	0
			3154	2125	505	518	6			

- Molecule 16 is a protein called NADH-quinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	H	353	Total	C	N	O	S	0	0	0
			2838	1943	431	457	7			
16	Q	353	Total	C	N	O	S	0	0	0
			2838	1943	431	457	7			

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



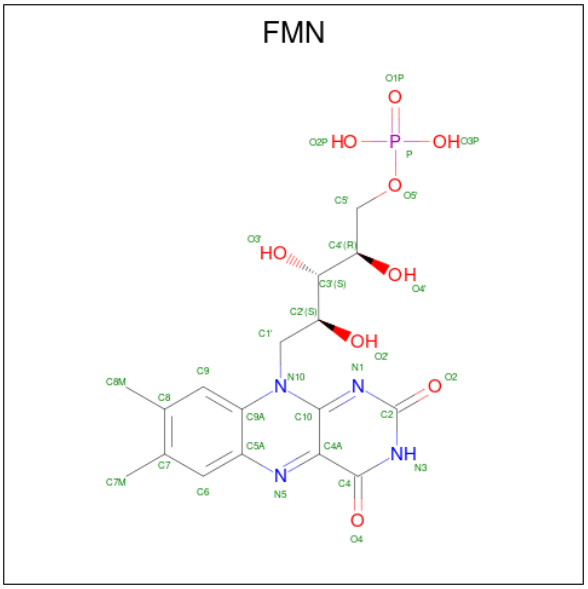
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	1	1	Total	Fe	S		0	0
			8	4	4			
17	3	1	Total	Fe	S		0	0
			8	4	4			
17	3	1	Total	Fe	S		0	0
			8	4	4			
17	3	1	Total	Fe	S		0	0
			8	4	4			
17	6	1	Total	Fe	S		0	0
			8	4	4			
17	9	1	Total	Fe	S		0	0
			8	4	4			
17	9	1	Total	Fe	S		0	0
			8	4	4			
17	B	1	Total	Fe	S		0	0
			8	4	4			
17	D	1	Total	Fe	S		0	0
			8	4	4			

Continued on next page...

Continued from previous page...

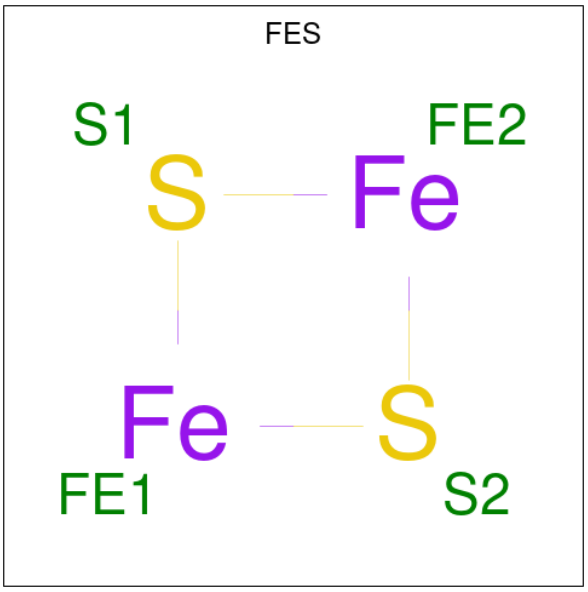
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total Fe S 8 4 4	0	0
17	D	1	Total Fe S 8 4 4	0	0
17	G	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0

- Molecule 18 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



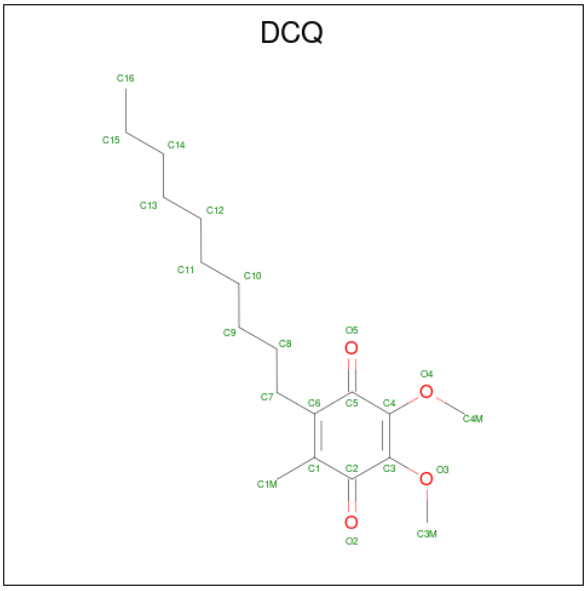
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	1	1	Total C N O P 31 17 4 9 1	0	0
18	B	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	2	1	Total Fe S 4 2 2	0	0
19	3	1	Total Fe S 4 2 2	0	0
19	C	1	Total Fe S 4 2 2	0	0
19	D	1	Total Fe S 4 2 2	0	0

- Molecule 20 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	4	1	Total	C	O	0	0
			23	19	4		
20	E	1	Total	C	O	0	0
			23	19	4		

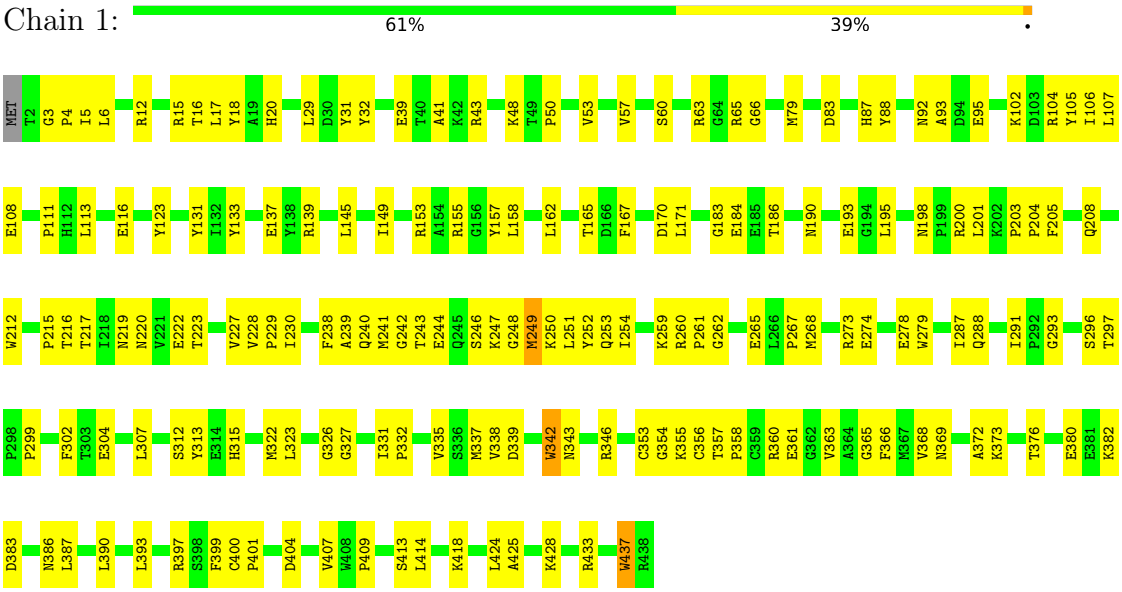
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

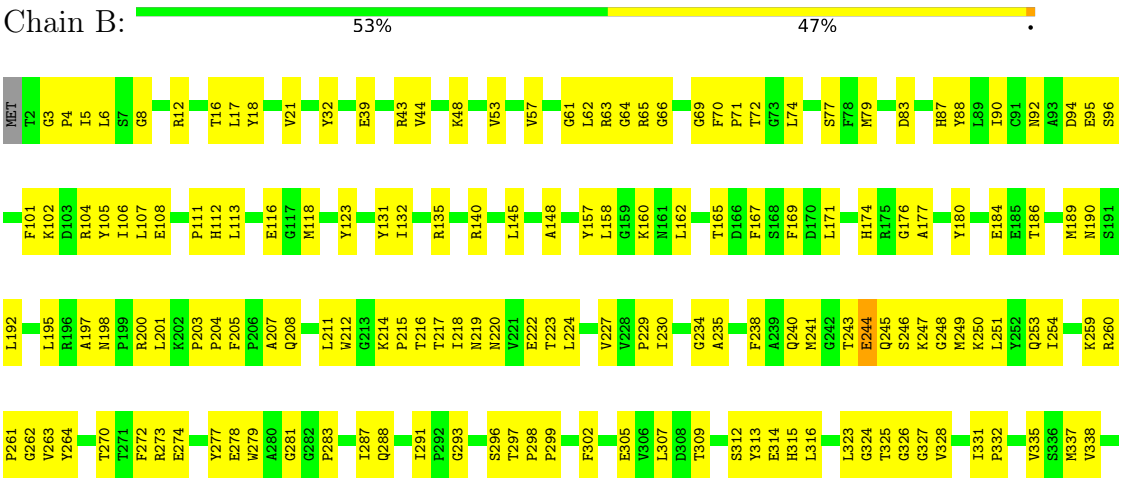
• Molecule 1: NADH-quinone oxidoreductase subunit 1

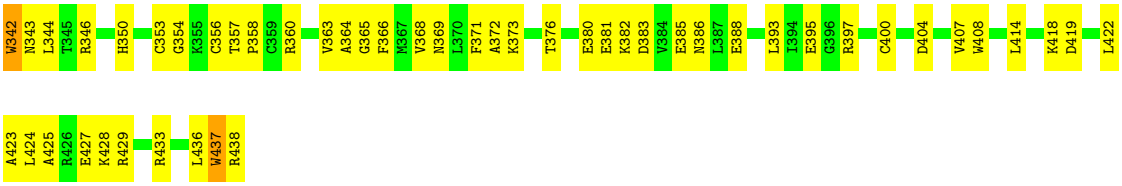
Chain 1:



• Molecule 1: NADH-quinone oxidoreductase subunit 1

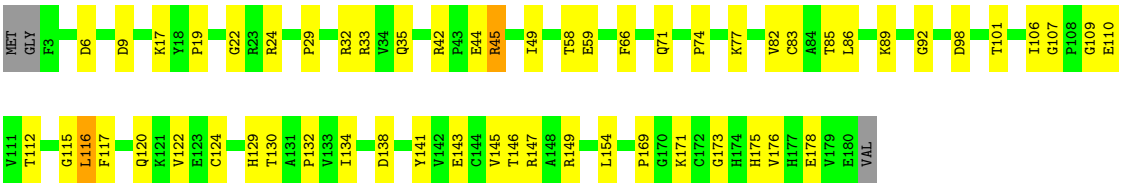
Chain B:





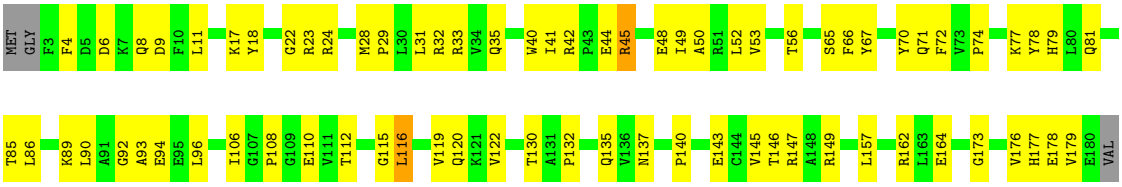
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2:



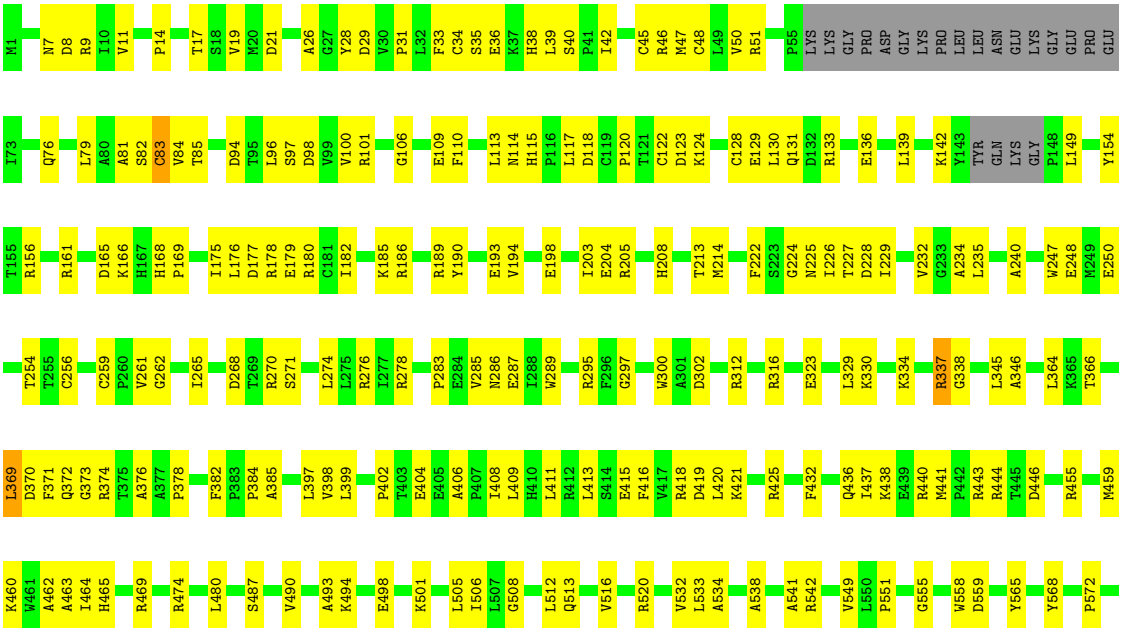
• Molecule 2: NADH-quinone oxidoreductase subunit 2

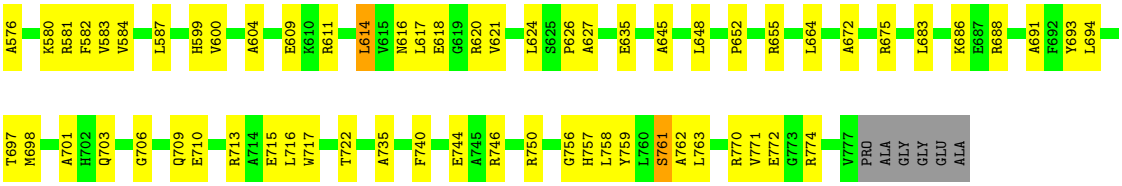
Chain C:



• Molecule 3: NADH-quinone oxidoreductase subunit 3

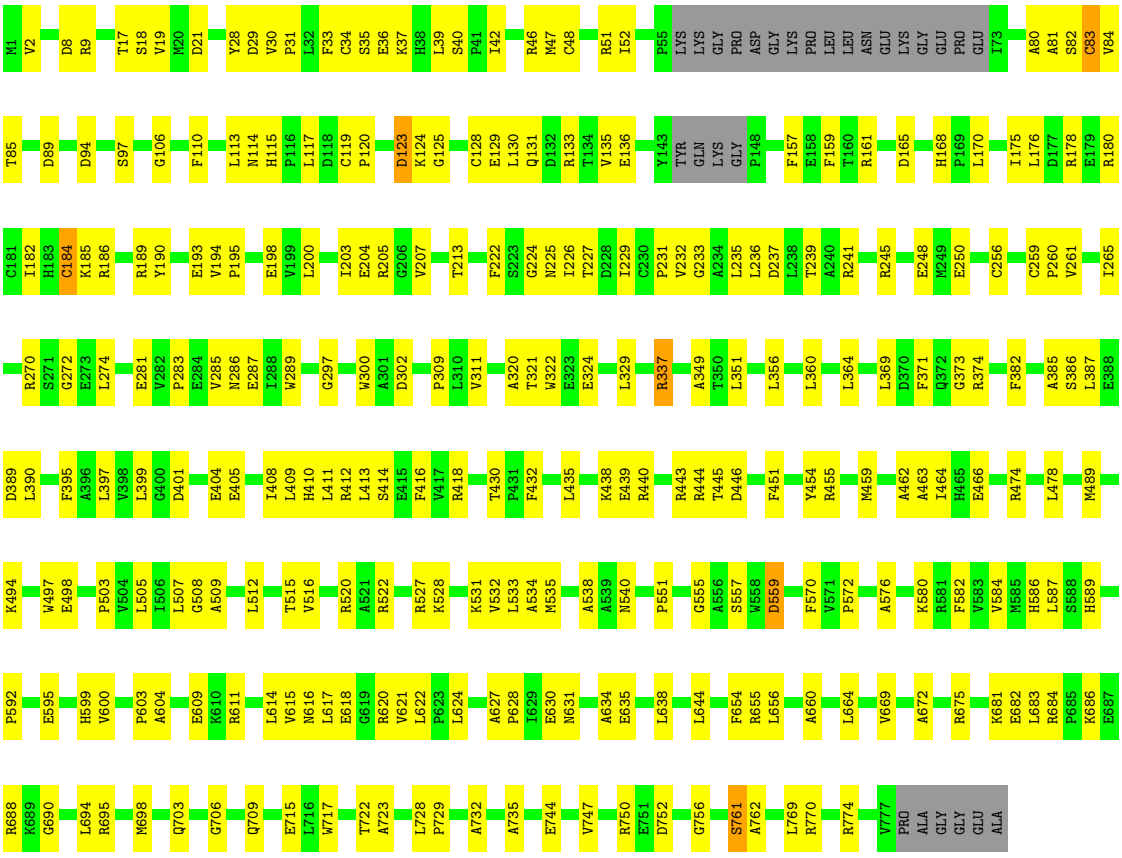
Chain 3:





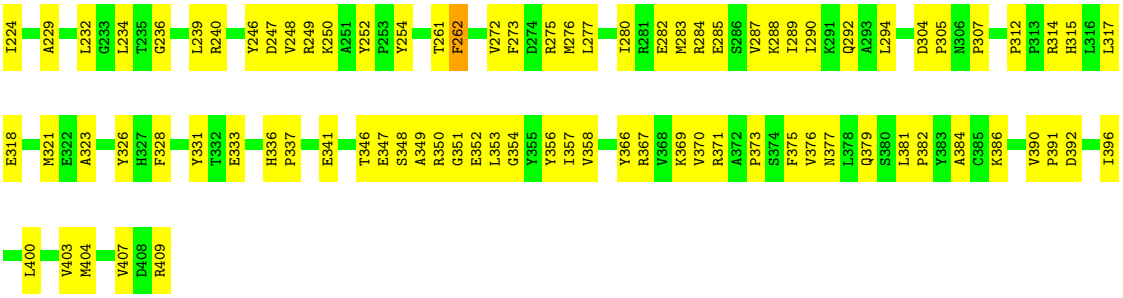
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain D:



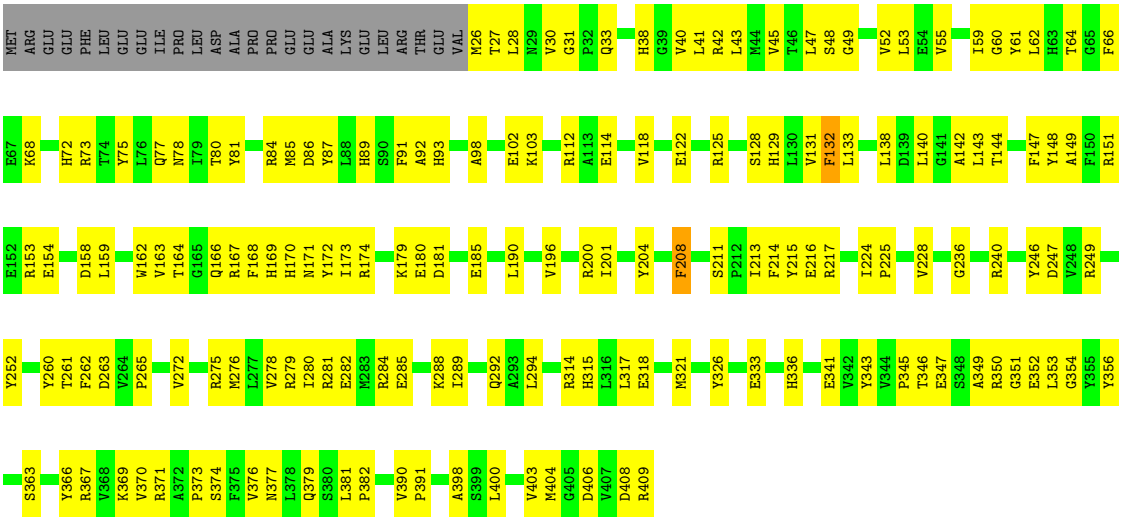
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4:



• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E:

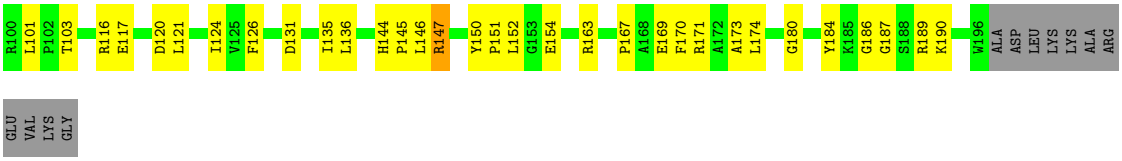


• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5:

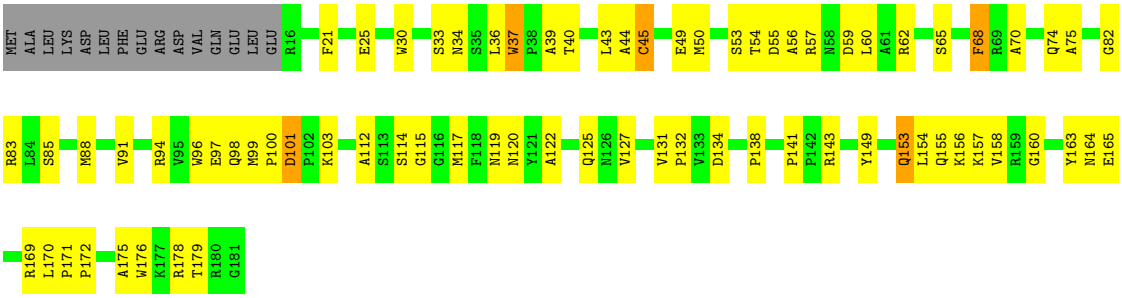
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F:



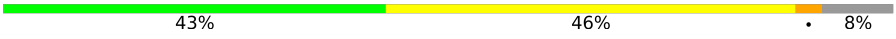
• Molecule 6: NADH-quinone oxidoreductase subunit 6

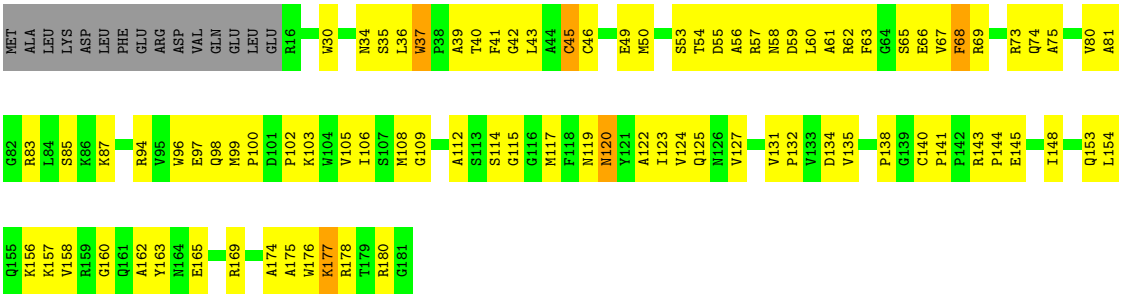
Chain 6:



• Molecule 6: NADH-quinone oxidoreductase subunit 6

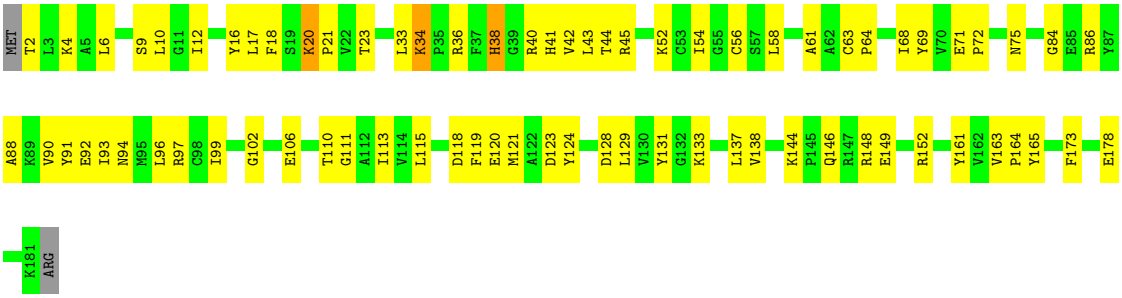
Chain G:





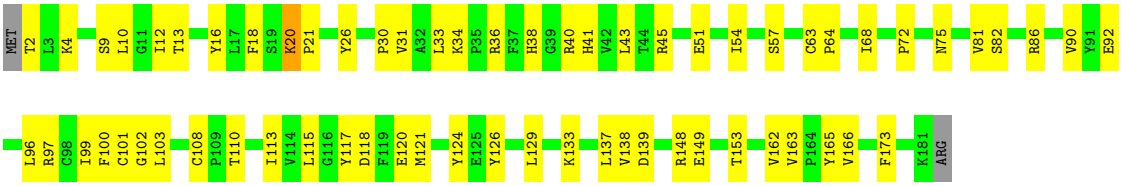
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9:

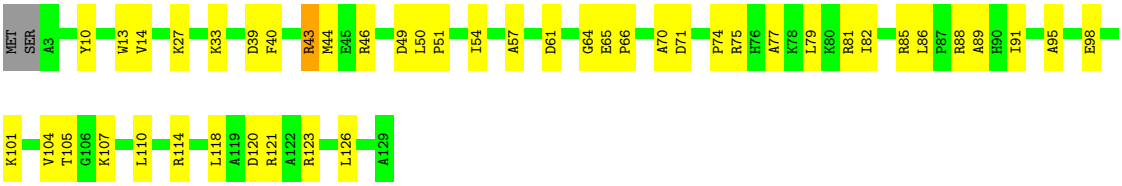


• Molecule 7: NADH-quinone oxidoreductase subunit 9

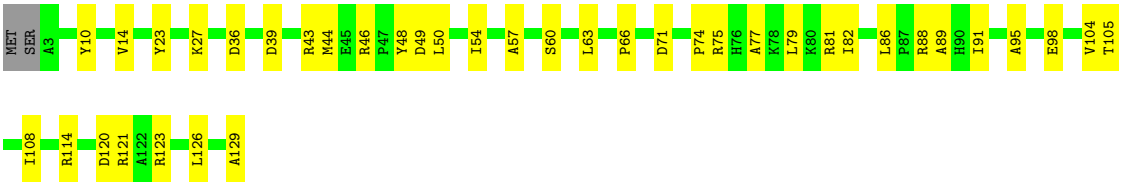
Chain O:



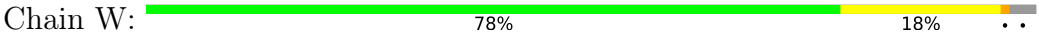
• Molecule 8: NADH-quinone oxidoreductase subunit 15

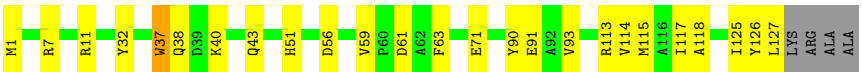


• Molecule 8: NADH-quinone oxidoreductase subunit 15



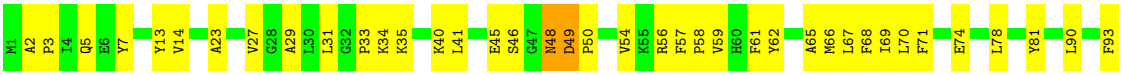
• Molecule 9: NADH-quinone oxidoreductase subunit 16





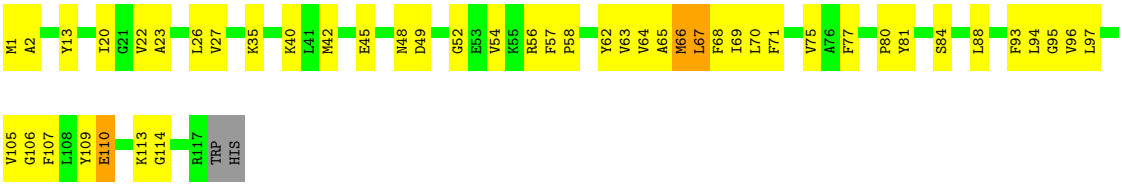
• Molecule 9: NADH-quinone oxidoreductase subunit 16

• Molecule 10: NADH-quinone oxidoreductase subunit 7



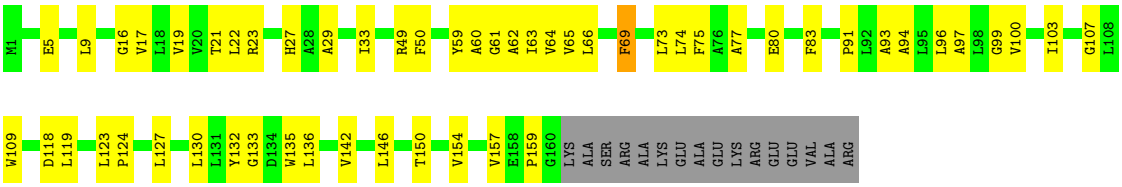
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:



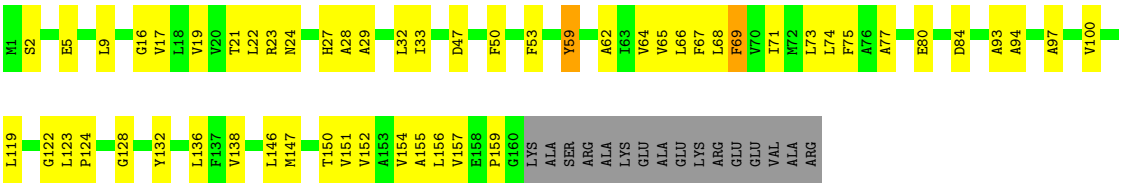
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



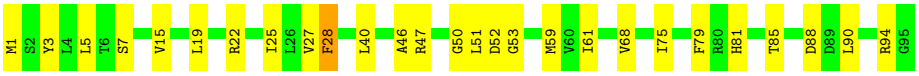
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



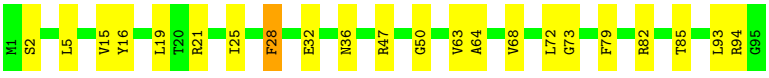
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



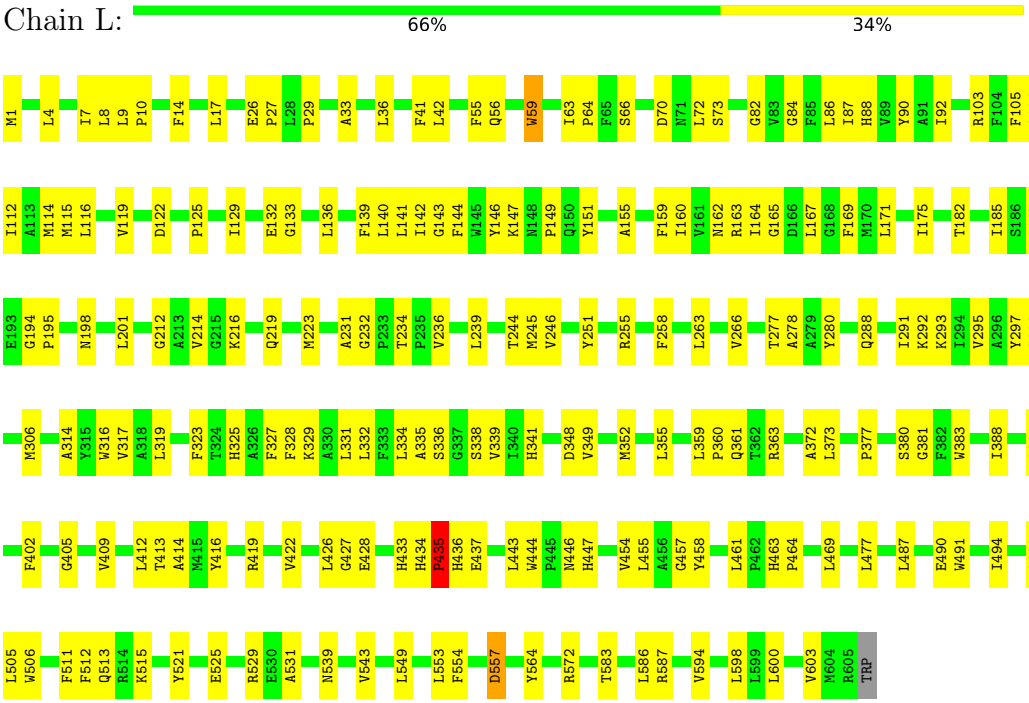
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:



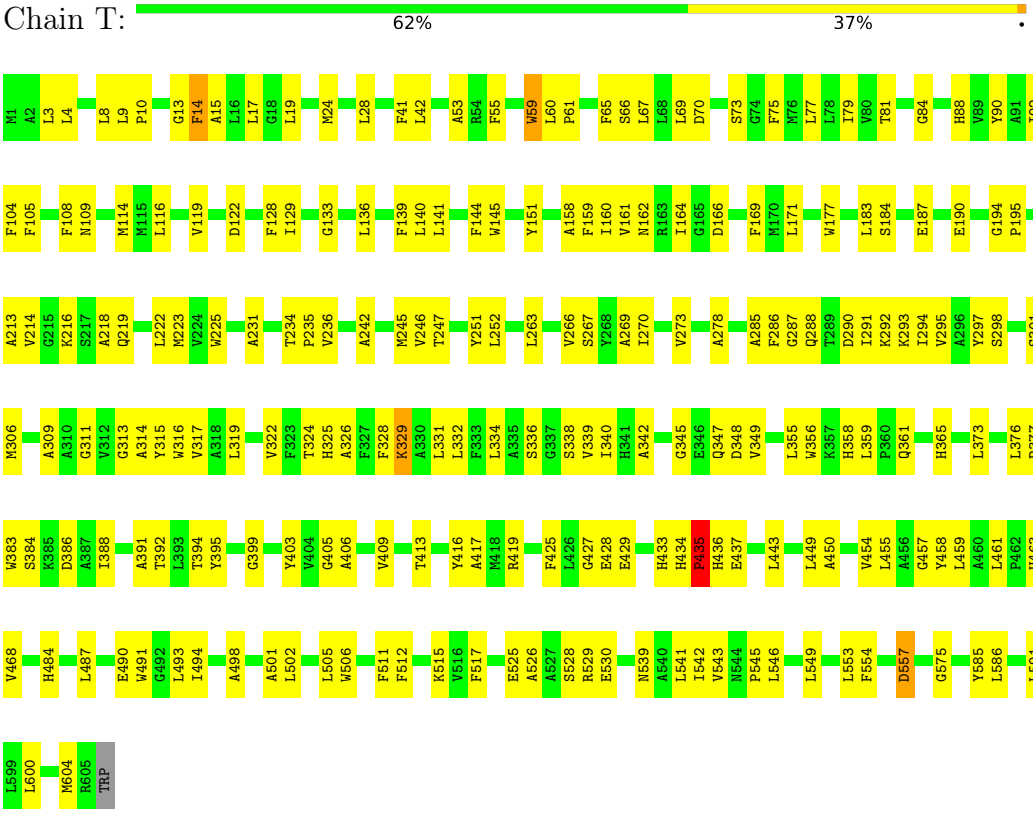
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:



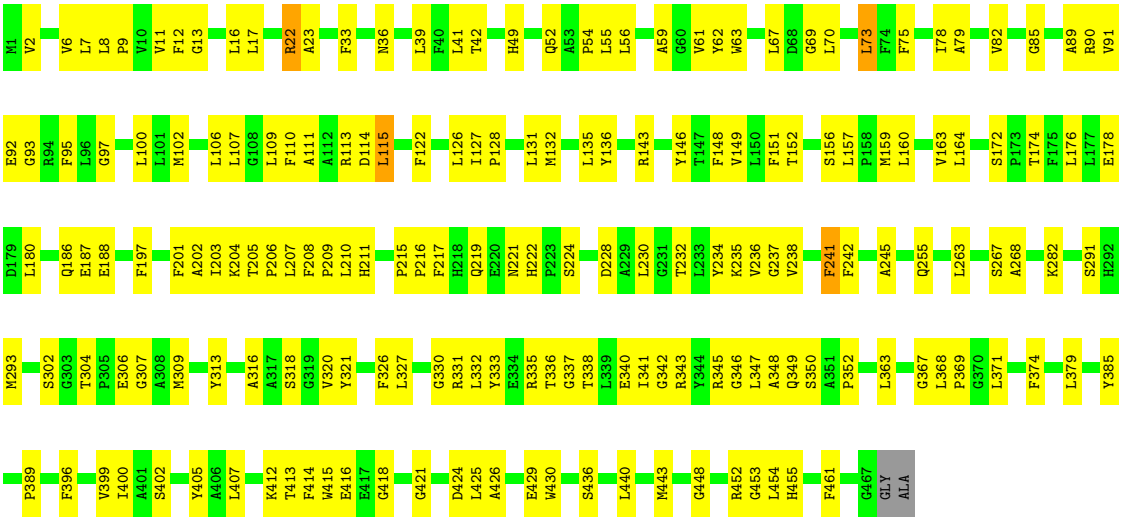
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain T:



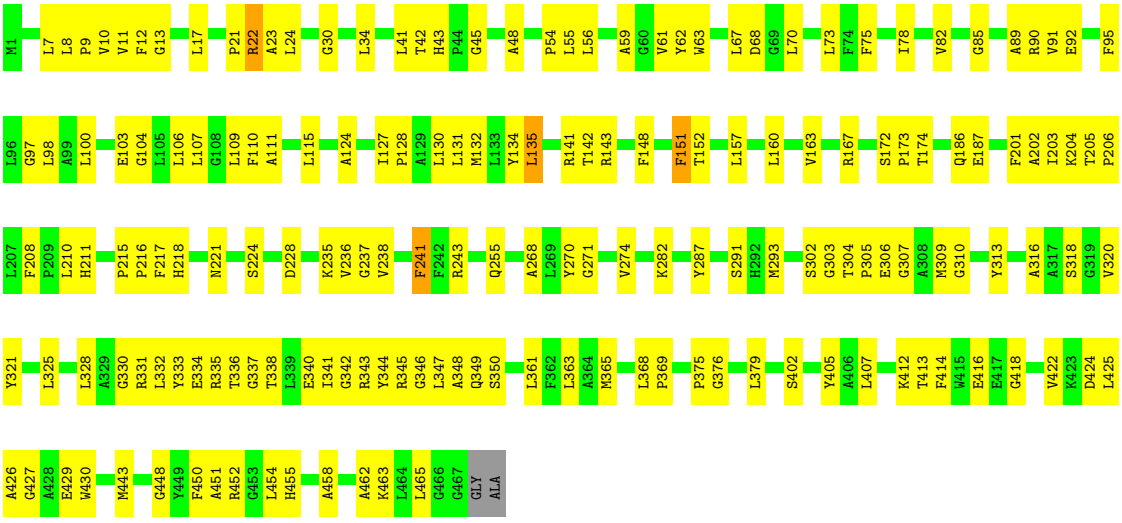
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain M:



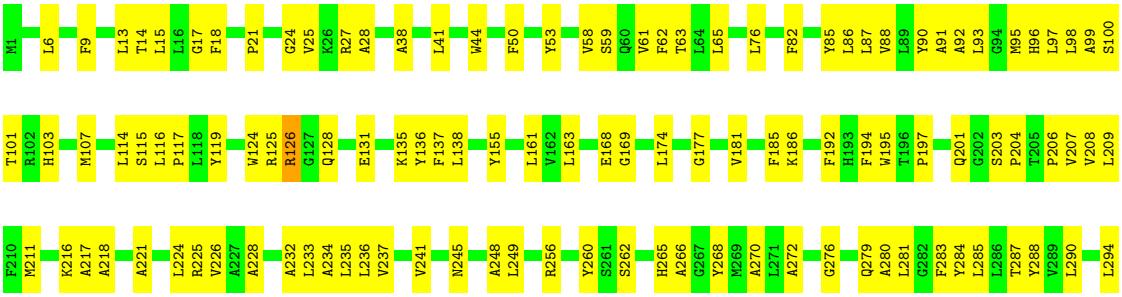
• Molecule 14: NADH-quinone oxidoreductase subunit 13

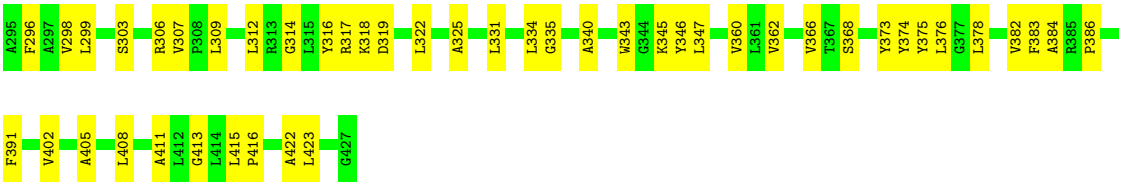
Chain U:



• Molecule 15: NADH-quinone oxidoreductase subunit 14

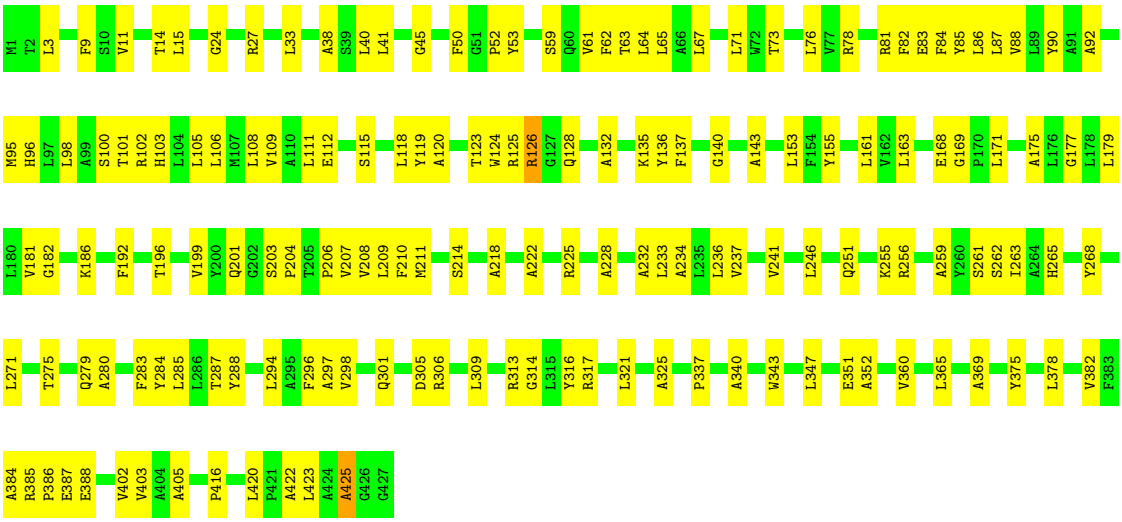
Chain N:





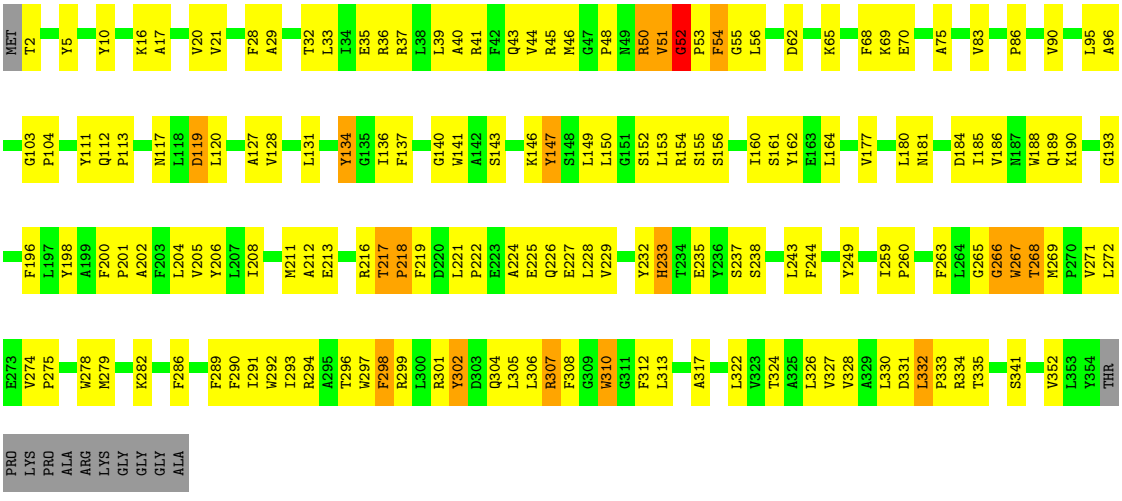
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V:



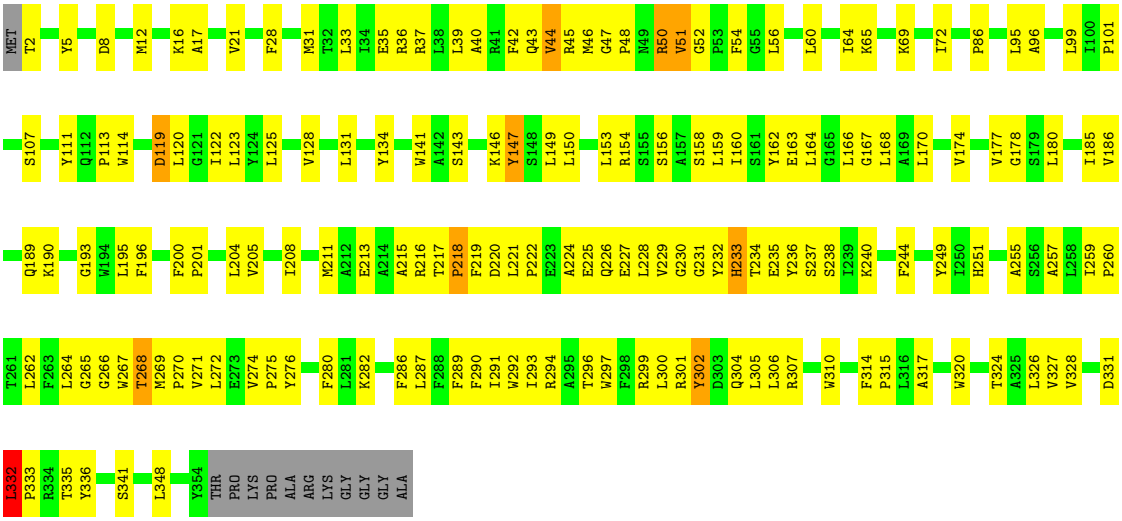
• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H:



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q:


MET T2 Y5 D8 M12 K16 A17 V21 F28 M31 T32 L33 I34 E35 R36 R37 L38 L39 A40 R41 F42 Q43 V44 R45 M46 G47 P48 N49 R50 V51 G52 P53 F54 G55 L56 L60 I64 K65 K69 I72 P86 L95 A96 L99 I100 P101
S107 Y111 Q112 P113 W114 D119 L120 G121 I122 L123 Y124 L125 V128 L131 Y134 W141 A142 S143 K146 Y147 S148 L149 L150 L153 R154 S155 S156 A157 S158 L159 I160 S161 Y162 E163 L164 G165 L166 G167 L168 A169 L170 V174 V177 G178 S179 L180 I185 V186
Q189 K190 G193 W194 L195 F196 P200 P201 L204 V205 I208 M211 A212 E213 A214 A215 R216 T217 P218 F219 D220 L221 P222 E223 A224 E225 Q226 E227 L228 V229 G230 G231 Y232 H233 T234 E235 Y236 S237 S238 I239 K240 F244 Y249 I250 H251 A255 S256 A257 L258 I259 P260
T261 L262 F263 L264 G265 G266 W267 T268 M269 P270 V271 L272 E273 V274 P275 Y276 F280 L281 K282 F286 L287 F288 F289 F290 I291 W292 I293 R294 A295 T296 W297 F298 R299 L300 R301 Y302 D303 Q304 L305 L306 R307 W310 F314 P315 L316 A317 W320 T324 A325 L326 V327 V328 D331
L332 P333 R334 T335 Y336 S341 L348 Y354 THR PRO LYS PRO ALA ARG LYS GLY GLY GLY ALA

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.70Å 328.00Å 260.90Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60	Depositor
% Data completeness (in resolution range)	76.5 (29.87-3.60)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.225	Depositor
Wilson B-factor (Å^2)	81.1	Xtriage
Anisotropy	0.034	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	0.337 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 137833 reflections	Xtriage
Total number of atoms	74132	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, FES, DCQ, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.27	0/3506	0.47	1/4745 (0.0%)
1	B	0.26	0/3506	0.48	1/4745 (0.0%)
2	2	0.28	0/1439	0.45	0/1953
2	C	0.27	0/1439	0.47	0/1953
3	3	0.28	0/6035	0.52	2/8185 (0.0%)
3	D	0.28	0/6035	0.50	1/8185 (0.0%)
4	4	0.28	0/3150	0.48	0/4284
4	E	0.28	0/3150	0.48	0/4284
5	5	0.28	0/1656	0.49	0/2246
5	F	0.28	0/1656	0.48	0/2246
6	6	0.30	0/1319	0.53	0/1786
6	G	0.30	0/1319	0.54	0/1786
7	9	0.31	0/1423	0.52	0/1933
7	O	0.31	0/1423	0.51	0/1933
8	7	0.27	0/1059	0.49	0/1429
8	I	0.26	0/1059	0.48	0/1429
9	W	0.27	0/985	0.49	0/1335
9	X	0.26	0/985	0.46	0/1335
10	A	0.29	0/940	0.49	0/1280
10	P	0.30	0/940	0.53	1/1280 (0.1%)
11	J	0.28	0/1206	0.45	0/1649
11	R	0.27	0/1206	0.45	0/1649
12	K	0.28	0/710	0.45	0/962
12	S	0.28	0/710	0.46	0/962
13	L	0.26	0/4741	0.45	0/6460
13	T	0.26	0/4741	0.44	0/6460
14	M	0.27	0/3591	0.47	0/4896
14	U	0.27	0/3591	0.47	0/4896
15	N	0.27	0/3238	0.43	0/4434
15	V	0.27	0/3238	0.42	0/4434
16	H	0.29	0/2935	0.52	0/4014
16	Q	0.29	0/2935	0.51	0/4014

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.28	0/75866	0.48	6/103182 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	9	0	2
7	O	0	2
12	K	0	1
12	S	0	1
13	L	0	1
13	T	0	1
16	H	0	4
16	Q	0	3
All	All	0	15

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	559	ASP	C-N-CA	-6.26	106.06	121.70
10	P	67	LEU	CA-CB-CG	6.00	129.09	115.30
1	1	296	SER	C-N-CA	-5.78	107.25	121.70
3	3	614	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	296	SER	C-N-CA	-5.27	108.53	121.70
3	3	626	PRO	C-N-CA	-5.25	108.58	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	20	LYS	Peptide
7	9	21	PRO	Peptide
16	H	217	THR	Peptide
16	H	266	GLY	Peptide
16	H	267	TRP	Peptide
16	H	52	GLY	Peptide
12	K	50	GLY	Peptide
13	L	435	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
7	O	20	LYS	Peptide
7	O	21	PRO	Peptide
16	Q	217	THR	Peptide
16	Q	266	GLY	Peptide
16	Q	332	LEU	Peptide
12	S	50	GLY	Peptide
13	T	435	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3388	127	0
1	B	3417	0	3389	162	0
2	2	1406	0	1373	49	0
2	C	1406	0	1373	62	0
3	3	5895	0	5931	192	0
3	D	5895	0	5931	193	0
4	4	3067	0	3049	181	0
4	E	3067	0	3049	172	0
5	5	1607	0	1574	66	0
5	F	1607	0	1574	61	0
6	6	1289	0	1298	75	0
6	G	1289	0	1298	88	0
7	9	1388	0	1383	74	0
7	O	1388	0	1383	57	0
8	7	1031	0	1029	38	0
8	I	1031	0	1029	30	0
9	W	967	0	1010	21	0
9	X	967	0	1010	26	0
10	A	910	0	939	59	0
10	P	910	0	939	59	0
11	J	1183	0	1286	61	0
11	R	1183	0	1286	52	0
12	K	703	0	747	26	0
12	S	703	0	747	23	0
13	L	4604	0	4734	153	0
13	T	4604	0	4734	157	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	3489	0	3606	136	0
14	U	3489	0	3606	126	0
15	N	3154	0	3343	111	0
15	V	3154	0	3343	114	0
16	H	2838	0	2903	157	0
16	Q	2838	0	2903	165	0
17	1	8	0	0	0	0
17	3	24	0	0	3	0
17	6	8	0	0	1	0
17	9	16	0	0	3	0
17	B	8	0	0	3	0
17	D	24	0	0	2	0
17	G	8	0	0	0	0
17	O	16	0	0	3	0
18	1	31	0	19	9	0
18	B	31	0	19	9	0
19	2	4	0	0	0	0
19	3	4	0	0	1	0
19	C	4	0	0	0	0
19	D	4	0	0	2	0
20	4	23	0	30	4	0
20	E	23	0	30	4	0
All	All	74132	0	75285	2642	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (2642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:162:TRP:CE2	7:9:34:LYS:HD2	1.87	1.09
12:S:28:PHE:CZ	12:S:68:VAL:HA	1.91	1.05
12:S:28:PHE:HZ	12:S:68:VAL:HA	1.16	1.04
4:E:138:LEU:CD1	4:E:143:LEU:HD23	1.89	1.02
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.45	0.97
4:E:143:LEU:HD21	16:Q:226:GLN:NE2	1.81	0.94
16:H:274:VAL:HG12	16:H:278:TRP:CD1	2.02	0.94
14:M:41:LEU:O	14:M:42:THR:HG22	1.69	0.91
3:3:259:CYS:HG	17:3:803:SF4:FE4	0.88	0.88
1:1:222:GLU:HG3	1:1:251:LEU:HD22	1.52	0.88
3:3:193:GLU:O	3:3:443:ARG:NH2	2.07	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:146:LYS:HA	16:Q:149:LEU:HB2	1.54	0.87
4:4:162:TRP:CD2	7:9:34:LYS:HD2	2.11	0.86
4:4:162:TRP:HA	7:9:34:LYS:HG3	1.58	0.85
14:M:69:GLY:O	14:M:73:LEU:HD23	1.76	0.85
13:L:557:ASP:OD1	14:M:211:HIS:NE2	2.10	0.84
6:G:56:ALA:HA	16:Q:45:ARG:HB2	1.59	0.84
16:H:302:TYR:HA	16:H:305:LEU:HB3	1.59	0.84
15:N:294:LEU:HD11	15:N:325:ALA:HB1	1.60	0.84
4:E:138:LEU:HD11	4:E:143:LEU:HD23	1.58	0.84
4:E:138:LEU:HD11	4:E:143:LEU:CD2	2.08	0.83
1:1:288:GLN:NE2	1:1:335:VAL:O	2.12	0.83
16:H:146:LYS:HA	16:H:149:LEU:HB2	1.61	0.83
3:D:259:CYS:HG	17:D:803:SF4:FE4	0.90	0.82
3:D:611:ARG:HA	3:D:624:LEU:O	1.79	0.82
4:E:85:MET:HE1	4:E:370:VAL:HG11	1.61	0.82
4:E:409:ARG:NH2	5:F:117:GLU:OE2	2.13	0.81
14:U:89:ALA:HB1	14:U:91:VAL:HG22	1.61	0.81
15:N:14:THR:HG1	15:N:90:TYR:HH	1.29	0.81
6:6:45:CYS:SG	6:6:83:ARG:NH2	2.55	0.80
14:U:115:LEU:HD13	14:U:163:VAL:HG23	1.63	0.80
14:U:217:PHE:O	14:U:221:ASN:ND2	2.14	0.80
3:3:286:ASN:ND2	3:3:289:TRP:O	2.14	0.80
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.15	0.80
1:1:92:ASN:ND2	18:1:502:FMN:O3'	2.15	0.79
4:4:128:SER:OG	4:4:350:ARG:NH2	2.15	0.79
6:6:149:TYR:O	6:6:153:GLN:NE2	2.15	0.79
15:N:280:ALA:HB1	15:N:347:LEU:HB3	1.64	0.79
15:V:73:THR:HG21	15:V:210:PHE:HB2	1.64	0.79
5:5:13:LYS:NZ	5:5:37:GLU:OE2	2.16	0.79
14:M:89:ALA:HB1	14:M:91:VAL:HG22	1.63	0.79
1:B:395:GLU:OE2	1:B:408:TRP:NE1	2.16	0.79
3:D:455:ARG:HH21	3:D:750:ARG:HH21	1.31	0.79
13:T:3:LEU:HD23	13:T:55:PHE:HB2	1.64	0.79
3:3:614:LEU:O	3:3:621:VAL:HA	1.82	0.78
13:L:278:ALA:HA	13:L:301:SER:HA	1.65	0.78
14:U:109:LEU:HD21	14:U:236:VAL:HG21	1.65	0.78
1:1:190:ASN:ND2	1:1:198:ASN:O	2.17	0.78
3:3:559:ASP:OD2	3:3:686:LYS:NZ	2.16	0.78
4:4:68:LYS:NZ	5:5:145:PRO:O	2.15	0.78
16:Q:327:VAL:O	16:Q:331:ASP:N	2.17	0.78
6:G:114:SER:HB2	7:O:97:ARG:HE	1.48	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:177:VAL:HG21	16:H:185:ILE:HG23	1.66	0.78
1:B:287:ILE:HA	1:B:332:PRO:HA	1.66	0.78
4:E:200:ARG:NH1	7:O:16:TYR:OH	2.16	0.78
16:Q:189:GLN:NE2	16:Q:264:LEU:O	2.16	0.78
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.66	0.77
16:Q:158:SER:HA	16:Q:306:LEU:HD21	1.66	0.77
14:U:124:ALA:HB2	15:V:337:PRO:HB2	1.66	0.77
3:D:614:LEU:O	3:D:621:VAL:HA	1.85	0.77
4:4:222:GLY:HA3	4:4:275:ARG:HH22	1.48	0.77
4:E:144:THR:HG22	4:E:148:TYR:HE1	1.47	0.77
6:G:62:ARG:HD2	16:Q:50:ARG:HH21	1.49	0.77
11:R:23:ARG:HG2	11:R:80:GLU:HG2	1.66	0.77
16:Q:292:TRP:O	16:Q:296:THR:OG1	2.03	0.76
14:M:208:PHE:O	14:M:211:HIS:ND1	2.16	0.76
14:M:217:PHE:O	14:M:221:ASN:ND2	2.18	0.76
1:B:63:ARG:H	1:B:65:ARG:HH21	1.32	0.76
4:E:166:GLN:NE2	7:O:100:PHE:O	2.18	0.76
6:G:160:GLY:O	6:G:169:ARG:NH1	2.17	0.76
15:V:280:ALA:HB1	15:V:347:LEU:HB3	1.67	0.76
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.68	0.76
13:T:340:ILE:O	13:T:345:GLY:N	2.19	0.76
1:1:220:ASN:ND2	18:1:502:FMN:O2	2.18	0.76
4:E:185:GLU:OE2	7:O:165:TYR:OH	2.03	0.76
1:1:287:ILE:HA	1:1:332:PRO:HA	1.67	0.76
2:2:132:PRO:HG2	2:2:145:VAL:HB	1.67	0.76
1:B:92:ASN:ND2	18:B:502:FMN:O3'	2.19	0.76
16:Q:291:ILE:HA	16:Q:294:ARG:HG3	1.66	0.76
4:4:26:MET:N	4:4:47:LEU:O	2.18	0.76
4:E:201:ILE:HG21	4:E:284:ARG:HG3	1.67	0.76
4:E:281:ARG:HD3	4:E:284:ARG:HH12	1.51	0.76
16:H:216:ARG:HD2	16:H:294:ARG:HA	1.68	0.75
3:D:401:ASP:OD2	3:D:454:TYR:OH	2.04	0.75
14:U:348:ALA:HB2	14:U:414:PHE:HB3	1.68	0.75
4:4:162:TRP:CA	7:9:34:LYS:HG3	2.16	0.75
16:H:265:GLY:O	16:H:282:LYS:NZ	2.18	0.75
14:U:22:ARG:HD2	14:U:23:ALA:N	2.02	0.75
16:Q:215:ALA:O	16:Q:294:ARG:NH1	2.16	0.75
1:B:88:TYR:HB2	1:B:216:THR:HG22	1.67	0.75
6:G:102:PRO:O	16:Q:69:LYS:NZ	2.19	0.75
12:S:64:ALA:O	12:S:68:VAL:HG23	1.86	0.75
16:H:219:PHE:HB3	16:H:299:ARG:HG2	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:62:ARG:HB3	16:Q:50:ARG:HB2	1.68	0.75
14:U:268:ALA:HA	14:U:291:SER:HA	1.69	0.75
5:5:35:LYS:NZ	5:5:103:THR:O	2.20	0.75
9:X:37:TRP:HD1	9:X:40:LYS:HB2	1.51	0.75
5:5:144:HIS:HB2	5:5:147:ARG:HD3	1.69	0.74
3:D:297:GLY:O	3:D:300:TRP:NE1	2.16	0.74
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.67	0.74
7:O:45:ARG:NH2	7:O:139:ASP:OD2	2.17	0.74
16:Q:302:TYR:HA	16:Q:305:LEU:HB3	1.68	0.74
1:1:131:TYR:OH	2:2:17:LYS:O	2.04	0.74
3:D:286:ASN:ND2	3:D:289:TRP:O	2.20	0.74
9:X:51:HIS:ND1	9:X:56:ASP:OD1	2.21	0.74
1:B:354:GLY:O	1:B:360:ARG:NH1	2.20	0.74
16:Q:219:PHE:HB3	16:Q:299:ARG:HG2	1.69	0.74
15:N:228:ALA:HB1	15:N:233:LEU:HD11	1.69	0.74
14:M:12:PHE:HB3	14:M:100:LEU:HD13	1.70	0.74
4:4:169:HIS:HD2	6:6:141:PRO:HD3	1.52	0.74
14:M:22:ARG:HD2	14:M:23:ALA:N	2.02	0.73
14:M:52:GLN:HE22	14:M:176:LEU:HD11	1.53	0.73
16:H:332:LEU:HB2	16:H:333:PRO:HD3	1.68	0.73
4:4:144:THR:HG22	4:4:148:TYR:HE1	1.54	0.73
1:B:353:CYS:HG	17:B:501:SF4:FE4	1.04	0.73
4:E:240:ARG:NH1	4:E:282:GLU:OE2	2.20	0.73
4:E:314:ARG:NH2	8:I:44:MET:SD	2.62	0.73
8:I:63:LEU:HD13	8:I:129:ALA:HB3	1.69	0.73
4:4:240:ARG:NH1	4:4:282:GLU:OE2	2.22	0.73
1:B:343:ASN:HB2	2:C:89:LYS:HZ2	1.51	0.73
4:E:45:VAL:HG13	4:E:55:VAL:HG22	1.69	0.73
13:L:458:TYR:HB3	13:L:461:LEU:HD11	1.69	0.73
14:M:348:ALA:HB2	14:M:414:PHE:HB3	1.69	0.73
14:M:363:LEU:HD22	14:M:368:LEU:HD13	1.71	0.73
6:G:74:GLN:HE22	16:Q:233:HIS:HB2	1.54	0.73
13:T:458:TYR:HB3	13:T:461:LEU:HD11	1.71	0.73
14:M:122:PHE:O	14:M:234:TYR:OH	2.04	0.73
8:7:120:ASP:OD1	8:7:123:ARG:NH1	2.22	0.73
2:C:132:PRO:HG2	2:C:145:VAL:HB	1.71	0.73
6:G:30:TRP:O	6:G:34:ASN:ND2	2.22	0.73
7:O:75:ASN:ND2	7:O:82:SER:OG	2.22	0.73
1:1:79:MET:SD	1:1:217:THR:OG1	2.46	0.73
3:D:722:THR:HG21	3:D:756:GLY:H	1.54	0.72
10:P:70:LEU:HD13	11:R:150:THR:HG22	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:26:TYR:OH	7:O:120:GLU:OE2	2.05	0.72
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.22	0.72
3:D:180:ARG:NH1	3:D:233:GLY:O	2.23	0.72
3:3:259:CYS:SG	17:3:803:SF4:FE4	1.81	0.72
14:U:346:GLY:HA3	14:U:418:GLY:HA2	1.70	0.72
2:2:110:GLU:HA	8:7:121:ARG:HH12	1.53	0.72
13:L:298:SER:OG	13:L:329:LYS:NZ	2.16	0.72
4:E:143:LEU:HD21	16:Q:226:GLN:HE22	1.55	0.72
4:E:143:LEU:CD2	16:Q:226:GLN:NE2	2.53	0.72
6:G:163:TYR:O	7:O:148:ARG:NH2	2.22	0.72
8:I:120:ASP:OD1	8:I:123:ARG:NH1	2.23	0.72
13:L:182:THR:HB	13:L:187:GLU:HG3	1.70	0.72
16:H:292:TRP:O	16:H:296:THR:OG1	2.06	0.72
2:2:109:GLY:O	8:7:121:ARG:NH2	2.21	0.71
16:H:43:GLN:O	16:H:45:ARG:N	2.23	0.71
11:R:50:PHE:HB2	11:R:124:PRO:HD3	1.71	0.71
16:H:52:GLY:HA3	16:H:55:GLY:H	1.53	0.71
15:V:14:THR:HA	15:V:86:LEU:HD21	1.71	0.71
4:4:236:GLY:HA2	4:4:351:GLY:HA3	1.72	0.71
6:G:119:ASN:HA	6:G:125:GLN:HE22	1.54	0.71
11:R:47:ASP:O	11:R:122:GLY:N	2.23	0.71
15:N:314:GLY:HA3	15:N:386:PRO:HG3	1.72	0.71
10:P:109:TYR:OH	10:P:113:LYS:NZ	2.20	0.71
12:S:28:PHE:CE1	12:S:68:VAL:HG22	2.26	0.71
16:H:226:GLN:HB2	16:H:299:ARG:HH22	1.54	0.71
1:B:16:THR:HG21	1:B:229:PRO:HB3	1.71	0.71
4:E:341:GLU:OE2	5:F:57:TYR:OH	2.08	0.71
14:U:54:PRO:HA	14:U:62:TYR:HD1	1.54	0.71
3:3:98:ASP:OD1	3:3:101:ARG:NH2	2.24	0.71
6:6:57:ARG:HA	7:9:23:THR:HA	1.72	0.71
11:J:49:ARG:NH1	16:H:119:ASP:OD2	2.23	0.71
4:E:240:ARG:NH2	4:E:347:GLU:OE2	2.23	0.71
10:A:35:LYS:O	10:A:40:LYS:NZ	2.23	0.71
12:K:94:ARG:NH1	13:L:583:THR:O	2.23	0.71
6:G:175:ALA:O	6:G:180:ARG:NH2	2.22	0.71
1:B:17:LEU:HD12	1:B:251:LEU:HD11	1.72	0.71
1:1:92:ASN:O	1:1:220:ASN:ND2	2.25	0.70
6:6:62:ARG:HB3	16:H:50:ARG:HB2	1.74	0.70
3:D:259:CYS:SG	17:D:803:SF4:FE4	1.84	0.70
4:E:154:GLU:HB3	6:G:57:ARG:HH11	1.56	0.70
8:7:54:ILE:HD11	8:7:57:ALA:HB2	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:327:VAL:O	16:H:331:ASP:N	2.18	0.70
3:3:40:SER:O	3:3:189:ARG:NE	2.22	0.70
14:M:203:ILE:HG13	14:M:210:LEU:HB3	1.73	0.70
3:D:193:GLU:O	3:D:443:ARG:NH2	2.22	0.70
11:R:157:VAL:HG12	11:R:159:PRO:HD3	1.74	0.70
3:3:701:ALA:N	3:3:763:LEU:O	2.21	0.70
13:T:328:PHE:O	13:T:332:LEU:HD12	1.92	0.70
3:3:117:LEU:H	4:4:321:MET:HE3	1.57	0.70
13:T:340:ILE:HB	13:T:345:GLY:HA2	1.73	0.70
13:L:426:LEU:HD23	13:L:513:GLN:HE21	1.56	0.70
8:I:54:ILE:HD11	8:I:57:ALA:HB2	1.71	0.70
15:V:317:ARG:NH1	15:V:384:ALA:O	2.25	0.70
3:3:203:ILE:HG22	3:3:204:GLU:HG3	1.74	0.70
4:4:240:ARG:NH2	4:4:347:GLU:OE2	2.22	0.70
16:Q:43:GLN:O	16:Q:45:ARG:N	2.24	0.70
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.73	0.70
15:V:314:GLY:HA3	15:V:386:PRO:HG3	1.74	0.70
13:L:167:LEU:HD21	14:M:396:PHE:HB3	1.74	0.69
3:D:194:VAL:HG12	3:D:411:LEU:HD22	1.74	0.69
15:V:136:TYR:OH	15:V:186:LYS:NZ	2.25	0.69
3:3:48:CYS:SG	3:3:83:CYS:N	2.65	0.69
1:B:192:LEU:HD22	1:B:211:LEU:HD21	1.74	0.69
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.75	0.69
3:3:609:GLU:HA	3:3:627:ALA:H	1.57	0.69
1:1:425:ALA:O	1:1:428:LYS:NZ	2.22	0.69
13:T:278:ALA:HA	13:T:301:SER:HA	1.73	0.69
3:3:261:VAL:HG21	3:3:408:ILE:HG12	1.75	0.69
3:3:373:GLY:HA3	3:3:538:ALA:HB2	1.75	0.69
14:M:2:VAL:HB	14:M:67:LEU:HD11	1.75	0.69
1:B:220:ASN:ND2	18:B:502:FMN:O2	2.25	0.69
3:D:584:VAL:HG12	3:D:600:VAL:HB	1.75	0.69
4:E:26:MET:N	4:E:47:LEU:O	2.25	0.69
5:F:144:HIS:HB2	5:F:147:ARG:HD3	1.74	0.69
10:A:65:ALA:HB3	11:J:66:LEU:HD13	1.75	0.69
1:B:131:TYR:OH	2:C:17:LYS:O	2.10	0.68
4:E:143:LEU:CD2	16:Q:226:GLN:HE22	2.05	0.68
12:S:28:PHE:HE1	12:S:68:VAL:HG22	1.56	0.68
9:W:51:HIS:ND1	9:W:56:ASP:OD1	2.26	0.68
16:H:50:ARG:O	16:H:52:GLY:N	2.21	0.68
3:D:117:LEU:HD23	4:E:321:MET:HE2	1.75	0.68
10:A:113:LYS:HD3	11:J:154:VAL:HG11	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:28:PHE:CZ	12:K:68:VAL:HA	2.28	0.68
3:D:682:GLU:OE1	3:D:684:ARG:NH2	2.26	0.68
1:1:312:SER:OG	1:1:315:HIS:ND1	2.22	0.68
11:J:130:LEU:CD1	12:K:51:LEU:CD2	2.70	0.68
15:N:13:LEU:HD22	15:N:25:VAL:HG13	1.74	0.68
15:N:228:ALA:HB1	15:N:233:LEU:CD1	2.23	0.68
9:X:98:GLU:OE2	9:X:113:ARG:NH1	2.26	0.68
3:3:149:LEU:HD11	4:4:304:ASP:HA	1.76	0.68
3:3:713:ARG:HH21	3:3:746:ARG:HH21	1.40	0.68
3:D:435:LEU:O	3:D:438:LYS:NZ	2.27	0.68
3:D:635:GLU:OE2	9:X:7:ARG:NH1	2.26	0.68
13:T:70:ASP:H	13:T:73:SER:HB2	1.58	0.68
13:T:213:ALA:HB2	13:T:252:LEU:HD23	1.76	0.68
14:U:56:LEU:HB2	14:U:61:VAL:HB	1.75	0.68
4:E:49:GLY:HA2	10:P:58:PRO:HD3	1.76	0.68
16:H:291:ILE:HA	16:H:294:ARG:HG3	1.74	0.68
1:B:79:MET:SD	1:B:217:THR:OG1	2.51	0.68
11:R:152:VAL:HG13	15:V:120:ALA:HB2	1.73	0.68
5:5:73:GLU:OE2	5:5:87:ARG:NH1	2.27	0.68
3:3:169:PRO:HA	3:3:175:ILE:HA	1.76	0.68
4:4:163:VAL:HG13	4:4:164:THR:HG23	1.76	0.68
16:H:143:SER:HB2	16:H:235:GLU:HG3	1.76	0.68
3:D:195:PRO:O	3:D:410:HIS:NE2	2.27	0.68
1:B:260:ARG:NH1	1:B:279:TRP:O	2.25	0.67
3:D:30:VAL:O	5:F:184:TYR:OH	2.12	0.67
13:T:355:LEU:HB3	13:T:359:LEU:HD12	1.76	0.67
13:L:132:GLU:OE2	13:L:163:ARG:NH1	2.27	0.67
13:L:355:LEU:HB3	13:L:359:LEU:HD12	1.76	0.67
13:L:572:ARG:NH2	15:N:373:TYR:OH	2.25	0.67
14:M:115:LEU:HD13	14:M:163:VAL:HG23	1.75	0.67
14:M:115:LEU:HD12	14:M:180:LEU:HD13	1.76	0.67
15:N:38:ALA:HA	15:N:41:LEU:HD12	1.77	0.67
3:3:551:PRO:HB2	3:3:555:GLY:HA2	1.75	0.67
6:6:138:PRO:HG2	7:9:121:MET:HG3	1.76	0.67
13:L:147:LYS:NZ	14:M:349:GLN:OE1	2.26	0.67
1:B:259:LYS:NZ	2:C:178:GLU:OE2	2.26	0.67
1:B:353:CYS:SG	17:B:501:SF4:FE4	1.86	0.67
5:F:35:LYS:NZ	5:F:103:THR:O	2.25	0.67
15:V:53:TYR:HA	15:V:101:THR:HG22	1.76	0.67
15:N:290:LEU:HD11	15:N:408:LEU:HD23	1.76	0.67
16:H:205:VAL:HG21	16:H:317:ALA:HB2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:168:GLU:HG2	15:V:169:GLY:H	1.59	0.67
10:P:35:LYS:O	10:P:40:LYS:NZ	2.24	0.67
1:1:165:THR:HG23	1:1:167:PHE:H	1.58	0.67
1:1:354:GLY:O	1:1:360:ARG:NH1	2.27	0.67
4:4:33:GLN:HE22	20:4:501:DCQ:H8A	1.59	0.67
14:U:208:PHE:O	14:U:211:HIS:ND1	2.27	0.67
4:4:205:GLU:OE1	4:4:284:ARG:NH2	2.27	0.67
3:D:186:ARG:HD3	3:D:229:ILE:HG22	1.75	0.67
10:P:95:GLY:HA3	11:R:136:LEU:HD11	1.77	0.67
10:A:41:LEU:HD22	16:H:75:ALA:H	1.59	0.67
6:G:143:ARG:NE	6:G:145:GLU:OE1	2.28	0.66
8:I:23:TYR:OH	8:I:123:ARG:NH1	2.24	0.66
6:6:62:ARG:HG2	16:H:48:PRO:HA	1.77	0.66
7:9:75:ASN:ND2	7:9:84:GLY:O	2.28	0.66
1:B:288:GLN:NE2	1:B:335:VAL:O	2.28	0.66
3:D:474:ARG:O	3:D:520:ARG:NH1	2.27	0.66
3:D:587:LEU:O	3:D:604:ALA:N	2.28	0.66
4:E:138:LEU:CD1	4:E:143:LEU:CD2	2.66	0.66
2:2:42:ARG:HB2	2:2:45:ARG:HG2	1.78	0.66
4:4:194:LEU:HD21	4:4:290:ILE:HG22	1.78	0.66
15:N:44:TRP:HE1	15:N:422:ALA:HB1	1.58	0.66
13:T:419:ARG:NH2	13:T:525:GLU:OE2	2.27	0.66
14:U:157:LEU:HB3	15:V:365:LEU:HB3	1.77	0.66
6:6:50:MET:O	6:6:53:SER:OG	2.13	0.66
13:L:70:ASP:H	13:L:73:SER:HB2	1.61	0.66
3:D:414:SER:OG	3:D:443:ARG:NH2	2.28	0.66
10:A:34:LYS:N	16:H:70:GLU:OE1	2.27	0.66
1:B:165:THR:HG23	1:B:167:PHE:H	1.61	0.66
15:N:309:LEU:HD22	15:N:378:LEU:HD11	1.78	0.66
13:T:328:PHE:O	13:T:332:LEU:CD1	2.44	0.66
4:4:147:PHE:HE2	16:H:45:ARG:HD3	1.60	0.66
15:N:128:GLN:OE1	15:N:306:ARG:NH2	2.29	0.66
2:2:77:LYS:H	2:2:116:LEU:HA	1.59	0.66
4:4:87:TYR:HB3	6:6:45:CYS:HB3	1.77	0.66
10:A:62:TYR:CD2	11:J:66:LEU:HD11	2.31	0.66
16:H:212:ALA:HA	16:H:218:PRO:HG3	1.77	0.66
13:T:214:VAL:HG13	13:T:219:GLN:HB2	1.77	0.66
13:T:359:LEU:HD23	13:T:437:GLU:HB3	1.79	0.66
3:D:723:ALA:HA	3:D:728:LEU:HD12	1.78	0.65
4:E:208:PHE:HE2	4:E:214:PHE:CZ	2.14	0.65
13:T:151:TYR:HB3	13:T:231:ALA:HB1	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:94:ASP:OD2	3:D:97:SER:OG	2.10	0.65
8:I:49:ASP:OD1	8:I:75:ARG:NE	2.28	0.65
16:Q:332:LEU:HB2	16:Q:333:PRO:HD3	1.78	0.65
7:9:40:ARG:NH2	7:9:118:ASP:OD1	2.29	0.65
11:J:157:VAL:HG12	11:J:159:PRO:HD3	1.79	0.65
13:L:325:HIS:NE2	13:L:329:LYS:HG3	2.11	0.65
15:N:168:GLU:HG2	15:N:169:GLY:H	1.61	0.65
3:D:373:GLY:HA3	3:D:538:ALA:HB2	1.77	0.65
14:U:332:LEU:O	14:U:336:THR:OG1	2.08	0.65
3:3:576:ALA:O	3:3:580:LYS:NZ	2.28	0.65
13:L:63:ILE:HG21	13:L:125:PRO:HG2	1.77	0.65
3:3:185:LYS:HB3	3:3:189:ARG:HH11	1.61	0.65
6:6:119:ASN:HA	6:6:125:GLN:HE22	1.61	0.65
13:L:422:VAL:HG22	13:L:426:LEU:HD22	1.77	0.65
15:N:136:TYR:OH	15:N:186:LYS:NZ	2.30	0.65
11:R:22:LEU:O	12:S:21:ARG:NH2	2.29	0.65
15:V:294:LEU:HD11	15:V:325:ALA:HB1	1.79	0.65
1:1:288:GLN:HE21	1:1:331:ILE:HG22	1.62	0.65
3:3:175:ILE:O	3:3:235:LEU:HA	1.96	0.65
7:9:43:LEU:HB2	7:9:137:LEU:HD12	1.78	0.65
13:L:105:PHE:O	13:L:109:ASN:ND2	2.30	0.65
4:E:163:VAL:HG13	4:E:164:THR:HG23	1.79	0.65
5:F:68:PHE:HB2	5:F:94:VAL:HB	1.77	0.65
6:G:106:ILE:HD11	6:G:154:LEU:HD22	1.79	0.65
11:J:130:LEU:HD12	12:K:51:LEU:CD2	2.26	0.65
13:T:334:LEU:HD12	13:T:449:LEU:HD11	1.78	0.65
13:L:214:VAL:HG13	13:L:219:GLN:HB2	1.79	0.65
4:4:161:GLU:HG2	7:9:34:LYS:HB2	1.79	0.65
1:B:380:GLU:N	1:B:383:ASP:OD2	2.30	0.65
7:O:117:TYR:HE2	7:O:166:VAL:HG12	1.62	0.65
15:N:262:SER:OG	15:N:288:TYR:OH	2.14	0.64
3:D:690:GLY:HA2	3:D:770:ARG:HB3	1.79	0.64
8:I:44:MET:HE2	8:I:46:ARG:HH22	1.62	0.64
14:U:151:PHE:HD1	14:U:203:ILE:HD11	1.61	0.64
3:D:233:GLY:HA2	3:D:236:LEU:HD21	1.79	0.64
3:D:621:VAL:HG23	3:D:672:ALA:HA	1.79	0.64
16:Q:216:ARG:HB2	16:Q:294:ARG:HD2	1.79	0.64
3:3:228:ASP:OD2	3:3:295:ARG:NH2	2.28	0.64
4:4:84:ARG:O	6:6:83:ARG:NH2	2.28	0.64
13:T:288:GLN:NE2	13:T:528:SER:O	2.31	0.64
13:T:314:ALA:HB1	13:T:317:VAL:HB	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:267:TRP:CG	16:Q:268:THR:N	2.66	0.64
3:3:285:VAL:HG13	3:3:286:ASN:H	1.61	0.64
3:D:34:CYS:O	3:D:189:ARG:NH2	2.30	0.64
4:E:208:PHE:CE2	4:E:214:PHE:CZ	2.86	0.64
14:U:12:PHE:HB3	14:U:100:LEU:HD13	1.79	0.64
1:1:5:ILE:H	1:1:12:ARG:HH22	1.45	0.64
1:1:104:ARG:NH1	1:1:108:GLU:OE2	2.31	0.64
4:4:81:TYR:OH	6:6:117:MET:O	2.12	0.64
7:9:71:GLU:HB2	7:9:90:VAL:HB	1.79	0.64
3:D:125:GLY:HA2	3:D:245:ARG:HH21	1.63	0.64
4:4:200:ARG:NH1	7:9:16:TYR:OH	2.31	0.64
4:E:138:LEU:HD12	4:E:143:LEU:HD23	1.77	0.64
13:T:246:VAL:HB	13:T:303:LEU:HD21	1.78	0.64
16:H:211:MET:HG3	16:H:218:PRO:HD3	1.80	0.64
1:B:190:ASN:ND2	1:B:198:ASN:O	2.30	0.64
5:F:31:ARG:NH2	5:F:98:ASP:OD2	2.31	0.64
8:I:74:PRO:HG2	8:I:77:ALA:HB2	1.78	0.64
8:I:98:GLU:HG2	8:I:104:VAL:HG21	1.79	0.64
4:4:40:VAL:HG21	6:6:88:MET:HE2	1.80	0.64
10:A:100:THR:HG21	16:H:322:LEU:HD11	1.79	0.64
16:H:267:TRP:CG	16:H:268:THR:N	2.66	0.64
8:7:88:ARG:HH21	8:7:126:LEU:HB3	1.63	0.63
14:U:235:LYS:HD3	14:U:293:MET:HG3	1.80	0.63
16:H:141:TRP:HE3	16:H:149:LEU:HD21	1.63	0.63
1:B:425:ALA:O	1:B:428:LYS:NZ	2.30	0.63
7:9:10:LEU:HD12	16:H:296:THR:HG21	1.81	0.63
6:G:50:MET:O	6:G:53:SER:OG	2.15	0.63
13:L:151:TYR:HB3	13:L:231:ALA:HB1	1.81	0.63
11:R:119:LEU:HD21	12:S:47:ARG:HA	1.81	0.63
13:T:305:TYR:OH	13:T:406:ALA:O	2.14	0.63
15:V:261:SER:HG	15:V:375:TYR:HH	1.44	0.63
15:V:343:TRP:CE2	15:V:416:PRO:HG3	2.34	0.63
3:D:226:ILE:HD12	3:D:235:LEU:HD13	1.80	0.63
10:P:62:TYR:HD2	11:R:66:LEU:HD11	1.64	0.63
11:R:64:VAL:HG13	16:Q:134:TYR:OH	1.97	0.63
11:J:130:LEU:HD11	12:K:51:LEU:HD22	1.81	0.63
4:E:173:ILE:O	4:E:174:ARG:NH1	2.31	0.63
13:T:105:PHE:O	13:T:109:ASN:ND2	2.32	0.63
15:V:103:HIS:CE1	15:V:161:LEU:HB2	2.34	0.63
4:4:333:GLU:OE2	4:4:336:HIS:NE2	2.32	0.63
13:L:359:LEU:HD23	13:L:437:GLU:HB3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:234:ALA:HB1	15:N:360:VAL:HG21	1.80	0.63
6:G:58:ASN:ND2	6:G:145:GLU:OE2	2.32	0.63
11:R:64:VAL:HA	11:R:67:PHE:HB2	1.81	0.63
15:V:92:ALA:HA	15:V:95:MET:HE2	1.79	0.63
1:1:184:GLU:OE1	1:1:186:THR:OG1	2.13	0.63
2:2:24:ARG:HH21	2:2:59:GLU:HB3	1.64	0.63
6:6:53:SER:O	6:6:60:LEU:N	2.31	0.63
6:6:94:ARG:O	6:6:98:GLN:N	2.32	0.63
3:D:203:ILE:HG22	3:D:204:GLU:HG3	1.80	0.63
11:J:130:LEU:CD1	12:K:51:LEU:HD23	2.29	0.62
14:M:268:ALA:HA	14:M:291:SER:HA	1.79	0.62
1:B:293:GLY:O	1:B:327:GLY:N	2.31	0.62
4:E:143:LEU:HD21	16:Q:226:GLN:HE21	1.63	0.62
7:O:18:PHE:O	7:O:20:LYS:NZ	2.32	0.62
4:4:261:THR:H	4:4:292:GLN:HE22	1.47	0.62
15:N:317:ARG:NH1	15:N:384:ALA:O	2.32	0.62
3:3:697:THR:OG1	3:3:762:ALA:O	2.16	0.62
14:M:16:LEU:HD22	14:M:97:GLY:H	1.65	0.62
3:3:120:PRO:HA	4:4:328:PHE:HE2	1.62	0.62
4:4:336:HIS:ND1	5:5:189:ARG:O	2.31	0.62
6:6:60:LEU:HG	6:6:65:SER:HB2	1.81	0.62
7:9:68:ILE:HG12	7:9:93:ILE:HG12	1.80	0.62
14:M:56:LEU:HD11	15:N:416:PRO:HG2	1.81	0.62
15:N:53:TYR:HA	15:N:101:THR:HG22	1.82	0.62
4:E:48:SER:H	4:E:53:LEU:HD23	1.64	0.62
4:E:73:ARG:NE	4:E:81:TYR:OH	2.33	0.62
4:E:343:TYR:HB2	4:E:356:TYR:HD1	1.63	0.62
13:T:278:ALA:HB1	13:T:409:VAL:HG11	1.79	0.62
13:T:291:ILE:HD12	13:T:336:SER:HB3	1.82	0.62
2:2:71:GLN:NE2	2:2:120:GLN:OE1	2.32	0.62
4:4:112:ARG:NH2	4:4:181:ASP:OD1	2.32	0.62
4:4:314:ARG:NH2	7:9:106:GLU:O	2.33	0.62
4:E:171:ASN:OD1	4:E:174:ARG:NH1	2.30	0.62
16:Q:227:GLU:HB2	16:Q:299:ARG:NH1	2.15	0.62
14:M:332:LEU:O	14:M:336:THR:OG1	2.10	0.62
11:R:29:ALA:O	11:R:33:ILE:HG13	2.00	0.62
13:L:359:LEU:O	13:L:363:ARG:NH1	2.32	0.62
16:H:29:ALA:O	16:H:32:THR:OG1	2.18	0.62
1:B:365:GLY:O	1:B:369:ASN:ND2	2.31	0.62
2:C:77:LYS:H	2:C:116:LEU:HA	1.65	0.62
6:G:37:TRP:CZ2	6:G:67:VAL:HB	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:114:ASN:HA	3:3:161:ARG:HG2	1.82	0.62
3:3:404:GLU:OE1	3:3:698:MET:N	2.20	0.62
2:C:56:THR:OG1	3:D:198:GLU:O	2.12	0.62
4:E:131:VAL:HG23	4:E:153:ARG:HD2	1.82	0.62
7:O:110:THR:OG1	17:O:202:SF4:S2	2.56	0.62
16:Q:332:LEU:HB2	16:Q:333:PRO:CD	2.29	0.62
3:3:346:ALA:HA	3:3:372:GLN:HB2	1.81	0.62
11:R:93:ALA:HB2	13:T:591:LEU:HD11	1.80	0.62
15:V:73:THR:HB	15:V:209:LEU:HD22	1.80	0.62
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.82	0.61
3:3:256:CYS:HB2	3:3:265:ILE:HD13	1.82	0.61
11:J:22:LEU:HD13	11:J:27:HIS:HB3	1.82	0.61
13:L:163:ARG:HE	14:M:399:VAL:HB	1.64	0.61
11:R:17:VAL:O	11:R:21:THR:OG1	2.16	0.61
15:V:279:GLN:NE2	15:V:420:LEU:O	2.32	0.61
1:1:404:ASP:HA	1:1:407:VAL:HG22	1.81	0.61
3:3:129:GLU:O	3:3:133:ARG:HG2	2.00	0.61
11:J:29:ALA:O	11:J:33:ILE:HG13	2.00	0.61
10:P:113:LYS:NZ	15:V:83:GLU:OE2	2.33	0.61
16:Q:290:PHE:O	16:Q:294:ARG:HG2	1.99	0.61
3:3:287:GLU:OE1	3:3:289:TRP:NE1	2.32	0.61
6:6:37:TRP:HB2	16:H:65:LYS:HE2	1.80	0.61
10:A:109:TYR:OH	10:A:113:LYS:NZ	2.26	0.61
15:N:24:GLY:HA2	15:N:27:ARG:HD2	1.81	0.61
1:B:241:MET:O	1:B:248:GLY:N	2.33	0.61
3:D:404:GLU:OE1	3:D:698:MET:N	2.31	0.61
4:E:315:HIS:HA	8:I:46:ARG:CZ	2.31	0.61
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.83	0.61
11:J:133:GLY:H	11:J:136:LEU:HB2	1.65	0.61
3:D:40:SER:O	3:D:189:ARG:NE	2.27	0.61
4:E:62:LEU:HD21	6:G:43:LEU:HB3	1.82	0.61
2:2:110:GLU:OE2	8:7:114:ARG:NE	2.26	0.61
5:5:121:LEU:HA	5:5:145:PRO:HD2	1.82	0.61
1:B:305:GLU:O	1:B:309:THR:OG1	2.17	0.61
3:D:29:ASP:OD2	5:F:187:GLY:N	2.28	0.61
3:3:42:ILE:HD12	3:3:42:ILE:O	2.00	0.61
13:L:502:LEU:HD23	13:L:505:LEU:HD12	1.82	0.61
6:G:69:ARG:NH2	16:Q:225:GLU:OE2	2.34	0.61
10:P:57:PHE:HB3	10:P:58:PRO:HD2	1.81	0.61
13:T:171:LEU:HB3	13:T:208:LEU:HD13	1.82	0.61
1:1:60:SER:HB2	1:1:230:ILE:HD13	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:59:ASP:OD1	6:6:62:ARG:NH2	2.33	0.61
16:H:198:TYR:O	16:H:341:SER:OG	2.17	0.61
8:7:98:GLU:HG2	8:7:104:VAL:HG21	1.83	0.61
10:A:105:VAL:HG13	15:N:15:LEU:HD21	1.81	0.61
14:M:304:THR:O	14:M:307:GLY:N	2.33	0.61
1:B:104:ARG:NH1	1:B:108:GLU:OE2	2.33	0.61
3:D:349:ALA:O	3:D:540:ASN:ND2	2.29	0.61
3:D:285:VAL:HG13	3:D:286:ASN:H	1.66	0.61
4:E:373:PRO:O	4:E:377:ASN:ND2	2.34	0.61
6:6:30:TRP:O	6:6:34:ASN:ND2	2.34	0.61
10:A:65:ALA:O	10:A:69:ILE:HG23	2.01	0.61
11:J:83:PHE:O	12:K:22:ARG:NH1	2.33	0.61
2:2:130:THR:HB	2:2:143:GLU:HB3	1.83	0.60
6:6:160:GLY:O	6:6:169:ARG:NH1	2.33	0.60
13:L:255:ARG:HA	13:L:477:LEU:HD23	1.83	0.60
2:C:28:MET:O	2:C:70:TYR:OH	2.17	0.60
3:D:46:ARG:HH22	3:D:81:ALA:HB2	1.66	0.60
4:E:72:HIS:HB3	5:F:171:ARG:HE	1.66	0.60
9:X:46:TYR:HB2	9:X:63:PHE:HB2	1.82	0.60
12:S:94:ARG:NH2	13:T:585:TYR:OH	2.28	0.60
1:1:212:TRP:HE1	2:2:22:GLY:HA3	1.66	0.60
3:3:382:PHE:HB3	3:3:532:VAL:HB	1.83	0.60
10:A:57:PHE:HB3	10:A:58:PRO:HD2	1.82	0.60
4:E:367:ARG:HH12	4:E:369:LYS:HB2	1.66	0.60
5:F:13:LYS:NZ	5:F:37:GLU:OE2	2.28	0.60
14:U:427:GLY:HA2	14:U:430:TRP:HD1	1.65	0.60
4:4:152:GLU:OE2	4:4:200:ARG:NE	2.34	0.60
10:A:3:PRO:HD2	16:H:2:THR:HB	1.83	0.60
6:G:74:GLN:NE2	16:Q:233:HIS:HB2	2.16	0.60
16:Q:17:ALA:O	16:Q:21:VAL:HG23	2.02	0.60
3:3:715:GLU:H	3:3:761:SER:HB2	1.65	0.60
6:6:56:ALA:HA	16:H:45:ARG:HB2	1.82	0.60
6:G:134:ASP:OD1	6:G:157:LYS:NZ	2.32	0.60
13:T:139:PHE:HB2	13:T:159:PHE:HB2	1.83	0.60
13:T:356:TRP:HB2	13:T:425:PHE:HB3	1.83	0.60
1:1:274:GLU:HG3	1:1:278:GLU:HG3	1.82	0.60
3:3:165:ASP:HB2	8:7:66:PRO:HG2	1.83	0.60
14:M:49:HIS:HD2	14:M:67:LEU:HD22	1.66	0.60
5:F:151:PRO:HD3	9:X:112:LYS:HE2	1.83	0.60
14:U:313:TYR:OH	14:U:443:MET:O	2.18	0.60
4:4:254:TYR:OH	4:4:346:THR:OG1	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:7:TYR:OH	16:H:119:ASP:OD1	2.20	0.60
11:J:50:PHE:HB2	11:J:124:PRO:HD3	1.83	0.60
1:B:63:ARG:O	1:B:65:ARG:NE	2.32	0.60
3:D:48:CYS:SG	3:D:83:CYS:N	2.75	0.60
16:Q:177:VAL:HG11	16:Q:185:ILE:HG12	1.83	0.60
6:6:39:ALA:HB2	6:6:75:ALA:HB3	1.84	0.60
1:B:372:ALA:O	1:B:376:THR:OG1	2.14	0.60
1:B:388:GLU:OE2	1:B:418:LYS:NZ	2.34	0.60
15:V:132:ALA:HB1	15:V:199:VAL:HA	1.84	0.60
1:1:92:ASN:HB3	1:1:220:ASN:HA	1.84	0.60
4:4:45:VAL:HG13	4:4:55:VAL:HG22	1.83	0.60
6:G:165:GLU:HG2	7:O:148:ARG:NH1	2.17	0.60
10:P:52:GLY:O	16:Q:146:LYS:NZ	2.27	0.60
15:V:33:LEU:HB2	15:V:71:LEU:HD21	1.82	0.60
3:3:587:LEU:O	3:3:604:ALA:N	2.35	0.60
3:3:611:ARG:HA	3:3:624:LEU:O	2.02	0.60
13:L:419:ARG:NH2	13:L:525:GLU:OE2	2.29	0.60
8:I:88:ARG:HH21	8:I:126:LEU:HB3	1.67	0.60
13:T:286:PHE:O	13:T:419:ARG:NH1	2.34	0.60
13:T:358:HIS:ND1	13:T:429:GLU:OE2	2.32	0.60
1:1:95:GLU:OE2	1:1:102:LYS:N	2.34	0.60
4:4:236:GLY:N	4:4:377:ASN:OD1	2.26	0.60
13:L:162:ASN:OD1	13:L:216:LYS:NZ	2.34	0.60
14:M:221:ASN:ND2	14:M:228:ASP:OD1	2.35	0.60
4:E:333:GLU:OE2	4:E:336:HIS:NE2	2.34	0.60
11:R:68:LEU:HD23	11:R:71:ILE:HD11	1.84	0.60
14:U:56:LEU:HD11	15:V:416:PRO:HG2	1.82	0.60
1:1:354:GLY:HA2	1:1:360:ARG:HB2	1.85	0.59
3:3:208:HIS:O	8:7:85:ARG:NH2	2.25	0.59
11:J:69:PHE:CZ	16:H:156:SER:HB3	2.38	0.59
13:L:17:LEU:HB2	13:L:106:ALA:HB2	1.84	0.59
16:H:17:ALA:O	16:H:21:VAL:HG23	2.02	0.59
14:U:304:THR:O	14:U:307:GLY:N	2.35	0.59
16:Q:39:LEU:O	16:Q:43:GLN:HG2	2.02	0.59
1:1:4:PRO:HA	1:1:12:ARG:HH12	1.68	0.59
2:2:107:GLY:H	2:2:110:GLU:HG3	1.66	0.59
3:D:551:PRO:HB2	3:D:555:GLY:HA2	1.83	0.59
14:U:157:LEU:HD12	15:V:369:ALA:HB2	1.84	0.59
16:Q:168:LEU:HD12	16:Q:314:PHE:HB3	1.84	0.59
1:1:15:ARG:HH22	1:1:279:TRP:HH2	1.50	0.59
4:E:87:TYR:CB	6:G:45:CYS:HB3	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:490:GLU:O	13:T:494:ILE:HG12	2.02	0.59
16:Q:189:GLN:HG2	16:Q:195:LEU:H	1.67	0.59
1:B:201:LEU:HG	1:B:203:PRO:HD2	1.84	0.59
4:4:201:ILE:HG21	4:4:284:ARG:HG3	1.83	0.59
13:L:314:ALA:HB1	13:L:317:VAL:HB	1.83	0.59
16:H:332:LEU:HB2	16:H:333:PRO:CD	2.31	0.59
1:B:338:VAL:HG21	1:B:424:LEU:HD22	1.85	0.59
3:D:190:TYR:OH	3:D:222:PHE:O	2.16	0.59
10:A:5:GLN:OE1	16:H:10:TYR:OH	2.19	0.59
3:D:8:ASP:OD2	3:D:28:TYR:OH	2.20	0.59
7:O:13:THR:HB	16:Q:42:PHE:CE1	2.38	0.59
13:T:487:LEU:HA	13:T:490:GLU:HG2	1.84	0.59
14:U:237:GLY:O	14:U:241:PHE:N	2.28	0.59
4:4:367:ARG:NH1	4:4:369:LYS:HB2	2.18	0.59
3:D:274:LEU:H	3:D:302:ASP:HB3	1.68	0.59
4:E:30:VAL:HB	4:E:43:LEU:HB2	1.84	0.59
6:G:73:ARG:NH2	10:P:42:MET:O	2.34	0.59
7:O:45:ARG:NH2	7:O:137:LEU:HD23	2.18	0.59
13:T:103:ARG:NH2	13:T:144:PHE:O	2.31	0.59
14:U:345:ARG:HG2	14:U:412:LYS:O	2.03	0.59
15:V:102:ARG:HD3	15:V:163:LEU:HB2	1.82	0.59
1:1:259:LYS:NZ	2:2:178:GLU:OE2	2.35	0.59
10:A:66:MET:O	10:A:69:ILE:HG12	2.03	0.59
1:B:316:LEU:HD13	1:B:323:LEU:HB2	1.83	0.59
6:G:61:ALA:HA	6:G:66:GLU:HB2	1.84	0.59
5:5:59:THR:O	5:5:59:THR:HG22	2.02	0.59
13:L:377:PRO:HG3	13:L:498:ALA:HB1	1.84	0.59
7:O:10:LEU:O	7:O:13:THR:OG1	2.20	0.59
16:Q:205:VAL:HG21	16:Q:317:ALA:HB2	1.85	0.59
1:1:365:GLY:O	1:1:369:ASN:ND2	2.35	0.59
3:3:34:CYS:O	3:3:189:ARG:NH2	2.34	0.59
3:D:297:GLY:O	3:D:703:GLN:NE2	2.34	0.59
14:U:85:GLY:O	14:U:89:ALA:HB2	2.01	0.59
4:4:87:TYR:CB	6:6:45:CYS:HB3	2.33	0.58
7:9:63:CYS:HA	17:9:201:SF4:S2	2.43	0.58
10:A:74:GLU:HB2	10:A:103:LEU:HD22	1.85	0.58
3:D:198:GLU:OE2	3:D:440:ARG:NH1	2.28	0.58
3:D:311:VAL:HG23	3:D:600:VAL:HG22	1.85	0.58
3:D:399:LEU:O	3:D:508:GLY:N	2.35	0.58
4:E:167:ARG:HD3	6:G:143:ARG:NH1	2.18	0.58
10:P:64:VAL:HA	10:P:67:LEU:HD22	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:234:ALA:HB1	15:V:360:VAL:HG21	1.85	0.58
16:Q:150:LEU:O	16:Q:154:ARG:HG3	2.03	0.58
1:1:239:ALA:HA	1:1:247:LYS:HB3	1.83	0.58
3:3:109:GLU:OE1	3:3:156:ARG:NH2	2.36	0.58
3:D:455:ARG:HH21	3:D:750:ARG:NH2	1.99	0.58
16:Q:271:VAL:HG12	16:Q:272:LEU:HG	1.83	0.58
13:L:149:PRO:HG3	14:M:416:GLU:HG2	1.84	0.58
14:M:338:THR:HG22	14:M:340:GLU:H	1.68	0.58
1:B:83:ASP:OD2	1:B:87:HIS:NE2	2.37	0.58
3:D:694:LEU:HB3	3:D:762:ALA:HB2	1.86	0.58
4:E:217:ARG:HD2	16:Q:301:ARG:HH11	1.68	0.58
15:V:119:TYR:CZ	15:V:137:PHE:HA	2.38	0.58
15:V:271:LEU:HD23	15:V:352:ALA:HB2	1.84	0.58
14:M:13:GLY:HA2	14:M:97:GLY:HA2	1.84	0.58
1:B:63:ARG:NE	1:B:69:GLY:O	2.37	0.58
3:D:615:VAL:HG22	3:D:621:VAL:HG12	1.85	0.58
14:U:402:SER:HA	14:U:405:TYR:CE2	2.38	0.58
1:1:241:MET:O	1:1:248:GLY:N	2.32	0.58
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.86	0.58
3:3:635:GLU:OE2	9:W:7:ARG:NH1	2.37	0.58
13:L:4:LEU:HG	13:L:8:LEU:HG	1.86	0.58
15:N:185:PHE:O	15:N:195:TRP:NE1	2.36	0.58
16:H:45:ARG:HG2	16:H:46:MET:N	2.18	0.58
6:G:54:THR:HA	6:G:60:LEU:H	1.69	0.58
13:T:502:LEU:HD23	13:T:505:LEU:HD12	1.86	0.58
16:Q:291:ILE:HA	16:Q:294:ARG:CG	2.33	0.58
4:4:341:GLU:HA	4:4:357:ILE:O	2.04	0.58
6:6:62:ARG:HD2	16:H:50:ARG:HH21	1.67	0.58
16:H:127:ALA:O	16:H:131:LEU:HG	2.03	0.58
4:E:403:VAL:HG12	4:E:406:ASP:H	1.67	0.58
11:R:119:LEU:HD11	12:S:47:ARG:HG3	1.85	0.58
13:T:234:THR:HG23	13:T:292:LYS:HE2	1.86	0.58
1:1:63:ARG:H	1:1:65:ARG:HH21	1.50	0.58
2:2:173:GLY:HA3	2:2:176:VAL:O	2.03	0.58
3:3:384:PRO:HG3	3:3:542:ARG:NH1	2.19	0.58
11:J:107:GLY:HA3	15:N:174:LEU:HD22	1.86	0.58
4:E:62:LEU:HD11	6:G:43:LEU:O	2.03	0.58
13:T:394:THR:HB	13:T:484:HIS:O	2.04	0.58
4:4:30:VAL:HB	4:4:43:LEU:HB2	1.85	0.58
9:W:71:GLU:OE1	3:D:527:ARG:HD3	2.03	0.58
11:J:135:TRP:HZ2	12:K:52:ASP:HB3	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:345:PRO:HB3	5:F:87:ARG:NH1	2.19	0.58
3:3:81:ALA:O	3:3:85:THR:OG1	2.15	0.58
3:3:94:ASP:OD2	3:3:97:SER:OG	2.17	0.58
5:5:68:PHE:HB2	5:5:94:VAL:HB	1.85	0.58
4:E:185:GLU:OE1	4:E:185:GLU:N	2.35	0.58
4:E:224:ILE:HD11	4:E:275:ARG:CZ	2.34	0.58
16:Q:96:ALA:HB1	16:Q:125:LEU:HD23	1.86	0.58
14:M:91:VAL:HG12	14:M:222:HIS:CE1	2.39	0.58
3:D:445:THR:HB	3:D:463:ALA:HB2	1.85	0.58
1:1:387:LEU:HA	1:1:390:LEU:HD12	1.86	0.57
3:3:462:ALA:O	3:3:465:HIS:ND1	2.37	0.57
15:N:6:LEU:HB3	15:N:93:LEU:HD12	1.85	0.57
6:G:37:TRP:HH2	16:Q:36:ARG:HH22	1.51	0.57
7:O:51:GLU:OE1	7:O:133:LYS:NZ	2.24	0.57
16:Q:120:LEU:HD22	16:Q:180:LEU:HD12	1.85	0.57
1:1:373:LYS:HA	8:7:79:LEU:HD11	1.86	0.57
3:3:271:SER:HG	7:9:69:TYR:HH	1.51	0.57
3:3:722:THR:HG21	3:3:756:GLY:H	1.69	0.57
7:9:110:THR:OG1	17:9:202:SF4:S2	2.56	0.57
10:A:69:ILE:HG22	11:J:62:ALA:HB1	1.85	0.57
14:M:91:VAL:HG23	14:M:92:GLU:H	1.69	0.57
14:M:333:TYR:O	14:M:337:GLY:N	2.37	0.57
1:B:8:GLY:HA2	1:B:270:THR:HG22	1.84	0.57
1:B:92:ASN:N	1:B:219:ASN:O	2.28	0.57
16:Q:101:PRO:HA	16:Q:114:TRP:HB3	1.86	0.57
1:1:32:TYR:OH	1:1:116:GLU:OE1	2.16	0.57
3:3:226:ILE:HD12	3:3:235:LEU:HD13	1.85	0.57
3:3:494:LYS:O	3:3:498:GLU:HG2	2.03	0.57
13:L:600:LEU:HD11	15:N:232:ALA:HB1	1.85	0.57
1:B:132:ILE:HD11	1:B:171:LEU:HD13	1.85	0.57
4:E:84:ARG:HG3	4:E:169:HIS:CE1	2.40	0.57
3:3:113:LEU:O	3:3:161:ARG:NH1	2.37	0.57
7:9:96:LEU:HD21	7:9:129:LEU:HD13	1.85	0.57
13:L:103:ARG:NH2	13:L:144:PHE:O	2.37	0.57
3:D:728:LEU:HB3	3:D:747:VAL:HG11	1.86	0.57
4:E:252:TYR:OH	5:F:85:GLY:O	2.19	0.57
5:F:2:ARG:NH2	5:F:82:ASP:O	2.37	0.57
2:2:146:THR:HG22	2:2:149:ARG:HB2	1.85	0.57
11:J:69:PHE:HZ	16:H:156:SER:HB3	1.69	0.57
13:L:234:THR:HG23	13:L:292:LYS:HE2	1.86	0.57
4:E:103:LYS:NZ	5:F:22:LEU:O	2.21	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:59:TYR:O	11:R:64:VAL:HG12	2.05	0.57
7:9:33:LEU:HD11	7:9:119:PHE:HE2	1.70	0.57
16:H:137:PHE:HA	16:H:152:SER:HB2	1.86	0.57
3:D:250:GLU:HG3	5:F:169:GLU:HG3	1.86	0.57
10:P:81:TYR:HB2	11:R:132:TYR:CZ	2.39	0.57
14:U:203:ILE:HG13	14:U:210:LEU:HB3	1.86	0.57
1:1:149:ILE:HG22	1:1:153:ARG:HE	1.70	0.57
3:3:248:GLU:HG2	5:5:170:PHE:CE1	2.40	0.57
5:5:75:VAL:HG13	5:5:87:ARG:HB2	1.87	0.57
13:L:490:GLU:O	13:L:494:ILE:HG12	2.04	0.57
4:E:31:GLY:HA3	10:P:45:GLU:OE2	2.05	0.57
16:Q:141:TRP:CE3	16:Q:149:LEU:HD11	2.40	0.57
3:3:397:LEU:HD21	3:3:480:LEU:HD13	1.87	0.57
15:N:98:LEU:HD23	15:N:218:ALA:HB1	1.87	0.57
15:N:343:TRP:CD1	15:N:413:GLY:HA2	2.39	0.57
7:O:41:HIS:HB3	7:O:113:ILE:HD11	1.86	0.57
13:T:55:PHE:O	13:T:66:SER:HA	2.04	0.57
13:T:557:ASP:OD1	14:U:211:HIS:NE2	2.32	0.57
15:V:340:ALA:HA	15:V:343:TRP:HD1	1.69	0.57
3:3:300:TRP:CD1	3:3:703:GLN:HA	2.39	0.57
4:4:181:ASP:O	7:9:36:ARG:NH2	2.29	0.57
6:6:134:ASP:OD1	6:6:157:LYS:NZ	2.38	0.57
16:H:227:GLU:HG2	16:H:228:LEU:H	1.70	0.57
1:B:189:MET:SD	1:B:216:THR:OG1	2.60	0.57
4:E:68:LYS:NZ	5:F:150:TYR:O	2.28	0.57
6:G:60:LEU:HG	6:G:65:SER:HB2	1.87	0.57
6:G:145:GLU:HG2	7:O:31:VAL:HG21	1.87	0.57
7:9:123:ASP:OD1	7:9:124:TYR:N	2.36	0.57
15:N:92:ALA:HA	15:N:95:MET:HE2	1.86	0.57
16:H:136:ILE:HG23	16:H:232:TYR:HD2	1.70	0.57
13:T:529:ARG:NH2	13:T:530:GLU:OE2	2.38	0.57
9:X:37:TRP:HE1	9:X:40:LYS:HD2	1.70	0.56
14:U:62:TYR:HE2	14:U:174:THR:HG21	1.69	0.56
1:1:238:PHE:CZ	1:1:248:GLY:HA3	2.41	0.56
13:L:66:SER:HB2	13:L:122:ASP:HB3	1.87	0.56
15:N:224:LEU:HD11	15:N:281:LEU:HD23	1.87	0.56
1:1:360:ARG:NE	1:1:361:GLU:OE2	2.38	0.56
1:1:437:TRP:O	2:2:147:ARG:NH2	2.38	0.56
3:3:506:ILE:HG12	3:3:533:LEU:HB2	1.87	0.56
3:3:740:PHE:HE2	3:3:771:VAL:HG11	1.70	0.56
4:4:48:SER:H	4:4:53:LEU:HD23	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:165:GLU:OE2	7:9:148:ARG:NH1	2.38	0.56
7:9:120:GLU:OE1	7:9:146:GLN:NE2	2.39	0.56
15:N:294:LEU:HD12	15:N:405:ALA:HB3	1.87	0.56
1:B:323:LEU:HD11	1:B:326:GLY:HA2	1.86	0.56
5:F:73:GLU:OE2	5:F:87:ARG:NH1	2.39	0.56
10:P:1:MET:O	16:Q:2:THR:N	2.39	0.56
10:P:105:VAL:HG11	15:V:11:VAL:HG13	1.87	0.56
14:U:328:LEU:HD23	14:U:332:LEU:HD23	1.87	0.56
16:Q:2:THR:HG23	16:Q:5:TYR:HD2	1.69	0.56
3:3:399:LEU:O	3:3:508:GLY:N	2.38	0.56
6:6:54:THR:HA	6:6:59:ASP:HA	1.87	0.56
13:L:328:PHE:O	13:L:332:LEU:CD1	2.54	0.56
15:V:203:SER:HB2	15:V:208:VAL:HG22	1.86	0.56
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.86	0.56
16:H:5:TYR:OH	16:H:184:ASP:OD1	2.19	0.56
16:H:186:VAL:HG11	16:H:267:TRP:CZ3	2.40	0.56
3:D:261:VAL:HG21	3:D:408:ILE:HG12	1.88	0.56
8:I:82:ILE:HG23	8:I:95:ALA:HB3	1.85	0.56
13:T:373:LEU:HD21	13:T:416:TYR:HE1	1.70	0.56
14:U:349:GLN:NE2	14:U:418:GLY:HA3	2.20	0.56
15:V:279:GLN:HG3	15:V:423:LEU:HB2	1.86	0.56
4:4:73:ARG:NH2	4:4:81:TYR:OH	2.38	0.56
3:D:51:ARG:HB3	3:D:94:ASP:HB3	1.87	0.56
3:D:261:VAL:O	3:D:616:ASN:ND2	2.35	0.56
7:O:30:PRO:HB2	7:O:162:VAL:HG22	1.87	0.56
15:V:115:SER:HA	15:V:118:LEU:HD12	1.88	0.56
1:1:343:ASN:HB2	2:2:89:LYS:HZ3	1.70	0.56
3:3:338:GLY:O	3:3:366:THR:HB	2.06	0.56
13:L:422:VAL:HA	13:L:426:LEU:HD13	1.86	0.56
3:D:256:CYS:HB2	3:D:265:ILE:HD13	1.88	0.56
3:D:494:LYS:O	3:D:498:GLU:HG2	2.05	0.56
11:R:146:LEU:O	11:R:150:THR:HG23	2.06	0.56
3:3:261:VAL:O	3:3:616:ASN:ND2	2.37	0.56
4:4:128:SER:HG	4:4:350:ARG:NH2	2.03	0.56
10:A:56:ARG:HD3	11:J:74:LEU:HA	1.88	0.56
1:B:274:GLU:HG3	1:B:278:GLU:HG3	1.86	0.56
9:X:74:LEU:HD21	9:X:126:TYR:HB3	1.86	0.56
13:T:177:TRP:HE3	13:T:183:LEU:HG	1.71	0.56
16:Q:45:ARG:HG2	16:Q:46:MET:N	2.21	0.56
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.86	0.56
16:H:131:LEU:HA	16:H:134:TYR:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:TRP:CD1	2:C:74:PRO:HA	2.41	0.56
3:D:559:ASP:OD2	3:D:686:LYS:NZ	2.38	0.56
3:D:664:LEU:HD22	3:D:669:VAL:HG11	1.87	0.56
4:E:236:GLY:HA2	4:E:351:GLY:HA3	1.87	0.56
6:G:178:ARG:NH1	9:X:122:ASP:OD2	2.38	0.56
10:P:68:PHE:CD2	16:Q:164:LEU:HB2	2.41	0.56
15:V:265:HIS:HA	15:V:268:TYR:CD2	2.41	0.56
3:3:474:ARG:O	3:3:520:ARG:NH1	2.39	0.56
4:4:352:GLU:CD	5:5:87:ARG:HH22	2.08	0.56
14:M:102:MET:HB3	14:M:230:LEU:HD23	1.88	0.56
10:P:109:TYR:HE1	15:V:82:PHE:HZ	1.54	0.56
14:U:333:TYR:O	14:U:337:GLY:N	2.39	0.56
15:V:33:LEU:HD22	15:V:67:LEU:HD22	1.87	0.56
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.88	0.55
3:3:710:GLU:O	3:3:713:ARG:NH1	2.35	0.55
1:B:203:PRO:HB2	1:B:204:PRO:HD3	1.88	0.55
3:D:185:LYS:HB3	3:D:189:ARG:HH11	1.71	0.55
13:T:247:THR:HG22	13:T:322:VAL:HG13	1.88	0.55
4:4:75:TYR:CZ	4:4:337:PRO:HG2	2.41	0.55
13:L:409:VAL:HA	13:L:412:LEU:HD12	1.87	0.55
14:M:54:PRO:HA	14:M:62:TYR:HD1	1.70	0.55
1:B:259:LYS:HB3	1:B:281:GLY:HA3	1.87	0.55
3:D:409:LEU:HD12	3:D:535:MET:HE3	1.88	0.55
4:E:84:ARG:CZ	4:E:169:HIS:HB3	2.35	0.55
11:R:151:VAL:HG11	15:V:90:TYR:HE2	1.71	0.55
13:T:463:HIS:CG	13:T:464:PRO:HD3	2.42	0.55
15:V:275:THR:OG1	15:V:351:GLU:OE1	2.20	0.55
4:4:185:GLU:OE2	7:9:165:TYR:OH	2.18	0.55
3:D:609:GLU:HA	3:D:627:ALA:H	1.71	0.55
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.87	0.55
9:W:43:GLN:NE2	3:D:522:ARG:HH22	2.05	0.55
10:A:67:LEU:HB3	16:H:310:TRP:HZ2	1.70	0.55
2:C:110:GLU:HA	8:I:121:ARG:HH12	1.71	0.55
10:P:71:PHE:CZ	10:P:107:PHE:HB2	2.41	0.55
1:1:219:ASN:ND2	18:1:502:FMN:O2P	2.40	0.55
9:W:37:TRP:CD1	9:W:40:LYS:HD2	2.42	0.55
14:M:126:LEU:HD11	14:M:149:VAL:HG22	1.89	0.55
15:N:209:LEU:HB2	15:N:296:PHE:HB3	1.88	0.55
4:E:114:GLU:O	4:E:118:VAL:HG13	2.06	0.55
4:E:376:VAL:HA	4:E:379:GLN:HE21	1.72	0.55
5:F:99:PRO:HB2	5:F:124:ILE:HA	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:40:ARG:NH2	7:O:118:ASP:OD1	2.38	0.55
8:I:60:SER:HA	8:I:66:PRO:HA	1.87	0.55
13:T:122:ASP:OD2	13:T:184:SER:OG	2.21	0.55
14:U:321:TYR:CE1	14:U:365:MET:HA	2.42	0.55
4:4:86:ASP:HB3	4:4:93:HIS:CD2	2.42	0.55
4:4:148:TYR:HB3	4:4:200:ARG:NH2	2.22	0.55
7:9:40:ARG:HH12	7:9:42:VAL:HG12	1.72	0.55
10:A:68:PHE:CD2	16:H:164:LEU:HB2	2.40	0.55
11:J:130:LEU:HD12	12:K:51:LEU:HD23	1.86	0.55
13:L:160:ILE:O	13:L:164:ILE:HG13	2.07	0.55
14:M:350:SER:HB3	14:M:421:GLY:HA2	1.88	0.55
2:2:74:PRO:HB2	8:7:121:ARG:HE	1.71	0.55
3:3:337:ARG:NH1	3:3:565:TYR:OH	2.38	0.55
3:3:713:ARG:NE	3:3:746:ARG:HE	2.04	0.55
1:B:90:ILE:HD11	1:B:211:LEU:HD22	1.89	0.55
4:E:28:LEU:HD21	16:Q:228:LEU:HD11	1.88	0.55
4:E:352:GLU:CD	5:F:87:ARG:HH22	2.10	0.55
6:G:53:SER:O	6:G:60:LEU:N	2.39	0.55
10:P:65:ALA:HB3	11:R:66:LEU:HD13	1.88	0.55
5:5:38:MET:HA	5:5:41:TYR:HD2	1.71	0.55
7:9:128:ASP:O	7:9:144:LYS:NZ	2.25	0.55
14:M:235:LYS:HD3	14:M:293:MET:HG3	1.88	0.55
3:D:592:PRO:HA	3:D:595:GLU:HG2	1.89	0.55
4:E:261:THR:H	4:E:292:GLN:HE22	1.55	0.55
6:G:132:PRO:HG2	6:G:175:ALA:HA	1.89	0.55
13:T:391:ALA:O	13:T:395:TYR:HB2	2.07	0.55
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.89	0.55
4:4:234:LEU:O	4:4:239:LEU:HB2	2.07	0.55
10:A:81:TYR:CE2	10:A:96:VAL:HG11	2.42	0.55
11:J:130:LEU:HD11	12:K:51:LEU:CD2	2.36	0.55
4:E:367:ARG:NH1	4:E:369:LYS:HB2	2.22	0.55
6:G:174:ALA:HA	6:G:177:LYS:HE2	1.88	0.55
15:V:98:LEU:HD23	15:V:218:ALA:HB1	1.89	0.55
15:V:294:LEU:HG	15:V:402:VAL:HG13	1.87	0.55
4:4:38:HIS:ND1	4:4:139:ASP:OD2	2.39	0.55
4:4:248:VAL:HG13	4:4:252:TYR:HD2	1.71	0.55
5:5:101:LEU:O	5:5:127:GLU:N	2.33	0.55
14:M:232:THR:HA	14:M:235:LYS:HZ2	1.71	0.55
1:B:95:GLU:OE2	1:B:102:LYS:N	2.40	0.55
2:C:85:THR:HG22	2:C:86:LEU:H	1.72	0.55
2:C:110:GLU:OE2	8:I:114:ARG:NE	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:160:ILE:O	13:T:164:ILE:HG13	2.07	0.55
16:Q:162:TYR:OH	16:Q:305:LEU:O	2.17	0.55
4:4:50:GLU:CD	16:H:154:ARG:HH12	2.10	0.54
5:5:100:ARG:NH1	5:5:127:GLU:OE1	2.40	0.54
10:A:61:PHE:HB2	11:J:73:LEU:HD11	1.89	0.54
12:K:25:ILE:HG12	12:K:75:ILE:HG21	1.89	0.54
1:B:72:THR:HG21	1:B:223:THR:HG21	1.90	0.54
2:C:130:THR:HB	2:C:143:GLU:HB3	1.90	0.54
6:G:114:SER:OG	7:O:96:LEU:O	2.24	0.54
7:O:33:LEU:HB2	7:O:163:VAL:HG12	1.89	0.54
9:X:29:ALA:HB1	9:X:50:LEU:HD11	1.89	0.54
5:5:120:ASP:OD2	5:5:136:LEU:N	2.39	0.54
13:T:61:PRO:HD3	14:U:448:GLY:HA2	1.88	0.54
13:T:162:ASN:OD1	13:T:216:LYS:NZ	2.38	0.54
2:2:9:ASP:N	2:2:9:ASP:OD1	2.40	0.54
13:L:55:PHE:O	13:L:66:SER:HA	2.08	0.54
13:L:463:HIS:CG	13:L:464:PRO:HD3	2.42	0.54
2:C:79:HIS:H	2:C:137:ASN:CG	2.10	0.54
3:D:557:SER:OG	3:D:559:ASP:OD1	2.21	0.54
13:T:325:HIS:NE2	13:T:329:LYS:HG3	2.23	0.54
4:4:375:PHE:HA	4:4:407:VAL:HG13	1.90	0.54
4:E:144:THR:HG22	4:E:148:TYR:CE1	2.36	0.54
13:T:119:VAL:O	13:T:251:TYR:OH	2.19	0.54
13:T:490:GLU:HG3	13:T:491:TRP:N	2.23	0.54
14:U:82:VAL:HG21	14:U:103:GLU:HB2	1.89	0.54
14:U:426:ALA:N	14:U:429:GLU:OE1	2.34	0.54
16:Q:122:ILE:HB	16:Q:170:LEU:HD13	1.90	0.54
1:1:293:GLY:O	1:1:327:GLY:N	2.40	0.54
14:M:215:PRO:HG2	14:M:216:PRO:HD3	1.89	0.54
16:H:150:LEU:O	16:H:154:ARG:HG3	2.07	0.54
12:S:93:LEU:HD21	15:V:128:GLN:HB2	1.90	0.54
16:Q:33:LEU:HD11	16:Q:56:LEU:HA	1.90	0.54
3:3:337:ARG:HH12	3:3:581:ARG:NH1	2.05	0.54
10:A:61:PHE:HD2	11:J:73:LEU:HD21	1.73	0.54
3:D:444:ARG:NH2	3:D:446:ASP:OD2	2.41	0.54
5:F:116:ARG:O	5:F:120:ASP:N	2.39	0.54
7:O:9:SER:O	7:O:12:ILE:HG13	2.07	0.54
7:O:96:LEU:HD21	7:O:129:LEU:HD13	1.88	0.54
3:3:118:ASP:OD2	3:3:180:ARG:NE	2.34	0.54
15:N:63:THR:HG22	15:N:96:HIS:HA	1.89	0.54
15:N:294:LEU:HG	15:N:402:VAL:HG13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASN:HD22	2:C:89:LYS:NZ	2.05	0.54
1:B:414:LEU:O	1:B:418:LYS:N	2.41	0.54
4:E:265:PRO:HB2	4:E:278:VAL:HG13	1.90	0.54
6:G:37:TRP:HH2	16:Q:36:ARG:NH2	2.06	0.54
4:4:129:HIS:HE1	4:4:349:ALA:HB1	1.73	0.54
16:H:149:LEU:O	16:H:153:LEU:HG	2.08	0.54
1:B:393:LEU:HD22	3:D:106:GLY:HA3	1.88	0.54
5:F:121:LEU:HA	5:F:145:PRO:HD2	1.89	0.54
10:P:107:PHE:HE1	16:Q:310:TRP:CD1	2.26	0.54
16:Q:149:LEU:O	16:Q:153:LEU:HG	2.08	0.54
1:1:139:ARG:HD2	2:2:138:ASP:O	2.08	0.54
5:5:31:ARG:HH21	5:5:100:ARG:HB2	1.73	0.54
11:J:59:TYR:O	11:J:64:VAL:HG12	2.08	0.54
2:C:79:HIS:N	2:C:137:ASN:OD1	2.40	0.54
2:C:106:ILE:HD11	2:C:112:THR:HB	1.90	0.54
3:D:2:VAL:HG13	3:D:89:ASP:HA	1.90	0.54
6:G:62:ARG:HG2	16:Q:48:PRO:HA	1.88	0.54
14:U:41:LEU:O	14:U:42:THR:HG22	2.07	0.54
16:Q:274:VAL:HG22	16:Q:275:PRO:HD2	1.88	0.54
3:3:268:ASP:OD2	3:3:278:ARG:NH1	2.40	0.54
6:6:21:PHE:O	6:6:25:GLU:HG2	2.07	0.54
13:L:328:PHE:O	13:L:332:LEU:HD13	2.08	0.54
1:B:61:GLY:HA3	1:B:247:LYS:HG3	1.88	0.54
1:B:201:LEU:HD13	3:D:42:ILE:HG22	1.89	0.54
3:D:688:ARG:HB3	3:D:770:ARG:HB2	1.90	0.54
11:R:152:VAL:O	11:R:156:LEU:HB2	2.07	0.54
13:T:600:LEU:HD13	15:V:236:LEU:HD21	1.89	0.54
15:V:38:ALA:HA	15:V:41:LEU:HD12	1.89	0.54
2:2:82:VAL:HG22	2:2:134:ILE:HG12	1.89	0.53
3:3:48:CYS:HB3	19:3:804:FES:S2	2.48	0.53
9:W:1:MET:HG3	9:W:56:ASP:HB2	1.89	0.53
13:L:163:ARG:NE	14:M:399:VAL:HB	2.23	0.53
13:L:413:THR:HA	13:L:416:TYR:CE2	2.43	0.53
5:F:163:ARG:NH2	7:O:92:GLU:OE2	2.40	0.53
13:T:316:TRP:HA	13:T:319:LEU:HD12	1.90	0.53
14:U:215:PRO:HG2	14:U:216:PRO:HD3	1.89	0.53
1:B:211:LEU:HB2	1:B:216:THR:HG21	1.90	0.53
2:C:9:ASP:OD1	2:C:9:ASP:N	2.40	0.53
2:C:110:GLU:HA	8:I:121:ARG:HH22	1.74	0.53
13:T:88:HIS:O	13:T:92:ILE:HG13	2.07	0.53
16:Q:260:PRO:HG3	16:Q:286:PHE:CD2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:350:ARG:O	4:4:373:PRO:HB2	2.08	0.53
13:L:490:GLU:HG3	13:L:491:TRP:N	2.22	0.53
14:M:22:ARG:HD2	14:M:22:ARG:C	2.28	0.53
15:N:85:TYR:O	15:N:88:VAL:HB	2.09	0.53
1:B:288:GLN:HE21	1:B:331:ILE:HG22	1.73	0.53
13:T:405:GLY:O	13:T:409:VAL:HG23	2.08	0.53
8:7:86:LEU:HD11	8:7:118:LEU:HD11	1.90	0.53
5:F:174:LEU:HD13	5:F:180:GLY:HA2	1.90	0.53
6:G:96:TRP:CE3	6:G:97:GLU:HG3	2.44	0.53
13:T:98:ASP:HB3	13:T:145:TRP:HE1	1.71	0.53
14:U:318:SER:HA	14:U:321:TYR:CZ	2.44	0.53
13:L:316:TRP:HA	13:L:319:LEU:HD12	1.91	0.53
14:M:49:HIS:HB2	14:M:67:LEU:HD13	1.91	0.53
14:M:205:THR:HG23	14:M:238:VAL:HG23	1.90	0.53
14:M:345:ARG:HG2	14:M:412:LYS:O	2.08	0.53
16:Q:8:ASP:OD2	16:Q:111:TYR:HB3	2.08	0.53
16:Q:170:LEU:HD21	16:Q:262:LEU:HD13	1.91	0.53
11:J:17:VAL:O	11:J:21:THR:OG1	2.18	0.53
16:H:291:ILE:HA	16:H:294:ARG:CG	2.37	0.53
10:P:65:ALA:O	10:P:69:ILE:HG23	2.08	0.53
14:U:13:GLY:HA2	14:U:97:GLY:HA2	1.91	0.53
14:U:56:LEU:HB3	14:U:59:ALA:HB3	1.91	0.53
1:1:260:ARG:NH1	1:1:279:TRP:O	2.36	0.53
1:1:382:LYS:O	1:1:386:ASN:ND2	2.42	0.53
13:L:380:SER:HA	13:L:383:TRP:HD1	1.73	0.53
14:M:56:LEU:HB3	14:M:59:ALA:HB3	1.90	0.53
1:B:63:ARG:H	1:B:65:ARG:NH2	2.05	0.53
13:T:141:LEU:HB3	13:T:236:VAL:HG11	1.91	0.53
15:V:128:GLN:OE1	15:V:306:ARG:NH2	2.42	0.53
15:V:259:ALA:O	15:V:263:ILE:HG13	2.09	0.53
16:Q:190:LYS:HD3	16:Q:268:THR:HG22	1.90	0.53
3:3:716:LEU:HD21	3:3:758:LEU:HD23	1.90	0.53
6:6:96:TRP:CZ2	6:6:103:LYS:HE3	2.43	0.53
10:A:81:TYR:HB2	11:J:132:TYR:CE1	2.43	0.53
11:J:64:VAL:HG13	16:H:134:TYR:OH	2.09	0.53
16:H:290:PHE:O	16:H:294:ARG:HG2	2.09	0.53
3:D:129:GLU:OE2	3:D:186:ARG:NH1	2.40	0.53
3:D:586:HIS:NE2	3:D:603:PRO:O	2.42	0.53
6:G:124:VAL:HG22	9:X:120:PRO:HD2	1.91	0.53
14:U:167:ARG:NH2	14:U:173:PRO:O	2.26	0.53
1:1:342:TRP:HZ3	1:1:346:ARG:HE	1.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:124:PRO:HA	11:J:127:LEU:HB2	1.90	0.53
13:T:386:ASP:OD2	13:T:494:ILE:HA	2.09	0.53
15:V:181:VAL:HA	15:V:192:PHE:CE2	2.44	0.53
15:V:207:VAL:O	15:V:211:MET:HG3	2.10	0.53
3:3:190:TYR:OH	3:3:222:PHE:O	2.20	0.52
4:4:232:LEU:HD23	5:5:109:GLY:HA3	1.90	0.52
14:M:318:SER:HA	14:M:321:TYR:CE1	2.44	0.52
16:H:37:ARG:NH2	16:H:54:PHE:O	2.41	0.52
1:B:63:ARG:HD3	1:B:313:TYR:HD2	1.75	0.52
4:E:201:ILE:HA	4:E:204:TYR:HD2	1.73	0.52
13:T:586:LEU:HB2	15:V:135:LYS:HZ2	1.74	0.52
14:U:90:ARG:HG2	14:U:334:GLU:HG3	1.91	0.52
14:U:151:PHE:CD1	14:U:203:ILE:HD11	2.41	0.52
1:1:243:THR:HG22	1:1:244:GLU:H	1.74	0.52
3:3:50:VAL:HG22	3:3:82:SER:HB3	1.91	0.52
8:7:74:PRO:HG2	8:7:77:ALA:HB2	1.92	0.52
1:B:238:PHE:CZ	1:B:248:GLY:HA3	2.44	0.52
2:C:108:PRO:HA	2:C:119:VAL:HG23	1.90	0.52
3:D:31:PRO:HB2	3:D:47:MET:HB3	1.92	0.52
4:E:128:SER:OG	4:E:350:ARG:NH2	2.42	0.52
4:E:128:SER:OG	4:E:350:ARG:NH1	2.41	0.52
6:G:40:THR:N	6:G:68:PHE:HE1	2.06	0.52
6:G:56:ALA:HB1	16:Q:44:VAL:HG12	1.91	0.52
1:1:288:GLN:NE2	1:1:332:PRO:O	2.42	0.52
2:2:110:GLU:HA	8:7:121:ARG:HH22	1.72	0.52
3:3:413:LEU:HA	3:3:416:PHE:HB3	1.90	0.52
3:3:444:ARG:NH2	3:3:446:ASP:OD2	2.42	0.52
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.89	0.52
11:J:123:LEU:HD22	16:H:120:LEU:HD21	1.91	0.52
1:B:96:SER:HB2	1:B:180:TYR:HD1	1.73	0.52
6:G:143:ARG:HG3	6:G:144:PRO:HD2	1.91	0.52
13:T:128:PHE:CZ	13:T:166:ASP:HB3	2.44	0.52
13:T:365:HIS:HD2	13:T:450:ALA:HB2	1.73	0.52
13:L:141:LEU:HB3	13:L:236:VAL:HG21	1.91	0.52
14:M:85:GLY:O	14:M:89:ALA:HB2	2.09	0.52
1:B:90:ILE:O	1:B:218:ILE:HA	2.10	0.52
1:B:373:LYS:HA	8:I:79:LEU:HD11	1.91	0.52
3:D:159:PHE:HE2	8:I:79:LEU:HD22	1.74	0.52
3:D:515:THR:HG23	3:D:683:LEU:HB3	1.91	0.52
5:F:38:MET:HA	5:F:41:TYR:HD2	1.74	0.52
16:Q:236:TYR:CD1	16:Q:240:LYS:HD2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:159:PHE:HD2	14:M:407:LEU:HD11	1.74	0.52
14:M:70:LEU:HD13	14:M:454:LEU:HD21	1.90	0.52
14:M:309:MET:HG3	14:M:454:LEU:HD12	1.92	0.52
15:N:14:THR:HA	15:N:86:LEU:HD21	1.92	0.52
16:H:224:ALA:HB2	16:H:233:HIS:CE1	2.44	0.52
4:E:208:PHE:CE2	4:E:214:PHE:CE2	2.98	0.52
6:G:81:ALA:HA	6:G:108:MET:HB3	1.90	0.52
13:T:434:HIS:HB3	13:T:435:PRO:HD3	1.91	0.52
15:V:283:PHE:O	15:V:287:THR:HG23	2.08	0.52
3:3:110:PHE:O	3:3:113:LEU:HB2	2.10	0.52
6:6:119:ASN:HA	6:6:125:GLN:NE2	2.25	0.52
7:9:54:ILE:HG12	7:9:110:THR:HG21	1.92	0.52
16:H:40:ALA:HB2	16:H:45:ARG:HH21	1.75	0.52
3:D:115:HIS:HB3	4:E:321:MET:HE3	1.92	0.52
10:P:68:PHE:CE2	16:Q:164:LEU:HB2	2.45	0.52
13:T:380:SER:HA	13:T:383:TRP:HD1	1.73	0.52
13:T:384:SER:O	13:T:388:ILE:HG13	2.10	0.52
15:V:102:ARG:NH1	15:V:225:ARG:O	2.42	0.52
13:L:360:PRO:HA	13:L:363:ARG:HH12	1.73	0.52
15:N:283:PHE:O	15:N:287:THR:HG23	2.08	0.52
16:H:90:VAL:HG21	16:H:243:LEU:HB3	1.90	0.52
13:T:324:THR:HG22	13:T:380:SER:HB2	1.90	0.52
3:3:115:HIS:HB3	4:4:321:MET:CE	2.40	0.52
6:6:40:THR:H	6:6:68:PHE:HE1	1.58	0.52
6:6:40:THR:HB	6:6:68:PHE:CZ	2.45	0.52
16:H:274:VAL:HG12	16:H:278:TRP:HD1	1.66	0.52
1:B:111:PRO:HB3	1:B:145:LEU:HD23	1.92	0.52
3:D:694:LEU:HD12	3:D:769:LEU:HB2	1.92	0.52
6:G:59:ASP:OD1	6:G:62:ARG:NH2	2.43	0.52
16:Q:300:LEU:O	16:Q:301:ARG:HG2	2.10	0.52
7:9:72:PRO:HG3	7:9:86:ARG:NH2	2.25	0.52
11:J:59:TYR:CE2	12:K:61:ILE:HG23	2.45	0.52
13:L:512:PHE:HE1	13:L:521:TYR:HH	1.57	0.52
13:L:564:TYR:OH	14:M:209:PRO:O	2.25	0.52
1:B:17:LEU:HD22	1:B:113:LEU:HD21	1.92	0.52
2:C:23:ARG:NH1	2:C:52:LEU:O	2.32	0.52
3:D:227:THR:HG21	3:D:237:ASP:HB2	1.90	0.52
4:E:211:SER:O	7:O:2:THR:OG1	2.27	0.52
10:P:23:ALA:O	10:P:27:VAL:HG23	2.09	0.52
13:T:361:GLN:HB2	13:T:443:LEU:HD23	1.91	0.52
13:T:459:LEU:O	13:T:468:VAL:N	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:6:LEU:HG	1:1:240:GLN:HE21	1.75	0.52
5:5:77:LEU:O	5:5:83:GLY:HA3	2.10	0.52
9:W:114:VAL:HA	9:W:117:ILE:HG12	1.93	0.52
14:M:41:LEU:O	14:M:42:THR:CG2	2.52	0.52
13:T:454:VAL:HB	13:T:455:LEU:HD22	1.91	0.52
1:1:287:ILE:HG22	1:1:302:PHE:HB2	1.92	0.51
4:4:222:GLY:HA3	4:4:275:ARG:NH2	2.23	0.51
10:A:71:PHE:CZ	10:A:107:PHE:HB2	2.45	0.51
13:L:291:ILE:O	13:L:295:VAL:HG23	2.10	0.51
4:E:341:GLU:OE1	4:E:356:TYR:OH	2.27	0.51
13:T:293:LYS:O	13:T:297:TYR:HD1	1.93	0.51
13:T:309:ALA:HB2	13:T:388:ILE:HD13	1.92	0.51
3:3:225:ASN:O	3:3:229:ILE:HG13	2.10	0.51
3:3:715:GLU:OE1	3:3:717:TRP:NE1	2.43	0.51
7:9:18:PHE:O	7:9:20:LYS:NZ	2.43	0.51
2:C:45:ARG:O	2:C:49:ILE:HG13	2.10	0.51
6:G:153:GLN:HG3	7:O:124:TYR:CZ	2.44	0.51
13:T:103:ARG:HH12	13:T:144:PHE:HA	1.75	0.51
14:U:9:PRO:HG2	14:U:107:LEU:HD12	1.92	0.51
2:2:85:THR:HG22	2:2:86:LEU:H	1.74	0.51
4:4:173:ILE:O	4:4:174:ARG:NH1	2.43	0.51
6:6:101:ASP:OD2	10:A:35:LYS:HB2	2.10	0.51
6:6:179:THR:HB	9:W:127:LEU:HB2	1.91	0.51
13:L:143:GLY:HA3	14:M:415:TRP:CH2	2.46	0.51
16:H:227:GLU:HB2	16:H:299:ARG:NH1	2.26	0.51
3:D:113:LEU:O	3:D:161:ARG:NH1	2.42	0.51
3:D:283:PRO:O	3:D:412:ARG:NH2	2.43	0.51
4:E:84:ARG:NH2	4:E:169:HIS:HB3	2.25	0.51
4:E:196:VAL:HG22	4:E:200:ARG:HG2	1.92	0.51
16:Q:221:LEU:N	16:Q:222:PRO:HA	2.24	0.51
1:1:297:THR:HG22	1:1:322:MET:HG3	1.92	0.51
2:2:83:CYS:HA	2:2:122:VAL:O	2.11	0.51
3:3:376:ALA:N	3:3:513:GLN:OE1	2.31	0.51
3:3:469:ARG:HD3	3:3:757:HIS:HE1	1.75	0.51
3:3:691:ALA:HB3	3:3:772:GLU:HA	1.93	0.51
16:H:86:PRO:HG3	16:H:244:PHE:CE2	2.45	0.51
1:B:106:ILE:HD11	1:B:251:LEU:HD21	1.92	0.51
1:B:219:ASN:HD22	18:B:502:FMN:P	2.33	0.51
1:B:297:THR:HG21	1:B:324:GLY:H	1.75	0.51
3:D:114:ASN:HA	3:D:161:ARG:HG2	1.92	0.51
4:E:98:ALA:O	4:E:102:GLU:HG3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:285:GLU:O	4:E:289:ILE:HG12	2.11	0.51
4:E:341:GLU:OE1	5:F:91:ARG:NH2	2.44	0.51
6:G:99:MET:HG2	6:G:100:PRO:HD2	1.91	0.51
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.92	0.51
3:3:248:GLU:HB3	3:3:270:ARG:NH1	2.26	0.51
4:4:35:PRO:HG3	16:H:147:TYR:OH	2.10	0.51
4:4:169:HIS:NE2	6:6:45:CYS:HB2	2.25	0.51
7:9:138:VAL:HA	7:9:173:PHE:HD1	1.75	0.51
11:J:59:TYR:CE1	11:J:63:ILE:HD12	2.46	0.51
13:L:331:LEU:HD12	13:L:446:ASN:OD1	2.10	0.51
13:L:600:LEU:HD13	15:N:236:LEU:HD21	1.93	0.51
1:B:63:ARG:HA	1:B:71:PRO:HA	1.92	0.51
14:U:91:VAL:HG23	14:U:92:GLU:H	1.75	0.51
2:2:98:ASP:HB3	8:7:107:LYS:NZ	2.26	0.51
13:L:87:ILE:HD12	13:L:239:LEU:HD13	1.92	0.51
14:M:219:GLN:HA	14:M:282:LYS:HG3	1.92	0.51
16:H:39:LEU:O	16:H:43:GLN:HG2	2.11	0.51
16:H:206:TYR:HE1	16:H:259:ILE:HG12	1.74	0.51
1:B:118:MET:HG2	1:B:224:LEU:HD13	1.92	0.51
4:E:43:LEU:HD13	4:E:55:VAL:HG11	1.92	0.51
8:I:10:TYR:O	8:I:14:VAL:HG23	2.11	0.51
13:T:53:ALA:HB3	13:T:69:LEU:HB3	1.91	0.51
14:U:201:PHE:O	14:U:205:THR:N	2.44	0.51
1:1:18:TYR:OH	1:1:102:LYS:O	2.27	0.51
3:3:455:ARG:HH21	3:3:750:ARG:NH2	2.09	0.51
3:3:706:GLY:O	3:3:709:GLN:HB2	2.11	0.51
4:4:26:MET:N	10:A:54:VAL:HG21	2.26	0.51
4:4:46:THR:O	4:4:53:LEU:HB2	2.10	0.51
12:K:79:PHE:CG	12:K:85:THR:HA	2.46	0.51
13:L:33:ALA:HA	13:L:36:LEU:HD12	1.91	0.51
13:L:246:VAL:HB	13:L:303:LEU:HD21	1.93	0.51
13:L:539:ASN:HA	13:L:543:VAL:HB	1.93	0.51
16:H:189:GLN:O	16:H:193:GLY:HA2	2.10	0.51
3:D:182:ILE:HG23	3:D:232:VAL:HG11	1.91	0.51
3:D:329:LEU:HD21	3:D:644:LEU:HA	1.93	0.51
4:E:129:HIS:CE1	4:E:349:ALA:HB1	2.46	0.51
6:G:36:LEU:HD13	6:G:154:LEU:HD23	1.91	0.51
7:O:45:ARG:HH21	7:O:137:LEU:HD23	1.75	0.51
14:U:91:VAL:HB	14:U:95:PHE:HE1	1.76	0.51
15:V:237:VAL:O	15:V:241:VAL:HG23	2.11	0.51
3:3:274:LEU:H	3:3:302:ASP:HB3	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:201:ILE:HA	4:4:204:TYR:HD2	1.76	0.51
5:5:154:GLU:OE2	5:5:167:PRO:HB2	2.11	0.51
11:J:146:LEU:O	11:J:150:THR:HG23	2.11	0.51
3:D:245:ARG:HG3	7:O:57:SER:HB3	1.92	0.51
3:D:451:PHE:CD1	3:D:466:GLU:HB3	2.46	0.51
6:G:80:VAL:HG11	6:G:127:VAL:HG21	1.93	0.51
10:P:105:VAL:HG13	15:V:15:LEU:HD21	1.93	0.51
14:U:331:ARG:HA	14:U:331:ARG:HH11	1.75	0.51
2:2:98:ASP:HB3	8:7:107:LYS:HZ2	1.75	0.51
3:3:198:GLU:OE2	3:3:440:ARG:NH1	2.44	0.51
3:3:438:LYS:O	3:3:441:MET:HG3	2.11	0.51
8:7:33:LYS:HG3	8:7:54:ILE:HD12	1.91	0.51
10:A:90:LEU:HD12	16:H:330:LEU:HD21	1.91	0.51
13:L:302:GLN:O	13:L:306:MET:HG3	2.11	0.51
15:N:207:VAL:O	15:N:211:MET:HG3	2.10	0.51
1:B:74:LEU:HD12	1:B:77:SER:OG	2.11	0.51
3:D:34:CYS:SG	3:D:35:SER:N	2.84	0.51
3:D:229:ILE:HD11	3:D:289:TRP:HZ3	1.76	0.51
10:P:88:LEU:HD23	11:R:132:TYR:HB2	1.93	0.51
14:U:128:PRO:O	14:U:132:MET:HG2	2.10	0.51
3:3:323:GLU:OE1	9:W:11:ARG:NH1	2.44	0.51
4:4:148:TYR:HB3	4:4:200:ARG:HH21	1.75	0.51
1:B:18:TYR:OH	1:B:102:LYS:O	2.27	0.51
11:R:94:ALA:O	11:R:97:ALA:HB3	2.11	0.51
13:T:373:LEU:HD21	13:T:416:TYR:CE1	2.46	0.51
15:V:73:THR:OG1	15:V:206:PRO:O	2.24	0.51
16:Q:174:VAL:O	16:Q:178:GLY:N	2.35	0.51
16:Q:189:GLN:O	16:Q:193:GLY:HA2	2.11	0.51
3:3:384:PRO:O	3:3:675:ARG:NH2	2.44	0.50
5:5:160:ARG:HB2	5:5:163:ARG:HH21	1.75	0.50
1:B:3:GLY:O	1:B:5:ILE:N	2.42	0.50
4:E:89:HIS:CE1	4:E:92:ALA:HB2	2.47	0.50
4:E:148:TYR:O	4:E:151:ARG:HB3	2.11	0.50
10:P:2:ALA:HB2	16:Q:119:ASP:HB3	1.92	0.50
14:U:221:ASN:ND2	14:U:228:ASP:OD1	2.44	0.50
1:1:66:GLY:HA3	18:1:502:FMN:H3'	1.92	0.50
1:1:323:LEU:HD11	1:1:326:GLY:HA2	1.93	0.50
4:4:87:TYR:CZ	4:4:403:VAL:HG13	2.47	0.50
12:K:46:ALA:HB2	12:K:53:GLY:HA3	1.93	0.50
1:B:6:LEU:HD11	1:B:240:GLN:HE21	1.75	0.50
3:D:715:GLU:OE1	3:D:717:TRP:NE1	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:29:LEU:HD23	1:1:155:ARG:NH1	2.25	0.50
1:1:87:HIS:HD2	1:1:215:PRO:HD2	1.75	0.50
2:2:110:GLU:HA	8:7:121:ARG:NH1	2.25	0.50
16:H:213:GLU:OE1	16:H:213:GLU:N	2.44	0.50
3:D:695:ARG:NH1	3:D:761:SER:OG	2.44	0.50
20:E:501:DCQ:H7	6:G:42:GLY:HA3	1.94	0.50
11:R:123:LEU:HD13	11:R:124:PRO:HD2	1.93	0.50
14:U:331:ARG:O	14:U:335:ARG:HG2	2.11	0.50
1:1:249:MET:HA	1:1:267:PRO:HA	1.93	0.50
4:4:285:GLU:O	4:4:289:ILE:HG12	2.12	0.50
4:E:47:LEU:HD13	4:E:52:VAL:HA	1.92	0.50
5:F:120:ASP:OD2	5:F:136:LEU:N	2.41	0.50
6:G:120:ASN:HD22	6:G:122:ALA:H	1.58	0.50
9:X:37:TRP:NE1	9:X:40:LYS:HD2	2.26	0.50
14:U:424:ASP:O	14:U:425:LEU:HD12	2.12	0.50
16:Q:232:TYR:HB2	16:Q:244:PHE:CE1	2.46	0.50
1:1:219:ASN:HD22	18:1:502:FMN:P	2.35	0.50
12:K:79:PHE:CD2	12:K:85:THR:HA	2.47	0.50
14:M:127:ILE:HB	14:M:128:PRO:HD3	1.93	0.50
15:N:181:VAL:HA	15:N:192:PHE:CE2	2.47	0.50
4:4:47:LEU:HD13	4:4:51:GLU:O	2.11	0.50
10:A:33:PRO:HD2	16:H:70:GLU:HB2	1.93	0.50
14:M:93:GLY:O	14:M:136:TYR:OH	2.20	0.50
3:D:123:ASP:OD2	3:D:241:ARG:HA	2.11	0.50
3:D:260:PRO:HB2	3:D:617:LEU:HB3	1.94	0.50
9:X:51:HIS:CE1	9:X:111:LEU:HD21	2.47	0.50
14:U:338:THR:HG22	14:U:340:GLU:H	1.75	0.50
4:4:162:TRP:N	7:9:34:LYS:HG3	2.25	0.50
9:W:7:ARG:NE	9:W:61:ASP:OD2	2.45	0.50
14:M:36:ASN:HD22	14:M:39:LEU:HD12	1.77	0.50
16:H:196:PHE:N	16:H:263:PHE:O	2.41	0.50
3:D:186:ARG:NH1	3:D:229:ILE:O	2.36	0.50
4:E:38:HIS:HA	20:E:501:DCQ:H8	1.94	0.50
4:E:390:VAL:HB	4:E:391:PRO:HD3	1.94	0.50
7:O:40:ARG:HH22	7:O:173:PHE:HE1	1.59	0.50
10:P:109:TYR:HE2	11:R:154:VAL:HG11	1.76	0.50
11:R:53:PHE:CE2	16:Q:120:LEU:HB2	2.47	0.50
14:U:350:SER:HB3	14:U:422:VAL:H	1.76	0.50
2:2:101:THR:HG23	2:2:106:ILE:O	2.12	0.50
3:3:21:ASP:OD1	3:3:432:PHE:N	2.32	0.50
3:3:166:LYS:NZ	3:3:179:GLU:OE1	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:156:ILE:O	4:4:159:LEU:HB2	2.12	0.50
11:J:93:ALA:O	11:J:97:ALA:N	2.30	0.50
16:H:119:ASP:OD1	16:H:120:LEU:HG	2.12	0.50
16:H:274:VAL:CG2	16:H:275:PRO:HD2	2.42	0.50
4:E:211:SER:HB3	4:E:214:PHE:HD2	1.77	0.50
15:V:95:MET:SD	15:V:214:SER:HB3	2.52	0.50
1:1:253:GLN:O	1:1:327:GLY:HA2	2.12	0.50
2:2:146:THR:HG23	2:2:149:ARG:H	1.77	0.50
3:3:459:MET:HA	3:3:462:ALA:HB3	1.94	0.50
4:4:122:GLU:HB2	4:4:290:ILE:HD11	1.94	0.50
4:4:250:LYS:HE2	4:4:262:PHE:HB3	1.92	0.50
5:5:113:PHE:O	5:5:116:ARG:HB2	2.12	0.50
11:J:99:GLY:O	11:J:103:ILE:HG22	2.12	0.50
13:L:84:GLY:O	13:L:88:HIS:ND1	2.39	0.50
14:M:90:ARG:HB2	14:M:331:ARG:CZ	2.42	0.50
3:D:157:PHE:CE1	3:D:159:PHE:HB2	2.46	0.50
5:F:186:GLY:HA2	5:F:190:LYS:HD3	1.93	0.50
8:I:89:ALA:O	8:I:91:ILE:HG13	2.12	0.50
16:Q:177:VAL:HG21	16:Q:185:ILE:HG12	1.94	0.50
16:Q:226:GLN:C	16:Q:299:ARG:HH12	2.16	0.50
1:1:250:LYS:HB3	1:1:252:TYR:CE1	2.47	0.49
7:9:9:SER:O	7:9:12:ILE:HG13	2.11	0.49
15:N:340:ALA:HA	15:N:343:TRP:HD1	1.77	0.49
1:B:260:ARG:HA	2:C:177:HIS:O	2.12	0.49
13:T:392:THR:HG22	13:T:399:GLY:HA3	1.94	0.49
1:1:259:LYS:HE3	1:1:260:ARG:HH21	1.76	0.49
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.52	0.49
6:6:37:TRP:HB3	6:6:75:ALA:HA	1.94	0.49
10:A:113:LYS:HG3	15:N:18:PHE:HE1	1.77	0.49
14:M:313:TYR:OH	14:M:443:MET:O	2.22	0.49
15:N:62:PHE:CE2	15:N:285:LEU:HD22	2.47	0.49
16:H:117:ASN:O	16:H:181:ASN:ND2	2.45	0.49
16:H:221:LEU:N	16:H:222:PRO:HA	2.26	0.49
16:H:224:ALA:HA	16:H:229:VAL:HA	1.93	0.49
3:D:576:ALA:O	3:D:580:LYS:NZ	2.42	0.49
15:V:24:GLY:HA2	15:V:27:ARG:HD2	1.93	0.49
16:Q:122:ILE:HA	16:Q:125:LEU:HD12	1.92	0.49
16:Q:213:GLU:N	16:Q:213:GLU:OE1	2.45	0.49
1:1:5:ILE:O	1:1:12:ARG:NH2	2.45	0.49
9:W:59:VAL:HG11	9:W:63:PHE:HE2	1.77	0.49
11:J:23:ARG:HD2	11:J:80:GLU:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:255:ARG:HD2	13:L:477:LEU:HD23	1.95	0.49
13:L:487:LEU:HA	13:L:490:GLU:HG2	1.95	0.49
14:M:131:LEU:O	14:M:135:LEU:HD23	2.11	0.49
15:N:87:LEU:O	15:N:91:ALA:N	2.26	0.49
16:H:185:ILE:HG22	16:H:189:GLN:OE1	2.12	0.49
1:B:264:TYR:CZ	2:C:176:VAL:HG11	2.47	0.49
1:B:356:CYS:N	17:B:501:SF4:S3	2.73	0.49
6:G:54:THR:HG22	6:G:60:LEU:HB3	1.94	0.49
15:V:204:PRO:O	15:V:208:VAL:HG23	2.12	0.49
16:Q:35:GLU:HG3	16:Q:291:ILE:HG23	1.94	0.49
1:1:201:LEU:HG	1:1:203:PRO:HD2	1.95	0.49
1:1:291:ILE:HD11	1:1:331:ILE:HD11	1.94	0.49
13:L:88:HIS:O	13:L:92:ILE:HG13	2.12	0.49
15:N:204:PRO:O	15:N:208:VAL:HG23	2.13	0.49
1:B:437:TRP:HB3	2:C:92:GLY:HA3	1.95	0.49
3:D:8:ASP:OD1	3:D:9:ARG:HG3	2.13	0.49
13:T:9:LEU:HB2	13:T:10:PRO:HD3	1.95	0.49
1:1:372:ALA:O	1:1:376:THR:OG1	2.20	0.49
2:2:74:PRO:HB2	8:7:121:ARG:NE	2.26	0.49
3:3:165:ASP:OD2	3:3:168:HIS:HB2	2.12	0.49
4:4:211:SER:HB3	4:4:214:PHE:HD2	1.78	0.49
7:9:164:PRO:HA	7:9:178:GLU:HB2	1.94	0.49
14:M:385:TYR:CE1	14:M:389:PRO:HB3	2.46	0.49
16:H:35:GLU:OE1	16:H:249:TYR:OH	2.19	0.49
16:H:161:SER:HG	16:H:310:TRP:HZ3	1.60	0.49
1:B:342:TRP:HE1	1:B:372:ALA:HA	1.77	0.49
10:P:22:VAL:O	10:P:26:LEU:HG	2.13	0.49
10:P:77:PHE:O	10:P:80:PRO:HD2	2.12	0.49
14:U:186:GLN:HG2	14:U:187:GLU:H	1.77	0.49
14:U:238:VAL:HA	14:U:241:PHE:HB2	1.93	0.49
16:Q:265:GLY:O	16:Q:282:LYS:NZ	2.28	0.49
4:4:103:LYS:HE3	5:5:22:LEU:HB3	1.94	0.49
4:4:158:ASP:OD1	6:6:57:ARG:NH1	2.46	0.49
7:9:111:GLY:N	8:7:44:MET:HG2	2.27	0.49
13:L:405:GLY:O	13:L:409:VAL:HG23	2.12	0.49
15:N:59:SER:OG	15:N:100:SER:OG	2.19	0.49
3:D:185:LYS:O	3:D:189:ARG:HB2	2.11	0.49
14:U:218:HIS:O	14:U:282:LYS:NZ	2.37	0.49
15:V:251:GLN:OE1	15:V:256:ARG:HD3	2.13	0.49
16:Q:154:ARG:HD3	16:Q:222:PRO:HG3	1.95	0.49
4:4:224:ILE:HG22	4:4:229:ALA:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.48	0.49
10:A:62:TYR:HD2	11:J:66:LEU:HD11	1.78	0.49
14:M:237:GLY:O	14:M:241:PHE:N	2.37	0.49
15:N:248:ALA:HB2	15:N:260:TYR:HB3	1.94	0.49
3:D:186:ARG:HD2	3:D:231:PRO:HD3	1.95	0.49
14:U:451:ALA:HA	14:U:454:LEU:HG	1.95	0.49
15:V:153:LEU:HD22	15:V:171:LEU:HD11	1.93	0.49
1:1:220:ASN:N	18:1:502:FMN:O3P	2.30	0.49
6:6:114:SER:OG	7:9:96:LEU:O	2.31	0.49
3:D:190:TYR:O	3:D:195:PRO:HD2	2.12	0.49
16:Q:236:TYR:HD1	16:Q:240:LYS:HD2	1.77	0.49
1:1:203:PRO:HB2	1:1:204:PRO:HD3	1.94	0.49
2:2:42:ARG:HB3	2:2:44:GLU:OE1	2.13	0.49
4:4:156:ILE:HA	4:4:159:LEU:HD12	1.95	0.49
13:L:325:HIS:CE1	13:L:329:LYS:HG3	2.48	0.49
2:C:4:PHE:N	2:C:48:GLU:OE2	2.38	0.49
3:D:300:TRP:CD1	3:D:703:GLN:HA	2.48	0.49
4:E:73:ARG:NH2	7:O:64:PRO:O	2.46	0.49
4:E:333:GLU:O	4:E:363:SER:OG	2.26	0.49
15:V:62:PHE:CE2	15:V:285:LEU:HD22	2.48	0.49
7:9:33:LEU:HD11	7:9:119:PHE:CE2	2.46	0.49
8:7:71:ASP:OD2	8:7:81:ARG:NH2	2.44	0.49
13:L:9:LEU:HB2	13:L:10:PRO:HD3	1.94	0.49
14:M:327:LEU:O	14:M:331:ARG:HG2	2.12	0.49
15:N:249:LEU:HD23	15:N:374:TYR:HD2	1.77	0.49
1:B:94:ASP:O	18:B:502:FMN:N3	2.38	0.49
1:B:291:ILE:O	1:B:328:VAL:HA	2.13	0.49
7:O:126:TYR:HB3	9:X:39:ASP:CG	2.34	0.49
11:R:100:VAL:HA	13:T:598:LEU:HD21	1.95	0.49
13:T:90:TYR:OH	13:T:338:SER:N	2.46	0.49
14:U:22:ARG:HD2	14:U:23:ALA:CA	2.42	0.49
14:M:224:SER:HA	14:M:330:GLY:HA3	1.94	0.48
15:N:217:ALA:HA	15:N:285:LEU:HD23	1.95	0.48
1:B:92:ASN:ND2	18:B:502:FMN:HO3'	2.08	0.48
3:D:631:ASN:HD22	3:D:634:ALA:HB3	1.78	0.48
7:O:43:LEU:O	7:O:138:VAL:HG13	2.13	0.48
9:X:78:VAL:HB	9:X:127:LEU:HD21	1.94	0.48
13:T:60:LEU:HD21	14:U:375:PRO:HB3	1.95	0.48
13:T:298:SER:O	13:T:302:GLN:HG2	2.13	0.48
16:Q:119:ASP:OD1	16:Q:120:LEU:HG	2.13	0.48
16:Q:186:VAL:HG11	16:Q:267:TRP:CZ3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:114:GLU:O	4:4:118:VAL:HG13	2.13	0.48
6:6:33:SER:O	6:6:36:LEU:HG	2.13	0.48
6:6:74:GLN:NE2	16:H:233:HIS:HB2	2.28	0.48
11:J:5:GLU:O	11:J:9:LEU:HG	2.13	0.48
11:J:63:ILE:O	11:J:66:LEU:N	2.46	0.48
4:E:26:MET:N	10:P:54:VAL:HG21	2.28	0.48
5:F:80:TRP:CE3	5:F:80:TRP:HA	2.47	0.48
8:I:86:LEU:HB2	8:I:91:ILE:HB	1.93	0.48
13:T:4:LEU:HG	13:T:8:LEU:HG	1.95	0.48
15:V:96:HIS:CE1	15:V:100:SER:HG	2.31	0.48
4:4:194:LEU:HD11	4:4:290:ILE:HG21	1.95	0.48
14:M:22:ARG:HD2	14:M:23:ALA:CA	2.42	0.48
15:N:163:LEU:HD13	15:N:226:VAL:HA	1.94	0.48
1:B:87:HIS:HD2	1:B:215:PRO:HD2	1.78	0.48
3:D:516:VAL:O	3:D:520:ARG:HG3	2.14	0.48
13:T:104:PHE:HZ	13:T:235:PRO:HG2	1.78	0.48
13:T:427:GLY:O	13:T:428:GLU:HG2	2.12	0.48
4:4:64:THR:HB	4:4:66:PHE:CE1	2.49	0.48
7:9:102:GLY:HA2	7:9:115:LEU:HD11	1.95	0.48
8:7:89:ALA:O	8:7:91:ILE:HG13	2.14	0.48
13:L:1:MET:HA	13:L:55:PHE:CD2	2.48	0.48
3:D:300:TRP:O	3:D:589:HIS:NE2	2.44	0.48
13:T:291:ILE:HG13	13:T:292:LYS:N	2.29	0.48
15:V:283:PHE:HB2	15:V:420:LEU:HD13	1.94	0.48
16:Q:146:LYS:CA	16:Q:149:LEU:HB2	2.37	0.48
16:Q:333:PRO:HG2	16:Q:336:TYR:CD1	2.48	0.48
1:1:339:ASP:OD1	1:1:433:ARG:NH2	2.46	0.48
2:2:112:THR:HG22	2:2:117:PHE:H	1.77	0.48
3:3:182:ILE:HG23	3:3:232:VAL:HG11	1.95	0.48
3:3:345:LEU:O	3:3:372:GLN:N	2.46	0.48
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.95	0.48
1:B:44:VAL:HG13	1:B:48:LYS:HD2	1.94	0.48
4:E:158:ASP:OD2	6:G:57:ARG:NH2	2.46	0.48
4:E:225:PRO:HG2	4:E:228:VAL:HB	1.95	0.48
10:P:62:TYR:CD2	11:R:66:LEU:HD11	2.47	0.48
10:P:93:PHE:O	10:P:96:VAL:HG12	2.14	0.48
13:T:214:VAL:O	13:T:218:ALA:N	2.47	0.48
13:T:313:GLY:HA2	13:T:315:TYR:CZ	2.49	0.48
13:T:328:PHE:O	13:T:331:LEU:HB3	2.14	0.48
13:T:501:ALA:O	13:T:505:LEU:HG	2.14	0.48
14:U:55:LEU:HD13	14:U:63:TRP:HE1	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:167:ARG:HG3	14:U:172:SER:HB3	1.95	0.48
16:Q:40:ALA:HB2	16:Q:45:ARG:HH21	1.78	0.48
1:1:363:VAL:O	1:1:368:VAL:HG12	2.13	0.48
13:L:90:TYR:CE2	13:L:334:LEU:HB3	2.49	0.48
14:M:33:PHE:HA	14:M:79:ALA:HB1	1.96	0.48
16:H:326:LEU:HD12	16:H:330:LEU:HD23	1.96	0.48
1:B:104:ARG:NH2	1:B:105:TYR:OH	2.41	0.48
3:D:497:TRP:O	3:D:528:LYS:HE3	2.14	0.48
4:E:64:THR:OG1	6:G:83:ARG:HD2	2.13	0.48
4:E:363:SER:HB3	5:F:173:ALA:HB1	1.94	0.48
10:P:68:PHE:HE1	11:R:62:ALA:HA	1.79	0.48
11:R:19:VAL:HG23	11:R:28:ALA:O	2.13	0.48
13:T:136:LEU:O	13:T:140:LEU:HG	2.13	0.48
13:T:219:GLN:O	13:T:223:MET:N	2.46	0.48
13:T:376:LEU:HB3	13:T:379:LEU:HD12	1.95	0.48
13:T:604:MET:HG2	15:V:232:ALA:HB2	1.95	0.48
14:U:346:GLY:HA2	14:U:416:GLU:O	2.13	0.48
1:1:39:GLU:O	1:1:43:ARG:HG2	2.14	0.48
5:5:99:PRO:HB2	5:5:124:ILE:HA	1.96	0.48
7:9:40:ARG:HH22	7:9:173:PHE:HZ	1.59	0.48
9:W:38:GLN:HG3	9:W:93:VAL:HG11	1.95	0.48
13:L:263:LEU:HB3	13:L:266:VAL:HB	1.95	0.48
14:M:187:GLU:HG2	14:M:188:GLU:N	2.28	0.48
16:H:177:VAL:HA	16:H:188:TRP:CD1	2.49	0.48
16:H:274:VAL:CG1	16:H:278:TRP:CD1	2.88	0.48
1:B:101:PHE:CE1	1:B:253:GLN:HB2	2.49	0.48
1:B:243:THR:HG21	1:B:315:HIS:HE1	1.79	0.48
3:D:413:LEU:HA	3:D:416:PHE:HB3	1.94	0.48
10:P:20:ILE:HD12	16:Q:21:VAL:HG11	1.95	0.48
14:U:443:MET:HA	14:U:450:PHE:CE2	2.49	0.48
1:1:106:ILE:HD11	1:1:251:LEU:HD21	1.94	0.48
3:3:36:GLU:HB3	3:3:39:LEU:HB2	1.96	0.48
3:3:185:LYS:O	3:3:189:ARG:HB2	2.14	0.48
3:3:316:ARG:HD3	3:D:675:ARG:HD3	1.96	0.48
3:3:568:TYR:CD1	3:3:572:PRO:HG3	2.49	0.48
4:4:288:LYS:HD3	4:4:288:LYS:HA	1.56	0.48
11:J:16:GLY:HA2	11:J:19:VAL:HG12	1.95	0.48
1:B:342:TRP:CD1	1:B:371:PHE:HB3	2.49	0.48
1:B:427:GLU:OE1	1:B:429:ARG:NH1	2.47	0.48
15:V:62:PHE:HE2	15:V:285:LEU:HD22	1.78	0.48
5:5:163:ARG:NH1	7:9:90:VAL:HG11	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LYS:NZ	1:B:325:THR:O	2.39	0.48
4:E:91:PHE:CZ	4:E:173:ILE:HB	2.49	0.48
4:E:168:PHE:CE1	6:G:141:PRO:HG3	2.49	0.48
4:E:352:GLU:HB3	4:E:371:ARG:NE	2.28	0.48
6:G:112:ALA:O	6:G:127:VAL:HG23	2.13	0.48
13:T:59:TRP:CH2	13:T:129:ILE:HD11	2.49	0.48
13:T:214:VAL:HG12	13:T:222:LEU:HB2	1.95	0.48
1:1:48:LYS:O	1:1:123:TYR:OH	2.13	0.48
3:3:168:HIS:N	3:3:176:LEU:O	2.36	0.48
4:4:143:LEU:H	4:4:143:LEU:HD23	1.78	0.48
13:L:90:TYR:OH	13:L:338:SER:OG	2.19	0.48
15:N:422:ALA:O	15:N:423:LEU:HD23	2.14	0.48
1:B:350:HIS:O	3:D:205:ARG:NH1	2.45	0.48
7:O:51:GLU:N	7:O:81:VAL:O	2.46	0.48
13:T:355:LEU:H	13:T:425:PHE:HA	1.78	0.48
15:V:103:HIS:HE1	15:V:161:LEU:HB2	1.76	0.48
16:Q:37:ARG:NH2	16:Q:54:PHE:O	2.41	0.48
5:5:105:THR:HA	5:5:108:TRP:O	2.13	0.47
6:6:120:ASN:HD22	6:6:122:ALA:H	1.62	0.47
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.49	0.47
7:9:6:LEU:HD23	16:H:297:TRP:CE2	2.48	0.47
14:M:109:LEU:HD21	14:M:236:VAL:HG21	1.96	0.47
14:M:335:ARG:NH2	14:M:429:GLU:OE2	2.47	0.47
15:N:216:LYS:NZ	15:N:266:ALA:HB2	2.29	0.47
16:H:293:ILE:HD12	16:H:297:TRP:CZ3	2.49	0.47
3:D:48:CYS:HB3	19:D:804:FES:S2	2.53	0.47
4:E:133:LEU:HD11	4:E:149:ALA:HB2	1.96	0.47
4:E:214:PHE:HA	4:E:217:ARG:HB2	1.96	0.47
16:Q:31:MET:SD	16:Q:287:LEU:HD13	2.54	0.47
18:1:502:FMN:H9	18:1:502:FMN:H1'1	1.60	0.47
4:4:208:PHE:CE2	4:4:276:MET:HG2	2.48	0.47
5:5:159:PHE:HB2	5:5:163:ARG:HB2	1.95	0.47
6:6:70:ALA:N	16:H:225:GLU:OE2	2.26	0.47
16:H:306:LEU:O	16:H:310:TRP:HB2	2.14	0.47
3:D:36:GLU:HB3	3:D:39:LEU:HB2	1.95	0.47
4:E:27:THR:H	10:P:54:VAL:HG11	1.79	0.47
4:E:33:GLN:HE22	20:E:501:DCQ:H10A	1.79	0.47
4:E:86:ASP:HB3	4:E:93:HIS:HD2	1.79	0.47
4:E:166:GLN:OE1	4:E:170:HIS:HA	2.14	0.47
4:E:318:GLU:HB2	8:I:39:ASP:HA	1.96	0.47
6:G:39:ALA:HB2	6:G:75:ALA:HB3	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:56:ARG:HD3	11:R:74:LEU:HA	1.96	0.47
11:R:16:GLY:HA2	11:R:19:VAL:HG12	1.96	0.47
11:R:147:MET:O	11:R:150:THR:OG1	2.26	0.47
14:U:172:SER:OG	14:U:174:THR:O	2.28	0.47
3:3:364:LEU:HD13	3:3:648:LEU:HD13	1.96	0.47
3:3:463:ALA:O	3:3:465:HIS:ND1	2.47	0.47
3:3:688:ARG:HD3	3:3:688:ARG:HA	1.49	0.47
4:4:384:ALA:HB1	4:4:396:ILE:HD11	1.96	0.47
4:4:390:VAL:HB	4:4:391:PRO:HD3	1.96	0.47
15:N:245:ASN:OD1	15:N:374:TYR:OH	2.32	0.47
16:H:216:ARG:CG	16:H:294:ARG:HD2	2.45	0.47
6:G:41:PHE:CE2	6:G:43:LEU:HD21	2.50	0.47
6:G:94:ARG:O	6:G:98:GLN:N	2.47	0.47
3:3:256:CYS:O	3:3:262:GLY:HA2	2.14	0.47
3:3:337:ARG:H	3:3:337:ARG:CD	2.26	0.47
13:L:372:ALA:O	13:L:381:GLY:HA3	2.14	0.47
14:M:148:PHE:O	14:M:152:THR:HG23	2.15	0.47
1:B:123:TYR:HA	1:B:167:PHE:CE1	2.48	0.47
1:B:205:PHE:HB2	1:B:208:GLN:OE1	2.14	0.47
1:B:230:ILE:HG23	1:B:235:ALA:HA	1.96	0.47
3:D:706:GLY:O	3:D:709:GLN:HB2	2.15	0.47
4:E:381:LEU:HB3	4:E:382:PRO:HD3	1.95	0.47
10:P:75:VAL:HG11	16:Q:167:GLY:HA3	1.95	0.47
14:U:43:HIS:NE2	14:U:67:LEU:O	2.32	0.47
14:U:306:GLU:O	14:U:379:LEU:HB3	2.14	0.47
14:U:325:LEU:HG	14:U:361:LEU:HB3	1.96	0.47
16:Q:65:LYS:HZ2	16:Q:69:LYS:HE2	1.79	0.47
3:3:40:SER:HB3	3:3:437:ILE:HG22	1.95	0.47
6:6:33:SER:HB2	6:6:155:GLN:HG2	1.97	0.47
13:L:380:SER:HB3	13:L:457:GLY:H	1.80	0.47
14:M:316:ALA:O	14:M:320:VAL:HG23	2.15	0.47
16:H:147:TYR:CD1	16:H:229:VAL:HG22	2.48	0.47
1:B:343:ASN:HD22	2:C:89:LYS:HZ2	1.61	0.47
13:T:263:LEU:HB3	13:T:266:VAL:HB	1.95	0.47
14:U:127:ILE:HB	14:U:128:PRO:HD3	1.94	0.47
3:3:371:PHE:CZ	3:3:374:ARG:HA	2.49	0.47
6:6:96:TRP:CE3	6:6:97:GLU:HG3	2.50	0.47
7:9:91:TYR:HB3	7:9:133:LYS:HB2	1.97	0.47
12:K:15:VAL:O	12:K:19:LEU:HG	2.14	0.47
13:L:444:TRP:O	13:L:447:HIS:HB2	2.14	0.47
16:H:111:TYR:O	16:H:112:GLN:NE2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:260:PRO:HG3	16:H:286:PHE:CD2	2.49	0.47
2:C:71:GLN:NE2	2:C:120:GLN:OE1	2.46	0.47
3:D:351:LEU:HD11	3:D:615:VAL:HG23	1.95	0.47
3:D:405:GLU:OE1	3:D:509:ALA:N	2.47	0.47
3:D:505:LEU:HD21	3:D:507:LEU:HD21	1.96	0.47
10:P:106:GLY:O	10:P:109:TYR:HB3	2.15	0.47
1:1:223:THR:O	1:1:227:VAL:HG23	2.14	0.47
3:3:177:ASP:HB3	3:3:234:ALA:HA	1.96	0.47
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.97	0.47
4:4:356:TYR:CE2	5:5:55:LEU:HD11	2.49	0.47
13:L:291:ILE:HD12	13:L:336:SER:HB3	1.97	0.47
13:L:293:LYS:O	13:L:297:TYR:HD1	1.98	0.47
16:H:225:GLU:HB3	16:H:226:GLN:HG2	1.97	0.47
16:H:274:VAL:HG22	16:H:275:PRO:HD2	1.95	0.47
1:B:291:ILE:HG12	1:B:299:PRO:HB3	1.97	0.47
6:G:35:SER:OG	16:Q:65:LYS:HD3	2.14	0.47
8:I:71:ASP:OD2	8:I:81:ARG:NH2	2.46	0.47
12:S:15:VAL:O	12:S:19:LEU:HG	2.14	0.47
13:T:512:PHE:HA	13:T:517:PHE:HE1	1.79	0.47
14:U:157:LEU:HD23	14:U:157:LEU:HA	1.70	0.47
15:V:108:LEU:HA	15:V:111:LEU:HD12	1.96	0.47
16:Q:65:LYS:NZ	16:Q:69:LYS:HE2	2.30	0.47
1:1:137:GLU:O	2:2:141:TYR:OH	2.26	0.47
3:3:29:ASP:OD1	3:3:29:ASP:N	2.48	0.47
4:4:148:TYR:O	4:4:151:ARG:HB3	2.15	0.47
4:4:254:TYR:HH	4:4:346:THR:HG1	1.51	0.47
11:J:61:GLY:O	11:J:65:VAL:HG21	2.15	0.47
13:L:26:GLU:HB3	13:L:27:PRO:HD3	1.97	0.47
16:H:70:GLU:O	16:H:237:SER:OG	2.28	0.47
16:H:260:PRO:HG3	16:H:286:PHE:CE2	2.49	0.47
3:D:459:MET:HA	3:D:462:ALA:HB3	1.97	0.47
13:T:433:HIS:CG	13:T:433:HIS:O	2.67	0.47
15:V:40:LEU:HD13	15:V:64:LEU:HB2	1.96	0.47
15:V:316:TYR:HB2	15:V:382:VAL:HG12	1.97	0.47
4:4:236:GLY:HA2	4:4:351:GLY:CA	2.41	0.47
7:9:149:GLU:HA	7:9:152:ARG:NE	2.29	0.47
9:W:91:GLU:OE1	9:W:126:TYR:OH	2.22	0.47
15:N:201:GLN:OE1	15:N:256:ARG:NH1	2.48	0.47
16:H:232:TYR:HB2	16:H:244:PHE:CD1	2.50	0.47
1:B:243:THR:HG22	1:B:244:GLU:H	1.80	0.47
1:B:344:LEU:HD21	2:C:86:LEU:HD22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LYS:O	1:B:386:ASN:ND2	2.48	0.47
3:D:19:VAL:HG23	3:D:85:THR:O	2.15	0.47
3:D:48:CYS:O	3:D:82:SER:OG	2.18	0.47
3:D:165:ASP:OD2	3:D:168:HIS:HB2	2.14	0.47
3:D:395:PHE:HB3	3:D:503:PRO:HB3	1.97	0.47
6:G:34:ASN:HB3	16:Q:51:VAL:HG21	1.96	0.47
10:P:66:MET:O	10:P:69:ILE:HG12	2.15	0.47
14:U:363:LEU:HD22	14:U:368:LEU:HD13	1.96	0.47
16:Q:227:GLU:HG2	16:Q:228:LEU:N	2.30	0.47
16:Q:324:THR:O	16:Q:328:VAL:HG23	2.15	0.47
3:3:115:HIS:HB3	4:4:321:MET:HE2	1.97	0.47
10:A:106:GLY:O	10:A:109:TYR:HB3	2.15	0.47
1:B:104:ARG:O	1:B:108:GLU:HG3	2.14	0.47
1:B:404:ASP:HA	1:B:407:VAL:HG22	1.95	0.47
3:D:36:GLU:OE1	3:D:37:LYS:N	2.46	0.47
3:D:387:LEU:O	3:D:390:LEU:HB3	2.14	0.47
3:D:439:GLU:HG2	3:D:440:ARG:HG2	1.97	0.47
3:D:582:PHE:HA	3:D:599:HIS:ND1	2.30	0.47
4:E:80:THR:HG21	7:O:64:PRO:HG3	1.97	0.47
4:E:118:VAL:O	4:E:122:GLU:HG2	2.15	0.47
6:G:63:PHE:HA	16:Q:50:ARG:HG2	1.97	0.47
11:R:24:ASN:HA	11:R:77:ALA:O	2.15	0.47
13:T:413:THR:HA	13:T:416:TYR:CE2	2.50	0.47
14:U:448:GLY:O	14:U:452:ARG:HG2	2.15	0.47
15:V:262:SER:OG	15:V:288:TYR:OH	2.27	0.47
1:1:63:ARG:O	1:1:65:ARG:NE	2.46	0.46
4:4:209:ALA:HB2	4:4:277:LEU:HD21	1.96	0.46
7:9:68:ILE:HD11	17:9:201:SF4:S1	2.55	0.46
12:K:90:LEU:HB3	15:N:131:GLU:HG3	1.96	0.46
13:L:586:LEU:HD13	15:N:138:LEU:HD12	1.96	0.46
14:M:75:PHE:CZ	14:M:111:ALA:HB2	2.50	0.46
14:M:204:LYS:HE3	14:M:234:TYR:O	2.14	0.46
14:M:371:LEU:HD12	14:M:440:LEU:HB3	1.96	0.46
15:N:87:LEU:HB3	15:N:117:PRO:HB2	1.96	0.46
3:D:133:ARG:NE	3:D:136:GLU:OE2	2.32	0.46
4:E:343:TYR:HB2	4:E:356:TYR:CD1	2.48	0.46
5:F:67:ARG:NH1	5:F:96:GLU:OE2	2.47	0.46
14:U:22:ARG:HD2	14:U:22:ARG:C	2.34	0.46
14:U:341:ILE:HG13	14:U:342:GLY:N	2.28	0.46
16:Q:72:ILE:HG22	16:Q:237:SER:HB3	1.97	0.46
1:1:53:VAL:O	1:1:57:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:63:HIS:O	6:6:122:ALA:HB1	2.14	0.46
12:K:88:ASP:OD1	13:L:587:ARG:HG3	2.15	0.46
13:L:142:ILE:HA	13:L:232:GLY:HA3	1.97	0.46
14:M:91:VAL:HB	14:M:95:PHE:CE1	2.50	0.46
15:N:299:LEU:HD21	15:N:312:LEU:HD11	1.97	0.46
15:N:318:LYS:HD3	15:N:391:PHE:CG	2.51	0.46
15:N:411:ALA:O	15:N:415:LEU:N	2.35	0.46
16:H:103:GLY:HA2	16:H:267:TRP:CE2	2.50	0.46
1:B:140:ARG:HB2	2:C:140:PRO:HG3	1.96	0.46
1:B:174:HIS:ND1	2:C:18:TYR:OH	2.42	0.46
3:D:170:LEU:HD11	3:D:176:LEU:HD22	1.97	0.46
4:E:38:HIS:HB2	20:E:501:DCQ:C4	2.44	0.46
5:F:71:VAL:HG11	5:F:89:PHE:HD2	1.79	0.46
6:G:138:PRO:HG2	7:O:121:MET:HG3	1.97	0.46
11:R:19:VAL:HG21	11:R:32:LEU:HB2	1.97	0.46
13:T:108:PHE:HE1	13:T:236:VAL:HG22	1.81	0.46
15:V:52:PRO:HB3	15:V:103:HIS:HB2	1.97	0.46
16:Q:143:SER:HB2	16:Q:235:GLU:HG3	1.98	0.46
3:3:232:VAL:HA	17:3:801:SF4:S2	2.56	0.46
4:4:112:ARG:NH1	4:4:181:ASP:OD2	2.46	0.46
4:4:127:ALA:HB1	4:4:153:ARG:NH1	2.30	0.46
5:5:28:VAL:HA	5:5:91:ARG:O	2.15	0.46
13:L:192:MET:SD	13:L:258:PHE:HE1	2.39	0.46
13:L:422:VAL:O	13:L:426:LEU:N	2.47	0.46
1:B:253:GLN:HA	1:B:262:GLY:O	2.15	0.46
4:E:213:ILE:O	4:E:217:ARG:HG2	2.16	0.46
11:R:138:VAL:HG22	15:V:106:LEU:HD22	1.98	0.46
1:1:93:ALA:HB3	1:1:133:TYR:O	2.16	0.46
3:3:722:THR:HG21	3:3:756:GLY:N	2.28	0.46
6:6:99:MET:HG2	6:6:100:PRO:HD2	1.98	0.46
13:L:163:ARG:HD3	14:M:399:VAL:O	2.15	0.46
14:M:7:LEU:O	14:M:11:VAL:HG12	2.16	0.46
14:M:349:GLN:NE2	14:M:418:GLY:HA3	2.30	0.46
15:N:61:VAL:O	15:N:65:LEU:HG	2.16	0.46
2:C:79:HIS:H	2:C:137:ASN:ND2	2.13	0.46
4:E:216:GLU:O	16:Q:301:ARG:NH1	2.48	0.46
5:F:82:ASP:OD1	5:F:82:ASP:N	2.49	0.46
12:S:28:PHE:CE1	12:S:68:VAL:HA	2.46	0.46
15:V:313:ARG:HB2	15:V:384:ALA:HB3	1.97	0.46
2:2:24:ARG:NH2	2:2:59:GLU:HB3	2.31	0.46
4:4:370:VAL:HB	4:4:409:ARG:HD2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:39:ALA:HB2	6:6:75:ALA:CB	2.46	0.46
6:6:158:VAL:HA	6:6:172:PRO:HB3	1.96	0.46
7:9:44:THR:HG22	7:9:138:VAL:HG11	1.96	0.46
8:7:40:PHE:HA	8:7:43:ARG:HG2	1.97	0.46
1:B:190:ASN:OD1	1:B:200:ARG:NE	2.43	0.46
3:D:356:LEU:HD13	3:D:654:PHE:HB2	1.97	0.46
13:T:77:LEU:HD12	13:T:116:LEU:HD22	1.98	0.46
13:T:90:TYR:OH	13:T:334:LEU:O	2.15	0.46
15:V:237:VAL:HG11	15:V:271:LEU:HD11	1.97	0.46
15:V:294:LEU:HD12	15:V:405:ALA:HB3	1.97	0.46
16:Q:131:LEU:HA	16:Q:134:TYR:HB2	1.98	0.46
16:Q:200:PHE:N	16:Q:341:SER:OG	2.46	0.46
1:1:373:LYS:NZ	1:1:383:ASP:OD1	2.44	0.46
3:3:139:LEU:HD12	4:4:326:TYR:CZ	2.51	0.46
4:4:154:GLU:OE2	4:4:167:ARG:NH2	2.47	0.46
14:M:206:PRO:HD2	14:M:293:MET:HG3	1.98	0.46
15:N:237:VAL:O	15:N:241:VAL:HG23	2.16	0.46
2:C:173:GLY:HA3	2:C:176:VAL:O	2.16	0.46
3:D:274:LEU:H	3:D:302:ASP:CB	2.27	0.46
13:T:461:LEU:N	13:T:467:ASN:OD1	2.45	0.46
3:3:38:HIS:ND1	3:3:287:GLU:OE2	2.48	0.46
4:4:80:THR:HG21	7:9:64:PRO:HG3	1.98	0.46
8:7:86:LEU:HB2	8:7:91:ILE:HB	1.96	0.46
11:J:97:ALA:O	11:J:100:VAL:HG12	2.16	0.46
13:L:433:HIS:O	13:L:433:HIS:CG	2.69	0.46
15:N:262:SER:HG	15:N:288:TYR:HH	1.57	0.46
15:N:317:ARG:NH2	15:N:383:PHE:O	2.49	0.46
16:H:190:LYS:HB2	16:H:268:THR:HG21	1.98	0.46
3:D:46:ARG:N	19:D:804:FES:S1	2.88	0.46
13:T:210:PHE:CD1	13:T:270:ILE:HG12	2.51	0.46
13:T:541:LEU:C	13:T:545:PRO:HG2	2.35	0.46
14:U:148:PHE:O	14:U:152:THR:HG23	2.16	0.46
1:1:409:PRO:O	1:1:413:SER:HB3	2.16	0.46
3:3:149:LEU:HD12	4:4:108:VAL:HG23	1.98	0.46
4:4:31:GLY:HA3	10:A:45:GLU:OE2	2.16	0.46
4:4:40:VAL:O	4:4:404:MET:HG3	2.16	0.46
4:4:379:GLN:HG2	5:5:113:PHE:CD2	2.51	0.46
5:5:82:ASP:OD1	5:5:82:ASP:N	2.47	0.46
10:A:2:ALA:HB3	16:H:119:ASP:OD2	2.16	0.46
10:A:29:ALA:O	10:A:34:LYS:NZ	2.28	0.46
10:A:67:LEU:HD23	16:H:310:TRP:CZ2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:586:LEU:HD11	15:N:135:LYS:HA	1.98	0.46
14:M:54:PRO:HA	14:M:62:TYR:CD1	2.50	0.46
15:N:115:SER:HB2	15:N:119:TYR:CZ	2.50	0.46
15:N:126:ARG:HD2	15:N:128:GLN:HG2	1.97	0.46
6:G:140:CYS:SG	7:O:99:ILE:HG13	2.55	0.46
9:X:48:LEU:O	9:X:58:LEU:HD12	2.16	0.46
13:T:90:TYR:CE2	13:T:334:LEU:HB3	2.51	0.46
15:V:63:THR:HG21	15:V:96:HIS:ND1	2.31	0.46
15:V:155:TYR:HB2	15:V:161:LEU:HD21	1.98	0.46
4:4:247:ASP:OD1	4:4:249:ARG:HG3	2.16	0.46
8:7:49:ASP:OD1	8:7:75:ARG:NE	2.38	0.46
13:L:469:LEU:HA	13:L:469:LEU:HD12	1.72	0.46
14:M:106:LEU:O	14:M:110:PHE:HD1	1.99	0.46
14:M:331:ARG:HA	14:M:331:ARG:HH11	1.81	0.46
16:H:333:PRO:HB2	16:H:335:THR:H	1.80	0.46
1:B:4:PRO:HA	1:B:12:ARG:HH22	1.80	0.46
2:C:78:TYR:CZ	2:C:157:LEU:HD22	2.50	0.46
2:C:162:ARG:NE	2:C:164:GLU:OE2	2.35	0.46
3:D:37:LYS:HB3	3:D:430:THR:HG21	1.97	0.46
3:D:119:CYS:HB2	3:D:120:PRO:HD3	1.97	0.46
3:D:454:TYR:HB2	3:D:752:ASP:OD2	2.16	0.46
4:E:366:TYR:HE1	5:F:59:THR:HB	1.80	0.46
7:O:117:TYR:CZ	7:O:163:VAL:HG11	2.51	0.46
1:1:291:ILE:HG12	1:1:299:PRO:HB3	1.97	0.46
2:2:58:THR:HG23	3:3:213:THR:HA	1.98	0.46
3:3:254:THR:OG1	3:3:624:LEU:HD23	2.16	0.46
4:4:352:GLU:OE2	5:5:87:ARG:NH1	2.42	0.46
13:L:198:ASN:ND2	13:L:201:LEU:HB2	2.31	0.46
13:L:291:ILE:HG13	13:L:292:LYS:N	2.31	0.46
14:M:186:GLN:HG2	14:M:187:GLU:H	1.81	0.46
4:E:66:PHE:HZ	6:G:83:ARG:HH12	1.63	0.46
13:T:84:GLY:O	13:T:88:HIS:ND1	2.45	0.46
13:T:348:ASP:OD1	13:T:349:VAL:N	2.47	0.46
13:T:403:TYR:CZ	13:T:493:LEU:HD13	2.51	0.46
14:U:78:ILE:HG22	14:U:103:GLU:HG3	1.98	0.46
3:3:464:ILE:HG21	3:3:493:ALA:HB2	1.97	0.45
3:3:735:ALA:HA	3:3:744:GLU:HA	1.98	0.45
4:4:356:TYR:HE2	5:5:55:LEU:HD11	1.81	0.45
7:9:33:LEU:HD12	7:9:161:TYR:CG	2.51	0.45
13:L:70:ASP:OD2	13:L:73:SER:OG	2.27	0.45
4:E:148:TYR:HE2	7:O:16:TYR:CG	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:190:LEU:HD23	4:E:294:LEU:HD12	1.97	0.45
4:E:246:TYR:HD1	5:F:78:PRO:HD2	1.81	0.45
7:O:102:GLY:HA2	7:O:115:LEU:HD11	1.97	0.45
16:Q:35:GLU:HA	16:Q:291:ILE:HD13	1.97	0.45
16:Q:35:GLU:OE1	16:Q:249:TYR:OH	2.26	0.45
16:Q:227:GLU:HG2	16:Q:228:LEU:H	1.80	0.45
16:Q:276:TYR:HD2	16:Q:280:PHE:HE2	1.64	0.45
16:Q:301:ARG:NH2	16:Q:304:GLN:HB2	2.31	0.45
1:1:157:TYR:O	1:1:158:LEU:HD23	2.16	0.45
1:1:222:GLU:OE2	1:1:250:LYS:HD2	2.16	0.45
3:3:115:HIS:O	3:3:161:ARG:HD3	2.15	0.45
4:4:367:ARG:HH12	4:4:369:LYS:HB2	1.79	0.45
13:L:414:ALA:HB1	13:L:505:LEU:HD23	1.96	0.45
15:N:17:GLY:HA3	15:N:82:PHE:CE2	2.51	0.45
16:H:308:PHE:O	16:H:312:PHE:HB3	2.16	0.45
1:B:18:TYR:CD2	1:B:21:VAL:HG21	2.51	0.45
3:D:281:GLU:HA	3:D:287:GLU:O	2.15	0.45
3:D:409:LEU:HA	3:D:409:LEU:HD23	1.59	0.45
11:R:65:VAL:HG11	16:Q:160:ILE:CD1	2.45	0.45
11:R:75:PHE:O	11:R:77:ALA:N	2.50	0.45
14:U:75:PHE:HZ	14:U:111:ALA:HB2	1.81	0.45
15:V:280:ALA:HA	15:V:347:LEU:HD13	1.98	0.45
16:Q:146:LYS:HG2	16:Q:149:LEU:HD12	1.98	0.45
16:Q:218:PRO:C	16:Q:220:ASP:H	2.20	0.45
1:1:254:ILE:HG23	1:1:261:PRO:HA	1.97	0.45
3:3:29:ASP:OD2	5:5:187:GLY:N	2.31	0.45
3:3:224:GLY:O	3:3:227:THR:HB	2.17	0.45
13:L:391:ALA:O	13:L:395:TYR:HB2	2.16	0.45
15:N:294:LEU:O	15:N:298:VAL:HG23	2.17	0.45
16:H:33:LEU:HD11	16:H:56:LEU:HA	1.98	0.45
1:B:197:ALA:HB3	2:C:66:PHE:CZ	2.51	0.45
4:E:112:ARG:NH2	4:E:181:ASP:OD1	2.49	0.45
4:E:261:THR:H	4:E:292:GLN:NE2	2.12	0.45
11:R:155:ALA:O	15:V:81:ARG:NH1	2.48	0.45
14:U:7:LEU:O	14:U:11:VAL:HG12	2.17	0.45
16:Q:216:ARG:CG	16:Q:294:ARG:HD2	2.46	0.45
1:1:195:LEU:HD23	2:2:24:ARG:HH12	1.81	0.45
1:1:401:PRO:HB2	18:1:502:FMN:HM82	1.98	0.45
3:3:33:PHE:HZ	3:3:130:LEU:HA	1.81	0.45
3:3:713:ARG:HE	3:3:746:ARG:HE	1.64	0.45
4:4:382:PRO:O	4:4:386:LYS:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:74:GLU:O	10:A:78:LEU:HG	2.16	0.45
11:J:33:ILE:HG12	11:J:64:VAL:HG11	1.97	0.45
13:L:263:LEU:HD13	13:L:266:VAL:HG21	1.99	0.45
13:L:380:SER:HA	13:L:457:GLY:HA2	1.99	0.45
14:M:113:ARG:HH21	14:M:178:GLU:HB2	1.82	0.45
1:B:18:TYR:CZ	1:B:263:VAL:HG11	2.52	0.45
4:E:211:SER:HB2	4:E:214:PHE:HB3	1.97	0.45
16:Q:204:LEU:HD12	16:Q:348:LEU:HD13	1.99	0.45
16:Q:234:THR:O	16:Q:234:THR:HG22	2.16	0.45
4:4:131:VAL:HG23	4:4:153:ARG:HD2	1.99	0.45
10:A:61:PHE:HB3	11:J:69:PHE:CD2	2.52	0.45
13:L:454:VAL:HB	13:L:455:LEU:HD22	1.98	0.45
14:M:302:SER:O	14:M:304:THR:HG23	2.16	0.45
15:N:237:VAL:HG22	15:N:270:ALA:HB3	1.98	0.45
1:B:184:GLU:OE1	1:B:186:THR:OG1	2.19	0.45
3:D:29:ASP:OD1	3:D:29:ASP:N	2.49	0.45
3:D:387:LEU:HD23	3:D:387:LEU:HA	1.76	0.45
4:E:247:ASP:OD1	4:E:249:ARG:HG3	2.16	0.45
14:U:318:SER:HA	14:U:321:TYR:CE1	2.51	0.45
4:4:211:SER:HB2	4:4:215:TYR:N	2.32	0.45
12:K:27:VAL:HG11	15:N:138:LEU:HD13	1.98	0.45
13:L:419:ARG:HD2	13:L:512:PHE:CZ	2.51	0.45
16:H:271:VAL:HG12	16:H:272:LEU:HG	1.99	0.45
1:B:53:VAL:O	1:B:57:VAL:HG23	2.16	0.45
4:E:371:ARG:HG3	5:F:51:ASP:OD1	2.15	0.45
5:F:64:ARG:HD3	5:F:64:ARG:HA	1.73	0.45
16:Q:163:GLU:O	16:Q:166:LEU:HB2	2.17	0.45
4:4:62:LEU:HD11	6:6:43:LEU:O	2.17	0.45
4:4:185:GLU:OE1	4:4:185:GLU:N	2.46	0.45
7:9:40:ARG:HH21	7:9:118:ASP:CG	2.18	0.45
10:A:65:ALA:HB1	11:J:66:LEU:HB2	1.99	0.45
11:J:75:PHE:O	11:J:77:ALA:N	2.50	0.45
13:L:328:PHE:O	13:L:331:LEU:HB3	2.16	0.45
14:M:208:PHE:N	14:M:267:SER:OG	2.48	0.45
14:M:318:SER:HA	14:M:321:TYR:CZ	2.51	0.45
16:H:103:GLY:O	16:H:113:PRO:HG2	2.15	0.45
16:H:331:ASP:CG	16:H:334:ARG:HH22	2.20	0.45
2:C:50:ALA:HA	2:C:53:VAL:HG12	1.99	0.45
4:E:217:ARG:HD2	16:Q:301:ARG:NH1	2.32	0.45
4:E:260:TYR:HA	4:E:292:GLN:NE2	2.32	0.45
4:E:400:LEU:HA	4:E:400:LEU:HD23	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:37:TRP:CH2	16:Q:36:ARG:NH2	2.85	0.45
16:Q:37:ARG:HD3	16:Q:47:GLY:HA3	1.98	0.45
4:4:349:ALA:HB3	4:4:350:ARG:HH12	1.82	0.45
5:5:153:GLY:HA2	9:W:113:ARG:NH2	2.31	0.45
13:L:427:GLY:O	13:L:428:GLU:HG2	2.17	0.45
14:M:385:TYR:CD1	14:M:389:PRO:HB3	2.52	0.45
16:H:32:THR:O	16:H:36:ARG:HG3	2.17	0.45
16:H:274:VAL:HG12	16:H:278:TRP:NE1	2.31	0.45
1:B:363:VAL:O	1:B:368:VAL:HG12	2.17	0.45
4:E:263:ASP:O	4:E:285:GLU:HG3	2.16	0.45
13:T:575:GLY:HA2	15:V:246:LEU:HB3	1.98	0.45
14:U:305:PRO:O	14:U:309:MET:HB3	2.17	0.45
15:V:76:LEU:HD12	15:V:206:PRO:HB3	1.99	0.45
15:V:340:ALA:HA	15:V:343:TRP:CD1	2.51	0.45
16:Q:216:ARG:NH1	16:Q:294:ARG:HB3	2.31	0.45
16:Q:332:LEU:H	16:Q:332:LEU:HD12	1.81	0.45
1:1:17:LEU:HD12	1:1:251:LEU:HD11	1.99	0.45
1:1:238:PHE:CE2	1:1:248:GLY:HA3	2.52	0.45
4:4:171:ASN:ND2	4:4:174:ARG:HH22	2.15	0.45
9:W:32:TYR:OH	9:W:115:MET:HG2	2.17	0.45
13:L:335:ALA:O	13:L:339:VAL:HG23	2.16	0.45
15:N:95:MET:HA	15:N:114:LEU:HD22	1.99	0.45
15:N:203:SER:HB2	15:N:208:VAL:HG22	1.98	0.45
16:H:140:GLY:HA3	16:H:152:SER:HB3	1.99	0.45
1:B:419:ASP:O	1:B:423:ALA:N	2.36	0.45
3:D:165:ASP:HB3	3:D:178:ARG:HD2	1.99	0.45
3:D:248:GLU:HB3	3:D:270:ARG:NH1	2.31	0.45
3:D:248:GLU:HG2	5:F:170:PHE:CE1	2.52	0.45
3:D:478:LEU:HD12	3:D:520:ARG:NH2	2.32	0.45
4:E:33:GLN:N	4:E:40:VAL:HG23	2.31	0.45
6:G:154:LEU:O	6:G:158:VAL:HG13	2.17	0.45
9:X:90:TYR:HB3	9:X:118:ALA:HB1	1.99	0.45
10:P:62:TYR:OH	12:S:73:GLY:N	2.50	0.45
10:P:105:VAL:HG22	15:V:15:LEU:HD11	1.99	0.45
13:T:41:PHE:HB2	13:T:81:THR:HB	1.98	0.45
14:U:68:ASP:OD2	14:U:243:ARG:NH2	2.50	0.45
14:U:347:LEU:HB2	14:U:414:PHE:HA	1.98	0.45
16:Q:237:SER:OG	16:Q:238:SER:N	2.49	0.45
4:4:283:MET:O	4:4:287:VAL:HG23	2.17	0.45
11:J:5:GLU:OE2	12:K:3:TYR:OH	2.31	0.45
13:L:108:PHE:CE1	13:L:236:VAL:HG22	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:69:GLY:O	14:M:73:LEU:CD2	2.57	0.45
14:M:114:ASP:HB3	14:M:176:LEU:HD23	1.99	0.45
1:B:107:LEU:O	1:B:111:PRO:HG3	2.17	0.45
1:B:157:TYR:O	1:B:158:LEU:HD23	2.17	0.45
2:C:146:THR:HG23	2:C:149:ARG:H	1.82	0.45
3:D:128:CYS:HB3	3:D:131:GLN:HB2	1.99	0.45
4:E:41:LEU:HD12	4:E:42:ARG:H	1.82	0.45
10:P:110:GLU:O	10:P:114:GLY:N	2.49	0.45
15:V:321:LEU:HD13	15:V:403:VAL:HG21	1.98	0.45
16:Q:267:TRP:O	16:Q:269:MET:N	2.50	0.45
4:4:381:LEU:HB3	4:4:382:PRO:HD3	1.98	0.44
10:A:96:VAL:HA	10:A:99:PHE:HB3	1.99	0.44
16:H:69:LYS:HB3	16:H:238:SER:HA	1.99	0.44
16:H:266:GLY:HA2	16:H:279:MET:HE1	1.98	0.44
1:B:96:SER:HA	1:B:135:ARG:NH1	2.31	0.44
1:B:243:THR:N	1:B:246:SER:O	2.50	0.44
2:C:93:ALA:HA	2:C:96:LEU:HB3	1.99	0.44
3:D:237:ASP:OD1	3:D:239:THR:HG22	2.17	0.44
3:D:618:GLU:OE2	3:D:620:ARG:NE	2.49	0.44
3:D:681:LYS:HE3	3:D:681:LYS:HB3	1.70	0.44
3:D:688:ARG:HD3	3:D:688:ARG:HA	1.76	0.44
4:E:288:LYS:HA	4:E:288:LYS:HD3	1.76	0.44
6:G:148:ILE:HG21	7:O:26:TYR:HD2	1.80	0.44
13:T:13:GLY:O	13:T:17:LEU:HG	2.17	0.44
13:T:549:LEU:O	13:T:553:LEU:HG	2.17	0.44
3:3:19:VAL:HG23	3:3:85:THR:O	2.17	0.44
3:3:378:PRO:HD2	3:3:683:LEU:HD23	1.99	0.44
3:3:421:LYS:N	3:3:436:GLN:OE1	2.46	0.44
4:4:72:HIS:HB3	5:5:171:ARG:CZ	2.47	0.44
4:4:193:LEU:HA	4:4:196:VAL:HG12	1.99	0.44
7:9:40:ARG:NH2	7:9:173:PHE:HZ	2.15	0.44
7:9:123:ASP:HB3	7:9:129:LEU:HG	1.98	0.44
10:A:56:ARG:HB3	11:J:73:LEU:O	2.17	0.44
16:H:304:GLN:HE22	16:H:307:ARG:HD2	1.81	0.44
1:B:62:LEU:HD11	1:B:223:THR:HG23	1.98	0.44
13:T:461:LEU:HB3	13:T:465:LEU:HB2	1.99	0.44
14:U:75:PHE:CZ	14:U:111:ALA:HB2	2.52	0.44
14:U:106:LEU:O	14:U:110:PHE:HD1	2.00	0.44
14:U:302:SER:O	14:U:304:THR:HG23	2.18	0.44
14:U:463:LYS:HD2	14:U:463:LYS:HA	1.77	0.44
1:1:241:MET:HG2	1:1:267:PRO:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:164:ASN:HD22	6:6:170:LEU:HD21	1.82	0.44
13:L:90:TYR:CD2	13:L:334:LEU:HD13	2.53	0.44
14:M:69:GLY:HA3	14:M:453:GLY:HA3	1.99	0.44
14:M:146:TYR:HE1	15:N:376:LEU:HB3	1.82	0.44
14:M:172:SER:OG	14:M:174:THR:O	2.33	0.44
16:H:36:ARG:NH2	16:H:62:ASP:OD2	2.50	0.44
1:B:259:LYS:O	2:C:179:VAL:N	2.35	0.44
6:G:105:VAL:HB	6:G:132:PRO:O	2.17	0.44
12:S:63:VAL:HG13	15:V:112:GLU:HG3	1.99	0.44
14:U:54:PRO:HA	14:U:62:TYR:CD1	2.43	0.44
16:Q:12:MET:HG2	16:Q:111:TYR:CD2	2.52	0.44
16:Q:147:TYR:CD1	16:Q:229:VAL:HG22	2.52	0.44
16:Q:222:PRO:HG2	16:Q:230:GLY:HA2	1.99	0.44
1:1:343:ASN:O	1:1:346:ARG:HG2	2.18	0.44
3:3:149:LEU:HG	4:4:305:PRO:HD2	2.00	0.44
3:3:406:ALA:O	3:3:409:LEU:HB2	2.18	0.44
4:4:73:ARG:HH11	5:5:171:ARG:HH21	1.66	0.44
12:K:1:MET:HG3	12:K:5:LEU:HD11	2.00	0.44
15:N:345:LYS:NZ	15:N:368:SER:OG	2.49	0.44
16:H:202:ALA:O	16:H:205:VAL:HG22	2.18	0.44
1:B:66:GLY:HA3	18:B:502:FMN:H3'	2.00	0.44
1:B:293:GLY:HA3	1:B:297:THR:HG21	1.98	0.44
1:B:364:ALA:HB3	3:D:207:VAL:HG13	2.00	0.44
2:C:31:LEU:HD22	2:C:41:ILE:HD13	2.00	0.44
4:E:180:GLU:HG3	7:O:36:ARG:HH12	1.83	0.44
11:R:97:ALA:HB2	12:S:16:TYR:HB2	2.00	0.44
15:V:175:ALA:O	15:V:179:LEU:HG	2.18	0.44
16:Q:226:GLN:HB2	16:Q:299:ARG:HH22	1.83	0.44
4:4:130:LEU:HD22	4:4:149:ALA:HB1	1.99	0.44
4:4:375:PHE:HB2	4:4:407:VAL:HA	1.98	0.44
5:5:75:VAL:HG21	5:5:87:ARG:HH21	1.82	0.44
11:J:23:ARG:HG2	11:J:80:GLU:HG2	1.99	0.44
14:M:402:SER:HA	14:M:405:TYR:CE2	2.52	0.44
2:C:81:GLN:NE2	2:C:135:GLN:OE1	2.50	0.44
3:D:729:PRO:HD2	3:D:732:ALA:HB3	1.98	0.44
4:E:353:LEU:HD12	4:E:354:GLY:H	1.82	0.44
13:T:129:ILE:HG12	14:U:369:PRO:HB2	1.98	0.44
13:T:365:HIS:CD2	13:T:450:ALA:HB2	2.52	0.44
15:V:95:MET:HB3	15:V:218:ALA:HB2	1.99	0.44
1:1:107:LEU:O	1:1:111:PRO:HG3	2.18	0.44
2:2:83:CYS:SG	2:2:124:CYS:HA	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:276:MET:O	4:4:280:ILE:HG13	2.18	0.44
10:A:70:LEU:HD13	11:J:150:THR:HG22	2.00	0.44
10:A:109:TYR:HE2	11:J:154:VAL:HG21	1.82	0.44
14:M:55:LEU:HD22	14:M:63:TRP:CE2	2.52	0.44
15:N:87:LEU:HB3	15:N:117:PRO:CB	2.47	0.44
15:N:362:VAL:O	15:N:366:VAL:HG23	2.17	0.44
3:D:337:ARG:CD	3:D:337:ARG:H	2.31	0.44
4:E:73:ARG:HG2	4:E:81:TYR:CE1	2.52	0.44
4:E:75:TYR:HA	4:E:78:ASN:HD22	1.83	0.44
4:E:147:PHE:HD2	6:G:56:ALA:HB2	1.82	0.44
4:E:158:ASP:CG	6:G:57:ARG:HH22	2.21	0.44
4:E:159:LEU:O	4:E:163:VAL:HG12	2.17	0.44
5:F:163:ARG:NH1	7:O:90:VAL:HG11	2.33	0.44
15:V:45:GLY:HA3	15:V:425:ALA:O	2.17	0.44
15:V:128:GLN:NE2	15:V:305:ASP:OD1	2.50	0.44
16:Q:96:ALA:HB2	16:Q:128:VAL:HG21	2.00	0.44
16:Q:260:PRO:HG3	16:Q:286:PHE:CE2	2.53	0.44
1:1:356:CYS:HB3	1:1:358:PRO:HG2	1.99	0.44
6:6:37:TRP:O	6:6:75:ALA:HB1	2.18	0.44
6:6:171:PRO:HA	6:6:172:PRO:HD3	1.87	0.44
11:J:109:TRP:HA	11:J:109:TRP:CE3	2.53	0.44
13:L:139:PHE:CD2	13:L:155:ALA:HB1	2.52	0.44
13:L:288:GLN:NE2	13:L:529:ARG:O	2.51	0.44
13:L:463:HIS:NE2	13:L:487:LEU:HD13	2.33	0.44
15:N:103:HIS:O	15:N:107:MET:HB2	2.17	0.44
16:Q:159:LEU:O	16:Q:163:GLU:HB2	2.18	0.44
16:Q:216:ARG:CB	16:Q:294:ARG:HD2	2.46	0.44
16:Q:269:MET:HG3	16:Q:270:PRO:HD2	2.00	0.44
3:3:616:ASN:OD1	3:3:617:LEU:HD23	2.18	0.44
4:4:346:THR:HG22	4:4:353:LEU:O	2.18	0.44
5:5:64:ARG:HA	5:5:64:ARG:HD3	1.64	0.44
6:6:44:ALA:CB	6:6:83:ARG:HE	2.31	0.44
7:9:33:LEU:HG	7:9:161:TYR:HB2	2.00	0.44
7:9:40:ARG:HD2	7:9:131:TYR:HE2	1.83	0.44
16:H:150:LEU:HD23	16:H:154:ARG:HD2	1.99	0.44
1:B:223:THR:O	1:B:227:VAL:HG23	2.17	0.44
1:B:381:GLU:HG3	1:B:422:LEU:HD22	2.00	0.44
5:F:167:PRO:HA	5:F:170:PHE:HB3	1.99	0.44
13:T:342:ALA:HA	13:T:436:HIS:CE1	2.53	0.44
13:T:491:TRP:HA	13:T:494:ILE:HG12	1.99	0.44
14:U:141:ARG:HG3	14:U:142:THR:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:343:ARG:HB3	14:U:344:TYR:HD1	1.83	0.44
15:V:3:LEU:HD13	15:V:96:HIS:HD2	1.83	0.44
4:4:134:GLY:HA3	4:4:146:PHE:HD1	1.82	0.44
4:4:358:VAL:O	4:4:366:TYR:N	2.51	0.44
10:A:23:ALA:O	10:A:27:VAL:HG23	2.18	0.44
13:L:115:MET:HG2	13:L:244:THR:HG22	1.99	0.44
13:L:323:PHE:CZ	13:L:327:PHE:HE2	2.36	0.44
3:D:110:PHE:O	3:D:113:LEU:HB2	2.17	0.44
3:D:135:VAL:HA	4:E:326:TYR:CZ	2.53	0.44
4:E:73:ARG:HG3	4:E:77:GLN:OE1	2.18	0.44
6:G:40:THR:HB	6:G:68:PHE:CZ	2.53	0.44
10:P:109:TYR:HE1	15:V:82:PHE:CZ	2.35	0.44
14:U:204:LYS:HD2	14:U:204:LYS:HA	1.77	0.44
14:U:271:GLY:HA2	14:U:287:TYR:HD1	1.83	0.44
14:U:347:LEU:HD13	14:U:422:VAL:HG21	1.99	0.44
15:V:196:THR:HG22	15:V:259:ALA:HB1	2.00	0.44
1:1:65:ARG:HB2	1:1:223:THR:OG1	2.17	0.43
1:1:393:LEU:HD22	3:3:106:GLY:HA3	2.00	0.43
4:4:353:LEU:HD12	4:4:354:GLY:H	1.82	0.43
5:5:163:ARG:NE	7:9:92:GLU:OE1	2.51	0.43
7:9:56:CYS:SG	7:9:58:LEU:HG	2.57	0.43
10:A:93:PHE:O	10:A:96:VAL:HG12	2.18	0.43
13:L:41:PHE:HD2	13:L:42:LEU:HD12	1.83	0.43
14:M:426:ALA:O	14:M:430:TRP:N	2.50	0.43
1:B:357:THR:N	1:B:358:PRO:HD2	2.32	0.43
3:D:21:ASP:OD1	3:D:432:PHE:N	2.44	0.43
4:E:276:MET:O	4:E:280:ILE:HG13	2.18	0.43
9:X:80:LEU:O	9:X:84:GLN:HG2	2.18	0.43
10:P:71:PHE:CE2	10:P:107:PHE:HB2	2.53	0.43
11:R:5:GLU:O	11:R:9:LEU:HG	2.18	0.43
15:V:201:GLN:HA	15:V:255:LYS:HE3	2.00	0.43
15:V:385:ARG:HH12	15:V:387:GLU:HG2	1.83	0.43
3:3:283:PRO:HA	3:3:287:GLU:HA	2.01	0.43
4:4:81:TYR:CZ	6:6:117:MET:HG3	2.53	0.43
4:4:221:VAL:HG11	4:4:392:ASP:CG	2.38	0.43
5:5:154:GLU:HG2	6:6:119:ASN:O	2.18	0.43
7:9:2:THR:OG1	7:9:2:THR:O	2.36	0.43
10:A:110:GLU:OE1	16:H:310:TRP:NE1	2.38	0.43
1:B:201:LEU:O	1:B:204:PRO:HD2	2.18	0.43
1:B:262:GLY:HA3	2:C:176:VAL:HG12	2.00	0.43
5:F:71:VAL:HA	5:F:90:VAL:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:21:LEU:HD12	9:X:24:LEU:HB3	1.98	0.43
10:P:93:PHE:CE2	16:Q:326:LEU:HD13	2.53	0.43
13:T:287:GLY:HA3	13:T:528:SER:HB2	2.01	0.43
13:T:463:HIS:CD2	13:T:464:PRO:HD3	2.52	0.43
1:1:41:ALA:HB2	1:1:116:GLU:HG3	2.01	0.43
1:1:205:PHE:HB2	1:1:208:GLN:HE22	1.83	0.43
1:1:273:ARG:NH2	1:1:304:GLU:OE1	2.44	0.43
3:3:370:ASP:OD2	3:3:558:TRP:HD1	2.02	0.43
3:3:415:GLU:HA	3:3:420:LEU:HD12	2.01	0.43
4:4:50:GLU:OE1	16:H:154:ARG:NH1	2.33	0.43
4:4:191:LYS:HE2	4:4:294:LEU:HD21	2.00	0.43
8:7:27:LYS:HA	8:7:27:LYS:HD3	1.91	0.43
10:A:48:ASN:OD1	10:A:49:ASP:HB2	2.18	0.43
1:B:112:HIS:CE1	1:B:148:ALA:HB1	2.54	0.43
1:B:184:GLU:HG2	18:B:502:FMN:C8	2.48	0.43
18:B:502:FMN:H1'1	18:B:502:FMN:H9	1.67	0.43
2:C:29:PRO:O	2:C:32:ARG:HB3	2.18	0.43
4:E:314:ARG:O	8:I:46:ARG:NH2	2.51	0.43
4:E:346:THR:HG22	4:E:353:LEU:O	2.19	0.43
5:F:49:LEU:HD21	5:F:52:ILE:HD11	1.99	0.43
5:F:163:ARG:CZ	7:O:90:VAL:HG11	2.48	0.43
6:G:39:ALA:HB2	6:G:75:ALA:CB	2.49	0.43
7:O:149:GLU:O	7:O:153:THR:CB	2.67	0.43
9:X:37:TRP:CD1	9:X:40:LYS:HB2	2.41	0.43
16:Q:141:TRP:HE3	16:Q:149:LEU:HD11	1.81	0.43
4:4:28:LEU:HA	10:A:50:PRO:O	2.19	0.43
13:L:219:GLN:NE2	13:L:277:THR:HG21	2.33	0.43
16:H:217:THR:HG23	16:H:298:PHE:O	2.19	0.43
16:H:267:TRP:O	16:H:269:MET:N	2.51	0.43
1:B:404:ASP:N	1:B:404:ASP:OD1	2.51	0.43
1:B:436:LEU:HD23	2:C:90:LEU:O	2.18	0.43
2:C:89:LYS:HA	2:C:93:ALA:HB3	2.00	0.43
3:D:184:CYS:SG	3:D:185:LYS:N	2.90	0.43
3:D:224:GLY:O	3:D:227:THR:HB	2.17	0.43
13:T:325:HIS:CD2	13:T:329:LYS:HG3	2.53	0.43
13:T:329:LYS:HA	13:T:332:LEU:HD13	2.00	0.43
14:U:21:PRO:HD2	14:U:24:LEU:HG	2.00	0.43
14:U:134:TYR:O	14:U:141:ARG:HD3	2.17	0.43
16:Q:224:ALA:HA	16:Q:229:VAL:HA	2.01	0.43
1:1:170:ASP:OD1	1:1:171:LEU:N	2.51	0.43
4:4:272:VAL:N	4:4:275:ARG:HH21	2.15	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:317:LEU:HD12	4:4:317:LEU:HA	1.81	0.43
6:6:62:ARG:HA	16:H:48:PRO:HA	2.00	0.43
14:M:209:PRO:HD3	14:M:263:LEU:HD22	1.99	0.43
14:M:367:GLY:O	14:M:374:PHE:HB2	2.18	0.43
15:N:13:LEU:HD21	15:N:28:ALA:HB3	2.00	0.43
2:C:42:ARG:HB2	2:C:45:ARG:HG2	2.00	0.43
4:E:72:HIS:ND1	5:F:152:LEU:HD22	2.33	0.43
4:E:148:TYR:HB3	4:E:200:ARG:NH2	2.33	0.43
5:F:101:LEU:HD23	5:F:126:PHE:CE2	2.53	0.43
11:R:2:SER:HA	11:R:5:GLU:HB3	2.00	0.43
13:T:328:PHE:O	13:T:332:LEU:HD13	2.18	0.43
13:T:586:LEU:HB2	15:V:135:LYS:NZ	2.33	0.43
14:U:43:HIS:NE2	14:U:45:GLY:O	2.51	0.43
14:U:43:HIS:CD2	14:U:48:ALA:HB2	2.54	0.43
14:U:331:ARG:HA	14:U:331:ARG:HD2	1.78	0.43
15:V:119:TYR:CE2	15:V:137:PHE:HA	2.53	0.43
15:V:124:TRP:O	15:V:125:ARG:HB2	2.19	0.43
16:Q:287:LEU:O	16:Q:291:ILE:HG13	2.18	0.43
3:3:297:GLY:O	3:3:300:TRP:NE1	2.50	0.43
10:A:71:PHE:HZ	10:A:107:PHE:HB2	1.83	0.43
13:L:107:TYR:CD2	13:L:140:LEU:HB3	2.53	0.43
14:M:452:ARG:HD3	14:M:452:ARG:HA	1.73	0.43
15:N:177:GLY:O	15:N:181:VAL:HG23	2.18	0.43
16:H:289:PHE:O	16:H:293:ILE:HG12	2.18	0.43
3:D:33:PHE:HZ	3:D:130:LEU:HA	1.84	0.43
3:D:414:SER:O	3:D:418:ARG:NE	2.33	0.43
6:G:46:CYS:SG	6:G:109:GLY:HA3	2.59	0.43
14:U:238:VAL:O	14:U:241:PHE:HB2	2.18	0.43
14:U:270:TYR:O	14:U:274:VAL:HG23	2.19	0.43
16:Q:333:PRO:HB2	16:Q:335:THR:H	1.83	0.43
3:3:118:ASP:O	3:3:122:CYS:N	2.52	0.43
3:3:385:ALA:O	3:3:533:LEU:HD21	2.18	0.43
4:4:41:LEU:HD13	4:4:59:ILE:HG22	2.00	0.43
4:4:183:PRO:HB2	4:4:185:GLU:OE1	2.19	0.43
4:4:214:PHE:HA	4:4:217:ARG:HB2	2.00	0.43
8:7:50:LEU:HA	8:7:51:PRO:HD3	1.88	0.43
13:L:119:VAL:O	13:L:251:TYR:OH	2.28	0.43
13:L:129:ILE:HG12	14:M:369:PRO:HB2	2.01	0.43
14:M:201:PHE:CE2	14:M:245:ALA:HB2	2.54	0.43
14:M:341:ILE:HG13	14:M:342:GLY:N	2.32	0.43
16:H:301:ARG:O	16:H:302:TYR:CD1	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:O	1:B:43:ARG:HG2	2.17	0.43
3:D:83:CYS:SG	3:D:84:VAL:HG13	2.58	0.43
3:D:129:GLU:O	3:D:133:ARG:HG2	2.19	0.43
3:D:133:ARG:HH21	3:D:136:GLU:CD	2.19	0.43
3:D:570:PHE:O	3:D:572:PRO:HD3	2.19	0.43
3:D:616:ASN:HD22	3:D:622:LEU:HD11	1.83	0.43
4:E:87:TYR:CZ	4:E:403:VAL:HG13	2.53	0.43
4:E:272:VAL:N	4:E:275:ARG:HH21	2.17	0.43
5:F:120:ASP:OD2	5:F:135:ILE:N	2.50	0.43
6:G:66:GLU:OE1	16:Q:45:ARG:NH1	2.52	0.43
12:S:25:ILE:H	12:S:25:ILE:HG13	1.61	0.43
13:T:373:LEU:HD23	13:T:417:ALA:HB2	2.00	0.43
14:U:316:ALA:O	14:U:320:VAL:HG23	2.18	0.43
16:Q:213:GLU:HG2	16:Q:251:HIS:CE1	2.53	0.43
2:2:129:HIS:CD2	2:2:130:THR:HG23	2.54	0.43
3:3:505:LEU:HB3	3:3:532:VAL:HG22	2.01	0.43
3:3:715:GLU:H	3:3:761:SER:CB	2.31	0.43
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.19	0.43
10:A:69:ILE:HA	11:J:62:ALA:HB1	2.01	0.43
11:J:23:ARG:HD2	11:J:80:GLU:H	1.84	0.43
13:L:317:VAL:HG12	13:L:388:ILE:HG12	2.01	0.43
13:L:341:HIS:O	13:L:436:HIS:HE1	2.01	0.43
15:N:21:PRO:O	15:N:25:VAL:HG23	2.18	0.43
1:B:245:GLN:HB2	1:B:314:GLU:OE2	2.19	0.43
3:D:17:THR:HG22	3:D:18:SER:O	2.18	0.43
3:D:654:PHE:CE2	3:D:660:ALA:HA	2.54	0.43
4:E:38:HIS:HE1	4:E:398:ALA:HA	1.84	0.43
4:E:72:HIS:HB3	5:F:171:ARG:HH21	1.84	0.43
10:P:62:TYR:CE2	12:S:72:LEU:HB3	2.54	0.43
14:U:305:PRO:HA	14:U:458:ALA:HB1	2.01	0.43
1:1:50:PRO:HA	1:1:53:VAL:HG12	2.01	0.43
3:3:178:ARG:HH22	8:7:65:GLU:CD	2.22	0.43
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.63	0.43
4:4:169:HIS:CD2	6:6:141:PRO:HD3	2.42	0.43
7:9:33:LEU:O	7:9:163:VAL:HG12	2.19	0.43
7:9:88:ALA:HB3	7:9:133:LYS:NZ	2.33	0.43
10:A:99:PHE:O	10:A:102:LEU:HB2	2.18	0.43
13:L:434:HIS:HB3	13:L:435:PRO:HD3	2.00	0.43
13:L:501:ALA:O	13:L:505:LEU:HG	2.19	0.43
14:M:347:LEU:HB2	14:M:414:PHE:HA	2.00	0.43
1:B:90:ILE:HA	1:B:131:TYR:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:112:THR:HG23	2:C:115:GLY:H	1.83	0.43
3:D:52:ILE:HD12	3:D:80:ALA:HB3	2.01	0.43
3:D:385:ALA:HB3	3:D:533:LEU:HG	2.01	0.43
5:F:74:LEU:HD12	5:F:88:PHE:CE1	2.53	0.43
8:I:27:LYS:HA	8:I:27:LYS:HD3	1.81	0.43
10:P:67:LEU:O	10:P:71:PHE:HD1	2.02	0.43
13:T:14:PHE:HB2	13:T:109:ASN:HB2	2.01	0.43
13:T:187:GLU:HA	13:T:190:GLU:HG2	2.01	0.43
14:U:17:LEU:HD11	14:U:98:LEU:HD23	2.01	0.43
15:V:143:ALA:HB1	15:V:182:GLY:HA2	2.00	0.43
16:Q:170:LEU:HA	16:Q:170:LEU:HD23	1.83	0.43
16:Q:257:ALA:O	16:Q:260:PRO:HD2	2.19	0.43
1:1:113:LEU:HD12	1:1:228:VAL:HG21	2.01	0.43
1:1:302:PHE:CZ	1:1:307:LEU:HD21	2.54	0.43
3:3:28:TYR:CE2	3:3:96:LEU:HD11	2.54	0.43
4:4:166:GLN:OE1	4:4:170:HIS:HA	2.18	0.43
14:M:36:ASN:HA	14:M:39:LEU:HD12	2.00	0.43
14:M:143:ARG:HD3	14:M:143:ARG:HA	1.81	0.43
14:M:352:PRO:HG3	14:M:424:ASP:OD2	2.19	0.43
14:M:424:ASP:O	14:M:425:LEU:HD12	2.18	0.43
15:N:194:PHE:O	15:N:197:PRO:HD2	2.19	0.43
15:N:331:LEU:O	15:N:335:GLY:N	2.51	0.43
16:H:267:TRP:HB3	16:H:279:MET:HB2	2.01	0.43
1:B:207:ALA:O	1:B:215:PRO:HB3	2.19	0.43
1:B:312:SER:O	1:B:316:LEU:HD12	2.17	0.43
1:B:433:ARG:NH1	2:C:94:GLU:HG3	2.33	0.43
3:D:735:ALA:HA	3:D:744:GLU:HA	2.01	0.43
4:E:61:TYR:O	6:G:85:SER:HB3	2.18	0.43
6:G:132:PRO:HG3	6:G:178:ARG:NE	2.33	0.43
7:O:54:ILE:HG12	7:O:110:THR:HG21	2.01	0.43
10:P:64:VAL:O	10:P:67:LEU:HB2	2.19	0.43
14:U:30:GLY:O	14:U:34:LEU:HG	2.19	0.43
16:Q:50:ARG:O	16:Q:52:GLY:N	2.52	0.43
3:3:487:SER:OG	3:3:490:VAL:HG23	2.19	0.42
4:4:249:ARG:HG3	4:4:347:GLU:HB3	2.00	0.42
13:L:399:GLY:HA2	13:L:402:PHE:CD2	2.53	0.42
16:H:156:SER:O	16:H:160:ILE:HB	2.19	0.42
1:B:273:ARG:O	1:B:277:TYR:HB2	2.19	0.42
3:D:464:ILE:HD12	3:D:464:ILE:H	1.83	0.42
4:E:162:TRP:NE1	7:O:34:LYS:HD2	2.34	0.42
4:E:172:TYR:O	4:E:179:LYS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:83:ARG:HB2	6:G:123:ILE:HD12	2.01	0.42
13:T:285:ALA:O	13:T:294:ILE:HG13	2.19	0.42
13:T:377:PRO:HG3	13:T:498:ALA:HB1	2.00	0.42
14:U:143:ARG:HD3	14:U:143:ARG:HA	1.65	0.42
14:U:218:HIS:HA	14:U:221:ASN:HD22	1.84	0.42
15:V:87:LEU:O	15:V:90:TYR:HB2	2.18	0.42
16:Q:224:ALA:O	16:Q:229:VAL:HG12	2.19	0.42
1:1:242:GLY:HA2	1:1:268:MET:O	2.18	0.42
4:4:213:ILE:O	4:4:217:ARG:HG2	2.19	0.42
5:5:163:ARG:HB3	7:9:69:TYR:CD2	2.53	0.42
10:A:67:LEU:HB3	16:H:310:TRP:CZ2	2.53	0.42
13:L:328:PHE:O	13:L:332:LEU:HD12	2.18	0.42
13:L:348:ASP:OD1	13:L:349:VAL:N	2.51	0.42
14:M:204:LYS:HD2	14:M:204:LYS:HA	1.88	0.42
14:M:306:GLU:O	14:M:379:LEU:HB3	2.20	0.42
16:H:120:LEU:HD22	16:H:180:LEU:HD12	2.02	0.42
16:H:200:PHE:HB3	16:H:201:PRO:HD3	2.00	0.42
16:H:205:VAL:HA	16:H:313:LEU:HD22	2.01	0.42
16:H:227:GLU:HG2	16:H:228:LEU:N	2.33	0.42
1:B:72:THR:HG21	1:B:223:THR:CG2	2.49	0.42
1:B:437:TRP:CH2	2:C:147:ARG:HG3	2.54	0.42
3:D:176:LEU:HD13	3:D:235:LEU:CD2	2.49	0.42
4:E:167:ARG:HH11	6:G:143:ARG:HH12	1.65	0.42
11:R:65:VAL:HG23	16:Q:134:TYR:CZ	2.54	0.42
15:V:422:ALA:O	15:V:423:LEU:HD23	2.18	0.42
3:3:83:CYS:SG	3:3:84:VAL:N	2.92	0.42
3:3:621:VAL:HG23	3:3:672:ALA:HA	2.00	0.42
4:4:39:GLY:H	20:4:501:DCQ:C2	2.32	0.42
4:4:314:ARG:HB3	8:7:44:MET:HE1	2.00	0.42
5:5:154:GLU:CD	5:5:171:ARG:HH22	2.23	0.42
6:6:178:ARG:NE	9:W:125:ILE:HG22	2.34	0.42
8:7:61:ASP:OD1	8:7:64:GLY:N	2.52	0.42
13:L:219:GLN:O	13:L:223:MET:N	2.52	0.42
13:L:413:THR:HA	13:L:416:TYR:CZ	2.53	0.42
16:H:83:VAL:O	16:H:86:PRO:HD2	2.19	0.42
1:B:162:LEU:O	1:B:165:THR:HG22	2.18	0.42
1:B:177:ALA:HB3	2:C:67:TYR:CG	2.54	0.42
2:C:8:GLN:HA	2:C:11:LEU:HD12	2.00	0.42
4:E:140:LEU:HG	16:Q:299:ARG:HH11	1.85	0.42
10:P:67:LEU:HD23	16:Q:310:TRP:NE1	2.33	0.42
15:V:61:VAL:O	15:V:65:LEU:HG	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:228:ALA:HB1	15:V:233:LEU:HD13	2.02	0.42
15:V:388:GLU:OE1	15:V:388:GLU:N	2.46	0.42
3:3:83:CYS:SG	3:3:84:VAL:HG13	2.59	0.42
11:J:65:VAL:HG11	16:H:160:ILE:CD1	2.49	0.42
12:K:28:PHE:CZ	15:N:137:PHE:HZ	2.38	0.42
14:M:95:PHE:HB3	14:M:136:TYR:CE2	2.54	0.42
16:H:190:LYS:HD3	16:H:268:THR:HG22	2.01	0.42
3:D:124:LYS:HG2	3:D:236:LEU:HD21	2.00	0.42
4:E:317:LEU:HD12	4:E:317:LEU:HA	1.82	0.42
8:I:36:ASP:HA	8:I:54:ILE:HA	2.01	0.42
11:R:100:VAL:HG23	13:T:598:LEU:HD21	2.01	0.42
13:T:65:PHE:CZ	13:T:67:LEU:HD21	2.54	0.42
15:V:294:LEU:O	15:V:298:VAL:HG23	2.20	0.42
3:3:460:LYS:HE2	3:3:460:LYS:HB2	1.80	0.42
4:4:61:TYR:O	6:6:85:SER:HB3	2.20	0.42
4:4:108:VAL:O	4:4:304:ASP:HB2	2.18	0.42
14:M:159:MET:HG3	14:M:197:PHE:CE1	2.55	0.42
16:H:155:SER:OG	16:H:156:SER:N	2.53	0.42
1:B:4:PRO:HA	1:B:12:ARG:NH2	2.35	0.42
3:D:356:LEU:HD22	3:D:638:LEU:HD12	2.00	0.42
4:E:246:TYR:CD1	5:F:78:PRO:HD2	2.54	0.42
5:F:121:LEU:HD13	5:F:146:LEU:HD12	2.00	0.42
9:X:21:LEU:HD21	9:X:26:LEU:HD11	2.01	0.42
9:X:31:VAL:O	9:X:90:TYR:N	2.45	0.42
11:R:69:PHE:CZ	16:Q:156:SER:HB3	2.54	0.42
13:T:388:ILE:O	13:T:392:THR:OG1	2.36	0.42
13:T:539:ASN:HA	13:T:543:VAL:HB	2.00	0.42
16:Q:201:PRO:HG2	16:Q:320:TRP:CE3	2.55	0.42
1:1:87:HIS:CD2	1:1:215:PRO:HD2	2.53	0.42
3:3:166:LYS:HG3	3:3:177:ASP:OD1	2.18	0.42
3:3:398:VAL:HG11	3:3:402:PRO:HG3	2.00	0.42
3:3:512:LEU:HD21	3:3:534:ALA:HB1	2.01	0.42
7:9:4:LYS:HB3	16:H:352:VAL:HG13	2.01	0.42
7:9:94:ASN:OD1	7:9:97:ARG:N	2.53	0.42
14:M:157:LEU:HD23	14:M:157:LEU:HA	1.82	0.42
15:N:138:LEU:HD23	15:N:138:LEU:HA	1.84	0.42
15:N:343:TRP:CE2	15:N:416:PRO:HG3	2.54	0.42
15:N:343:TRP:NE1	15:N:413:GLY:O	2.29	0.42
4:E:336:HIS:ND1	5:F:189:ARG:O	2.52	0.42
6:G:135:VAL:HG22	7:O:124:TYR:CD2	2.55	0.42
10:P:13:TYR:CZ	16:Q:95:LEU:HA	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:57:PHE:HB2	11:R:73:LEU:HD23	2.01	0.42
13:T:114:MET:HG3	13:T:133:GLY:HA3	2.02	0.42
15:V:85:TYR:O	15:V:88:VAL:HB	2.20	0.42
15:V:309:LEU:HD22	15:V:378:LEU:HD11	2.00	0.42
3:3:154:TYR:CE1	4:4:307:PRO:HB3	2.54	0.42
3:3:693:TYR:HD1	3:3:770:ARG:HG2	1.83	0.42
4:4:43:LEU:HD13	4:4:55:VAL:HG11	2.02	0.42
4:4:98:ALA:O	4:4:102:GLU:HG3	2.18	0.42
4:4:114:GLU:HA	4:4:117:ARG:HD3	2.02	0.42
13:L:114:MET:HG3	13:L:133:GLY:HA3	2.01	0.42
13:L:136:LEU:O	13:L:140:LEU:HG	2.20	0.42
13:L:164:ILE:HG12	14:M:400:ILE:HG12	2.02	0.42
13:L:477:LEU:HA	13:L:477:LEU:HD12	1.71	0.42
14:M:78:ILE:O	14:M:82:VAL:HG23	2.19	0.42
14:M:306:GLU:H	14:M:306:GLU:HG3	1.70	0.42
15:N:279:GLN:HG3	15:N:423:LEU:HB2	2.02	0.42
16:H:96:ALA:CB	16:H:128:VAL:HG21	2.49	0.42
16:H:224:ALA:O	16:H:229:VAL:HG12	2.19	0.42
1:B:197:ALA:HB3	2:C:66:PHE:CE2	2.55	0.42
3:D:165:ASP:HB2	8:I:66:PRO:HG2	2.01	0.42
10:P:57:PHE:CE2	16:Q:146:LYS:HD2	2.55	0.42
13:T:380:SER:HB3	13:T:457:GLY:H	1.84	0.42
16:Q:231:GLY:C	16:Q:233:HIS:H	2.23	0.42
1:1:198:ASN:HB3	1:1:355:LYS:HD2	2.01	0.42
1:1:380:GLU:N	1:1:383:ASP:OD2	2.41	0.42
3:3:7:ASN:OD1	3:3:94:ASP:HA	2.18	0.42
20:4:501:DCQ:H7	20:4:501:DCQ:H1M	1.76	0.42
6:6:163:TYR:HD1	7:9:152:ARG:HD2	1.82	0.42
8:7:105:THR:HG23	8:7:110:LEU:HB2	2.02	0.42
13:L:171:LEU:O	13:L:175:ILE:HG13	2.19	0.42
13:L:373:LEU:HD21	13:L:416:TYR:HE1	1.85	0.42
14:M:56:LEU:HB2	14:M:61:VAL:HB	2.00	0.42
14:M:202:ALA:HB1	14:M:207:LEU:HD12	2.02	0.42
15:N:99:ALA:O	15:N:225:ARG:NH1	2.52	0.42
15:N:334:LEU:HD13	15:N:375:TYR:CD2	2.55	0.42
16:H:208:ILE:O	16:H:211:MET:HG2	2.19	0.42
3:D:656:LEU:HD21	9:X:3:ARG:HD3	2.02	0.42
4:E:142:ALA:HB2	16:Q:297:TRP:O	2.20	0.42
5:F:53:VAL:HG13	5:F:71:VAL:HB	2.01	0.42
5:F:75:VAL:HG13	5:F:87:ARG:HB2	2.02	0.42
13:T:70:ASP:OD2	13:T:73:SER:OG	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:515:LYS:HA	13:T:517:PHE:CZ	2.54	0.42
14:U:407:LEU:HD23	14:U:407:LEU:HA	1.84	0.42
15:V:177:GLY:O	15:V:181:VAL:HG23	2.20	0.42
15:V:297:ALA:O	15:V:301:GLN:HG3	2.20	0.42
16:Q:224:ALA:HA	16:Q:230:GLY:H	1.84	0.42
2:2:29:PRO:O	2:2:32:ARG:HB3	2.20	0.42
4:4:91:PHE:HD2	4:4:121:ASN:HB2	1.85	0.42
4:4:159:LEU:O	4:4:163:VAL:HG12	2.20	0.42
4:4:352:GLU:O	4:4:373:PRO:HB3	2.20	0.42
5:5:75:VAL:HG21	5:5:87:ARG:NH2	2.34	0.42
5:5:101:LEU:HD23	5:5:126:PHE:CE2	2.55	0.42
6:6:112:ALA:O	6:6:127:VAL:HG23	2.20	0.42
13:L:194:GLY:HA3	13:L:195:PRO:HD3	1.93	0.42
13:L:513:GLN:O	13:L:515:LYS:HG3	2.20	0.42
15:N:265:HIS:HA	15:N:268:TYR:CD2	2.54	0.42
2:C:110:GLU:OE2	8:I:114:ARG:NH2	2.52	0.42
3:D:272:GLY:O	3:D:630:GLU:N	2.41	0.42
4:E:374:SER:HA	4:E:377:ASN:HB2	2.01	0.42
10:P:63:VAL:O	10:P:67:LEU:HD13	2.20	0.42
10:P:71:PHE:HZ	10:P:107:PHE:HB2	1.83	0.42
15:V:201:GLN:O	15:V:255:LYS:NZ	2.46	0.42
1:1:338:VAL:HG11	1:1:424:LEU:HD22	2.02	0.42
2:2:154:LEU:HD23	2:2:154:LEU:HA	1.95	0.42
5:5:57:TYR:OH	5:5:91:ARG:NH1	2.52	0.42
9:W:43:GLN:HE21	3:D:522:ARG:HH22	1.68	0.42
14:M:8:LEU:HB3	14:M:9:PRO:HD3	2.02	0.42
15:N:116:LEU:HA	15:N:119:TYR:CD2	2.55	0.42
1:B:167:PHE:CE2	1:B:169:PHE:HB2	2.55	0.42
1:B:254:ILE:HG23	1:B:261:PRO:HA	2.02	0.42
1:B:298:PRO:HG3	1:B:408:TRP:HB3	2.01	0.42
2:C:65:SER:HA	2:C:72:PHE:CZ	2.55	0.42
13:T:267:SER:HB3	13:T:311:GLY:O	2.20	0.42
13:T:290:ASP:OD1	13:T:347:GLN:HG2	2.20	0.42
14:U:160:LEU:O	14:U:163:VAL:HG12	2.19	0.42
14:U:202:ALA:O	14:U:206:PRO:HA	2.19	0.42
2:2:66:PHE:CZ	3:3:205:ARG:HD3	2.55	0.41
3:3:79:LEU:HD22	3:3:100:VAL:HG22	2.02	0.41
4:4:321:MET:HE2	4:4:321:MET:HB2	1.78	0.41
4:4:376:VAL:O	4:4:379:GLN:HG3	2.20	0.41
5:5:3:LEU:HB2	5:5:86:SER:HB2	2.02	0.41
13:L:433:HIS:O	13:L:433:HIS:ND1	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:216:ARG:NH1	16:H:294:ARG:O	2.50	0.41
1:B:212:TRP:CZ2	2:C:22:GLY:HA3	2.55	0.41
3:D:371:PHE:CZ	3:D:374:ARG:HA	2.54	0.41
3:D:464:ILE:HA	3:D:489:MET:SD	2.59	0.41
11:R:93:ALA:O	11:R:97:ALA:N	2.44	0.41
13:T:309:ALA:HB2	13:T:388:ILE:CD1	2.50	0.41
14:U:55:LEU:HD22	14:U:63:TRP:CE2	2.54	0.41
16:Q:289:PHE:O	16:Q:293:ILE:HG12	2.19	0.41
1:1:18:TYR:OH	1:1:105:TYR:HB2	2.20	0.41
2:2:45:ARG:O	2:2:49:ILE:HG13	2.20	0.41
2:2:149:ARG:NE	2:2:169:PRO:O	2.53	0.41
3:3:8:ASP:OD1	3:3:9:ARG:HG3	2.20	0.41
3:3:114:ASN:OD1	3:3:161:ARG:HA	2.20	0.41
5:5:71:VAL:HG11	5:5:89:PHE:HD2	1.85	0.41
10:A:74:GLU:HB2	10:A:103:LEU:CD2	2.49	0.41
13:L:90:TYR:CG	13:L:334:LEU:HD13	2.55	0.41
13:L:598:LEU:HD23	13:L:598:LEU:HA	1.91	0.41
14:M:128:PRO:O	14:M:132:MET:HG2	2.20	0.41
16:H:104:PRO:HD3	16:H:267:TRP:HE1	1.85	0.41
1:B:176:GLY:HA2	2:C:28:MET:HE2	2.02	0.41
3:D:309:PRO:HG2	3:D:320:ALA:O	2.19	0.41
13:T:339:VAL:HG22	13:T:359:LEU:HD13	2.02	0.41
14:U:131:LEU:O	14:U:135:LEU:HD23	2.20	0.41
15:V:84:PHE:HZ	15:V:123:THR:O	2.03	0.41
15:V:105:LEU:O	15:V:109:VAL:HG23	2.21	0.41
16:Q:16:LYS:HB2	16:Q:16:LYS:HE3	1.88	0.41
16:Q:208:ILE:O	16:Q:211:MET:HG2	2.20	0.41
1:1:104:ARG:O	1:1:108:GLU:HG3	2.20	0.41
1:1:162:LEU:O	1:1:165:THR:HG22	2.19	0.41
1:1:212:TRP:HE1	2:2:22:GLY:CA	2.32	0.41
4:4:147:PHE:O	4:4:151:ARG:N	2.38	0.41
4:4:161:GLU:OE2	6:6:143:ARG:NH2	2.51	0.41
5:5:147:ARG:H	5:5:147:ARG:HG2	1.65	0.41
9:W:90:TYR:HB3	9:W:118:ALA:HB1	2.01	0.41
11:J:96:LEU:HD22	13:L:594:VAL:HG12	2.01	0.41
13:L:187:GLU:HA	13:L:190:GLU:HG2	2.02	0.41
14:M:242:PHE:CZ	14:M:461:PHE:HD2	2.39	0.41
15:N:280:ALA:HA	15:N:347:LEU:HD13	2.03	0.41
1:B:160:LYS:H	1:B:160:LYS:HG2	1.66	0.41
1:B:343:ASN:O	1:B:346:ARG:HG2	2.20	0.41
4:E:38:HIS:CE1	4:E:398:ALA:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:366:TYR:OH	5:F:56:ASP:O	2.24	0.41
6:G:37:TRP:CE2	6:G:67:VAL:HB	2.55	0.41
9:X:110:LEU:HD12	9:X:110:LEU:O	2.20	0.41
12:S:2:SER:HA	12:S:5:LEU:HD12	2.02	0.41
13:T:24:MET:SD	13:T:28:LEU:HD23	2.60	0.41
13:T:161:VAL:HG21	13:T:225:TRP:HB3	2.03	0.41
13:T:526:ALA:HB1	13:T:529:ARG:HH22	1.86	0.41
13:T:542:ILE:O	13:T:546:LEU:HG	2.20	0.41
1:1:183:GLY:HA3	18:1:502:FMN:O4	2.20	0.41
1:1:212:TRP:CZ2	2:2:19:PRO:HD2	2.55	0.41
1:1:356:CYS:SG	1:1:399:PHE:HB2	2.59	0.41
1:1:357:THR:N	1:1:358:PRO:HD2	2.35	0.41
3:3:247:TRP:NE1	7:9:61:ALA:HB2	2.35	0.41
3:3:369:LEU:HD13	3:3:549:VAL:HA	2.03	0.41
4:4:62:LEU:HD23	4:4:62:LEU:HA	1.77	0.41
4:4:72:HIS:HB3	5:5:171:ARG:NE	2.35	0.41
5:5:140:ASP:OD2	9:W:90:TYR:OH	2.33	0.41
8:7:10:TYR:O	8:7:14:VAL:HG23	2.20	0.41
13:L:361:GLN:HB2	13:L:443:LEU:HD23	2.02	0.41
13:L:549:LEU:O	13:L:553:LEU:HG	2.20	0.41
16:H:45:ARG:HG2	16:H:46:MET:H	1.85	0.41
16:H:217:THR:HA	16:H:219:PHE:HB2	2.01	0.41
1:B:219:ASN:ND2	18:B:502:FMN:O2P	2.53	0.41
1:B:230:ILE:HA	1:B:234:GLY:O	2.21	0.41
1:B:381:GLU:HG2	1:B:385:GLU:OE2	2.20	0.41
3:D:175:ILE:HG22	3:D:236:LEU:HB2	2.02	0.41
3:D:225:ASN:O	3:D:229:ILE:HG13	2.20	0.41
4:E:75:TYR:HA	4:E:78:ASN:ND2	2.35	0.41
4:E:125:ARG:HG3	4:E:349:ALA:HB2	2.01	0.41
4:E:201:ILE:HA	4:E:204:TYR:CD2	2.54	0.41
4:E:236:GLY:HA2	4:E:351:GLY:CA	2.49	0.41
6:G:162:ALA:HB1	7:O:124:TYR:CZ	2.56	0.41
14:U:224:SER:HA	14:U:330:GLY:CA	2.50	0.41
15:V:126:ARG:HD2	15:V:126:ARG:HA	1.46	0.41
16:Q:120:LEU:HA	16:Q:180:LEU:HB3	2.01	0.41
16:Q:255:ALA:O	16:Q:259:ILE:HG13	2.20	0.41
1:1:3:GLY:HA2	1:1:4:PRO:HD3	1.86	0.41
3:3:14:PRO:HG2	3:3:17:THR:OG1	2.20	0.41
3:3:312:ARG:HA	3:3:316:ARG:O	2.21	0.41
3:3:618:GLU:OE2	3:3:620:ARG:NE	2.44	0.41
4:4:84:ARG:O	6:6:83:ARG:NH1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:132:LEU:HD23	5:5:132:LEU:HA	1.86	0.41
6:6:34:ASN:HA	6:6:155:GLN:HE21	1.85	0.41
7:9:163:VAL:O	7:9:178:GLU:N	2.53	0.41
8:7:101:LYS:H	8:7:101:LYS:HG2	1.68	0.41
10:A:31:LEU:HD13	16:H:68:PHE:CZ	2.56	0.41
12:K:7:SER:HB3	12:K:40:LEU:HD23	2.02	0.41
13:L:112:ILE:O	13:L:116:LEU:HG	2.21	0.41
14:M:164:LEU:HD21	15:N:346:TYR:HE1	1.85	0.41
14:M:436:SER:O	14:M:440:LEU:HD13	2.21	0.41
1:B:32:TYR:OH	1:B:116:GLU:OE1	2.24	0.41
2:C:81:GLN:HB3	2:C:122:VAL:HG21	2.01	0.41
4:E:60:GLY:N	4:E:408:ASP:OD1	2.50	0.41
4:E:350:ARG:O	4:E:373:PRO:HB2	2.21	0.41
6:G:99:MET:HB3	6:G:103:LYS:HD3	2.02	0.41
7:O:108:CYS:HB2	7:O:113:ILE:HG22	2.03	0.41
9:X:7:ARG:NH2	9:X:61:ASP:OD1	2.53	0.41
13:T:242:ALA:HB1	13:T:326:ALA:HA	2.02	0.41
16:Q:123:LEU:HD13	16:Q:180:LEU:HD13	2.01	0.41
1:1:83:ASP:OD2	1:1:87:HIS:NE2	2.54	0.41
2:2:66:PHE:O	3:3:205:ARG:NE	2.54	0.41
3:3:136:GLU:HG2	5:5:186:GLY:O	2.20	0.41
4:4:38:HIS:HB2	20:4:501:DCQ:C4	2.50	0.41
4:4:312:PRO:HG3	4:4:323:ALA:O	2.19	0.41
6:6:127:VAL:HG12	6:6:131:VAL:HG22	2.02	0.41
6:6:132:PRO:HG2	6:6:175:ALA:HA	2.03	0.41
11:J:142:VAL:HG21	12:K:59:MET:SD	2.61	0.41
13:L:7:ILE:HG12	13:L:116:LEU:HB2	2.02	0.41
13:L:70:ASP:OD1	13:L:72:LEU:N	2.54	0.41
13:L:463:HIS:CD2	13:L:464:PRO:HD3	2.56	0.41
14:M:151:PHE:HD1	14:M:151:PHE:HA	1.74	0.41
14:M:448:GLY:O	14:M:452:ARG:HG2	2.19	0.41
15:N:97:LEU:HD23	15:N:97:LEU:HA	1.93	0.41
15:N:155:TYR:HB2	15:N:161:LEU:HD21	2.01	0.41
15:N:299:LEU:HD22	15:N:307:VAL:HG11	2.02	0.41
15:N:316:TYR:HB2	15:N:382:VAL:CG1	2.51	0.41
1:B:214:LYS:O	1:B:216:THR:HG23	2.21	0.41
3:D:320:ALA:HB1	3:D:324:GLU:HB2	2.02	0.41
12:S:19:LEU:HD11	13:T:594:VAL:HG21	2.02	0.41
13:T:183:LEU:HD23	13:T:183:LEU:HA	1.82	0.41
13:T:302:GLN:O	13:T:306:MET:HG3	2.20	0.41
13:T:433:HIS:O	13:T:433:HIS:ND1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:8:LEU:HB3	14:U:9:PRO:HD3	2.03	0.41
14:U:303:GLY:HA3	14:U:465:LEU:HD11	2.03	0.41
3:3:330:LYS:O	3:3:334:LYS:HB2	2.20	0.41
3:3:582:PHE:HA	3:3:599:HIS:ND1	2.36	0.41
3:3:583:VAL:HG23	3:3:599:HIS:H	1.85	0.41
4:4:67:GLU:OE2	4:4:409:ARG:NE	2.54	0.41
4:4:331:TYR:OH	7:9:106:GLU:OE2	2.39	0.41
11:J:91:PRO:O	11:J:94:ALA:HB3	2.20	0.41
13:L:187:GLU:O	13:L:190:GLU:HG2	2.21	0.41
13:L:349:VAL:O	13:L:352:MET:HB2	2.20	0.41
14:M:338:THR:HG21	14:M:343:ARG:NH1	2.35	0.41
1:B:211:LEU:CB	1:B:216:THR:HG21	2.50	0.41
3:D:512:LEU:HD21	3:D:534:ALA:HB1	2.03	0.41
4:E:260:TYR:HA	4:E:292:GLN:HE22	1.86	0.41
6:G:115:GLY:HA3	6:G:125:GLN:OE1	2.20	0.41
7:O:72:PRO:HG3	7:O:86:ARG:NH2	2.35	0.41
7:O:101:CYS:SG	7:O:103:LEU:HD12	2.61	0.41
10:P:56:ARG:HD3	11:R:73:LEU:O	2.20	0.41
14:U:313:TYR:HE1	14:U:450:PHE:HB2	1.85	0.41
16:Q:60:LEU:O	16:Q:64:ILE:HG13	2.20	0.41
1:1:193:GLU:OE1	1:1:200:ARG:NH2	2.54	0.41
2:2:112:THR:HG23	2:2:115:GLY:H	1.84	0.41
3:3:34:CYS:SG	3:3:35:SER:N	2.94	0.41
3:3:128:CYS:HB3	3:3:131:GLN:HB2	2.02	0.41
3:3:516:VAL:O	3:3:520:ARG:HG3	2.21	0.41
4:4:167:ARG:HD3	6:6:143:ARG:NH1	2.35	0.41
4:4:246:TYR:HD1	5:5:78:PRO:HD2	1.85	0.41
6:6:117:MET:CE	7:9:99:ILE:HG12	2.51	0.41
10:A:14:VAL:HG22	16:H:95:LEU:HD22	2.03	0.41
13:L:1:MET:HA	13:L:55:PHE:HD2	1.86	0.41
13:L:82:GLY:O	13:L:86:LEU:HG	2.21	0.41
13:L:426:LEU:HD23	13:L:513:GLN:NE2	2.28	0.41
14:M:332:LEU:HA	14:M:335:ARG:HG2	2.02	0.41
14:M:347:LEU:HB2	14:M:413:THR:O	2.21	0.41
1:B:272:PHE:HB2	1:B:307:LEU:HA	2.03	0.41
1:B:283:PRO:HB3	1:B:287:ILE:HD13	2.03	0.41
3:D:42:ILE:HG21	3:D:439:GLU:OE1	2.21	0.41
4:E:42:ARG:O	4:E:43:LEU:HD23	2.21	0.41
5:F:116:ARG:HD2	5:F:131:ASP:O	2.21	0.41
13:T:291:ILE:O	13:T:295:VAL:HG23	2.20	0.41
14:U:10:VAL:HG23	14:U:104:GLY:HA3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:127:ILE:O	14:U:130:LEU:HG	2.20	0.41
16:Q:120:LEU:HA	16:Q:180:LEU:CB	2.51	0.41
1:1:338:VAL:O	1:1:342:TRP:HB2	2.21	0.41
1:1:414:LEU:O	1:1:418:LYS:N	2.54	0.41
3:3:11:VAL:HG21	3:3:26:ALA:HB2	2.02	0.41
3:3:297:GLY:HA3	3:3:703:GLN:NE2	2.36	0.41
3:3:329:LEU:CD1	3:3:584:VAL:HG11	2.51	0.41
4:4:42:ARG:O	4:4:43:LEU:HD23	2.21	0.41
4:4:400:LEU:HD23	4:4:400:LEU:HA	1.89	0.41
6:6:82:GLY:HA2	17:6:201:SF4:S4	2.60	0.41
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.21	0.41
6:6:154:LEU:O	6:6:158:VAL:HG13	2.21	0.41
7:9:17:LEU:HA	16:H:41:ARG:O	2.20	0.41
9:W:59:VAL:HG11	9:W:63:PHE:CE2	2.55	0.41
10:A:59:VAL:HG13	10:A:62:TYR:HB3	2.03	0.41
12:K:81:HIS:CD2	12:K:81:HIS:H	2.39	0.41
13:L:159:PHE:CD2	14:M:407:LEU:HD11	2.54	0.41
14:M:238:VAL:O	14:M:241:PHE:HB2	2.21	0.41
15:N:17:GLY:HA3	15:N:82:PHE:CD2	2.55	0.41
15:N:58:VAL:O	15:N:62:PHE:HD1	2.04	0.41
15:N:232:ALA:O	15:N:236:LEU:HG	2.21	0.41
15:N:272:ALA:O	15:N:276:GLY:N	2.47	0.41
16:H:16:LYS:O	16:H:20:VAL:HG23	2.21	0.41
16:H:52:GLY:HA3	16:H:53:PRO:C	2.41	0.41
16:H:65:LYS:O	16:H:69:LYS:HB2	2.21	0.41
16:H:204:LEU:HA	16:H:204:LEU:HD23	1.79	0.41
16:H:330:LEU:HB3	16:H:332:LEU:HD11	2.03	0.41
1:B:195:LEU:HD23	2:C:24:ARG:HH12	1.85	0.41
1:B:369:ASN:HB3	3:D:159:PHE:CE2	2.56	0.41
3:D:360:LEU:O	3:D:364:LEU:HB3	2.20	0.41
4:E:86:ASP:HB3	4:E:93:HIS:CD2	2.55	0.41
8:I:105:THR:HG1	8:I:108:ILE:HB	1.85	0.41
10:P:40:LYS:HB2	10:P:40:LYS:HE3	1.78	0.41
10:P:94:LEU:O	10:P:97:LEU:HB3	2.20	0.41
11:R:22:LEU:HD13	11:R:27:HIS:HB3	2.02	0.41
13:T:158:ALA:HA	13:T:225:TRP:HB2	2.03	0.41
13:T:269:ALA:O	13:T:273:VAL:HG23	2.21	0.41
14:U:103:GLU:O	14:U:107:LEU:HG	2.20	0.41
14:U:307:GLY:HA2	14:U:379:LEU:O	2.21	0.41
14:U:347:LEU:HB2	14:U:413:THR:O	2.21	0.41
15:V:119:TYR:OH	15:V:140:GLY:HA3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:201:PRO:HD2	16:Q:320:TRP:CE2	2.56	0.41
1:1:145:LEU:HD23	1:1:145:LEU:HA	1.88	0.41
1:1:373:LYS:N	8:7:79:LEU:HD21	2.36	0.41
3:3:645:ALA:HB3	3:3:652:PRO:HD3	2.03	0.41
4:4:218:ALA:HB1	4:4:273:PHE:N	2.36	0.41
5:5:153:GLY:HA2	9:W:113:ARG:HH21	1.86	0.41
7:9:36:ARG:O	7:9:38:HIS:ND1	2.52	0.41
13:L:17:LEU:HD22	13:L:29:PRO:HB3	2.02	0.41
15:N:76:LEU:HD12	15:N:206:PRO:HB3	2.03	0.41
1:B:3:GLY:HA2	1:B:4:PRO:HD3	1.94	0.41
2:C:24:ARG:HA	2:C:53:VAL:CG2	2.51	0.41
4:E:40:VAL:O	4:E:404:MET:HG3	2.20	0.41
4:E:211:SER:CB	4:E:214:PHE:HB3	2.50	0.41
5:F:154:GLU:CD	5:F:171:ARG:HH22	2.25	0.41
7:O:2:THR:OG1	7:O:2:THR:O	2.38	0.41
10:P:1:MET:HG2	10:P:2:ALA:H	1.86	0.41
13:T:75:PHE:CZ	13:T:79:ILE:HD11	2.56	0.41
13:T:194:GLY:HA3	13:T:195:PRO:HD3	1.86	0.41
15:V:98:LEU:HG	15:V:222:ALA:HB2	2.03	0.41
16:Q:107:SER:OG	16:Q:113:PRO:HG3	2.21	0.41
3:3:168:HIS:O	3:3:176:LEU:N	2.51	0.40
3:3:250:GLU:HG3	5:5:169:GLU:HG3	2.03	0.40
4:4:315:HIS:HA	8:7:46:ARG:CZ	2.50	0.40
8:7:13:TRP:HZ3	8:7:70:ALA:HB1	1.86	0.40
11:J:60:ALA:O	11:J:65:VAL:HG23	2.21	0.40
12:K:47:ARG:HE	12:K:47:ARG:HB3	1.69	0.40
13:L:165:GLY:CA	13:L:212:GLY:HA2	2.52	0.40
14:M:17:LEU:HD23	14:M:17:LEU:HA	1.88	0.40
15:N:124:TRP:O	15:N:125:ARG:HB2	2.21	0.40
16:H:232:TYR:HB2	16:H:244:PHE:CE1	2.56	0.40
1:B:222:GLU:HG3	1:B:251:LEU:HD22	2.03	0.40
1:B:438:ARG:O	2:C:147:ARG:HB2	2.20	0.40
3:D:200:LEU:HD12	3:D:213:THR:HB	2.02	0.40
4:E:132:PHE:CE2	4:E:279:ARG:HD2	2.55	0.40
6:G:40:THR:HB	6:G:68:PHE:CE1	2.56	0.40
7:O:68:ILE:HD11	17:O:201:SF4:S1	2.61	0.40
7:O:101:CYS:HB2	7:O:103:LEU:H	1.86	0.40
7:O:117:TYR:CE2	7:O:163:VAL:HG11	2.56	0.40
12:S:32:GLU:O	12:S:36:ASN:ND2	2.42	0.40
12:S:47:ARG:HE	12:S:47:ARG:HB3	1.68	0.40
12:S:79:PHE:CD2	12:S:85:THR:HA	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:20:HIS:CG	1:1:31:TYR:HE1	2.39	0.40
3:3:418:ARG:HG2	3:3:443:ARG:HG2	2.03	0.40
3:3:701:ALA:HB2	3:3:763:LEU:HB2	2.01	0.40
4:4:49:GLY:HA2	10:A:58:PRO:HD3	2.02	0.40
4:4:89:HIS:ND1	4:4:348:SER:HB2	2.35	0.40
5:5:163:ARG:CZ	7:9:90:VAL:HG11	2.51	0.40
5:5:167:PRO:HA	5:5:170:PHE:HB3	2.02	0.40
7:9:34:LYS:HA	7:9:34:LYS:HD3	1.48	0.40
13:L:280:TYR:OH	13:L:531:ALA:HB1	2.20	0.40
14:M:6:VAL:HG22	14:M:107:LEU:HB3	2.03	0.40
14:M:160:LEU:O	14:M:163:VAL:HG12	2.21	0.40
14:M:331:ARG:HA	14:M:331:ARG:HD2	1.77	0.40
15:N:14:THR:OG1	15:N:90:TYR:OH	2.10	0.40
15:N:95:MET:HE3	15:N:95:MET:HB2	1.87	0.40
16:H:162:TYR:OH	16:H:305:LEU:O	2.36	0.40
16:H:237:SER:OG	16:H:238:SER:N	2.53	0.40
1:B:64:GLY:N	1:B:70:PHE:O	2.37	0.40
3:D:321:THR:HG22	3:D:322:TRP:H	1.85	0.40
3:D:418:ARG:HD3	3:D:443:ARG:CZ	2.52	0.40
5:F:147:ARG:H	5:F:147:ARG:HG2	1.72	0.40
12:S:19:LEU:HD21	13:T:594:VAL:HG21	2.04	0.40
13:T:15:ALA:O	13:T:19:LEU:HG	2.21	0.40
16:Q:96:ALA:HA	16:Q:99:LEU:HD13	2.04	0.40
3:3:46:ARG:NH2	3:3:81:ALA:HB2	2.37	0.40
3:3:329:LEU:HD12	3:3:329:LEU:HA	1.85	0.40
3:3:418:ARG:O	3:3:419:ASP:HB2	2.22	0.40
6:6:91:VAL:HG22	10:A:46:SER:HB3	2.02	0.40
6:6:94:ARG:HB3	6:6:98:GLN:NE2	2.37	0.40
7:9:45:ARG:HH21	7:9:137:LEU:HD23	1.85	0.40
13:L:59:TRP:HB3	13:L:64:PRO:HA	2.03	0.40
13:L:122:ASP:O	13:L:185:ILE:N	2.52	0.40
14:M:346:GLY:HA3	14:M:418:GLY:HA2	2.02	0.40
15:N:62:PHE:CD2	15:N:221:ALA:HB2	2.55	0.40
15:N:319:ASP:HB3	15:N:322:LEU:HB2	2.03	0.40
2:C:42:ARG:HB3	2:C:44:GLU:OE1	2.22	0.40
3:D:382:PHE:HB3	3:D:532:VAL:HB	2.03	0.40
3:D:386:SER:HB3	3:D:389:ASP:OD2	2.21	0.40
4:E:80:THR:O	4:E:84:ARG:NH1	2.54	0.40
5:F:103:THR:HG22	5:F:126:PHE:HB3	2.03	0.40
10:P:84:SER:OG	11:R:128:GLY:HA3	2.21	0.40
13:T:41:PHE:HD2	13:T:42:LEU:HD12	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:310:GLY:HA2	14:U:376:GLY:HA2	2.03	0.40
1:1:246:SER:OG	1:1:313:TYR:HB2	2.21	0.40
1:1:262:GLY:HA3	2:2:175:HIS:O	2.21	0.40
3:3:38:HIS:CD2	3:3:287:GLU:HB3	2.56	0.40
3:3:142:LYS:HE2	3:3:142:LYS:HB2	1.87	0.40
3:3:240:ALA:CB	3:3:276:ARG:HB2	2.51	0.40
3:3:664:LEU:HD23	3:3:664:LEU:HA	1.96	0.40
4:4:341:GLU:OE2	5:5:57:TYR:OH	2.28	0.40
6:6:30:TRP:O	6:6:33:SER:OG	2.36	0.40
11:J:94:ALA:O	11:J:97:ALA:HB3	2.22	0.40
13:L:603:VAL:HG21	15:N:235:LEU:HD22	2.03	0.40
14:M:135:LEU:HD23	14:M:135:LEU:H	1.87	0.40
15:N:303:SER:HB3	15:N:307:VAL:HG22	2.01	0.40
16:H:51:VAL:H	16:H:51:VAL:HG23	1.59	0.40
3:D:136:GLU:HG2	5:F:189:ARG:HG2	2.02	0.40
3:D:385:ALA:HA	3:D:531:LYS:HB3	2.02	0.40
3:D:397:LEU:O	3:D:505:LEU:HD12	2.21	0.40
7:O:63:CYS:HA	17:O:201:SF4:S2	2.62	0.40
9:X:37:TRP:CD1	9:X:40:LYS:HD2	2.56	0.40
13:T:586:LEU:HD12	15:V:135:LYS:HG2	2.03	0.40
14:U:70:LEU:O	14:U:73:LEU:HD23	2.21	0.40
15:V:209:LEU:HB2	15:V:296:PHE:HB3	2.03	0.40
16:Q:86:PRO:HG3	16:Q:244:PHE:CE2	2.56	0.40
16:Q:226:GLN:HB2	16:Q:299:ARG:NH2	2.37	0.40
1:1:16:THR:H	1:1:265:GLU:CD	2.21	0.40
4:4:162:TRP:CD2	7:9:34:LYS:CD	2.95	0.40
4:4:234:LEU:HD12	4:4:377:ASN:O	2.22	0.40
4:4:246:TYR:CD1	5:5:78:PRO:HD2	2.56	0.40
4:4:371:ARG:HG3	5:5:51:ASP:OD1	2.22	0.40
10:A:95:GLY:HA3	11:J:136:LEU:HD11	2.02	0.40
13:L:586:LEU:CD1	15:N:135:LYS:HA	2.51	0.40
14:M:156:SER:O	14:M:159:MET:HB3	2.21	0.40
16:H:147:TYR:CE1	16:H:228:LEU:HD13	2.57	0.40
16:H:324:THR:O	16:H:328:VAL:HG23	2.22	0.40
1:B:176:GLY:O	2:C:32:ARG:NH2	2.30	0.40
3:D:176:LEU:HD13	3:D:235:LEU:HD23	2.02	0.40
4:E:59:ILE:O	6:G:87:LYS:NZ	2.42	0.40
4:E:211:SER:HB2	4:E:215:TYR:N	2.36	0.40
5:F:55:LEU:HB2	5:F:69:ALA:O	2.21	0.40
5:F:145:PRO:HA	5:F:150:TYR:CD1	2.56	0.40
6:G:105:VAL:HG11	6:G:131:VAL:HG23	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:119:ASN:HA	6:G:125:GLN:NE2	2.31	0.40
8:I:48:TYR:CE2	8:I:50:LEU:HB2	2.57	0.40
14:U:78:ILE:O	14:U:82:VAL:HG23	2.21	0.40
14:U:305:PRO:HD3	14:U:462:ALA:CB	2.52	0.40
14:U:343:ARG:HB3	14:U:344:TYR:CD1	2.57	0.40
15:V:59:SER:OG	15:V:100:SER:OG	2.25	0.40
16:Q:314:PHE:HB2	16:Q:315:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	408 (94%)	27 (6%)	0	100	100
1	B	435/438 (99%)	407 (94%)	28 (6%)	0	100	100
2	2	176/181 (97%)	165 (94%)	11 (6%)	0	100	100
2	C	176/181 (97%)	165 (94%)	11 (6%)	0	100	100
3	3	750/783 (96%)	695 (93%)	55 (7%)	0	100	100
3	D	750/783 (96%)	698 (93%)	52 (7%)	0	100	100
4	4	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
4	E	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
5	5	194/207 (94%)	183 (94%)	11 (6%)	0	100	100
5	F	194/207 (94%)	180 (93%)	14 (7%)	0	100	100
6	6	164/181 (91%)	149 (91%)	15 (9%)	0	100	100
6	G	164/181 (91%)	152 (93%)	12 (7%)	0	100	100
7	9	178/182 (98%)	170 (96%)	8 (4%)	0	100	100
7	O	178/182 (98%)	169 (95%)	9 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
8	I	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
9	W	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
9	X	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
10	A	115/119 (97%)	103 (90%)	12 (10%)	0	100	100
10	P	115/119 (97%)	104 (90%)	11 (10%)	0	100	100
11	J	158/176 (90%)	146 (92%)	12 (8%)	0	100	100
11	R	158/176 (90%)	145 (92%)	13 (8%)	0	100	100
12	K	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
12	S	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
13	L	603/606 (100%)	562 (93%)	40 (7%)	1 (0%)	47	79
13	T	603/606 (100%)	568 (94%)	34 (6%)	1 (0%)	47	79
14	M	465/469 (99%)	436 (94%)	29 (6%)	0	100	100
14	U	465/469 (99%)	439 (94%)	26 (6%)	0	100	100
15	N	425/427 (100%)	399 (94%)	26 (6%)	0	100	100
15	V	425/427 (100%)	397 (93%)	27 (6%)	1 (0%)	47	79
16	H	351/365 (96%)	302 (86%)	43 (12%)	6 (2%)	9	45
16	Q	351/365 (96%)	307 (88%)	39 (11%)	5 (1%)	11	48
All	All	9478/9796 (97%)	8820 (93%)	644 (7%)	14 (0%)	51	83

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	51	VAL
16	H	44	VAL
16	Q	51	VAL
16	H	268	THR
16	Q	44	VAL
16	Q	268	THR
16	H	50	ARG
13	T	435	PRO
16	Q	50	ARG
13	L	435	PRO
15	V	425	ALA
16	H	52	GLY
16	Q	218	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	H	218	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	355/356 (100%)	347 (98%)	8 (2%)	50	76
1	B	355/356 (100%)	346 (98%)	9 (2%)	47	75
2	2	150/152 (99%)	144 (96%)	6 (4%)	31	65
2	C	150/152 (99%)	145 (97%)	5 (3%)	38	69
3	3	609/628 (97%)	597 (98%)	12 (2%)	55	79
3	D	609/628 (97%)	600 (98%)	9 (2%)	65	84
4	4	332/355 (94%)	325 (98%)	7 (2%)	53	78
4	E	332/355 (94%)	329 (99%)	3 (1%)	78	90
5	5	167/175 (95%)	162 (97%)	5 (3%)	41	71
5	F	167/175 (95%)	164 (98%)	3 (2%)	59	81
6	6	135/149 (91%)	126 (93%)	9 (7%)	16	50
6	G	135/149 (91%)	125 (93%)	10 (7%)	13	46
7	9	148/150 (99%)	146 (99%)	2 (1%)	67	85
7	O	148/150 (99%)	146 (99%)	2 (1%)	67	85
8	7	104/106 (98%)	103 (99%)	1 (1%)	76	88
8	I	104/106 (98%)	103 (99%)	1 (1%)	76	88
9	W	99/101 (98%)	98 (99%)	1 (1%)	76	88
9	X	99/101 (98%)	98 (99%)	1 (1%)	76	88
10	A	90/92 (98%)	87 (97%)	3 (3%)	38	69
10	P	90/92 (98%)	86 (96%)	4 (4%)	28	63
11	J	118/130 (91%)	115 (98%)	3 (2%)	47	75
11	R	118/130 (91%)	115 (98%)	3 (2%)	47	75
12	K	71/71 (100%)	70 (99%)	1 (1%)	67	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	S	71/71 (100%)	69 (97%)	2 (3%)	43	72
13	L	453/454 (100%)	443 (98%)	10 (2%)	52	77
13	T	453/454 (100%)	444 (98%)	9 (2%)	55	79
14	M	332/332 (100%)	325 (98%)	7 (2%)	53	78
14	U	332/332 (100%)	326 (98%)	6 (2%)	59	81
15	N	302/302 (100%)	298 (99%)	4 (1%)	69	86
15	V	302/302 (100%)	297 (98%)	5 (2%)	60	82
16	H	293/300 (98%)	282 (96%)	11 (4%)	33	66
16	Q	293/300 (98%)	285 (97%)	8 (3%)	44	73
All	All	7516/7706 (98%)	7346 (98%)	170 (2%)	50	76

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	249	MET
1	1	337	MET
1	1	342	TRP
1	1	353	CYS
1	1	366	PHE
1	1	397	ARG
1	1	400	CYS
1	1	437	TRP
2	2	6	ASP
2	2	33	ARG
2	2	35	GLN
2	2	45	ARG
2	2	116	LEU
2	2	171	LYS
3	3	76	GLN
3	3	83	CYS
3	3	123	ASP
3	3	124	LYS
3	3	214	MET
3	3	337	ARG
3	3	369	LEU
3	3	425	ARG
3	3	501	LYS
3	3	655	ARG
3	3	761	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	774	ARG
4	4	68	LYS
4	4	87	TYR
4	4	129	HIS
4	4	132	PHE
4	4	152	GLU
4	4	208	PHE
4	4	262	PHE
5	5	31	ARG
5	5	38	MET
5	5	147	ARG
5	5	178	ASP
5	5	183	PHE
6	6	37	TRP
6	6	45	CYS
6	6	49	GLU
6	6	55	ASP
6	6	68	PHE
6	6	101	ASP
6	6	153	GLN
6	6	156	LYS
6	6	176	TRP
7	9	34	LYS
7	9	38	HIS
8	7	43	ARG
9	W	37	TRP
10	A	13	TYR
10	A	48	ASN
10	A	49	ASP
11	J	69	PHE
11	J	118	ASP
11	J	119	LEU
12	K	28	PHE
13	L	14	PHE
13	L	56	GLN
13	L	59	TRP
13	L	146	TYR
13	L	169	PHE
13	L	245	MET
13	L	506	TRP
13	L	511	PHE
13	L	554	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	L	557	ASP
14	M	22	ARG
14	M	73	LEU
14	M	115	LEU
14	M	241	PHE
14	M	255	GLN
14	M	326	PHE
14	M	455	HIS
15	N	9	PHE
15	N	50	PHE
15	N	126	ARG
15	N	284	TYR
16	H	28	PHE
16	H	54	PHE
16	H	119	ASP
16	H	134	TYR
16	H	147	TYR
16	H	233	HIS
16	H	298	PHE
16	H	302	TYR
16	H	307	ARG
16	H	310	TRP
16	H	332	LEU
1	B	244	GLU
1	B	249	MET
1	B	302	PHE
1	B	337	MET
1	B	342	TRP
1	B	366	PHE
1	B	397	ARG
1	B	400	CYS
1	B	437	TRP
2	C	6	ASP
2	C	33	ARG
2	C	35	GLN
2	C	45	ARG
2	C	116	LEU
3	D	83	CYS
3	D	123	ASP
3	D	184	CYS
3	D	337	ARG
3	D	369	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	628	PRO
3	D	655	ARG
3	D	761	SER
3	D	774	ARG
4	E	132	PHE
4	E	208	PHE
4	E	262	PHE
5	F	31	ARG
5	F	97	GLU
5	F	147	ARG
6	G	37	TRP
6	G	45	CYS
6	G	49	GLU
6	G	55	ASP
6	G	68	PHE
6	G	117	MET
6	G	120	ASN
6	G	156	LYS
6	G	176	TRP
6	G	177	LYS
7	O	4	LYS
7	O	38	HIS
8	I	43	ARG
9	X	37	TRP
10	P	48	ASN
10	P	49	ASP
10	P	66	MET
10	P	110	GLU
11	R	59	TYR
11	R	69	PHE
11	R	84	ASP
12	S	28	PHE
12	S	82	ARG
13	T	14	PHE
13	T	59	TRP
13	T	169	PHE
13	T	245	MET
13	T	329	LYS
13	T	506	TRP
13	T	511	PHE
13	T	554	PHE
13	T	557	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	U	22	ARG
14	U	135	LEU
14	U	151	PHE
14	U	241	PHE
14	U	255	GLN
14	U	455	HIS
15	V	9	PHE
15	V	50	PHE
15	V	78	ARG
15	V	126	ARG
15	V	284	TYR
16	Q	28	PHE
16	Q	119	ASP
16	Q	147	TYR
16	Q	196	PHE
16	Q	233	HIS
16	Q	302	TYR
16	Q	307	ARG
16	Q	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	240	GLN
1	1	288	GLN
2	2	35	GLN
2	2	71	GLN
2	2	120	GLN
3	3	25	HIS
3	3	104	GLN
3	3	168	HIS
3	3	347	HIS
3	3	709	GLN
4	4	33	GLN
4	4	129	HIS
4	4	169	HIS
4	4	292	GLN
5	5	129	HIS
6	6	98	GLN
6	6	120	ASN
6	6	155	GLN
8	7	76	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	43	GLN
10	A	60	HIS
11	J	117	GLN
11	J	125	GLN
13	L	432	HIS
13	L	436	HIS
13	L	447	HIS
13	L	513	GLN
14	M	49	HIS
14	M	52	GLN
14	M	221	ASN
15	N	245	ASN
15	N	277	ASN
16	H	49	ASN
16	H	117	ASN
16	H	181	ASN
16	H	183	ASN
16	H	233	HIS
16	H	304	GLN
1	B	20	HIS
1	B	161	ASN
1	B	219	ASN
1	B	240	GLN
1	B	245	GLN
1	B	288	GLN
1	B	343	ASN
1	B	350	HIS
1	B	386	ASN
2	C	35	GLN
3	D	104	GLN
3	D	208	HIS
3	D	347	HIS
3	D	468	HIS
3	D	631	ASN
3	D	709	GLN
4	E	78	ASN
4	E	379	GLN
5	F	112	ASN
5	F	129	HIS
6	G	74	GLN
6	G	120	ASN
6	G	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	76	HIS
9	X	43	GLN
9	X	84	GLN
10	P	60	HIS
11	R	55	GLN
12	S	81	HIS
13	T	150	GLN
13	T	302	GLN
13	T	325	HIS
13	T	365	HIS
14	U	221	ASN
14	U	349	GLN
15	V	103	HIS
15	V	245	ASN
15	V	277	ASN
16	Q	112	GLN
16	Q	226	GLN
16	Q	233	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SF4	D	801	3	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.37	11 (22%)
17	SF4	9	201	7	0,12,12	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		
19	FES	3	804	3	0,4,4	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
20	DCQ	E	501	-	23,23,23	0.18	0	26,29,29	0.86	1 (3%)
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	O	202	7	0,12,12	-	-	-		
19	FES	2	201	2	0,4,4	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		
20	DCQ	4	501	-	23,23,23	0.22	0	26,29,29	0.84	1 (3%)
17	SF4	6	201	6	0,12,12	-	-	-		
18	FMN	1	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.37	12 (25%)
17	SF4	G	201	6	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	D	801	3	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	9	201	7	-	-	0/6/5/5
17	SF4	D	803	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
19	FES	3	804	3	-	-	0/1/1/1
20	DCQ	E	501	-	-	4/14/38/38	0/1/1/1
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	O	202	7	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
20	DCQ	4	501	-	-	4/14/38/38	0/1/1/1
17	SF4	D	802	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C4A-N5	3.82	1.38	1.30
18	B	502	FMN	C4A-N5	3.70	1.37	1.30
18	B	502	FMN	C10-N1	2.54	1.38	1.33
18	1	502	FMN	C10-N1	2.51	1.38	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	502	FMN	C4-N3-C2	-3.34	119.47	125.64
18	1	502	FMN	C4-N3-C2	-3.26	119.62	125.64
18	B	502	FMN	C5'-C4'-C3'	-2.90	106.61	112.20
18	B	502	FMN	C4A-C4-N3	2.81	120.32	113.19
18	B	502	FMN	C4A-C10-N1	-2.80	118.22	124.73
18	1	502	FMN	C4A-C10-N1	-2.75	118.34	124.73
18	1	502	FMN	C5A-C9A-N10	2.71	120.75	117.95
18	B	502	FMN	O4-C4-C4A	-2.70	119.44	126.60
18	1	502	FMN	C4A-C4-N3	2.69	120.03	113.19
18	1	502	FMN	C5'-C4'-C3'	-2.69	107.01	112.20
18	1	502	FMN	O4-C4-C4A	-2.49	120.00	126.60
18	B	502	FMN	C5A-C9A-N10	2.39	120.42	117.95
18	1	502	FMN	C4A-C10-N10	2.34	119.89	116.48
18	B	502	FMN	C4A-C10-N10	2.31	119.86	116.48
20	4	501	DCQ	C4M-O4-C4	2.31	124.66	116.47
20	E	501	DCQ	C4M-O4-C4	2.28	124.55	116.47
18	B	502	FMN	C10-N1-C2	2.26	121.42	116.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	502	FMN	C4-C4A-C10	2.22	120.53	116.79
18	B	502	FMN	C4-C4A-C10	2.22	120.53	116.79
18	1	502	FMN	C9A-C5A-N5	-2.16	120.09	122.43
18	1	502	FMN	C10-C4A-N5	-2.12	120.35	124.86
18	1	502	FMN	C10-N1-C2	2.10	121.11	116.90
18	B	502	FMN	C9A-C5A-N5	-2.10	120.14	122.43
18	1	502	FMN	C1'-N10-C9A	-2.09	117.03	120.51
18	B	502	FMN	C10-C4A-N5	-2.07	120.47	124.86

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	502	FMN	N10-C1'-C2'-O2'
18	1	502	FMN	N10-C1'-C2'-C3'
18	1	502	FMN	C1'-C2'-C3'-O3'
18	1	502	FMN	C1'-C2'-C3'-C4'
18	1	502	FMN	C3'-C4'-C5'-O5'
18	1	502	FMN	O4'-C4'-C5'-O5'
18	B	502	FMN	N10-C1'-C2'-O2'
18	B	502	FMN	N10-C1'-C2'-C3'
18	B	502	FMN	C1'-C2'-C3'-O3'
18	B	502	FMN	C1'-C2'-C3'-C4'
18	B	502	FMN	C3'-C4'-C5'-O5'
18	B	502	FMN	O4'-C4'-C5'-O5'
20	4	501	DCQ	C6-C7-C8-C9
20	E	501	DCQ	C6-C7-C8-C9
18	B	502	FMN	O2'-C2'-C3'-C4'
18	B	502	FMN	O2'-C2'-C3'-O3'
18	1	502	FMN	O2'-C2'-C3'-C4'
20	4	501	DCQ	C9-C10-C11-C12
20	E	501	DCQ	C9-C10-C11-C12
20	4	501	DCQ	C12-C13-C14-C15
20	E	501	DCQ	C12-C13-C14-C15
18	1	502	FMN	O2'-C2'-C3'-O3'
20	E	501	DCQ	C11-C10-C9-C8
20	4	501	DCQ	C11-C10-C9-C8

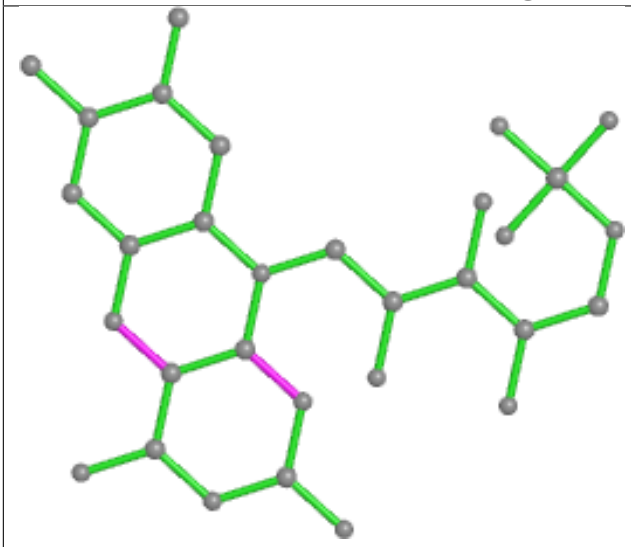
There are no ring outliers.

15 monomers are involved in 44 short contacts:

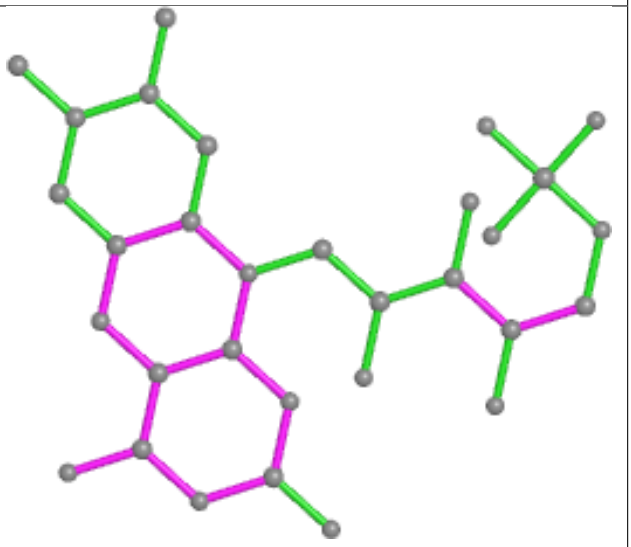
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	502	FMN	9	0
17	9	201	SF4	2	0
17	D	803	SF4	2	0
19	3	804	FES	1	0
17	B	501	SF4	3	0
20	E	501	DCQ	4	0
17	O	202	SF4	1	0
17	3	803	SF4	2	0
17	3	801	SF4	1	0
19	D	804	FES	2	0
20	4	501	DCQ	4	0
17	6	201	SF4	1	0
18	1	502	FMN	9	0
17	9	202	SF4	1	0
17	O	201	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

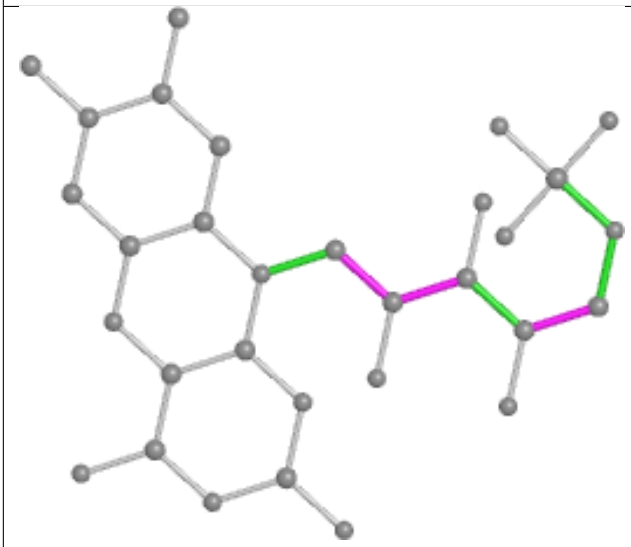
Ligand FMN B 502



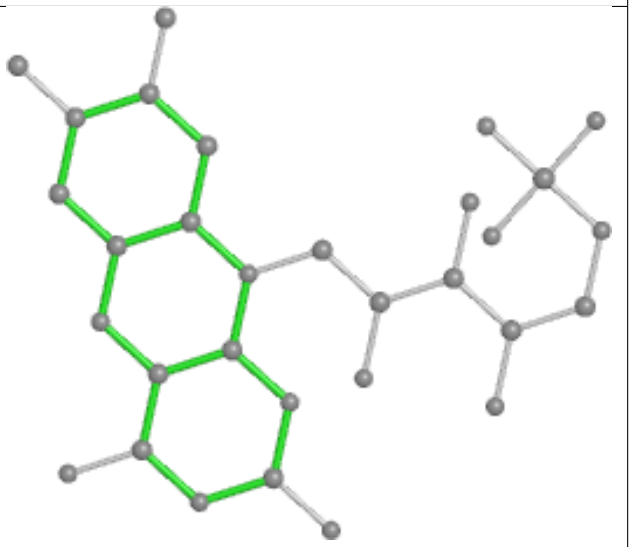
Bond lengths



Bond angles

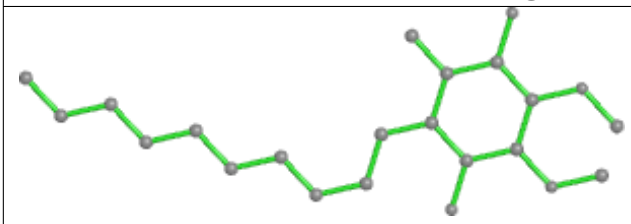


Torsions

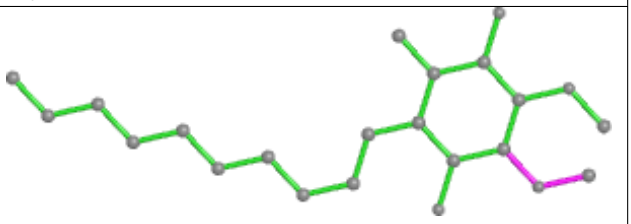


Rings

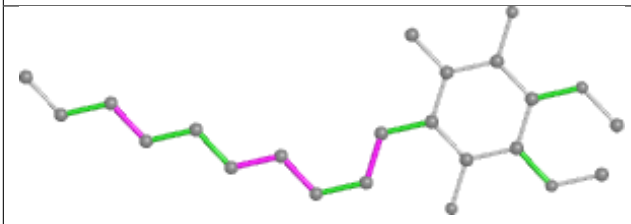
Ligand DCQ E 501



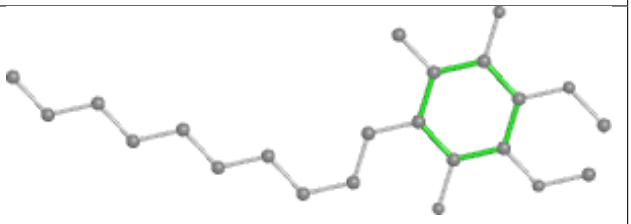
Bond lengths



Bond angles

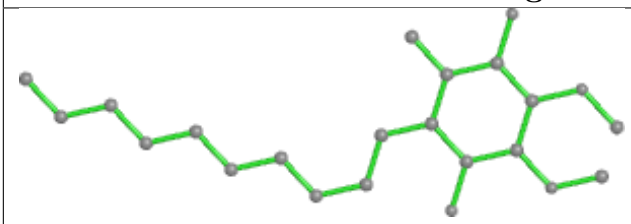


Torsions

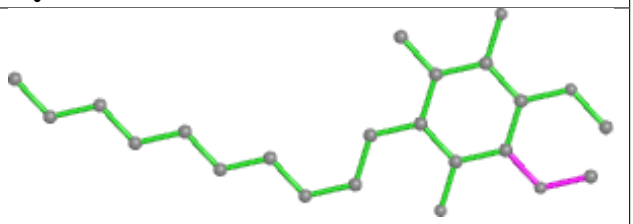


Rings

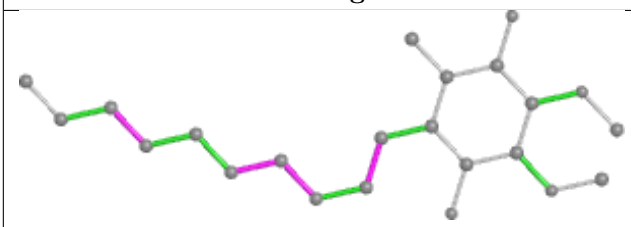
Ligand DCQ 4 501



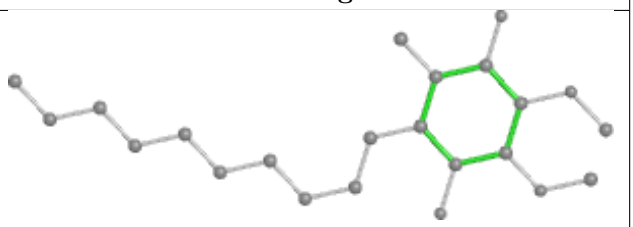
Bond lengths



Bond angles

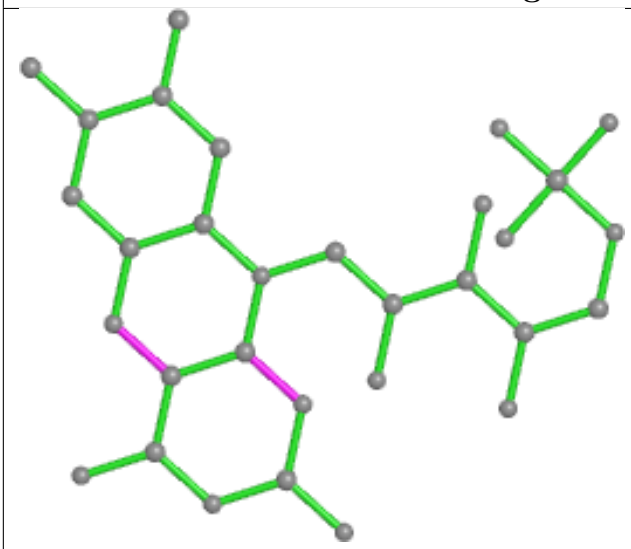


Torsions

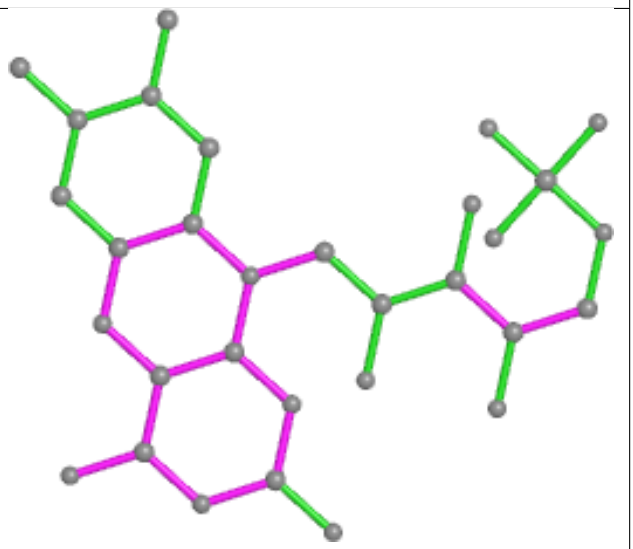


Rings

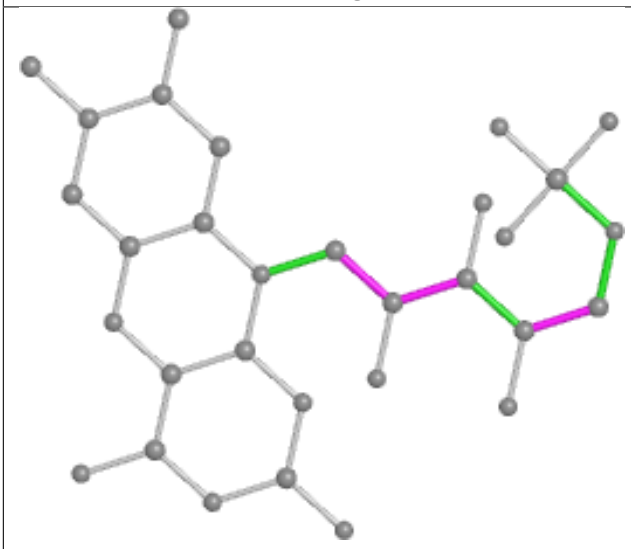
Ligand FMN 1 502



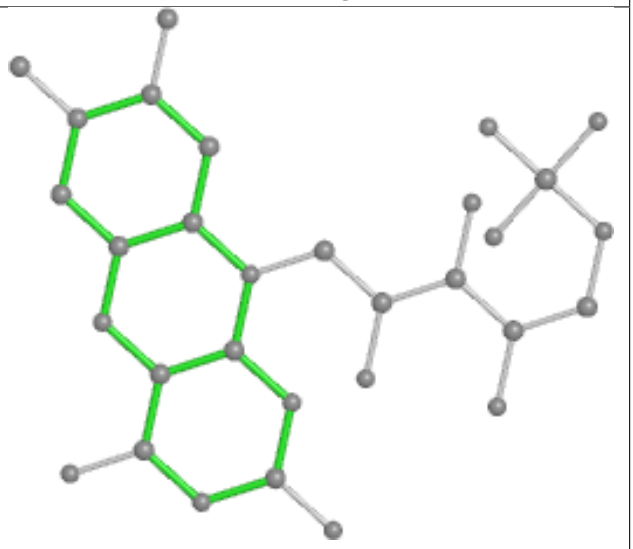
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.