Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 12:43 PM EDT

PDB ID	:	5W1S
Title	:	X-ray crystal structure of Escherichia coli RNA polymerase and TraR complex
Authors	:	Murakami, K.S.; Molodtsov, V.
Deposited on	:	2017-06-04
Resolution	:	3.81 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:

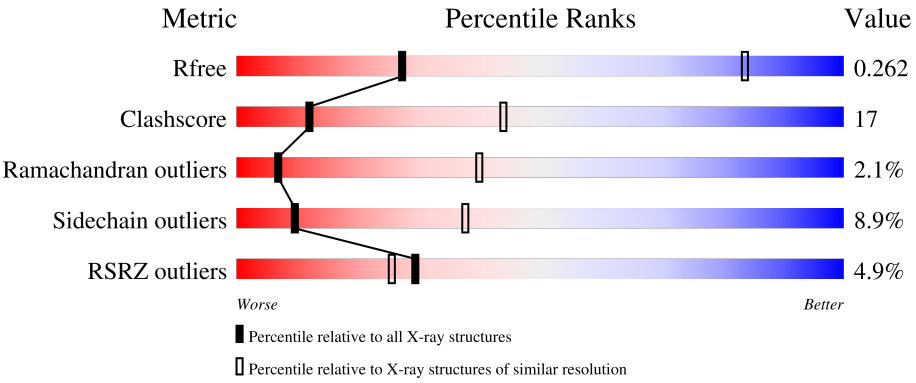
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.81 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))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	2% 45% 41% 10%
1	B	329	3% 40% 24% 34%
1	G	329	2% 37% 27% 31%
1	H	329	6% 42% 22% 34%
2	C	1342	6% 57% 38%

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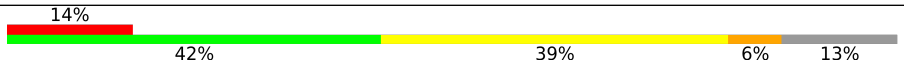
Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	
6	M	79	
6	N	79	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 56825 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10564	6628	1838	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1173	Total	C	N	O	S	0	0	0
			9095	5718	1628	1703	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	72	Total	C	N	O	S	0	0	0
			573	350	110	112	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	70	Total	C	N	O	S	0	0	0
			557	346	103	103	5			
6	N	69	Total	C	N	O	S	0	0	0
			552	343	102	102	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	74	HIS	-	expression tag	UNP P41065
M	75	HIS	-	expression tag	UNP P41065
M	76	HIS	-	expression tag	UNP P41065
M	77	HIS	-	expression tag	UNP P41065
M	78	HIS	-	expression tag	UNP P41065
M	79	HIS	-	expression tag	UNP P41065
N	74	HIS	-	expression tag	UNP P41065
N	75	HIS	-	expression tag	UNP P41065
N	76	HIS	-	expression tag	UNP P41065
N	77	HIS	-	expression tag	UNP P41065
N	78	HIS	-	expression tag	UNP P41065
N	79	HIS	-	expression tag	UNP P41065

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	J	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

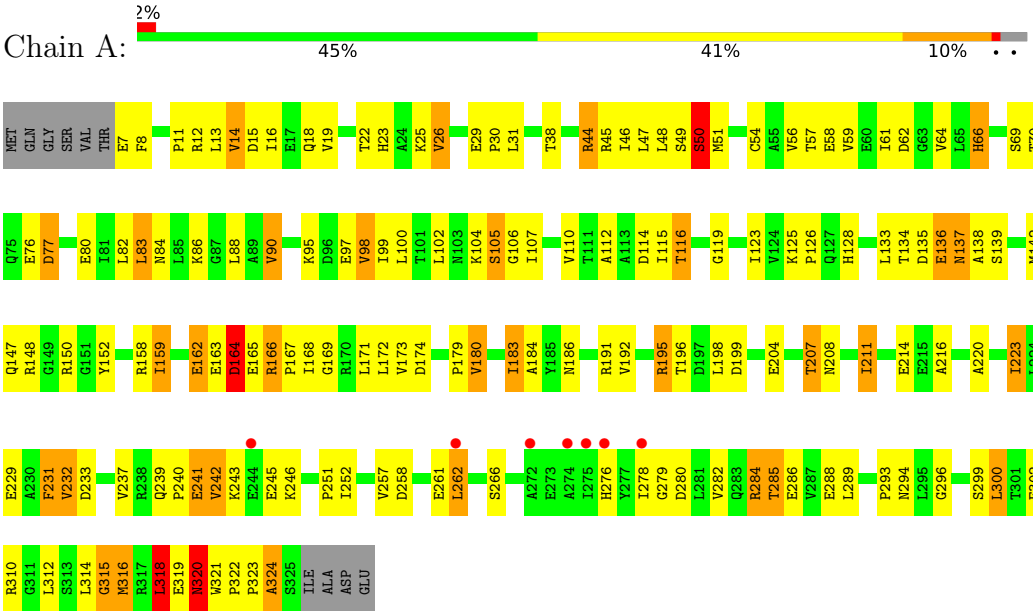
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	2	Total Zn 2 2	0	0
8	J	2	Total Zn 2 2	0	0
8	M	1	Total Zn 1 1	0	0
8	N	1	Total Zn 1 1	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

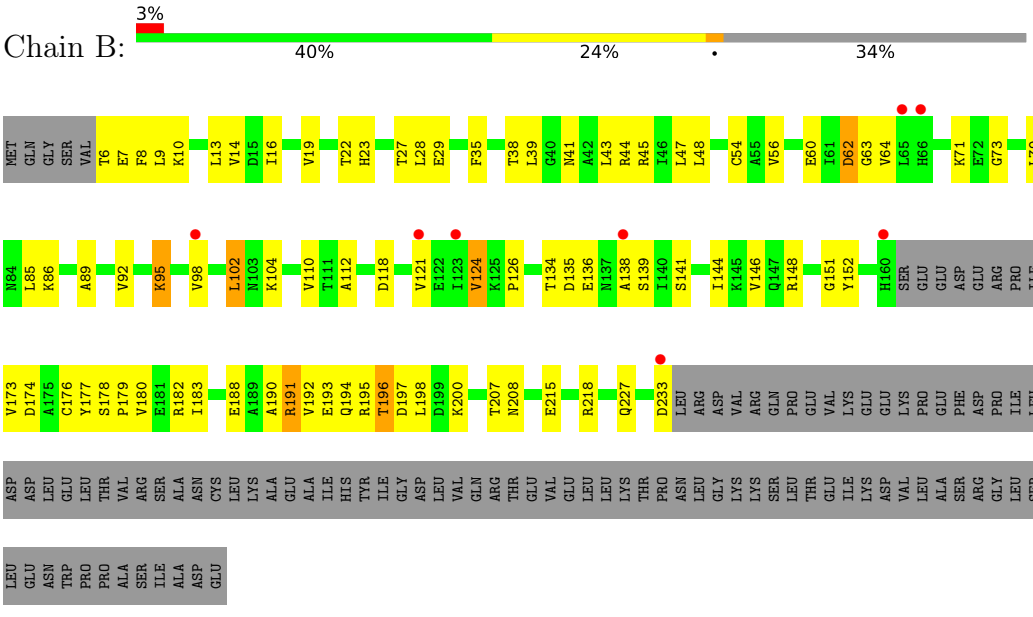
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



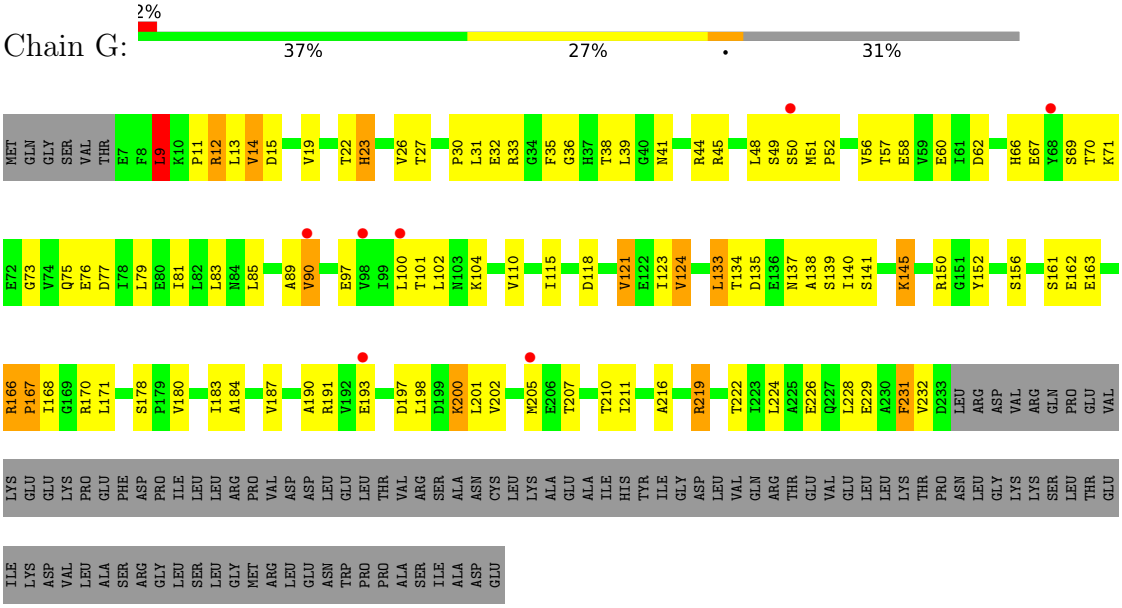
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



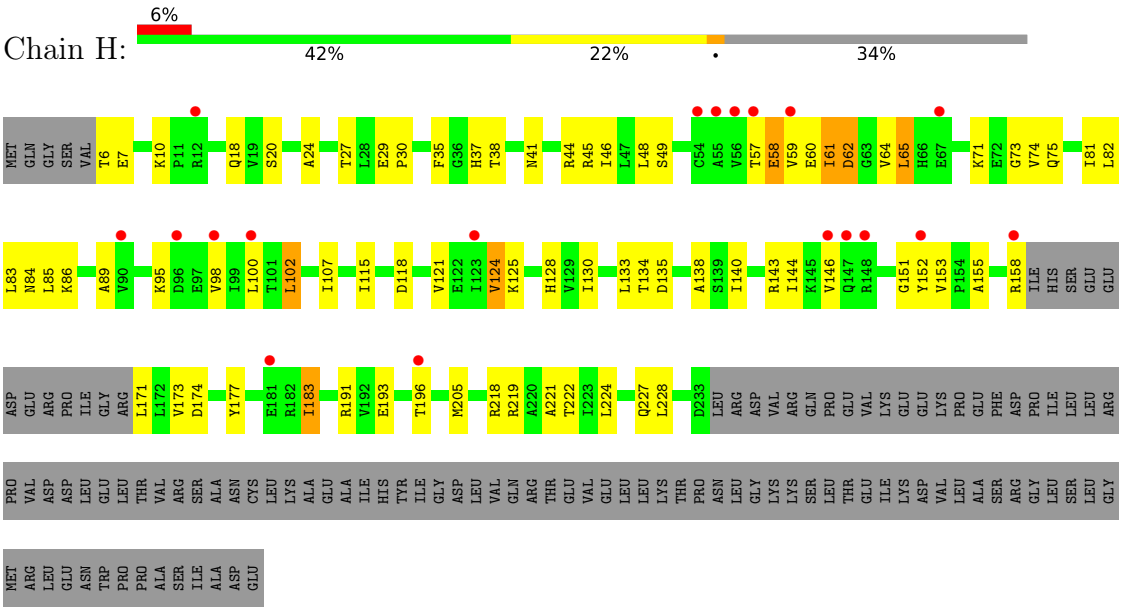
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



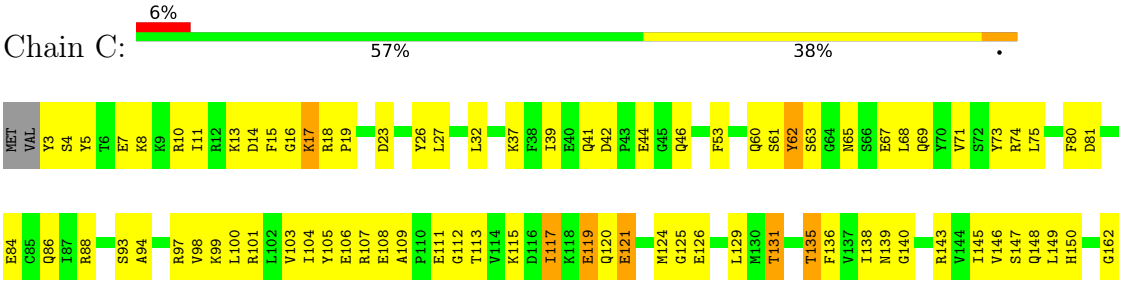
• Molecule 1: DNA-directed RNA polymerase subunit alpha

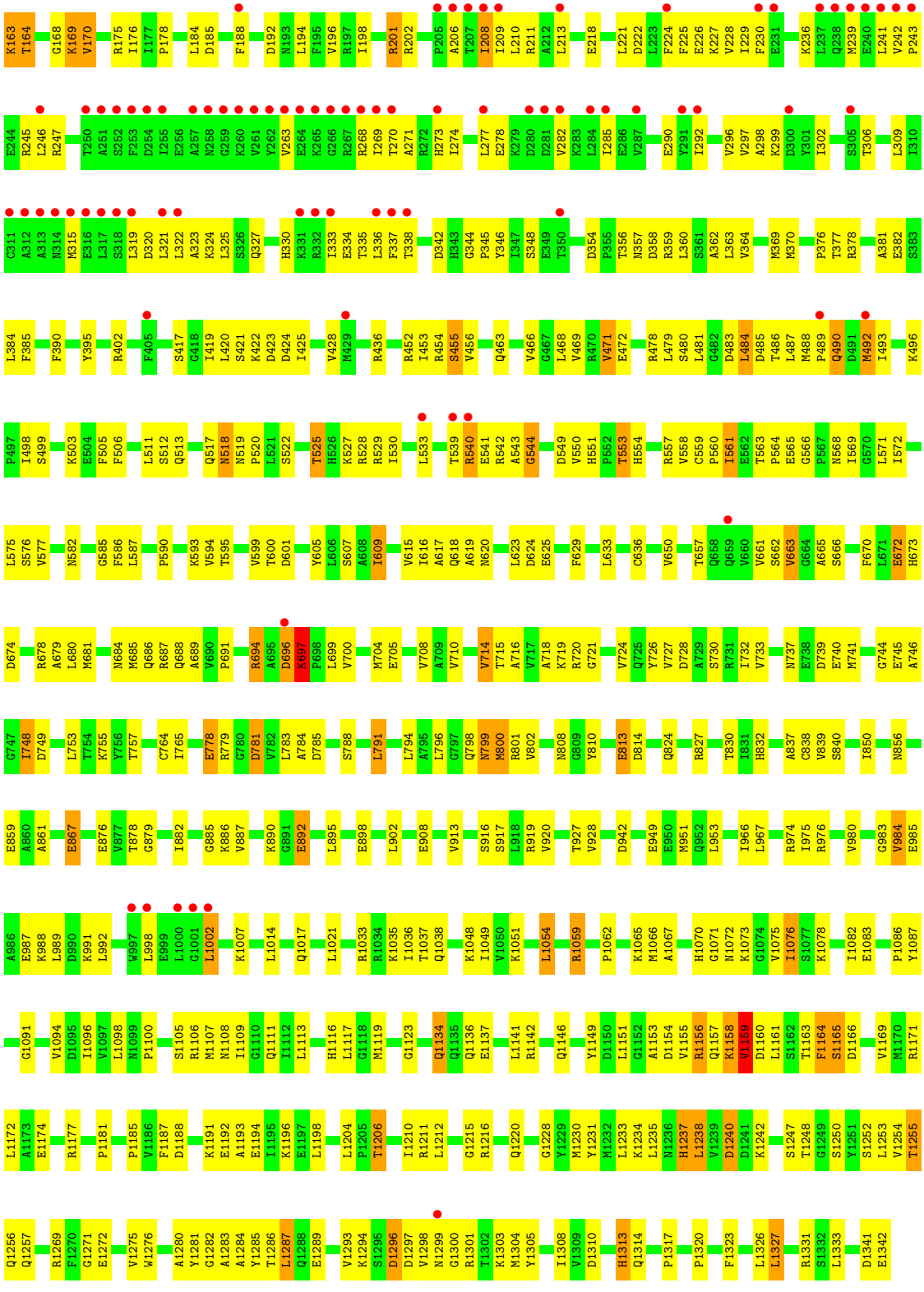
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

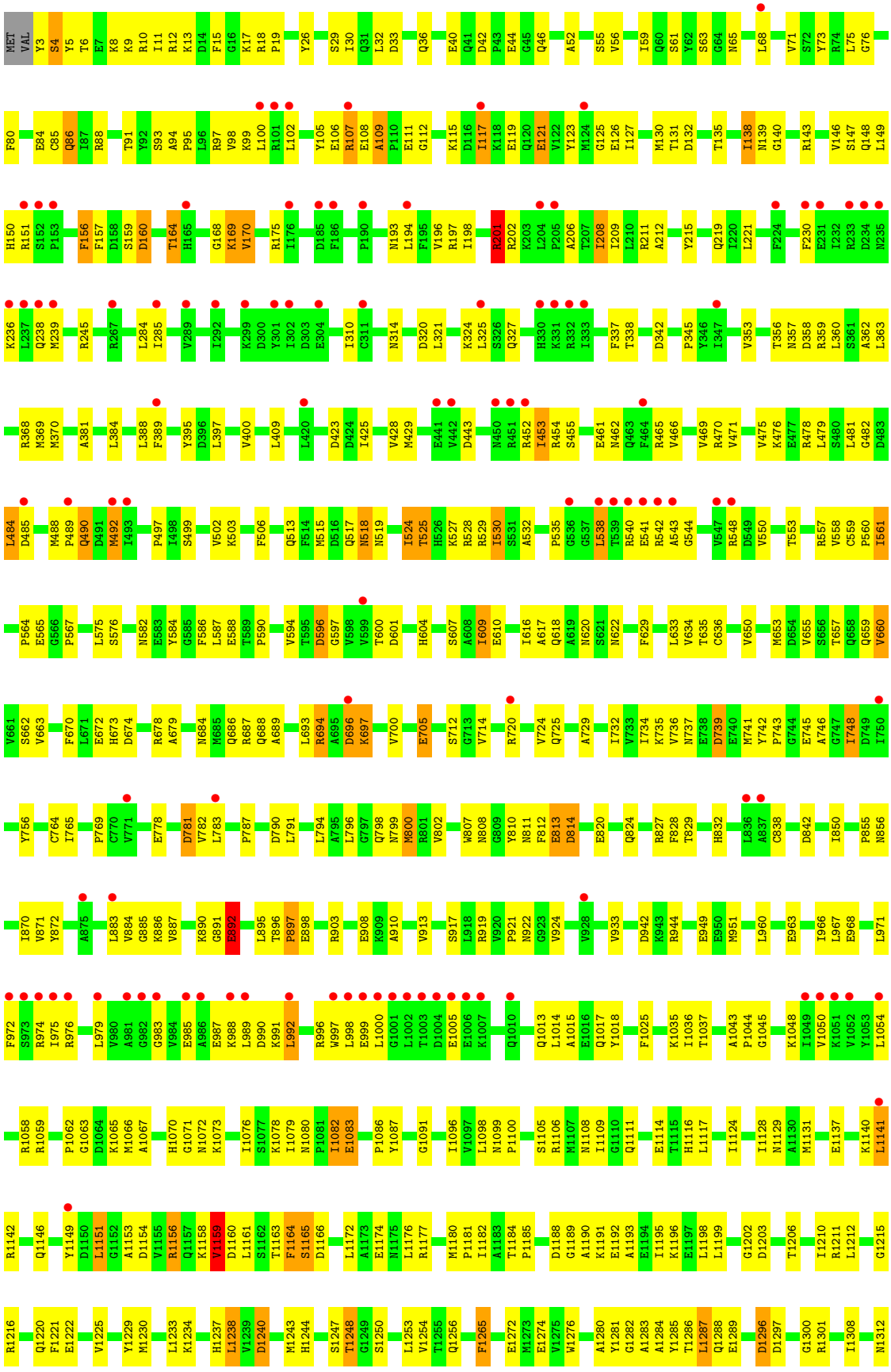
Chain C:

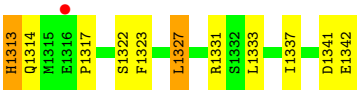




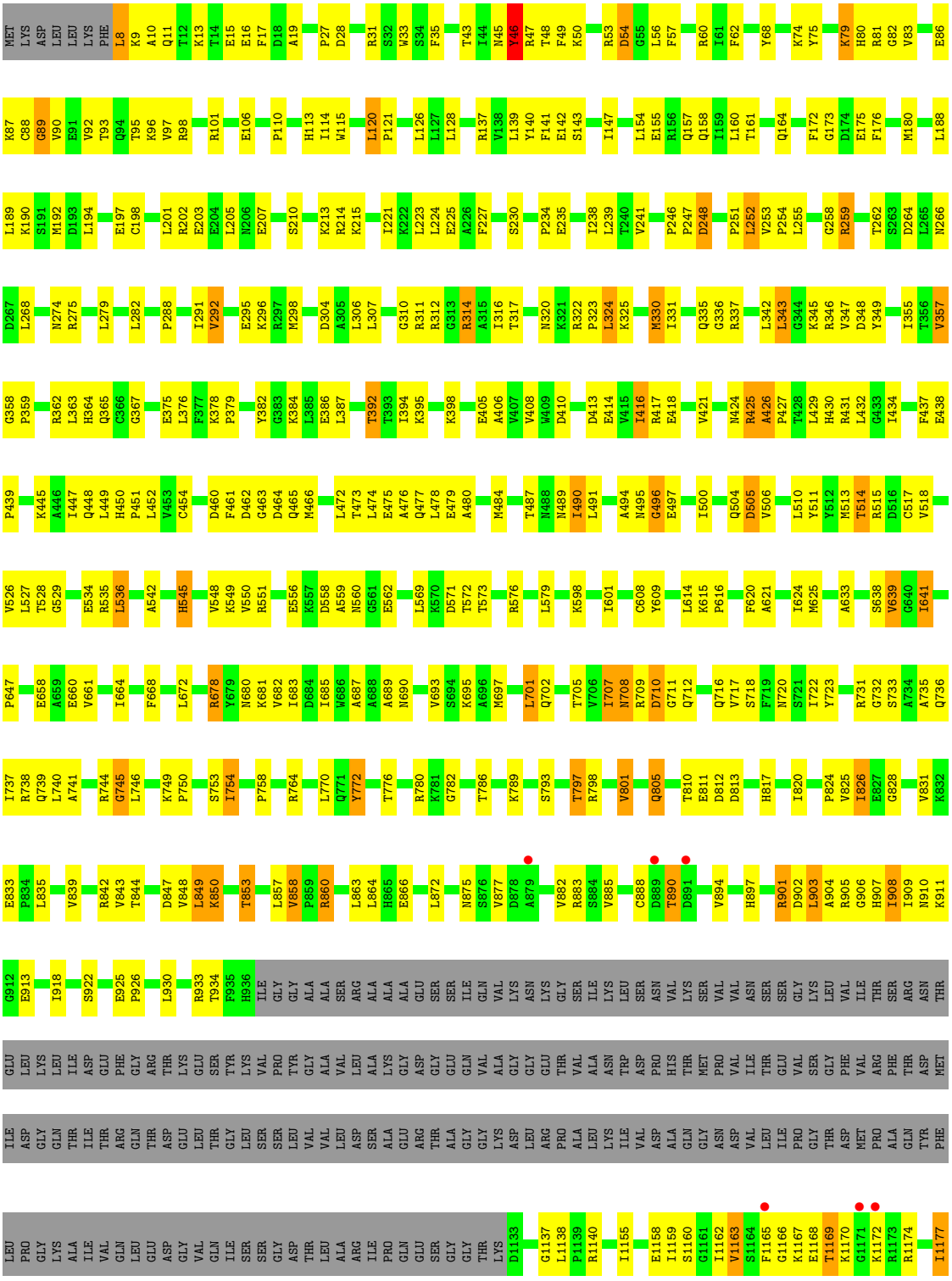
• Molecule 2: DNA-directed RNA polymerase subunit beta

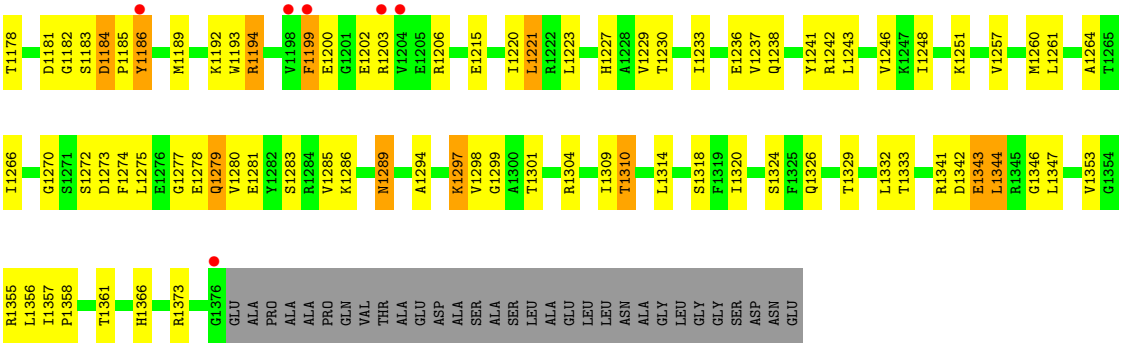
Chain I:



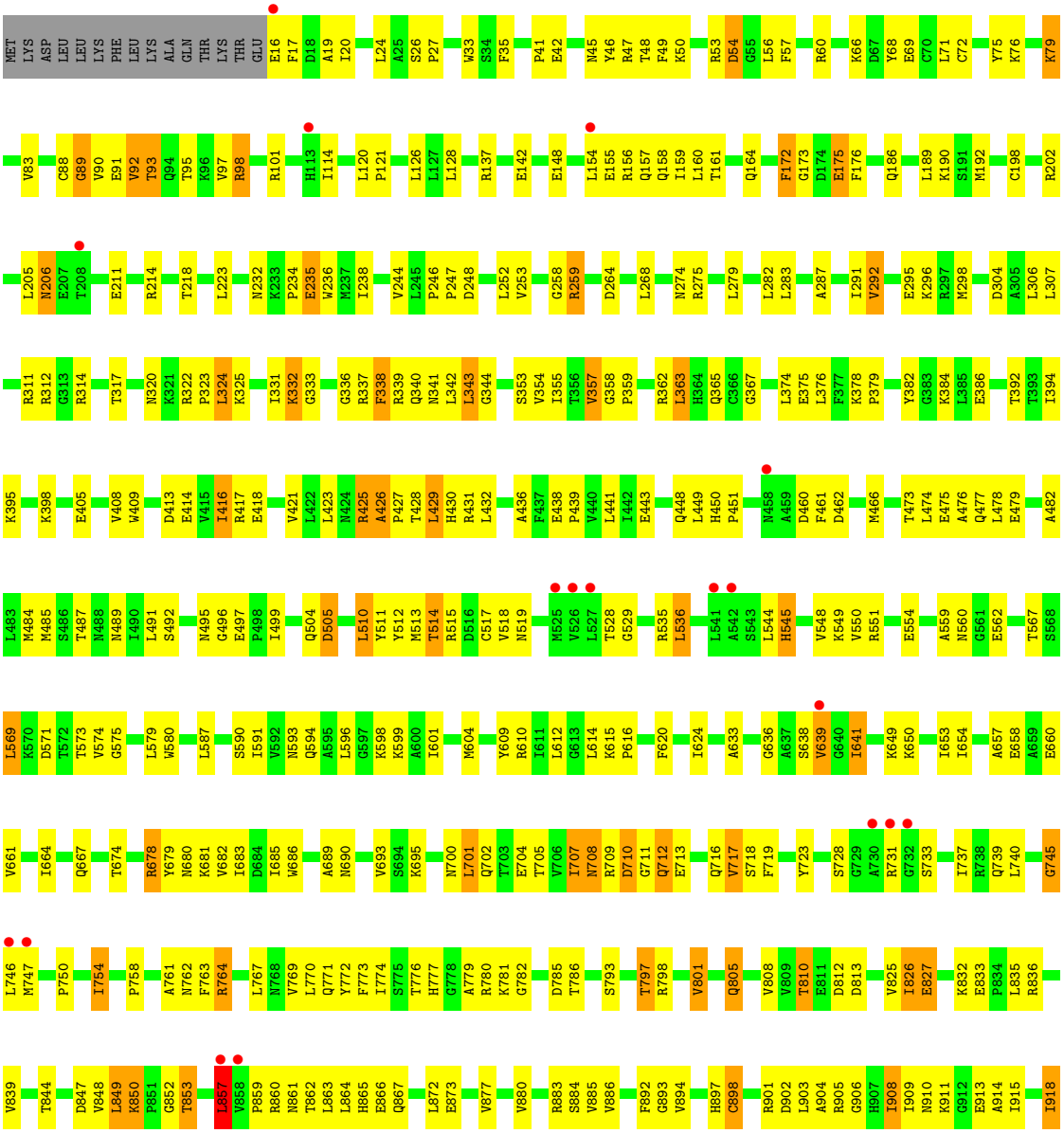


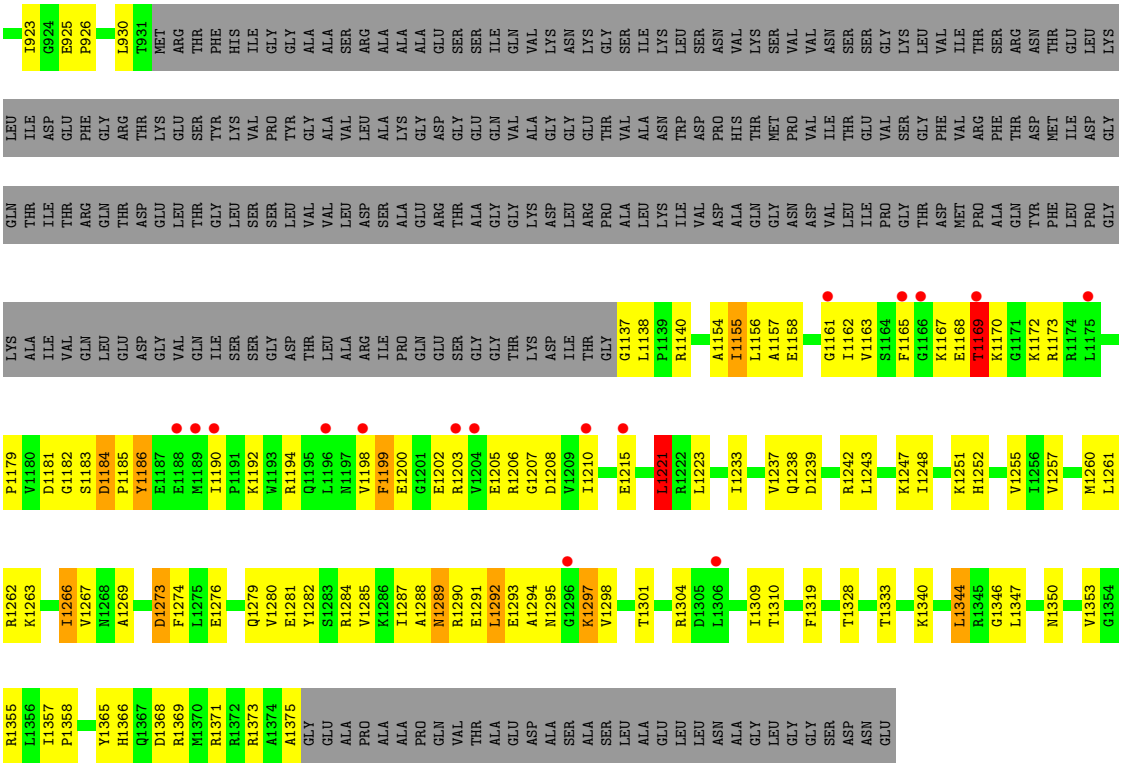
• Molecule 3: DNA-directed RNA polymerase subunit beta'



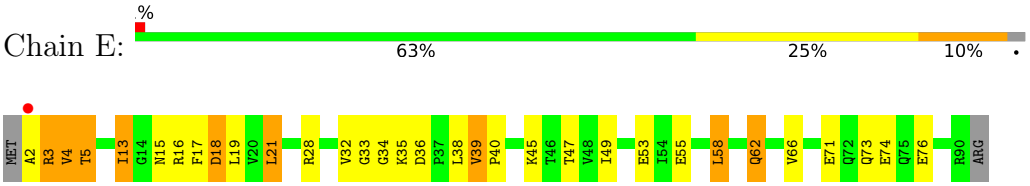


• Molecule 3: DNA-directed RNA polymerase subunit beta'

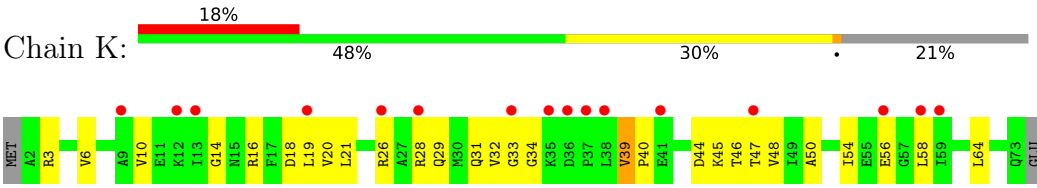


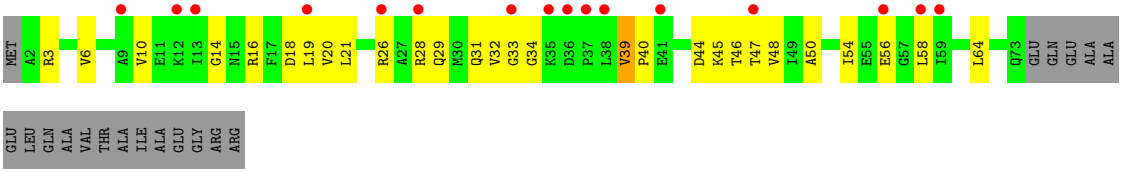


• Molecule 4: DNA-directed RNA polymerase subunit omega

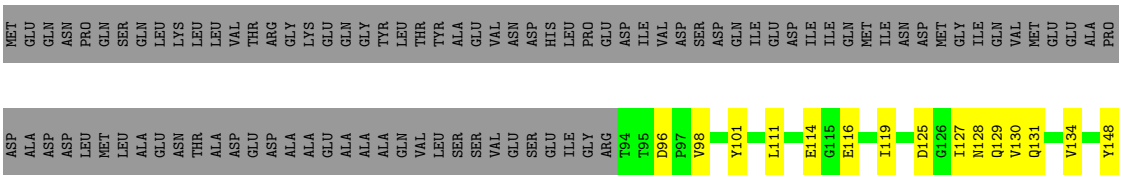


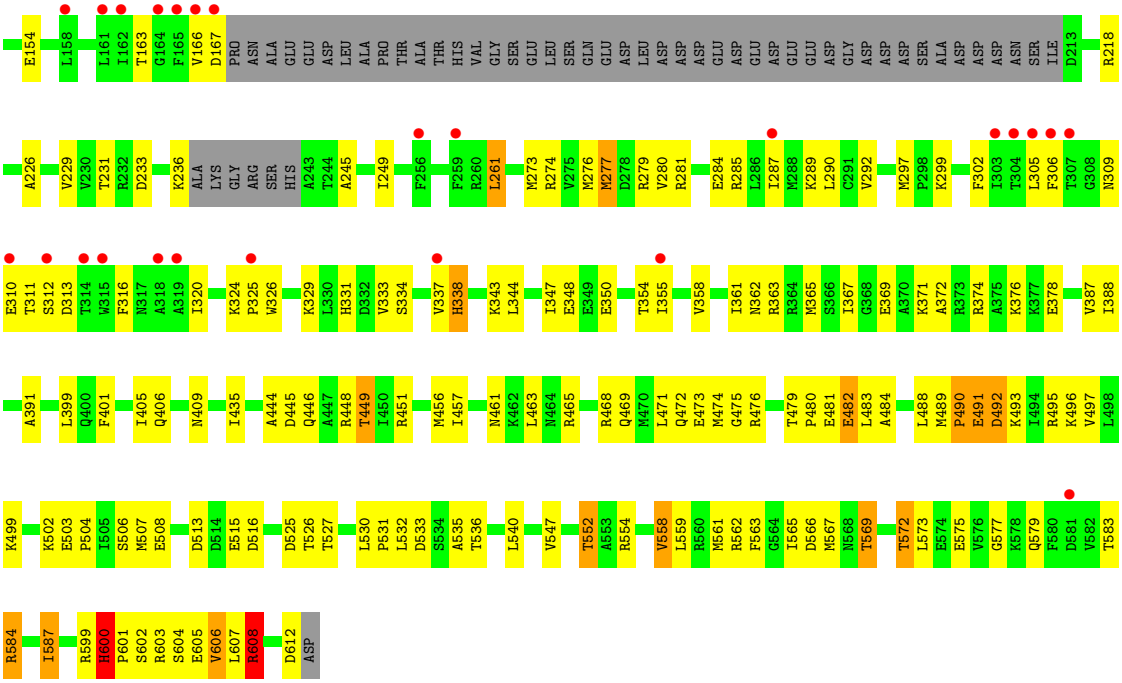
• Molecule 4: DNA-directed RNA polymerase subunit omega





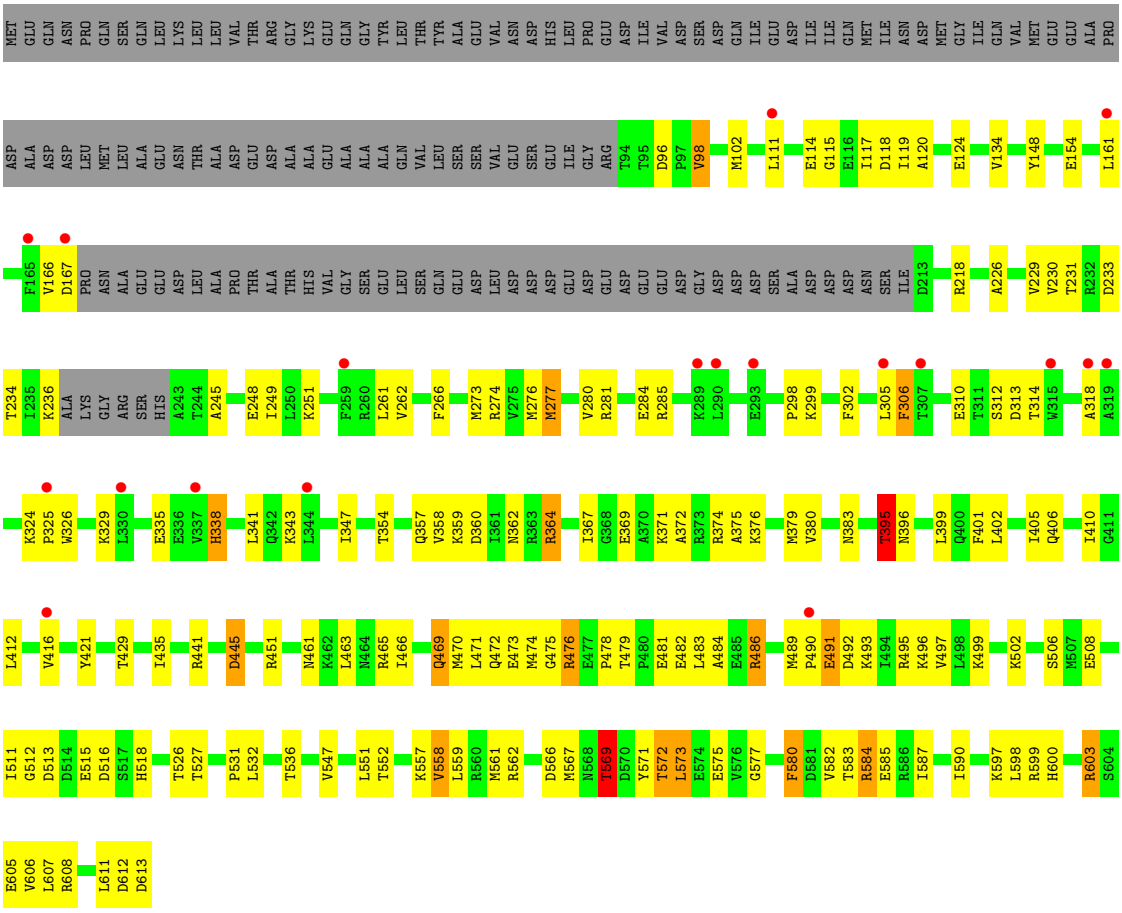
• Molecule 5: RNA polymerase sigma factor RpoD





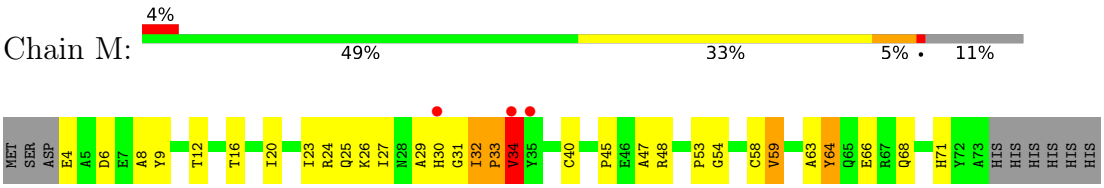
• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:



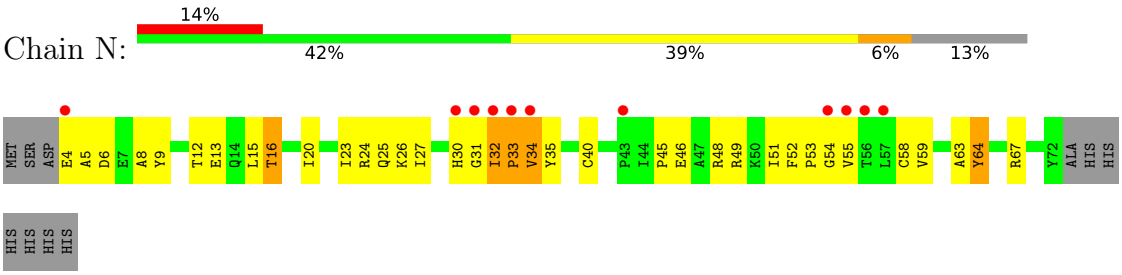
• Molecule 6: Protein TraR

Chain M:



• Molecule 6: Protein TraR

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	186.48Å 206.04Å 310.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.81 49.84 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.84-3.81) 86.5 (49.84-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.60 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.208 , 0.262 0.208 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å^2)	156.4	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 180.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	56825	wwPDB-VP
Average B, all atoms (Å^2)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: ZN, MG

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	A	0.29	0/2524	0.63	1/3421 (0.0%)
1	B	0.30	0/1697	0.60	0/2300
1	G	0.28	0/1777	0.59	0/2408
1	H	0.29	0/1681	0.63	2/2278 (0.1%)
2	C	0.30	0/10733	0.58	1/14482 (0.0%)
2	I	0.29	0/10735	0.56	0/14484
3	D	0.31	0/9235	0.59	0/12472
3	J	0.29	0/9140	0.56	2/12341 (0.0%)
4	E	0.27	0/693	0.52	0/935
4	K	0.26	0/575	0.43	0/774
5	F	0.28	0/3864	0.54	1/5194 (0.0%)
5	L	0.27	0/3872	0.53	0/5205
6	M	0.34	0/567	0.64	1/766 (0.1%)
6	N	0.37	0/562	0.64	1/759 (0.1%)
All	All	0.29	0/57655	0.57	9/77819 (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
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
5	F	0	1
All	All	0	9

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	LEU	CA-CB-CG	6.11	129.35	115.30
6	M	32	ILE	C-N-CD	-6.10	107.18	120.60
1	H	29	GLU	C-N-CD	-5.98	107.44	120.60
3	J	1221	LEU	CA-CB-CG	5.83	128.71	115.30
6	N	32	ILE	C-N-CD	-5.66	108.16	120.60
1	H	65	LEU	CA-CB-CG	5.50	127.95	115.30
3	J	857	LEU	CA-CB-CG	5.21	127.28	115.30
2	C	544	GLY	N-CA-C	-5.21	100.09	113.10
5	F	608	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	600	HIS	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	853	THR	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	A	2490	0	2542	120	0
1	B	1677	0	1703	61	0
1	G	1755	0	1773	78	0
1	H	1662	0	1687	59	0
2	C	10564	0	10571	426	0
2	I	10566	0	10576	351	0
3	D	9095	0	9222	385	0
3	J	9001	0	9167	375	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	691	0	695	26	0
4	K	573	0	587	20	0
5	F	3813	0	3880	119	0
5	L	3821	0	3884	109	0
6	M	557	0	547	31	0
6	N	552	0	542	44	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	56825	0	57376	1966	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 17.

All (1966) 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)
1:A:45:ARG:HG2	1:B:38:THR:HB	1.42	1.02
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.42	1.01
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.38	1.00
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.44	0.99
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.46	0.96
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.49	0.94
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.50	0.91
6:M:31:GLY:H	6:M:53:PRO:HB2	1.34	0.89
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.35	0.89
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.19	0.89
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.55	0.88
3:J:739:GLN:NE2	6:N:9:TYR:OH	2.07	0.88
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.16	0.87
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.40	0.87
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.57	0.87
3:J:754:ILE:HD12	6:N:20:ILE:HG12	1.55	0.86
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.58	0.85
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.59	0.84
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.60	0.84
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.60	0.84
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.60	0.83
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.60	0.82
1:A:296:GLY:H	1:A:299:SER:HB2	1.44	0.82
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.45	0.82
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.62	0.82
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.62	0.82
3:J:782:GLY:HA3	6:N:12:THR:HG22	1.63	0.81
6:N:31:GLY:H	6:N:53:PRO:HB2	1.45	0.81
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.63	0.80
2:C:678:ARG:NH2	6:M:6:ASP:OD1	2.13	0.80
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.63	0.80
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.61	0.80
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.15	0.80
2:C:168:GLY:O	2:C:170:VAL:N	2.13	0.79
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.63	0.79
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.64	0.79
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.45	0.79
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.63	0.79
2:C:41:GLN:NE2	2:C:73:TYR:O	2.16	0.79
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.64	0.78
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.16	0.78
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.15	0.78
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.48	0.78
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.49	0.78
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.67	0.77
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.65	0.77
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.67	0.77
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.66	0.77
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.50	0.77
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.66	0.77
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.66	0.77
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.66	0.77
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.17	0.77
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.67	0.76
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.02	0.76
3:J:48:THR:O	3:J:50:LYS:N	2.17	0.76
1:A:51:MET:HE1	1:A:220:ALA:HB2	1.68	0.76
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.20	0.76
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.17	0.76
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.68	0.76
2:I:705:GLU:HB2	2:I:794:LEU:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:GLU:HB3	1:H:10:LYS:HE3	1.67	0.75
3:J:709:ARG:O	3:J:711:GLY:N	2.18	0.75
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.50	0.75
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.69	0.75
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.68	0.75
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.66	0.75
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.67	0.74
5:L:481:GLU:OE1	5:L:495:ARG:NH2	2.20	0.74
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.69	0.74
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.68	0.74
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.67	0.74
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.70	0.74
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.67	0.74
2:I:1276:TRP:HH2	3:J:798:ARG:HG3	1.52	0.74
2:I:1287:LEU:HD22	3:J:1357:ILE:HG13	1.70	0.74
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.68	0.74
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.68	0.73
2:I:30:ILE:HD12	2:I:30:ILE:H	1.51	0.73
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.52	0.73
3:D:495:ASN:O	3:D:497:GLU:N	2.21	0.73
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.71	0.73
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.70	0.73
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.71	0.73
1:H:134:THR:HG23	1:H:135:ASP:H	1.53	0.73
1:A:191:ARG:NH1	1:A:198:LEU:O	2.22	0.73
3:D:252:LEU:HD23	3:D:262:THR:HB	1.71	0.73
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.24	0.73
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.71	0.73
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.71	0.73
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.71	0.72
3:D:395:LYS:HG2	5:F:536:THR:HG21	1.71	0.72
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.72	0.72
3:J:460:ASP:OD1	3:J:462:ASP:OD1	2.07	0.72
2:C:356:THR:HG21	2:C:362:ALA:HA	1.70	0.72
3:D:418:GLU:OE1	4:E:3:ARG:NH2	2.23	0.72
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.21	0.72
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.71	0.72
3:D:709:ARG:O	3:D:711:GLY:N	2.23	0.72
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.71	0.71
2:C:201:ARG:NH2	2:C:370:MET:O	2.23	0.71
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.55	0.71
3:D:739:GLN:NE2	6:M:9:TYR:OH	2.23	0.71
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.23	0.71
1:A:226:GLU:HB3	1:B:10:LYS:HE2	1.72	0.71
1:A:77:ASP:OD1	1:A:77:ASP:N	2.24	0.71
2:C:721:GLY:N	2:C:740:GLU:OE1	2.22	0.71
1:B:62:ASP:OD1	1:B:62:ASP:N	2.21	0.71
5:L:561:MET:HA	5:L:567:MET:HE1	1.73	0.70
1:A:14:VAL:HG22	1:A:15:ASP:H	1.56	0.70
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.23	0.70
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.55	0.70
3:D:746:LEU:HB2	3:D:754:ILE:HD11	1.72	0.70
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.72	0.70
3:D:362:ARG:H	3:D:365:GLN:HE21	1.39	0.70
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.74	0.70
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.56	0.70
2:I:1116:HIS:HE1	3:J:641:ILE:N	1.89	0.70
3:D:490:ILE:H	3:D:490:ILE:HD13	1.55	0.70
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.07	0.70
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.23	0.70
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.74	0.70
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.74	0.70
2:C:143:ARG:NH2	2:C:512:SER:O	2.25	0.70
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.74	0.70
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.24	0.70
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.22	0.70
2:I:528:ARG:NH2	2:I:576:SER:O	2.25	0.70
5:L:573:LEU:HD23	5:L:573:LEU:H	1.57	0.69
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.74	0.69
3:D:786:THR:HG21	6:M:8:ALA:HA	1.72	0.69
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.57	0.69
1:A:227:GLN:HG3	1:B:39:LEU:HD11	1.74	0.69
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.74	0.69
2:I:168:GLY:O	2:I:170:VAL:N	2.24	0.69
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.26	0.69
2:I:9:LYS:HD2	2:I:791:LEU:HD21	1.75	0.69
3:D:473:THR:HG23	3:D:476:ALA:H	1.58	0.69
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.93	0.69
4:E:38:LEU:HB3	4:E:58:LEU:HD22	1.74	0.69
3:J:473:THR:HG23	3:J:476:ALA:H	1.57	0.68
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.25	0.68
2:I:4:SER:OG	2:I:5:TYR:N	2.26	0.68
3:J:808:VAL:HG13	3:J:914:ALA:HA	1.76	0.68
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.75	0.68
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.74	0.68
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.76	0.68
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.57	0.68
4:E:4:VAL:HG13	4:E:5:THR:H	1.59	0.68
1:G:150:ARG:NH1	1:H:7:GLU:O	2.20	0.68
2:C:1161:LEU:HD21	2:C:1165:SER:HB3	1.76	0.68
3:D:749:LYS:HB2	3:D:750:PRO:HD2	1.75	0.68
3:J:418:GLU:HG3	4:K:45:LYS:H	1.59	0.68
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.76	0.68
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.29	0.68
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.74	0.68
4:E:32:VAL:O	4:E:34:GLY:N	2.26	0.67
3:J:683:ILE:HD13	6:N:23:ILE:HG21	1.76	0.67
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.59	0.67
6:N:33:PRO:HG3	6:N:54:GLY:HA2	1.77	0.67
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.74	0.67
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.76	0.67
2:I:739:ASP:OD1	2:I:739:ASP:N	2.26	0.67
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.60	0.67
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.76	0.67
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.60	0.67
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.77	0.67
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.77	0.67
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.24	0.67
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.76	0.67
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.28	0.67
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.60	0.67
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.76	0.66
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.76	0.66
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.75	0.66
3:D:48:THR:O	3:D:50:LYS:N	2.28	0.66
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.77	0.66
2:I:148:GLN:NE2	2:I:535:PRO:O	2.28	0.66
2:I:678:ARG:NH2	6:N:6:ASP:OD1	2.29	0.66
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.77	0.66
3:J:1233:ILE:O	3:J:1237:VAL:HG12	1.94	0.66
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:668:PHE:HB2	3:D:678:ARG:HG3	1.78	0.66
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.10	0.66
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.21	0.66
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.60	0.66
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	1.78	0.66
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.60	0.66
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.60	0.66
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.77	0.66
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.30	0.66
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.76	0.66
5:L:493:LYS:O	5:L:497:VAL:N	2.22	0.66
1:B:35:PHE:HA	1:B:38:THR:HG22	1.77	0.66
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.78	0.66
3:D:746:LEU:CB	3:D:754:ILE:HD11	2.25	0.66
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.78	0.66
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.78	0.66
3:J:901:ARG:HD2	3:J:906:GLY:O	1.96	0.66
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.30	0.65
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.78	0.65
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.16	0.65
1:G:9:LEU:O	1:H:227:GLN:NE2	2.29	0.65
2:I:1327:LEU:O	2:I:1331:ARG:HB2	1.97	0.65
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.78	0.65
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.30	0.65
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.78	0.65
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.30	0.65
2:C:705:GLU:HB2	2:C:794:LEU:H	1.61	0.65
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.79	0.65
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.79	0.65
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.77	0.65
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.62	0.65
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.79	0.64
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.80	0.64
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.78	0.64
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.61	0.64
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.78	0.64
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.28	0.64
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.79	0.64
2:I:452:ARG:NH1	2:I:584:TYR:O	2.31	0.64
1:A:97:GLU:HB3	1:A:147:GLN:HG2	1.80	0.64
2:C:297:VAL:HG12	2:C:315:MET:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.29	0.64
3:D:708:ASN:OD1	3:D:708:ASN:N	2.31	0.64
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.28	0.64
3:J:259:ARG:HD3	5:L:502:LYS:HD2	1.79	0.64
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.78	0.64
2:C:563:THR:HG22	2:C:680:LEU:HD11	1.77	0.64
1:G:45:ARG:HG2	1:H:38:THR:HB	1.80	0.64
3:J:797:THR:O	3:J:801:VAL:HG12	1.98	0.64
3:D:43:THR:OG1	5:F:449:THR:O	2.10	0.64
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.80	0.64
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.79	0.64
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.30	0.64
5:L:493:LYS:HG2	5:L:496:LYS:HE2	1.79	0.64
2:C:93:SER:OG	2:C:126:GLU:OE1	2.12	0.63
1:A:289:LEU:HD13	1:A:300:LEU:HD21	1.78	0.63
2:C:297:VAL:HG23	2:C:333:ILE:HG23	1.80	0.63
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.80	0.63
3:J:844:THR:OG1	3:J:860:ARG:O	2.11	0.63
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.62	0.63
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.79	0.63
2:I:30:ILE:HD11	2:I:575:LEU:HD22	1.80	0.63
2:C:105:TYR:HD1	2:C:112:GLY:H	1.45	0.63
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.81	0.63
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.80	0.63
2:I:560:PRO:O	3:J:780:ARG:NH2	2.30	0.63
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.30	0.63
2:C:617:ALA:HA	2:C:636:CYS:SG	2.38	0.63
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.79	0.63
2:I:992:LEU:HD11	2:I:1000:LEU:HD11	1.81	0.63
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.34	0.63
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.81	0.63
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.79	0.62
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.64	0.62
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.62	0.62
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.30	0.62
2:I:596:ASP:CG	2:I:597:GLY:H	2.03	0.62
2:C:119:GLU:HG3	2:C:489:PRO:HD2	1.82	0.62
2:C:246:LEU:HB2	2:C:269:ILE:HG21	1.81	0.62
1:G:14:VAL:HG13	1:G:15:ASP:H	1.62	0.62
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.81	0.62
1:B:63:GLY:HA3	1:B:71:LYS:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:479:THR:HG23	5:F:481:GLU:H	1.64	0.62
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.81	0.62
2:I:206:ALA:O	2:I:209:ILE:HG22	1.99	0.62
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.81	0.62
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.81	0.62
1:G:161:SER:O	1:G:163:GLU:N	2.33	0.62
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.81	0.62
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.09	0.62
3:J:79:LYS:HB2	5:L:569:THR:H	1.64	0.62
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.29	0.62
1:B:118:ASP:HB2	1:B:121:VAL:HB	1.81	0.61
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.63	0.61
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.25	0.61
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.82	0.61
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.81	0.61
1:G:12:ARG:H	1:G:30:PRO:HD2	1.64	0.61
3:J:495:ASN:O	3:J:497:GLU:N	2.32	0.61
3:J:1365:TYR:OH	3:J:1369:ARG:NH1	2.32	0.61
1:A:251:PRO:HD2	5:F:605:GLU:HG3	1.83	0.61
2:C:1164:PHE:O	2:C:1166:ASP:N	2.33	0.61
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.82	0.61
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.81	0.61
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.64	0.61
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.65	0.61
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.16	0.61
1:B:191:ARG:NH2	3:D:410:ASP:OD2	2.33	0.61
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.81	0.61
2:C:125:GLY:HA3	2:C:499:SER:HB2	1.81	0.61
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.83	0.61
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.82	0.61
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.83	0.61
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.66	0.61
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.83	0.61
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.83	0.61
3:J:16:GLU:HG3	3:J:17:PHE:H	1.66	0.61
3:J:786:THR:HG21	6:N:8:ALA:HA	1.82	0.61
6:N:46:GLU:HB3	6:N:49:ARG:HH21	1.66	0.61
2:I:998:LEU:H	2:I:998:LEU:HD12	1.65	0.60
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.83	0.60
3:J:128:LEU:HA	3:J:192:MET:HE1	1.83	0.60
3:J:460:ASP:OD1	6:N:4:GLU:OE2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.83	0.60
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.65	0.60
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.83	0.60
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	1.82	0.60
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.83	0.60
4:K:26:ARG:HD3	4:K:64:LEU:HD21	1.84	0.60
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.84	0.60
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.83	0.60
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.82	0.60
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.82	0.60
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.65	0.60
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.83	0.60
1:A:135:ASP:O	1:A:137:ASN:N	2.35	0.60
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.34	0.60
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.82	0.60
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.67	0.60
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.17	0.60
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.84	0.60
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.84	0.60
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.66	0.60
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.82	0.60
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.83	0.60
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.83	0.60
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.83	0.60
3:J:658:GLU:O	3:J:661:VAL:HG22	2.01	0.60
6:M:31:GLY:O	6:M:32:ILE:HG13	2.02	0.60
6:M:45:PRO:HD2	6:M:48:ARG:CZ	2.32	0.60
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.84	0.59
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.34	0.59
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.83	0.59
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.85	0.59
3:D:849:LEU:H	3:D:849:LEU:HD22	1.67	0.59
3:J:761:ALA:H	3:J:771:GLN:HE22	1.50	0.59
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.17	0.59
3:D:786:THR:HA	3:D:789:LYS:HG3	1.82	0.59
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.83	0.59
2:C:360:LEU:HD11	2:C:378:ARG:HA	1.83	0.59
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.68	0.59
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.37	0.59
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.31	0.59
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:470:MET:HB2	5:L:478:PRO:HG3	1.82	0.59
1:A:310:ARG:O	5:F:608:ARG:NH2	2.35	0.59
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.85	0.59
1:B:215:GLU:HA	1:B:218:ARG:HG3	1.85	0.59
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.85	0.59
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.35	0.59
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.83	0.59
1:A:211:ILE:HG21	1:A:216:ALA:HB2	1.84	0.59
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.67	0.59
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.68	0.59
5:L:469:GLN:O	5:L:473:GLU:HB2	2.03	0.59
2:C:1282:GLY:O	2:C:1284:ALA:N	2.35	0.59
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.84	0.59
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.35	0.59
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.85	0.59
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.85	0.59
3:D:515:ARG:O	3:D:545:HIS:HB3	2.02	0.59
3:D:1167:LYS:HZ2	3:D:1168:GLU:H	1.50	0.59
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.84	0.59
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.85	0.59
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.84	0.59
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.38	0.59
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.85	0.59
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.83	0.59
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.03	0.59
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.85	0.58
2:C:802:VAL:HG11	2:C:1230:MET:HB3	1.85	0.58
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.22	0.58
6:M:48:ARG:NH2	6:M:58:CYS:HA	2.18	0.58
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.68	0.58
3:D:259:ARG:HG3	5:F:502:LYS:HD2	1.86	0.58
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.84	0.58
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.03	0.58
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.39	0.58
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.84	0.58
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.38	0.58
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.85	0.58
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.84	0.58
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.86	0.58
1:G:166:ARG:HD3	1:G:168:ILE:HG23	1.85	0.58
4:K:26:ARG:NH1	4:K:29:GLN:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:379:MET:O	5:L:383:ASN:ND2	2.36	0.58
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.86	0.58
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.84	0.58
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.85	0.58
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.85	0.58
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	1.86	0.58
3:J:504:GLN:HG3	3:J:505:ASP:H	1.69	0.58
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.85	0.58
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.85	0.58
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.84	0.58
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.84	0.58
2:C:360:LEU:HD22	2:C:378:ARG:HE	1.68	0.58
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.85	0.58
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.38	0.58
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.30	0.58
6:M:25:GLN:O	6:M:27:ILE:N	2.35	0.58
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.39	0.57
2:C:471:VAL:HG21	2:C:498:ILE:HD11	1.85	0.57
5:F:469:GLN:O	5:F:473:GLU:HB2	2.04	0.57
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.85	0.57
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.86	0.57
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.86	0.57
3:D:264:ASP:OD2	5:F:506:SER:OG	2.17	0.57
3:D:414:GLU:O	4:E:45:LYS:NZ	2.36	0.57
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.86	0.57
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.85	0.57
2:I:808:ASN:H	3:J:633:ALA:HB2	1.69	0.57
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.85	0.57
3:D:705:THR:OG1	3:D:718:SER:HA	2.04	0.57
2:I:324:LYS:O	2:I:327:GLN:NE2	2.37	0.57
6:M:63:ALA:O	6:M:66:GLU:N	2.36	0.57
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.11	0.57
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.86	0.57
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.68	0.57
6:N:16:THR:O	6:N:20:ILE:HG13	2.05	0.57
1:A:241:GLU:HG3	1:A:242:VAL:H	1.70	0.57
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.33	0.57
2:C:1326:LEU:HD11	3:D:331:ILE:HG23	1.86	0.57
3:D:317:THR:HG22	3:D:322:ARG:O	2.04	0.57
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.39	0.57
2:C:1107:MET:HG2	3:D:740:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.85	0.57
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.87	0.57
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.38	0.57
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.86	0.57
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.85	0.57
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.85	0.57
3:J:317:THR:HB	3:J:324:LEU:HB3	1.86	0.57
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.69	0.57
3:D:418:GLU:HG3	4:E:45:LYS:H	1.70	0.57
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.86	0.57
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.87	0.57
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.86	0.57
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.86	0.57
3:J:1319:PHE:HB3	3:J:1340:LYS:HD2	1.86	0.57
5:L:148:TYR:OH	5:L:218:ARG:HA	2.05	0.57
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.87	0.57
1:A:82:LEU:HB3	1:A:173:VAL:HG12	1.87	0.56
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.40	0.56
2:C:1106:ARG:NE	6:M:6:ASP:OD2	2.36	0.56
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.86	0.56
6:N:31:GLY:O	6:N:32:ILE:HG13	2.04	0.56
1:B:192:VAL:O	1:B:194:GLN:N	2.38	0.56
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.86	0.56
5:F:612:ASP:OD1	5:F:612:ASP:N	2.37	0.56
1:H:191:ARG:HH22	3:J:409:TRP:HB3	1.69	0.56
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.06	0.56
1:A:47:LEU:O	1:A:180:VAL:HG21	2.04	0.56
2:C:13:LYS:HD3	2:C:1149:TYR:HA	1.87	0.56
2:C:324:LYS:O	2:C:327:GLN:NE2	2.38	0.56
3:D:75:TYR:OH	3:D:86:GLU:OE1	2.21	0.56
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.85	0.56
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.88	0.56
2:I:168:GLY:C	2:I:170:VAL:H	2.08	0.56
2:I:169:LYS:O	2:I:170:VAL:HG22	2.05	0.56
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.88	0.56
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.87	0.56
2:C:778:GLU:O	2:C:781:ASP:HB2	2.05	0.56
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.87	0.56
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.87	0.56
2:I:208:ILE:HG12	2:I:362:ALA:CB	2.35	0.56
2:I:1243:MET:HA	3:J:353:SER:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HB3	2:C:694:ARG:HH21	1.70	0.56
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.40	0.56
2:I:1129:ASN:OD1	2:I:1177:ARG:NH2	2.37	0.56
3:J:205:LEU:HD22	3:J:214:ARG:HB2	1.87	0.56
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.88	0.56
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.87	0.56
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.88	0.56
2:I:798:GLN:OE1	2:I:827:ARG:HB2	2.06	0.56
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.35	0.56
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.86	0.56
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.71	0.56
3:J:1239:ASP:O	3:J:1243:LEU:HB2	2.06	0.56
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.19	0.56
1:A:137:ASN:N	1:A:137:ASN:OD1	2.36	0.56
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.70	0.56
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.38	0.56
3:J:657:ALA:HA	3:J:660:GLU:HB2	1.88	0.56
3:J:705:THR:HG21	3:J:719:PHE:H	1.71	0.56
5:L:470:MET:O	5:L:478:PRO:HD3	2.06	0.56
1:A:45:ARG:HG3	1:A:46:ILE:HD13	1.88	0.56
2:C:1298:VAL:HG11	3:D:96:LYS:HZ1	1.69	0.56
2:I:356:THR:HG21	2:I:362:ALA:HA	1.88	0.56
3:J:311:ARG:O	3:J:312:ARG:HD3	2.06	0.56
3:J:761:ALA:H	3:J:771:GLN:NE2	2.04	0.56
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.88	0.56
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.21	0.56
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.10	0.56
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.88	0.56
5:L:508:GLU:HG3	5:L:518:HIS:ND1	2.21	0.56
6:N:35:TYR:OH	6:N:49:ARG:NE	2.39	0.56
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.88	0.55
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.05	0.55
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.87	0.55
2:I:924:VAL:HG12	2:I:1058:ARG:HH21	1.71	0.55
2:I:1247:SER:HB3	3:J:375:GLU:O	2.05	0.55
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.88	0.55
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.37	0.55
6:N:48:ARG:HD3	6:N:59:VAL:HG23	1.87	0.55
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.06	0.55
3:D:844:THR:HG21	3:D:858:VAL:HG21	1.87	0.55
4:K:32:VAL:O	4:K:34:GLY:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HG22	1:A:116:THR:H	1.69	0.55
2:C:744:GLY:C	2:C:746:ALA:H	2.09	0.55
2:C:1075:VAL:HG21	3:D:463:GLY:HA2	1.88	0.55
3:D:205:LEU:HD22	3:D:214:ARG:HB2	1.88	0.55
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.41	0.55
2:I:1106:ARG:HG3	6:N:6:ASP:OD1	2.06	0.55
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.71	0.55
5:F:575:GLU:O	5:F:579:GLN:HG2	2.07	0.55
2:I:462:ASN:O	2:I:466:VAL:HG23	2.07	0.55
3:J:91:GLU:OE1	3:J:93:THR:OG1	2.24	0.55
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.89	0.55
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.88	0.55
5:F:312:SER:OG	5:F:313:ASP:N	2.40	0.55
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.88	0.55
3:J:549:LYS:HD3	3:J:569:LEU:HD23	1.88	0.55
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.34	0.55
1:A:166:ARG:O	1:A:168:ILE:N	2.40	0.55
3:D:203:GLU:O	3:D:207:GLU:HG2	2.07	0.55
3:D:1165:PHE:HE1	3:D:1200:GLU:HB2	1.71	0.55
3:D:1227:HIS:HB2	3:J:1293:GLU:OE1	2.07	0.55
5:F:292:VAL:HG11	5:F:299:LYS:HG3	1.87	0.55
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.88	0.55
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.47	0.55
1:A:44:ARG:HB2	1:A:183:ILE:HG21	1.89	0.55
1:A:223:ILE:HD13	1:B:8:PHE:CZ	2.42	0.55
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.21	0.55
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.30	0.55
2:I:475:VAL:HG22	2:I:492:MET:HB2	1.89	0.55
2:I:655:VAL:N	2:I:659:GLN:OE1	2.40	0.55
2:I:814:ASP:HB3	2:I:1073:LYS:O	2.07	0.55
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.87	0.55
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.72	0.55
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.21	0.55
3:D:683:ILE:HD13	6:M:23:ILE:HG21	1.87	0.55
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.72	0.55
5:F:316:PHE:CZ	5:F:338:HIS:HB2	2.41	0.55
2:I:807:TRP:HE1	2:I:1086:PRO:HD3	1.71	0.55
5:L:515:GLU:HG2	5:L:516:ASP:N	2.22	0.55
2:C:395:TYR:HD2	2:C:419:ILE:HG22	1.71	0.55
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.89	0.55
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.40	0.55
5:L:124:GLU:OE1	5:L:421:TYR:OH	2.22	0.55
5:L:479:THR:HG23	5:L:481:GLU:H	1.72	0.55
2:C:323:ALA:O	2:C:327:GLN:HG3	2.07	0.55
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.88	0.55
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.72	0.55
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.42	0.55
3:D:88:CYS:O	3:D:90:VAL:N	2.39	0.55
5:F:561:MET:HA	5:F:567:MET:HE1	1.89	0.55
1:H:151:GLY:O	1:H:177:TYR:HB2	2.06	0.55
2:I:135:THR:HG22	2:I:527:LYS:HE2	1.88	0.55
2:I:678:ARG:NH1	2:I:1071:GLY:O	2.33	0.55
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.39	0.55
5:L:551:LEU:HD23	5:L:597:LYS:HD2	1.88	0.55
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.22	0.54
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.88	0.54
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.89	0.54
2:C:1272:GLU:H	3:D:342:LEU:CB	2.20	0.54
3:D:680:ASN:OD1	6:M:23:ILE:HG23	2.07	0.54
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.89	0.54
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.27	0.54
1:H:18:GLN:HA	1:H:24:ALA:HA	1.90	0.54
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.89	0.54
3:J:782:GLY:HA3	6:N:12:THR:CG2	2.35	0.54
2:C:453:ILE:HD12	2:C:587:LEU:HG	1.89	0.54
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.89	0.54
5:F:261:LEU:H	5:F:261:LEU:HD12	1.71	0.54
5:L:612:ASP:N	5:L:612:ASP:OD1	2.39	0.54
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.89	0.54
3:D:658:GLU:O	3:D:661:VAL:HG22	2.08	0.54
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.90	0.54
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.08	0.54
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.22	0.54
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.90	0.54
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.38	0.54
2:C:686:GLN:HG2	2:C:796:LEU:HD22	1.90	0.54
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.73	0.54
3:J:436:ALA:HB3	3:J:485:MET:HA	1.90	0.54
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.89	0.54
5:L:354:THR:O	5:L:358:VAL:HG23	2.08	0.54
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.73	0.54
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.28	0.54
2:I:84:GLU:OE1	2:I:1035:LYS:HD2	2.08	0.54
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.90	0.54
3:J:332:LYS:HA	3:J:337:ARG:H	1.73	0.54
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.90	0.54
2:C:802:VAL:HG21	2:C:1098:LEU:HD22	1.90	0.54
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.89	0.54
2:C:1247:SER:HB3	3:D:375:GLU:O	2.08	0.54
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.08	0.54
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.90	0.54
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.54
3:D:438:GLU:OE1	4:E:3:ARG:NH1	2.35	0.54
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.73	0.54
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.72	0.54
5:L:245:ALA:O	5:L:249:ILE:HG13	2.08	0.54
1:A:14:VAL:HG22	1:A:15:ASP:N	2.23	0.53
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.72	0.53
2:C:1255:THR:O	2:C:1257:GLN:N	2.40	0.53
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.90	0.53
3:D:201:LEU:HB2	3:D:221:ILE:HD13	1.90	0.53
5:F:280:VAL:HG13	5:F:355:ILE:HD12	1.90	0.53
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.89	0.53
2:C:61:SER:O	2:C:63:SER:N	2.41	0.53
2:C:243:PRO:HB3	2:C:277:LEU:HB3	1.90	0.53
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.90	0.53
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.41	0.53
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.33	0.53
3:D:1270:GLY:HA3	3:D:1297:LYS:C	2.28	0.53
5:F:343:LYS:H	5:F:343:LYS:HD2	1.73	0.53
2:I:106:GLU:O	2:I:109:ALA:HB2	2.08	0.53
2:I:201:ARG:NH2	2:I:370:MET:O	2.37	0.53
2:I:810:TYR:HD2	3:J:359:PRO:HG2	1.74	0.53
2:I:975:ILE:O	2:I:979:LEU:HB2	2.09	0.53
3:J:492:SER:HB2	3:J:499:ILE:HB	1.90	0.53
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.22	0.53
1:A:98:VAL:HG22	1:A:100:LEU:HD12	1.89	0.53
3:D:833:GLU:OE1	3:D:1242:ARG:HD3	2.09	0.53
3:D:848:VAL:HG13	3:D:857:LEU:HB2	1.89	0.53
1:G:67:GLU:HB3	1:G:171:LEU:HG	1.89	0.53
2:I:156:PHE:CD2	2:I:175:ARG:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.74	0.53
3:J:287:ALA:HB3	3:J:292:VAL:HG12	1.91	0.53
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.91	0.53
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.90	0.53
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.91	0.53
3:D:325:LYS:HE2	3:D:330:MET:HG3	1.90	0.53
3:D:425:ARG:HG2	3:D:426:ALA:H	1.73	0.53
3:J:449:LEU:HD22	3:J:466:MET:SD	2.49	0.53
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.90	0.53
2:C:98:VAL:O	2:C:121:GLU:HA	2.09	0.53
3:D:1221:LEU:HB2	3:D:1229:VAL:HG11	1.91	0.53
5:F:354:THR:O	5:F:358:VAL:HG23	2.07	0.53
2:I:588:GLU:HB3	2:I:607:SER:HA	1.90	0.53
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.91	0.53
3:J:708:ASN:OD1	3:J:708:ASN:N	2.36	0.53
2:C:228:VAL:HG22	2:C:245:ARG:HE	1.74	0.53
1:G:52:PRO:HG3	1:H:6:THR:HG21	1.90	0.53
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.91	0.53
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.43	0.53
2:I:1067:ALA:HB2	2:I:1073:LYS:HA	1.91	0.53
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.24	0.53
3:D:54:ASP:OD1	3:D:54:ASP:N	2.42	0.53
5:F:245:ALA:O	5:F:249:ILE:HG13	2.09	0.53
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.08	0.53
3:J:683:ILE:HD11	3:J:754:ILE:HD13	1.90	0.53
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.44	0.53
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.74	0.53
1:A:237:VAL:HG12	1:B:14:VAL:HG12	1.91	0.53
2:C:243:PRO:HB3	2:C:277:LEU:CB	2.38	0.53
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.90	0.53
2:I:149:LEU:O	2:I:532:ALA:HA	2.08	0.53
2:I:409:LEU:HD21	2:I:428:VAL:HA	1.91	0.53
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.89	0.53
4:K:39:VAL:HG21	4:K:56:GLU:HG3	1.90	0.53
1:A:12:ARG:H	1:A:30:PRO:HD2	1.74	0.53
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.91	0.53
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.40	0.53
1:G:27:THR:HG23	1:G:202:VAL:HG22	1.90	0.53
1:G:32:GLU:HB2	1:G:35:PHE:CD2	2.44	0.53
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.49	0.53
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.41	0.53
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.40	0.53
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.92	0.52
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.90	0.52
1:G:49:SER:HB3	2:I:1083:GLU:CD	2.30	0.52
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.74	0.52
2:I:384:LEU:O	2:I:388:LEU:HG	2.09	0.52
3:J:908:ILE:HG12	3:J:909:ILE:N	2.24	0.52
5:L:281:ARG:O	5:L:285:ARG:HG3	2.09	0.52
1:A:318:LEU:O	1:A:320:ASN:N	2.38	0.52
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.73	0.52
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.40	0.52
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.40	0.52
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.73	0.52
3:J:901:ARG:HA	3:J:908:ILE:HA	1.90	0.52
5:L:395:THR:OG1	5:L:396:ASN:N	2.42	0.52
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.24	0.52
3:D:1314:LEU:O	3:D:1326:GLN:NE2	2.42	0.52
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.91	0.52
3:J:793:SER:O	3:J:797:THR:HG23	2.08	0.52
3:J:1184:ASP:O	3:J:1186:TYR:N	2.43	0.52
1:A:257:VAL:HG13	1:A:276:HIS:O	2.09	0.52
2:C:582:ASN:HB3	2:C:586:PHE:H	1.74	0.52
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.25	0.52
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.39	0.52
2:I:678:ARG:NH2	6:N:5:ALA:HB3	2.24	0.52
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.44	0.52
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.92	0.52
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.37	0.52
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.91	0.52
3:J:42:GLU:OE2	5:L:451:ARG:NE	2.31	0.52
5:L:234:THR:O	5:L:245:ALA:HB2	2.09	0.52
5:L:312:SER:OG	5:L:313:ASP:N	2.42	0.52
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.91	0.52
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.92	0.52
3:D:1347:LEU:HD12	3:D:1358:PRO:HG2	1.92	0.52
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.91	0.52
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.90	0.52
6:M:29:ALA:O	6:M:53:PRO:HG2	2.09	0.52
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.39	0.52
1:A:86:LYS:HE2	1:A:174:ASP:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:928:VAL:HG22	2:C:1054:LEU:HD11	1.92	0.52
2:C:1211:ARG:HE	2:C:1220:GLN:NE2	2.07	0.52
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.92	0.52
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.44	0.52
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.08	0.52
1:G:231:PHE:HB3	1:H:218:ARG:HB3	1.92	0.52
3:J:438:GLU:OE1	4:K:3:ARG:NH2	2.43	0.52
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.92	0.52
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.25	0.52
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.91	0.52
5:F:513:ASP:C	5:F:515:GLU:H	2.12	0.52
4:K:44:ASP:HB3	4:K:48:VAL:HB	1.91	0.52
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.92	0.52
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.10	0.52
3:D:903:LEU:HD22	3:D:909:ILE:HD12	1.91	0.52
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.46	0.52
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.45	0.52
3:J:770:LEU:H	3:J:770:LEU:HD22	1.74	0.52
2:C:885:GLY:HA2	2:C:917:SER:HB3	1.93	0.51
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.43	0.51
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.92	0.51
3:D:909:ILE:HD11	3:D:913:GLU:HG2	1.91	0.51
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.10	0.51
3:J:700:ASN:O	3:J:704:GLU:HB2	2.10	0.51
2:C:298:ALA:HB3	2:C:334:GLU:HB2	1.91	0.51
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.92	0.51
3:D:506:VAL:HG21	3:D:625:MET:HA	1.92	0.51
4:E:13:ILE:HD12	4:E:19:LEU:HA	1.91	0.51
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.49	0.51
2:C:1271:GLY:HA3	3:D:343:LEU:HD12	1.91	0.51
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.29	0.51
2:I:156:PHE:HD2	2:I:175:ARG:HB3	1.76	0.51
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.08	0.51
3:J:598:LYS:O	3:J:601:ILE:HG22	2.09	0.51
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.31	0.51
3:J:903:LEU:HD22	3:J:909:ILE:HD12	1.92	0.51
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	1.92	0.51
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.10	0.51
2:C:808:ASN:H	3:D:633:ALA:HB2	1.75	0.51
2:I:138:ILE:O	2:I:139:ASN:ND2	2.43	0.51
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:88:CYS:O	3:J:90:VAL:N	2.44	0.51
3:J:517:CYS:HA	3:J:716:GLN:NE2	2.24	0.51
3:J:1290:ARG:HD2	3:J:1298:VAL:HG12	1.92	0.51
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.93	0.51
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	1.92	0.51
3:D:11:GLN:HG2	3:D:15:GLU:CD	2.31	0.51
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.93	0.51
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.43	0.51
3:J:460:ASP:CG	3:J:462:ASP:OD1	2.48	0.51
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.75	0.51
2:C:211:ARG:NH1	2:C:357:ASN:O	2.44	0.51
2:C:338:THR:HG22	2:C:345:PRO:HB3	1.92	0.51
3:D:227:PHE:O	3:D:230:SER:HB3	2.10	0.51
3:D:901:ARG:HA	3:D:908:ILE:HA	1.93	0.51
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.92	0.51
2:I:813:GLU:HG3	3:J:460:ASP:HA	1.92	0.51
2:I:1282:GLY:O	2:I:1284:ALA:N	2.44	0.51
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.74	0.51
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.91	0.51
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.43	0.51
2:C:624:ASP:OD1	2:C:625:GLU:N	2.38	0.51
2:C:1289:GLU:OE1	2:C:1294:LYS:HE2	2.11	0.51
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.93	0.51
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.41	0.51
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.93	0.51
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.11	0.51
3:J:398:LYS:HE2	5:L:532:LEU:HD23	1.93	0.51
5:L:483:LEU:HD12	5:L:483:LEU:H	1.75	0.51
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.43	0.51
3:D:687:ALA:HB1	6:M:24:ARG:NE	2.25	0.51
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.26	0.51
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.93	0.51
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.93	0.51
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.92	0.51
5:L:314:THR:O	5:L:318:ALA:HB3	2.11	0.51
1:A:289:LEU:HD11	1:A:314:LEU:HD21	1.93	0.51
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.46	0.51
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.46	0.51
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.93	0.51
2:I:36:GLN:O	2:I:40:GLU:HB2	2.11	0.51
2:I:620:ASN:O	2:I:620:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.93	0.51
3:J:705:THR:OG1	3:J:718:SER:HA	2.10	0.51
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.92	0.51
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.76	0.51
5:F:489:MET:O	5:F:491:GLU:N	2.44	0.51
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.93	0.51
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.93	0.51
3:J:690:ASN:ND2	3:J:745:GLY:HA2	2.26	0.51
4:E:2:ALA:HB2	4:E:55:GLU:CD	2.31	0.50
1:A:44:ARG:HB2	1:A:183:ILE:CG2	2.41	0.50
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	1.92	0.50
1:H:107:ILE:HG23	1:H:134:THR:O	2.11	0.50
2:I:208:ILE:HG12	2:I:362:ALA:HB1	1.91	0.50
2:I:524:ILE:HD12	2:I:712:SER:HB2	1.93	0.50
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.93	0.50
1:A:95:LYS:O	1:A:148:ARG:NH2	2.45	0.50
1:A:169:GLY:O	1:A:171:LEU:HD22	2.11	0.50
1:A:225:ALA:O	1:A:229:GLU:N	2.44	0.50
1:A:285:THR:OG1	1:A:286:GLU:N	2.44	0.50
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.26	0.50
3:D:709:ARG:HD2	3:D:710:ASP:N	2.26	0.50
3:D:903:LEU:HB3	3:D:905:ARG:HG3	1.94	0.50
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.92	0.50
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.26	0.50
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.44	0.50
1:B:102:LEU:O	1:B:141:SER:HA	2.11	0.50
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.93	0.50
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.41	0.50
5:F:148:TYR:OH	5:F:218:ARG:HA	2.11	0.50
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.23	0.50
3:J:682:VAL:HG13	3:J:685:ILE:HD11	1.93	0.50
3:J:930:LEU:HB2	3:J:1138:LEU:HB2	1.92	0.50
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.94	0.50
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.92	0.50
1:B:188:GLU:O	1:B:200:LYS:N	2.37	0.50
2:C:395:TYR:HB3	2:C:419:ILE:HG22	1.93	0.50
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	1.94	0.50
3:D:491:LEU:HD22	3:D:496:GLY:O	2.11	0.50
2:I:52:ALA:HB2	2:I:461:GLU:HG3	1.94	0.50
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.46	0.50
2:I:998:LEU:HD23	2:I:1015:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:HG21	2:C:727:VAL:O	2.11	0.50
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.93	0.50
3:D:258:GLY:HA3	5:F:499:LYS:HE2	1.93	0.50
5:F:531:PRO:O	5:F:535:ALA:N	2.37	0.50
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.94	0.50
2:I:1296:ASP:OD2	2:I:1322:SER:HB3	2.11	0.50
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.94	0.50
2:C:710:VAL:HA	2:C:715:THR:HG21	1.94	0.50
5:F:292:VAL:HG13	5:F:297:MET:O	2.11	0.50
5:F:391:ALA:HB3	5:F:405:ILE:HG22	1.93	0.50
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.92	0.50
1:A:150:ARG:NH1	1:B:7:GLU:O	2.45	0.50
2:C:549:ASP:OD1	3:D:750:PRO:HG3	2.11	0.50
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.92	0.50
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.42	0.50
5:F:111:LEU:HD13	5:F:116:GLU:HA	1.94	0.50
2:I:810:TYR:HE1	2:I:1078:LYS:HD2	1.76	0.50
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.77	0.50
3:J:833:GLU:OE1	3:J:1242:ARG:HD3	2.11	0.50
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.47	0.50
2:C:225:PHE:HZ	2:C:348:SER:H	1.60	0.50
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.26	0.50
3:D:478:LEU:HG	4:E:47:THR:HG23	1.94	0.50
2:I:515:MET:HG2	2:I:517:GLN:HB2	1.93	0.50
2:I:921:PRO:O	2:I:924:VAL:HG22	2.11	0.50
2:C:208:ILE:HG13	2:C:354:ASP:OD1	2.12	0.49
2:C:213:LEU:HD23	2:C:385:PHE:HE2	1.77	0.49
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.94	0.49
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.93	0.49
2:C:1116:HIS:HE1	3:D:641:ILE:N	1.99	0.49
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.77	0.49
5:F:310:GLU:OE2	5:F:355:ILE:HG21	2.12	0.49
2:I:151:ARG:HH22	2:I:175:ARG:NH1	2.10	0.49
2:I:778:GLU:O	2:I:781:ASP:HB2	2.12	0.49
6:M:25:GLN:C	6:M:27:ILE:H	2.16	0.49
1:A:23:HIS:HE1	1:A:204:GLU:HG2	1.76	0.49
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.78	0.49
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.37	0.49
2:C:325:LEU:O	2:C:330:HIS:HB2	2.12	0.49
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.94	0.49
3:D:709:ARG:HD2	3:D:710:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.44	0.49
1:G:23:HIS:HB2	1:G:205:MET:O	2.12	0.49
1:G:31:LEU:HD21	1:G:39:LEU:HD12	1.94	0.49
2:I:820:GLU:N	2:I:1080:ASN:O	2.45	0.49
3:J:661:VAL:HG12	3:J:685:ILE:HD11	1.94	0.49
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.45	0.49
2:C:488:MET:O	2:C:490:GLN:N	2.40	0.49
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.48	0.49
3:D:56:LEU:H	3:D:56:LEU:HD12	1.76	0.49
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.12	0.49
2:I:963:GLU:O	2:I:967:LEU:HB2	2.12	0.49
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.95	0.49
1:G:140:ILE:HG13	1:G:140:ILE:O	2.12	0.49
2:I:1174:GLU:OE2	2:I:1177:ARG:NH1	2.45	0.49
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.94	0.49
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.78	0.49
2:C:10:ARG:HA	2:C:1172:LEU:HD23	1.93	0.49
2:C:149:LEU:HD12	2:C:452:ARG:O	2.12	0.49
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.94	0.49
2:C:708:VAL:CG1	2:C:794:LEU:HD22	2.42	0.49
3:D:744:ARG:HG3	3:D:744:ARG:O	2.13	0.49
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.12	0.49
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.45	0.49
3:J:680:ASN:O	3:J:683:ILE:HG22	2.13	0.49
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.78	0.49
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.94	0.49
3:J:554:GLU:HA	3:J:580:TRP:HZ2	1.78	0.49
2:C:80:PHE:HB3	2:C:84:GLU:HB2	1.94	0.49
2:C:298:ALA:N	2:C:334:GLU:O	2.35	0.49
2:C:402:ARG:NE	2:C:417:SER:O	2.46	0.49
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.43	0.49
3:D:392:THR:HG21	5:F:606:VAL:HA	1.95	0.49
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.44	0.49
2:I:1066:MET:HG2	2:I:1234:LYS:HA	1.95	0.49
6:N:25:GLN:O	6:N:27:ILE:N	2.42	0.49
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.48	0.49
1:B:35:PHE:HA	1:B:38:THR:CG2	2.43	0.49
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.94	0.49
4:E:15:ASN:HB3	4:E:18:ASP:H	1.77	0.49
1:G:102:LEU:HD11	1:G:110:VAL:HG11	1.95	0.49
2:I:91:THR:HG21	2:I:503:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.95	0.49
3:J:48:THR:C	3:J:50:LYS:H	2.12	0.49
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.95	0.49
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.94	0.49
1:A:76:GLU:N	1:A:76:GLU:OE2	2.46	0.49
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.94	0.49
2:C:131:THR:OG1	2:C:135:THR:O	2.28	0.49
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.48	0.49
1:H:60:GLU:HA	1:H:171:LEU:HD12	1.94	0.49
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.48	0.49
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.13	0.49
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.95	0.49
5:F:532:LEU:O	5:F:536:THR:HG23	2.13	0.49
5:F:552:THR:OG1	5:F:554:ARG:HG2	2.13	0.49
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.78	0.49
2:I:202:ARG:HB2	2:I:369:MET:HG2	1.94	0.49
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.77	0.49
3:J:425:ARG:HG2	3:J:426:ALA:H	1.77	0.49
6:M:20:ILE:HG22	6:M:24:ARG:HE	1.78	0.49
6:M:48:ARG:NH1	6:M:59:VAL:HB	2.27	0.49
6:M:63:ALA:O	6:M:64:TYR:C	2.51	0.49
1:A:115:ILE:HG22	1:A:116:THR:N	2.28	0.48
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.93	0.48
2:C:796:LEU:H	2:C:796:LEU:HD12	1.77	0.48
1:G:45:ARG:HH22	1:H:37:HIS:CB	2.25	0.48
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.48	0.48
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.95	0.48
3:J:903:LEU:HD21	3:J:913:GLU:OE1	2.12	0.48
5:L:166:VAL:O	5:L:167:ASP:HB2	2.13	0.48
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.96	0.48
2:C:520:PRO:HB3	2:C:714:VAL:HG21	1.94	0.48
2:C:998:LEU:H	2:C:998:LEU:HD12	1.79	0.48
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.95	0.48
1:H:49:SER:O	1:H:151:GLY:HA2	2.13	0.48
2:I:737:ASN:O	2:I:741:MET:HB2	2.13	0.48
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.78	0.48
5:L:343:LYS:O	5:L:347:ILE:HG13	2.13	0.48
1:B:6:THR:OG1	1:B:7:GLU:N	2.41	0.48
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.12	0.48
5:F:279:ARG:HB3	5:F:347:ILE:HD11	1.95	0.48
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.53	0.48
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.95	0.48
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	1.95	0.48
5:F:363:ARG:O	5:F:367:ILE:HG13	2.14	0.48
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.49	0.48
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.48	0.48
2:C:138:ILE:O	2:C:139:ASN:ND2	2.46	0.48
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.48	0.48
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.48
1:A:266:SER:HB3	1:A:303:ILE:HD11	1.95	0.48
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.49	0.48
2:C:620:ASN:ND2	2:C:620:ASN:O	2.46	0.48
2:C:739:ASP:N	2:C:739:ASP:OD1	2.46	0.48
3:D:1285:VAL:HG23	3:D:1286:LYS:HG3	1.94	0.48
4:E:49:ILE:O	4:E:53:GLU:HG3	2.13	0.48
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.29	0.48
2:I:453:ILE:HD12	2:I:587:LEU:HG	1.96	0.48
2:I:812:PHE:O	3:J:504:GLN:NE2	2.45	0.48
2:I:1156:ARG:HB2	2:I:1156:ARG:HH11	1.78	0.48
2:I:1253:LEU:HD11	3:J:253:VAL:HG11	1.96	0.48
3:J:519:ASN:HB2	3:J:709:ARG:HB2	1.96	0.48
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.27	0.48
5:L:489:MET:O	5:L:491:GLU:N	2.47	0.48
6:N:52:PHE:HB2	6:N:55:VAL:HG23	1.95	0.48
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.44	0.48
2:C:192:ASP:HB3	2:C:346:TYR:CE1	2.49	0.48
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.48	0.48
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.95	0.48
2:C:861:ALA:HB1	2:C:882:ILE:HD13	1.96	0.48
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.78	0.48
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.96	0.48
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.49	0.48
3:D:905:ARG:NH1	4:E:16:ARG:HB2	2.29	0.48
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.28	0.48
2:I:18:ARG:HH12	2:I:622:ASN:HA	1.78	0.48
2:I:198:ILE:O	2:I:201:ARG:HB2	2.14	0.48
3:J:148:GLU:H	3:J:156:ARG:HG3	1.79	0.48
3:J:489:ASN:HA	3:J:904:ALA:CB	2.44	0.48
2:C:566:GLY:O	2:C:569:ILE:HG13	2.14	0.48
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.48
3:D:793:SER:O	3:D:797:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.49	0.48
3:D:1158:GLU:HG3	3:D:1186:TYR:CZ	2.48	0.48
5:F:483:LEU:H	5:F:483:LEU:HD12	1.79	0.48
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.95	0.48
1:A:163:GLU:O	1:A:164:ASP:HB2	2.12	0.48
2:C:53:PHE:CZ	2:C:98:VAL:HG21	2.49	0.48
2:C:1111:GLN:HB2	2:C:1230:MET:HE1	1.96	0.48
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.27	0.48
3:D:154:LEU:HD22	3:D:160:LEU:HD11	1.96	0.48
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.96	0.48
2:I:61:SER:O	2:I:63:SER:N	2.47	0.48
2:I:616:ILE:HG22	2:I:617:ALA:O	2.14	0.48
2:I:872:TYR:HA	2:I:944:ARG:HH12	1.79	0.48
3:J:429:LEU:HD13	3:J:429:LEU:HA	1.73	0.48
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.14	0.48
3:J:1156:LEU:HA	3:J:1208:ASP:O	2.13	0.48
5:L:338:HIS:CE1	5:L:341:LEU:HD13	2.49	0.48
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.14	0.48
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.49	0.48
1:B:81:ILE:O	1:B:85:LEU:HG	2.14	0.48
2:C:209:ILE:HD13	2:C:425:ILE:HG21	1.96	0.48
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.94	0.48
2:C:691:PRO:HA	2:C:788:SER:OG	2.14	0.48
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.47	0.48
3:D:678:ARG:O	3:D:682:VAL:HG23	2.14	0.48
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.96	0.48
5:F:562:ARG:HH21	5:F:573:LEU:HD23	1.78	0.48
1:G:89:ALA:HB1	1:G:210:THR:HG23	1.96	0.48
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.96	0.48
6:M:68:GLN:HA	6:M:71:HIS:HD2	1.77	0.48
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.76	0.47
3:D:598:LYS:O	3:D:601:ILE:HG22	2.14	0.47
1:G:51:MET:HE1	1:G:216:ALA:HA	1.96	0.47
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.13	0.47
3:J:883:ARG:HB3	3:J:898:CYS:SG	2.54	0.47
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.95	0.47
2:C:68:LEU:HD11	2:C:100:LEU:HB3	1.95	0.47
2:C:421:SER:H	2:C:424:ASP:HB2	1.79	0.47
2:C:551:HIS:H	2:C:554:HIS:CD2	2.31	0.47
3:D:835:LEU:O	3:D:839:VAL:HG23	2.13	0.47
5:F:281:ARG:O	5:F:285:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.71	0.47
2:I:518:ASN:OD1	2:I:518:ASN:N	2.46	0.47
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.47	0.47
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.95	0.47
2:C:719:LYS:O	2:C:779:ARG:HG3	2.14	0.47
3:D:365:GLN:O	3:D:437:PHE:HD1	1.97	0.47
5:F:348:GLU:HG2	5:F:354:THR:HA	1.96	0.47
2:I:119:GLU:HG3	2:I:488:MET:HB3	1.96	0.47
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.95	0.47
5:L:476:ARG:HB3	5:L:476:ARG:HH11	1.79	0.47
2:C:1164:PHE:HD1	2:C:1164:PHE:HA	1.56	0.47
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.45	0.47
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.44	0.47
3:J:342:LEU:HA	3:J:343:LEU:HA	1.66	0.47
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.96	0.47
3:J:649:LYS:O	3:J:653:ILE:HG13	2.14	0.47
3:D:74:LYS:HD2	3:D:87:LYS:HZ3	1.80	0.47
3:D:664:ILE:HG21	3:D:681:LYS:HB3	1.97	0.47
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.97	0.47
3:J:56:LEU:HD12	3:J:56:LEU:H	1.79	0.47
3:J:1203:ARG:NH2	3:J:1205:GLU:HG2	2.30	0.47
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.30	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.75	0.47
2:C:468:LEU:O	2:C:472:GLU:N	2.41	0.47
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.44	0.47
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.49	0.47
3:D:48:THR:C	3:D:50:LYS:H	2.17	0.47
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.95	0.47
3:D:1257:VAL:HA	3:D:1260:MET:HG3	1.95	0.47
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.95	0.47
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.96	0.47
2:I:1276:TRP:CH2	3:J:798:ARG:HG3	2.41	0.47
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.97	0.47
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.45	0.47
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.95	0.47
1:A:80:GLU:O	1:A:84:ASN:ND2	2.48	0.47
2:C:245:ARG:HG2	2:C:337:PHE:CE2	2.49	0.47
2:C:363:LEU:C	2:C:381:ALA:HB1	2.35	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.49	0.47
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.80	0.47
3:D:384:LYS:HD2	3:D:387:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:425:ARG:HG2	3:D:426:ALA:N	2.29	0.47
3:D:504:GLN:HG3	3:D:505:ASP:H	1.79	0.47
3:D:901:ARG:HD2	3:D:906:GLY:O	2.15	0.47
5:F:608:ARG:HB2	5:F:608:ARG:HH11	1.80	0.47
1:G:75:GLN:HA	2:I:729:ALA:N	2.30	0.47
1:G:167:PRO:HB2	1:G:170:ARG:HG3	1.96	0.47
1:H:153:VAL:HG11	1:H:158:ARG:HH11	1.79	0.47
2:I:564:PRO:HA	2:I:684:ASN:HD21	1.79	0.47
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.95	0.47
2:I:1283:ALA:HB1	2:I:1286:THR:HB	1.97	0.47
2:I:1327:LEU:HG	2:I:1337:ILE:HG23	1.96	0.47
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.15	0.47
4:K:19:LEU:HD13	4:K:54:ILE:HG21	1.95	0.47
4:K:50:ALA:O	4:K:54:ILE:HG12	2.14	0.47
2:C:104:ILE:O	2:C:113:THR:HA	2.15	0.47
2:C:730:SER:O	2:C:753:LEU:HB2	2.15	0.47
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.76	0.47
1:G:56:VAL:HG11	1:G:85:LEU:HB3	1.96	0.47
1:H:102:LEU:HD11	1:H:130:ILE:HG21	1.97	0.47
2:I:601:ASP:OD1	2:I:601:ASP:N	2.45	0.47
2:I:617:ALA:HA	2:I:636:CYS:SG	2.55	0.47
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.50	0.47
3:J:1347:LEU:HD12	3:J:1358:PRO:HG2	1.97	0.47
6:M:33:PRO:HG3	6:M:54:GLY:HA2	1.96	0.47
6:N:9:TYR:O	6:N:12:THR:OG1	2.18	0.47
6:N:25:GLN:C	6:N:27:ILE:H	2.18	0.47
6:N:48:ARG:HB3	6:N:55:VAL:HG11	1.97	0.47
6:N:63:ALA:HB1	6:N:67:ARG:NE	2.30	0.47
1:A:228:LEU:HD21	1:B:43:LEU:HD11	1.97	0.47
2:C:15:PHE:CE1	2:C:1194:GLU:HB3	2.50	0.47
2:C:105:TYR:CE1	2:C:111:GLU:HB3	2.50	0.47
2:C:247:ARG:CZ	2:C:274:ILE:HD12	2.45	0.47
3:D:689:ALA:O	3:D:693:VAL:HG23	2.15	0.47
1:G:31:LEU:HD12	1:G:201:LEU:HB2	1.97	0.47
3:J:128:LEU:HB3	3:J:157:GLN:HE22	1.80	0.47
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.14	0.47
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.97	0.47
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.47
3:D:609:TYR:CE2	3:D:614:LEU:HD12	2.49	0.47
5:F:101:TYR:HE2	5:F:388:ILE:HD11	1.80	0.47
1:G:31:LEU:HD23	1:G:31:LEU:HA	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.97	0.47
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.80	0.47
3:J:172:PHE:HB3	3:J:175:GLU:OE2	2.15	0.47
5:L:233:ASP:O	5:L:236:LYS:HE2	2.14	0.47
1:A:22:THR:O	1:A:207:THR:N	2.36	0.46
3:D:53:ARG:HA	3:D:54:ASP:HA	1.58	0.46
3:D:687:ALA:HB1	6:M:24:ARG:CZ	2.46	0.46
1:G:83:LEU:HD23	2:I:694:ARG:NE	2.27	0.46
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.97	0.46
6:M:48:ARG:HD3	6:M:59:VAL:HG23	1.96	0.46
2:C:5:TYR:O	2:C:8:LYS:HG2	2.15	0.46
2:C:213:LEU:HD13	2:C:422:LYS:HG2	1.96	0.46
2:C:685:MET:HE1	2:C:1071:GLY:HA2	1.97	0.46
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.80	0.46
2:I:607:SER:OG	2:I:609:ILE:HG13	2.15	0.46
2:I:1272:GLU:HB2	3:J:342:LEU:CB	2.45	0.46
2:I:1285:TYR:CD1	3:J:475:GLU:HG2	2.50	0.46
2:I:1287:LEU:HD22	3:J:1357:ILE:CG1	2.42	0.46
3:J:518:VAL:HG12	3:J:707:ILE:HD13	1.97	0.46
3:J:709:ARG:NE	3:J:710:ASP:OD2	2.48	0.46
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.51	0.46
3:D:13:LYS:HA	3:D:13:LYS:HD3	1.75	0.46
3:D:291:ILE:HG23	5:F:406:GLN:HE22	1.80	0.46
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.31	0.46
4:E:15:ASN:C	4:E:17:PHE:H	2.19	0.46
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.97	0.46
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.63	0.46
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.31	0.46
3:J:716:GLN:HG3	3:J:717:VAL:O	2.16	0.46
3:J:733:SER:O	3:J:737:ILE:HG12	2.15	0.46
2:C:882:ILE:HD12	2:C:882:ILE:H	1.80	0.46
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.96	0.46
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.51	0.46
3:D:255:LEU:HD13	3:D:255:LEU:HA	1.79	0.46
3:D:500:ILE:HG22	3:D:500:ILE:O	2.15	0.46
1:G:13:LEU:HD23	1:G:13:LEU:H	1.80	0.46
1:G:152:TYR:CZ	2:I:824:GLN:HA	2.50	0.46
2:I:465:ARG:O	2:I:469:VAL:HG13	2.16	0.46
3:J:615:LYS:HE2	3:J:616:PRO:HD3	1.98	0.46
1:A:54:CYS:HB3	1:A:148:ARG:HB2	1.97	0.46
2:C:222:ASP:HA	2:C:227:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:PHE:CB	2:C:336:LEU:HD22	2.45	0.46
2:C:541:GLU:OE1	2:C:541:GLU:N	2.49	0.46
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.81	0.46
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.30	0.46
3:D:311:ARG:NH2	3:D:1329:THR:HG21	2.31	0.46
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.96	0.46
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.31	0.46
2:I:215:TYR:HD1	2:I:219:GLN:HB3	1.80	0.46
2:I:960:LEU:HB3	2:I:1025:PHE:CE2	2.51	0.46
3:J:358:GLY:N	3:J:359:PRO:HD3	2.30	0.46
3:J:559:ALA:HB3	3:J:562:GLU:HB3	1.98	0.46
3:J:801:VAL:O	3:J:805:GLN:HB2	2.16	0.46
3:J:1290:ARG:HD2	3:J:1295:ASN:HD22	1.81	0.46
6:N:35:TYR:OH	6:N:46:GLU:HG2	2.16	0.46
1:A:179:PRO:HA	1:A:208:ASN:ND2	2.30	0.46
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.51	0.46
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.46	0.46
3:D:572:THR:OG1	3:D:576:ARG:HB2	2.16	0.46
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.51	0.46
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	1.97	0.46
3:J:580:TRP:HH2	3:J:587:LEU:O	1.97	0.46
3:J:683:ILE:HD11	3:J:754:ILE:HG23	1.97	0.46
2:C:296:VAL:O	2:C:335:THR:HA	2.16	0.46
2:C:452:ARG:HH12	2:C:585:GLY:HA3	1.81	0.46
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.81	0.46
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.97	0.46
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	2.31	0.46
3:D:1178:THR:HG23	3:D:1184:ASP:HB3	1.98	0.46
2:I:617:ALA:HB3	2:I:653:MET:HB2	1.98	0.46
2:I:996:ARG:NH1	2:I:999:GLU:OE1	2.39	0.46
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.98	0.46
3:J:513:MET:O	3:J:575:GLY:HA3	2.16	0.46
3:J:848:VAL:HG21	3:J:880:VAL:HG22	1.97	0.46
3:J:1257:VAL:HA	3:J:1260:MET:HG3	1.98	0.46
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.98	0.46
5:L:584:ARG:HA	5:L:584:ARG:HD2	1.78	0.46
1:B:56:VAL:HG21	1:B:144:ILE:HD11	1.97	0.46
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.48	0.46
2:C:228:VAL:HB	2:C:335:THR:OG1	2.15	0.46
2:C:263:VAL:HG21	2:C:273:HIS:CG	2.51	0.46
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1304:MET:HE2	3:D:472:LEU:HB3	1.98	0.46
3:D:405:GLU:O	3:D:408:VAL:HG22	2.15	0.46
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.16	0.46
2:I:13:LYS:NZ	2:I:1151:LEU:HB2	2.30	0.46
2:I:688:GLN:OE1	2:I:1237:HIS:HE1	1.99	0.46
3:J:587:LEU:HD23	3:J:591:ILE:HG21	1.97	0.46
3:J:667:GLN:NE2	6:N:51:ILE:HD11	2.30	0.46
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.97	0.46
6:M:45:PRO:HD2	6:M:48:ARG:NH2	2.31	0.46
1:A:158:ARG:NH2	1:A:172:LEU:HB3	2.30	0.46
1:A:232:VAL:O	1:B:218:ARG:HA	2.16	0.46
3:D:27:PRO:O	3:D:31:ARG:HG3	2.16	0.46
3:D:310:GLY:CA	3:D:314:ARG:HH11	2.29	0.46
3:D:697:MET:SD	3:D:741:ALA:HB3	2.56	0.46
3:D:1273:ASP:O	3:D:1275:LEU:N	2.47	0.46
1:G:137:ASN:OD1	1:G:137:ASN:N	2.43	0.46
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.46	0.46
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.96	0.46
3:J:515:ARG:NH2	3:J:717:VAL:O	2.48	0.46
1:A:59:VAL:HG22	1:A:144:ILE:HG12	1.99	0.46
1:A:195:ARG:HD2	1:A:196:THR:H	1.81	0.46
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.51	0.46
2:C:1149:TYR:CB	2:C:1159:VAL:HG21	2.46	0.46
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.81	0.46
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.30	0.46
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.98	0.46
1:G:62:ASP:HB2	1:G:141:SER:O	2.16	0.46
1:G:219:ARG:HA	1:G:222:THR:HB	1.98	0.46
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.80	0.46
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.98	0.46
3:J:258:GLY:HA3	5:L:499:LYS:HE2	1.96	0.46
1:A:195:ARG:HG3	1:A:198:LEU:HD11	1.98	0.45
1:B:194:GLN:NE2	3:D:406:ALA:HB2	2.30	0.45
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.97	0.45
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.98	0.45
5:F:309:ASN:ND2	5:F:312:SER:HB3	2.29	0.45
1:H:62:ASP:OD1	1:H:62:ASP:N	2.31	0.45
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.44	0.45
3:J:205:LEU:CD2	3:J:214:ARG:HB2	2.46	0.45
3:J:322:ARG:HG3	3:J:323:PRO:HD2	1.98	0.45
3:J:680:ASN:HD22	6:N:27:ILE:HD11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:HG2	1:A:13:LEU:H	1.82	0.45
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.97	0.45
2:C:681:MET:HE2	2:C:1073:LYS:HD2	1.98	0.45
2:C:733:VAL:CG1	2:C:748:ILE:HG13	2.45	0.45
3:D:194:LEU:O	3:D:198:CYS:N	2.45	0.45
3:D:746:LEU:HB3	3:D:754:ILE:HD11	1.98	0.45
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.98	0.45
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.97	0.45
5:F:461:ASN:O	5:F:465:ARG:HG2	2.15	0.45
1:G:9:LEU:HD13	1:G:32:GLU:HG2	1.98	0.45
1:H:98:VAL:O	1:H:146:VAL:HG22	2.15	0.45
1:H:155:ALA:HB2	1:H:174:ASP:N	2.31	0.45
2:I:80:PHE:HB3	2:I:84:GLU:HB2	1.97	0.45
2:I:107:ARG:HA	2:I:108:GLU:HA	1.65	0.45
3:J:849:LEU:H	3:J:849:LEU:HD22	1.81	0.45
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.97	0.45
2:C:247:ARG:HB2	2:C:274:ILE:CD1	2.47	0.45
3:D:197:GLU:O	3:D:201:LEU:HG	2.16	0.45
3:D:672:LEU:HD23	6:M:47:ALA:HB1	1.97	0.45
3:D:680:ASN:O	3:D:683:ILE:HG22	2.17	0.45
3:D:1170:LYS:C	3:D:1172:LYS:H	2.19	0.45
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.16	0.45
4:K:6:VAL:O	4:K:10:VAL:HG23	2.15	0.45
1:B:92:VAL:CG1	1:B:95:LYS:HB3	2.47	0.45
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.99	0.45
2:C:106:GLU:HG3	2:C:107:ARG:N	2.32	0.45
2:C:213:LEU:HD22	2:C:422:LYS:HG2	1.99	0.45
2:C:359:ARG:NH1	2:C:382:GLU:OE2	2.50	0.45
2:C:492:MET:H	2:C:492:MET:HG2	1.61	0.45
3:D:316:ILE:HA	3:D:323:PRO:HA	1.99	0.45
3:D:647:PRO:CG	3:D:697:MET:HB3	2.44	0.45
1:H:102:LEU:HG	1:H:115:ILE:HG12	1.97	0.45
2:I:17:LYS:NZ	2:I:1154:ASP:OD1	2.49	0.45
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.97	0.45
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.17	0.45
3:J:812:ASP:HB2	3:J:911:LYS:HE3	1.99	0.45
3:D:528:THR:O	3:D:551:ARG:HB3	2.17	0.45
5:F:226:ALA:O	5:F:229:VAL:HG22	2.17	0.45
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.32	0.45
2:I:842:ASP:N	2:I:1045:GLY:O	2.49	0.45
3:J:478:LEU:HG	4:K:47:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:810:THR:HG21	3:J:893:GLY:HA3	1.98	0.45
2:C:540:ARG:HB2	2:C:540:ARG:HH11	1.82	0.45
1:G:166:ARG:HH11	1:G:168:ILE:H	1.65	0.45
2:I:13:LYS:HD3	2:I:1149:TYR:HA	1.99	0.45
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.98	0.45
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.50	0.45
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.32	0.45
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.81	0.45
1:A:252:ILE:HG21	1:A:312:LEU:HD11	1.98	0.45
1:B:98:VAL:O	1:B:146:VAL:HG13	2.17	0.45
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.97	0.45
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.47	0.45
2:C:1296:ASP:HB3	2:C:1320:PRO:HB3	1.99	0.45
3:D:903:LEU:HD23	3:D:905:ARG:HD3	1.99	0.45
3:D:1301:THR:HA	3:J:1297:LYS:HE2	1.99	0.45
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.17	0.45
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	1.98	0.45
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.75	0.45
3:J:1173:ARG:HB2	3:J:1192:LYS:HB3	1.99	0.45
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.32	0.45
2:C:247:ARG:HH22	2:C:271:ALA:HA	1.82	0.45
3:D:495:ASN:C	3:D:497:GLU:H	2.18	0.45
3:D:735:ALA:O	3:D:738:ARG:HB3	2.16	0.45
3:D:770:LEU:H	3:D:770:LEU:HD22	1.80	0.45
3:D:826:ILE:HD12	3:D:826:ILE:O	2.17	0.45
3:J:69:GLU:HG3	3:J:76:LYS:HG2	1.97	0.45
3:J:186:GLN:HB2	3:J:238:ILE:HG21	1.99	0.45
3:J:279:LEU:HD12	3:J:295:GLU:HG3	1.99	0.45
3:J:902:ASP:OD1	3:J:903:LEU:N	2.50	0.45
2:C:601:ASP:OD1	2:C:601:ASP:N	2.49	0.45
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.45	0.45
3:J:317:THR:HG22	3:J:322:ARG:O	2.17	0.45
3:J:740:LEU:HA	3:J:763:PHE:HB2	1.99	0.45
3:J:826:ILE:HD12	3:J:826:ILE:O	2.17	0.45
6:N:48:ARG:CZ	6:N:59:VAL:H	2.29	0.45
1:B:22:THR:OG1	1:B:207:THR:O	2.35	0.45
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.31	0.45
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.45
2:C:1187:PHE:HZ	3:D:772:TYR:HD2	1.65	0.45
3:D:529:GLY:HA2	3:D:551:ARG:O	2.17	0.45
5:F:608:ARG:HH11	5:F:608:ARG:CG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:THR:HG21	1:H:46:ILE:HG13	1.99	0.45
2:I:548:ARG:NH2	2:I:567:PRO:O	2.50	0.45
2:I:1106:ARG:O	2:I:1108:ASN:N	2.44	0.45
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.42	0.45
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.43	0.45
5:L:161:LEU:C	5:L:262:VAL:HG23	2.37	0.45
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.30	0.45
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.16	0.45
5:L:513:ASP:C	5:L:515:GLU:H	2.19	0.45
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.99	0.44
2:I:160:ASP:HB3	2:I:164:THR:HG21	1.99	0.44
2:I:1244:HIS:HD2	2:I:1265:PHE:HB2	1.82	0.44
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.82	0.44
2:C:395:TYR:CD2	2:C:419:ILE:HG22	2.52	0.44
2:C:1062:PRO:HA	2:C:1076:ILE:HG13	1.97	0.44
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.99	0.44
3:D:45:ASN:O	3:D:46:TYR:HD2	2.00	0.44
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.98	0.44
3:D:342:LEU:HA	3:D:343:LEU:HA	1.69	0.44
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.68	0.44
3:D:480:ALA:HA	3:D:484:MET:HG3	1.98	0.44
3:D:1167:LYS:HE3	3:D:1174:ARG:HD2	1.98	0.44
1:G:71:LYS:HE2	1:G:139:SER:O	2.17	0.44
1:G:97:GLU:OE2	1:G:145:LYS:HE2	2.16	0.44
1:H:85:LEU:HD23	1:H:85:LEU:HA	1.84	0.44
2:I:151:ARG:HH22	2:I:175:ARG:HH11	1.64	0.44
2:I:596:ASP:CG	2:I:597:GLY:N	2.69	0.44
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	2.00	0.44
3:J:161:THR:H	3:J:164:GLN:HB2	1.82	0.44
3:J:590:SER:HA	3:J:593:ASN:HB2	1.98	0.44
4:K:14:GLY:C	4:K:16:ARG:H	2.20	0.44
5:L:380:VAL:HG13	5:L:412:LEU:HD23	1.99	0.44
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.52	0.44
1:B:71:LYS:HA	1:B:71:LYS:HD2	1.77	0.44
1:B:178:SER:HA	1:B:179:PRO:HD3	1.86	0.44
2:C:1253:LEU:CD1	3:D:253:VAL:HG11	2.45	0.44
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.52	0.44
1:G:152:TYR:CG	2:I:824:GLN:HG2	2.52	0.44
2:I:29:SER:O	2:I:33:ASP:HB2	2.17	0.44
2:I:211:ARG:NH1	2:I:357:ASN:O	2.51	0.44
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:503:LYS:HA	2:I:503:LYS:HD2	1.74	0.44
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.32	0.44
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.17	0.44
3:J:264:ASP:HB3	3:J:324:LEU:HB2	1.99	0.44
3:J:650:LYS:HZ2	3:J:762:ASN:HD22	1.65	0.44
3:J:689:ALA:O	3:J:693:VAL:HG23	2.16	0.44
5:L:461:ASN:HB3	5:L:465:ARG:NH2	2.32	0.44
5:L:515:GLU:HG2	5:L:516:ASP:H	1.82	0.44
6:N:20:ILE:HG22	6:N:24:ARG:HE	1.82	0.44
6:N:45:PRO:HD2	6:N:48:ARG:CZ	2.47	0.44
1:B:54:CYS:SG	1:B:148:ARG:HG3	2.58	0.44
2:C:117:ILE:H	2:C:117:ILE:HG12	1.61	0.44
2:C:145:ILE:HA	2:C:511:LEU:O	2.18	0.44
2:C:533:LEU:HD11	2:C:540:ARG:HD2	1.99	0.44
2:C:737:ASN:O	2:C:741:MET:HB2	2.17	0.44
2:C:1298:VAL:HG11	3:D:96:LYS:NZ	2.33	0.44
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.32	0.44
3:D:262:THR:HG1	3:D:266:ASN:ND2	2.15	0.44
1:G:73:GLY:C	1:G:134:THR:HG22	2.37	0.44
1:H:84:ASN:O	1:H:128:HIS:HE1	2.01	0.44
3:J:50:LYS:HD3	3:J:71:LEU:HD21	2.00	0.44
3:J:495:ASN:C	3:J:497:GLU:H	2.21	0.44
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.53	0.44
5:L:478:PRO:HG2	5:L:483:LEU:HD11	2.00	0.44
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.98	0.44
2:C:517:GLN:O	2:C:517:GLN:HG2	2.16	0.44
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.99	0.44
3:D:60:ARG:HA	3:D:89:GLY:O	2.18	0.44
3:D:110:PRO:HB3	3:D:238:ILE:CG2	2.47	0.44
3:D:449:LEU:HD22	3:D:466:MET:SD	2.58	0.44
5:F:134:VAL:HA	5:F:273:MET:HE1	2.00	0.44
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.98	0.44
5:F:530:LEU:HD12	5:F:533:ASP:H	1.82	0.44
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.82	0.44
1:H:59:VAL:HG12	1:H:61:ILE:HD13	1.98	0.44
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.99	0.44
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	2.00	0.44
2:I:1111:GLN:HB2	2:I:1230:MET:CE	2.48	0.44
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.17	0.44
3:J:292:VAL:O	3:J:296:LYS:HG3	2.18	0.44
5:L:463:LEU:HA	5:L:466:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:561:MET:HA	5:L:567:MET:CE	2.45	0.44
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.47	0.44
2:C:666:SER:OG	2:C:704:MET:HG3	2.17	0.44
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.57	0.44
3:D:81:ARG:C	3:D:83:VAL:H	2.20	0.44
4:E:73:GLN:HA	4:E:76:GLU:HB2	2.00	0.44
5:F:166:VAL:O	5:F:167:ASP:HB2	2.17	0.44
1:G:77:ASP:O	1:G:81:ILE:HG13	2.17	0.44
2:I:519:ASN:ND2	2:I:689:ALA:HB3	2.33	0.44
2:I:871:VAL:HG11	2:I:883:LEU:HD22	2.00	0.44
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.98	0.44
3:J:514:THR:O	3:J:514:THR:OG1	2.35	0.44
6:M:4:GLU:C	6:M:6:ASP:H	2.21	0.44
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.99	0.44
1:A:102:LEU:HB3	1:A:142:MET:HG2	2.00	0.44
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.89	0.44
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.17	0.44
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.98	0.44
3:D:215:LYS:HE2	3:D:215:LYS:HB3	1.83	0.44
5:F:372:ALA:O	5:F:376:LYS:HG3	2.17	0.44
5:F:572:THR:HG23	5:F:575:GLU:HG3	2.00	0.44
1:G:89:ALA:HB1	1:G:210:THR:CG2	2.47	0.44
2:I:490:GLN:HG3	5:L:472:GLN:HG3	1.99	0.44
5:L:277:MET:CG	5:L:362:ASN:HD21	2.29	0.44
1:A:166:ARG:NH1	1:A:168:ILE:HG12	2.32	0.44
1:A:239:GLN:HG3	1:A:240:PRO:HD2	2.00	0.44
2:C:62:TYR:HD1	2:C:480:SER:HB2	1.82	0.44
2:C:221:LEU:HD12	2:C:298:ALA:O	2.18	0.44
2:C:528:ARG:NH2	2:C:576:SER:O	2.51	0.44
2:C:949:GLU:HG2	2:C:1036:ILE:CG2	2.48	0.44
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.18	0.44
2:C:1240:ASP:OD1	2:C:1240:ASP:N	2.51	0.44
3:D:128:LEU:HD23	3:D:192:MET:HE3	2.00	0.44
3:D:274:ASN:OD1	5:F:446:GLN:NE2	2.50	0.44
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.51	0.44
2:I:800:MET:O	2:I:1229:TYR:HA	2.18	0.44
3:J:712:GLN:HB2	3:J:713:GLU:H	1.56	0.44
3:J:761:ALA:N	3:J:771:GLN:HE22	2.15	0.44
5:L:372:ALA:O	5:L:376:LYS:HG3	2.18	0.44
6:M:68:GLN:HA	6:M:71:HIS:CD2	2.52	0.44
1:A:162:GLU:HB3	1:A:163:GLU:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:TYR:CD1	2:C:480:SER:HB2	2.53	0.44
2:C:139:ASN:HD22	2:C:139:ASN:HA	1.64	0.44
2:C:363:LEU:HD13	2:C:382:GLU:HA	2.00	0.44
2:C:720:ARG:HH21	2:C:741:MET:HA	1.81	0.44
2:C:1087:TYR:CE1	2:C:1215:GLY:HA2	2.51	0.44
2:C:1187:PHE:CZ	3:D:772:TYR:HD2	2.36	0.44
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.18	0.44
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.00	0.44
3:D:739:GLN:OE1	3:D:744:ARG:HB2	2.17	0.44
2:I:543:ALA:HA	2:I:544:GLY:HA3	1.74	0.44
2:I:700:VAL:HG21	2:I:1114:GLU:HG2	2.00	0.44
2:I:975:ILE:CD1	2:I:998:LEU:HG	2.47	0.44
2:I:1082:ILE:H	2:I:1082:ILE:CD1	2.27	0.44
2:I:1313:HIS:HB2	3:J:474:LEU:HD13	2.00	0.44
3:J:1319:PHE:HB3	3:J:1340:LYS:CD	2.48	0.44
1:A:38:THR:HG1	1:B:45:ARG:NH1	2.16	0.43
1:B:195:ARG:CB	1:B:198:LEU:HD21	2.48	0.43
2:C:247:ARG:NH2	2:C:274:ILE:HD12	2.32	0.43
3:D:1283:SER:O	3:D:1286:LYS:N	2.50	0.43
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.83	0.43
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.00	0.43
1:G:76:GLU:OE2	1:G:76:GLU:N	2.51	0.43
2:I:891:GLY:O	2:I:892:GLU:HG3	2.17	0.43
3:J:650:LYS:NZ	3:J:762:ASN:HD22	2.17	0.43
3:J:678:ARG:HG3	3:J:679:TYR:N	2.32	0.43
3:J:682:VAL:O	3:J:685:ILE:HG12	2.18	0.43
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.46	0.43
1:A:88:LEU:HA	1:A:128:HIS:CD2	2.53	0.43
3:D:147:ILE:HG13	3:D:147:ILE:O	2.18	0.43
3:D:251:PRO:HD2	5:F:507:MET:SD	2.58	0.43
3:D:279:LEU:HD12	3:D:295:GLU:HG3	2.00	0.43
3:D:1344:LEU:O	3:D:1346:GLY:N	2.43	0.43
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.53	0.43
2:I:150:HIS:CE1	2:I:454:ARG:HH21	2.36	0.43
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.52	0.43
2:I:693:LEU:HD12	2:I:829:THR:HB	2.00	0.43
3:J:53:ARG:HA	3:J:54:ASP:HA	1.55	0.43
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.99	0.43
3:J:779:ALA:HA	6:N:12:THR:HG21	2.00	0.43
3:J:782:GLY:CA	6:N:12:THR:HG22	2.43	0.43
1:A:112:ALA:O	1:A:115:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.51	0.43
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.33	0.43
1:G:57:THR:HG22	1:G:58:GLU:HG3	2.00	0.43
2:I:42:ASP:O	2:I:44:GLU:N	2.44	0.43
2:I:151:ARG:NH2	2:I:175:ARG:HD2	2.34	0.43
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.99	0.43
5:L:280:VAL:O	5:L:284:GLU:HG3	2.18	0.43
6:M:33:PRO:HB2	6:M:34:VAL:H	1.67	0.43
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.53	0.43
1:A:316:MET:SD	5:F:600:HIS:CE1	3.12	0.43
2:C:577:VAL:HG23	2:C:661:VAL:O	2.18	0.43
2:C:1066:MET:HG2	2:C:1234:LYS:HA	2.00	0.43
3:D:137:ARG:HD3	3:D:143:SER:HB2	2.00	0.43
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.77	0.43
3:D:812:ASP:HB2	3:D:911:LYS:HE3	2.00	0.43
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.85	0.43
2:I:1124:ILE:HG21	2:I:1180:MET:CE	2.48	0.43
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.89	0.43
3:J:425:ARG:HB2	3:J:466:MET:HG2	2.00	0.43
4:K:31:GLN:HB2	4:K:46:THR:HG21	2.01	0.43
5:L:573:LEU:H	5:L:573:LEU:CD2	2.29	0.43
1:A:49:SER:O	1:A:51:MET:N	2.50	0.43
1:B:104:LYS:HG2	1:B:110:VAL:HG13	2.00	0.43
2:C:107:ARG:HA	2:C:108:GLU:HA	1.38	0.43
2:C:131:THR:H	2:C:131:THR:HG1	1.42	0.43
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.18	0.43
3:D:161:THR:HG23	3:D:164:GLN:H	1.84	0.43
3:D:824:PRO:HD3	3:D:835:LEU:HB2	2.01	0.43
5:F:276:MET:O	5:F:280:VAL:HG23	2.18	0.43
1:H:152:TYR:CZ	3:J:536:LEU:HD21	2.53	0.43
2:I:582:ASN:HB3	2:I:586:PHE:H	1.83	0.43
2:I:896:THR:HB	2:I:897:PRO:HD2	2.01	0.43
3:J:850:LYS:HB2	3:J:852:GLY:O	2.18	0.43
5:L:230:VAL:HG22	5:L:248:GLU:OE2	2.18	0.43
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.81	0.43
6:M:48:ARG:CZ	6:M:59:VAL:H	2.32	0.43
1:A:315:GLY:C	1:A:316:MET:HG3	2.39	0.43
1:B:134:THR:OG1	1:B:135:ASP:N	2.50	0.43
3:D:19:ALA:HB2	3:D:1373:ARG:NH2	2.33	0.43
3:D:489:ASN:HA	3:D:904:ALA:CB	2.44	0.43
5:F:127:ILE:O	5:F:130:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:445:ASP:OD2	5:F:451:ARG:HD2	2.18	0.43
2:I:5:TYR:O	2:I:8:LYS:HG2	2.18	0.43
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.89	0.43
2:I:149:LEU:HB2	2:I:530:ILE:HG22	2.00	0.43
2:I:1129:ASN:CB	2:I:1177:ARG:HB2	2.47	0.43
3:J:159:ILE:O	3:J:159:ILE:HG13	2.18	0.43
3:J:1266:ILE:HD11	3:J:1276:GLU:HB2	2.01	0.43
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.19	0.43
3:J:1344:LEU:O	3:J:1346:GLY:N	2.43	0.43
1:B:191:ARG:O	1:B:191:ARG:HG2	2.18	0.43
2:C:136:PHE:HE2	2:C:456:VAL:HG11	1.83	0.43
2:C:607:SER:OG	2:C:609:ILE:HG13	2.19	0.43
2:C:830:THR:HG23	2:C:832:HIS:NE2	2.33	0.43
3:D:81:ARG:HG3	3:D:82:GLY:H	1.84	0.43
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.52	0.43
3:D:1166:GLY:O	3:D:1174:ARG:HB2	2.18	0.43
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.84	0.43
5:F:456:MET:HE1	5:F:497:VAL:HG13	2.00	0.43
1:H:35:PHE:HA	1:H:38:THR:HG22	2.00	0.43
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.54	0.43
3:J:19:ALA:HB2	3:J:1373:ARG:NH2	2.33	0.43
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.54	0.43
3:J:1170:LYS:C	3:J:1172:LYS:H	2.22	0.43
5:L:119:ILE:HG23	5:L:375:ALA:HB1	2.00	0.43
1:A:159:ILE:HG13	1:A:162:GLU:HG3	2.01	0.43
2:C:42:ASP:C	2:C:44:GLU:H	2.22	0.43
2:C:178:PRO:HG3	2:C:395:TYR:CE1	2.54	0.43
2:C:230:PHE:CE1	2:C:239:MET:HB2	2.54	0.43
2:C:560:PRO:O	3:D:780:ARG:NH2	2.49	0.43
2:C:670:PHE:CD1	2:C:1113:LEU:HD23	2.53	0.43
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.53	0.43
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.00	0.43
3:D:733:SER:O	3:D:737:ILE:HG12	2.17	0.43
3:D:860:ARG:HD2	3:D:860:ARG:HA	1.83	0.43
3:D:1168:GLU:O	3:D:1170:LYS:N	2.52	0.43
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.70	0.43
2:I:565:GLU:HG2	2:I:565:GLU:O	2.19	0.43
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.34	0.43
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.79	0.43
3:J:827:GLU:HB3	3:J:832:LYS:HD2	2.00	0.43
2:C:17:LYS:NZ	2:C:1194:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:247:ARG:HB2	2:C:274:ILE:HD11	2.01	0.43
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	2.00	0.43
2:I:97:ARG:HB3	2:I:121:GLU:HB3	2.00	0.43
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.59	0.43
3:J:785:ASP:OD2	6:N:15:LEU:HD11	2.19	0.43
3:J:923:ILE:O	3:J:926:PRO:HD2	2.19	0.43
6:M:9:TYR:O	6:M:12:THR:OG1	2.21	0.43
1:A:57:THR:O	1:A:158:ARG:NH2	2.51	0.43
1:A:104:LYS:HD3	1:A:114:ASP:OD2	2.19	0.43
1:A:211:ILE:CG2	1:A:216:ALA:HB2	2.48	0.43
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.92	0.43
2:C:856:ASN:ND2	2:C:908:GLU:OE1	2.52	0.43
2:C:886:LYS:H	2:C:917:SER:HB3	1.84	0.43
3:D:682:VAL:O	3:D:685:ILE:HG12	2.19	0.43
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.83	0.43
3:D:1183:SER:HA	3:J:206:ASN:ND2	2.33	0.43
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.86	0.43
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.19	0.43
2:I:93:SER:HB2	2:I:126:GLU:HB3	2.00	0.43
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.00	0.43
3:J:865:HIS:HE1	3:J:867:GLN:HB2	1.84	0.43
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.33	0.43
3:J:1165:PHE:HE1	3:J:1200:GLU:HB2	1.83	0.43
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.68	0.43
6:N:48:ARG:NH2	6:N:58:CYS:HA	2.34	0.43
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.84	0.42
1:A:284:ARG:HG3	1:A:288:GLU:HG3	2.01	0.42
2:C:209:ILE:HG13	2:C:385:PHE:CE1	2.54	0.42
2:C:519:ASN:ND2	2:C:796:LEU:HD23	2.33	0.42
2:C:519:ASN:HD22	2:C:689:ALA:HB3	1.83	0.42
3:D:292:VAL:O	3:D:296:LYS:HG3	2.18	0.42
3:D:702:GLN:O	3:D:718:SER:N	2.38	0.42
4:E:15:ASN:O	4:E:16:ARG:HB3	2.19	0.42
5:F:233:ASP:O	5:F:236:LYS:HE2	2.19	0.42
1:G:22:THR:OG1	1:G:23:HIS:N	2.52	0.42
1:H:183:ILE:HG23	1:H:205:MET:HG3	2.01	0.42
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.83	0.42
3:J:279:LEU:HD23	3:J:283:LEU:HG	2.01	0.42
3:J:482:ALA:HB3	4:K:20:VAL:HG22	2.01	0.42
2:C:135:THR:HG22	2:C:527:LYS:HE2	2.00	0.42
2:C:518:ASN:OD1	2:C:518:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	2.00	0.42
5:F:125:ASP:O	5:F:129:GLN:HG3	2.19	0.42
5:F:310:GLU:O	5:F:344:LEU:HD21	2.19	0.42
1:H:134:THR:HG23	1:H:135:ASP:N	2.28	0.42
1:H:196:THR:HG23	3:J:443:GLU:HG3	2.01	0.42
2:I:55:SER:OG	2:I:56:VAL:N	2.52	0.42
2:I:105:TYR:HD1	2:I:112:GLY:H	1.67	0.42
2:I:151:ARG:HH12	2:I:175:ARG:NH1	2.17	0.42
2:I:1164:PHE:O	2:I:1166:ASP:N	2.53	0.42
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.49	0.42
3:J:528:THR:O	3:J:551:ARG:HB3	2.19	0.42
6:N:20:ILE:HG22	6:N:24:ARG:NE	2.34	0.42
1:A:315:GLY:O	1:A:316:MET:HG3	2.20	0.42
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.62	0.42
2:I:32:LEU:HD23	2:I:130:MET:SD	2.59	0.42
2:I:76:GLY:O	2:I:94:ALA:HB1	2.19	0.42
3:J:511:TYR:CG	3:J:728:SER:HB3	2.55	0.42
3:J:594:GLN:HG3	3:J:596:LEU:HD22	2.00	0.42
3:J:747:MET:HB2	3:J:774:ILE:CG2	2.45	0.42
6:M:48:ARG:HH21	6:M:58:CYS:HA	1.83	0.42
1:A:261:GLU:CD	2:C:859:GLU:HB2	2.39	0.42
2:C:4:SER:OG	2:C:5:TYR:N	2.52	0.42
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	2.00	0.42
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	2.20	0.42
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.51	0.42
2:I:933:VAL:HG22	2:I:1050:VAL:HG13	2.02	0.42
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.34	0.42
3:J:701:LEU:HD22	3:J:701:LEU:HA	1.91	0.42
5:L:547:VAL:HG22	5:L:603:ARG:HD3	2.01	0.42
1:A:73:GLY:O	1:A:134:THR:HG22	2.19	0.42
2:C:229:ILE:CD1	2:C:334:GLU:HG2	2.50	0.42
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.84	0.42
2:C:800:MET:HE3	2:C:800:MET:HB3	1.89	0.42
2:C:813:GLU:HG3	3:D:460:ASP:HA	2.01	0.42
5:F:130:VAL:HB	5:F:365:MET:HG3	2.02	0.42
5:F:449:THR:OG1	5:F:503:GLU:OE1	2.37	0.42
5:F:563:PHE:HB2	5:F:565:ILE:HG13	2.02	0.42
1:G:89:ALA:O	1:G:124:VAL:HG12	2.20	0.42
1:G:197:ASP:O	1:G:198:LEU:HD23	2.20	0.42
3:J:60:ARG:HA	3:J:89:GLY:O	2.19	0.42
3:J:654:ILE:O	3:J:658:GLU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:925:GLU:HB3	3:J:926:PRO:HD3	2.01	0.42
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.89	0.42
1:A:104:LYS:HG3	1:A:105:SER:N	2.33	0.42
2:C:198:ILE:O	2:C:201:ARG:HB2	2.20	0.42
2:C:277:LEU:HD23	2:C:282:VAL:HG21	2.01	0.42
2:C:338:THR:CG2	2:C:345:PRO:HB3	2.49	0.42
2:C:1035:LYS:O	2:C:1038:GLN:HG2	2.20	0.42
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.47	0.42
3:D:1264:ALA:O	3:D:1277:GLY:HA2	2.20	0.42
5:F:448:ARG:HE	5:F:448:ARG:HB3	1.60	0.42
1:H:219:ARG:HA	1:H:222:THR:HB	2.02	0.42
2:I:194:LEU:HD12	2:I:194:LEU:HA	1.79	0.42
3:J:517:CYS:CA	3:J:716:GLN:HE22	2.31	0.42
1:B:151:GLY:O	1:B:177:TYR:HB2	2.20	0.42
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.29	0.42
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.41	0.42
3:D:291:ILE:HD13	5:F:409:ASN:HB3	2.01	0.42
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.84	0.42
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	2.02	0.42
3:J:839:VAL:HG12	3:J:864:LEU:HD12	2.01	0.42
3:J:903:LEU:HD12	3:J:903:LEU:HA	1.83	0.42
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.02	0.42
5:L:557:LYS:HG3	5:L:561:MET:HE3	2.01	0.42
1:A:13:LEU:H	1:A:13:LEU:HD23	1.85	0.42
2:C:417:SER:OG	2:C:419:ILE:O	2.31	0.42
2:C:879:GLY:HA2	2:C:920:VAL:HG12	2.01	0.42
3:D:16:GLU:HA	3:D:16:GLU:OE2	2.20	0.42
3:D:155:GLU:HB2	3:D:158:GLN:HB2	2.01	0.42
3:D:288:PRO:O	3:D:292:VAL:HG13	2.19	0.42
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.95	0.42
3:D:451:PRO:O	3:D:454:CYS:HB2	2.20	0.42
3:D:526:VAL:HA	3:D:549:LYS:O	2.20	0.42
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.34	0.42
1:G:133:LEU:HD12	1:G:138:ALA:HB3	2.01	0.42
1:H:118:ASP:HB2	1:H:121:VAL:CB	2.42	0.42
2:I:820:GLU:HA	2:I:1079:ILE:HD11	2.02	0.42
2:I:1131:MET:HE1	2:I:1141:LEU:HA	2.02	0.42
3:J:45:ASN:HB3	3:J:48:THR:O	2.20	0.42
3:J:1291:GLU:HG2	3:J:1297:LYS:HD2	2.02	0.42
5:L:226:ALA:O	5:L:229:VAL:HG22	2.19	0.42
6:N:35:TYR:CE1	6:N:49:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:CYS:HA	1:A:148:ARG:HA	2.00	0.42
1:A:257:VAL:HG12	1:A:278:ILE:HG22	2.00	0.42
2:C:533:LEU:CD1	2:C:540:ARG:HD2	2.50	0.42
3:D:8:LEU:HD23	3:D:9:LYS:N	2.35	0.42
3:D:347:VAL:HG12	3:D:348:ASP:O	2.19	0.42
3:D:494:ALA:HA	3:D:922:SER:HB3	2.02	0.42
3:D:732:GLY:HA2	3:D:736:GLN:OE1	2.19	0.42
3:D:902:ASP:OD1	3:D:903:LEU:N	2.53	0.42
3:D:926:PRO:CB	3:D:1246:VAL:HG11	2.50	0.42
1:G:104:LYS:HG2	1:G:110:VAL:HG22	2.02	0.42
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	2.01	0.42
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.66	0.42
3:J:649:LYS:HA	3:J:649:LYS:HD3	1.84	0.42
3:J:681:LYS:HE3	6:N:51:ILE:CG2	2.50	0.42
5:L:248:GLU:HG2	5:L:251:LYS:HZ1	1.85	0.42
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.72	0.42
1:B:196:THR:HG22	1:B:197:ASP:N	2.35	0.42
2:C:225:PHE:HZ	2:C:348:SER:N	2.18	0.42
2:C:800:MET:HG3	2:C:1096:ILE:CD1	2.49	0.42
2:C:1298:VAL:CG1	3:D:96:LYS:HZ1	2.33	0.42
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.01	0.42
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.54	0.42
3:D:1298:VAL:H	3:D:1299:GLY:CA	2.31	0.42
5:F:279:ARG:NH2	5:F:350:GLU:OE2	2.36	0.42
5:F:463:LEU:HD23	5:F:463:LEU:HA	1.82	0.42
2:I:538:LEU:HD13	2:I:543:ALA:HB3	2.02	0.42
2:I:1274:GLU:HA	3:J:428:THR:HG21	2.02	0.42
3:J:198:CYS:O	3:J:202:ARG:HG3	2.20	0.42
5:L:276:MET:O	5:L:280:VAL:HG23	2.20	0.42
5:L:380:VAL:HG22	5:L:416:VAL:HG21	2.02	0.42
2:C:785:ASP:OD2	2:C:791:LEU:N	2.50	0.41
3:D:282:LEU:HD23	3:D:282:LEU:HA	1.89	0.41
3:D:317:THR:HA	3:D:324:LEU:HD23	2.02	0.41
3:D:608:CYS:HG	3:D:620:PHE:HD2	1.66	0.41
5:F:274:ARG:NH2	5:F:369:GLU:OE2	2.52	0.41
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.01	0.41
3:J:425:ARG:HG2	3:J:426:ALA:N	2.35	0.41
3:J:441:LEU:HD13	3:J:441:LEU:HA	1.91	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.77	0.41
5:L:412:LEU:HD13	5:L:435:ILE:HD11	2.01	0.41
5:L:441:ARG:NH1	5:L:445:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:12:THR:OG1	6:N:13:GLU:N	2.53	0.41
6:N:48:ARG:NH1	6:N:59:VAL:HB	2.35	0.41
1:A:195:ARG:HD2	1:A:196:THR:N	2.35	0.41
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.50	0.41
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.02	0.41
2:C:210:LEU:HD13	2:C:224:PHE:HE2	1.86	0.41
2:C:357:ASN:ND2	2:C:358:ASP:OD2	2.53	0.41
2:C:487:LEU:HD23	2:C:487:LEU:H	1.85	0.41
2:C:1107:MET:HG2	3:D:740:LEU:CD1	2.48	0.41
3:D:224:LEU:O	3:D:227:PHE:N	2.53	0.41
3:D:357:VAL:HB	3:D:358:GLY:H	1.71	0.41
3:D:452:LEU:HD23	3:D:452:LEU:HA	1.88	0.41
3:D:1361:THR:HG22	4:E:21:LEU:HD22	2.02	0.41
5:F:572:THR:O	5:F:575:GLU:HB2	2.20	0.41
1:G:166:ARG:O	1:G:167:PRO:C	2.58	0.41
2:I:561:ILE:HD12	2:I:679:ALA:HB1	2.02	0.41
2:I:1114:GLU:OE1	2:I:1230:MET:HA	2.20	0.41
2:I:1140:LYS:HD2	2:I:1140:LYS:HA	1.83	0.41
3:J:529:GLY:HA2	3:J:551:ARG:O	2.21	0.41
1:A:23:HIS:HE1	1:A:204:GLU:CG	2.33	0.41
2:C:519:ASN:HB3	2:C:522:SER:HB2	2.02	0.41
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.01	0.41
2:C:616:ILE:HG22	2:C:617:ALA:O	2.20	0.41
2:C:720:ARG:HB2	2:C:749:ASP:OD1	2.19	0.41
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.76	0.41
3:D:888:CYS:SG	3:D:890:THR:HB	2.60	0.41
5:F:284:GLU:HG2	5:F:310:GLU:OE1	2.21	0.41
1:H:46:ILE:HD11	1:H:224:LEU:HD13	2.02	0.41
3:J:515:ARG:O	3:J:545:HIS:HB3	2.20	0.41
3:J:517:CYS:HB3	3:J:719:PHE:CZ	2.56	0.41
5:L:474:MET:C	5:L:476:ARG:H	2.24	0.41
6:N:35:TYR:HE1	6:N:49:ARG:HB2	1.84	0.41
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.75	0.41
2:C:876:GLU:HG2	2:C:927:THR:OG1	2.21	0.41
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	2.03	0.41
3:D:801:VAL:O	3:D:805:GLN:HB2	2.21	0.41
3:D:903:LEU:HD12	3:D:903:LEU:HA	1.94	0.41
2:I:541:GLU:OE1	2:I:541:GLU:N	2.52	0.41
2:I:1220:GLN:HG2	2:I:1221:PHE:N	2.36	0.41
2:I:1225:VAL:HG12	3:J:636:GLY:O	2.20	0.41
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:405:GLU:O	3:J:408:VAL:HG22	2.20	0.41
4:K:26:ARG:HB2	4:K:64:LEU:HD11	2.02	0.41
5:L:511:ILE:HD12	5:L:511:ILE:HA	1.86	0.41
5:L:572:THR:HG23	5:L:575:GLU:HB2	2.03	0.41
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.20	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.91	0.41
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.20	0.41
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.84	0.41
4:E:58:LEU:HD12	4:E:58:LEU:H	1.85	0.41
5:F:280:VAL:HG21	5:F:358:VAL:HG11	2.03	0.41
2:I:499:SER:HA	2:I:502:VAL:HG12	2.03	0.41
2:I:850:ILE:O	2:I:850:ILE:HG22	2.21	0.41
3:J:362:ARG:H	3:J:365:GLN:HE21	1.68	0.41
3:J:416:ILE:HD12	3:J:416:ILE:HA	1.85	0.41
3:J:544:LEU:O	3:J:574:VAL:HB	2.20	0.41
4:K:14:GLY:O	4:K:16:ARG:N	2.50	0.41
5:L:511:ILE:HG13	5:L:512:GLY:H	1.85	0.41
2:C:176:ILE:HB	2:C:184:LEU:HB3	2.01	0.41
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.52	0.41
3:D:262:THR:HG22	5:F:504:PRO:HB2	2.03	0.41
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.35	0.41
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.21	0.41
5:F:387:VAL:HG22	5:F:435:ILE:HD13	2.01	0.41
5:F:465:ARG:HD2	5:F:468:ARG:HH22	1.86	0.41
5:F:577:GLY:HA3	5:F:583:THR:HG23	2.03	0.41
5:F:599:ARG:O	5:F:604:SER:HB2	2.20	0.41
2:I:212:ALA:HA	2:I:359:ARG:HG3	2.03	0.41
2:I:607:SER:N	2:I:610:GLU:HB2	2.35	0.41
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.20	0.41
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.56	0.41
3:J:268:LEU:HD11	3:J:324:LEU:HD13	2.03	0.41
3:J:1167:LYS:HG2	3:J:1168:GLU:H	1.84	0.41
1:A:45:ARG:NE	2:C:1083:GLU:HB3	2.33	0.41
1:B:47:LEU:O	1:B:180:VAL:HG21	2.21	0.41
2:C:53:PHE:HZ	2:C:98:VAL:HG21	1.85	0.41
2:C:364:VAL:HG22	2:C:376:PRO:HB2	2.01	0.41
2:C:499:SER:O	2:C:503:LYS:HB2	2.21	0.41
2:C:1164:PHE:C	2:C:1166:ASP:H	2.24	0.41
3:D:101:ARG:O	3:D:246:PRO:HG3	2.20	0.41
3:D:268:LEU:HD11	3:D:324:LEU:HD13	2.02	0.41
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:678:ARG:CZ	6:N:5:ALA:HB3	2.51	0.41
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.56	0.41
3:J:686:TRP:HB3	3:J:758:PRO:HG2	2.03	0.41
3:J:835:LEU:O	3:J:839:VAL:HG23	2.20	0.41
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.80	0.41
5:L:605:GLU:HA	5:L:608:ARG:HH12	1.84	0.41
2:C:119:GLU:HG3	2:C:488:MET:HB3	2.02	0.41
2:C:176:ILE:HD11	2:C:428:VAL:HG21	2.02	0.41
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.86	0.41
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.30	0.41
2:I:93:SER:OG	2:I:126:GLU:OE1	2.18	0.41
2:I:202:ARG:NH2	2:I:368:ARG:HH12	2.19	0.41
2:I:1161:LEU:HA	2:I:1161:LEU:HD12	1.81	0.41
2:I:1327:LEU:CD2	2:I:1331:ARG:HH21	2.33	0.41
3:J:781:LYS:HE2	6:N:15:LEU:HD13	2.03	0.41
3:J:850:LYS:HG2	3:J:857:LEU:CD2	2.51	0.41
1:A:102:LEU:HD11	1:A:110:VAL:HG11	2.03	0.41
1:A:135:ASP:O	1:A:138:ALA:N	2.38	0.41
1:A:293:PRO:O	1:A:294:ASN:HB2	2.20	0.41
1:B:190:ALA:O	1:B:198:LEU:HB2	2.20	0.41
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.91	0.41
2:C:520:PRO:HG3	2:C:714:VAL:HG21	2.02	0.41
2:C:618:GLN:CG	3:D:770:LEU:HD21	2.48	0.41
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.77	0.41
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	2.02	0.41
2:C:1252:SER:HB3	2:C:1255:THR:O	2.20	0.41
2:C:1276:TRP:HH2	3:D:798:ARG:HG3	1.86	0.41
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	2.03	0.41
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.55	0.41
3:D:510:LEU:O	3:D:514:THR:HG22	2.21	0.41
3:D:1278:GLU:OE1	3:D:1279:GLN:HG2	2.21	0.41
4:E:62:GLN:O	4:E:66:VAL:HG23	2.21	0.41
5:F:558:VAL:HG22	5:F:587:ILE:HD11	2.03	0.41
1:G:85:LEU:HD23	1:G:85:LEU:HA	1.85	0.41
1:H:155:ALA:HB2	1:H:173:VAL:C	2.41	0.41
2:I:147:SER:HB2	2:I:529:ARG:O	2.20	0.41
2:I:660:VAL:HG11	3:J:769:VAL:HG13	2.03	0.41
2:I:725:GLN:HE22	2:I:966:ILE:HG23	1.86	0.41
2:I:732:ILE:HD11	2:I:769:PRO:HB3	2.01	0.41
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.86	0.41
3:J:211:GLU:OE2	3:J:214:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:514:THR:HG21	3:J:596:LEU:HG	2.03	0.41
3:J:591:ILE:HD12	3:J:591:ILE:HA	1.89	0.41
3:J:836:ARG:HD2	3:J:873:GLU:OE1	2.21	0.41
3:J:1263:LYS:HE2	3:J:1279:GLN:NE2	2.36	0.41
3:J:1292:LEU:O	3:J:1293:GLU:HB2	2.20	0.41
6:N:6:ASP:OD1	6:N:6:ASP:N	2.52	0.41
1:A:262:LEU:HD12	1:A:262:LEU:H	1.86	0.41
2:C:867:GLU:H	2:C:867:GLU:HG3	1.46	0.41
2:C:902:LEU:HD12	5:F:607:LEU:HD23	2.02	0.41
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.54	0.41
3:D:782:GLY:HA3	6:M:12:THR:CG2	2.51	0.41
5:F:309:ASN:HB3	5:F:310:GLU:H	1.71	0.41
5:F:320:ILE:HG21	5:F:331:HIS:CE1	2.56	0.41
2:I:193:ASN:ND2	2:I:353:VAL:HG21	2.36	0.41
2:I:425:ILE:O	2:I:429:MET:HG3	2.21	0.41
2:I:714:VAL:HB	2:I:787:PRO:HD2	2.03	0.41
2:I:1063:GLY:O	3:J:354:VAL:HG11	2.21	0.41
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.86	0.41
3:J:638:SER:OG	3:J:639:VAL:N	2.53	0.41
3:J:1155:ILE:H	3:J:1155:ILE:HG13	1.75	0.41
1:A:13:LEU:HD11	1:A:214:GLU:HG3	2.02	0.40
1:A:31:LEU:HA	1:A:31:LEU:HD23	1.78	0.40
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.51	0.40
2:C:243:PRO:O	2:C:274:ILE:HG12	2.21	0.40
2:C:525:THR:HG21	2:C:687:ARG:CD	2.29	0.40
2:C:1285:TYR:CD1	3:D:475:GLU:HG2	2.56	0.40
3:D:336:GLY:HA3	3:D:1324:SER:O	2.21	0.40
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.85	0.40
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.96	0.40
1:G:35:PHE:HD1	1:G:35:PHE:HA	1.76	0.40
2:I:238:GLN:OE1	2:I:284:LEU:HD21	2.21	0.40
2:I:1086:PRO:HB3	2:I:1212:LEU:HD23	2.03	0.40
3:J:114:ILE:HD11	3:J:311:ARG:HB2	2.02	0.40
3:J:275:ARG:HH11	3:J:298:MET:HB3	1.86	0.40
5:L:324:LYS:HB3	5:L:325:PRO:HD2	2.04	0.40
5:L:558:VAL:HG11	5:L:590:ILE:HG22	2.02	0.40
1:A:45:ARG:HG2	1:B:38:THR:CB	2.30	0.40
2:C:88:ARG:HB2	2:C:88:ARG:HH11	1.84	0.40
2:C:162:GLY:O	2:C:164:THR:N	2.54	0.40
2:C:226:GLU:HB2	2:C:245:ARG:HH22	1.85	0.40
2:C:837:ALA:HB2	2:C:1051:LYS:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:638:SER:OG	3:D:639:VAL:N	2.52	0.40
3:D:710:ASP:OD1	3:D:711:GLY:N	2.54	0.40
3:D:797:THR:O	3:D:801:VAL:HG12	2.20	0.40
5:F:316:PHE:CZ	5:F:334:SER:HA	2.57	0.40
1:G:232:VAL:C	1:H:218:ARG:HH12	2.24	0.40
2:I:157:PHE:O	2:I:443:ASP:N	2.48	0.40
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.56	0.40
3:J:264:ASP:OD2	5:L:506:SER:OG	2.23	0.40
3:J:338:PHE:O	3:J:340:GLN:N	2.54	0.40
3:J:510:LEU:HD22	3:J:601:ILE:HD11	2.02	0.40
3:J:517:CYS:HB3	3:J:719:PHE:CE2	2.55	0.40
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.22	0.40
2:C:27:LEU:O	2:C:528:ARG:NH1	2.47	0.40
2:C:1293:VAL:HG13	2:C:1301:ARG:HA	2.04	0.40
3:D:45:ASN:O	3:D:46:TYR:CD2	2.74	0.40
3:D:239:LEU:HD23	3:D:239:LEU:HA	1.89	0.40
3:D:355:ILE:HG12	3:D:464:ASP:O	2.21	0.40
3:D:430:HIS:CE1	3:D:925:GLU:HG3	2.54	0.40
3:D:614:LEU:HD23	4:E:5:THR:HB	2.03	0.40
5:F:119:ILE:HD13	5:F:378:GLU:HG2	2.03	0.40
1:H:57:THR:HG22	1:H:58:GLU:OE1	2.22	0.40
2:I:576:SER:HA	2:I:662:SER:HA	2.02	0.40
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.86	0.40
3:J:155:GLU:HB2	3:J:158:GLN:HB2	2.03	0.40
3:J:773:PHE:O	3:J:776:THR:HB	2.20	0.40
3:J:884:SER:OG	3:J:886:VAL:HG12	2.21	0.40
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.37	0.40
1:A:106:GLY:HA2	1:A:136:GLU:O	2.21	0.40
2:C:14:ASP:OD2	2:C:1156:ARG:NE	2.55	0.40
2:C:18:ARG:HA	2:C:19:PRO:HD3	1.92	0.40
2:C:147:SER:OG	2:C:455:SER:HB3	2.21	0.40
2:C:560:PRO:HB3	3:D:776:THR:HG21	2.04	0.40
2:C:565:GLU:OE1	2:C:681:MET:HE3	2.21	0.40
2:C:619:ALA:HB1	2:C:657:THR:HA	2.03	0.40
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.52	0.40
3:D:707:ILE:HD12	3:D:707:ILE:H	1.87	0.40
1:H:125:LYS:HE2	1:H:128:HIS:HB2	2.04	0.40
2:I:159:SER:O	2:I:160:ASP:HB2	2.21	0.40
2:I:686:GLN:HG2	2:I:796:LEU:HD22	2.04	0.40
2:I:1124:ILE:O	2:I:1128:ILE:HG13	2.21	0.40
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:63:ALA:O	6:N:64:TYR:C	2.60	0.40
1:A:31:LEU:HB2	1:A:199:ASP:O	2.22	0.40
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.53	0.40
2:C:681:MET:O	2:C:685:MET:HE2	2.22	0.40
3:D:621:ALA:HA	3:D:624:ILE:HD12	2.02	0.40
3:D:825:VAL:C	3:D:826:ILE:HG13	2.42	0.40
5:F:316:PHE:HZ	5:F:334:SER:HA	1.86	0.40
5:F:474:MET:O	5:F:476:ARG:N	2.49	0.40
1:G:228:LEU:HG	1:H:221:ALA:HB1	2.03	0.40
2:I:95:PRO:CA	2:I:126:GLU:HG2	2.48	0.40
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.86	0.40
2:I:657:THR:HG21	2:I:1188:ASP:HB2	2.03	0.40
2:I:1286:THR:N	3:J:479:GLU:OE2	2.42	0.40
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.57	0.40
3:J:674:THR:HG22	6:N:59:VAL:HG22	2.03	0.40
3:J:825:VAL:C	3:J:826:ILE:HG13	2.42	0.40
3:J:1173:ARG:N	3:J:1190:ILE:O	2.54	0.40
3:J:1269:ALA:HB2	3:J:1274:PHE:CD1	2.56	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	A	317/329 (96%)	247 (78%)	52 (16%)	18 (6%)	1 21
1	B	213/329 (65%)	194 (91%)	15 (7%)	4 (2%)	8 42
1	G	225/329 (68%)	199 (88%)	20 (9%)	6 (3%)	5 35
1	H	212/329 (64%)	196 (92%)	12 (6%)	4 (2%)	8 42
2	C	1338/1342 (100%)	1201 (90%)	118 (9%)	19 (1%)	11 46
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	9 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1169/1407 (83%)	1038 (89%)	104 (9%)	27 (2%)	6	38
3	J	1151/1407 (82%)	1026 (89%)	99 (9%)	26 (2%)	6	38
4	E	87/91 (96%)	80 (92%)	5 (6%)	2 (2%)	6	38
4	K	70/91 (77%)	61 (87%)	8 (11%)	1 (1%)	11	46
5	F	462/613 (75%)	426 (92%)	28 (6%)	8 (2%)	9	43
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	9	43
6	M	68/79 (86%)	56 (82%)	7 (10%)	5 (7%)	1	16
6	N	67/79 (85%)	56 (84%)	6 (9%)	5 (8%)	1	15
All	All	7180/8380 (86%)	6402 (89%)	624 (9%)	154 (2%)	7	40

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO
1	A	242	VAL
1	B	193	GLU
2	C	169	LYS
2	C	170	VAL
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1153	ALA
2	C	1154	ASP
2	C	1159	VAL
2	C	1165	SER
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY

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Mol	Chain	Res	Type
5	F	490	PRO
5	F	569	THR
1	G	167	PRO
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	49	PHE
3	J	341	ASN
3	J	426	ALA
3	J	710	ASP
3	J	712	GLN
3	J	850	LYS
3	J	1294	ALA
4	K	33	GLY
5	L	584	ARG
6	M	26	LYS
6	M	33	PRO
6	M	64	TYR
6	N	26	LYS
6	N	33	PRO
6	N	64	TYR
1	A	50	SER
1	A	62	ASP
1	A	119	GLY
1	A	164	ASP
1	A	232	VAL
1	A	315	GLY
1	A	320	ASN
1	B	13	LEU
2	C	121	GLU
3	D	89	GLY
3	D	805	GLN
3	D	1274	PHE
5	F	566	ASP

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Mol	Chain	Res	Type
5	F	584	ARG
1	G	162	GLU
1	H	138	ALA
2	I	1059	ARG
2	I	1165	SER
3	J	89	GLY
3	J	314	ARG
3	J	339	ARG
3	J	496	GLY
3	J	745	GLY
3	J	805	GLN
3	J	826	ILE
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP
5	L	490	PRO
5	L	566	ASP
5	L	569	THR
6	M	30	HIS
6	N	30	HIS
1	A	324	ALA
1	B	136	GLU
2	C	163	LYS
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	173	GLY
3	D	417	ARG
3	D	933	ARG
3	D	934	THR
3	D	1344	LEU
1	G	229	GLU
1	H	193	GLU
2	I	813	GLU
2	I	983	GLY
2	I	1317	PRO
3	J	332	LYS
3	J	417	ARG
1	A	319	GLU
1	B	138	ALA
2	C	813	GLU
2	C	1059	ARG

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Mol	Chain	Res	Type
3	D	314	ARG
3	D	1297	LYS
1	H	20	SER
2	I	696	ASP
2	I	892	GLU
3	J	344	GLY
3	J	1344	LEU
1	A	318	LEU
2	C	62	TYR
2	C	983	GLY
2	C	1158	LYS
3	D	46	TYR
3	D	345	LYS
5	F	602	SER
2	I	201	ARG
3	J	338	PHE
3	J	357	VAL
5	L	585	GLU
1	A	241	GLU
3	D	357	VAL
5	F	96	ASP
1	G	9	LEU
2	I	160	ASP
2	I	756	TYR
3	J	333	GLY
5	L	395	THR
1	A	19	VAL
3	D	826	ILE
3	J	173	GLY
6	M	34	VAL
3	D	828	GLY
3	J	336	GLY
5	L	475	GLY
6	N	34	VAL
3	D	831	VAL
5	F	361	ILE
3	J	639	VAL
3	D	120	LEU
2	I	1202	GLY
3	D	850	LYS
4	E	4	VAL
5	F	475	GLY

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Mol	Chain	Res	Type
1	G	14	VAL
1	H	30	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	A	278/286 (97%)	226 (81%)	52 (19%)	1 11
1	B	186/286 (65%)	171 (92%)	15 (8%)	11 41
1	G	193/286 (68%)	169 (88%)	24 (12%)	4 24
1	H	183/286 (64%)	172 (94%)	11 (6%)	19 50
2	C	1154/1157 (100%)	1052 (91%)	102 (9%)	10 38
2	I	1154/1157 (100%)	1058 (92%)	96 (8%)	11 40
3	D	962/1168 (82%)	882 (92%)	80 (8%)	11 40
3	J	960/1168 (82%)	876 (91%)	84 (9%)	10 38
4	E	72/75 (96%)	63 (88%)	9 (12%)	4 24
4	K	62/75 (83%)	59 (95%)	3 (5%)	25 56
5	F	417/540 (77%)	387 (93%)	30 (7%)	14 45
5	L	418/540 (77%)	380 (91%)	38 (9%)	9 36
6	M	59/68 (87%)	55 (93%)	4 (7%)	16 47
6	N	59/68 (87%)	56 (95%)	3 (5%)	24 54
All	All	6157/7160 (86%)	5606 (91%)	551 (9%)	9 38

All (551) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	18	GLN
1	A	26	VAL
1	A	29	GLU

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Mol	Chain	Res	Type
1	A	44	ARG
1	A	50	SER
1	A	56	VAL
1	A	66	HIS
1	A	70	THR
1	A	71	LYS
1	A	72	GLU
1	A	74	VAL
1	A	77	ASP
1	A	83	LEU
1	A	90	VAL
1	A	98	VAL
1	A	99	ILE
1	A	105	SER
1	A	116	THR
1	A	125	LYS
1	A	133	LEU
1	A	137	ASN
1	A	139	SER
1	A	159	ILE
1	A	164	ASP
1	A	165	GLU
1	A	166	ARG
1	A	180	VAL
1	A	183	ILE
1	A	186	ASN
1	A	192	VAL
1	A	195	ARG
1	A	207	THR
1	A	211	ILE
1	A	223	ILE
1	A	231	PHE
1	A	243	LYS
1	A	245	GLU
1	A	246	LYS
1	A	258	ASP
1	A	262	LEU
1	A	280	ASP
1	A	282	VAL
1	A	284	ARG
1	A	285	THR
1	A	300	LEU

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Mol	Chain	Res	Type
1	A	302	GLU
1	A	306	VAL
1	A	316	MET
1	A	318	LEU
1	A	320	ASN
1	B	9	LEU
1	B	16	ILE
1	B	27	THR
1	B	60	GLU
1	B	62	ASP
1	B	64	VAL
1	B	79	LEU
1	B	95	LYS
1	B	102	LEU
1	B	124	VAL
1	B	139	SER
1	B	183	ILE
1	B	191	ARG
1	B	196	THR
1	B	233	ASP
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS
2	C	23	ASP
2	C	46	GLN
2	C	81	ASP
2	C	103	VAL
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	131	THR
2	C	135	THR
2	C	150	HIS
2	C	164	THR
2	C	201	ARG
2	C	208	ILE
2	C	285	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP

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Mol	Chain	Res	Type
2	C	377	THR
2	C	384	LEU
2	C	423	ASP
2	C	455	SER
2	C	471	VAL
2	C	481	LEU
2	C	484	LEU
2	C	485	ASP
2	C	490	GLN
2	C	492	MET
2	C	518	ASN
2	C	525	THR
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	553	THR
2	C	558	VAL
2	C	561	ILE
2	C	575	LEU
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	663	VAL
2	C	672	GLU
2	C	694	ARG
2	C	697	LYS
2	C	714	VAL
2	C	748	ILE
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	778	GLU
2	C	781	ASP
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	867	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU

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Mol	Chain	Res	Type
2	C	895	LEU
2	C	919	ARG
2	C	951	MET
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1037	THR
2	C	1054	LEU
2	C	1059	ARG
2	C	1076	ILE
2	C	1082	ILE
2	C	1134	GLN
2	C	1141	LEU
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1233	LEU
2	C	1237	HIS
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1250	SER
2	C	1254	VAL
2	C	1255	THR
2	C	1287	LEU
2	C	1296	ASP
2	C	1310	ASP
2	C	1313	HIS
2	C	1327	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	46	TYR
3	D	47	ARG
3	D	54	ASP

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Mol	Chain	Res	Type
3	D	79	LYS
3	D	93	THR
3	D	95	THR
3	D	97	VAL
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	248	ASP
3	D	252	LEU
3	D	259	ARG
3	D	292	VAL
3	D	324	LEU
3	D	330	MET
3	D	335	GLN
3	D	343	LEU
3	D	376	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	413	ASP
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	490	ILE
3	D	505	ASP
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	560	ASN
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	639	VAL
3	D	641	ILE
3	D	678	ARG
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	717	VAL
3	D	753	SER
3	D	754	ILE
3	D	764	ARG

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Mol	Chain	Res	Type
3	D	772	TYR
3	D	797	THR
3	D	801	VAL
3	D	810	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG
3	D	890	THR
3	D	897	HIS
3	D	903	LEU
3	D	908	ILE
3	D	910	ASN
3	D	918	ILE
3	D	1155	ILE
3	D	1162	ILE
3	D	1163	VAL
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1199	PHE
3	D	1221	LEU
3	D	1251	LYS
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1289	ASN
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1366	HIS
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	18	ASP
4	E	21	LEU
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU

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Mol	Chain	Res	Type
4	E	62	GLN
5	F	98	VAL
5	F	114	GLU
5	F	154	GLU
5	F	163	THR
5	F	261	LEU
5	F	277	MET
5	F	305	LEU
5	F	306	PHE
5	F	338	HIS
5	F	401	PHE
5	F	449	THR
5	F	471	LEU
5	F	472	GLN
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	516	ASP
5	F	526	THR
5	F	527	THR
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	569	THR
5	F	572	THR
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	33	ARG
1	G	50	SER
1	G	70	THR
1	G	79	LEU
1	G	90	VAL
1	G	101	THR

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Mol	Chain	Res	Type
1	G	121	VAL
1	G	124	VAL
1	G	133	LEU
1	G	145	LYS
1	G	156	SER
1	G	166	ARG
1	G	178	SER
1	G	187	VAL
1	G	200	LYS
1	G	207	THR
1	G	211	ILE
1	G	219	ARG
1	G	231	PHE
1	H	27	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	95	LYS
1	H	102	LEU
1	H	124	VAL
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	46	GLN
2	I	86	GLN
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE
2	I	131	THR
2	I	132	ASP
2	I	138	ILE
2	I	156	PHE
2	I	164	THR
2	I	197	ARG
2	I	201	ARG
2	I	208	ILE
2	I	285	ILE
2	I	320	ASP

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Mol	Chain	Res	Type
2	I	321	LEU
2	I	342	ASP
2	I	360	LEU
2	I	423	ASP
2	I	453	ILE
2	I	455	SER
2	I	471	VAL
2	I	481	LEU
2	I	484	LEU
2	I	485	ASP
2	I	490	GLN
2	I	492	MET
2	I	518	ASN
2	I	524	ILE
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	540	ARG
2	I	542	ARG
2	I	553	THR
2	I	558	VAL
2	I	561	ILE
2	I	596	ASP
2	I	600	THR
2	I	604	HIS
2	I	609	ILE
2	I	633	LEU
2	I	635	THR
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	694	ARG
2	I	705	GLU
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	764	CYS
2	I	765	ILE
2	I	781	ASP
2	I	782	VAL
2	I	799	ASN
2	I	800	MET

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Mol	Chain	Res	Type
2	I	814	ASP
2	I	828	PHE
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	919	ARG
2	I	922	ASN
2	I	951	MET
2	I	992	LEU
2	I	1005	GLU
2	I	1037	THR
2	I	1054	LEU
2	I	1082	ILE
2	I	1083	GLU
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1198	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1250	SER
2	I	1254	VAL
2	I	1265	PHE
2	I	1287	LEU
2	I	1296	ASP
2	I	1313	HIS
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	46	TYR
3	J	47	ARG
3	J	54	ASP
3	J	79	LYS
3	J	92	VAL

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Mol	Chain	Res	Type
3	J	93	THR
3	J	95	THR
3	J	97	VAL
3	J	98	ARG
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	206	ASN
3	J	218	THR
3	J	235	GLU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	259	ARG
3	J	292	VAL
3	J	324	LEU
3	J	343	LEU
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	386	GLU
3	J	392	THR
3	J	394	ILE
3	J	413	ASP
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG
3	J	429	LEU
3	J	505	ASP
3	J	510	LEU
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	560	ASN
3	J	567	THR
3	J	569	LEU
3	J	571	ASP
3	J	573	THR
3	J	641	ILE
3	J	678	ARG
3	J	701	LEU
3	J	707	ILE

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Mol	Chain	Res	Type
3	J	708	ASN
3	J	717	VAL
3	J	754	ILE
3	J	764	ARG
3	J	772	TYR
3	J	797	THR
3	J	801	VAL
3	J	810	THR
3	J	827	GLU
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	897	HIS
3	J	898	CYS
3	J	908	ILE
3	J	910	ASN
3	J	918	ILE
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1186	TYR
3	J	1194	ARG
3	J	1199	PHE
3	J	1221	LEU
3	J	1251	LYS
3	J	1261	LEU
3	J	1266	ILE
3	J	1273	ASP
3	J	1282	TYR
3	J	1285	VAL
3	J	1289	ASN
3	J	1292	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	18	ASP
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	102	MET
5	L	114	GLU

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Mol	Chain	Res	Type
5	L	154	GLU
5	L	261	LEU
5	L	266	PHE
5	L	277	MET
5	L	305	LEU
5	L	306	PHE
5	L	335	GLU
5	L	338	HIS
5	L	364	ARG
5	L	395	THR
5	L	401	PHE
5	L	405	ILE
5	L	429	THR
5	L	445	ASP
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	486	ARG
5	L	491	GLU
5	L	492	ASP
5	L	526	THR
5	L	527	THR
5	L	552	THR
5	L	558	VAL
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
6	M	16	THR
6	M	34	VAL
6	M	40	CYS
6	M	59	VAL
6	N	16	THR
6	N	34	VAL
6	N	40	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	128	HIS
1	A	320	ASN
1	B	23	HIS
1	B	132	HIS
2	C	46	GLN
2	C	69	GLN
2	C	139	ASN
2	C	343	HIS
2	C	513	GLN
2	C	554	HIS
2	C	620	ASN
2	C	725	GLN
2	C	760	ASN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1220	GLN
2	C	1236	ASN
2	C	1237	HIS
2	C	1288	GLN
2	C	1299	ASN
2	C	1314	GLN
3	D	200	GLN
3	D	320	ASN
3	D	365	GLN
3	D	424	ASN
3	D	690	ASN
3	D	716	GLN
3	D	739	GLN
3	D	817	HIS
3	D	910	ASN
5	F	129	GLN
5	F	131	GLN
5	F	147	GLN
5	F	406	GLN
5	F	446	GLN
5	F	469	GLN
5	F	472	GLN
5	F	579	GLN
1	G	66	HIS

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Mol	Chain	Res	Type
1	H	128	HIS
2	I	139	ASN
2	I	150	HIS
2	I	343	HIS
2	I	357	ASN
2	I	620	ASN
2	I	628	HIS
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1146	GLN
2	I	1220	GLN
2	I	1237	HIS
2	I	1288	GLN
2	I	1314	GLN
3	J	200	GLN
3	J	206	ASN
3	J	667	GLN
3	J	680	ASN
3	J	690	ASN
3	J	716	GLN
3	J	771	GLN
3	J	817	HIS
3	J	861	ASN
3	J	1295	ASN
5	L	131	GLN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	579	GLN
6	M	71	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	319/329 (96%)	-0.01	8 (2%) 57 49	152, 220, 344, 468	0
1	B	217/329 (65%)	-0.05	9 (4%) 37 31	140, 238, 332, 383	0
1	G	227/329 (68%)	-0.06	7 (3%) 49 40	204, 264, 358, 416	0
1	H	216/329 (65%)	0.41	19 (8%) 10 8	204, 298, 387, 432	0
2	C	1340/1342 (99%)	0.23	83 (6%) 20 16	104, 197, 403, 528	0
2	I	1340/1342 (99%)	0.38	109 (8%) 12 10	127, 264, 377, 485	0
3	D	1173/1407 (83%)	-0.07	12 (1%) 82 76	101, 174, 294, 419	0
3	J	1155/1407 (82%)	0.07	34 (2%) 51 42	125, 213, 329, 431	0
4	E	89/91 (97%)	-0.34	1 (1%) 80 74	160, 216, 269, 393	0
4	K	72/91 (79%)	1.28	16 (22%) 0 0	227, 323, 429, 470	0
5	F	468/613 (76%)	0.08	25 (5%) 26 23	137, 239, 365, 477	0
5	L	469/613 (76%)	-0.06	19 (4%) 37 31	162, 251, 379, 489	0
6	M	70/79 (88%)	0.12	3 (4%) 35 30	226, 315, 399, 479	0
6	N	69/79 (87%)	0.45	11 (15%) 1 2	325, 403, 501, 568	0
All	All	7224/8380 (86%)	0.14	356 (4%) 29 25	101, 230, 372, 568	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	338	THR	14.4
2	C	252	SER	10.7
2	C	241	LEU	9.4
3	J	1198	VAL	9.2
2	C	251	ALA	9.1
2	C	207	THR	8.9
5	F	305	LEU	8.5
2	C	253	PHE	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	7.6
2	C	261	VAL	7.4
2	I	231	GLU	7.0
2	I	998	LEU	6.9
2	C	332	ARG	6.9
2	I	1004	ASP	6.8
2	C	264	GLU	6.8
2	I	975	ILE	6.7
2	C	206	ALA	6.6
5	F	167	ASP	6.6
5	F	165	PHE	6.5
2	C	255	ILE	6.4
3	J	542	ALA	6.2
2	C	265	LYS	6.2
1	H	56	VAL	6.1
1	H	152	TYR	6.1
2	C	230	PHE	6.1
1	B	233	ASP	5.8
2	I	230	PHE	5.7
2	C	239	MET	5.6
2	I	979	LEU	5.5
2	C	313	ALA	5.5
5	L	315	TRP	5.5
2	I	239	MET	5.4
2	I	1005	GLU	5.3
5	F	259	PHE	5.2
5	F	314	THR	5.1
4	K	12	LYS	5.1
1	H	12	ARG	5.1
2	C	1000	LEU	5.0
2	C	317	LEU	5.0
4	K	13	ILE	4.9
2	C	254	ASP	4.8
2	C	205	PRO	4.8
2	C	263	VAL	4.8
2	I	492	MET	4.8
5	F	319	ALA	4.7
2	C	318	SER	4.7
2	I	420	LEU	4.7
2	I	1003	THR	4.7
2	C	242	VAL	4.7
2	I	972	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
3	J	747	MET	4.6
1	H	158	ARG	4.6
1	H	146	VAL	4.6
2	C	292	ILE	4.6
2	C	312	ALA	4.6
2	C	260	LYS	4.5
2	I	1006	GLU	4.5
2	C	231	GLU	4.5
6	N	32	ILE	4.5
1	H	55	ALA	4.5
2	C	267	ARG	4.5
5	F	315	TRP	4.5
2	I	540	ARG	4.5
2	C	209	ILE	4.4
2	C	266	GLY	4.4
2	C	257	ALA	4.3
2	C	331	LYS	4.3
3	D	1198	VAL	4.3
3	J	541	LEU	4.3
1	H	59	VAL	4.3
1	A	303	ILE	4.3
2	I	450	ASN	4.2
4	K	26	ARG	4.2
2	C	250	THR	4.2
5	F	162	ILE	4.2
2	C	258	ASN	4.1
5	F	164	GLY	4.1
2	I	1000	LEU	4.1
2	I	536	GLY	4.1
3	J	746	LEU	4.0
4	K	38	LEU	4.0
2	C	282	VAL	4.0
5	L	290	LEU	3.9
2	C	333	ILE	3.9
2	I	204	LEU	3.9
2	I	976	ARG	3.9
2	I	299	LYS	3.9
6	N	33	PRO	3.9
2	C	350	THR	3.9
1	B	160	HIS	3.9
4	K	47	THR	3.9
2	C	269	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
5	F	310	GLU	3.9
2	I	194	LEU	3.9
2	C	1001	GLY	3.8
2	I	236	LYS	3.8
5	F	304	THR	3.8
2	I	301	TYR	3.8
2	C	429	MET	3.8
2	I	451	ARG	3.8
5	F	161	LEU	3.8
2	I	489	PRO	3.7
2	C	243	PRO	3.7
2	I	538	LEU	3.7
2	C	268	ARG	3.7
2	I	973	SER	3.7
2	I	539	THR	3.7
1	G	98	VAL	3.7
2	I	267	ARG	3.7
2	I	330	HIS	3.7
2	C	208	ILE	3.6
1	A	275	ILE	3.6
1	H	123	ILE	3.6
2	C	240	GLU	3.6
2	C	311	CYS	3.6
2	I	332	ARG	3.6
2	I	442	VAL	3.5
2	I	982	GLY	3.5
2	C	539	THR	3.5
6	M	35	TYR	3.5
2	I	1050	VAL	3.5
4	K	58	LEU	3.5
2	C	540	ARG	3.5
2	C	273	HIS	3.5
2	C	246	LEU	3.5
2	I	541	GLU	3.5
2	C	224	PHE	3.5
2	I	165	HIS	3.5
2	C	259	GLY	3.4
2	C	337	PHE	3.4
5	L	305	LEU	3.4
3	J	857	LEU	3.4
2	I	333	ILE	3.4
3	J	732	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	I	1007	LYS	3.4
2	C	322	LEU	3.4
3	J	1215	GLU	3.4
2	C	281	ASP	3.3
3	J	1296	GLY	3.3
2	I	836	LEU	3.3
4	K	36	ASP	3.3
2	I	311	CYS	3.3
2	I	234	ASP	3.3
2	I	981	ALA	3.3
6	N	34	VAL	3.3
3	J	1196	LEU	3.3
2	I	235	ASN	3.2
2	C	336	LEU	3.2
4	K	37	PRO	3.2
5	L	490	PRO	3.2
5	L	325	PRO	3.2
5	F	306	PHE	3.2
2	I	102	LEU	3.2
3	J	1165	PHE	3.2
2	C	277	LEU	3.2
2	C	314	ASN	3.2
2	I	100	LEU	3.1
5	L	161	LEU	3.1
2	I	238	GLN	3.1
2	C	262	TYR	3.1
2	I	986	ALA	3.1
2	I	485	ASP	3.1
1	H	67	GLU	3.1
2	I	124	MET	3.1
2	I	1149	TYR	3.0
1	B	98	VAL	3.0
2	I	441	GLU	3.0
2	C	319	LEU	3.0
1	B	138	ALA	3.0
2	I	325	LEU	3.0
2	C	188	PHE	3.0
2	I	988	LYS	3.0
5	L	165	PHE	3.0
2	I	331	LYS	3.0
4	K	33	GLY	3.0
2	I	1001	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	997	TRP	2.9
2	I	543	ALA	2.9
5	F	355	ILE	2.9
2	I	1141	LEU	2.9
2	I	837	ALA	2.9
3	J	1175	LEU	2.9
4	K	56	GLU	2.9
1	H	57	THR	2.9
3	J	1190	ILE	2.9
6	N	56	THR	2.8
1	H	96	ASP	2.8
3	J	1161	GLY	2.8
2	I	985	GLU	2.8
3	D	1186	TYR	2.8
5	L	416	VAL	2.8
6	N	43	PRO	2.8
2	I	389	PHE	2.8
2	I	974	ARG	2.8
2	I	928	VAL	2.8
1	A	278	ILE	2.8
3	J	1210	ILE	2.8
1	H	54	CYS	2.8
2	I	548	ARG	2.8
5	F	287	ILE	2.8
2	I	983	GLY	2.8
6	N	4	GLU	2.7
2	I	205	PRO	2.7
2	C	287	VAL	2.7
2	I	233	ARG	2.7
3	J	731	ARG	2.7
3	J	526	VAL	2.7
1	H	148	ARG	2.7
2	I	1002	LEU	2.7
2	C	291	TYR	2.7
2	I	542	ARG	2.7
2	C	321	LEU	2.7
3	D	1204	VAL	2.7
3	J	730	ALA	2.7
4	K	9	ALA	2.7
1	B	65	LEU	2.7
3	J	16	GLU	2.7
2	C	237	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	66	HIS	2.6
3	D	1165	PHE	2.6
2	I	992	LEU	2.6
6	N	54	GLY	2.6
5	L	337	VAL	2.6
1	A	274	ALA	2.6
2	I	599	VAL	2.6
2	C	300	ASP	2.6
1	H	90	VAL	2.6
2	I	186	PHE	2.6
5	F	337	VAL	2.6
2	I	1051	LYS	2.6
3	J	1188	GLU	2.5
1	H	98	VAL	2.5
5	F	325	PRO	2.5
1	H	181	GLU	2.5
2	I	151	ARG	2.5
2	I	452	ARG	2.5
5	L	259	PHE	2.5
5	F	318	ALA	2.5
1	B	121	VAL	2.5
2	I	68	LEU	2.5
6	M	34	VAL	2.5
3	D	1376	GLY	2.5
2	I	464	PHE	2.5
2	I	285	ILE	2.5
5	F	303	ILE	2.5
3	J	113	HIS	2.5
5	F	307	THR	2.5
2	I	1054	LEU	2.5
6	N	31	GLY	2.5
6	N	55	VAL	2.5
3	J	154	LEU	2.4
3	J	858	VAL	2.4
3	D	889	ASP	2.4
3	J	1204	VAL	2.4
5	L	319	ALA	2.4
3	J	208	THR	2.4
1	B	172	LEU	2.4
2	C	1002	LEU	2.4
2	I	883	LEU	2.4
2	C	492	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	493	ILE	2.4
4	E	2	ALA	2.4
2	I	1049	ILE	2.4
5	L	167	ASP	2.4
5	L	307	THR	2.4
2	I	117	ILE	2.4
2	C	998	LEU	2.4
2	I	989	LEU	2.4
4	K	41	GLU	2.4
2	C	270	THR	2.4
5	L	289	LYS	2.3
2	I	1052	VAL	2.3
5	L	111	LEU	2.3
3	J	1203	ARG	2.3
2	I	302	ILE	2.3
3	J	1166	GLY	2.3
2	C	1299	ASN	2.3
5	L	344	LEU	2.3
2	C	280	ASP	2.3
2	I	347	ILE	2.3
2	I	720	ARG	2.3
2	I	771	VAL	2.3
3	J	1189	MET	2.3
2	I	185	ASP	2.3
3	J	1169	THR	2.3
5	L	293	GLU	2.3
5	F	256	PHE	2.3
3	D	1171	GLY	2.3
5	F	166	VAL	2.3
5	L	330	LEU	2.3
2	C	316	GLU	2.3
5	F	158	LEU	2.3
2	I	696	ASP	2.3
1	G	100	LEU	2.2
4	K	28	ARG	2.2
2	C	305	SER	2.2
2	I	1010	GLN	2.2
2	I	237	LEU	2.2
4	K	59	ILE	2.2
3	J	639	VAL	2.2
2	I	107	ARG	2.2
3	D	1203	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	999	GLU	2.2
2	I	292	ILE	2.2
1	G	193	GLU	2.2
1	A	244	GLU	2.2
2	I	875	ALA	2.2
2	I	153	PRO	2.2
2	I	750	ILE	2.2
2	C	285	ILE	2.2
1	G	205	MET	2.2
5	F	312	SER	2.2
2	C	213	LEU	2.2
1	B	123	ILE	2.2
2	C	315	MET	2.1
5	F	581	ASP	2.1
2	C	284	LEU	2.1
2	C	533	LEU	2.1
6	N	57	LEU	2.1
3	D	1199	PHE	2.1
2	I	152	SER	2.1
1	H	196	THR	2.1
4	K	35	LYS	2.1
3	J	458	ASN	2.1
1	G	50	SER	2.1
2	C	659	GLN	2.1
3	D	879	ALA	2.1
3	J	525	MET	2.1
2	I	1316	GLU	2.1
1	G	90	VAL	2.1
1	H	147	GLN	2.1
2	C	405	PHE	2.1
6	M	30	HIS	2.1
1	H	100	LEU	2.1
2	C	997	TRP	2.1
2	I	224	PHE	2.1
2	I	190	PRO	2.1
2	C	238	GLN	2.1
3	D	891	ASP	2.1
1	G	68	TYR	2.1
2	C	489	PRO	2.1
2	I	304	GLU	2.1
3	J	1306	LEU	2.1
6	N	30	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	272	ALA	2.1
2	C	696	ASP	2.1
2	I	783	LEU	2.1
3	J	527	LEU	2.0
3	D	1172	LYS	2.0
5	L	318	ALA	2.0
2	I	289	VAL	2.0
2	I	101	ARG	2.0
2	I	176	ILE	2.0
1	A	276	HIS	2.0
2	I	547	VAL	2.0
4	K	19	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	D	2001	1/1	0.42	0.18	251,251,251,251	0
8	ZN	N	101	1/1	0.78	0.06	465,465,465,465	0
8	ZN	M	101	1/1	0.84	0.04	468,468,468,468	0
8	ZN	J	2002	1/1	0.87	0.15	229,229,229,229	0
8	ZN	D	2002	1/1	0.94	0.15	182,182,182,182	0
8	ZN	D	2003	1/1	0.97	0.49	334,334,334,334	0
7	MG	J	2001	1/1	0.98	0.47	170,170,170,170	0
8	ZN	J	2003	1/1	0.99	0.24	126,126,126,126	0

6.5 Other polymers (i)

There are no such residues in this entry.