Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2024 – 06:11 PM EDT

PDB ID	:	5WKO
Title	:	Crystal structure of antibody 27F3 recognizing the HA from A/California/04/2009 (H1N1) influenza virus
Authors	:	Wilson, I.A.; Lang, S.; Zhu, X.
Deposited on	:	2017-07-25
Resolution	:	3.49 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:

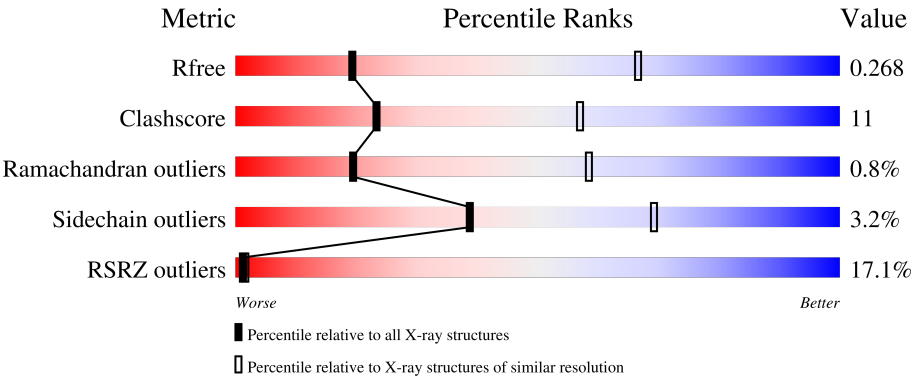
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	225	6% 74% 21% 5%
1	C	225	5% 70% 26% ·
1	E	225	4% 74% 23% ·
1	G	225	5% 70% 25% 5%
1	I	225	15% 72% 25% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	225	6% 74% 23%
2	B	213	72% 23%
2	D	213	68% 29%
2	F	213	78% 21%
2	H	213	% 75% 23%
2	J	213	2% 72% 25%
2	L	213	76% 21%
3	M	331	44% 77% 20%
3	N	331	41% 81% 16%
3	O	331	50% 76% 21%
3	S	331	34% 79% 18%
3	T	331	34% 83% 13%
3	U	331	35% 79% 18%
4	P	177	6% 79% 20%
4	Q	177	6% 80% 17%
4	R	177	5% 76% 19%
4	V	177	6% 80% 19%
4	W	177	7% 81% 15%
4	X	177	6% 80% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 43322 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 Antibody 27F3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	C	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	E	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	G	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	I	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	K	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			

- Molecule 2 is a protein called Antibody 27F3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	D	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	F	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	H	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	J	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	L	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	THR	SER	conflict	UNP Q9UL78

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	83	PHE	CYS	conflict	UNP Q9UL78
B	92	VAL	GLY	conflict	UNP Q9UL78
B	94	THR	SER	conflict	UNP Q9UL78
D	76	THR	SER	conflict	UNP Q9UL78
D	83	PHE	CYS	conflict	UNP Q9UL78
D	92	VAL	GLY	conflict	UNP Q9UL78
D	94	THR	SER	conflict	UNP Q9UL78
F	76	THR	SER	conflict	UNP Q9UL78
F	83	PHE	CYS	conflict	UNP Q9UL78
F	92	VAL	GLY	conflict	UNP Q9UL78
F	94	THR	SER	conflict	UNP Q9UL78
H	76	THR	SER	conflict	UNP Q9UL78
H	83	PHE	CYS	conflict	UNP Q9UL78
H	92	VAL	GLY	conflict	UNP Q9UL78
H	94	THR	SER	conflict	UNP Q9UL78
J	76	THR	SER	conflict	UNP Q9UL78
J	83	PHE	CYS	conflict	UNP Q9UL78
J	92	VAL	GLY	conflict	UNP Q9UL78
J	94	THR	SER	conflict	UNP Q9UL78
L	76	THR	SER	conflict	UNP Q9UL78
L	83	PHE	CYS	conflict	UNP Q9UL78
L	92	VAL	GLY	conflict	UNP Q9UL78
L	94	THR	SER	conflict	UNP Q9UL78

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	324	Total	C	N	O	S	0	0	0
			2529	1599	436	483	11			
3	N	323	Total	C	N	O	S	0	0	0
			2523	1596	435	481	11			
3	O	326	Total	C	N	O	S	0	0	0
			2544	1608	438	487	11			
3	S	324	Total	C	N	O	S	0	0	0
			2529	1599	436	483	11			
3	T	323	Total	C	N	O	S	0	0	0
			2523	1596	435	481	11			
3	U	326	Total	C	N	O	S	0	0	0
			2544	1608	438	487	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	7	ALA	-	expression tag	UNP C3W5S1
M	8	ASP	-	expression tag	UNP C3W5S1
M	9	PRO	-	expression tag	UNP C3W5S1
M	10	GLY	-	expression tag	UNP C3W5S1
N	7	ALA	-	expression tag	UNP C3W5S1
N	8	ASP	-	expression tag	UNP C3W5S1
N	9	PRO	-	expression tag	UNP C3W5S1
N	10	GLY	-	expression tag	UNP C3W5S1
O	7	ALA	-	expression tag	UNP C3W5S1
O	8	ASP	-	expression tag	UNP C3W5S1
O	9	PRO	-	expression tag	UNP C3W5S1
O	10	GLY	-	expression tag	UNP C3W5S1
S	7	ALA	-	expression tag	UNP C3W5S1
S	8	ASP	-	expression tag	UNP C3W5S1
S	9	PRO	-	expression tag	UNP C3W5S1
S	10	GLY	-	expression tag	UNP C3W5S1
T	7	ALA	-	expression tag	UNP C3W5S1
T	8	ASP	-	expression tag	UNP C3W5S1
T	9	PRO	-	expression tag	UNP C3W5S1
T	10	GLY	-	expression tag	UNP C3W5S1
U	7	ALA	-	expression tag	UNP C3W5S1
U	8	ASP	-	expression tag	UNP C3W5S1
U	9	PRO	-	expression tag	UNP C3W5S1
U	10	GLY	-	expression tag	UNP C3W5S1

- Molecule 4 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			
4	Q	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	R	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	V	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			
4	W	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	X	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			

There are 24 discrepancies between the modelled and reference sequences:

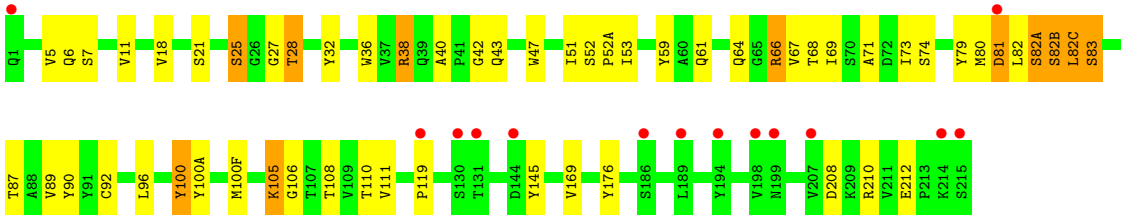
Chain	Residue	Modelled	Actual	Comment	Reference
P	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
P	175	SER	-	expression tag	UNP A0A023ZYH9
P	176	GLY	-	expression tag	UNP A0A023ZYH9
P	177	ARG	-	expression tag	UNP A0A023ZYH9
Q	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
Q	175	SER	-	expression tag	UNP A0A023ZYH9
Q	176	GLY	-	expression tag	UNP A0A023ZYH9
Q	177	ARG	-	expression tag	UNP A0A023ZYH9
R	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
R	175	SER	-	expression tag	UNP A0A023ZYH9
R	176	GLY	-	expression tag	UNP A0A023ZYH9
R	177	ARG	-	expression tag	UNP A0A023ZYH9
V	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
V	175	SER	-	expression tag	UNP A0A023ZYH9
V	176	GLY	-	expression tag	UNP A0A023ZYH9
V	177	ARG	-	expression tag	UNP A0A023ZYH9
W	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
W	175	SER	-	expression tag	UNP A0A023ZYH9
W	176	GLY	-	expression tag	UNP A0A023ZYH9
W	177	ARG	-	expression tag	UNP A0A023ZYH9
X	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
X	175	SER	-	expression tag	UNP A0A023ZYH9
X	176	GLY	-	expression tag	UNP A0A023ZYH9
X	177	ARG	-	expression tag	UNP A0A023ZYH9

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.

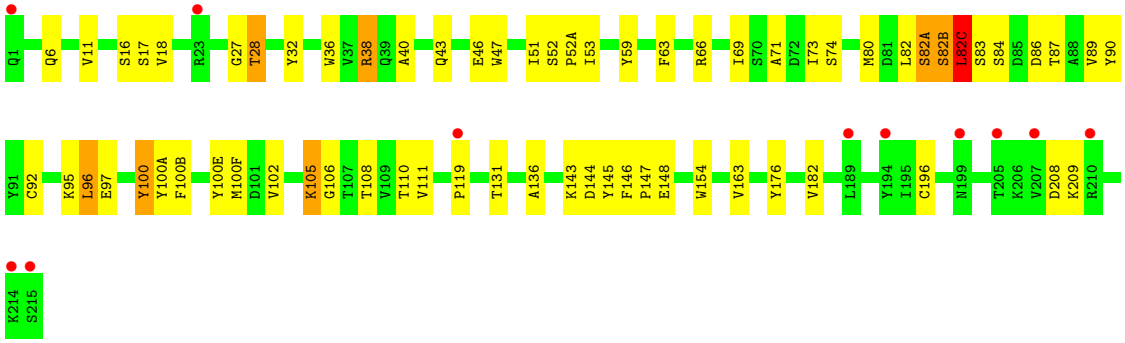
• Molecule 1: Antibody 27F3 heavy chain

Chain A:



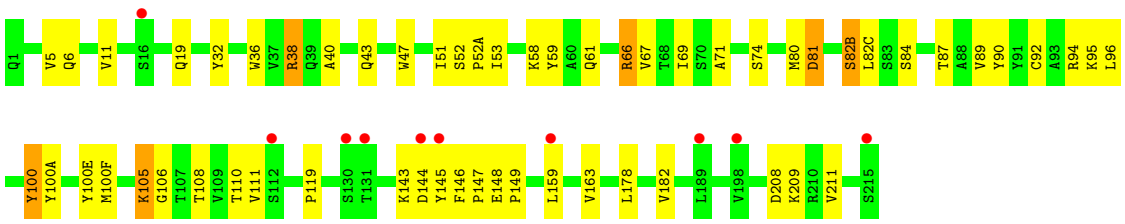
• Molecule 1: Antibody 27F3 heavy chain

Chain C:



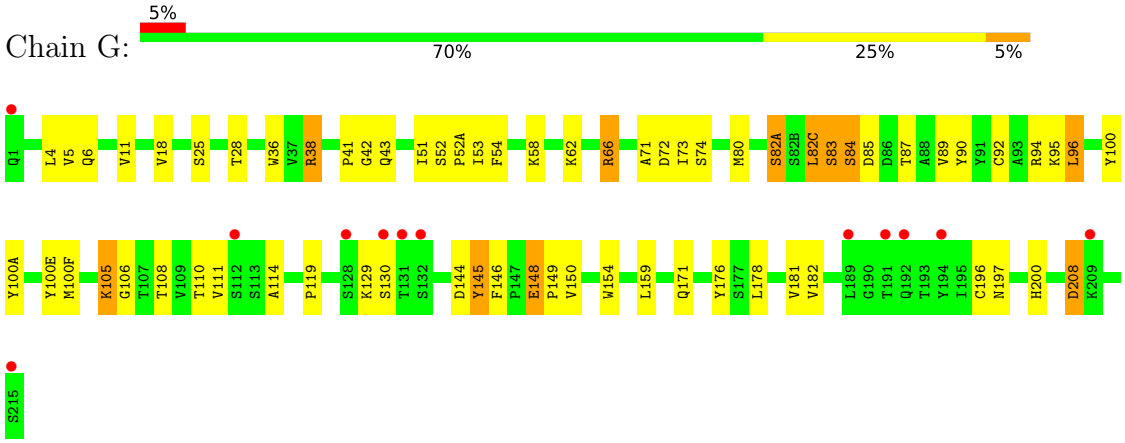
• Molecule 1: Antibody 27F3 heavy chain

Chain E:



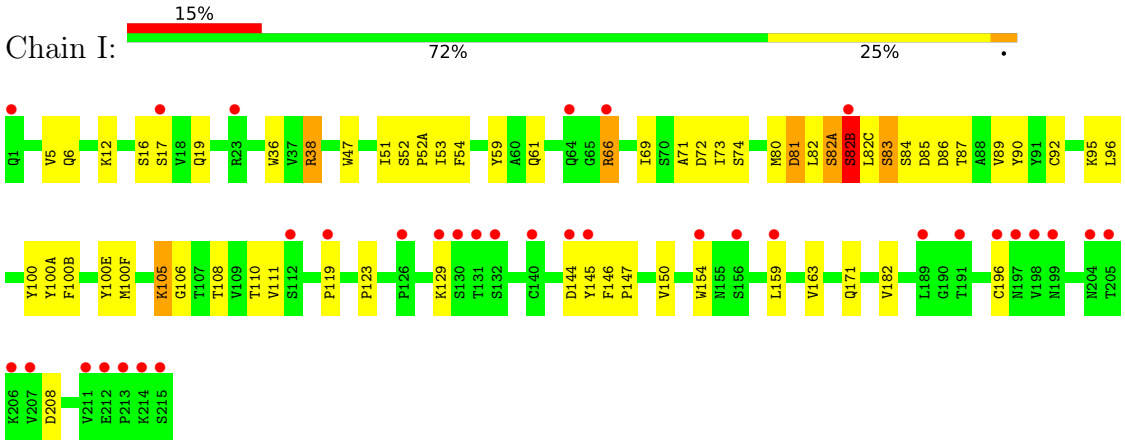
• Molecule 1: Antibody 27F3 heavy chain

Chain G:



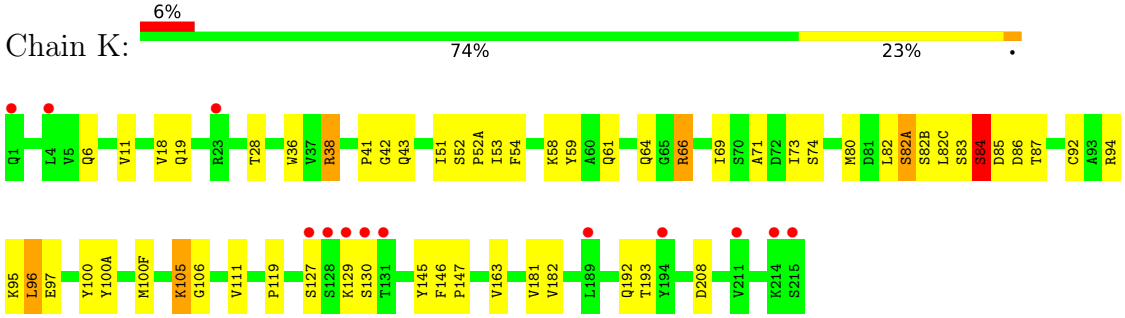
• Molecule 1: Antibody 27F3 heavy chain

Chain I:



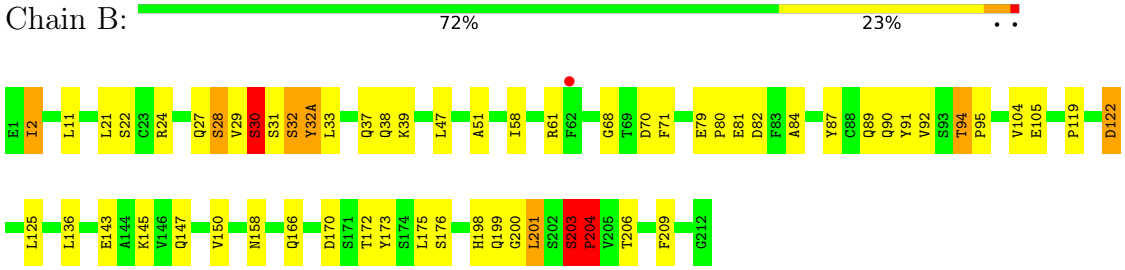
• Molecule 1: Antibody 27F3 heavy chain

Chain K:



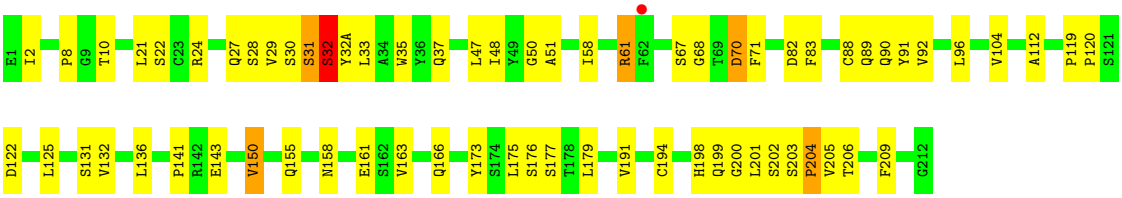
• Molecule 2: Antibody 27F3 light chain

Chain B:



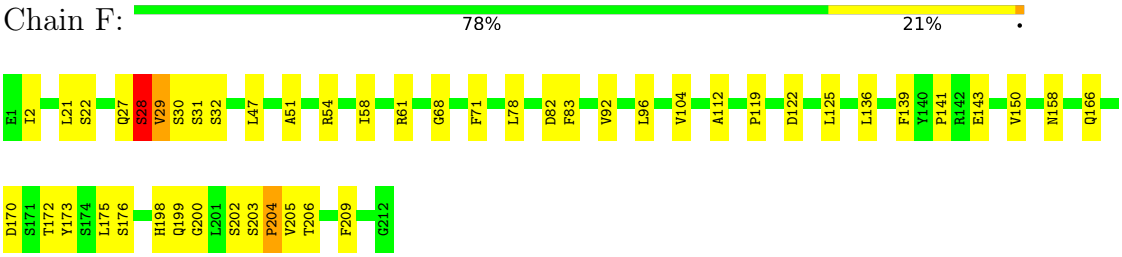
• Molecule 2: Antibody 27F3 light chain

Chain D:



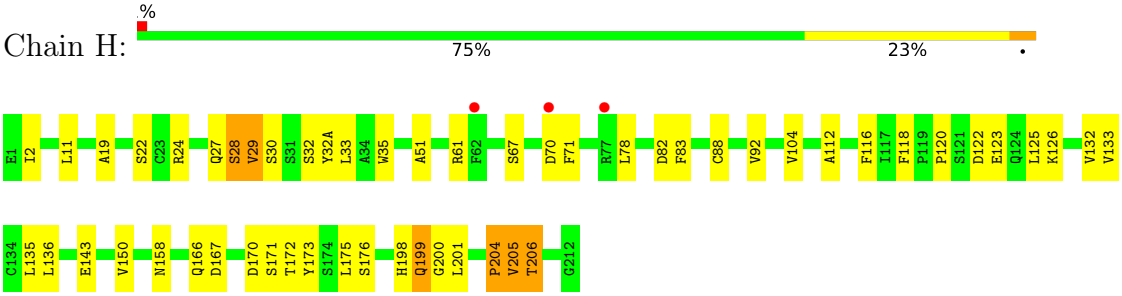
• Molecule 2: Antibody 27F3 light chain

Chain F:



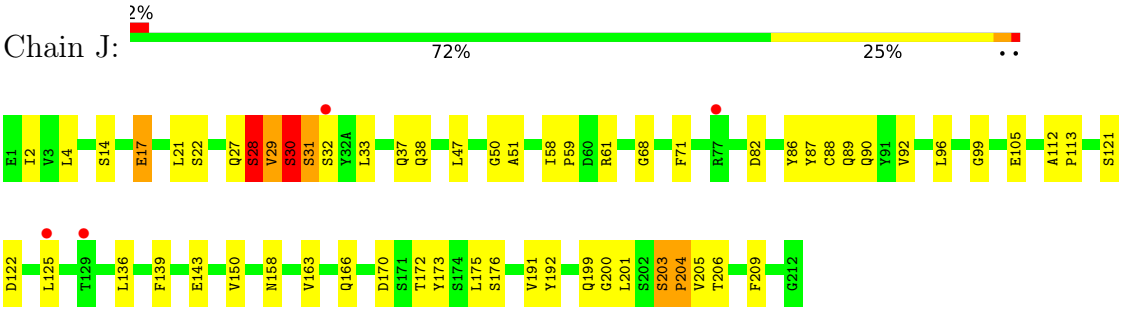
• Molecule 2: Antibody 27F3 light chain

Chain H:



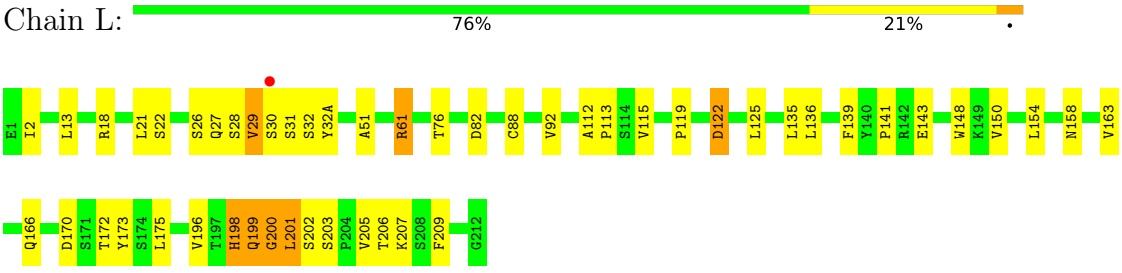
• Molecule 2: Antibody 27F3 light chain

Chain J:



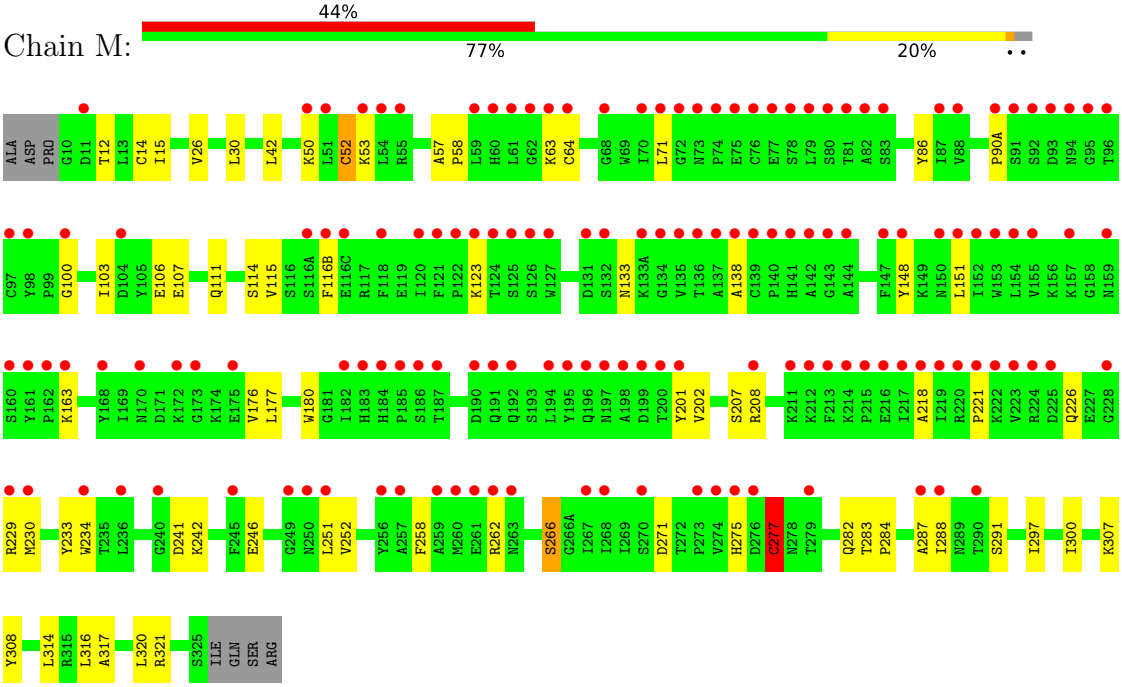
• Molecule 2: Antibody 27F3 light chain

Chain L:



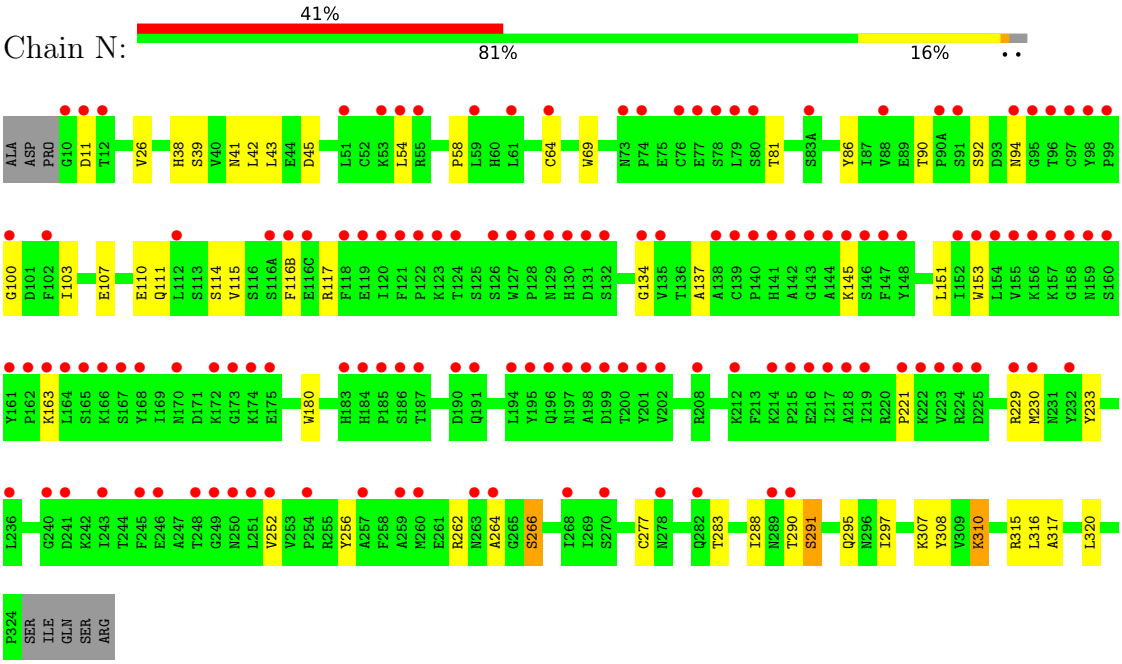
• Molecule 3: Hemagglutinin

Chain M:



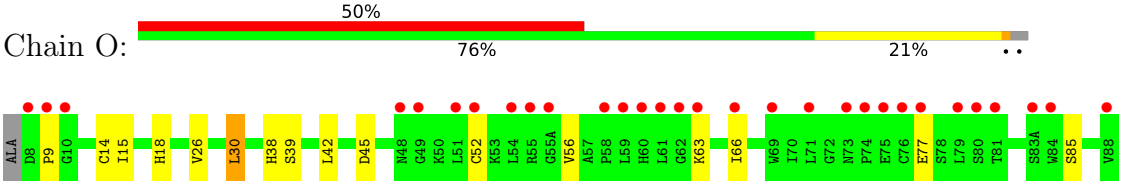
• Molecule 3: Hemagglutinin

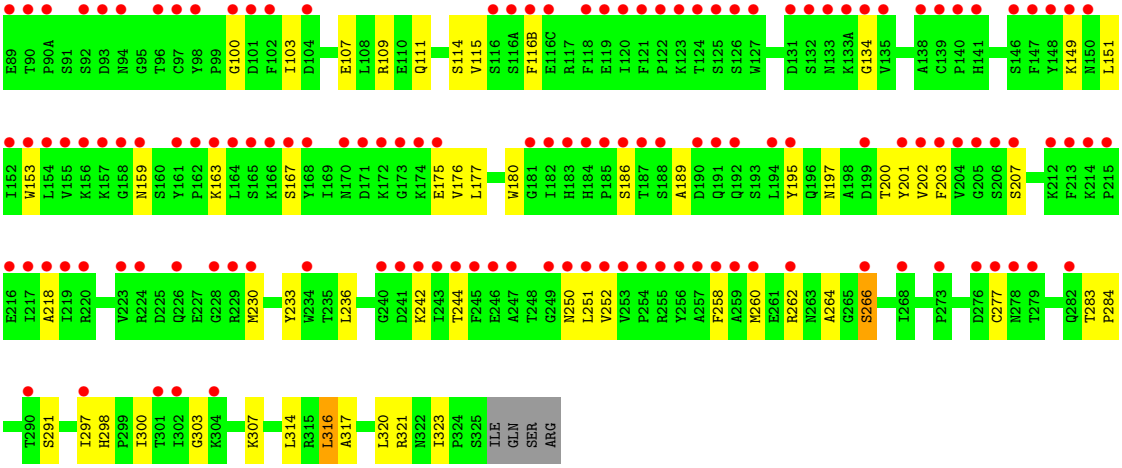
Chain N:



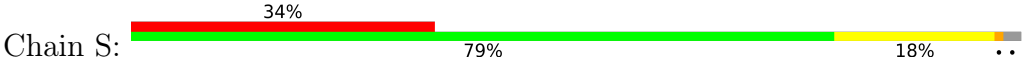
• Molecule 3: Hemagglutinin

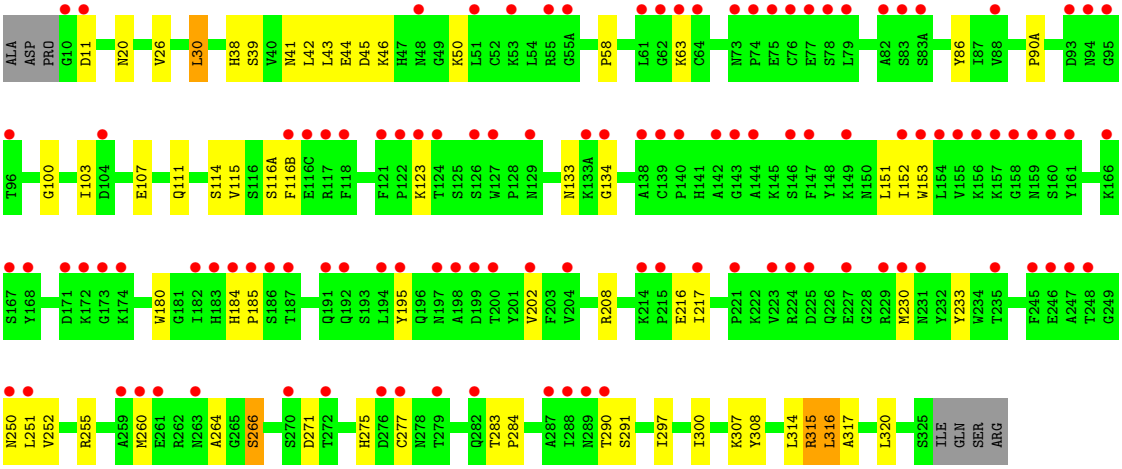
Chain O:



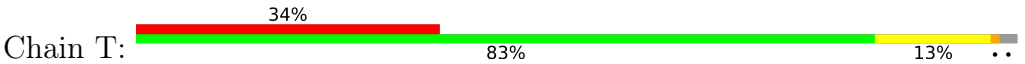


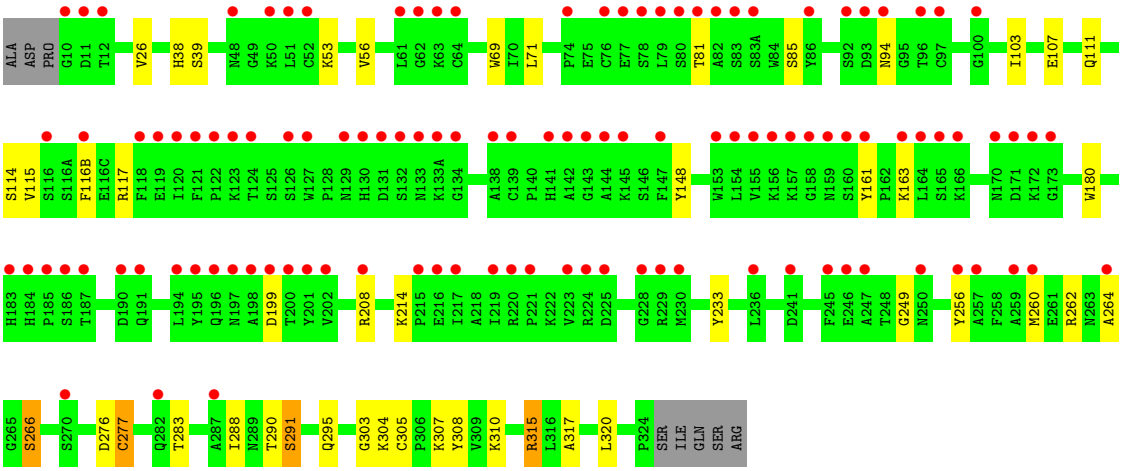
• Molecule 3: Hemagglutinin





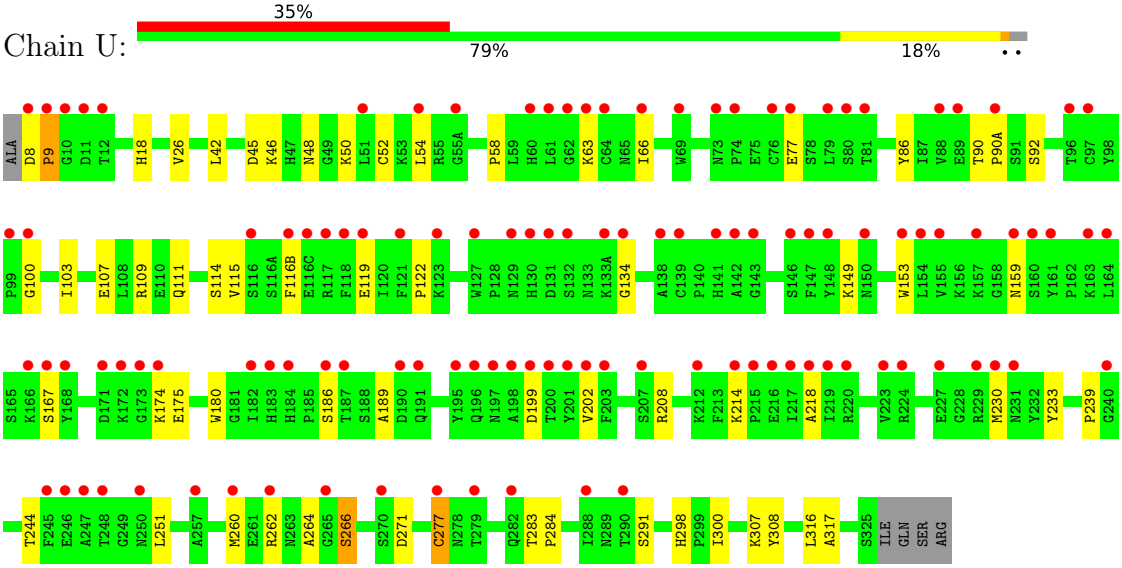
• Molecule 3: Hemagglutinin





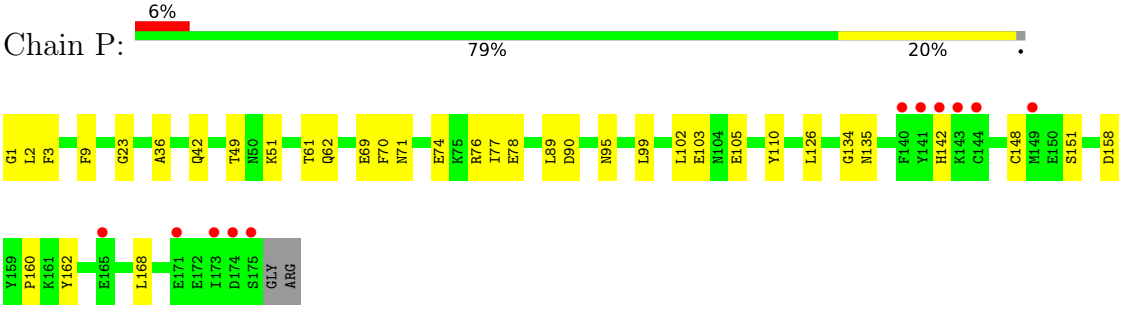
• Molecule 3: Hemagglutinin

Chain U:



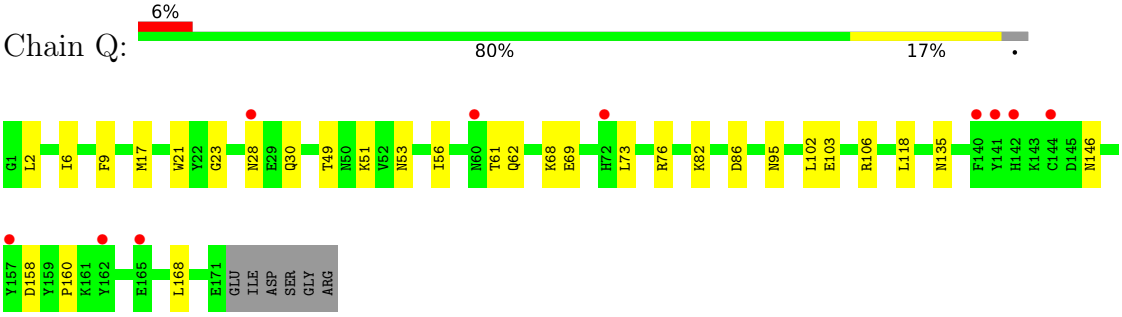
• Molecule 4: Hemagglutinin

Chain P:



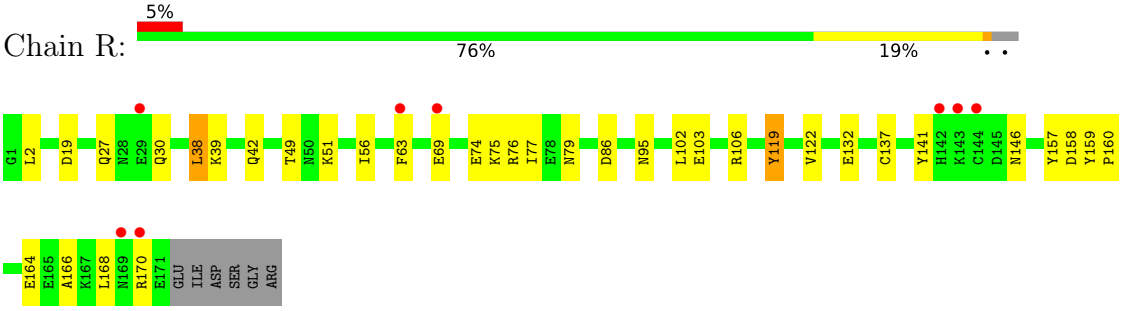
• Molecule 4: Hemagglutinin

Chain Q:



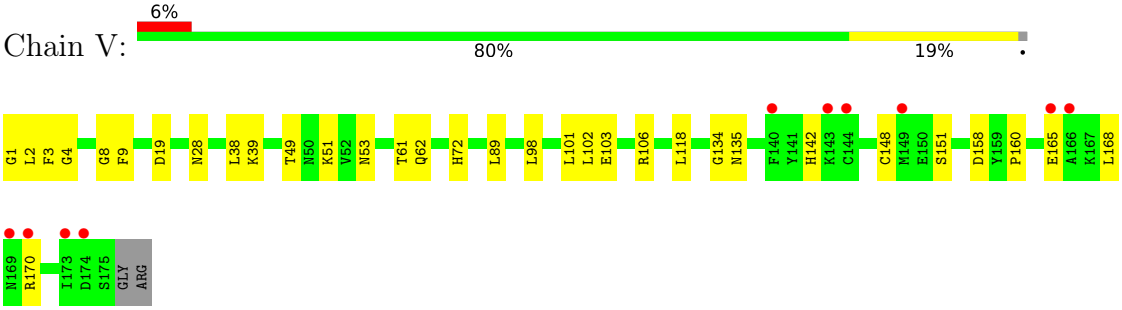
• Molecule 4: Hemagglutinin

Chain R:



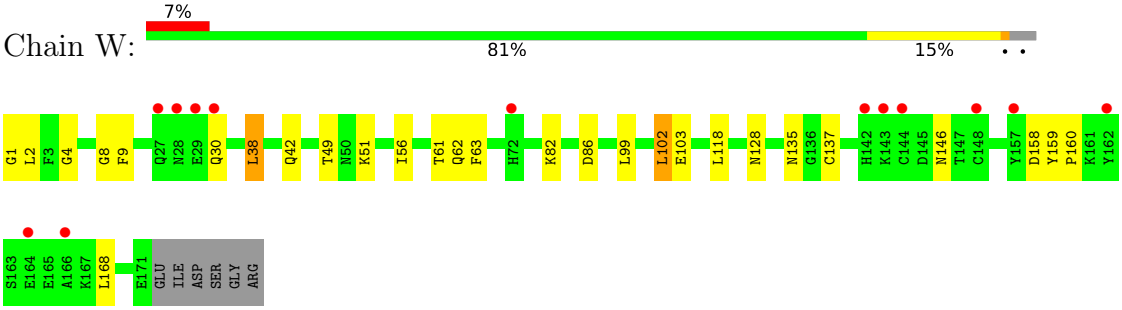
• Molecule 4: Hemagglutinin

Chain V:



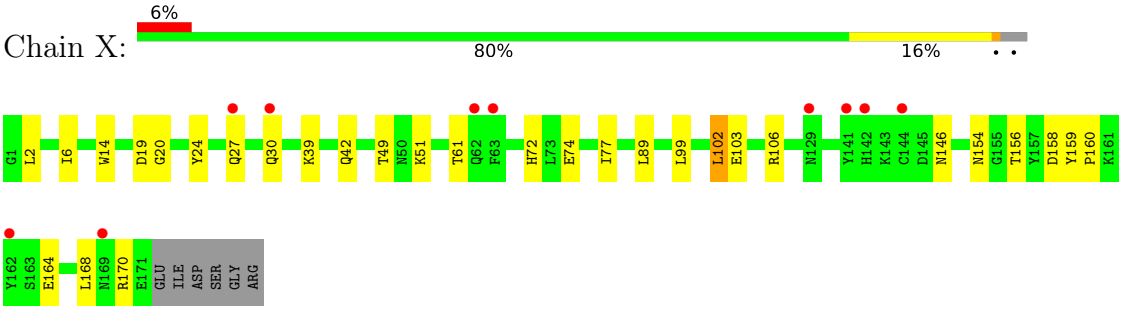
• Molecule 4: Hemagglutinin

Chain W:



• Molecule 4: Hemagglutinin

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	190.58Å 191.49Å 391.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 3.49 49.45 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.45-3.49) 98.1 (49.45-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.246 , 0.268 0.246 , 0.268	Depositor DCC
R_{free} test set	8910 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	90.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	43322	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.16% 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 (i)

5.1 Standard geometry (i)

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	1.09	3/1719 (0.2%)	0.83	2/2344 (0.1%)
1	C	0.92	0/1719	0.82	1/2344 (0.0%)
1	E	0.96	1/1719 (0.1%)	0.81	2/2344 (0.1%)
1	G	0.92	1/1719 (0.1%)	0.81	2/2344 (0.1%)
1	I	0.83	0/1719	0.75	1/2344 (0.0%)
1	K	1.05	1/1719 (0.1%)	0.82	1/2344 (0.0%)
2	B	1.19	0/1663	0.93	4/2260 (0.2%)
2	D	0.98	1/1663 (0.1%)	0.85	2/2260 (0.1%)
2	F	0.99	0/1663	0.83	0/2260
2	H	1.00	0/1663	0.84	0/2260
2	J	0.99	1/1663 (0.1%)	0.87	1/2260 (0.0%)
2	L	1.14	1/1663 (0.1%)	0.88	2/2260 (0.1%)
3	M	0.62	3/2593 (0.1%)	0.72	3/3524 (0.1%)
3	N	0.62	0/2587	0.79	3/3516 (0.1%)
3	O	0.57	1/2609 (0.0%)	0.74	2/3547 (0.1%)
3	S	0.62	0/2593	0.73	4/3524 (0.1%)
3	T	0.64	1/2587 (0.0%)	0.83	6/3516 (0.2%)
3	U	0.60	0/2609	0.75	1/3547 (0.0%)
4	P	1.01	1/1434 (0.1%)	0.87	0/1932
4	Q	1.04	1/1403 (0.1%)	0.86	2/1890 (0.1%)
4	R	0.94	2/1403 (0.1%)	0.86	1/1890 (0.1%)
4	V	0.99	0/1434	0.90	3/1932 (0.2%)
4	W	0.96	1/1403 (0.1%)	0.84	3/1890 (0.2%)
4	X	0.90	1/1403 (0.1%)	0.89	3/1890 (0.2%)
All	All	0.88	20/44350 (0.0%)	0.82	49/60222 (0.1%)

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
1	G	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
All	All	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	TYR	CE1-CZ	-8.04	1.28	1.38
1	E	211	VAL	C-N	7.65	1.51	1.34
2	J	17	GLU	CB-CG	-7.09	1.38	1.52
3	M	14	CYS	CB-SG	-6.31	1.71	1.82
4	Q	21	TRP	CB-CG	-6.09	1.39	1.50
2	L	88	CYS	CB-SG	-6.09	1.72	1.82
4	W	137	CYS	CB-SG	-6.07	1.72	1.82
2	D	194	CYS	CB-SG	-5.88	1.72	1.81
3	O	14	CYS	CB-SG	-5.87	1.72	1.81
4	R	119	TYR	CD1-CE1	-5.47	1.31	1.39
1	A	100(A)	TYR	CE1-CZ	-5.34	1.31	1.38
1	A	79	TYR	CE2-CZ	-5.24	1.31	1.38
1	K	96	LEU	C-N	-5.17	1.22	1.34
4	P	110	TYR	CE1-CZ	-5.16	1.31	1.38
4	R	137	CYS	CB-SG	-5.13	1.73	1.81
3	T	305	CYS	CB-SG	-5.12	1.73	1.81
1	G	96	LEU	C-N	-5.10	1.22	1.34
3	M	64	CYS	CB-SG	-5.10	1.73	1.81
3	M	52	CYS	CB-SG	-5.09	1.73	1.81
4	X	14	TRP	CB-CG	-5.06	1.41	1.50

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	277	CYS	CA-CB-SG	-15.68	85.77	114.00
3	S	277	CYS	CA-CB-SG	-8.97	97.85	114.00
3	T	320	LEU	CB-CG-CD2	-8.45	96.64	111.00
1	I	82(B)	SER	N-CA-C	-8.29	88.63	111.00
3	S	30	LEU	CB-CG-CD2	-7.80	97.73	111.00
2	B	30	SER	N-CA-CB	7.50	121.75	110.50
4	V	106	ARG	NE-CZ-NH1	-7.27	116.67	120.30
3	N	277	CYS	CA-CB-SG	-6.82	101.72	114.00
2	B	32	SER	N-CA-C	-6.72	92.85	111.00
2	B	201	LEU	CA-CB-CG	6.65	130.60	115.30
3	T	315	ARG	NE-CZ-NH1	-6.57	117.01	120.30
3	S	315	ARG	NE-CZ-NH1	-6.48	117.06	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	200	GLY	N-CA-C	-6.41	97.08	113.10
2	L	201	LEU	N-CA-C	-6.28	94.04	111.00
3	O	316	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	A	96	LEU	CA-CB-CG	-6.21	101.02	115.30
1	E	58	LYS	CD-CE-NZ	6.15	125.84	111.70
3	M	30	LEU	CB-CG-CD2	-6.01	100.78	111.00
3	O	30	LEU	CB-CG-CD2	-5.94	100.90	111.00
2	J	17	GLU	N-CA-CB	-5.84	100.08	110.60
2	B	32(A)	TYR	N-CA-C	-5.83	95.27	111.00
2	D	32	SER	N-CA-C	-5.82	95.27	111.00
4	V	39	LYS	CD-CE-NZ	5.76	124.95	111.70
3	M	277	CYS	CA-CB-SG	-5.67	103.80	114.00
4	Q	118	LEU	CB-CG-CD1	-5.67	101.37	111.00
4	Q	106	ARG	NE-CZ-NH1	-5.63	117.49	120.30
3	T	310	LYS	CD-CE-NZ	5.60	124.57	111.70
3	T	320	LEU	CB-CG-CD1	-5.59	101.50	111.00
4	W	1	GLY	N-CA-C	-5.58	99.14	113.10
4	X	102	LEU	CB-CG-CD2	-5.57	101.54	111.00
4	X	106	ARG	NE-CZ-NH1	-5.48	117.56	120.30
4	V	118	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	K	58	LYS	CD-CE-NZ	5.46	124.25	111.70
1	C	82(C)	LEU	N-CA-C	5.45	125.71	111.00
3	T	304	LYS	CG-CD-CE	5.37	128.00	111.90
4	W	102	LEU	CB-CG-CD2	-5.33	101.94	111.00
4	X	24	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	G	58	LYS	CD-CE-NZ	5.24	123.74	111.70
4	R	38	LEU	CB-CG-CD2	-5.22	102.12	111.00
4	W	38	LEU	CB-CG-CD2	-5.19	102.18	111.00
3	M	12	THR	CA-CB-CG2	-5.18	105.14	112.40
2	D	70	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	G	62	LYS	CD-CE-NZ	5.07	123.36	111.70
3	N	320	LEU	CA-CB-CG	5.07	126.96	115.30
1	E	94	ARG	NE-CZ-NH1	-5.06	117.77	120.30
3	N	315	ARG	NE-CZ-NH1	-5.03	117.79	120.30
3	S	316	LEU	CB-CG-CD2	-5.02	102.46	111.00
3	U	277	CYS	N-CA-CB	-5.02	101.56	110.60
1	A	82(A)	SER	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	148	GLU	Peptide
2	L	198	HIS	Mainchain

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	1675	0	1642	62	0
1	C	1675	0	1642	67	0
1	E	1675	0	1643	43	0
1	G	1675	0	1643	77	0
1	I	1675	0	1643	69	0
1	K	1675	0	1642	45	0
2	B	1628	0	1592	63	0
2	D	1628	0	1591	65	0
2	F	1628	0	1592	30	0
2	H	1628	0	1592	35	0
2	J	1628	0	1590	63	0
2	L	1628	0	1592	36	0
3	M	2529	0	2479	46	0
3	N	2523	0	2474	37	0
3	O	2544	0	2490	54	0
3	S	2529	0	2479	43	0
3	T	2523	0	2474	30	0
3	U	2544	0	2490	47	0
4	P	1406	0	1326	32	0
4	Q	1375	0	1300	28	0
4	R	1375	0	1300	32	0
4	V	1406	0	1326	33	0
4	W	1375	0	1300	23	0
4	X	1375	0	1300	26	0
All	All	43322	0	42142	966	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 11.

All (966) 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)
2:J:30:SER:OG	2:J:92:VAL:CG1	1.64	1.44
2:B:94:THR:CB	2:B:95:PRO:HD3	1.33	1.34
1:I:66:ARG:HB3	1:I:82(B):SER:CB	1.59	1.33
2:B:94:THR:CB	2:B:95:PRO:CD	2.07	1.32
1:I:17:SER:CB	1:I:82(A):SER:OG	1.76	1.31
1:A:68:THR:O	1:A:81:ASP:CB	1.78	1.29
1:I:17:SER:CA	1:I:82(A):SER:OG	1.83	1.25
1:I:83:SER:O	1:I:111:VAL:HG11	1.33	1.24
1:C:83:SER:O	1:C:111:VAL:HG11	1.27	1.24
2:D:29:VAL:HG11	2:D:71:PHE:CZ	1.71	1.24
1:A:83:SER:O	1:A:111:VAL:HG11	1.38	1.23
1:A:68:THR:O	1:A:81:ASP:HB2	1.08	1.23
2:D:112:ALA:HB2	2:D:200:GLY:O	1.36	1.23
1:G:145:TYR:CE2	1:G:150:VAL:CG2	2.22	1.21
2:J:30:SER:OG	2:J:92:VAL:HG11	1.17	1.19
2:F:29:VAL:HG23	2:F:68:GLY:O	1.38	1.19
1:G:145:TYR:CE1	1:G:176:TYR:HB2	1.78	1.18
1:G:145:TYR:HE2	1:G:150:VAL:CG2	1.56	1.16
1:G:145:TYR:HE1	1:G:176:TYR:CB	1.56	1.16
1:G:83:SER:O	1:G:111:VAL:HG11	1.46	1.15
1:I:66:ARG:HB3	1:I:82(B):SER:HB2	1.20	1.14
1:I:66:ARG:CB	1:I:82(B):SER:HB3	1.76	1.14
1:I:17:SER:HA	1:I:82(A):SER:OG	1.42	1.14
1:G:145:TYR:CE2	1:G:150:VAL:HG23	1.80	1.13
2:B:94:THR:HB	2:B:95:PRO:CD	1.71	1.13
2:B:94:THR:OG1	2:B:95:PRO:CD	2.00	1.10
1:A:67:VAL:HG23	1:A:81:ASP:O	1.51	1.08
2:J:29:VAL:CG2	2:J:68:GLY:O	2.01	1.08
1:I:66:ARG:CB	1:I:82(B):SER:CB	2.29	1.07
2:D:29:VAL:HG11	2:D:71:PHE:CE2	1.89	1.06
2:J:29:VAL:HG23	2:J:68:GLY:O	1.54	1.05
1:G:145:TYR:CE1	1:G:176:TYR:CB	2.37	1.05
1:A:68:THR:H	1:A:81:ASP:HB3	1.20	1.04
2:B:31:SER:OG	2:B:32(A):TYR:HD2	1.41	1.03
2:J:32:SER:O	2:J:50:GLY:O	1.76	1.03
1:A:18:VAL:HG23	1:A:82(C):LEU:HD21	1.38	1.02
1:K:66:ARG:O	1:K:82(A):SER:N	1.86	1.02
1:G:145:TYR:CE2	1:G:150:VAL:HG21	1.90	1.02
1:I:83:SER:O	1:I:111:VAL:CG1	2.09	1.01
1:E:66:ARG:NH1	1:E:82(B):SER:OG	1.90	1.01
2:B:94:THR:OG1	2:B:95:PRO:HD2	1.61	1.01
1:G:145:TYR:HE1	1:G:176:TYR:HB3	1.22	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:ARG:HB3	1:I:82(B):SER:HB3	1.37	1.00
1:I:17:SER:HA	1:I:82(A):SER:HG	1.16	0.99
1:G:28:THR:HG22	4:V:53:ASN:ND2	1.78	0.98
1:C:83:SER:O	1:C:111:VAL:CG1	2.11	0.98
1:A:68:THR:OG1	1:A:81:ASP:CG	2.03	0.97
3:M:221:PRO:HG3	3:O:242:LYS:HB3	1.46	0.97
1:A:74:SER:HB3	3:N:291:SER:HB3	1.43	0.97
2:D:29:VAL:CG1	2:D:71:PHE:CZ	2.48	0.97
1:I:66:ARG:HB2	1:I:82(B):SER:HB3	1.47	0.97
1:C:27:GLY:O	1:C:28:THR:HG23	1.65	0.96
1:A:68:THR:OG1	1:A:81:ASP:CB	2.14	0.96
1:I:17:SER:HB3	1:I:82(A):SER:OG	1.64	0.96
2:B:31:SER:OG	2:B:32(A):TYR:CD2	2.16	0.95
2:D:33:LEU:HD12	2:D:89:GLN:O	1.67	0.95
1:A:18:VAL:CG2	1:A:82(C):LEU:HD21	1.97	0.94
2:B:29:VAL:HG11	2:B:71:PHE:CZ	2.02	0.94
3:M:229:ARG:HH21	3:O:207:SER:HA	1.33	0.94
1:G:83:SER:O	1:G:111:VAL:CG1	2.16	0.93
2:D:29:VAL:CG1	2:D:71:PHE:HZ	1.80	0.93
2:B:94:THR:OG1	2:B:95:PRO:HD3	1.64	0.93
1:K:18:VAL:HG23	1:K:82(C):LEU:HD11	1.49	0.93
1:C:66:ARG:HB2	1:C:82(B):SER:HB2	1.48	0.93
1:I:17:SER:CA	1:I:82(A):SER:HG	1.73	0.92
1:A:68:THR:C	1:A:81:ASP:HB2	1.90	0.92
1:G:28:THR:HG22	4:V:53:ASN:HD21	1.35	0.91
1:G:145:TYR:CD2	1:G:150:VAL:CG2	2.52	0.91
1:A:68:THR:N	1:A:81:ASP:HB3	1.85	0.91
1:G:28:THR:CG2	4:V:53:ASN:ND2	2.34	0.90
1:C:27:GLY:C	1:C:28:THR:HG23	1.92	0.90
1:A:83:SER:O	1:A:111:VAL:CG1	2.20	0.90
1:G:145:TYR:CD2	1:G:150:VAL:HG21	2.06	0.90
1:C:27:GLY:O	1:C:28:THR:CB	2.20	0.89
2:D:29:VAL:HG11	2:D:71:PHE:HZ	1.34	0.89
2:D:32:SER:CB	2:D:51:ALA:HB2	2.02	0.88
2:J:30:SER:OG	2:J:92:VAL:CB	2.20	0.88
1:A:67:VAL:CG2	1:A:81:ASP:O	2.22	0.88
1:G:145:TYR:CD1	1:G:176:TYR:HB2	2.08	0.88
1:C:27:GLY:O	1:C:28:THR:OG1	1.91	0.88
2:J:30:SER:OG	2:J:92:VAL:HG12	1.74	0.88
1:C:27:GLY:O	1:C:28:THR:CG2	2.22	0.87
4:X:51:LYS:HE3	4:X:103:GLU:OE1	1.75	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:THR:HG22	4:Q:53:ASN:HD22	1.41	0.86
1:A:28:THR:HG22	4:Q:53:ASN:ND2	1.90	0.86
1:A:18:VAL:HG23	1:A:82(C):LEU:CD2	2.06	0.85
2:D:112:ALA:CB	2:D:200:GLY:O	2.24	0.85
2:J:112:ALA:HB2	2:J:200:GLY:O	1.76	0.85
2:B:94:THR:HB	2:B:95:PRO:HD3	0.85	0.84
1:I:96:LEU:HD12	1:I:96:LEU:O	1.77	0.84
1:I:17:SER:HB2	1:I:82(A):SER:OG	1.77	0.82
2:D:29:VAL:HG12	2:D:68:GLY:O	1.80	0.82
4:R:51:LYS:HE3	4:R:103:GLU:OE1	1.80	0.82
3:N:114:SER:HB2	3:N:266:SER:HB2	1.62	0.81
1:K:38:ARG:NH2	1:K:86:ASP:OD1	2.13	0.81
1:G:28:THR:CG2	4:V:53:ASN:HD22	1.93	0.81
1:A:47:TRP:CZ3	2:B:95:PRO:HA	2.14	0.81
1:C:66:ARG:HB2	1:C:82(B):SER:CB	2.11	0.80
2:B:29:VAL:HG11	2:B:71:PHE:HZ	1.46	0.80
2:B:39:LYS:NZ	2:B:81:GLU:O	2.14	0.80
3:M:242:LYS:HB3	3:N:221:PRO:HG3	1.63	0.80
2:J:112:ALA:HB1	2:J:201:LEU:HD13	1.63	0.80
2:F:31:SER:OG	2:F:32:SER:N	2.16	0.79
1:I:66:ARG:CB	1:I:82(B):SER:HB2	2.02	0.78
3:O:298:HIS:HE1	3:O:300:ILE:HD12	1.47	0.78
2:J:29:VAL:HG22	2:J:68:GLY:O	1.84	0.77
1:E:6:GLN:NE2	1:E:92:CYS:SG	2.58	0.77
2:J:61:ARG:NH1	2:J:82:ASP:OD2	2.18	0.77
2:L:112:ALA:HB2	2:L:200:GLY:O	1.85	0.77
1:A:6:GLN:NE2	1:A:92:CYS:SG	2.58	0.77
3:T:114:SER:HB2	3:T:266:SER:HB2	1.67	0.76
4:P:51:LYS:HE3	4:P:103:GLU:OE1	1.84	0.76
1:I:83:SER:OG	1:I:85:ASP:OD1	2.02	0.76
2:B:198:HIS:CD2	2:B:200:GLY:H	2.04	0.75
1:G:74:SER:HB3	3:S:291:SER:CB	2.16	0.75
2:J:31:SER:OG	2:J:32:SER:N	2.18	0.75
2:B:33:LEU:HD22	2:B:71:PHE:CD2	2.22	0.74
1:G:18:VAL:HG23	1:G:82(C):LEU:CD2	2.17	0.74
4:R:119:TYR:OH	4:R:132:GLU:OE2	2.04	0.74
1:A:68:THR:O	1:A:81:ASP:N	2.20	0.74
1:G:18:VAL:HG23	1:G:82(C):LEU:HD21	1.69	0.74
2:J:29:VAL:HG21	2:J:71:PHE:HE2	1.52	0.73
2:D:32:SER:OG	2:D:51:ALA:CB	2.36	0.73
1:E:6:GLN:HG3	1:E:106:GLY:H	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:89:VAL:HG22	1:I:108:THR:HG22	1.70	0.73
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.21	0.73
3:U:116(B):PHE:HE1	3:U:260:MET:HE1	1.53	0.73
1:G:74:SER:HB3	3:S:291:SER:OG	1.89	0.73
1:C:74:SER:HB3	3:U:291:SER:HB2	1.69	0.72
3:T:117:ARG:HD3	3:T:256:TYR:CD1	2.23	0.72
1:G:83:SER:OG	1:G:85:ASP:OD1	2.06	0.72
1:I:6:GLN:NE2	1:I:92:CYS:SG	2.62	0.72
1:C:6:GLN:HG3	1:C:106:GLY:H	1.54	0.72
1:G:6:GLN:NE2	1:G:92:CYS:SG	2.63	0.72
1:A:66:ARG:HD2	1:A:82(B):SER:OG	1.90	0.72
2:B:38:GLN:HE21	2:B:87:TYR:HE2	1.38	0.72
2:L:32:SER:HB2	2:L:51:ALA:HB2	1.70	0.71
2:B:198:HIS:HD2	2:B:200:GLY:H	1.36	0.71
2:F:29:VAL:HG21	2:F:71:PHE:HE2	1.54	0.70
1:G:145:TYR:CE1	1:G:176:TYR:HB3	2.15	0.70
2:H:204:PRO:O	2:H:206:THR:HG22	1.91	0.70
2:D:32:SER:HB2	2:D:51:ALA:HB2	1.71	0.70
1:K:18:VAL:CG2	1:K:82(C):LEU:HD11	2.21	0.70
3:M:114:SER:HB2	3:M:266:SER:HB2	1.73	0.70
1:C:18:VAL:HG23	1:C:82(C):LEU:HD21	1.74	0.70
2:D:32:SER:CB	2:D:51:ALA:CB	2.70	0.70
2:B:29:VAL:HG11	2:B:71:PHE:CE2	2.26	0.69
1:E:66:ARG:NH1	1:E:82(B):SER:HG	1.88	0.69
1:G:74:SER:HB3	3:S:291:SER:HB2	1.73	0.69
2:J:27:GLN:O	2:J:28:SER:O	2.09	0.69
1:A:89:VAL:HG22	1:A:108:THR:HG22	1.75	0.68
3:N:117:ARG:HD3	3:N:256:TYR:CD1	2.28	0.68
2:B:27:GLN:O	2:B:28:SER:C	2.30	0.68
1:I:74:SER:HB2	4:R:56:ILE:HG21	1.75	0.68
3:U:298:HIS:HE1	3:U:300:ILE:HD12	1.58	0.68
4:W:103:GLU:OE2	4:X:102:LEU:HD21	1.93	0.68
2:D:32:SER:HB2	2:D:51:ALA:CB	2.24	0.68
2:L:31:SER:OG	2:L:32:SER:N	2.24	0.68
1:I:82(B):SER:O	1:I:86:ASP:OD2	2.11	0.68
3:N:107:GLU:O	3:N:111:GLN:HG2	1.93	0.68
1:E:82(B):SER:HB2	1:E:82(C):LEU:HA	1.75	0.68
1:G:6:GLN:HG3	1:G:106:GLY:H	1.58	0.68
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.76	0.68
2:J:112:ALA:HB1	2:J:201:LEU:CD1	2.23	0.68
1:A:68:THR:O	1:A:81:ASP:CA	2.42	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:30:SER:O	2:J:31:SER:CB	2.41	0.67
1:I:163:VAL:HG22	1:I:182:VAL:HG22	1.76	0.67
1:K:74:SER:HB3	3:T:291:SER:HB3	1.75	0.67
1:C:66:ARG:CB	1:C:82(B):SER:HB2	2.23	0.67
3:T:107:GLU:O	3:T:111:GLN:HG2	1.95	0.67
2:B:38:GLN:NE2	2:B:87:TYR:HE2	1.91	0.66
1:C:18:VAL:HG23	1:C:82(C):LEU:CD2	2.25	0.66
2:D:32:SER:OG	2:D:51:ALA:HB2	1.93	0.66
3:O:134:GLY:HA3	3:O:153:TRP:HB3	1.77	0.66
1:K:119:PRO:HB3	1:K:145:TYR:HB3	1.77	0.66
1:E:119:PRO:HB3	1:E:145:TYR:HB3	1.78	0.66
1:A:68:THR:OG1	1:A:81:ASP:OD2	2.13	0.66
2:J:29:VAL:HG21	2:J:71:PHE:CE2	2.30	0.66
3:N:111:GLN:HE22	3:N:262:ARG:NH1	1.92	0.66
4:W:51:LYS:HE3	4:W:103:GLU:OE1	1.95	0.66
2:J:30:SER:OG	2:J:92:VAL:HB	1.96	0.66
4:Q:51:LYS:HE3	4:Q:103:GLU:OE1	1.96	0.66
1:C:16:SER:O	1:C:82(C):LEU:HB2	1.97	0.65
2:J:201:LEU:HD21	2:J:205:VAL:HG12	1.79	0.65
2:B:29:VAL:CG1	2:B:71:PHE:HZ	2.10	0.65
1:A:67:VAL:HA	1:A:81:ASP:O	1.96	0.65
1:C:53:ILE:HD13	4:X:49:THR:HA	1.79	0.65
2:D:141:PRO:HG3	2:D:199:GLN:NE2	2.12	0.65
2:B:29:VAL:CG1	2:B:71:PHE:CZ	2.78	0.64
3:O:26:VAL:HG21	3:O:317:ALA:HB2	1.78	0.64
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.78	0.64
1:I:82(B):SER:O	1:I:82(B):SER:OG	2.09	0.64
3:N:163:LYS:HB3	3:U:159:ASN:ND2	2.13	0.64
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.33	0.64
4:Q:69:GLU:O	4:R:76:ARG:NH1	2.28	0.64
2:B:94:THR:HG1	2:B:95:PRO:CD	2.09	0.64
1:C:36:TRP:CE2	1:C:80:MET:HB2	2.32	0.64
1:I:66:ARG:O	1:I:82:LEU:HD12	1.98	0.64
4:P:69:GLU:O	4:Q:76:ARG:NH1	2.31	0.64
2:H:112:ALA:HB2	2:H:200:GLY:O	1.98	0.64
2:F:170:ASP:OD1	2:F:172:THR:HG22	1.98	0.63
2:H:61:ARG:NH1	2:H:82:ASP:OD2	2.32	0.63
3:S:115:VAL:HG11	3:S:116(B):PHE:HB2	1.80	0.63
2:F:29:VAL:HG21	2:F:71:PHE:CE2	2.34	0.63
1:G:18:VAL:CG2	1:G:82(C):LEU:HD21	2.28	0.63
3:U:116(B):PHE:CE1	3:U:260:MET:HE1	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:154:ASN:OD1	4:X:156:THR:OG1	2.06	0.63
2:L:158:ASN:OD1	2:L:158:ASN:N	2.28	0.63
4:Q:30:GLN:OE1	4:Q:146:ASN:N	2.29	0.63
3:S:307:LYS:HE2	4:V:61:THR:HG22	1.81	0.63
1:I:52:SER:OG	1:I:54:PHE:HB3	1.99	0.63
3:U:115:VAL:HG11	3:U:116(B):PHE:HB2	1.79	0.63
2:B:170:ASP:OD1	2:B:172:THR:HG22	1.99	0.63
1:G:145:TYR:CD2	1:G:150:VAL:HG23	2.26	0.62
2:J:32:SER:HB2	2:J:51:ALA:HB2	1.80	0.62
2:B:32:SER:HB2	2:B:51:ALA:HB2	1.81	0.62
3:N:90:THR:OG1	3:N:92:SER:OG	2.10	0.62
1:G:83:SER:O	1:G:111:VAL:CB	2.48	0.62
3:M:115:VAL:HG11	3:M:116(B):PHE:HB2	1.80	0.62
1:K:6:GLN:NE2	1:K:92:CYS:SG	2.73	0.62
1:A:87:THR:OG1	1:A:110:THR:HA	1.99	0.62
1:C:27:GLY:C	1:C:28:THR:CG2	2.61	0.62
3:O:202:VAL:HG11	3:O:251:LEU:HD13	1.80	0.62
2:L:141:PRO:HG3	2:L:199:GLN:NE2	2.15	0.61
3:O:114:SER:HB2	3:O:266:SER:HB2	1.82	0.61
4:R:30:GLN:OE1	4:R:146:ASN:N	2.31	0.61
1:A:74:SER:HB2	4:Q:56:ILE:HG21	1.81	0.61
3:O:38:HIS:CD2	3:O:39:SER:N	2.68	0.61
1:K:6:GLN:HG3	1:K:106:GLY:H	1.63	0.61
3:N:111:GLN:NE2	3:N:262:ARG:NH1	2.48	0.61
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.82	0.61
2:D:61:ARG:NH1	2:D:82:ASP:OD1	2.33	0.61
2:F:166:GLN:HG3	2:F:173:TYR:CZ	2.35	0.60
1:G:36:TRP:CE2	1:G:80:MET:HB2	2.36	0.60
1:I:74:SER:HB3	3:O:291:SER:CB	2.31	0.60
3:M:229:ARG:NH2	3:O:207:SER:HA	2.10	0.60
3:O:42:LEU:HD11	3:O:316:LEU:HD22	1.82	0.60
1:I:74:SER:HB3	3:O:291:SER:HB2	1.83	0.60
4:V:158:ASP:OD1	4:V:160:PRO:HD2	2.01	0.60
1:E:74:SER:HB3	3:M:291:SER:OG	2.01	0.60
1:A:74:SER:HB3	3:N:291:SER:CB	2.25	0.60
2:H:32:SER:HB2	2:H:51:ALA:HB2	1.84	0.60
1:G:89:VAL:HG22	1:G:108:THR:HG22	1.83	0.60
3:U:90:THR:OG1	3:U:92:SER:OG	2.08	0.60
4:W:30:GLN:OE1	4:W:146:ASN:N	2.32	0.60
1:A:68:THR:CA	1:A:81:ASP:HB3	2.30	0.60
1:E:36:TRP:CZ3	1:E:92:CYS:HB3	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:201:TYR:OH	3:M:246:GLU:OE2	2.15	0.60
1:K:42:GLY:O	1:K:43:GLN:NE2	2.30	0.60
4:P:103:GLU:OE2	4:Q:102:LEU:HD21	2.01	0.60
2:D:30:SER:OG	2:D:92:VAL:CG1	2.50	0.60
1:A:61:GLN:N	1:A:61:GLN:OE1	2.35	0.60
1:E:66:ARG:HH11	1:E:82(B):SER:HG	1.42	0.60
2:D:27:GLN:O	2:D:28:SER:C	2.35	0.60
1:E:36:TRP:CE2	1:E:80:MET:HB2	2.36	0.59
2:J:205:VAL:HG13	2:J:205:VAL:O	2.02	0.59
1:A:6:GLN:HG3	1:A:106:GLY:H	1.67	0.59
2:B:158:ASN:N	2:B:158:ASN:OD1	2.33	0.59
3:U:308:TYR:CD2	4:X:89:LEU:HD13	2.38	0.59
2:D:29:VAL:HG22	2:D:29:VAL:O	2.03	0.59
2:L:29:VAL:O	2:L:29:VAL:HG12	2.02	0.59
4:V:51:LYS:HE3	4:V:103:GLU:OE1	2.03	0.59
1:E:40:ALA:HB3	1:E:43:GLN:HG3	1.85	0.58
1:G:36:TRP:CZ3	1:G:92:CYS:HB3	2.37	0.58
2:H:27:GLN:O	2:H:28:SER:C	2.41	0.58
2:J:30:SER:O	2:J:31:SER:OG	2.20	0.58
4:V:9:PHE:O	4:V:135:ASN:HA	2.03	0.58
1:G:87:THR:OG1	1:G:110:THR:HA	2.02	0.58
2:J:32:SER:O	2:J:50:GLY:C	2.40	0.58
1:I:5:VAL:HA	1:I:105:LYS:NZ	2.19	0.58
2:J:61:ARG:NH1	2:J:82:ASP:CG	2.57	0.58
1:K:36:TRP:CE2	1:K:80:MET:HB2	2.38	0.58
2:F:158:ASN:OD1	2:F:158:ASN:N	2.35	0.58
2:F:27:GLN:O	2:F:28:SER:C	2.41	0.58
1:G:53:ILE:HD13	4:V:49:THR:HA	1.85	0.58
2:H:158:ASN:OD1	2:H:158:ASN:N	2.36	0.58
1:I:74:SER:HB3	3:O:291:SER:OG	2.03	0.58
3:S:42:LEU:HD11	3:S:316:LEU:HD22	1.86	0.58
1:C:63:PHE:HD2	1:C:66:ARG:HD2	1.68	0.58
1:C:95:LYS:HE3	1:C:100(E):TYR:CZ	2.39	0.58
3:S:44:GLU:OE2	3:S:46:LYS:HG2	2.02	0.58
1:A:28:THR:CG2	4:Q:53:ASN:HD22	2.13	0.58
1:A:68:THR:OG1	1:A:81:ASP:HB2	2.02	0.58
2:D:32(A):TYR:HD1	2:D:91:TYR:CE2	2.22	0.58
2:D:158:ASN:OD1	2:D:158:ASN:N	2.37	0.58
2:D:112:ALA:HB1	2:D:201:LEU:CD2	2.34	0.58
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.86	0.58
2:J:201:LEU:HD21	2:J:205:VAL:CG1	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:95:ASN:ND2	4:R:95:ASN:HD21	2.01	0.58
4:P:134:GLY:O	4:P:135:ASN:OD1	2.23	0.57
3:S:39:SER:OG	3:S:315:ARG:NE	2.32	0.57
1:G:83:SER:OG	1:G:84:SER:N	2.35	0.57
2:J:61:ARG:NH1	2:J:82:ASP:OD1	2.37	0.57
3:U:199:ASP:OD1	3:U:214:LYS:NZ	2.37	0.57
1:K:83:SER:O	1:K:83:SER:OG	2.17	0.57
1:A:68:THR:C	1:A:81:ASP:CB	2.59	0.57
3:U:114:SER:HB2	3:U:266:SER:HB2	1.86	0.57
4:W:82:LYS:NZ	4:W:86:ASP:OD2	2.34	0.57
1:C:96:LEU:CD1	1:C:102:VAL:HG21	2.35	0.57
2:L:198:HIS:CG	2:L:199:GLN:H	2.23	0.57
3:T:115:VAL:HG11	3:T:116(B):PHE:HB2	1.87	0.57
2:D:166:GLN:HG3	2:D:173:TYR:CZ	2.39	0.57
3:S:103:ILE:HG13	3:S:233:TYR:CE2	2.40	0.57
3:O:163:LYS:NZ	3:O:201:TYR:OH	2.38	0.57
3:S:114:SER:HB2	3:S:266:SER:HB2	1.86	0.56
3:S:180:TRP:CE2	3:S:233:TYR:HB2	2.40	0.56
1:G:5:VAL:HA	1:G:105:LYS:NZ	2.20	0.56
3:N:42:LEU:HD11	3:N:316:LEU:HD22	1.87	0.56
3:S:307:LYS:HE2	4:V:61:THR:CG2	2.36	0.56
3:N:180:TRP:CE2	3:N:233:TYR:HB2	2.40	0.56
1:I:159:LEU:HD21	1:I:182:VAL:HG11	1.88	0.56
2:H:166:GLN:HG3	2:H:173:TYR:CZ	2.40	0.56
1:I:36:TRP:CE2	1:I:80:MET:HB2	2.40	0.56
3:N:26:VAL:HG21	3:N:317:ALA:HB2	1.88	0.56
1:A:105:LYS:HE2	1:A:105:LYS:H	1.69	0.56
1:E:87:THR:OG1	1:E:110:THR:HA	2.05	0.56
3:M:207:SER:HA	3:N:229:ARG:HH21	1.71	0.56
3:M:221:PRO:HG2	3:O:242:LYS:O	2.06	0.56
1:C:66:ARG:HB3	1:C:82(B):SER:OG	2.06	0.56
3:S:151:LEU:HB3	3:S:252:VAL:HG12	1.87	0.56
3:T:180:TRP:CE2	3:T:233:TYR:HB2	2.41	0.56
3:O:175:GLU:OE1	3:O:262:ARG:NH1	2.39	0.55
4:P:76:ARG:NH1	4:R:69:GLU:O	2.39	0.55
1:C:73:ILE:HD12	1:C:73:ILE:H	1.71	0.55
1:G:5:VAL:HA	1:G:105:LYS:HZ3	1.71	0.55
3:N:288:ILE:HG22	3:N:290:THR:HG22	1.88	0.55
1:I:105:LYS:H	1:I:105:LYS:HE2	1.71	0.55
3:U:42:LEU:HD11	3:U:316:LEU:HD22	1.87	0.55
3:M:221:PRO:CG	3:O:242:LYS:HB3	2.28	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:LEU:N	2:B:136:LEU:HD23	2.22	0.55
1:K:83:SER:O	1:K:85:ASP:N	2.36	0.55
2:B:94:THR:HG1	2:B:95:PRO:HD3	1.68	0.55
2:F:29:VAL:CG2	2:F:68:GLY:O	2.33	0.55
2:L:170:ASP:OD1	2:L:172:THR:HG22	2.06	0.55
2:D:206:THR:O	2:D:206:THR:OG1	2.22	0.55
2:J:14:SER:N	2:J:17:GLU:OE2	2.39	0.55
2:H:24:ARG:NH1	2:H:70:ASP:OD1	2.40	0.55
3:S:26:VAL:HG21	3:S:317:ALA:HB2	1.89	0.55
1:E:52:SER:O	1:E:53:ILE:N	2.40	0.54
1:E:67:VAL:HA	1:E:81:ASP:O	2.08	0.54
1:I:19:GLN:HG3	1:I:81:ASP:OD2	2.08	0.54
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.88	0.54
1:C:66:ARG:CB	1:C:82(B):SER:CB	2.82	0.54
2:F:136:LEU:HD23	2:F:136:LEU:N	2.22	0.54
1:E:19:GLN:HG3	1:E:81:ASP:OD2	2.06	0.54
2:H:204:PRO:O	2:H:206:THR:CG2	2.56	0.54
3:M:52:CYS:HB3	3:M:277:CYS:O	2.07	0.54
3:O:18:HIS:O	3:O:320:LEU:HD11	2.07	0.54
3:U:175:GLU:OE1	3:U:262:ARG:NH1	2.41	0.54
2:B:38:GLN:NE2	2:B:87:TYR:CE2	2.75	0.54
4:P:148:CYS:O	4:P:151:SER:OG	2.23	0.54
3:T:277:CYS:O	3:T:277:CYS:SG	2.55	0.54
1:I:38:ARG:HG3	1:I:90:TYR:CE1	2.43	0.54
3:N:115:VAL:HG11	3:N:116(B):PHE:HB2	1.90	0.54
1:K:163:VAL:HG22	1:K:182:VAL:HG22	1.90	0.53
3:N:295:GLN:O	3:N:308:TYR:HA	2.08	0.53
3:O:77:GLU:HG3	3:O:149:LYS:HE3	1.90	0.53
4:Q:82:LYS:NZ	4:Q:86:ASP:OD2	2.36	0.53
1:C:66:ARG:HD3	1:C:82(B):SER:HB2	1.89	0.53
1:K:59:TYR:HE1	1:K:69:ILE:HG13	1.74	0.53
3:U:202:VAL:HG11	3:U:251:LEU:HD13	1.90	0.53
1:E:84:SER:HA	1:E:111:VAL:HB	1.90	0.53
3:N:103:ILE:HG13	3:N:233:TYR:CE2	2.44	0.53
2:J:201:LEU:CD2	2:J:205:VAL:HG12	2.38	0.53
3:O:111:GLN:OE1	3:O:262:ARG:NE	2.42	0.53
4:X:27:GLN:O	4:X:27:GLN:HG3	2.08	0.53
1:C:74:SER:CB	3:U:291:SER:HB2	2.37	0.53
2:D:29:VAL:CG1	2:D:71:PHE:CE2	2.76	0.53
2:H:136:LEU:N	2:H:136:LEU:HD23	2.24	0.53
1:I:105:LYS:H	1:I:105:LYS:CE	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:GLN:O	2:F:28:SER:O	2.27	0.53
1:G:114:ALA:HB3	1:G:146:PHE:CE2	2.43	0.53
1:I:96:LEU:HD12	1:I:96:LEU:C	2.22	0.53
3:N:58:PRO:HB3	3:N:86:TYR:CZ	2.44	0.53
2:D:30:SER:OG	2:D:92:VAL:HG12	2.09	0.53
2:L:32(A):TYR:HB2	2:L:92:VAL:HG12	1.91	0.53
4:V:103:GLU:OE2	4:W:102:LEU:HD21	2.09	0.53
2:B:32:SER:HB2	2:B:51:ALA:CB	2.39	0.52
1:I:6:GLN:HG3	1:I:106:GLY:H	1.74	0.52
2:J:158:ASN:OD1	2:J:158:ASN:N	2.40	0.52
3:U:180:TRP:CE2	3:U:233:TYR:HB2	2.44	0.52
4:V:62:GLN:H	4:V:62:GLN:CD	2.13	0.52
3:O:115:VAL:HG11	3:O:116(B):PHE:HB2	1.91	0.52
2:L:136:LEU:HD21	2:L:196:VAL:HG21	1.90	0.52
3:T:307:LYS:HE2	4:W:61:THR:HG22	1.90	0.52
2:D:30:SER:OG	2:D:92:VAL:HG11	2.10	0.52
2:F:119:PRO:HB3	2:F:209:PHE:CE2	2.44	0.52
3:T:307:LYS:HE2	4:W:61:THR:CG2	2.40	0.52
3:M:26:VAL:HG21	3:M:317:ALA:HB2	1.92	0.52
4:P:62:GLN:NE2	4:Q:86:ASP:HB3	2.24	0.52
4:V:134:GLY:O	4:V:135:ASN:OD1	2.27	0.52
1:K:84:SER:H	1:K:111:VAL:HG11	1.75	0.52
3:O:38:HIS:CD2	3:O:39:SER:H	2.26	0.52
1:I:5:VAL:HA	1:I:105:LYS:HZ1	1.75	0.52
1:A:68:THR:H	1:A:81:ASP:CB	2.08	0.52
1:A:210:ARG:HH12	1:A:212:GLU:HB3	1.75	0.52
2:J:37:GLN:HG3	2:J:86:TYR:CE2	2.45	0.52
3:N:134:GLY:HA3	3:N:153:TRP:HB3	1.92	0.52
1:C:96:LEU:HD13	1:C:102:VAL:CG2	2.40	0.51
2:H:170:ASP:OD1	2:H:172:THR:HG22	2.09	0.51
1:G:52:SER:O	1:G:53:ILE:N	2.43	0.51
3:M:284:PRO:HD3	3:M:300:ILE:O	2.09	0.51
2:J:27:GLN:O	2:J:28:SER:C	2.44	0.51
3:N:163:LYS:HB3	3:U:159:ASN:HD21	1.74	0.51
1:I:154:TRP:CH2	1:I:196:CYS:HB3	2.45	0.51
1:A:52:SER:O	1:A:53:ILE:N	2.44	0.51
1:C:52:SER:O	1:C:53:ILE:N	2.43	0.51
1:E:5:VAL:HA	1:E:105:LYS:NZ	2.24	0.51
1:C:163:VAL:HG22	1:C:182:VAL:HG22	1.93	0.51
1:I:87:THR:OG1	1:I:110:THR:HA	2.11	0.51
3:M:288:ILE:HG21	3:M:297:ILE:HG13	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:GLN:HG3	2:B:173:TYR:CZ	2.46	0.51
2:D:141:PRO:O	2:D:198:HIS:HE1	1.93	0.51
1:E:148:GLU:OE1	1:E:149:PRO:HA	2.11	0.51
3:N:100:GLY:HA3	3:N:230:MET:O	2.10	0.51
2:B:32:SER:O	2:B:32:SER:OG	2.21	0.51
2:D:112:ALA:HB1	2:D:201:LEU:HD23	1.93	0.51
1:G:38:ARG:HG3	1:G:90:TYR:CE1	2.46	0.50
1:C:38:ARG:HG3	1:C:90:TYR:CE1	2.46	0.50
1:K:100(A):TYR:HD2	4:W:42:GLN:OE1	1.93	0.50
1:A:59:TYR:HE1	1:A:69:ILE:HG13	1.77	0.50
1:C:74:SER:HB3	3:U:291:SER:CB	2.38	0.50
2:H:175:LEU:HD12	2:H:176:SER:H	1.77	0.50
3:M:103:ILE:HG13	3:M:233:TYR:CE2	2.47	0.50
1:E:32:TYR:HB3	1:E:100:TYR:CD1	2.46	0.50
1:G:28:THR:HG21	4:V:53:ASN:HD22	1.71	0.50
3:T:69:TRP:HE1	3:T:81:THR:HG21	1.77	0.50
1:A:68:THR:CA	1:A:81:ASP:CB	2.89	0.50
2:D:29:VAL:HG11	2:D:71:PHE:HE2	1.69	0.50
2:F:47:LEU:HD23	2:F:58:ILE:HD12	1.94	0.50
2:J:32:SER:HB2	2:J:51:ALA:CB	2.42	0.50
2:L:115:VAL:HG22	2:L:136:LEU:HD22	1.93	0.50
3:O:100:GLY:HA3	3:O:230:MET:O	2.11	0.50
4:Q:95:ASN:HD21	4:R:95:ASN:HD21	1.58	0.50
4:V:98:LEU:O	4:V:102:LEU:HG	2.11	0.50
1:A:105:LYS:H	1:A:105:LYS:CE	2.25	0.50
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.46	0.50
3:M:151:LEU:HB3	3:M:252:VAL:HG12	1.94	0.50
3:U:77:GLU:HG3	3:U:149:LYS:HE3	1.94	0.50
1:E:59:TYR:HE1	1:E:69:ILE:HG13	1.76	0.49
4:P:158:ASP:OD1	4:P:160:PRO:HD2	2.12	0.49
1:K:74:SER:HB2	4:W:56:ILE:HG21	1.93	0.49
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.47	0.49
3:N:11:ASP:OD1	4:Q:28:ASN:HA	2.11	0.49
4:P:70:PHE:CE2	4:P:78:GLU:HA	2.47	0.49
3:S:134:GLY:HA3	3:S:153:TRP:HB3	1.93	0.49
4:W:62:GLN:CD	4:W:62:GLN:H	2.14	0.49
3:O:189:ALA:HA	3:U:189:ALA:CB	2.42	0.49
3:M:111:GLN:OE1	3:M:262:ARG:NH1	2.41	0.49
2:B:32(A):TYR:HD1	2:B:91:TYR:CE2	2.30	0.49
2:J:170:ASP:OD1	2:J:172:THR:HG22	2.12	0.49
2:D:24:ARG:NH1	2:D:70:ASP:OD1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:74:SER:HB3	3:T:291:SER:CB	2.40	0.49
4:P:9:PHE:O	4:P:135:ASN:HA	2.12	0.49
1:E:36:TRP:CH2	1:E:92:CYS:HB3	2.47	0.49
1:G:145:TYR:HD2	1:G:150:VAL:CG2	2.19	0.49
3:S:50:LYS:HD2	3:S:275:HIS:HB2	1.94	0.49
1:G:145:TYR:CD1	1:G:145:TYR:C	2.85	0.49
1:I:83:SER:O	1:I:111:VAL:CB	2.59	0.49
3:U:284:PRO:HD3	3:U:300:ILE:O	2.13	0.49
1:C:66:ARG:CB	1:C:82(B):SER:OG	2.61	0.49
1:I:52:SER:O	1:I:53:ILE:N	2.46	0.49
3:T:103:ILE:HG13	3:T:233:TYR:CE2	2.47	0.49
2:B:30:SER:OG	2:B:92:VAL:HG11	2.12	0.48
2:D:67:SER:HA	2:D:71:PHE:CE1	2.47	0.48
2:B:29:VAL:CG1	2:B:71:PHE:CE2	2.95	0.48
1:C:47:TRP:CG	2:D:96:LEU:HB2	2.48	0.48
2:F:32:SER:HB2	2:F:51:ALA:HB2	1.95	0.48
1:K:84:SER:O	1:K:87:THR:HG22	2.13	0.48
1:E:95:LYS:HE3	1:E:100(E):TYR:CZ	2.48	0.48
1:G:42:GLY:O	1:G:43:GLN:NE2	2.43	0.48
1:G:145:TYR:HD1	1:G:145:TYR:O	1.97	0.48
3:O:284:PRO:HD3	3:O:300:ILE:O	2.14	0.48
2:B:105:GLU:OE1	2:B:173:TYR:OH	2.26	0.48
1:C:87:THR:OG1	1:C:110:THR:HA	2.13	0.48
1:G:25:SER:O	1:G:25:SER:OG	2.19	0.48
2:J:4:LEU:HD11	2:J:90:GLN:HB3	1.96	0.48
2:L:141:PRO:O	2:L:198:HIS:HE1	1.97	0.48
3:S:123:LYS:NZ	3:S:133:ASN:HD21	2.10	0.48
1:E:74:SER:HB3	3:M:291:SER:CB	2.43	0.48
1:K:52:SER:O	1:K:53:ILE:N	2.46	0.48
3:O:186:SER:HA	3:O:218:ALA:O	2.12	0.48
2:F:83:PHE:HA	2:F:104:VAL:HG23	1.96	0.48
1:G:73:ILE:H	1:G:73:ILE:HD12	1.79	0.48
1:I:123:PRO:HD2	2:J:121:SER:HB3	1.94	0.48
3:T:199:ASP:OD1	3:T:214:LYS:NZ	2.42	0.48
4:X:158:ASP:OD1	4:X:160:PRO:HD2	2.13	0.48
4:X:159:TYR:HB3	4:X:160:PRO:HD3	1.95	0.48
2:D:61:ARG:NH1	2:D:82:ASP:OD2	2.47	0.48
1:E:38:ARG:HG3	1:E:90:TYR:CE1	2.48	0.48
2:L:198:HIS:CG	2:L:199:GLN:N	2.81	0.48
3:O:66:ILE:HD12	3:O:109:ARG:CZ	2.44	0.48
2:D:30:SER:OG	2:D:31:SER:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:TRP:CG	1:E:80:MET:HG3	2.48	0.48
1:E:53:ILE:HD13	4:P:49:THR:HA	1.96	0.48
3:O:307:LYS:NZ	4:P:90:ASP:OD2	2.41	0.48
1:C:40:ALA:HB3	1:C:43:GLN:HB2	1.95	0.48
2:D:163:VAL:HG22	2:D:175:LEU:HD13	1.96	0.48
1:I:47:TRP:CG	2:J:96:LEU:HB2	2.49	0.48
1:I:82(C):LEU:HD12	1:I:82(C):LEU:HA	1.53	0.48
1:I:95:LYS:HE3	1:I:100(E):TYR:CZ	2.49	0.48
4:R:164:GLU:O	4:R:168:LEU:HD13	2.13	0.48
1:A:7:SER:HB3	1:A:21:SER:OG	2.14	0.47
1:C:6:GLN:NE2	1:C:92:CYS:SG	2.87	0.47
2:D:32:SER:C	2:D:50:GLY:O	2.52	0.47
1:I:47:TRP:CD2	2:J:96:LEU:HB2	2.49	0.47
3:U:100:GLY:HA3	3:U:230:MET:O	2.14	0.47
1:C:100(B):PHE:CE1	4:X:19:ASP:HA	2.49	0.47
1:K:51:ILE:HD11	1:K:71:ALA:HB2	1.96	0.47
3:O:159:ASN:ND2	3:T:163:LYS:NZ	2.62	0.47
3:T:288:ILE:HG22	3:T:290:THR:HG22	1.96	0.47
1:C:47:TRP:NE1	2:D:96:LEU:HD12	2.29	0.47
1:E:143:LYS:HE3	1:E:144:ASP:OD1	2.14	0.47
1:K:105:LYS:HE2	1:K:105:LYS:H	1.80	0.47
2:L:141:PRO:CG	2:L:199:GLN:NE2	2.77	0.47
3:S:44:GLU:HG2	3:S:290:THR:HG21	1.97	0.47
4:V:102:LEU:CD2	4:X:103:GLU:OE2	2.62	0.47
1:I:100(B):PHE:CE1	4:R:19:ASP:HA	2.49	0.47
3:M:307:LYS:HE2	4:P:61:THR:HG22	1.97	0.47
3:T:111:GLN:HE22	3:T:262:ARG:NH1	2.11	0.47
3:U:48:ASN:O	3:U:50:LYS:HG2	2.14	0.47
2:D:8:PRO:HG2	2:D:10:THR:O	2.14	0.47
1:G:129:LYS:HE2	1:G:129:LYS:HA	1.96	0.47
2:L:136:LEU:N	2:L:136:LEU:HD23	2.28	0.47
1:C:59:TYR:HE1	1:C:69:ILE:HG13	1.80	0.47
2:D:47:LEU:O	2:D:48:ILE:HD13	2.15	0.47
3:S:123:LYS:HZ1	3:S:133:ASN:ND2	2.12	0.47
1:A:32:TYR:HB3	1:A:100:TYR:CD1	2.50	0.47
1:A:38:ARG:HG3	1:A:90:TYR:CE1	2.50	0.47
1:G:159:LEU:HD21	1:G:182:VAL:HG11	1.96	0.47
3:M:100:GLY:HA3	3:M:230:MET:O	2.15	0.47
3:S:185:PRO:O	3:S:217:ILE:HA	2.15	0.47
3:U:262:ARG:HG3	3:U:262:ARG:HH11	1.78	0.47
3:U:307:LYS:HE2	4:X:61:THR:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:TRP:NE1	2:J:96:LEU:HD12	2.30	0.47
3:N:307:LYS:HE2	4:Q:61:THR:CG2	2.45	0.47
3:O:195:TYR:CZ	3:O:250:ASN:HA	2.49	0.47
3:T:38:HIS:CD2	3:T:39:SER:N	2.83	0.47
2:B:175:LEU:HD12	2:B:176:SER:H	1.79	0.47
1:C:38:ARG:NH2	1:C:86:ASP:OD1	2.48	0.47
3:S:202:VAL:HG11	3:S:251:LEU:HD13	1.97	0.47
1:I:144:ASP:OD1	1:I:171:GLN:NE2	2.43	0.46
3:O:56:VAL:HB	3:O:85:SER:HB3	1.98	0.46
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.97	0.46
3:S:100:GLY:HA3	3:S:230:MET:O	2.15	0.46
1:A:61:GLN:HA	1:A:64:GLN:HB2	1.98	0.46
3:M:50:LYS:HD2	3:M:275:HIS:HB2	1.97	0.46
3:M:58:PRO:HB3	3:M:86:TYR:CZ	2.51	0.46
1:C:105:LYS:HE2	1:C:105:LYS:H	1.80	0.46
1:G:105:LYS:H	1:G:105:LYS:HE2	1.80	0.46
1:K:94:ARG:NE	1:K:95:LYS:O	2.41	0.46
4:X:30:GLN:OE1	4:X:146:ASN:N	2.42	0.46
2:B:21:LEU:N	2:B:21:LEU:HD12	2.31	0.46
1:K:129:LYS:HE2	1:K:129:LYS:HA	1.96	0.46
3:M:114:SER:HB2	3:M:266:SER:CB	2.44	0.46
3:N:110:GLU:HG3	4:R:75:LYS:HE3	1.96	0.46
3:U:58:PRO:HB3	3:U:86:TYR:CZ	2.50	0.46
4:V:142:HIS:HB2	4:V:165:GLU:CD	2.36	0.46
2:F:30:SER:HB2	2:F:92:VAL:CG1	2.46	0.46
2:H:67:SER:HA	2:H:71:PHE:CE1	2.51	0.46
3:N:163:LYS:CB	3:U:159:ASN:ND2	2.78	0.46
4:P:102:LEU:HD23	4:P:102:LEU:HA	1.77	0.46
3:S:107:GLU:O	3:S:111:GLN:HG2	2.15	0.46
3:S:123:LYS:NZ	3:S:133:ASN:ND2	2.64	0.46
3:T:111:GLN:NE2	3:T:262:ARG:NH1	2.63	0.46
1:A:67:VAL:CA	1:A:81:ASP:O	2.63	0.46
2:B:89:GLN:HG2	2:B:90:GLN:N	2.31	0.46
1:C:154:TRP:CH2	1:C:196:CYS:HB3	2.50	0.46
2:J:47:LEU:HD11	2:J:86:TYR:HE2	1.81	0.46
2:J:89:GLN:HG2	2:J:90:GLN:N	2.31	0.46
2:J:192:TYR:HB2	2:J:209:PHE:CE1	2.51	0.46
1:K:84:SER:H	1:K:111:VAL:CG1	2.29	0.46
3:U:208:ARG:NH1	4:V:72:HIS:CD2	2.83	0.46
2:B:206:THR:O	2:B:206:THR:OG1	2.26	0.46
1:G:52:SER:OG	1:G:54:PHE:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:202:VAL:HG11	3:M:251:LEU:HD13	1.96	0.46
4:R:158:ASP:OD1	4:R:160:PRO:HD2	2.16	0.46
1:C:53:ILE:CD1	4:X:49:THR:HA	2.46	0.46
2:F:119:PRO:HB3	2:F:209:PHE:CZ	2.51	0.46
1:I:59:TYR:HE1	1:I:69:ILE:HG13	1.81	0.46
2:L:21:LEU:HD12	2:L:21:LEU:N	2.30	0.46
3:O:107:GLU:O	3:O:111:GLN:HG2	2.16	0.46
3:O:303:GLY:HA2	4:R:63:PHE:CE2	2.50	0.46
4:W:4:GLY:O	4:W:8:GLY:HA3	2.15	0.46
2:D:141:PRO:CG	2:D:199:GLN:NE2	2.77	0.46
1:E:47:TRP:CG	2:F:96:LEU:HB2	2.51	0.46
2:H:198:HIS:CD2	2:H:199:GLN:O	2.68	0.46
3:O:167:SER:OG	3:O:244:THR:HG22	2.16	0.46
3:S:284:PRO:HD3	3:S:300:ILE:O	2.15	0.46
2:D:136:LEU:N	2:D:136:LEU:HD23	2.31	0.45
2:D:150:VAL:HG13	2:D:155:GLN:HG2	1.98	0.45
2:H:200:GLY:O	2:H:201:LEU:HD23	2.16	0.45
3:S:38:HIS:CD2	3:S:39:SER:N	2.84	0.45
1:A:36:TRP:CD2	1:A:80:MET:HG3	2.52	0.45
3:N:38:HIS:CD2	3:N:39:SER:N	2.84	0.45
1:A:47:TRP:HZ3	2:B:95:PRO:HA	1.75	0.45
1:E:96:LEU:HD12	1:E:96:LEU:HA	1.75	0.45
1:G:4:LEU:HD11	1:G:94:ARG:HG2	1.99	0.45
1:G:87:THR:HG1	1:G:110:THR:HA	1.81	0.45
1:G:145:TYR:CD1	1:G:145:TYR:O	2.70	0.45
3:U:107:GLU:O	3:U:111:GLN:HG2	2.17	0.45
4:V:102:LEU:HD21	4:X:103:GLU:OE2	2.16	0.45
2:D:175:LEU:HD12	2:D:176:SER:H	1.81	0.45
2:J:136:LEU:N	2:J:136:LEU:HD23	2.31	0.45
4:W:9:PHE:O	4:W:135:ASN:HA	2.16	0.45
1:G:95:LYS:HE3	1:G:100(E):TYR:CZ	2.51	0.45
1:I:72:ASP:OD1	3:O:291:SER:OG	2.30	0.45
2:J:33:LEU:HD22	2:J:71:PHE:CG	2.52	0.45
2:J:203:SER:OG	2:J:203:SER:O	2.34	0.45
3:N:69:TRP:HE1	3:N:81:THR:HG21	1.81	0.45
4:R:74:GLU:HB3	4:R:77:ILE:HD11	1.98	0.45
3:U:134:GLY:HA3	3:U:153:TRP:HB3	1.98	0.45
2:F:141:PRO:HG3	2:F:199:GLN:NE2	2.31	0.45
2:H:32(A):TYR:HB2	2:H:92:VAL:HG12	1.99	0.45
2:J:38:GLN:NE2	2:J:87:TYR:HE2	2.14	0.45
2:L:112:ALA:CB	2:L:200:GLY:O	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:39:LYS:HB2	4:X:39:LYS:HE3	1.69	0.45
1:A:5:VAL:HA	1:A:105:LYS:NZ	2.32	0.45
1:C:83:SER:O	1:C:111:VAL:CB	2.64	0.45
2:J:21:LEU:HD12	2:J:21:LEU:N	2.32	0.45
1:C:131:THR:HA	1:C:136:ALA:HA	1.97	0.45
2:F:139:PHE:HD2	2:F:198:HIS:CE1	2.34	0.45
1:G:83:SER:O	1:G:111:VAL:HB	2.17	0.45
2:J:105:GLU:OE1	2:J:173:TYR:OH	2.27	0.45
3:O:321:ARG:HD2	3:O:323:ILE:HD11	1.98	0.45
2:L:148:TRP:O	2:L:154:LEU:HD12	2.17	0.45
3:M:282:GLN:OE1	3:M:287:ALA:HB2	2.17	0.45
3:O:45:ASP:C	3:O:297:ILE:HD11	2.36	0.45
4:W:158:ASP:OD1	4:W:160:PRO:HD2	2.17	0.45
4:X:6:ILE:HD13	4:X:6:ILE:HG21	1.73	0.45
2:D:33:LEU:HD12	2:D:89:GLN:C	2.33	0.45
2:J:113:PRO:HB3	2:J:139:PHE:HB3	1.99	0.45
2:L:32(A):TYR:HB2	2:L:92:VAL:CG1	2.47	0.45
3:M:221:PRO:HG3	3:O:242:LYS:CB	2.32	0.45
4:V:4:GLY:O	4:V:8:GLY:HA3	2.17	0.45
4:V:38:LEU:HA	4:V:38:LEU:HD23	1.77	0.45
1:C:96:LEU:CD1	1:C:102:VAL:CG2	2.95	0.44
4:V:2:LEU:HD12	4:V:2:LEU:HA	1.69	0.44
1:G:66:ARG:HB3	1:G:82(A):SER:O	2.18	0.44
2:J:166:GLN:HG3	2:J:173:TYR:CZ	2.52	0.44
1:K:66:ARG:HB3	1:K:82(A):SER:HB2	1.03	0.44
3:N:137:ALA:HA	3:N:145:LYS:HG2	1.99	0.44
4:Q:9:PHE:O	4:Q:135:ASN:HA	2.18	0.44
3:U:90(A):PRO:HD2	3:U:271:ASP:OD1	2.17	0.44
4:V:3:PHE:CZ	4:W:2:LEU:HG	2.52	0.44
1:C:209:LYS:HD2	1:C:209:LYS:HA	1.86	0.44
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.98	0.44
1:G:53:ILE:CD1	4:V:49:THR:HA	2.47	0.44
1:G:197:ASN:ND2	1:G:208:ASP:OD2	2.45	0.44
3:M:314:LEU:HD23	3:M:314:LEU:HA	1.85	0.44
3:T:69:TRP:HE1	3:T:81:THR:CG2	2.31	0.44
3:T:295:GLN:O	3:T:308:TYR:HA	2.17	0.44
4:V:1:GLY:O	4:V:2:LEU:C	2.56	0.44
2:B:145:LYS:HE2	2:B:147:GLN:NE2	2.32	0.44
1:C:66:ARG:CD	1:C:82(B):SER:HB2	2.47	0.44
2:D:47:LEU:HD23	2:D:58:ILE:HD12	1.98	0.44
2:D:161:GLU:HA	2:D:177:SER:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:LEU:HD22	2:J:71:PHE:CD2	2.52	0.44
3:U:111:GLN:OE1	3:U:262:ARG:NE	2.50	0.44
1:A:53:ILE:HD13	4:Q:49:THR:HA	1.98	0.44
1:A:66:ARG:HB3	1:A:82(B):SER:OG	2.18	0.44
2:D:33:LEU:HD12	2:D:33:LEU:HA	1.70	0.44
2:J:163:VAL:HG22	2:J:175:LEU:HD13	1.99	0.44
2:J:175:LEU:HD12	2:J:176:SER:H	1.82	0.44
1:K:73:ILE:HD12	1:K:73:ILE:H	1.81	0.44
3:M:90(A):PRO:HD2	3:M:271:ASP:OD1	2.18	0.44
3:O:180:TRP:CE2	3:O:233:TYR:HB2	2.52	0.44
3:S:30:LEU:HD23	3:S:30:LEU:HA	1.61	0.44
3:T:56:VAL:HB	3:T:85:SER:HB3	1.99	0.44
4:X:2:LEU:HD12	4:X:2:LEU:HA	1.75	0.44
1:C:32:TYR:HB3	1:C:100:TYR:CD1	2.53	0.44
1:C:63:PHE:CD2	1:C:66:ARG:HD2	2.51	0.44
1:C:154:TRP:CZ3	1:C:196:CYS:HB3	2.52	0.44
2:F:78:LEU:HD23	2:F:78:LEU:HA	1.73	0.44
2:F:175:LEU:HD12	2:F:176:SER:H	1.83	0.44
2:H:118:PHE:HB2	2:H:133:VAL:HB	2.00	0.44
2:L:18:ARG:HG2	2:L:76:THR:HA	1.99	0.44
3:O:52:CYS:HB3	3:O:277:CYS:O	2.16	0.44
2:B:11:LEU:O	2:B:104:VAL:HA	2.18	0.44
2:B:39:LYS:HG2	2:B:84:ALA:HB2	1.98	0.44
2:F:21:LEU:N	2:F:21:LEU:HD12	2.33	0.44
1:G:36:TRP:CH2	1:G:92:CYS:HB3	2.52	0.44
1:G:178:LEU:C	1:G:178:LEU:HD12	2.38	0.44
3:M:71:LEU:O	3:M:148:TYR:HB3	2.18	0.44
3:S:314:LEU:HD23	3:S:314:LEU:HA	1.71	0.44
3:U:45:ASP:O	3:U:46:LYS:HD2	2.18	0.44
1:A:51:ILE:HD11	1:A:71:ALA:HB2	2.00	0.44
1:A:73:ILE:HD12	1:A:73:ILE:H	1.82	0.44
2:B:31:SER:HB2	2:B:32:SER:H	1.63	0.44
2:B:33:LEU:HD12	2:B:89:GLN:O	2.18	0.44
4:R:102:LEU:HD23	4:R:102:LEU:HA	1.73	0.44
3:T:53:LYS:HE3	3:T:276:ASP:OD1	2.18	0.44
2:H:175:LEU:HD12	2:H:176:SER:N	2.32	0.44
1:I:53:ILE:HD13	4:R:49:THR:HA	2.00	0.44
1:I:100(A):TYR:HD2	4:R:42:GLN:OE1	2.01	0.44
2:L:202:SER:O	2:L:202:SER:OG	2.30	0.44
3:M:107:GLU:O	3:M:111:GLN:HG2	2.17	0.44
3:M:138:ALA:HB2	3:M:226:GLN:HE21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:SER:O	1:I:82(C):LEU:HB2	2.17	0.43
1:I:73:ILE:HD12	1:I:73:ILE:H	1.83	0.43
2:J:14:SER:O	2:J:17:GLU:OE2	2.36	0.43
3:O:15:ILE:HD11	4:R:122:VAL:HG21	2.00	0.43
3:O:151:LEU:HB3	3:O:252:VAL:HG12	1.99	0.43
1:A:51:ILE:CD1	1:A:71:ALA:HB2	2.48	0.43
2:D:191:VAL:O	2:D:191:VAL:HG13	2.18	0.43
3:M:163:LYS:HE3	3:M:246:GLU:OE2	2.18	0.43
3:N:45:ASP:C	3:N:297:ILE:HD11	2.39	0.43
3:O:197:ASN:HB2	3:O:200:THR:HG22	2.00	0.43
4:Q:17:MET:SD	4:Q:23:GLY:HA3	2.58	0.43
1:A:169:VAL:O	1:A:176:TYR:HA	2.18	0.43
2:B:33:LEU:CD2	2:B:71:PHE:CD2	2.97	0.43
1:G:41:PRO:O	1:G:43:GLN:HG2	2.18	0.43
2:J:37:GLN:HG3	2:J:86:TYR:CZ	2.54	0.43
3:M:218:ALA:HB3	3:O:203:PHE:CE2	2.53	0.43
3:N:64:CYS:O	3:N:92:SER:HB3	2.18	0.43
4:Q:6:ILE:HD13	4:Q:6:ILE:HG21	1.79	0.43
4:R:2:LEU:HA	4:R:2:LEU:HD12	1.58	0.43
3:S:195:TYR:CZ	3:S:250:ASN:HA	2.53	0.43
4:W:128:ASN:ND2	4:W:159:TYR:OH	2.47	0.43
4:X:164:GLU:O	4:X:168:LEU:HD13	2.18	0.43
4:P:126:LEU:HA	4:P:126:LEU:HD23	1.70	0.43
4:X:74:GLU:HB3	4:X:77:ILE:HD11	2.00	0.43
1:G:51:ILE:HD11	1:G:71:ALA:HB2	1.99	0.43
1:G:130:SER:HA	2:H:116:PHE:HD1	1.83	0.43
4:W:2:LEU:HD12	4:W:2:LEU:HA	1.54	0.43
2:D:32:SER:O	2:D:50:GLY:O	2.36	0.43
2:D:61:ARG:NH1	2:D:82:ASP:CG	2.72	0.43
1:K:105:LYS:H	1:K:105:LYS:CE	2.32	0.43
1:K:192:GLN:OE1	1:K:193:THR:N	2.51	0.43
3:M:176:VAL:HA	3:M:258:PHE:O	2.18	0.43
3:O:189:ALA:HA	3:U:189:ALA:HB1	2.00	0.43
3:T:208:ARG:HH11	4:X:72:HIS:CE1	2.37	0.43
2:B:31:SER:OG	2:B:32(A):TYR:CE2	2.69	0.43
1:C:18:VAL:CG2	1:C:82(C):LEU:HD21	2.44	0.43
1:E:82(B):SER:CB	1:E:82(C):LEU:HA	2.46	0.43
1:G:145:TYR:CD1	1:G:176:TYR:O	2.72	0.43
4:P:62:GLN:CD	4:P:62:GLN:H	2.22	0.43
4:P:102:LEU:HD21	4:R:103:GLU:OE2	2.18	0.43
4:P:105:GLU:CG	4:R:106:ARG:HH12	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:315:ARG:HH11	3:S:315:ARG:HD2	1.62	0.43
1:C:84:SER:HA	1:C:111:VAL:HB	2.00	0.43
1:E:32:TYR:HB3	1:E:100:TYR:CE1	2.53	0.43
1:K:53:ILE:HD13	4:W:49:THR:HA	2.01	0.43
3:T:161:TYR:CZ	3:T:249:GLY:HA2	2.54	0.43
3:T:315:ARG:HH11	3:T:315:ARG:HD2	1.60	0.43
2:J:88:CYS:O	2:J:99:GLY:N	2.51	0.43
3:M:53:LYS:HG2	3:M:57:ALA:HA	2.00	0.43
3:O:314:LEU:HD23	3:O:314:LEU:HA	1.76	0.43
4:P:95:ASN:ND2	4:Q:95:ASN:HD21	2.17	0.43
3:U:308:TYR:HD2	4:X:89:LEU:HD13	1.81	0.43
4:W:99:LEU:HD12	4:W:99:LEU:HA	1.78	0.43
2:B:175:LEU:HD12	2:B:176:SER:N	2.33	0.43
1:E:159:LEU:HD21	1:E:182:VAL:HG11	2.01	0.43
2:H:201:LEU:HD23	2:H:201:LEU:HA	1.73	0.43
3:O:177:LEU:HA	3:O:236:LEU:HD23	2.01	0.43
4:Q:68:LYS:HE3	4:R:79:ASN:HB2	2.00	0.43
4:R:27:GLN:O	4:R:27:GLN:HG3	2.18	0.43
3:U:167:SER:OG	3:U:244:THR:HG22	2.18	0.43
1:C:82(C):LEU:HD12	1:C:82(C):LEU:HA	1.55	0.42
1:G:146:PHE:O	1:G:200:HIS:HE1	2.02	0.42
1:G:154:TRP:CZ3	1:G:196:CYS:HB3	2.53	0.42
1:I:83:SER:OG	1:I:84:SER:N	2.51	0.42
2:B:58:ILE:HD13	2:B:58:ILE:HA	1.83	0.42
1:C:89:VAL:HG22	1:C:108:THR:HG22	2.02	0.42
2:L:136:LEU:CD2	2:L:196:VAL:HG21	2.48	0.42
3:M:123:LYS:HZ2	3:M:133:ASN:HD21	1.66	0.42
4:Q:158:ASP:OD1	4:Q:160:PRO:HD2	2.19	0.42
2:B:122:ASP:O	2:B:125:LEU:N	2.51	0.42
2:B:203:SER:HA	2:B:204:PRO:HD3	1.53	0.42
1:E:178:LEU:C	1:E:178:LEU:HD12	2.39	0.42
2:F:61:ARG:NH1	2:F:82:ASP:OD1	2.52	0.42
2:H:204:PRO:O	2:H:205:VAL:C	2.55	0.42
4:Q:103:GLU:OE2	4:R:102:LEU:HD21	2.19	0.42
3:U:26:VAL:HG21	3:U:317:ALA:HB2	2.00	0.42
4:W:102:LEU:HD23	4:W:102:LEU:HA	1.60	0.42
2:D:29:VAL:O	2:D:29:VAL:HG13	2.18	0.42
2:F:198:HIS:CD2	2:F:200:GLY:H	2.37	0.42
2:H:205:VAL:O	2:H:205:VAL:HG12	2.18	0.42
1:I:123:PRO:HD2	2:J:121:SER:CB	2.49	0.42
1:I:154:TRP:CZ3	1:I:196:CYS:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:SER:OG	1:K:54:PHE:HB3	2.20	0.42
3:O:30:LEU:HA	3:O:30:LEU:HD23	1.82	0.42
4:P:70:PHE:CD2	4:P:78:GLU:HA	2.53	0.42
3:S:116(A):SER:O	3:S:260:MET:HA	2.20	0.42
3:T:116(B):PHE:HE1	3:T:260:MET:HE1	1.84	0.42
3:U:103:ILE:N	3:U:103:ILE:HD12	2.34	0.42
1:A:25:SER:O	1:A:25:SER:OG	2.24	0.42
1:A:40:ALA:HB3	1:A:43:GLN:HB2	2.01	0.42
2:B:29:VAL:HG12	2:B:68:GLY:O	2.20	0.42
1:C:143:LYS:HE3	1:C:144:ASP:OD1	2.20	0.42
1:E:100(A):TYR:HD2	4:P:42:GLN:OE1	2.03	0.42
2:F:54:ARG:HG2	2:F:58:ILE:HB	2.02	0.42
2:J:191:VAL:HG13	2:J:191:VAL:O	2.19	0.42
1:K:181:VAL:HG11	2:L:135:LEU:CD2	2.50	0.42
3:M:177:LEU:HD11	3:M:234:TRP:HB2	2.01	0.42
3:O:298:HIS:CE1	3:O:300:ILE:HD12	2.38	0.42
4:W:118:LEU:HA	4:W:118:LEU:HD12	1.75	0.42
2:B:2:ILE:HG12	2:B:27:GLN:HB2	2.02	0.42
1:E:5:VAL:HA	1:E:105:LYS:HZ1	1.83	0.42
1:K:127:SER:H	1:K:130:SER:HB2	1.83	0.42
2:L:32:SER:HB2	2:L:51:ALA:CB	2.46	0.42
2:L:198:HIS:CD2	2:L:199:GLN:O	2.72	0.42
3:N:137:ALA:HB2	3:N:145:LYS:HE3	2.01	0.42
3:O:103:ILE:N	3:O:103:ILE:HD12	2.34	0.42
4:P:168:LEU:HD23	4:P:168:LEU:HA	1.78	0.42
3:T:26:VAL:HG21	3:T:317:ALA:HB2	2.00	0.42
3:U:8:ASP:N	3:U:9:PRO:HD2	2.33	0.42
2:H:32(A):TYR:HB2	2:H:92:VAL:CG1	2.49	0.42
1:I:51:ILE:CD1	1:I:71:ALA:HB2	2.50	0.42
2:J:206:THR:O	2:J:206:THR:OG1	2.32	0.42
3:M:106:GLU:CD	4:P:71:ASN:HB3	2.39	0.42
3:U:66:ILE:HD12	3:U:109:ARG:HG2	2.00	0.42
1:E:163:VAL:HG22	1:E:182:VAL:HG22	2.01	0.42
2:F:203:SER:HA	2:F:204:PRO:HD3	1.78	0.42
1:K:51:ILE:HD13	1:K:51:ILE:HG21	1.68	0.42
3:M:123:LYS:NZ	3:M:133:ASN:HD21	2.17	0.42
4:V:168:LEU:HA	4:V:168:LEU:HD23	1.80	0.42
1:A:210:ARG:NH1	1:A:212:GLU:HB3	2.35	0.42
2:F:141:PRO:O	2:F:198:HIS:HE1	2.02	0.42
2:F:198:HIS:HD2	2:F:200:GLY:H	1.68	0.42
1:G:18:VAL:HG23	1:G:82(C):LEU:HD22	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:HG11	2:H:135:LEU:HD22	2.02	0.42
2:H:120:PRO:HD3	2:H:132:VAL:HG22	2.02	0.42
1:A:82(C):LEU:HD12	1:A:82(C):LEU:HA	1.75	0.42
1:C:146:PHE:HA	1:C:147:PRO:HA	1.79	0.42
1:K:181:VAL:HG11	2:L:135:LEU:HD22	2.02	0.42
2:L:163:VAL:HG22	2:L:175:LEU:HD13	2.02	0.42
2:L:198:HIS:CD2	2:L:199:GLN:H	2.37	0.42
3:U:119:GLU:CD	3:U:122:PRO:HA	2.39	0.42
2:B:24:ARG:NH1	2:B:70:ASP:OD1	2.53	0.41
1:C:17:SER:HA	1:C:82(A):SER:HA	1.96	0.41
1:C:51:ILE:HG21	1:C:51:ILE:HD13	1.71	0.41
2:H:29:VAL:O	2:H:29:VAL:CG1	2.68	0.41
1:K:61:GLN:N	1:K:61:GLN:OE1	2.52	0.41
1:K:95:LYS:HE2	1:K:97:GLU:O	2.19	0.41
3:O:116(B):PHE:CE1	3:O:260:MET:HE2	2.54	0.41
3:S:45:ASP:C	3:S:297:ILE:HD11	2.40	0.41
2:B:32(A):TYR:CD1	2:B:91:TYR:CE2	3.08	0.41
2:D:29:VAL:CG1	2:D:68:GLY:O	2.61	0.41
1:E:61:GLN:OE1	1:E:61:GLN:N	2.54	0.41
2:H:32:SER:HB2	2:H:51:ALA:CB	2.49	0.41
2:H:123:GLU:HA	2:H:126:LYS:HE2	2.03	0.41
2:J:205:VAL:HG12	2:J:205:VAL:H	1.59	0.41
4:P:95:ASN:HD21	4:R:95:ASN:ND2	2.17	0.41
4:P:99:LEU:HA	4:P:99:LEU:HD12	1.86	0.41
3:S:58:PRO:HB3	3:S:86:TYR:CZ	2.55	0.41
3:S:152:ILE:HD11	3:S:255:ARG:HD2	2.02	0.41
1:E:51:ILE:HG21	1:E:51:ILE:HD13	1.72	0.41
1:E:209:LYS:HD2	1:E:209:LYS:HA	1.77	0.41
2:F:112:ALA:HB2	2:F:200:GLY:HA3	2.02	0.41
1:G:72:ASP:OD1	3:S:291:SER:OG	2.28	0.41
2:H:33:LEU:HD22	2:H:71:PHE:CG	2.55	0.41
2:H:35:TRP:CZ3	2:H:88:CYS:HB3	2.55	0.41
2:H:78:LEU:HD23	2:H:78:LEU:HA	1.83	0.41
1:I:129:LYS:HE2	1:I:129:LYS:HA	2.03	0.41
1:K:18:VAL:HG12	1:K:19:GLN:N	2.35	0.41
3:N:151:LEU:HB3	3:N:252:VAL:HG12	2.02	0.41
4:R:170:ARG:HH11	4:R:170:ARG:HD2	1.72	0.41
3:S:11:ASP:OD1	4:V:28:ASN:HA	2.20	0.41
3:U:8:ASP:N	3:U:9:PRO:CD	2.84	0.41
3:U:174:LYS:CA	3:U:239:PRO:HG3	2.50	0.41
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:LYS:HE2	1:E:105:LYS:H	1.84	0.41
3:M:207:SER:OG	3:M:241:ASP:OD1	2.27	0.41
3:S:90(A):PRO:HD2	3:S:271:ASP:OD1	2.19	0.41
3:U:186:SER:HA	3:U:218:ALA:O	2.20	0.41
4:X:102:LEU:HD23	4:X:102:LEU:HA	1.87	0.41
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.56	0.41
1:C:148:GLU:HG2	1:C:176:TYR:CD2	2.55	0.41
1:K:6:GLN:HG3	1:K:106:GLY:N	2.33	0.41
4:P:3:PHE:CZ	4:Q:2:LEU:HG	2.55	0.41
4:R:159:TYR:HB3	4:R:160:PRO:HD3	2.01	0.41
2:B:79:GLU:HB3	2:B:80:PRO:HD2	2.02	0.41
2:B:95:PRO:O	2:B:95:PRO:CG	2.69	0.41
2:D:120:PRO:HD3	2:D:132:VAL:HG22	2.01	0.41
2:D:201:LEU:HD23	2:D:201:LEU:HA	1.85	0.41
1:G:74:SER:CB	3:S:291:SER:HB2	2.45	0.41
1:G:144:ASP:OD1	1:G:171:GLN:NE2	2.52	0.41
3:O:195:TYR:O	3:O:197:ASN:N	2.49	0.41
4:R:38:LEU:HA	4:R:38:LEU:HD23	1.61	0.41
3:S:308:TYR:CD2	4:V:89:LEU:HD13	2.56	0.41
4:V:1:GLY:O	4:V:4:GLY:N	2.51	0.41
1:G:100(A):TYR:OH	4:V:19:ASP:O	2.32	0.41
1:K:100(A):TYR:HB3	4:W:42:GLN:OE1	2.20	0.41
3:M:15:ILE:N	3:M:15:ILE:HD12	2.35	0.41
3:M:180:TRP:CE2	3:M:233:TYR:HB2	2.56	0.41
3:N:94:ASN:HD22	3:N:94:ASN:HA	1.69	0.41
1:A:53:ILE:CD1	4:Q:49:THR:HA	2.50	0.41
2:B:32(A):TYR:CB	2:B:92:VAL:HG12	2.51	0.41
2:B:61:ARG:NH1	2:B:82:ASP:OD1	2.54	0.41
1:C:38:ARG:NH1	1:C:46:GLU:OE2	2.48	0.41
1:C:51:ILE:HD11	1:C:71:ALA:HB2	2.03	0.41
1:G:96:LEU:HA	1:G:96:LEU:HD12	1.84	0.41
1:K:129:LYS:HZ3	2:L:207:LYS:HD3	1.85	0.41
1:K:146:PHE:CE1	1:K:147:PRO:HB3	2.56	0.41
3:S:41:ASN:ND2	3:S:43:LEU:O	2.54	0.41
3:S:184:HIS:HB3	3:S:216:GLU:O	2.21	0.41
3:U:262:ARG:NH1	3:U:262:ARG:HG3	2.36	0.41
1:C:36:TRP:CZ2	1:C:80:MET:HB2	2.55	0.41
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.55	0.41
2:D:83:PHE:HA	2:D:104:VAL:HG23	2.03	0.41
2:D:131:SER:HA	2:D:179:LEU:O	2.21	0.41
1:E:89:VAL:HG22	1:E:108:THR:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:LEU:O	2:H:104:VAL:HA	2.20	0.41
1:I:47:TRP:HB3	2:J:96:LEU:O	2.21	0.41
1:K:61:GLN:HA	1:K:64:GLN:HB2	2.02	0.41
1:K:96:LEU:HA	1:K:96:LEU:HD12	1.82	0.41
2:L:122:ASP:O	2:L:125:LEU:N	2.54	0.41
3:M:308:TYR:CD2	4:P:89:LEU:HD13	2.56	0.41
3:N:54:LEU:HA	3:N:54:LEU:HD12	1.82	0.41
3:O:176:VAL:HA	3:O:258:PHE:O	2.20	0.41
4:P:1:GLY:O	4:P:2:LEU:C	2.57	0.41
4:P:2:LEU:HD12	4:P:2:LEU:HA	1.62	0.41
4:P:74:GLU:HB3	4:P:77:ILE:HD11	2.03	0.41
4:R:39:LYS:HE3	4:R:39:LYS:HB2	1.79	0.41
3:U:18:HIS:HB2	4:X:20:GLY:O	2.21	0.41
4:V:170:ARG:HH11	4:V:170:ARG:HD2	1.74	0.41
4:X:170:ARG:HH11	4:X:170:ARG:HD2	1.72	0.41
3:N:310:LYS:HD3	3:N:310:LYS:HA	1.90	0.41
3:O:262:ARG:HH11	3:O:262:ARG:HG3	1.85	0.41
4:P:142:HIS:CE1	4:P:162:TYR:CG	3.09	0.41
4:Q:62:GLN:NE2	4:R:86:ASP:HB3	2.35	0.41
3:T:303:GLY:HA2	4:W:63:PHE:CE2	2.56	0.41
4:V:101:LEU:HD23	4:V:101:LEU:HA	1.75	0.41
4:X:99:LEU:HA	4:X:99:LEU:HD12	1.87	0.41
1:C:100(A):TYR:HD2	4:X:42:GLN:OE1	2.04	0.40
2:D:89:GLN:HG2	2:D:90:GLN:N	2.35	0.40
2:H:19:ALA:HB2	2:H:78:LEU:HD11	2.03	0.40
1:I:61:GLN:N	1:I:61:GLN:OE1	2.54	0.40
1:I:146:PHE:HA	1:I:147:PRO:HA	1.90	0.40
3:M:42:LEU:HD11	3:M:316:LEU:HD22	2.03	0.40
3:M:321:ARG:HH11	3:M:321:ARG:HD2	1.75	0.40
4:P:23:GLY:HA3	4:P:36:ALA:HA	2.02	0.40
4:Q:62:GLN:H	4:Q:62:GLN:CD	2.24	0.40
3:U:52:CYS:HB3	3:U:277:CYS:O	2.20	0.40
4:V:148:CYS:O	4:V:151:SER:OG	2.29	0.40
1:C:47:TRP:CD1	2:D:96:LEU:HD12	2.57	0.40
1:E:146:PHE:HA	1:E:147:PRO:HA	1.91	0.40
1:G:89:VAL:HA	1:G:108:THR:HA	2.03	0.40
1:I:38:ARG:NH2	1:I:86:ASP:OD1	2.55	0.40
1:I:145:TYR:CE1	1:I:150:VAL:HG23	2.57	0.40
2:L:13:LEU:HD23	2:L:13:LEU:HA	1.75	0.40
2:L:141:PRO:HG3	2:L:199:GLN:HE22	1.82	0.40
3:T:71:LEU:O	3:T:148:TYR:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:LEU:HD12	2:D:21:LEU:N	2.36	0.40
1:I:12:LYS:HD2	1:I:12:LYS:HA	1.94	0.40
2:J:203:SER:HA	2:J:204:PRO:HD3	1.63	0.40
1:K:41:PRO:O	1:K:43:GLN:HG2	2.21	0.40
4:Q:73:LEU:HD23	4:Q:73:LEU:HA	1.84	0.40
4:R:141:TYR:O	4:R:166:ALA:HA	2.21	0.40
4:R:157:TYR:CE2	4:R:159:TYR:HA	2.56	0.40
4:W:38:LEU:HA	4:W:38:LEU:HD23	1.82	0.40
1:E:51:ILE:HD11	1:E:71:ALA:HB2	2.03	0.40
2:H:83:PHE:HA	2:H:104:VAL:HG23	2.04	0.40
3:N:41:ASN:ND2	3:N:43:LEU:O	2.53	0.40
3:S:20:ASN:C	3:S:20:ASN:OD1	2.60	0.40
3:T:94:ASN:HD22	3:T:94:ASN:HA	1.75	0.40
1:A:42:GLY:O	1:A:43:GLN:NE2	2.44	0.40
1:C:105:LYS:H	1:C:105:LYS:CE	2.35	0.40
2:D:203:SER:HB3	2:D:204:PRO:HD2	2.02	0.40
1:G:82(C):LEU:HD12	1:G:82(C):LEU:HA	1.81	0.40
2:H:167:ASP:O	2:H:171:SER:HA	2.22	0.40
2:J:47:LEU:HD11	2:J:86:TYR:CE2	2.57	0.40
2:J:58:ILE:HA	2:J:59:PRO:HD2	1.89	0.40
3:S:42:LEU:HA	3:S:42:LEU:HD23	1.67	0.40
3:U:54:LEU:HD12	3:U:54:LEU:HA	1.92	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	223/225 (99%)	204 (92%)	16 (7%)	3 (1%)	12	48
1	C	223/225 (99%)	200 (90%)	20 (9%)	3 (1%)	12	48
1	E	223/225 (99%)	207 (93%)	15 (7%)	1 (0%)	34	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	223/225 (99%)	203 (91%)	18 (8%)	2 (1%)	17	56
1	I	223/225 (99%)	205 (92%)	17 (8%)	1 (0%)	34	72
1	K	223/225 (99%)	203 (91%)	17 (8%)	3 (1%)	12	48
2	B	211/213 (99%)	189 (90%)	16 (8%)	6 (3%)	5	32
2	D	211/213 (99%)	191 (90%)	17 (8%)	3 (1%)	11	46
2	F	211/213 (99%)	192 (91%)	16 (8%)	3 (1%)	11	46
2	H	211/213 (99%)	192 (91%)	17 (8%)	2 (1%)	17	56
2	J	211/213 (99%)	190 (90%)	15 (7%)	6 (3%)	5	32
2	L	211/213 (99%)	193 (92%)	15 (7%)	3 (1%)	11	46
3	M	322/331 (97%)	312 (97%)	10 (3%)	0	100	100
3	N	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	41	75
3	O	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	25	64
3	S	322/331 (97%)	312 (97%)	9 (3%)	1 (0%)	41	75
3	T	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	41	75
3	U	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	25	64
4	P	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
4	Q	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
4	R	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
4	V	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
4	W	169/177 (96%)	166 (98%)	3 (2%)	0	100	100
4	X	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
All	All	5560/5676 (98%)	5246 (94%)	271 (5%)	43 (1%)	19	58

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82(B)	SER
2	B	30	SER
2	B	94	THR
1	C	28	THR
1	G	149	PRO
2	J	30	SER
1	K	82(A)	SER
1	A	27	GLY
2	D	31	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	204	PRO
2	H	204	PRO
2	J	28	SER
2	B	204	PRO
1	C	82(C)	LEU
2	J	31	SER
1	K	84	SER
2	B	201	LEU
2	B	203	SER
2	J	203	SER
2	L	203	SER
2	F	28	SER
2	L	201	LEU
3	O	264	ALA
3	U	264	ALA
3	N	264	ALA
3	O	9	PRO
3	S	264	ALA
3	T	264	ALA
3	U	9	PRO
2	D	204	PRO
1	E	52(A)	PRO
1	G	52(A)	PRO
2	J	204	PRO
1	A	52(A)	PRO
2	B	2	ILE
1	C	52(A)	PRO
2	D	2	ILE
2	F	2	ILE
2	H	2	ILE
2	J	2	ILE
1	K	52(A)	PRO
2	L	2	ILE
1	I	52(A)	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	189/189 (100%)	175 (93%)	14 (7%)	13	44
1	C	189/189 (100%)	177 (94%)	12 (6%)	18	51
1	E	189/189 (100%)	180 (95%)	9 (5%)	25	60
1	G	189/189 (100%)	176 (93%)	13 (7%)	15	47
1	I	189/189 (100%)	179 (95%)	10 (5%)	22	55
1	K	189/189 (100%)	178 (94%)	11 (6%)	20	53
2	B	184/184 (100%)	176 (96%)	8 (4%)	29	62
2	D	184/184 (100%)	175 (95%)	9 (5%)	25	59
2	F	184/184 (100%)	174 (95%)	10 (5%)	22	55
2	H	184/184 (100%)	173 (94%)	11 (6%)	19	52
2	J	184/184 (100%)	175 (95%)	9 (5%)	25	59
2	L	184/184 (100%)	171 (93%)	13 (7%)	14	46
3	M	284/290 (98%)	278 (98%)	6 (2%)	53	79
3	N	283/290 (98%)	279 (99%)	4 (1%)	67	85
3	O	286/290 (99%)	283 (99%)	3 (1%)	76	88
3	S	284/290 (98%)	279 (98%)	5 (2%)	59	81
3	T	283/290 (98%)	280 (99%)	3 (1%)	73	88
3	U	286/290 (99%)	283 (99%)	3 (1%)	76	88
4	P	150/151 (99%)	150 (100%)	0	100	100
4	Q	146/151 (97%)	145 (99%)	1 (1%)	84	93
4	R	146/151 (97%)	146 (100%)	0	100	100
4	V	150/151 (99%)	150 (100%)	0	100	100
4	W	146/151 (97%)	145 (99%)	1 (1%)	84	93
4	X	146/151 (97%)	146 (100%)	0	100	100
All	All	4828/4884 (99%)	4673 (97%)	155 (3%)	39	69

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	25	SER
1	A	28	THR
1	A	38	ARG
1	A	66	ARG
1	A	81	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	LEU
1	A	82(A)	SER
1	A	82(C)	LEU
1	A	83	SER
1	A	100	TYR
1	A	100(F)	MET
1	A	105	LYS
1	A	208	ASP
2	B	22	SER
2	B	28	SER
2	B	122	ASP
2	B	143	GLU
2	B	150	VAL
2	B	199	GLN
2	B	203	SER
2	B	204	PRO
1	C	11	VAL
1	C	38	ARG
1	C	82	LEU
1	C	82(A)	SER
1	C	82(B)	SER
1	C	82(C)	LEU
1	C	96	LEU
1	C	97	GLU
1	C	100	TYR
1	C	100(F)	MET
1	C	105	LYS
1	C	208	ASP
2	D	22	SER
2	D	32	SER
2	D	61	ARG
2	D	122	ASP
2	D	125	LEU
2	D	143	GLU
2	D	150	VAL
2	D	202	SER
2	D	205	VAL
1	E	11	VAL
1	E	38	ARG
1	E	66	ARG
1	E	81	ASP
1	E	82(B)	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	100	TYR
1	E	100(F)	MET
1	E	105	LYS
1	E	208	ASP
2	F	22	SER
2	F	28	SER
2	F	29	VAL
2	F	122	ASP
2	F	125	LEU
2	F	143	GLU
2	F	150	VAL
2	F	202	SER
2	F	205	VAL
2	F	206	THR
1	G	11	VAL
1	G	38	ARG
1	G	66	ARG
1	G	82(A)	SER
1	G	82(C)	LEU
1	G	83	SER
1	G	84	SER
1	G	100	TYR
1	G	100(F)	MET
1	G	105	LYS
1	G	145	TYR
1	G	148	GLU
1	G	208	ASP
2	H	22	SER
2	H	28	SER
2	H	29	VAL
2	H	30	SER
2	H	122	ASP
2	H	125	LEU
2	H	143	GLU
2	H	150	VAL
2	H	199	GLN
2	H	205	VAL
2	H	206	THR
1	I	38	ARG
1	I	66	ARG
1	I	81	ASP
1	I	82(A)	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	82(B)	SER
1	I	83	SER
1	I	100	TYR
1	I	100(F)	MET
1	I	105	LYS
1	I	208	ASP
2	J	22	SER
2	J	28	SER
2	J	29	VAL
2	J	30	SER
2	J	122	ASP
2	J	125	LEU
2	J	143	GLU
2	J	150	VAL
2	J	199	GLN
1	K	11	VAL
1	K	28	THR
1	K	38	ARG
1	K	66	ARG
1	K	82	LEU
1	K	82(B)	SER
1	K	84	SER
1	K	100	TYR
1	K	100(F)	MET
1	K	105	LYS
1	K	208	ASP
2	L	22	SER
2	L	26	SER
2	L	27	GLN
2	L	28	SER
2	L	29	VAL
2	L	30	SER
2	L	61	ARG
2	L	122	ASP
2	L	143	GLU
2	L	150	VAL
2	L	199	GLN
2	L	205	VAL
2	L	206	THR
3	M	63	LYS
3	M	208	ARG
3	M	266	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	277	CYS
3	M	283	THR
3	M	320	LEU
3	N	266	SER
3	N	283	THR
3	N	291	SER
3	N	310	LYS
3	O	63	LYS
3	O	266	SER
3	O	283	THR
4	Q	168	LEU
3	S	63	LYS
3	S	208	ARG
3	S	266	SER
3	S	283	THR
3	S	320	LEU
3	T	266	SER
3	T	283	THR
3	T	291	SER
3	U	63	LYS
3	U	266	SER
3	U	283	THR
4	W	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	B	38	GLN
2	B	198	HIS
2	B	199	GLN
2	D	38	GLN
2	D	198	HIS
2	D	199	GLN
1	E	39	GLN
1	E	199	ASN
2	F	38	GLN
2	F	198	HIS
2	H	198	HIS
1	I	39	GLN
2	J	38	GLN
2	J	199	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	6	GLN
2	L	198	HIS
2	L	199	GLN
3	M	94	ASN
3	M	133	ASN
3	M	226	GLN
3	N	94	ASN
3	N	111	GLN
3	O	38	HIS
3	O	94	ASN
3	O	159	ASN
3	O	226	GLN
4	P	43	ASN
4	P	95	ASN
4	Q	53	ASN
4	Q	95	ASN
4	Q	154	ASN
4	R	25	HIS
4	R	79	ASN
3	S	94	ASN
3	S	133	ASN
3	T	111	GLN
3	T	226	GLN
3	U	94	ASN
3	U	159	ASN
3	U	226	GLN
3	U	275	HIS
4	V	43	ASN
4	V	53	ASN
4	V	95	ASN
4	W	25	HIS
4	W	95	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	225/225 (100%)	0.56	14 (6%) 20 18	51, 74, 96, 116	0
1	C	225/225 (100%)	0.53	11 (4%) 29 26	59, 78, 95, 114	0
1	E	225/225 (100%)	0.54	10 (4%) 34 30	55, 79, 99, 111	0
1	G	225/225 (100%)	0.64	12 (5%) 26 24	54, 81, 105, 124	0
1	I	225/225 (100%)	0.92	34 (15%) 2 3	59, 91, 116, 128	0
1	K	225/225 (100%)	0.55	13 (5%) 23 20	51, 72, 98, 114	0
2	B	213/213 (100%)	0.23	1 (0%) 91 88	53, 61, 76, 85	0
2	D	213/213 (100%)	0.38	1 (0%) 91 88	62, 71, 83, 94	0
2	F	213/213 (100%)	0.30	0 100 100	58, 68, 83, 92	0
2	H	213/213 (100%)	0.29	3 (1%) 75 69	54, 68, 86, 98	0
2	J	213/213 (100%)	0.33	4 (1%) 66 61	55, 71, 89, 106	0
2	L	213/213 (100%)	0.17	1 (0%) 91 88	51, 61, 76, 88	0
3	M	324/331 (97%)	2.28	146 (45%) 0 0	55, 175, 212, 218	0
3	N	323/331 (97%)	2.01	137 (42%) 0 0	50, 168, 205, 211	0
3	O	326/331 (98%)	2.48	165 (50%) 0 0	54, 196, 228, 232	0
3	S	324/331 (97%)	1.69	114 (35%) 0 0	55, 153, 182, 186	0
3	T	323/331 (97%)	1.72	114 (35%) 0 0	52, 157, 192, 196	0
3	U	326/331 (98%)	1.73	116 (35%) 0 0	55, 159, 190, 197	0
4	P	175/177 (98%)	0.62	11 (6%) 20 18	51, 73, 141, 170	0
4	Q	171/177 (96%)	0.53	10 (5%) 23 20	50, 72, 133, 157	0
4	R	171/177 (96%)	0.51	8 (4%) 31 28	51, 74, 134, 156	0
4	V	175/177 (98%)	0.57	10 (5%) 23 21	52, 77, 128, 147	0
4	W	171/177 (96%)	0.57	13 (7%) 13 14	51, 72, 113, 141	0
4	X	171/177 (96%)	0.52	10 (5%) 23 20	53, 77, 116, 142	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	5608/5676 (98%)	1.01	958 (17%) 1 1	50, 80, 199, 232	0

All (958) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	165	SER	13.2
3	O	164	LEU	11.8
3	N	198	ALA	11.7
3	O	250	ASN	10.9
3	M	127	TRP	9.4
3	O	138	ALA	9.4
3	O	154	LEU	9.2
3	M	187	THR	9.1
3	M	250	ASN	8.9
1	A	215	SER	8.7
3	M	76	CYS	8.6
3	M	224	ARG	8.6
3	N	186	SER	8.5
3	N	138	ALA	8.5
3	N	127	TRP	8.4
3	M	225	ASP	8.2
3	M	195	TYR	8.1
3	M	74	PRO	8.1
3	S	183	HIS	8.0
3	M	154	LEU	7.8
3	O	123	LYS	7.8
3	O	8	ASP	7.7
3	S	154	LEU	7.7
3	O	246	GLU	7.6
3	M	260	MET	7.6
3	M	142	ALA	7.6
3	O	247	ALA	7.6
3	N	167	SER	7.4
3	O	243	ILE	7.3
1	G	215	SER	7.3
3	N	199	ASP	7.3
3	O	205	GLY	7.2
3	T	173	GLY	7.2
3	M	55	ARG	7.0
3	T	154	LEU	6.9
3	O	155	VAL	6.9
3	M	172	LYS	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	163	LYS	6.8
3	M	155	VAL	6.8
3	U	81	THR	6.8
3	M	123	LYS	6.7
1	I	131	THR	6.7
1	I	215	SER	6.7
3	M	217	ILE	6.7
3	O	127	TRP	6.7
3	O	133(A)	LYS	6.7
3	N	77	GLU	6.6
3	T	132	SER	6.6
3	S	134	GLY	6.6
3	T	224	ARG	6.5
3	O	141	HIS	6.5
3	O	199	ASP	6.5
3	O	101	ASP	6.4
3	N	224	ARG	6.4
3	T	250	ASN	6.4
3	O	76	CYS	6.3
3	O	159	ASN	6.3
3	S	138	ALA	6.3
3	O	213	PHE	6.2
3	O	132	SER	6.2
3	M	143	GLY	6.2
3	U	154	LEU	6.2
3	M	229	ARG	6.2
3	U	138	ALA	6.2
3	O	74	PRO	6.1
3	O	79	LEU	6.1
3	N	216	GLU	6.1
3	O	148	TYR	6.1
3	U	163	LYS	6.1
3	U	76	CYS	6.1
3	N	154	LEU	6.0
3	S	155	VAL	6.0
4	P	175	SER	6.0
3	U	134	GLY	6.0
3	N	116(C)	GLU	6.0
3	S	153	TRP	5.9
3	U	153	TRP	5.9
3	N	76	CYS	5.9
3	T	198	ALA	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	155	VAL	5.8
3	O	173	GLY	5.8
3	M	134	GLY	5.8
3	O	77	GLU	5.8
3	O	216	GLU	5.8
3	T	155	VAL	5.8
3	O	187	THR	5.8
3	T	160	SER	5.8
4	P	174	ASP	5.8
3	N	187	THR	5.7
3	M	213	PHE	5.7
3	T	123	LYS	5.7
3	T	142	ALA	5.7
3	M	186	SER	5.7
3	M	230	MET	5.7
3	M	197	ASN	5.7
3	O	116(C)	GLU	5.7
3	N	250	ASN	5.7
3	U	139	CYS	5.6
3	M	80	SER	5.6
3	N	223	VAL	5.6
3	O	153	TRP	5.6
3	O	139	CYS	5.6
3	S	172	LYS	5.6
3	M	147	PHE	5.5
3	M	93	ASP	5.5
3	U	142	ALA	5.5
3	O	195	TYR	5.5
3	U	250	ASN	5.5
3	M	138	ALA	5.5
3	M	135	VAL	5.4
3	M	161	TYR	5.4
3	T	153	TRP	5.4
1	K	215	SER	5.4
3	T	195	TYR	5.4
3	O	245	PHE	5.4
3	S	64	CYS	5.3
3	M	150	ASN	5.3
3	N	96	THR	5.3
3	S	116(C)	GLU	5.3
3	O	241	ASP	5.3
3	M	144	ALA	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	93	ASP	5.1
3	M	75	GLU	5.1
3	M	97	CYS	5.1
3	N	159	ASN	5.1
3	U	61	LEU	5.0
3	U	63	LYS	5.0
3	M	215	PRO	5.0
3	O	203	PHE	5.0
3	M	82	ALA	5.0
3	M	153	TRP	4.9
3	M	163	LYS	4.9
3	N	132	SER	4.9
3	M	139	CYS	4.9
3	M	200	THR	4.9
3	O	88	VAL	4.9
3	N	141	HIS	4.9
3	O	251	LEU	4.9
3	N	126	SER	4.9
3	T	161	TYR	4.9
3	U	116(C)	GLU	4.9
3	T	196	GLN	4.8
3	M	133(A)	LYS	4.8
1	K	130	SER	4.8
3	U	8	ASP	4.8
3	U	160	SER	4.8
3	O	194	LEU	4.8
3	N	251	LEU	4.8
3	O	181	GLY	4.8
3	T	127	TRP	4.8
3	S	127	TRP	4.7
3	M	51	LEU	4.7
3	M	116(B)	PHE	4.7
3	S	152	ILE	4.7
3	O	9	PRO	4.7
3	T	97	CYS	4.7
3	T	228	GLY	4.7
3	U	223	VAL	4.7
3	M	183	HIS	4.7
3	N	246	GLU	4.7
3	T	78	SER	4.7
3	M	121	PHE	4.7
3	U	216	GLU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	228	GLY	4.7
3	N	158	GLY	4.7
3	O	62	GLY	4.7
3	O	73	ASN	4.7
3	M	132	SER	4.6
3	S	230	MET	4.6
3	O	229	ARG	4.6
3	O	116(B)	PHE	4.6
3	M	220	ARG	4.6
4	P	173	ILE	4.6
3	O	214	LYS	4.6
3	N	173	GLY	4.6
3	T	129	ASN	4.6
3	T	122	PRO	4.6
3	T	141	HIS	4.6
3	N	153	TRP	4.6
3	S	197	ASN	4.6
3	U	217	ILE	4.6
3	O	172	LYS	4.5
3	O	201	TYR	4.5
3	U	260	MET	4.5
3	N	194	LEU	4.5
3	N	260	MET	4.5
3	U	127	TRP	4.5
3	O	61	LEU	4.5
3	T	229	ARG	4.4
3	O	80	SER	4.4
3	O	249	GLY	4.4
3	O	204	VAL	4.4
3	N	197	ASN	4.4
3	M	141	HIS	4.4
3	O	166	LYS	4.4
3	M	287	ALA	4.4
3	O	90(A)	PRO	4.4
1	G	130	SER	4.4
3	O	152	ILE	4.4
1	G	131	THR	4.4
3	T	172	LYS	4.3
3	M	140	PRO	4.3
3	T	126	SER	4.3
3	U	55(A)	GLY	4.3
3	S	79	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	121	PHE	4.3
3	O	131	ASP	4.3
3	N	160	SER	4.3
3	O	134	GLY	4.3
3	T	138	ALA	4.3
3	N	163	LYS	4.3
3	T	185	PRO	4.3
3	U	230	MET	4.3
3	S	156	LYS	4.3
3	U	161	TYR	4.3
3	N	245	PHE	4.2
4	V	174	ASP	4.2
3	T	77	GLU	4.2
3	O	51	LEU	4.2
3	O	81	THR	4.2
3	O	215	PRO	4.2
3	M	162	PRO	4.2
3	T	80	SER	4.2
3	M	219	ILE	4.2
3	O	252	VAL	4.2
3	S	198	ALA	4.2
3	S	248	THR	4.2
3	N	229	ARG	4.1
3	N	161	TYR	4.1
1	A	131	THR	4.1
3	M	73	ASN	4.1
3	N	79	LEU	4.1
3	N	201	TYR	4.1
3	N	241	ASP	4.1
3	T	216	GLU	4.1
3	N	157	LYS	4.1
3	N	185	PRO	4.1
3	O	162	PRO	4.1
3	O	207	SER	4.1
3	M	173	GLY	4.1
3	M	126	SER	4.1
3	T	79	LEU	4.1
3	M	122	PRO	4.1
3	M	77	GLU	4.1
3	M	196	GLN	4.1
3	T	100	GLY	4.1
3	N	97	CYS	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	152	ILE	4.1
4	X	144	CYS	4.1
3	M	288	ILE	4.0
3	M	72	GLY	4.0
3	M	96	THR	4.0
3	O	104	ASP	4.0
3	N	191	GLN	4.0
3	M	245	PHE	4.0
3	S	247	ALA	4.0
3	M	94	ASN	4.0
3	O	191	GLN	4.0
3	T	120	ILE	4.0
3	S	166	LYS	4.0
3	N	129	ASN	4.0
3	U	215	PRO	4.0
3	M	223	VAL	4.0
3	M	81	THR	4.0
3	T	260	MET	4.0
3	T	223	VAL	3.9
1	I	214	LYS	3.9
3	M	118	PHE	3.9
3	O	171	ASP	3.9
1	I	132	SER	3.9
3	N	156	LYS	3.9
3	S	63	LYS	3.9
3	T	134	GLY	3.9
3	U	116(B)	PHE	3.9
4	V	143	LYS	3.9
3	O	122	PRO	3.9
3	U	123	LYS	3.9
3	N	83(A)	SER	3.9
3	O	185	PRO	3.9
3	S	168	TYR	3.9
3	O	224	ARG	3.9
1	I	130	SER	3.9
3	O	223	VAL	3.9
1	K	214	LYS	3.9
3	S	157	LYS	3.9
3	M	92	SER	3.9
3	T	220	ARG	3.9
3	N	221	PRO	3.8
3	U	214	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	270	SER	3.8
3	S	123	LYS	3.8
3	T	156	LYS	3.8
1	I	196	CYS	3.8
3	M	64	CYS	3.8
3	T	11	ASP	3.8
3	N	166	LYS	3.8
3	T	157	LYS	3.8
3	M	190	ASP	3.8
3	S	76	CYS	3.8
1	C	215	SER	3.8
3	O	266	SER	3.8
3	S	160	SER	3.8
3	U	157	LYS	3.8
3	O	156	LYS	3.8
3	U	77	GLU	3.8
1	I	198	VAL	3.8
3	M	152	ILE	3.8
3	S	139	CYS	3.8
3	S	161	TYR	3.8
3	M	198	ALA	3.7
3	T	63	LYS	3.7
3	T	159	ASN	3.7
3	M	120	ILE	3.7
3	U	148	TYR	3.7
3	M	124	THR	3.7
3	M	191	GLN	3.7
3	N	134	GLY	3.7
3	N	184	HIS	3.7
3	S	118	PHE	3.7
1	E	215	SER	3.7
3	O	279	THR	3.7
3	U	224	ARG	3.7
4	Q	142	HIS	3.7
3	U	164	LEU	3.6
3	M	116(A)	SER	3.6
3	M	87	ILE	3.6
3	O	116(A)	SER	3.6
3	O	228	GLY	3.6
3	N	78	SER	3.6
3	O	83(A)	SER	3.6
3	O	98	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	58	PRO	3.6
3	O	124	THR	3.6
3	N	183	HIS	3.6
3	S	77	GLU	3.6
3	S	174	LYS	3.6
3	U	11	ASP	3.6
3	U	80	SER	3.6
3	O	150	ASN	3.6
3	T	147	PHE	3.6
4	V	173	ILE	3.6
3	T	200	THR	3.6
3	N	195	TYR	3.6
3	T	116	SER	3.6
3	M	62	GLY	3.5
3	N	55	ARG	3.5
3	N	172	LYS	3.5
3	M	60	HIS	3.5
3	O	59	LEU	3.5
3	M	83	SER	3.5
3	N	165	SER	3.5
3	N	259	ALA	3.5
3	N	140	PRO	3.5
3	T	62	GLY	3.5
3	M	276	ASP	3.5
3	O	244	THR	3.5
3	S	261	GLU	3.5
3	T	197	ASN	3.5
3	O	97	CYS	3.5
3	U	196	GLN	3.5
3	M	100	GLY	3.5
3	N	170	ASN	3.5
3	U	62	GLY	3.5
1	I	112	SER	3.5
3	N	121	PHE	3.5
3	U	229	ARG	3.4
3	N	74	PRO	3.4
3	S	74	PRO	3.4
3	U	79	LEU	3.4
3	S	62	GLY	3.4
4	V	140	PHE	3.4
3	M	137	ALA	3.4
3	S	117	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	151	LEU	3.4
3	O	146	SER	3.4
3	S	187	THR	3.4
1	A	214	LYS	3.4
3	U	173	GLY	3.4
3	N	175	GLU	3.4
1	E	189	LEU	3.4
3	N	202	VAL	3.4
4	X	129	ASN	3.4
1	K	131	THR	3.4
3	O	183	HIS	3.4
3	O	157	LYS	3.4
3	U	133(A)	LYS	3.4
3	M	216	GLU	3.4
3	T	230	MET	3.4
1	I	82(B)	SER	3.4
3	U	247	ALA	3.4
3	M	218	ALA	3.4
3	O	125	SER	3.4
4	P	144	CYS	3.4
3	S	171	ASP	3.4
3	O	220	ARG	3.4
3	S	10	GLY	3.4
3	S	55	ARG	3.4
3	S	224	ARG	3.4
3	S	195	TYR	3.3
3	O	126	SER	3.3
3	M	54	LEU	3.3
3	N	122	PRO	3.3
3	U	97	CYS	3.3
3	U	147	PHE	3.3
3	S	173	GLY	3.3
3	U	199	ASP	3.3
3	M	251	LEU	3.3
3	N	88	VAL	3.3
3	O	259	ALA	3.3
3	S	245	PHE	3.3
3	N	139	CYS	3.3
1	E	198	VAL	3.3
3	M	257	ALA	3.3
3	N	11	ASP	3.3
3	T	139	CYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	S	147	PHE	3.3
3	O	260	MET	3.3
3	O	161	TYR	3.3
1	K	129	LYS	3.3
3	M	270	SER	3.3
3	O	174	LYS	3.3
1	K	189	LEU	3.3
3	M	79	LEU	3.3
3	S	251	LEU	3.3
3	T	245	PHE	3.3
4	W	144	CYS	3.3
3	U	171	ASP	3.3
3	N	123	LYS	3.2
3	S	199	ASP	3.2
3	T	76	CYS	3.2
3	U	197	ASN	3.2
3	T	219	ILE	3.2
1	E	131	THR	3.2
3	O	202	VAL	3.2
3	T	96	THR	3.2
3	O	218	ALA	3.2
4	P	143	LYS	3.2
3	M	70	ILE	3.2
3	U	90(A)	PRO	3.2
3	O	116	SER	3.2
3	O	167	SER	3.2
3	S	246	GLU	3.2
3	O	282	GLN	3.2
1	I	159	LEU	3.2
4	R	144	CYS	3.2
3	M	50	LYS	3.2
3	O	94	ASN	3.2
3	N	118	PHE	3.2
3	O	192	GLN	3.2
3	S	96	THR	3.2
3	M	98	TYR	3.2
4	X	141	TYR	3.2
3	O	182	ILE	3.2
3	T	124	THR	3.2
3	O	273	PRO	3.1
3	N	289	ASN	3.1
3	S	194	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	V	144	CYS	3.1
3	S	260	MET	3.1
1	I	207	VAL	3.1
3	S	95	GLY	3.1
3	T	247	ALA	3.1
3	T	187	THR	3.1
3	O	158	GLY	3.1
3	O	240	GLY	3.1
3	N	61	LEU	3.1
3	S	94	ASN	3.1
3	M	104	ASP	3.1
3	N	263	ASN	3.1
1	I	212	GLU	3.1
3	O	206	SER	3.1
3	O	254	PRO	3.1
3	O	90	THR	3.1
3	M	240	GLY	3.1
3	U	73	ASN	3.1
3	O	147	PHE	3.1
3	M	221	PRO	3.0
3	M	160	SER	3.0
3	N	219	ILE	3.0
3	O	186	SER	3.0
3	U	155	VAL	3.0
3	U	279	THR	3.0
4	Q	162	TYR	3.0
3	S	93	ASP	3.0
3	T	131	ASP	3.0
3	O	257	ALA	3.0
3	T	130	HIS	3.0
3	T	201	TYR	3.0
1	I	144	ASP	3.0
3	S	121	PHE	3.0
1	C	210	ARG	3.0
3	S	51	LEU	3.0
3	O	102	PHE	3.0
3	M	259	ALA	3.0
3	O	188	SER	3.0
3	T	165	SER	3.0
3	M	116(C)	GLU	3.0
3	T	143	GLY	3.0
3	O	60	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	221	PRO	3.0
1	G	191	THR	3.0
3	S	290	THR	3.0
3	N	94	ASN	3.0
3	S	250	ASN	3.0
3	U	219	ILE	3.0
3	S	61	LEU	3.0
3	O	149	LYS	3.0
3	O	48	ASN	3.0
3	S	167	SER	3.0
3	U	231	ASN	3.0
4	R	143	LYS	3.0
3	N	64	CYS	3.0
3	S	277	CYS	3.0
1	I	154	TRP	2.9
3	S	133(A)	LYS	2.9
3	M	68	GLY	2.9
3	M	136	THR	2.9
1	A	189	LEU	2.9
4	W	27	GLN	2.9
3	U	288	ILE	2.9
3	N	142	ALA	2.9
3	N	100	GLY	2.9
3	O	226	GLN	2.9
3	U	207	SER	2.9
3	O	96	THR	2.9
3	O	290	THR	2.9
3	U	246	GLU	2.9
3	U	182	ILE	2.9
3	S	263	ASN	2.9
3	T	74	PRO	2.9
3	U	150	ASN	2.9
3	S	88	VAL	2.9
1	A	130	SER	2.9
3	S	122	PRO	2.9
3	S	215	PRO	2.9
3	U	195	TYR	2.9
3	N	119	GLU	2.9
3	O	118	PHE	2.9
3	M	159	ASN	2.9
3	N	208	ARG	2.9
3	S	124	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	S	229	ARG	2.9
3	S	184	HIS	2.9
3	N	249	GLY	2.9
3	T	144	ALA	2.9
3	M	95	GLY	2.9
3	S	55(A)	GLY	2.9
3	M	236	LEU	2.9
3	U	186	SER	2.9
3	M	71	LEU	2.9
3	T	61	LEU	2.9
3	O	92	SER	2.8
3	U	159	ASN	2.8
3	O	190	ASP	2.8
3	T	158	GLY	2.8
3	U	141	HIS	2.8
3	M	212	LYS	2.8
3	N	257	ALA	2.8
3	S	73	ASN	2.8
3	T	81	THR	2.8
4	R	63	PHE	2.8
3	S	186	SER	2.8
3	S	231	ASN	2.8
3	O	69	TRP	2.8
3	N	144	ALA	2.8
3	T	82	ALA	2.8
3	O	100	GLY	2.8
3	M	263	ASN	2.8
3	N	190	ASP	2.8
3	O	140	PRO	2.8
4	Q	141	TYR	2.8
1	E	16	SER	2.8
3	S	83(A)	SER	2.8
3	U	245	PHE	2.8
3	T	170	ASN	2.8
3	M	194	LEU	2.8
3	O	168	TYR	2.8
4	W	142	HIS	2.8
3	M	91	SER	2.8
3	O	277	CYS	2.8
3	S	282	GLN	2.8
1	K	194	TYR	2.8
3	T	118	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	171	ASP	2.8
3	S	78	SER	2.8
3	T	64	CYS	2.8
3	T	191	GLN	2.7
3	S	146	SER	2.7
3	O	121	PHE	2.7
3	U	60	HIS	2.7
3	T	92	SER	2.7
3	M	90(A)	PRO	2.7
3	N	254	PRO	2.7
3	T	241	ASP	2.7
3	U	200	THR	2.7
3	U	248	THR	2.7
3	U	168	TYR	2.7
3	U	201	TYR	2.7
3	U	51	LEU	2.7
3	N	268	ILE	2.7
3	N	90(A)	PRO	2.7
1	I	145	TYR	2.7
3	S	287	ALA	2.7
1	I	66	ARG	2.7
3	U	166	LYS	2.7
3	N	51	LEU	2.7
3	S	83	SER	2.7
3	T	215	PRO	2.7
3	M	214	LYS	2.7
4	Q	144	CYS	2.7
1	E	130	SER	2.7
3	M	63	LYS	2.7
3	N	124	THR	2.7
3	N	200	THR	2.7
3	S	202	VAL	2.7
3	S	272	THR	2.7
3	T	202	VAL	2.7
3	N	164	LEU	2.7
3	M	78	SER	2.7
3	U	99	PRO	2.7
4	W	148	CYS	2.7
3	S	223	VAL	2.7
3	N	218	ALA	2.7
3	N	174	LYS	2.7
3	N	282	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	U	10	GLY	2.7
4	V	149	MET	2.7
3	O	75	GLU	2.7
3	M	53	LYS	2.7
3	M	157	LYS	2.7
1	K	128	SER	2.7
3	S	200	THR	2.7
3	N	147	PHE	2.7
3	M	261	GLU	2.7
4	P	142	HIS	2.7
2	L	30	SER	2.6
3	M	222	LYS	2.6
1	I	206	LYS	2.6
3	O	212	LYS	2.6
3	U	74	PRO	2.6
3	T	184	HIS	2.6
3	U	146	SER	2.6
1	I	1	GLN	2.6
3	O	10	GLY	2.6
3	O	242	LYS	2.6
3	N	162	PRO	2.6
3	N	212	LYS	2.6
3	S	129	ASN	2.6
3	T	50	LYS	2.6
4	W	143	LYS	2.6
3	M	59	LEU	2.6
3	T	52	CYS	2.6
3	S	185	PRO	2.6
3	N	145	LYS	2.6
2	J	77	ARG	2.6
3	O	63	LYS	2.6
3	S	270	SER	2.6
3	N	217	ILE	2.6
3	N	278	ASN	2.6
3	N	148	TYR	2.6
3	N	102	PHE	2.6
3	M	184	HIS	2.6
3	S	75	GLU	2.6
3	T	270	SER	2.6
3	O	120	ILE	2.6
3	N	73	ASN	2.6
3	S	289	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	194	TYR	2.6
1	E	144	ASP	2.6
3	U	218	ALA	2.6
1	I	199	ASN	2.6
3	M	275	HIS	2.6
3	S	11	ASP	2.6
3	S	214	LYS	2.6
3	O	219	ILE	2.6
1	I	64	GLN	2.6
3	N	99	PRO	2.6
3	U	118	PHE	2.6
3	S	149	LYS	2.6
1	I	119	PRO	2.6
3	U	9	PRO	2.6
3	N	196	GLN	2.5
3	N	264	ALA	2.5
1	I	23	ARG	2.5
3	S	48	ASN	2.5
3	M	256	TYR	2.5
3	S	192	GLN	2.5
3	O	49	GLY	2.5
3	M	131	ASP	2.5
3	N	116(B)	PHE	2.5
3	U	172	LYS	2.5
2	J	129	THR	2.5
3	O	119	GLU	2.5
3	S	82	ALA	2.5
3	T	133(A)	LYS	2.5
2	B	62	PHE	2.5
3	U	184	HIS	2.5
3	N	236	LEU	2.5
3	U	270	SER	2.5
4	P	165	GLU	2.5
3	U	190	ASP	2.5
3	M	192	GLN	2.5
3	M	170	ASN	2.5
1	I	191	THR	2.5
3	N	54	LEU	2.5
3	S	140	PRO	2.5
3	M	182	ILE	2.5
3	U	12	THR	2.5
3	U	89	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	208	ARG	2.5
1	C	189	LEU	2.5
3	S	158	GLY	2.5
3	U	262	ARG	2.5
3	M	290	THR	2.5
3	U	187	THR	2.5
3	U	198	ALA	2.5
4	W	164	GLU	2.5
3	M	274	VAL	2.5
3	T	12	THR	2.5
3	N	131	ASP	2.5
3	T	246	GLU	2.5
3	N	230	MET	2.4
3	N	143	GLY	2.4
3	T	259	ALA	2.4
1	I	126	PRO	2.4
3	S	191	GLN	2.4
3	S	221	PRO	2.4
3	O	175	GLU	2.4
1	G	112	SER	2.4
3	U	167	SER	2.4
3	U	54	LEU	2.4
3	M	148	TYR	2.4
1	I	129	LYS	2.4
3	S	225	ASP	2.4
3	U	116	SER	2.4
3	U	220	ARG	2.4
1	I	204	ASN	2.4
3	U	88	VAL	2.4
3	N	80	SER	2.4
3	O	55	ARG	2.4
3	U	129	ASN	2.4
4	W	162	TYR	2.4
3	N	98	TYR	2.4
3	S	143	GLY	2.4
3	U	290	THR	2.4
1	G	194	TYR	2.4
3	M	11	ASP	2.4
3	O	71	LEU	2.4
3	U	183	HIS	2.4
1	G	132	SER	2.4
3	O	52	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	130	HIS	2.4
3	U	131	ASP	2.4
3	T	194	LEU	2.4
1	G	192	GLN	2.4
1	I	211	VAL	2.4
2	D	62	PHE	2.4
3	T	186	SER	2.4
3	M	185	PRO	2.4
3	N	215	PRO	2.4
3	N	12	THR	2.4
3	N	120	ILE	2.4
3	T	163	LYS	2.4
3	T	257	ALA	2.4
4	P	141	TYR	2.4
3	T	93	ASP	2.4
3	M	88	VAL	2.4
1	E	112	SER	2.4
1	G	1	GLN	2.4
4	Q	157	TYR	2.4
1	I	205	THR	2.4
3	U	66	ILE	2.4
3	N	135	VAL	2.3
3	T	217	ILE	2.3
3	U	100	GLY	2.3
3	M	175	GLU	2.3
4	W	166	ALA	2.3
3	O	84	TRP	2.3
3	U	64	CYS	2.3
3	O	268	ILE	2.3
1	A	207	VAL	2.3
1	K	1	GLN	2.3
3	M	168	TYR	2.3
3	T	133	ASN	2.3
3	T	183	HIS	2.3
3	O	217	ILE	2.3
3	O	258	PHE	2.3
1	G	209	LYS	2.3
3	O	135	VAL	2.3
3	S	204	VAL	2.3
4	V	165	GLU	2.3
4	X	30	GLN	2.3
4	X	62	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	60	ASN	2.3
1	C	214	LYS	2.3
3	N	128	PRO	2.3
3	N	222	LYS	2.3
1	A	1	GLN	2.3
3	U	130	HIS	2.3
3	T	86	TYR	2.3
3	T	287	ALA	2.3
3	N	243	ILE	2.3
3	O	304	LYS	2.3
3	T	225	ASP	2.3
1	K	4	LEU	2.3
3	U	191	GLN	2.3
3	O	55(A)	GLY	2.3
3	S	288	ILE	2.3
3	N	91	SER	2.3
3	N	95	GLY	2.2
1	C	23	ARG	2.2
3	O	302	ILE	2.2
1	K	211	VAL	2.2
1	C	199	ASN	2.2
4	X	63	PHE	2.2
3	T	264	ALA	2.2
3	U	282	GLN	2.2
4	R	29	GLU	2.2
4	X	162	TYR	2.2
3	M	234	TRP	2.2
3	T	51	LEU	2.2
3	O	230	MET	2.2
1	A	81	ASP	2.2
4	Q	140	PHE	2.2
3	N	252	VAL	2.2
3	T	145	LYS	2.2
3	U	174	LYS	2.2
1	I	17	SER	2.2
3	S	276	ASP	2.2
3	O	301	THR	2.2
4	R	142	HIS	2.2
1	A	186	SER	2.2
3	T	83(A)	SER	2.2
3	O	255	ARG	2.2
3	M	249	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	140	CYS	2.2
4	W	72	HIS	2.2
3	O	262	ARG	2.2
1	C	119	PRO	2.2
1	I	197	ASN	2.2
3	T	116(B)	PHE	2.2
3	T	208	ARG	2.2
3	M	267	ILE	2.2
1	I	189	LEU	2.2
2	H	70	ASP	2.2
3	T	190	ASP	2.2
3	S	227	GLU	2.2
3	T	10	GLY	2.2
3	U	132	SER	2.2
1	A	198	VAL	2.2
3	N	10	GLY	2.2
3	S	126	SER	2.2
1	C	1	GLN	2.2
3	T	282	GLN	2.2
3	O	170	ASN	2.2
3	S	235	THR	2.2
3	M	262	ARG	2.2
3	U	117	ARG	2.2
1	E	159	LEU	2.2
3	U	212	LYS	2.2
4	Q	165	GLU	2.2
3	N	290	THR	2.2
3	U	121	PHE	2.1
1	I	213	PRO	2.1
3	M	199	ASP	2.1
3	S	104	ASP	2.1
3	U	202	VAL	2.1
4	P	140	PHE	2.1
3	N	146	SER	2.1
3	O	276	ASP	2.1
3	T	236	LEU	2.1
1	C	205	THR	2.1
3	M	211	LYS	2.1
4	W	28	ASN	2.1
3	T	199	ASP	2.1
3	T	256	TYR	2.1
3	U	69	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	V	169	ASN	2.1
4	V	170	ARG	2.1
4	X	142	HIS	2.1
3	O	297	ILE	2.1
3	S	217	ILE	2.1
3	T	48	ASN	2.1
3	U	265	GLY	2.1
4	R	170	ARG	2.1
3	N	168	TYR	2.1
3	O	89	GLU	2.1
3	U	227	GLU	2.1
3	M	279	THR	2.1
3	N	240	GLY	2.1
3	S	159	ASN	2.1
3	S	279	THR	2.1
3	T	166	LYS	2.1
1	A	194	TYR	2.1
1	G	128	SER	2.1
3	U	257	ALA	2.1
3	O	184	HIS	2.1
3	O	234	TRP	2.1
4	Q	72	HIS	2.1
3	U	143	GLY	2.1
1	A	199	ASN	2.1
4	P	149	MET	2.1
4	Q	28	ASN	2.1
1	E	145	TYR	2.1
1	C	207	VAL	2.1
2	H	77	ARG	2.1
3	N	225	ASP	2.1
2	H	62	PHE	2.1
3	U	203	PHE	2.1
3	N	248	THR	2.1
3	M	201	TYR	2.1
3	M	273	PRO	2.1
4	R	69	GLU	2.1
3	O	253	VAL	2.1
3	S	142	ALA	2.1
4	V	166	ALA	2.1
3	N	59	LEU	2.1
3	N	116(A)	SER	2.1
4	W	30	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	256	TYR	2.1
3	S	144	ALA	2.1
3	U	96	THR	2.1
4	P	171	GLU	2.1
3	N	53	LYS	2.0
3	S	116(B)	PHE	2.0
1	A	119	PRO	2.0
3	T	94	ASN	2.0
4	R	169	ASN	2.0
3	M	268	ILE	2.0
3	N	112	LEU	2.0
2	J	32	SER	2.0
4	X	27	GLN	2.0
3	U	277	CYS	2.0
2	J	125	LEU	2.0
3	O	278	ASN	2.0
3	T	164	LEU	2.0
3	N	214	LYS	2.0
4	W	29	GLU	2.0
4	W	157	TYR	2.0
1	G	189	LEU	2.0
3	O	133	ASN	2.0
3	U	119	GLU	2.0
3	N	232	TYR	2.0
3	O	54	LEU	2.0
3	O	66	ILE	2.0
3	S	259	ALA	2.0
4	X	169	ASN	2.0
1	A	144	ASP	2.0
1	I	156	SER	2.0
1	K	127	SER	2.0
3	M	125	SER	2.0
3	S	53	LYS	2.0
3	T	83	SER	2.0
3	S	182	ILE	2.0
3	U	240	GLY	2.0
3	T	119	GLU	2.0
1	K	23	ARG	2.0
3	M	61	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.