Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 04:46 PM EDT

PDB ID	:	1T60
Title	:	Crystal structure of Type IV collagen NC1 domain from bovine lens capsule
Authors	:	Vanacore, R.M.; Shanmugasundararaj, S.; Friedman, D.B.; Bondar, O.; Hudson, B.G.; Sundaramoorthy, M.
Deposited on	:	2004-05-05
Resolution	:	1.50 Å(reported)

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

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

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

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

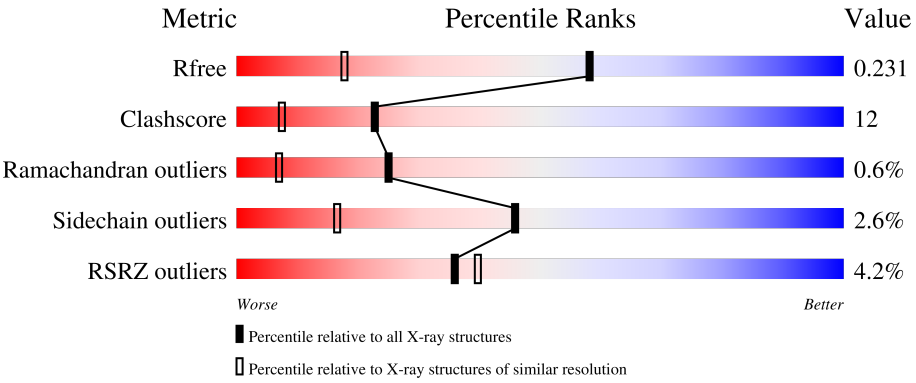
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	229	78% 19%
1	B	229	7% 75% 22%
1	D	229	2% 76% 20%
1	E	229	3% 79% 18%
1	G	229	3% 81% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	229	5% 76% 22%
1	J	229	5% 75% 21%
1	K	229	7% 79% 17%
1	M	229	5% 73% 21%
1	N	229	5% 75% 23%
1	P	229	% 78% 19%
1	Q	229	3% 78% 18%
1	S	229	2% 79% 18%
1	T	229	4% 76% 21%
1	V	229	5% 69% 27%
1	W	229	5% 75% 22%
2	C	227	6% 73% 24%
2	F	227	6% 76% 21%
2	I	227	4% 77% 21%
2	L	227	4% 75% 22%
2	O	227	4% 76% 22%
2	R	227	5% 73% 24%
2	U	227	4% 76% 21%
2	X	227	5% 76% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	J	5009	-	-	-	X
4	MPD	P	5006	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 44599 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 type iv collagen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1724	1085	300	318	21			
1	B	225	Total	C	N	O	S	0	0	0
			1745	1097	307	320	21			
1	D	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	E	224	Total	C	N	O	S	0	0	0
			1735	1091	304	319	21			
1	G	228	Total	C	N	O	S	0	0	0
			1767	1110	310	326	21			
1	H	227	Total	C	N	O	S	0	0	0
			1760	1105	309	325	21			
1	J	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	K	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	M	223	Total	C	N	O	S	0	0	0
			1724	1085	300	318	21			
1	N	224	Total	C	N	O	S	0	0	0
			1738	1093	304	320	21			
1	P	225	Total	C	N	O	S	0	0	0
			1745	1097	307	320	21			
1	Q	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	S	225	Total	C	N	O	S	0	0	0
			1745	1097	307	320	21			
1	T	227	Total	C	N	O	S	0	0	0
			1760	1105	309	325	21			
1	V	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			
1	W	224	Total	C	N	O	S	0	0	0
			1734	1091	303	319	21			

- Molecule 2 is a protein called type iv collagen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	0	0
			1724	1093	291	321	19			
2	F	222	Total	C	N	O	S	0	0	0
			1720	1089	291	321	19			
2	I	225	Total	C	N	O	S	0	0	0
			1738	1100	294	325	19			
2	L	221	Total	C	N	O	S	0	0	0
			1708	1080	290	319	19			
2	O	224	Total	C	N	O	S	0	0	0
			1732	1097	293	323	19			
2	R	224	Total	C	N	O	S	0	0	0
			1732	1097	293	323	19			
2	U	224	Total	C	N	O	S	0	0	0
			1732	1097	293	323	19			
2	X	223	Total	C	N	O	S	0	0	0
			1724	1091	292	322	19			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

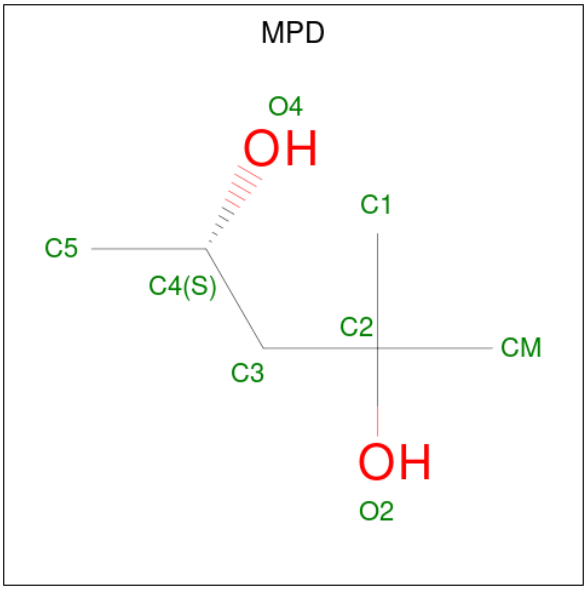
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	I	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	L	1	Total	Cl	0	0
			1	1		
3	M	1	Total	Cl	0	0
			1	1		
3	O	1	Total	Cl	0	0
			1	1		
3	P	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	R	1	Total Cl 1 1	0	0
3	S	1	Total Cl 1 1	0	0
3	U	1	Total Cl 1 1	0	0
3	V	1	Total Cl 1 1	0	0
3	X	1	Total Cl 1 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	J	1	Total C O 8 6 2	0	0
4	M	1	Total C O 8 6 2	0	0
4	M	1	Total C O 8 6 2	0	0
4	P	1	Total C O 8 6 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total C O 8 6 2	0	0
4	S	1	Total C O 8 6 2	0	0
4	T	1	Total C O 8 6 2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	C	2	Total K 2 2	0	0
5	D	1	Total K 1 1	0	0
5	G	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0
5	I	1	Total K 1 1	0	0
5	L	1	Total K 1 1	0	0
5	M	1	Total K 1 1	0	0
5	N	1	Total K 1 1	0	0
5	O	1	Total K 1 1	0	0
5	P	1	Total K 1 1	0	0
5	T	1	Total K 1 1	0	0
5	U	2	Total K 2 2	0	0
5	V	1	Total K 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	112	Total O 112 112	0	0
6	B	101	Total O 101 101	0	0
6	C	116	Total O 116 116	0	0
6	D	134	Total O 134 134	0	0
6	E	127	Total O 127 127	0	0
6	F	117	Total O 117 117	0	0
6	G	144	Total O 144 144	0	0
6	H	104	Total O 104 104	0	0
6	I	121	Total O 121 121	0	0
6	J	97	Total O 97 97	0	0
6	K	102	Total O 102 102	0	0
6	L	111	Total O 111 111	0	0
6	M	118	Total O 118 118	0	0
6	N	113	Total O 113 113	0	0
6	O	125	Total O 125 125	0	0
6	P	133	Total O 133 133	0	0
6	Q	108	Total O 108 108	0	0
6	R	129	Total O 129 129	0	0
6	S	137	Total O 137 137	0	0
6	T	127	Total O 127 127	0	0
6	U	139	Total O 139 139	0	0
6	V	110	Total O 110 110	0	0

Continued on next page...

Continued from previous page...

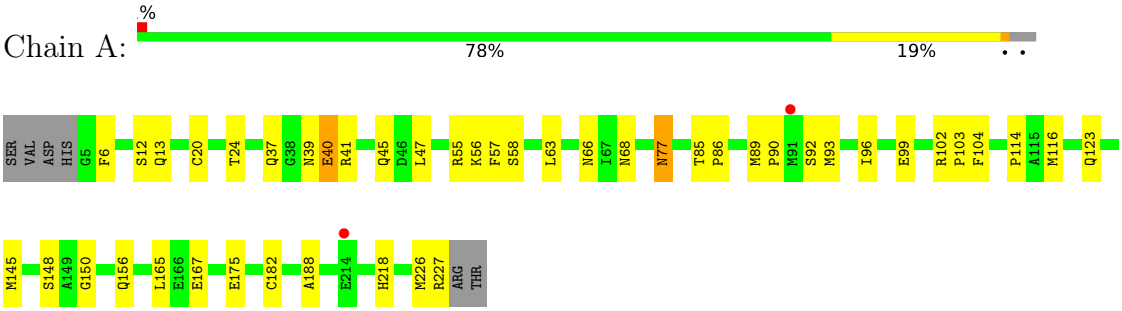
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	W	103	Total O 103 103	0	0
6	X	110	Total O 110 110	0	0

3 Residue-property plots (i)

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

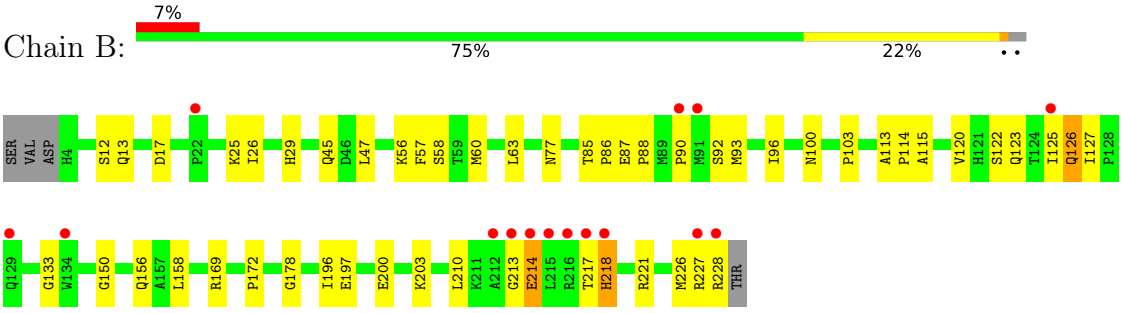
• Molecule 1: type iv collagen

Chain A:



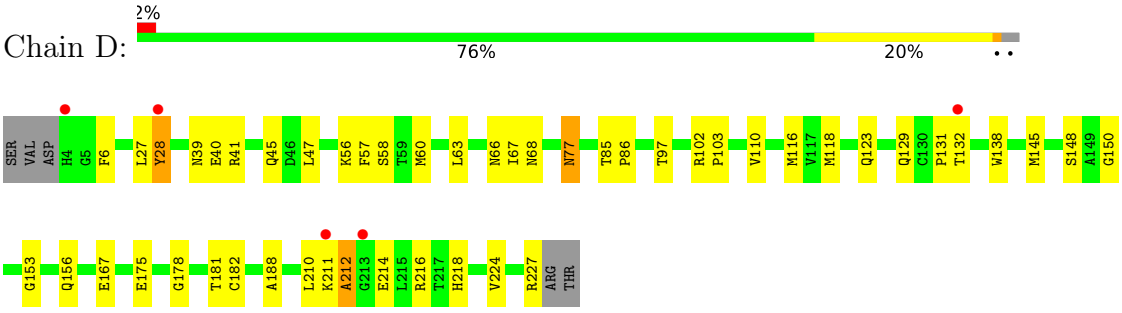
• Molecule 1: type iv collagen

Chain B:



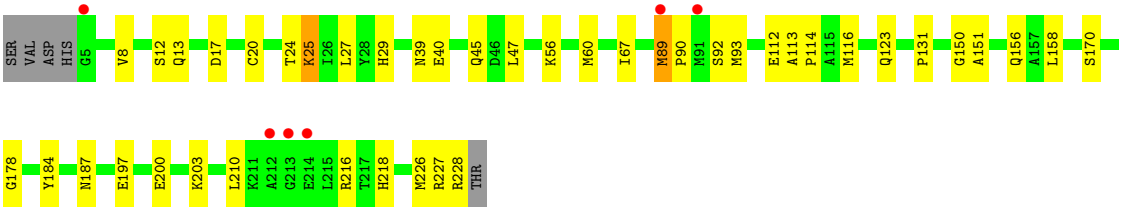
• Molecule 1: type iv collagen

Chain D:



• Molecule 1: type iv collagen

Chain E:

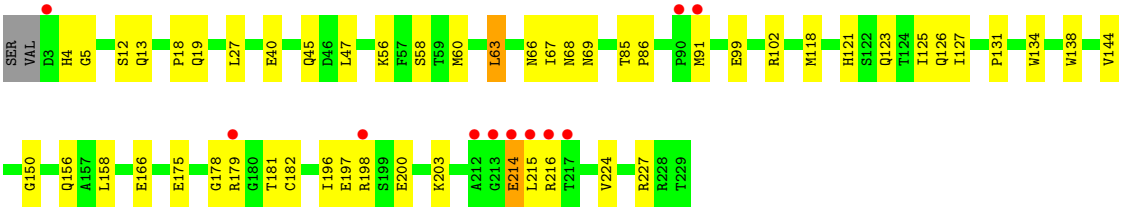


• Molecule 1: type iv collagen

Chain G:

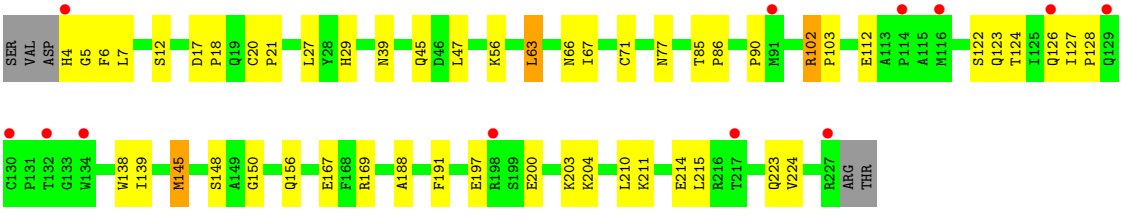
• Molecule 1: type iv collagen

Chain H:



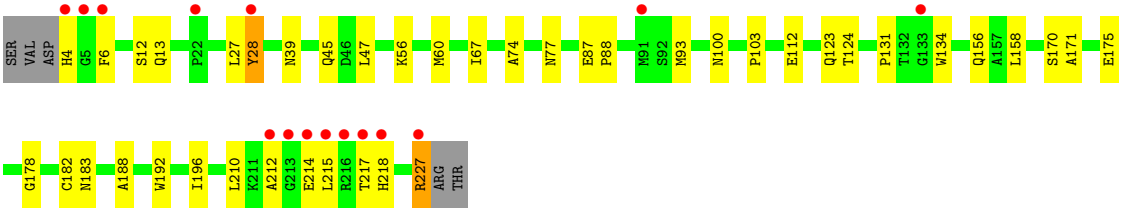
• Molecule 1: type iv collagen

Chain J:



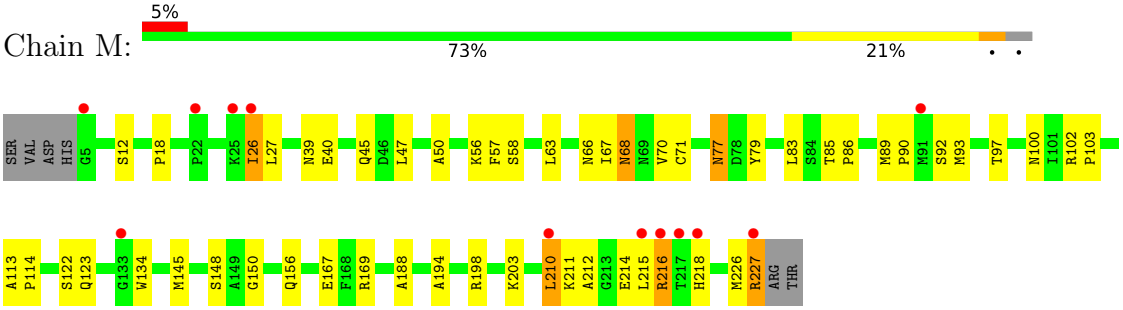
• Molecule 1: type iv collagen

Chain K:



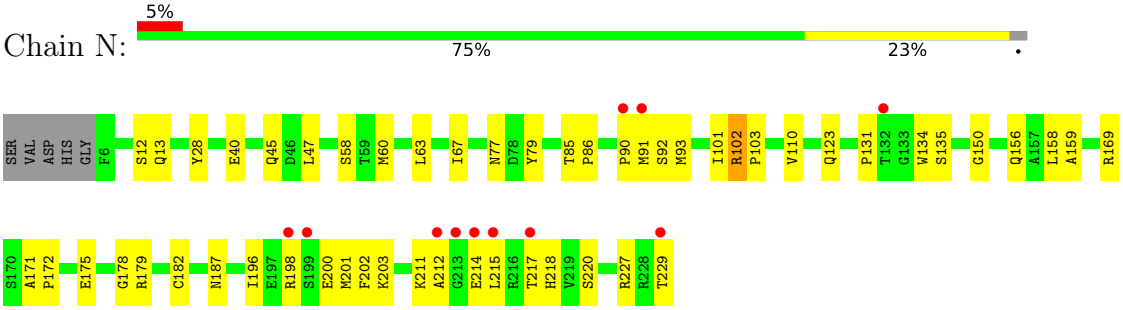
• Molecule 1: type iv collagen

Chain M:



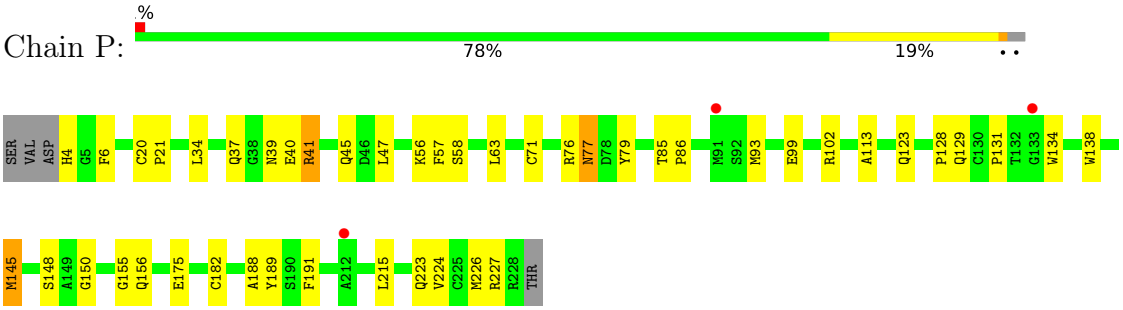
• Molecule 1: type iv collagen

Chain N:



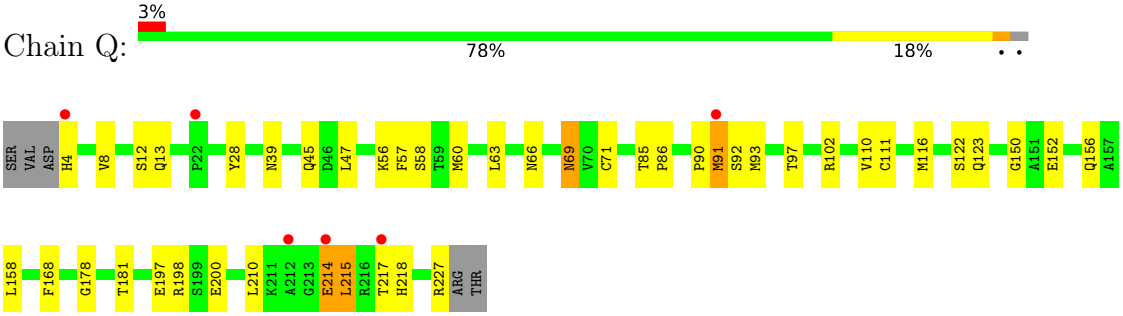
• Molecule 1: type iv collagen

Chain P:



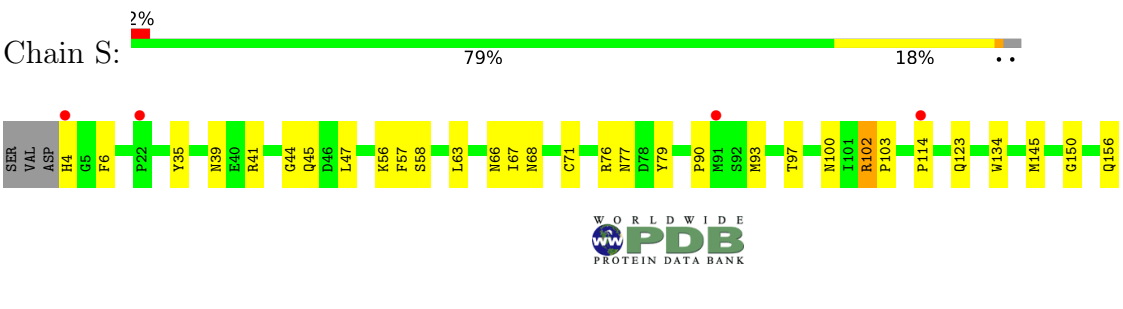
• Molecule 1: type iv collagen

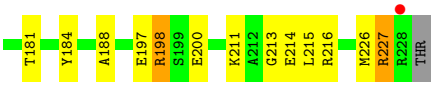
Chain Q:



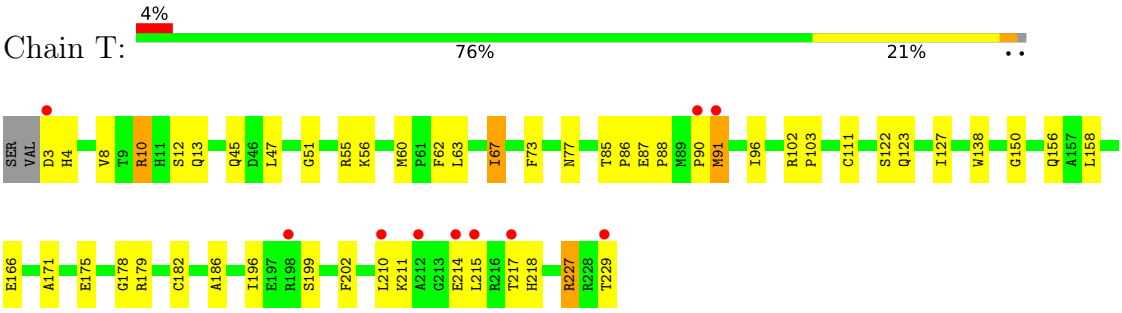
• Molecule 1: type iv collagen

Chain S:

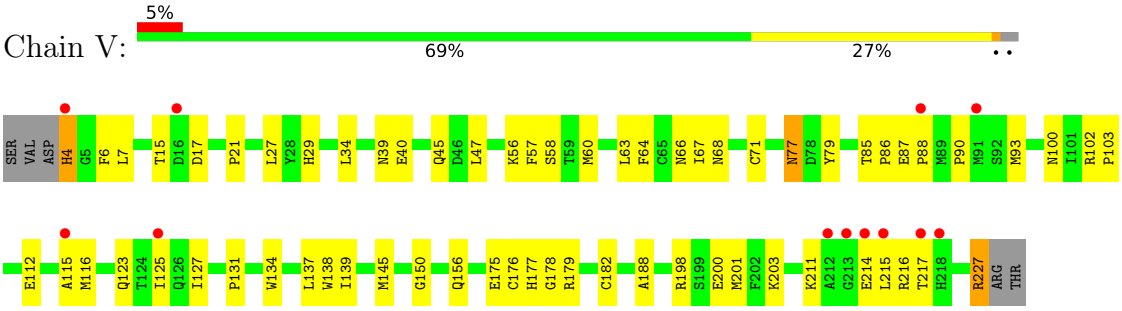




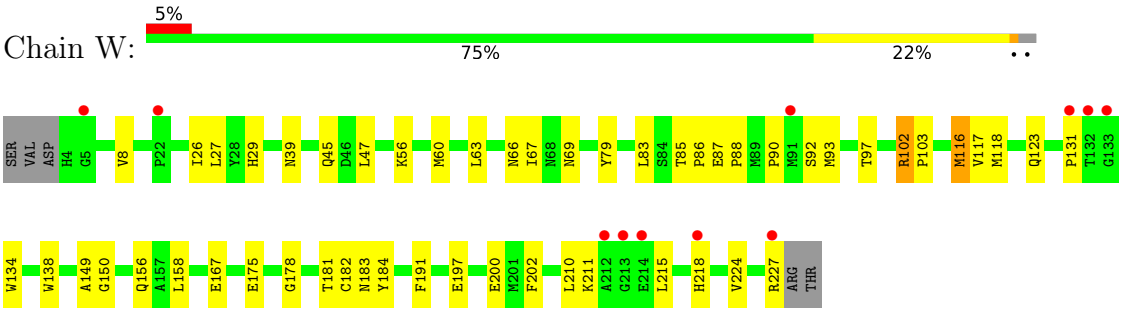
• Molecule 1: type iv collagen



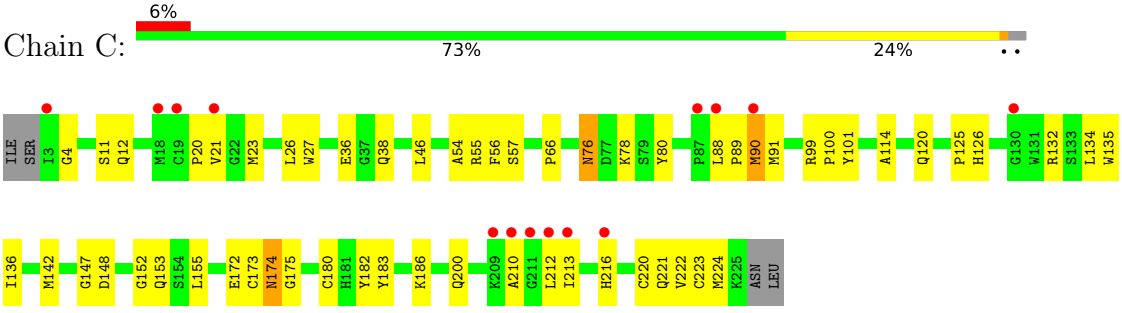
• Molecule 1: type iv collagen



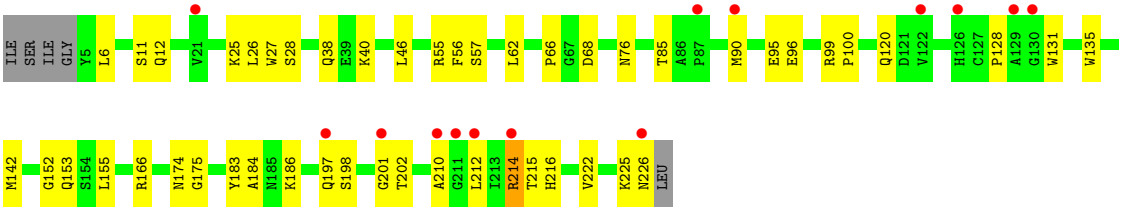
• Molecule 1: type iv collagen



• Molecule 2: type iv collagen

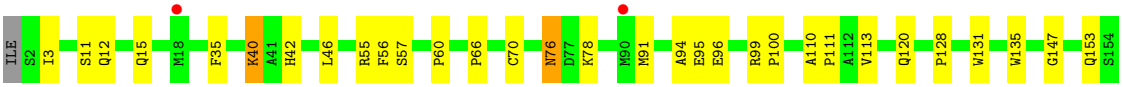


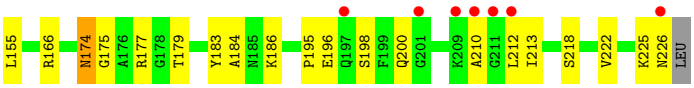
• Molecule 2: type iv collagen



• Molecule 2: type iv collagen

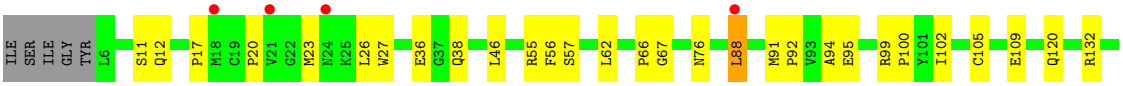
Chain I:





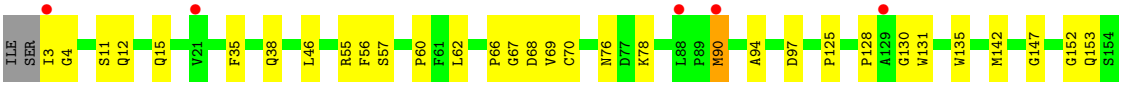
• Molecule 2: type iv collagen

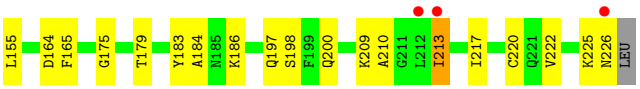
Chain L:



• Molecule 2: type iv collagen

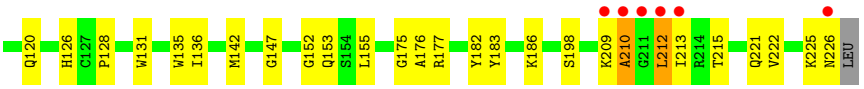
Chain O:





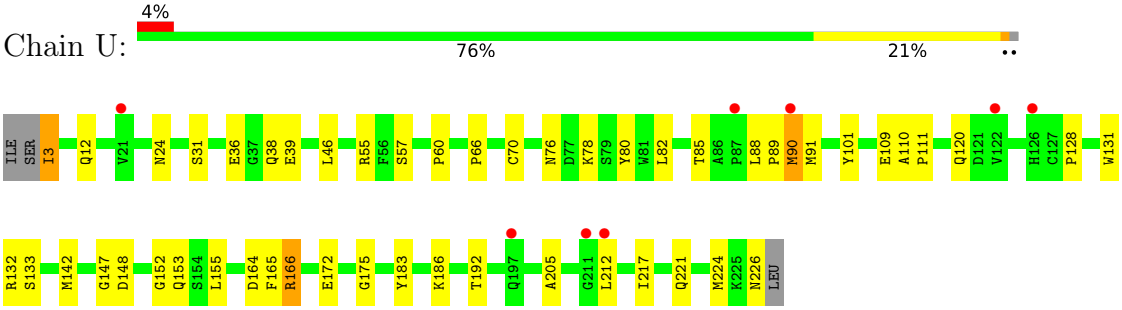
• Molecule 2: type iv collagen

Chain R:



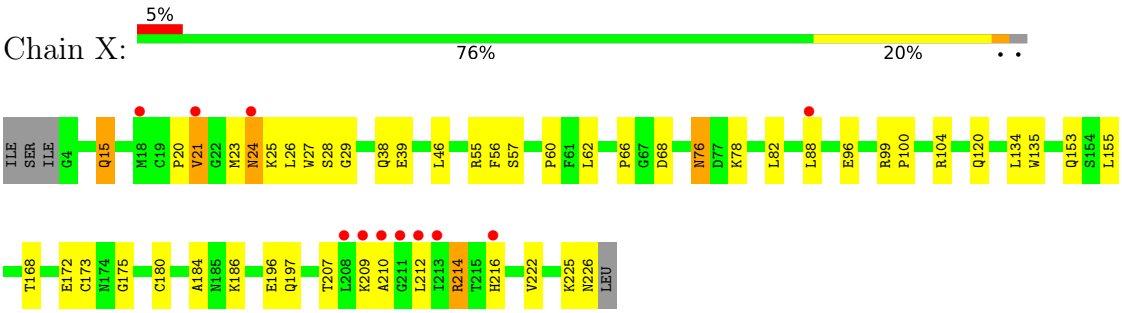
• Molecule 2: type iv collagen

Chain U:



• Molecule 2: type iv collagen

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.88Å 140.13Å 160.69Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	8.00 – 1.50 50.02 – 1.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.50) 89.5 (50.02-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.216 0.205 , 0.231	Depositor DCC
R_{free} test set	39655 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	44599	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9581e-04.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, CL, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/1774	0.62	0/2410
1	B	0.34	0/1796	0.61	0/2439
1	D	0.36	0/1785	0.63	0/2425
1	E	0.35	0/1785	0.61	0/2424
1	G	0.36	0/1818	0.62	0/2470
1	H	0.34	0/1811	0.60	0/2460
1	J	0.34	0/1785	0.62	0/2425
1	K	0.34	0/1785	0.61	0/2425
1	M	0.35	0/1774	0.61	0/2410
1	N	0.33	0/1788	0.61	0/2429
1	P	0.35	0/1796	0.61	0/2439
1	Q	0.35	0/1785	0.61	0/2425
1	S	0.34	0/1796	0.60	0/2439
1	T	0.34	0/1811	0.61	0/2460
1	V	0.33	0/1785	0.59	0/2425
1	W	0.33	0/1785	0.59	0/2425
2	C	0.36	0/1775	0.65	0/2415
2	F	0.36	0/1771	0.63	0/2410
2	I	0.34	0/1789	0.63	0/2434
2	L	0.35	0/1758	0.64	0/2392
2	O	0.35	0/1783	0.63	0/2426
2	R	0.35	0/1783	0.63	0/2426
2	U	0.35	0/1783	0.64	0/2426
2	X	0.34	0/1775	0.63	0/2415
All	All	0.35	0/42876	0.62	0/58274

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1724	0	1640	45	0
1	B	1745	0	1661	56	0
1	D	1734	0	1647	56	0
1	E	1735	0	1654	39	0
1	G	1767	0	1680	41	0
1	H	1760	0	1672	48	0
1	J	1734	0	1647	55	0
1	K	1734	0	1648	49	0
1	M	1724	0	1640	65	0
1	N	1738	0	1658	49	0
1	P	1745	0	1660	44	0
1	Q	1734	0	1648	41	0
1	S	1745	0	1661	48	0
1	T	1760	0	1672	55	0
1	V	1734	0	1647	57	0
1	W	1734	0	1648	49	0
2	C	1724	0	1637	54	0
2	F	1720	0	1629	39	0
2	I	1738	0	1648	54	0
2	L	1708	0	1619	40	0
2	O	1732	0	1643	43	0
2	R	1732	0	1643	56	0
2	U	1732	0	1643	48	0
2	X	1724	0	1631	51	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	X	1	0	0	0	0
4	A	8	0	14	0	0
4	D	8	0	14	1	0
4	J	8	0	14	3	0
4	M	16	0	28	1	0
4	P	8	0	14	6	0
4	S	16	0	28	5	0
4	T	8	0	14	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	T	1	0	0	0	0
5	U	2	0	0	0	0
5	V	1	0	0	0	0
6	A	112	0	0	4	0
6	B	101	0	0	1	0
6	C	116	0	0	0	0
6	D	134	0	0	3	0
6	E	127	0	0	1	0
6	F	117	0	0	0	0
6	G	144	0	0	1	0
6	H	104	0	0	2	0
6	I	121	0	0	2	0
6	J	97	0	0	1	0
6	K	102	0	0	1	0
6	L	111	0	0	0	0
6	M	118	0	0	2	0
6	N	113	0	0	5	0
6	O	125	0	0	1	0
6	P	133	0	0	3	0
6	Q	108	0	0	1	0
6	R	129	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	137	0	0	4	0
6	T	127	0	0	5	0
6	U	139	0	0	1	0
6	V	110	0	0	3	0
6	W	103	0	0	2	0
6	X	110	0	0	5	0
All	All	44599	0	39702	939	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 12.

All (939) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:HE2	1:B:203:LYS:HA	1.40	1.03
1:E:27:LEU:HD21	1:E:112:GLU:HG3	1.40	1.00
1:V:123:GLN:HE22	2:X:55:ARG:H	1.20	0.89
1:N:200:GLU:HA	1:N:203:LYS:HE2	1.56	0.87
1:J:45:GLN:HE22	1:K:158:LEU:H	1.22	0.85
1:W:45:GLN:HE22	2:X:155:LEU:H	1.23	0.85
1:P:123:GLN:HE22	2:R:55:ARG:H	1.23	0.84
1:M:67:ILE:HG22	1:N:171:ALA:HB2	1.57	0.84
2:C:136:ILE:HG22	2:C:221:GLN:HG2	1.58	0.83
4:P:5006:MPD:O4	2:R:27:TRP:HB3	1.77	0.83
1:J:67:ILE:HD12	1:J:67:ILE:H	1.43	0.82
2:I:94:ALA:HB2	2:I:179:THR:HG22	1.61	0.82
1:M:123:GLN:HE22	2:O:55:ARG:H	1.27	0.82
1:T:217:THR:HG23	1:T:218:HIS:ND1	1.95	0.82
1:A:123:GLN:HE22	2:C:55:ARG:H	1.24	0.82
1:P:45:GLN:HE22	1:Q:158:LEU:H	1.27	0.82
1:Q:217:THR:HG23	1:Q:218:HIS:ND1	1.95	0.81
1:S:123:GLN:HE22	2:U:55:ARG:H	1.28	0.80
1:N:217:THR:HG23	1:N:218:HIS:ND1	1.95	0.80
1:Q:45:GLN:HE22	2:R:155:LEU:H	1.29	0.80
1:V:200:GLU:HG2	1:V:203:LYS:HE3	1.62	0.80
1:M:67:ILE:HG23	6:N:5149:HOH:O	1.80	0.79
2:F:25:LYS:HE3	2:F:28:SER:HB3	1.65	0.78
1:T:214:GLU:O	1:T:217:THR:HG22	1.82	0.78
1:J:211:LYS:O	1:J:214:GLU:HG2	1.84	0.78
1:S:216:ARG:HH11	4:S:5005:MPD:H52	1.48	0.78
1:W:47:LEU:H	1:W:156:GLN:HE22	1.29	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLN:HE22	2:F:55:ARG:H	1.27	0.77
1:V:45:GLN:HE22	1:W:158:LEU:H	1.31	0.77
1:M:210:LEU:HD21	2:O:70:CYS:HB2	1.65	0.77
1:B:93:MET:SD	1:D:211:LYS:NZ	2.56	0.76
2:C:90:MET:HG2	2:C:91:MET:N	2.00	0.76
1:J:47:LEU:H	1:J:156:GLN:HE22	1.33	0.76
1:Q:69:ASN:HB3	2:R:210:ALA:HB2	1.67	0.76
2:O:38:GLN:NE2	1:Q:150:GLY:H	1.84	0.75
1:T:47:LEU:H	1:T:156:GLN:HE22	1.34	0.75
1:S:67:ILE:HG23	6:T:5155:HOH:O	1.85	0.75
2:I:12:GLN:HE21	2:I:166:ARG:HH11	1.35	0.75
2:C:174:ASN:C	2:C:174:ASN:HD22	1.90	0.75
2:I:95:GLU:CG	2:I:96:GLU:H	2.00	0.74
2:U:38:GLN:NE2	1:W:150:GLY:H	1.84	0.74
1:D:41:ARG:HG2	6:D:5233:HOH:O	1.87	0.74
1:B:45:GLN:HE22	2:C:155:LEU:H	1.33	0.74
1:M:56:LYS:H	1:N:123:GLN:HE22	1.35	0.74
1:G:47:LEU:H	1:G:156:GLN:HE22	1.36	0.73
1:S:4:HIS:HE1	1:T:227:ARG:HH11	1.35	0.73
1:E:47:LEU:H	1:E:156:GLN:HE22	1.36	0.73
1:N:211:LYS:HE2	1:P:93:MET:HE2	1.70	0.73
1:D:45:GLN:HE22	1:E:158:LEU:H	1.37	0.73
1:J:5:GLY:HA3	1:K:227:ARG:HG3	1.70	0.73
1:M:210:LEU:CD2	2:O:70:CYS:HB2	2.19	0.73
1:D:47:LEU:H	1:D:156:GLN:HE22	1.35	0.72
1:G:123:GLN:HE22	2:I:55:ARG:H	1.35	0.72
1:J:67:ILE:HD12	1:J:67:ILE:N	2.03	0.72
1:M:210:LEU:HD13	1:M:210:LEU:H	1.52	0.72
1:G:103:PRO:HG3	6:G:5323:HOH:O	1.88	0.72
1:T:10:ARG:HD3	1:T:166:GLU:OE1	1.88	0.72
1:V:7:LEU:HD11	1:W:118:MET:HE2	1.71	0.72
1:J:67:ILE:H	1:J:67:ILE:CD1	2.03	0.72
1:P:47:LEU:H	1:P:156:GLN:HE22	1.38	0.71
1:K:47:LEU:H	1:K:156:GLN:HE22	1.38	0.71
1:M:67:ILE:HG22	1:N:171:ALA:CB	2.20	0.71
1:W:56:LYS:H	2:X:120:GLN:HE22	1.38	0.71
1:A:47:LEU:H	1:A:156:GLN:HE22	1.35	0.70
1:D:56:LYS:H	1:E:123:GLN:HE22	1.39	0.70
1:G:45:GLN:HE22	1:H:158:LEU:H	1.38	0.70
1:E:56:LYS:H	2:F:120:GLN:HE22	1.38	0.70
2:C:20:PRO:HB2	2:C:23:MET:HE3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:210:LEU:HB2	1:M:214:GLU:HG3	1.73	0.70
2:U:132:ARG:HH11	2:U:226:ASN:HD22	1.40	0.70
1:S:71:CYS:SG	1:T:215:LEU:HG	2.31	0.70
1:S:45:GLN:HE22	1:T:158:LEU:H	1.38	0.70
2:L:209:LYS:HD3	2:L:210:ALA:H	1.57	0.70
2:L:11:SER:HB3	2:L:17:PRO:HG3	1.74	0.70
1:M:45:GLN:HE22	1:N:158:LEU:H	1.39	0.69
2:R:26:LEU:HD11	2:R:109:GLU:HB2	1.74	0.69
2:C:90:MET:HG2	2:C:91:MET:H	1.57	0.69
2:F:225:LYS:O	2:F:226:ASN:HB2	1.91	0.69
1:H:56:LYS:H	2:I:120:GLN:HE22	1.40	0.69
1:K:217:THR:HG23	1:K:218:HIS:H	1.55	0.69
1:S:103:PRO:HG2	6:S:5314:HOH:O	1.91	0.69
1:K:45:GLN:HE22	2:L:155:LEU:H	1.39	0.69
1:S:197:GLU:HB2	1:S:200:GLU:HG2	1.73	0.69
1:E:200:GLU:OE1	1:E:203:LYS:HD2	1.93	0.68
1:A:150:GLY:H	1:D:39:ASN:ND2	1.91	0.68
1:V:47:LEU:H	1:V:156:GLN:HE22	1.41	0.68
1:P:56:LYS:H	1:Q:123:GLN:HE22	1.40	0.68
2:C:90:MET:CG	2:C:91:MET:H	2.05	0.68
1:K:217:THR:HG23	1:K:218:HIS:N	2.09	0.68
1:M:215:LEU:HD22	2:O:70:CYS:SG	2.34	0.68
1:M:47:LEU:H	1:M:156:GLN:HE22	1.41	0.68
2:C:183:TYR:H	2:C:186:LYS:HZ2	1.40	0.68
1:G:56:LYS:H	1:H:123:GLN:HE22	1.42	0.68
2:R:11:SER:HB3	2:R:17:PRO:HG3	1.76	0.67
1:V:6:PHE:CE2	1:V:116:MET:HB3	2.29	0.67
1:S:39:ASN:ND2	1:V:150:GLY:H	1.92	0.67
1:H:67:ILE:HG12	2:I:184:ALA:HA	1.76	0.67
1:D:28:TYR:HE1	1:D:110:VAL:HG21	1.60	0.67
2:I:174:ASN:C	2:I:174:ASN:HD22	1.98	0.67
1:S:4:HIS:CE1	1:T:227:ARG:HH11	2.13	0.67
1:G:167:GLU:OE1	1:M:198:ARG:NH1	2.28	0.66
1:E:45:GLN:HE22	2:F:155:LEU:H	1.41	0.66
1:J:123:GLN:HE22	2:L:55:ARG:H	1.43	0.66
2:F:183:TYR:H	2:F:186:LYS:HZ2	1.42	0.66
1:S:56:LYS:H	1:T:123:GLN:HE22	1.43	0.66
2:R:88:LEU:HD11	2:R:182:TYR:HB2	1.78	0.66
1:J:67:ILE:HG13	1:K:171:ALA:HB2	1.77	0.66
1:P:215:LEU:HD22	2:R:70:CYS:SG	2.36	0.66
1:T:45:GLN:HE22	2:U:155:LEU:H	1.43	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:LEU:H	1:H:156:GLN:HE22	1.44	0.66
2:U:91:MET:HE3	2:X:207:THR:H	1.61	0.65
2:I:225:LYS:O	2:I:226:ASN:HB2	1.95	0.65
1:B:114:PRO:HB2	1:B:228:ARG:HH22	1.60	0.65
1:J:211:LYS:HB2	1:J:211:LYS:NZ	2.12	0.65
2:I:95:GLU:CD	2:I:96:GLU:H	2.00	0.65
2:R:183:TYR:H	2:R:186:LYS:HZ2	1.42	0.65
1:H:56:LYS:H	2:I:120:GLN:NE2	1.95	0.65
1:H:5:GLY:O	2:I:113:VAL:HG21	1.97	0.64
1:S:47:LEU:H	1:S:156:GLN:HE22	1.43	0.64
1:B:47:LEU:H	1:B:156:GLN:HE22	1.44	0.64
1:V:87:GLU:OE1	1:V:88:PRO:HD2	1.98	0.64
1:H:45:GLN:HE22	2:I:155:LEU:H	1.45	0.64
1:H:200:GLU:HG2	1:H:203:LYS:CE	2.28	0.64
1:M:210:LEU:HD23	1:M:215:LEU:HA	1.79	0.64
2:U:90:MET:SD	2:U:90:MET:N	2.71	0.64
1:N:47:LEU:H	1:N:156:GLN:HE22	1.45	0.64
2:O:147:GLY:H	1:Q:39:ASN:HD21	1.46	0.63
2:L:183:TYR:H	2:L:186:LYS:HZ2	1.46	0.63
1:E:25:LYS:HG3	1:E:112:GLU:HB2	1.81	0.63
1:J:45:GLN:NE2	1:K:158:LEU:H	1.95	0.63
1:V:71:CYS:SG	1:W:215:LEU:HD22	2.38	0.63
2:L:225:LYS:O	2:L:226:ASN:HB2	1.98	0.63
1:V:67:ILE:HD12	1:W:184:TYR:HB3	1.81	0.63
2:C:90:MET:CG	2:C:91:MET:N	2.62	0.63
2:O:147:GLY:H	1:Q:39:ASN:ND2	1.97	0.63
1:S:67:ILE:HG22	1:T:171:ALA:HB2	1.81	0.63
1:S:211:LYS:O	1:S:214:GLU:HG2	1.98	0.63
2:F:96:GLU:CD	2:F:96:GLU:H	2.03	0.62
1:M:89:MET:SD	4:M:5008:MPD:H13	2.38	0.62
1:Q:47:LEU:H	1:Q:156:GLN:HE22	1.46	0.62
2:U:88:LEU:H	2:U:88:LEU:HD22	1.64	0.62
1:M:40:GLU:OE1	1:P:37:GLN:NE2	2.32	0.62
1:M:150:GLY:H	1:P:39:ASN:ND2	1.97	0.62
1:T:10:ARG:HG3	1:T:138:TRP:CZ3	2.34	0.62
1:B:150:GLY:H	2:F:38:GLN:NE2	1.97	0.62
1:P:45:GLN:NE2	1:Q:158:LEU:H	1.94	0.62
1:V:56:LYS:H	1:W:123:GLN:HE22	1.48	0.62
1:G:150:GLY:H	1:J:39:ASN:ND2	1.97	0.62
2:L:88:LEU:HD11	2:L:182:TYR:HB2	1.82	0.62
1:A:45:GLN:HE22	1:B:158:LEU:H	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:ARG:HB3	2:C:100:PRO:HD3	1.82	0.61
2:C:126:HIS:HE1	1:H:18:PRO:HA	1.65	0.61
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.64	0.61
1:T:127:ILE:N	1:T:127:ILE:HD12	2.15	0.61
2:C:147:GLY:H	1:E:39:ASN:ND2	1.99	0.61
1:J:56:LYS:H	1:K:123:GLN:HE22	1.48	0.61
1:V:7:LEU:HD11	1:W:118:MET:CE	2.30	0.61
1:W:197:GLU:HB2	1:W:200:GLU:HG3	1.82	0.61
1:A:39:ASN:ND2	1:D:150:GLY:H	1.99	0.61
1:V:21:PRO:HB2	1:V:137:LEU:HD22	1.82	0.61
2:O:225:LYS:O	2:O:226:ASN:HB2	2.00	0.61
1:V:45:GLN:NE2	1:W:158:LEU:H	1.99	0.61
1:W:56:LYS:H	2:X:120:GLN:NE2	1.97	0.61
2:F:85:THR:HG23	2:F:166:ARG:NH2	2.16	0.61
1:H:200:GLU:HG2	1:H:203:LYS:NZ	2.15	0.60
1:K:27:LEU:HD11	1:K:112:GLU:HG3	1.82	0.60
1:A:47:LEU:H	1:A:156:GLN:NE2	2.00	0.60
2:R:225:LYS:O	2:R:226:ASN:HB2	2.01	0.60
1:S:6:PHE:HZ	2:U:3:ILE:HD13	1.66	0.60
1:W:118:MET:HG2	1:W:134:TRP:CZ3	2.37	0.60
2:L:26:LEU:HD11	2:L:109:GLU:HB2	1.83	0.60
1:V:6:PHE:CD2	1:W:116:MET:HE3	2.36	0.60
1:V:102:ARG:HB3	1:V:103:PRO:HD3	1.84	0.60
1:G:211:LYS:HE3	1:K:93:MET:HE2	1.84	0.60
1:D:129:GLN:HG2	6:D:5298:HOH:O	2.01	0.60
1:G:39:ASN:ND2	1:J:150:GLY:H	2.00	0.59
2:U:85:THR:HG23	2:U:166:ARG:NH2	2.18	0.59
2:X:225:LYS:O	2:X:226:ASN:HB2	2.02	0.59
4:P:5006:MPD:HO4	2:R:27:TRP:HB3	1.66	0.59
2:U:164:ASP:HB2	2:U:166:ARG:HH11	1.67	0.59
1:V:211:LYS:O	1:V:214:GLU:HG2	2.01	0.59
1:K:217:THR:HG23	1:K:218:HIS:ND1	2.18	0.59
2:X:24:ASN:OD1	2:X:24:ASN:N	2.30	0.59
1:D:6:PHE:CE2	1:D:116:MET:HG2	2.37	0.59
2:U:132:ARG:HH11	2:U:226:ASN:ND2	2.01	0.59
1:W:47:LEU:H	1:W:156:GLN:NE2	1.99	0.59
2:O:46:LEU:H	2:O:153:GLN:HE22	1.50	0.59
1:A:90:PRO:HD2	6:A:5229:HOH:O	2.03	0.59
1:D:123:GLN:NE2	2:F:55:ARG:H	2.00	0.59
2:I:40:LYS:HD2	6:I:5302:HOH:O	2.02	0.59
2:O:78:LYS:HE3	6:O:5332:HOH:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:95:GLU:CG	2:I:96:GLU:N	2.66	0.58
1:V:85:THR:HB	1:V:86:PRO:HD2	1.84	0.58
2:F:46:LEU:H	2:F:153:GLN:HE22	1.48	0.58
1:M:39:ASN:ND2	1:P:150:GLY:H	2.00	0.58
1:M:210:LEU:HD23	1:M:215:LEU:HD23	1.86	0.58
1:T:211:LYS:HE2	1:V:93:MET:HE2	1.85	0.58
2:X:214:ARG:HG2	2:X:214:ARG:HH21	1.67	0.58
2:C:147:GLY:H	1:E:39:ASN:HD21	1.51	0.58
2:R:99:ARG:HB3	2:R:100:PRO:HD3	1.85	0.58
2:R:136:ILE:HG22	2:R:221:GLN:HG2	1.85	0.58
1:A:150:GLY:H	1:D:39:ASN:HD21	1.49	0.58
1:E:56:LYS:H	2:F:120:GLN:NE2	2.01	0.58
2:I:183:TYR:H	2:I:186:LYS:HZ2	1.52	0.58
1:K:28:TYR:CD1	1:K:28:TYR:C	2.77	0.58
1:B:228:ARG:HG3	1:B:228:ARG:HH11	1.68	0.58
1:H:179:ARG:HH11	2:L:176:ALA:CB	2.17	0.58
1:Q:71:CYS:SG	2:R:213:ILE:HG21	2.43	0.58
1:W:45:GLN:NE2	2:X:155:LEU:H	1.97	0.58
1:N:60:MET:HB2	1:N:178:GLY:HA2	1.85	0.58
2:U:183:TYR:H	2:U:186:LYS:HZ2	1.51	0.58
1:A:40:GLU:HG3	1:D:150:GLY:HA3	1.86	0.57
1:B:56:LYS:H	2:C:120:GLN:HE22	1.50	0.57
1:J:7:LEU:HD21	1:J:27:LEU:HD11	1.87	0.57
2:C:183:TYR:H	2:C:186:LYS:NZ	2.02	0.57
1:A:85:THR:HB	1:A:86:PRO:CD	2.34	0.57
1:B:213:GLY:O	1:B:214:GLU:HB2	2.04	0.57
2:R:177:ARG:HD3	6:R:5336:HOH:O	2.05	0.57
1:S:90:PRO:HD2	6:S:5249:HOH:O	2.04	0.57
2:L:99:ARG:HB3	2:L:100:PRO:HD3	1.85	0.57
2:R:183:TYR:H	2:R:186:LYS:NZ	2.01	0.57
1:S:150:GLY:H	1:V:39:ASN:ND2	2.02	0.57
2:R:128:PRO:HB2	2:R:131:TRP:CD1	2.40	0.57
1:A:37:GLN:OE1	1:D:40:GLU:OE2	2.22	0.57
1:A:55:ARG:NH2	1:B:120:VAL:HB	2.19	0.57
2:X:135:TRP:CE2	2:X:222:VAL:HG21	2.40	0.57
1:Q:92:SER:O	1:Q:93:MET:HB2	2.05	0.57
1:G:28:TYR:CD1	1:G:28:TYR:C	2.77	0.57
1:H:125:ILE:HD12	1:H:125:ILE:C	2.25	0.57
1:J:47:LEU:H	1:J:156:GLN:NE2	2.00	0.56
2:U:147:GLY:H	1:W:39:ASN:ND2	2.02	0.56
1:B:12:SER:O	1:B:13:GLN:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:91:MET:SD	1:T:91:MET:N	2.62	0.56
2:O:135:TRP:CZ2	2:O:222:VAL:HG21	2.41	0.56
1:S:39:ASN:HD21	1:V:150:GLY:H	1.54	0.56
1:S:215:LEU:HB2	4:S:5005:MPD:H11	1.88	0.56
1:T:102:ARG:HB3	1:T:103:PRO:HD3	1.88	0.56
1:H:131:PRO:HB2	1:H:134:TRP:CD1	2.41	0.56
1:A:150:GLY:HA3	1:D:40:GLU:HG3	1.86	0.56
1:G:202:PHE:O	2:I:95:GLU:HG2	2.06	0.56
1:H:150:GLY:H	2:L:38:GLN:NE2	2.03	0.56
2:U:12:GLN:HB3	2:U:166:ARG:NH1	2.21	0.56
1:B:133:GLY:O	1:B:228:ARG:N	2.39	0.56
1:B:197:GLU:HB2	1:B:200:GLU:HG2	1.88	0.56
2:C:89:PRO:HD2	2:C:182:TYR:HD1	1.71	0.56
1:N:169:ARG:O	1:N:172:PRO:HD3	2.05	0.56
1:N:214:GLU:O	1:N:217:THR:HG22	2.04	0.56
1:W:67:ILE:HG12	2:X:184:ALA:HA	1.88	0.56
1:D:56:LYS:H	1:E:123:GLN:NE2	2.04	0.56
1:K:100:ASN:O	1:K:103:PRO:HD2	2.06	0.56
1:N:67:ILE:HD13	2:O:184:ALA:HA	1.88	0.56
1:K:47:LEU:H	1:K:156:GLN:NE2	2.04	0.56
1:N:45:GLN:HE22	2:O:155:LEU:H	1.54	0.56
2:C:36:GLU:OE1	1:E:40:GLU:OE2	2.24	0.56
1:D:28:TYR:CE1	1:D:110:VAL:HB	2.41	0.55
1:H:200:GLU:HA	1:H:203:LYS:HE2	1.87	0.55
1:P:56:LYS:H	1:Q:123:GLN:NE2	2.04	0.55
1:B:25:LYS:HD2	6:H:5211:HOH:O	2.04	0.55
1:B:197:GLU:O	1:B:200:GLU:HG2	2.06	0.55
1:D:131:PRO:HB3	2:F:26:LEU:HD22	1.87	0.55
1:E:47:LEU:H	1:E:156:GLN:NE2	2.02	0.55
2:O:62:LEU:C	2:O:62:LEU:HD12	2.26	0.55
2:I:210:ALA:C	2:I:212:LEU:H	2.09	0.55
1:V:4:HIS:CE1	1:V:6:PHE:HE1	2.23	0.55
1:M:56:LYS:H	1:N:123:GLN:NE2	2.02	0.55
1:M:210:LEU:HD13	1:M:210:LEU:N	2.20	0.55
1:P:47:LEU:H	1:P:156:GLN:NE2	2.04	0.55
2:U:46:LEU:H	2:U:153:GLN:HE22	1.54	0.55
2:X:135:TRP:CZ2	2:X:222:VAL:HG21	2.41	0.55
1:N:200:GLU:CA	1:N:203:LYS:HE2	2.35	0.55
2:R:96:GLU:OE2	2:R:99:ARG:HD2	2.06	0.55
2:C:132:ARG:HH22	2:C:224:MET:HE3	1.71	0.55
2:O:135:TRP:CE2	2:O:222:VAL:HG21	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:MET:HB2	1:B:178:GLY:HA2	1.88	0.54
2:I:174:ASN:CG	2:I:177:ARG:HB3	2.28	0.54
1:K:215:LEU:C	1:K:217:THR:H	2.10	0.54
2:O:183:TYR:H	2:O:186:LYS:NZ	2.06	0.54
1:S:114:PRO:HD2	1:S:226:MET:SD	2.46	0.54
2:U:12:GLN:HB3	2:U:166:ARG:HH12	1.71	0.54
1:B:45:GLN:NE2	2:C:155:LEU:H	2.04	0.54
2:O:3:ILE:HG13	2:O:4:GLY:N	2.22	0.54
1:T:55:ARG:NH1	6:T:5241:HOH:O	2.41	0.54
1:V:56:LYS:H	1:W:123:GLN:NE2	2.04	0.54
1:Q:45:GLN:NE2	2:R:155:LEU:H	2.00	0.54
2:C:135:TRP:CZ2	2:C:222:VAL:HG21	2.41	0.54
1:G:41:ARG:HD3	1:G:42:ALA:N	2.22	0.54
1:G:45:GLN:NE2	1:H:158:LEU:H	2.05	0.54
1:J:86:PRO:HD3	1:J:169:ARG:NH2	2.22	0.54
4:P:5006:MPD:O4	2:R:27:TRP:CB	2.53	0.54
2:U:85:THR:CG2	2:U:166:ARG:NH2	2.71	0.54
1:A:55:ARG:HH22	1:B:120:VAL:HB	1.73	0.54
2:I:94:ALA:CB	2:I:179:THR:HG22	2.36	0.54
1:J:124:THR:OG1	1:J:126:GLN:HG2	2.07	0.54
1:G:91:MET:CE	2:O:97:ASP:HA	2.38	0.54
2:I:96:GLU:OE2	2:I:99:ARG:HD2	2.08	0.54
1:K:28:TYR:C	1:K:28:TYR:HD1	2.12	0.54
2:U:36:GLU:OE2	2:U:78:LYS:HE3	2.07	0.54
1:W:102:ARG:HB3	1:W:103:PRO:HD3	1.90	0.54
1:K:214:GLU:O	1:K:217:THR:HG22	2.08	0.53
1:M:45:GLN:NE2	1:N:158:LEU:H	2.04	0.53
1:N:47:LEU:H	1:N:156:GLN:NE2	2.06	0.53
1:P:188:ALA:O	2:R:66:PRO:HD3	2.08	0.53
1:V:47:LEU:H	1:V:156:GLN:NE2	2.05	0.53
1:W:26:ILE:CD1	1:W:29:HIS:CE1	2.91	0.53
1:B:227:ARG:HD2	1:B:228:ARG:H	1.73	0.53
1:M:188:ALA:O	2:O:66:PRO:HD3	2.08	0.53
1:T:229:THR:HG22	6:T:5238:HOH:O	2.09	0.53
2:U:147:GLY:H	1:W:39:ASN:HD21	1.56	0.53
1:B:90:PRO:CD	1:B:96:ILE:HD11	2.38	0.53
1:H:4:HIS:CE1	2:I:3:ILE:HG23	2.43	0.53
1:J:5:GLY:CA	1:K:227:ARG:HG3	2.39	0.53
2:L:62:LEU:C	2:L:62:LEU:HD12	2.29	0.53
2:O:183:TYR:H	2:O:186:LYS:HZ2	1.55	0.53
1:J:211:LYS:H	1:J:214:GLU:CG	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:215:LEU:HD22	2:U:70:CYS:SG	2.49	0.53
1:N:179:ARG:NH1	6:N:5221:HOH:O	2.35	0.53
1:Q:60:MET:HB2	1:Q:178:GLY:HA2	1.91	0.53
2:C:46:LEU:H	2:C:153:GLN:HE22	1.56	0.53
1:S:215:LEU:HB2	4:S:5005:MPD:C1	2.38	0.53
1:V:17:ASP:HB3	1:V:29:HIS:CD2	2.44	0.53
1:M:114:PRO:HD2	1:M:226:MET:SD	2.48	0.53
1:P:85:THR:HB	1:P:86:PRO:HD2	1.91	0.53
1:P:129:GLN:O	4:P:5006:MPD:HM3	2.08	0.53
1:Q:210:LEU:HD13	1:Q:217:THR:HG22	1.91	0.53
1:B:214:GLU:HG2	1:B:214:GLU:O	2.09	0.52
1:D:47:LEU:H	1:D:156:GLN:NE2	2.04	0.52
1:K:56:LYS:H	2:L:120:GLN:HE22	1.57	0.52
1:N:92:SER:O	1:N:93:MET:HB2	2.08	0.52
2:X:46:LEU:H	2:X:153:GLN:HE22	1.55	0.52
1:G:55:ARG:NH1	1:H:121:HIS:O	2.42	0.52
1:G:215:LEU:HD22	2:I:70:CYS:SG	2.49	0.52
1:Q:91:MET:HE2	1:Q:92:SER:HA	1.92	0.52
1:B:92:SER:O	1:B:93:MET:HB2	2.09	0.52
1:K:60:MET:HB2	1:K:178:GLY:HA2	1.91	0.52
1:A:150:GLY:CA	1:D:40:GLU:HG3	2.40	0.52
2:C:38:GLN:NE2	1:E:150:GLY:H	2.07	0.52
1:D:211:LYS:O	1:D:214:GLU:HG2	2.10	0.52
1:D:214:GLU:O	1:D:218:HIS:CD2	2.63	0.52
1:E:89:MET:H	1:E:89:MET:CE	2.22	0.52
1:H:67:ILE:HD12	1:H:68:ASN:N	2.24	0.52
1:T:67:ILE:N	1:T:67:ILE:HD13	2.24	0.52
1:W:26:ILE:HD12	1:W:29:HIS:CE1	2.44	0.52
1:A:102:ARG:HB3	1:A:103:PRO:HD3	1.91	0.52
1:H:125:ILE:HD12	1:H:126:GLN:N	2.25	0.52
1:J:203:LYS:HD2	1:J:204:LYS:N	2.25	0.52
2:O:67:GLY:O	2:O:69:VAL:HG23	2.09	0.52
1:V:90:PRO:HD2	6:V:5261:HOH:O	2.10	0.52
1:W:60:MET:HB2	1:W:178:GLY:HA2	1.91	0.52
1:J:56:LYS:HE3	1:K:124:THR:CG2	2.40	0.52
2:L:26:LEU:HD12	2:L:26:LEU:N	2.25	0.52
1:T:150:GLY:H	2:X:38:GLN:NE2	2.07	0.52
2:U:164:ASP:HB2	2:U:166:ARG:NH1	2.24	0.52
1:G:47:LEU:H	1:G:156:GLN:NE2	2.06	0.51
1:S:45:GLN:NE2	1:T:158:LEU:H	2.06	0.51
1:H:214:GLU:O	1:H:214:GLU:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:177:ARG:NH1	1:K:74:ALA:O	2.43	0.51
1:Q:90:PRO:HD2	6:Q:314:HOH:O	2.09	0.51
2:R:210:ALA:O	2:R:212:LEU:N	2.40	0.51
1:A:56:LYS:H	1:B:123:GLN:HE22	1.58	0.51
2:C:126:HIS:CE1	1:H:19:GLN:H	2.28	0.51
1:N:85:THR:HB	1:N:86:PRO:CD	2.40	0.51
1:N:102:ARG:HB3	1:N:103:PRO:HD3	1.92	0.51
1:T:56:LYS:H	2:U:120:GLN:NE2	2.08	0.51
2:C:142:MET:HA	2:C:152:GLY:HA2	1.93	0.51
2:C:20:PRO:HB2	2:C:23:MET:CE	2.41	0.51
1:N:150:GLY:H	2:R:38:GLN:NE2	2.08	0.51
1:S:188:ALA:O	2:U:66:PRO:HD3	2.10	0.51
1:A:45:GLN:NE2	1:B:158:LEU:H	2.09	0.51
1:G:214:GLU:HG3	1:G:217:THR:HG21	1.91	0.51
1:J:4:HIS:HB2	1:J:6:PHE:CE1	2.45	0.51
2:C:174:ASN:C	2:C:174:ASN:ND2	2.62	0.51
1:K:214:GLU:O	1:K:214:GLU:HG2	2.11	0.51
2:L:91:MET:HB2	2:L:92:PRO:HD2	1.93	0.51
1:M:26:ILE:HD13	1:M:27:LEU:N	2.26	0.51
1:P:155:GLY:HA3	2:R:42:HIS:CE1	2.46	0.51
1:V:188:ALA:O	2:X:66:PRO:HD3	2.11	0.51
1:K:210:LEU:HD13	1:K:217:THR:CG2	2.41	0.51
1:M:47:LEU:H	1:M:156:GLN:NE2	2.09	0.51
2:R:26:LEU:N	2:R:26:LEU:HD12	2.26	0.51
2:U:183:TYR:H	2:U:186:LYS:NZ	2.08	0.51
1:P:6:PHE:CE2	1:Q:116:MET:HE1	2.46	0.50
1:T:77:ASN:ND2	2:X:78:LYS:HD3	2.26	0.50
2:X:186:LYS:NZ	2:X:186:LYS:HB3	2.26	0.50
1:A:39:ASN:C	1:A:40:GLU:HG2	2.31	0.50
2:C:11:SER:O	2:C:12:GLN:HB2	2.11	0.50
1:G:58:SER:HB2	1:H:196:ILE:HD13	1.93	0.50
2:L:183:TYR:H	2:L:186:LYS:NZ	2.09	0.50
1:T:47:LEU:H	1:T:156:GLN:NE2	2.04	0.50
2:U:80:TYR:CE1	2:U:172:GLU:HB2	2.45	0.50
1:D:63:LEU:C	1:D:63:LEU:HD12	2.31	0.50
1:E:27:LEU:CD2	1:E:112:GLU:HG3	2.29	0.50
2:C:89:PRO:HG3	2:C:101:TYR:CZ	2.46	0.50
1:S:197:GLU:CB	1:S:200:GLU:HG2	2.42	0.50
1:T:210:LEU:HD11	1:T:218:HIS:ND1	2.26	0.50
1:A:188:ALA:O	2:C:66:PRO:HD3	2.12	0.50
1:B:125:ILE:HD11	1:B:217:THR:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:PHE:CD1	2:O:57:SER:N	2.80	0.50
1:S:47:LEU:H	1:S:156:GLN:NE2	2.08	0.50
1:H:27:LEU:HD22	2:I:128:PRO:HB3	1.93	0.50
1:M:150:GLY:H	1:P:39:ASN:HD21	1.60	0.50
1:Q:28:TYR:CZ	1:Q:110:VAL:HG21	2.46	0.50
2:R:91:MET:HB2	2:R:92:PRO:HD2	1.94	0.50
2:F:214:ARG:HD3	2:F:215:THR:N	2.27	0.50
1:G:56:LYS:H	1:H:123:GLN:NE2	2.08	0.50
2:I:46:LEU:H	2:I:153:GLN:HE22	1.58	0.50
1:J:63:LEU:C	1:J:63:LEU:HD22	2.30	0.50
1:M:40:GLU:CG	1:P:40:GLU:OE2	2.60	0.50
1:M:212:ALA:HB2	2:O:68:ASP:HB3	1.92	0.50
1:S:58:SER:HB2	1:T:196:ILE:HD13	1.93	0.50
1:J:203:LYS:HD2	1:J:204:LYS:H	1.76	0.50
1:V:27:LEU:HD22	1:W:131:PRO:HB3	1.94	0.50
2:L:94:ALA:HB2	2:L:179:THR:HG22	1.94	0.49
1:D:210:LEU:N	1:D:210:LEU:HD22	2.27	0.49
2:L:46:LEU:H	2:L:153:GLN:HE22	1.59	0.49
1:Q:56:LYS:H	2:R:120:GLN:HE22	1.59	0.49
1:Q:214:GLU:OE2	1:Q:217:THR:HG21	2.12	0.49
1:D:28:TYR:HE1	1:D:110:VAL:CG2	2.24	0.49
1:D:188:ALA:O	2:F:66:PRO:HD3	2.13	0.49
1:K:45:GLN:NE2	2:L:155:LEU:H	2.08	0.49
2:R:135:TRP:CZ2	2:R:222:VAL:HG21	2.48	0.49
1:W:138:TRP:CE2	1:W:224:VAL:HG21	2.47	0.49
1:S:67:ILE:HG22	1:T:171:ALA:CB	2.42	0.49
1:B:115:ALA:HB1	1:B:227:ARG:HB3	1.94	0.49
2:I:99:ARG:HB3	2:I:100:PRO:HD3	1.93	0.49
1:J:203:LYS:HD2	2:L:95:GLU:OE2	2.12	0.49
2:F:99:ARG:HB3	2:F:100:PRO:HD3	1.94	0.49
1:P:41:ARG:NH2	6:P:5270:HOH:O	2.46	0.49
1:S:93:MET:CE	1:W:211:LYS:HE3	2.43	0.49
1:D:67:ILE:HD12	1:E:184:TYR:HB3	1.94	0.49
2:C:135:TRP:CE2	2:C:222:VAL:HG21	2.48	0.49
1:E:8:VAL:HG23	1:E:113:ALA:HB2	1.95	0.49
2:O:210:ALA:HA	2:O:213:ILE:HD12	1.95	0.49
1:J:102:ARG:HB3	1:J:103:PRO:HD3	1.95	0.49
1:M:71:CYS:SG	1:N:215:LEU:HG	2.53	0.49
1:M:100:ASN:O	1:M:103:PRO:HD2	2.13	0.49
1:M:167:GLU:CD	1:M:169:ARG:HH21	2.15	0.49
1:E:17:ASP:HB3	1:E:29:HIS:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:47:LEU:H	1:Q:156:GLN:NE2	2.09	0.49
2:C:80:TYR:CE1	2:C:172:GLU:HB2	2.47	0.48
1:J:188:ALA:O	2:L:66:PRO:HD3	2.13	0.48
1:M:134:TRP:CE2	1:M:227:ARG:HG2	2.48	0.48
1:M:211:LYS:O	1:M:214:GLU:HG2	2.13	0.48
2:O:142:MET:HA	2:O:152:GLY:HA2	1.95	0.48
1:T:56:LYS:H	2:U:120:GLN:HE22	1.60	0.48
1:G:71:CYS:SG	1:H:215:LEU:HD22	2.53	0.48
2:I:210:ALA:HA	2:I:213:ILE:HG13	1.95	0.48
1:J:4:HIS:HB2	1:J:6:PHE:HE1	1.78	0.48
1:J:210:LEU:HB3	1:J:215:LEU:HD23	1.95	0.48
2:O:15:GLN:HE21	2:O:15:GLN:HA	1.78	0.48
1:E:67:ILE:HD13	2:F:184:ALA:HA	1.96	0.48
1:B:56:LYS:H	2:C:120:GLN:NE2	2.11	0.48
1:J:17:ASP:HB3	1:J:29:HIS:CD2	2.49	0.48
1:J:145:MET:HG2	1:J:191:PHE:HB2	1.95	0.48
1:M:66:ASN:HB3	1:M:68:ASN:ND2	2.28	0.48
1:Q:56:LYS:HG2	2:R:198:SER:HA	1.94	0.48
2:R:88:LEU:CD1	2:R:182:TYR:HB2	2.43	0.48
1:T:45:GLN:HE21	1:T:51:GLY:HA3	1.78	0.48
1:W:210:LEU:HD11	1:W:218:HIS:CG	2.49	0.48
1:D:153:GLY:H	2:F:40:LYS:NZ	2.11	0.48
1:K:214:GLU:O	1:K:217:THR:CG2	2.62	0.48
1:V:123:GLN:NE2	2:X:55:ARG:H	2.00	0.48
2:L:102:ILE:CD1	2:L:102:ILE:N	2.76	0.48
1:N:77:ASN:ND2	2:R:78:LYS:HD3	2.29	0.48
1:N:175:GLU:O	1:N:182:CYS:HA	2.14	0.48
1:Q:198:ARG:HD2	1:Q:198:ARG:C	2.34	0.48
2:U:24:ASN:OD1	2:U:109:GLU:HB3	2.12	0.48
2:L:11:SER:O	2:L:12:GLN:HB2	2.13	0.48
1:M:12:SER:HB3	1:M:18:PRO:HB3	1.95	0.48
1:S:216:ARG:NH1	4:S:5005:MPD:H52	2.23	0.48
1:W:175:GLU:O	1:W:182:CYS:HA	2.14	0.48
1:B:77:ASN:ND2	2:F:174:ASN:OD1	2.47	0.48
1:D:97:THR:HG22	1:D:181:THR:HG22	1.94	0.48
1:D:211:LYS:O	1:D:212:ALA:C	2.51	0.48
1:T:90:PRO:HG2	1:T:96:ILE:CD1	2.44	0.48
2:U:31:SER:HB2	2:U:82:LEU:HB2	1.95	0.48
1:D:216:ARG:HH21	1:S:197:GLU:HG3	1.78	0.48
4:D:5007:MPD:H11	2:F:66:PRO:HB2	1.96	0.48
1:G:188:ALA:O	2:I:66:PRO:HD3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:40:GLU:HG2	1:P:40:GLU:OE2	2.14	0.48
1:N:179:ARG:NH2	2:R:75:ARG:O	2.47	0.48
1:W:197:GLU:HB2	1:W:200:GLU:CG	2.44	0.48
2:X:96:GLU:HB2	6:X:5308:HOH:O	2.14	0.48
1:A:175:GLU:O	1:A:182:CYS:HA	2.13	0.47
1:Q:197:GLU:HB2	1:Q:200:GLU:HG2	1.95	0.47
1:Q:198:ARG:HD2	1:Q:198:ARG:O	2.13	0.47
1:T:4:HIS:HD2	6:U:5327:HOH:O	1.96	0.47
1:T:85:THR:HB	1:T:86:PRO:CD	2.44	0.47
1:G:7:LEU:HD11	1:H:118:MET:SD	2.54	0.47
2:X:168:THR:CG2	2:X:186:LYS:HZ2	2.27	0.47
1:J:71:CYS:SG	1:K:215:LEU:HG	2.54	0.47
1:N:229:THR:C	2:X:197:GLN:HB3	2.34	0.47
1:S:66:ASN:HB3	1:S:68:ASN:OD1	2.14	0.47
2:X:15:GLN:HA	2:X:15:GLN:HE21	1.78	0.47
1:E:45:GLN:NE2	2:F:155:LEU:H	2.09	0.47
1:T:175:GLU:O	1:T:182:CYS:HA	2.12	0.47
4:J:5009:MPD:H52	2:L:67:GLY:HA2	1.97	0.47
1:M:50:ALA:HB3	1:N:159:ALA:HB2	1.96	0.47
1:P:34:LEU:HD12	6:P:5255:HOH:O	2.13	0.47
1:S:56:LYS:H	1:T:123:GLN:NE2	2.09	0.47
2:U:91:MET:HG2	2:X:207:THR:HB	1.96	0.47
1:D:45:GLN:NE2	1:E:158:LEU:H	2.07	0.47
1:Q:85:THR:HB	1:Q:86:PRO:CD	2.44	0.47
1:V:63:LEU:HD12	1:V:63:LEU:C	2.35	0.47
1:B:228:ARG:HG3	1:B:228:ARG:NH1	2.30	0.47
2:C:210:ALA:HA	2:C:213:ILE:HD12	1.97	0.47
1:G:12:SER:O	1:G:13:GLN:HB2	2.14	0.47
1:G:25:LYS:HB2	1:G:25:LYS:NZ	2.29	0.47
1:J:167:GLU:CD	1:J:169:ARG:HE	2.15	0.47
1:K:217:THR:CG2	1:K:218:HIS:H	2.26	0.47
2:O:125:PRO:HG3	2:O:220:CYS:HA	1.97	0.47
1:P:4:HIS:HB2	1:P:6:PHE:CE1	2.50	0.47
1:P:77:ASN:HD22	1:P:77:ASN:HA	1.56	0.47
2:R:46:LEU:H	2:R:153:GLN:HE22	1.60	0.47
2:U:165:PHE:CE2	2:U:217:ILE:HD13	2.50	0.47
1:V:115:ALA:HB1	1:V:227:ARG:HB3	1.97	0.47
1:B:126:GLN:H	1:B:126:GLN:NE2	2.12	0.47
2:F:11:SER:O	2:F:12:GLN:HB2	2.15	0.47
1:H:58:SER:OG	2:I:200:GLN:NE2	2.48	0.47
1:P:99:GLU:OE1	1:P:102:ARG:NE	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:39:GLU:OE1	1:W:79:TYR:OH	2.26	0.47
1:W:63:LEU:C	1:W:63:LEU:HD12	2.36	0.47
1:D:118:MET:SD	2:F:6:LEU:HD11	2.55	0.47
2:I:147:GLY:H	1:K:39:ASN:ND2	2.13	0.47
1:J:7:LEU:CD2	1:J:27:LEU:HD11	2.45	0.47
1:J:67:ILE:HD11	1:K:188:ALA:HB3	1.97	0.47
1:M:86:PRO:HG3	1:M:169:ARG:NH2	2.30	0.47
2:U:57:SER:O	2:U:60:PRO:HD3	2.15	0.47
1:B:203:LYS:HE2	1:B:203:LYS:CA	2.27	0.47
2:C:148:ASP:C	2:C:148:ASP:OD2	2.54	0.47
1:K:56:LYS:H	2:L:120:GLN:NE2	2.12	0.47
1:M:56:LYS:NZ	1:N:198:ARG:HB2	2.30	0.47
1:P:131:PRO:HB2	1:P:134:TRP:CD1	2.50	0.47
1:T:10:ARG:HG2	6:T:5133:HOH:O	2.15	0.47
1:V:123:GLN:HE22	2:X:55:ARG:N	2.01	0.47
1:W:90:PRO:HD2	6:W:282:HOH:O	2.13	0.47
1:B:100:ASN:O	1:B:103:PRO:HD2	2.14	0.46
1:G:167:GLU:OE2	1:M:198:ARG:HD2	2.14	0.46
6:P:5324:HOH:O	2:R:40:LYS:HD2	2.15	0.46
1:Q:214:GLU:O	1:Q:217:THR:HG22	2.15	0.46
1:W:85:THR:HB	1:W:86:PRO:CD	2.45	0.46
2:X:168:THR:HG23	2:X:186:LYS:HZ2	1.79	0.46
1:B:169:ARG:O	1:B:172:PRO:HD3	2.14	0.46
1:B:228:ARG:HG3	1:B:228:ARG:O	2.15	0.46
1:H:125:ILE:HD12	1:H:126:GLN:HG2	1.96	0.46
1:J:197:GLU:HB2	1:J:200:GLU:HG2	1.97	0.46
1:T:77:ASN:HD22	2:X:78:LYS:HD3	1.79	0.46
1:J:90:PRO:HD2	6:J:5246:HOH:O	2.15	0.46
1:J:127:ILE:HD13	1:J:139:ILE:HD12	1.97	0.46
1:N:12:SER:O	1:N:13:GLN:HB2	2.15	0.46
1:P:71:CYS:SG	1:Q:215:LEU:HG	2.56	0.46
2:C:173:CYS:HA	2:C:180:CYS:HA	1.98	0.46
1:D:138:TRP:CE2	1:D:224:VAL:HG21	2.51	0.46
2:I:183:TYR:H	2:I:186:LYS:NZ	2.12	0.46
2:L:26:LEU:O	2:L:27:TRP:HB3	2.14	0.46
1:V:200:GLU:HG2	1:V:203:LYS:CE	2.38	0.46
2:F:215:THR:HG23	2:F:216:HIS:ND1	2.31	0.46
1:N:40:GLU:OE2	2:R:36:GLU:OE1	2.33	0.46
1:V:127:ILE:CD1	1:V:139:ILE:HD12	2.45	0.46
2:F:183:TYR:H	2:F:186:LYS:NZ	2.12	0.46
1:A:227:ARG:CD	2:C:4:GLY:HA3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:195:PRO:HG2	2:I:196:GLU:OE1	2.15	0.46
1:V:34:LEU:HD12	6:V:5292:HOH:O	2.15	0.46
2:C:132:ARG:NH2	2:C:224:MET:HE3	2.30	0.46
1:J:211:LYS:HB2	1:J:211:LYS:HZ2	1.80	0.46
1:Q:63:LEU:HD12	1:Q:63:LEU:C	2.36	0.46
1:S:63:LEU:C	1:S:63:LEU:HD12	2.36	0.46
1:A:39:ASN:HD21	1:D:150:GLY:H	1.64	0.46
2:C:90:MET:HG2	2:C:91:MET:HG3	1.98	0.46
1:J:85:THR:HB	1:J:86:PRO:HD2	1.98	0.46
2:F:142:MET:HA	2:F:152:GLY:HA2	1.98	0.46
2:F:212:LEU:N	2:F:212:LEU:HD22	2.31	0.46
1:H:138:TRP:CE2	1:H:224:VAL:HG21	2.51	0.46
2:L:102:ILE:N	2:L:102:ILE:HD12	2.30	0.46
1:M:102:ARG:HA	1:N:202:PHE:CE2	2.50	0.46
2:R:40:LYS:HB2	2:R:40:LYS:NZ	2.32	0.46
1:S:213:GLY:C	4:S:5005:MPD:HM3	2.36	0.46
1:T:60:MET:HB2	1:T:178:GLY:HA2	1.98	0.46
2:U:46:LEU:H	2:U:153:GLN:NE2	2.13	0.46
2:X:29:GLY:O	2:X:104:ARG:NH1	2.49	0.46
2:X:56:PHE:CD1	2:X:57:SER:N	2.84	0.46
1:E:90:PRO:HD2	6:E:277:HOH:O	2.16	0.45
2:L:20:PRO:HB2	2:L:23:MET:CE	2.46	0.45
1:Q:97:THR:HG22	1:Q:181:THR:HG22	1.98	0.45
2:I:135:TRP:CE2	2:I:222:VAL:HG21	2.50	0.45
1:J:67:ILE:HG13	1:K:171:ALA:CB	2.46	0.45
1:N:229:THR:HG23	1:W:102:ARG:HH22	1.82	0.45
1:P:175:GLU:O	1:P:182:CYS:HA	2.17	0.45
2:U:132:ARG:NH1	2:U:226:ASN:HD22	2.10	0.45
2:I:210:ALA:O	2:I:212:LEU:N	2.45	0.45
1:P:145:MET:HG2	1:P:191:PHE:HB2	1.97	0.45
2:R:62:LEU:C	2:R:62:LEU:HD12	2.37	0.45
1:H:99:GLU:CD	1:H:102:ARG:HH21	2.19	0.45
2:I:128:PRO:HB2	2:I:131:TRP:CD1	2.52	0.45
1:K:12:SER:O	1:K:13:GLN:HB2	2.15	0.45
1:K:182:CYS:O	1:K:183:ASN:HB2	2.16	0.45
1:A:63:LEU:C	1:A:63:LEU:HD12	2.37	0.45
1:A:92:SER:O	1:A:93:MET:HB2	2.17	0.45
1:B:122:SER:O	1:B:123:GLN:HB2	2.17	0.45
1:J:122:SER:HB3	1:J:128:PRO:HB3	1.98	0.45
1:M:102:ARG:HB3	1:M:103:PRO:HD3	1.99	0.45
2:R:135:TRP:CE2	2:R:222:VAL:HG21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:12:SER:O	1:T:13:GLN:HB2	2.16	0.45
1:V:57:PHE:CG	1:V:58:SER:N	2.84	0.45
1:B:47:LEU:H	1:B:156:GLN:NE2	2.13	0.45
2:C:210:ALA:HA	2:C:213:ILE:CD1	2.47	0.45
1:H:47:LEU:H	1:H:156:GLN:NE2	2.12	0.45
2:L:91:MET:HB2	2:L:92:PRO:CD	2.47	0.45
1:M:63:LEU:HD12	1:M:63:LEU:C	2.37	0.45
2:O:90:MET:HG3	2:R:209:LYS:HE2	1.99	0.45
2:O:213:ILE:O	2:O:217:ILE:HD13	2.17	0.45
1:W:8:VAL:HG22	1:W:117:VAL:HG21	1.98	0.45
2:X:25:LYS:HE2	2:X:28:SER:OG	2.16	0.45
1:H:45:GLN:NE2	2:I:155:LEU:H	2.12	0.45
1:H:216:ARG:NH1	6:H:5182:HOH:O	2.50	0.45
2:I:56:PHE:CD1	2:I:57:SER:N	2.85	0.45
2:I:76:ASN:HD22	2:I:76:ASN:HA	1.62	0.45
1:T:211:LYS:HE2	1:V:93:MET:CE	2.47	0.45
2:U:148:ASP:C	2:U:148:ASP:OD1	2.55	0.45
1:D:77:ASN:HD22	1:D:77:ASN:HA	1.60	0.45
1:M:113:ALA:HA	1:M:114:PRO:HD3	1.83	0.45
1:P:227:ARG:HD2	2:R:3:ILE:HG22	1.99	0.45
2:R:91:MET:HB2	2:R:92:PRO:CD	2.46	0.45
2:X:173:CYS:HA	2:X:180:CYS:HA	1.99	0.45
1:A:89:MET:HE2	6:A:5229:HOH:O	2.17	0.45
1:G:102:ARG:HB3	1:G:103:PRO:HD3	1.98	0.45
6:N:5214:HOH:O	2:R:147:GLY:HA3	2.17	0.45
1:Q:152:GLU:HA	1:Q:152:GLU:OE1	2.17	0.45
1:Q:12:SER:O	1:Q:13:GLN:HB2	2.18	0.44
1:S:197:GLU:HB2	1:S:200:GLU:CG	2.45	0.44
2:X:168:THR:CG2	2:X:186:LYS:NZ	2.80	0.44
1:G:39:ASN:HD21	1:J:150:GLY:H	1.65	0.44
2:I:210:ALA:C	2:I:212:LEU:N	2.71	0.44
1:M:216:ARG:H	1:M:216:ARG:HD2	1.82	0.44
1:N:101:ILE:HD13	1:N:182:CYS:SG	2.57	0.44
2:U:88:LEU:HD22	2:U:88:LEU:N	2.32	0.44
2:U:132:ARG:HB3	2:U:226:ASN:HD21	1.82	0.44
1:E:92:SER:O	1:E:93:MET:HB2	2.17	0.44
1:T:45:GLN:NE2	2:U:155:LEU:H	2.13	0.44
2:X:96:GLU:HG2	6:X:5311:HOH:O	2.18	0.44
1:B:133:GLY:HA3	1:B:227:ARG:NH1	2.32	0.44
1:J:12:SER:HB3	1:J:18:PRO:HB3	1.99	0.44
1:M:83:LEU:HD12	1:M:83:LEU:HA	1.89	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:203:LYS:HA	1:M:203:LYS:HD3	1.80	0.44
2:O:128:PRO:HB2	2:O:131:TRP:CD1	2.53	0.44
1:S:57:PHE:CD1	1:S:58:SER:N	2.86	0.44
1:A:96:ILE:HD13	1:A:104:PHE:CE1	2.53	0.44
2:C:125:PRO:HG3	2:C:220:CYS:HA	1.99	0.44
2:F:135:TRP:CZ2	2:F:222:VAL:HG21	2.53	0.44
1:G:57:PHE:CG	1:G:58:SER:N	2.86	0.44
1:G:85:THR:HB	1:G:86:PRO:CD	2.47	0.44
1:H:175:GLU:O	1:H:182:CYS:HA	2.16	0.44
1:P:227:ARG:HD2	2:R:3:ILE:CG2	2.48	0.44
2:X:76:ASN:HD22	2:X:76:ASN:HA	1.61	0.44
1:G:155:GLY:HA3	2:I:42:HIS:CE1	2.52	0.44
1:K:175:GLU:O	1:K:182:CYS:HA	2.17	0.44
1:N:67:ILE:CD1	2:O:184:ALA:HA	2.48	0.44
1:N:198:ARG:HA	1:N:201:MET:HG3	2.00	0.44
1:S:102:ARG:HA	1:T:202:PHE:CE2	2.52	0.44
1:T:67:ILE:H	1:T:67:ILE:CD1	2.31	0.44
2:X:56:PHE:CG	2:X:57:SER:N	2.84	0.44
1:A:40:GLU:HG3	1:D:150:GLY:CA	2.47	0.44
1:D:66:ASN:HB3	1:D:68:ASN:OD1	2.17	0.44
1:E:210:LEU:HD11	1:E:218:HIS:HB2	2.00	0.44
1:H:99:GLU:OE1	1:H:102:ARG:NH2	2.49	0.44
2:I:135:TRP:CZ2	2:I:222:VAL:HG21	2.52	0.44
4:J:5009:MPD:H4	2:L:66:PRO:HB2	1.99	0.44
1:K:4:HIS:HB3	6:K:318:HOH:O	2.18	0.44
1:S:57:PHE:CG	1:S:58:SER:N	2.86	0.44
1:S:134:TRP:CE2	1:S:227:ARG:HG2	2.52	0.44
1:W:26:ILE:HG12	1:W:27:LEU:N	2.32	0.44
1:E:60:MET:HB2	1:E:178:GLY:HA2	2.00	0.44
2:F:62:LEU:HD12	2:F:62:LEU:C	2.37	0.44
2:L:135:TRP:CE2	2:L:222:VAL:HG21	2.52	0.44
1:B:26:ILE:HG21	1:H:127:ILE:HG13	2.00	0.44
2:C:76:ASN:HD22	2:C:76:ASN:HA	1.64	0.44
1:D:210:LEU:O	1:D:211:LYS:HD3	2.18	0.44
1:J:211:LYS:H	1:J:214:GLU:CD	2.21	0.44
1:M:57:PHE:CG	1:M:58:SER:N	2.86	0.44
1:V:66:ASN:HB3	1:V:68:ASN:OD1	2.17	0.44
2:X:172:GLU:O	2:X:180:CYS:HA	2.18	0.44
1:A:6:PHE:CE2	1:A:116:MET:SD	3.11	0.43
1:B:113:ALA:HB1	1:B:226:MET:SD	2.58	0.43
1:B:133:GLY:HA3	1:B:227:ARG:HH12	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:120:GLN:HA	2:I:218:SER:HB2	2.00	0.43
1:J:63:LEU:HD13	1:K:192:TRP:O	2.18	0.43
1:K:87:GLU:HA	1:K:88:PRO:HD3	1.86	0.43
1:M:210:LEU:HD22	2:O:70:CYS:HB2	1.99	0.43
2:R:56:PHE:CD1	2:R:57:SER:N	2.86	0.43
2:X:214:ARG:NH1	6:X:5326:HOH:O	2.50	0.43
1:A:12:SER:O	1:A:13:GLN:HB2	2.17	0.43
1:D:41:ARG:HG3	1:E:151:ALA:O	2.17	0.43
2:F:56:PHE:CD1	2:F:57:SER:N	2.85	0.43
1:G:197:GLU:OE1	1:G:197:GLU:HA	2.18	0.43
1:H:40:GLU:OE2	2:L:36:GLU:OE1	2.36	0.43
1:V:175:GLU:O	1:V:182:CYS:HA	2.18	0.43
1:E:20:CYS:HB3	1:E:24:THR:OG1	2.18	0.43
1:H:60:MET:HB2	1:H:178:GLY:HA2	2.00	0.43
1:H:85:THR:HB	1:H:86:PRO:CD	2.48	0.43
2:I:95:GLU:HG2	2:I:96:GLU:N	2.32	0.43
1:J:66:ASN:O	1:K:170:SER:HB3	2.18	0.43
4:J:5009:MPD:H4	2:L:66:PRO:CB	2.47	0.43
1:M:194:ALA:HA	1:M:218:HIS:O	2.18	0.43
2:R:210:ALA:HA	2:R:213:ILE:HD11	1.99	0.43
1:T:87:GLU:HA	1:T:88:PRO:HD3	1.91	0.43
2:U:89:PRO:HD3	2:U:101:TYR:CE1	2.53	0.43
2:O:38:GLN:HE22	1:Q:150:GLY:H	1.64	0.43
1:P:20:CYS:HA	1:P:21:PRO:HD3	1.92	0.43
1:A:41:ARG:HG2	6:B:5198:HOH:O	2.19	0.43
1:A:57:PHE:CG	1:A:58:SER:N	2.86	0.43
2:C:134:LEU:O	2:C:135:TRP:HB3	2.17	0.43
2:I:174:ASN:C	2:I:174:ASN:ND2	2.71	0.43
1:J:56:LYS:HD3	1:K:196:ILE:O	2.17	0.43
1:M:210:LEU:HD22	1:M:210:LEU:O	2.19	0.43
1:S:67:ILE:HD11	1:T:186:ALA:HA	2.01	0.43
2:U:88:LEU:H	2:U:88:LEU:CD2	2.30	0.43
2:C:56:PHE:CD1	2:C:57:SER:N	2.86	0.43
2:C:89:PRO:HD2	2:C:182:TYR:CD1	2.53	0.43
2:C:212:LEU:HB3	2:C:216:HIS:HE1	1.82	0.43
1:H:138:TRP:CD1	1:H:166:GLU:HG2	2.53	0.43
2:L:214:ARG:HH21	2:L:214:ARG:HG3	1.83	0.43
2:O:209:LYS:O	2:O:213:ILE:HG13	2.19	0.43
1:V:177:HIS:HB2	1:V:179:ARG:HG2	2.00	0.43
1:B:63:LEU:C	1:B:63:LEU:HD12	2.39	0.43
2:C:26:LEU:O	2:C:27:TRP:HB3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:PRO:HB2	2:F:131:TRP:CD1	2.54	0.43
1:M:77:ASN:HD22	1:M:77:ASN:HA	1.57	0.43
6:S:5276:HOH:O	1:V:40:GLU:HG2	2.18	0.43
2:U:110:ALA:HA	2:U:111:PRO:HD3	1.83	0.43
1:A:77:ASN:HD22	1:A:77:ASN:HA	1.60	0.43
1:B:58:SER:OG	2:C:200:GLN:NE2	2.49	0.43
1:D:28:TYR:CE1	1:D:110:VAL:CB	3.02	0.43
1:G:211:LYS:CE	1:K:93:MET:HE2	2.48	0.43
2:I:147:GLY:H	1:K:39:ASN:HD21	1.65	0.43
1:K:215:LEU:C	1:K:217:THR:N	2.71	0.43
2:O:165:PHE:CZ	2:O:213:ILE:HG21	2.54	0.43
4:P:5006:MPD:HO4	2:R:27:TRP:CB	2.30	0.43
1:V:100:ASN:O	1:V:103:PRO:HD2	2.19	0.43
2:X:62:LEU:C	2:X:62:LEU:HD12	2.38	0.43
2:F:56:PHE:CG	2:F:57:SER:N	2.86	0.43
1:G:175:GLU:O	1:G:182:CYS:HA	2.18	0.43
2:L:211:GLY:O	2:L:213:ILE:N	2.51	0.43
1:N:200:GLU:HG2	1:N:203:LYS:NZ	2.33	0.43
1:S:93:MET:HE2	1:W:211:LYS:HE3	2.01	0.43
1:T:179:ARG:HD3	6:X:5318:HOH:O	2.18	0.43
1:V:127:ILE:HD11	1:V:139:ILE:HD12	2.00	0.43
1:A:58:SER:HB2	1:B:196:ILE:HD13	2.00	0.43
2:I:56:PHE:CG	2:I:57:SER:N	2.87	0.43
2:I:78:LYS:HG2	1:K:77:ASN:ND2	2.34	0.43
1:Q:168:PHE:CD1	1:Q:168:PHE:C	2.92	0.43
2:X:99:ARG:HB3	2:X:100:PRO:HD3	2.01	0.43
2:X:212:LEU:O	2:X:216:HIS:ND1	2.52	0.43
1:A:56:LYS:H	1:B:123:GLN:NE2	2.16	0.42
1:A:114:PRO:HD2	1:A:226:MET:SD	2.59	0.42
1:B:197:GLU:H	1:B:200:GLU:CG	2.32	0.42
1:D:28:TYR:CE1	1:D:110:VAL:HG21	2.48	0.42
1:D:57:PHE:CG	1:D:58:SER:N	2.86	0.42
1:G:28:TYR:C	1:G:28:TYR:HD1	2.19	0.42
1:M:40:GLU:CD	1:P:40:GLU:OE2	2.57	0.42
1:M:58:SER:HB2	1:N:196:ILE:HD13	2.01	0.42
2:O:11:SER:O	2:O:12:GLN:HB2	2.19	0.42
1:P:123:GLN:NE2	2:R:55:ARG:H	2.03	0.42
1:Q:122:SER:O	1:Q:123:GLN:HB2	2.19	0.42
2:R:21:VAL:O	2:R:21:VAL:HG13	2.18	0.42
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.89	0.42
1:E:56:LYS:HG2	2:F:198:SER:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:138:TRP:CE2	1:J:224:VAL:HG21	2.55	0.42
2:L:135:TRP:CZ2	2:L:222:VAL:HG21	2.53	0.42
1:T:63:LEU:HD12	1:T:63:LEU:C	2.39	0.42
1:V:215:LEU:C	1:V:217:THR:H	2.22	0.42
1:W:182:CYS:O	1:W:183:ASN:HB2	2.19	0.42
2:F:201:GLY:O	2:F:202:THR:C	2.57	0.42
1:G:123:GLN:NE2	2:I:55:ARG:H	2.09	0.42
1:K:4:HIS:HB2	1:K:6:PHE:CE1	2.54	0.42
1:K:131:PRO:HB2	1:K:134:TRP:CD1	2.55	0.42
1:N:58:SER:OG	2:O:200:GLN:NE2	2.51	0.42
1:P:113:ALA:HB1	1:P:226:MET:SD	2.58	0.42
1:V:60:MET:HB2	1:V:178:GLY:HA2	2.00	0.42
1:A:66:ASN:HB3	1:A:68:ASN:OD1	2.19	0.42
1:B:197:GLU:H	1:B:200:GLU:CD	2.22	0.42
1:D:66:ASN:O	1:E:170:SER:HB3	2.19	0.42
1:M:97:THR:O	1:M:100:ASN:HB2	2.19	0.42
1:T:127:ILE:N	1:T:127:ILE:CD1	2.82	0.42
1:V:217:THR:HG22	1:V:217:THR:O	2.19	0.42
1:E:197:GLU:HB2	1:E:200:GLU:HG2	2.01	0.42
1:G:63:LEU:C	1:G:63:LEU:HD12	2.39	0.42
1:H:63:LEU:HD12	1:H:63:LEU:C	2.39	0.42
1:M:85:THR:HB	1:M:86:PRO:CD	2.49	0.42
2:U:111:PRO:HD2	2:U:224:MET:SD	2.60	0.42
2:X:209:LYS:O	2:X:210:ALA:C	2.58	0.42
1:B:210:LEU:HD11	1:B:218:HIS:HB2	2.00	0.42
1:D:85:THR:HB	1:D:86:PRO:CD	2.49	0.42
1:E:12:SER:O	1:E:13:GLN:HB2	2.19	0.42
2:F:26:LEU:O	2:F:27:TRP:HB3	2.18	0.42
1:J:211:LYS:HB2	1:J:211:LYS:HZ3	1.85	0.42
2:O:130:GLY:O	2:O:226:ASN:N	2.42	0.42
1:B:85:THR:HB	1:B:86:PRO:CD	2.50	0.42
2:C:38:GLN:NE2	1:E:187:ASN:ND2	2.67	0.42
1:D:60:MET:HB2	1:D:178:GLY:HA2	2.02	0.42
1:M:57:PHE:CD1	1:M:58:SER:N	2.88	0.42
2:O:209:LYS:HE2	2:O:209:LYS:HB3	1.92	0.42
1:P:138:TRP:CE2	1:P:224:VAL:HG21	2.54	0.42
1:Q:8:VAL:HG13	1:Q:111:CYS:HB2	2.02	0.42
1:W:167:GLU:HB3	6:W:302:HOH:O	2.20	0.42
2:X:20:PRO:HB2	2:X:23:MET:CE	2.50	0.42
2:X:196:GLU:OE2	2:X:196:GLU:N	2.46	0.42
1:B:17:ASP:HB3	1:B:29:HIS:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LYS:O	1:D:212:ALA:O	2.38	0.42
1:D:227:ARG:HG2	1:D:227:ARG:NH1	2.32	0.42
1:H:66:ASN:HB2	6:I:5235:HOH:O	2.19	0.42
1:N:187:ASN:HB3	1:P:189:TYR:CZ	2.55	0.42
2:O:46:LEU:H	2:O:153:GLN:NE2	2.15	0.42
1:V:198:ARG:HA	1:V:201:MET:HG3	2.01	0.42
1:W:92:SER:O	1:W:93:MET:HB2	2.19	0.42
1:D:27:LEU:HD22	1:E:131:PRO:HB3	2.01	0.42
1:H:12:SER:O	1:H:13:GLN:HB2	2.19	0.42
1:M:216:ARG:HD2	1:M:216:ARG:N	2.35	0.42
1:N:211:LYS:HE2	1:P:93:MET:CE	2.44	0.42
1:S:35:TYR:CB	1:S:44:GLY:HA2	2.49	0.42
1:T:73:PHE:O	2:U:205:ALA:HA	2.20	0.42
1:D:175:GLU:O	1:D:182:CYS:HA	2.20	0.42
1:G:77:ASN:HD22	1:G:77:ASN:HA	1.57	0.42
1:P:129:GLN:O	4:P:5006:MPD:CM	2.68	0.42
1:S:97:THR:HG22	1:S:181:THR:HG22	2.00	0.42
1:S:100:ASN:O	1:S:103:PRO:HD2	2.20	0.42
2:U:38:GLN:HE22	1:W:149:ALA:HA	1.84	0.42
1:A:57:PHE:CD1	1:A:58:SER:N	2.88	0.41
1:D:86:PRO:HG2	1:S:198:ARG:HG2	2.02	0.41
2:F:95:GLU:HB2	2:F:96:GLU:OE2	2.21	0.41
1:N:135:SER:HB3	6:N:5178:HOH:O	2.19	0.41
1:P:63:LEU:C	1:P:63:LEU:HD12	2.40	0.41
1:S:184:TYR:HA	6:S:5338:HOH:O	2.20	0.41
2:X:21:VAL:O	2:X:21:VAL:HG13	2.20	0.41
6:A:5252:HOH:O	2:C:54:ALA:HB3	2.19	0.41
1:T:214:GLU:O	1:T:214:GLU:HG2	2.20	0.41
2:U:142:MET:HA	2:U:152:GLY:HA2	2.02	0.41
1:V:131:PRO:HB2	1:V:134:TRP:CD1	2.55	0.41
1:V:215:LEU:O	1:V:217:THR:N	2.52	0.41
2:X:96:GLU:OE2	2:X:99:ARG:NH1	2.46	0.41
1:A:56:LYS:HD2	1:B:123:GLN:HB2	2.02	0.41
2:I:91:MET:HE3	2:L:207:THR:HB	2.02	0.41
1:M:218:HIS:HB3	6:M:5317:HOH:O	2.20	0.41
1:W:87:GLU:HA	1:W:88:PRO:HD3	1.87	0.41
2:O:225:LYS:O	2:O:226:ASN:CB	2.67	0.41
1:W:97:THR:HG22	1:W:181:THR:HG22	2.02	0.41
2:X:96:GLU:OE1	2:X:99:ARG:NH1	2.53	0.41
1:P:128:PRO:O	1:P:223:GLN:NE2	2.53	0.41
1:T:67:ILE:N	1:T:67:ILE:CD1	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:102:ARG:HA	1:W:202:PHE:CE2	2.55	0.41
1:A:167:GLU:HG3	6:A:5270:HOH:O	2.20	0.41
2:C:21:VAL:HG13	2:C:21:VAL:O	2.21	0.41
1:D:167:GLU:HG3	6:D:5284:HOH:O	2.21	0.41
1:G:41:ARG:HD3	1:G:41:ARG:C	2.41	0.41
1:G:66:ASN:HB3	1:G:68:ASN:OD1	2.20	0.41
2:I:110:ALA:HA	2:I:111:PRO:HD3	1.80	0.41
1:J:20:CYS:HA	1:J:21:PRO:HD3	1.88	0.41
2:R:3:ILE:N	2:R:5:TYR:CE2	2.89	0.41
1:V:112:GLU:OE2	1:W:227:ARG:NE	2.54	0.41
2:X:26:LEU:O	2:X:27:TRP:HB3	2.21	0.41
2:X:57:SER:O	2:X:60:PRO:HD3	2.20	0.41
1:B:87:GLU:HA	1:B:88:PRO:HD3	1.87	0.41
2:L:56:PHE:CD1	2:L:57:SER:N	2.89	0.41
1:Q:4:HIS:HB2	6:R:5319:HOH:O	2.20	0.41
2:R:212:LEU:HD11	2:R:215:THR:OG1	2.20	0.41
1:T:62:PHE:HA	2:U:192:THR:HG23	2.02	0.41
2:X:214:ARG:HG2	2:X:214:ARG:NH2	2.33	0.41
2:F:135:TRP:CE2	2:F:222:VAL:HG21	2.55	0.41
1:M:70:VAL:HG21	1:P:93:MET:HE1	2.03	0.41
1:M:122:SER:O	1:M:123:GLN:HB2	2.20	0.41
1:N:179:ARG:HD2	6:N:5197:HOH:O	2.19	0.41
1:N:214:GLU:O	1:N:214:GLU:HG2	2.21	0.41
1:B:127:ILE:HD13	1:B:221:ARG:HB3	2.03	0.41
1:D:28:TYR:CE1	1:D:110:VAL:CG2	3.03	0.41
1:D:102:ARG:HB3	1:D:103:PRO:HD3	2.02	0.41
1:E:25:LYS:CG	1:E:112:GLU:HB2	2.50	0.41
1:E:114:PRO:HG2	1:E:228:ARG:HD2	2.02	0.41
1:E:226:MET:CE	1:E:228:ARG:HD3	2.51	0.41
2:I:174:ASN:ND2	2:I:177:ARG:H	2.18	0.41
1:J:63:LEU:HD13	1:J:63:LEU:H	1.86	0.41
1:J:128:PRO:O	1:J:223:GLN:NE2	2.53	0.41
1:K:67:ILE:CD1	2:L:184:ALA:HA	2.51	0.41
1:M:68:ASN:N	1:M:68:ASN:HD22	2.18	0.41
1:N:131:PRO:HB2	1:N:134:TRP:CD1	2.56	0.41
2:O:35:PHE:CE1	2:O:60:PRO:HG2	2.56	0.41
1:P:57:PHE:CG	1:P:58:SER:N	2.89	0.41
1:P:57:PHE:CD1	1:P:58:SER:N	2.89	0.41
2:R:11:SER:O	2:R:12:GLN:HB2	2.21	0.41
2:R:45:ASP:HB3	2:R:48:LEU:HD12	2.03	0.41
1:T:122:SER:O	1:T:123:GLN:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:133:SER:OG	2:U:221:GLN:NE2	2.54	0.41
2:X:78:LYS:HB2	2:X:173:CYS:O	2.21	0.41
2:X:82:LEU:HD23	2:X:82:LEU:HA	1.96	0.41
1:A:20:CYS:HB3	1:A:24:THR:OG1	2.21	0.41
2:C:114:ALA:HA	2:C:223:CYS:O	2.21	0.41
1:H:197:GLU:HA	1:H:197:GLU:OE2	2.21	0.41
2:I:11:SER:O	2:I:12:GLN:HB2	2.20	0.41
1:K:134:TRP:CE2	1:K:227:ARG:HG2	2.56	0.41
1:M:90:PRO:HD2	6:M:5260:HOH:O	2.21	0.41
1:N:28:TYR:CZ	1:N:110:VAL:HG21	2.55	0.41
1:N:63:LEU:C	1:N:63:LEU:HD12	2.42	0.41
1:N:123:GLN:HA	1:N:220:SER:HB2	2.03	0.41
2:O:94:ALA:HB2	2:O:179:THR:HG22	2.02	0.41
1:T:8:VAL:CG1	1:T:111:CYS:HB2	2.51	0.41
2:U:128:PRO:HB2	2:U:131:TRP:CD1	2.56	0.41
2:C:23:MET:HE2	2:C:224:MET:HE3	2.03	0.40
2:F:46:LEU:H	2:F:153:GLN:NE2	2.17	0.40
1:Q:57:PHE:CG	1:Q:58:SER:N	2.88	0.40
1:T:3:ASP:N	6:T:5221:HOH:O	2.53	0.40
1:V:137:LEU:O	1:V:138:TRP:HB3	2.21	0.40
1:V:176:CYS:HA	1:V:182:CYS:HA	2.03	0.40
1:W:66:ASN:HB2	6:X:5219:HOH:O	2.20	0.40
1:A:99:GLU:OE1	1:A:102:ARG:HD2	2.20	0.40
1:H:144:VAL:HG22	1:H:158:LEU:HD21	2.02	0.40
1:H:179:ARG:HH21	1:H:181:THR:CB	2.35	0.40
2:L:17:PRO:HG2	2:L:105:CYS:HA	2.03	0.40
1:M:92:SER:O	1:M:93:MET:HB2	2.21	0.40
2:R:142:MET:HA	2:R:152:GLY:HA2	2.04	0.40
1:S:102:ARG:HB3	1:S:103:PRO:HD3	2.02	0.40
1:V:4:HIS:CE1	1:V:6:PHE:CE1	3.07	0.40
2:X:134:LEU:O	2:X:135:TRP:HB3	2.22	0.40
1:A:96:ILE:HD13	1:A:104:PHE:CZ	2.56	0.40
1:B:90:PRO:HD3	1:B:96:ILE:HD11	2.01	0.40
2:I:35:PHE:CE1	2:I:60:PRO:HG2	2.56	0.40
1:J:27:LEU:HD21	1:J:112:GLU:HB2	2.03	0.40
1:N:179:ARG:HH11	2:R:176:ALA:HB1	1.86	0.40
1:V:64:PHE:HB3	1:W:191:PHE:CD1	2.56	0.40
1:V:77:ASN:HD22	1:V:77:ASN:HA	1.56	0.40
1:V:125:ILE:HG23	6:V:5289:HOH:O	2.21	0.40
1:A:85:THR:HB	1:A:86:PRO:HD2	2.03	0.40
2:F:214:ARG:HD3	2:F:214:ARG:C	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:56:PHE:CG	2:R:57:SER:N	2.89	0.40
2:R:212:LEU:HD13	2:R:212:LEU:C	2.42	0.40
1:T:8:VAL:HG13	1:T:111:CYS:HB2	2.04	0.40
1:B:57:PHE:CG	1:B:58:SER:N	2.90	0.40
1:B:126:GLN:H	1:B:126:GLN:HE21	1.70	0.40
2:C:224:MET:HE2	2:C:224:MET:HB3	1.81	0.40
1:E:226:MET:HE3	1:E:228:ARG:HD3	2.03	0.40
1:G:57:PHE:CD1	1:G:58:SER:N	2.89	0.40
2:I:40:LYS:NZ	2:I:40:LYS:HB2	2.37	0.40
1:Q:66:ASN:HB2	6:R:5227:HOH:O	2.21	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	221/229 (96%)	214 (97%)	6 (3%)	1 (0%)	29 9
1	B	223/229 (97%)	213 (96%)	9 (4%)	1 (0%)	34 13
1	D	222/229 (97%)	211 (95%)	9 (4%)	2 (1%)	17 3
1	E	222/229 (97%)	213 (96%)	9 (4%)	0	100 100
1	G	226/229 (99%)	218 (96%)	6 (3%)	2 (1%)	17 3
1	H	225/229 (98%)	215 (96%)	9 (4%)	1 (0%)	34 13
1	J	222/229 (97%)	213 (96%)	8 (4%)	1 (0%)	29 9
1	K	222/229 (97%)	211 (95%)	10 (4%)	1 (0%)	29 9
1	M	221/229 (96%)	210 (95%)	10 (4%)	1 (0%)	29 9
1	N	222/229 (97%)	213 (96%)	7 (3%)	2 (1%)	17 3
1	P	223/229 (97%)	217 (97%)	4 (2%)	2 (1%)	17 3
1	Q	222/229 (97%)	212 (96%)	10 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	S	223/229 (97%)	215 (96%)	7 (3%)	1 (0%)	34 13
1	T	225/229 (98%)	212 (94%)	13 (6%)	0	100 100
1	V	222/229 (97%)	209 (94%)	12 (5%)	1 (0%)	29 9
1	W	222/229 (97%)	210 (95%)	12 (5%)	0	100 100
2	C	221/227 (97%)	203 (92%)	17 (8%)	1 (0%)	29 9
2	F	220/227 (97%)	205 (93%)	13 (6%)	2 (1%)	17 3
2	I	223/227 (98%)	211 (95%)	10 (4%)	2 (1%)	17 3
2	L	219/227 (96%)	203 (93%)	15 (7%)	1 (0%)	29 9
2	O	222/227 (98%)	208 (94%)	11 (5%)	3 (1%)	11 1
2	R	222/227 (98%)	208 (94%)	12 (5%)	2 (1%)	17 3
2	U	222/227 (98%)	212 (96%)	9 (4%)	1 (0%)	29 9
2	X	221/227 (97%)	200 (90%)	19 (9%)	2 (1%)	17 3
All	All	5333/5480 (97%)	5056 (95%)	247 (5%)	30 (1%)	25 7

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	GLU
1	D	212	ALA
2	F	175	GLY
1	H	214	GLU
2	L	175	GLY
2	O	213	ILE
2	R	210	ALA
2	C	175	GLY
2	F	210	ALA
1	N	212	ALA
2	R	175	GLY
1	V	216	ARG
2	X	21	VAL
2	X	175	GLY
2	O	175	GLY
1	P	76	ARG
2	U	175	GLY
1	M	148	SER
2	O	198	SER
1	P	148	SER
1	S	76	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	76	ARG
1	G	148	SER
2	I	198	SER
1	J	148	SER
1	K	212	ALA
1	A	148	SER
1	D	148	SER
2	I	175	GLY
1	N	90	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	189/195 (97%)	185 (98%)	4 (2%)	53	23
1	B	191/195 (98%)	189 (99%)	2 (1%)	76	57
1	D	190/195 (97%)	186 (98%)	4 (2%)	53	23
1	E	190/195 (97%)	185 (97%)	5 (3%)	46	16
1	G	194/195 (100%)	188 (97%)	6 (3%)	40	11
1	H	193/195 (99%)	188 (97%)	5 (3%)	46	16
1	J	190/195 (97%)	186 (98%)	4 (2%)	53	23
1	K	190/195 (97%)	188 (99%)	2 (1%)	73	53
1	M	189/195 (97%)	181 (96%)	8 (4%)	30	6
1	N	191/195 (98%)	187 (98%)	4 (2%)	53	23
1	P	191/195 (98%)	187 (98%)	4 (2%)	53	23
1	Q	190/195 (97%)	184 (97%)	6 (3%)	39	10
1	S	191/195 (98%)	184 (96%)	7 (4%)	34	8
1	T	193/195 (99%)	188 (97%)	5 (3%)	46	16
1	V	190/195 (97%)	184 (97%)	6 (3%)	39	10
1	W	190/195 (97%)	186 (98%)	4 (2%)	53	23
2	C	187/191 (98%)	182 (97%)	5 (3%)	44	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	187/191 (98%)	182 (97%)	5 (3%)	44 15
2	I	189/191 (99%)	185 (98%)	4 (2%)	53 23
2	L	186/191 (97%)	181 (97%)	5 (3%)	44 15
2	O	188/191 (98%)	184 (98%)	4 (2%)	53 23
2	R	188/191 (98%)	182 (97%)	6 (3%)	39 10
2	U	188/191 (98%)	183 (97%)	5 (3%)	44 15
2	X	187/191 (98%)	180 (96%)	7 (4%)	34 8
All	All	4552/4648 (98%)	4435 (97%)	117 (3%)	46 16

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	77	ASN
1	A	145	MET
1	A	218	HIS
1	B	126	GLN
1	B	218	HIS
2	C	76	ASN
2	C	78	LYS
2	C	88	LEU
2	C	90	MET
2	C	174	ASN
1	D	28	TYR
1	D	77	ASN
1	D	132	THR
1	D	145	MET
1	E	25	LYS
1	E	89	MET
1	E	116	MET
1	E	216	ARG
1	E	227	ARG
2	F	68	ASP
2	F	76	ASN
2	F	90	MET
2	F	197	GLN
2	F	214	ARG
1	G	3	ASP
1	G	25	LYS
1	G	28	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	41	ARG
1	G	77	ASN
1	G	145	MET
1	H	63	LEU
1	H	69	ASN
1	H	91	MET
1	H	198	ARG
1	H	227	ARG
2	I	15	GLN
2	I	40	LYS
2	I	76	ASN
2	I	174	ASN
1	J	63	LEU
1	J	77	ASN
1	J	102	ARG
1	J	145	MET
1	K	28	TYR
1	K	227	ARG
2	L	76	ASN
2	L	88	LEU
2	L	132	ARG
2	L	136	ILE
2	L	212	LEU
1	M	26	ILE
1	M	68	ASN
1	M	77	ASN
1	M	79	TYR
1	M	145	MET
1	M	210	LEU
1	M	216	ARG
1	M	227	ARG
1	N	79	TYR
1	N	91	MET
1	N	102	ARG
1	N	227	ARG
2	O	76	ASN
2	O	90	MET
2	O	164	ASP
2	O	197	GLN
1	P	41	ARG
1	P	77	ASN
1	P	79	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	145	MET
1	Q	69	ASN
1	Q	91	MET
1	Q	102	ARG
1	Q	214	GLU
1	Q	215	LEU
1	Q	227	ARG
2	R	40	LYS
2	R	68	ASP
2	R	76	ASN
2	R	88	LEU
2	R	126	HIS
2	R	212	LEU
1	S	41	ARG
1	S	77	ASN
1	S	79	TYR
1	S	102	ARG
1	S	145	MET
1	S	198	ARG
1	S	227	ARG
1	T	10	ARG
1	T	67	ILE
1	T	91	MET
1	T	199	SER
1	T	227	ARG
2	U	3	ILE
2	U	76	ASN
2	U	90	MET
2	U	166	ARG
2	U	212	LEU
1	V	4	HIS
1	V	15	THR
1	V	77	ASN
1	V	79	TYR
1	V	145	MET
1	V	227	ARG
1	W	69	ASN
1	W	83	LEU
1	W	102	ARG
1	W	116	MET
2	X	15	GLN
2	X	24	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	39	GLU
2	X	68	ASP
2	X	76	ASN
2	X	88	LEU
2	X	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	39	ASN
1	A	45	GLN
1	A	66	ASN
1	A	77	ASN
1	A	100	ASN
1	A	123	GLN
1	A	156	GLN
1	B	37	GLN
1	B	45	GLN
1	B	77	ASN
1	B	100	ASN
1	B	123	GLN
1	B	126	GLN
1	B	129	GLN
1	B	156	GLN
2	C	38	GLN
2	C	76	ASN
2	C	120	GLN
2	C	126	HIS
2	C	153	GLN
2	C	174	ASN
2	C	200	GLN
1	D	19	GLN
1	D	39	ASN
1	D	45	GLN
1	D	66	ASN
1	D	77	ASN
1	D	123	GLN
1	D	126	GLN
1	D	156	GLN
1	D	218	HIS
1	E	29	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	37	GLN
1	E	39	ASN
1	E	45	GLN
1	E	77	ASN
1	E	123	GLN
1	E	156	GLN
2	F	15	GLN
2	F	38	GLN
2	F	76	ASN
2	F	120	GLN
2	F	153	GLN
2	F	174	ASN
2	F	200	GLN
2	F	221	GLN
1	G	39	ASN
1	G	45	GLN
1	G	66	ASN
1	G	77	ASN
1	G	100	ASN
1	G	123	GLN
1	G	129	GLN
1	G	156	GLN
1	H	37	GLN
1	H	45	GLN
1	H	100	ASN
1	H	123	GLN
1	H	129	GLN
1	H	156	GLN
2	I	12	GLN
2	I	15	GLN
2	I	76	ASN
2	I	120	GLN
2	I	153	GLN
2	I	174	ASN
2	I	200	GLN
2	I	221	GLN
2	I	226	ASN
1	J	29	HIS
1	J	39	ASN
1	J	45	GLN
1	J	66	ASN
1	J	77	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	100	ASN
1	J	123	GLN
1	J	156	GLN
1	K	29	HIS
1	K	37	GLN
1	K	39	ASN
1	K	45	GLN
1	K	77	ASN
1	K	123	GLN
1	K	156	GLN
2	L	15	GLN
2	L	38	GLN
2	L	76	ASN
2	L	120	GLN
2	L	153	GLN
2	L	174	ASN
2	L	221	GLN
2	L	226	ASN
1	M	37	GLN
1	M	39	ASN
1	M	45	GLN
1	M	66	ASN
1	M	68	ASN
1	M	77	ASN
1	M	123	GLN
1	M	156	GLN
1	N	37	GLN
1	N	45	GLN
1	N	77	ASN
1	N	100	ASN
1	N	123	GLN
1	N	129	GLN
1	N	156	GLN
2	O	15	GLN
2	O	38	GLN
2	O	76	ASN
2	O	120	GLN
2	O	153	GLN
2	O	197	GLN
2	O	200	GLN
2	O	221	GLN
1	P	29	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	39	ASN
1	P	45	GLN
1	P	66	ASN
1	P	77	ASN
1	P	123	GLN
1	P	156	GLN
1	P	218	HIS
1	Q	4	HIS
1	Q	37	GLN
1	Q	39	ASN
1	Q	45	GLN
1	Q	77	ASN
1	Q	123	GLN
1	Q	156	GLN
2	R	15	GLN
2	R	38	GLN
2	R	76	ASN
2	R	120	GLN
2	R	153	GLN
2	R	221	GLN
2	R	226	ASN
1	S	4	HIS
1	S	37	GLN
1	S	39	ASN
1	S	45	GLN
1	S	66	ASN
1	S	77	ASN
1	S	100	ASN
1	S	123	GLN
1	S	156	GLN
1	T	4	HIS
1	T	29	HIS
1	T	37	GLN
1	T	45	GLN
1	T	69	ASN
1	T	77	ASN
1	T	123	GLN
1	T	126	GLN
1	T	129	GLN
1	T	156	GLN
2	U	38	GLN
2	U	76	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	U	120	GLN
2	U	153	GLN
2	U	200	GLN
2	U	221	GLN
2	U	226	ASN
1	V	19	GLN
1	V	29	HIS
1	V	39	ASN
1	V	45	GLN
1	V	66	ASN
1	V	77	ASN
1	V	123	GLN
1	V	156	GLN
1	V	218	HIS
1	V	223	GLN
1	W	29	HIS
1	W	37	GLN
1	W	39	ASN
1	W	45	GLN
1	W	77	ASN
1	W	123	GLN
1	W	126	GLN
1	W	156	GLN
1	W	223	GLN
2	X	15	GLN
2	X	38	GLN
2	X	76	ASN
2	X	120	GLN
2	X	153	GLN
2	X	200	GLN
2	X	226	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 32 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MPD	D	5007	-	7,7,7	0.94	0	9,10,10	0.50	0
4	MPD	M	5008	-	7,7,7	0.62	0	9,10,10	0.48	0
4	MPD	M	5003	-	7,7,7	0.61	0	9,10,10	0.55	0
4	MPD	S	5004	-	7,7,7	0.53	0	9,10,10	0.50	0
4	MPD	S	5005	-	7,7,7	0.80	0	9,10,10	0.70	0
4	MPD	J	5009	-	7,7,7	0.57	0	9,10,10	0.57	0
4	MPD	A	5001	-	7,7,7	0.53	0	9,10,10	0.52	0
4	MPD	P	5006	-	7,7,7	0.61	0	9,10,10	0.55	0
4	MPD	T	5002	-	7,7,7	1.60	2 (28%)	9,10,10	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	D	5007	-	-	3/5/5/5	-
4	MPD	M	5008	-	-	0/5/5/5	-
4	MPD	M	5003	-	-	1/5/5/5	-
4	MPD	S	5004	-	-	0/5/5/5	-
4	MPD	S	5005	-	-	0/5/5/5	-
4	MPD	J	5009	-	-	0/5/5/5	-
4	MPD	A	5001	-	-	0/5/5/5	-
4	MPD	P	5006	-	-	0/5/5/5	-
4	MPD	T	5002	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	5002	MPD	CM-C2	-2.52	1.44	1.52
4	T	5002	MPD	C3-C2	-2.06	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	5007	MPD	C1-C2-C3-C4
4	D	5007	MPD	O2-C2-C3-C4
4	M	5003	MPD	C1-C2-C3-C4
4	D	5007	MPD	CM-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5007	MPD	1	0
4	M	5008	MPD	1	0
4	S	5005	MPD	5	0
4	J	5009	MPD	3	0
4	P	5006	MPD	6	0

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	223/229 (97%)	-0.00	2 (0%)	84 87	10, 18, 33, 42	0
1	B	225/229 (98%)	0.20	15 (6%)	17 19	11, 19, 41, 49	0
1	D	224/229 (97%)	-0.17	5 (2%)	62 67	8, 14, 33, 49	0
1	E	224/229 (97%)	-0.08	6 (2%)	54 59	9, 16, 35, 45	0
1	G	228/229 (99%)	-0.11	6 (2%)	56 61	9, 15, 39, 47	0
1	H	227/229 (99%)	0.09	11 (4%)	30 33	10, 18, 39, 50	0
1	J	224/229 (97%)	0.14	12 (5%)	25 28	10, 20, 41, 49	0
1	K	224/229 (97%)	0.13	15 (6%)	17 19	10, 18, 41, 50	0
1	M	223/229 (97%)	0.17	12 (5%)	25 28	10, 20, 38, 50	0
1	N	224/229 (97%)	0.24	11 (4%)	29 32	10, 19, 41, 49	0
1	P	225/229 (98%)	-0.15	3 (1%)	77 81	10, 18, 32, 45	0
1	Q	224/229 (97%)	-0.04	6 (2%)	54 59	10, 18, 39, 47	0
1	S	225/229 (98%)	-0.05	5 (2%)	62 67	10, 17, 32, 42	0
1	T	227/229 (99%)	0.13	10 (4%)	34 38	10, 18, 42, 49	0
1	V	224/229 (97%)	0.30	12 (5%)	25 28	12, 22, 42, 50	0
1	W	224/229 (97%)	0.17	11 (4%)	29 32	10, 21, 43, 49	0
2	C	223/227 (98%)	0.27	14 (6%)	20 21	10, 20, 40, 50	0
2	F	222/227 (97%)	0.25	14 (6%)	20 21	9, 19, 38, 50	0
2	I	225/227 (99%)	0.20	9 (4%)	38 42	9, 20, 36, 48	0
2	L	221/227 (97%)	0.21	10 (4%)	33 36	11, 20, 41, 50	0
2	O	224/227 (98%)	0.05	8 (3%)	42 47	9, 17, 34, 45	0
2	R	224/227 (98%)	0.04	12 (5%)	25 28	9, 17, 37, 50	0
2	U	224/227 (98%)	0.09	8 (3%)	42 47	9, 16, 37, 47	0
2	X	223/227 (98%)	0.21	11 (4%)	29 32	10, 20, 41, 50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	5381/5480 (98%)	0.09	228 (4%)	36	40	8, 18, 39, 50	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	212	LEU	12.5
2	X	21	VAL	11.6
2	L	212	LEU	10.7
2	X	212	LEU	9.9
2	R	211	GLY	8.5
2	R	212	LEU	8.1
2	F	212	LEU	7.4
2	L	21	VAL	6.3
2	F	210	ALA	6.2
2	L	210	ALA	6.2
1	G	2	VAL	6.2
2	R	210	ALA	6.1
2	U	212	LEU	6.1
2	C	213	ILE	6.0
2	R	3	ILE	5.8
1	B	217	THR	5.7
1	N	229	THR	5.7
1	T	91	MET	5.7
1	B	213	GLY	5.7
1	V	4	HIS	5.7
1	V	217	THR	5.6
1	D	213	GLY	5.5
2	C	210	ALA	5.5
1	T	212	ALA	5.4
1	K	217	THR	5.4
1	V	91	MET	5.4
2	I	212	LEU	5.3
2	C	21	VAL	5.3
2	O	3	ILE	5.2
2	X	210	ALA	5.0
1	W	212	ALA	5.0
1	J	132	THR	4.9
2	L	211	GLY	4.7
2	U	21	VAL	4.7
1	G	229	THR	4.7
1	J	4	HIS	4.6
2	R	209	LYS	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	213	GLY	4.5
1	K	212	ALA	4.5
1	B	228	ARG	4.4
2	R	213	ILE	4.4
1	M	217	THR	4.4
1	V	213	GLY	4.4
1	Q	91	MET	4.4
1	K	91	MET	4.3
1	D	28	TYR	4.3
1	N	91	MET	4.2
1	M	210	LEU	4.1
1	H	217	THR	4.1
2	R	5	TYR	4.1
2	U	90	MET	4.1
1	M	215	LEU	4.0
1	N	213	GLY	4.0
2	I	210	ALA	3.9
1	B	91	MET	3.9
2	X	18	MET	3.9
2	I	90	MET	3.9
1	E	91	MET	3.8
1	K	215	LEU	3.7
1	T	215	LEU	3.7
2	X	88	LEU	3.7
2	C	18	MET	3.7
1	N	217	THR	3.7
1	K	214	GLU	3.7
1	H	212	ALA	3.7
1	E	89	MET	3.7
1	J	91	MET	3.7
2	C	90	MET	3.6
1	H	91	MET	3.6
2	C	211	GLY	3.5
2	O	21	VAL	3.5
1	N	215	LEU	3.3
1	K	28	TYR	3.3
2	F	214	ARG	3.3
1	W	91	MET	3.3
2	O	212	LEU	3.3
1	P	91	MET	3.3
2	I	197	GLN	3.3
1	D	211	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	212	ALA	3.3
1	K	133	GLY	3.2
2	L	18	MET	3.2
2	R	21	VAL	3.2
1	B	214	GLU	3.2
1	B	125	ILE	3.2
2	X	24	ASN	3.2
2	L	209	LYS	3.1
1	N	214	GLU	3.1
1	H	216	ARG	3.1
1	G	217	THR	3.1
1	H	215	LEU	3.1
1	M	26	ILE	3.1
2	F	201	GLY	3.1
2	F	90	MET	3.0
2	U	122	VAL	3.0
1	H	214	GLU	3.0
2	C	3	ILE	3.0
1	J	198	ARG	2.9
1	J	217	THR	2.9
1	E	213	GLY	2.9
1	K	218	HIS	2.9
1	V	214	GLU	2.9
2	I	201	GLY	2.9
1	T	217	THR	2.9
2	U	87	PRO	2.9
2	O	90	MET	2.9
1	K	213	GLY	2.9
1	M	5	GLY	2.8
1	T	210	LEU	2.8
2	L	88	LEU	2.8
1	M	133	GLY	2.8
2	U	211	GLY	2.8
1	Q	217	THR	2.8
2	X	209	LYS	2.8
1	W	132	THR	2.8
1	S	22	PRO	2.8
1	N	132	THR	2.8
2	C	88	LEU	2.7
1	G	28	TYR	2.7
1	S	4	HIS	2.7
1	B	212	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	215	LEU	2.7
2	X	213	ILE	2.7
2	I	211	GLY	2.7
1	G	91	MET	2.7
1	E	212	ALA	2.7
1	Q	214	GLU	2.7
2	O	226	ASN	2.7
1	M	218	HIS	2.6
1	Q	4	HIS	2.6
1	V	212	ALA	2.6
1	W	213	GLY	2.6
2	R	90	MET	2.6
1	K	5	GLY	2.6
1	K	22	PRO	2.6
1	V	215	LEU	2.6
1	W	218	HIS	2.6
1	B	22	PRO	2.6
1	T	229	THR	2.6
2	X	211	GLY	2.5
1	N	90	PRO	2.5
1	B	216	ARG	2.5
2	R	226	ASN	2.5
1	H	3	ASP	2.5
1	K	4	HIS	2.5
1	V	16	ASP	2.5
1	H	198	ARG	2.5
1	B	134	TRP	2.5
1	W	133	GLY	2.4
1	A	91	MET	2.4
2	X	216	HIS	2.4
2	I	209	LYS	2.4
2	F	87	PRO	2.4
2	F	211	GLY	2.4
1	P	212	ALA	2.4
1	V	125	ILE	2.4
1	K	227	ARG	2.4
1	E	214	GLU	2.4
1	Q	212	ALA	2.4
1	B	129	GLN	2.4
2	I	18	MET	2.4
2	F	226	ASN	2.3
1	T	3	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	5	GLY	2.3
2	L	24	ASN	2.3
1	J	227	ARG	2.3
1	M	216	ARG	2.3
1	J	129	GLN	2.3
1	D	132	THR	2.3
1	V	88	PRO	2.3
1	H	179	ARG	2.3
1	J	126	GLN	2.3
2	F	197	GLN	2.3
2	F	130	GLY	2.3
1	J	134	TRP	2.3
2	C	209	LYS	2.3
1	K	216	ARG	2.3
1	S	228	ARG	2.3
2	C	130	GLY	2.3
1	D	4	HIS	2.2
2	C	87	PRO	2.2
2	U	126	HIS	2.2
1	J	130	CYS	2.2
2	R	22	GLY	2.2
2	F	21	VAL	2.2
2	C	216	HIS	2.2
1	Q	22	PRO	2.2
1	T	90	PRO	2.2
2	F	122	VAL	2.2
1	W	5	GLY	2.2
2	U	197	GLN	2.2
1	H	90	PRO	2.2
1	W	22	PRO	2.2
1	J	116	MET	2.2
1	V	115	ALA	2.2
2	O	129	ALA	2.2
2	L	213	ILE	2.2
1	T	214	GLU	2.2
2	F	129	ALA	2.1
1	B	227	ARG	2.1
1	W	227	ARG	2.1
2	F	126	HIS	2.1
2	O	88	LEU	2.1
1	P	133	GLY	2.1
1	W	214	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	226	ASN	2.1
1	M	22	PRO	2.1
1	B	218	HIS	2.1
1	T	198	ARG	2.1
1	A	214	GLU	2.1
1	K	6	PHE	2.1
2	C	19	CYS	2.1
1	B	90	PRO	2.1
1	M	91	MET	2.1
1	S	114	PRO	2.1
1	M	227	ARG	2.1
1	V	218	HIS	2.0
1	N	199	SER	2.0
1	W	131	PRO	2.0
1	G	214	GLU	2.0
1	N	198	ARG	2.0
1	S	91	MET	2.0
1	J	114	PRO	2.0
1	M	25	LYS	2.0
2	X	208	LEU	2.0
2	O	213	ILE	2.0
2	R	18	MET	2.0
2	I	226	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MPD	P	5006	8/8	0.59	0.34	42,45,49,50	0
4	MPD	S	5005	8/8	0.62	0.33	47,49,49,50	0
4	MPD	J	5009	8/8	0.64	0.47	46,48,50,50	0
4	MPD	M	5008	8/8	0.70	0.22	38,40,44,46	0
4	MPD	D	5007	8/8	0.71	0.30	42,44,44,46	0
4	MPD	S	5004	8/8	0.75	0.18	45,45,46,47	0
4	MPD	A	5001	8/8	0.82	0.14	37,40,41,44	0
4	MPD	T	5002	8/8	0.84	0.33	45,46,47,47	0
5	K	M	5105	1/1	0.90	0.08	42,42,42,42	0
4	MPD	M	5003	8/8	0.92	0.08	24,29,31,33	0
5	K	D	5102	1/1	0.95	0.06	35,35,35,35	0
5	K	V	5108	1/1	0.96	0.06	36,36,36,36	0
5	K	H	5111	1/1	0.98	0.04	21,21,21,21	0
5	K	C	5101	1/1	0.98	0.04	26,26,26,26	0
5	K	P	5106	1/1	0.98	0.07	33,33,33,33	0
5	K	B	5109	1/1	0.98	0.05	20,20,20,20	0
3	CL	L	5209	1/1	0.99	0.03	15,15,15,15	0
3	CL	M	5208	1/1	0.99	0.03	15,15,15,15	0
3	CL	O	5210	1/1	0.99	0.05	13,13,13,13	0
3	CL	P	5211	1/1	0.99	0.04	13,13,13,13	0
3	CL	R	5212	1/1	0.99	0.04	14,14,14,14	0
3	CL	S	5213	1/1	0.99	0.03	16,16,16,16	0
3	CL	V	5215	1/1	0.99	0.04	17,17,17,17	0
5	K	C	5110	1/1	0.99	0.03	19,19,19,19	0
3	CL	X	5216	1/1	0.99	0.05	18,18,18,18	0
5	K	G	5103	1/1	0.99	0.06	34,34,34,34	0
3	CL	A	5201	1/1	0.99	0.03	13,13,13,13	0
5	K	I	5112	1/1	0.99	0.04	21,21,21,21	0
5	K	L	5104	1/1	0.99	0.04	27,27,27,27	0
3	CL	C	5202	1/1	0.99	0.05	15,15,15,15	0
3	CL	F	5204	1/1	0.99	0.05	14,14,14,14	0
5	K	T	5115	1/1	0.99	0.04	17,17,17,17	0
5	K	U	5107	1/1	0.99	0.05	30,30,30,30	0
5	K	U	5116	1/1	0.99	0.04	18,18,18,18	0
3	CL	G	5205	1/1	0.99	0.05	14,14,14,14	0
5	K	O	5114	1/1	1.00	0.03	16,16,16,16	0
3	CL	D	5203	1/1	1.00	0.03	13,13,13,13	0
3	CL	I	5206	1/1	1.00	0.02	11,11,11,11	0
3	CL	J	5207	1/1	1.00	0.03	13,13,13,13	0
3	CL	U	5214	1/1	1.00	0.04	12,12,12,12	0
5	K	N	5113	1/1	1.00	0.03	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.