



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:13 PM UTC

PDB ID : 6TQO / pdb_00006tqo
EMDB ID : EMD-10548
Title : rrn anti-termination complex
Authors : Huang, Y.H.; Wahl, M.C.; Loll, B.; Hilal, T.; Said, N.
Deposited on : 2019-12-17
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

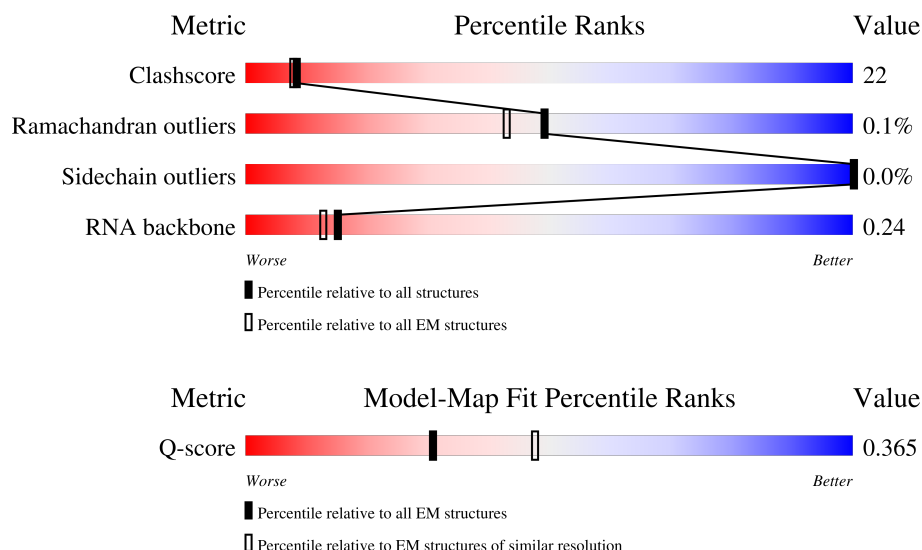
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	267	
2	S	271	
3	A	497	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	141	
5	E	106	
6	G	184	
7	U	329	
7	V	329	
8	W	91	
9	X	1342	
10	Y	1417	
11	C	208	
12	R	85	
13	L	35	
14	K	35	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 40993 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Inositol monophosphatase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	255	Total	C	N	O	S	0	0
			1966	1239	349	371	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-3	GLY	-	expression tag	UNP A0A5B7PBT3
T	-2	ALA	-	expression tag	UNP A0A5B7PBT3
T	-1	MET	-	expression tag	UNP A0A5B7PBT3
T	0	ALA	-	expression tag	UNP A0A5B7PBT3

- Molecule 2 is a protein called Inositol-1-monophosphatase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	267	Total	C	N	O	S	0	0
			2048	1289	364	388	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-3	GLY	-	expression tag	UNP P0ADG4
S	-2	ALA	-	expression tag	UNP P0ADG4
S	-1	MET	-	expression tag	UNP P0ADG4
S	0	ALA	-	expression tag	UNP P0ADG4

- Molecule 3 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	495	Total	C	N	O	S	0	0
			3850	2395	669	773	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A4P8BVH6
A	0	ALA	-	expression tag	UNP A0A4P8BVH6
A	358	ALA	THR	conflict	UNP A0A4P8BVH6

- Molecule 4 is a protein called Transcription antitermination protein NusB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	134	Total	C	N	O	S	0	0
			1063	677	183	201	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A4P8C5Y7
B	0	ALA	-	expression tag	UNP A0A4P8C5Y7

- Molecule 5 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	98	Total	C	N	O	S	0	0
			783	490	149	143	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	LEU	-	expression tag	UNP A0A073G203
E	-1	GLY	-	expression tag	UNP A0A073G203
E	0	SER	-	expression tag	UNP A0A073G203

- Molecule 6 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	178	Total	C	N	O	S	0	0
			1421	900	253	261	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	LEU	-	expression tag	UNP V0ZS55
G	-1	GLY	-	expression tag	UNP V0ZS55
G	0	SER	-	expression tag	UNP V0ZS55

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	322	Total	C	N	O	S	0	0
			2510	1569	442	491	8		
7	V	222	Total	C	N	O	S	0	0
			1715	1072	303	334	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	W	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	1342	Total	C	N	O	S	0	0
			10585	6641	1843	2057	44		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	1337	Total	C	N	O	S	0	0
			10394	6530	1853	1961	50		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1408	HIS	-	expression tag	UNP S1HM87
Y	1409	HIS	-	expression tag	UNP S1HM87
Y	1410	HIS	-	expression tag	UNP S1HM87
Y	1411	HIS	-	expression tag	UNP S1HM87
Y	1412	HIS	-	expression tag	UNP S1HM87
Y	1413	HIS	-	expression tag	UNP S1HM87
Y	1414	HIS	-	expression tag	UNP S1HM87
Y	1415	HIS	-	expression tag	UNP S1HM87
Y	1416	HIS	-	expression tag	UNP S1HM87
Y	1417	HIS	-	expression tag	UNP S1HM87

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP I2X692
C	0	ALA	-	expression tag	UNP I2X692
C	106	ALA	GLY	conflict	UNP I2X692

- Molecule 12 is a RNA chain called rrnGnut RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	45	Total	C	N	O	P	0	0
			955	426	161	323	45		

- Molecule 13 is a DNA chain called tDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	34	Total	C	N	O	P	0	0
			689	327	123	205	34		

- Molecule 14 is a DNA chain called ntDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	32	Total	C	N	O	P	0	0
			657	312	123	190	32		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	T	1	Total	Mg	0
			1	1	
15	S	1	Total	Mg	0
			1	1	
15	Y	1	Total	Mg	0
			1	1	

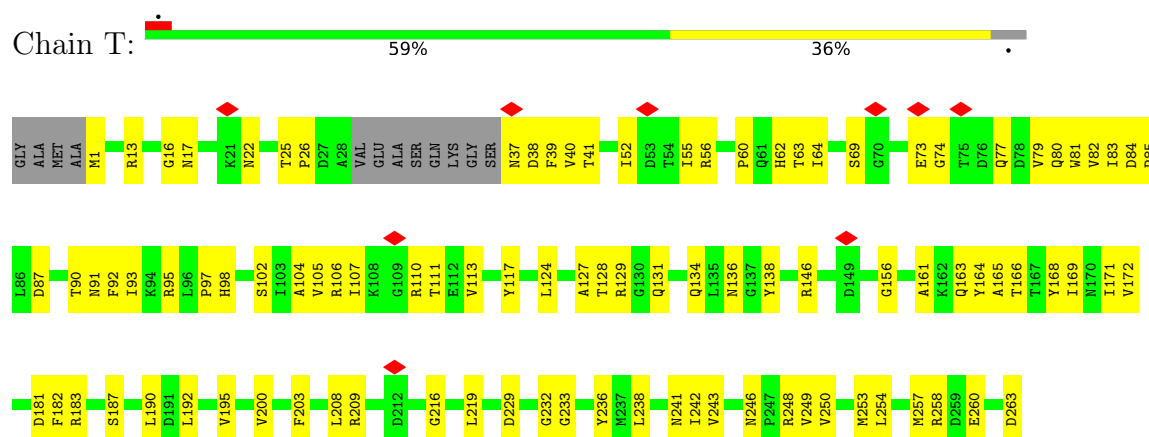
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	Y	2	Total	Zn	0
			2	2	

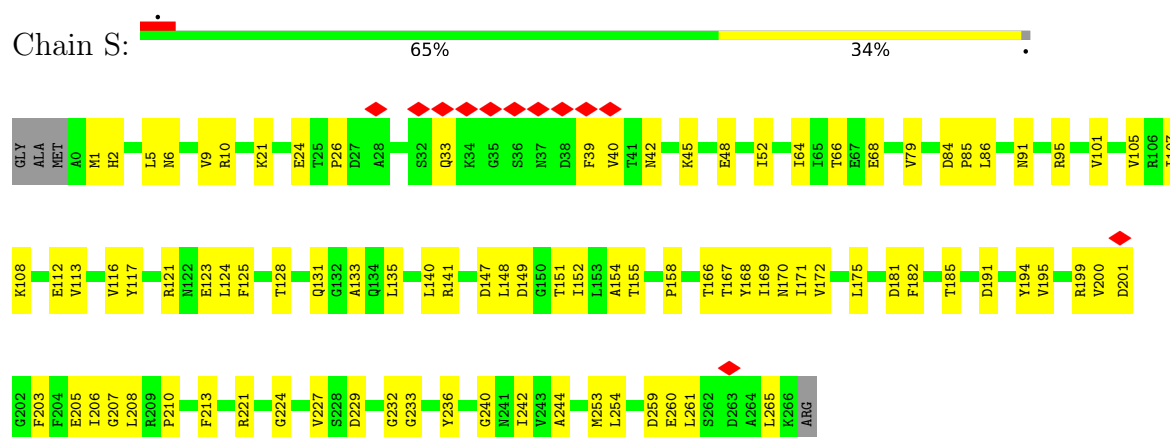
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

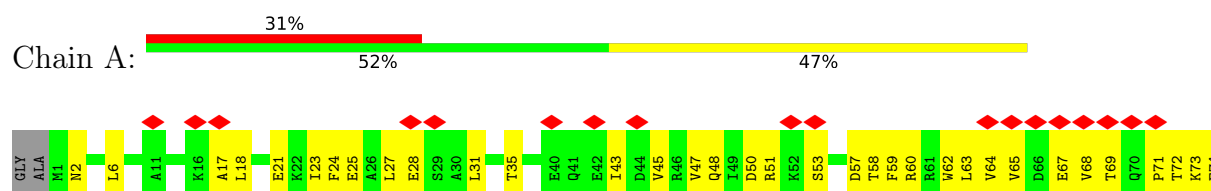
• Molecule 1: Inositol monophosphatase

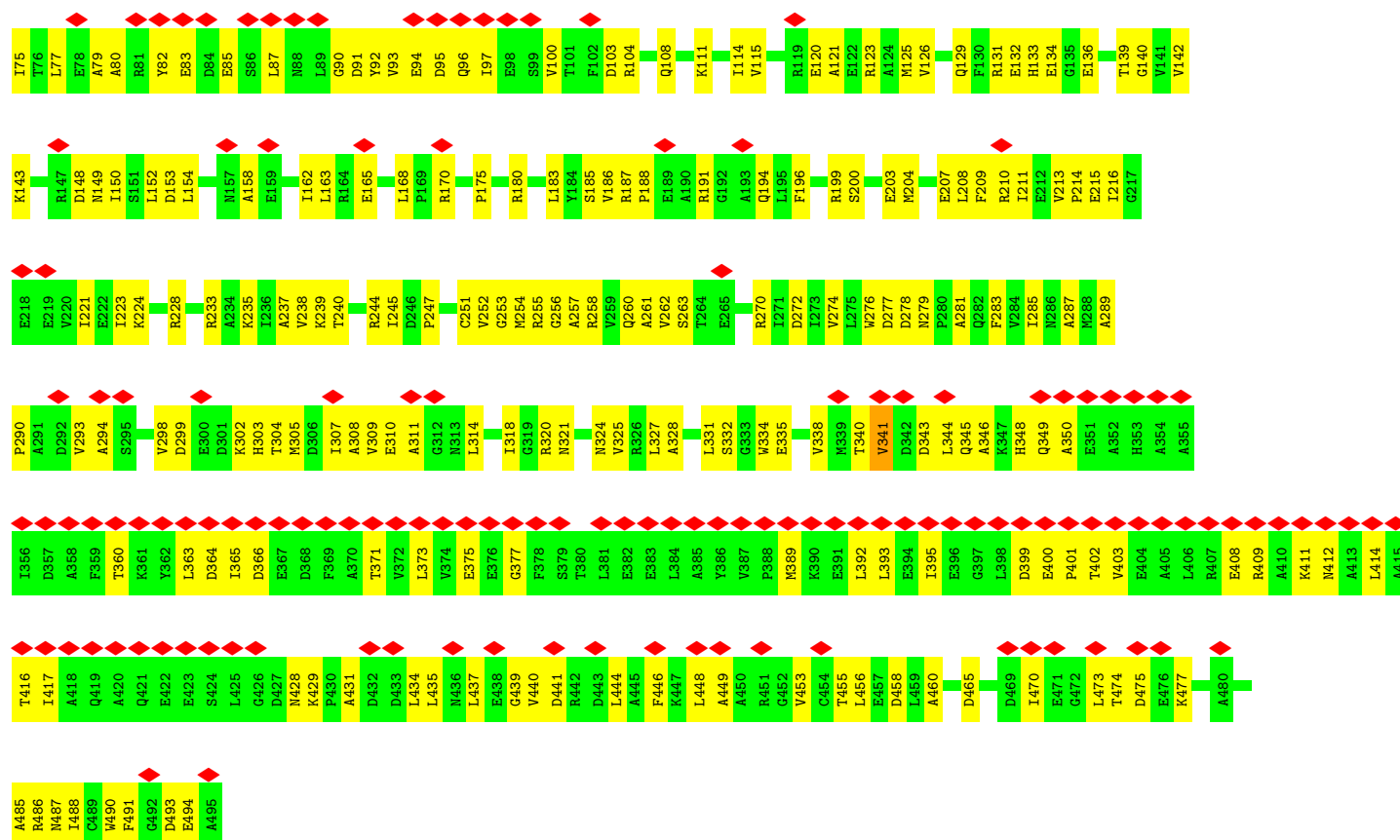


• Molecule 2: Inositol-1-monophosphatase

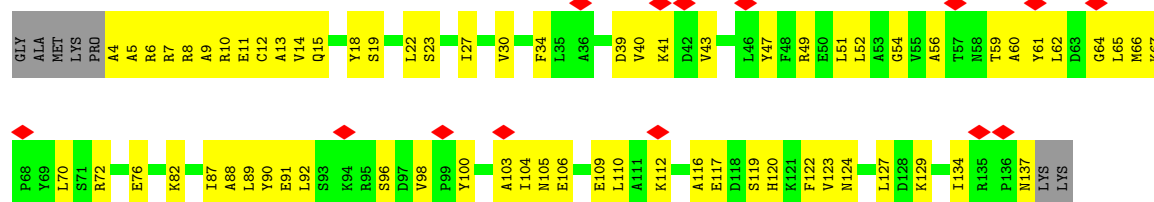


• Molecule 3: Transcription termination/antitermination protein NusA

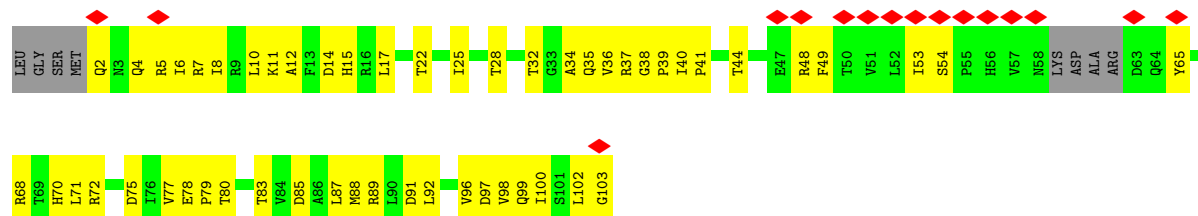




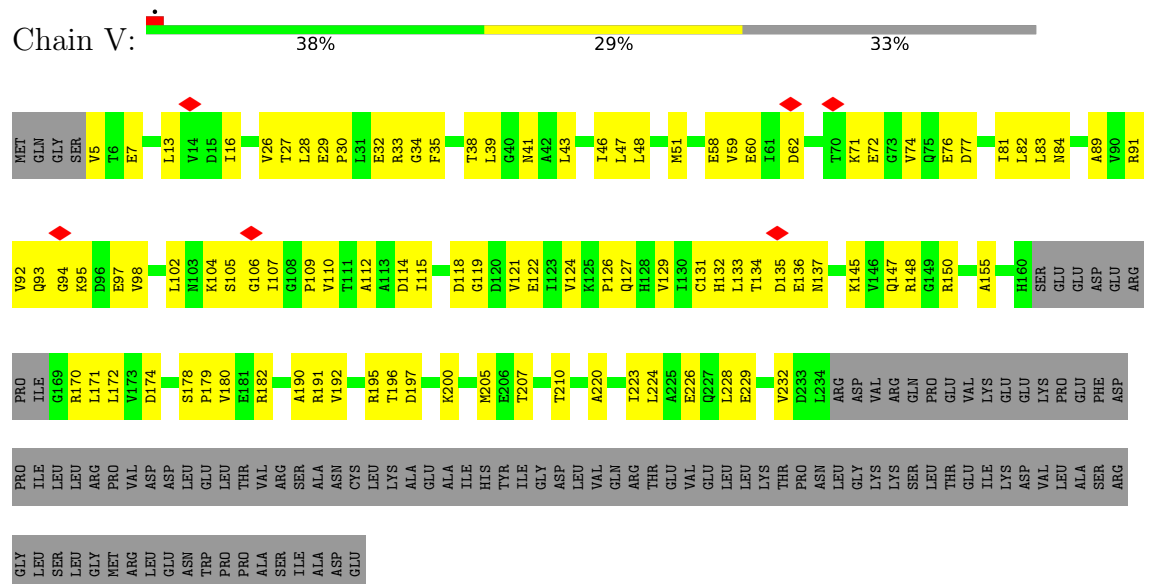
• Molecule 4: Transcription antitermination protein NusB

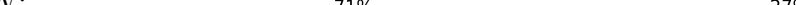


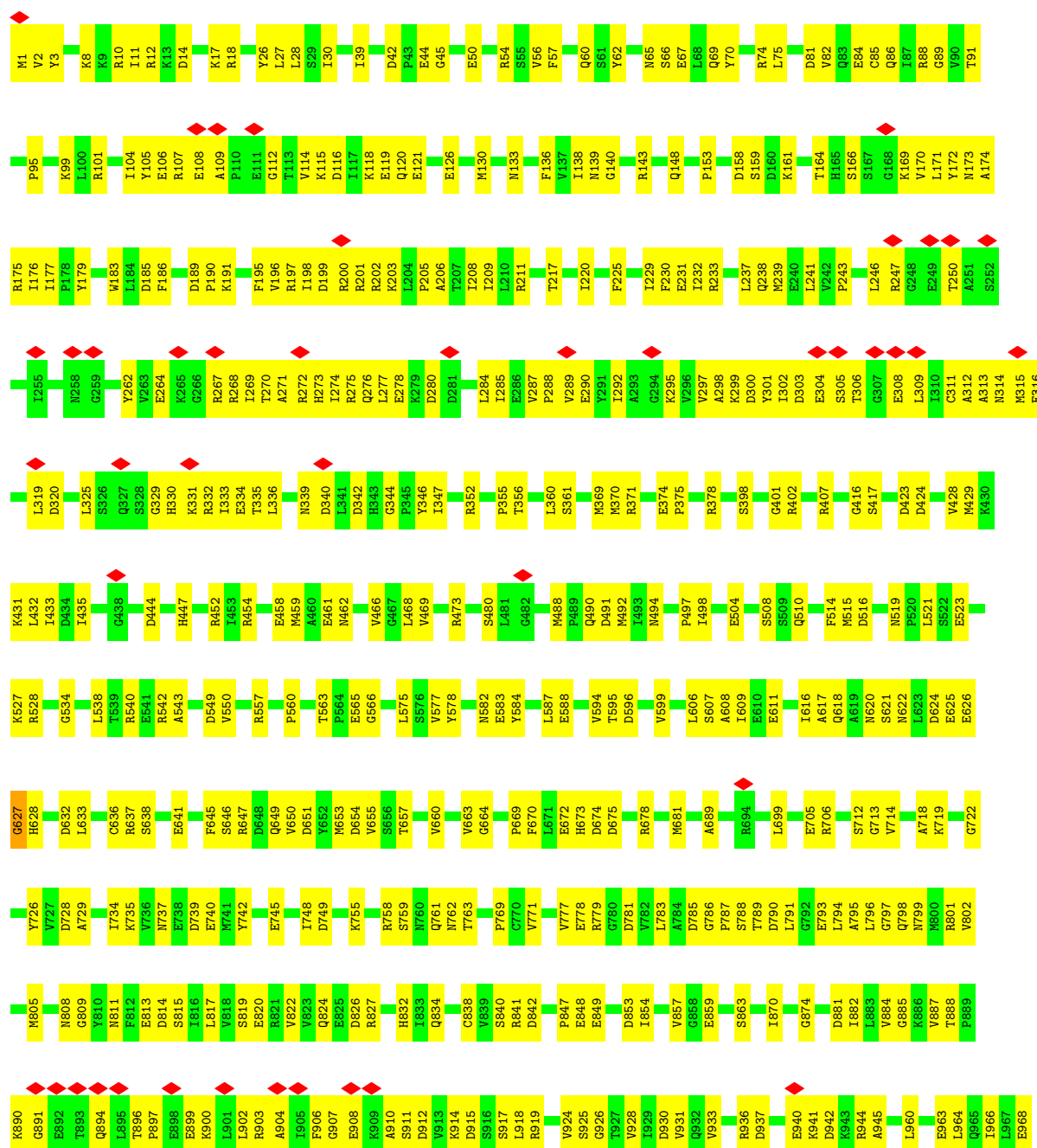
• Molecule 5: 30S ribosomal protein S10



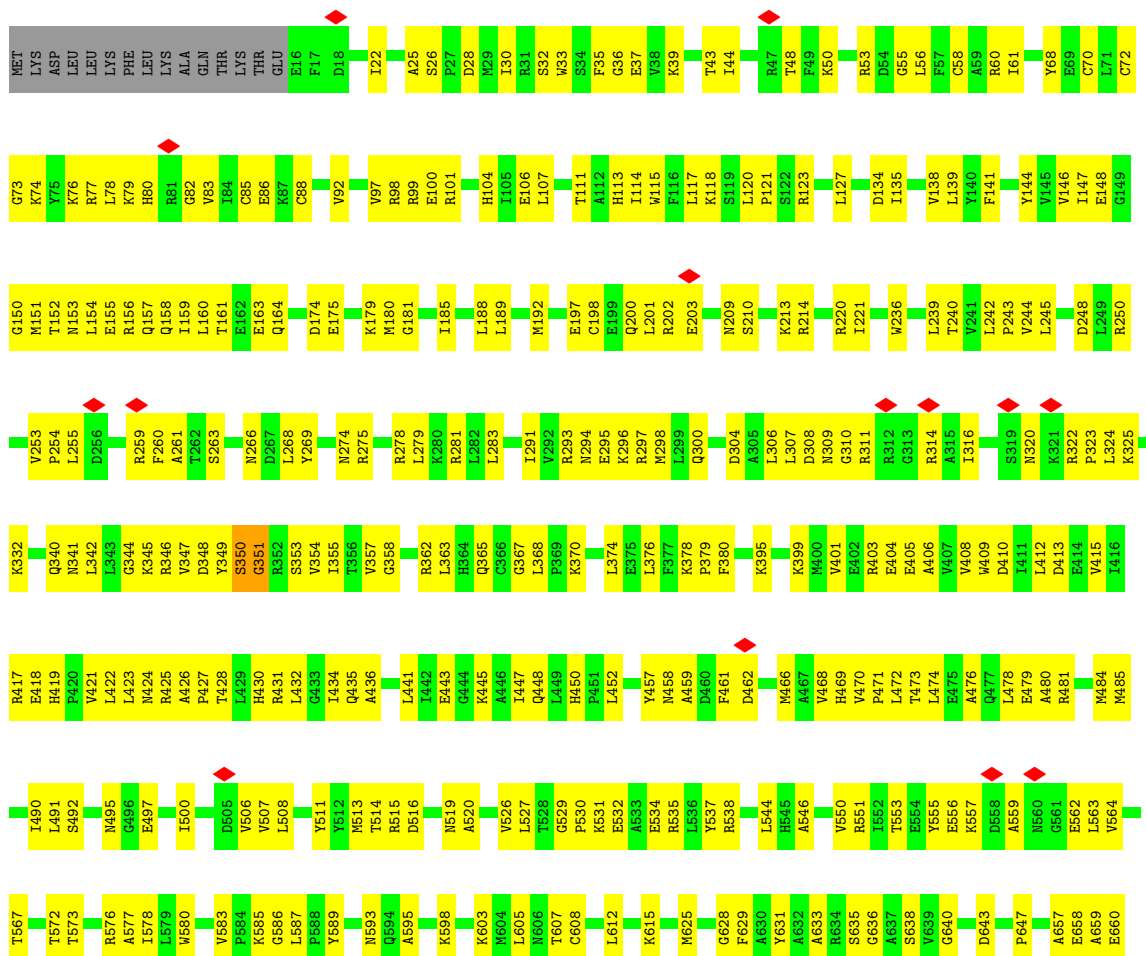
• Molecule 6: Transcription termination/antitermination protein NusG

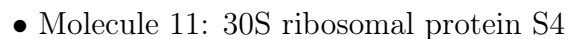


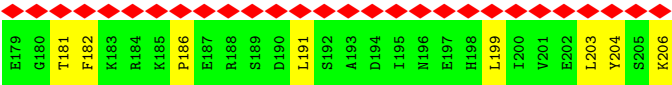
- Chain W:  21% 71% 27%



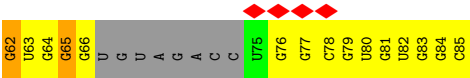
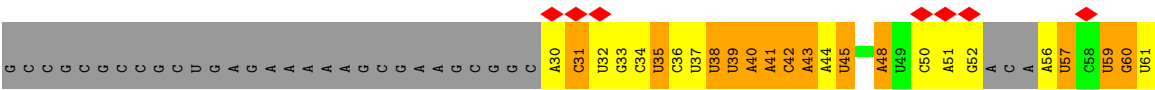
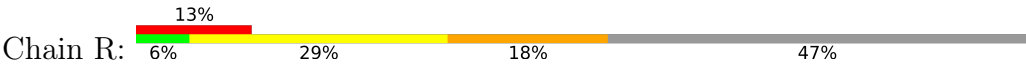
- Molecule 10: DNA-directed RNA polymerase subunit beta'



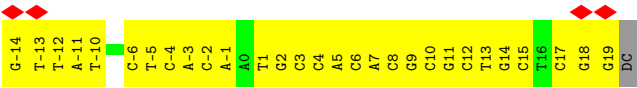




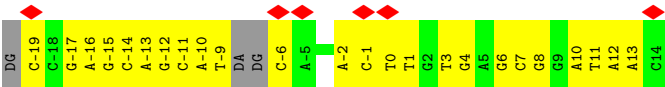
• Molecule 12: rrnGnut RNA



• Molecule 13: tDNA



• Molecule 14: ntDNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.990	Depositor
Minimum map value	-3.689	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.454	Depositor
Recommended contour level	3	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T	0.21	0/2001	0.38	0/2711
2	S	0.28	0/2084	0.37	0/2823
3	A	0.19	0/3895	0.40	0/5270
4	B	0.20	0/1080	0.45	0/1462
5	E	0.22	0/792	0.45	0/1071
6	G	0.22	0/1452	0.44	0/1956
7	U	0.25	0/2544	0.42	0/3449
7	V	0.26	0/1735	0.44	0/2351
8	W	0.22	0/711	0.36	0/956
9	X	0.28	0/10754	0.41	0/14509
10	Y	0.27	0/10551	0.43	0/14246
11	C	0.16	0/1665	0.41	0/2227
12	R	0.16	0/1063	0.29	0/1649
13	L	0.31	0/770	0.47	0/1184
14	K	0.26	0/736	0.59	2/1131 (0.2%)
All	All	0.25	0/41833	0.42	2/56995 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	Y	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K	0	DT	OP1-P-O3'	-8.70	81.89	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K	0	DT	OP2-P-O3'	-8.66	82.01	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	Y	350	SER	Peptide
10	Y	852	GLY	Peptide

5.2 Too-close contacts ⓘ

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	T	1966	0	1951	75	0
2	S	2048	0	2040	72	0
3	A	3850	0	3833	205	0
4	B	1063	0	1071	64	0
5	E	783	0	817	52	0
6	G	1421	0	1416	90	0
7	U	2510	0	2563	107	0
7	V	1715	0	1750	75	0
8	W	709	0	719	22	0
9	X	10585	0	10603	500	0
10	Y	10394	0	10614	484	0
11	C	1643	0	1705	61	0
12	R	955	0	481	51	0
13	L	689	0	382	38	0
14	K	657	0	361	28	0
15	S	1	0	0	0	0
15	T	1	0	0	0	0
15	Y	1	0	0	0	0
16	Y	2	0	0	0	0
All	All	40993	0	40306	1749	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 22.

All (1749) 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)
5:E:5:ARG:HD2	5:E:7:ARG:HE	1.33	0.92
3:A:298:VAL:HA	3:A:305:MET:HG2	1.53	0.89
10:Y:1266:ILE:HD13	10:Y:1274:PHE:HB3	1.55	0.88
11:C:102:VAL:HG13	11:C:107:PHE:HB2	1.57	0.87
10:Y:885:VAL:HG12	10:Y:1254:GLU:HG2	1.56	0.86
2:S:84:ASP:OD1	2:S:86:LEU:O	1.94	0.86
10:Y:1173:ARG:HB2	10:Y:1192:LYS:HB3	1.58	0.86
9:X:560:PRO:HB2	10:Y:776:THR:HG21	1.57	0.84
6:G:30:ILE:HG12	6:G:39:PHE:HD2	1.41	0.84
4:B:61:TYR:O	4:B:65:LEU:N	2.12	0.83
7:V:48:LEU:HD22	10:Y:535:ARG:HG3	1.61	0.83
3:A:133:HIS:ND1	3:A:136:GLU:OE1	2.11	0.82
9:X:143:ARG:HA	9:X:514:PHE:HA	1.60	0.82
10:Y:120:LEU:HD11	14:K:6:DG:H4'	1.63	0.81
10:Y:973:LEU:HB3	10:Y:1003:LEU:HB2	1.62	0.80
9:X:65:ASN:HB3	9:X:105:TYR:HB2	1.62	0.80
3:A:487:ASN:HA	3:A:491:PHE:HB2	1.64	0.80
7:U:321:TRP:HA	7:U:323:PRO:HD3	1.63	0.79
9:X:82:VAL:O	9:X:86:GLN:HB2	1.82	0.79
7:U:273:GLU:O	7:U:284:ARG:NH1	2.15	0.79
10:Y:422:LEU:HB3	10:Y:434:ILE:HD11	1.65	0.79
9:X:10:ARG:NH2	9:X:790:ASP:OD2	2.16	0.79
3:A:207:GLU:O	3:A:210:ARG:HB2	1.83	0.79
10:Y:120:LEU:HD12	10:Y:121:PRO:HA	1.65	0.79
10:Y:1163:VAL:HG13	10:Y:1175:LEU:HD11	1.65	0.79
10:Y:978:ARG:NH2	10:Y:1202:GLU:OE2	2.17	0.78
3:A:377:GLY:H	11:C:22:LYS:HE2	1.47	0.78
5:E:44:THR:HB	5:E:68:ARG:HH11	1.49	0.78
3:A:299:ASP:OD2	3:A:302:LYS:NZ	2.16	0.78
7:U:269:CYS:HB3	7:U:292:THR:HG21	1.65	0.78
3:A:453:VAL:HG13	3:A:458:ASP:HB3	1.66	0.77
13:L:6:DC:H2'	13:L:7:DA:H8	1.49	0.77
4:B:100:TYR:HH	12:R:35:U:H3	1.33	0.76
5:E:2:GLN:HB2	5:E:79:PRO:HG2	1.66	0.76
9:X:988:LYS:HB3	9:X:992:LEU:HD12	1.67	0.76
1:T:106:ARG:HA	1:T:111:THR:HA	1.66	0.76
9:X:74:ARG:HH11	9:X:121:GLU:HG2	1.49	0.76
9:X:891:GLY:H	9:X:912:ASP:HB2	1.49	0.76
10:Y:1093:THR:HG22	10:Y:1094:ASP:H	1.51	0.76
9:X:897:PRO:HA	9:X:900:LYS:HB2	1.68	0.75
1:T:258:ARG:NH2	3:A:493:ASP:OD2	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:258:ARG:NH2	5:E:14:ASP:OD2	2.20	0.74
9:X:890:LYS:HB2	9:X:914:LYS:HB2	1.69	0.74
10:Y:702:GLN:HG3	10:Y:703:THR:HG23	1.67	0.74
3:A:71:PRO:HA	3:A:74:GLU:HB2	1.69	0.74
10:Y:883:ARG:NH2	10:Y:898:CYS:SG	2.60	0.74
4:B:9:ALA:HB1	4:B:43:VAL:HG23	1.69	0.74
7:U:284:ARG:NH2	7:U:288:GLU:O	2.21	0.74
9:X:940:GLU:HG3	9:X:941:LYS:H	1.52	0.73
9:X:618:GLN:HE22	10:Y:770:LEU:H	1.35	0.73
10:Y:789:LYS:NZ	10:Y:930:LEU:O	2.18	0.73
11:C:104:ARG:HH22	11:C:166:GLU:HG3	1.53	0.73
9:X:1058:ARG:HD3	9:X:1238:LEU:HD11	1.71	0.73
9:X:12:ARG:NH2	9:X:793:GLU:OE1	2.22	0.73
9:X:243:PRO:HG2	9:X:278:GLU:HG3	1.71	0.73
9:X:882:ILE:HG12	9:X:919:ARG:HG2	1.69	0.73
9:X:267:ARG:HG2	9:X:268:ARG:HG2	1.69	0.72
9:X:617:ALA:HB3	9:X:653:MET:HA	1.71	0.72
10:Y:985:ILE:HA	10:Y:991:THR:HA	1.71	0.72
10:Y:72:CYS:HB3	10:Y:88:CYS:SG	2.28	0.72
3:A:486:ARG:O	3:A:491:PHE:N	2.22	0.72
10:Y:975:ILE:HG23	10:Y:980:THR:HG21	1.70	0.72
5:E:102:LEU:O	6:G:157:ARG:NH2	2.23	0.72
9:X:133:ASN:O	9:X:527:LYS:NZ	2.20	0.72
10:Y:156:ARG:HH11	10:Y:157:GLN:HE22	1.37	0.72
10:Y:490:ILE:HG13	10:Y:491:LEU:HD12	1.72	0.72
7:U:58:GLU:HB3	7:U:145:LYS:HB3	1.71	0.72
9:X:1246:ARG:NH2	9:X:1250:SER:O	2.23	0.72
11:C:74:ASN:HA	11:C:77:LYS:HE3	1.72	0.72
1:T:73:GLU:HB2	8:W:90:ARG:HH22	1.53	0.72
9:X:201:ARG:NH1	9:X:370:MET:SD	2.63	0.72
3:A:62:TRP:HD1	3:A:92:TYR:HA	1.55	0.71
12:R:78:C:H2'	12:R:79:G:H8	1.55	0.71
7:U:59:VAL:HG11	7:U:85:LEU:HD13	1.72	0.71
4:B:64:GLY:HA2	4:B:67:LYS:HB2	1.73	0.71
7:U:182:ARG:NH1	9:X:1090:ASN:O	2.23	0.71
10:Y:85:CYS:SG	10:Y:86:GLU:N	2.64	0.71
10:Y:418:GLU:O	10:Y:481:ARG:NH2	2.23	0.71
9:X:758:ARG:NH1	9:X:762:ASN:OD1	2.23	0.71
10:Y:1160:SER:OG	10:Y:1203:ARG:NH1	2.24	0.71
9:X:894:GLN:NE2	9:X:899:GLU:OE1	2.23	0.71
10:Y:1174:ARG:NH2	10:Y:1187:GLU:OE1	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:106:GLU:HG2	4:B:110:LEU:HD12	1.73	0.71
9:X:271:ALA:HA	9:X:274:ILE:HD12	1.73	0.71
9:X:1211:ARG:NH1	9:X:1220:GLN:OE1	2.24	0.70
10:Y:370:LYS:HG2	10:Y:441:LEU:HD12	1.73	0.70
5:E:34:ALA:HA	5:E:78:GLU:HB3	1.71	0.70
9:X:1105:SER:HB3	10:Y:731:ARG:HG3	1.72	0.70
10:Y:121:PRO:HG2	10:Y:123:ARG:HH22	1.56	0.70
10:Y:1140:ARG:HH12	10:Y:1144:LEU:HD13	1.57	0.70
9:X:842:ASP:HA	9:X:847:PRO:HA	1.73	0.70
9:X:1117:LEU:HD13	9:X:1195:ILE:HG12	1.72	0.70
7:V:58:GLU:HB3	7:V:145:LYS:HB3	1.72	0.70
10:Y:739:GLN:OE1	10:Y:744:ARG:NH1	2.23	0.70
8:W:31:GLN:HB2	8:W:46:THR:HG21	1.74	0.70
3:A:59:PHE:HA	3:A:94:GLU:HA	1.74	0.70
6:G:21:ARG:NH2	13:L:15:DC:OP1	2.23	0.70
1:T:90:THR:HA	1:T:93:ILE:HD12	1.74	0.69
6:G:11:VAL:HG21	10:Y:291:ILE:HD11	1.72	0.69
9:X:719:LYS:O	9:X:779:ARG:NH1	2.26	0.69
13:L:6:DC:H2'	13:L:7:DA:C8	2.27	0.69
4:B:100:TYR:OH	12:R:35:U:N3	2.23	0.69
7:U:214:GLU:OE2	7:U:218:ARG:NH1	2.25	0.69
7:U:233:ASP:HB2	7:U:235:ARG:HH21	1.58	0.69
3:A:363:LEU:HA	3:A:366:ASP:HB2	1.74	0.69
6:G:150:GLU:HB3	6:G:159:LYS:HB3	1.75	0.69
10:Y:1171:GLY:O	10:Y:1192:LYS:NZ	2.26	0.69
7:U:252:ILE:HA	7:U:255:ARG:HD3	1.73	0.69
9:X:116:ASP:OD2	9:X:118:LYS:NZ	2.19	0.69
9:X:995:ASP:O	9:X:996:ARG:NE	2.24	0.69
9:X:314:ASN:O	9:X:352:ARG:NH1	2.25	0.69
9:X:903:ARG:HD3	9:X:907:GLY:HA3	1.75	0.69
10:Y:1064:SER:HB2	10:Y:1072:LYS:HG3	1.74	0.69
4:B:22:LEU:HD23	5:E:39:PRO:HG3	1.75	0.68
7:U:167:PRO:HG2	7:U:170:ARG:HG2	1.75	0.68
10:Y:117:LEU:HD23	10:Y:118:LYS:HG2	1.74	0.68
10:Y:814:CYS:SG	10:Y:883:ARG:NH2	2.66	0.68
9:X:808:ASN:H	10:Y:633:ALA:HB2	1.58	0.68
10:Y:968:ASN:ND2	10:Y:970:SER:OG	2.26	0.68
11:C:140:ASN:HA	11:C:182:PHE:O	1.94	0.68
9:X:1065:LYS:NZ	10:Y:462:ASP:O	2.27	0.68
10:Y:511:TYR:OH	10:Y:515:ARG:NH1	2.27	0.68
9:X:492:MET:SD	9:X:492:MET:N	2.65	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:595:THR:HG22	9:X:596:ASP:H	1.58	0.68
9:X:1072:ASN:ND2	9:X:1111:GLN:OE1	2.27	0.68
10:Y:268:LEU:HD13	10:Y:306:LEU:HA	1.75	0.68
10:Y:1179:PRO:HD2	10:Y:1184:ASP:HB3	1.75	0.68
10:Y:56:LEU:O	10:Y:250:ARG:NH2	2.26	0.68
10:Y:848:VAL:HB	10:Y:858:VAL:HG22	1.75	0.68
10:Y:890:THR:OG1	10:Y:893:GLY:O	2.12	0.68
7:V:74:VAL:HG23	7:V:76:GLU:H	1.59	0.68
7:V:84:ASN:ND2	7:V:129:VAL:O	2.26	0.68
9:X:894:GLN:NE2	9:X:896:THR:OG1	2.26	0.68
1:T:79:VAL:HG22	1:T:107:ILE:HG12	1.75	0.68
7:U:284:ARG:NH2	7:U:288:GLU:OE1	2.27	0.68
9:X:1243:MET:HE2	10:Y:445:LYS:HD2	1.74	0.67
12:R:78:C:H2'	12:R:79:G:C8	2.29	0.67
13:L:9:DG:H2'	13:L:10:DC:C6	2.29	0.67
3:A:441:ASP:OD1	3:A:444:LEU:N	2.27	0.67
9:X:1004:ASP:HA	9:X:1008:GLN:HB3	1.76	0.67
10:Y:1307:LEU:HB2	10:Y:1312:ALA:HB2	1.75	0.67
11:C:28:ILE:HG22	11:C:34:ILE:HD13	1.74	0.67
9:X:874:GLY:H	9:X:928:VAL:HG13	1.59	0.67
9:X:890:LYS:N	9:X:912:ASP:O	2.23	0.67
6:G:13:GLN:HB3	6:G:90:MET:HB2	1.77	0.67
6:G:103:ILE:HG12	6:G:107:GLU:HG3	1.77	0.67
10:Y:245:LEU:O	10:Y:250:ARG:NH1	2.27	0.67
11:C:95:GLU:HG2	11:C:186:PRO:HD2	1.75	0.67
7:U:27:THR:HG22	7:U:202:VAL:HG22	1.76	0.67
1:T:243:VAL:HG13	1:T:253:MET:HE3	1.77	0.66
9:X:104:ILE:HB	9:X:115:LYS:HB2	1.76	0.66
3:A:93:VAL:HG21	7:U:297:LYS:HE2	1.78	0.66
9:X:161:LYS:HA	9:X:170:VAL:HG12	1.77	0.66
9:X:516:ASP:HA	9:X:761:GLN:HE22	1.58	0.66
13:L:9:DG:H2'	13:L:10:DC:H6	1.59	0.66
3:A:58:THR:OG1	3:A:96:GLN:O	2.13	0.66
11:C:174:ASP:O	11:C:178:MET:N	2.28	0.66
13:L:12:DC:H2''	13:L:13:DT:C5	2.30	0.66
4:B:66:MET:O	4:B:70:LEU:HG	1.94	0.66
7:U:320:ASN:OD1	7:U:321:TRP:N	2.28	0.66
9:X:638:SER:N	9:X:641:GLU:OE2	2.28	0.66
10:Y:1061:VAL:HB	10:Y:1105:ALA:HB3	1.78	0.66
13:L:1:DT:H2'	13:L:2:DG:C8	2.31	0.66
13:L:12:DC:H2''	13:L:13:DT:C6	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:223:ILE:HA	3:A:238:VAL:HG12	1.78	0.66
7:U:86:LYS:NZ	9:X:826:ASP:OD1	2.28	0.66
7:U:278:ILE:HA	7:U:281:LEU:HG	1.77	0.66
10:Y:180:MET:SD	10:Y:293:ARG:NH1	2.68	0.66
2:S:128:THR:HG23	2:S:131:GLN:HB2	1.77	0.66
3:A:233:ARG:HH21	3:A:270:ARG:HH11	1.44	0.66
4:B:100:TYR:HD2	4:B:137:ASN:HD21	1.44	0.66
7:U:304:LYS:HA	7:U:314:LEU:HD21	1.78	0.66
9:X:968:GLU:OE2	9:X:994:ARG:NH1	2.28	0.66
11:C:98:LEU:HD21	11:C:123:ILE:HG21	1.76	0.66
6:G:49:VAL:HG13	6:G:124:PRO:HA	1.77	0.66
7:U:45:ARG:HE	7:V:38:THR:HB	1.62	0.65
9:X:900:LYS:O	9:X:904:ALA:N	2.30	0.65
10:Y:148:GLU:H	10:Y:156:ARG:HG3	1.59	0.65
4:B:122:PHE:HB3	12:R:39:U:H5'	1.77	0.65
9:X:211:ARG:NH2	9:X:217:THR:OG1	2.29	0.65
9:X:179:TYR:HB2	9:X:398:SER:HB2	1.78	0.65
10:Y:973:LEU:O	10:Y:1003:LEU:N	2.26	0.65
2:S:155:THR:OG1	2:S:168:TYR:OH	2.14	0.65
9:X:1296:ASP:OD1	9:X:1297:ASP:N	2.27	0.65
10:Y:111:THR:OG1	10:Y:300:GLN:OE1	2.12	0.65
4:B:13:ALA:HB3	4:B:51:LEU:HD13	1.79	0.65
9:X:1258:PRO:HG3	10:Y:348:ASP:HB3	1.78	0.65
9:X:398:SER:HB3	9:X:401:GLY:H	1.60	0.65
10:Y:278:ARG:NH2	14:K:-12:DG:OP1	2.30	0.65
12:R:76:G:H2'	12:R:77:G:C8	2.31	0.65
1:T:97:PRO:O	2:S:121:ARG:NH2	2.29	0.65
1:T:138:TYR:OH	3:A:320:ARG:NH2	2.29	0.65
4:B:6:ARG:HG2	4:B:47:TYR:HE2	1.61	0.65
8:W:42:GLU:O	10:Y:417:ARG:NH2	2.30	0.65
10:Y:1043:GLY:N	10:Y:1046:ILE:O	2.30	0.65
13:L:5:DA:H2'	13:L:6:DC:C6	2.32	0.65
2:S:5:LEU:HB2	2:S:113:VAL:HG21	1.79	0.65
3:A:213:VAL:HG22	3:A:258:ARG:HH11	1.61	0.65
1:T:87:ASP:OD2	1:T:187:SER:OG	2.14	0.65
3:A:185:SER:OG	3:A:187:ARG:NE	2.29	0.65
7:V:71:LYS:NZ	7:V:72:GLU:O	2.30	0.65
1:T:1:MET:SD	1:T:128:THR:OG1	2.54	0.64
3:A:277:ASP:HB3	3:A:283:PHE:HA	1.77	0.64
6:G:174:ASP:OD1	6:G:175:PHE:N	2.30	0.64
10:Y:587:LEU:H	10:Y:587:LEU:HD12	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:82:U:H2'	12:R:83:G:C8	2.30	0.64
6:G:173:LEU:HD21	6:G:177:GLN:HB2	1.79	0.64
9:X:735:LYS:HA	9:X:748:ILE:HD12	1.79	0.64
10:Y:127:LEU:O	10:Y:220:ARG:NH2	2.30	0.64
10:Y:253:VAL:HG21	12:R:76:G:H1'	1.79	0.64
10:Y:519:ASN:HD22	10:Y:709:ARG:HA	1.61	0.64
3:A:327:LEU:O	3:A:331:LEU:N	2.29	0.64
7:V:91:ARG:NH1	7:V:210:THR:O	2.31	0.64
8:W:4:VAL:HG13	8:W:5:THR:HG23	1.78	0.64
9:X:859:GLU:O	9:X:863:SER:N	2.31	0.64
4:B:116:ALA:O	4:B:117:GLU:HG3	1.97	0.64
9:X:99:LYS:NZ	9:X:121:GLU:OE2	2.31	0.64
9:X:262:TYR:HB3	9:X:276:GLN:HE22	1.62	0.64
2:S:26:PRO:HG3	2:S:95:ARG:HH11	1.61	0.64
12:R:76:G:H2'	12:R:77:G:H8	1.63	0.64
1:T:129:ARG:NH2	3:A:465:ASP:O	2.30	0.64
8:W:26:ARG:HG3	8:W:30:MET:HE2	1.79	0.64
9:X:473:ARG:NH2	14:K:-6:DC:O2	2.31	0.64
9:X:1025:PHE:HD1	9:X:1028:LYS:HD3	1.63	0.64
3:A:348:HIS:O	3:A:349:GLN:NE2	2.31	0.64
9:X:993:PRO:O	9:X:997:TRP:NE1	2.30	0.64
9:X:1275:VAL:HG13	9:X:1287:LEU:HD11	1.79	0.64
2:S:42:ASN:HA	2:S:45:LYS:HE2	1.81	0.63
9:X:3:TYR:O	9:X:8:LYS:NZ	2.30	0.63
10:Y:425:ARG:HG3	10:Y:427:PRO:HD2	1.79	0.63
6:G:138:ASP:HB2	6:G:177:GLN:HB3	1.80	0.63
6:G:155:LYS:HG2	6:G:157:ARG:HG2	1.79	0.63
9:X:674:ASP:OD1	9:X:675:ASP:N	2.31	0.63
10:Y:824:PRO:HD3	10:Y:835:LEU:HD12	1.81	0.63
10:Y:1116:SER:HB3	10:Y:1119:ASP:HB3	1.80	0.63
10:Y:1167:LYS:NZ	14:K:13:DA:OP1	2.31	0.63
4:B:60:ALA:O	4:B:64:GLY:N	2.23	0.63
7:V:134:THR:HG22	7:V:136:GLU:H	1.63	0.63
9:X:1042:LEU:HB3	9:X:1046:VAL:HG23	1.79	0.63
10:Y:1169:THR:HG22	10:Y:1192:LYS:HE2	1.81	0.63
3:A:276:TRP:NE1	3:A:278:ASP:OD1	2.26	0.63
6:G:68:TYR:OH	10:Y:294:ASN:ND2	2.32	0.63
3:A:272:ASP:OD1	12:R:44:A:O2'	2.17	0.63
9:X:811:ASN:O	9:X:1099:ASN:ND2	2.28	0.63
1:T:161:ALA:HB1	1:T:163:GLN:HE22	1.64	0.63
3:A:209:PHE:HE1	3:A:262:VAL:HG11	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:190:ALA:HB2	7:V:200:LYS:HB2	1.81	0.63
10:Y:424:ASN:HB2	10:Y:434:ILE:HD13	1.80	0.63
7:U:263:THR:HG22	7:U:265:ARG:H	1.64	0.63
9:X:617:ALA:HA	9:X:636:CYS:SG	2.39	0.63
10:Y:975:ILE:HD12	10:Y:1001:ALA:HB3	1.81	0.63
3:A:60:ARG:N	3:A:93:VAL:O	2.32	0.62
7:U:60:GLU:OE2	7:U:143:ARG:NH2	2.32	0.62
7:V:226:GLU:HA	7:V:229:GLU:HG2	1.80	0.62
10:Y:73:GLY:O	10:Y:76:LYS:NZ	2.32	0.62
10:Y:1174:ARG:HG2	10:Y:1189:MET:HG2	1.79	0.62
1:T:82:VAL:HB	1:T:104:ALA:HB3	1.81	0.62
1:T:241:ASN:ND2	1:T:263:ASP:OD2	2.32	0.62
3:A:168:LEU:HD21	3:A:228:ARG:HH21	1.64	0.62
4:B:91:GLU:O	4:B:96:SER:N	2.33	0.62
9:X:1119:MET:HB2	9:X:1228:GLY:HA2	1.80	0.62
3:A:254:MET:SD	12:R:40:A:O2'	2.53	0.62
10:Y:857:LEU:HG	10:Y:858:VAL:HG13	1.81	0.62
3:A:289:ALA:HB1	12:R:44:A:H2	1.63	0.62
7:U:252:ILE:HG22	7:U:278:ILE:HG21	1.81	0.62
7:U:297:LYS:O	7:U:301:THR:N	2.32	0.62
9:X:18:ARG:NH1	9:X:620:ASN:O	2.32	0.62
10:Y:121:PRO:O	10:Y:123:ARG:NH1	2.32	0.62
3:A:186:VAL:HG22	3:A:188:PRO:HD3	1.81	0.62
10:Y:527:LEU:HB2	10:Y:550:VAL:HG22	1.81	0.62
10:Y:768:ASN:N	10:Y:771:GLN:OE1	2.29	0.62
10:Y:809:VAL:HG13	10:Y:912:GLY:H	1.65	0.62
10:Y:1292:LEU:HD22	10:Y:1297:LYS:HD2	1.80	0.62
13:L:7:DA:H2'	13:L:8:DC:C6	2.35	0.62
7:U:110:VAL:HG21	7:U:140:ILE:HD11	1.81	0.62
9:X:1297:ASP:OD2	9:X:1319:MET:N	2.31	0.62
10:Y:353:SER:OG	10:Y:354:VAL:N	2.31	0.62
5:E:96:VAL:O	6:G:167:ARG:NH2	2.32	0.62
6:G:128:PHE:HD2	6:G:158:LEU:HD11	1.65	0.62
7:V:112:ALA:HB3	7:V:126:PRO:HA	1.82	0.62
9:X:273:HIS:O	9:X:276:GLN:NE2	2.32	0.62
9:X:301:TYR:HB2	9:X:311:CYS:HB2	1.82	0.62
10:Y:520:ALA:HB3	10:Y:546:ALA:HB2	1.82	0.62
10:Y:951:GLN:HE22	10:Y:1016:THR:HG1	1.48	0.62
9:X:657:THR:HB	9:X:1187:PHE:HB2	1.80	0.61
3:A:18:LEU:HD13	3:A:23:ILE:HD11	1.82	0.61
3:A:289:ALA:HB3	3:A:290:PRO:HD3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:46:THR:HA	6:G:63:LYS:HA	1.82	0.61
9:X:402:ARG:NE	9:X:417:SER:O	2.30	0.61
10:Y:966:VAL:HG12	10:Y:976:THR:HG21	1.82	0.61
10:Y:1238:GLN:NE2	10:Y:1250:ASP:OD1	2.33	0.61
3:A:104:ARG:NH2	9:X:853:ASP:OD1	2.33	0.61
7:U:102:LEU:HB2	7:U:115:ILE:HG22	1.81	0.61
1:T:181:ASP:OD1	1:T:182:PHE:N	2.30	0.61
2:S:24:GLU:OE2	3:A:170:ARG:NH1	2.34	0.61
2:S:172:VAL:HG13	2:S:182:PHE:HE2	1.64	0.61
9:X:303:ASP:HB3	9:X:306:THR:HG22	1.80	0.61
9:X:1069:ARG:NH2	9:X:1114:GLU:OE2	2.31	0.61
1:T:13:ARG:O	1:T:17:ASN:ND2	2.33	0.61
3:A:45:VAL:HG13	3:A:59:PHE:H	1.65	0.61
9:X:1088:ASP:OD1	9:X:1089:GLU:N	2.32	0.61
6:G:152:ASP:CG	6:G:157:ARG:H	2.08	0.61
7:U:312:LEU:HG	7:U:313:SER:H	1.65	0.61
9:X:1290:MET:HA	9:X:1294:LYS:HD2	1.82	0.61
10:Y:885:VAL:HG11	10:Y:1255:VAL:HG12	1.82	0.61
3:A:43:ILE:HD11	3:A:72:THR:HB	1.83	0.61
10:Y:968:ASN:OD1	10:Y:972:LYS:N	2.34	0.61
1:T:16:GLY:HA3	1:T:117:TYR:HE2	1.66	0.61
2:S:116:VAL:HG22	2:S:125:PHE:HB2	1.82	0.61
4:B:15:GLN:HE22	5:E:41:PRO:C	2.08	0.61
9:X:528:ARG:HD3	9:X:663:VAL:HG11	1.82	0.61
9:X:933:VAL:HG22	9:X:1050:VAL:HG12	1.81	0.61
1:T:182:PHE:O	1:T:183:ARG:NH1	2.32	0.61
3:A:213:VAL:HG12	3:A:215:GLU:H	1.64	0.61
5:E:80:THR:O	5:E:83:THR:OG1	2.19	0.61
7:U:270:LEU:HB3	7:U:275:ILE:HB	1.82	0.61
9:X:264:GLU:OE1	9:X:264:GLU:N	2.31	0.61
9:X:726:TYR:OH	9:X:728:ASP:OD2	2.17	0.61
10:Y:1038:THR:OG1	10:Y:1077:ALA:O	2.18	0.61
7:U:92:VAL:O	7:U:148:ARG:NH2	2.34	0.60
9:X:549:ASP:OD1	9:X:550:VAL:N	2.33	0.60
10:Y:996:LYS:NZ	10:Y:997:VAL:O	2.34	0.60
10:Y:1219:ASP:OD1	10:Y:1222:ARG:NH2	2.34	0.60
10:Y:1114:GLN:NE2	10:Y:1115:ILE:O	2.33	0.60
1:T:81:TRP:HE1	1:T:105:VAL:HG13	1.66	0.60
9:X:30:ILE:HD11	9:X:575:LEU:HD22	1.84	0.60
12:R:83:G:H2'	12:R:84:G:H8	1.66	0.60
1:T:91:ASN:ND2	1:T:98:HIS:O	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:5:THR:OG1	10:Y:615:LYS:NZ	2.33	0.60
9:X:148:GLN:OE1	9:X:454:ARG:NH2	2.32	0.60
9:X:1237:HIS:HE1	12:R:84:G:H4'	1.67	0.60
3:A:221:ILE:HG12	3:A:240:THR:HG23	1.83	0.60
9:X:238:GLN:HE22	9:X:285:ILE:H	1.49	0.60
11:C:67:VAL:HG11	11:C:97:ARG:HH22	1.66	0.60
1:T:40:VAL:HG12	1:T:92:PHE:HD2	1.65	0.60
3:A:64:VAL:HG21	3:A:90:GLY:H	1.67	0.60
3:A:204:MET:HE2	3:A:208:LEU:HD12	1.82	0.60
5:E:70:HIS:HB3	5:E:72:ARG:HH12	1.66	0.60
10:Y:799:ARG:NH1	10:Y:1146:GLU:OE2	2.34	0.60
1:T:229:ASP:OD1	1:T:233:GLY:N	2.35	0.60
3:A:346:ALA:HB1	3:A:350:ALA:HB3	1.84	0.60
14:K:10:DA:H2'	14:K:11:DT:H71	1.83	0.60
7:U:290:LEU:HA	7:U:295:LEU:HD12	1.82	0.60
10:Y:972:LYS:HD2	10:Y:1004:ALA:HA	1.84	0.60
10:Y:1313:SER:O	10:Y:1316:THR:OG1	2.18	0.60
9:X:515:MET:SD	9:X:523:GLU:HG3	2.42	0.60
10:Y:789:LYS:NZ	10:Y:928:THR:O	2.35	0.60
12:R:60:G:H22	12:R:62:G:H8	1.48	0.60
9:X:176:ILE:HD11	9:X:428:VAL:HG21	1.83	0.60
9:X:275:ARG:NH2	9:X:278:GLU:OE1	2.35	0.60
9:X:1269:ARG:NH2	10:Y:344:GLY:O	2.31	0.60
10:Y:255:LEU:HB2	10:Y:259:ARG:HB3	1.83	0.60
3:A:470:ILE:HB	3:A:473:LEU:HB3	1.84	0.59
6:G:42:VAL:HG12	6:G:71:VAL:HG12	1.84	0.59
9:X:1192:GLU:OE2	10:Y:764:ARG:NH2	2.36	0.59
11:C:171:LEU:HD13	11:C:182:PHE:HD2	1.67	0.59
9:X:331:LYS:O	9:X:332:ARG:NE	2.35	0.59
10:Y:515:ARG:NH2	10:Y:718:SER:O	2.36	0.59
7:V:84:ASN:OD1	10:Y:551:ARG:NH2	2.35	0.59
10:Y:1067:ARG:NH1	10:Y:1071:GLY:O	2.35	0.59
7:V:196:THR:HB	10:Y:443:GLU:HG3	1.83	0.59
3:A:65:VAL:HG13	3:A:67:GLU:H	1.67	0.59
6:G:135:ARG:HG2	6:G:145:ASN:HB3	1.83	0.59
9:X:1281:TYR:CZ	10:Y:431:ARG:HG2	2.37	0.59
10:Y:308:ASP:OD2	10:Y:311:ARG:NH1	2.36	0.59
3:A:108:GLN:NE2	9:X:910:ALA:O	2.35	0.59
8:W:3:ARG:NH2	8:W:5:THR:OG1	2.36	0.59
10:Y:1271:SER:HB2	10:Y:1292:LEU:HD13	1.84	0.59
2:S:185:THR:OG1	2:S:191:ASP:OD1	2.19	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:49:ARG:HE	4:B:52:LEU:HD21	1.66	0.59
10:Y:1044:GLN:NE2	10:Y:1070:GLY:O	2.33	0.59
10:Y:1172:LYS:HB2	10:Y:1189:MET:HE2	1.85	0.59
3:A:428:ASN:HD21	3:A:446:PHE:HA	1.66	0.59
9:X:881:ASP:OD1	9:X:882:ILE:N	2.35	0.59
3:A:180:ARG:O	3:A:199:ARG:NH1	2.30	0.59
7:V:74:VAL:HG12	7:V:133:LEU:HD12	1.84	0.59
7:V:182:ARG:HD2	10:Y:531:LYS:HG2	1.85	0.59
9:X:714:VAL:HB	9:X:787:PRO:HD2	1.85	0.59
9:X:44:GLU:O	9:X:54:ARG:NH1	2.36	0.59
9:X:270:THR:HG22	9:X:272:ARG:H	1.66	0.59
10:Y:1003:LEU:HD23	10:Y:1018:ALA:HB2	1.85	0.59
9:X:95:PRO:HA	9:X:126:GLU:HG2	1.84	0.58
9:X:309:LEU:HD12	9:X:312:ALA:HB2	1.85	0.58
10:Y:197:GLU:OE2	10:Y:220:ARG:NH1	2.32	0.58
10:Y:586:GLY:HA3	10:Y:612:LEU:HD11	1.84	0.58
10:Y:984:LEU:HB3	10:Y:993:GLU:HB2	1.84	0.58
12:R:80:U:H2'	12:R:81:G:C8	2.38	0.58
4:B:98:VAL:HG23	4:B:103:ALA:HB2	1.86	0.58
8:W:16:ARG:HE	10:Y:905:ARG:HE	1.51	0.58
9:X:632:ASP:HA	9:X:647:ARG:HD2	1.85	0.58
9:X:1083:GLU:OE1	9:X:1083:GLU:N	2.23	0.58
2:S:105:VAL:HB	2:S:113:VAL:HG12	1.85	0.58
9:X:196:VAL:H	9:X:206:ALA:HA	1.66	0.58
10:Y:450:HIS:CE1	10:Y:625:MET:HE2	2.38	0.58
10:Y:950:ILE:HD13	10:Y:997:VAL:HG12	1.86	0.58
10:Y:1176:VAL:HB	10:Y:1187:GLU:HG2	1.85	0.58
4:B:109:GLU:HB2	12:R:36:C:H42	1.69	0.58
7:U:270:LEU:HD22	7:U:275:ILE:HD12	1.84	0.58
7:U:289:LEU:O	7:U:292:THR:OG1	2.20	0.58
7:V:136:GLU:OE1	7:V:137:ASN:ND2	2.37	0.58
9:X:811:ASN:ND2	9:X:1098:LEU:O	2.35	0.58
10:Y:77:ARG:HG3	10:Y:79:LYS:H	1.67	0.58
10:Y:310:GLY:O	10:Y:314:ARG:NH1	2.36	0.58
1:T:195:VAL:HG12	1:T:200:VAL:HG13	1.86	0.58
3:A:417:ILE:HD11	11:C:5:LEU:HD12	1.85	0.58
6:G:51:GLU:O	6:G:58:ARG:N	2.33	0.58
9:X:11:ILE:O	9:X:1149:TYR:OH	2.15	0.58
9:X:39:ILE:HD11	9:X:75:LEU:HD11	1.85	0.58
9:X:158:ASP:OD1	9:X:159:SER:N	2.36	0.58
9:X:239:MET:HE2	9:X:285:ILE:HD11	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:426:ALA:HB3	10:Y:427:PRO:HD3	1.85	0.58
10:Y:1165:PHE:HZ	10:Y:1196:LEU:HD22	1.69	0.58
12:R:83:G:H2'	12:R:84:G:C8	2.38	0.58
6:G:27:ARG:HA	6:G:30:ILE:HD12	1.86	0.58
10:Y:863:LEU:HD11	10:Y:901:ARG:HB2	1.85	0.58
1:T:165:ALA:O	1:T:169:ILE:N	2.28	0.58
7:U:231:PHE:HB2	7:U:234:LEU:HB3	1.85	0.58
8:W:28:ARG:HH12	9:X:1314:GLN:HB2	1.68	0.58
9:X:1280:ALA:HB1	10:Y:918:ILE:HG22	1.85	0.58
10:Y:37:GLU:OE1	10:Y:39:LYS:NZ	2.27	0.58
12:R:40:A:O2'	12:R:41:A:O5'	2.20	0.58
7:U:100:LEU:HD23	7:U:115:ILE:HD12	1.85	0.58
9:X:801:ARG:HH11	9:X:1229:TYR:HE1	1.52	0.58
9:X:1116:HIS:HD2	9:X:1208:GLY:HA3	1.67	0.58
2:S:66:THR:HG22	2:S:68:GLU:H	1.69	0.58
6:G:47:GLU:N	6:G:62:ARG:O	2.33	0.58
9:X:300:ASP:HB2	9:X:313:ALA:HB2	1.86	0.58
9:X:794:LEU:HD21	9:X:796:LEU:HG	1.86	0.58
7:V:41:ASN:ND2	9:X:1217:THR:O	2.37	0.58
9:X:1268:GLN:NE2	10:Y:350:SER:O	2.37	0.58
6:G:148:VAL:HA	6:G:160:VAL:HG22	1.86	0.57
7:V:110:VAL:N	7:V:131:CYS:O	2.32	0.57
9:X:211:ARG:HH22	9:X:217:THR:HG1	1.49	0.57
9:X:119:GLU:OE1	9:X:490:GLN:NE2	2.28	0.57
4:B:112:LYS:HA	4:B:120:HIS:CE1	2.39	0.57
9:X:1126:ASP:OD1	9:X:1127:LYS:N	2.37	0.57
10:Y:201:LEU:HB2	10:Y:221:ILE:HD13	1.86	0.57
10:Y:311:ARG:NH2	13:L:-2:DC:OP1	2.38	0.57
10:Y:842:ARG:HH21	10:Y:1251:LYS:HG3	1.70	0.57
13:L:7:DA:H2'	13:L:8:DC:H6	1.68	0.57
9:X:820:GLU:HB3	9:X:824:GLN:HE21	1.69	0.57
2:S:259:ASP:OD1	2:S:260:GLU:N	2.38	0.57
3:A:377:GLY:HA3	11:C:22:LYS:HG3	1.85	0.57
3:A:414:LEU:HA	3:A:417:ILE:HD12	1.85	0.57
7:U:59:VAL:HG12	7:U:144:ILE:HG23	1.86	0.57
10:Y:134:ASP:HB3	10:Y:159:ILE:HG21	1.85	0.57
10:Y:1046:ILE:HG12	10:Y:1061:VAL:HG22	1.85	0.57
3:A:281:ALA:O	3:A:285:ILE:HG12	2.04	0.57
3:A:449:ALA:HA	3:A:453:VAL:H	1.70	0.57
7:V:192:VAL:HB	7:V:195:ARG:HB2	1.86	0.57
9:X:107:ARG:HD2	9:X:108:GLU:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:1257:GLN:NE2	10:Y:341:ASN:OD1	2.38	0.57
10:Y:141:PHE:HB3	10:Y:180:MET:HE2	1.86	0.57
2:S:147:ASP:OD1	2:S:149:ASP:N	2.38	0.57
4:B:124:ASN:ND2	12:R:37:U:O4'	2.37	0.57
7:U:135:ASP:OD1	7:U:136:GLU:N	2.36	0.57
9:X:56:VAL:HG11	9:X:468:LEU:HD21	1.85	0.57
9:X:189:ASP:HB2	9:X:195:PHE:HE2	1.69	0.57
10:Y:481:ARG:HA	10:Y:485:MET:HE3	1.87	0.57
3:A:274:VAL:HG21	3:A:287:ALA:HA	1.86	0.57
9:X:582:ASN:OD1	9:X:583:GLU:N	2.33	0.57
9:X:884:VAL:O	9:X:918:LEU:N	2.29	0.57
9:X:1331:ARG:HD3	10:Y:33:TRP:CE2	2.40	0.57
4:B:62:LEU:HA	4:B:65:LEU:HB2	1.87	0.57
9:X:705:GLU:OE1	9:X:705:GLU:N	2.35	0.57
10:Y:156:ARG:NH2	10:Y:188:LEU:O	2.37	0.57
10:Y:202:ARG:HH21	10:Y:221:ILE:HG13	1.70	0.57
9:X:241:LEU:HD11	9:X:246:LEU:HD23	1.87	0.56
9:X:1292:THR:HG21	9:X:1317:PRO:HB3	1.87	0.56
12:R:80:U:H2'	12:R:81:G:H8	1.69	0.56
1:T:254:LEU:HA	1:T:257:MET:HG3	1.87	0.56
10:Y:1165:PHE:HA	10:Y:1175:LEU:HA	1.87	0.56
1:T:80:GLN:HB2	1:T:106:ARG:HG3	1.87	0.56
7:V:77:ASP:N	7:V:77:ASP:OD1	2.36	0.56
9:X:175:ARG:NE	14:K:-1:DC:N3	2.53	0.56
9:X:225:PHE:HE2	9:X:347:ILE:HB	1.69	0.56
10:Y:147:ILE:HG22	10:Y:188:LEU:HD13	1.87	0.56
10:Y:430:HIS:HD2	10:Y:432:LEU:H	1.54	0.56
7:U:101:THR:HG22	7:U:143:ARG:HG3	1.87	0.56
9:X:198:ILE:HG22	9:X:199:ASP:H	1.70	0.56
10:Y:146:VAL:HG11	10:Y:154:LEU:HD12	1.87	0.56
10:Y:263:SER:OG	10:Y:266:ASN:OD1	2.22	0.56
11:C:140:ASN:CA	11:C:182:PHE:O	2.52	0.56
9:X:57:PHE:CD2	9:X:70:TYR:HB3	2.40	0.56
9:X:521:LEU:HB2	9:X:794:LEU:HD11	1.88	0.56
9:X:908:GLU:OE1	9:X:908:GLU:N	2.36	0.56
9:X:1006:GLU:HA	9:X:1009:ASN:HB3	1.88	0.56
10:Y:978:ARG:NE	10:Y:1197:ASN:O	2.37	0.56
12:R:43:A:H2'	12:R:44:A:O4'	2.04	0.56
9:X:201:ARG:NH1	9:X:370:MET:O	2.39	0.56
9:X:1291:LEU:HD11	10:Y:1351:VAL:HG13	1.88	0.56
10:Y:316:ILE:HA	10:Y:323:PRO:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:1208:ASP:OD1	10:Y:1209:VAL:N	2.39	0.56
3:A:213:VAL:HG22	3:A:258:ARG:HD3	1.87	0.56
9:X:979:LEU:HD11	9:X:1002:LEU:HD13	1.88	0.56
10:Y:980:THR:OG1	10:Y:997:VAL:O	2.23	0.56
10:Y:1079:LYS:HD2	10:Y:1087:ASP:HB2	1.87	0.56
3:A:309:VAL:HG22	3:A:310:GLU:H	1.69	0.56
10:Y:850:LYS:N	10:Y:855:ASP:O	2.39	0.56
10:Y:1045:THR:HA	10:Y:1067:ARG:HD3	1.87	0.56
11:C:203:LEU:HA	11:C:206:LYS:HE3	1.88	0.56
4:B:105:ASN:ND2	12:R:34:C:O3'	2.39	0.56
9:X:107:ARG:NH1	9:X:109:ALA:O	2.38	0.56
10:Y:86:GLU:N	10:Y:86:GLU:OE1	2.39	0.56
2:S:2:HIS:NE2	2:S:112:GLU:OE1	2.38	0.56
3:A:131:ARG:HG2	3:A:186:VAL:HG11	1.88	0.56
5:E:36:VAL:HG22	5:E:37:ARG:O	2.06	0.56
7:U:45:ARG:NH1	9:X:1084:ASP:OD1	2.26	0.56
10:Y:930:LEU:HD11	10:Y:1241:TYR:HE1	1.69	0.56
3:A:43:ILE:HG23	3:A:73:LYS:HB3	1.87	0.55
6:G:158:LEU:HB2	6:G:173:LEU:O	2.06	0.55
7:U:255:ARG:HE	7:U:259:ASP:HB3	1.71	0.55
9:X:199:ASP:OD1	9:X:199:ASP:N	2.36	0.55
10:Y:26:SER:HB2	10:Y:236:TRP:CZ2	2.41	0.55
10:Y:104:HIS:NE2	10:Y:106:GLU:OE1	2.36	0.55
10:Y:452:LEU:HB3	10:Y:500:ILE:HG13	1.88	0.55
3:A:21:GLU:O	3:A:25:GLU:HG2	2.06	0.55
9:X:706:ARG:NH2	9:X:793:GLU:OE2	2.38	0.55
10:Y:1072:LYS:NZ	10:Y:1169:THR:OG1	2.39	0.55
1:T:258:ARG:NH2	3:A:490:TRP:O	2.40	0.55
3:A:389:MET:O	3:A:393:LEU:N	2.32	0.55
6:G:173:LEU:HD11	6:G:177:GLN:HG3	1.87	0.55
9:X:60:GLN:HA	9:X:67:GLU:HG3	1.88	0.55
9:X:814:ASP:N	9:X:814:ASP:OD1	2.38	0.55
3:A:244:ARG:HH11	3:A:245:ILE:HD11	1.70	0.55
4:B:10:ARG:NH2	4:B:91:GLU:HG2	2.22	0.55
7:U:56:VAL:HG22	7:U:146:VAL:HG22	1.87	0.55
9:X:288:PRO:HB2	9:X:290:GLU:CD	2.32	0.55
12:R:81:G:H2'	12:R:82:U:C6	2.42	0.55
3:A:154:LEU:HB2	3:A:158:ALA:HB3	1.88	0.55
7:V:92:VAL:O	7:V:148:ARG:NH2	2.37	0.55
9:X:538:LEU:H	9:X:538:LEU:HD23	1.72	0.55
9:X:739:ASP:OD1	9:X:740:GLU:N	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:165:GLU:OE1	3:A:165:GLU:N	2.39	0.55
6:G:157:ARG:HB3	6:G:172:GLU:HG3	1.89	0.55
7:V:170:ARG:NH2	7:V:172:LEU:HD21	2.22	0.55
9:X:50:GLU:OE2	9:X:70:TYR:OH	2.24	0.55
9:X:596:ASP:N	9:X:596:ASP:OD1	2.40	0.55
12:R:81:G:H2'	12:R:82:U:H6	1.72	0.55
2:S:191:ASP:O	2:S:195:VAL:HG23	2.06	0.55
3:A:360:THR:HA	3:A:363:LEU:HB2	1.87	0.55
9:X:238:GLN:HE22	9:X:285:ILE:N	2.04	0.55
10:Y:1371:ARG:HG3	10:Y:1372:ARG:HG2	1.89	0.55
9:X:778:GLU:N	9:X:781:ASP:OD2	2.40	0.55
10:Y:847:ASP:OD1	10:Y:847:ASP:N	2.39	0.55
3:A:289:ALA:HB1	12:R:44:A:C2	2.42	0.55
3:A:303:HIS:HB3	3:A:334:TRP:HA	1.89	0.55
7:U:195:ARG:HG2	7:U:196:THR:H	1.71	0.55
8:W:13:ILE:HD12	8:W:19:LEU:HA	1.89	0.55
13:L:8:DC:H2'	13:L:9:DG:C8	2.41	0.55
2:S:167:THR:O	2:S:170:ASN:HB2	2.07	0.54
3:A:199:ARG:O	3:A:228:ARG:NH2	2.38	0.54
8:W:20:VAL:HG21	10:Y:479:GLU:HA	1.89	0.54
13:L:-6:DC:H1'	13:L:-5:DT:H5'	1.89	0.54
1:T:56:ARG:NH2	1:T:60:PRO:O	2.40	0.54
2:S:155:THR:HG1	2:S:168:TYR:HH	1.53	0.54
6:G:26:LEU:O	6:G:30:ILE:HG13	2.06	0.54
1:T:192:LEU:HD13	1:T:216:GLY:HA3	1.90	0.54
3:A:148:ASP:OD1	3:A:148:ASP:N	2.37	0.54
3:A:208:LEU:HD22	3:A:262:VAL:HG23	1.89	0.54
3:A:224:LYS:HD3	3:A:239:LYS:HG2	1.89	0.54
7:V:46:ILE:HD11	7:V:224:LEU:HD13	1.89	0.54
9:X:169:LYS:NZ	9:X:190:PRO:O	2.36	0.54
3:A:279:ASN:O	3:A:283:PHE:N	2.36	0.54
6:G:30:ILE:HG12	6:G:39:PHE:CD2	2.33	0.54
6:G:128:PHE:HZ	6:G:178:VAL:HG21	1.73	0.54
7:U:182:ARG:HG2	7:U:206:GLU:HB3	1.90	0.54
7:V:220:ALA:O	7:V:223:ILE:HG22	2.06	0.54
9:X:202:ARG:HE	9:X:369:MET:HA	1.71	0.54
9:X:303:ASP:OD1	9:X:304:GLU:N	2.40	0.54
9:X:488:MET:O	9:X:490:GLN:N	2.40	0.54
9:X:712:SER:OG	9:X:713:GLY:N	2.41	0.54
10:Y:1279:GLN:NE2	10:Y:1305:ASP:OD2	2.41	0.54
9:X:158:ASP:HB3	9:X:173:ASN:OD1	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:538:LEU:HD12	9:X:543:ALA:HA	1.89	0.54
9:X:1289:GLU:HB3	9:X:1315:MET:HE3	1.89	0.54
10:Y:1215:GLU:HB3	10:Y:1220:ILE:HD11	1.89	0.54
11:C:132:ILE:HB	11:C:135:TYR:CE2	2.43	0.54
9:X:788:SER:OG	9:X:795:ALA:O	2.23	0.54
7:V:92:VAL:HG13	7:V:121:VAL:HG12	1.88	0.54
9:X:231:GLU:HG3	9:X:332:ARG:HH12	1.73	0.54
9:X:915:ASP:N	9:X:915:ASP:OD1	2.36	0.54
10:Y:506:VAL:HG23	10:Y:628:GLY:HA3	1.90	0.54
12:R:82:U:H2'	12:R:83:G:H8	1.71	0.54
14:K:-10:DA:O3'	14:K:-6:DC:N4	2.41	0.54
3:A:434:LEU:HD21	3:A:448:LEU:HD11	1.89	0.54
5:E:49:PHE:N	5:E:65:TYR:O	2.30	0.54
12:R:36:C:O2'	12:R:37:U:H5'	2.07	0.54
9:X:198:ILE:HG21	9:X:370:MET:HE1	1.90	0.54
10:Y:36:GLY:O	10:Y:104:HIS:ND1	2.41	0.54
10:Y:472:LEU:HD23	10:Y:472:LEU:H	1.72	0.54
11:C:62:ARG:HD2	11:C:67:VAL:HG23	1.90	0.54
1:T:146:ARG:HA	1:T:248:ARG:HB3	1.90	0.54
7:V:27:THR:OG1	7:V:200:LYS:NZ	2.41	0.54
8:W:28:ARG:NH1	9:X:1314:GLN:OE1	2.41	0.54
9:X:66:SER:HB3	9:X:104:ILE:HG23	1.88	0.54
9:X:925:SER:OG	9:X:926:GLY:N	2.41	0.54
10:Y:274:ASN:ND2	14:K:-12:DG:OP2	2.34	0.54
10:Y:657:ALA:O	10:Y:660:GLU:HB3	2.08	0.54
10:Y:1284:ARG:NH1	10:Y:1317:GLU:OE1	2.41	0.54
10:Y:255:LEU:N	10:Y:259:ARG:O	2.41	0.53
7:U:196:THR:HG22	7:U:197:ASP:H	1.72	0.53
10:Y:998:PRO:HG2	10:Y:1020:TRP:CE2	2.43	0.53
2:S:166:THR:HG23	2:S:167:THR:H	1.74	0.53
2:S:221:ARG:NH1	10:Y:28:ASP:OD1	2.42	0.53
7:V:98:VAL:HG11	7:V:121:VAL:HG11	1.89	0.53
10:Y:412:LEU:HA	10:Y:415:VAL:HG12	1.90	0.53
9:X:987:GLU:OE2	9:X:988:LYS:NZ	2.32	0.53
10:Y:915:ILE:HA	10:Y:918:ILE:HG12	1.90	0.53
9:X:183:TRP:CH2	14:K:-2:DA:H2''	2.44	0.53
10:Y:350:SER:HB2	10:Y:469:HIS:HA	1.91	0.53
3:A:215:GLU:N	3:A:215:GLU:OE1	2.41	0.53
5:E:15:HIS:CD2	5:E:70:HIS:CE1	2.96	0.53
7:V:93:GLN:O	7:V:95:LYS:N	2.42	0.53
9:X:42:ASP:OD2	9:X:45:GLY:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:175:ARG:HG3	9:X:177:ILE:HD11	1.89	0.53
9:X:246:LEU:HD13	9:X:269:ILE:HD13	1.89	0.53
9:X:678:ARG:NH1	9:X:681:MET:SD	2.81	0.53
9:X:1252:SER:OG	9:X:1255:THR:O	2.19	0.53
10:Y:798:ARG:NH2	10:Y:1325:PHE:O	2.42	0.53
11:C:40:GLN:O	11:C:47:ARG:NH1	2.42	0.53
14:K:7:DC:H2"	14:K:8:DG:C8	2.44	0.53
3:A:90:GLY:HA2	3:A:92:TYR:CZ	2.44	0.53
3:A:412:ASN:O	3:A:416:THR:OG1	2.23	0.53
4:B:56:ALA:O	4:B:59:THR:HG23	2.07	0.53
7:V:118:ASP:HB3	7:V:121:VAL:HG22	1.90	0.53
9:X:130:MET:HB2	9:X:136:PHE:HE1	1.74	0.53
9:X:491:ASP:N	9:X:491:ASP:OD1	2.40	0.53
1:T:55:ILE:HG12	1:T:81:TRP:HZ3	1.72	0.53
9:X:205:PRO:HG2	9:X:355:PRO:HD3	1.89	0.53
10:Y:35:PHE:CG	10:Y:101:ARG:HD3	2.44	0.53
3:A:93:VAL:HG13	3:A:95:ASP:H	1.74	0.53
9:X:370:MET:HG3	9:X:371:ARG:HG3	1.91	0.53
2:S:229:ASP:OD1	2:S:233:GLY:N	2.41	0.53
3:A:31:LEU:O	3:A:35:THR:HG23	2.09	0.53
5:E:5:ARG:HD2	5:E:7:ARG:NE	2.14	0.53
10:Y:515:ARG:HG2	10:Y:516:ASP:H	1.74	0.53
11:C:152:GLN:HB2	11:C:155:VAL:HG22	1.91	0.53
1:T:183:ARG:HH21	2:S:91:ASN:CG	2.17	0.52
6:G:14:ALA:N	6:G:67:GLY:O	2.40	0.52
7:V:60:GLU:OE2	7:V:171:LEU:N	2.42	0.52
10:Y:556:GLU:OE2	10:Y:557:LYS:N	2.41	0.52
10:Y:1154:ALA:N	10:Y:1214:PRO:O	2.36	0.52
2:S:207:GLY:N	2:S:240:GLY:O	2.42	0.52
3:A:254:MET:C	3:A:255:ARG:HD3	2.34	0.52
3:A:255:ARG:N	12:R:42:C:OP2	2.39	0.52
7:U:69:SER:OG	7:U:70:THR:N	2.39	0.52
9:X:292:ILE:HG23	9:X:295:LYS:HB2	1.91	0.52
9:X:672:GLU:OE1	9:X:672:GLU:N	2.40	0.52
9:X:847:PRO:HB2	9:X:1047:LEU:HD11	1.92	0.52
10:Y:886:VAL:HA	10:Y:1258:ARG:HG3	1.89	0.52
9:X:314:ASN:OD1	9:X:352:ARG:NH1	2.42	0.52
9:X:975:ILE:HD11	9:X:1011:LEU:HD12	1.91	0.52
10:Y:1080:ILE:HD11	10:Y:1097:ALA:HB3	1.92	0.52
9:X:402:ARG:HG2	9:X:416:GLY:H	1.74	0.52
9:X:785:ASP:OD2	9:X:791:LEU:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:1307:ASN:HD21	9:X:1312:ASN:HD22	1.57	0.52
10:Y:144:TYR:O	10:Y:160:LEU:N	2.41	0.52
10:Y:357:VAL:HG23	10:Y:358:GLY:H	1.72	0.52
10:Y:1319:PHE:O	10:Y:1323:ALA:N	2.35	0.52
13:L:5:DA:H2'	13:L:6:DC:H6	1.74	0.52
3:A:111:LYS:HD3	9:X:903:ARG:HD2	1.90	0.52
6:G:135:ARG:HH12	6:G:143:ASP:HB3	1.75	0.52
7:U:95:LYS:NZ	7:U:120:ASP:OD2	2.27	0.52
9:X:742:TYR:N	9:X:745:GLU:OE2	2.42	0.52
10:Y:1140:ARG:NH2	10:Y:1236:GLU:OE2	2.43	0.52
11:C:104:ARG:HH21	11:C:168:PRO:HG3	1.74	0.52
1:T:40:VAL:HG11	1:T:93:ILE:HG13	1.91	0.52
5:E:98:VAL:HG11	6:G:165:PHE:CZ	2.44	0.52
6:G:24:THR:O	6:G:28:GLU:HG2	2.10	0.52
9:X:1268:GLN:O	10:Y:347:VAL:N	2.43	0.52
10:Y:977:SER:OG	10:Y:978:ARG:N	2.40	0.52
11:C:104:ARG:NH2	11:C:166:GLU:O	2.43	0.52
13:L:4:DC:H3'	13:L:5:DA:H8	1.75	0.52
4:B:8:ARG:NE	4:B:11:GLU:OE2	2.43	0.52
7:U:74:VAL:HG21	7:U:81:ILE:HD11	1.92	0.52
7:U:158:ARG:HH12	7:U:174:ASP:HA	1.75	0.52
7:U:303:ILE:HG23	7:U:307:LEU:HD22	1.90	0.52
8:W:15:ASN:OD1	8:W:18:ASP:N	2.32	0.52
9:X:101:ARG:HG2	9:X:118:LYS:HG3	1.92	0.52
9:X:300:ASP:CG	9:X:313:ALA:H	2.17	0.52
9:X:431:LYS:O	9:X:435:ILE:HG12	2.10	0.52
10:Y:430:HIS:CD2	10:Y:432:LEU:H	2.28	0.52
10:Y:507:VAL:HG21	10:Y:598:LYS:HB2	1.92	0.52
9:X:360:LEU:HD11	9:X:378:ARG:HA	1.92	0.52
10:Y:362:ARG:N	10:Y:365:GLN:OE1	2.35	0.52
10:Y:811:GLU:HB2	10:Y:890:THR:HG21	1.92	0.52
9:X:618:GLN:NE2	10:Y:770:LEU:H	2.07	0.52
9:X:813:GLU:OE2	10:Y:461:PHE:N	2.40	0.52
10:Y:357:VAL:HG23	10:Y:358:GLY:N	2.25	0.52
10:Y:670:SER:OG	10:Y:672:LEU:HD23	2.09	0.52
1:T:63:THR:HG21	1:T:77:GLN:HG2	1.91	0.51
1:T:165:ALA:O	1:T:168:TYR:HB3	2.10	0.51
2:S:194:TYR:CD1	2:S:199:ARG:HD2	2.45	0.51
3:A:58:THR:H	3:A:97:ILE:HG22	1.74	0.51
9:X:841:ARG:HD2	9:X:1046:VAL:HG12	1.92	0.51
3:A:60:ARG:NH1	3:A:95:ASP:OD2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:105:SER:OG	7:V:106:GLY:N	2.44	0.51
9:X:230:PHE:N	9:X:333:ILE:O	2.41	0.51
9:X:504:GLU:OE2	9:X:508:SER:OG	2.27	0.51
10:Y:1148:ARG:NH1	14:K:3:DT:O3'	2.44	0.51
12:R:65:G:N3	12:R:66:G:N2	2.58	0.51
2:S:147:ASP:HB3	9:X:1341:ASP:OD2	2.10	0.51
6:G:50:VAL:O	6:G:124:PRO:HB3	2.10	0.51
9:X:183:TRP:HH2	14:K:-2:DA:H2''	1.75	0.51
9:X:976:ARG:HG3	9:X:989:LEU:HD13	1.91	0.51
9:X:1313:HIS:HB2	10:Y:474:LEU:HB2	1.93	0.51
10:Y:640:GLY:N	10:Y:643:ASP:OD2	2.31	0.51
11:C:114:ALA:O	11:C:118:VAL:HG23	2.10	0.51
11:C:132:ILE:HB	11:C:135:TYR:HE2	1.75	0.51
6:G:9:TRP:NE1	6:G:72:GLN:HG3	2.25	0.51
7:U:281:LEU:O	7:U:284:ARG:HB2	2.09	0.51
7:U:233:ASP:N	7:U:233:ASP:OD1	2.40	0.51
10:Y:367:GLY:HA3	10:Y:448:GLN:HB2	1.92	0.51
11:C:22:LYS:HG2	11:C:24:GLY:H	1.75	0.51
1:T:107:ILE:N	1:T:110:ARG:O	2.33	0.51
9:X:171:LEU:HD23	9:X:171:LEU:H	1.75	0.51
9:X:809:GLY:HA3	10:Y:629:PHE:CD2	2.45	0.51
9:X:1101:LEU:HD11	10:Y:508:LEU:HD22	1.92	0.51
9:X:1269:ARG:HA	10:Y:346:ARG:HA	1.93	0.51
9:X:1274:GLU:HG3	10:Y:428:THR:HG21	1.92	0.51
1:T:52:ILE:HD13	1:T:55:ILE:HD12	1.93	0.51
3:A:208:LEU:O	3:A:211:ILE:HG22	2.11	0.51
6:G:20:GLY:O	6:G:24:THR:HG23	2.11	0.51
6:G:98:ASP:HB2	9:X:375:PRO:HB3	1.91	0.51
13:L:1:DT:H2'	13:L:2:DG:H8	1.74	0.51
3:A:343:ASP:N	3:A:343:ASP:OD1	2.42	0.51
3:A:474:THR:HG23	3:A:477:LYS:H	1.75	0.51
9:X:174:ALA:HB2	9:X:432:LEU:HD13	1.93	0.51
10:Y:572:THR:HG21	10:Y:589:TYR:CE1	2.46	0.51
13:L:3:DC:H3'	13:L:4:DC:H6	1.76	0.51
5:E:4:GLN:O	5:E:77:VAL:HA	2.11	0.51
5:E:41:PRO:HB3	5:E:72:ARG:HD3	1.93	0.51
6:G:81:HIS:HE1	9:X:375:PRO:HG2	1.76	0.51
7:U:15:ASP:OD1	7:U:16:ILE:N	2.44	0.51
7:U:193:GLU:HG2	7:U:194:GLN:H	1.76	0.51
9:X:289:VAL:HG12	9:X:319:LEU:HD23	1.92	0.51
9:X:817:LEU:HD11	9:X:1080:ASN:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:937:ASP:N	9:X:937:ASP:OD1	2.42	0.51
7:V:32:GLU:HB2	7:V:35:PHE:CG	2.46	0.51
7:V:180:VAL:O	10:Y:535:ARG:NH1	2.44	0.51
9:X:56:VAL:HG13	9:X:57:PHE:CD1	2.45	0.51
9:X:870:ILE:HG21	9:X:931:VAL:HG11	1.93	0.51
3:A:203:GLU:N	3:A:203:GLU:OE1	2.38	0.50
3:A:340:THR:HG21	3:A:344:LEU:HB2	1.92	0.50
7:V:62:ASP:OD1	7:V:62:ASP:N	2.43	0.50
10:Y:956:GLY:HA3	10:Y:985:ILE:O	2.11	0.50
10:Y:1259:GLN:HE22	10:Y:1262:ARG:NH1	2.09	0.50
3:A:67:GLU:HB3	3:A:69:THR:HG23	1.92	0.50
3:A:247:PRO:HA	3:A:251:CYS:HB3	1.93	0.50
4:B:54:GLY:HA2	4:B:90:TYR:CZ	2.46	0.50
6:G:128:PHE:CZ	6:G:178:VAL:HG21	2.46	0.50
9:X:982:GLY:O	9:X:984:VAL:HA	2.12	0.50
9:X:1222:GLU:OE1	9:X:1222:GLU:N	2.34	0.50
10:Y:72:CYS:N	10:Y:88:CYS:SG	2.84	0.50
10:Y:468:VAL:O	10:Y:469:HIS:ND1	2.44	0.50
10:Y:1034:PHE:HD1	10:Y:1114:GLN:HA	1.76	0.50
11:C:82:LEU:HD22	11:C:89:ASN:HD22	1.76	0.50
11:C:89:ASN:OD1	11:C:90:LEU:N	2.44	0.50
1:T:127:ALA:HB2	1:T:219:LEU:HD13	1.93	0.50
3:A:87:LEU:HD13	3:A:91:ASP:HA	1.91	0.50
9:X:1288:GLN:O	9:X:1292:THR:HG22	2.10	0.50
3:A:440:VAL:HG22	3:A:444:LEU:HD23	1.92	0.50
4:B:89:LEU:HD21	4:B:127:LEU:HD21	1.93	0.50
10:Y:850:LYS:C	10:Y:852:GLY:H	2.20	0.50
13:L:-2:DC:H2''	13:L:-1:DA:C8	2.46	0.50
2:S:33:GLN:HA	2:S:39:PHE:HA	1.94	0.50
3:A:363:LEU:HD21	3:A:371:THR:HA	1.94	0.50
7:V:102:LEU:HD13	7:V:115:ILE:HD13	1.92	0.50
9:X:189:ASP:HB2	9:X:195:PHE:CE2	2.46	0.50
9:X:1307:ASN:HD21	9:X:1312:ASN:ND2	2.10	0.50
10:Y:26:SER:HB2	10:Y:236:TRP:CE2	2.47	0.50
10:Y:419:HIS:HE1	10:Y:471:PRO:O	1.94	0.50
14:K:-14:DC:H2''	14:K:-13:DA:N7	2.27	0.50
2:S:158:PRO:HB3	2:S:206:ILE:HG23	1.93	0.50
3:A:62:TRP:CD1	3:A:92:TYR:HA	2.43	0.50
6:G:18:PHE:CD2	6:G:88:ARG:HD3	2.46	0.50
9:X:89:GLY:HA2	9:X:140:GLY:HA2	1.94	0.50
9:X:306:THR:HG23	9:X:308:GLU:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:339:ASN:OD1	9:X:340:ASP:N	2.44	0.50
9:X:1225:VAL:HG23	10:Y:638:SER:HB2	1.92	0.50
3:A:2:ASN:O	3:A:6:LEU:HB2	2.11	0.50
9:X:819:SER:O	9:X:822:VAL:HG12	2.12	0.50
9:X:1214:ASP:HB2	9:X:1221:PHE:CE1	2.47	0.50
10:Y:242:LEU:HD12	10:Y:243:PRO:HD2	1.93	0.50
10:Y:244:VAL:HG23	10:Y:269:TYR:CZ	2.47	0.50
10:Y:320:ASN:ND2	10:Y:322:ARG:HE	2.09	0.50
3:A:474:THR:OG1	3:A:475:ASP:N	2.44	0.50
4:B:120:HIS:HA	4:B:123:VAL:HG22	1.92	0.50
5:E:91:ASP:HA	6:G:165:PHE:HB2	1.94	0.50
10:Y:350:SER:OG	10:Y:470:VAL:HG12	2.12	0.50
10:Y:697:MET:HE2	10:Y:738:ARG:HA	1.93	0.50
10:Y:1027:VAL:HB	10:Y:1121:LEU:HB2	1.94	0.50
1:T:134:GLN:HA	1:T:138:TYR:O	2.12	0.50
3:A:294:ALA:H	3:A:341:VAL:HG21	1.77	0.50
6:G:10:TYR:CE1	6:G:102:PRO:HB3	2.47	0.50
6:G:15:PHE:HD2	14:K:-11:DC:H4'	1.77	0.50
7:U:111:THR:OG1	7:U:126:PRO:O	2.29	0.50
9:X:225:PHE:CE2	9:X:347:ILE:HB	2.47	0.50
9:X:557:ARG:NH2	9:X:607:SER:O	2.44	0.50
9:X:940:GLU:O	9:X:941:LYS:HG3	2.11	0.50
10:Y:114:ILE:HB	10:Y:304:ASP:OD1	2.11	0.50
10:Y:527:LEU:HD12	10:Y:532:GLU:HG3	1.93	0.50
10:Y:1323:ALA:HA	10:Y:1331:VAL:HG11	1.92	0.50
9:X:88:ARG:NH2	9:X:1035:LYS:O	2.45	0.49
9:X:344:GLY:HA3	9:X:346:TYR:CZ	2.46	0.49
12:R:40:A:H3'	12:R:41:A:H8	1.77	0.49
12:R:40:A:H3'	12:R:41:A:C8	2.47	0.49
4:B:19:SER:O	4:B:23:SER:N	2.33	0.49
7:U:174:ASP:OD1	7:U:174:ASP:N	2.41	0.49
7:U:207:THR:HG23	7:U:209:GLY:H	1.77	0.49
9:X:179:TYR:OH	9:X:462:ASN:ND2	2.45	0.49
10:Y:161:THR:HG22	10:Y:164:GLN:CD	2.36	0.49
11:C:48:LEU:HD11	11:C:199:LEU:HG	1.94	0.49
1:T:168:TYR:O	1:T:172:VAL:HG23	2.11	0.49
3:A:24:PHE:CD2	3:A:51:ARG:HA	2.47	0.49
3:A:80:ALA:HB1	3:A:85:GLU:HG3	1.94	0.49
3:A:318:ILE:HA	3:A:325:VAL:HG23	1.94	0.49
6:G:79:SER:O	6:G:83:VAL:HG23	2.12	0.49
9:X:81:ASP:O	9:X:85:CYS:N	2.35	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:805:MET:HE3	10:Y:636:GLY:HA2	1.93	0.49
9:X:1288:GLN:HE21	10:Y:1355:ARG:HA	1.77	0.49
9:X:1297:ASP:O	9:X:1300:GLY:N	2.45	0.49
10:Y:859:PRO:HD2	10:Y:862:THR:HG21	1.93	0.49
1:T:105:VAL:HB	1:T:113:VAL:HB	1.95	0.49
2:S:205:GLU:OE1	2:S:208:LEU:HB2	2.12	0.49
3:A:343:ASP:O	3:A:345:GLN:N	2.45	0.49
3:A:346:ALA:O	3:A:350:ALA:N	2.46	0.49
4:B:100:TYR:HB3	4:B:137:ASN:OD1	2.13	0.49
7:U:303:ILE:O	7:U:307:LEU:HB2	2.12	0.49
7:V:81:ILE:HG12	7:V:131:CYS:HB2	1.93	0.49
9:X:200:ARG:NH1	14:K:-1:DC:OP1	2.44	0.49
9:X:510:GLN:HG2	9:X:534:GLY:HA2	1.94	0.49
9:X:521:LEU:HD11	9:X:664:GLY:HA2	1.93	0.49
9:X:1103:VAL:HG21	9:X:1112:ILE:HD11	1.95	0.49
10:Y:35:PHE:CD1	10:Y:101:ARG:HD3	2.47	0.49
10:Y:141:PHE:H	10:Y:297:ARG:HG3	1.76	0.49
10:Y:1163:VAL:HG22	10:Y:1177:ILE:HG12	1.94	0.49
13:L:8:DC:H2'	13:L:9:DG:H8	1.75	0.49
3:A:28:GLU:HG2	3:A:47:VAL:HB	1.93	0.49
6:G:63:LYS:O	10:Y:281:ARG:NH1	2.36	0.49
7:V:155:ALA:N	7:V:174:ASP:OD1	2.29	0.49
9:X:942:ASP:H	9:X:945:ALA:HB3	1.77	0.49
10:Y:209:ASN:HA	10:Y:214:ARG:HD2	1.94	0.49
10:Y:844:THR:HA	10:Y:882:VAL:HG23	1.94	0.49
10:Y:1266:ILE:HD12	10:Y:1278:GLU:HB3	1.95	0.49
1:T:37:ASN:O	1:T:41:THR:HG23	2.13	0.49
3:A:45:VAL:HG11	3:A:58:THR:HB	1.95	0.49
5:E:88:MET:HG3	6:G:164:ILE:HG23	1.94	0.49
9:X:494:ASN:O	9:X:497:PRO:HD2	2.12	0.49
9:X:636:CYS:HB2	9:X:645:PHE:HD2	1.77	0.49
9:X:838:CYS:HB3	9:X:1050:VAL:HG23	1.94	0.49
9:X:1146:GLN:NE2	9:X:1150:ASP:OD2	2.45	0.49
10:Y:141:PHE:CE2	10:Y:181:GLY:HA3	2.47	0.49
10:Y:423:LEU:HD11	10:Y:447:ILE:HG21	1.93	0.49
10:Y:733:SER:OG	10:Y:734:ALA:N	2.45	0.49
12:R:84:G:H2'	12:R:85:C:C6	2.48	0.49
3:A:213:VAL:HB	3:A:216:ILE:HG22	1.95	0.49
6:G:19:GLU:OE2	6:G:67:GLY:N	2.46	0.49
9:X:488:MET:O	9:X:492:MET:HE1	2.11	0.49
9:X:995:ASP:N	9:X:995:ASP:OD1	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:1089:GLU:HB3	9:X:1213:TYR:HE2	1.77	0.49
9:X:1295:SER:OG	10:Y:348:ASP:N	2.46	0.49
10:Y:1158:GLU:HA	10:Y:1223:LEU:HD11	1.93	0.49
11:C:76:TYR:CZ	11:C:204:TYR:HB3	2.48	0.49
1:T:246:ASN:OD1	1:T:249:VAL:HG12	2.13	0.49
2:S:152:ILE:N	2:S:201:ASP:OD2	2.35	0.49
3:A:82:TYR:CD2	3:A:83:GLU:HG3	2.48	0.49
4:B:8:ARG:HA	4:B:110:LEU:HD13	1.95	0.49
9:X:65:ASN:OD1	9:X:107:ARG:NE	2.46	0.49
13:L:13:DT:H1'	13:L:14:DG:C4	2.48	0.49
7:U:8:PHE:HD1	7:V:150:ARG:CZ	2.26	0.49
7:U:242:VAL:HG22	7:U:243:LYS:H	1.78	0.49
7:V:170:ARG:HH21	7:V:172:LEU:HD21	1.78	0.49
8:W:52:ARG:O	8:W:55:GLU:HG3	2.12	0.49
9:X:542:ARG:HH12	14:K:1:DT:H72	1.78	0.49
9:X:594:VAL:HG11	9:X:650:VAL:HG23	1.94	0.49
9:X:718:ALA:HB2	9:X:783:LEU:HG	1.95	0.49
2:S:2:HIS:HB3	2:S:5:LEU:HB3	1.95	0.49
5:E:11:LYS:HB2	5:E:97:ASP:HB2	1.94	0.49
5:E:37:ARG:HB2	5:E:75:ASP:HB2	1.93	0.49
9:X:1:MET:HG2	9:X:2:VAL:HG13	1.94	0.49
10:Y:37:GLU:HG3	10:Y:106:GLU:HG2	1.94	0.49
10:Y:720:ASN:OD1	10:Y:722:ILE:N	2.46	0.49
11:C:142:VAL:HG12	11:C:181:THR:HG22	1.95	0.49
3:A:244:ARG:NE	4:B:72:ARG:HH11	2.09	0.48
7:U:39:LEU:HD21	7:V:228:LEU:HD21	1.95	0.48
9:X:239:MET:SD	9:X:287:VAL:HG21	2.53	0.48
9:X:312:ALA:H	9:X:315:MET:HE2	1.77	0.48
9:X:670:PHE:CE2	9:X:1113:LEU:HB3	2.48	0.48
9:X:887:VAL:HG12	9:X:915:ASP:HA	1.95	0.48
10:Y:659:ALA:O	10:Y:662:ALA:HB3	2.13	0.48
10:Y:709:ARG:NE	10:Y:710:ASP:OD2	2.46	0.48
13:L:4:DC:H2'	13:L:5:DA:C8	2.47	0.48
2:S:224:GLY:O	10:Y:32:SER:OG	2.16	0.48
3:A:27:LEU:HD21	3:A:114:ILE:HD11	1.94	0.48
3:A:308:ALA:HB3	3:A:340:THR:O	2.13	0.48
3:A:400:GLU:HB2	3:A:401:PRO:HD3	1.94	0.48
10:Y:155:GLU:HB2	10:Y:158:GLN:HB2	1.94	0.48
10:Y:1061:VAL:O	10:Y:1104:LYS:N	2.46	0.48
2:S:79:VAL:HG22	2:S:107:ILE:HG12	1.95	0.48
9:X:81:ASP:H	9:X:84:GLU:HB2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:626:GLU:O	9:X:628:HIS:ND1	2.45	0.48
10:Y:1078:LEU:HD21	10:Y:1107:VAL:HG21	1.95	0.48
13:L:18:DG:H2''	13:L:19:DG:O4'	2.13	0.48
7:U:62:ASP:N	7:U:62:ASP:OD1	2.44	0.48
7:U:104:LYS:HG2	7:U:110:VAL:HG22	1.94	0.48
9:X:237:LEU:HD22	9:X:289:VAL:HA	1.95	0.48
10:Y:1368:ASP:HA	10:Y:1371:ARG:HG2	1.96	0.48
12:R:30:A:C8	12:R:31:C:H2'	2.49	0.48
2:S:48:GLU:HG3	2:S:66:THR:HG21	1.96	0.48
3:A:318:ILE:HG12	3:A:338:VAL:HG11	1.95	0.48
3:A:411:LYS:HD2	3:A:414:LEU:HD11	1.95	0.48
9:X:262:TYR:OH	9:X:280:ASP:OD2	2.31	0.48
2:S:133:ALA:HB1	2:S:140:LEU:HD12	1.95	0.48
4:B:59:THR:O	4:B:62:LEU:HG	2.14	0.48
9:X:557:ARG:HH12	9:X:611:GLU:CD	2.21	0.48
10:Y:1064:SER:HA	10:Y:1072:LYS:HA	1.95	0.48
10:Y:1157:ALA:O	10:Y:1207:GLY:N	2.29	0.48
4:B:119:SER:HA	4:B:122:PHE:CE1	2.49	0.48
7:U:227:GLN:HG3	7:V:35:PHE:CE2	2.48	0.48
9:X:444:ASP:OD2	9:X:447:HIS:N	2.46	0.48
9:X:599:VAL:N	9:X:627:GLY:O	2.47	0.48
9:X:759:SER:OG	9:X:763:THR:N	2.33	0.48
9:X:1184:THR:OG1	9:X:1189:GLY:HA2	2.14	0.48
10:Y:1364:ALA:O	10:Y:1367:GLN:NE2	2.47	0.48
2:S:1:MET:HB2	6:G:133:MET:HE2	1.96	0.48
2:S:40:VAL:HG12	2:S:45:LYS:HZ3	1.77	0.48
9:X:197:ARG:HE	9:X:201:ARG:H	1.62	0.48
9:X:217:THR:HA	9:X:220:ILE:HD12	1.96	0.48
11:C:113:GLU:HA	11:C:116:GLN:CD	2.39	0.48
2:S:40:VAL:HG12	2:S:45:LYS:NZ	2.28	0.48
3:A:253:GLY:HA3	3:A:258:ARG:HE	1.79	0.48
3:A:431:ALA:O	3:A:435:LEU:N	2.47	0.48
3:A:437:LEU:HB2	3:A:440:VAL:HG21	1.96	0.48
3:A:455:THR:HG23	3:A:458:ASP:H	1.79	0.48
9:X:796:LEU:HD23	9:X:796:LEU:HA	1.63	0.48
9:X:1126:ASP:O	9:X:1129:ASN:HB3	2.14	0.48
10:Y:661:VAL:HG23	10:Y:682:VAL:HG22	1.96	0.48
10:Y:743:MET:HG2	10:Y:745:GLY:H	1.79	0.48
10:Y:1368:ASP:HB3	10:Y:1373:ARG:HH12	1.78	0.48
1:T:26:PRO:HA	1:T:95:ARG:HH21	1.79	0.48
9:X:196:VAL:HG23	9:X:206:ALA:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:786:GLY:N	9:X:789:THR:OG1	2.46	0.48
9:X:930:ASP:OD1	9:X:931:VAL:N	2.47	0.48
10:Y:56:LEU:HB3	10:Y:250:ARG:HH21	1.79	0.48
10:Y:692:ARG:O	10:Y:695:LYS:HG2	2.14	0.48
9:X:312:ALA:O	9:X:315:MET:HG2	2.14	0.47
10:Y:72:CYS:SG	10:Y:74:LYS:HB2	2.53	0.47
10:Y:1037:PHE:CD1	10:Y:1040:MET:HG3	2.49	0.47
11:C:32:CYS:O	11:C:34:ILE:HD12	2.14	0.47
3:A:439:GLY:O	3:A:477:LYS:NZ	2.46	0.47
4:B:112:LYS:HD3	4:B:120:HIS:CE1	2.49	0.47
5:E:91:ASP:OD1	5:E:92:LEU:N	2.39	0.47
7:U:260:LEU:HB3	7:U:306:VAL:HB	1.95	0.47
7:V:83:LEU:HD13	10:Y:526:VAL:HG12	1.96	0.47
9:X:1290:MET:HA	9:X:1294:LYS:HB2	1.94	0.47
1:T:38:ASP:OD1	1:T:39:PHE:N	2.44	0.47
3:A:191:ARG:NE	12:R:59:U:OP2	2.45	0.47
4:B:123:VAL:O	4:B:127:LEU:HB2	2.13	0.47
6:G:92:PHE:HD2	6:G:100:PRO:HG3	1.79	0.47
9:X:1130:ALA:O	9:X:1134:GLN:NE2	2.47	0.47
10:Y:261:ALA:HB2	12:R:76:G:H21	1.79	0.47
13:L:-2:DC:N3	13:L:-1:DA:N6	2.62	0.47
7:U:15:ASP:OD1	7:U:17:GLU:N	2.47	0.47
9:X:942:ASP:OD1	9:X:944:ARG:N	2.37	0.47
10:Y:563:LEU:HD23	10:Y:563:LEU:HA	1.78	0.47
10:Y:965:SER:HB2	10:Y:973:LEU:HD21	1.96	0.47
13:L:11:DG:C8	13:L:11:DG:H5'	2.50	0.47
7:U:321:TRP:NE1	7:U:325:SER:OG	2.47	0.47
9:X:74:ARG:NH1	9:X:121:GLU:HG2	2.25	0.47
9:X:164:THR:C	9:X:166:SER:H	2.23	0.47
9:X:299:LYS:NZ	9:X:300:ASP:O	2.29	0.47
10:Y:399:LYS:HB3	10:Y:403:ARG:HH12	1.79	0.47
10:Y:1350:ASN:HB3	10:Y:1356:LEU:O	2.14	0.47
2:S:229:ASP:OD1	2:S:232:GLY:N	2.47	0.47
3:A:321:ASN:N	12:R:48:A:OP1	2.38	0.47
4:B:72:ARG:HB2	4:B:76:GLU:OE2	2.12	0.47
7:V:178:SER:OG	7:V:180:VAL:HG12	2.14	0.47
9:X:320:ASP:OD1	9:X:320:ASP:N	2.46	0.47
9:X:339:ASN:HB3	9:X:342:ASP:O	2.15	0.47
9:X:466:VAL:O	9:X:469:VAL:HG12	2.15	0.47
10:Y:1257:VAL:HA	10:Y:1260:MET:HG2	1.96	0.47
10:Y:1284:ARG:NH2	10:Y:1317:GLU:OE2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:79:G:H2'	12:R:80:U:C6	2.49	0.47
2:S:148:LEU:O	2:S:151:THR:OG1	2.21	0.47
2:S:236:TYR:HB2	2:S:242:ILE:HD13	1.97	0.47
4:B:8:ARG:O	4:B:11:GLU:HG3	2.15	0.47
5:E:8:ILE:HG23	5:E:100:ILE:HG22	1.96	0.47
6:G:96:THR:HG23	6:G:99:ARG:HB3	1.94	0.47
7:U:284:ARG:HH21	7:U:288:GLU:HB3	1.79	0.47
9:X:247:ARG:HG3	9:X:274:ILE:HD11	1.95	0.47
9:X:398:SER:HB3	9:X:401:GLY:N	2.27	0.47
9:X:542:ARG:HB2	14:K:1:DT:P	2.55	0.47
9:X:542:ARG:HH11	14:K:1:DT:P	2.37	0.47
9:X:678:ARG:NH2	9:X:1106:ARG:HG2	2.30	0.47
9:X:1042:LEU:HB3	9:X:1046:VAL:CG2	2.44	0.47
9:X:1245:ALA:HA	10:Y:351:GLY:HA2	1.97	0.47
9:X:1273:MET:HE3	9:X:1273:MET:HB2	1.79	0.47
10:Y:113:HIS:CE1	10:Y:115:TRP:HB2	2.50	0.47
10:Y:986:ASP:OD1	10:Y:990:ARG:N	2.47	0.47
10:Y:1323:ALA:O	10:Y:1328:THR:HB	2.14	0.47
4:B:4:ALA:HA	4:B:8:ARG:HH11	1.79	0.47
4:B:15:GLN:HB2	4:B:34:PHE:HE1	1.80	0.47
6:G:136:VAL:O	6:G:143:ASP:N	2.43	0.47
7:V:16:ILE:HG23	7:V:26:VAL:HG12	1.96	0.47
9:X:172:TYR:O	9:X:432:LEU:HD11	2.14	0.47
9:X:988:LYS:O	9:X:992:LEU:HB2	2.15	0.47
10:Y:163:GLU:H	10:Y:163:GLU:CD	2.23	0.47
10:Y:544:LEU:HD21	10:Y:631:TYR:HD2	1.79	0.47
10:Y:826:ILE:HG12	10:Y:831:VAL:HG22	1.95	0.47
1:T:195:VAL:HG11	1:T:203:PHE:HB2	1.97	0.47
3:A:340:THR:OG1	3:A:343:ASP:OD1	2.33	0.47
3:A:373:LEU:HB3	3:A:395:ILE:HG21	1.96	0.47
3:A:428:ASN:ND2	3:A:449:ALA:HB3	2.29	0.47
6:G:115:LEU:HA	6:G:118:VAL:HG12	1.95	0.47
9:X:458:GLU:O	9:X:461:GLU:HG3	2.15	0.47
9:X:468:LEU:HA	9:X:498:ILE:HD11	1.97	0.47
9:X:885:GLY:H	9:X:917:SER:HB2	1.79	0.47
9:X:1009:ASN:O	9:X:1013:GLN:HG2	2.15	0.47
10:Y:511:TYR:CD2	10:Y:728:SER:HB3	2.50	0.47
10:Y:706:VAL:HG12	10:Y:715:LYS:HG2	1.96	0.47
10:Y:979:ASN:HA	10:Y:996:LYS:HE2	1.97	0.47
3:A:304:THR:HA	3:A:335:GLU:O	2.15	0.47
5:E:99:GLN:HA	6:G:170:PRO:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:60:GLU:OE1	7:U:170:ARG:NH1	2.47	0.47
7:V:191:ARG:HH22	10:Y:413:ASP:HB2	1.79	0.47
7:V:196:THR:OG1	7:V:197:ASP:N	2.48	0.47
9:X:809:GLY:HA3	10:Y:629:PHE:CE2	2.50	0.47
9:X:888:THR:OG1	9:X:914:LYS:O	2.27	0.47
10:Y:58:CYS:SG	10:Y:60:ARG:HB3	2.55	0.47
10:Y:783:LEU:HA	10:Y:783:LEU:HD23	1.79	0.47
10:Y:865:HIS:CE1	10:Y:868:TRP:CD1	3.03	0.47
10:Y:1184:ASP:OD1	10:Y:1184:ASP:N	2.47	0.47
13:L:-4:DC:H2'	13:L:-3:DA:C8	2.50	0.47
3:A:294:ALA:N	3:A:341:VAL:HG21	2.30	0.46
6:G:24:THR:HA	6:G:27:ARG:NH2	2.30	0.46
7:V:51:MET:HG3	7:V:179:PRO:HD2	1.97	0.46
10:Y:432:LEU:HD22	10:Y:435:GLN:HE21	1.80	0.46
10:Y:1069:ALA:HA	10:Y:1072:LYS:HB3	1.96	0.46
6:G:39:PHE:CE1	6:G:79:SER:HB2	2.50	0.46
7:U:82:LEU:HD21	7:U:171:LEU:HD23	1.97	0.46
9:X:172:TYR:CD2	9:X:435:ILE:HG22	2.50	0.46
9:X:848:GLU:OE1	9:X:888:THR:HG22	2.14	0.46
9:X:1286:THR:HG22	10:Y:476:ALA:HB1	1.96	0.46
10:Y:325:LYS:NZ	12:R:79:G:H5'	2.30	0.46
11:C:41:HIS:O	11:C:45:LYS:HD2	2.15	0.46
1:T:165:ALA:HA	1:T:168:TYR:HB3	1.98	0.46
3:A:343:ASP:HB2	3:A:344:LEU:HG	1.97	0.46
3:A:373:LEU:HB2	3:A:375:GLU:OE1	2.15	0.46
9:X:243:PRO:HG3	9:X:277:LEU:HG	1.97	0.46
9:X:594:VAL:HG22	9:X:599:VAL:HG22	1.96	0.46
9:X:1088:ASP:OD1	9:X:1089:GLU:HG2	2.16	0.46
10:Y:635:SER:OG	10:Y:636:GLY:N	2.48	0.46
3:A:82:TYR:HD2	3:A:83:GLU:HG3	1.80	0.46
3:A:235:LYS:HZ2	3:A:328:ALA:N	2.14	0.46
6:G:86:VAL:HB	6:G:87:PRO:HD2	1.98	0.46
9:X:27:LEU:O	9:X:528:ARG:NH1	2.49	0.46
9:X:1308:ILE:HD11	10:Y:380:PHE:CZ	2.51	0.46
13:L:11:DG:H5'	13:L:11:DG:H8	1.81	0.46
4:B:27:ILE:HD12	4:B:30:VAL:HB	1.97	0.46
6:G:156:SER:O	6:G:157:ARG:HD2	2.14	0.46
9:X:195:PHE:HB3	9:X:203:LYS:HG2	1.96	0.46
9:X:565:GLU:OE2	9:X:566:GLY:N	2.48	0.46
10:Y:150:GLY:HA3	10:Y:175:GLU:O	2.14	0.46
10:Y:425:ARG:NH1	10:Y:458:ASN:O	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:587:LEU:HD11	10:Y:608:CYS:HB2	1.97	0.46
10:Y:814:CYS:SG	10:Y:816:THR:OG1	2.61	0.46
11:C:86:THR:HG22	11:C:90:LEU:HD23	1.97	0.46
3:A:82:TYR:OH	7:U:294:ASN:ND2	2.47	0.46
3:A:134:GLU:HA	3:A:183:LEU:HD23	1.98	0.46
3:A:142:VAL:HG13	3:A:175:PRO:HA	1.98	0.46
3:A:270:ARG:NE	12:R:45:U:OP1	2.48	0.46
3:A:428:ASN:ND2	3:A:446:PHE:HA	2.29	0.46
4:B:18:TYR:CD1	5:E:41:PRO:HD3	2.51	0.46
7:U:55:ALA:H	7:U:177:TYR:HB3	1.80	0.46
7:V:35:PHE:HA	7:V:38:THR:HG22	1.98	0.46
9:X:699:LEU:HG	9:X:799:ASN:HD22	1.81	0.46
9:X:840:SER:HB2	9:X:848:GLU:HB2	1.98	0.46
9:X:902:LEU:HB3	9:X:903:ARG:NH2	2.30	0.46
10:Y:135:ILE:HA	10:Y:138:VAL:HG12	1.97	0.46
10:Y:332:LYS:HA	10:Y:1328:THR:HG21	1.96	0.46
10:Y:1094:ASP:OD1	10:Y:1094:ASP:N	2.48	0.46
13:L:-3:DA:H2"	13:L:-2:DC:H6	1.80	0.46
14:K:-17:DG:H2"	14:K:-16:DA:H8	1.81	0.46
3:A:311:ALA:HA	3:A:314:LEU:HD13	1.97	0.46
4:B:66:MET:HG3	4:B:129:LYS:HG2	1.98	0.46
7:U:305:ASP:HA	7:U:309:SER:HB2	1.97	0.46
7:V:59:VAL:HG21	7:V:82:LEU:HD22	1.98	0.46
9:X:57:PHE:HD2	9:X:70:TYR:HB3	1.79	0.46
9:X:262:TYR:CG	9:X:277:LEU:HD13	2.51	0.46
9:X:903:ARG:HA	9:X:907:GLY:N	2.31	0.46
9:X:1308:ILE:HD11	10:Y:380:PHE:CE2	2.51	0.46
10:Y:1044:GLN:O	10:Y:1067:ARG:HD3	2.15	0.46
3:A:494:GLU:N	3:A:494:GLU:OE1	2.49	0.46
4:B:49:ARG:O	4:B:52:LEU:HG	2.16	0.46
5:E:5:ARG:HB2	5:E:103:GLY:H	1.81	0.46
5:E:48:ARG:HD2	5:E:65:TYR:O	2.16	0.46
5:E:85:ASP:O	5:E:89:ARG:HD3	2.15	0.46
7:U:192:VAL:HG21	7:U:198:LEU:HD12	1.97	0.46
8:W:31:GLN:HE21	9:X:1312:ASN:HA	1.81	0.46
9:X:423:ASP:OD1	9:X:424:ASP:N	2.48	0.46
9:X:616:ILE:HB	9:X:637:ARG:HG3	1.98	0.46
9:X:669:PRO:HG3	9:X:1069:ARG:NH2	2.31	0.46
10:Y:147:ILE:HD11	10:Y:179:LYS:HD2	1.98	0.46
10:Y:309:ASN:ND2	10:Y:324:LEU:H	2.13	0.46
10:Y:349:TYR:OH	10:Y:379:PRO:HG2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:374:LEU:HD11	10:Y:401:VAL:HG23	1.98	0.46
3:A:186:VAL:C	3:A:187:ARG:HD2	2.41	0.46
6:G:10:TYR:CZ	6:G:102:PRO:HB3	2.51	0.46
9:X:563:THR:OG1	10:Y:780:ARG:NH2	2.49	0.46
9:X:735:LYS:HA	9:X:748:ILE:HG23	1.97	0.46
10:Y:68:TYR:HD2	10:Y:78:LEU:HA	1.81	0.46
10:Y:909:ILE:HD11	10:Y:913:GLU:HB2	1.97	0.46
11:C:113:GLU:HA	11:C:116:GLN:OE1	2.16	0.46
11:C:140:ASN:N	11:C:182:PHE:O	2.49	0.46
7:V:89:ALA:HB3	7:V:124:VAL:HG21	1.98	0.46
7:V:104:LYS:HG3	7:V:114:ASP:CG	2.41	0.46
9:X:138:ILE:HG22	9:X:139:ASN:H	1.80	0.46
9:X:849:GLU:OE2	9:X:887:VAL:HG23	2.16	0.46
10:Y:342:LEU:HD12	10:Y:1352:ILE:HG23	1.98	0.46
10:Y:412:LEU:O	10:Y:415:VAL:HG12	2.15	0.46
10:Y:1046:ILE:HG21	10:Y:1059:LEU:HB3	1.98	0.46
2:S:85:PRO:HA	2:S:101:VAL:HG23	1.97	0.45
2:S:154:ALA:HB2	2:S:200:VAL:HG11	1.98	0.45
3:A:125:MET:HE2	3:A:129:GLN:NE2	2.31	0.45
3:A:364:ASP:OD1	3:A:365:ILE:N	2.49	0.45
6:G:152:ASP:OD1	6:G:152:ASP:N	2.47	0.45
8:W:47:THR:HG23	10:Y:478:LEU:HD13	1.99	0.45
9:X:195:PHE:CG	9:X:203:LYS:HE3	2.51	0.45
10:Y:430:HIS:ND1	10:Y:925:GLU:HG3	2.31	0.45
10:Y:480:ALA:HA	10:Y:484:MET:HG2	1.98	0.45
11:C:65:TYR:CZ	11:C:94:LEU:HB3	2.51	0.45
3:A:251:CYS:O	3:A:258:ARG:HD2	2.16	0.45
6:G:22:VAL:O	6:G:26:LEU:HD23	2.16	0.45
7:U:302:GLU:O	7:U:306:VAL:HG22	2.16	0.45
9:X:626:GLU:O	9:X:628:HIS:N	2.49	0.45
9:X:660:VAL:HG21	10:Y:769:VAL:HG11	1.99	0.45
9:X:903:ARG:HE	9:X:906:PHE:HB2	1.81	0.45
9:X:1116:HIS:CD2	9:X:1208:GLY:HA3	2.49	0.45
1:T:16:GLY:HA3	1:T:117:TYR:CE2	2.50	0.45
1:T:166:THR:O	1:T:169:ILE:HB	2.16	0.45
3:A:237:ALA:HA	3:A:274:VAL:O	2.16	0.45
9:X:1333:LEU:HD22	10:Y:307:LEU:HD22	1.98	0.45
10:Y:80:HIS:O	10:Y:83:VAL:HG12	2.16	0.45
10:Y:261:ALA:HB2	12:R:76:G:N2	2.31	0.45
10:Y:405:GLU:O	10:Y:408:VAL:HG12	2.15	0.45
10:Y:406:ALA:HA	10:Y:409:TRP:HD1	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:603:LYS:O	10:Y:607:THR:HG22	2.16	0.45
14:K:-9:DT:H5''	14:K:-6:DC:C4	2.51	0.45
3:A:63:LEU:HB2	3:A:73:LYS:O	2.17	0.45
7:V:91:ARG:HG3	7:V:122:GLU:HB3	1.98	0.45
9:X:734:ILE:HB	9:X:749:ASP:OD1	2.17	0.45
9:X:903:ARG:HA	9:X:907:GLY:H	1.82	0.45
9:X:1336:ASN:HB2	10:Y:25:ALA:HB2	1.99	0.45
10:Y:185:ILE:O	10:Y:189:LEU:HG	2.15	0.45
2:S:6:ASN:O	2:S:9:VAL:HG12	2.16	0.45
5:E:11:LYS:HG2	5:E:71:LEU:CD1	2.47	0.45
5:E:88:MET:HA	6:G:165:PHE:H	1.81	0.45
9:X:1054:LEU:HD23	9:X:1054:LEU:HA	1.73	0.45
10:Y:1263:LYS:HZ1	10:Y:1279:GLN:HB3	1.81	0.45
1:T:62:HIS:CG	1:T:79:VAL:HB	2.52	0.45
3:A:57:ASP:N	3:A:57:ASP:OD1	2.50	0.45
7:V:107:ILE:HD12	7:V:135:ASP:O	2.17	0.45
9:X:722:GLY:HA2	9:X:737:ASN:CG	2.42	0.45
9:X:971:LEU:HD12	9:X:971:LEU:HA	1.78	0.45
9:X:1292:THR:HG23	9:X:1293:VAL:N	2.32	0.45
10:Y:146:VAL:HG13	10:Y:155:GLU:O	2.16	0.45
10:Y:200:GLN:O	10:Y:203:GLU:HG2	2.17	0.45
10:Y:325:LYS:HZ1	12:R:79:G:H5'	1.81	0.45
10:Y:555:TYR:HD2	10:Y:585:LYS:HB3	1.81	0.45
10:Y:1051:ASP:HB2	10:Y:1056:LEU:HB3	1.98	0.45
10:Y:1063:ASP:CG	10:Y:1064:SER:H	2.24	0.45
10:Y:1369:ARG:HG3	10:Y:1373:ARG:HD2	1.99	0.45
11:C:60:LYS:HA	11:C:63:ARG:HG2	1.99	0.45
2:S:135:LEU:HB2	2:S:140:LEU:HD21	1.99	0.45
9:X:176:ILE:O	9:X:183:TRP:HB2	2.17	0.45
9:X:189:ASP:OD2	9:X:191:LYS:N	2.45	0.45
9:X:540:ARG:HA	9:X:543:ALA:HB2	1.98	0.45
9:X:854:ILE:HB	9:X:857:VAL:HG22	1.99	0.45
9:X:1025:PHE:CD1	9:X:1028:LYS:HD3	2.47	0.45
9:X:1085:MET:HE3	9:X:1085:MET:HB3	1.77	0.45
10:Y:53:ARG:HD2	10:Y:60:ARG:NH1	2.31	0.45
10:Y:759:ILE:HG23	10:Y:771:GLN:HB3	1.99	0.45
1:T:52:ILE:HD11	1:T:64:ILE:HG21	1.98	0.45
1:T:192:LEU:O	1:T:195:VAL:HG22	2.16	0.45
3:A:252:VAL:HG12	3:A:256:GLY:HA2	1.98	0.45
4:B:18:TYR:HH	5:E:72:ARG:HE	1.61	0.45
5:E:80:THR:OG1	5:E:83:THR:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:47:LEU:HD23	7:V:47:LEU:HA	1.71	0.45
10:Y:22:ILE:O	10:Y:1339:GLY:HA2	2.17	0.45
10:Y:275:ARG:HE	10:Y:298:MET:HG2	1.82	0.45
10:Y:457:TYR:HB2	10:Y:459:ALA:HB2	1.97	0.45
10:Y:514:THR:OG1	10:Y:595:ALA:O	2.35	0.45
10:Y:658:GLU:O	10:Y:661:VAL:HG12	2.16	0.45
10:Y:1268:ASN:ND2	10:Y:1270:GLY:H	2.15	0.45
11:C:91:LEU:HD13	11:C:191:LEU:HD23	1.99	0.45
14:K:-13:DA:H1'	14:K:-12:DG:C4	2.52	0.45
1:T:195:VAL:HA	1:T:200:VAL:O	2.16	0.45
2:S:170:ASN:HB3	2:S:260:GLU:OE2	2.17	0.45
3:A:63:LEU:HD13	3:A:73:LYS:HB2	1.99	0.45
3:A:429:LYS:HD3	3:A:429:LYS:HA	1.71	0.45
9:X:17:LYS:H	9:X:17:LYS:HD2	1.82	0.45
9:X:91:THR:HG22	9:X:139:ASN:N	2.32	0.45
9:X:371:ARG:NH1	9:X:374:GLU:OE1	2.50	0.45
9:X:970:GLY:O	9:X:973:SER:OG	2.24	0.45
9:X:1106:ARG:HH12	10:Y:731:ARG:HH22	1.64	0.45
10:Y:410:ASP:N	10:Y:410:ASP:OD1	2.47	0.45
10:Y:1157:ALA:HB2	10:Y:1210:ILE:HD11	1.99	0.45
13:L:-3:DA:C4	13:L:-2:DC:C5	3.05	0.45
2:S:52:ILE:HD12	2:S:64:ILE:HD13	1.97	0.45
6:G:33:HIS:HB3	6:G:35:MET:HG2	1.99	0.45
6:G:81:HIS:O	6:G:85:SER:N	2.47	0.45
9:X:618:GLN:O	9:X:621:SER:OG	2.28	0.45
9:X:1256:GLN:HE21	10:Y:99:ARG:NH2	2.15	0.45
10:Y:955:LYS:HB3	10:Y:1010:GLN:HG3	1.99	0.45
12:R:63:U:O2'	12:R:64:G:O4'	2.34	0.45
3:A:408:GLU:HB3	3:A:409:ARG:NH2	2.31	0.44
4:B:88:ALA:HA	4:B:91:GLU:CD	2.42	0.44
5:E:99:GLN:H	5:E:99:GLN:CD	2.24	0.44
6:G:47:GLU:O	6:G:62:ARG:N	2.48	0.44
7:U:280:ASP:O	7:U:284:ARG:HG2	2.17	0.44
9:X:233:ARG:HE	9:X:238:GLN:HG3	1.82	0.44
9:X:1305:TYR:HE1	10:Y:379:PRO:HG3	1.82	0.44
10:Y:221:ILE:HA	10:Y:221:ILE:HD12	1.84	0.44
10:Y:744:ARG:NH2	10:Y:775:SER:OG	2.50	0.44
12:R:79:G:H2'	12:R:80:U:H6	1.82	0.44
1:T:69:SER:O	1:T:69:SER:OG	2.28	0.44
2:S:261:LEU:HD11	2:S:265:LEU:HB2	1.99	0.44
3:A:214:PRO:HD3	5:E:17:LEU:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:12:CYS:HB3	4:B:40:VAL:HG21	1.99	0.44
9:X:673:HIS:O	9:X:1109:ILE:HG22	2.17	0.44
9:X:1134:GLN:HG2	9:X:1136:GLN:HG2	1.99	0.44
9:X:1160:ASP:C	9:X:1162:SER:H	2.25	0.44
10:Y:395:LYS:O	10:Y:399:LYS:HG2	2.17	0.44
10:Y:534:GLU:HA	10:Y:578:ILE:HD11	1.99	0.44
10:Y:1272:SER:HB2	10:Y:1292:LEU:HD11	2.00	0.44
3:A:143:LYS:HB2	3:A:153:ASP:CG	2.42	0.44
4:B:91:GLU:OE1	4:B:103:ALA:HB1	2.17	0.44
5:E:12:ALA:HB2	5:E:96:VAL:HG12	1.99	0.44
9:X:891:GLY:N	9:X:912:ASP:HB2	2.24	0.44
10:Y:492:SER:OG	10:Y:495:ASN:O	2.35	0.44
10:Y:538:ARG:HD3	10:Y:538:ARG:HA	1.83	0.44
10:Y:556:GLU:HB3	10:Y:564:VAL:HG23	1.98	0.44
10:Y:768:ASN:HB2	10:Y:771:GLN:CD	2.42	0.44
11:C:19:LEU:HD23	11:C:21:LEU:HD11	1.98	0.44
11:C:130:VAL:O	11:C:130:VAL:HG23	2.18	0.44
1:T:161:ALA:HB1	1:T:163:GLN:NE2	2.31	0.44
3:A:310:GLU:HA	3:A:341:VAL:HG12	1.99	0.44
7:U:107:ILE:HA	7:U:133:LEU:O	2.17	0.44
7:V:205:MET:HE2	7:V:207:THR:HG22	1.98	0.44
9:X:588:GLU:HA	9:X:606:LEU:O	2.17	0.44
10:Y:37:GLU:HB2	10:Y:104:HIS:CE1	2.52	0.44
10:Y:78:LEU:H	10:Y:78:LEU:HD12	1.82	0.44
10:Y:576:ARG:HD3	10:Y:593:ASN:HA	2.00	0.44
2:S:206:ILE:HD12	2:S:265:LEU:HD11	1.98	0.44
3:A:111:LYS:O	3:A:115:VAL:HG23	2.18	0.44
3:A:304:THR:HG22	3:A:335:GLU:HB3	1.99	0.44
5:E:38:GLY:C	5:E:40:ILE:HG13	2.43	0.44
5:E:53:ILE:HG12	5:E:54:SER:H	1.82	0.44
7:U:100:LEU:HD21	7:U:121:VAL:HG21	2.00	0.44
9:X:69:GLN:HE21	9:X:101:ARG:NH1	2.15	0.44
9:X:452:ARG:NH2	9:X:584:TYR:O	2.30	0.44
9:X:577:VAL:HG13	9:X:578:TYR:H	1.83	0.44
9:X:933:VAL:HG11	9:X:945:ALA:HB2	1.99	0.44
9:X:994:ARG:HA	9:X:997:TRP:CE2	2.52	0.44
10:Y:423:LEU:O	10:Y:434:ILE:HD12	2.18	0.44
10:Y:513:MET:HE2	10:Y:631:TYR:CG	2.53	0.44
10:Y:770:LEU:HD23	10:Y:770:LEU:HA	1.87	0.44
11:C:121:LYS:HA	11:C:131:ASN:HD21	1.82	0.44
13:L:-11:DA:H2"	13:L:-10:DT:H71	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:46:THR:OG1	6:G:62:ARG:O	2.24	0.44
7:U:61:ILE:HG12	7:U:142:MET:HB3	1.99	0.44
7:V:104:LYS:HD2	7:V:105:SER:O	2.18	0.44
9:X:728:ASP:O	9:X:769:PRO:HG3	2.18	0.44
9:X:960:LEU:HD23	9:X:960:LEU:HA	1.78	0.44
9:X:1001:GLY:C	9:X:1002:LEU:HD12	2.42	0.44
9:X:1217:THR:OG1	9:X:1219:GLU:HG2	2.16	0.44
10:Y:378:LYS:HB3	10:Y:379:PRO:HD3	2.00	0.44
10:Y:876:SER:O	10:Y:876:SER:OG	2.36	0.44
10:Y:1062:LEU:O	10:Y:1067:ARG:NH2	2.49	0.44
13:L:-4:DC:H2''	13:L:-3:DA:H8	1.83	0.44
2:S:33:GLN:HG2	2:S:39:PHE:CD1	2.52	0.44
3:A:50:ASP:HB3	3:A:53:SER:OG	2.18	0.44
3:A:214:PRO:HD2	3:A:258:ARG:HH12	1.82	0.44
7:U:314:LEU:HD23	7:U:314:LEU:HA	1.83	0.44
7:V:29:GLU:HA	7:V:30:PRO:HA	1.79	0.44
7:V:39:LEU:HA	7:V:39:LEU:HD23	1.69	0.44
9:X:454:ARG:HG2	9:X:459:MET:HG3	2.00	0.44
9:X:788:SER:OG	9:X:788:SER:O	2.35	0.44
10:Y:58:CYS:O	10:Y:61:ILE:HG22	2.17	0.44
10:Y:495:ASN:C	10:Y:497:GLU:H	2.26	0.44
10:Y:647:PRO:HD3	10:Y:697:MET:HG2	1.98	0.44
10:Y:751:ASP:OD1	10:Y:752:GLY:N	2.51	0.44
10:Y:782:GLY:O	10:Y:786:THR:HG23	2.18	0.44
10:Y:1250:ASP:O	10:Y:1254:GLU:HB2	2.18	0.44
11:C:117:LEU:HD23	11:C:117:LEU:HA	1.83	0.44
11:C:160:GLU:HG2	12:R:57:U:OP2	2.18	0.44
2:S:33:GLN:HG2	2:S:39:PHE:HD1	1.83	0.44
3:A:17:ALA:HB2	3:A:125:MET:SD	2.58	0.44
3:A:93:VAL:HG11	7:U:297:LYS:HD2	2.00	0.44
4:B:5:ALA:O	4:B:9:ALA:HB2	2.18	0.44
4:B:122:PHE:HA	12:R:38:U:H4'	1.98	0.44
6:G:135:ARG:HA	6:G:145:ASN:HA	1.99	0.44
9:X:202:ARG:HG3	9:X:369:MET:HG2	2.00	0.44
9:X:670:PHE:HZ	9:X:1195:ILE:HD11	1.81	0.44
9:X:728:ASP:OD1	9:X:729:ALA:N	2.48	0.44
9:X:797:GLY:N	9:X:1231:TYR:OH	2.50	0.44
9:X:1223:ARG:HB3	9:X:1223:ARG:CZ	2.48	0.44
9:X:1259:LEU:HD11	12:R:76:G:H5''	2.00	0.44
9:X:1261:GLY:HA2	13:L:5:DA:OP1	2.17	0.44
10:Y:174:ASP:O	10:Y:175:GLU:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:121:ARG:HB2	2:S:123:GLU:HG3	2.00	0.44
6:G:52:ILE:HG13	6:G:53:ARG:HG3	2.00	0.44
7:U:231:PHE:HE2	7:V:39:LEU:HD13	1.82	0.44
9:X:250:THR:OG1	9:X:267:ARG:HB2	2.17	0.44
9:X:557:ARG:NH1	9:X:611:GLU:OE1	2.50	0.44
10:Y:70:CYS:SG	10:Y:85:CYS:HB2	2.57	0.44
10:Y:320:ASN:O	10:Y:322:ARG:N	2.50	0.44
10:Y:903:LEU:C	10:Y:905:ARG:H	2.26	0.44
1:T:98:HIS:CE1	1:T:190:LEU:HD13	2.53	0.43
2:S:210:PRO:HA	2:S:213:PHE:CE2	2.53	0.43
5:E:4:GLN:O	5:E:6:ILE:HD12	2.18	0.43
7:U:222:THR:HA	7:V:232:VAL:HG12	2.00	0.43
7:V:5:VAL:HG23	7:V:7:GLU:H	1.83	0.43
7:V:33:ARG:HD2	7:V:33:ARG:O	2.18	0.43
8:W:12:LYS:HD3	8:W:12:LYS:HA	1.83	0.43
9:X:62:TYR:CD1	9:X:480:SER:HA	2.53	0.43
9:X:232:ILE:HD11	9:X:333:ILE:HD12	2.00	0.43
9:X:315:MET:HG3	9:X:316:GLU:H	1.82	0.43
9:X:646:SER:OG	9:X:649:GLN:HB2	2.18	0.43
10:Y:298:MET:HE3	10:Y:298:MET:HB2	1.90	0.43
10:Y:1027:VAL:HG21	10:Y:1101:LEU:HD22	2.00	0.43
3:A:75:ILE:HG21	3:A:80:ALA:HB2	2.00	0.43
9:X:519:ASN:ND2	9:X:689:ALA:HB3	2.33	0.43
9:X:587:LEU:HD23	9:X:587:LEU:HA	1.88	0.43
9:X:815:SER:HB2	9:X:1077:SER:HB2	1.99	0.43
10:Y:1259:GLN:HE22	10:Y:1262:ARG:CZ	2.31	0.43
10:Y:1311:LYS:HE3	10:Y:1311:LYS:HB2	1.87	0.43
11:C:3:ARG:HD3	11:C:3:ARG:HA	1.72	0.43
1:T:62:HIS:CD2	1:T:79:VAL:HB	2.53	0.43
2:S:84:ASP:CG	2:S:86:LEU:O	2.59	0.43
3:A:140:GLY:HA3	3:A:152:LEU:HD21	2.00	0.43
3:A:149:ASN:HB3	3:A:163:LEU:HA	2.00	0.43
6:G:33:HIS:CD2	6:G:82:LEU:HD21	2.53	0.43
9:X:69:GLN:HE21	9:X:101:ARG:CZ	2.32	0.43
9:X:229:ILE:HG23	9:X:334:GLU:HG3	1.99	0.43
9:X:231:GLU:HG3	9:X:332:ARG:NH1	2.33	0.43
9:X:297:VAL:HA	9:X:335:THR:HG22	1.99	0.43
9:X:1117:LEU:HD12	9:X:1117:LEU:HA	1.84	0.43
10:Y:980:THR:OG1	10:Y:997:VAL:HG23	2.18	0.43
10:Y:1082:ASP:C	10:Y:1084:GLN:H	2.26	0.43
10:Y:1160:SER:HB2	10:Y:1205:GLU:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:154:ALA:O	2:S:203:PHE:HA	2.17	0.43
2:S:169:ILE:O	2:S:172:VAL:HB	2.19	0.43
2:S:181:ASP:OD1	2:S:182:PHE:N	2.51	0.43
3:A:456:LEU:HD21	3:A:488:ILE:HG21	1.99	0.43
5:E:25:ILE:O	5:E:28:THR:OG1	2.33	0.43
6:G:8:ARG:NH1	6:G:103:ILE:O	2.51	0.43
7:U:236:ASP:C	7:U:238:ARG:H	2.26	0.43
9:X:301:TYR:OH	9:X:333:ILE:HA	2.18	0.43
9:X:674:ASP:O	10:Y:772:TYR:HE1	2.02	0.43
9:X:1106:ARG:NH1	10:Y:731:ARG:HH22	2.17	0.43
9:X:1332:SER:HB3	10:Y:245:LEU:HD13	2.00	0.43
1:T:183:ARG:HE	2:S:91:ASN:HD21	1.66	0.43
2:S:254:LEU:HA	2:S:254:LEU:HD23	1.77	0.43
3:A:126:VAL:HA	3:A:129:GLN:OE1	2.19	0.43
3:A:183:LEU:HD12	3:A:196:PHE:O	2.18	0.43
3:A:308:ALA:HB2	3:A:338:VAL:HA	1.99	0.43
9:X:185:ASP:OD1	9:X:197:ARG:HB3	2.17	0.43
9:X:802:VAL:HG23	9:X:1096:ILE:HG22	1.99	0.43
10:Y:822:MET:SD	10:Y:838:ARG:NH2	2.92	0.43
11:C:106:ALA:CA	11:C:162:ALA:HB2	2.48	0.43
11:C:132:ILE:HG22	11:C:134:SER:H	1.83	0.43
13:L:2:DG:H2'	13:L:3:DC:C6	2.53	0.43
1:T:63:THR:HG22	1:T:74:GLY:H	1.83	0.43
2:S:24:GLU:OE1	2:S:24:GLU:N	2.52	0.43
3:A:43:ILE:HG21	3:A:60:ARG:HG3	2.00	0.43
7:U:273:GLU:HG3	7:U:292:THR:OG1	2.18	0.43
9:X:329:GLY:HA3	9:X:330:HIS:CG	2.53	0.43
9:X:557:ARG:NH2	9:X:608:ALA:HA	2.33	0.43
10:Y:77:ARG:HB3	10:Y:80:HIS:ND1	2.33	0.43
10:Y:1149:ARG:NH1	10:Y:1218:HIS:HB2	2.34	0.43
10:Y:1273:ASP:OD1	10:Y:1273:ASP:N	2.50	0.43
1:T:52:ILE:O	1:T:56:ARG:HG2	2.19	0.43
1:T:209:ARG:HH22	1:T:238:LEU:C	2.26	0.43
2:S:166:THR:HG23	2:S:167:THR:N	2.33	0.43
3:A:100:VAL:HG23	3:A:103:ASP:OD2	2.18	0.43
7:U:249:PHE:CE2	7:U:321:TRP:HZ3	2.36	0.43
7:U:292:THR:HB	7:U:295:LEU:HG	2.01	0.43
9:X:298:ALA:HB2	9:X:336:LEU:HD21	2.00	0.43
9:X:1222:GLU:HG2	9:X:1223:ARG:HG3	2.00	0.43
9:X:1271:GLY:O	9:X:1275:VAL:HG23	2.19	0.43
10:Y:511:TYR:CG	10:Y:728:SER:HB3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:770:LEU:O	10:Y:774:ILE:HG13	2.18	0.43
10:Y:1044:GLN:HG2	10:Y:1045:THR:HG23	1.99	0.43
10:Y:1169:THR:HA	10:Y:1192:LYS:HE2	2.01	0.43
10:Y:1271:SER:OG	10:Y:1298:VAL:O	2.26	0.43
1:T:246:ASN:O	1:T:250:VAL:HG23	2.18	0.43
2:S:107:ILE:HG22	2:S:108:LYS:HG2	2.00	0.43
3:A:60:ARG:HG2	3:A:62:TRP:CE2	2.53	0.43
3:A:257:ALA:O	3:A:261:ALA:N	2.48	0.43
4:B:6:ARG:NH1	4:B:7:ARG:HG3	2.34	0.43
4:B:39:ASP:O	4:B:41:LYS:NZ	2.38	0.43
5:E:83:THR:O	5:E:87:LEU:HD23	2.19	0.43
10:Y:151:MET:N	10:Y:175:GLU:OE1	2.52	0.43
13:L:17:DC:H2''	13:L:18:DG:H8	1.84	0.43
3:A:63:LEU:HD13	3:A:73:LYS:HD2	2.00	0.43
3:A:340:THR:HG21	3:A:344:LEU:C	2.44	0.43
7:U:6:THR:OG1	7:U:7:GLU:OE1	2.30	0.43
9:X:186:PHE:CD1	9:X:196:VAL:HG22	2.54	0.43
10:Y:55:GLY:H	10:Y:58:CYS:HB2	1.83	0.43
10:Y:82:GLY:H	10:Y:92:VAL:HG13	1.84	0.43
10:Y:139:LEU:HD21	10:Y:185:ILE:HG13	1.99	0.43
10:Y:198:CYS:O	10:Y:221:ILE:HD11	2.19	0.43
10:Y:436:ALA:HB3	10:Y:485:MET:HA	2.01	0.43
10:Y:980:THR:O	10:Y:996:LYS:NZ	2.27	0.43
11:C:79:ALA:HB2	11:C:93:LEU:HD12	2.01	0.43
1:T:52:ILE:HA	1:T:55:ILE:HD12	2.00	0.43
2:S:210:PRO:HA	2:S:213:PHE:CZ	2.53	0.43
3:A:340:THR:HG23	3:A:345:GLN:HB3	2.00	0.43
6:G:80:TRP:CH2	6:G:84:ARG:HG3	2.54	0.43
6:G:138:ASP:HB2	6:G:177:GLN:CB	2.48	0.43
7:U:229:GLU:HA	7:U:232:VAL:HB	2.01	0.43
9:X:1111:GLN:HG3	9:X:1112:ILE:N	2.34	0.43
9:X:1239:VAL:HG23	10:Y:354:VAL:HG12	2.00	0.43
10:Y:495:ASN:ND2	10:Y:1247:LYS:O	2.36	0.43
10:Y:805:GLN:CD	10:Y:1348:LYS:HB2	2.44	0.43
10:Y:884:SER:OG	10:Y:887:SER:N	2.51	0.43
10:Y:1179:PRO:CD	10:Y:1184:ASP:HB3	2.45	0.43
10:Y:1284:ARG:O	10:Y:1287:ILE:HG12	2.18	0.43
14:K:7:DC:H2''	14:K:8:DG:N7	2.34	0.43
1:T:232:GLY:HA3	3:A:491:PHE:CE1	2.54	0.42
4:B:122:PHE:HB3	12:R:39:U:C5'	2.48	0.42
6:G:149:GLU:OE1	6:G:161:SER:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:70:THR:OG1	7:U:71:LYS:N	2.52	0.42
7:V:13:LEU:HB3	7:V:28:LEU:HD23	2.01	0.42
9:X:66:SER:HA	9:X:104:ILE:HA	2.01	0.42
9:X:670:PHE:CD2	9:X:1113:LEU:HB3	2.54	0.42
9:X:1096:ILE:HD13	9:X:1232:MET:HE2	2.01	0.42
10:Y:202:ARG:HE	10:Y:221:ILE:HG12	1.84	0.42
10:Y:749:LYS:O	10:Y:781:LYS:NZ	2.52	0.42
10:Y:1251:LYS:O	10:Y:1255:VAL:HG13	2.18	0.42
14:K:-15:DG:C2	14:K:-14:DC:C2	3.07	0.42
2:S:10:ARG:HH22	6:G:147:VAL:HG11	1.83	0.42
3:A:150:ILE:HD11	3:A:162:ILE:HD12	2.00	0.42
3:A:235:LYS:NZ	3:A:324:ASN:O	2.49	0.42
8:W:15:ASN:OD1	8:W:17:PHE:N	2.52	0.42
8:W:16:ARG:NE	10:Y:905:ARG:HE	2.15	0.42
9:X:153:PRO:O	9:X:401:GLY:HA2	2.19	0.42
9:X:302:ILE:HG22	9:X:309:LEU:HA	2.00	0.42
9:X:796:LEU:HB3	9:X:1233:LEU:HD22	2.00	0.42
10:Y:48:THR:O	10:Y:50:LYS:N	2.48	0.42
10:Y:156:ARG:NH1	10:Y:157:GLN:HE22	2.12	0.42
10:Y:210:SER:HB2	10:Y:213:LYS:HE2	2.01	0.42
10:Y:516:ASP:OD1	10:Y:516:ASP:N	2.51	0.42
10:Y:774:ILE:O	10:Y:777:HIS:HB2	2.19	0.42
1:T:128:THR:HG23	1:T:131:GLN:HB2	2.01	0.42
1:T:236:TYR:HB2	1:T:242:ILE:HD13	2.01	0.42
2:S:167:THR:O	2:S:171:ILE:HG13	2.19	0.42
7:U:265:ARG:HH11	7:U:294:ASN:HB3	1.84	0.42
9:X:241:LEU:HD12	9:X:241:LEU:HA	1.84	0.42
9:X:369:MET:HE3	9:X:369:MET:HB3	1.93	0.42
10:Y:279:LEU:O	10:Y:283:LEU:HD23	2.18	0.42
10:Y:705:THR:OG1	10:Y:716:GLN:O	2.37	0.42
10:Y:902:ASP:HB2	10:Y:909:ILE:HA	2.01	0.42
10:Y:1077:ALA:HB2	10:Y:1100:PHE:CE1	2.54	0.42
11:C:71:GLN:HA	11:C:74:ASN:ND2	2.34	0.42
13:L:6:DC:C2	13:L:7:DA:C8	3.07	0.42
1:T:22:ASN:O	1:T:25:THR:HG22	2.20	0.42
2:S:171:ILE:HG22	2:S:175:LEU:HD23	2.00	0.42
3:A:58:THR:OG1	3:A:97:ILE:HA	2.18	0.42
3:A:120:GLU:OE2	3:A:123:ARG:NH1	2.29	0.42
5:E:10:LEU:HD21	5:E:98:VAL:HG13	2.01	0.42
7:V:127:GLN:H	7:V:127:GLN:CD	2.26	0.42
9:X:510:GLN:O	9:X:510:GLN:NE2	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:594:VAL:HB	9:X:651:ASP:C	2.44	0.42
9:X:624:ASP:CG	9:X:628:HIS:HB2	2.44	0.42
10:Y:404:GLU:HA	10:Y:408:VAL:HG11	2.01	0.42
10:Y:790:THR:HG23	10:Y:791:ALA:N	2.35	0.42
10:Y:1051:ASP:N	10:Y:1056:LEU:O	2.43	0.42
1:T:83:ILE:HG22	1:T:85:PRO:HD3	2.00	0.42
3:A:247:PRO:CA	3:A:251:CYS:HB3	2.49	0.42
4:B:112:LYS:HE2	4:B:120:HIS:CD2	2.54	0.42
5:E:22:THR:HG21	5:E:72:ARG:HG3	2.00	0.42
7:U:45:ARG:NH2	7:V:34:GLY:O	2.50	0.42
9:X:1004:ASP:HA	9:X:1008:GLN:CB	2.48	0.42
9:X:1209:GLN:HE21	10:Y:640:GLY:HA3	1.85	0.42
10:Y:368:LEU:HD12	10:Y:368:LEU:HA	1.83	0.42
4:B:11:GLU:HG2	4:B:110:LEU:HB3	2.00	0.42
7:U:195:ARG:HG2	7:U:196:THR:N	2.34	0.42
7:V:118:ASP:OD1	7:V:119:GLY:N	2.47	0.42
9:X:75:LEU:HD23	9:X:75:LEU:HA	1.72	0.42
9:X:624:ASP:O	9:X:625:GLU:HB3	2.19	0.42
9:X:654:ASP:OD1	9:X:655:VAL:N	2.52	0.42
9:X:907:GLY:O	9:X:911:SER:OG	2.14	0.42
9:X:964:LEU:HA	9:X:1025:PHE:HE2	1.85	0.42
9:X:972:PHE:O	9:X:975:ILE:HG22	2.20	0.42
10:Y:664:ILE:HD13	10:Y:664:ILE:HA	1.86	0.42
10:Y:816:THR:HG21	10:Y:889:ASP:HB2	2.01	0.42
10:Y:1036:ARG:HE	10:Y:1085:GLY:C	2.27	0.42
11:C:110:THR:O	11:C:114:ALA:N	2.48	0.42
3:A:460:ALA:HB2	3:A:485:ALA:HB1	2.02	0.42
6:G:56:GLN:OE1	6:G:57:ARG:N	2.49	0.42
7:U:33:ARG:C	7:U:35:PHE:H	2.27	0.42
7:V:109:PRO:HA	7:V:132:HIS:HA	2.02	0.42
9:X:28:LEU:HD23	9:X:28:LEU:HA	1.80	0.42
9:X:523:GLU:HG2	9:X:527:LYS:HE3	2.00	0.42
9:X:990:ASP:OD1	9:X:990:ASP:N	2.53	0.42
6:G:108:VAL:O	6:G:112:MET:HG2	2.20	0.42
7:U:233:ASP:O	7:U:235:ARG:NE	2.52	0.42
9:X:56:VAL:HG21	9:X:468:LEU:HG	2.01	0.42
9:X:65:ASN:O	9:X:105:TYR:N	2.35	0.42
9:X:305:SER:O	9:X:305:SER:OG	2.38	0.42
9:X:1212:LEU:HD23	9:X:1212:LEU:HA	1.82	0.42
9:X:1274:GLU:OE1	9:X:1274:GLU:N	2.44	0.42
10:Y:254:PRO:HA	10:Y:260:PHE:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:555:TYR:CD2	10:Y:585:LYS:HB3	2.55	0.42
10:Y:818:GLU:OE1	10:Y:818:GLU:N	2.51	0.42
10:Y:1215:GLU:OE1	10:Y:1215:GLU:N	2.52	0.42
3:A:48:GLN:HB2	3:A:59:PHE:CZ	2.55	0.42
3:A:200:SER:HA	3:A:228:ARG:NH2	2.35	0.42
3:A:332:SER:C	3:A:334:TRP:H	2.27	0.42
3:A:335:GLU:OE2	12:R:50:C:O2'	2.37	0.42
7:U:133:LEU:HD11	7:U:140:ILE:HG12	2.01	0.42
7:U:278:ILE:HG12	7:U:281:LEU:HD21	2.02	0.42
7:V:182:ARG:HB3	10:Y:531:LYS:HB3	2.02	0.42
9:X:771:VAL:HG11	9:X:783:LEU:HD22	2.01	0.42
9:X:1291:LEU:HA	9:X:1291:LEU:HD23	1.85	0.42
10:Y:107:LEU:HD12	10:Y:240:THR:C	2.45	0.42
10:Y:127:LEU:HG	10:Y:192:MET:HE1	2.02	0.42
2:S:148:LEU:HA	2:S:148:LEU:HD23	1.79	0.42
3:A:260:GLN:O	3:A:263:SER:OG	2.30	0.42
5:E:37:ARG:HH21	5:E:77:VAL:HG21	1.84	0.42
6:G:29:HIS:O	6:G:32:LEU:HB3	2.20	0.42
6:G:136:VAL:HG12	6:G:138:ASP:H	1.84	0.42
7:U:43:LEU:HD23	7:U:43:LEU:HA	1.91	0.42
7:U:304:LYS:HB3	7:U:314:LEU:HD11	2.01	0.42
7:V:43:LEU:HD13	7:V:43:LEU:HA	1.94	0.42
9:X:832:HIS:ND1	9:X:1058:ARG:HD2	2.35	0.42
9:X:963:GLU:HA	9:X:966:ILE:HG22	2.02	0.42
10:Y:964:LYS:O	10:Y:976:THR:OG1	2.31	0.42
10:Y:1072:LYS:NZ	10:Y:1168:GLU:HB2	2.35	0.42
11:C:104:ARG:HE	11:C:168:PRO:HG3	1.84	0.42
14:K:12:DA:H2''	14:K:13:DA:C8	2.55	0.42
1:T:156:GLY:O	1:T:168:TYR:OH	2.34	0.41
3:A:48:GLN:C	3:A:50:ASP:H	2.28	0.41
5:E:4:GLN:O	5:E:6:ILE:N	2.51	0.41
5:E:6:ILE:HG13	5:E:102:LEU:HD13	2.02	0.41
5:E:7:ARG:HG2	5:E:75:ASP:HB3	2.01	0.41
5:E:14:ASP:OD1	5:E:15:HIS:N	2.53	0.41
5:E:32:THR:HG21	5:E:83:THR:N	2.35	0.41
6:G:68:TYR:OH	10:Y:295:GLU:OE1	2.25	0.41
7:U:262:LEU:HB3	7:U:306:VAL:HG21	2.01	0.41
7:V:107:ILE:O	7:V:133:LEU:HB3	2.19	0.41
9:X:105:TYR:HD2	9:X:112:GLY:H	1.68	0.41
9:X:106:GLU:OE1	9:X:114:VAL:HG13	2.20	0.41
9:X:899:GLU:HA	9:X:902:LEU:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:1332:SER:O	10:Y:243:PRO:HG2	2.19	0.41
10:Y:97:VAL:HG22	10:Y:101:ARG:HG3	2.00	0.41
10:Y:789:LYS:HZ3	10:Y:928:THR:C	2.27	0.41
10:Y:1045:THR:HA	10:Y:1067:ARG:CD	2.49	0.41
11:C:103:TYR:HB2	11:C:111:ARG:HG2	2.01	0.41
2:S:141:ARG:HD2	2:S:141:ARG:HA	1.70	0.41
3:A:208:LEU:HD22	3:A:262:VAL:CG2	2.49	0.41
6:G:68:TYR:CD2	10:Y:291:ILE:HD12	2.55	0.41
9:X:1014:LEU:HA	9:X:1017:GLN:OE1	2.20	0.41
10:Y:580:TRP:CZ3	10:Y:583:VAL:HG21	2.55	0.41
10:Y:1161:GLY:HA3	10:Y:1178:THR:O	2.20	0.41
10:Y:1234:VAL:HA	10:Y:1253:ILE:HD12	2.01	0.41
2:S:21:LYS:HE3	2:S:21:LYS:HB3	1.93	0.41
2:S:253:MET:HB3	2:S:253:MET:HE2	1.78	0.41
6:G:80:TRP:CZ3	6:G:84:ARG:HG3	2.56	0.41
7:U:158:ARG:NH2	7:U:173:VAL:O	2.53	0.41
9:X:99:LYS:HG2	9:X:120:GLN:HB3	2.01	0.41
9:X:196:VAL:HG23	9:X:206:ALA:CA	2.50	0.41
9:X:599:VAL:H	9:X:627:GLY:CA	2.33	0.41
9:X:622:ASN:OD1	9:X:622:ASN:N	2.53	0.41
9:X:633:LEU:HD13	9:X:633:LEU:HA	1.93	0.41
9:X:834:GLN:NE2	9:X:924:VAL:HG21	2.35	0.41
9:X:1109:ILE:HD12	9:X:1109:ILE:HA	1.86	0.41
9:X:1333:LEU:C	9:X:1335:ILE:H	2.28	0.41
10:Y:347:VAL:HG22	10:Y:348:ASP:H	1.85	0.41
10:Y:421:VAL:HG22	10:Y:422:LEU:H	1.86	0.41
10:Y:664:ILE:O	10:Y:667:GLN:HB2	2.20	0.41
11:C:171:LEU:HD13	11:C:182:PHE:CD2	2.51	0.41
3:A:341:VAL:C	3:A:345:GLN:HG2	2.45	0.41
9:X:577:VAL:HG13	9:X:578:TYR:N	2.34	0.41
9:X:783:LEU:HD23	9:X:783:LEU:HA	1.83	0.41
9:X:798:GLN:OE1	9:X:827:ARG:NE	2.39	0.41
10:Y:98:ARG:O	10:Y:248:ASP:HB2	2.21	0.41
10:Y:350:SER:HA	10:Y:376:LEU:CD2	2.51	0.41
10:Y:1079:LYS:HE2	10:Y:1079:LYS:HB2	1.83	0.41
2:S:227:VAL:HG12	2:S:244:ALA:HB2	2.02	0.41
5:E:88:MET:HG2	6:G:164:ILE:HA	2.03	0.41
9:X:838:CYS:HB2	9:X:918:LEU:HD22	2.02	0.41
9:X:994:ARG:HA	9:X:997:TRP:NE1	2.35	0.41
10:Y:36:GLY:HA3	10:Y:61:ILE:HG13	2.02	0.41
10:Y:553:THR:HG22	10:Y:567:THR:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:605:LEU:HD23	10:Y:605:LEU:HA	1.80	0.41
10:Y:1035:VAL:HG11	10:Y:1109:LEU:HB3	2.02	0.41
3:A:31:LEU:HB3	3:A:47:VAL:HG21	2.02	0.41
3:A:293:VAL:HG11	3:A:307:ILE:HA	2.03	0.41
6:G:111:ILE:HD13	6:G:111:ILE:HA	1.92	0.41
6:G:157:ARG:NH2	6:G:172:GLU:O	2.53	0.41
9:X:429:MET:O	9:X:433:ILE:HG13	2.21	0.41
9:X:936:ARG:HB2	9:X:1047:LEU:HA	2.02	0.41
9:X:972:PHE:HD2	9:X:994:ARG:CZ	2.34	0.41
10:Y:245:LEU:HD12	10:Y:245:LEU:HA	1.96	0.41
10:Y:462:ASP:OD1	10:Y:462:ASP:N	2.50	0.41
10:Y:1033:GLY:O	10:Y:1115:ILE:HG12	2.20	0.41
1:T:208:LEU:HG	1:T:209:ARG:H	1.85	0.41
6:G:116:GLN:O	6:G:120:ASP:HB2	2.20	0.41
6:G:129:GLU:N	6:G:132:GLU:OE2	2.31	0.41
7:U:13:LEU:HD21	7:U:16:ILE:HG13	2.02	0.41
7:V:35:PHE:O	7:V:38:THR:HG22	2.21	0.41
7:V:136:GLU:HG3	7:V:137:ASN:HB2	2.03	0.41
9:X:105:TYR:HA	9:X:112:GLY:O	2.20	0.41
9:X:777:VAL:HG11	9:X:783:LEU:HD21	2.03	0.41
9:X:801:ARG:HB2	9:X:1229:TYR:CZ	2.55	0.41
9:X:982:GLY:C	9:X:984:VAL:HA	2.46	0.41
10:Y:43:THR:OG1	10:Y:44:ILE:N	2.52	0.41
10:Y:1050:THR:HA	10:Y:1057:SER:HA	2.02	0.41
7:U:39:LEU:HA	7:U:39:LEU:HD23	1.88	0.41
7:U:155:ALA:HA	7:U:158:ARG:CZ	2.49	0.41
7:V:97:GLU:OE2	7:V:147:GLN:NE2	2.54	0.41
9:X:238:GLN:NE2	9:X:284:LEU:HB2	2.35	0.41
9:X:407:ARG:NE	9:X:609:ILE:HD12	2.36	0.41
9:X:542:ARG:HD3	14:K:1:DT:P	2.60	0.41
9:X:755:LYS:HA	9:X:755:LYS:HD2	1.76	0.41
10:Y:530:PRO:HB3	10:Y:577:ALA:O	2.20	0.41
10:Y:573:THR:HG23	10:Y:576:ARG:H	1.85	0.41
10:Y:827:GLU:N	10:Y:827:GLU:OE2	2.53	0.41
10:Y:1143:ASP:CG	10:Y:1148:ARG:HE	2.27	0.41
10:Y:1325:PHE:CE2	10:Y:1326:GLN:HB2	2.56	0.41
11:C:172:GLU:HB2	11:C:181:THR:OG1	2.20	0.41
13:L:-14:DG:H2'	13:L:-13:DT:H71	2.02	0.41
1:T:84:ASP:HB3	1:T:102:SER:OG	2.21	0.41
1:T:254:LEU:HD22	1:T:258:ARG:HG3	2.03	0.41
3:A:24:PHE:O	3:A:28:GLU:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:58:THR:C	3:A:59:PHE:HD1	2.29	0.41
3:A:139:THR:HG22	3:A:180:ARG:HG2	2.02	0.41
4:B:11:GLU:HB3	4:B:110:LEU:HB3	2.03	0.41
4:B:87:ILE:O	4:B:91:GLU:HG3	2.21	0.41
4:B:100:TYR:CE1	4:B:104:ILE:HG13	2.56	0.41
6:G:128:PHE:HE2	6:G:178:VAL:HG11	1.85	0.41
9:X:12:ARG:HG3	9:X:1181:PRO:HB2	2.01	0.41
9:X:196:VAL:HG21	9:X:209:ILE:HG22	2.03	0.41
9:X:315:MET:HG3	9:X:316:GLU:N	2.36	0.41
9:X:510:GLN:OE1	12:R:81:G:H5"	2.21	0.41
9:X:542:ARG:NH1	14:K:1:DT:H72	2.35	0.41
9:X:841:ARG:O	9:X:848:GLU:HG2	2.21	0.41
9:X:1113:LEU:HD23	9:X:1113:LEU:HA	1.84	0.41
9:X:1320:PRO:HB3	10:Y:345:LYS:NZ	2.35	0.41
10:Y:347:VAL:HG11	10:Y:469:HIS:CE1	2.56	0.41
10:Y:350:SER:CB	10:Y:469:HIS:HA	2.50	0.41
10:Y:355:ILE:HG21	10:Y:466:MET:SD	2.61	0.41
10:Y:363:LEU:HA	10:Y:450:HIS:CD2	2.56	0.41
10:Y:405:GLU:O	10:Y:408:VAL:N	2.42	0.41
10:Y:529:GLY:O	10:Y:532:GLU:HB3	2.21	0.41
10:Y:625:MET:HE3	10:Y:625:MET:HB3	1.77	0.41
10:Y:1267:VAL:HB	10:Y:1301:THR:OG1	2.21	0.41
11:C:149:ALA:HB1	11:C:152:GLN:OE1	2.20	0.41
13:L:-12:DT:H2"	13:L:-11:DA:O5'	2.19	0.41
1:T:163:GLN:HG2	1:T:164:TYR:N	2.36	0.41
3:A:18:LEU:HD22	3:A:23:ILE:HD11	2.03	0.41
3:A:129:GLN:O	3:A:132:GLU:HB2	2.21	0.41
3:A:399:ASP:N	3:A:402:THR:HB	2.36	0.41
4:B:18:TYR:OH	5:E:72:ARG:NE	2.38	0.41
6:G:105:ASP:OD1	6:G:106:LYS:N	2.54	0.41
7:U:61:ILE:HG22	7:U:62:ASP:OD1	2.21	0.41
7:U:262:LEU:HA	7:U:302:GLU:OE1	2.21	0.41
8:W:56:GLU:HB3	8:W:58:LEU:HD22	2.03	0.41
9:X:62:TYR:H	9:X:62:TYR:HD1	1.67	0.41
9:X:356:THR:HB	9:X:361:SER:OG	2.21	0.41
9:X:1132:LEU:HA	9:X:1132:LEU:HD23	1.86	0.41
10:Y:97:VAL:C	10:Y:99:ARG:H	2.29	0.41
10:Y:537:TYR:CZ	10:Y:544:LEU:HD13	2.56	0.41
10:Y:1177:ILE:HB	10:Y:1186:TYR:OH	2.20	0.41
11:C:6:GLY:HA3	11:C:7:PRO:HD3	1.84	0.41
11:C:39:GLY:O	11:C:42:GLY:N	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:64:VAL:HG12	3:A:77:LEU:HD23	2.04	0.40
3:A:188:PRO:O	3:A:194:GLN:NE2	2.53	0.40
4:B:92:LEU:HD23	4:B:134:ILE:HG13	2.03	0.40
7:U:167:PRO:HG2	7:U:170:ARG:CG	2.49	0.40
7:V:82:LEU:HD23	7:V:82:LEU:HA	1.87	0.40
9:X:308:GLU:HG2	9:X:309:LEU:HD23	2.02	0.40
9:X:980:VAL:HG23	9:X:986:ALA:HB2	2.03	0.40
9:X:1306:LYS:HB2	9:X:1306:LYS:HE3	1.86	0.40
10:Y:559:ALA:HB3	10:Y:562:GLU:CD	2.47	0.40
11:C:161:LEU:HG	12:R:56:A:OP1	2.20	0.40
1:T:171:ILE:HD11	1:T:260:GLU:HB2	2.02	0.40
2:S:117:TYR:HD2	2:S:124:LEU:HD13	1.85	0.40
3:A:79:ALA:HB2	7:U:287:VAL:HG22	2.03	0.40
3:A:392:LEU:HA	3:A:392:LEU:HD23	1.86	0.40
7:U:275:ILE:HG13	7:U:284:ARG:NH1	2.36	0.40
9:X:208:ILE:HG23	9:X:209:ILE:N	2.37	0.40
9:X:577:VAL:HG13	9:X:578:TYR:HD1	1.86	0.40
9:X:660:VAL:HG21	10:Y:769:VAL:CG1	2.51	0.40
9:X:811:ASN:HA	9:X:815:SER:OG	2.21	0.40
9:X:1256:GLN:HE21	10:Y:99:ARG:HH22	1.68	0.40
10:Y:100:GLU:N	10:Y:100:GLU:OE1	2.54	0.40
10:Y:152:THR:OG1	10:Y:153:ASN:N	2.53	0.40
10:Y:473:THR:HG23	10:Y:476:ALA:H	1.85	0.40
10:Y:828:GLY:HA2	10:Y:994:SER:O	2.20	0.40
10:Y:1369:ARG:HA	10:Y:1373:ARG:HD2	2.04	0.40
10:Y:1370:MET:HA	10:Y:1374:ALA:HB3	2.03	0.40
11:C:55:LEU:HD23	11:C:55:LEU:HA	1.95	0.40
3:A:244:ARG:HE	4:B:72:ARG:HD2	1.85	0.40
4:B:82:LYS:HE2	4:B:82:LYS:HB2	1.86	0.40
6:G:32:LEU:HD13	9:X:62:TYR:HD2	1.86	0.40
6:G:135:ARG:HB2	6:G:179:GLU:CB	2.52	0.40
9:X:1162:SER:C	9:X:1164:PHE:H	2.29	0.40
10:Y:113:HIS:HB2	10:Y:239:LEU:HD23	2.03	0.40
10:Y:141:PHE:CZ	10:Y:296:LYS:HB3	2.57	0.40
14:K:-19:DC:C6	14:K:-19:DC:H5'	2.57	0.40
3:A:6:LEU:HD23	3:A:6:LEU:HA	1.89	0.40
3:A:114:ILE:HD13	3:A:114:ILE:HA	1.91	0.40
3:A:392:LEU:HD21	3:A:403:VAL:HG21	2.04	0.40
6:G:163:SER:O	6:G:163:SER:OG	2.40	0.40
7:V:104:LYS:HE3	7:V:104:LYS:HB3	1.84	0.40
8:W:24:ALA:HA	10:Y:478:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:43:ASN:HB3	10:Y:417:ARG:NH2	2.37	0.40
9:X:26:TYR:CE2	9:X:28:LEU:HB2	2.56	0.40
9:X:169:LYS:HD2	9:X:169:LYS:HA	1.79	0.40
9:X:577:VAL:HG13	9:X:578:TYR:CD1	2.56	0.40
9:X:645:PHE:HB3	9:X:649:GLN:HB3	2.03	0.40
9:X:1225:VAL:HG22	9:X:1226:THR:N	2.36	0.40
9:X:1269:ARG:NH1	10:Y:340:GLN:HA	2.37	0.40
9:X:1331:ARG:HE	9:X:1331:ARG:HB2	1.58	0.40
10:Y:30:ILE:HA	10:Y:33:TRP:CE3	2.56	0.40
10:Y:135:ILE:O	10:Y:139:LEU:HD23	2.21	0.40
10:Y:1196:LEU:HD13	10:Y:1198:VAL:O	2.22	0.40
11:C:86:THR:HA	11:C:89:ASN:CG	2.46	0.40
11:C:101:VAL:O	11:C:105:MET:HG2	2.22	0.40
11:C:163:GLU:HG2	11:C:167:LYS:HZ1	1.86	0.40
14:K:3:DT:H2''	14:K:4:DG:H8	1.86	0.40
1:T:124:LEU:HB3	1:T:136:ASN:OD1	2.22	0.40
3:A:17:ALA:HB1	3:A:121:ALA:HB1	2.03	0.40
3:A:224:LYS:HA	3:A:224:LYS:HD2	1.92	0.40
3:A:409:ARG:HD3	3:A:409:ARG:HA	1.84	0.40
4:B:10:ARG:O	4:B:14:VAL:HG13	2.22	0.40
5:E:35:GLN:H	5:E:78:GLU:HB3	1.85	0.40
7:U:256:PRO:HD2	7:U:259:ASP:OD2	2.21	0.40
9:X:14:ASP:HA	9:X:1183:ALA:HB3	2.03	0.40
9:X:297:VAL:HG21	9:X:301:TYR:HE2	1.87	0.40
9:X:311:CYS:SG	9:X:325:LEU:HB3	2.61	0.40
10:Y:707:ILE:O	10:Y:714:GLU:N	2.45	0.40
13:L:4:DC:C3'	13:L:5:DA:H8	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	T	251/267 (94%)	228 (91%)	23 (9%)	0	100	100
2	S	265/271 (98%)	248 (94%)	17 (6%)	0	100	100
3	A	493/497 (99%)	414 (84%)	79 (16%)	0	100	100
4	B	132/141 (94%)	116 (88%)	16 (12%)	0	100	100
5	E	94/106 (89%)	81 (86%)	13 (14%)	0	100	100
6	G	176/184 (96%)	153 (87%)	23 (13%)	0	100	100
7	U	320/329 (97%)	274 (86%)	46 (14%)	0	100	100
7	V	218/329 (66%)	189 (87%)	28 (13%)	1 (0%)	24	57
8	W	88/91 (97%)	80 (91%)	8 (9%)	0	100	100
9	X	1340/1342 (100%)	1197 (89%)	142 (11%)	1 (0%)	48	79
10	Y	1331/1417 (94%)	1189 (89%)	141 (11%)	1 (0%)	48	79
11	C	203/208 (98%)	188 (93%)	15 (7%)	0	100	100
All	All	4911/5182 (95%)	4357 (89%)	551 (11%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	V	94	GLY
9	X	627	GLY
10	Y	351	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	T	202/209 (97%)	202 (100%)	0	100	100
2	S	210/212 (99%)	210 (100%)	0	100	100
3	A	408/408 (100%)	406 (100%)	2 (0%)	81	81
4	B	111/116 (96%)	111 (100%)	0	100	100
5	E	86/92 (94%)	86 (100%)	0	100	100
6	G	155/160 (97%)	155 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	281/286 (98%)	281 (100%)	0	100	100
7	V	190/286 (66%)	190 (100%)	0	100	100
8	W	74/75 (99%)	74 (100%)	0	100	100
9	X	1157/1157 (100%)	1157 (100%)	0	100	100
10	Y	1120/1178 (95%)	1120 (100%)	0	100	100
11	C	172/173 (99%)	172 (100%)	0	100	100
All	All	4166/4352 (96%)	4164 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	68	VAL
3	A	341	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	42	ASN
1	T	62	HIS
1	T	98	HIS
1	T	177	ASN
2	S	37	ASN
3	A	146	ASN
3	A	172	ASN
3	A	241	ASN
3	A	337	ASN
3	A	349	GLN
3	A	419	GLN
3	A	428	ASN
4	B	58	ASN
5	E	3	ASN
5	E	4	GLN
5	E	35	GLN
5	E	70	HIS
6	G	13	GLN
6	G	33	HIS
6	G	81	HIS
6	G	177	GLN
7	U	23	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	128	HIS
7	U	227	GLN
7	U	294	ASN
7	V	137	ASN
8	W	31	GLN
9	X	193	ASN
9	X	238	GLN
9	X	330	HIS
9	X	494	ASN
9	X	613	ASN
9	X	686	GLN
9	X	824	GLN
9	X	834	GLN
9	X	894	GLN
9	X	1116	HIS
9	X	1129	ASN
9	X	1146	GLN
9	X	1157	GLN
9	X	1237	HIS
9	X	1256	GLN
9	X	1257	GLN
9	X	1268	GLN
9	X	1307	ASN
10	Y	157	GLN
10	Y	196	GLN
10	Y	209	ASN
10	Y	294	ASN
10	Y	320	ASN
10	Y	340	GLN
10	Y	341	ASN
10	Y	364	HIS
10	Y	435	GLN
10	Y	488	ASN
10	Y	489	ASN
10	Y	519	ASN
10	Y	560	ASN
10	Y	951	GLN
10	Y	1259	GLN
10	Y	1350	ASN
10	Y	1366	HIS
11	C	140	ASN
11	C	198	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	42/85 (49%)	20 (47%)	1 (2%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	31	C
12	R	32	U
12	R	33	G
12	R	35	U
12	R	38	U
12	R	39	U
12	R	40	A
12	R	41	A
12	R	42	C
12	R	43	A
12	R	45	U
12	R	48	A
12	R	51	A
12	R	52	G
12	R	57	U
12	R	59	U
12	R	60	G
12	R	61	U
12	R	62	G
12	R	65	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	R	31	C

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

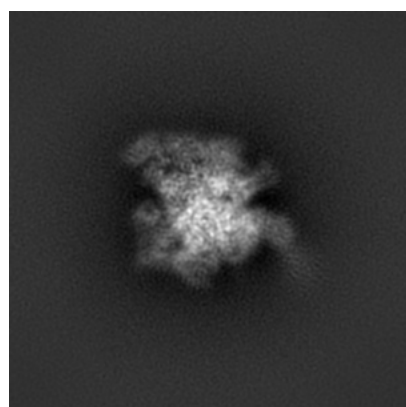
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10548. These allow visual inspection of the internal detail of the map and identification of artifacts.

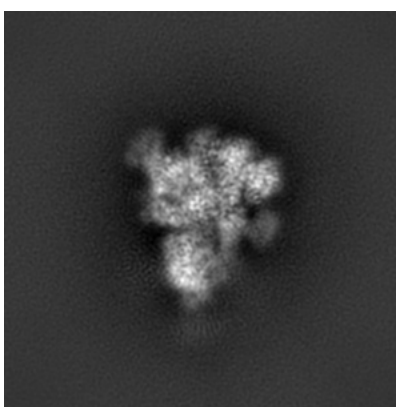
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

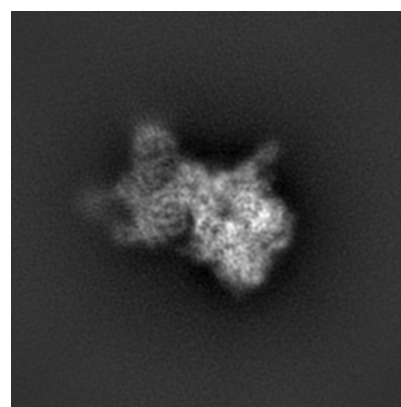
6.1.1 Primary map



X



Y

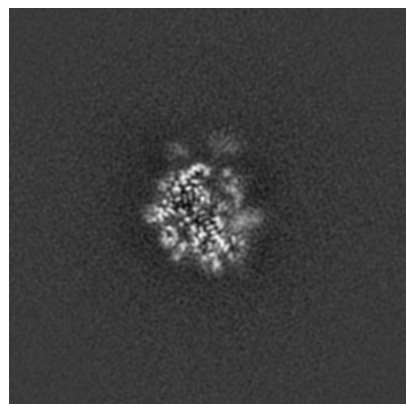


Z

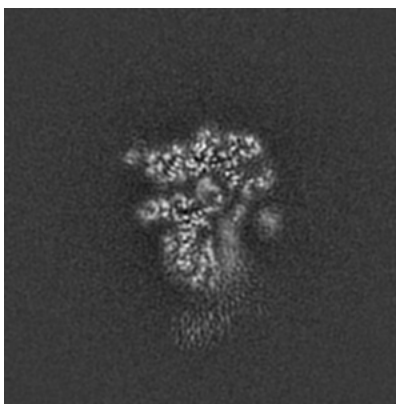
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

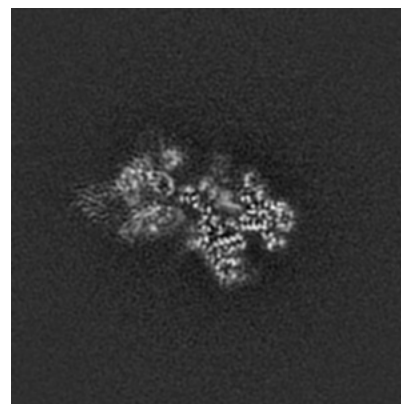
6.2.1 Primary map



X Index: 150



Y Index: 150

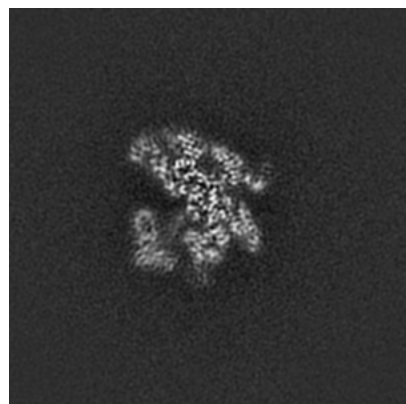


Z Index: 150

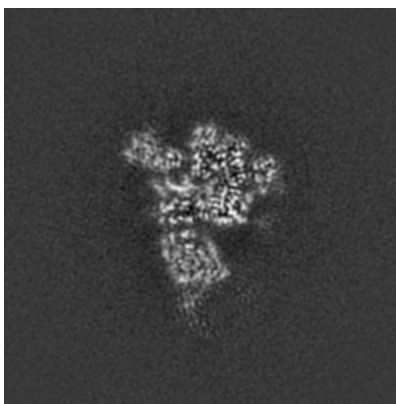
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

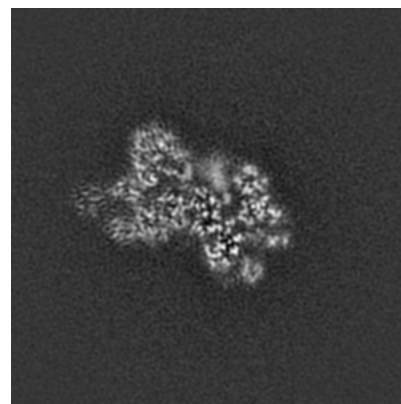
6.3.1 Primary map



X Index: 181



Y Index: 140

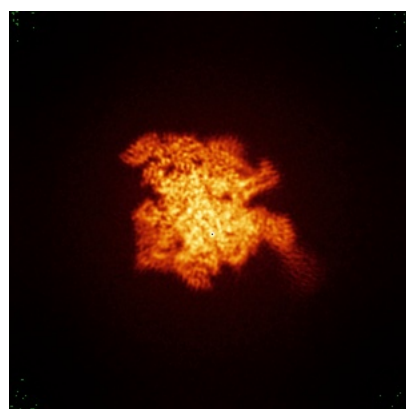


Z Index: 141

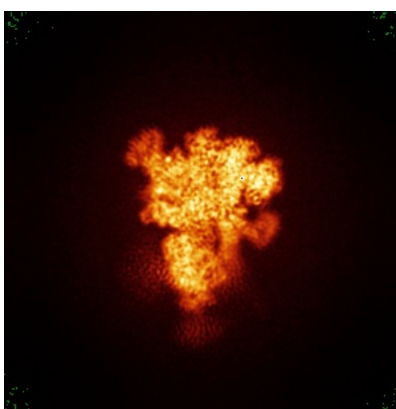
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

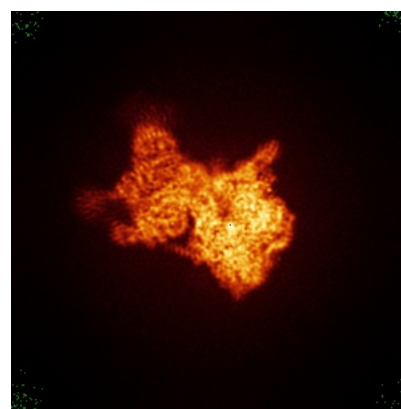
6.4.1 Primary map



X



Y

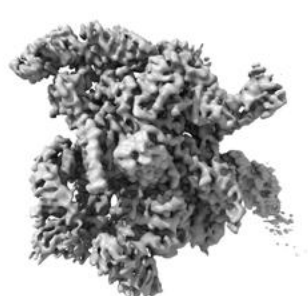


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

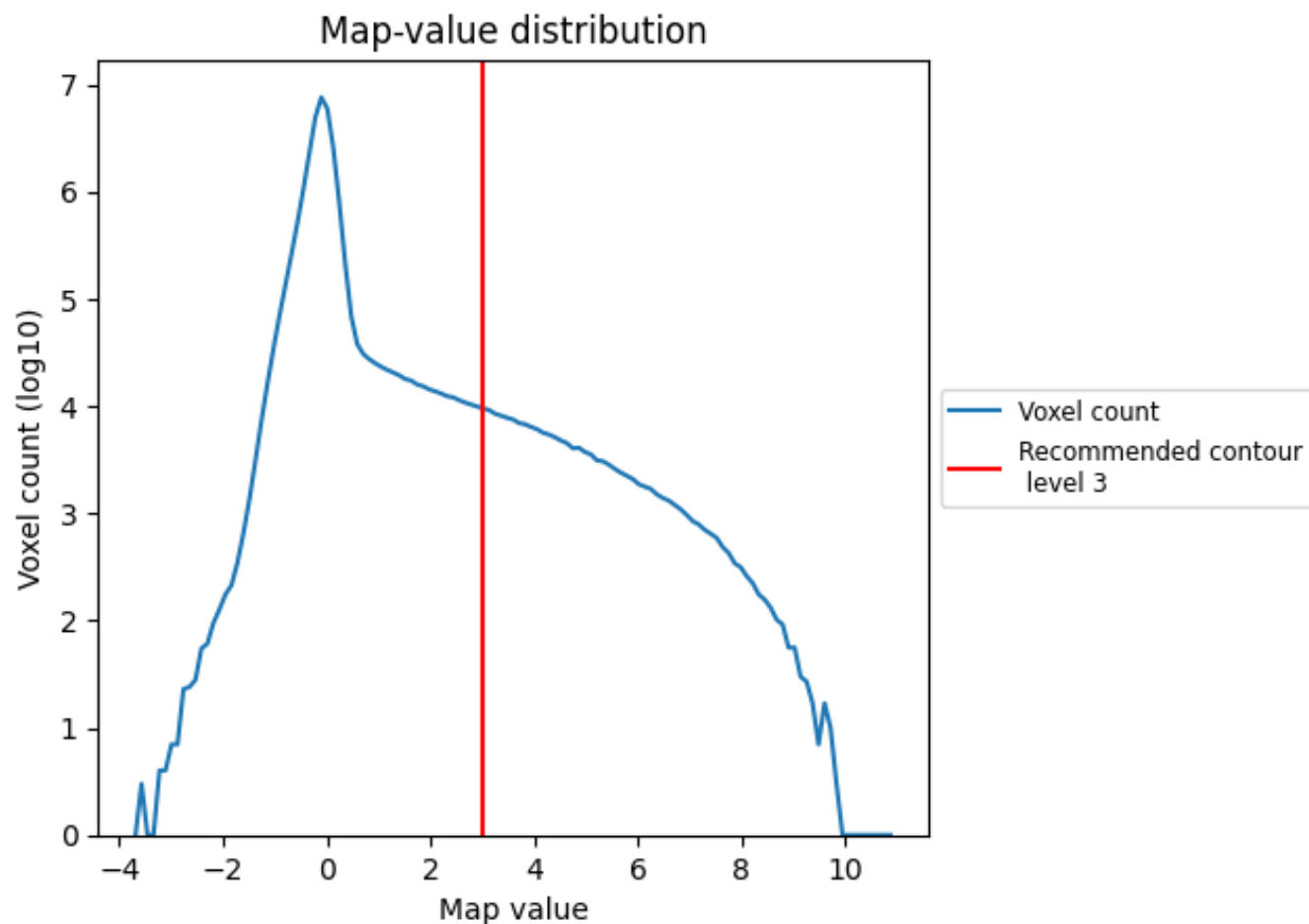
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

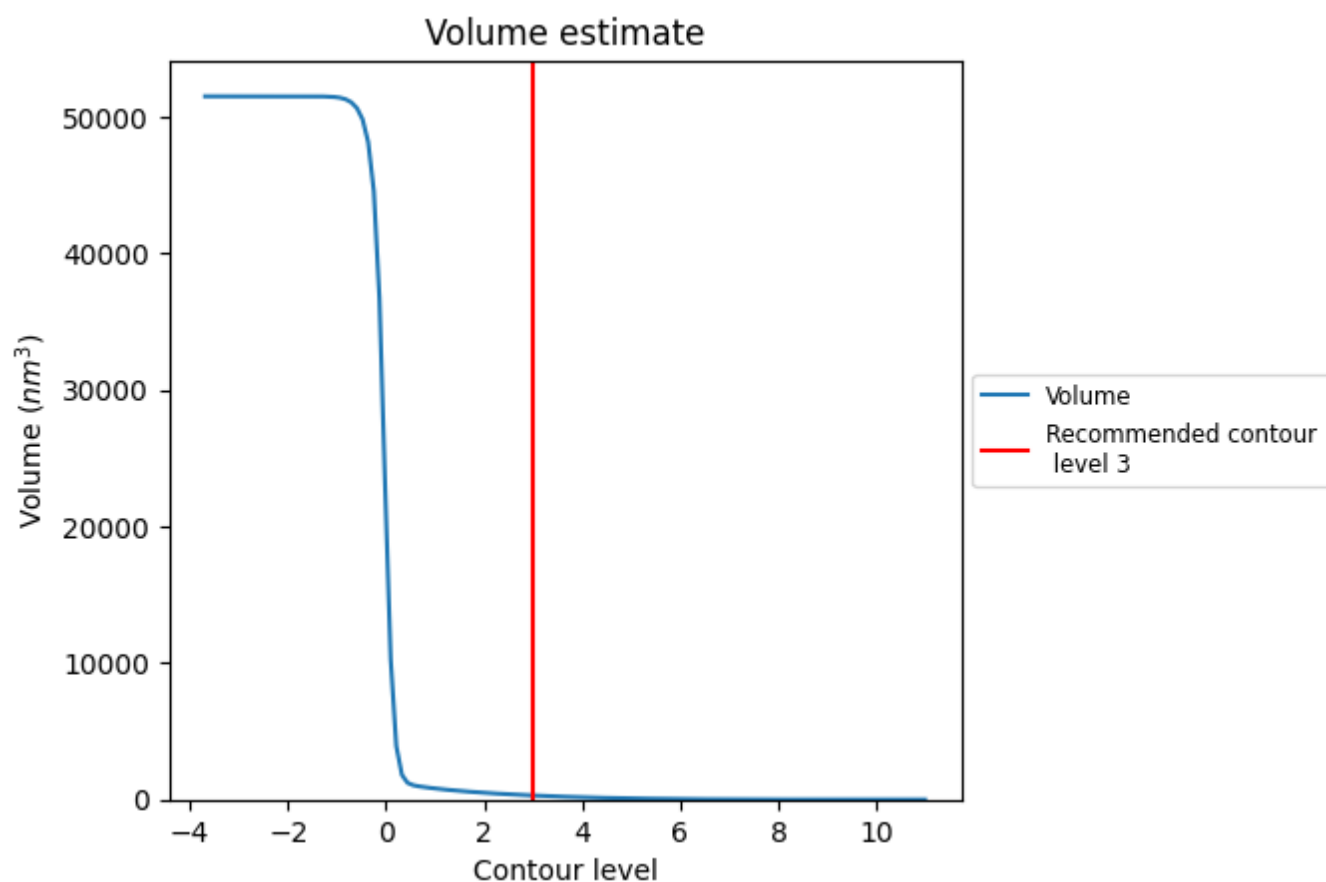
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

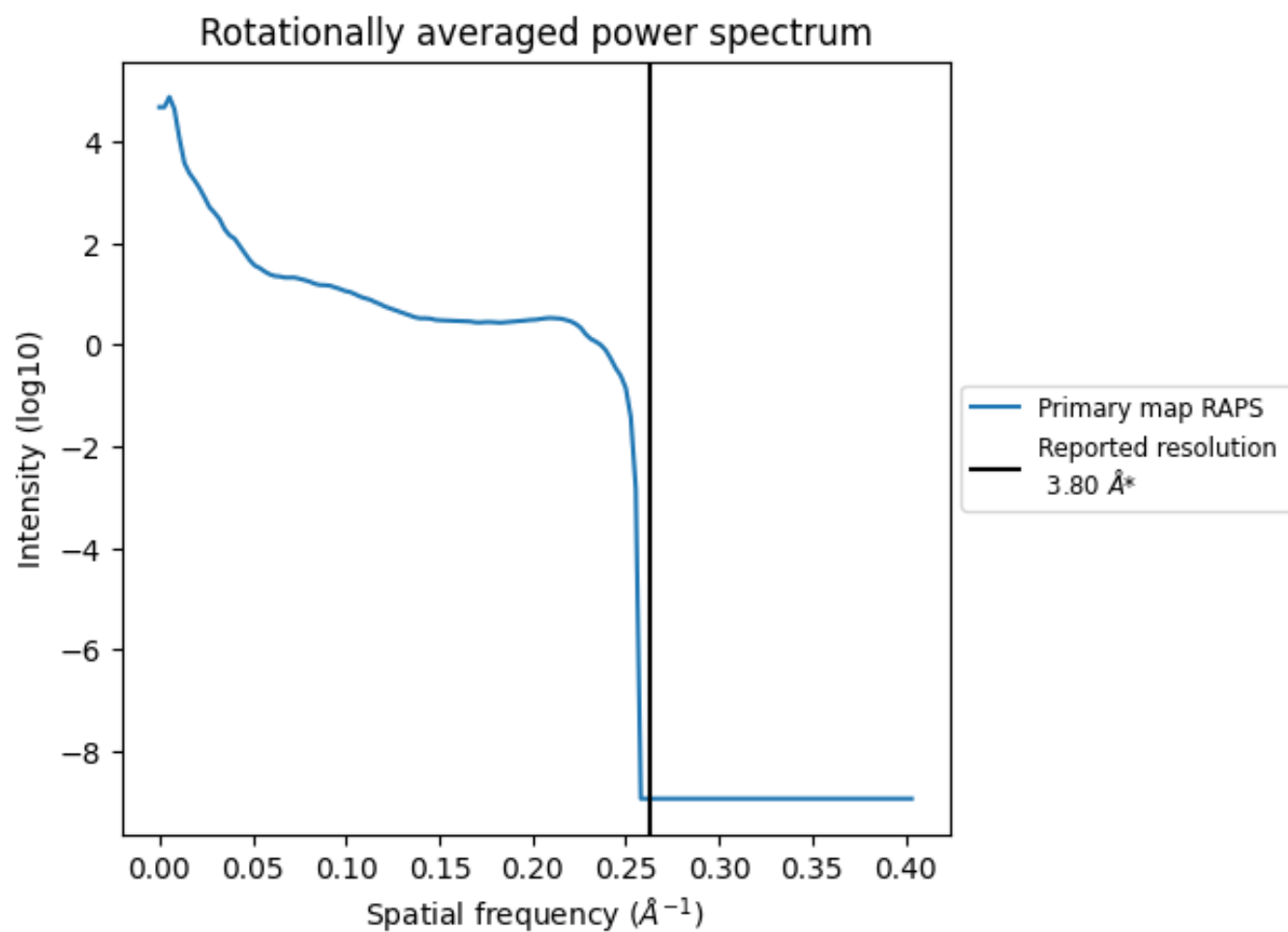
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm³; this corresponds to an approximate mass of 270 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

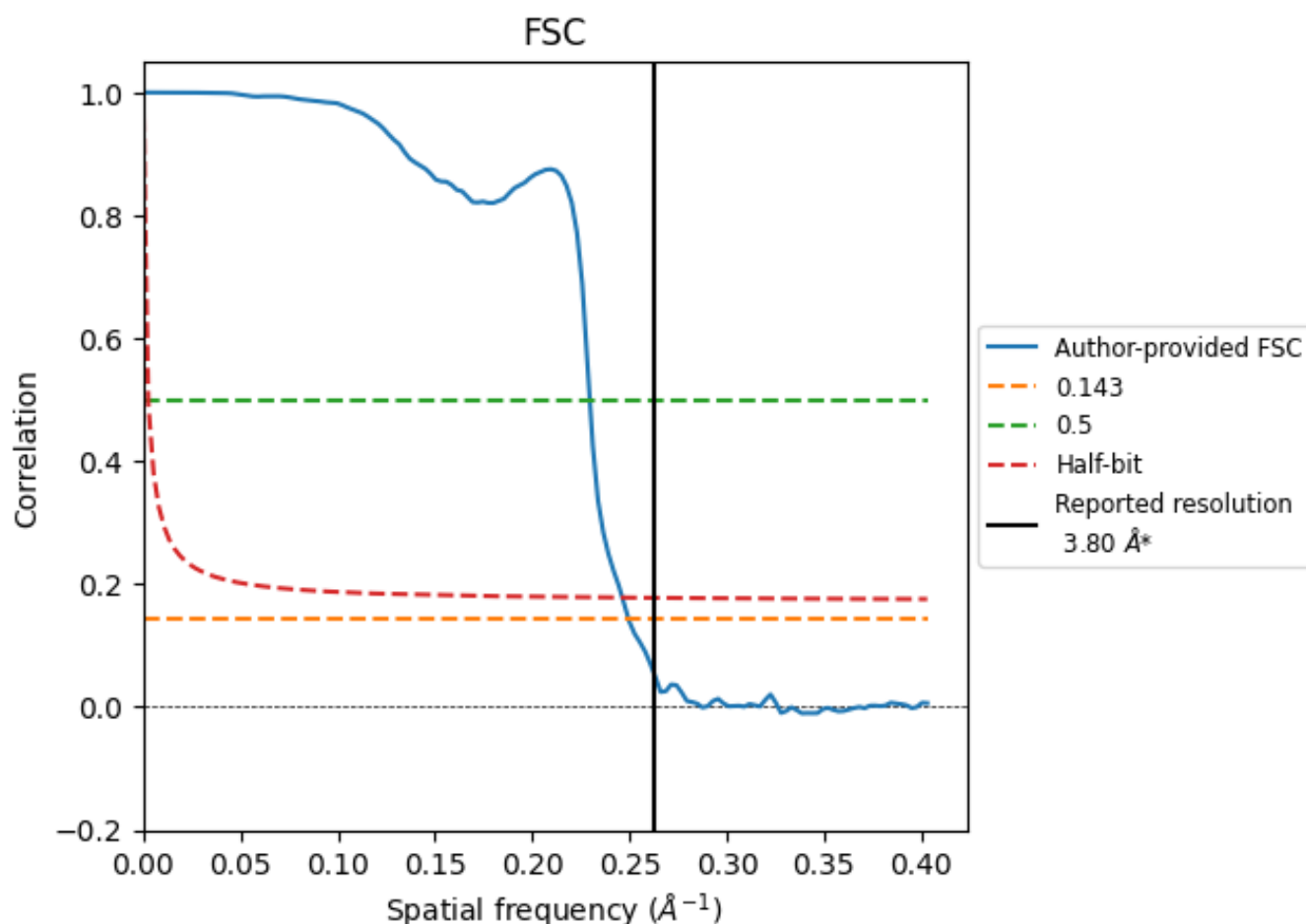


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	4.01	4.35	4.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

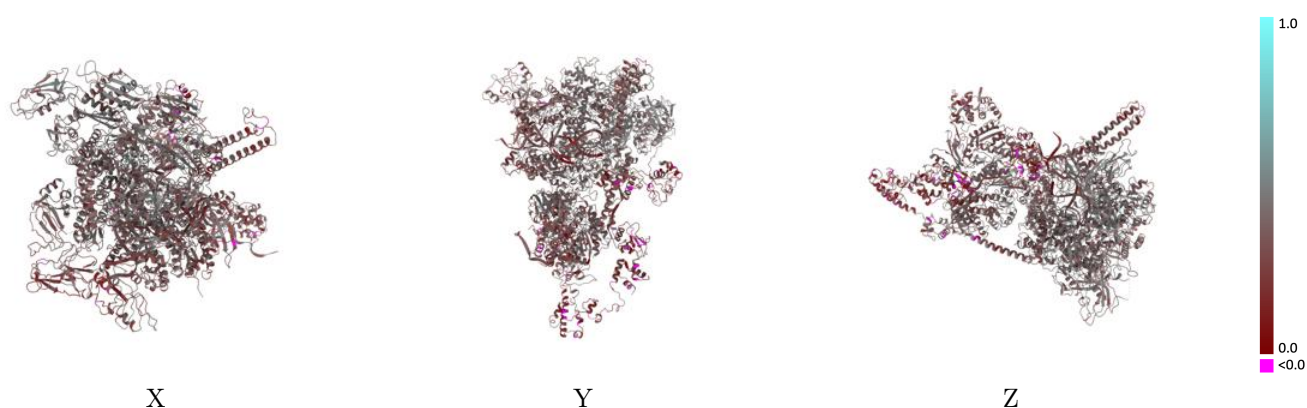
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10548 and PDB model 6TQO. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

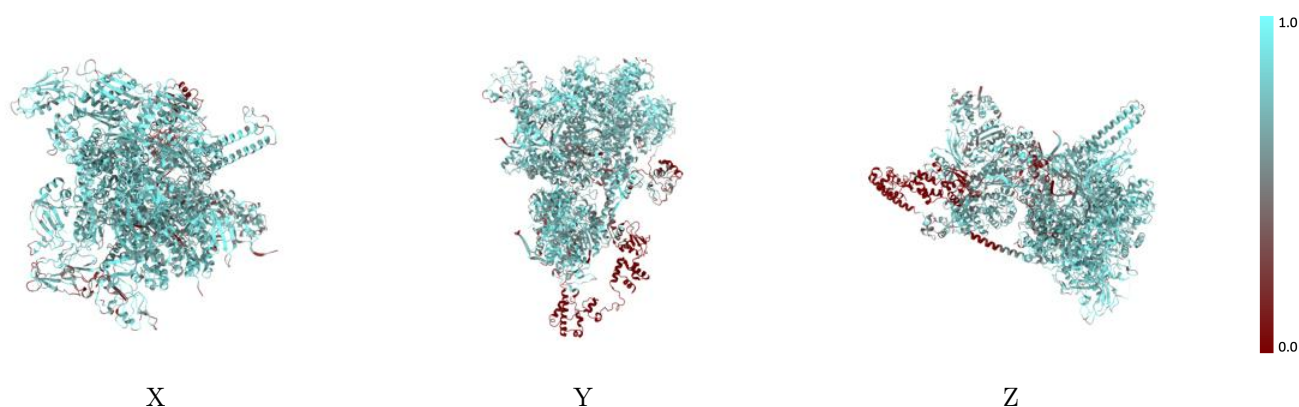
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



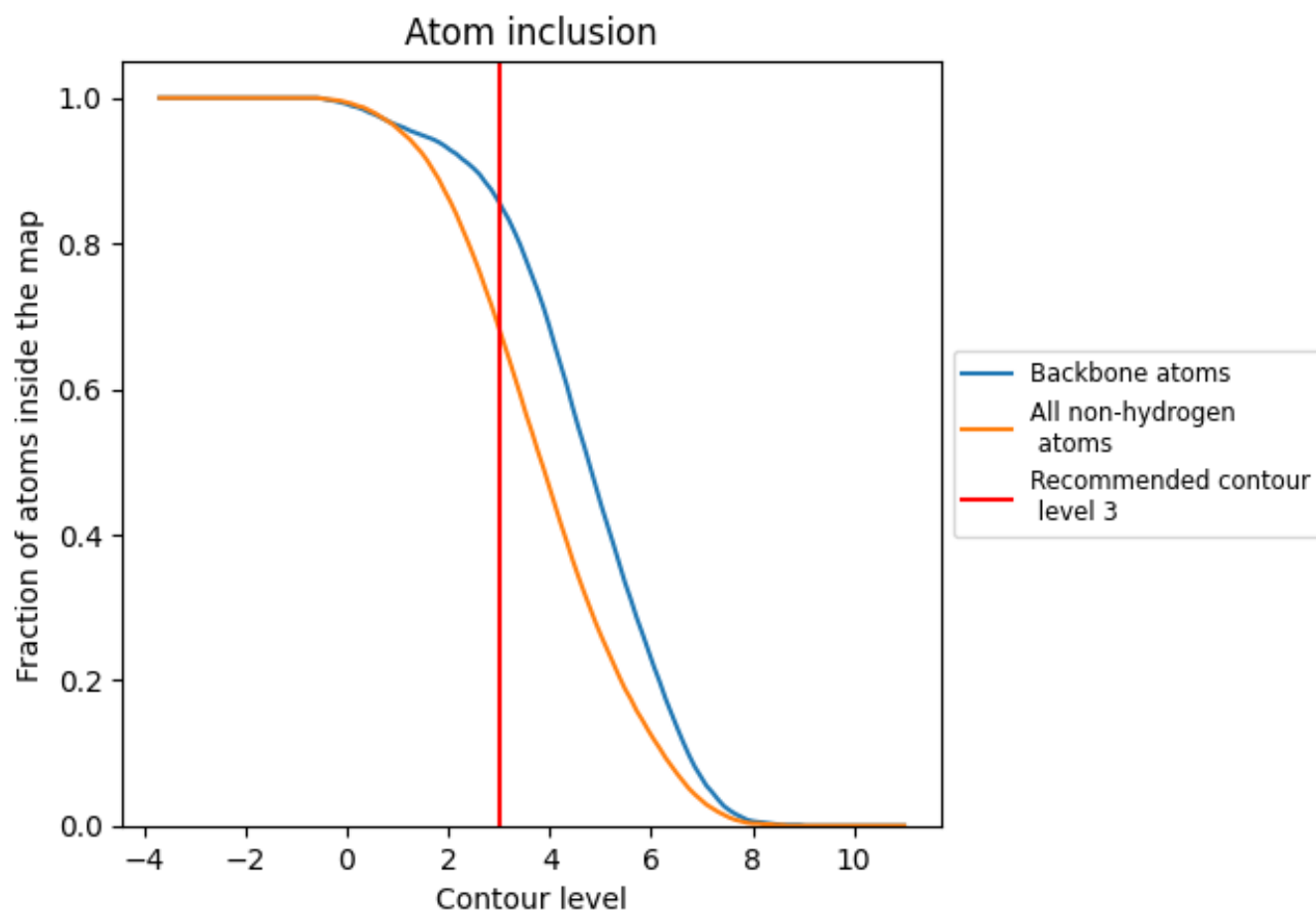
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6840	 0.3650
A	 0.5500	 0.3140
B	 0.6890	 0.2920
C	 0.0370	 0.2380
E	 0.6210	 0.3380
G	 0.7410	 0.3440
K	 0.6480	 0.2630
L	 0.7500	 0.2770
R	 0.6590	 0.3030
S	 0.7520	 0.3960
T	 0.7440	 0.3710
U	 0.6240	 0.3790
V	 0.7670	 0.4120
W	 0.5850	 0.3630
X	 0.7590	 0.3930
Y	 0.7390	 0.3870

