



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 11:38 am BST

PDB ID : 9FRL / pdb_00009frl
EMDB ID : EMD-50717
Title : Cryo-EM structure of *Saccharolobus solfataricus* 30S initiation complex bound to SD mRNA with h44 in up position
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2024-06-19
Resolution : 2.97 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:

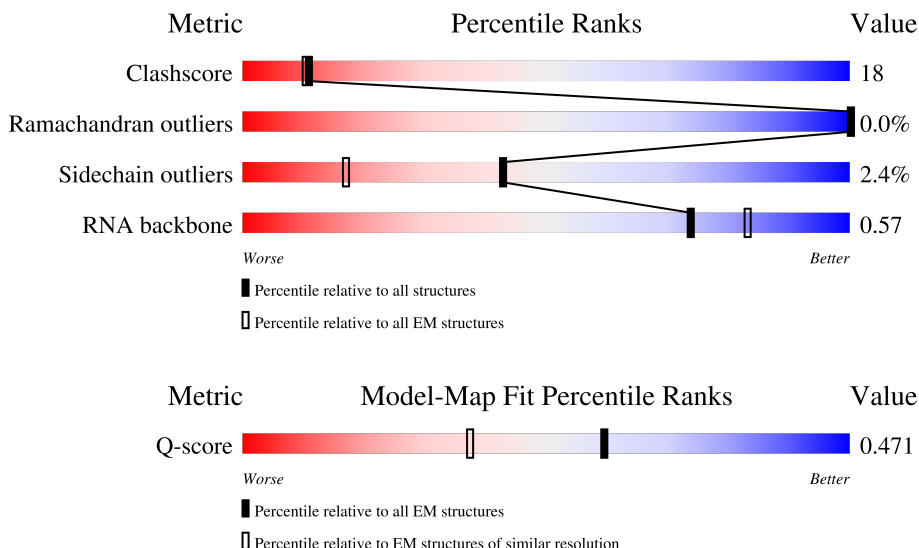
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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

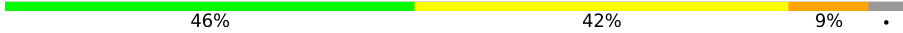
The reported resolution of this entry is 2.97 Å.

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.



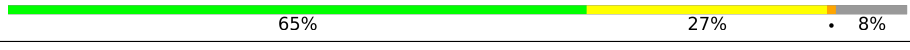
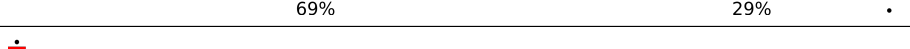
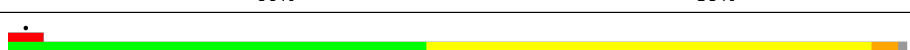
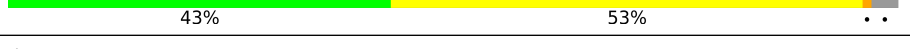
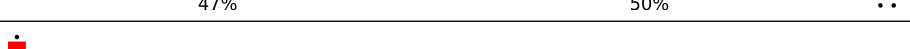
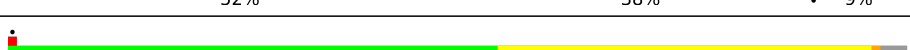
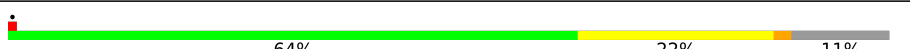
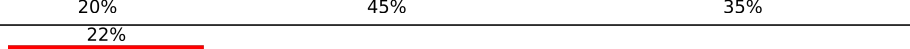
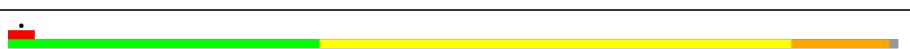
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13205 (2.47 - 3.47)

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	2	1497	
2	A	208	
3	B	231	

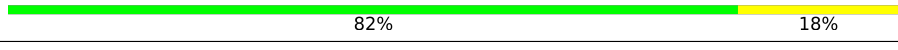
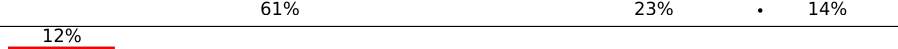
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	65	
5	D	181	
6	F	214	
7	G	214	
8	H	193	
9	I	133	
10	J	133	
11	K	137	
12	L	102	
13	M	132	
14	N	147	
15	O	165	
16	Q	152	
17	S	79	
18	T	140	
19	U	158	
20	V	120	
21	W	66	
22	X	83	
23	Y	75	
24	3	127	
25	a	72	
26	e	52	
27	4	77	
28	5	28	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	P	54	
30	R	114	
31	Z	229	
32	d	72	
33	c	110	
34	E	239	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	SPM	2	1567	-	-	X	-
36	SPM	2	1576	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 65224 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 RNA chain called rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1443	Total	C	N	O	P	0	0
			31042	13845	5740	10014	1443		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	843	4AC	C	conflict	GB AE006641.1
2	930	C4J	U	conflict	GB AE006641.1
2	1466	4AC	C	conflict	GB AE006641.1
2	1467	4AC	C	conflict	GB AE006641.1
2	1477	4AC	C	conflict	GB AE006641.1
2	1478	4AC	C	conflict	GB AE006641.1
2	1496	C	A	conflict	GB AE006641.1

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	186	Total	C	N	O	S	0	0
			1515	974	261	278	2		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	215	Total	C	N	O	S	0	0
			1698	1092	291	312	3		

- Molecule 4 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	58	Total	C	N	O	S	0	0
			455	282	84	81	8		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	166	Total	C	N	O	S	0	0
			1354	864	249	240	1		

- Molecule 6 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	210	Total	C	N	O	S	0	0
			1625	1041	275	303	6		

- Molecule 7 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	213	Total	C	N	O	S	0	0
			1661	1052	292	315	2		

- Molecule 8 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	192	Total	C	N	O	S	0	0
			1543	983	283	274	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	132	Total	C	N	O	S	0	0
			1050	675	187	182	6		

- Molecule 10 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	127	Total	C	N	O	0	0
			982	617	186	179		

- Molecule 11 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	133	Total	C	N	O	S	0	0
			1068	675	201	185	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	101	Total	C	N	O	S	0	0
			840	536	157	142	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	127	Total	C	N	O	S	0	0
			944	587	184	170	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1140	723	220	193	4		

- Molecule 15 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	140	Total	C	N	O	S	0	0
			1124	708	210	202	4		

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	145	Total	C	N	O	S	0	0
			1185	753	224	205	3		

- Molecule 17 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	66	Total	C	N	O	S	0	0
			571	364	101	105	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	128	Total	C	N	O	S	0	0
			1064	684	192	184	4		

- Molecule 19 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	154	Total	C	N	O	S	0	0
			1247	805	223	217	2		

- Molecule 20 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	107	Total	C	N	O	S	0	0
			836	524	154	156	2		

- Molecule 21 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	65	Total	C	N	O	S	0	0
			503	319	93	84	7		

- Molecule 22 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	67	Total	C	N	O		0	0
			535	335	103	97			

- Molecule 23 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	49	Total	C	N	O	S	0	0
			395	252	73	65	5		

- Molecule 24 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	117	Total	C	N	O	S	0	0
			893	567	149	175	2		

- Molecule 25 is a protein called aS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	71	Total	C	N	O	S	0	0
			562	361	98	96	7		

- Molecule 26 is a protein called LSU ribosomal protein S30E (Rps30E).

Mol	Chain	Residues	Atoms				AltConf	Trace
26	e	43	Total	C	N	O	0	0
			354	220	74	60		

- Molecule 27 is a RNA chain called tRNA Met initiator.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	4	77	Total	C	N	O	P	S	0	0
			1645	734	296	537	77	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	A	C	engineered mutation	GB 1334604293
4	72	U	A	engineered mutation	GB 1334604293

- Molecule 28 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 29 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	53	Total	C	N	O	S	0	0
			440	282	80	74	4		

- Molecule 30 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R	113	Total	C	N	O	S	0	0
			901	570	166	161	4		

- Molecule 31 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	196	Total	C	N	O	S	0	0
			1561	1009	274	272	6		

- Molecule 32 is a protein called aS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	70	Total	C	N	O	S	0	0
			570	370	92	105	3		

- Molecule 33 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	109	Total	C	N	O	S	0	0
			856	539	152	164	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	E	238	Total	C	N	O	S	0	0
			1930	1238	342	344	6		

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	2	47	Total	Mg	0
			47	47	
35	F	2	Total	Mg	0
			2	2	
35	K	1	Total	Mg	0
			1	1	
35	5	1	Total	Mg	0
			1	1	
35	P	1	Total	Mg	0
			1	1	
35	R	1	Total	Mg	0
			1	1	

- Molecule 36 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	C	2	Total	Zn	0
			2	2	
37	F	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
37	W	1	Total 1	Zn 1	0
37	a	2	Total 2	Zn 2	0
37	P	1	Total 1	Zn 1	0
37	R	1	Total 1	Zn 1	0

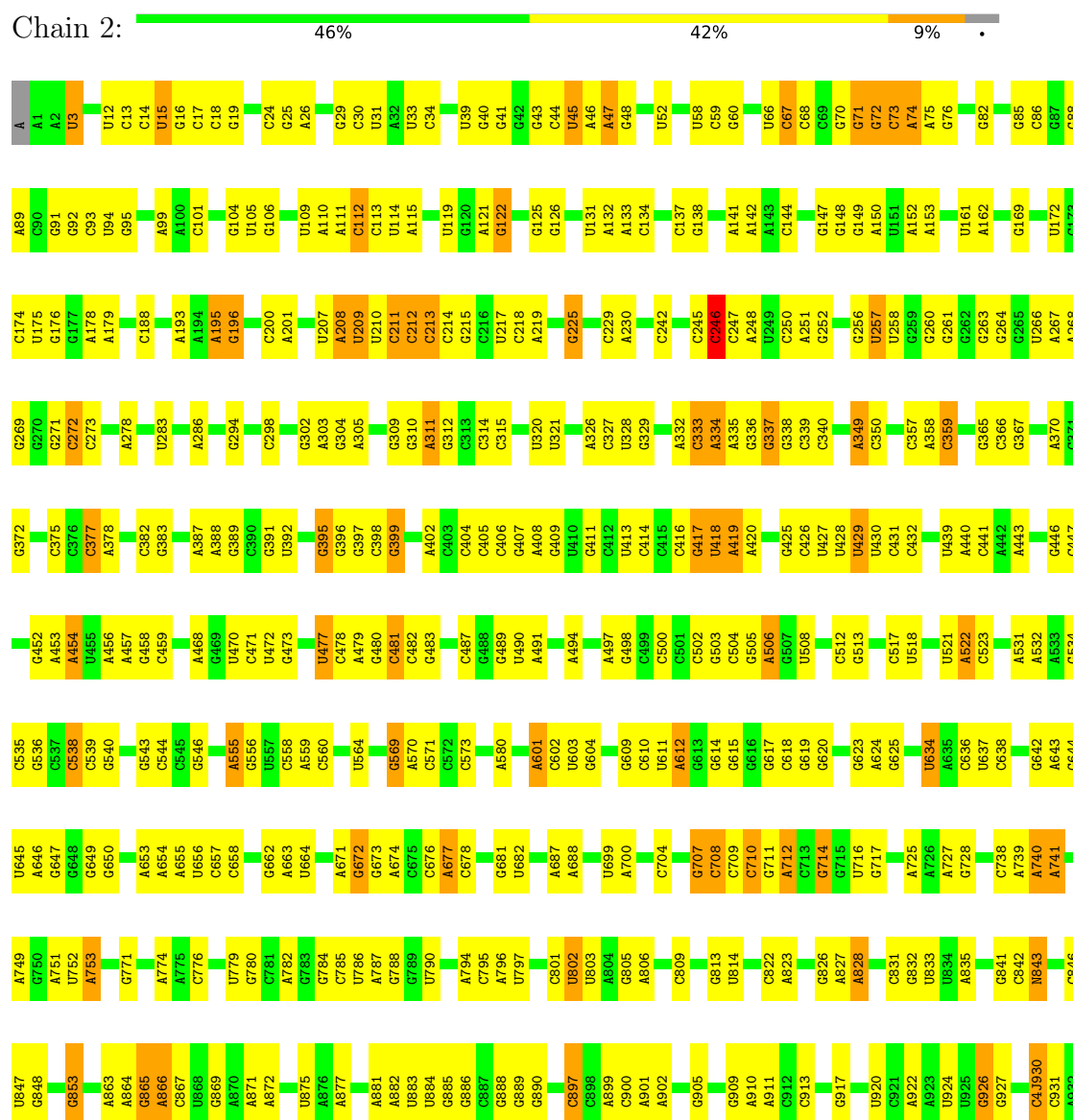
- Molecule 38 is water.

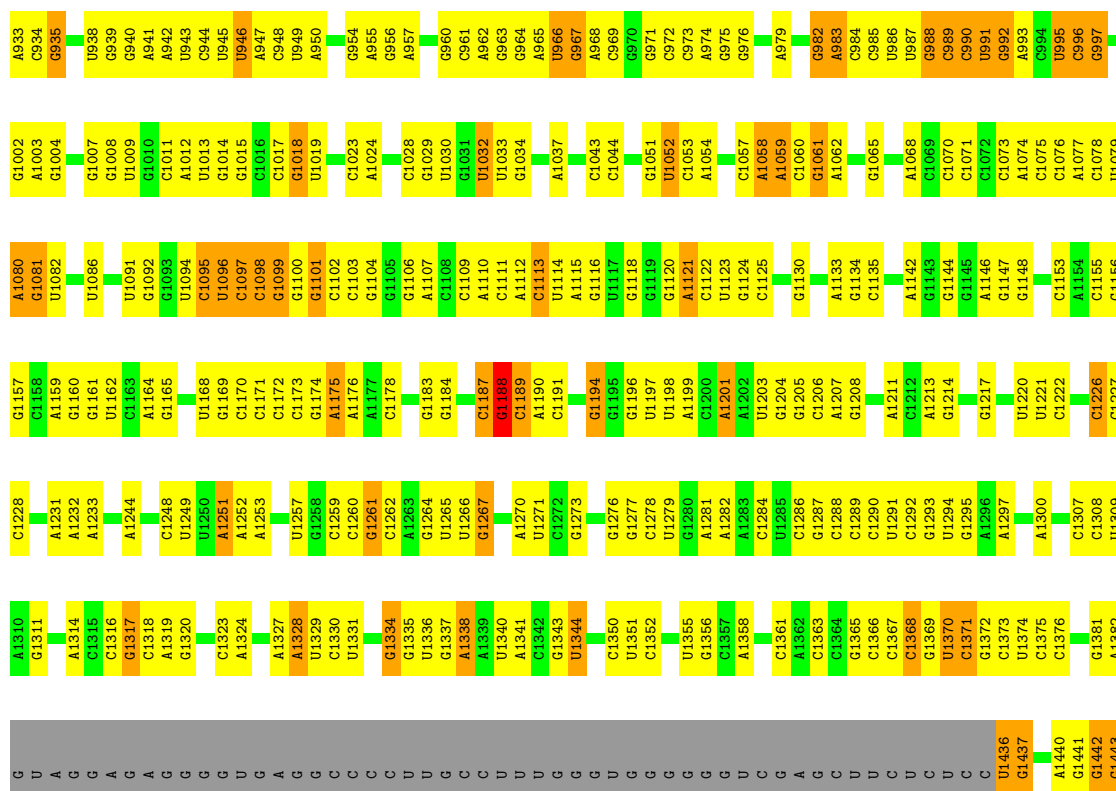
Mol	Chain	Residues	Atoms		AltConf
38	2	192	Total 192	O 192	0
38	D	1	Total 1	O 1	0
38	H	1	Total 1	O 1	0
38	I	2	Total 2	O 2	0
38	K	3	Total 3	O 3	0
38	4	3	Total 3	O 3	0
38	5	4	Total 4	O 4	0
38	P	1	Total 1	O 1	0
38	R	2	Total 2	O 2	0
38	E	1	Total 1	O 1	0

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: rRNA 16S





• Molecule 2: Small ribosomal subunit protein eS1

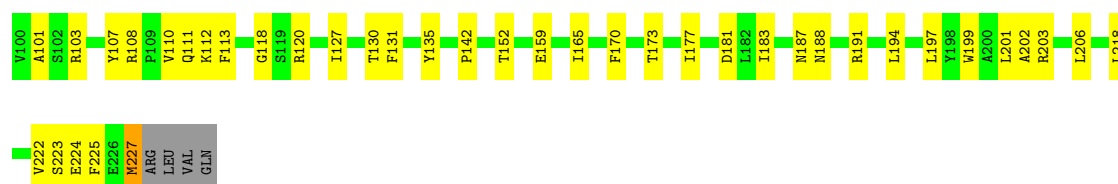
Chain A: 53% 34% 11%



• Molecule 3: Small ribosomal subunit protein uS2

Chain B: 64% 29% 7%





- Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein



- Molecule 5: Small ribosomal subunit protein uS4



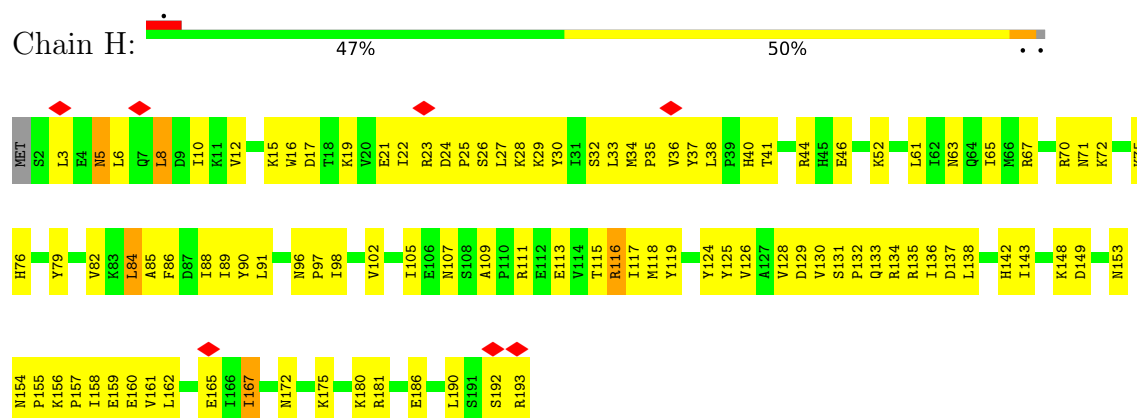
- Molecule 6: Small ribosomal subunit protein uS5



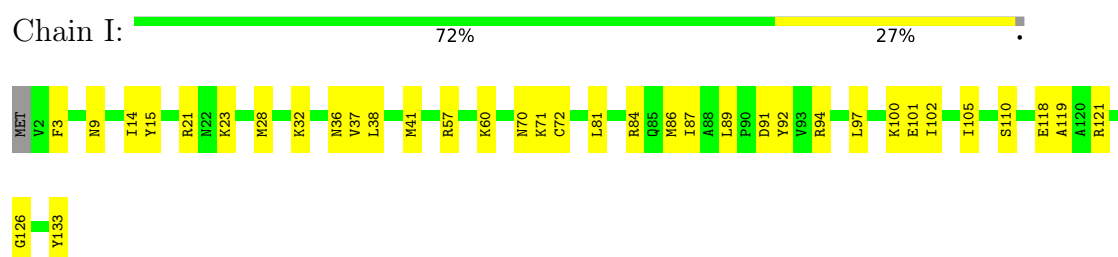
- Molecule 7: Small ribosomal subunit protein eS6



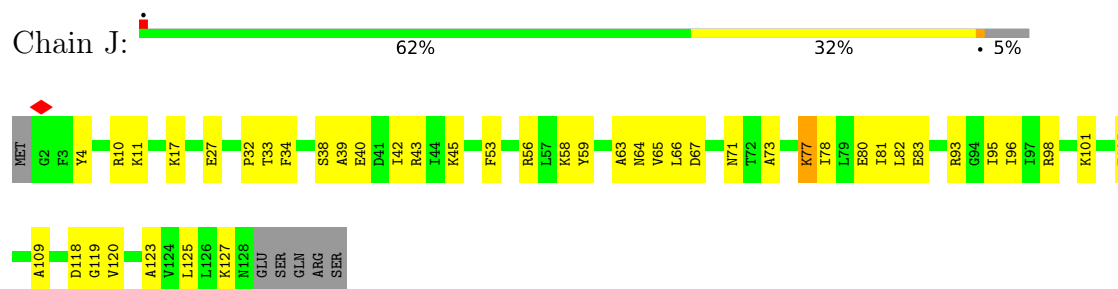
- Molecule 8: Small ribosomal subunit protein uS7



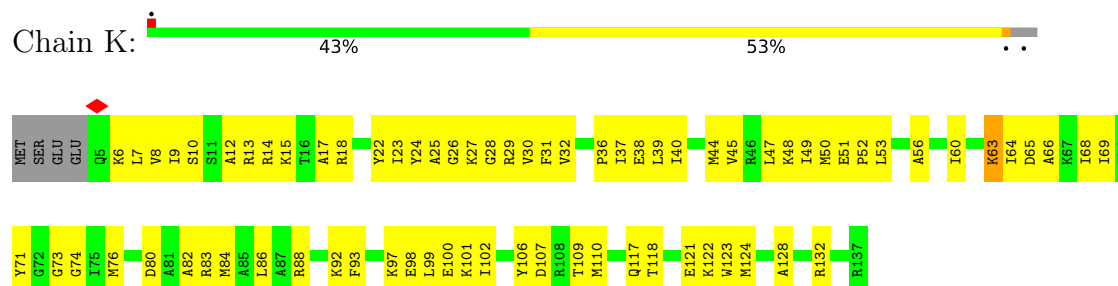
• Molecule 9: Small ribosomal subunit protein uS8



• Molecule 10: Small ribosomal subunit protein eS8

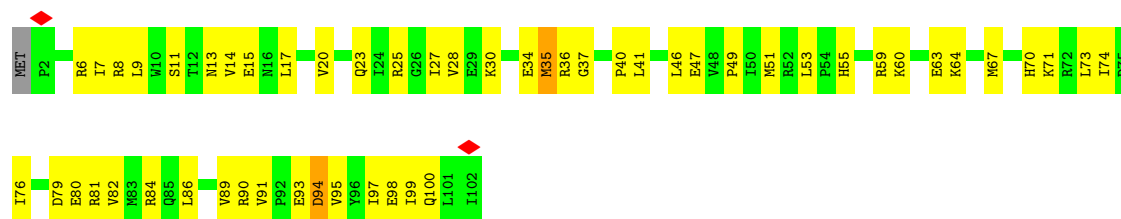


• Molecule 11: Small ribosomal subunit protein uS9

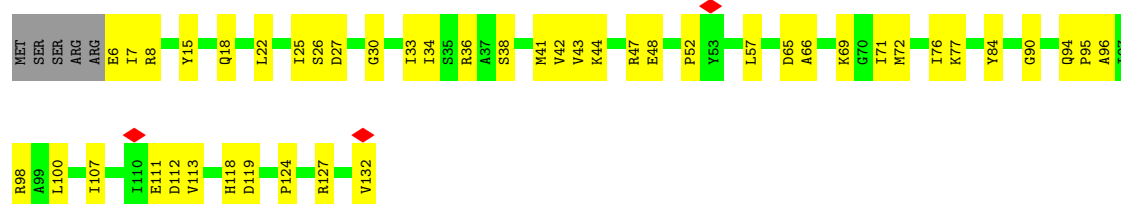


• Molecule 12: Small ribosomal subunit protein uS10

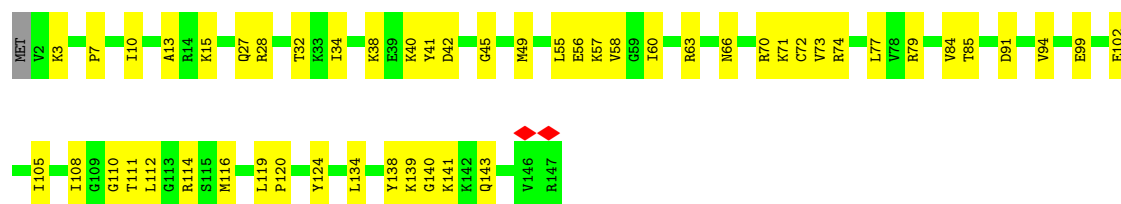




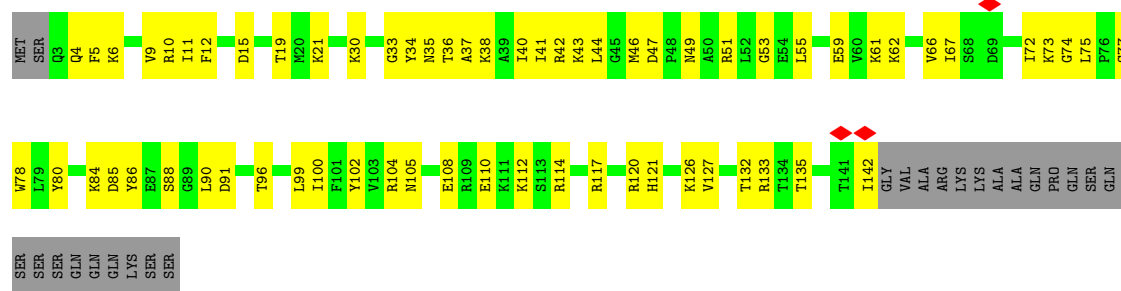
- Molecule 13: Small ribosomal subunit protein uS11



- Molecule 14: Small ribosomal subunit protein uS12

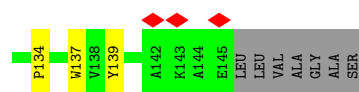


- Molecule 15: Small ribosomal subunit protein uS13

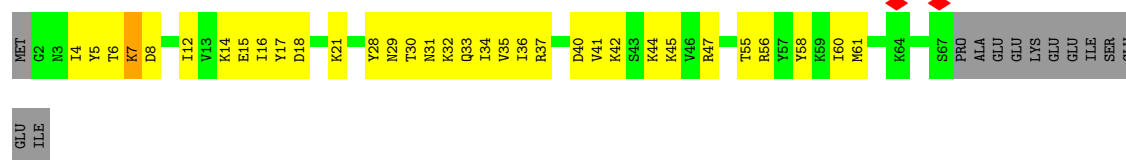


- Molecule 16: Small ribosomal subunit protein uS15

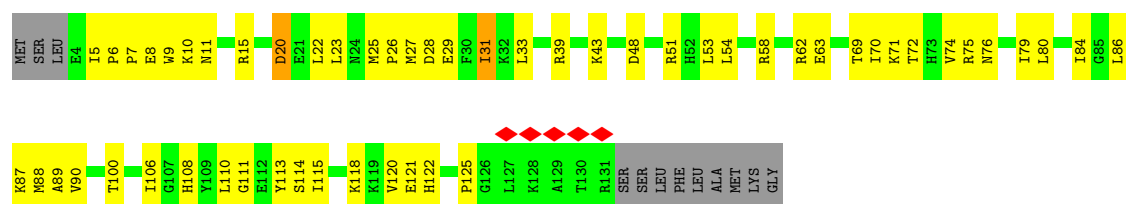




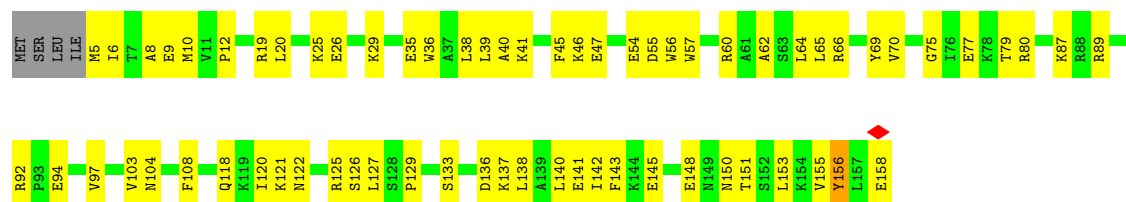
- Molecule 17: Small ribosomal subunit protein eS17



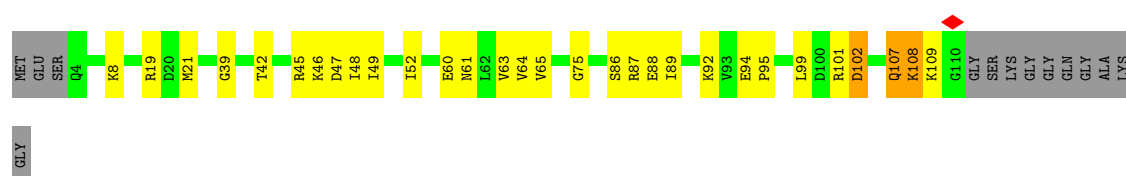
- Molecule 18: Small ribosomal subunit protein uS19



- Molecule 19: Small ribosomal subunit protein eS19



- Molecule 20: Small ribosomal subunit protein eS24

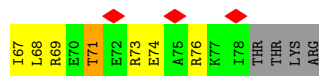


- Molecule 21: Small ribosomal subunit protein eS27

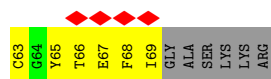
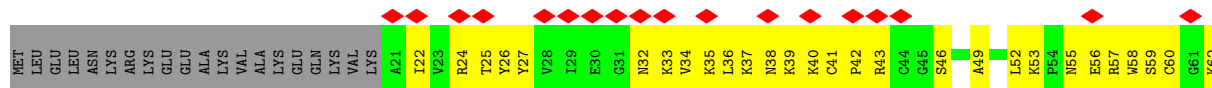
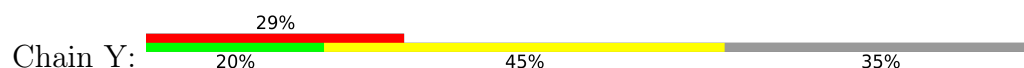




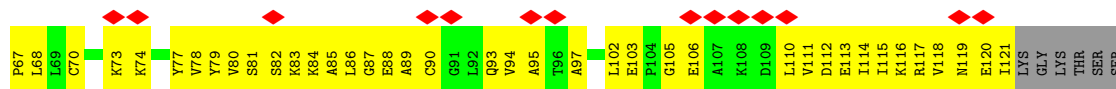
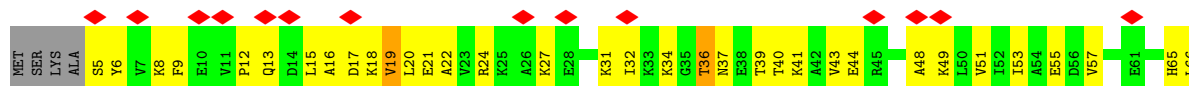
- Molecule 22: Small ribosomal subunit protein eS28



- Molecule 23: Small ribosomal subunit protein eS31



- Molecule 24: Large ribosomal subunit protein eL8



- Molecule 25: aS34

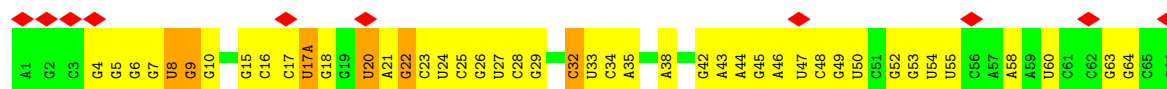


- Molecule 26: LSU ribosomal protein S30E (Rps30E)





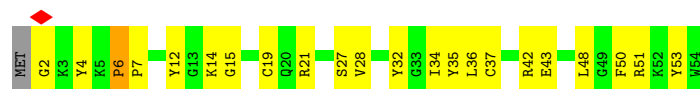
• Molecule 27: tRNA Met initiator



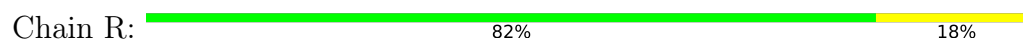
• Molecule 28: mRNA



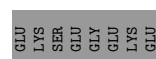
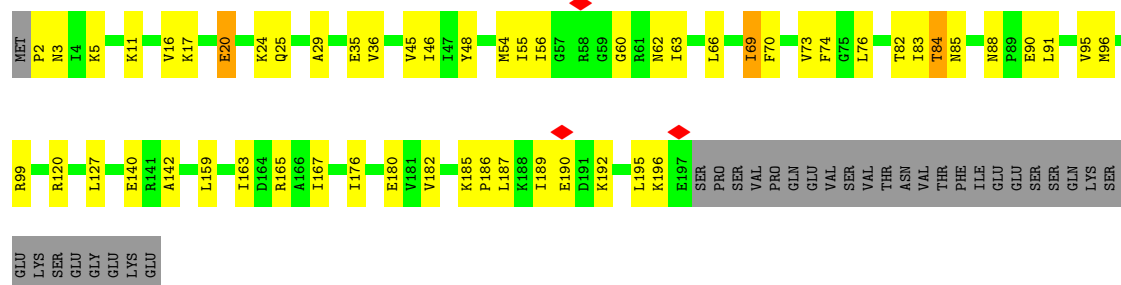
• Molecule 29: Small ribosomal subunit protein uS14



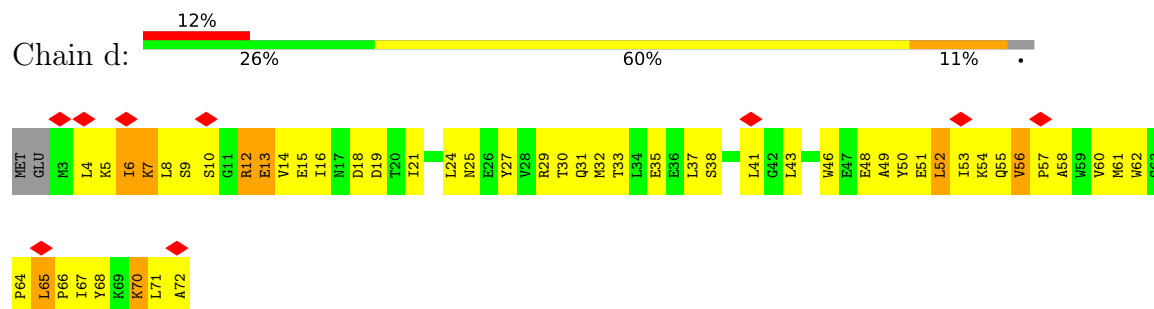
• Molecule 30: Small ribosomal subunit protein uS17



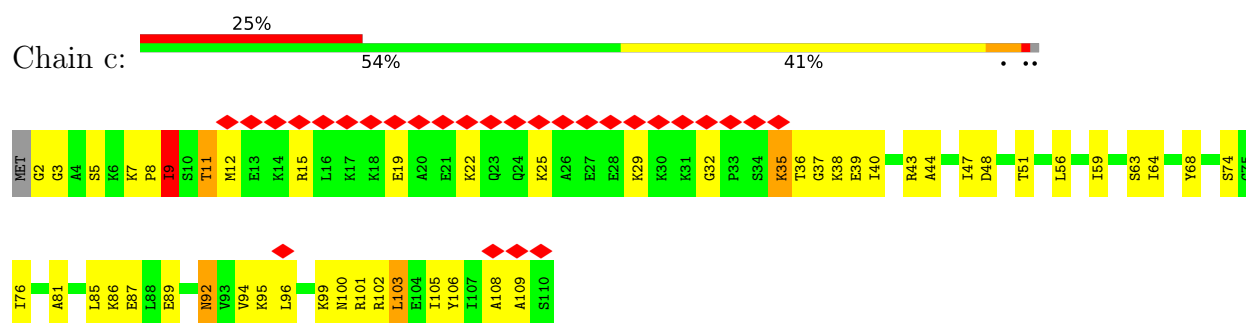
• Molecule 31: Small ribosomal subunit protein uS3



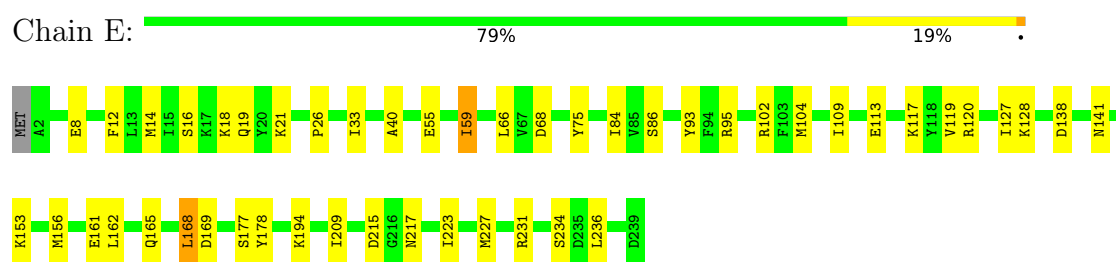
- Molecule 32: aS33



- Molecule 33: Small ribosomal subunit protein eS25



- Molecule 34: Small ribosomal subunit protein eS4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	366.444, 366.444, 366.444	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, OMG, SPM, H2U, 4SU, MG, 5MU, MA6, OMC, PSU, OMU, ZN, 5MC, 6MZ, 4AC, C4J

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	2	0.20	0/33909	0.33	7/52900 (0.0%)
2	A	0.23	0/1543	0.52	0/2077
3	B	0.22	0/1731	0.47	0/2349
4	C	0.24	0/466	0.55	1/625 (0.2%)
5	D	0.20	0/1380	0.37	0/1859
6	F	0.21	0/1654	0.42	0/2240
7	G	0.19	0/1684	0.43	0/2265
8	H	0.24	0/1571	0.58	0/2116
9	I	0.22	0/1070	0.39	0/1444
10	J	0.20	0/994	0.40	0/1337
11	K	0.28	0/1084	0.67	1/1450 (0.1%)
12	L	0.26	0/856	0.61	0/1154
13	M	0.27	0/960	0.61	0/1294
14	N	0.21	0/1155	0.44	0/1540
15	O	0.26	0/1142	0.60	0/1532
16	Q	0.20	0/1206	0.42	0/1618
17	S	0.30	0/578	0.64	1/770 (0.1%)
18	T	0.21	0/1087	0.49	0/1456
19	U	0.22	0/1270	0.50	0/1710
20	V	0.23	0/843	0.50	1/1124 (0.1%)
21	W	0.26	0/511	0.68	0/684
22	X	0.29	0/538	0.72	0/722
23	Y	0.31	0/404	0.78	0/540
24	3	0.29	0/902	0.65	0/1216
25	a	0.45	0/574	1.17	2/770 (0.3%)
26	e	0.36	0/360	0.64	1/477 (0.2%)
27	4	0.16	1/1725 (0.1%)	0.21	0/2687
28	5	0.26	0/481	0.38	0/748
29	P	0.26	0/451	0.59	2/600 (0.3%)
30	R	0.32	0/918	0.44	0/1236
31	Z	0.25	0/1584	0.42	0/2124
32	d	0.24	0/581	0.59	0/786

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.36	1/861 (0.1%)	0.63	3/1143 (0.3%)
34	E	0.31	0/1965	0.48	0/2644
All	All	0.23	2/68038 (0.0%)	0.43	19/99237 (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
8	H	0	1
25	a	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	9	ILE	CA-C	-6.84	1.44	1.52
27	4	8	4SU	O3'-P	5.05	1.61	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1370	U	P-O3'-C3'	-27.41	79.09	120.20
1	2	1370	U	OP1-P-O3'	-14.58	64.27	108.00
1	2	1370	U	OP2-P-O3'	10.83	140.49	108.00
25	a	26	ARG	CA-C-N	-7.35	111.04	121.99
25	a	26	ARG	C-N-CA	-7.35	111.04	121.99
33	c	9	ILE	N-CA-C	6.99	117.13	110.42
1	2	942	A	C4'-C3'-O3'	-6.48	103.29	113.00
1	2	942	A	C2'-C3'-O3'	6.34	123.20	113.70
29	P	6	PRO	CA-C-N	6.25	126.22	119.78
29	P	6	PRO	C-N-CA	6.25	126.22	119.78
33	c	103	LEU	N-CA-C	6.08	118.09	108.79
33	c	9	ILE	O-C-N	5.55	127.35	121.91
26	e	31	ARG	CG-CD-NE	-5.49	99.91	112.00
1	2	1188	G	C3'-C2'-O2'	5.43	118.85	110.70
4	C	21	LYS	CG-CD-CE	-5.37	98.95	111.30
20	V	107	GLN	CA-CB-CG	5.29	124.67	114.10
11	K	63	LYS	CA-CB-CG	5.24	124.59	114.10
17	S	7	LYS	CG-CD-CE	5.10	123.02	111.30
1	2	1095	C	O4'-C1'-N1	5.10	115.84	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	116	ARG	Sidechain
25	a	36	TYR	Sidechain

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	2	31042	0	15709	709	0
2	A	1515	0	1565	69	0
3	B	1698	0	1753	59	0
4	C	455	0	437	33	0
5	D	1354	0	1419	46	0
6	F	1625	0	1689	63	0
7	G	1661	0	1737	69	0
8	H	1543	0	1611	142	0
9	I	1050	0	1100	32	0
10	J	982	0	1046	35	0
11	K	1068	0	1125	98	0
12	L	840	0	893	61	0
13	M	944	0	978	42	0
14	N	1140	0	1244	47	0
15	O	1124	0	1162	66	0
16	Q	1185	0	1260	30	0
17	S	571	0	598	43	0
18	T	1064	0	1107	47	0
19	U	1247	0	1329	76	0
20	V	836	0	894	29	0
21	W	503	0	532	35	0
22	X	535	0	572	48	0
23	Y	395	0	405	40	0
24	3	893	0	940	77	0
25	a	562	0	575	83	0
26	e	354	0	386	22	0
27	4	1645	0	840	41	0
28	5	430	0	215	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	P	440	0	436	45	0
30	R	901	0	935	17	0
31	Z	1561	0	1667	62	0
32	d	570	0	590	98	0
33	c	856	0	941	75	0
34	E	1930	0	2013	32	0
35	2	47	0	0	0	0
35	5	1	0	0	0	0
35	F	2	0	0	0	0
35	K	1	0	0	0	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
36	2	434	0	805	74	0
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	W	1	0	0	0	0
37	a	2	0	0	0	0
38	2	192	0	0	9	0
38	4	3	0	0	0	0
38	5	4	0	0	0	0
38	D	1	0	0	0	0
38	E	1	0	0	0	0
38	H	1	0	0	1	0
38	I	2	0	0	0	0
38	K	3	0	0	0	0
38	P	1	0	0	0	0
38	R	2	0	0	0	0
All	All	65224	0	50508	2105	0

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

All (2105) 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)
8:H:3:LEU:HD21	32:d:70:LYS:CE	1.37	1.50
8:H:3:LEU:CD2	32:d:70:LYS:HE3	1.03	1.50
1:2:927:G:OP1	36:2:1576:SPM:C12	1.67	1.43
8:H:3:LEU:CD2	32:d:70:LYS:CE	1.89	1.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:51:GLU:OE2	25:a:54:LYS:HD3	1.30	1.29
32:d:56:VAL:HG22	32:d:57:PRO:CD	1.69	1.23
25:a:53:ASP:O	25:a:57:LEU:HD23	1.36	1.22
1:2:809:C:OP1	36:2:1575:SPM:C9	1.86	1.22
1:2:125:G:OP2	36:2:1567:SPM:C7	1.89	1.19
1:2:125:G:OP2	36:2:1567:SPM:H72	1.02	1.18
8:H:84:LEU:HD11	33:c:100:ASN:HB2	1.21	1.17
25:a:21:CYS:SG	25:a:53:ASP:OD2	2.02	1.17
8:H:159:GLU:OE2	33:c:100:ASN:ND2	1.81	1.13
15:O:30:LYS:NZ	33:c:9:ILE:O	1.82	1.11
8:H:88:ILE:CD1	33:c:105:ILE:CD1	2.28	1.11
8:H:88:ILE:CD1	33:c:105:ILE:HD11	1.81	1.09
8:H:88:ILE:HD11	33:c:105:ILE:HD11	1.16	1.08
1:2:483:G:OP2	36:2:1549:SPM:H132	1.51	1.08
8:H:84:LEU:CD1	33:c:100:ASN:HB2	1.82	1.08
1:2:809:C:OP1	36:2:1575:SPM:H92	1.49	1.07
1:2:1496:C:O2	28:5:806:G:N2	1.87	1.07
4:C:16:CYS:HB3	4:C:19:CYS:SG	1.95	1.07
32:d:56:VAL:HG22	32:d:57:PRO:HD2	1.32	1.07
25:a:51:GLU:O	25:a:54:LYS:HG2	1.55	1.06
1:2:1451:G:C5	1:2:1452:U:C5	2.44	1.05
8:H:3:LEU:HD23	32:d:70:LYS:CE	1.75	1.04
25:a:51:GLU:OE2	25:a:54:LYS:CD	2.04	1.04
1:2:1451:G:C6	1:2:1452:U:C4	2.45	1.04
25:a:14:LEU:HG	31:Z:24:LYS:HG2	1.36	1.03
8:H:3:LEU:HD23	32:d:70:LYS:HE3	1.31	1.02
1:2:1451:G:C4	1:2:1452:U:C5	2.47	1.02
36:2:1553:SPM:H31	36:2:1553:SPM:H71	1.41	1.01
32:d:7:LYS:HA	32:d:7:LYS:HE3	1.43	1.01
1:2:1053:C:H5'	17:S:7:LYS:HE3	1.43	0.99
1:2:949:U:H3	1:2:1183:G:H1	1.06	0.99
1:2:920:U:H1'	1:2:1188:G:N2	1.77	0.98
1:2:927:G:P	36:2:1576:SPM:C12	2.51	0.98
8:H:193:ARG:HH12	22:X:73:ARG:HD3	1.28	0.97
32:d:56:VAL:HG22	32:d:57:PRO:HD3	1.45	0.96
11:K:8:VAL:HG22	11:K:23:ILE:HD11	1.44	0.96
25:a:53:ASP:O	25:a:57:LEU:CD2	2.14	0.95
6:F:128:CYS:SG	6:F:132:HIS:HD2	1.89	0.95
18:T:5:ILE:HD12	18:T:6:PRO:HD2	1.49	0.94
1:2:1003:A:O2'	25:a:26:ARG:NH1	2.01	0.94
1:2:1189:C:HO2'	33:c:2:GLY:N	1.67	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:51:GLU:CD	25:a:54:LYS:HD3	1.93	0.92
32:d:12:ARG:HG2	32:d:12:ARG:HH11	1.35	0.91
8:H:88:ILE:HD11	33:c:105:ILE:CD1	1.94	0.91
15:O:12:PHE:O	15:O:96:THR:HG21	1.70	0.91
1:2:1495:C:O2	28:5:807:G:N2	2.03	0.91
1:2:927:G:OP1	36:2:1576:SPM:C13	2.19	0.90
1:2:1453:C:H2'	1:2:1454:G:O4'	1.71	0.90
1:2:1495:C:N3	28:5:807:G:N1	2.20	0.90
19:U:5:MET:N	19:U:5:MET:SD	2.46	0.89
1:2:1324:A:C8	29:P:12:TYR:HB3	2.07	0.88
1:2:1453:C:C4	1:2:1454:G:N7	2.41	0.88
24:3:115:ILE:O	24:3:119:ASN:ND2	2.07	0.88
1:2:1009:U:OP2	36:2:1576:SPM:N5	2.07	0.87
36:2:1573:SPM:H42	36:2:1573:SPM:H82	1.57	0.87
25:a:30:ILE:HG21	31:Z:73:VAL:HG21	1.56	0.86
25:a:45:TYR:CE1	29:P:6:PRO:HB2	2.10	0.86
25:a:40:LYS:NZ	25:a:64:CYS:SG	2.49	0.86
33:c:7:LYS:HB2	33:c:9:ILE:HG22	1.58	0.85
6:F:121:CYS:SG	6:F:128:CYS:HB3	2.13	0.84
8:H:88:ILE:CD1	33:c:105:ILE:HD13	2.06	0.84
8:H:3:LEU:HD23	32:d:70:LYS:NZ	1.92	0.84
8:H:159:GLU:OE1	33:c:102:ARG:NE	2.10	0.84
1:2:809:C:OP1	36:2:1575:SPM:H91	1.76	0.84
25:a:51:GLU:O	25:a:54:LYS:CG	2.26	0.84
22:X:44:GLU:OE2	32:d:50:TYR:OH	1.95	0.84
7:G:57:ASP:OD2	7:G:58:THR:N	2.12	0.83
16:Q:97:ARG:NH2	16:Q:139:TYR:OH	2.10	0.83
32:d:25:ASN:ND2	32:d:64:PRO:HA	1.93	0.83
1:2:440:A:H2	20:V:109:LYS:HE3	1.44	0.83
18:T:7:PRO:HA	18:T:10:LYS:HD3	1.59	0.83
1:2:125:G:P	36:2:1567:SPM:H92	2.18	0.83
27:4:50:U:H3	27:4:64:G:H1	0.86	0.83
32:d:56:VAL:CG2	32:d:57:PRO:CD	2.56	0.82
11:K:30:VAL:HG12	11:K:66:ALA:HB3	1.62	0.82
24:3:19:VAL:HG12	24:3:114:ILE:HG12	1.60	0.82
1:2:309:G:N2	5:D:3:ASP:OD2	2.12	0.82
17:S:36:ILE:HG22	17:S:47:ARG:HD2	1.60	0.81
8:H:3:LEU:CG	32:d:70:LYS:HE3	2.07	0.81
11:K:27:LYS:NZ	19:U:155:VAL:O	2.14	0.80
11:K:101:LYS:CE	32:d:66:PRO:HB3	2.11	0.80
8:H:113:GLU:OE1	8:H:113:GLU:N	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:71:G:N1	1:2:213:C:N3	2.29	0.79
36:2:1553:SPM:H31	36:2:1553:SPM:C7	2.12	0.79
1:2:920:U:H1'	1:2:1188:G:H21	1.44	0.79
13:M:77:LYS:HD2	13:M:111:GLU:OE2	1.83	0.79
25:a:21:CYS:SG	25:a:24:CYS:HB3	2.23	0.79
32:d:56:VAL:CG2	32:d:57:PRO:HD3	2.12	0.79
36:2:1566:SPM:H31	36:2:1566:SPM:H72	1.63	0.79
2:A:19:TRP:CE2	2:A:37:PRO:HG3	2.18	0.79
24:3:49:LYS:HZ1	24:3:103:GLU:H	1.30	0.79
32:d:71:LEU:HD13	32:d:72:ALA:N	1.98	0.78
1:2:1091:U:H3	1:2:1104:G:H1	1.32	0.78
18:T:53:LEU:HD21	18:T:88:MET:HE1	1.65	0.78
25:a:6:ARG:O	31:Z:165:ARG:NH1	2.17	0.78
2:A:16:MET:N	2:A:16:MET:SD	2.57	0.78
1:2:1012:A:O2'	31:Z:140:GLU:O	2.03	0.77
25:a:40:LYS:CE	25:a:64:CYS:SG	2.73	0.77
8:H:193:ARG:NH1	22:X:73:ARG:HD3	1.98	0.77
11:K:101:LYS:HE3	32:d:66:PRO:HB3	1.65	0.77
12:L:63:GLU:OE2	29:P:42:ARG:NE	2.18	0.77
1:2:1451:G:C6	1:2:1452:U:O4	2.38	0.76
9:I:97:LEU:HD21	9:I:105:ILE:HG12	1.67	0.76
1:2:1451:G:C4	1:2:1452:U:C6	2.72	0.76
2:A:23:ILE:HD11	2:A:80:ILE:HG22	1.65	0.76
1:2:18:C:H5''	14:N:112:LEU:HD21	1.66	0.76
1:2:920:U:O2	1:2:1188:G:C2	2.38	0.76
1:2:310:G:HO2'	5:D:2:GLY:N	1.84	0.76
31:Z:36:VAL:HG12	31:Z:45:VAL:HG22	1.68	0.76
1:2:822:C:O3'	4:C:50:LYS:NZ	2.18	0.76
1:2:71:G:N2	1:2:213:C:O2	2.16	0.75
25:a:28:LEU:HB3	25:a:35:LEU:HD23	1.67	0.75
1:2:17:C:H2'	1:2:18:C:H6	1.51	0.75
1:2:1008:G:OP1	36:2:1576:SPM:H72	1.86	0.75
1:2:1217:G:OP1	29:P:32:TYR:OH	2.02	0.75
3:B:101:ALA:HB2	3:B:110:VAL:HG21	1.69	0.75
8:H:10:ILE:HD12	8:H:37:TYR:CE1	2.22	0.75
16:Q:134:PRO:HG2	16:Q:137:TRP:HB2	1.69	0.75
1:2:39:U:O4	34:E:18:LYS:NZ	2.20	0.75
7:G:23:VAL:HG22	7:G:92:VAL:HB	1.69	0.75
15:O:66:VAL:HG12	15:O:72:ILE:HD12	1.68	0.75
11:K:102:ILE:CD1	32:d:67:ILE:HD13	2.16	0.74
12:L:7:ILE:HD13	12:L:74:ILE:HG22	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:21:CYS:HB3	25:a:26:ARG:H	1.52	0.74
4:C:34:CYS:SG	4:C:57:CYS:HB2	2.26	0.74
8:H:88:ILE:HD12	33:c:105:ILE:CD1	2.17	0.74
1:2:337:OMG:HM22	1:2:338:G:H5'	1.70	0.74
1:2:1295:G:H4'	33:c:8:PRO:HG2	1.70	0.74
8:H:67:ARG:HG3	8:H:148:LYS:HD3	1.70	0.74
11:K:53:LEU:HB2	11:K:86:LEU:HD11	1.68	0.74
21:W:20:LYS:NZ	21:W:25:GLY:O	2.20	0.74
31:Z:63:ILE:H	31:Z:63:ILE:HD12	1.53	0.73
3:B:224:GLU:OE1	3:B:224:GLU:N	2.21	0.73
8:H:22:ILE:O	8:H:28:LYS:NZ	2.21	0.73
15:O:6:LYS:HE3	15:O:9:VAL:HG22	1.67	0.73
31:Z:70:PHE:HB3	31:Z:76:LEU:HD12	1.71	0.73
29:P:19:CYS:SG	29:P:36:LEU:HA	2.28	0.73
32:d:52:LEU:C	32:d:52:LEU:HD12	2.13	0.73
16:Q:36:GLU:OE1	16:Q:76:ARG:NH1	2.20	0.73
5:D:154:ASP:OD1	5:D:155:TYR:N	2.21	0.73
8:H:90:TYR:HB2	8:H:97:PRO:HG3	1.69	0.73
5:D:31:GLY:HA3	26:e:38:TYR:CD2	2.24	0.73
15:O:44:LEU:HD21	15:O:66:VAL:HG21	1.70	0.73
8:H:130:VAL:HG12	8:H:135:ARG:HG3	1.71	0.73
2:A:16:MET:O	2:A:18:LYS:NZ	2.21	0.72
32:d:64:PRO:HG2	32:d:67:ILE:HB	1.69	0.72
12:L:11:SER:HB3	12:L:17:LEU:HG	1.70	0.72
13:M:25:ILE:HG22	13:M:34:ILE:HB	1.71	0.72
12:L:7:ILE:HD11	12:L:76:ILE:HG12	1.71	0.72
1:2:809:C:OP1	36:2:1575:SPM:C8	2.38	0.72
11:K:84:MET:O	11:K:88:ARG:HD2	1.90	0.72
32:d:24:LEU:HD21	32:d:53:ILE:HD11	1.71	0.72
1:2:1453:C:H2'	1:2:1454:G:C1'	2.19	0.72
7:G:137:VAL:HG12	7:G:151:LYS:HG3	1.71	0.72
1:2:973:C:N4	1:2:982:G:O6	2.18	0.72
1:2:1053:C:H5'	17:S:7:LYS:CE	2.18	0.72
17:S:15:GLU:OE1	31:Z:195:LEU:HD11	1.90	0.72
25:a:57:LEU:CD1	29:P:4:TYR:CE1	2.73	0.72
1:2:885:G:H2'	1:2:886:G:C8	2.24	0.72
4:C:9:GLU:N	4:C:9:GLU:OE2	2.22	0.72
5:D:116:SER:HB2	5:D:121:GLN:HG2	1.71	0.72
6:F:126:CYS:SG	6:F:128:CYS:CB	2.78	0.72
1:2:983:A:OP1	29:P:2:GLY:HA2	1.90	0.71
25:a:57:LEU:HD11	29:P:4:TYR:CE1	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:619:G:H2'	1:2:620:G:C8	2.26	0.71
11:K:27:LYS:HZ2	19:U:155:VAL:HG22	1.55	0.71
12:L:46:LEU:HD22	29:P:32:TYR:CD1	2.25	0.71
24:3:18:LYS:NZ	24:3:110:LEU:O	2.22	0.71
4:C:16:CYS:CB	4:C:19:CYS:SG	2.65	0.71
7:G:45:LYS:HB2	7:G:93:TRP:HB2	1.72	0.71
13:M:44:LYS:HA	13:M:44:LYS:HE3	1.72	0.71
25:a:37:LYS:HD3	25:a:71:ILE:HB	1.72	0.71
1:2:409:G:OP1	26:e:31:ARG:NH1	2.23	0.71
1:2:1032:OMU:HM22	1:2:1033:U:H5'	1.72	0.71
21:W:18:ARG:HB3	21:W:62:VAL:HG22	1.73	0.71
1:2:1253:A:OP1	36:2:1578:SPM:C9	2.38	0.71
7:G:142:GLN:CD	7:G:142:GLN:H	1.99	0.71
1:2:965:A:H2'	24:3:94:VAL:HG11	1.73	0.71
1:2:967:G:N7	24:3:37:ASN:ND2	2.38	0.71
1:2:983:A:OP2	29:P:2:GLY:HA3	1.91	0.71
5:D:40:GLU:OE1	5:D:40:GLU:N	2.23	0.71
22:X:73:ARG:NH1	22:X:73:ARG:HA	2.06	0.71
13:M:48:GLU:OE2	13:M:48:GLU:N	2.21	0.70
1:2:920:U:C1'	1:2:1188:G:N2	2.53	0.70
1:2:1365:G:N7	38:2:1611:HOH:O	2.23	0.70
21:W:15:ARG:HG3	21:W:64:ILE:HD11	1.73	0.70
1:2:1451:G:H2'	1:2:1452:U:H6	1.56	0.70
25:a:16:TRP:CD2	31:Z:17:LYS:HG3	2.27	0.70
11:K:107:ASP:OD1	11:K:109:THR:OG1	2.09	0.70
12:L:6:ARG:HD2	12:L:100:GLN:HE21	1.55	0.70
7:G:203:GLN:OE1	7:G:203:GLN:N	2.19	0.70
14:N:102:GLU:N	14:N:102:GLU:OE2	2.25	0.70
22:X:14:GLU:OE2	22:X:14:GLU:N	2.25	0.70
24:3:12:PRO:HG3	24:3:117:ARG:CZ	2.22	0.70
8:H:89:ILE:HD11	8:H:97:PRO:HA	1.73	0.70
8:H:84:LEU:CD1	33:c:100:ASN:CB	2.68	0.70
32:d:12:ARG:HG2	32:d:12:ARG:NH1	2.07	0.70
33:c:96:LEU:HD13	33:c:96:LEU:C	2.17	0.70
1:2:872:A:OP1	14:N:28:ARG:NH2	2.24	0.69
1:2:644:G:N3	13:M:36:ARG:NH2	2.37	0.69
1:2:1352:C:H4'	36:2:1577:SPM:H42	1.74	0.69
5:D:143:TYR:OH	5:D:149:GLU:OE2	2.08	0.69
3:B:34:GLU:N	3:B:34:GLU:OE1	2.24	0.69
27:4:32:OMC:HM22	27:4:33:U:H5'	1.75	0.69
25:a:57:LEU:HD22	25:a:57:LEU:N	2.08	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:88:G:N1	7:G:187:GLU:OE2	2.20	0.69
1:2:1112:A:O2'	11:K:71:TYR:OH	2.11	0.69
16:Q:95:ASN:OD1	16:Q:98:ARG:NH2	2.22	0.69
1:2:910:A:H2'	1:2:911:A:C8	2.28	0.69
1:2:1253:A:OP1	36:2:1578:SPM:N10	2.25	0.69
4:C:57:CYS:CB	4:C:60:CYS:SG	2.78	0.69
6:F:141:LYS:NZ	6:F:143:GLY:O	2.25	0.69
8:H:118:MET:HE2	8:H:118:MET:HA	1.73	0.69
25:a:40:LYS:HE3	25:a:64:CYS:SG	2.33	0.69
1:2:1489:U:H2'	1:2:1490:C:H6	1.56	0.69
8:H:134:ARG:O	8:H:138:LEU:HD12	1.92	0.69
8:H:159:GLU:CD	33:c:102:ARG:HE	2.00	0.69
9:I:86:MET:HE3	9:I:119:ALA:HB3	1.73	0.69
19:U:35:GLU:N	19:U:35:GLU:OE1	2.24	0.69
22:X:61:ARG:HD2	32:d:31:GLN:HG3	1.74	0.69
25:a:63:TYR:CD1	29:P:6:PRO:HB3	2.28	0.69
31:Z:163:ILE:C	31:Z:163:ILE:HD12	2.17	0.69
1:2:1198:U:OP1	38:2:1601:HOH:O	2.11	0.69
22:X:34:GLU:OE1	22:X:34:GLU:N	2.24	0.69
32:d:71:LEU:HD13	32:d:71:LEU:C	2.18	0.68
1:2:30:C:O3'	14:N:141:LYS:NZ	2.25	0.68
1:2:603:U:OP1	36:2:1574:SPM:H81	1.93	0.68
8:H:23:ARG:H	8:H:23:ARG:HD2	1.58	0.68
12:L:94:ASP:N	12:L:94:ASP:OD1	2.24	0.68
3:B:98:ILE:HG12	3:B:142:PRO:HB3	1.74	0.68
11:K:102:ILE:HD13	32:d:67:ILE:HD13	1.74	0.68
27:4:9:G:O2'	27:4:10:G:N7	2.25	0.68
32:d:7:LYS:HE2	32:d:55:GLN:HG3	1.73	0.68
1:2:1034:G:N2	1:2:1037:A:OP2	2.21	0.68
1:2:409:G:OP2	26:e:31:ARG:NH2	2.26	0.68
2:A:161:GLU:OE2	2:A:166:ARG:NH1	2.27	0.68
3:B:49:ILE:O	3:B:187:ASN:ND2	2.26	0.68
8:H:26:SER:HB3	22:X:67:ILE:HD11	1.74	0.68
1:2:983:A:P	29:P:2:GLY:HA3	2.34	0.68
2:A:119:ARG:HB2	2:A:192:LEU:HD21	1.76	0.68
13:M:22:LEU:HD13	13:M:38:SER:HB3	1.76	0.68
25:a:36:TYR:CZ	25:a:54:LYS:NZ	2.62	0.68
1:2:1054:A:OP2	17:S:7:LYS:NZ	2.27	0.68
6:F:123:SER:O	9:I:100:LYS:NZ	2.23	0.68
20:V:52:ILE:HG21	20:V:63:VAL:HG11	1.75	0.68
23:Y:26:TYR:CE1	23:Y:37:LYS:HB3	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:7:LYS:HE3	32:d:7:LYS:CA	2.14	0.68
1:2:672:OMG:H2'	1:2:673:G:C8	2.29	0.68
23:Y:41:CYS:HB3	23:Y:46:SER:H	1.57	0.68
6:F:126:CYS:SG	6:F:128:CYS:HB3	2.33	0.68
16:Q:98:ARG:NH1	16:Q:102:GLU:OE2	2.24	0.68
15:O:30:LYS:HZ2	33:c:9:ILE:C	1.94	0.67
15:O:72:ILE:HG21	15:O:75:LEU:HD23	1.73	0.67
25:a:17:LEU:HB3	25:a:30:ILE:HB	1.76	0.67
12:L:30:LYS:HZ1	12:L:82:VAL:HG12	1.59	0.67
1:2:71:G:O6	1:2:213:C:N4	2.26	0.67
1:2:1489:U:H2'	1:2:1490:C:C6	2.29	0.67
1:2:714:G:H21	9:I:3:PHE:HZ	1.41	0.67
12:L:46:LEU:HD22	29:P:32:TYR:CE1	2.30	0.67
1:2:634:U:OP1	2:A:188:LYS:NZ	2.28	0.67
1:2:1374:U:C2	1:2:1448:G:N2	2.63	0.67
2:A:116:TYR:CE1	2:A:195:PRO:HD2	2.29	0.67
36:2:1573:SPM:H82	36:2:1573:SPM:C4	2.24	0.67
33:c:96:LEU:HB2	33:c:106:TYR:CE1	2.30	0.67
34:E:153:LYS:H	34:E:156:MET:HE2	1.60	0.67
1:2:900:C:H2'	1:2:901:A:H8	1.59	0.67
4:C:47:MET:HE2	4:C:51:GLN:HG2	1.77	0.67
12:L:46:LEU:HD22	29:P:32:TYR:CG	2.30	0.67
32:d:4:LEU:O	32:d:6:ILE:HD13	1.95	0.67
11:K:32:VAL:HG13	11:K:37:ILE:HG22	1.77	0.67
12:L:90:ARG:NH2	12:L:91:VAL:O	2.23	0.67
18:T:5:ILE:HD11	18:T:9:TRP:HE1	1.60	0.67
1:2:1453:C:C5	1:2:1454:G:N7	2.63	0.67
22:X:76:ARG:H	22:X:76:ARG:HD3	1.59	0.67
27:4:22:G:H2'	27:4:23:C:H6	1.60	0.67
1:2:481:OMC:HM22	1:2:482:C:H5'	1.77	0.67
1:2:1451:G:N3	1:2:1452:U:C6	2.63	0.67
10:J:63:ALA:HB2	10:J:78:ILE:HG13	1.75	0.67
12:L:41:LEU:HD11	12:L:73:LEU:HB2	1.76	0.67
32:d:4:LEU:HD13	32:d:4:LEU:C	2.19	0.67
8:H:41:THR:O	8:H:44:ARG:NH1	2.27	0.66
36:2:1563:SPM:N1	38:2:1621:HOH:O	2.27	0.66
7:G:167:VAL:HG21	7:G:196:ILE:HD11	1.77	0.66
8:H:156:LYS:HE3	33:c:68:TYR:CE2	2.31	0.66
1:2:1292:C:OP1	15:O:35:ASN:ND2	2.28	0.66
19:U:137:LYS:HD3	19:U:137:LYS:N	2.10	0.66
20:V:19:ARG:HE	20:V:21:MET:HE2	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:29:LYS:NZ	32:d:27:TYR:O	2.28	0.66
17:S:31:ASN:O	17:S:35:VAL:HG23	1.95	0.66
15:O:84:LYS:O	18:T:15:ARG:NH1	2.29	0.66
4:C:21:LYS:HZ1	9:I:21:ARG:HG2	1.59	0.66
15:O:47:ASP:OD1	15:O:49:ASN:ND2	2.28	0.66
6:F:206:THR:OG1	6:F:209:ASP:OD1	2.11	0.66
7:G:49:LYS:HD3	7:G:50:THR:N	2.11	0.66
11:K:60:ILE:O	11:K:64:ILE:HG13	1.96	0.66
19:U:143:PHE:HD2	19:U:143:PHE:O	1.79	0.66
2:A:19:TRP:CZ2	2:A:37:PRO:HG3	2.30	0.66
3:B:112:LYS:NZ	3:B:224:GLU:O	2.29	0.66
8:H:34:MET:HE3	8:H:35:PRO:HD2	1.78	0.66
1:2:16:G:H2'	1:2:17:C:C6	2.31	0.65
6:F:3:GLU:OE1	6:F:3:GLU:N	2.29	0.65
8:H:138:LEU:HB3	8:H:142:HIS:NE2	2.11	0.65
10:J:81:ILE:HD11	10:J:96:ILE:HG12	1.77	0.65
19:U:94:GLU:N	19:U:94:GLU:OE2	2.27	0.65
1:2:17:C:H2'	1:2:18:C:C6	2.30	0.65
19:U:45:PHE:HB2	19:U:87:LYS:HB2	1.77	0.65
1:2:218:C:H2'	1:2:219:A:H8	1.60	0.65
21:W:49:TYR:HB2	21:W:56:LYS:HG2	1.76	0.65
32:d:7:LYS:HE2	32:d:55:GLN:CG	2.27	0.65
4:C:21:LYS:NZ	9:I:21:ARG:HG2	2.12	0.65
31:Z:56:ILE:HG23	31:Z:63:ILE:HD11	1.78	0.65
32:d:12:ARG:HD3	32:d:12:ARG:C	2.21	0.65
1:2:349:A:H5''	1:2:350:C:H5	1.61	0.65
15:O:11:ILE:HG22	15:O:12:PHE:CD1	2.31	0.65
23:Y:32:ASN:HA	24:3:68:LEU:HB2	1.79	0.65
25:a:36:TYR:OH	25:a:54:LYS:NZ	2.30	0.65
1:2:1081:G:H5''	12:L:36:ARG:HB3	1.79	0.65
21:W:33:HIS:CD2	21:W:54:LYS:HG3	2.32	0.65
1:2:610:C:N4	1:2:712:A:OP2	2.29	0.65
1:2:790:U:O2'	1:2:1496:C:OP1	2.15	0.65
11:K:50:MET:HA	11:K:50:MET:HE3	1.77	0.65
1:2:794:A:OP2	36:2:1575:SPM:H31	1.97	0.65
1:2:409:G:O2'	1:2:456:A:N1	2.30	0.64
1:2:1081:G:N2	1:2:1082:U:O4	2.30	0.64
3:B:29:LYS:HA	3:B:29:LYS:HE2	1.78	0.64
21:W:20:LYS:HE2	21:W:20:LYS:HA	1.77	0.64
1:2:375:C:O2'	20:V:109:LYS:NZ	2.28	0.64
10:J:93:ARG:HB2	10:J:95:ILE:HD13	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:15:ARG:HG3	18:T:33:LEU:HB3	1.79	0.64
22:X:22:VAL:HG23	22:X:62:VAL:HA	1.79	0.64
24:3:112:ASP:O	24:3:115:ILE:HG12	1.97	0.64
32:d:65:LEU:O	32:d:65:LEU:HD22	1.97	0.64
7:G:164:ARG:NH1	7:G:181:PRO:O	2.29	0.64
25:a:57:LEU:HD22	25:a:57:LEU:H	1.62	0.64
18:T:27:MET:N	18:T:27:MET:SD	2.70	0.64
21:W:26:ASN:OD1	21:W:27:GLU:N	2.31	0.64
1:2:1251:A:H2'	1:2:1252:A:C8	2.32	0.64
1:2:1451:G:N1	1:2:1452:U:C4	2.66	0.64
22:X:23:ILE:HA	22:X:62:VAL:HG23	1.79	0.64
24:3:55:GLU:HB2	24:3:80:VAL:HG21	1.79	0.64
3:B:99:VAL:HG23	3:B:110:VAL:HG13	1.79	0.64
32:d:7:LYS:HE2	32:d:55:GLN:CD	2.23	0.64
8:H:88:ILE:HD13	33:c:105:ILE:HD13	1.79	0.64
19:U:142:ILE:O	19:U:145:GLU:HG2	1.98	0.64
22:X:22:VAL:HG12	22:X:40:VAL:HG12	1.79	0.64
32:d:21:ILE:HD11	32:d:60:VAL:HB	1.79	0.64
1:2:487:C:H41	14:N:66:ASN:ND2	1.97	0.63
3:B:188:ASN:HA	3:B:194:LEU:HD13	1.80	0.63
1:2:1034:G:H4'	36:2:1560:SPM:H42	1.81	0.63
18:T:84:ILE:HD11	18:T:106:ILE:HG22	1.79	0.63
25:a:36:TYR:CE2	25:a:54:LYS:HD2	2.33	0.63
8:H:3:LEU:O	32:d:70:LYS:NZ	2.31	0.63
1:2:1287:G:H2'	1:2:1288:C:C6	2.33	0.63
1:2:505:G:O6	26:e:33:ARG:HD2	1.98	0.63
1:2:418:U:H1'	1:2:419:A:C5	2.34	0.63
17:S:31:ASN:OD1	17:S:55:THR:OG1	2.14	0.63
19:U:77:GLU:OE1	19:U:77:GLU:N	2.29	0.63
5:D:97:THR:HG23	5:D:99:GLN:H	1.63	0.63
24:3:20:LEU:O	24:3:24:ARG:NH1	2.31	0.63
24:3:27:LYS:HD2	24:3:90:CYS:HB2	1.80	0.63
1:2:506:A:OP2	5:D:37:ASN:ND2	2.32	0.62
14:N:91:ASP:N	14:N:138:TYR:OH	2.28	0.62
1:2:1443:G:H3'	1:2:1444:G:H8	1.64	0.62
24:3:79:TYR:OH	24:3:121:ILE:HG21	1.98	0.62
32:d:29:ARG:HH12	32:d:62:TRP:HA	1.62	0.62
1:2:885:G:H2'	1:2:886:G:H8	1.64	0.62
1:2:147:G:H4'	7:G:153:THR:OG1	1.99	0.62
8:H:21:GLU:OE1	32:d:58:ALA:N	2.33	0.62
23:Y:27:TYR:O	23:Y:37:LYS:NZ	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:ARG:HG2	7:G:112:TYR:HD1	1.64	0.62
11:K:63:LYS:O	11:K:63:LYS:HD2	1.99	0.62
34:E:66:LEU:HB2	34:E:86:SER:HB2	1.81	0.62
1:2:920:U:C2	1:2:1188:G:C2	2.87	0.62
1:2:1328:A:OP2	19:U:89:ARG:NH2	2.30	0.62
4:C:47:MET:HA	4:C:47:MET:HE3	1.82	0.62
8:H:115:THR:HG21	22:X:57:LYS:HD2	1.80	0.62
1:2:125:G:OP2	36:2:1567:SPM:C8	2.47	0.62
5:D:158:THR:HG21	20:V:39:GLY:HA3	1.82	0.62
11:K:13:ARG:HG2	11:K:18:ARG:HD3	1.81	0.62
16:Q:28:ARG:HG3	16:Q:65:VAL:HA	1.82	0.62
21:W:14:SER:O	21:W:15:ARG:HD3	1.99	0.62
25:a:51:GLU:C	25:a:54:LYS:HG2	2.24	0.62
1:2:962:A:H2'	1:2:963:G:C8	2.34	0.62
24:3:88:GLU:OE2	24:3:94:VAL:N	2.32	0.62
19:U:108:PHE:CD2	19:U:125:ARG:HD3	2.35	0.62
1:2:500:C:OP2	26:e:25:LYS:NZ	2.21	0.62
1:2:1318:C:H2'	1:2:1319:A:H8	1.64	0.62
11:K:29:ARG:HH12	19:U:156:TYR:HA	1.64	0.62
14:N:119:LEU:HD12	14:N:120:PRO:HD2	1.82	0.62
33:c:35:LYS:O	33:c:38:LYS:HG2	2.00	0.61
1:2:927:G:P	36:2:1576:SPM:H121	2.38	0.61
6:F:79:LEU:HD11	6:F:188:GLU:HA	1.81	0.61
8:H:102:VAL:O	8:H:105:ILE:HG22	2.00	0.61
11:K:123:TRP:HE3	11:K:124:MET:HG3	1.65	0.61
1:2:1015:G:OP1	36:2:1562:SPM:N14	2.33	0.61
2:A:116:TYR:HE1	2:A:194:VAL:HG22	1.64	0.61
21:W:47:LEU:HA	21:W:58:VAL:HG22	1.83	0.61
26:e:13:VAL:HA	26:e:16:GLN:HG2	1.82	0.61
32:d:12:ARG:HD3	32:d:13:GLU:N	2.15	0.61
32:d:18:ASP:OD1	32:d:19:ASP:N	2.32	0.61
33:c:22:LYS:HD3	33:c:25:LYS:HD2	1.81	0.61
1:2:1188:G:H2'	1:2:1188:G:N3	2.15	0.61
1:2:1213:A:H2'	1:2:1214:G:C8	2.36	0.61
1:2:1134:G:OP2	17:S:56:ARG:NH2	2.19	0.61
7:G:41:VAL:HG11	7:G:146:LEU:HD21	1.83	0.61
34:E:109:ILE:HB	34:E:113:GLU:HG3	1.83	0.61
1:2:502:C:OP1	26:e:41:ARG:NH1	2.34	0.61
4:C:22:ILE:HD11	6:F:209:ASP:HB3	1.81	0.61
1:2:983:A:OP1	29:P:2:GLY:CA	2.49	0.61
8:H:38:LEU:HD22	11:K:47:LEU:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:47:GLU:N	19:U:47:GLU:OE2	2.33	0.61
19:U:66:ARG:O	19:U:70:VAL:HG13	2.01	0.61
1:2:1451:G:C5	1:2:1452:U:C4	2.82	0.61
1:2:272:C:H2'	1:2:273:C:H6	1.66	0.61
32:d:65:LEU:HD22	32:d:65:LEU:C	2.26	0.61
1:2:1076:C:H2'	1:2:1077:A:H8	1.66	0.60
7:G:28:GLN:OE1	7:G:28:GLN:N	2.34	0.60
1:2:749:A:OP1	27:4:38:A:O2'	2.19	0.60
8:H:157:PRO:HB3	33:c:102:ARG:HB3	1.83	0.60
16:Q:25:ARG:HA	16:Q:25:ARG:HE	1.64	0.60
1:2:1004:G:HO2'	1:2:1178:C:HO2'	1.49	0.60
5:D:21:GLU:OE1	5:D:21:GLU:N	2.20	0.60
32:d:16:ILE:CG2	32:d:21:ILE:HD13	2.31	0.60
1:2:272:C:H2'	1:2:273:C:C6	2.36	0.60
8:H:3:LEU:HD21	32:d:70:LYS:CD	2.26	0.60
11:K:26:GLY:HA3	11:K:65:ASP:HB2	1.83	0.60
11:K:38:GLU:OE2	11:K:38:GLU:N	2.33	0.60
12:L:46:LEU:HD22	29:P:32:TYR:CD2	2.36	0.60
13:M:6:GLU:OE1	13:M:7:ILE:N	2.34	0.60
1:2:655:A:H2'	1:2:656:U:H6	1.66	0.60
8:H:107:ASN:ND2	8:H:172:ASN:OD1	2.35	0.60
31:Z:127:LEU:HG	31:Z:186:PRO:HA	1.84	0.60
1:2:1436:U:H2'	1:2:1437:G:C8	2.37	0.60
7:G:42:PRO:HB2	7:G:79:PHE:HD2	1.65	0.60
8:H:19:LYS:HZ1	32:d:71:LEU:HD21	1.66	0.60
18:T:87:LYS:HE2	18:T:100:THR:OG1	2.02	0.60
18:T:121:GLU:OE1	18:T:121:GLU:N	2.28	0.60
20:V:64:VAL:HG21	20:V:94:GLU:HG2	1.84	0.60
1:2:1206:C:H5''	19:U:47:GLU:OE1	2.02	0.60
2:A:183:LYS:HD3	2:A:184:ALA:H	1.67	0.60
18:T:115:ILE:HD12	18:T:115:ILE:O	2.01	0.60
1:2:962:A:H2'	1:2:963:G:H8	1.67	0.60
6:F:126:CYS:SG	6:F:128:CYS:HB2	2.41	0.60
6:F:183:GLU:OE2	6:F:185:ARG:HB2	2.02	0.60
8:H:23:ARG:HD2	8:H:23:ARG:N	2.17	0.60
10:J:40:GLU:N	10:J:40:GLU:OE2	2.31	0.60
12:L:46:LEU:HD22	29:P:32:TYR:CZ	2.37	0.60
13:M:6:GLU:OE1	13:M:7:ILE:HG23	2.02	0.60
18:T:20:ASP:HA	18:T:23:LEU:HD12	1.83	0.60
1:2:1370:U:C2'	1:2:1371:C:H5'	2.31	0.60
15:O:112:LYS:O	15:O:114:ARG:NH1	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:24:LEU:CD2	32:d:53:ILE:HD11	2.32	0.60
1:2:1444:G:N2	1:2:1445:G:O6	2.34	0.59
13:M:18:GLN:HE22	13:M:90:GLY:HA2	1.67	0.59
26:e:43:VAL:HG23	26:e:44:LYS:HE2	1.84	0.59
27:4:69:C:H2'	27:4:70:G:H8	1.66	0.59
1:2:636:C:H2'	1:2:637:U:C6	2.36	0.59
1:2:886:G:O2'	1:2:1363:C:OP2	2.18	0.59
1:2:1368:5MC:H2'	1:2:1369:G:C8	2.36	0.59
3:B:135:TYR:CE1	6:F:16:ARG:CZ	2.85	0.59
11:K:23:ILE:HG22	11:K:66:ALA:HB2	1.83	0.59
25:a:62:PRO:HB3	29:P:4:TYR:HD1	1.67	0.59
1:2:1443:G:H3'	1:2:1444:G:C8	2.37	0.59
3:B:170:PHE:HE1	3:B:197:LEU:HB3	1.67	0.59
1:2:458:G:H2'	1:2:459:C:C6	2.37	0.59
8:H:85:ALA:O	8:H:89:ILE:HG23	2.03	0.59
15:O:132:THR:OG1	33:c:3:GLY:HA3	2.02	0.59
17:S:21:LYS:HZ1	17:S:58:TYR:HE1	1.50	0.59
19:U:20:LEU:HD21	19:U:65:LEU:HD12	1.84	0.59
19:U:69:TYR:HA	19:U:127:LEU:HD13	1.85	0.59
1:2:534:G:O6	14:N:3:LYS:NZ	2.35	0.59
10:J:42:ILE:HD12	10:J:59:TYR:HD1	1.67	0.59
27:4:24:U:H2'	27:4:25:C:H6	1.66	0.59
16:Q:13:ILE:HG21	21:W:10:PRO:HB2	1.84	0.59
18:T:54:LEU:O	18:T:58:ARG:HD3	2.02	0.59
21:W:38:VAL:H	21:W:48:VAL:HG12	1.67	0.59
34:E:161:GLU:HB2	34:E:168:LEU:HD21	1.85	0.59
1:2:1451:G:H2'	1:2:1452:U:C6	2.37	0.59
8:H:117:ILE:HD13	8:H:126:VAL:HB	1.84	0.59
15:O:42:ARG:NH1	19:U:38:LEU:HB3	2.16	0.59
17:S:40:ASP:CG	31:Z:196:LYS:HB3	2.27	0.59
32:d:65:LEU:N	32:d:66:PRO:HD2	2.17	0.59
1:2:573:C:H4'	5:D:72:GLN:HG2	1.83	0.59
1:2:866:A:H2'	1:2:867:C:H6	1.67	0.59
13:M:8:ARG:HG2	13:M:71:ILE:HD13	1.85	0.59
1:2:902:A:N3	1:2:1340:U:O2'	2.31	0.59
5:D:133:VAL:HG22	5:D:153:ILE:HD13	1.84	0.59
16:Q:61:VAL:HG11	16:Q:69:VAL:HG23	1.83	0.59
16:Q:102:GLU:HG3	16:Q:103:TYR:CD1	2.38	0.59
1:2:602:C:OP1	36:2:1574:SPM:H42	2.02	0.59
1:2:12:U:H2'	1:2:13:C:C6	2.38	0.58
1:2:704:C:OP1	1:2:814:U:O2'	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:875:U:OP1	14:N:63:ARG:NH1	2.36	0.58
19:U:143:PHE:CZ	19:U:156:TYR:HB3	2.37	0.58
19:U:145:GLU:HA	19:U:148:GLU:HG3	1.86	0.58
27:4:58:A:O2'	27:4:60:U:OP2	2.16	0.58
32:d:7:LYS:CG	32:d:16:ILE:HD11	2.33	0.58
33:c:56:LEU:O	33:c:59:ILE:HG22	2.03	0.58
2:A:68:TYR:OH	2:A:87:GLU:OE1	2.21	0.58
15:O:100:ILE:HG22	15:O:104:ARG:HH22	1.67	0.58
22:X:44:GLU:CD	32:d:50:TYR:HH	2.06	0.58
1:2:1446:G:H2'	1:2:1447:A:H8	1.67	0.58
3:B:18:GLU:OE2	3:B:66:ARG:NH2	2.36	0.58
3:B:170:PHE:O	3:B:188:ASN:ND2	2.33	0.58
22:X:61:ARG:CD	32:d:31:GLN:HG3	2.33	0.58
1:2:611:U:O4	1:2:711:G:O2'	2.21	0.58
1:2:673:G:H2'	1:2:674:A:H8	1.69	0.58
1:2:1374:U:N3	1:2:1448:G:C2	2.71	0.58
8:H:19:LYS:NZ	32:d:71:LEU:HD11	2.19	0.58
8:H:132:PRO:HA	8:H:135:ARG:HD3	1.84	0.58
10:J:38:SER:OG	10:J:39:ALA:N	2.36	0.58
14:N:70:ARG:HG3	14:N:119:LEU:HD13	1.86	0.58
15:O:4:GLN:HE22	15:O:6:LYS:HG2	1.68	0.58
20:V:107:GLN:C	20:V:108:LYS:HD3	2.28	0.58
34:E:120:ARG:HG3	34:E:227:MET:HE2	1.85	0.58
1:2:938:U:H2'	29:P:27:SER:OG	2.03	0.58
1:2:1081:G:N7	1:2:1109:C:O2'	2.35	0.58
25:a:57:LEU:CD2	25:a:57:LEU:H	2.16	0.58
8:H:3:LEU:CD2	32:d:70:LYS:HE2	2.21	0.58
5:D:19:ILE:HG22	5:D:22:ARG:H	1.68	0.58
8:H:30:TYR:OH	22:X:61:ARG:NH1	2.37	0.58
25:a:38:CYS:SG	25:a:66:THR:OG1	2.60	0.58
3:B:21:LYS:C	3:B:21:LYS:HZ2	2.12	0.58
11:K:12:ALA:HB1	11:K:84:MET:HE2	1.85	0.58
27:4:22:G:H2'	27:4:23:C:C6	2.39	0.58
32:d:54:LYS:HG2	32:d:54:LYS:O	2.03	0.58
1:2:16:G:N7	36:2:1548:SPM:N14	2.52	0.58
1:2:1201:A:H2	1:2:1204:G:N3	2.02	0.58
12:L:7:ILE:HD13	12:L:74:ILE:CG2	2.33	0.58
1:2:1204:G:H2'	1:2:1205:G:H8	1.69	0.58
11:K:102:ILE:HD12	32:d:67:ILE:HD13	1.85	0.58
25:a:62:PRO:HB2	29:P:4:TYR:HB2	1.86	0.58
34:E:40:ALA:HB2	34:E:75:TYR:HB2	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:983:A:P	29:P:2:GLY:CA	2.92	0.57
8:H:96:ASN:OD1	8:H:98:ILE:HD12	2.04	0.57
8:H:116:ARG:HH11	8:H:125:TYR:HD2	1.51	0.57
23:Y:35:LYS:HD3	23:Y:35:LYS:N	2.18	0.57
24:3:86:LEU:HD23	24:3:87:GLY:H	1.69	0.57
25:a:44:LYS:HG2	25:a:45:TYR:CE2	2.39	0.57
27:4:17:C:OP2	27:4:17(A):U:O2'	2.20	0.57
32:d:52:LEU:HD12	32:d:52:LEU:O	2.04	0.57
18:T:31:ILE:HG23	18:T:39:ARG:HG2	1.84	0.57
33:c:100:ASN:ND2	33:c:102:ARG:HH21	2.01	0.57
1:2:1282:A:O2'	18:T:76:ASN:ND2	2.35	0.57
2:A:20:TYR:CE2	2:A:41:ILE:HD12	2.39	0.57
13:M:72:MET:SD	13:M:72:MET:N	2.77	0.57
24:3:114:ILE:O	24:3:118:VAL:HG23	2.04	0.57
33:c:39:GLU:HB2	33:c:76:ILE:HA	1.84	0.57
1:2:1311:G:N2	1:2:1338:A:OP2	2.29	0.57
3:B:95:GLN:OE1	3:B:120:ARG:NH1	2.36	0.57
24:3:31:LYS:C	24:3:32:ILE:HD12	2.30	0.57
25:a:14:LEU:CG	31:Z:24:LYS:HG2	2.23	0.57
27:4:43:A:H2'	27:4:44:A:C8	2.39	0.57
1:2:1068:A:N7	38:2:1632:HOH:O	2.32	0.57
1:2:1370:U:H2'	1:2:1371:C:O4'	2.04	0.57
3:B:191:ARG:NH1	3:B:227:MET:SD	2.77	0.57
8:H:19:LYS:HZ1	32:d:71:LEU:HD11	1.70	0.57
17:S:40:ASP:OD1	31:Z:196:LYS:CB	2.53	0.57
19:U:60:ARG:HH11	19:U:104:ASN:HD21	1.51	0.57
20:V:61:ASN:O	20:V:87:ARG:NH1	2.36	0.57
23:Y:24:ARG:HD3	24:3:37:ASN:HB3	1.84	0.57
1:2:425:G:H2'	1:2:426:C:H6	1.69	0.57
1:2:1481:C:H2'	1:2:1482:G:H8	1.70	0.57
8:H:24:ASP:HB2	22:X:16:PHE:HE2	1.70	0.57
11:K:29:ARG:N	11:K:65:ASP:OD1	2.35	0.57
23:Y:36:LEU:HB3	23:Y:38:ASN:O	2.04	0.57
32:d:51:GLU:HA	32:d:51:GLU:OE1	2.05	0.57
1:2:1260:C:H5'	15:O:21:LYS:HZ3	1.69	0.57
6:F:205:VAL:H	9:I:70:ASN:HD21	1.53	0.57
9:I:92:TYR:CE1	30:R:68:LYS:HD3	2.40	0.57
1:2:263:G:H2'	1:2:264:G:H8	1.70	0.57
1:2:1287:G:H2'	1:2:1288:C:H6	1.69	0.57
3:B:142:PRO:HG2	3:B:165:ILE:HD13	1.85	0.57
15:O:37:ALA:O	15:O:41:ILE:HG23	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:57:ARG:HB2	23:Y:66:THR:HG22	1.87	0.57
1:2:676:C:H4'	13:M:119:ASP:OD1	2.04	0.57
5:D:81:GLY:O	5:D:84:LYS:NZ	2.38	0.56
17:S:17:TYR:OH	17:S:61:MET:SD	2.62	0.56
19:U:20:LEU:HD22	19:U:62:ALA:HA	1.85	0.56
1:2:1043:C:H2'	1:2:1044:C:H6	1.70	0.56
1:2:1355:U:H2'	1:2:1356:G:C8	2.40	0.56
15:O:85:ASP:OD2	15:O:86:TYR:N	2.38	0.56
1:2:93:C:H1'	1:2:359:C:H5'	1.88	0.56
1:2:809:C:OP1	36:2:1575:SPM:H81	2.04	0.56
1:2:1204:G:H2'	1:2:1205:G:C8	2.41	0.56
1:2:1318:C:H2'	1:2:1319:A:C8	2.40	0.56
5:D:123:ARG:HH21	26:e:31:ARG:NH2	2.03	0.56
7:G:80:LYS:NZ	7:G:145:GLY:O	2.35	0.56
8:H:16:TRP:CZ3	8:H:86:PHE:HB3	2.41	0.56
8:H:76:HIS:CD2	11:K:44:MET:HG3	2.39	0.56
15:O:75:LEU:HD12	19:U:39:LEU:HD13	1.86	0.56
20:V:107:GLN:O	20:V:108:LYS:HD3	2.05	0.56
23:Y:57:ARG:HA	23:Y:68:PHE:HA	1.86	0.56
1:2:1203:U:H5'	33:c:102:ARG:HD3	1.87	0.56
2:A:155:PHE:O	2:A:159:THR:OG1	2.22	0.56
6:F:160:VAL:HG12	6:F:178:SER:HB3	1.87	0.56
9:I:37:VAL:O	9:I:41:MET:HG3	2.05	0.56
12:L:46:LEU:CD2	29:P:32:TYR:CE1	2.87	0.56
23:Y:38:ASN:HD22	23:Y:58:TRP:HH2	1.52	0.56
23:Y:39:LYS:NZ	23:Y:67:GLU:OE2	2.33	0.56
3:B:40:ASP:OD1	3:B:41:THR:N	2.38	0.56
34:E:117:LYS:HB2	34:E:162:LEU:HD11	1.87	0.56
1:2:975:G:H2'	1:2:976:G:H8	1.70	0.56
3:B:43:LEU:HD13	3:B:48:HIS:CE1	2.40	0.56
12:L:46:LEU:HD22	29:P:32:TYR:CE2	2.41	0.56
15:O:34:TYR:CE1	15:O:38:LYS:HG3	2.41	0.56
17:S:40:ASP:OD1	31:Z:196:LYS:HG2	2.05	0.56
24:3:15:LEU:HD13	24:3:117:ARG:HE	1.70	0.56
32:d:50:TYR:CZ	32:d:54:LYS:HE3	2.40	0.56
13:M:113:VAL:O	13:M:113:VAL:HG12	2.05	0.56
25:a:42:GLU:OE1	25:a:43:LYS:HB3	2.05	0.56
1:2:392:U:O4	36:2:1564:SPM:N14	2.38	0.56
1:2:612:A:H5''	9:I:57:ARG:HE	1.70	0.56
1:2:920:U:C2	1:2:1188:G:N2	2.74	0.56
8:H:107:ASN:HD22	8:H:172:ASN:CG	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:98:ARG:N	13:M:98:ARG:HD3	2.21	0.56
15:O:4:GLN:NE2	15:O:4:GLN:O	2.38	0.56
17:S:30:THR:O	17:S:34:ILE:HG12	2.05	0.56
18:T:5:ILE:HD12	18:T:6:PRO:CD	2.30	0.56
20:V:19:ARG:NE	20:V:21:MET:HE2	2.21	0.56
1:2:642:G:H2'	1:2:643:A:C8	2.40	0.56
1:2:917:G:N7	15:O:133:ARG:NH2	2.49	0.56
8:H:142:HIS:CG	8:H:181:ARG:HD2	2.41	0.56
23:Y:22:ILE:HD12	23:Y:22:ILE:O	2.06	0.56
31:Z:185:LYS:HB3	31:Z:187:LEU:HD13	1.88	0.56
1:2:125:G:OP2	36:2:1567:SPM:H92	2.06	0.55
1:2:943:U:H4'	36:2:1561:SPM:H92	1.88	0.55
1:2:1453:C:C4	1:2:1454:G:C5	2.94	0.55
2:A:126:THR:OG1	2:A:128:TYR:O	2.23	0.55
8:H:91:LEU:O	33:c:63:SER:OG	2.15	0.55
14:N:143:GLN:OE1	14:N:143:GLN:N	2.38	0.55
24:3:12:PRO:HG3	24:3:117:ARG:NH1	2.21	0.55
1:2:95:G:OP2	36:2:1554:SPM:N5	2.38	0.55
1:2:504:C:H41	26:e:33:ARG:NH1	2.03	0.55
1:2:965:A:O4'	1:2:993:A:N6	2.40	0.55
1:2:1479:U:H2'	1:2:1480:G:H8	1.70	0.55
3:B:63:TYR:CD2	3:B:64:ARG:HG2	2.41	0.55
7:G:80:LYS:HE3	7:G:146:LEU:HD13	1.88	0.55
15:O:19:THR:CG2	33:c:40:ILE:HD12	2.36	0.55
19:U:120:ILE:HD13	19:U:126:SER:HB3	1.88	0.55
32:d:7:LYS:HG2	32:d:16:ILE:HD11	1.87	0.55
3:B:199:TRP:CD2	3:B:222:VAL:HG22	2.42	0.55
25:a:9:ASN:ND2	29:P:43:GLU:O	2.39	0.55
25:a:28:LEU:HD12	25:a:35:LEU:HB3	1.88	0.55
25:a:57:LEU:HD13	29:P:4:TYR:HE1	1.71	0.55
27:4:50:U:O2	27:4:64:G:N2	2.26	0.55
1:2:1343:G:H2'	1:2:1344:OMU:H6	1.88	0.55
12:L:27:ILE:O	12:L:30:LYS:HG2	2.07	0.55
14:N:60:ILE:HG12	14:N:72:CYS:SG	2.47	0.55
17:S:40:ASP:OD1	31:Z:196:LYS:N	2.39	0.55
8:H:113:GLU:OE1	8:H:130:VAL:HG23	2.07	0.55
8:H:193:ARG:HH12	22:X:73:ARG:CD	2.10	0.55
14:N:40:LYS:HG2	14:N:41:TYR:CZ	2.42	0.55
1:2:152:A:H2'	1:2:153:A:C8	2.42	0.55
1:2:428:U:O2'	1:2:430:U:O4	2.18	0.55
3:B:81:ARG:O	3:B:84:ILE:HG22	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:PRO:HA	8:H:28:LYS:HE2	1.88	0.55
23:Y:52:LEU:HB2	23:Y:53:LYS:HE2	1.88	0.55
1:2:1116:G:OP1	12:L:70:HIS:ND1	2.40	0.55
7:G:157:ASP:HA	7:G:205:ILE:HA	1.89	0.55
15:O:44:LEU:HB3	15:O:46:MET:HE3	1.89	0.55
19:U:158:GLU:OE1	19:U:158:GLU:N	2.38	0.55
25:a:22:ARG:NH1	25:a:45:TYR:O	2.28	0.55
1:2:1030:U:H4'	3:B:135:TYR:CE2	2.42	0.55
12:L:46:LEU:CD2	29:P:32:TYR:CD1	2.90	0.55
27:4:4:G:H2'	27:4:5:G:H8	1.71	0.55
1:2:1451:G:C6	1:2:1452:U:C5	2.82	0.55
5:D:44:ALA:HA	5:D:101:LEU:HD13	1.88	0.55
15:O:12:PHE:HE2	15:O:67:ILE:HG22	1.72	0.54
25:a:50:CYS:SG	25:a:53:ASP:CG	2.90	0.54
1:2:119:U:O2	34:E:141:ASN:ND2	2.36	0.54
1:2:966:U:C4	24:3:57:VAL:HG13	2.42	0.54
1:2:1257:U:OP1	33:c:99:LYS:NZ	2.41	0.54
4:C:37:CYS:SG	4:C:38:GLY:N	2.80	0.54
7:G:79:PHE:HE2	7:G:98:MET:HG2	1.71	0.54
14:N:7:PRO:HG3	14:N:15:LYS:HB3	1.90	0.54
21:W:40:CYS:HB3	21:W:44:GLY:H	1.72	0.54
31:Z:165:ARG:HB2	31:Z:182:VAL:HG22	1.89	0.54
1:2:521:U:C4	14:N:27:GLN:HG2	2.42	0.54
1:2:1003:A:H2'	1:2:1004:G:C8	2.43	0.54
8:H:24:ASP:HB2	22:X:16:PHE:CE2	2.43	0.54
12:L:6:ARG:HD2	12:L:100:GLN:NE2	2.22	0.54
15:O:43:LYS:HZ1	15:O:74:GLY:H	1.55	0.54
33:c:59:ILE:HG21	33:c:108:ALA:HB2	1.90	0.54
1:2:457:A:OP1	26:e:26:HIS:HE1	1.90	0.54
1:2:1194:OMG:OP1	38:2:1602:HOH:O	2.18	0.54
1:2:1451:G:O6	1:2:1452:U:O4	2.25	0.54
2:A:18:LYS:HG3	2:A:20:TYR:CE1	2.42	0.54
3:B:95:GLN:O	3:B:120:ARG:NH2	2.40	0.54
6:F:11:GLU:HG2	6:F:12:GLU:OE1	2.07	0.54
21:W:2:MET:SD	21:W:6:ARG:HB3	2.48	0.54
11:K:29:ARG:NH1	19:U:156:TYR:HA	2.22	0.54
24:3:27:LYS:O	24:3:32:ILE:HD11	2.07	0.54
24:3:51:VAL:HG23	24:3:77:TYR:HB2	1.89	0.54
1:2:1191:C:OP2	33:c:2:GLY:N	2.41	0.54
11:K:23:ILE:HG22	11:K:66:ALA:CB	2.37	0.54
17:S:17:TYR:CZ	17:S:21:LYS:HE2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3:18:LYS:NZ	24:3:113:GLU:HB3	2.22	0.54
1:2:125:G:P	36:2:1567:SPM:H72	2.33	0.54
1:2:910:A:O2'	1:2:1297:A:N3	2.40	0.54
1:2:1015:G:H5''	31:Z:167:ILE:HD13	1.90	0.54
6:F:188:GLU:HG3	6:F:189:ASN:N	2.22	0.54
8:H:143:ILE:HA	8:H:165:GLU:OE2	2.08	0.54
11:K:27:LYS:NZ	19:U:155:VAL:HG22	2.22	0.54
12:L:93:GLU:OE1	12:L:93:GLU:N	2.40	0.54
1:2:1453:C:C6	1:2:1454:G:C8	2.95	0.54
3:B:227:MET:HA	3:B:227:MET:HE3	1.88	0.54
4:C:47:MET:HG2	9:I:21:ARG:CZ	2.38	0.54
8:H:3:LEU:HD21	32:d:70:LYS:HE3	0.54	0.54
15:O:62:LYS:O	15:O:66:VAL:HG23	2.06	0.54
19:U:36:TRP:CD1	19:U:36:TRP:H	2.26	0.54
23:Y:55:ASN:ND2	23:Y:57:ARG:HG2	2.23	0.54
25:a:6:ARG:HB3	31:Z:165:ARG:HD3	1.89	0.54
27:4:52:G:H2'	27:4:53:G:H8	1.73	0.54
27:4:74:C:H4'	27:4:75:C:O5'	2.06	0.54
5:D:16:HIS:HB3	5:D:19:ILE:HD13	1.90	0.54
11:K:45:VAL:O	11:K:49:ILE:HG12	2.07	0.54
24:3:116:LYS:HA	24:3:116:LYS:HE3	1.89	0.54
1:2:979:A:H4'	18:T:72:THR:HA	1.90	0.54
1:2:1095:C:O2'	1:2:1096:U:OP2	2.23	0.54
1:2:1096:U:P	19:U:137:LYS:HZ2	2.31	0.54
1:2:1481:C:H2'	1:2:1482:G:C8	2.43	0.54
1:2:263:G:H5''	10:J:98:ARG:HB3	1.90	0.53
1:2:617:G:H2'	1:2:618:C:C6	2.43	0.53
6:F:59:VAL:HG11	6:F:81:ILE:HD12	1.90	0.53
8:H:10:ILE:HA	8:H:37:TYR:CZ	2.43	0.53
10:J:45:LYS:NZ	10:J:53:PHE:HB3	2.23	0.53
13:M:42:VAL:HG23	13:M:43:VAL:HG13	1.89	0.53
20:V:45:ARG:NH1	20:V:65:VAL:O	2.40	0.53
1:2:1495:C:H2'	1:2:1496:C:C6	2.43	0.53
5:D:28:GLU:HA	26:e:38:TYR:CE2	2.43	0.53
6:F:68:THR:HG22	6:F:69:ASP:H	1.72	0.53
1:2:1095:C:H1'	1:2:1096:U:H5'	1.89	0.53
8:H:26:SER:HA	22:X:65:ILE:HB	1.90	0.53
13:M:65:ASP:O	13:M:69:LYS:HG2	2.09	0.53
33:c:64:ILE:HG23	33:c:105:ILE:HG23	1.90	0.53
1:2:440:A:C2	20:V:109:LYS:HE3	2.33	0.53
1:2:1475:MA6:H2'	1:2:1476:A:C8	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:147:VAL:HG23	6:F:180:THR:HG22	1.90	0.53
8:H:17:ASP:OD2	8:H:19:LYS:HE2	2.09	0.53
8:H:85:ALA:CB	8:H:162:LEU:HD22	2.38	0.53
8:H:130:VAL:CG1	8:H:135:ARG:HG3	2.38	0.53
15:O:72:ILE:CG2	15:O:75:LEU:HD23	2.39	0.53
29:P:21:ARG:NE	31:Z:20:GLU:OE1	2.30	0.53
33:c:35:LYS:O	33:c:38:LYS:CG	2.57	0.53
1:2:1253:A:N1	1:2:1335:G:O2'	2.37	0.53
3:B:181:ASP:OD1	4:C:44:ARG:NH1	2.40	0.53
4:C:45:ASP:OD1	4:C:48:CYS:HB2	2.08	0.53
14:N:140:GLY:O	14:N:141:LYS:HG3	2.09	0.53
20:V:46:LYS:O	20:V:49:ILE:HG13	2.08	0.53
23:Y:41:CYS:SG	23:Y:43:ARG:HD2	2.49	0.53
24:3:27:LYS:HA	24:3:32:ILE:HD11	1.90	0.53
3:B:82:LEU:HD23	3:B:201:LEU:HD23	1.89	0.53
5:D:107:GLN:HE21	5:D:119:ILE:HG13	1.74	0.53
8:H:37:TYR:HB2	11:K:51:GLU:OE1	2.08	0.53
10:J:43:ARG:NE	10:J:119:GLY:O	2.37	0.53
12:L:13:ASN:HB3	12:L:94:ASP:OD2	2.08	0.53
11:K:123:TRP:CE3	11:K:124:MET:HG3	2.43	0.53
22:X:29:THR:OG1	22:X:30:GLY:N	2.42	0.53
22:X:54:ARG:NH1	22:X:73:ARG:HB2	2.23	0.53
1:2:17:C:H4'	1:2:848:G:C8	2.43	0.53
6:F:132:HIS:ND1	6:F:175:ASP:OD2	2.42	0.53
12:L:8:ARG:HG2	12:L:73:LEU:HD12	1.91	0.53
22:X:12:ILE:O	22:X:15:GLU:HG3	2.08	0.53
22:X:66:LEU:HD12	22:X:67:ILE:H	1.74	0.53
23:Y:41:CYS:CB	23:Y:46:SER:H	2.21	0.53
33:c:103:LEU:HD12	33:c:103:LEU:O	2.09	0.53
2:A:193:LYS:NZ	2:A:195:PRO:HA	2.24	0.53
6:F:85:MET:N	6:F:85:MET:SD	2.82	0.53
6:F:198:LEU:O	6:F:201:THR:OG1	2.19	0.53
8:H:192:SER:O	8:H:192:SER:OG	2.27	0.53
17:S:40:ASP:OD1	31:Z:196:LYS:HB3	2.09	0.53
21:W:24:CYS:SG	21:W:40:CYS:SG	3.07	0.53
21:W:50:SER:O	21:W:51:MET:HE2	2.08	0.53
25:a:62:PRO:HB3	29:P:4:TYR:CD1	2.44	0.53
1:2:827:A:H2'	1:2:828:A:C8	2.44	0.53
2:A:196:GLU:HA	2:A:196:GLU:OE2	2.08	0.53
5:D:86:GLU:OE1	5:D:86:GLU:N	2.21	0.53
8:H:27:LEU:HD21	8:H:135:ARG:HH21	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:40:ASP:OD2	31:Z:196:LYS:HB3	2.09	0.53
18:T:84:ILE:HD11	18:T:106:ILE:CG2	2.39	0.53
1:2:910:A:H2'	1:2:911:A:H8	1.72	0.52
1:2:1008:G:OP2	36:2:1576:SPM:H21	2.09	0.52
36:2:1573:SPM:C4	36:2:1573:SPM:C8	2.86	0.52
3:B:57:TYR:OH	4:C:65:PRO:O	2.25	0.52
10:J:45:LYS:HZ3	10:J:53:PHE:HB3	1.74	0.52
11:K:17:ALA:HB2	11:K:73:GLY:HA3	1.89	0.52
1:2:25:G:H2'	1:2:26:A:C8	2.45	0.52
1:2:558:C:H2'	1:2:559:A:H8	1.74	0.52
1:2:1070:C:H2'	1:2:1071:C:H6	1.75	0.52
1:2:1453:C:N3	1:2:1454:G:C5	2.78	0.52
14:N:110:GLY:HA3	14:N:114:ARG:O	2.09	0.52
23:Y:27:TYR:HE2	24:3:44:GLU:OE2	1.92	0.52
27:4:15:G:N2	27:4:48:C:O2	2.39	0.52
1:2:257:U:H2'	1:2:258:U:C6	2.45	0.52
1:2:483:G:OP2	36:2:1549:SPM:C13	2.40	0.52
7:G:3:ASP:OD1	7:G:3:ASP:N	2.41	0.52
7:G:98:MET:HE2	7:G:98:MET:H	1.75	0.52
8:H:190:LEU:HD12	8:H:193:ARG:HD3	1.91	0.52
14:N:108:ILE:HD12	14:N:116:MET:HB3	1.90	0.52
17:S:17:TYR:OH	17:S:21:LYS:HE2	2.08	0.52
20:V:60:GLU:H	20:V:60:GLU:CD	2.16	0.52
1:2:1189:C:O2	18:T:122:HIS:CE1	2.62	0.52
7:G:19:ILE:HD12	7:G:20:LYS:H	1.74	0.52
10:J:67:ASP:HB2	10:J:125:LEU:HD12	1.92	0.52
1:2:687:A:H2'	1:2:688:A:C8	2.44	0.52
9:I:81:LEU:O	9:I:81:LEU:HD12	2.10	0.52
1:2:1187:C:H3'	1:2:1188:G:H5''	1.91	0.52
1:2:468:A:H61	36:2:1549:SPM:H22	1.75	0.52
1:2:888:G:C2	1:2:890:G:C8	2.98	0.52
1:2:1369:G:O2'	1:2:1370:U:H5'	2.10	0.52
1:2:1491:A:H2'	1:2:1492:C:C6	2.45	0.52
2:A:19:TRP:CD1	2:A:37:PRO:HB3	2.45	0.52
3:B:103:ARG:NH1	3:B:152:THR:HB	2.24	0.52
8:H:32:SER:HA	32:d:62:TRP:CE2	2.45	0.52
11:K:23:ILE:HD13	11:K:93:PHE:CD1	2.44	0.52
15:O:10:ARG:NH2	15:O:15:ASP:OD1	2.36	0.52
31:Z:17:LYS:HD2	31:Z:74:PHE:CE1	2.44	0.52
1:2:82:G:O2'	1:2:132:A:N3	2.41	0.52
7:G:22:LYS:HE2	7:G:22:LYS:N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:88:ILE:HD12	33:c:105:ILE:HG12	1.92	0.52
9:I:118:GLU:OE2	9:I:121:ARG:NH2	2.28	0.52
24:3:93:GLN:HG2	24:3:93:GLN:O	2.09	0.52
36:2:1562:SPM:N14	31:Z:180:GLU:OE1	2.41	0.52
25:a:57:LEU:HD13	29:P:4:TYR:CE1	2.44	0.52
1:2:479:A:OP1	14:N:71:LYS:NZ	2.43	0.52
1:2:601:A:N7	9:I:110:SER:HA	2.25	0.52
2:A:116:TYR:CD2	2:A:155:PHE:HB2	2.45	0.52
8:H:84:LEU:HD11	33:c:100:ASN:CB	2.15	0.52
23:Y:65:TYR:O	23:Y:65:TYR:CD1	2.63	0.52
1:2:195:A:N1	1:2:225:G:O2'	2.40	0.51
1:2:133:A:OP2	1:2:134:C:N4	2.30	0.51
1:2:1207:A:H2'	1:2:1208:G:H8	1.76	0.51
1:2:1260:C:H5'	15:O:21:LYS:NZ	2.25	0.51
1:2:1334:G:OP2	11:K:118:THR:HG21	2.10	0.51
2:A:27:ALA:HB2	2:A:156:ASP:HB2	1.91	0.51
2:A:145:THR:HG21	2:A:170:GLU:OE1	2.10	0.51
6:F:11:GLU:H	6:F:11:GLU:CD	2.18	0.51
15:O:104:ARG:O	15:O:108:GLU:HG2	2.09	0.51
30:R:25:ASP:OD2	30:R:28:CYS:HB2	2.09	0.51
1:2:93:C:H2'	1:2:94:U:C6	2.45	0.51
1:2:699:U:H2'	1:2:700:A:H8	1.74	0.51
1:2:1028:C:H2'	1:2:1029:G:H8	1.75	0.51
7:G:43:GLN:NE2	7:G:82:ASP:OD2	2.44	0.51
32:d:7:LYS:HB3	32:d:55:GLN:NE2	2.26	0.51
1:2:409:G:H4'	1:2:429:U:O2	2.11	0.51
1:2:1077:A:H2'	1:2:1078:C:C6	2.44	0.51
1:2:1260:C:H4'	1:2:1266:U:O4	2.09	0.51
3:B:223:SER:OG	3:B:224:GLU:OE1	2.25	0.51
23:Y:37:LYS:HZ2	23:Y:37:LYS:HB2	1.75	0.51
28:5:823:C:O2	28:5:823:C:H2'	2.11	0.51
29:P:50:PHE:O	29:P:51:ARG:NH1	2.41	0.51
1:2:196:G:OP1	36:2:1567:SPM:H22	2.10	0.51
1:2:218:C:H2'	1:2:219:A:C8	2.43	0.51
1:2:263:G:H2'	1:2:264:G:C8	2.46	0.51
1:2:521:U:H4'	1:2:522:A:H5'	1.93	0.51
1:2:784:G:O2'	9:I:9:ASN:OD1	2.26	0.51
1:2:826:G:O6	36:2:1560:SPM:H81	2.11	0.51
1:2:866:A:H2'	1:2:867:C:C6	2.45	0.51
1:2:949:U:H2'	1:2:950:A:C8	2.46	0.51
1:2:1291:U:OP1	19:U:41:LYS:NZ	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:205:VAL:N	9:I:70:ASN:HD21	2.08	0.51
10:J:109:ALA:HB1	10:J:123:ALA:HB1	1.93	0.51
28:5:822:C:O2	28:5:822:C:O2'	2.25	0.51
1:2:302:G:N2	1:2:305:A:OP2	2.39	0.51
1:2:452:G:O2'	1:2:454:A:H1'	2.11	0.51
1:2:1057:C:N4	1:2:1060:OMC:OP2	2.43	0.51
1:2:1253:A:OP1	36:2:1578:SPM:H91	2.09	0.51
2:A:14:TRP:CD1	2:A:17:LYS:HD2	2.45	0.51
7:G:49:LYS:HD3	7:G:50:THR:H	1.74	0.51
11:K:23:ILE:HD12	11:K:23:ILE:O	2.11	0.51
24:3:22:ALA:HB1	24:3:111:VAL:HG23	1.92	0.51
25:a:41:CYS:HA	25:a:44:LYS:HE3	1.92	0.51
1:2:406:C:O2'	1:2:580:A:N3	2.37	0.51
1:2:864:A:C5	1:2:865:OMG:H1'	2.45	0.51
3:B:165:ILE:O	4:C:49:ARG:NH2	2.43	0.51
4:C:37:CYS:HB3	4:C:60:CYS:HB3	1.92	0.51
8:H:111:ARG:N	8:H:186:GLU:OE2	2.37	0.51
15:O:9:VAL:HG12	15:O:11:ILE:HD11	1.93	0.51
21:W:33:HIS:HD2	21:W:54:LYS:HG3	1.71	0.51
1:2:479:A:H1'	26:e:13:VAL:HG23	1.93	0.51
3:B:113:PHE:HD1	3:B:202:ALA:HB2	1.76	0.51
6:F:14:LYS:HD3	6:F:14:LYS:N	2.26	0.51
8:H:119:TYR:HB2	8:H:124:TYR:CE2	2.46	0.51
9:I:23:LYS:HA	9:I:23:LYS:HE2	1.92	0.51
22:X:46:ARG:NH2	22:X:71:THR:HB	2.25	0.51
31:Z:84:THR:OG1	31:Z:85:ASN:N	2.42	0.51
32:d:25:ASN:HD21	32:d:64:PRO:HA	1.74	0.51
1:2:1316:C:H2'	1:2:1317:G:C8	2.46	0.51
1:2:71:G:H2'	1:2:72:G:C8	2.46	0.51
1:2:673:G:H2'	1:2:674:A:C8	2.45	0.51
1:2:900:C:C2	1:2:901:A:C8	2.98	0.51
1:2:991:U:H2'	1:2:992:G:C4	2.45	0.51
1:2:1451:G:C5	1:2:1452:U:H5	2.18	0.51
36:2:1563:SPM:N14	11:K:122:LYS:O	2.44	0.51
7:G:142:GLN:HG2	7:G:143:LEU:HD22	1.93	0.51
24:3:31:LYS:NZ	24:3:102:LEU:HB3	2.26	0.51
1:2:614:G:H2'	1:2:615:G:H8	1.75	0.50
1:2:1164:A:OP1	36:2:1576:SPM:N1	2.43	0.50
5:D:91:ASP:OD1	6:F:128:CYS:HA	2.11	0.50
1:2:654:A:H2'	1:2:655:A:C8	2.46	0.50
1:2:828:A:OP2	1:2:828:A:H8	1.95	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1013:U:OP1	31:Z:142:ALA:N	2.33	0.50
1:2:1097:C:O2'	1:2:1099:G:N1	2.40	0.50
1:2:1287:G:OP2	38:2:1604:HOH:O	2.19	0.50
2:A:80:ILE:HD12	2:A:80:ILE:O	2.12	0.50
7:G:49:LYS:NZ	7:G:89:ASP:HA	2.26	0.50
24:3:20:LEU:O	24:3:24:ARG:HD2	2.10	0.50
24:3:24:ARG:HG3	24:3:89:ALA:HB1	1.93	0.50
1:2:25:G:H2'	1:2:26:A:H8	1.76	0.50
1:2:407:G:O3'	5:D:140:SER:OG	2.29	0.50
1:2:1078:C:H2'	1:2:1079:U:C6	2.46	0.50
1:2:1369:G:H2'	1:2:1370:U:H6	1.75	0.50
1:2:1453:C:C2'	1:2:1454:G:O4'	2.54	0.50
17:S:33:GLN:O	17:S:36:ILE:HG13	2.11	0.50
24:3:24:ARG:NH2	24:3:85:ALA:O	2.44	0.50
31:Z:62:ASN:O	31:Z:66:LEU:HG	2.11	0.50
33:c:103:LEU:HD12	33:c:103:LEU:C	2.36	0.50
1:2:897:C:O2'	1:2:1308:C:OP2	2.24	0.50
1:2:1120:G:N7	17:S:44:LYS:NZ	2.55	0.50
5:D:36:ARG:HG3	26:e:31:ARG:HG3	1.93	0.50
11:K:9:ILE:HD12	11:K:22:TYR:CD2	2.46	0.50
27:4:69:C:H2'	27:4:70:G:C8	2.46	0.50
1:2:260:G:H2'	1:2:261:G:H8	1.76	0.50
1:2:478:C:H2'	1:2:479:A:O4'	2.11	0.50
1:2:871:A:H2'	1:2:872:A:H8	1.77	0.50
1:2:1053:C:OP1	17:S:7:LYS:HG2	2.11	0.50
1:2:1096:U:H2'	1:2:1098:C:C5	2.47	0.50
3:B:36:LEU:O	3:B:203:ARG:NH2	2.43	0.50
27:4:4:G:H2'	27:4:5:G:C8	2.46	0.50
1:2:727:A:H4'	1:2:1480:G:N2	2.27	0.50
1:2:1231:A:H4'	19:U:36:TRP:CE3	2.47	0.50
7:G:60:LEU:HD21	7:G:111:ALA:HB1	1.93	0.50
11:K:52:PRO:HG2	11:K:86:LEU:HD12	1.93	0.50
25:a:61:CYS:O	25:a:65:GLY:N	2.45	0.50
34:E:215:ASP:OD2	34:E:217:ASN:ND2	2.45	0.50
34:E:234:SER:OG	34:E:236:LEU:O	2.28	0.50
1:2:137:C:O2'	7:G:118:GLN:HB2	2.12	0.50
1:2:973:C:C2	1:2:974:A:C8	2.99	0.50
2:A:14:TRP:NE1	2:A:17:LYS:HD2	2.26	0.50
8:H:116:ARG:C	8:H:117:ILE:HD12	2.37	0.50
19:U:45:PHE:HB3	19:U:97:VAL:HB	1.93	0.50
1:2:739:A:OP1	36:2:1559:SPM:N14	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1100:G:H1'	19:U:5:MET:HE1	1.94	0.50
5:D:56:ARG:HE	6:F:125:GLN:NE2	2.10	0.50
8:H:115:THR:CG2	22:X:57:LYS:HD2	2.42	0.50
16:Q:33:MET:SD	16:Q:33:MET:N	2.84	0.50
17:S:44:LYS:HG3	17:S:47:ARG:NH2	2.26	0.50
1:2:505:G:OP2	5:D:37:ASN:HB2	2.12	0.50
1:2:1461:G:OP1	1:2:1464:A:H4'	2.12	0.50
8:H:40:HIS:HD2	11:K:48:LYS:HE2	1.77	0.50
9:I:91:ASP:OD1	9:I:94:ARG:NH2	2.45	0.50
21:W:28:GLN:HG3	21:W:29:THR:N	2.27	0.50
24:3:55:GLU:N	24:3:80:VAL:HG21	2.27	0.50
25:a:60:LYS:HB3	25:a:65:GLY:HA2	1.94	0.50
32:d:38:SER:HB2	32:d:43:LEU:HD23	1.94	0.50
1:2:872:A:P	14:N:28:ARG:HH22	2.34	0.49
1:2:968:A:H62	1:2:992:G:H21	1.59	0.49
1:2:996:C:O2'	1:2:997:G:H8	1.95	0.49
1:2:1043:C:H2'	1:2:1044:C:C6	2.47	0.49
1:2:1314:A:H1'	8:H:72:LYS:HG2	1.94	0.49
1:2:1374:U:C2	1:2:1448:G:C2	3.00	0.49
1:2:1445:G:H2'	1:2:1446:G:H8	1.75	0.49
2:A:110:VAL:HG11	2:A:146:VAL:HG12	1.94	0.49
7:G:45:LYS:NZ	7:G:82:ASP:OD1	2.43	0.49
8:H:111:ARG:HD2	22:X:69:ARG:HD3	1.92	0.49
12:L:35:MET:HE2	12:L:74:ILE:HD12	1.93	0.49
15:O:30:LYS:HE3	15:O:100:ILE:HD11	1.93	0.49
19:U:64:LEU:HB3	19:U:108:PHE:HE1	1.77	0.49
24:3:16:ALA:O	24:3:19:VAL:HG22	2.11	0.49
33:c:29:LYS:HB3	33:c:39:GLU:OE2	2.12	0.49
1:2:29:G:H2'	1:2:30:C:C6	2.47	0.49
1:2:126:G:OP2	36:2:1567:SPM:H71	2.12	0.49
1:2:417:G:H21	1:2:419:A:H1'	1.77	0.49
1:2:1070:C:H2'	1:2:1071:C:C6	2.47	0.49
1:2:1226:C:H2'	1:2:1227:C:H6	1.77	0.49
2:A:183:LYS:HE3	2:A:183:LYS:HA	1.94	0.49
6:F:98:GLN:HE21	6:F:100:ARG:NH1	2.10	0.49
11:K:101:LYS:NZ	32:d:66:PRO:HB3	2.27	0.49
16:Q:29:GLU:OE1	16:Q:29:GLU:N	2.39	0.49
33:c:8:PRO:HA	33:c:11:THR:HB	1.93	0.49
1:2:47:A:OP2	38:2:1603:HOH:O	2.19	0.49
1:2:1470:A:H2'	1:2:1471:G:C8	2.47	0.49
2:A:24:THR:OG1	2:A:28:PHE:HB2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:99:ARG:HG2	2:A:99:ARG:HH11	1.76	0.49
14:N:28:ARG:O	14:N:32:THR:HG22	2.12	0.49
16:Q:71:GLN:HA	16:Q:74:GLU:OE1	2.12	0.49
19:U:19:ARG:HH12	19:U:141:GLU:CD	2.19	0.49
21:W:40:CYS:CB	21:W:43:CYS:SG	3.00	0.49
22:X:47:ASP:OD1	22:X:50:ARG:NE	2.45	0.49
22:X:56:VAL:HG21	22:X:60:VAL:HG21	1.92	0.49
23:Y:34:VAL:C	23:Y:35:LYS:HD3	2.37	0.49
24:3:53:ILE:HD13	24:3:67:PRO:HD3	1.94	0.49
25:a:36:TYR:CE2	25:a:54:LYS:NZ	2.77	0.49
25:a:45:TYR:CD1	29:P:6:PRO:HB2	2.46	0.49
1:2:899:A:H2'	1:2:900:C:C6	2.47	0.49
1:2:956:G:H22	1:2:1175:A:P	2.35	0.49
6:F:147:VAL:HG21	6:F:164:LEU:HD11	1.95	0.49
11:K:102:ILE:HG23	32:d:67:ILE:CD1	2.42	0.49
19:U:92:ARG:HH11	19:U:92:ARG:HG3	1.76	0.49
21:W:27:GLU:HA	21:W:27:GLU:OE2	2.12	0.49
24:3:13:GLN:OE1	24:3:13:GLN:HA	2.11	0.49
27:4:23:C:H2'	27:4:24:U:C6	2.47	0.49
32:d:4:LEU:C	32:d:4:LEU:CD1	2.86	0.49
33:c:29:LYS:NZ	33:c:40:ILE:HD11	2.27	0.49
1:2:1096:U:O2'	1:2:1099:G:O6	2.25	0.49
1:2:1295:G:H4'	33:c:8:PRO:CG	2.42	0.49
1:2:1367:C:N4	28:5:821:G:OP1	2.41	0.49
8:H:33:LEU:H	32:d:62:TRP:CG	2.30	0.49
8:H:52:LYS:NZ	8:H:137:ASP:OD2	2.44	0.49
10:J:80:GLU:OE1	10:J:82:LEU:HD23	2.13	0.49
21:W:23:ASN:HD22	21:W:45:THR:HG21	1.78	0.49
21:W:30:ILE:HD11	21:W:38:VAL:HG11	1.94	0.49
22:X:34:GLU:H	22:X:34:GLU:CD	2.20	0.49
25:a:16:TRP:CG	31:Z:17:LYS:HG3	2.47	0.49
1:2:413:U:H2'	1:2:414:C:C6	2.48	0.49
1:2:1024:A:OP1	36:2:1577:SPM:N14	2.46	0.49
1:2:1077:A:H2'	1:2:1078:C:H6	1.77	0.49
1:2:1370:U:H2'	1:2:1371:C:H5'	1.94	0.49
30:R:23:CYS:HB2	30:R:83:PRO:HG2	1.94	0.49
1:2:408:A:O5'	5:D:141:PRO:HD2	2.12	0.49
1:2:418:U:O2	1:2:419:A:N6	2.46	0.49
1:2:961:C:H2'	1:2:962:A:H8	1.78	0.49
1:2:964:G:N2	1:2:965:A:N1	2.60	0.49
1:2:964:G:O2'	1:2:967:G:O2'	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2:1562:SPM:C13	31:Z:180:GLU:OE1	2.61	0.49
4:C:47:MET:HE2	4:C:51:GLN:CG	2.41	0.49
6:F:141:LYS:HG3	6:F:146:GLU:OE2	2.11	0.49
8:H:24:ASP:OD1	8:H:26:SER:N	2.45	0.49
8:H:84:LEU:HB2	8:H:159:GLU:HG2	1.93	0.49
8:H:156:LYS:HE3	33:c:68:TYR:CD2	2.48	0.49
12:L:79:ASP:O	12:L:82:VAL:HG22	2.13	0.49
19:U:45:PHE:CE1	19:U:46:LYS:HE2	2.47	0.49
19:U:75:GLY:O	19:U:79:THR:HG23	2.12	0.49
19:U:142:ILE:HA	19:U:145:GLU:OE1	2.13	0.49
22:X:25:ILE:HA	22:X:38:VAL:HG23	1.95	0.49
24:3:43:VAL:HG12	24:3:73:LYS:HE3	1.94	0.49
1:2:990:C:H4'	23:Y:62:LYS:HE2	1.95	0.49
1:2:1262:C:C4	8:H:155:PRO:HA	2.47	0.49
17:S:56:ARG:O	17:S:60:ILE:HG13	2.12	0.49
20:V:94:GLU:HG3	20:V:95:PRO:HD2	1.94	0.49
29:P:19:CYS:HA	29:P:35:TYR:O	2.13	0.49
1:2:382:C:H2'	1:2:383:G:H8	1.78	0.49
1:2:1343:G:H2'	1:2:1344:OMU:C6	2.42	0.49
8:H:40:HIS:HD2	11:K:48:LYS:CE	2.25	0.49
8:H:156:LYS:HD3	8:H:161:VAL:HG12	1.94	0.49
19:U:77:GLU:HA	19:U:80:ARG:HG3	1.94	0.49
21:W:24:CYS:HG	21:W:42:SER:HG	1.61	0.49
25:a:51:GLU:OE2	25:a:54:LYS:HD2	2.07	0.49
25:a:57:LEU:O	25:a:58:LYS:HB2	2.13	0.49
1:2:913:C:OP2	15:O:135:THR:HG21	2.13	0.49
8:H:89:ILE:HD11	8:H:97:PRO:CA	2.42	0.49
11:K:24:TYR:HE2	11:K:65:ASP:HB3	1.77	0.49
20:V:86:SER:HB3	20:V:89:ILE:HD12	1.94	0.49
23:Y:60:CYS:HB3	23:Y:63:CYS:HB3	1.95	0.49
24:3:83:LYS:HD3	24:3:95:ALA:HB1	1.94	0.49
1:2:555:A:OP2	1:2:556:G:OP2	2.30	0.48
1:2:1442:G:N3	1:2:1443:G:C8	2.81	0.48
1:2:1460:A:H2	28:5:815:U:C5	2.31	0.48
8:H:84:LEU:HD12	33:c:100:ASN:CB	2.42	0.48
11:K:39:LEU:HD22	19:U:12:PRO:HD3	1.95	0.48
11:K:49:ILE:HD12	11:K:82:ALA:HB3	1.95	0.48
13:M:26:SER:OG	13:M:30:GLY:HA2	2.13	0.48
18:T:79:ILE:HD11	18:T:110:LEU:HD23	1.95	0.48
25:a:44:LYS:HG2	25:a:45:TYR:CD2	2.47	0.48
1:2:636:C:H2'	1:2:637:U:H6	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:922:A:N3	1:2:949:U:O2'	2.40	0.48
1:2:1011:C:N4	28:5:824:A:C6	2.81	0.48
1:2:1207:A:H2'	1:2:1208:G:C8	2.48	0.48
1:2:1328:A:P	19:U:89:ARG:HH22	2.36	0.48
2:A:14:TRP:HE1	2:A:17:LYS:HD2	1.77	0.48
6:F:12:GLU:OE1	6:F:12:GLU:N	2.44	0.48
7:G:42:PRO:HB2	7:G:79:PHE:CD2	2.47	0.48
11:K:8:VAL:HG21	11:K:92:LYS:HD2	1.94	0.48
1:2:989:C:OP1	23:Y:49:ALA:HA	2.13	0.48
1:2:1282:A:HO2'	18:T:76:ASN:HD22	1.59	0.48
5:D:86:GLU:H	5:D:86:GLU:CD	2.16	0.48
6:F:187:THR:O	6:F:191:VAL:HG23	2.13	0.48
10:J:66:LEU:HA	10:J:73:ALA:HA	1.95	0.48
22:X:37:GLN:OE1	22:X:37:GLN:HA	2.12	0.48
25:a:57:LEU:CD2	25:a:57:LEU:N	2.73	0.48
1:2:74:A:N1	1:2:213:C:O2'	2.41	0.48
1:2:504:C:O2'	1:2:508:U:OP1	2.30	0.48
1:2:716:U:H2'	1:2:717:G:O4'	2.13	0.48
1:2:1024:A:N1	1:2:1065:G:O2'	2.36	0.48
1:2:1189:C:O2'	33:c:2:GLY:N	2.40	0.48
1:2:1311:G:O6	11:K:14:ARG:NH2	2.46	0.48
6:F:188:GLU:OE1	6:F:192:ARG:NH2	2.47	0.48
8:H:36:VAL:HG23	11:K:106:TYR:CZ	2.49	0.48
8:H:89:ILE:HB	8:H:167:ILE:HD11	1.95	0.48
12:L:30:LYS:HE3	12:L:81:ARG:CZ	2.43	0.48
13:M:76:ILE:HD12	13:M:76:ILE:N	2.27	0.48
23:Y:38:ASN:HB3	23:Y:58:TRP:HZ3	1.78	0.48
23:Y:53:LYS:HE2	23:Y:53:LYS:N	2.27	0.48
30:R:26:GLU:OE1	30:R:33:SER:OG	2.31	0.48
31:Z:55:ILE:HG22	31:Z:83:ILE:HD13	1.95	0.48
1:2:200:C:H2'	1:2:201:A:H8	1.78	0.48
1:2:949:U:H2'	1:2:950:A:H8	1.79	0.48
1:2:1165:G:OP2	12:L:55:HIS:ND1	2.42	0.48
1:2:1259:C:O3'	15:O:21:LYS:NZ	2.46	0.48
8:H:109:ALA:HB1	8:H:135:ARG:HB3	1.95	0.48
8:H:131:SER:HB2	22:X:60:VAL:HG22	1.95	0.48
3:B:22:GLU:O	3:B:26:LYS:HD2	2.13	0.48
5:D:36:ARG:CG	26:e:31:ARG:HE	2.26	0.48
7:G:177:LEU:CD1	7:G:194:LYS:HB2	2.44	0.48
7:G:180:PRO:O	7:G:182:GLY:N	2.47	0.48
10:J:77:LYS:HD2	10:J:78:ILE:N	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:56:ALA:HB1	11:K:60:ILE:HG21	1.95	0.48
14:N:57:LYS:HD2	14:N:94:VAL:HG22	1.95	0.48
19:U:143:PHE:HE2	19:U:153:LEU:HB3	1.78	0.48
27:4:24:U:H2'	27:4:25:C:C6	2.48	0.48
31:Z:46:ILE:HA	31:Z:82:THR:O	2.13	0.48
1:2:871:A:H2'	1:2:872:A:C8	2.49	0.48
1:2:965:A:H8	24:3:34:LYS:HE2	1.78	0.48
1:2:1053:C:C5'	17:S:7:LYS:HE3	2.28	0.48
1:2:1078:C:H2'	1:2:1079:U:H6	1.79	0.48
1:2:1188:G:H2'	18:T:120:VAL:HG21	1.96	0.48
2:A:112:THR:OG1	2:A:116:TYR:HB2	2.14	0.48
7:G:65:THR:OG1	7:G:72:LYS:HE3	2.14	0.48
14:N:13:ALA:HB2	30:R:69:ARG:HB2	1.95	0.48
1:2:149:G:H2'	1:2:150:A:H8	1.77	0.48
1:2:217:U:H2'	1:2:218:C:H6	1.78	0.48
1:2:229:C:H2'	1:2:230:A:H8	1.78	0.48
15:O:114:ARG:HH11	15:O:114:ARG:HG2	1.79	0.48
18:T:62:ARG:HG2	18:T:63:GLU:OE1	2.13	0.48
19:U:5:MET:O	19:U:6:ILE:HD13	2.13	0.48
1:2:40:G:H2'	1:2:41:G:C8	2.48	0.48
11:K:31:PHE:HE1	19:U:156:TYR:CE1	2.31	0.48
14:N:91:ASP:H	14:N:138:TYR:HH	1.59	0.48
17:S:15:GLU:HA	17:S:18:ASP:OD2	2.14	0.48
1:2:397:G:O6	36:2:1555:SPM:N1	2.47	0.48
1:2:413:U:H2'	1:2:414:C:H6	1.79	0.48
1:2:517:C:N3	38:2:1636:HOH:O	2.35	0.48
7:G:22:LYS:HD3	7:G:108:GLU:HG3	1.95	0.48
11:K:36:PRO:HD3	19:U:10:MET:HG2	1.95	0.48
12:L:30:LYS:HE3	12:L:81:ARG:NH1	2.28	0.48
25:a:14:LEU:O	25:a:18:THR:OG1	2.31	0.48
1:2:468:A:N6	36:2:1549:SPM:H22	2.28	0.47
1:2:961:C:C2	1:2:962:A:C8	3.02	0.47
1:2:1121:A:OP2	17:S:32:LYS:NZ	2.46	0.47
3:B:84:ILE:HD11	4:C:36:ASN:HB2	1.96	0.47
3:B:108:ARG:NH1	3:B:227:MET:O	2.47	0.47
3:B:113:PHE:CD1	3:B:202:ALA:HB2	2.49	0.47
8:H:88:ILE:HD12	33:c:105:ILE:CG1	2.44	0.47
10:J:38:SER:OG	10:J:40:GLU:OE2	2.30	0.47
14:N:38:LYS:O	14:N:42:ASP:HB3	2.14	0.47
16:Q:112:GLY:O	16:Q:116:ILE:HD12	2.14	0.47
17:S:42:LYS:N	17:S:42:LYS:HE2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:6:PRO:HB2	18:T:8:GLU:OE1	2.13	0.47
1:2:131:U:H2'	1:2:132:A:H8	1.79	0.47
1:2:741:A:H4'	1:2:1471:G:O2'	2.14	0.47
1:2:985:C:C2	1:2:986:U:H5	2.32	0.47
1:2:1371:C:H2'	1:2:1372:G:O4'	2.14	0.47
2:A:94:ARG:CZ	2:A:94:ARG:HB2	2.44	0.47
3:B:95:GLN:NE2	3:B:118:GLY:O	2.47	0.47
6:F:121:CYS:SG	6:F:126:CYS:HB3	2.55	0.47
13:M:27:ASP:OD1	13:M:27:ASP:N	2.47	0.47
15:O:10:ARG:O	15:O:11:ILE:HD13	2.14	0.47
18:T:70:ILE:HD12	18:T:87:LYS:O	2.14	0.47
19:U:143:PHE:CE2	19:U:153:LEU:HB3	2.49	0.47
33:c:96:LEU:HB2	33:c:106:TYR:HE1	1.76	0.47
1:2:1445:G:H2'	1:2:1446:G:C8	2.49	0.47
6:F:98:GLN:HE21	6:F:100:ARG:HH12	1.62	0.47
8:H:21:GLU:HB3	8:H:23:ARG:HH12	1.78	0.47
16:Q:33:MET:O	16:Q:37:GLU:HG2	2.15	0.47
32:d:4:LEU:O	32:d:6:ILE:CD1	2.61	0.47
32:d:71:LEU:C	32:d:71:LEU:CD1	2.86	0.47
33:c:25:LYS:O	33:c:29:LYS:HG3	2.14	0.47
1:2:40:G:H2'	1:2:41:G:H8	1.78	0.47
1:2:439:U:OP2	20:V:101:ARG:NH1	2.38	0.47
1:2:1470:A:H2'	1:2:1471:G:H8	1.79	0.47
6:F:28:ILE:HG22	6:F:30:SER:H	1.78	0.47
6:F:82:MET:HG2	6:F:83:GLY:N	2.29	0.47
12:L:23:GLN:O	12:L:27:ILE:HG12	2.14	0.47
21:W:28:GLN:HA	21:W:28:GLN:HE21	1.78	0.47
24:3:27:LYS:HG3	24:3:32:ILE:HG12	1.94	0.47
1:2:398:C:C2	1:2:399:OMG:C8	3.02	0.47
1:2:699:U:H2'	1:2:700:A:C8	2.49	0.47
8:H:125:TYR:O	8:H:192:SER:OG	2.32	0.47
12:L:46:LEU:CD2	31:Z:5:LYS:HD3	2.44	0.47
12:L:47:GLU:OE1	12:L:49:PRO:HD3	2.13	0.47
17:S:41:VAL:HG11	17:S:47:ARG:HB2	1.96	0.47
25:a:5:ASN:HD21	29:P:42:ARG:HG2	1.79	0.47
1:2:725:A:OP2	1:2:771:G:N2	2.47	0.47
1:2:1171:C:H2'	1:2:1172:C:H6	1.79	0.47
14:N:91:ASP:OD2	26:e:14:ARG:HB2	2.15	0.47
18:T:118:LYS:CD	18:T:118:LYS:H	2.28	0.47
24:3:80:VAL:HG22	24:3:81:SER:O	2.14	0.47
32:d:61:MET:HE3	32:d:61:MET:HB2	1.68	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:17:C:C2	1:2:18:C:C5	3.02	0.47
1:2:92:G:OP1	34:E:21:LYS:NZ	2.44	0.47
1:2:106:G:OP1	1:2:564:U:O2'	2.23	0.47
1:2:176:G:N1	1:2:179:A:OP2	2.46	0.47
1:2:489:G:N3	1:2:489:G:H2'	2.30	0.47
1:2:518:U:OP2	36:2:1548:SPM:N5	2.47	0.47
1:2:1226:C:H2'	1:2:1227:C:C6	2.50	0.47
1:2:1337:G:N7	11:K:15:LYS:NZ	2.63	0.47
1:2:1371:C:C2	1:2:1372:G:C8	3.03	0.47
2:A:183:LYS:HD3	2:A:184:ALA:N	2.28	0.47
3:B:98:ILE:CG1	3:B:142:PRO:HB3	2.44	0.47
6:F:91:ILE:HD11	6:F:192:ARG:HD3	1.96	0.47
8:H:180:LYS:HE2	8:H:180:LYS:HB2	1.66	0.47
11:K:48:LYS:HD3	11:K:83:ARG:NH2	2.30	0.47
11:K:84:MET:HB3	11:K:88:ARG:HE	1.78	0.47
12:L:86:LEU:HD13	12:L:99:ILE:HG13	1.96	0.47
13:M:25:ILE:O	13:M:34:ILE:N	2.33	0.47
14:N:84:VAL:HG21	14:N:124:TYR:CE1	2.50	0.47
14:N:139:LYS:HB3	14:N:139:LYS:HE2	1.65	0.47
22:X:21:GLU:HG3	22:X:65:ILE:HD12	1.96	0.47
22:X:27:ASP:OD2	22:X:27:ASP:N	2.47	0.47
23:Y:26:TYR:OH	23:Y:38:ASN:OD1	2.31	0.47
31:Z:90:GLU:OE2	31:Z:120:ARG:NH2	2.47	0.47
32:d:25:ASN:HD22	32:d:64:PRO:HA	1.76	0.47
33:c:29:LYS:HE2	33:c:39:GLU:OE2	2.15	0.47
33:c:86:LYS:O	33:c:89:GLU:HG3	2.14	0.47
1:2:188:C:O2'	10:J:64:ASN:OD1	2.29	0.47
1:2:539:C:H2'	1:2:540:G:O4'	2.14	0.47
1:2:954:G:H2'	1:2:955:A:C8	2.50	0.47
1:2:1451:G:C2	1:2:1452:U:C6	3.03	0.47
5:D:36:ARG:HG3	26:e:31:ARG:HE	1.79	0.47
7:G:57:ASP:HB3	7:G:113:ARG:NH2	2.30	0.47
19:U:118:GLN:OE1	19:U:129:PRO:HD3	2.15	0.47
21:W:63:ARG:NH1	21:W:65:MET:HB2	2.30	0.47
25:a:30:ILE:HD12	25:a:35:LEU:HD21	1.97	0.47
32:d:57:PRO:O	32:d:60:VAL:HG22	2.15	0.47
32:d:68:TYR:CD1	32:d:68:TYR:C	2.92	0.47
1:2:72:G:N1	1:2:209:U:O2'	2.45	0.47
1:2:212:C:H2'	1:2:213:C:C6	2.50	0.47
1:2:349:A:H5''	1:2:350:C:C5	2.48	0.47
1:2:935:G:OP2	11:K:132:ARG:NH2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1017:C:H2'	1:2:1018:OMG:H8	1.80	0.47
1:2:1252:A:H2'	1:2:1253:A:C8	2.50	0.47
1:2:1335:G:O3'	11:K:74:GLY:HA3	2.15	0.47
7:G:47:ASN:O	7:G:50:THR:OG1	2.30	0.47
18:T:53:LEU:HD12	18:T:74:VAL:CG1	2.45	0.47
19:U:64:LEU:HD22	19:U:108:PHE:CZ	2.50	0.47
21:W:23:ASN:HD22	21:W:45:THR:CG2	2.28	0.47
27:4:15:G:N2	27:4:48:C:C2	2.80	0.47
1:2:637:U:H2'	1:2:638:C:C6	2.50	0.47
1:2:653:A:H5''	13:M:47:ARG:CG	2.45	0.47
1:2:965:A:C8	24:3:34:LYS:HE2	2.49	0.47
1:2:1491:A:H2'	1:2:1492:C:H6	1.80	0.47
1:2:1496:C:N3	28:5:806:G:N1	2.52	0.47
6:F:91:ILE:HG21	6:F:191:VAL:HG12	1.97	0.47
7:G:4:PHE:HB2	7:G:121:VAL:HG13	1.96	0.47
11:K:30:VAL:O	11:K:37:ILE:HG23	2.15	0.47
13:M:15:TYR:HB3	13:M:22:LEU:HB2	1.97	0.47
33:c:96:LEU:C	33:c:96:LEU:CD1	2.86	0.47
1:2:601:A:H2'	1:2:602:C:H6	1.79	0.46
1:2:1329:U:OP1	36:2:1570:SPM:N14	2.48	0.46
7:G:23:VAL:C	7:G:24:LYS:HD2	2.39	0.46
8:H:12:VAL:HG12	8:H:16:TRP:O	2.15	0.46
18:T:48:ASP:HA	18:T:51:ARG:NH1	2.30	0.46
32:d:32:MET:HE3	32:d:32:MET:HB3	1.79	0.46
1:2:426:C:H2'	1:2:427:U:C6	2.48	0.46
1:2:637:U:H2'	1:2:638:C:H6	1.81	0.46
1:2:863:A:H2'	1:2:864:A:C8	2.50	0.46
1:2:1113:C:OP1	11:K:18:ARG:NE	2.48	0.46
1:2:1350:C:H2'	1:2:1351:U:H6	1.80	0.46
12:L:80:GLU:O	12:L:84:ARG:HG3	2.15	0.46
15:O:59:GLU:O	15:O:62:LYS:HG2	2.14	0.46
22:X:54:ARG:CZ	22:X:68:LEU:HD12	2.46	0.46
30:R:21:LYS:HD2	30:R:84:CYS:HA	1.97	0.46
30:R:92:LYS:HG2	30:R:113:VAL:HG13	1.98	0.46
34:E:177:SER:HA	34:E:231:ARG:O	2.15	0.46
1:2:382:C:H2'	1:2:383:G:C8	2.50	0.46
1:2:809:C:P	36:2:1575:SPM:H81	2.56	0.46
1:2:975:G:H2'	1:2:976:G:C8	2.50	0.46
3:B:191:ARG:NH2	3:B:227:MET:H	2.13	0.46
4:C:25:PRO:HB3	6:F:35:PHE:CD1	2.50	0.46
12:L:53:LEU:HD11	12:L:60:LYS:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:36:GLU:HG2	16:Q:40:LYS:HZ3	1.81	0.46
19:U:9:GLU:OE1	19:U:9:GLU:HA	2.16	0.46
3:B:58:MET:HE1	3:B:183:ILE:HD13	1.97	0.46
3:B:73:LEU:HD21	3:B:173:THR:HG22	1.98	0.46
10:J:101:LYS:HE3	10:J:101:LYS:HB2	1.78	0.46
15:O:36:THR:O	15:O:40:ILE:HG23	2.16	0.46
19:U:25:LYS:HB3	19:U:26:GLU:OE1	2.14	0.46
19:U:150:ASN:OD1	19:U:153:LEU:HG	2.14	0.46
24:3:66:LEU:O	24:3:70:CYS:N	2.48	0.46
28:5:808:A:H2'	28:5:808:A:N3	2.30	0.46
34:E:14:MET:SD	34:E:102:ARG:HG3	2.54	0.46
1:2:131:U:H2'	1:2:132:A:C8	2.51	0.46
36:2:1578:SPM:H32	33:c:101:ARG:HH12	1.80	0.46
7:G:72:LYS:HD2	7:G:72:LYS:HA	1.64	0.46
7:G:157:ASP:HB3	7:G:197:ARG:HD3	1.97	0.46
8:H:88:ILE:HG23	33:c:64:ILE:HG21	1.97	0.46
11:K:68:ILE:C	11:K:69:ILE:HD12	2.41	0.46
15:O:38:LYS:O	15:O:41:ILE:HG13	2.16	0.46
15:O:66:VAL:O	15:O:73:LYS:NZ	2.45	0.46
18:T:10:LYS:N	18:T:10:LYS:HD2	2.31	0.46
21:W:14:SER:HB3	21:W:33:HIS:CE1	2.51	0.46
32:d:46:TRP:HA	32:d:49:ALA:HB3	1.97	0.46
1:2:614:G:H2'	1:2:615:G:C8	2.51	0.46
1:2:645:U:O4	1:2:662:G:O2'	2.17	0.46
1:2:883:U:H2'	1:2:884:U:C6	2.51	0.46
12:L:93:GLU:N	12:L:93:GLU:CD	2.73	0.46
21:W:4:LYS:HD3	21:W:5:LEU:HD22	1.98	0.46
25:a:40:LYS:HD2	25:a:40:LYS:C	2.41	0.46
1:2:12:U:OP1	6:F:62:LYS:NZ	2.33	0.46
1:2:266:U:OP1	10:J:56:ARG:NH2	2.49	0.46
1:2:646:A:C2	1:2:663:A:C5	3.03	0.46
1:2:1490:C:C2	1:2:1491:A:C8	3.04	0.46
2:A:25:PRO:HD3	2:A:81:THR:HG23	1.98	0.46
3:B:29:LYS:HB2	3:B:76:ARG:HH11	1.81	0.46
10:J:4:TYR:HE1	10:J:27:GLU:OE2	1.99	0.46
23:Y:25:THR:HG23	24:3:65:HIS:CE1	2.51	0.46
32:d:43:LEU:HD21	32:d:48:GLU:HG2	1.98	0.46
1:2:112:C:H2'	1:2:113:OMC:C6	2.50	0.46
1:2:311:A:O2'	1:2:312:G:H5'	2.16	0.46
1:2:329:G:N1	1:2:332:A:OP2	2.49	0.46
1:2:801:C:H2'	1:2:802:U:O4'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:909:G:C2	1:2:910:A:C8	3.04	0.46
2:A:114:ASP:O	2:A:195:PRO:HG3	2.16	0.46
7:G:46:VAL:HG22	7:G:50:THR:OG1	2.16	0.46
17:S:32:LYS:O	17:S:36:ILE:HG23	2.15	0.46
20:V:88:GLU:H	20:V:88:GLU:CD	2.18	0.46
33:c:92:ASN:O	33:c:92:ASN:CG	2.57	0.46
1:2:3:U:H5'	6:F:159:VAL:HG12	1.98	0.46
1:2:602:C:H2'	1:2:603:U:H6	1.81	0.46
1:2:796:A:H2'	1:2:797:U:C6	2.51	0.46
1:2:949:U:C2	1:2:1184:G:N2	2.84	0.46
1:2:1294:U:H2'	1:2:1295:G:O4'	2.15	0.46
7:G:79:PHE:HZ	7:G:102:PHE:CZ	2.33	0.46
8:H:15:LYS:HG2	8:H:16:TRP:CE2	2.50	0.46
10:J:11:LYS:HG2	10:J:17:LYS:HD3	1.98	0.46
11:K:27:LYS:HZ1	11:K:29:ARG:CZ	2.29	0.46
20:V:19:ARG:HG3	20:V:19:ARG:NH1	2.31	0.46
33:c:7:LYS:HB2	33:c:9:ILE:CG2	2.37	0.46
33:c:15:ARG:O	33:c:19:GLU:HB2	2.15	0.46
1:2:367:G:N1	1:2:370:A:OP2	2.49	0.46
1:2:927:G:OP1	36:2:1576:SPM:H131	2.11	0.46
2:A:22:VAL:O	2:A:33:LEU:N	2.40	0.46
8:H:3:LEU:HD23	32:d:70:LYS:HZ1	1.75	0.46
9:I:14:ILE:HD11	9:I:38:LEU:HD21	1.98	0.46
11:K:37:ILE:HD13	11:K:50:MET:SD	2.56	0.46
16:Q:25:ARG:HA	16:Q:25:ARG:NE	2.30	0.46
20:V:99:LEU:HA	20:V:102:ASP:OD1	2.16	0.46
27:4:34:C:H2'	27:4:35:A:H8	1.80	0.46
30:R:92:LYS:HG2	30:R:113:VAL:CG1	2.46	0.46
1:2:125:G:OP2	36:2:1567:SPM:C9	2.62	0.45
1:2:728:G:H4'	1:2:1470:A:H4'	1.99	0.45
1:2:954:G:H2'	1:2:955:A:H8	1.82	0.45
1:2:1188:G:N3	1:2:1188:G:C2'	2.79	0.45
1:2:1369:G:H2'	1:2:1370:U:C6	2.50	0.45
6:F:9:ASN:HB2	6:F:12:GLU:CD	2.41	0.45
10:J:58:LYS:HD2	10:J:58:LYS:HA	1.66	0.45
11:K:28:GLY:N	11:K:64:ILE:O	2.49	0.45
14:N:45:GLY:HA3	14:N:79:ARG:NH2	2.31	0.45
22:X:56:VAL:CG2	22:X:60:VAL:HG21	2.46	0.45
23:Y:65:TYR:O	23:Y:65:TYR:HD1	1.99	0.45
24:3:6:TYR:CZ	24:3:8:LYS:HD2	2.50	0.45
25:a:60:LYS:HA	25:a:60:LYS:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1061:OMG:HM22	1:2:1062:A:H5'	1.98	0.45
1:2:1484:C:H2'	1:2:1485:U:C6	2.51	0.45
2:A:36:THR:OG1	2:A:47:ARG:NH1	2.49	0.45
2:A:41:ILE:HG12	2:A:74:ASN:ND2	2.31	0.45
5:D:123:ARG:HE	26:e:31:ARG:NH1	2.14	0.45
11:K:102:ILE:HG23	32:d:67:ILE:HD11	1.98	0.45
15:O:38:LYS:HB3	15:O:38:LYS:HE3	1.72	0.45
24:3:20:LEU:HG	24:3:24:ARG:NH2	2.31	0.45
31:Z:96:MET:HA	31:Z:96:MET:HE3	1.98	0.45
1:2:251:A:N1	1:2:283:U:O2'	2.40	0.45
1:2:395:G:H2'	1:2:396:G:C8	2.52	0.45
1:2:477:U:H2'	1:2:489:G:C8	2.51	0.45
1:2:617:G:H2'	1:2:618:C:H6	1.80	0.45
1:2:681:G:N7	2:A:129:LYS:NZ	2.65	0.45
1:2:1293:G:H5''	15:O:33:GLY:H	1.81	0.45
1:2:1363:C:O2	1:2:1459:A:N6	2.49	0.45
8:H:124:TYR:HB2	8:H:126:VAL:HG23	1.96	0.45
14:N:56:GLU:HA	14:N:99:GLU:OE2	2.16	0.45
17:S:40:ASP:OD1	31:Z:196:LYS:CG	2.63	0.45
19:U:6:ILE:HA	19:U:10:MET:HE1	1.98	0.45
22:X:44:GLU:OE1	32:d:50:TYR:CE2	2.70	0.45
33:c:47:ILE:HD11	33:c:87:GLU:HB3	1.99	0.45
1:2:398:C:O2	1:2:398:C:H2'	2.17	0.45
1:2:458:G:H2'	1:2:459:C:H6	1.81	0.45
1:2:782:A:N6	1:2:841:G:O6	2.49	0.45
1:2:944:C:O2	29:P:15:GLY:N	2.45	0.45
1:2:1013:U:H4'	31:Z:142:ALA:HB2	1.98	0.45
1:2:1095:C:O2'	1:2:1096:U:P	2.75	0.45
1:2:1477:4AC:O7	1:2:1477:4AC:H5	2.16	0.45
2:A:25:PRO:HG3	2:A:81:THR:O	2.16	0.45
11:K:36:PRO:HB3	19:U:156:TYR:CE2	2.50	0.45
12:L:11:SER:HB2	12:L:95:VAL:HG22	1.98	0.45
15:O:72:ILE:O	15:O:80:TYR:OH	2.30	0.45
17:S:6:THR:OG1	17:S:8:ASP:OD1	2.26	0.45
24:3:36:THR:HB	24:3:97:ALA:HB3	1.97	0.45
24:3:88:GLU:OE2	24:3:93:GLN:HA	2.16	0.45
25:a:72:LEU:HD21	31:Z:73:VAL:HG23	1.98	0.45
1:2:91:G:O6	36:2:1552:SPM:N1	2.50	0.45
1:2:425:G:H2'	1:2:426:C:C6	2.50	0.45
1:2:677:A:H5''	1:2:678:C:OP2	2.16	0.45
1:2:926:OMG:HM22	1:2:927:G:H5'	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:53:LEU:HD13	2:A:67:LEU:HD11	1.99	0.45
3:B:103:ARG:NE	3:B:103:ARG:HA	2.31	0.45
5:D:87:THR:O	5:D:87:THR:OG1	2.32	0.45
6:F:205:VAL:H	9:I:70:ASN:ND2	2.14	0.45
7:G:24:LYS:HE3	7:G:106:ASP:OD2	2.16	0.45
9:I:32:LYS:O	9:I:36:ASN:ND2	2.46	0.45
12:L:63:GLU:CD	29:P:42:ARG:HE	2.18	0.45
22:X:53:THR:OG1	22:X:74:GLU:OE2	2.32	0.45
31:Z:35:GLU:HG3	31:Z:48:TYR:HE1	1.81	0.45
32:d:24:LEU:HB3	32:d:61:MET:HG2	1.99	0.45
1:2:257:U:H5''	10:J:10:ARG:HG2	1.98	0.45
1:2:1130:G:N2	1:2:1133:A:OP2	2.45	0.45
1:2:1161:G:H2'	1:2:1162:U:C6	2.51	0.45
1:2:1232:A:H2'	1:2:1233:A:C8	2.52	0.45
5:D:83:LEU:HA	5:D:83:LEU:HD13	1.68	0.45
6:F:17:THR:OG1	6:F:43:GLU:OE2	2.26	0.45
7:G:139:GLU:HB3	7:G:141:ASN:OD1	2.17	0.45
8:H:63:ASN:OD1	8:H:75:LYS:HE3	2.16	0.45
14:N:63:ARG:NH1	14:N:120:PRO:HA	2.31	0.45
15:O:5:PHE:CE2	15:O:53:GLY:HA3	2.52	0.45
17:S:40:ASP:OD1	17:S:40:ASP:N	2.47	0.45
22:X:12:ILE:HD12	22:X:13:ILE:N	2.32	0.45
34:E:194:LYS:HD2	34:E:194:LYS:HA	1.70	0.45
1:2:246:OMC:HM22	1:2:247:C:H5'	1.97	0.45
1:2:409:G:OP2	26:e:31:ARG:CZ	2.65	0.45
1:2:1277:G:H2'	1:2:1278:C:H6	1.82	0.45
2:A:14:TRP:CH2	13:M:69:LYS:HE3	2.51	0.45
27:4:25:C:C2	27:4:26:G:C8	3.04	0.45
29:P:48:LEU:HD23	31:Z:16:VAL:HG21	1.99	0.45
31:Z:63:ILE:HD12	31:Z:63:ILE:N	2.28	0.45
33:c:81:ALA:O	33:c:85:LEU:HD23	2.16	0.45
34:E:209:ILE:HD11	34:E:223:ILE:HD12	1.98	0.45
1:2:901:A:H4'	22:X:32:THR:HG21	1.99	0.45
2:A:14:TRP:HH2	13:M:69:LYS:O	1.99	0.45
8:H:175:LYS:HE2	8:H:175:LYS:N	2.31	0.45
11:K:29:ARG:HH12	19:U:156:TYR:CA	2.30	0.45
25:a:6:ARG:HG3	25:a:6:ARG:NH1	2.32	0.45
27:4:27:U:H2'	27:4:28:C:C6	2.52	0.45
27:4:44:A:H2'	27:4:45:G:O4'	2.16	0.45
1:2:377:C:O2'	36:2:1564:SPM:N14	2.49	0.45
1:2:426:C:H2'	1:2:427:U:H6	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1075:C:H1'	1:2:1142:A:C4	2.52	0.45
1:2:1124:G:C2	1:2:1125:C:C6	3.05	0.45
1:2:1134:G:H2'	1:2:1135:C:C6	2.52	0.45
1:2:1370:U:H2'	1:2:1371:C:C5'	2.46	0.45
5:D:65:GLU:CD	9:I:84:ARG:HH22	2.25	0.45
10:J:105:GLU:OE2	10:J:105:GLU:N	2.50	0.45
11:K:8:VAL:HG22	11:K:23:ILE:CD1	2.32	0.45
16:Q:100:ILE:HD13	16:Q:110:LYS:HG2	1.98	0.45
24:3:41:LYS:HA	24:3:44:GLU:OE1	2.16	0.45
25:a:28:LEU:HD21	25:a:50:CYS:HB3	1.99	0.45
1:2:147:G:H2'	1:2:148:G:H8	1.82	0.45
1:2:217:U:H2'	1:2:218:C:C6	2.52	0.45
1:2:822:C:H2'	1:2:823:A:H8	1.82	0.45
1:2:826:G:N7	36:2:1560:SPM:H111	2.32	0.45
1:2:853:G:O2'	1:2:869:G:O6	2.29	0.45
1:2:949:U:C2	1:2:1184:G:C2	3.04	0.45
5:D:123:ARG:O	5:D:127:THR:HG23	2.17	0.45
6:F:146:GLU:OE2	6:F:146:GLU:HA	2.17	0.45
17:S:33:GLN:O	17:S:37:ARG:HG3	2.16	0.45
18:T:69:THR:HA	18:T:87:LYS:HB3	1.99	0.45
20:V:19:ARG:HG3	20:V:19:ARG:HH11	1.82	0.45
27:4:23:C:H2'	27:4:24:U:H6	1.82	0.45
27:4:63:G:H2'	27:4:64:G:H8	1.82	0.45
31:Z:2:PRO:HB2	31:Z:3:ASN:H	1.62	0.45
31:Z:29:ALA:HB2	31:Z:54:MET:HG3	1.98	0.45
1:2:416:C:H2'	1:2:417:G:O4'	2.16	0.44
1:2:446:G:H21	20:V:42:THR:HG21	1.82	0.44
1:2:813:G:H2'	1:2:814:U:C6	2.52	0.44
1:2:991:U:H2'	1:2:992:G:C5	2.52	0.44
13:M:94:GLN:O	13:M:98:ARG:HG2	2.17	0.44
32:d:12:ARG:NH1	32:d:12:ARG:CG	2.73	0.44
1:2:242:C:OP1	30:R:75:SER:HB2	2.15	0.44
1:2:643:A:H2'	1:2:644:G:O4'	2.17	0.44
1:2:657:C:C2	1:2:658:C:C5	3.05	0.44
1:2:710:OMC:HM22	1:2:711:G:H5'	2.00	0.44
1:2:1341:A:N6	8:H:46:GLU:OE2	2.40	0.44
4:C:55:TYR:CZ	4:C:64:GLY:HA3	2.52	0.44
10:J:33:THR:HG21	10:J:56:ARG:HD3	1.99	0.44
11:K:10:SER:OG	11:K:88:ARG:HB2	2.17	0.44
15:O:126:LYS:HG2	33:c:5:SER:HB3	1.97	0.44
16:Q:85:ASP:OD1	16:Q:85:ASP:N	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3:78:VAL:HG13	24:3:114:ILE:HG21	1.99	0.44
32:d:50:TYR:O	32:d:50:TYR:CG	2.70	0.44
33:c:94:VAL:HB	33:c:106:TYR:HB3	1.98	0.44
1:2:260:G:H2'	1:2:261:G:C8	2.52	0.44
1:2:366:C:H2'	1:2:367:G:C8	2.52	0.44
1:2:803:U:O4	2:A:127:THR:HG21	2.16	0.44
1:2:971:G:H2'	1:2:972:C:O4'	2.17	0.44
1:2:1074:A:H5'	11:K:117:GLN:HE21	1.83	0.44
1:2:1122:C:OP2	17:S:45:LYS:HG3	2.17	0.44
1:2:1287:G:OP2	38:2:1605:HOH:O	2.21	0.44
1:2:1466:4AC:HM73	1:2:1467:4AC:HM72	1.99	0.44
36:2:1563:SPM:H91	11:K:121:GLU:OE1	2.16	0.44
5:D:55:ALA:HB1	5:D:90:VAL:HG13	1.98	0.44
6:F:118:ARG:NH1	6:F:201:THR:O	2.50	0.44
7:G:197:ARG:HG2	7:G:205:ILE:HD11	1.99	0.44
13:M:94:GLN:HA	13:M:94:GLN:OE1	2.17	0.44
18:T:90:VAL:CG2	18:T:114:SER:HB2	2.47	0.44
22:X:25:ILE:HD12	22:X:25:ILE:O	2.17	0.44
23:Y:26:TYR:HH	23:Y:38:ASN:CG	2.26	0.44
23:Y:33:LYS:HA	23:Y:33:LYS:HE3	1.98	0.44
24:3:82:SER:O	24:3:82:SER:OG	2.34	0.44
28:5:817:A:H3'	28:5:818:A:H8	1.82	0.44
33:c:103:LEU:C	33:c:103:LEU:CD1	2.90	0.44
1:2:1110:A:H5'	1:2:1111:C:OP2	2.16	0.44
1:2:1293:G:H5''	15:O:33:GLY:N	2.33	0.44
11:K:29:ARG:HH12	19:U:156:TYR:C	2.25	0.44
13:M:52:PRO:HB3	13:M:95:PRO:HG2	2.00	0.44
15:O:61:LYS:HD2	15:O:61:LYS:N	2.33	0.44
18:T:90:VAL:HG23	18:T:114:SER:HB2	1.98	0.44
19:U:56:TRP:CH2	19:U:103:VAL:HG11	2.51	0.44
23:Y:58:TRP:N	23:Y:67:GLU:O	2.50	0.44
31:Z:29:ALA:CB	31:Z:55:ILE:HG13	2.48	0.44
1:2:113:OMC:HM22	1:2:114:U:H5'	2.00	0.44
1:2:430:U:C4	1:2:431:C:C5	3.06	0.44
1:2:796:A:O3'	21:W:53:GLY:HA3	2.18	0.44
1:2:813:G:H5''	21:W:2:MET:O	2.18	0.44
1:2:1097:C:C2	19:U:140:LEU:HD13	2.53	0.44
1:2:1121:A:N3	1:2:1144:G:C2	2.85	0.44
1:2:1382:A:P	1:2:1382:A:H8	2.41	0.44
1:2:1453:C:C2	1:2:1454:G:C8	3.05	0.44
2:A:116:TYR:CD1	2:A:195:PRO:CD	3.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:86:MET:HE3	9:I:119:ALA:CB	2.44	0.44
11:K:36:PRO:HB3	19:U:156:TYR:CZ	2.53	0.44
19:U:54:GLU:OE1	19:U:54:GLU:N	2.37	0.44
33:c:95:LYS:HZ2	33:c:109:ALA:HA	1.82	0.44
1:2:172:U:OP2	30:R:2:VAL:HG12	2.17	0.44
1:2:246:OMC:HM21	14:N:34:ILE:HA	2.00	0.44
2:A:54:TYR:CE2	2:A:60:PHE:HA	2.53	0.44
6:F:54:LEU:HD23	6:F:54:LEU:HA	1.83	0.44
6:F:121:CYS:SG	6:F:126:CYS:CB	3.04	0.44
7:G:148:VAL:HB	7:G:212:ILE:HG23	2.00	0.44
13:M:41:MET:HE2	13:M:41:MET:HA	1.98	0.44
20:V:92:LYS:HE2	20:V:92:LYS:HB2	1.80	0.44
24:3:105:GLY:C	24:3:106:GLU:HG3	2.43	0.44
34:E:169:ASP:CG	34:E:231:ARG:HH22	2.25	0.44
1:2:457:A:P	26:e:26:HIS:HE1	2.40	0.44
1:2:677:A:C4	1:2:678:C:C5	3.06	0.44
1:2:707:G:C8	16:Q:59:PRO:HB2	2.52	0.44
5:D:55:ALA:O	5:D:58:LEU:HB2	2.17	0.44
7:G:90:ASN:C	7:G:90:ASN:OD1	2.61	0.44
8:H:61:LEU:O	8:H:65:ILE:HG12	2.18	0.44
8:H:79:TYR:O	8:H:82:VAL:HG12	2.17	0.44
16:Q:94:VAL:HA	16:Q:97:ARG:NH1	2.32	0.44
21:W:15:ARG:HD2	21:W:66:GLY:HA2	2.00	0.44
21:W:40:CYS:SG	21:W:42:SER:OG	2.75	0.44
24:3:43:VAL:HG22	24:3:48:ALA:HB3	1.99	0.44
29:P:28:VAL:HA	29:P:37:CYS:HA	2.00	0.44
31:Z:25:GLN:HA	31:Z:25:GLN:OE1	2.18	0.44
1:2:200:C:H2'	1:2:201:A:C8	2.53	0.44
1:2:431:C:C2	1:2:432:C:C5	3.05	0.44
1:2:947:A:O2'	1:2:1007:G:OP2	2.22	0.44
1:2:1092:G:C6	1:2:1104:G:C6	3.05	0.44
3:B:58:MET:HE3	3:B:177:ILE:HG21	2.00	0.44
3:B:131:PHE:HB2	3:B:159:GLU:HB3	2.00	0.44
3:B:194:LEU:HD12	3:B:194:LEU:HA	1.82	0.44
8:H:128:VAL:HG23	22:X:55:ASN:HB2	1.99	0.44
23:Y:33:LYS:HB3	23:Y:35:LYS:HE3	1.99	0.44
24:3:41:LYS:HE3	24:3:41:LYS:HB3	1.80	0.44
31:Z:95:VAL:O	31:Z:99:ARG:HG3	2.17	0.44
34:E:12:PHE:CE1	34:E:104:MET:HE2	2.52	0.44
1:2:334:A:OP2	36:2:1556:SPM:N5	2.38	0.44
1:2:708:C:H2'	1:2:709:C:H6	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:846:C:O2'	1:2:847:U:H5'	2.17	0.44
1:2:1276:G:P	18:T:39:ARG:HH22	2.41	0.44
2:A:50:GLU:HG2	2:A:68:TYR:CE1	2.53	0.44
6:F:56:TYR:HB3	6:F:82:MET:HG3	2.00	0.44
8:H:8:LEU:HD22	32:d:70:LYS:HB3	2.00	0.44
12:L:46:LEU:HB2	12:L:67:MET:HB3	1.99	0.44
13:M:96:ALA:O	13:M:100:LEU:HD12	2.17	0.44
16:Q:52:LEU:HB3	16:Q:58:ILE:HB	1.99	0.44
27:4:22:G:C4	27:4:23:C:C5	3.06	0.44
1:2:479:A:O2'	14:N:91:ASP:OD1	2.24	0.43
1:2:988:G:O2'	1:2:989:C:O5'	2.31	0.43
1:2:1019:U:OP1	12:L:59:ARG:NE	2.39	0.43
1:2:1494:U:C2	1:2:1495:C:C5	3.06	0.43
2:A:23:ILE:O	2:A:81:THR:HG22	2.18	0.43
2:A:148:LYS:NZ	2:A:149:LYS:HE2	2.32	0.43
3:B:127:ILE:O	3:B:130:THR:OG1	2.25	0.43
6:F:9:ASN:HB2	6:F:12:GLU:OE1	2.18	0.43
10:J:118:ASP:HB3	10:J:120:VAL:HG22	2.00	0.43
11:K:76:MET:HE2	11:K:76:MET:HB2	1.83	0.43
14:N:45:GLY:HA3	14:N:79:ARG:HH22	1.82	0.43
14:N:134:LEU:O	14:N:138:TYR:HB2	2.17	0.43
15:O:55:LEU:HG	15:O:59:GLU:HG3	2.00	0.43
17:S:8:ASP:OD1	17:S:8:ASP:N	2.49	0.43
24:3:17:ASP:HA	24:3:20:LEU:HB2	1.99	0.43
27:4:52:G:H2'	27:4:53:G:C8	2.52	0.43
1:2:207:U:H2'	1:2:208:A:C8	2.53	0.43
1:2:229:C:H2'	1:2:230:A:C8	2.54	0.43
1:2:264:G:O2'	10:J:32:PRO:HB3	2.18	0.43
1:2:268:A:H2'	1:2:269:G:C8	2.53	0.43
8:H:70:ARG:HG2	8:H:71:ASN:N	2.32	0.43
10:J:83:GLU:HG3	10:J:101:LYS:HB3	2.00	0.43
13:M:66:ALA:HA	13:M:69:LYS:HB2	2.00	0.43
16:Q:76:ARG:HB2	16:Q:78:LEU:HD12	2.00	0.43
24:3:70:CYS:SG	24:3:77:TYR:HB3	2.57	0.43
1:2:119:U:O2'	34:E:165:GLN:OE1	2.27	0.43
1:2:298:C:H5'	1:2:569:G:N3	2.33	0.43
1:2:327:C:H2'	1:2:328:U:C6	2.53	0.43
1:2:784:G:H2'	1:2:785:C:H6	1.83	0.43
1:2:1261:G:OP1	15:O:51:ARG:NH2	2.51	0.43
1:2:1307:C:H2'	1:2:1308:C:C6	2.53	0.43
1:2:1336:U:H2'	1:2:1337:G:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:9:LEU:HD23	12:L:9:LEU:HA	1.74	0.43
13:M:111:GLU:C	13:M:111:GLU:OE1	2.61	0.43
15:O:11:ILE:HD12	15:O:11:ILE:HG23	1.79	0.43
21:W:43:CYS:SG	21:W:45:THR:HG23	2.58	0.43
24:3:27:LYS:NZ	24:3:89:ALA:HB3	2.33	0.43
24:3:119:ASN:HD22	24:3:119:ASN:N	2.16	0.43
27:4:67:C:H2'	27:4:68:C:C6	2.53	0.43
1:2:1340:U:H2'	1:2:1341:A:C8	2.53	0.43
7:G:17:LYS:HZ3	7:G:19:ILE:HG22	1.82	0.43
7:G:139:GLU:O	7:G:142:GLN:NE2	2.51	0.43
11:K:40:ILE:HD13	11:K:40:ILE:HA	1.76	0.43
11:K:124:MET:CE	12:L:60:LYS:H	2.32	0.43
14:N:57:LYS:HG2	14:N:73:VAL:HG12	2.00	0.43
24:3:79:TYR:CE1	24:3:118:VAL:HG22	2.54	0.43
25:a:51:GLU:HA	25:a:54:LYS:CD	2.48	0.43
32:d:24:LEU:HD23	32:d:24:LEU:HA	1.68	0.43
1:2:31:U:P	14:N:141:LYS:NZ	2.91	0.43
1:2:339:C:H2'	1:2:340:C:H6	1.83	0.43
1:2:413:U:H5''	5:D:118:THR:HG23	2.00	0.43
1:2:558:C:H2'	1:2:559:A:C8	2.53	0.43
1:2:603:U:C2	1:2:604:G:C8	3.06	0.43
1:2:987:U:H2'	1:2:988:G:C8	2.53	0.43
4:C:34:CYS:SG	4:C:57:CYS:CB	2.96	0.43
6:F:148:ASP:OD1	6:F:148:ASP:N	2.50	0.43
7:G:16:PRO:HB2	7:G:112:TYR:HB2	2.00	0.43
7:G:175:ILE:HD11	7:G:177:LEU:HG	2.00	0.43
8:H:30:TYR:CE2	8:H:132:PRO:HG2	2.52	0.43
13:M:111:GLU:OE1	13:M:113:VAL:HG23	2.17	0.43
15:O:77:SER:OG	15:O:91:ASP:OD2	2.33	0.43
16:Q:123:LEU:HD23	16:Q:123:LEU:HA	1.86	0.43
19:U:121:LYS:HD2	19:U:122:ASN:OD1	2.18	0.43
19:U:137:LYS:HD3	19:U:137:LYS:H	1.83	0.43
32:d:65:LEU:HB3	32:d:66:PRO:HD3	2.01	0.43
1:2:24:C:H2'	1:2:25:G:H8	1.84	0.43
1:2:58:U:H2'	1:2:59:C:C6	2.54	0.43
1:2:655:A:H2'	1:2:656:U:C6	2.50	0.43
1:2:749:A:N6	1:2:1455:U:OP1	2.52	0.43
1:2:1097:C:N3	19:U:140:LEU:HD13	2.34	0.43
1:2:1155:C:H2'	1:2:1156:G:O4'	2.18	0.43
1:2:1289:C:H2'	1:2:1290:C:H6	1.84	0.43
2:A:19:TRP:HA	2:A:37:PRO:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:116:TYR:HB3	2:A:155:PHE:HD1	1.82	0.43
2:A:123:LEU:HD11	2:A:125:LEU:HD21	1.99	0.43
3:B:191:ARG:NH2	3:B:227:MET:SD	2.89	0.43
3:B:199:TRP:NE1	3:B:218:LEU:HD23	2.34	0.43
11:K:13:ARG:O	11:K:84:MET:HE1	2.19	0.43
11:K:23:ILE:HD12	11:K:23:ILE:C	2.44	0.43
12:L:25:ARG:HA	12:L:28:VAL:HG12	2.01	0.43
14:N:91:ASP:N	14:N:138:TYR:HH	2.14	0.43
23:Y:43:ARG:HD2	23:Y:43:ARG:H	1.83	0.43
23:Y:56:GLU:HB3	23:Y:69:ILE:HB	2.00	0.43
27:4:23:C:C2	27:4:24:U:C5	3.07	0.43
32:d:37:LEU:O	32:d:41:LEU:HG	2.18	0.43
32:d:65:LEU:C	32:d:65:LEU:CD2	2.90	0.43
1:2:310:G:H5''	1:2:311:A:OP1	2.19	0.43
1:2:418:U:H4'	1:2:419:A:H5'	2.00	0.43
1:2:1189:C:O2	18:T:122:HIS:HE1	2.00	0.43
2:A:40:ASP:C	2:A:40:ASP:OD1	2.61	0.43
4:C:19:CYS:SG	4:C:20:GLY:N	2.91	0.43
8:H:34:MET:SD	32:d:29:ARG:NH2	2.91	0.43
8:H:142:HIS:ND1	8:H:181:ARG:HD2	2.33	0.43
18:T:72:THR:OG1	18:T:74:VAL:HG12	2.19	0.43
19:U:108:PHE:HD2	19:U:125:ARG:HD3	1.79	0.43
22:X:18:PHE:HB2	22:X:68:LEU:O	2.18	0.43
22:X:73:ARG:HA	22:X:73:ARG:HH11	1.82	0.43
1:2:18:C:C2	1:2:19:G:C8	3.07	0.43
1:2:91:G:OP1	36:2:1551:SPM:H111	2.19	0.43
1:2:995:U:H2'	1:2:996:C:C5	2.54	0.43
1:2:1366:OMC:HM22	1:2:1367:C:H5'	2.01	0.43
7:G:32:ILE:HG23	7:G:35:GLU:HG3	2.01	0.43
7:G:59:LEU:HB3	7:G:114:THR:HB	1.99	0.43
17:S:16:ILE:HD11	31:Z:195:LEU:HD21	2.01	0.43
18:T:86:LEU:HD13	18:T:86:LEU:HA	1.90	0.43
21:W:40:CYS:C	21:W:42:SER:H	2.26	0.43
30:R:37:ARG:HD3	30:R:37:ARG:N	2.33	0.43
31:Z:60:GLY:HA2	31:Z:63:ILE:HD13	2.01	0.43
32:d:12:ARG:C	32:d:12:ARG:CD	2.86	0.43
33:c:11:THR:O	33:c:12:MET:C	2.60	0.43
33:c:35:LYS:HB2	33:c:36:THR:H	1.65	0.43
1:2:45:U:O2'	1:2:46:A:H2'	2.18	0.43
1:2:569:G:C2	1:2:570:A:C8	3.06	0.43
1:2:740:A:OP1	36:2:1559:SPM:H112	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:779:U:H4'	1:2:780:G:OP2	2.19	0.43
1:2:1350:C:H2'	1:2:1351:U:C6	2.54	0.43
1:2:1478:4AC:O7	1:2:1478:4AC:H5	2.18	0.43
1:2:1488:A:C4	1:2:1489:U:C5	3.06	0.43
3:B:33:ILE:CD1	3:B:76:ARG:HG2	2.49	0.43
8:H:5:ASN:N	8:H:5:ASN:OD1	2.50	0.43
9:I:84:ARG:O	9:I:87:ILE:HG22	2.19	0.43
9:I:101:GLU:HG2	9:I:102:ILE:HD12	2.01	0.43
11:K:27:LYS:HD2	11:K:27:LYS:C	2.44	0.43
16:Q:91:ARG:HB3	16:Q:91:ARG:HH11	1.84	0.43
25:a:63:TYR:CE1	29:P:4:TYR:O	2.72	0.43
1:2:44:C:H3'	1:2:45:U:H5''	2.01	0.43
1:2:210:U:H5''	1:2:211:C:H5'	2.00	0.43
1:2:497:A:H2'	1:2:498:G:H8	1.84	0.43
1:2:504:C:H41	26:e:33:ARG:CZ	2.31	0.43
1:2:751:A:O2'	1:2:753:A:N7	2.47	0.43
1:2:1057:C:C4	1:2:1059:A:H5''	2.54	0.43
2:A:101:SER:O	2:A:126:THR:OG1	2.37	0.43
8:H:24:ASP:OD1	8:H:27:LEU:N	2.38	0.43
15:O:99:LEU:HD12	15:O:99:LEU:O	2.18	0.43
18:T:22:LEU:HA	18:T:25:MET:HE2	2.01	0.43
18:T:53:LEU:O	18:T:53:LEU:HD23	2.19	0.43
23:Y:27:TYR:CE1	23:Y:36:LEU:HA	2.53	0.43
25:a:63:TYR:CE1	29:P:6:PRO:HB3	2.54	0.43
31:Z:88:ASN:HB3	31:Z:91:LEU:HB2	2.00	0.43
32:d:12:ARG:HD3	32:d:13:GLU:O	2.18	0.43
1:2:109:U:H5'	30:R:37:ARG:HG3	2.01	0.42
1:2:125:G:OP1	36:2:1567:SPM:H92	2.19	0.42
1:2:339:C:H2'	1:2:340:C:C6	2.54	0.42
1:2:397:G:H2'	1:2:398:C:O4'	2.19	0.42
1:2:543:G:H2'	1:2:544:C:C6	2.54	0.42
1:2:663:A:C5	1:2:664:U:C5	3.07	0.42
1:2:1115:A:O4'	12:L:40:PRO:HB2	2.18	0.42
1:2:1277:G:H2'	1:2:1278:C:C6	2.54	0.42
2:A:19:TRP:NE1	2:A:37:PRO:HB3	2.34	0.42
5:D:80:MET:HE2	5:D:80:MET:HB3	1.83	0.42
6:F:126:CYS:HB2	6:F:153:PRO:HA	2.00	0.42
14:N:40:LYS:HG2	14:N:41:TYR:CE1	2.54	0.42
25:a:40:LYS:C	25:a:40:LYS:CD	2.92	0.42
32:d:64:PRO:HG2	32:d:67:ILE:CB	2.45	0.42
1:2:913:C:H5'	1:2:1328:A:N6	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1116:G:O5'	12:L:14:VAL:HG21	2.19	0.42
1:2:1121:A:C2	1:2:1144:G:C4	3.07	0.42
2:A:39:TYR:N	2:A:43:GLN:OE1	2.51	0.42
16:Q:32:GLU:HB3	16:Q:76:ARG:NH2	2.34	0.42
18:T:28:ASP:OD1	18:T:29:GLU:N	2.51	0.42
18:T:48:ASP:OD2	18:T:51:ARG:NH1	2.52	0.42
20:V:88:GLU:OE2	20:V:88:GLU:N	2.31	0.42
25:a:7:GLY:O	25:a:9:ASN:N	2.53	0.42
25:a:22:ARG:HB3	25:a:49:PHE:CE1	2.54	0.42
27:4:20:H2U:O2'	27:4:22:G:OP1	2.33	0.42
29:P:34:ILE:H	29:P:34:ILE:HG13	1.65	0.42
1:2:391:G:OP2	36:2:1564:SPM:H42	2.18	0.42
1:2:946:U:H4'	1:2:947:A:O4'	2.19	0.42
1:2:1329:U:H2'	1:2:1330:C:H6	1.84	0.42
1:2:1464:A:H2'	1:2:1465:G:C8	2.54	0.42
3:B:29:LYS:HB2	3:B:76:ARG:HD2	2.01	0.42
7:G:173:ARG:HG3	7:G:174:LYS:N	2.33	0.42
10:J:66:LEU:HD12	10:J:73:ALA:HB2	2.01	0.42
13:M:112:ASP:OD2	13:M:112:ASP:C	2.62	0.42
15:O:100:ILE:HG22	15:O:104:ARG:NH2	2.32	0.42
16:Q:62:LYS:HD2	16:Q:62:LYS:O	2.18	0.42
23:Y:59:SER:HB3	23:Y:66:THR:HG23	2.01	0.42
24:3:34:LYS:O	24:3:39:THR:HG23	2.18	0.42
25:a:51:GLU:OE2	25:a:51:GLU:HA	2.18	0.42
27:4:9:G:H1'	27:4:45:G:H2'	2.01	0.42
1:2:569:G:C4	1:2:570:A:C8	3.07	0.42
1:2:620:G:N2	1:2:795:C:H4'	2.35	0.42
1:2:831:C:H2'	1:2:832:G:O4'	2.19	0.42
1:2:881:A:H2'	1:2:882:A:C8	2.54	0.42
1:2:1122:C:H6	17:S:28:TYR:CZ	2.37	0.42
1:2:1319:A:H2'	1:2:1320:G:H8	1.84	0.42
7:G:157:ASP:OD1	7:G:161:PHE:N	2.51	0.42
21:W:18:ARG:HD3	21:W:65:MET:HE2	2.01	0.42
27:4:10:G:N2	27:4:26:G:H1'	2.34	0.42
32:d:35:GLU:N	32:d:35:GLU:OE2	2.52	0.42
34:E:84:ILE:HD11	34:E:95:ARG:NH1	2.34	0.42
1:2:784:G:H2'	1:2:785:C:C6	2.54	0.42
1:2:965:A:O2'	24:3:34:LYS:HD3	2.20	0.42
1:2:1168:U:H4'	31:Z:176:ILE:HD11	2.00	0.42
1:2:1273:G:OP1	15:O:117:ARG:NH1	2.48	0.42
2:A:53:LEU:HB3	2:A:62:GLN:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:116:TYR:CD1	2:A:195:PRO:HD2	2.53	0.42
4:C:19:CYS:HB2	4:C:21:LYS:HZ1	1.84	0.42
7:G:10:ASP:OD2	7:G:113:ARG:NH1	2.52	0.42
7:G:142:GLN:CD	7:G:142:GLN:N	2.75	0.42
8:H:154:ASN:HD21	8:H:156:LYS:HB3	1.84	0.42
9:I:15:TYR:CZ	9:I:71:LYS:HD2	2.55	0.42
11:K:36:PRO:HB2	11:K:39:LEU:CD1	2.49	0.42
14:N:56:GLU:HG2	14:N:74:ARG:HG3	2.01	0.42
15:O:142:ILE:HD12	18:T:125:PRO:HG3	2.02	0.42
22:X:76:ARG:HD3	22:X:76:ARG:N	2.29	0.42
24:3:40:THR:HG22	24:3:66:LEU:HD11	2.00	0.42
34:E:68:ASP:HA	34:E:162:LEU:HD13	2.01	0.42
34:E:95:ARG:NH2	34:E:113:GLU:O	2.49	0.42
1:2:88:G:H1	7:G:187:GLU:CD	2.20	0.42
1:2:326:A:O2'	7:G:191:ARG:NH2	2.53	0.42
1:2:504:C:H2'	1:2:505:G:O4'	2.20	0.42
1:2:644:G:H1'	13:M:33:ILE:HD11	2.02	0.42
1:2:967:G:O6	24:3:37:ASN:HB2	2.20	0.42
1:2:1059:A:H2'	1:2:1060:OMC:C6	2.54	0.42
1:2:1175:A:O2'	1:2:1176:A:OP2	2.33	0.42
2:A:156:ASP:O	2:A:160:GLN:HG2	2.20	0.42
3:B:107:TYR:O	3:B:111:GLN:HG3	2.20	0.42
5:D:145:VAL:HG13	5:D:149:GLU:HG3	2.01	0.42
8:H:34:MET:HA	8:H:35:PRO:HD3	1.93	0.42
25:a:8:SER:HA	31:Z:167:ILE:HD12	2.01	0.42
33:c:32:GLY:HA3	33:c:35:LYS:HE3	2.01	0.42
1:2:141:A:H2'	1:2:142:A:O4'	2.20	0.42
1:2:623:G:C6	36:2:1558:SPM:H22	2.54	0.42
1:2:671:A:H2'	1:2:672:OMG:C8	2.54	0.42
1:2:1073:C:O2'	11:K:117:GLN:HG3	2.20	0.42
1:2:1278:C:H2'	1:2:1279:U:C6	2.55	0.42
1:2:1323:C:H5''	29:P:14:LYS:HA	2.00	0.42
2:A:96:LEU:HB3	2:A:125:LEU:HD11	2.02	0.42
2:A:162:VAL:HG12	2:A:167:LEU:HD23	2.01	0.42
3:B:199:TRP:HD1	3:B:225:PHE:CE1	2.38	0.42
4:C:37:CYS:SG	4:C:39:GLU:HG2	2.60	0.42
11:K:29:ARG:NH2	19:U:158:GLU:C	2.77	0.42
13:M:77:LYS:HE2	13:M:113:VAL:HG21	2.00	0.42
16:Q:13:ILE:CG2	21:W:10:PRO:HB2	2.49	0.42
32:d:65:LEU:HB3	32:d:66:PRO:CD	2.48	0.42
1:2:121:A:H2'	1:2:122:G:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:178:A:O2'	30:R:10:ASP:O	2.36	0.42
1:2:314:C:H2'	1:2:315:C:H6	1.84	0.42
1:2:333:C:H4'	1:2:334:A:H5''	2.01	0.42
1:2:395:G:H2'	1:2:396:G:H8	1.85	0.42
3:B:84:ILE:HD11	4:C:36:ASN:CB	2.50	0.42
7:G:79:PHE:CE2	7:G:98:MET:HG2	2.53	0.42
8:H:3:LEU:CD2	32:d:70:LYS:NZ	2.61	0.42
12:L:9:LEU:HD11	12:L:20:VAL:CG1	2.49	0.42
18:T:63:GLU:OE1	18:T:63:GLU:N	2.53	0.42
18:T:108:HIS:ND1	18:T:113:TYR:OH	2.51	0.42
27:4:68:C:H2'	27:4:69:C:C6	2.55	0.42
1:2:387:A:H2'	1:2:388:A:C8	2.54	0.42
1:2:899:A:H2'	1:2:900:C:H6	1.85	0.42
1:2:1080:A:H4'	12:L:37:GLY:HA3	2.02	0.42
1:2:1189:C:H2'	15:O:132:THR:HG23	2.01	0.42
2:A:22:VAL:HG12	2:A:79:LEU:HB2	2.02	0.42
8:H:25:PRO:O	8:H:28:LYS:HG3	2.20	0.42
8:H:38:LEU:HD23	11:K:48:LYS:HG2	2.02	0.42
12:L:86:LEU:O	12:L:89:VAL:HG23	2.19	0.42
20:V:47:ASP:OD2	20:V:48:ILE:N	2.53	0.42
24:3:79:TYR:OH	24:3:118:VAL:HG13	2.20	0.42
27:4:27:U:H2'	27:4:28:C:H6	1.83	0.42
31:Z:63:ILE:H	31:Z:63:ILE:CD1	2.27	0.42
33:c:96:LEU:HD22	33:c:105:ILE:O	2.19	0.42
34:E:127:ILE:HG13	34:E:128:LYS:H	1.84	0.42
1:2:72:G:H2'	1:2:209:U:O2	2.18	0.42
1:2:1271:U:H4'	33:c:5:SER:HB2	2.00	0.42
1:2:1436:U:O2'	1:2:1437:G:OP1	2.36	0.42
3:B:33:ILE:HD11	3:B:76:ARG:HG2	2.01	0.42
8:H:158:ILE:HG22	33:c:102:ARG:CD	2.50	0.42
9:I:71:LYS:HB3	9:I:133:TYR:CZ	2.54	0.42
10:J:65:VAL:HG22	10:J:123:ALA:HB3	2.02	0.42
10:J:127:LYS:HB3	10:J:127:LYS:HE3	1.69	0.42
12:L:51:MET:HE3	12:L:51:MET:HB2	1.94	0.42
13:M:33:ILE:HD12	13:M:33:ILE:C	2.45	0.42
17:S:12:ILE:HD12	17:S:12:ILE:HA	1.94	0.42
19:U:29:LYS:HA	19:U:29:LYS:HE3	2.01	0.42
31:Z:54:MET:H	31:Z:54:MET:HG2	1.67	0.42
1:2:175:U:H2'	1:2:176:G:O4'	2.20	0.41
1:2:1201:A:N3	1:2:1201:A:H2'	2.35	0.41
1:2:1319:A:H2'	1:2:1320:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1331:U:OP2	36:2:1563:SPM:H132	2.19	0.41
4:C:28:LYS:HD2	4:C:28:LYS:HA	1.82	0.41
6:F:13:TRP:C	6:F:14:LYS:HD3	2.45	0.41
13:M:42:VAL:HG21	13:M:57:LEU:HB2	2.00	0.41
14:N:84:VAL:HG22	14:N:85:THR:N	2.35	0.41
17:S:29:ASN:OD1	17:S:29:ASN:N	2.53	0.41
27:4:6:G:H2'	27:4:7:G:C8	2.55	0.41
27:4:34:C:H2'	27:4:35:A:C8	2.54	0.41
27:4:43:A:H2'	27:4:44:A:H8	1.85	0.41
1:2:66:U:H2'	1:2:67:C:O4'	2.20	0.41
1:2:169:G:H1'	10:J:71:ASN:ND2	2.35	0.41
1:2:404:C:H2'	1:2:405:C:C6	2.55	0.41
1:2:472:U:H2'	1:2:473:G:H8	1.84	0.41
1:2:512:OMC:HM22	1:2:513:G:H5'	2.02	0.41
1:2:1014:G:H2'	1:2:1015:G:O4'	2.20	0.41
1:2:1052:U:O2	17:S:4:ILE:HG13	2.20	0.41
1:2:1096:U:OP1	19:U:137:LYS:NZ	2.50	0.41
1:2:1114:U:O2'	12:L:40:PRO:O	2.29	0.41
4:C:40:VAL:HG21	4:C:58:PRO:HD2	2.01	0.41
6:F:9:ASN:OD1	6:F:9:ASN:N	2.53	0.41
15:O:11:ILE:HG22	15:O:12:PHE:CE1	2.54	0.41
18:T:25:MET:HG3	18:T:26:PRO:HD2	2.02	0.41
24:3:74:LYS:HD2	24:3:74:LYS:HA	1.83	0.41
25:a:72:LEU:HD11	31:Z:69:ILE:HG12	2.03	0.41
1:2:12:U:H2'	1:2:13:C:H6	1.84	0.41
1:2:338:G:H2'	1:2:339:C:H6	1.86	0.41
1:2:413:U:C2	1:2:425:G:N2	2.88	0.41
1:2:625:G:OP1	36:2:1558:SPM:N5	2.52	0.41
1:2:1446:G:H2'	1:2:1447:A:C8	2.51	0.41
36:2:1553:SPM:H111	36:2:1553:SPM:H81	1.83	0.41
4:C:8:ARG:NE	4:C:9:GLU:OE2	2.54	0.41
5:D:11:TRP:HB3	5:D:43:ILE:HG13	2.01	0.41
6:F:209:ASP:OD1	6:F:209:ASP:N	2.53	0.41
11:K:30:VAL:HA	11:K:66:ALA:O	2.20	0.41
11:K:107:ASP:O	11:K:110:MET:HG3	2.20	0.41
14:N:49:MET:HE2	14:N:49:MET:HB3	1.88	0.41
24:3:18:LYS:HZ1	24:3:113:GLU:HB3	1.85	0.41
24:3:55:GLU:HB2	24:3:80:VAL:HG11	2.01	0.41
34:E:55:GLU:O	34:E:59:ILE:HG23	2.19	0.41
1:2:29:G:H2'	1:2:30:C:H6	1.84	0.41
1:2:46:A:H1'	1:2:48:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:842:C:H2'	1:2:843:4AC:H6	2.02	0.41
2:A:72:ILE:HG21	2:A:82:ARG:HD3	2.02	0.41
2:A:99:ARG:HG2	2:A:99:ARG:NH1	2.35	0.41
4:C:55:TYR:C	4:C:56:ILE:HD12	2.45	0.41
7:G:65:THR:HA	7:G:74:LYS:HA	2.02	0.41
7:G:144:ILE:HG22	7:G:146:LEU:HD23	2.01	0.41
12:L:11:SER:HA	12:L:94:ASP:O	2.19	0.41
12:L:74:ILE:HD12	12:L:74:ILE:HG23	1.73	0.41
14:N:10:ILE:O	14:N:10:ILE:HG13	2.20	0.41
15:O:102:TYR:HA	15:O:105:ASN:OD1	2.20	0.41
19:U:133:SER:HA	19:U:136:ASP:OD1	2.20	0.41
19:U:143:PHE:HZ	19:U:156:TYR:HB3	1.85	0.41
23:Y:42:PRO:HD2	23:Y:43:ARG:NE	2.34	0.41
25:a:36:TYR:HE2	25:a:51:GLU:OE2	2.02	0.41
25:a:45:TYR:HB3	29:P:7:PRO:HG2	2.03	0.41
27:4:29:G:C6	27:4:42:G:C6	3.09	0.41
27:4:50:U:O4	27:4:64:G:O6	2.37	0.41
34:E:119:VAL:HG21	34:E:138:ASP:OD1	2.21	0.41
1:2:172:U:P	30:R:2:VAL:HG12	2.60	0.41
1:2:303:A:H2'	1:2:304:G:O4'	2.20	0.41
1:2:649:G:H2'	1:2:650:G:C8	2.55	0.41
1:2:677:A:C5	13:M:118:HIS:CD2	3.09	0.41
1:2:782:A:C6	1:2:841:G:C6	3.09	0.41
3:B:64:ARG:CZ	3:B:64:ARG:HB3	2.50	0.41
8:H:30:TYR:HE2	8:H:132:PRO:HG2	1.84	0.41
9:I:28:MET:HE2	9:I:60:LYS:HE3	2.02	0.41
12:L:15:GLU:C	12:L:15:GLU:OE1	2.64	0.41
14:N:84:VAL:HG21	14:N:124:TYR:CD1	2.56	0.41
15:O:121:HIS:CE1	15:O:127:VAL:HG11	2.56	0.41
20:V:8:LYS:HE2	20:V:8:LYS:N	2.36	0.41
22:X:20:ALA:O	22:X:66:LEU:N	2.49	0.41
23:Y:56:GLU:O	23:Y:58:TRP:HD1	2.04	0.41
25:a:69:VAL:HA	25:a:70:PRO:HD2	1.68	0.41
34:E:169:ASP:OD1	34:E:231:ARG:NH2	2.53	0.41
1:2:569:G:C5	1:2:570:A:N7	2.89	0.41
1:2:934:C:OP1	12:L:60:LYS:NZ	2.48	0.41
1:2:1169:G:H2'	1:2:1170:C:C6	2.55	0.41
1:2:1173:C:H2'	1:2:1174:G:O4'	2.20	0.41
6:F:68:THR:HG22	6:F:69:ASP:N	2.36	0.41
8:H:40:HIS:CD2	11:K:48:LYS:HE2	2.55	0.41
11:K:98:GLU:OE1	11:K:102:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:9:LEU:HD11	12:L:20:VAL:HG11	2.02	0.41
19:U:6:ILE:HA	19:U:10:MET:CE	2.51	0.41
24:3:114:ILE:HD12	24:3:114:ILE:H	1.86	0.41
25:a:72:LEU:HG	31:Z:73:VAL:CG2	2.51	0.41
34:E:178:TYR:CD1	34:E:234:SER:HB2	2.56	0.41
1:2:85:G:H2'	1:2:86:C:C6	2.54	0.41
1:2:261:G:OP1	30:R:52:LYS:NZ	2.54	0.41
1:2:677:A:C5	1:2:678:C:C5	3.09	0.41
1:2:1003:A:H2'	1:2:1004:G:O4'	2.21	0.41
1:2:1101:G:H2'	1:2:1102:C:H6	1.86	0.41
1:2:1365:G:H2'	1:2:1366:OMC:O4'	2.21	0.41
1:2:1490:C:H2'	1:2:1491:A:C8	2.55	0.41
6:F:138:VAL:HG11	6:F:201:THR:HG22	2.02	0.41
8:H:133:GLN:O	8:H:136:ILE:HG13	2.20	0.41
9:I:71:LYS:HG3	9:I:72:CYS:N	2.36	0.41
9:I:81:LEU:HD12	9:I:126:GLY:H	1.86	0.41
13:M:26:SER:HA	13:M:33:ILE:HA	2.03	0.41
14:N:111:THR:O	14:N:114:ARG:HB2	2.21	0.41
24:3:9:PHE:CZ	24:3:121:ILE:HG23	2.56	0.41
1:2:483:G:N2	36:2:1549:SPM:H112	2.36	0.41
1:2:602:C:C2	1:2:603:U:C5	3.09	0.41
1:2:681:G:OP1	2:A:99:ARG:NH1	2.54	0.41
1:2:786:U:H2'	1:2:833:U:O4	2.21	0.41
1:2:974:A:H1'	23:Y:57:ARG:CZ	2.50	0.41
1:2:1442:G:C2	1:2:1443:G:C8	3.09	0.41
5:D:28:GLU:HA	26:e:38:TYR:HE2	1.85	0.41
8:H:85:ALA:HB3	8:H:162:LEU:HD22	2.03	0.41
12:L:93:GLU:O	31:Z:11:LYS:NZ	2.52	0.41
25:a:34:ILE:CD1	25:a:51:GLU:HB2	2.51	0.41
25:a:34:ILE:HD12	25:a:34:ILE:O	2.21	0.41
31:Z:189:ILE:HG21	31:Z:192:LYS:HG3	2.03	0.41
32:d:4:LEU:O	32:d:4:LEU:HD13	2.21	0.41
34:E:16:SER:HB2	34:E:19:GLN:HB2	2.03	0.41
1:2:431:C:H2'	1:2:432:C:H6	1.85	0.41
1:2:534:G:O2'	1:2:780:G:H5'	2.20	0.41
1:2:538:OMC:HM22	1:2:539:C:O4'	2.21	0.41
1:2:709:C:OP2	16:Q:14:ARG:NH2	2.52	0.41
1:2:1058:A:H4'	1:2:1059:A:H5'	2.03	0.41
1:2:1074:A:C5'	11:K:117:GLN:HE21	2.34	0.41
1:2:1076:C:H2'	1:2:1077:A:C8	2.52	0.41
3:B:15:GLU:HB3	3:B:66:ARG:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:10:LYS:HA	5:D:10:LYS:HD2	1.89	0.41
5:D:12:GLU:HA	5:D:12:GLU:OE2	2.20	0.41
6:F:22:LEU:HB3	6:F:28:ILE:HD13	2.02	0.41
6:F:154:LYS:HA	6:F:175:ASP:OD2	2.21	0.41
7:G:31:SER:OG	7:G:97:THR:HG21	2.20	0.41
8:H:129:ASP:OD1	8:H:130:VAL:N	2.54	0.41
8:H:190:LEU:HD12	8:H:190:LEU:HA	1.93	0.41
10:J:63:ALA:HB2	10:J:78:ILE:CG1	2.47	0.41
11:K:24:TYR:CE2	11:K:65:ASP:HB3	2.55	0.41
11:K:88:ARG:NE	11:K:110:MET:O	2.53	0.41
12:L:46:LEU:HD21	31:Z:5:LYS:HD3	2.03	0.41
13:M:33:ILE:HD12	13:M:33:ILE:O	2.21	0.41
14:N:58:VAL:HG23	14:N:72:CYS:SG	2.61	0.41
15:O:72:ILE:HD12	15:O:72:ILE:HG23	1.81	0.41
15:O:126:LYS:CG	33:c:5:SER:HB3	2.51	0.41
18:T:39:ARG:O	18:T:43:LYS:HB2	2.20	0.41
18:T:75:ARG:HB3	18:T:111:GLY:HA3	2.03	0.41
19:U:138:LEU:O	19:U:142:ILE:HG13	2.20	0.41
24:3:21:GLU:C	24:3:21:GLU:OE2	2.64	0.41
24:3:84:LYS:HA	24:3:84:LYS:HD3	1.85	0.41
25:a:9:ASN:HD22	29:P:43:GLU:HB3	1.86	0.41
29:P:51:ARG:HB2	29:P:53:TYR:CE1	2.56	0.41
30:R:37:ARG:HD3	30:R:37:ARG:H	1.86	0.41
34:E:14:MET:HE3	34:E:14:MET:HB3	1.86	0.41
34:E:102:ARG:HD3	34:E:102:ARG:HA	1.90	0.41
1:2:738:C:H5''	13:M:124:PRO:HB3	2.03	0.41
1:2:1146:A:O2'	1:2:1148:G:OP2	2.28	0.41
1:2:1174:G:H5'	1:2:1176:A:H1'	2.02	0.41
1:2:1196:G:H2'	1:2:1197:U:C6	2.56	0.41
1:2:1288:C:H2'	1:2:1289:C:H6	1.86	0.41
1:2:1372:G:H1'	1:2:1451:G:N2	2.35	0.41
1:2:1483:G:N7	13:M:127:ARG:NH2	2.68	0.41
2:A:91:ASP:OD1	2:A:91:ASP:C	2.64	0.41
3:B:56:LYS:HA	3:B:56:LYS:HD3	1.58	0.41
6:F:146:GLU:O	6:F:180:THR:HA	2.21	0.41
7:G:49:LYS:HZ3	7:G:89:ASP:HA	1.84	0.41
8:H:153:ASN:OD1	38:H:201:HOH:O	2.21	0.41
10:J:38:SER:HB3	10:J:59:TYR:HB3	2.02	0.41
11:K:6:LYS:HD3	11:K:93:PHE:CE1	2.55	0.41
11:K:83:ARG:HG2	11:K:84:MET:N	2.36	0.41
11:K:107:ASP:OD1	11:K:107:ASP:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:77:LEU:HD21	14:N:105:ILE:HD11	2.03	0.41
31:Z:189:ILE:CG2	31:Z:192:LYS:HG3	2.51	0.41
1:2:44:C:H3'	1:2:45:U:C5'	2.51	0.40
1:2:73:C:OP2	1:2:209:U:N3	2.40	0.40
1:2:161:U:H2'	1:2:162:A:C8	2.56	0.40
1:2:570:A:C5	1:2:571:C:C5	3.09	0.40
1:2:843:4AC:H5	1:2:843:4AC:O7	2.21	0.40
1:2:940:G:H21	1:2:1327:A:H5'	1.86	0.40
2:A:69:PHE:HB3	2:A:81:THR:OG1	2.22	0.40
7:G:141:ASN:ND2	7:G:147:PRO:HA	2.36	0.40
8:H:24:ASP:OD1	8:H:27:LEU:HD22	2.21	0.40
11:K:18:ARG:HB2	11:K:71:TYR:CE1	2.57	0.40
11:K:51:GLU:OE2	11:K:51:GLU:HA	2.19	0.40
15:O:120:ARG:NH1	15:O:126:LYS:O	2.54	0.40
20:V:52:ILE:HD12	20:V:52:ILE:HA	1.92	0.40
22:X:53:THR:H	22:X:74:GLU:CD	2.28	0.40
24:3:5:SER:O	24:3:5:SER:OG	2.35	0.40
24:3:117:ARG:HA	24:3:120:GLU:OE1	2.21	0.40
25:a:57:LEU:HD11	29:P:4:TYR:CD1	2.56	0.40
28:5:808:A:H3'	28:5:809:G:H8	1.85	0.40
30:R:3:SER:OG	30:R:4:LYS:N	2.55	0.40
33:c:43:ARG:HG3	33:c:44:ALA:N	2.36	0.40
1:2:14:C:H2'	1:2:15:OMU:H6	2.03	0.40
1:2:365:G:H2'	1:2:366:C:C6	2.56	0.40
1:2:506:A:P	5:D:36:ARG:HH21	2.44	0.40
1:2:794:A:H2'	1:2:795:C:C6	2.56	0.40
1:2:985:C:C2	1:2:986:U:C5	3.09	0.40
1:2:1070:C:C2	1:2:1071:C:C5	3.08	0.40
1:2:1111:C:H2'	1:2:1112:A:O4'	2.21	0.40
1:2:1290:C:C2	1:2:1291:U:C5	3.09	0.40
4:C:21:LYS:HE3	4:C:21:LYS:HB2	1.80	0.40
6:F:207:LEU:HD22	6:F:210:TRP:CZ2	2.56	0.40
8:H:156:LYS:HE2	8:H:160:GLU:CD	2.46	0.40
9:I:89:LEU:H	9:I:89:LEU:HD12	1.86	0.40
11:K:97:LYS:HA	11:K:100:GLU:HG3	2.02	0.40
18:T:71:LYS:HA	18:T:89:ALA:O	2.22	0.40
24:3:34:LYS:C	24:3:34:LYS:HD2	2.47	0.40
34:E:26:PRO:HG2	34:E:33:ILE:HG12	2.03	0.40
1:2:85:G:H2'	1:2:86:C:H6	1.87	0.40
1:2:104:G:H2'	1:2:105:U:C6	2.56	0.40
1:2:441:C:P	20:V:101:ARG:HH21	2.44	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:443:A:OP2	36:2:1565:SPM:N14	2.53	0.40
1:2:447:C:H4'	20:V:75:GLY:HA2	2.03	0.40
1:2:559:A:H2'	1:2:560:C:C6	2.56	0.40
1:2:822:C:H2'	1:2:823:A:C8	2.56	0.40
1:2:1134:G:OP1	17:S:5:TYR:HD1	2.05	0.40
1:2:1228:C:P	19:U:125:ARG:HH12	2.44	0.40
1:2:1253:A:OP1	36:2:1578:SPM:C11	2.70	0.40
7:G:46:VAL:CG1	7:G:81:VAL:HG23	2.52	0.40
8:H:6:LEU:HD21	8:H:8:LEU:HD13	2.03	0.40
12:L:41:LEU:HD12	12:L:71:LYS:HG2	2.04	0.40
15:O:78:TRP:CH2	19:U:40:ALA:HB2	2.55	0.40
15:O:88:SER:C	15:O:90:LEU:H	2.29	0.40
25:a:31:GLY:HA3	31:Z:69:ILE:HD11	2.03	0.40
1:2:503:G:H2'	1:2:504:C:C6	2.57	0.40
1:2:569:G:N3	1:2:569:G:H2'	2.36	0.40
1:2:787:A:H2'	1:2:788:G:O4'	2.20	0.40
1:2:945:U:H2'	1:2:946:U:C5	2.57	0.40
1:2:947:A:H5'	1:2:948:C:OP2	2.21	0.40
1:2:984:C:H2'	1:2:985:C:C6	2.57	0.40
1:2:1153:C:P	25:a:2:SER:HB2	2.62	0.40
1:2:1201:A:C8	1:2:1267:G:H1'	2.56	0.40
1:2:1466:4AC:O7	1:2:1466:4AC:H5	2.22	0.40
2:A:96:LEU:HB3	2:A:125:LEU:CD1	2.51	0.40
5:D:65:GLU:OE1	9:I:84:ARG:NH2	2.54	0.40
7:G:135:GLY:HA2	7:G:151:LYS:HZ2	1.87	0.40
7:G:204:GLU:OE1	7:G:204:GLU:N	2.26	0.40
8:H:115:THR:HA	8:H:116:ARG:CZ	2.51	0.40
8:H:149:ASP:OD1	8:H:149:ASP:N	2.53	0.40
10:J:34:PHE:HB3	10:J:95:ILE:CG1	2.51	0.40
11:K:25:ALA:HA	11:K:63:LYS:HZ3	1.87	0.40
11:K:121:GLU:HA	11:K:128:ALA:HA	2.03	0.40
12:L:97:ILE:HD12	12:L:98:GLU:H	1.86	0.40
16:Q:29:GLU:N	16:Q:29:GLU:CD	2.79	0.40
19:U:8:ALA:HB3	19:U:69:TYR:CE2	2.57	0.40
23:Y:40:LYS:HA	23:Y:40:LYS:HD2	1.84	0.40
24:3:27:LYS:CD	24:3:90:CYS:HB2	2.48	0.40
24:3:65:HIS:CD2	24:3:66:LEU:HD12	2.56	0.40
32:d:12:ARG:HD3	32:d:13:GLU:C	2.47	0.40
33:c:37:GLY:O	33:c:38:LYS:C	2.64	0.40
33:c:47:ILE:HG23	33:c:51:THR:CG2	2.51	0.40
34:E:93:TYR:HB2	34:E:109:ILE:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:72:G:C2	1:2:209:U:H1'	2.56	0.40
1:2:174:C:H2'	1:2:175:U:C6	2.57	0.40
1:2:822:C:C2	1:2:823:A:C8	3.10	0.40
2:A:140:LYS:HE3	2:A:140:LYS:HB2	1.53	0.40
4:C:14:PRO:HB2	4:C:23:ILE:HD12	2.02	0.40
12:L:7:ILE:HB	12:L:74:ILE:HB	2.02	0.40
17:S:14:LYS:HG3	17:S:15:GLU:N	2.35	0.40
19:U:57:TRP:CZ3	19:U:103:VAL:HG13	2.56	0.40
31:Z:159:LEU:HD22	31:Z:163:ILE:HG12	2.04	0.40
33:c:89:GLU:HB3	33:c:94:VAL:HG23	2.03	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	
2	A	184/208 (88%)	179 (97%)	5 (3%)	0	100	100
3	B	213/231 (92%)	208 (98%)	5 (2%)	0	100	100
4	C	56/65 (86%)	54 (96%)	2 (4%)	0	100	100
5	D	164/181 (91%)	161 (98%)	3 (2%)	0	100	100
6	F	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
7	G	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
8	H	190/193 (98%)	183 (96%)	7 (4%)	0	100	100
9	I	130/133 (98%)	126 (97%)	4 (3%)	0	100	100
10	J	125/133 (94%)	123 (98%)	2 (2%)	0	100	100
11	K	131/137 (96%)	122 (93%)	9 (7%)	0	100	100
12	L	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
13	M	125/132 (95%)	114 (91%)	11 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	144/147 (98%)	137 (95%)	7 (5%)	0	100	100
15	O	138/165 (84%)	132 (96%)	6 (4%)	0	100	100
16	Q	143/152 (94%)	143 (100%)	0	0	100	100
17	S	64/79 (81%)	62 (97%)	2 (3%)	0	100	100
18	T	126/140 (90%)	126 (100%)	0	0	100	100
19	U	152/158 (96%)	147 (97%)	5 (3%)	0	100	100
20	V	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
21	W	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
22	X	65/83 (78%)	57 (88%)	8 (12%)	0	100	100
23	Y	47/75 (63%)	39 (83%)	8 (17%)	0	100	100
24	3	115/127 (91%)	99 (86%)	16 (14%)	0	100	100
25	a	69/72 (96%)	63 (91%)	5 (7%)	1 (1%)	9	34
26	e	41/52 (79%)	40 (98%)	1 (2%)	0	100	100
29	P	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
30	R	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
31	Z	194/229 (85%)	189 (97%)	5 (3%)	0	100	100
32	d	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
33	c	107/110 (97%)	99 (92%)	8 (8%)	0	100	100
34	E	236/239 (99%)	228 (97%)	8 (3%)	0	100	100
All	All	3875/4197 (92%)	3709 (96%)	165 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	a	58	LYS

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	
2	A	168/184 (91%)	162 (96%)	6 (4%)	31	63
3	B	182/198 (92%)	180 (99%)	2 (1%)	65	82
4	C	51/58 (88%)	50 (98%)	1 (2%)	48	75
5	D	147/158 (93%)	146 (99%)	1 (1%)	76	87
6	F	180/184 (98%)	180 (100%)	0	100	100
7	G	186/187 (100%)	182 (98%)	4 (2%)	45	73
8	H	166/167 (99%)	162 (98%)	4 (2%)	43	72
9	I	113/114 (99%)	113 (100%)	0	100	100
10	J	104/110 (94%)	103 (99%)	1 (1%)	68	83
11	K	109/113 (96%)	106 (97%)	3 (3%)	38	69
12	L	93/94 (99%)	89 (96%)	4 (4%)	26	58
13	M	93/98 (95%)	90 (97%)	3 (3%)	34	65
14	N	122/123 (99%)	121 (99%)	1 (1%)	73	86
15	O	121/142 (85%)	120 (99%)	1 (1%)	73	86
16	Q	125/129 (97%)	125 (100%)	0	100	100
17	S	63/75 (84%)	63 (100%)	0	100	100
18	T	116/126 (92%)	112 (97%)	4 (3%)	32	64
19	U	134/138 (97%)	131 (98%)	3 (2%)	45	73
20	V	92/99 (93%)	90 (98%)	2 (2%)	45	73
21	W	57/58 (98%)	56 (98%)	1 (2%)	51	76
22	X	58/73 (80%)	56 (97%)	2 (3%)	32	64
23	Y	43/65 (66%)	43 (100%)	0	100	100
24	3	97/105 (92%)	95 (98%)	2 (2%)	47	74
25	a	61/62 (98%)	56 (92%)	5 (8%)	10	35
26	e	40/46 (87%)	39 (98%)	1 (2%)	42	71
29	P	45/46 (98%)	45 (100%)	0	100	100
30	R	101/102 (99%)	100 (99%)	1 (1%)	68	83
31	Z	163/195 (84%)	159 (98%)	4 (2%)	42	71
32	d	63/65 (97%)	47 (75%)	16 (25%)	0	3
33	c	95/96 (99%)	89 (94%)	6 (6%)	16	46
34	E	214/215 (100%)	211 (99%)	3 (1%)	59	80
All	All	3402/3625 (94%)	3321 (98%)	81 (2%)	43	72

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	18	LYS
2	A	60	PHE
2	A	87	GLU
2	A	105	ASN
2	A	127	THR
2	A	157	ASP
3	B	206	LEU
3	B	227	MET
4	C	59	ASN
5	D	83	LEU
7	G	54	LEU
7	G	56	VAL
7	G	141	ASN
7	G	152	ILE
8	H	5	ASN
8	H	8	LEU
8	H	84	LEU
8	H	167	ILE
10	J	77	LYS
11	K	7	LEU
11	K	80	ASP
11	K	99	LEU
12	L	34	GLU
12	L	35	MET
12	L	64	LYS
12	L	94	ASP
13	M	84	TYR
13	M	107	ILE
13	M	132	VAL
14	N	55	LEU
15	O	110	GLU
18	T	11	ASN
18	T	20	ASP
18	T	31	ILE
18	T	80	LEU
19	U	55	ASP
19	U	151	THR
19	U	156	TYR
20	V	102	ASP
20	V	108	LYS
21	W	17	LEU
22	X	12	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	X	71	THR
24	3	19	VAL
24	3	36	THR
25	a	40	LYS
25	a	41	CYS
25	a	57	LEU
25	a	69	VAL
25	a	72	LEU
26	e	29	VAL
30	R	94	ILE
31	Z	20	GLU
31	Z	69	ILE
31	Z	84	THR
31	Z	190	GLU
32	d	5	LYS
32	d	6	ILE
32	d	7	LYS
32	d	8	LEU
32	d	9	SER
32	d	10	SER
32	d	12	ARG
32	d	13	GLU
32	d	14	VAL
32	d	15	GLU
32	d	30	THR
32	d	33	THR
32	d	52	LEU
32	d	56	VAL
32	d	65	LEU
32	d	70	LYS
33	c	9	ILE
33	c	11	THR
33	c	35	LYS
33	c	48	ASP
33	c	74	SER
33	c	92	ASN
34	E	8	GLU
34	E	59	ILE
34	E	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	62	GLN
2	A	105	ASN
3	B	187	ASN
4	C	36	ASN
6	F	98	GLN
6	F	125	GLN
7	G	142	GLN
8	H	71	ASN
8	H	76	HIS
9	I	64	GLN
9	I	70	ASN
10	J	52	ASN
11	K	33	ASN
12	L	100	GLN
13	M	18	GLN
14	N	66	ASN
14	N	95	ASN
15	O	4	GLN
15	O	121	HIS
19	U	102	HIS
20	V	59	GLN
21	W	23	ASN
23	Y	32	ASN
24	3	119	ASN
25	a	25	ASN
26	e	26	HIS
31	Z	62	ASN
32	d	55	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1442/1497 (96%)	226 (15%)	4 (0%)
27	4	76/77 (98%)	13 (17%)	1 (1%)
28	5	19/28 (67%)	10 (52%)	0
All	All	1537/1602 (95%)	249 (16%)	5 (0%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	33	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	34	C
1	2	43	G
1	2	45	U
1	2	47	A
1	2	60	G
1	2	67	C
1	2	68	C
1	2	70	G
1	2	71	G
1	2	72	G
1	2	73	C
1	2	74	A
1	2	75	A
1	2	76	G
1	2	89	A
1	2	99	A
1	2	101	C
1	2	110	A
1	2	111	A
1	2	112	C
1	2	115	A
1	2	122	G
1	2	138	G
1	2	144	C
1	2	193	A
1	2	195	A
1	2	196	G
1	2	208	A
1	2	209	U
1	2	211	C
1	2	212	C
1	2	213	C
1	2	214	C
1	2	215	G
1	2	225	G
1	2	245	C
1	2	246	OMC
1	2	248	A
1	2	250	C
1	2	252	G
1	2	256	G
1	2	257	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	267	A
1	2	271	G
1	2	272	C
1	2	278	A
1	2	286	A
1	2	294	G
1	2	311	A
1	2	320	U
1	2	321	U
1	2	333	C
1	2	334	A
1	2	335	A
1	2	336	G
1	2	349	A
1	2	357	C
1	2	358	A
1	2	359	C
1	2	372	G
1	2	377	C
1	2	378	A
1	2	389	G
1	2	395	G
1	2	402	A
1	2	411	G
1	2	417	G
1	2	418	U
1	2	419	A
1	2	420	A
1	2	429	U
1	2	453	A
1	2	454	A
1	2	470	U
1	2	471	C
1	2	477	U
1	2	480	G
1	2	490	U
1	2	491	A
1	2	506	A
1	2	522	A
1	2	523	C
1	2	531	A
1	2	532	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	535	C
1	2	536	G
1	2	555	A
1	2	569	G
1	2	601	A
1	2	609	G
1	2	612	A
1	2	624	A
1	2	634	U
1	2	647	G
1	2	677	A
1	2	682	U
1	2	707	G
1	2	708	C
1	2	712	A
1	2	714	G
1	2	740	A
1	2	741	A
1	2	752	U
1	2	753	A
1	2	774	A
1	2	776	C
1	2	802	U
1	2	805	G
1	2	806	A
1	2	828	A
1	2	835	A
1	2	853	G
1	2	866	A
1	2	877	A
1	2	889	G
1	2	897	C
1	2	924	U
1	2	930	C4J
1	2	931	C
1	2	933	A
1	2	935	G
1	2	939	G
1	2	941	A
1	2	946	U
1	2	957	A
1	2	960	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	966	U
1	2	967	G
1	2	969	C
1	2	982	G
1	2	983	A
1	2	988	G
1	2	989	C
1	2	990	C
1	2	991	U
1	2	992	G
1	2	995	U
1	2	996	C
1	2	997	G
1	2	1002	G
1	2	1023	C
1	2	1051	G
1	2	1052	U
1	2	1058	A
1	2	1059	A
1	2	1080	A
1	2	1081	G
1	2	1086	U
1	2	1094	U
1	2	1096	U
1	2	1097	C
1	2	1098	C
1	2	1099	G
1	2	1101	G
1	2	1103	C
1	2	1106	G
1	2	1107	A
1	2	1113	C
1	2	1118	G
1	2	1121	A
1	2	1123	U
1	2	1147	G
1	2	1157	G
1	2	1159	A
1	2	1160	G
1	2	1175	A
1	2	1187	C
1	2	1188	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1189	C
1	2	1190	A
1	2	1199	A
1	2	1201	A
1	2	1211	A
1	2	1220	U
1	2	1221	U
1	2	1222	C
1	2	1226	C
1	2	1244	A
1	2	1248	C
1	2	1249	U
1	2	1251	A
1	2	1261	G
1	2	1264	G
1	2	1265	U
1	2	1267	G
1	2	1270	A
1	2	1281	A
1	2	1284	C
1	2	1286	C
1	2	1300	A
1	2	1309	U
1	2	1317	G
1	2	1328	A
1	2	1334	G
1	2	1338	A
1	2	1358	A
1	2	1361	C
1	2	1371	C
1	2	1373	C
1	2	1375	C
1	2	1376	C
1	2	1381	G
1	2	1437	G
1	2	1440	A
1	2	1441	G
1	2	1442	G
1	2	1443	G
1	2	1444	G
1	2	1448	G
1	2	1449	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1450	A
1	2	1453	C
1	2	1454	G
1	2	1455	U
1	2	1456	A
1	2	1459	A
1	2	1460	A
1	2	1461	G
1	2	1463	U
1	2	1474	G
1	2	1476	A
1	2	1486	G
1	2	1487	G
1	2	1493	C
27	4	8	4SU
27	4	9	G
27	4	16	C
27	4	17(A)	U
27	4	18	G
27	4	20	H2U
27	4	21	A
27	4	22	G
27	4	46	A
27	4	47	U
27	4	49	G
27	4	74	C
27	4	75	C
28	5	807	G
28	5	808	A
28	5	809	G
28	5	812	G
28	5	813	A
28	5	815	U
28	5	818	A
28	5	822	C
28	5	823	C
28	5	824	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	256	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1187	C
1	2	1188	G
1	2	1436	U
27	4	74	C

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

38 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMC	2	710	1	19,22,23	0.83	0	26,31,34	0.91	1 (3%)
27	H2U	4	20	27	18,21,22	0.30	0	21,30,33	0.43	0
1	OMC	2	1366	1	19,22,23	0.81	0	26,31,34	0.77	0
1	4AC	2	1477	1	21,24,25	1.04	2 (9%)	29,34,37	1.53	5 (17%)
1	OMC	2	246	1	19,22,23	0.84	0	26,31,34	0.99	1 (3%)
1	MA6	2	1475	1	23,26,27	1.48	4 (17%)	34,38,41	2.08	10 (29%)
1	4AC	2	843	1	21,24,25	1.05	2 (9%)	29,34,37	1.34	4 (13%)
1	OMG	2	1018	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
27	OMC	4	32	27	19,22,23	0.86	0	26,31,34	1.04	2 (7%)
1	OMC	2	313	1	19,22,23	0.84	0	26,31,34	0.85	0
1	C4J	2	930	1	24,29,30	0.67	1 (4%)	29,42,45	0.57	0
27	4SU	4	8	27	18,21,22	0.27	0	26,30,33	0.34	0
27	5MU	4	54	27	19,22,23	1.37	5 (26%)	28,32,35	2.07	8 (28%)
1	4AC	2	1478	1	21,24,25	1.00	2 (9%)	29,34,37	1.40	4 (13%)
1	OMG	2	337	1	23,26,27	1.21	3 (13%)	33,38,41	1.96	6 (18%)
1	OMG	2	905	1	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
1	OMC	2	512	1	19,22,23	0.82	0	26,31,34	0.81	0
1	OMG	2	672	1	23,26,27	1.23	3 (13%)	33,38,41	1.94	6 (18%)
1	6MZ	2	1457	1,35	22,25,26	1.47	4 (18%)	30,36,39	2.21	10 (33%)
1	5MC	2	1368	1	18,22,23	0.91	2 (11%)	26,32,35	1.04	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	2	1467	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	OMC	2	1060	1	19,22,23	0.81	0	26,31,34	0.72	0
1	OMG	2	865	1	23,26,27	1.23	3 (13%)	33,38,41	1.98	7 (21%)
1	OMU	2	1032	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	4 (15%)
1	OMG	2	399	1	23,26,27	1.24	3 (13%)	33,38,41	1.91	6 (18%)
1	OMC	2	538	1	19,22,23	0.81	0	26,31,34	0.87	1 (3%)
1	OMC	2	481	1	19,22,23	0.88	1 (5%)	26,31,34	0.98	1 (3%)
1	OMU	2	15	1	19,22,23	1.21	3 (15%)	26,31,34	1.72	4 (15%)
27	PSU	4	55	27	18,21,22	1.32	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	2	494	1	22,25,26	1.45	4 (18%)	31,36,39	2.09	9 (29%)
1	OMG	2	1061	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	OMU	2	1344	1	19,22,23	1.22	3 (15%)	26,31,34	1.70	6 (23%)
1	OMC	2	113	1	19,22,23	0.83	0	26,31,34	0.84	0
1	OMG	2	1194	1	23,26,27	1.19	3 (13%)	33,38,41	1.96	7 (21%)
1	OMG	2	926	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	OMU	2	52	1	19,22,23	1.24	3 (15%)	26,31,34	1.72	4 (15%)
1	OMG	2	546	1	23,26,27	1.20	3 (13%)	33,38,41	1.90	6 (18%)
1	4AC	2	1466	1	21,24,25	1.00	2 (9%)	29,34,37	1.29	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2	710	1	-	0/9/27/28	0/2/2/2
27	H2U	4	20	27	-	3/7/38/39	0/2/2/2
1	OMC	2	1366	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1477	1	-	0/11/29/30	0/2/2/2
1	OMC	2	246	1	-	3/9/27/28	0/2/2/2
1	MA6	2	1475	1	-	0/11/29/30	0/3/3/3
1	4AC	2	843	1	-	0/11/29/30	0/2/2/2
1	OMG	2	1018	1	-	0/9/27/28	0/3/3/3
27	OMC	4	32	27	-	3/9/27/28	0/2/2/2
1	OMC	2	313	1	-	0/9/27/28	0/2/2/2
1	C4J	2	930	1	-	2/16/34/35	0/2/2/2
27	4SU	4	8	27	-	0/7/25/26	0/2/2/2
27	5MU	4	54	27	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	1478	1	-	0/11/29/30	0/2/2/2
1	OMG	2	337	1	-	1/9/27/28	0/3/3/3
1	OMG	2	905	1	-	0/9/27/28	0/3/3/3
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2
1	OMG	2	672	1	-	0/9/27/28	0/3/3/3
1	6MZ	2	1457	1,35	-	0/9/27/28	0/3/3/3
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2
1	OMG	2	865	1	-	0/9/27/28	0/3/3/3
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2
1	OMG	2	399	1	-	0/9/27/28	0/3/3/3
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2
1	OMU	2	15	1	-	0/9/27/28	0/2/2/2
27	PSU	4	55	27	-	2/7/25/26	0/2/2/2
1	A2M	2	494	1	-	0/9/27/28	0/3/3/3
1	OMG	2	1061	1	-	0/9/27/28	0/3/3/3
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	OMC	2	113	1	-	0/9/27/28	0/2/2/2
1	OMG	2	1194	1	-	0/9/27/28	0/3/3/3
1	OMG	2	926	1	-	0/9/27/28	0/3/3/3
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	OMG	2	546	1	-	0/9/27/28	0/3/3/3
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1475	MA6	C5-C4	4.57	1.47	1.39
1	2	1457	6MZ	C5-C4	4.49	1.47	1.39
1	2	494	A2M	C5-C4	4.30	1.47	1.39
27	4	55	PSU	C6-C5	3.22	1.39	1.35
1	2	865	OMG	C5-C4	3.10	1.47	1.38
1	2	672	OMG	C5-C4	3.05	1.47	1.38
1	2	1061	OMG	C5-C4	2.98	1.47	1.38
1	2	926	OMG	C5-C4	2.98	1.47	1.38
1	2	905	OMG	C5-C4	2.96	1.47	1.38
1	2	399	OMG	C5-C4	2.96	1.47	1.38
1	2	546	OMG	C5-C4	2.95	1.47	1.38
1	2	1018	OMG	C5-C4	2.95	1.47	1.38
1	2	337	OMG	C5-C4	2.93	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	843	4AC	C5-C4	2.91	1.47	1.40
1	2	1194	OMG	C5-C4	2.88	1.46	1.38
1	2	1477	4AC	C5-C4	2.81	1.46	1.40
1	2	930	C4J	O4'-C1'	-2.80	1.40	1.43
1	2	1466	4AC	C5-C4	2.77	1.46	1.40
1	2	1475	MA6	C5-C6	2.76	1.48	1.41
1	2	1478	4AC	C5-C4	2.76	1.46	1.40
1	2	1467	4AC	C5-C4	2.75	1.46	1.40
1	2	1457	6MZ	C5-C6	2.74	1.49	1.41
1	2	399	OMG	C6-N1	-2.73	1.33	1.38
1	2	1018	OMG	C6-N1	-2.68	1.33	1.38
1	2	337	OMG	C6-N1	-2.68	1.33	1.38
1	2	672	OMG	C6-N1	-2.65	1.33	1.38
1	2	52	OMU	C4-N3	-2.63	1.33	1.38
1	2	1061	OMG	C6-N1	-2.62	1.34	1.38
27	4	55	PSU	C4-N3	-2.62	1.34	1.38
1	2	905	OMG	C6-N1	-2.62	1.34	1.38
1	2	1344	OMU	C4-N3	-2.61	1.33	1.38
1	2	1032	OMU	C4-N3	-2.60	1.33	1.38
1	2	926	OMG	C6-N1	-2.59	1.34	1.38
1	2	494	A2M	C5-C6	2.56	1.48	1.41
1	2	1194	OMG	C6-N1	-2.55	1.34	1.38
27	4	54	5MU	C6-C5	2.54	1.38	1.34
1	2	15	OMU	C4-N3	-2.53	1.34	1.38
27	4	54	5MU	C4-N3	-2.51	1.34	1.38
1	2	546	OMG	C6-N1	-2.51	1.34	1.38
1	2	865	OMG	C6-N1	-2.49	1.34	1.38
1	2	843	4AC	C4-N3	-2.44	1.28	1.32
1	2	399	OMG	C5-N7	-2.44	1.34	1.39
1	2	1368	5MC	C6-C5	2.40	1.38	1.34
27	4	54	5MU	C4-C5	2.40	1.48	1.44
1	2	1467	4AC	C4-N3	-2.39	1.28	1.32
1	2	494	A2M	C5-N7	-2.37	1.34	1.39
1	2	52	OMU	C2-N3	-2.34	1.33	1.38
1	2	1368	5MC	C6-N1	-2.32	1.34	1.38
1	2	672	OMG	C5-N7	-2.31	1.34	1.39
1	2	1032	OMU	C2-N3	-2.29	1.33	1.38
1	2	15	OMU	C2-N3	-2.28	1.33	1.38
1	2	1457	6MZ	C8-N7	2.28	1.35	1.31
27	4	54	5MU	C6-N1	-2.28	1.34	1.38
1	2	1018	OMG	C5-N7	-2.27	1.34	1.39
1	2	926	OMG	C5-N7	-2.26	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	337	OMG	C5-N7	-2.26	1.34	1.39
1	2	1475	MA6	C8-N7	2.25	1.35	1.31
1	2	494	A2M	C8-N7	2.25	1.35	1.31
1	2	1466	4AC	C4-N3	-2.24	1.28	1.32
1	2	1194	OMG	C5-N7	-2.24	1.34	1.39
1	2	1061	OMG	C5-N7	-2.21	1.34	1.39
1	2	905	OMG	C5-N7	-2.18	1.34	1.39
1	2	1344	OMU	C2-N3	-2.17	1.34	1.38
1	2	15	OMU	C5-C4	-2.16	1.38	1.43
1	2	1475	MA6	C5-N7	-2.16	1.34	1.39
1	2	1344	OMU	C5-C4	-2.15	1.38	1.43
1	2	865	OMG	C5-N7	-2.15	1.34	1.39
1	2	1457	6MZ	C5-N7	-2.10	1.35	1.39
1	2	481	OMC	C6-C5	2.10	1.39	1.35
1	2	1477	4AC	C4-N3	-2.10	1.29	1.32
1	2	546	OMG	C5-N7	-2.08	1.35	1.39
27	4	54	5MU	C2-N1	2.08	1.41	1.38
1	2	1032	OMU	C5-C4	-2.07	1.39	1.43
1	2	1478	4AC	C4-N3	-2.07	1.29	1.32
1	2	52	OMU	C5-C4	-2.05	1.39	1.43

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	672	OMG	C5-C4-N3	-6.28	118.27	128.46
1	2	494	A2M	C5-C4-N3	-6.24	118.60	126.75
1	2	399	OMG	C5-C4-N3	-6.14	118.50	128.46
1	2	1018	OMG	C5-C4-N3	-6.11	118.55	128.46
1	2	1061	OMG	C5-C4-N3	-6.09	118.58	128.46
1	2	926	OMG	C5-C4-N3	-6.04	118.66	128.46
1	2	865	OMG	C5-C4-N3	-6.04	118.66	128.46
1	2	337	OMG	C5-C4-N3	-6.03	118.68	128.46
1	2	905	OMG	C5-C4-N3	-6.02	118.69	128.46
1	2	1194	OMG	C5-C4-N3	-6.02	118.70	128.46
1	2	1457	6MZ	C5-C4-N3	-5.96	118.98	126.75
27	4	55	PSU	N1-C2-N3	5.78	121.68	115.13
1	2	1475	MA6	C5-C4-N3	-5.69	119.32	126.75
1	2	546	OMG	C5-C4-N3	-5.64	119.31	128.46
27	4	54	5MU	C4-N3-C2	-5.11	120.74	127.35
1	2	1194	OMG	C2-N3-C4	5.01	121.22	112.30
1	2	672	OMG	C2-N3-C4	4.90	121.02	112.30
1	2	337	OMG	C2-N3-C4	4.89	121.02	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	494	A2M	N3-C4-N9	4.87	135.11	127.08
1	2	1061	OMG	C2-N3-C4	4.87	120.98	112.30
1	2	905	OMG	C2-N3-C4	4.87	120.97	112.30
1	2	926	OMG	C2-N3-C4	4.86	120.95	112.30
1	2	865	OMG	C2-N3-C4	4.86	120.95	112.30
1	2	399	OMG	C2-N3-C4	4.81	120.87	112.30
1	2	1018	OMG	C2-N3-C4	4.81	120.87	112.30
27	4	54	5MU	N3-C2-N1	4.74	121.18	114.89
1	2	672	OMG	N9-C4-N3	4.70	135.38	125.94
1	2	546	OMG	C2-N3-C4	4.66	120.60	112.30
1	2	1018	OMG	N9-C4-N3	4.60	135.18	125.94
1	2	399	OMG	N9-C4-N3	4.58	135.13	125.94
1	2	1032	OMU	C4-N3-C2	-4.58	120.54	126.58
1	2	1475	MA6	C2-N1-C6	4.57	122.56	111.75
1	2	1061	OMG	N9-C4-N3	4.53	135.04	125.94
1	2	926	OMG	N9-C4-N3	4.53	135.03	125.94
1	2	1478	4AC	O7-C7-N4	4.52	129.13	121.82
1	2	1467	4AC	O7-C7-N4	4.51	129.11	121.82
1	2	1194	OMG	N9-C4-N3	4.51	134.99	125.94
1	2	865	OMG	N9-C4-N3	4.50	134.97	125.94
1	2	1477	4AC	O7-C7-N4	4.48	129.08	121.82
1	2	52	OMU	C4-N3-C2	-4.48	120.68	126.58
1	2	15	OMU	C4-N3-C2	-4.48	120.68	126.58
1	2	905	OMG	N9-C4-N3	4.44	134.85	125.94
1	2	1457	6MZ	C6-C5-N7	4.42	137.18	132.39
1	2	1466	4AC	O7-C7-N4	4.42	128.97	121.82
1	2	1457	6MZ	N3-C4-N9	4.37	134.28	127.08
1	2	337	OMG	N9-C4-N3	4.36	134.69	125.94
27	4	54	5MU	C5-C4-N3	4.35	119.02	115.31
1	2	1344	OMU	C4-N3-C2	-4.33	120.86	126.58
1	2	1475	MA6	N3-C4-N9	4.30	134.16	127.08
1	2	843	4AC	O7-C7-N4	4.26	128.71	121.82
1	2	1344	OMU	N3-C2-N1	4.13	120.38	114.89
1	2	52	OMU	N3-C2-N1	4.07	120.30	114.89
1	2	546	OMG	N9-C4-N3	4.07	134.10	125.94
27	4	55	PSU	C4-N3-C2	-3.98	120.60	126.34
1	2	1032	OMU	N3-C2-N1	3.94	120.12	114.89
1	2	1457	6MZ	C4-C5-N7	-3.92	105.85	110.62
1	2	1457	6MZ	C2-N3-C4	3.91	120.98	111.75
1	2	494	A2M	C2-N3-C4	3.88	120.92	111.75
1	2	15	OMU	N3-C2-N1	3.82	119.96	114.89
1	2	15	OMU	C5-C4-N3	3.79	120.51	114.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1032	OMU	C5-C4-N3	3.78	120.49	114.84
1	2	1475	MA6	C4-C5-N7	-3.75	106.05	110.62
1	2	1475	MA6	C2-N3-C4	3.72	120.54	111.75
1	2	52	OMU	C5-C4-N3	3.64	120.29	114.84
27	4	54	5MU	O4-C4-C5	-3.64	120.69	124.90
27	4	54	5MU	C5-C6-N1	-3.59	119.65	123.34
1	2	1344	OMU	C5-C4-N3	3.53	120.12	114.84
1	2	1477	4AC	N4-C4-N3	3.51	119.74	113.85
1	2	546	OMG	C6-C5-N7	3.44	136.64	130.25
1	2	1478	4AC	N4-C4-N3	3.41	119.58	113.85
1	2	1457	6MZ	N1-C2-N3	-3.37	123.33	128.60
1	2	1467	4AC	CM7-C7-N4	-3.37	109.47	115.29
1	2	905	OMG	C6-C5-N7	3.33	136.43	130.25
1	2	337	OMG	C6-C5-N7	3.31	136.41	130.25
1	2	1477	4AC	C5-C4-N4	-3.31	117.17	122.92
1	2	15	OMU	O4-C4-C5	-3.30	119.35	125.16
1	2	865	OMG	C6-C5-N7	3.27	136.33	130.25
1	2	1194	OMG	C6-C5-N7	3.22	136.24	130.25
1	2	1475	MA6	N1-C2-N3	-3.22	123.56	128.60
1	2	1061	OMG	C6-C5-N7	3.22	136.24	130.25
1	2	494	A2M	C4-C5-N7	-3.21	106.71	110.62
27	4	55	PSU	O2-C2-N1	-3.20	119.27	122.79
1	2	926	OMG	C6-C5-N7	3.19	136.18	130.25
1	2	1478	4AC	C5-C4-N4	-3.18	117.39	122.92
1	2	494	A2M	N3-C2-N1	-3.15	123.67	128.60
1	2	1368	5MC	C5-C6-N1	-3.14	120.11	123.34
1	2	1457	6MZ	C5-N7-C8	3.11	107.92	103.51
1	2	1032	OMU	O4-C4-C5	-3.11	119.70	125.16
1	2	1018	OMG	C6-C5-N7	3.09	136.00	130.25
1	2	52	OMU	O4-C4-C5	-3.04	119.82	125.16
1	2	1466	4AC	N4-C4-N3	3.03	118.94	113.85
1	2	672	OMG	C6-C5-N7	3.02	135.87	130.25
1	2	1475	MA6	C5-N7-C8	3.02	107.80	103.51
1	2	399	OMG	C6-C5-N7	3.02	135.86	130.25
1	2	1344	OMU	O4-C4-C5	-3.00	119.88	125.16
1	2	865	OMG	C2'-C1'-N9	-2.97	108.45	114.22
1	2	1467	4AC	C5-C4-N4	-2.93	117.82	122.92
1	2	1467	4AC	N4-C4-N3	2.85	118.64	113.85
27	4	32	OMC	O2-C2-N3	-2.75	117.85	122.33
1	2	494	A2M	C5-N7-C8	2.74	107.40	103.51
1	2	1466	4AC	C5-C4-N4	-2.72	118.19	122.92
1	2	1475	MA6	C4-N9-C8	2.72	108.68	105.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	843	4AC	C5-C4-N4	-2.70	118.22	122.92
1	2	843	4AC	N4-C4-N3	2.70	118.39	113.85
1	2	843	4AC	CM7-C7-N4	-2.69	110.63	115.29
1	2	905	OMG	C4-C5-N7	-2.67	106.50	110.72
1	2	337	OMG	C4-C5-N7	-2.65	106.52	110.72
1	2	546	OMG	C4-C5-N7	-2.65	106.53	110.72
1	2	865	OMG	C4-C5-N7	-2.64	106.53	110.72
1	2	1478	4AC	CM7-C7-N4	-2.64	110.73	115.29
1	2	1477	4AC	CM7-C7-N4	-2.62	110.76	115.29
1	2	1061	OMG	C4-C5-N7	-2.61	106.59	110.72
1	2	1466	4AC	CM7-C7-N4	-2.60	110.80	115.29
1	2	1457	6MZ	C4-N9-C8	2.59	108.53	105.73
1	2	672	OMG	C4-C5-N7	-2.58	106.64	110.72
1	2	246	OMC	O2-C2-N3	-2.56	118.17	122.33
1	2	1018	OMG	C4-C5-N7	-2.55	106.68	110.72
1	2	926	OMG	C4-C5-N7	-2.55	106.69	110.72
1	2	399	OMG	C4-C5-N7	-2.52	106.73	110.72
1	2	1194	OMG	C4-C5-N7	-2.50	106.76	110.72
1	2	494	A2M	C4-N9-C8	2.50	108.44	105.73
27	4	54	5MU	O2-C2-N1	-2.45	119.52	122.79
1	2	1368	5MC	C5-C4-N3	-2.42	119.06	121.67
27	4	54	5MU	C5M-C5-C4	2.34	121.35	118.77
1	2	1194	OMG	O6-C6-C5	-2.23	120.68	126.60
1	2	1477	4AC	C1'-N1-C2	2.21	123.35	118.42
1	2	1475	MA6	C6-C5-N7	2.20	136.97	133.28
1	2	1018	OMG	O6-C6-C5	-2.19	120.79	126.60
27	4	32	OMC	C1'-N1-C2	2.17	123.27	118.42
1	2	1457	6MZ	C2-N1-C6	2.17	122.54	115.25
1	2	1457	6MZ	N9-C8-N7	-2.17	110.95	113.91
1	2	1475	MA6	N9-C8-N7	-2.17	110.95	113.91
1	2	1061	OMG	O6-C6-C5	-2.16	120.87	126.60
1	2	926	OMG	O6-C6-C5	-2.14	120.92	126.60
1	2	865	OMG	O6-C6-C5	-2.12	120.99	126.60
1	2	710	OMC	O2-C2-N3	-2.12	118.89	122.33
1	2	494	A2M	C6-C5-N7	2.11	135.95	132.02
1	2	1344	OMU	C1'-N1-C2	2.11	121.38	117.57
1	2	905	OMG	O6-C6-C5	-2.10	121.02	126.60
1	2	1344	OMU	O2-C2-N1	-2.09	120.01	122.79
1	2	672	OMG	O6-C6-C5	-2.09	121.07	126.60
1	2	546	OMG	O6-C6-C5	-2.07	121.12	126.60
1	2	399	OMG	O6-C6-C5	-2.06	121.13	126.60
27	4	54	5MU	C5M-C5-C6	-2.06	120.10	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	538	OMC	O2-C2-N3	-2.03	119.02	122.33
1	2	481	OMC	O2-C2-N3	-2.02	119.05	122.33
1	2	494	A2M	N9-C8-N7	-2.01	111.17	113.91
1	2	337	OMG	O6-C6-C5	-2.00	121.28	126.60
1	2	1194	OMG	C5-C6-N1	2.00	118.27	113.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	246	OMC	C3'-C4'-C5'-O5'
27	4	20	H2U	O4'-C1'-N1-C6
1	2	930	C4J	C4'-C5'-O5'-P
1	2	246	OMC	O4'-C4'-C5'-O5'
27	4	20	H2U	O4'-C1'-N1-C2
1	2	930	C4J	C3'-C4'-C5'-O5'
27	4	20	H2U	C4'-C5'-O5'-P
1	2	337	OMG	C4'-C5'-O5'-P
27	4	32	OMC	C3'-C2'-O2'-CM2
27	4	32	OMC	C2'-C1'-N1-C6
27	4	55	PSU	O4'-C1'-C5-C4
1	2	246	OMC	C2'-C1'-N1-C2
27	4	55	PSU	O4'-C1'-C5-C6
27	4	32	OMC	C2'-C1'-N1-C2

There are no ring outliers.

28 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	710	OMC	1	0
27	4	20	H2U	1	0
1	2	1366	OMC	2	0
1	2	1477	4AC	1	0
1	2	246	OMC	2	0
1	2	1475	MA6	1	0
1	2	843	4AC	2	0
1	2	1018	OMG	1	0
27	4	32	OMC	1	0
1	2	1478	4AC	1	0
1	2	337	OMG	1	0
1	2	512	OMC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	672	OMG	2	0
1	2	1368	5MC	1	0
1	2	1467	4AC	1	0
1	2	1060	OMC	2	0
1	2	865	OMG	1	0
1	2	1032	OMU	1	0
1	2	399	OMG	1	0
1	2	538	OMC	1	0
1	2	481	OMC	1	0
1	2	15	OMU	1	0
1	2	1061	OMG	1	0
1	2	1344	OMU	2	0
1	2	113	OMC	2	0
1	2	1194	OMG	1	0
1	2	926	OMG	1	0
1	2	1466	4AC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 61 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
36	SPM	2	1570	-	13,13,13	0.09	0	12,12,12	0.11	0
36	SPM	2	1553	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1559	-	13,13,13	0.12	0	12,12,12	0.10	0
36	SPM	2	1563	-	13,13,13	0.08	0	12,12,12	0.12	0
36	SPM	2	1555	-	13,13,13	0.12	0	12,12,12	0.09	0
36	SPM	2	1565	-	13,13,13	0.09	0	12,12,12	0.10	0
36	SPM	2	1569	-	13,13,13	0.12	0	12,12,12	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	SPM	2	1551	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1568	-	13,13,13	0.11	0	12,12,12	0.08	0
36	SPM	2	1556	-	13,13,13	0.09	0	12,12,12	0.12	0
36	SPM	2	1557	-	13,13,13	0.10	0	12,12,12	0.09	0
36	SPM	2	1574	-	13,13,13	0.12	0	12,12,12	0.06	0
36	SPM	2	1548	-	13,13,13	0.08	0	12,12,12	0.11	0
36	SPM	2	1552	-	13,13,13	0.07	0	12,12,12	0.12	0
36	SPM	2	1566	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1577	-	13,13,13	0.14	0	12,12,12	0.10	0
36	SPM	2	1567	-	13,13,13	0.12	0	12,12,12	0.07	0
36	SPM	2	1549	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1575	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1561	-	13,13,13	0.12	0	12,12,12	0.09	0
36	SPM	2	1550	-	13,13,13	0.10	0	12,12,12	0.11	0
36	SPM	2	1576	-	13,13,13	0.12	0	12,12,12	0.07	0
36	SPM	2	1558	-	13,13,13	0.08	0	12,12,12	0.13	0
36	SPM	2	1554	-	13,13,13	0.07	0	12,12,12	0.15	0
36	SPM	2	1578	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1564	-	13,13,13	0.08	0	12,12,12	0.09	0
36	SPM	2	1560	-	13,13,13	0.11	0	12,12,12	0.11	0
36	SPM	2	1572	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1573	-	13,13,13	0.12	0	12,12,12	0.06	0
36	SPM	2	1562	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1571	-	13,13,13	0.09	0	12,12,12	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	2	1570	-	-	3/11/11/11	-
36	SPM	2	1553	-	-	4/11/11/11	-
36	SPM	2	1559	-	-	4/11/11/11	-
36	SPM	2	1563	-	-	1/11/11/11	-
36	SPM	2	1555	-	-	2/11/11/11	-
36	SPM	2	1565	-	-	3/11/11/11	-
36	SPM	2	1569	-	-	3/11/11/11	-
36	SPM	2	1551	-	-	2/11/11/11	-
36	SPM	2	1568	-	-	3/11/11/11	-
36	SPM	2	1556	-	-	2/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	2	1557	-	-	2/11/11/11	-
36	SPM	2	1574	-	-	3/11/11/11	-
36	SPM	2	1548	-	-	2/11/11/11	-
36	SPM	2	1552	-	-	2/11/11/11	-
36	SPM	2	1566	-	-	3/11/11/11	-
36	SPM	2	1577	-	-	1/11/11/11	-
36	SPM	2	1567	-	-	4/11/11/11	-
36	SPM	2	1549	-	-	2/11/11/11	-
36	SPM	2	1575	-	-	2/11/11/11	-
36	SPM	2	1561	-	-	2/11/11/11	-
36	SPM	2	1550	-	-	3/11/11/11	-
36	SPM	2	1576	-	-	3/11/11/11	-
36	SPM	2	1558	-	-	2/11/11/11	-
36	SPM	2	1554	-	-	1/11/11/11	-
36	SPM	2	1578	-	-	4/11/11/11	-
36	SPM	2	1564	-	-	5/11/11/11	-
36	SPM	2	1560	-	-	1/11/11/11	-
36	SPM	2	1572	-	-	3/11/11/11	-
36	SPM	2	1573	-	-	3/11/11/11	-
36	SPM	2	1562	-	-	2/11/11/11	-
36	SPM	2	1571	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	2	1556	SPM	C12-C11-N10-C9
36	2	1565	SPM	C7-C6-N5-C4
36	2	1569	SPM	C3-C4-N5-C6
36	2	1573	SPM	C7-C6-N5-C4
36	2	1575	SPM	C3-C4-N5-C6
36	2	1553	SPM	C12-C11-N10-C9
36	2	1565	SPM	C3-C4-N5-C6
36	2	1566	SPM	C3-C4-N5-C6
36	2	1566	SPM	C7-C6-N5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	2	1573	SPM	C8-C9-N10-C11
36	2	1574	SPM	C7-C6-N5-C4
36	2	1548	SPM	C8-C9-N10-C11
36	2	1550	SPM	C12-C11-N10-C9
36	2	1551	SPM	C3-C4-N5-C6
36	2	1554	SPM	C12-C11-N10-C9
36	2	1556	SPM	C8-C9-N10-C11
36	2	1557	SPM	C3-C4-N5-C6
36	2	1562	SPM	C12-C11-N10-C9
36	2	1566	SPM	C12-C11-N10-C9
36	2	1568	SPM	C7-C6-N5-C4
36	2	1570	SPM	C12-C11-N10-C9
36	2	1567	SPM	C3-C4-N5-C6
36	2	1571	SPM	C7-C6-N5-C4
36	2	1559	SPM	C7-C6-N5-C4
36	2	1568	SPM	C8-C9-N10-C11
36	2	1576	SPM	C3-C4-N5-C6
36	2	1576	SPM	C12-C11-N10-C9
36	2	1578	SPM	C7-C6-N5-C4
36	2	1553	SPM	C8-C9-N10-C11
36	2	1548	SPM	C12-C11-N10-C9
36	2	1550	SPM	C3-C4-N5-C6
36	2	1550	SPM	C8-C9-N10-C11
36	2	1555	SPM	C7-C6-N5-C4
36	2	1557	SPM	C7-C6-N5-C4
36	2	1558	SPM	C7-C6-N5-C4
36	2	1559	SPM	C3-C4-N5-C6
36	2	1560	SPM	C8-C9-N10-C11
36	2	1564	SPM	C3-C4-N5-C6
36	2	1571	SPM	C8-C9-N10-C11
36	2	1574	SPM	C8-C9-N10-C11
36	2	1561	SPM	C12-C11-N10-C9
36	2	1558	SPM	C3-C4-N5-C6
36	2	1564	SPM	C7-C6-N5-C4
36	2	1559	SPM	C8-C9-N10-C11
36	2	1562	SPM	C7-C6-N5-C4
36	2	1567	SPM	C7-C6-N5-C4
36	2	1564	SPM	N10-C11-C12-C13
36	2	1563	SPM	C3-C4-N5-C6
36	2	1570	SPM	C7-C6-N5-C4
36	2	1575	SPM	C7-C6-N5-C4
36	2	1552	SPM	C8-C9-N10-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	2	1551	SPM	C8-C9-N10-C11
36	2	1569	SPM	C12-C11-N10-C9
36	2	1570	SPM	C3-C4-N5-C6
36	2	1549	SPM	C3-C4-N5-C6
36	2	1555	SPM	C3-C4-N5-C6
36	2	1569	SPM	C7-C6-N5-C4
36	2	1559	SPM	C12-C11-N10-C9
36	2	1561	SPM	C7-C6-N5-C4
36	2	1572	SPM	C6-C7-C8-C9
36	2	1564	SPM	C8-C9-N10-C11
36	2	1564	SPM	C12-C11-N10-C9
36	2	1567	SPM	C8-C9-N10-C11
36	2	1577	SPM	C7-C6-N5-C4
36	2	1578	SPM	C3-C4-N5-C6
36	2	1573	SPM	C6-C7-C8-C9
36	2	1578	SPM	C6-C7-C8-C9
36	2	1552	SPM	C7-C6-N5-C4
36	2	1572	SPM	C3-C4-N5-C6
36	2	1553	SPM	C6-C7-C8-C9
36	2	1549	SPM	C8-C9-N10-C11
36	2	1567	SPM	C12-C11-N10-C9
36	2	1568	SPM	C12-C11-N10-C9
36	2	1574	SPM	C12-C11-N10-C9
36	2	1576	SPM	C8-C9-N10-C11
36	2	1578	SPM	C12-C11-N10-C9
36	2	1565	SPM	C6-C7-C8-C9
36	2	1553	SPM	C7-C6-N5-C4
36	2	1572	SPM	C12-C11-N10-C9

There are no ring outliers.

25 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	2	1570	SPM	1	0
36	2	1553	SPM	3	0
36	2	1559	SPM	2	0
36	2	1563	SPM	4	0
36	2	1555	SPM	1	0
36	2	1565	SPM	1	0
36	2	1551	SPM	1	0
36	2	1556	SPM	1	0
36	2	1574	SPM	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	2	1548	SPM	2	0
36	2	1552	SPM	1	0
36	2	1566	SPM	1	0
36	2	1577	SPM	2	0
36	2	1567	SPM	10	0
36	2	1549	SPM	5	0
36	2	1575	SPM	7	0
36	2	1561	SPM	1	0
36	2	1576	SPM	9	0
36	2	1558	SPM	2	0
36	2	1554	SPM	1	0
36	2	1578	SPM	5	0
36	2	1564	SPM	3	0
36	2	1560	SPM	3	0
36	2	1573	SPM	3	0
36	2	1562	SPM	3	0

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.

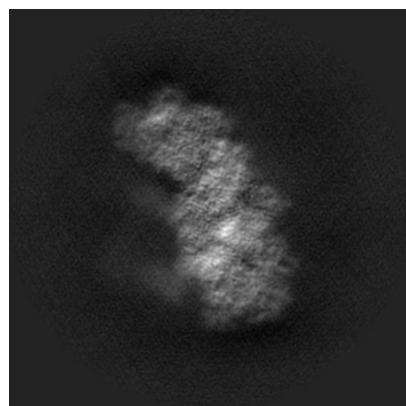
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50717. These allow visual inspection of the internal detail of the map and identification of artifacts.

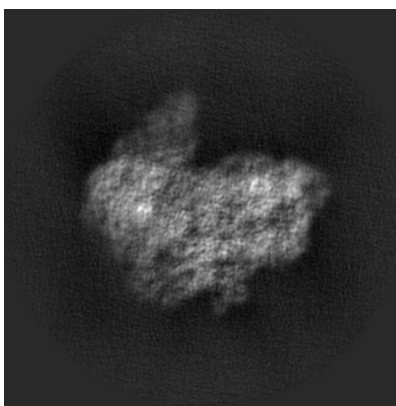
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

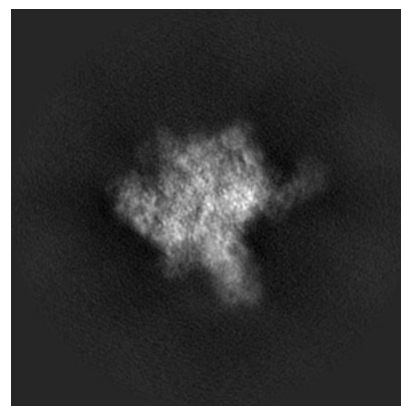
6.1.1 Primary map



X

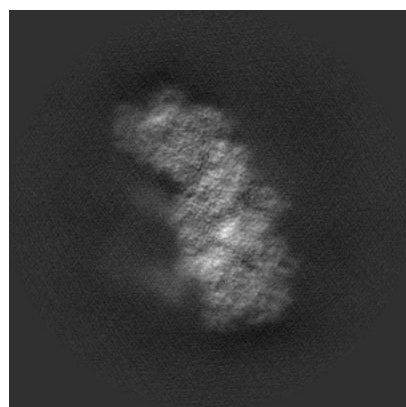


Y

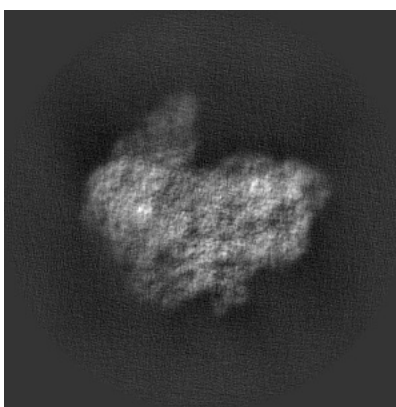


Z

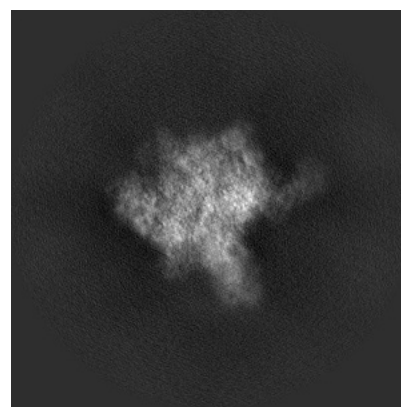
6.1.2 Raw map



X



Y

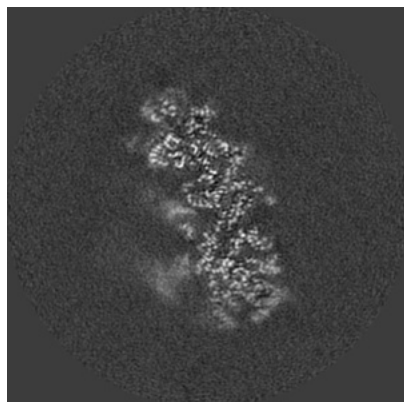


Z

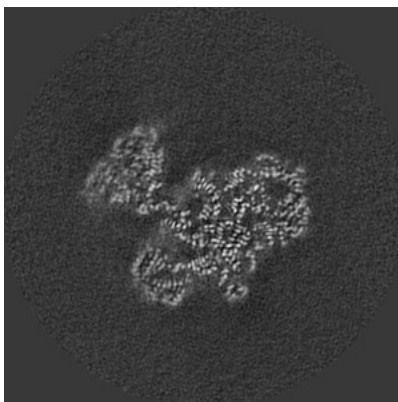
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

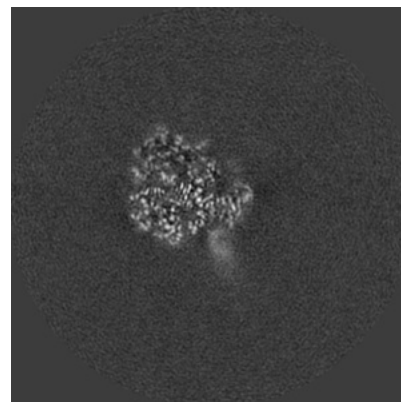
6.2.1 Primary map



X Index: 174

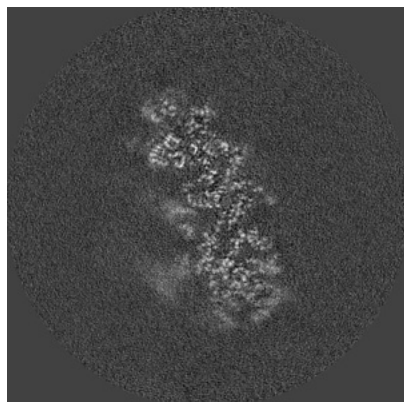


Y Index: 174

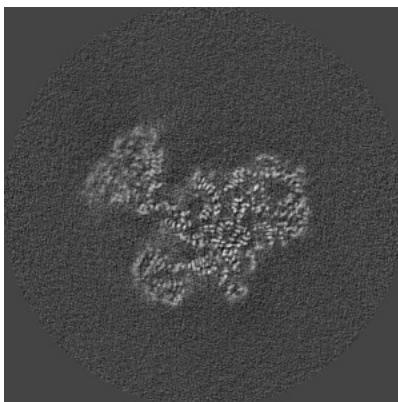


Z Index: 174

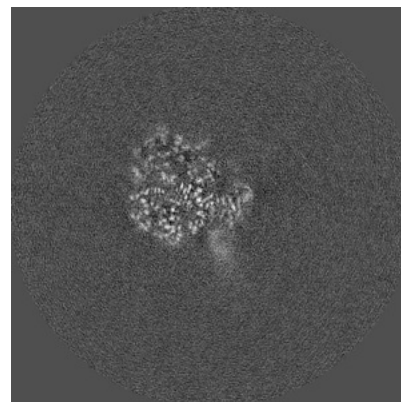
6.2.2 Raw map



X Index: 174



Y Index: 174

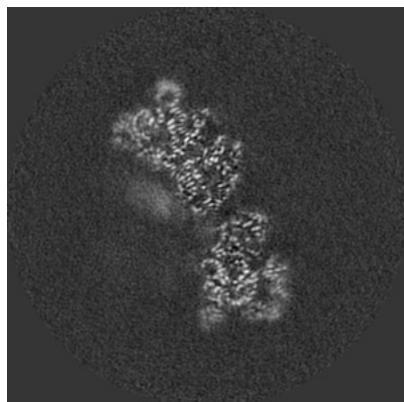


Z Index: 174

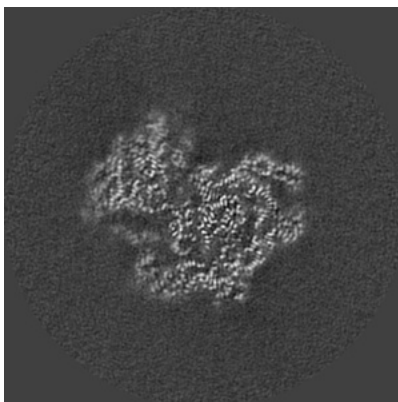
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

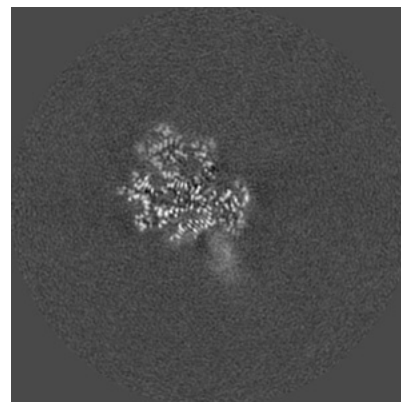
6.3.1 Primary map



X Index: 187

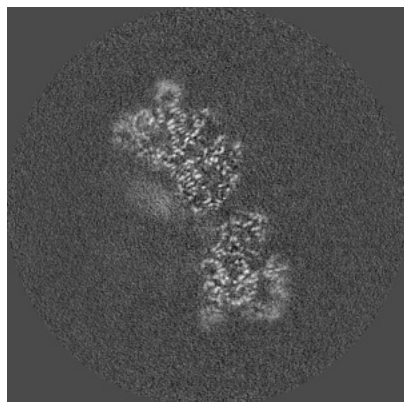


Y Index: 181

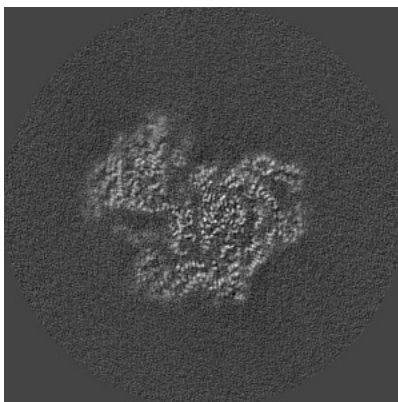


Z Index: 179

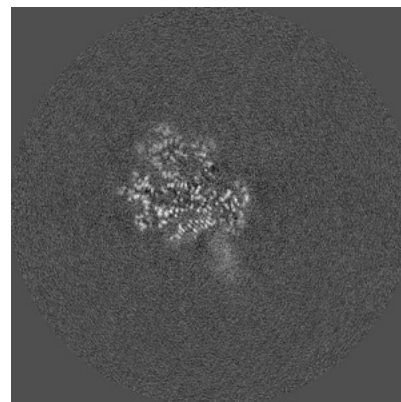
6.3.2 Raw map



X Index: 187



Y Index: 180

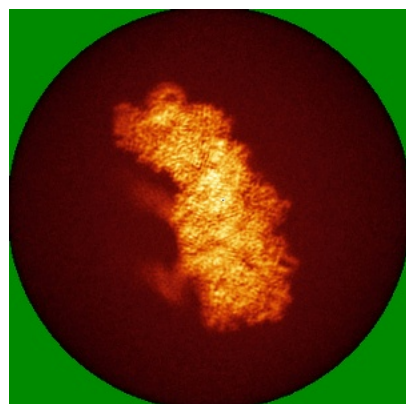


Z Index: 179

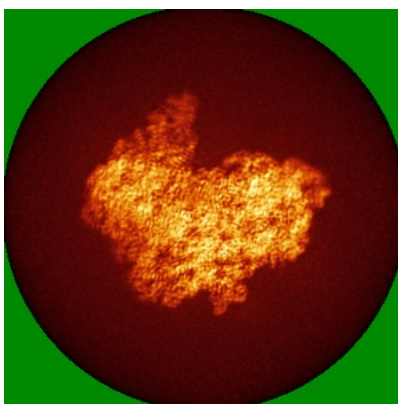
The images above show the largest variance slices of the map in three orthogonal directions.

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

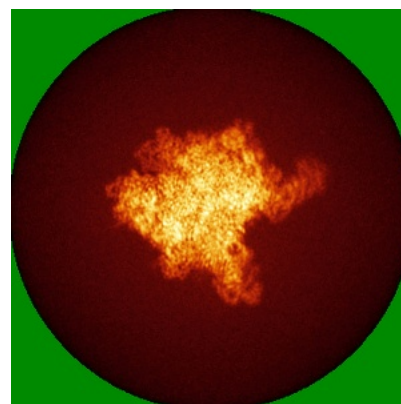
6.4.1 Primary map



X

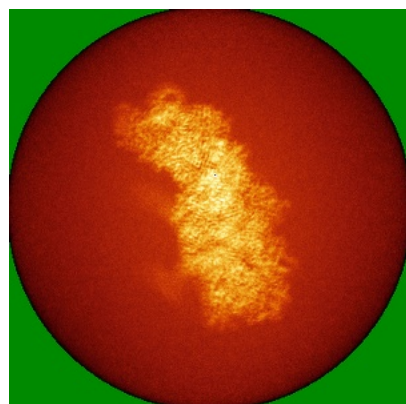


Y

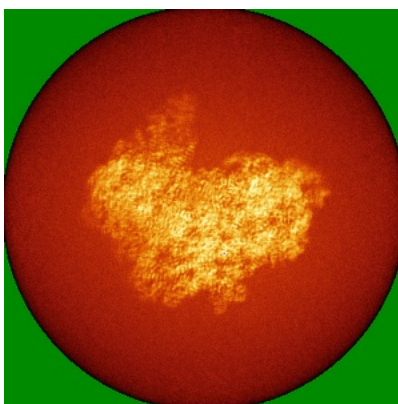


Z

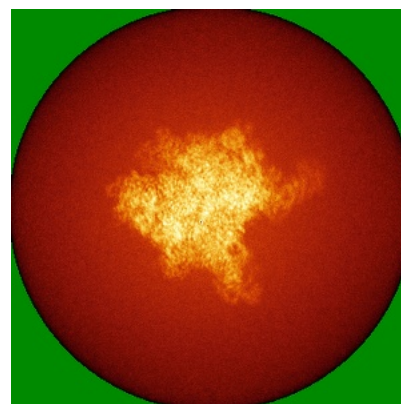
6.4.2 Raw map



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



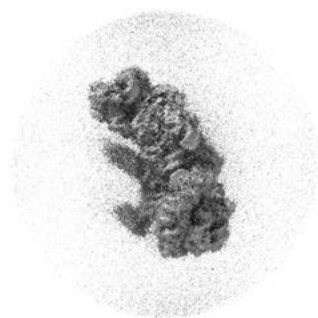
Y



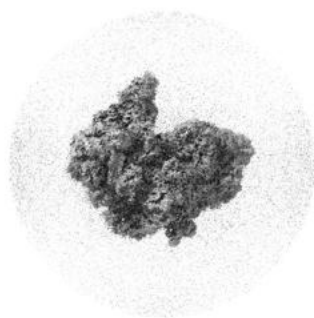
Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

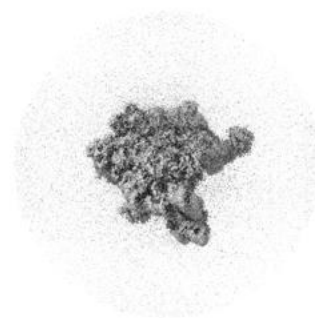
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

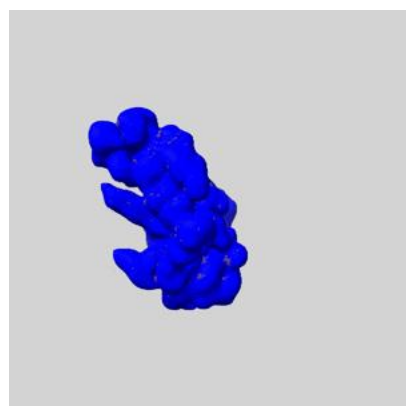
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

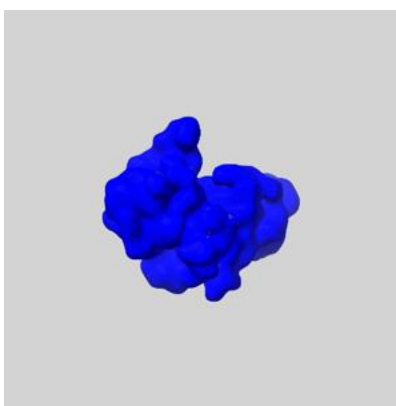
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

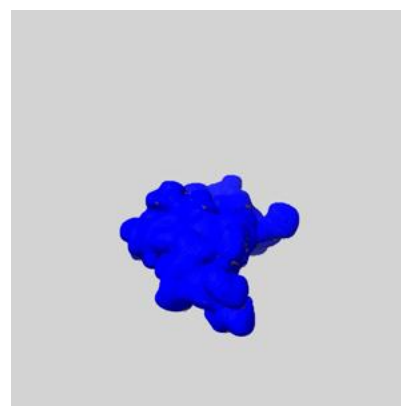
6.6.1 emd_50717_msk_1.map [i](#)



X



Y

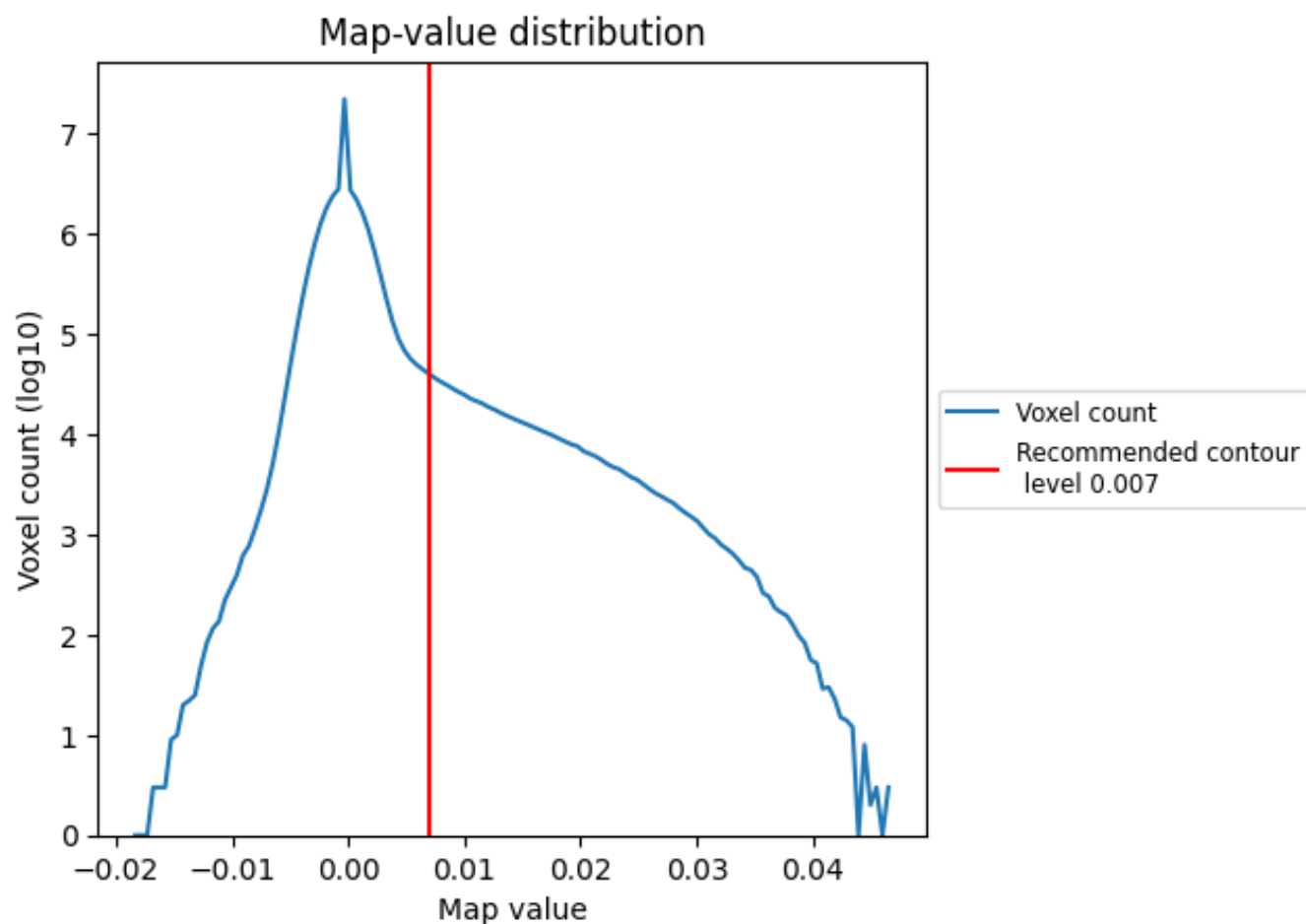


Z

7 Map analysis [i](#)

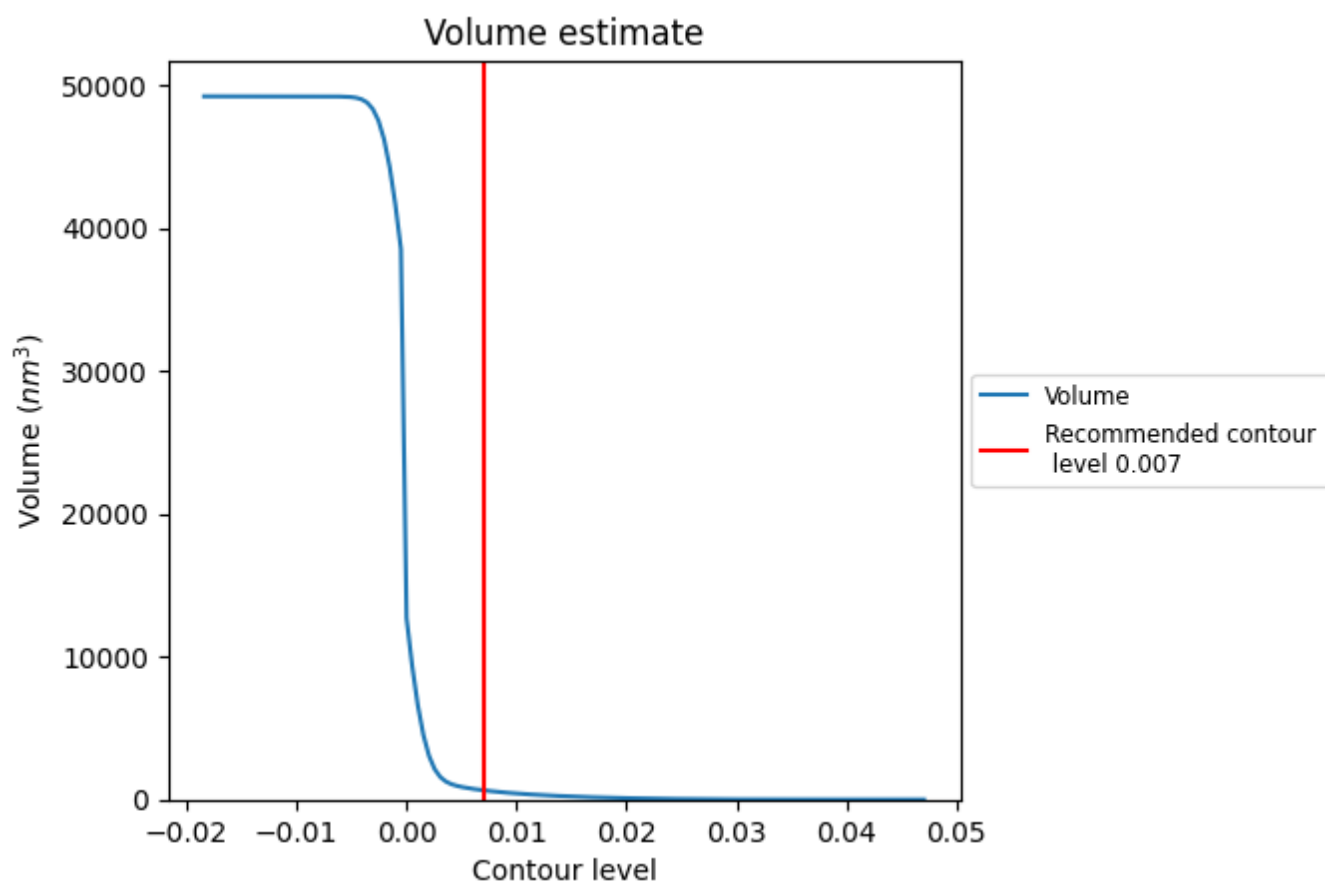
This section contains the results of statistical analysis of the map.

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.

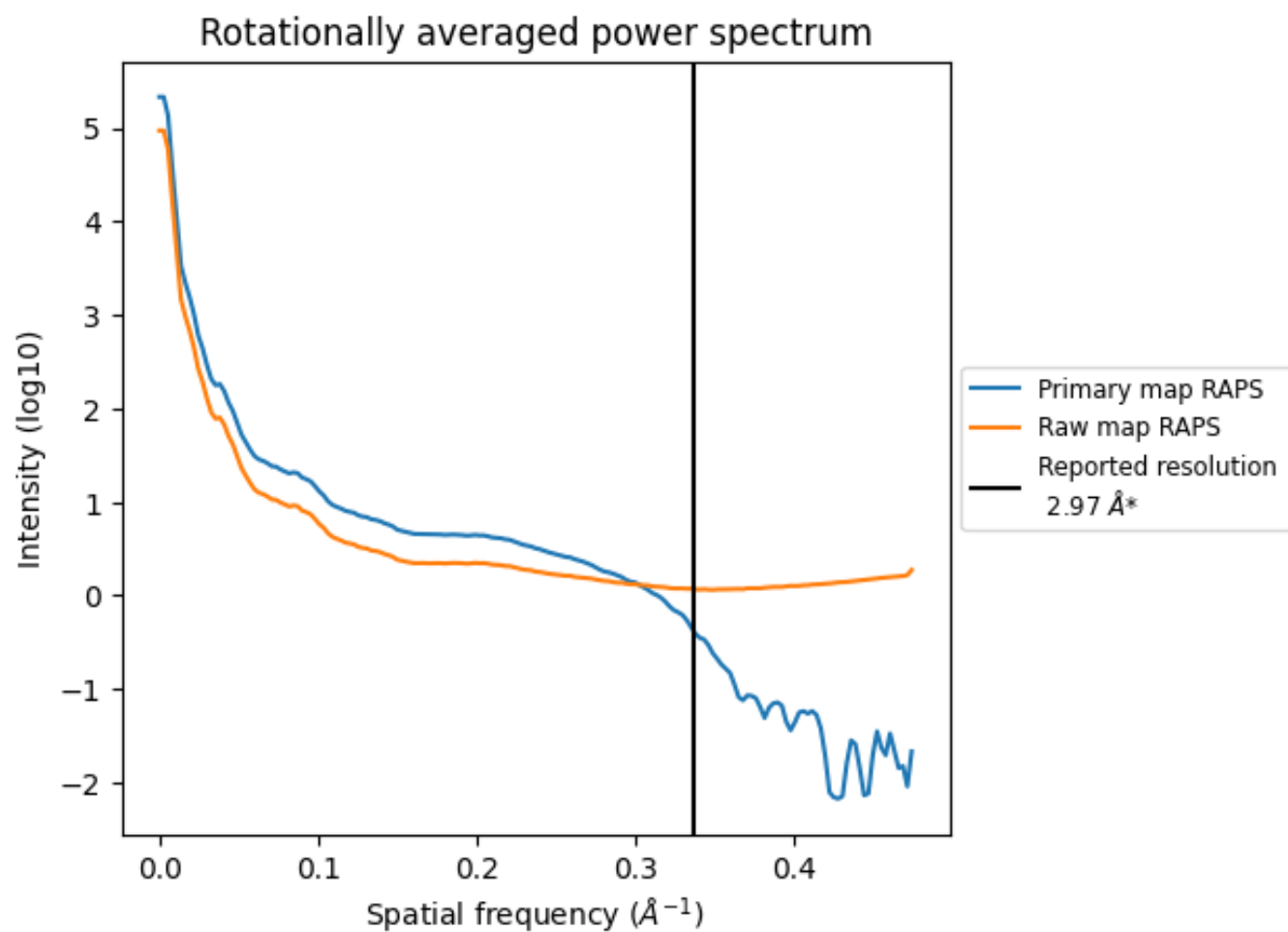
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 651 nm³; this corresponds to an approximate mass of 588 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 ⓘ

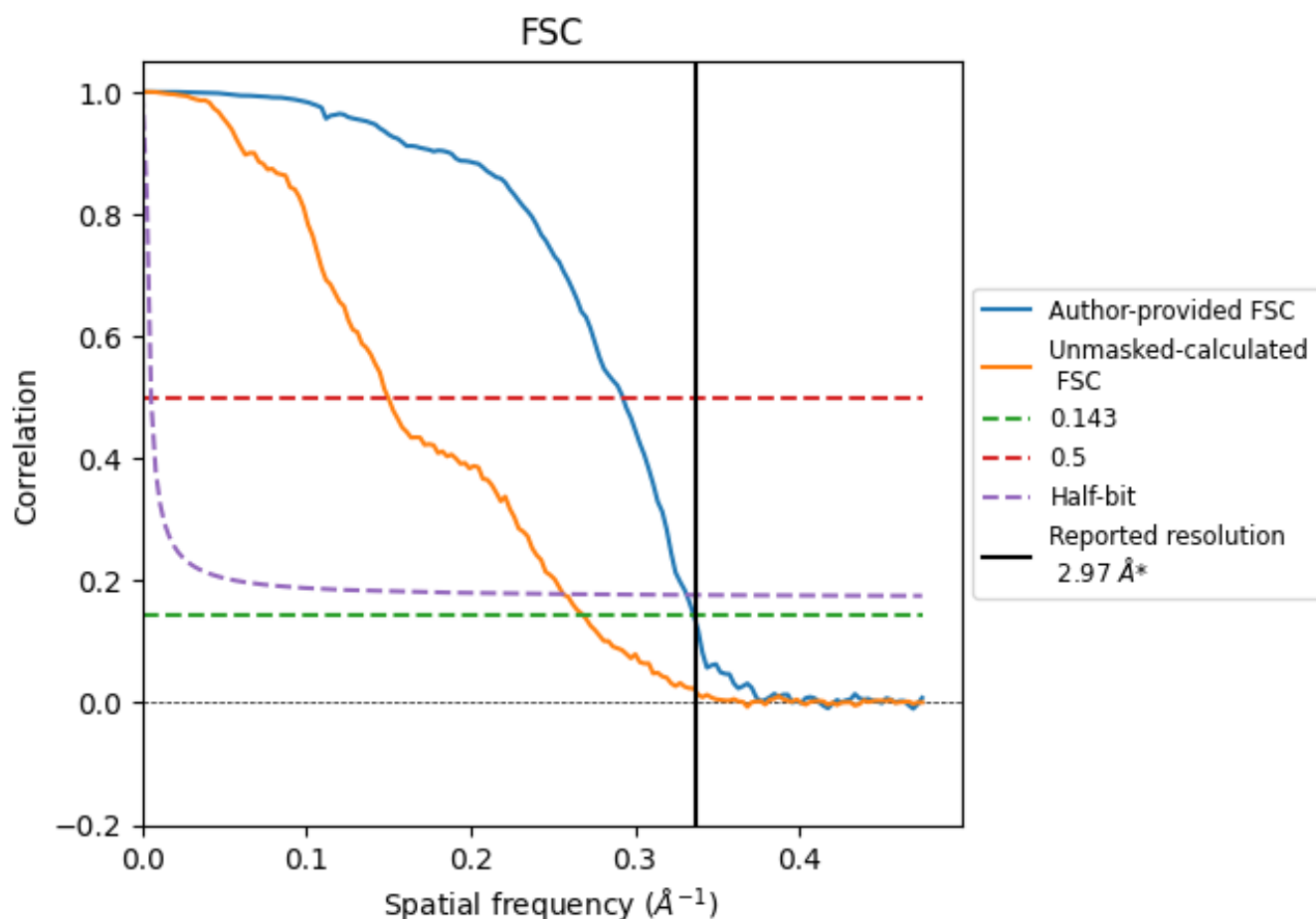


*Reported resolution corresponds to spatial frequency of $0.337 \text{ \AA}^{-1}$

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 0.337 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

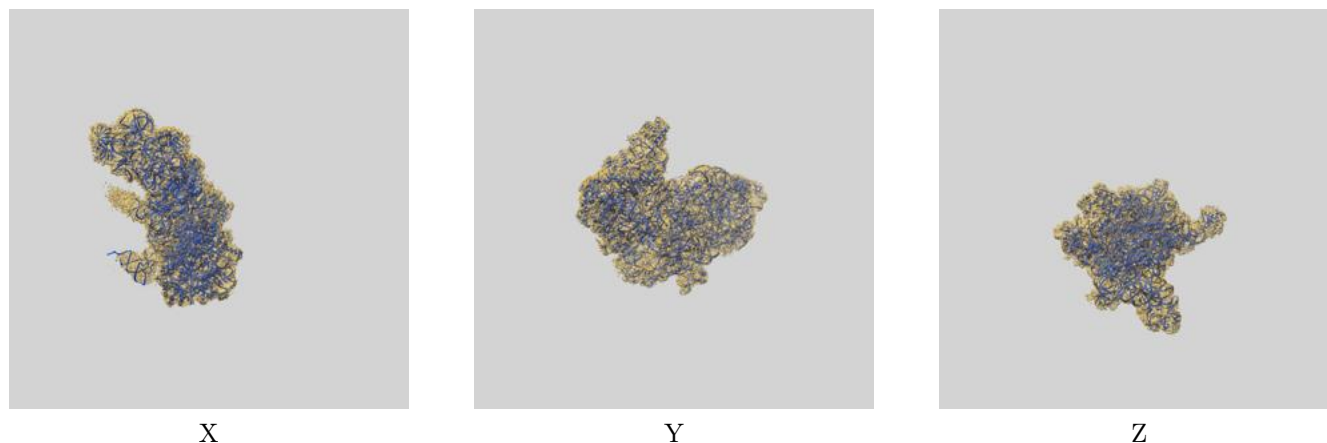
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.98	3.42	3.02
Unmasked-calculated*	3.73	6.68	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 2.97 by more than 10 %

9 Map-model fit [i](#)

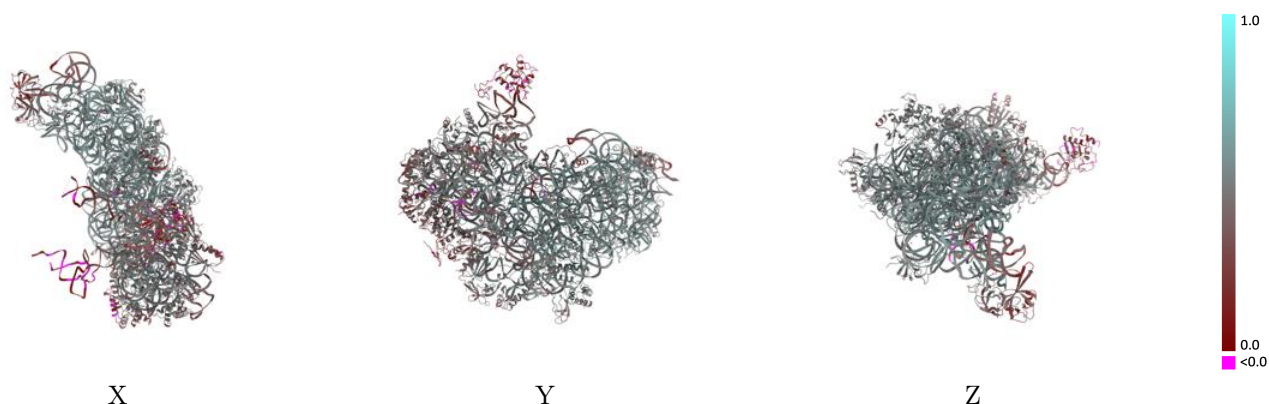
This section contains information regarding the fit between EMDB map EMD-50717 and PDB model 9FRL. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



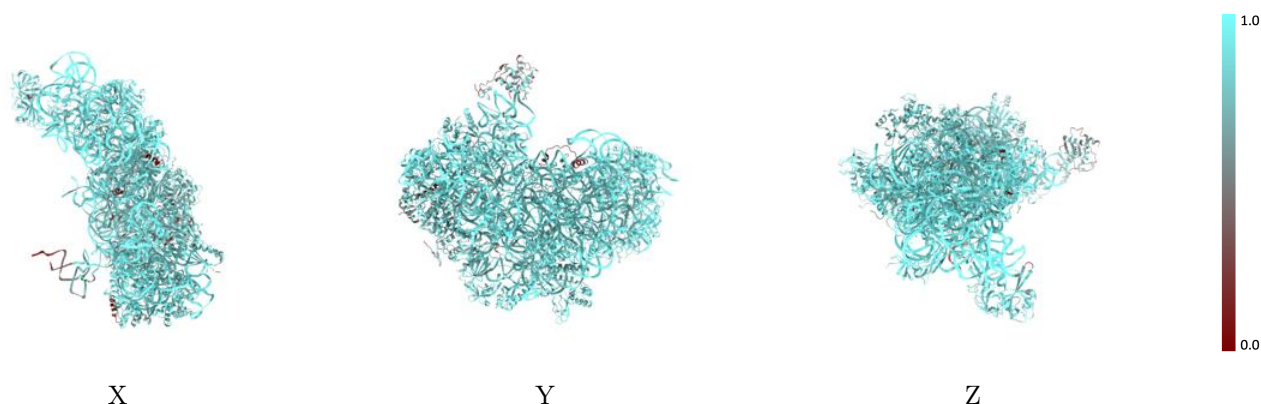
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



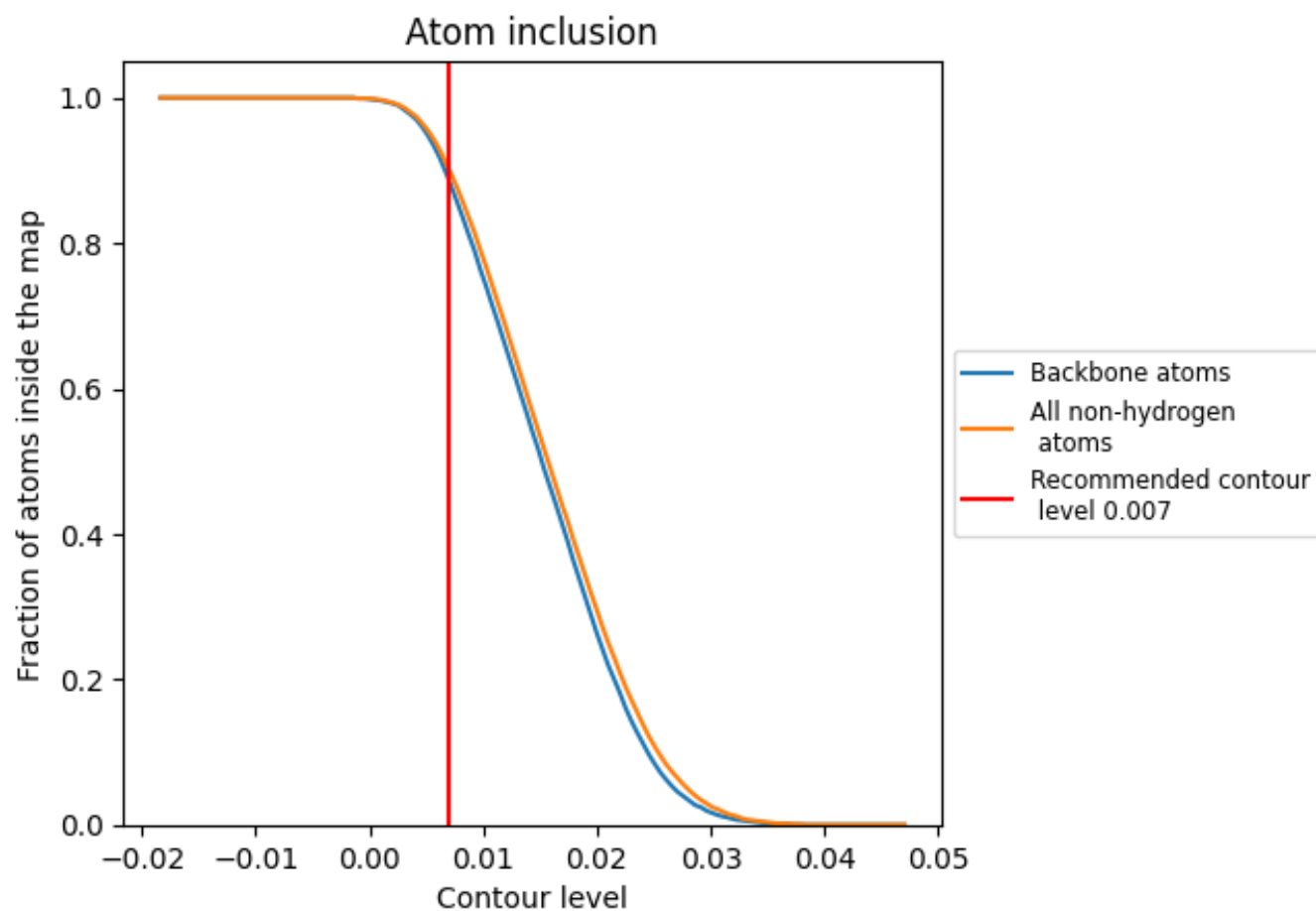
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.4710
2	 0.9800	 0.5140
3	 0.5890	 0.1590
4	 0.6660	 0.1740
5	 0.8140	 0.3810
A	 0.8900	 0.4550
B	 0.8250	 0.4780
C	 0.8970	 0.5090
D	 0.9290	 0.5260
E	 0.9190	 0.5220
F	 0.8990	 0.5330
G	 0.8480	 0.3680
H	 0.8170	 0.3990
I	 0.9370	 0.5410
J	 0.9300	 0.5150
K	 0.8700	 0.4510
L	 0.8570	 0.4080
M	 0.8720	 0.4630
N	 0.8950	 0.5180
O	 0.8790	 0.4400
P	 0.8890	 0.4940
Q	 0.8730	 0.4980
R	 0.9140	 0.5320
S	 0.8530	 0.4450
T	 0.8430	 0.4270
U	 0.8880	 0.4560
V	 0.8960	 0.4890
W	 0.8620	 0.4450
X	 0.7770	 0.3680
Y	 0.4340	 0.1830
Z	 0.8610	 0.4540
a	 0.8620	 0.4140
c	 0.5430	 0.2660
d	 0.6940	 0.2830
e	 0.1140	 0.2440

