



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:48 PM UTC

PDB ID : 5LMP / pdb_00005lmp
EMDB ID : EMD-4075
Title : Structure of bacterial 30S-IF1-IF3-mRNA translation pre-initiation complex (state-1C)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 5.35 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

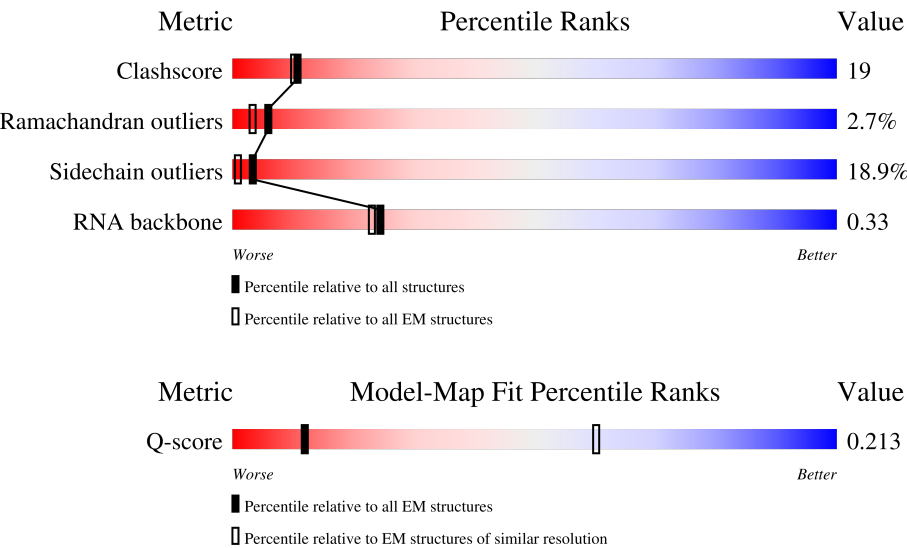
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.35 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	505 (4.85 - 5.85)

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	A	1522	 26% 54% 17% ..
2	B	256	 23% 50% 31% 9% . 9%
3	C	239	 55% 28% . 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	72	
23	X	171	
24	Y	39	

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
26	ZN	D	300	-	-	X	-
26	ZN	N	101	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 54132 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0
			32525	14481	6019	10514	1511		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			933	577	192	162	2		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

- Molecule 23 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	168	Total	C	N	O	S	0	0
			1356	853	249	245	9		

- Molecule 24 is a RNA chain called mRNA.

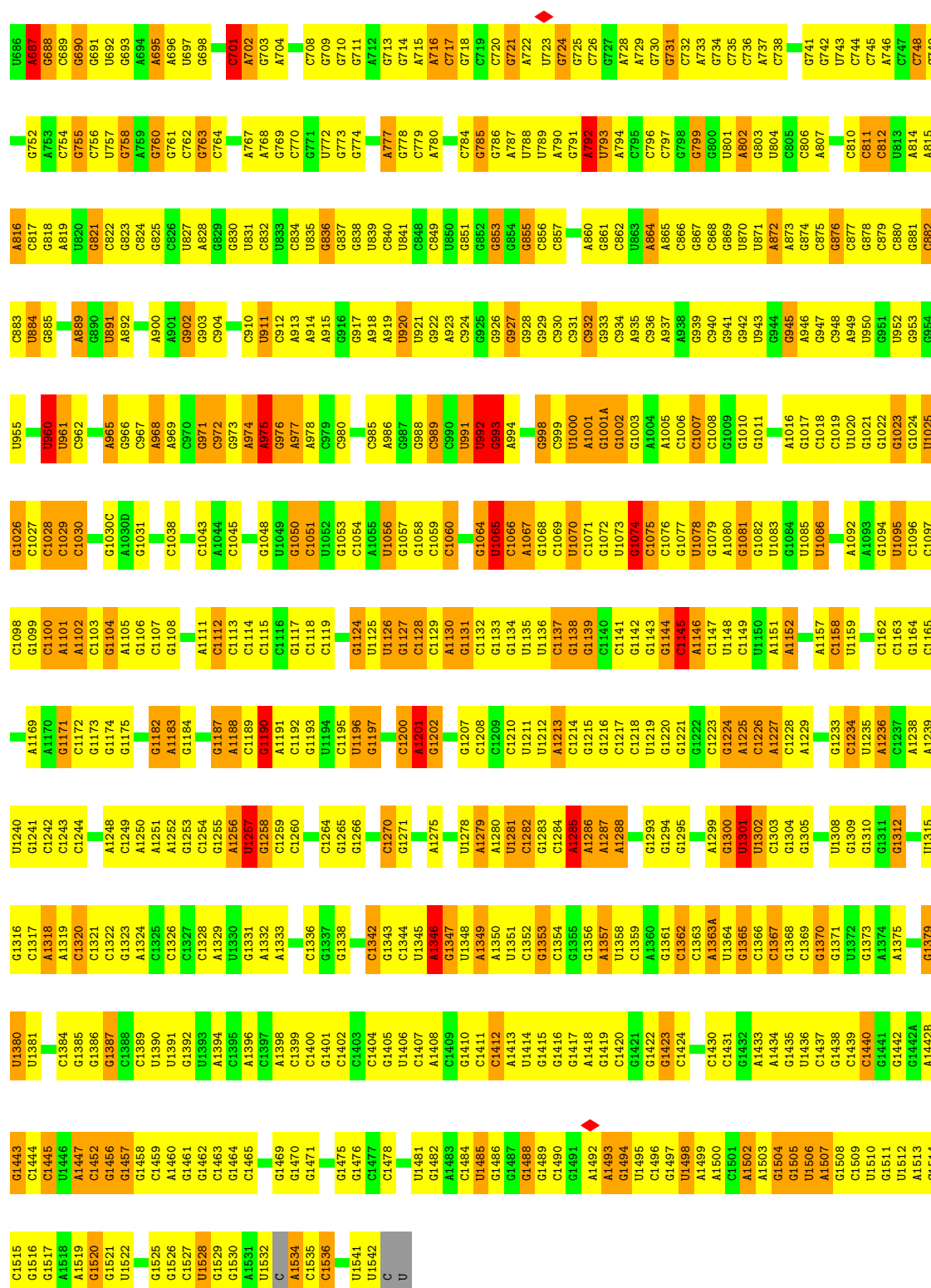
Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	20	Total	C	N	O	P	0	0
			439	196	89	134	20		

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	A	108	Total	Mg	0
			108	108	

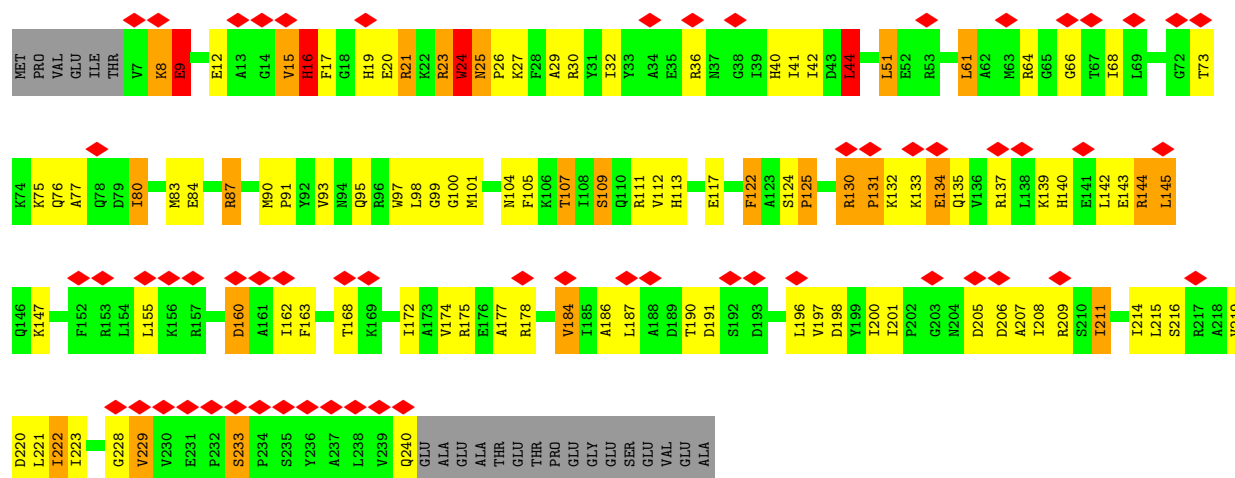
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Zn	0
			1	1	
26	N	1	Total	Zn	0
			1	1	

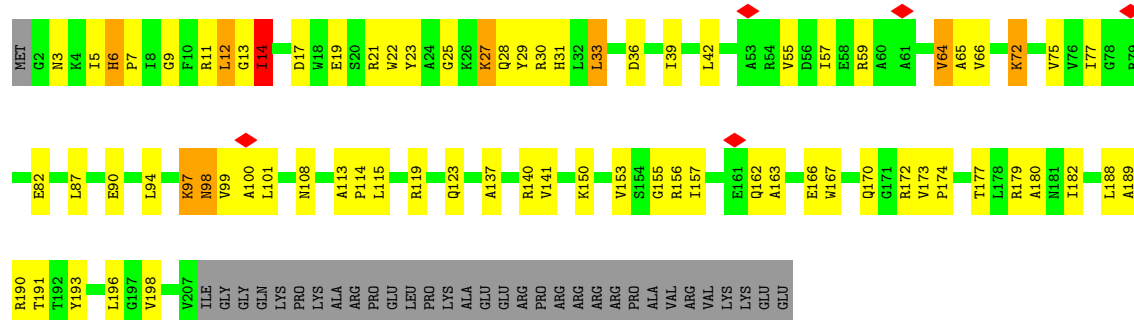


• Molecule 2: 30S ribosomal protein S2

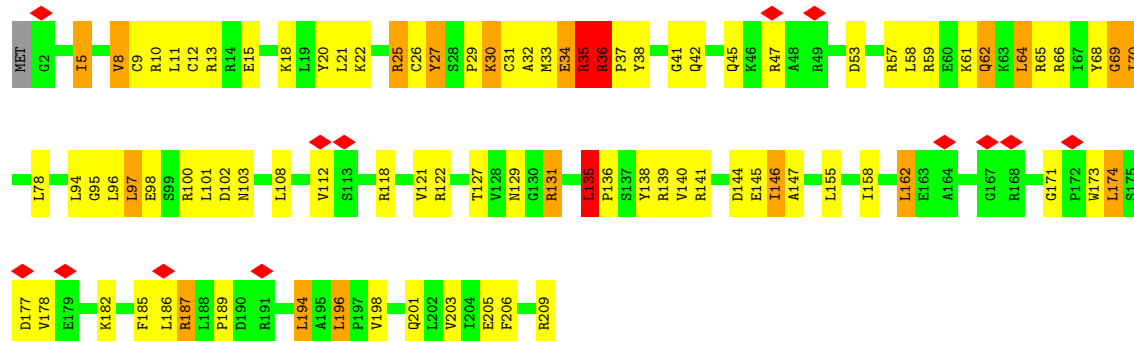




• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

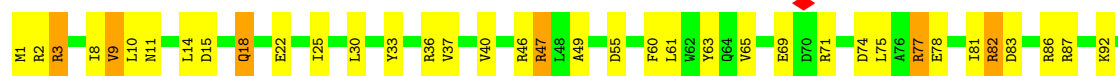


• Molecule 5: 30S ribosomal protein S5

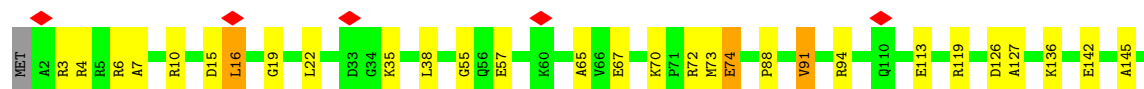
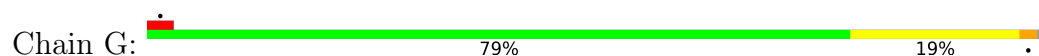




• Molecule 6: 30S ribosomal protein S6



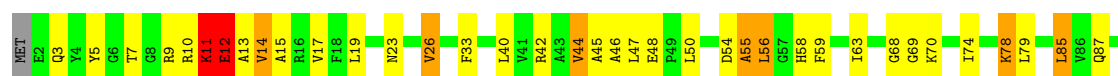
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

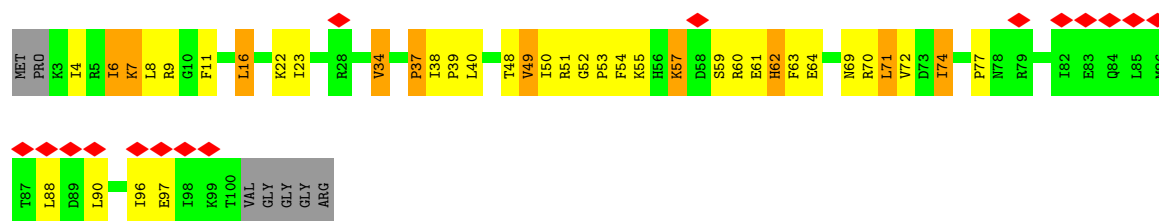


• Molecule 9: 30S ribosomal protein S9

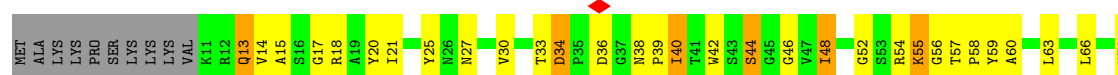


• Molecule 10: 30S ribosomal protein S10

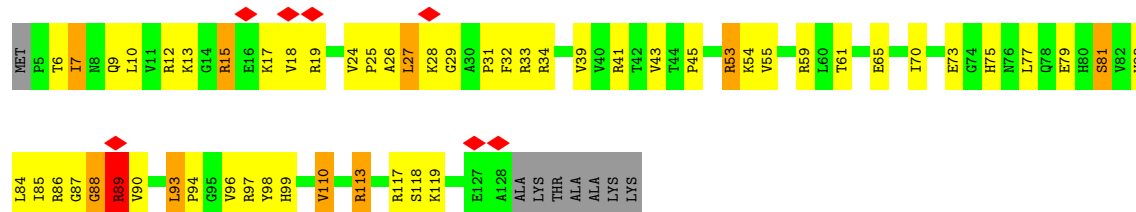




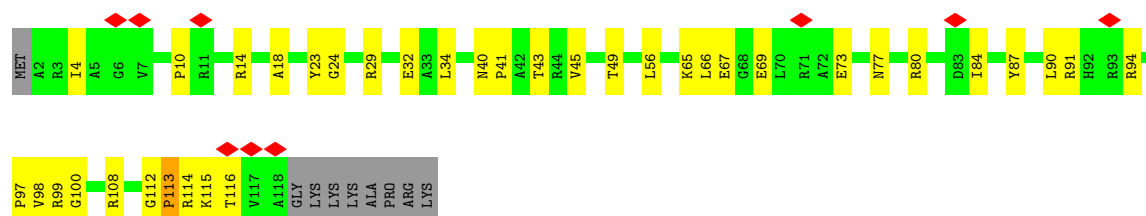
- Molecule 11: 30S ribosomal protein S11



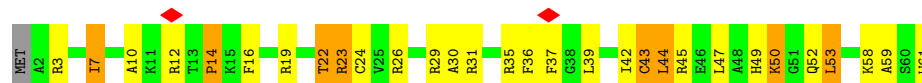
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

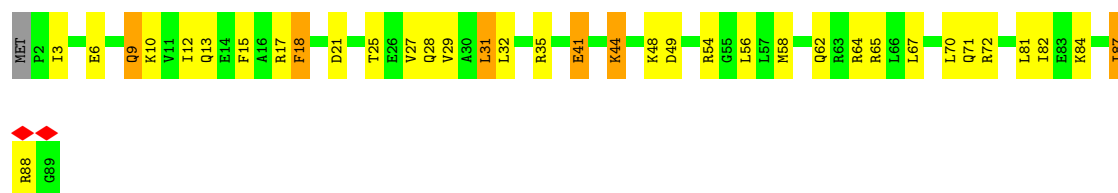


- Molecule 14: 30S ribosomal protein S14 type Z



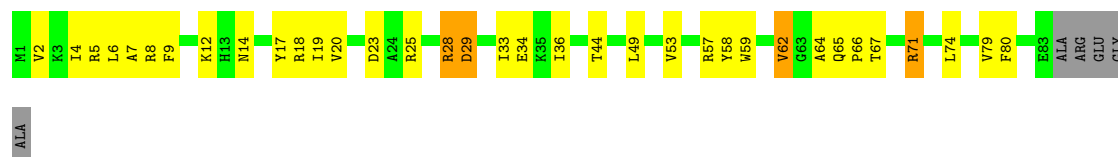
- Molecule 15: 30S ribosomal protein S15

Chain O: 



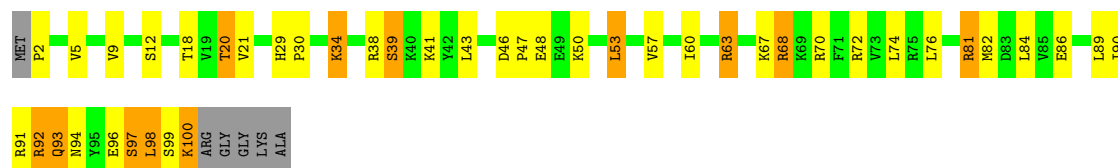
- Molecule 16: 30S ribosomal protein S16

Chain P: 



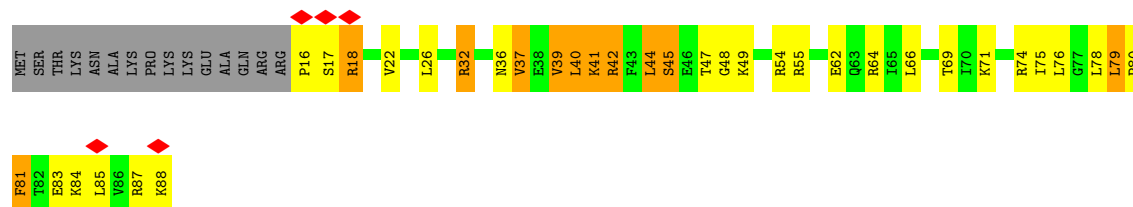
- Molecule 17: 30S ribosomal protein S17

Chain Q: 



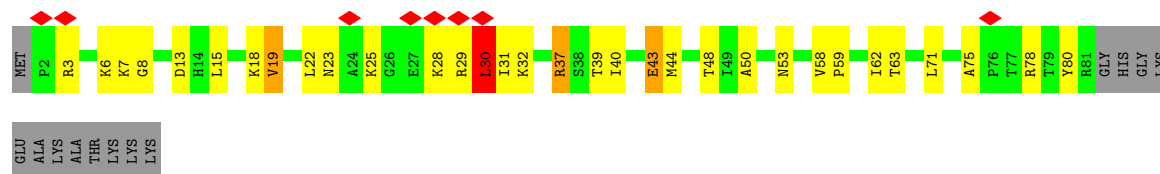
- Molecule 18: 30S ribosomal protein S18

Chain R: 



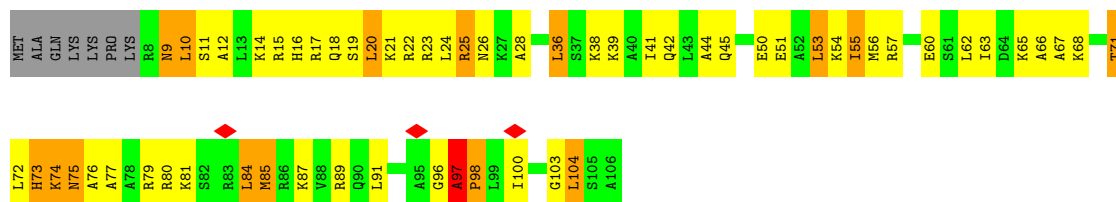
- Molecule 19: 30S ribosomal protein S19

Chain S: 



- Molecule 20: 30S ribosomal protein S20

Chain T: 



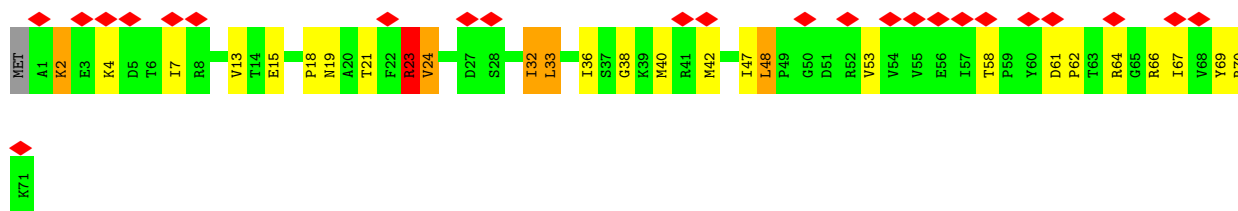
- Molecule 21: 30S ribosomal protein Thx

Chain V: 



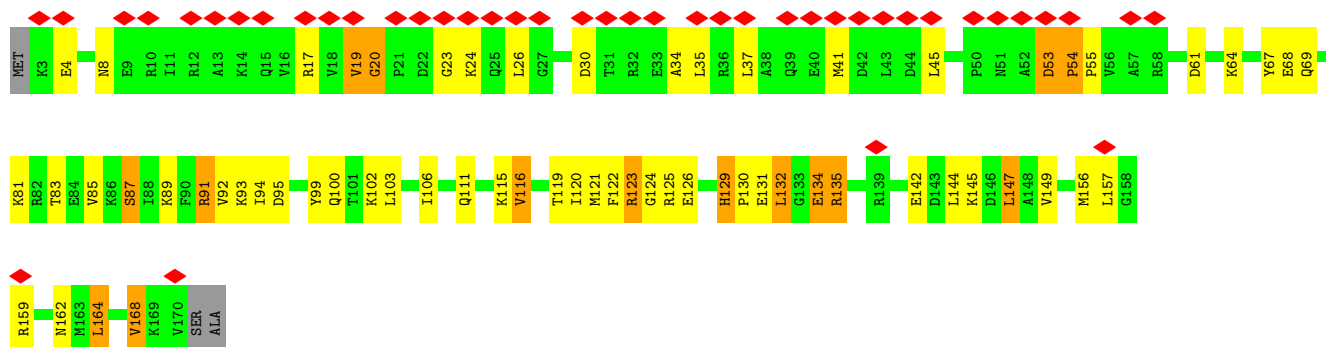
- Molecule 22: Translation initiation factor IF-1

Chain W: 



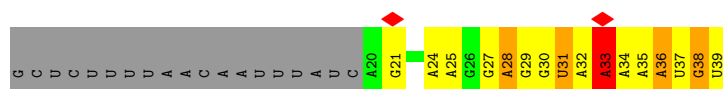
- Molecule 23: Translation initiation factor IF-3

Chain X: 



- Molecule 24: mRNA

Chain Y: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.301	Depositor
Minimum map value	-0.090	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	348.4, 348.4, 348.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	1/36397 (0.0%)	0.84	76/56783 (0.1%)
2	B	0.94	0/1935	1.22	5/2609 (0.2%)
3	C	0.71	0/1636	1.15	6/2205 (0.3%)
4	D	0.72	1/1733 (0.1%)	1.27	9/2318 (0.4%)
5	E	0.67	0/1162	1.34	9/1564 (0.6%)
6	F	0.58	0/856	1.08	0/1154
7	G	0.79	0/1276	1.18	0/1709
8	H	0.66	0/1136	1.13	3/1527 (0.2%)
9	I	0.73	0/1029	1.20	3/1379 (0.2%)
10	J	0.91	0/805	1.05	1/1082 (0.1%)
11	K	0.77	0/900	1.16	3/1213 (0.2%)
12	L	0.63	0/986	1.08	2/1320 (0.2%)
13	M	0.94	0/943	1.22	2/1265 (0.2%)
14	N	0.72	0/501	1.09	3/664 (0.5%)
15	O	0.68	0/745	1.27	2/992 (0.2%)
16	P	0.57	0/716	1.00	0/963
17	Q	0.60	0/836	1.04	2/1117 (0.2%)
18	R	0.79	0/604	1.18	3/801 (0.4%)
19	S	1.02	0/661	1.02	0/890
20	T	0.70	0/765	1.38	4/1007 (0.4%)
21	V	1.10	1/212 (0.5%)	1.03	0/277
22	W	1.01	0/580	1.28	3/782 (0.4%)
23	X	1.00	0/1375	1.29	9/1844 (0.5%)
24	Y	0.62	0/494	1.00	3/770 (0.4%)
All	All	0.61	3/58283 (0.0%)	0.97	148/86235 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
9	I	1	0
23	X	0	1
All	All	1	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	2	GLY	N-CA	11.65	1.64	1.45
4	D	30	LYS	CA-C	5.24	1.57	1.52
1	A	1074	G	O5'-C5'	5.22	1.50	1.42

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	11	LYS	CB-CA-C	20.57	151.36	110.42
5	E	15	ARG	N-CA-C	-17.31	80.73	109.46
5	E	16	THR	N-CA-CB	-14.21	86.10	110.83
22	W	23	ARG	N-CA-C	-13.58	88.17	109.76
1	A	266	G	C2'-C3'-O3'	13.29	129.44	109.50
4	D	35	ARG	N-CA-C	11.90	129.17	112.04
22	W	23	ARG	CB-CA-C	-11.77	90.66	109.84
1	A	1498	U	C2'-C3'-O3'	10.89	125.83	109.50
1	A	792	A	C2'-C3'-O3'	10.88	125.82	109.50
1	A	1145	C	C2'-C3'-O3'	10.77	125.65	109.50
9	I	12	GLU	N-CA-C	-9.82	97.71	112.54
1	A	181	G	C2'-C3'-O3'	9.51	123.77	109.50
1	A	115	G	C4'-C3'-O3'	9.28	123.31	109.40
1	A	1301	U	C2'-C3'-O3'	9.04	123.06	109.50
1	A	328	C	C2'-C3'-O3'	9.02	123.03	109.50
1	A	1182	G	C2'-C3'-O3'	8.80	122.71	109.50
1	A	960	U	C2'-C3'-O3'	8.67	122.51	109.50
1	A	748	C	C2'-C3'-O3'	8.58	122.37	109.50
1	A	1346	A	C2'-C3'-O3'	8.57	122.36	109.50
22	W	24	VAL	N-CA-CB	-8.53	99.64	111.41
1	A	965	A	C2'-C3'-O3'	8.26	121.89	109.50
1	A	1257	U	C2'-C3'-O3'	8.10	121.66	109.50
1	A	1101	A	C2'-C3'-O3'	8.06	121.59	109.50
1	A	1534	A	C2'-C3'-O3'	8.04	125.76	113.70
1	A	701	C	C2'-C3'-O3'	7.82	121.23	109.50
1	A	197	A	C2'-C3'-O3'	7.79	121.18	109.50
20	T	97	ALA	CA-C-N	7.72	129.49	119.84
20	T	97	ALA	C-N-CA	7.72	129.49	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	G	C2'-C3'-O3'	7.63	125.15	113.70
23	X	54	PRO	CA-C-N	7.53	129.25	119.84
23	X	54	PRO	C-N-CA	7.53	129.25	119.84
24	Y	33	A	C2'-C3'-O3'	7.51	120.77	109.50
1	A	1190	G	C2'-C3'-O3'	7.45	124.88	113.70
1	A	518	C	C2'-C3'-O3'	7.34	120.51	109.50
3	C	13	GLY	N-CA-C	7.27	122.08	112.77
24	Y	33	A	C4'-C3'-O3'	7.25	120.28	109.40
1	A	1065	U	C2'-C3'-O3'	7.22	120.33	109.50
24	Y	31	U	C4'-C3'-O3'	7.16	120.14	109.40
1	A	1300	G	C2'-C3'-O3'	7.12	120.19	109.50
1	A	1201	A	C4'-C3'-O3'	7.06	120.00	109.40
1	A	51	A	C4'-C3'-O3'	7.02	119.93	109.40
23	X	91	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	A	1285	A	C4'-C3'-O3'	6.94	119.82	109.40
1	A	509	A	C4'-C3'-O3'	6.91	123.36	113.00
4	D	36	ARG	N-CA-C	-6.89	98.76	109.79
23	X	53	ASP	CA-C-N	6.84	127.42	120.38
23	X	53	ASP	C-N-CA	6.84	127.42	120.38
13	M	4	ILE	N-CA-C	6.75	116.76	110.42
1	A	1380	U	C2'-C3'-O3'	6.53	119.30	109.50
1	A	559	A	C2'-C3'-O3'	6.53	123.49	113.70
1	A	484	G	C2'-C3'-O3'	6.52	119.28	109.50
1	A	484	G	C4'-C3'-O3'	6.52	119.18	109.40
8	H	53	VAL	N-CA-C	-6.52	98.35	107.80
1	A	562	C	C2'-C3'-O3'	6.46	119.19	109.50
1	A	17	U	N1-C1'-C2'	6.42	121.63	112.00
1	A	1101	A	C4'-C3'-O3'	6.42	119.03	109.40
4	D	36	ARG	N-CA-CB	-6.35	100.78	110.75
1	A	372	C	C2'-C3'-O3'	6.35	119.03	109.50
1	A	993	G	C4'-C3'-O3'	6.29	118.84	109.40
1	A	428	G	C2'-C3'-O3'	6.28	118.92	109.50
1	A	60	A	C4'-C3'-O3'	6.27	118.81	109.40
13	M	99	ARG	N-CA-C	6.27	121.00	113.23
18	R	37	VAL	N-CA-C	6.27	117.83	111.00
1	A	1504	G	C4'-C3'-O3'	6.21	118.71	109.40
5	E	78	HIS	N-CA-C	6.17	118.16	108.96
11	K	101	SER	N-CA-C	6.08	118.69	111.33
1	A	181	G	C4'-C3'-O3'	6.08	118.52	109.40
1	A	1504	G	C2'-C3'-O3'	6.06	118.58	109.50
23	X	129	HIS	O-C-N	6.03	125.84	120.48
9	I	11	LYS	N-CA-C	-6.02	97.98	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	119	LEU	N-CA-C	5.99	117.34	108.60
1	A	1380	U	C4'-C3'-O3'	5.99	118.38	109.40
5	E	117	ASP	N-CA-C	5.98	118.97	107.44
1	A	1197	G	C4'-C3'-O3'	-5.92	104.12	113.00
1	A	6	G	C4'-C3'-O3'	-5.89	104.17	113.00
5	E	15	ARG	CB-CA-C	-5.88	100.16	109.80
1	A	115	G	C2'-C3'-O3'	5.87	118.30	109.50
1	A	991	U	C4'-C3'-O3'	-5.86	104.20	113.00
10	J	6	ILE	N-CA-C	5.86	115.18	106.85
1	A	960	U	C4'-C3'-O3'	5.83	118.15	109.40
1	A	1285	A	C2'-C3'-O3'	5.83	118.24	109.50
1	A	202	U	C4'-C3'-O3'	5.82	118.14	109.40
1	A	1200	C	C4'-C3'-O3'	-5.82	104.27	113.00
1	A	412	A	C2'-C3'-O3'	5.79	118.19	109.50
1	A	243	A	C2'-C3'-O3'	5.78	118.17	109.50
5	E	118	ILE	N-CA-C	5.77	115.84	107.88
3	C	12	LEU	N-CA-C	5.73	118.30	111.71
1	A	1196	U	C4'-C3'-O3'	5.73	117.99	109.40
15	O	18	PHE	N-CA-C	5.72	113.16	108.07
1	A	428	G	C4'-C3'-O3'	5.72	117.98	109.40
1	A	60	A	C2'-C3'-O3'	5.71	118.06	109.50
1	A	811	C	C2'-C3'-O3'	-5.70	105.15	113.70
1	A	351	G	C2'-C3'-O3'	5.67	118.00	109.50
12	L	93	LEU	CA-C-N	5.67	125.42	119.76
12	L	93	LEU	C-N-CA	5.67	125.42	119.76
1	A	1145	C	C4'-C3'-O3'	-5.59	101.01	109.40
1	A	508	C	C4'-C3'-O3'	5.59	117.79	109.40
17	Q	63	ARG	CA-C-N	5.58	125.58	119.89
17	Q	63	ARG	C-N-CA	5.58	125.58	119.89
4	D	171	GLY	CA-C-N	5.57	125.28	119.82
4	D	171	GLY	C-N-CA	5.57	125.28	119.82
23	X	116	VAL	N-CA-C	5.55	116.11	107.28
2	B	27	LYS	N-CA-C	-5.55	106.46	113.18
1	A	812	C	C4'-C3'-O3'	-5.51	104.73	113.00
15	O	12	ILE	CB-CA-C	-5.49	104.94	111.97
1	A	1183	A	C2'-C3'-O3'	5.48	121.92	113.70
20	T	71	THR	N-CA-C	5.46	116.91	111.07
11	K	80	VAL	N-CA-C	5.46	115.72	107.75
1	A	288	A	C2'-C3'-O3'	5.45	121.88	113.70
1	A	758	G	C4'-C3'-O3'	-5.44	104.83	113.00
1	A	687	A	C4'-C3'-O3'	5.44	117.56	109.40
2	B	66	GLY	N-CA-C	5.44	120.09	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14	ILE	N-CA-C	5.43	120.63	109.34
5	E	61	TYR	CB-CA-C	-5.42	102.36	110.88
1	A	992	U	C2'-C3'-O3'	5.42	117.63	109.50
1	A	429	U	C4'-C3'-O3'	5.41	117.51	109.40
2	B	44	LEU	N-CA-C	5.40	119.98	113.17
1	A	7	G	C4'-C3'-O3'	5.39	117.48	109.40
8	H	54	ASP	CB-CA-C	-5.39	110.38	116.63
1	A	1493	A	C4'-C3'-O3'	5.37	121.06	113.00
2	B	223	ILE	CB-CA-C	5.37	118.85	111.97
1	A	1196	U	C2'-C3'-O3'	5.36	117.54	109.50
1	A	1183	A	C4'-C3'-O3'	-5.35	104.98	113.00
2	B	24	TRP	N-CA-C	5.35	122.19	110.80
20	T	12	ALA	N-CA-C	-5.32	106.17	113.30
1	A	372	C	C4'-C3'-O3'	5.29	117.34	109.40
3	C	98	ASN	N-CA-C	-5.29	101.53	109.15
1	A	251	G	C4'-C3'-O3'	5.26	117.30	109.40
4	D	155	LEU	CA-C-N	5.24	127.73	120.29
4	D	155	LEU	C-N-CA	5.24	127.73	120.29
14	N	22	THR	N-CA-C	5.23	121.93	110.80
23	X	20	GLY	CA-C-N	5.20	126.34	119.84
23	X	20	GLY	C-N-CA	5.20	126.34	119.84
1	A	975	A	C2'-C3'-O3'	5.15	117.23	109.50
5	E	48	ALA	CA-C-N	5.15	126.28	119.84
5	E	48	ALA	C-N-CA	5.15	126.28	119.84
1	A	882	C	C4'-C3'-O3'	-5.14	105.29	113.00
1	A	119	A	C4'-C3'-O3'	5.10	117.06	109.40
18	R	79	LEU	CA-C-N	5.08	125.08	119.90
18	R	79	LEU	C-N-CA	5.08	125.08	119.90
3	C	6	HIS	CA-C-N	5.07	124.38	118.85
3	C	6	HIS	C-N-CA	5.07	124.38	118.85
11	K	17	GLY	N-CA-C	5.05	116.84	110.38
1	A	243	A	C4'-C3'-O3'	5.02	116.93	109.40
4	D	135	LEU	CA-C-N	5.02	124.51	119.19
4	D	135	LEU	C-N-CA	5.02	124.51	119.19
14	N	53	LEU	CA-C-N	5.01	125.01	119.90
14	N	53	LEU	C-N-CA	5.01	125.01	119.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	I	11	LYS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1445	C	Sidechain
1	A	218	C	Sidechain
23	X	53	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32525	0	16434	1098	0
2	B	1900	0	1951	50	0
3	C	1612	0	1677	84	0
4	D	1703	0	1766	94	0
5	E	1146	0	1207	59	0
6	F	843	0	857	19	0
7	G	1257	0	1296	18	0
8	H	1116	0	1177	39	0
9	I	1010	0	1035	26	0
10	J	792	0	835	38	0
11	K	885	0	904	33	0
12	L	970	0	1057	36	0
13	M	933	0	992	17	0
14	N	492	0	533	42	0
15	O	734	0	771	13	0
16	P	700	0	720	23	0
17	Q	823	0	888	40	0
18	R	598	0	670	23	0
19	S	647	0	673	20	0
20	T	763	0	861	84	0
21	V	208	0	221	3	0
22	W	570	0	598	22	0
23	X	1356	0	1401	30	0
24	Y	439	0	218	10	0
25	A	108	0	0	0	0
26	D	1	0	0	3	0
26	N	1	0	0	2	0
All	All	54132	0	38742	1710	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 19.

All (1710) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:A:H3'	3:C:27:LYS:NZ	1.22	1.48
1:A:1256:A:C3'	3:C:27:LYS:HZ1	1.25	1.47
4:D:36:ARG:HD2	4:D:38:TYR:CZ	1.47	1.46
17:Q:41:LYS:NZ	17:Q:92:ARG:NH2	1.65	1.44
3:C:57:ILE:HG12	3:C:66:VAL:CG2	1.51	1.39
3:C:57:ILE:CG1	3:C:66:VAL:HG22	1.59	1.31
5:E:15:ARG:NE	5:E:26:PHE:CE2	1.99	1.31
5:E:79:GLU:OE1	8:H:105:ARG:HG2	1.27	1.30
1:A:413:G:O6	4:D:35:ARG:CD	1.79	1.30
1:A:1366:C:O2'	10:J:60:ARG:NH1	1.63	1.30
3:C:29:TYR:CD2	14:N:36:PHE:CE2	2.21	1.28
5:E:15:ARG:NH2	5:E:26:PHE:CZ	2.04	1.25
4:D:36:ARG:CD	4:D:38:TYR:OH	1.85	1.25
5:E:16:THR:HG22	5:E:27:ARG:O	1.34	1.25
4:D:36:ARG:CD	4:D:38:TYR:CZ	2.22	1.22
1:A:413:G:O6	4:D:35:ARG:NE	1.70	1.21
1:A:426:G:OP1	4:D:36:ARG:NE	1.72	1.20
20:T:73:HIS:CE1	20:T:76:ALA:H	1.59	1.19
1:A:247:G:OP2	17:Q:100:LYS:HD2	1.41	1.18
4:D:36:ARG:HD2	4:D:38:TYR:OH	1.02	1.18
3:C:29:TYR:HD2	14:N:36:PHE:CE2	1.58	1.16
4:D:36:ARG:HG3	4:D:38:TYR:CE2	1.80	1.15
1:A:827:U:O4	1:A:872:A:N1	1.82	1.12
5:E:18:ARG:HB3	5:E:25:ARG:O	1.50	1.12
1:A:439:A:OP2	1:A:493:G:N1	1.84	1.11
10:J:38:ILE:HG23	10:J:71:LEU:HB3	1.33	1.11
1:A:92:C:H2'	1:A:93:G:H8	1.11	1.11
20:T:38:LYS:O	20:T:41:ILE:HG22	1.49	1.11
20:T:66:ALA:CB	20:T:72:LEU:HD22	1.81	1.10
8:H:53:VAL:HG12	8:H:54:ASP:OD1	1.52	1.08
1:A:413:G:O6	4:D:35:ARG:HD3	1.53	1.07
1:A:439:A:OP2	1:A:493:G:N2	1.88	1.06
1:A:18:C:H2'	1:A:19:C:O4'	1.56	1.04
1:A:45:U:H2'	1:A:46:G:C8	1.93	1.03
3:C:29:TYR:CE2	14:N:36:PHE:CE2	2.46	1.03
5:E:79:GLU:OE1	8:H:105:ARG:CG	2.07	1.02
3:C:29:TYR:CD2	14:N:36:PHE:CZ	2.47	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:U:N3	1:A:872:A:N6	2.07	1.01
1:A:558:G:H3'	1:A:559:A:H5''	1.38	1.01
3:C:59:ARG:HG2	3:C:64:VAL:HG22	1.35	1.01
20:T:66:ALA:HB3	20:T:72:LEU:HD22	1.43	1.01
20:T:67:ALA:N	20:T:72:LEU:HD21	1.75	1.01
1:A:45:U:H2'	1:A:46:G:H8	1.23	1.00
3:C:29:TYR:HD2	14:N:36:PHE:CZ	1.80	1.00
20:T:73:HIS:HE1	20:T:76:ALA:N	1.58	1.00
3:C:64:VAL:HG23	3:C:97:LYS:HD2	1.39	0.99
4:D:26:CYS:SG	26:D:300:ZN:ZN	1.51	0.98
4:D:36:ARG:HD2	4:D:38:TYR:HH	1.27	0.98
20:T:73:HIS:CE1	20:T:76:ALA:N	2.30	0.98
1:A:439:A:OP2	1:A:493:G:C2	2.16	0.98
1:A:920:U:H2'	1:A:921:U:C6	1.98	0.97
4:D:13:ARG:NH2	4:D:36:ARG:CZ	2.27	0.97
1:A:560:U:H2'	5:E:123:LEU:HD22	1.47	0.97
1:A:80:G:H3'	1:A:81:U:H5''	1.46	0.96
1:A:827:U:H3	1:A:872:A:N6	1.60	0.96
3:C:59:ARG:HG2	3:C:64:VAL:CG2	1.94	0.96
20:T:41:ILE:HD11	20:T:87:LYS:HE2	1.44	0.96
5:E:16:THR:CG2	5:E:27:ARG:O	2.14	0.95
14:N:24:CYS:HG	26:N:101:ZN:ZN	0.66	0.95
1:A:92:C:H2'	1:A:93:G:C8	2.01	0.95
4:D:36:ARG:HG3	4:D:38:TYR:CZ	2.01	0.95
4:D:36:ARG:CG	4:D:38:TYR:CZ	2.50	0.94
1:A:246:A:H3'	17:Q:100:LYS:HA	1.46	0.94
1:A:1081:G:OP2	1:A:1081:G:H8	1.49	0.94
5:E:15:ARG:CZ	5:E:26:PHE:CE2	2.52	0.93
1:A:262:A:H5'	20:T:73:HIS:NE2	1.85	0.92
4:D:13:ARG:HH21	4:D:36:ARG:CZ	1.81	0.92
1:A:664:G:H22	1:A:741:G:H1	1.08	0.91
1:A:1219:U:H2'	1:A:1220:G:H8	1.36	0.91
1:A:10:A:H2'	1:A:11:G:C8	2.04	0.91
20:T:67:ALA:N	20:T:72:LEU:CD2	2.34	0.91
1:A:920:U:C2	1:A:1080:A:C2	2.58	0.91
20:T:72:LEU:HD11	20:T:77:ALA:HB2	1.51	0.90
1:A:19:C:H2'	1:A:20:U:C6	2.07	0.90
17:Q:41:LYS:HZ3	17:Q:92:ARG:NH2	1.42	0.90
1:A:914:A:H2'	1:A:915:A:H8	1.36	0.89
4:D:9:CYS:HG	26:D:300:ZN:ZN	0.88	0.88
1:A:955:U:H1'	1:A:1227:A:H61	1.39	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:90:ILE:HA	17:Q:93:GLN:NE2	1.89	0.87
23:X:130:PRO:O	23:X:134:GLU:HB2	1.74	0.87
5:E:15:ARG:NH2	5:E:26:PHE:CE2	2.43	0.87
1:A:16:A:H2	1:A:1079:G:N3	1.72	0.87
3:C:55:VAL:HG13	3:C:66:VAL:HG11	1.57	0.87
1:A:558:G:H3'	1:A:559:A:C5'	2.05	0.87
1:A:123:C:H2'	1:A:124:G:H8	1.40	0.86
10:J:16:LEU:HD23	10:J:70:ARG:HG2	1.56	0.86
1:A:15:G:H2'	1:A:16:A:C8	2.11	0.86
1:A:662:G:H2'	1:A:663:A:C8	2.11	0.86
3:C:29:TYR:CE2	14:N:36:PHE:HE2	1.86	0.86
14:N:24:CYS:SG	26:N:101:ZN:ZN	1.62	0.86
1:A:15:G:H2'	1:A:16:A:H8	1.41	0.85
1:A:973:G:H3'	1:A:974:A:H5''	1.58	0.85
1:A:18:C:O4'	1:A:1078:U:C2	2.30	0.85
20:T:41:ILE:HD13	20:T:87:LYS:HD3	1.57	0.85
1:A:1077:G:N2	1:A:1079:G:H3'	1.91	0.85
10:J:50:ILE:HG13	10:J:60:ARG:HG2	1.59	0.85
1:A:1219:U:H2'	1:A:1220:G:C8	2.12	0.84
1:A:10:A:H2'	1:A:11:G:H8	1.42	0.84
4:D:36:ARG:CG	4:D:38:TYR:CE2	2.61	0.84
3:C:30:ARG:HD3	14:N:35:ARG:O	1.77	0.83
1:A:18:C:H2'	1:A:19:C:C1'	2.06	0.83
4:D:162:LEU:HD12	4:D:178:VAL:HG23	1.61	0.82
1:A:914:A:H2'	1:A:915:A:C8	2.13	0.82
1:A:920:U:H2'	1:A:921:U:H6	1.39	0.82
16:P:59:TRP:O	16:P:62:VAL:HG22	1.79	0.82
1:A:247:G:P	17:Q:100:LYS:HD2	2.19	0.82
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.14	0.82
1:A:316:G:H1	1:A:337:C:H42	1.26	0.81
1:A:917:G:H2'	1:A:918:A:C8	2.14	0.81
1:A:1079:G:H5'	5:E:14:ARG:NH2	1.95	0.81
4:D:36:ARG:HB2	4:D:36:ARG:HH11	1.45	0.81
1:A:17:U:O2'	1:A:1078:U:O2	1.98	0.81
1:A:17:U:C2'	1:A:1078:U:O2	2.29	0.80
1:A:656:C:H4'	15:O:62:GLN:HE22	1.45	0.80
1:A:743:U:H2'	1:A:744:C:C6	2.17	0.80
1:A:1081:G:OP2	1:A:1081:G:C8	2.33	0.80
1:A:123:C:H2'	1:A:124:G:C8	2.14	0.80
1:A:674:G:H2'	1:A:675:A:H8	1.45	0.80
7:G:74:GLU:HG2	7:G:91:VAL:HG13	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:66:ALA:C	20:T:72:LEU:CD2	2.54	0.80
1:A:46:G:H2'	1:A:366:C:C5	2.17	0.80
1:A:361:G:H2'	1:A:362:G:O4'	1.82	0.80
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.64	0.80
4:D:36:ARG:O	4:D:38:TYR:N	2.15	0.79
1:A:1367:C:H4'	10:J:48:THR:HG21	1.64	0.79
1:A:78:G:H2'	1:A:79:G:O4'	1.82	0.79
1:A:814:A:H2'	1:A:816:A:H5''	1.64	0.79
3:C:64:VAL:CG2	3:C:97:LYS:HD2	2.12	0.79
3:C:64:VAL:O	3:C:99:VAL:HG23	1.83	0.79
1:A:745:C:H2'	1:A:746:A:C8	2.18	0.78
22:W:32:ILE:O	22:W:32:ILE:HD13	1.81	0.78
1:A:665:A:N6	1:A:724:G:O6	2.17	0.78
17:Q:41:LYS:HZ3	17:Q:92:ARG:HH22	1.28	0.78
20:T:66:ALA:HB1	20:T:72:LEU:HD22	1.62	0.78
1:A:18:C:C2'	1:A:19:C:O4'	2.32	0.78
1:A:426:G:OP1	4:D:36:ARG:CD	2.31	0.77
1:A:562:C:H41	1:A:884:U:H2'	1.50	0.77
1:A:584:G:H2'	1:A:585:G:H8	1.50	0.77
1:A:544:G:OP1	4:D:62:GLN:HG3	1.84	0.77
20:T:41:ILE:HD12	20:T:91:LEU:CD1	2.14	0.77
1:A:269:C:H2'	1:A:270:A:C8	2.20	0.76
4:D:13:ARG:NH2	4:D:36:ARG:NE	2.32	0.76
1:A:69:G:H1	1:A:100:C:H42	1.32	0.76
1:A:222:U:H2'	1:A:223:U:C6	2.20	0.76
1:A:1255:G:H2'	1:A:1279:A:N6	2.00	0.76
1:A:16:A:H1'	1:A:1080:A:O4'	1.85	0.76
3:C:29:TYR:HE2	14:N:36:PHE:HE2	1.34	0.76
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.66	0.76
3:C:97:LYS:HB2	3:C:97:LYS:HZ3	1.50	0.75
23:X:92:VAL:HG13	23:X:132:LEU:HD13	1.67	0.75
23:X:102:LYS:O	23:X:106:ILE:HG13	1.84	0.75
2:B:61:LEU:HD11	2:B:160:ASP:HB3	1.67	0.75
1:A:99:U:H2'	1:A:100:C:C6	2.22	0.75
3:C:30:ARG:HG3	14:N:36:PHE:O	1.87	0.75
4:D:36:ARG:HH11	4:D:36:ARG:CB	2.00	0.75
1:A:67:C:H2'	1:A:68:G:C8	2.22	0.75
1:A:584:G:H2'	1:A:585:G:C8	2.21	0.75
1:A:926:G:H8	1:A:926:G:O5'	1.69	0.75
4:D:98:GLU:HA	4:D:103:ASN:HD22	1.50	0.75
1:A:1356:G:H2'	1:A:1357:A:C8	2.21	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:G:H2'	1:A:22:G:C8	2.22	0.74
8:H:53:VAL:C	8:H:54:ASP:OD1	2.31	0.74
1:A:1256:A:H3'	3:C:27:LYS:CE	2.17	0.74
1:A:1256:A:C3'	3:C:27:LYS:NZ	2.07	0.74
17:Q:94:ASN:O	17:Q:97:SER:HB3	1.85	0.74
20:T:72:LEU:HD11	20:T:77:ALA:CB	2.18	0.74
1:A:919:A:C2	1:A:1079:G:N2	2.55	0.74
4:D:34:GLU:OE1	4:D:34:GLU:HA	1.86	0.74
10:J:50:ILE:HG23	10:J:59:SER:O	1.87	0.74
1:A:1099:G:C6	1:A:1100:C:N3	2.56	0.73
3:C:25:GLY:O	3:C:29:TYR:HB2	1.88	0.73
1:A:729:A:H2'	1:A:730:G:H8	1.53	0.73
1:A:952:U:H2'	1:A:953:G:H8	1.54	0.73
1:A:662:G:H2'	1:A:663:A:H8	1.50	0.73
20:T:38:LYS:O	20:T:41:ILE:CG2	2.31	0.73
1:A:830:G:H4'	2:B:23:ARG:HA	1.71	0.73
1:A:1152:A:OP1	10:J:70:ARG:NH2	2.21	0.73
1:A:926:G:H3'	1:A:1505:G:H21	1.54	0.72
5:E:16:THR:CG2	5:E:27:ARG:HG2	2.19	0.72
5:E:27:ARG:NH1	5:E:27:ARG:HB2	2.04	0.72
8:H:12:ARG:HD2	8:H:26:VAL:HG12	1.72	0.72
23:X:61:ASP:HB3	23:X:64:LYS:HB3	1.70	0.72
1:A:1386:G:H2'	1:A:1387:G:H8	1.54	0.72
11:K:15:ALA:HA	11:K:77:MET:HA	1.70	0.72
1:A:61:G:H2'	1:A:62:U:O4'	1.90	0.72
1:A:790:A:H2'	1:A:791:G:C8	2.25	0.72
4:D:95:GLY:HA2	4:D:189:PRO:HG2	1.70	0.72
20:T:66:ALA:CB	20:T:72:LEU:CD2	2.66	0.72
20:T:41:ILE:CD1	20:T:91:LEU:HD11	2.20	0.72
4:D:13:ARG:CZ	4:D:36:ARG:HG2	2.19	0.71
8:H:82:HIS:HE1	8:H:84:ARG:HB2	1.54	0.71
1:A:277:C:H5'	17:Q:68:ARG:NH2	2.03	0.71
4:D:36:ARG:HG3	4:D:38:TYR:CD2	2.25	0.71
1:A:1127:G:H21	1:A:1147:C:H41	1.36	0.71
3:C:55:VAL:HG13	3:C:66:VAL:CG1	2.20	0.71
3:C:65:ALA:HB1	3:C:100:ALA:O	1.90	0.71
1:A:1435:G:H2'	1:A:1436:U:C6	2.26	0.71
8:H:82:HIS:CE1	8:H:84:ARG:HB2	2.25	0.71
1:A:1086:U:H5''	1:A:1389:C:H5''	1.73	0.71
1:A:1359:C:H3'	14:N:35:ARG:HH21	1.54	0.71
1:A:1475:G:H2'	1:A:1476:G:H8	1.53	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:U:N3	1:A:915:A:N6	2.38	0.71
1:A:188:C:H5'	20:T:89:ARG:HD3	1.73	0.71
5:E:15:ARG:NE	5:E:26:PHE:HE2	1.57	0.70
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.72	0.70
1:A:90:U:H2'	1:A:91:C:C6	2.27	0.70
1:A:262:A:C5'	20:T:73:HIS:NE2	2.55	0.70
1:A:398:C:H2'	1:A:399:G:H8	1.56	0.70
1:A:1422:G:H1	1:A:1478:C:H42	1.39	0.70
3:C:64:VAL:HG23	3:C:97:LYS:CD	2.17	0.70
4:D:9:CYS:SG	26:D:300:ZN:ZN	1.79	0.70
1:A:278:G:C8	17:Q:92:ARG:NH1	2.59	0.70
16:P:58:TYR:O	16:P:62:VAL:HG13	1.92	0.70
1:A:17:U:H2'	1:A:1078:U:O2	1.92	0.69
1:A:69:G:H1	1:A:100:C:N4	1.89	0.69
5:E:16:THR:HG21	5:E:27:ARG:HG2	1.73	0.69
1:A:426:G:OP1	4:D:36:ARG:CZ	2.38	0.69
20:T:74:LYS:HB3	20:T:74:LYS:NZ	2.07	0.69
1:A:920:U:O2	1:A:1080:A:C2	2.45	0.69
20:T:41:ILE:HD11	20:T:91:LEU:HD11	1.74	0.69
1:A:266:G:C8	1:A:266:G:H5''	2.27	0.69
1:A:124:G:H2'	1:A:125:U:O4'	1.92	0.69
1:A:1392:G:N2	1:A:1502:A:H8	1.89	0.69
1:A:170:U:H2'	1:A:171:A:H8	1.55	0.69
1:A:313:A:H2'	1:A:314:C:C6	2.27	0.69
1:A:737:A:H2'	1:A:738:C:C6	2.28	0.69
1:A:864:A:H2'	1:A:865:A:C8	2.28	0.69
1:A:1342:C:H2'	1:A:1343:G:H8	1.58	0.69
4:D:36:ARG:HD2	4:D:38:TYR:CE1	2.22	0.69
1:A:524:G:C6	1:A:525:C:N4	2.60	0.69
1:A:955:U:H1'	1:A:1227:A:N6	2.07	0.68
1:A:1079:G:H2'	1:A:1080:A:C8	2.28	0.68
1:A:1443:G:C6	1:A:1444:C:N4	2.62	0.68
11:K:90:GLY:O	11:K:93:GLN:N	2.26	0.68
1:A:1097:C:H5'	2:B:140:HIS:HE1	1.56	0.68
1:A:392:G:H2'	1:A:393:A:C8	2.28	0.68
1:A:1095:U:H2'	1:A:1096:C:C6	2.28	0.68
1:A:560:U:H5'	1:A:566:G:N2	2.08	0.68
1:A:1022:G:H2'	1:A:1023:G:H8	1.57	0.68
1:A:883:C:H2'	1:A:884:U:C6	2.28	0.68
1:A:1475:G:H2'	1:A:1476:G:C8	2.28	0.68
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.75	0.68
20:T:73:HIS:CE1	20:T:75:ASN:HB3	2.28	0.68
1:A:277:C:H5'	17:Q:68:ARG:HH22	1.59	0.68
1:A:376:G:H2'	1:A:377:G:H8	1.58	0.68
1:A:555:C:H2'	1:A:556:C:C6	2.28	0.68
1:A:674:G:H2'	1:A:675:A:C8	2.28	0.68
1:A:1358:U:H3	1:A:1363(A):A:H61	1.41	0.68
6:F:78:GLU:HA	6:F:81:ILE:HD12	1.76	0.68
1:A:233:C:H2'	1:A:234:C:H6	1.58	0.67
1:A:524:G:C2	1:A:525:C:N3	2.62	0.67
2:B:174:VAL:HG22	2:B:184:VAL:HG21	1.76	0.67
1:A:397:A:N3	1:A:397:A:H5''	2.10	0.67
1:A:779:C:O2'	11:K:120:ARG:HD2	1.94	0.67
1:A:1281:U:H5'	1:A:1282:C:H5	1.57	0.67
18:R:36:ASN:O	18:R:40:LEU:HD12	1.93	0.67
23:X:34:ALA:HB1	23:X:45:LEU:HD13	1.76	0.67
4:D:64:LEU:HD11	4:D:198:VAL:HG23	1.76	0.67
5:E:83:GLU:HG2	5:E:88:LYS:HA	1.77	0.67
1:A:1126:U:O2	1:A:1126:U:H2'	1.93	0.67
1:A:46:G:H2'	1:A:366:C:H5	1.60	0.67
4:D:22:LYS:HG3	4:D:26:CYS:SG	2.34	0.67
19:S:19:VAL:HG21	19:S:44:MET:HG2	1.76	0.67
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.76	0.67
5:E:18:ARG:CB	5:E:25:ARG:O	2.38	0.67
1:A:247:G:OP2	17:Q:100:LYS:CD	2.33	0.67
1:A:1105:A:H2'	1:A:1106:G:H8	1.60	0.67
5:E:15:ARG:HE	5:E:26:PHE:HE2	0.73	0.67
9:I:50:LEU:HD21	9:I:85:LEU:HD11	1.76	0.67
20:T:66:ALA:HB3	20:T:72:LEU:CD2	2.22	0.67
1:A:299:G:H2'	1:A:300:A:C8	2.29	0.67
1:A:1158:C:H5'	2:B:132:LYS:HG2	1.75	0.66
1:A:521:G:N2	1:A:522:C:C2	2.64	0.66
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.76	0.66
11:K:33:THR:HA	11:K:39:PRO:HA	1.77	0.66
1:A:316:G:H1	1:A:337:C:N4	1.93	0.66
1:A:868:C:H2'	1:A:869:G:O4'	1.95	0.66
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.77	0.66
1:A:34:C:H2'	1:A:35:G:C8	2.30	0.66
1:A:671:G:N2	1:A:736:C:C2	2.62	0.66
4:D:129:ASN:HD21	4:D:145:GLU:H	1.43	0.66
1:A:262:A:H4'	20:T:75:ASN:HB3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:G:O6	4:D:35:ARG:CZ	2.44	0.66
1:A:1366:C:H2'	1:A:1367:C:C6	2.31	0.66
1:A:729:A:H2'	1:A:730:G:C8	2.30	0.66
1:A:1128:C:H2'	1:A:1139:G:N7	2.11	0.66
2:B:111:ARG:HD3	2:B:145:LEU:HD21	1.78	0.66
3:C:30:ARG:CD	14:N:35:ARG:O	2.43	0.66
10:J:22:LYS:HE2	10:J:90:LEU:HD12	1.77	0.66
1:A:543:C:H2'	1:A:544:G:H8	1.60	0.66
1:A:673:G:H2'	1:A:674:G:C8	2.31	0.66
1:A:16:A:C2	1:A:1079:G:N2	2.64	0.65
1:A:1264:C:H2'	1:A:1265:G:H8	1.61	0.65
1:A:1342:C:H2'	1:A:1343:G:C8	2.30	0.65
1:A:377:G:H2'	1:A:378:G:C8	2.32	0.65
4:D:98:GLU:HB3	4:D:189:PRO:HG3	1.78	0.65
1:A:15:G:C2'	1:A:16:A:H8	2.08	0.65
1:A:736:C:H2'	1:A:737:A:C8	2.31	0.65
1:A:946:A:H2'	1:A:947:G:C8	2.31	0.65
1:A:1457:G:H5''	1:A:1457:G:C8	2.32	0.65
5:E:102:ALA:O	5:E:107:ARG:NH1	2.30	0.65
1:A:757:U:H2'	1:A:758:G:O4'	1.96	0.65
1:A:1218:C:H2'	1:A:1219:U:C6	2.31	0.65
1:A:1386:G:H2'	1:A:1387:G:C8	2.31	0.65
4:D:8:VAL:HG12	4:D:9:CYS:N	2.11	0.65
8:H:52:ASP:OD1	8:H:54:ASP:O	2.15	0.65
20:T:41:ILE:HD11	20:T:87:LYS:CE	2.21	0.65
1:A:1077:G:H2'	1:A:1079:G:N7	2.11	0.65
4:D:13:ARG:HH21	4:D:36:ARG:NH2	1.94	0.65
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.78	0.65
1:A:269:C:H2'	1:A:270:A:H8	1.61	0.65
3:C:30:ARG:CZ	14:N:35:ARG:O	2.44	0.64
11:K:109:VAL:HG13	18:R:84:LYS:HB3	1.78	0.64
15:O:64:ARG:HA	15:O:67:LEU:HD12	1.77	0.64
20:T:66:ALA:C	20:T:72:LEU:HD23	2.20	0.64
1:A:952:U:H2'	1:A:953:G:C8	2.32	0.64
8:H:86:ILE:HD11	8:H:136:GLU:HB2	1.79	0.64
1:A:671:G:C2	1:A:736:C:N3	2.66	0.64
1:A:1536:C:H42	24:Y:29:G:H1	1.45	0.64
5:E:27:ARG:CB	5:E:27:ARG:HH11	2.11	0.64
11:K:52:GLY:O	11:K:55:LYS:HB2	1.98	0.64
20:T:41:ILE:CD1	20:T:87:LYS:HE2	2.22	0.64
1:A:1079:G:H5'	5:E:14:ARG:HH22	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:THR:HG23	3:C:180:ALA:HB2	1.79	0.64
14:N:24:CYS:HB3	14:N:29:ARG:H	1.61	0.64
1:A:224:C:H2'	1:A:225:C:C6	2.32	0.64
1:A:792:A:H4'	1:A:793:U:C5'	2.28	0.64
2:B:36:ARG:HB2	2:B:41:ILE:HD12	1.80	0.64
20:T:72:LEU:CD1	20:T:77:ALA:HB2	2.27	0.64
1:A:774:G:N2	1:A:806:C:C2	2.66	0.64
1:A:1225:A:H4'	19:S:78:ARG:HD3	1.79	0.64
1:A:1410:G:H2'	1:A:1411:C:C6	2.32	0.64
1:A:1445:C:C2	1:A:1458:G:C2	2.86	0.64
1:A:1520:G:H2'	1:A:1521:G:C8	2.33	0.64
10:J:4:ILE:HD11	10:J:77:PRO:HB3	1.80	0.64
8:H:104:ARG:HG3	8:H:138:TRP:CD1	2.33	0.63
1:A:67:C:H2'	1:A:68:G:H8	1.64	0.63
12:L:73:GLU:H	12:L:110:VAL:HG21	1.62	0.63
1:A:919:A:H2	1:A:1079:G:N2	1.95	0.63
20:T:41:ILE:CD1	20:T:91:LEU:CD1	2.76	0.63
1:A:13:U:H3	1:A:915:A:N6	1.95	0.63
1:A:1022:G:H2'	1:A:1023:G:C8	2.33	0.63
1:A:1416:G:H2'	1:A:1417:G:O4'	1.99	0.63
1:A:1422:G:H1	1:A:1478:C:N4	1.96	0.63
1:A:56:U:H2'	1:A:57:G:C8	2.34	0.63
1:A:398:C:H2'	1:A:399:G:C8	2.34	0.63
5:E:15:ARG:NH2	5:E:26:PHE:CE1	2.55	0.63
10:J:38:ILE:CG2	10:J:71:LEU:O	2.47	0.63
1:A:917:G:H2'	1:A:918:A:H8	1.60	0.62
1:A:1073:U:H3	1:A:1102:A:H61	1.46	0.62
1:A:1077:G:H22	1:A:1079:G:H3'	1.64	0.62
3:C:57:ILE:CG1	3:C:66:VAL:CG2	2.42	0.62
1:A:17:U:H2'	1:A:18:C:C5	2.35	0.62
1:A:18:C:C4	1:A:19:C:C4	2.86	0.62
1:A:148:G:H2'	1:A:149:A:C8	2.35	0.62
1:A:194:C:H5''	20:T:65:LYS:HE2	1.80	0.62
1:A:827:U:C4	1:A:872:A:N1	2.65	0.62
1:A:392:G:H2'	1:A:393:A:H8	1.63	0.62
20:T:41:ILE:HD13	20:T:87:LYS:CD	2.27	0.62
1:A:588:G:N2	1:A:589:C:C2	2.67	0.62
1:A:170:U:H2'	1:A:171:A:C8	2.35	0.62
1:A:457:C:H2'	1:A:458:C:C6	2.35	0.61
2:B:76:GLN:HB3	2:B:208:ILE:HG12	1.80	0.61
3:C:97:LYS:HB2	3:C:97:LYS:NZ	2.11	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:C:O2	1:A:564:C:H2'	1.99	0.61
5:E:27:ARG:HB2	5:E:27:ARG:HH11	1.64	0.61
1:A:1016:A:H2'	1:A:1017:G:O4'	2.00	0.61
1:A:1437:C:H2'	1:A:1438:G:H8	1.64	0.61
1:A:1488:G:H2'	1:A:1489:G:H8	1.65	0.61
24:Y:27:G:H2'	24:Y:28:A:O4'	1.99	0.61
1:A:1342:C:H5''	9:I:125:TYR:CZ	2.35	0.61
1:A:1390:U:H2'	1:A:1391:U:C6	2.35	0.61
1:A:512:U:H2'	1:A:513:C:C6	2.35	0.61
20:T:41:ILE:CD1	20:T:87:LYS:CE	2.77	0.61
20:T:51:GLU:HA	20:T:54:LYS:HE3	1.82	0.61
1:A:128:G:N2	1:A:234:C:C2	2.68	0.61
1:A:391:G:H2'	1:A:392:G:O4'	2.00	0.61
2:B:68:ILE:HD12	2:B:222:ILE:HD11	1.83	0.61
4:D:68:TYR:HB2	4:D:70:ILE:HD11	1.83	0.61
23:X:123:ARG:HG3	23:X:124:GLY:H	1.66	0.61
1:A:602:A:H2'	1:A:603:U:O4'	2.00	0.61
18:R:32:ARG:HA	18:R:69:THR:HG21	1.80	0.61
10:J:53:PRO:HB3	14:N:42:ILE:HG12	1.82	0.61
20:T:73:HIS:CE1	20:T:75:ASN:CB	2.83	0.61
1:A:224:C:OP1	20:T:74:LYS:HD2	2.00	0.61
9:I:44:VAL:HG12	9:I:47:LEU:HD12	1.82	0.60
20:T:74:LYS:HB3	20:T:74:LYS:HZ3	1.65	0.60
4:D:201:GLN:NE2	5:E:116:THR:OG1	2.34	0.60
8:H:54:ASP:OD1	8:H:54:ASP:N	2.34	0.60
11:K:18:ARG:HG3	11:K:81:ASP:HB3	1.82	0.60
1:A:967:C:H2'	1:A:968:A:C8	2.36	0.60
1:A:543:C:H2'	1:A:544:G:C8	2.37	0.60
1:A:920:U:O2'	1:A:1081:G:O2'	2.16	0.60
1:A:998:G:N2	1:A:999:C:C2	2.70	0.60
1:A:1103:C:H2'	1:A:1104:G:O4'	2.01	0.60
1:A:1255:G:H2'	1:A:1279:A:H62	1.66	0.60
4:D:31:CYS:C	4:D:33:MET:H	2.09	0.60
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.82	0.60
1:A:233:C:H2'	1:A:234:C:C6	2.37	0.60
1:A:262:A:C5'	20:T:73:HIS:CE1	2.84	0.60
1:A:860:A:H3'	1:A:861:G:H8	1.65	0.60
1:A:1071:C:H2'	1:A:1072:G:H8	1.67	0.60
22:W:36:ILE:HG12	22:W:40:MET:HB2	1.84	0.60
3:C:55:VAL:CG1	3:C:66:VAL:HG11	2.30	0.60
1:A:16:A:H2	1:A:1079:G:C2	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:A:H4'	1:A:975:A:H3'	1.83	0.60
3:C:22:TRP:HB3	3:C:59:ARG:H	1.67	0.60
1:A:18:C:N4	1:A:19:C:N4	2.50	0.60
1:A:718:G:H5'	11:K:117:ASN:HB2	1.83	0.60
2:B:84:GLU:HG2	2:B:87:ARG:HH21	1.67	0.60
4:D:31:CYS:HB3	4:D:33:MET:HB2	1.83	0.60
1:A:262:A:H5'	20:T:73:HIS:CE1	2.36	0.59
1:A:424:G:H2'	1:A:425:G:H8	1.67	0.59
1:A:918:A:H2'	1:A:919:A:O4'	2.02	0.59
1:A:1077:G:C5	1:A:1079:G:OP2	2.55	0.59
3:C:30:ARG:CG	14:N:36:PHE:O	2.50	0.59
1:A:962:C:H1'	1:A:1201:A:N6	2.17	0.59
1:A:1521:G:H2'	1:A:1522:U:C6	2.37	0.59
1:A:664:G:N2	1:A:741:G:H1	1.89	0.59
2:B:15:VAL:HG11	2:B:209:ARG:HB3	1.84	0.59
1:A:501:C:OP1	12:L:117:ARG:NH2	2.35	0.59
1:A:19:C:C2'	1:A:20:U:C6	2.83	0.59
1:A:568:G:N2	1:A:883:C:C2	2.71	0.59
1:A:1081:G:OP1	5:E:17:ALA:O	2.21	0.59
20:T:38:LYS:C	20:T:41:ILE:HG22	2.24	0.59
1:A:302:G:H2'	1:A:303:A:C8	2.38	0.59
1:A:1264:C:H2'	1:A:1265:G:C8	2.37	0.59
1:A:1542:U:H4'	18:R:18:ARG:H	1.67	0.59
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.84	0.59
1:A:224:C:OP1	20:T:74:LYS:CD	2.51	0.59
1:A:1370:G:H5'	9:I:12:GLU:HG3	1.85	0.59
1:A:33:A:H2'	1:A:34:C:C6	2.38	0.59
1:A:376:G:H5''	16:P:5:ARG:HB2	1.85	0.59
1:A:216:G:C6	1:A:217:C:N4	2.71	0.58
1:A:921:U:H4'	1:A:1082:G:H5'	1.85	0.58
1:A:955:U:C1'	1:A:1227:A:H61	2.13	0.58
1:A:1353:G:N2	1:A:1354:C:C2	2.70	0.58
8:H:28:ALA:HA	8:H:59:LEU:HD12	1.85	0.58
1:A:1151:A:HO2'	1:A:1152:A:H8	1.52	0.58
7:G:73:MET:HE3	7:G:145:ALA:HB1	1.85	0.58
17:Q:90:ILE:HA	17:Q:93:GLN:HE21	1.64	0.58
20:T:53:LEU:HD11	20:T:104:LEU:HD11	1.84	0.58
1:A:735:C:H5'	18:R:71:LYS:HD3	1.86	0.58
1:A:881:G:OP2	12:L:12:ARG:NH2	2.34	0.58
1:A:389:A:H3'	1:A:390:C:C6	2.38	0.58
1:A:521:G:N1	1:A:522:C:C4	2.71	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:G:H2'	1:A:425:G:C8	2.39	0.58
4:D:13:ARG:NH2	4:D:36:ARG:NH2	2.51	0.58
1:A:1312:G:C2	1:A:1326:C:C2	2.91	0.58
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.85	0.58
1:A:335:C:H2'	1:A:336:C:C6	2.39	0.58
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.85	0.58
11:K:60:ALA:HA	11:K:63:LEU:HD12	1.86	0.58
20:T:10:LEU:HD12	20:T:11:SER:N	2.19	0.58
1:A:56:U:H2'	1:A:57:G:H8	1.68	0.58
1:A:279:A:C6	17:Q:98:LEU:HD12	2.39	0.58
1:A:303:A:H2'	1:A:304:U:H6	1.69	0.58
1:A:1241:G:N2	1:A:1242:C:C2	2.72	0.58
10:J:38:ILE:HG22	10:J:71:LEU:O	2.04	0.58
13:M:65:LYS:HG3	13:M:69:GLU:HB3	1.84	0.58
1:A:234:C:H2'	1:A:235:C:C6	2.39	0.57
1:A:457:C:H2'	1:A:458:C:H6	1.68	0.57
1:A:1488:G:H2'	1:A:1489:G:C8	2.39	0.57
1:A:430:A:P	4:D:8:VAL:H	2.27	0.57
1:A:530:G:H8	22:W:38:GLY:HA3	1.69	0.57
1:A:443:C:C2	1:A:492:G:N2	2.72	0.57
1:A:701:C:H4'	1:A:702:A:O5'	2.04	0.57
1:A:1287:A:H2'	1:A:1288:A:C8	2.39	0.57
1:A:1405:G:H2'	1:A:1406:U:C6	2.39	0.57
1:A:1513:A:H2'	1:A:1514:C:C6	2.39	0.57
4:D:194:LEU:CD2	4:D:196:LEU:HG	2.35	0.57
20:T:63:ILE:CG2	20:T:77:ALA:HB1	2.35	0.57
23:X:85:VAL:HA	23:X:115:LYS:O	2.04	0.57
1:A:253:U:H2'	1:A:254:G:H8	1.70	0.57
1:A:918:A:H2'	1:A:919:A:C8	2.40	0.57
1:A:17:U:N3	1:A:1079:G:N2	2.53	0.57
1:A:28:G:H2'	1:A:29:G:O4'	2.04	0.57
1:A:109:A:H5'	1:A:110:C:H5	1.69	0.57
1:A:1114:C:H2'	1:A:1115:C:C6	2.40	0.57
1:A:18:C:H5'	1:A:1078:U:H1'	1.86	0.57
1:A:184:G:H2'	1:A:185:A:H8	1.70	0.57
1:A:1233:G:C6	1:A:1234:C:N4	2.72	0.57
1:A:1389:C:H2'	1:A:1390:U:C6	2.39	0.57
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.86	0.57
1:A:259:G:H2'	1:A:260:G:C8	2.39	0.57
1:A:1515:C:H2'	1:A:1516:G:C8	2.39	0.57
1:A:10:A:H61	1:A:24:U:H3	1.50	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1500:A:H5''	1:A:1508:G:H5''	1.86	0.57
1:A:1536:C:N4	24:Y:29:G:H1	2.02	0.57
16:P:9:PHE:CE2	16:P:18:ARG:HG3	2.39	0.57
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.86	0.56
10:J:37:PRO:HA	10:J:72:VAL:HG22	1.85	0.56
15:O:6:GLU:HA	15:O:9:GLN:HB2	1.86	0.56
1:A:636:U:H2'	1:A:637:G:C8	2.39	0.56
1:A:988:G:N1	1:A:989:C:C2	2.73	0.56
1:A:1106:G:N2	1:A:1107:C:C2	2.73	0.56
1:A:1164:G:N2	1:A:1165:C:C2	2.73	0.56
1:A:1391:U:H2'	1:A:1392:G:C8	2.40	0.56
1:A:1443:G:C2	1:A:1444:C:N3	2.73	0.56
7:G:150:ALA:HA	11:K:59:TYR:CG	2.39	0.56
15:O:31:LEU:O	15:O:35:ARG:HG3	2.05	0.56
1:A:216:G:C2	1:A:217:C:N3	2.74	0.56
1:A:589:C:O2	1:A:651:C:O2	2.24	0.56
1:A:648:A:H2'	1:A:649:G:C8	2.41	0.56
1:A:836:G:H2'	1:A:837:G:C8	2.39	0.56
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.87	0.56
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.87	0.56
1:A:1464:G:N2	1:A:1465:C:C2	2.73	0.56
1:A:1495:U:H5'	23:X:93:LYS:HB2	1.87	0.56
1:A:662:G:C2	1:A:744:C:O2	2.59	0.56
1:A:701:C:N4	23:X:67:TYR:HB2	2.20	0.56
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.86	0.56
16:P:28:ARG:HD2	16:P:29:ASP:OD1	2.04	0.56
5:E:87:SER:HA	5:E:125:SER:HB3	1.88	0.56
1:A:18:C:C4	1:A:19:C:N4	2.73	0.56
1:A:34:C:H2'	1:A:35:G:H8	1.70	0.56
1:A:197:A:C6	1:A:221:C:H4'	2.40	0.56
1:A:377:G:H2'	1:A:378:G:H8	1.70	0.56
1:A:389:A:H3'	1:A:390:C:H6	1.70	0.56
10:J:38:ILE:O	10:J:71:LEU:N	2.23	0.56
11:K:90:GLY:O	11:K:91:ARG:C	2.47	0.55
1:A:500:G:H2'	1:A:501:C:C6	2.42	0.55
1:A:1097:C:H5'	2:B:140:HIS:CE1	2.39	0.55
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.87	0.55
20:T:63:ILE:HG23	20:T:77:ALA:HB1	1.88	0.55
20:T:67:ALA:CA	20:T:72:LEU:HD21	2.35	0.55
22:W:2:LYS:HD3	22:W:4:LYS:HE2	1.88	0.55
23:X:131:GLU:O	23:X:135:ARG:HB2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:U:O4	1:A:752:G:O2'	2.22	0.55
1:A:397:A:N3	1:A:397:A:H3'	2.22	0.55
1:A:725:G:N2	1:A:726:C:C2	2.75	0.55
1:A:1162:C:C2	1:A:1175:G:N2	2.74	0.55
1:A:1456:G:N2	1:A:1457:G:C8	2.75	0.55
1:A:522:C:H41	12:L:53:ARG:HH21	1.54	0.55
1:A:777:A:H2'	1:A:778:G:C8	2.42	0.55
1:A:975:A:H5''	1:A:975:A:C8	2.41	0.55
4:D:13:ARG:HH22	4:D:36:ARG:NE	2.03	0.55
8:H:49:GLU:HG2	8:H:60:ARG:HB2	1.89	0.55
20:T:42:GLN:O	20:T:45:GLN:HB2	2.07	0.55
1:A:769:G:N2	1:A:770:C:C2	2.74	0.55
1:A:920:U:C2	1:A:921:U:C5	2.94	0.55
1:A:1048:G:N2	1:A:1210:C:C2	2.75	0.55
1:A:582:U:H2'	1:A:583:A:C8	2.42	0.55
1:A:745:C:H2'	1:A:746:A:H8	1.69	0.55
1:A:1505:G:H4'	1:A:1506:U:H5''	1.88	0.55
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.88	0.55
22:W:32:ILE:H	22:W:32:ILE:CD1	2.19	0.55
1:A:683:G:N2	1:A:708:C:C2	2.75	0.55
1:A:1431:C:H42	1:A:1469:G:H1	1.54	0.55
7:G:150:ALA:HA	11:K:59:TYR:HB2	1.88	0.55
16:P:2:VAL:HG13	16:P:64:ALA:HA	1.89	0.55
1:A:19:C:H2'	1:A:20:U:H6	1.65	0.54
2:B:130:ARG:HG2	3:C:179:ARG:CZ	2.37	0.54
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.88	0.54
1:A:217:C:O2'	1:A:470:C:N4	2.41	0.54
1:A:436:C:H2'	1:A:437:U:H6	1.71	0.54
1:A:71:C:H2'	1:A:72:C:O4'	2.08	0.54
1:A:263:A:OP1	20:T:79:ARG:HD3	2.08	0.54
1:A:413:G:C6	4:D:35:ARG:HD3	2.38	0.54
4:D:201:GLN:HE21	5:E:100:VAL:HG23	1.72	0.54
6:F:11:ASN:HD22	6:F:86:ARG:HH12	1.55	0.54
8:H:32:LYS:HA	8:H:35:ILE:HD12	1.89	0.54
14:N:7:ILE:HG23	14:N:10:ALA:HB3	1.89	0.54
1:A:318:G:N2	1:A:336:C:C2	2.75	0.54
1:A:1078:U:H2'	1:A:1079:G:C8	2.42	0.54
23:X:20:GLY:HA3	23:X:24:LYS:HB2	1.88	0.54
1:A:192:U:H1'	20:T:103:GLY:HA2	1.90	0.54
1:A:500:G:C6	1:A:501:C:N4	2.75	0.54
1:A:767:A:H2'	1:A:768:A:O4'	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:110:LEU:HD22	5:E:118:ILE:HG13	1.89	0.54
1:A:109:A:H5'	1:A:110:C:C5	2.42	0.54
1:A:878:G:H5'	8:H:89:PRO:HG2	1.89	0.54
1:A:998:G:N1	1:A:999:C:C4	2.76	0.54
6:F:8:ILE:HA	6:F:87:ARG:O	2.06	0.54
17:Q:93:GLN:O	17:Q:96:GLU:HB2	2.08	0.54
1:A:17:U:C2	1:A:1079:G:N2	2.76	0.54
1:A:25:C:H5'	1:A:524:G:H1'	1.89	0.54
1:A:975:A:H4'	1:A:976:G:O5'	2.07	0.54
1:A:1128:C:H1'	1:A:1146:A:H61	1.73	0.54
14:N:59:ALA:HB1	14:N:61:TRP:HZ3	1.73	0.54
1:A:76:C:H2'	1:A:77:G:H5'	1.90	0.54
1:A:590:C:C2	1:A:650:G:C2	2.96	0.54
10:J:40:LEU:HG	10:J:71:LEU:HB2	1.90	0.54
1:A:18:C:H6	1:A:18:C:O5'	1.90	0.54
1:A:354:G:N2	1:A:355:C:C2	2.75	0.54
1:A:399:G:H2'	1:A:400:C:C6	2.43	0.54
1:A:681:C:C2	1:A:710:G:N2	2.76	0.54
1:A:1459:C:H2'	1:A:1460:A:H8	1.71	0.54
1:A:525:C:H2'	1:A:526:C:C6	2.43	0.54
1:A:1438:G:N2	1:A:1439:C:C2	2.75	0.54
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.90	0.54
1:A:1163:C:C2	1:A:1174:G:N2	2.76	0.53
2:B:184:VAL:HG13	2:B:198:ASP:H	1.72	0.53
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.89	0.53
1:A:16:A:HO2'	1:A:1079:G:HO2'	1.57	0.53
1:A:101:A:H2'	1:A:102:G:H8	1.73	0.53
1:A:184:G:H2'	1:A:185:A:C8	2.43	0.53
1:A:612:C:H2'	1:A:613:C:C6	2.43	0.53
4:D:108:LEU:HD11	4:D:146:ILE:HD13	1.88	0.53
22:W:32:ILE:HD13	22:W:32:ILE:H	1.73	0.53
1:A:113:G:H2'	1:A:114:U:C6	2.43	0.53
1:A:1112:C:H5'	2:B:131:PRO:HG3	1.90	0.53
1:A:1301:U:H1'	1:A:1302:U:OP1	2.09	0.53
1:A:1312:G:N2	1:A:1326:C:C2	2.76	0.53
5:E:103:GLY:O	5:E:106:PRO:HD2	2.08	0.53
18:R:41:LYS:HA	18:R:79:LEU:HD21	1.91	0.53
24:Y:24:A:H2'	24:Y:25:A:C8	2.43	0.53
1:A:509:A:H4'	1:A:510:A:OP1	2.09	0.53
1:A:1070:U:H2'	1:A:1071:C:C6	2.44	0.53
1:A:928:G:H1	1:A:1389:C:H42	1.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:ARG:NE	14:N:35:ARG:O	2.40	0.53
3:C:123:GLN:HE22	3:C:140:ARG:HH22	1.57	0.53
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.90	0.53
22:W:32:ILE:HD13	22:W:32:ILE:C	2.32	0.53
22:W:42:MET:HE2	22:W:42:MET:HA	1.91	0.53
1:A:22:G:C2	1:A:23:C:C2	2.97	0.53
1:A:1257:U:OP2	3:C:27:LYS:HE3	2.08	0.53
1:A:1347:G:O6	9:I:10:ARG:NH2	2.41	0.53
3:C:59:ARG:HG2	3:C:64:VAL:HG21	1.88	0.53
1:A:129(A):G:HO2'	1:A:189(F):U:H2'	1.74	0.53
1:A:568:G:C2	1:A:883:C:N3	2.77	0.53
1:A:648:A:H2'	1:A:649:G:H8	1.74	0.53
1:A:720:C:H2'	1:A:721:G:C8	2.44	0.53
2:B:15:VAL:HG21	2:B:209:ARG:HG2	1.91	0.53
6:F:47:ARG:HB2	6:F:47:ARG:HH11	1.73	0.53
15:O:18:PHE:O	15:O:21:ASP:HB3	2.09	0.53
20:T:26:ASN:CB	20:T:71:THR:HG23	2.39	0.53
1:A:17:U:C2	1:A:18:C:C4	2.97	0.53
1:A:258:G:N2	1:A:269:C:C2	2.77	0.53
1:A:316:G:H2'	1:A:317:G:C8	2.43	0.53
1:A:370:C:C2	1:A:392:G:N2	2.77	0.53
1:A:501:C:H2'	1:A:502:G:C8	2.42	0.53
1:A:1132:C:H2'	1:A:1133:G:C8	2.44	0.53
1:A:1459:C:H2'	1:A:1460:A:O4'	2.09	0.53
1:A:1520:G:H2'	1:A:1521:G:H8	1.72	0.53
1:A:803:G:H2'	1:A:804:U:O4'	2.08	0.53
1:A:1256:A:C2'	3:C:27:LYS:NZ	2.71	0.53
1:A:1270:C:H2'	1:A:1271:G:H8	1.72	0.53
1:A:1366:C:C2'	10:J:60:ARG:HH12	2.18	0.53
1:A:1494:G:C8	22:W:18:PRO:HG3	2.43	0.53
2:B:29:ALA:HA	2:B:32:ILE:HD12	1.91	0.53
1:A:774:G:C2	1:A:806:C:C2	2.96	0.52
1:A:524:G:H8	1:A:524:G:OP1	1.93	0.52
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.90	0.52
24:Y:33:A:H2'	24:Y:33:A:N3	2.23	0.52
1:A:218:C:H2'	1:A:219:C:C6	2.44	0.52
1:A:1104:G:OP1	2:B:144:ARG:NH1	2.42	0.52
1:A:22:G:C6	1:A:23:C:C4	2.97	0.52
1:A:430:A:OP2	4:D:8:VAL:HB	2.10	0.52
1:A:939:G:C6	1:A:940:C:N4	2.77	0.52
1:A:1029:C:H2'	1:A:1030:C:C6	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:C:C2	1:A:1502:A:N6	2.78	0.52
3:C:30:ARG:NH1	14:N:35:ARG:O	2.43	0.52
12:L:24:VAL:HG12	12:L:26:ALA:H	1.74	0.52
19:S:23:ASN:HD21	19:S:43:GLU:HB2	1.74	0.52
1:A:110:C:H2'	1:A:111:G:O4'	2.09	0.52
1:A:253:U:H2'	1:A:254:G:C8	2.45	0.52
1:A:1141:C:H2'	1:A:1142:G:H8	1.74	0.52
1:A:1284:C:H2'	1:A:1285:A:C8	2.45	0.52
1:A:1308:U:OP1	13:M:97:PRO:HA	2.09	0.52
19:S:30:LEU:H	19:S:48:THR:HB	1.74	0.52
1:A:80:G:H3'	1:A:81:U:C5'	2.31	0.52
1:A:552:U:H5'	12:L:86:ARG:HH11	1.75	0.52
1:A:678:U:H2'	1:A:679:C:C6	2.45	0.52
20:T:41:ILE:CD1	20:T:87:LYS:CD	2.87	0.52
1:A:571:U:H2'	1:A:572:A:H5''	1.90	0.52
1:A:1010:G:H2'	1:A:1011:G:H8	1.74	0.52
1:A:1437:C:H2'	1:A:1438:G:C8	2.44	0.52
4:D:194:LEU:HD23	4:D:196:LEU:HG	1.91	0.52
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.45	0.52
1:A:333:G:N2	1:A:334:C:C2	2.78	0.52
1:A:379:C:H2'	1:A:380:G:O4'	2.09	0.52
1:A:538:G:OP1	12:L:113:ARG:HA	2.10	0.52
1:A:623:C:H2'	1:A:624:C:O4'	2.09	0.52
1:A:921:U:H6	1:A:921:U:O5'	1.93	0.52
1:A:1079:G:C5'	5:E:14:ARG:NH2	2.71	0.52
1:A:1096:C:H2'	1:A:1097:C:C6	2.44	0.52
12:L:10:LEU:HD21	12:L:15:ARG:HE	1.74	0.52
20:T:14:LYS:HG2	20:T:18:GLN:HE21	1.74	0.52
22:W:32:ILE:CD1	22:W:32:ILE:N	2.73	0.52
1:A:661:G:C2	1:A:745:C:N3	2.78	0.52
1:A:792:A:H4'	1:A:793:U:H5'	1.92	0.52
1:A:980:C:H1'	14:N:19:ARG:HG2	1.92	0.52
1:A:1099:G:C2	1:A:1100:C:O2	2.63	0.52
1:A:1102:A:H2'	1:A:1103:C:C6	2.44	0.52
11:K:36:ASP:OD2	11:K:38:ASN:ND2	2.43	0.52
11:K:121:PRO:HG2	11:K:126:ARG:HG2	1.92	0.52
1:A:122:G:N1	1:A:123:C:C2	2.78	0.52
1:A:785:G:H1	1:A:797:C:H42	1.58	0.52
3:C:28:GLN:HA	3:C:31:HIS:CD2	2.45	0.52
1:A:1072:G:H21	2:B:107:THR:HG21	1.72	0.51
16:P:74:LEU:HD13	16:P:80:PHE:HE2	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:74:LYS:NZ	20:T:74:LYS:CB	2.73	0.51
1:A:270:A:H2'	1:A:271:C:C6	2.45	0.51
1:A:824:C:H2'	1:A:825:G:C8	2.45	0.51
1:A:1086:U:C5'	1:A:1389:C:H5''	2.39	0.51
1:A:1359:C:H3'	14:N:35:ARG:NH2	2.25	0.51
1:A:1365:G:C2	1:A:1366:C:C2	2.98	0.51
9:I:7:THR:HG23	9:I:15:ALA:O	2.11	0.51
1:A:568:G:C6	1:A:569:C:N4	2.79	0.51
1:A:946:A:H2'	1:A:947:G:H8	1.73	0.51
1:A:1081:G:H3'	1:A:1082:G:H8	1.75	0.51
24:Y:28:A:H3'	24:Y:29:G:C8	2.44	0.51
1:A:416:G:C6	1:A:417:C:N3	2.78	0.51
1:A:914:A:C4	1:A:915:A:N7	2.78	0.51
1:A:1050:G:C6	1:A:1051:C:N4	2.78	0.51
1:A:1077:G:C6	1:A:1079:G:OP2	2.64	0.51
1:A:1164:G:N1	1:A:1165:C:C4	2.78	0.51
1:A:1223:C:H5''	1:A:1224:G:H5''	1.91	0.51
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.76	0.51
2:B:134:GLU:CD	3:C:179:ARG:HH12	2.19	0.51
3:C:39:ILE:HG21	3:C:66:VAL:HG21	1.91	0.51
11:K:70:LYS:HA	11:K:73:MET:HE3	1.92	0.51
1:A:568:G:H2'	1:A:569:C:C6	2.46	0.51
1:A:755:G:N2	1:A:756:C:C2	2.78	0.51
1:A:7:G:H5'	1:A:298:A:O4'	2.11	0.51
1:A:63:C:H42	1:A:104:G:H1	1.59	0.51
1:A:972:C:H4'	10:J:57:LYS:HD2	1.93	0.51
1:A:1081:G:H2'	1:A:1082:G:H8	1.76	0.51
1:A:1358:U:H3	1:A:1363(A):A:N6	2.08	0.51
1:A:1391:U:H2'	1:A:1392:G:H8	1.75	0.51
1:A:1440:C:H42	1:A:1461:G:H1	1.57	0.51
19:S:30:LEU:HD23	19:S:50:ALA:HB2	1.91	0.51
1:A:122:G:C2	1:A:123:C:C2	2.99	0.51
1:A:243:A:H4'	1:A:244:U:O5'	2.10	0.51
8:H:91:ARG:HD3	12:L:7:ILE:HG21	1.93	0.51
9:I:50:LEU:CD2	9:I:85:LEU:HD11	2.41	0.51
1:A:286:G:H2'	1:A:287:U:O4'	2.10	0.51
1:A:309:G:H2'	1:A:310:G:H8	1.75	0.51
1:A:681:C:H42	1:A:709:G:H1	1.58	0.51
1:A:921:U:O4'	1:A:1081:G:O2'	2.28	0.51
1:A:1114:C:C2	1:A:1187:G:C2	2.99	0.51
1:A:1430:C:C2	1:A:1471:G:N2	2.79	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:106:PRO:HA	5:E:109:ILE:HD12	1.93	0.51
16:P:71:ARG:HA	16:P:74:LEU:HD12	1.93	0.51
1:A:279:A:H5''	1:A:280:C:H3'	1.92	0.51
1:A:1216:G:N2	1:A:1217:C:C2	2.78	0.51
1:A:1225:A:H2'	1:A:1225:A:N3	2.26	0.51
4:D:13:ARG:NH1	4:D:38:TYR:O	2.42	0.51
12:L:54:LYS:HG2	12:L:75:HIS:HE1	1.76	0.51
1:A:110:C:H4'	16:P:25:ARG:HB3	1.92	0.51
1:A:189:G:C2	1:A:189(A):C:C2	2.99	0.51
1:A:437:U:H3'	1:A:438:G:H8	1.75	0.51
1:A:1118:C:H2'	1:A:1119:C:C6	2.45	0.51
1:A:1162:C:C2	1:A:1175:G:C2	2.99	0.51
1:A:1525:G:H2'	1:A:1526:G:H8	1.76	0.51
5:E:58:ALA:O	5:E:61:TYR:HB2	2.10	0.51
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.46	0.51
24:Y:24:A:H2'	24:Y:25:A:H8	1.76	0.51
1:A:16:A:N1	1:A:1080:A:C2	2.80	0.50
1:A:255:G:C2	1:A:272:C:C2	2.99	0.50
1:A:643:C:H2'	1:A:644:G:H8	1.76	0.50
1:A:875:C:O2'	8:H:14:ARG:HD2	2.11	0.50
1:A:926:G:H3'	1:A:1505:G:N2	2.24	0.50
1:A:1366:C:HO2'	10:J:60:ARG:NH1	1.98	0.50
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.93	0.50
1:A:128:G:C2	1:A:234:C:C2	2.99	0.50
1:A:542:G:H2'	1:A:543:C:C6	2.46	0.50
1:A:1000:U:H2'	1:A:1001:A:H1'	1.93	0.50
1:A:1025:U:H2'	1:A:1026:G:C8	2.46	0.50
1:A:1106:G:C6	1:A:1107:C:N4	2.79	0.50
1:A:1365:G:C6	1:A:1366:C:C4	3.00	0.50
1:A:1464:G:N1	1:A:1465:C:C4	2.79	0.50
2:B:122:PHE:HZ	2:B:135:GLN:O	1.95	0.50
8:H:87:SER:HB2	8:H:133:LEU:O	2.12	0.50
20:T:36:LEU:HD12	20:T:55:ILE:HG23	1.94	0.50
23:X:89:LYS:HG3	23:X:119:THR:HG23	1.93	0.50
1:A:16:A:C2	1:A:1079:G:C2	2.99	0.50
1:A:661:G:N2	1:A:745:C:C2	2.80	0.50
2:B:42:ILE:HD11	2:B:190:THR:HB	1.93	0.50
1:A:125:U:H2'	1:A:126:G:C8	2.47	0.50
1:A:148:G:C2	1:A:175:C:C2	3.00	0.50
1:A:643:C:H2'	1:A:644:G:C8	2.46	0.50
1:A:647:C:H2'	1:A:648:A:H8	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:G:N2	1:A:875:C:C2	2.80	0.50
1:A:1081:G:H2'	1:A:1082:G:C8	2.46	0.50
3:C:97:LYS:NZ	3:C:97:LYS:CB	2.73	0.50
23:X:130:PRO:O	23:X:134:GLU:CB	2.52	0.50
1:A:45:U:C2'	1:A:46:G:H8	2.11	0.50
1:A:130:A:H8	1:A:130:A:OP1	1.95	0.50
1:A:437:U:H3'	1:A:438:G:C8	2.47	0.50
1:A:519:C:OP1	22:W:66:ARG:HD3	2.11	0.50
1:A:779:C:H2'	1:A:780:A:O4'	2.12	0.50
1:A:924:C:H5'	1:A:1399:C:OP2	2.11	0.50
1:A:1105:A:H2'	1:A:1106:G:C8	2.43	0.50
1:A:1220:G:H2'	1:A:1221:G:O4'	2.12	0.50
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.94	0.50
1:A:59:A:H5''	1:A:387:U:H5''	1.94	0.50
1:A:301:G:H2'	1:A:302:G:C8	2.47	0.50
1:A:921:U:H2'	1:A:922:G:O4'	2.12	0.50
1:A:1048:G:H5''	14:N:3:ARG:HG2	1.94	0.50
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.93	0.50
1:A:15:G:O4'	1:A:1396:A:O2'	2.30	0.50
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.11	0.50
11:K:86:GLY:HA2	11:K:112:THR:HG23	1.94	0.50
11:K:109:VAL:CG1	18:R:84:LYS:HB3	2.41	0.50
20:T:67:ALA:H	20:T:72:LEU:HD21	1.69	0.50
1:A:14:U:H1'	1:A:17:U:H5	1.77	0.50
1:A:889:A:OP2	1:A:1488:G:H5''	2.12	0.50
1:A:1010:G:H2'	1:A:1011:G:C8	2.46	0.50
1:A:1027:C:H2'	1:A:1028:C:H5'	1.92	0.50
2:B:186:ALA:O	2:B:201:ILE:HB	2.12	0.50
20:T:73:HIS:CE1	20:T:75:ASN:CA	2.95	0.50
1:A:303:A:H2'	1:A:304:U:C6	2.46	0.50
1:A:568:G:C2	1:A:883:C:C2	2.99	0.50
1:A:617:G:C6	1:A:618:C:N4	2.80	0.50
1:A:1390:U:H2'	1:A:1391:U:H6	1.75	0.50
1:A:533:A:O2'	1:A:535:A:OP1	2.29	0.49
1:A:786:G:N2	1:A:797:C:C2	2.80	0.49
3:C:9:GLY:HA2	3:C:12:LEU:HG	1.94	0.49
21:V:10:ARG:HA	21:V:13:ILE:HD12	1.93	0.49
1:A:445:G:H1	1:A:489:C:H42	1.59	0.49
1:A:479:C:H2'	1:A:480:U:O4'	2.11	0.49
1:A:932:C:H5'	7:G:3:ARG:HB3	1.94	0.49
12:L:25:PRO:C	12:L:27:LEU:H	2.18	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:7:ALA:HB3	16:P:18:ARG:HB2	1.93	0.49
17:Q:94:ASN:O	17:Q:97:SER:N	2.45	0.49
22:W:13:VAL:HG22	22:W:24:VAL:HG22	1.94	0.49
1:A:376:G:H2'	1:A:377:G:C8	2.44	0.49
1:A:553:A:O4'	12:L:31:PRO:HA	2.12	0.49
1:A:1494:G:H21	23:X:95:ASP:CB	2.26	0.49
1:A:1515:C:H2'	1:A:1516:G:H8	1.76	0.49
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.94	0.49
4:D:62:GLN:OE1	4:D:62:GLN:HA	2.11	0.49
5:E:139:LEU:O	5:E:142:LEU:HB2	2.11	0.49
18:R:74:ARG:HB3	18:R:81:PHE:CE2	2.48	0.49
1:A:189:G:C6	1:A:189(A):C:C4	3.00	0.49
1:A:516:U:O3'	22:W:2:LYS:HE3	2.11	0.49
1:A:761:G:C2	1:A:762:C:C2	3.00	0.49
1:A:910:C:H4'	1:A:1413:A:H4'	1.95	0.49
1:A:1069:C:H42	1:A:1106:G:H1	1.60	0.49
1:A:1092:A:H5''	7:G:4:ARG:CZ	2.43	0.49
1:A:1348:U:H2'	1:A:1349:A:H8	1.76	0.49
20:T:44:ALA:HB3	20:T:91:LEU:HD13	1.95	0.49
1:A:169:C:H2'	1:A:170:U:C6	2.48	0.49
1:A:946:A:O2'	1:A:1333:A:N3	2.37	0.49
1:A:1017:G:C2	1:A:1018:C:C2	3.00	0.49
1:A:1508:G:C2	1:A:1509:C:C2	3.00	0.49
2:B:23:ARG:HD3	2:B:24:TRP:H	1.78	0.49
19:S:32:LYS:HA	19:S:50:ALA:HB3	1.94	0.49
1:A:17:U:H2'	1:A:18:C:C6	2.47	0.49
1:A:397:A:H5'	1:A:398:C:OP1	2.12	0.49
1:A:502:G:H5''	12:L:119:LYS:HE3	1.95	0.49
1:A:579:G:H2'	1:A:580:U:C6	2.48	0.49
1:A:860:A:H3'	1:A:861:G:C8	2.45	0.49
3:C:59:ARG:CG	3:C:64:VAL:HG22	2.25	0.49
8:H:113:SER:HB3	8:H:132:GLU:HB3	1.93	0.49
1:A:189(K):U:H2'	1:A:189(L):G:H8	1.77	0.49
1:A:1256:A:H3'	3:C:27:LYS:HZ1	0.39	0.49
1:A:1433:A:H2'	1:A:1434:A:O4'	2.13	0.49
1:A:1508:G:H2'	1:A:1509:C:C6	2.48	0.49
13:M:108:ARG:O	13:M:112:GLY:O	2.31	0.49
15:O:41:GLU:HA	15:O:44:LYS:HD2	1.95	0.49
1:A:999:C:O2	1:A:1043:C:O2	2.30	0.49
1:A:1023:G:H2'	1:A:1023:G:N3	2.28	0.49
1:A:1251:A:H2'	1:A:1252:A:O4'	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:C2	1:A:1444:C:C4	3.01	0.49
4:D:201:GLN:CD	5:E:116:THR:OG1	2.56	0.49
6:F:74:ASP:HA	6:F:77:ARG:HD2	1.95	0.49
11:K:58:PRO:HB3	11:K:93:GLN:HG3	1.95	0.49
1:A:225:C:H2'	1:A:226:G:H8	1.78	0.49
1:A:302:G:H2'	1:A:303:A:H8	1.77	0.49
1:A:1073:U:O2'	2:B:104:ASN:OD1	2.27	0.49
1:A:1106:G:C2	1:A:1107:C:C4	3.01	0.49
1:A:1418:A:H2'	1:A:1418:A:N3	2.28	0.49
1:A:236:G:C2	1:A:237:C:C2	3.01	0.48
1:A:827:U:N3	1:A:872:A:C6	2.72	0.48
1:A:992:U:H4'	1:A:993:G:O5'	2.12	0.48
3:C:33:LEU:HD21	14:N:39:LEU:HD11	1.93	0.48
4:D:36:ARG:CB	4:D:36:ARG:NH1	2.73	0.48
1:A:127:G:N2	1:A:235:C:C2	2.81	0.48
1:A:363:A:OP1	12:L:33:ARG:HA	2.12	0.48
1:A:741:G:H2'	1:A:742:G:O4'	2.13	0.48
1:A:774:G:C2	1:A:806:C:N3	2.81	0.48
1:A:824:C:H2'	1:A:825:G:H8	1.78	0.48
1:A:1459:C:H2'	1:A:1460:A:C8	2.48	0.48
12:L:9:GLN:O	12:L:13:LYS:HB2	2.13	0.48
1:A:551:U:O2'	12:L:86:ARG:HD2	2.13	0.48
1:A:588:G:N1	1:A:589:C:C4	2.81	0.48
1:A:625:G:OP1	16:P:9:PHE:HB3	2.12	0.48
1:A:675:A:H1'	11:K:116:HIS:CG	2.48	0.48
1:A:1163:C:N3	1:A:1174:G:C2	2.82	0.48
1:A:1286:A:H2'	1:A:1287:A:H4'	1.94	0.48
1:A:1320:C:H5'	19:S:3:ARG:HH12	1.79	0.48
1:A:1323:G:H2'	1:A:1324:A:C8	2.49	0.48
2:B:77:ALA:HA	2:B:80:ILE:HD12	1.94	0.48
3:C:137:ALA:O	3:C:141:VAL:HG23	2.12	0.48
1:A:357:G:OP1	1:A:367:U:H5''	2.12	0.48
1:A:474:G:H2'	1:A:475:G:C8	2.48	0.48
1:A:834:C:C2	1:A:853:G:C2	3.02	0.48
1:A:1414:U:H2'	1:A:1415:G:C8	2.49	0.48
1:A:505:G:H2'	1:A:506:G:H8	1.78	0.48
5:E:41:VAL:HG21	5:E:139:LEU:HD13	1.95	0.48
1:A:79:G:H2'	1:A:80:G:H8	1.78	0.48
1:A:375:U:H5''	16:P:6:LEU:HD22	1.95	0.48
1:A:520:A:N1	1:A:536:C:H1'	2.29	0.48
1:A:920:U:C2	1:A:1080:A:H2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:G:H1	1:A:1389:C:N4	2.12	0.48
7:G:88:PRO:HG3	7:G:149:ARG:HA	1.95	0.48
9:I:19:LEU:HD22	9:I:59:PHE:HB3	1.95	0.48
1:A:17:U:C2	1:A:1079:G:C2	3.01	0.48
1:A:17:U:H1'	1:A:1079:G:H1'	1.96	0.48
1:A:122:G:C6	1:A:123:C:C4	3.02	0.48
1:A:301:G:H2'	1:A:302:G:H8	1.77	0.48
1:A:416:G:C6	1:A:417:C:C4	3.01	0.48
1:A:948:C:H42	1:A:1233:G:H1	1.62	0.48
1:A:1073:U:H3	1:A:1102:A:N6	2.11	0.48
1:A:1103:C:H5''	2:B:98:LEU:HD22	1.95	0.48
1:A:1163:C:H2'	1:A:1164:G:H8	1.79	0.48
1:A:1235:U:H2'	1:A:1236:A:O4'	2.14	0.48
1:A:1384:C:H2'	1:A:1385:G:C8	2.49	0.48
1:A:18:C:C5	1:A:19:C:C5	3.02	0.48
1:A:778:G:O2'	11:K:119:CYS:SG	2.66	0.48
1:A:832:C:C2	1:A:855:G:C2	3.01	0.48
1:A:878:G:H2'	1:A:879:C:C6	2.48	0.48
1:A:945:G:H2'	1:A:945:G:N3	2.28	0.48
1:A:1202:G:N2	14:N:43:CYS:SG	2.86	0.48
1:A:1257:U:OP2	3:C:27:LYS:CE	2.61	0.48
1:A:278:G:N7	17:Q:92:ARG:NH1	2.62	0.48
1:A:564:C:O2	1:A:564:C:C2'	2.62	0.48
1:A:877:C:H2'	1:A:878:G:H8	1.78	0.48
1:A:1225:A:H4'	19:S:78:ARG:HH11	1.79	0.48
16:P:33:ILE:HG22	16:P:34:GLU:HB2	1.94	0.48
23:X:115:LYS:HB3	23:X:164:LEU:HD21	1.94	0.48
1:A:1351:U:H2'	1:A:1352:C:H6	1.79	0.48
3:C:57:ILE:HG12	3:C:66:VAL:HG22	0.62	0.48
8:H:127:LEU:HB3	8:H:129:VAL:HG13	1.95	0.48
17:Q:9:VAL:O	17:Q:21:VAL:HA	2.14	0.48
1:A:377:G:H1	1:A:386:C:H42	1.61	0.47
1:A:590:C:N3	1:A:650:G:C2	2.82	0.47
1:A:985:C:C2	1:A:1221:G:N2	2.82	0.47
1:A:1067:A:H8	1:A:1067:A:OP2	1.97	0.47
1:A:1283:G:C6	1:A:1284:C:N4	2.82	0.47
4:D:64:LEU:HD13	4:D:203:VAL:HG21	1.96	0.47
15:O:82:ILE:HA	15:O:87:ILE:HD12	1.94	0.47
16:P:57:ARG:HD2	16:P:79:VAL:HG13	1.96	0.47
20:T:54:LYS:HA	20:T:57:ARG:HH11	1.79	0.47
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:G:H5''	1:A:451:A:H3'	1.96	0.47
1:A:718:G:H21	18:R:49:LYS:HE2	1.78	0.47
1:A:769:G:H4'	1:A:1513:A:H4'	1.96	0.47
1:A:866:C:C4	1:A:867:G:H1'	2.49	0.47
1:A:1106:G:N1	1:A:1107:C:C4	2.82	0.47
1:A:1118:C:H2'	1:A:1119:C:H6	1.78	0.47
1:A:1373:G:N7	9:I:11:LYS:NZ	2.61	0.47
1:A:1419:G:C2	1:A:1420:C:C2	3.02	0.47
2:B:19:HIS:CG	2:B:20:GLU:N	2.83	0.47
3:C:65:ALA:CB	3:C:100:ALA:O	2.61	0.47
8:H:88:LYS:HB3	8:H:91:ARG:HB3	1.96	0.47
1:A:247:G:OP2	17:Q:100:LYS:N	2.47	0.47
1:A:259:G:H2'	1:A:260:G:H8	1.78	0.47
1:A:356:A:H2'	1:A:357:G:O4'	2.14	0.47
1:A:728:A:H2'	1:A:729:A:H8	1.79	0.47
3:C:174:PRO:HD2	3:C:182:ILE:HD11	1.95	0.47
16:P:9:PHE:CD2	16:P:18:ARG:HG3	2.49	0.47
17:Q:43:LEU:HD13	17:Q:68:ARG:HE	1.79	0.47
1:A:685:G:H4'	11:K:40:ILE:O	2.15	0.47
1:A:975:A:C8	1:A:975:A:C5'	2.97	0.47
1:A:1048:G:C2	1:A:1210:C:C2	3.03	0.47
1:A:1192:C:H2'	1:A:1193:G:O4'	2.14	0.47
1:A:1361:G:C6	1:A:1362:C:N3	2.82	0.47
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.96	0.47
10:J:7:LYS:HE2	10:J:9:ARG:HH21	1.80	0.47
10:J:38:ILE:HG23	10:J:71:LEU:O	2.13	0.47
16:P:12:LYS:C	16:P:14:ASN:H	2.22	0.47
1:A:105:G:C2	1:A:106:C:C2	3.02	0.47
1:A:157:G:C6	1:A:165:C:N3	2.83	0.47
1:A:200:G:C2	1:A:218:C:C2	3.02	0.47
1:A:401:C:H2'	1:A:402:G:H8	1.79	0.47
1:A:558:G:C6	1:A:559:A:C6	3.03	0.47
1:A:743:U:H2'	1:A:744:C:H6	1.71	0.47
1:A:1366:C:H2'	1:A:1367:C:H6	1.77	0.47
4:D:36:ARG:HD3	4:D:38:TYR:OH	2.00	0.47
4:D:206:PHE:CD1	4:D:206:PHE:C	2.92	0.47
7:G:15:ASP:HB3	7:G:19:GLY:H	1.80	0.47
23:X:111:GLN:HG3	23:X:147:LEU:HD21	1.97	0.47
1:A:778:G:C2	1:A:779:C:C2	3.03	0.47
1:A:941:G:H2'	1:A:942:G:O4'	2.14	0.47
3:C:55:VAL:CG1	3:C:66:VAL:CG1	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:14:ARG:HA	13:M:43:THR:O	2.14	0.47
16:P:8:ARG:HB3	16:P:28:ARG:NE	2.30	0.47
18:R:47:THR:O	18:R:49:LYS:N	2.47	0.47
20:T:14:LYS:HA	20:T:17:ARG:HD2	1.96	0.47
1:A:13:U:C4	1:A:915:A:N6	2.82	0.47
1:A:20:U:H2'	1:A:21:G:O4'	2.15	0.47
1:A:24:U:H2'	1:A:25:C:C6	2.49	0.47
1:A:54:C:H42	1:A:357:G:H1	1.63	0.47
1:A:137:C:C2	1:A:227:G:C2	3.03	0.47
1:A:262:A:C4'	20:T:73:HIS:NE2	2.77	0.47
1:A:327:A:N3	1:A:329:A:H1'	2.30	0.47
1:A:542:G:C6	1:A:543:C:N4	2.83	0.47
1:A:553:A:O2'	12:L:29:GLY:O	2.31	0.47
1:A:670:G:H1	1:A:736:C:H42	1.62	0.47
1:A:717:C:H2'	1:A:734:G:H5'	1.95	0.47
1:A:728:A:H2'	1:A:729:A:C8	2.50	0.47
1:A:761:G:C6	1:A:762:C:C4	3.03	0.47
1:A:778:G:C6	1:A:779:C:C4	3.03	0.47
1:A:778:G:C6	1:A:779:C:N3	2.82	0.47
1:A:902:G:H2'	1:A:903:G:H8	1.79	0.47
1:A:939:G:H2'	1:A:940:C:C6	2.50	0.47
1:A:1000:U:H2'	1:A:1001:A:C1'	2.45	0.47
1:A:1065:U:H4'	1:A:1066:C:O5'	2.15	0.47
1:A:1217:C:N4	1:A:1218:C:N4	2.62	0.47
1:A:1353:G:N1	1:A:1354:C:C4	2.82	0.47
3:C:97:LYS:HZ3	3:C:97:LYS:CB	2.25	0.47
6:F:97:PHE:HE2	18:R:62:GLU:HG3	1.79	0.47
23:X:126:GLU:HA	23:X:129:HIS:HB3	1.96	0.47
1:A:823:G:N2	1:A:824:C:C2	2.83	0.47
1:A:1447:A:H4'	1:A:1452:C:OP2	2.15	0.47
1:A:1485:U:H2'	1:A:1486:G:H8	1.80	0.47
1:A:1507:A:H2'	1:A:1508:G:C8	2.50	0.47
1:A:1527:C:H2'	1:A:1528:U:C6	2.50	0.47
7:G:148:ASN:C	7:G:150:ALA:N	2.73	0.47
8:H:4:ASP:HB3	8:H:7:ALA:HB3	1.97	0.47
17:Q:92:ARG:HD3	17:Q:92:ARG:HA	1.50	0.47
18:R:16:PRO:HD3	24:Y:24:A:H1'	1.97	0.47
1:A:911:U:H2'	1:A:912:C:C6	2.50	0.47
5:E:17:ALA:HA	5:E:26:PHE:CD2	2.50	0.47
7:G:150:ALA:HA	11:K:59:TYR:CD1	2.48	0.47
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:149:VAL:HG13	23:X:168:VAL:HG22	1.96	0.47
1:A:183:G:H2'	1:A:184:G:O4'	2.15	0.47
1:A:390:C:O3'	16:P:28:ARG:NH2	2.48	0.47
1:A:585:G:C6	1:A:586:C:C4	3.03	0.47
1:A:861:G:C2	1:A:862:C:C2	3.03	0.47
1:A:1405:G:H2'	1:A:1406:U:H6	1.79	0.47
1:A:1525:G:H2'	1:A:1526:G:C8	2.49	0.47
3:C:113:ALA:N	3:C:114:PRO:CD	2.78	0.47
4:D:31:CYS:C	4:D:33:MET:N	2.72	0.47
5:E:15:ARG:NE	5:E:26:PHE:CD2	2.72	0.47
5:E:40:ARG:HB3	5:E:66:MET:SD	2.56	0.47
11:K:21:ILE:HG12	11:K:30:VAL:HG13	1.97	0.47
15:O:62:GLN:HA	15:O:65:ARG:HH11	1.79	0.47
1:A:109:A:H2'	1:A:326:G:N2	2.30	0.46
1:A:265:G:H2'	1:A:267:C:H5	1.79	0.46
1:A:399:G:C6	1:A:400:C:N4	2.83	0.46
1:A:977:A:H2'	1:A:978:A:H5''	1.97	0.46
1:A:1059:C:H2'	1:A:1060:C:C6	2.50	0.46
1:A:1293:G:H2'	1:A:1294:G:C8	2.50	0.46
3:C:57:ILE:CD1	3:C:66:VAL:CG2	2.93	0.46
5:E:27:ARG:NH1	5:E:27:ARG:CB	2.73	0.46
12:L:43:VAL:HA	22:W:64:ARG:NE	2.30	0.46
18:R:37:VAL:HG21	18:R:78:LEU:HB3	1.97	0.46
1:A:79:G:N1	1:A:91:C:C2	2.82	0.46
1:A:289:G:C2	1:A:290:C:C2	3.03	0.46
1:A:353:A:H8	1:A:353:A:OP1	1.97	0.46
1:A:960:U:H4'	1:A:961:U:H5''	1.98	0.46
1:A:1346:A:C8	1:A:1348:U:C2	3.03	0.46
1:A:1368:G:N2	1:A:1369:C:C2	2.83	0.46
20:T:41:ILE:HG23	20:T:42:GLN:N	2.28	0.46
23:X:123:ARG:HB2	24:Y:38:G:O5'	2.15	0.46
1:A:25:C:H2'	1:A:26:A:C8	2.50	0.46
1:A:394:G:N2	1:A:395:C:C2	2.84	0.46
1:A:576:G:H3'	1:A:577:G:H5''	1.98	0.46
1:A:830:G:C2	1:A:857:C:C2	3.03	0.46
1:A:939:G:H1'	1:A:1375:A:C2	2.50	0.46
6:F:25:ILE:HG21	6:F:82:ARG:HD2	1.96	0.46
1:A:784:C:C2	1:A:799:G:N2	2.84	0.46
1:A:1080:A:OP1	5:E:16:THR:HG21	2.16	0.46
1:A:1106:G:H5''	3:C:172:ARG:HG3	1.97	0.46
1:A:1211:U:H1'	1:A:1213:A:C2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:G:H2'	1:A:1294:G:H8	1.81	0.46
5:E:16:THR:HG22	5:E:27:ARG:HG2	1.97	0.46
20:T:73:HIS:C	20:T:73:HIS:ND1	2.73	0.46
1:A:522:C:H41	12:L:53:ARG:NH2	2.14	0.46
1:A:548:G:C2	1:A:549:C:C2	3.03	0.46
1:A:577:G:C2	1:A:578:C:C2	3.03	0.46
1:A:629:G:H2'	1:A:630:G:O4'	2.16	0.46
1:A:673:G:H1	1:A:717:C:H42	1.63	0.46
1:A:912:C:H2'	1:A:913:A:C8	2.50	0.46
1:A:1316:G:N2	1:A:1318:A:H3'	2.30	0.46
2:B:19:HIS:CG	2:B:20:GLU:H	2.34	0.46
4:D:8:VAL:CG1	4:D:9:CYS:N	2.77	0.46
4:D:98:GLU:HA	4:D:103:ASN:ND2	2.24	0.46
11:K:14:VAL:HG21	11:K:34:ASP:HB2	1.97	0.46
1:A:500:G:C2	1:A:501:C:N3	2.84	0.46
1:A:598:U:H2'	1:A:599:C:C6	2.51	0.46
1:A:974:A:H8	1:A:974:A:OP1	1.99	0.46
1:A:1130:A:H4'	9:I:3:GLN:OE1	2.16	0.46
1:A:1343:G:C6	1:A:1344:C:N3	2.83	0.46
1:A:1419:G:C6	1:A:1420:C:C4	3.03	0.46
1:A:1457:G:H5''	1:A:1457:G:H8	1.80	0.46
6:F:30:LEU:HD22	6:F:65:VAL:HG11	1.97	0.46
11:K:123:LYS:HA	11:K:126:ARG:HB2	1.96	0.46
13:M:24:GLY:O	13:M:29:ARG:NH1	2.49	0.46
20:T:84:LEU:HD23	20:T:85:MET:HG3	1.97	0.46
1:A:70:G:C2	1:A:100:C:O2	2.69	0.46
1:A:542:G:C2	1:A:543:C:C2	3.04	0.46
1:A:1308:U:OP1	13:M:98:VAL:N	2.48	0.46
3:C:72:LYS:HD3	3:C:75:VAL:HG23	1.98	0.46
8:H:60:ARG:HD2	8:H:62:TYR:CZ	2.51	0.46
11:K:48:ILE:HG21	11:K:63:LEU:HB3	1.98	0.46
13:M:94:ARG:HH12	19:S:80:TYR:HD2	1.63	0.46
19:S:23:ASN:ND2	19:S:43:GLU:HB2	2.31	0.46
1:A:73:G:N1	1:A:76:C:C2	2.84	0.46
1:A:97:G:H2'	1:A:98:G:C8	2.51	0.46
1:A:338:A:H2'	1:A:339:C:O4'	2.16	0.46
1:A:734:G:C2	1:A:735:C:C2	3.03	0.46
1:A:920:U:H1'	1:A:1080:A:C6	2.51	0.46
1:A:1321:C:H42	19:S:37:ARG:HH22	1.64	0.46
1:A:1392:G:H21	1:A:1502:A:H8	1.59	0.46
5:E:33:VAL:HG21	5:E:109:ILE:HG12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:35:LYS:HE2	7:G:38:LEU:HD22	1.97	0.46
9:I:112:LYS:HE3	9:I:117:HIS:C	2.41	0.46
1:A:289:G:N2	1:A:290:C:C2	2.84	0.46
1:A:369:C:H2'	1:A:370:C:C6	2.51	0.46
1:A:436:C:H2'	1:A:437:U:C6	2.49	0.46
1:A:585:G:C2	1:A:586:C:C2	3.04	0.46
1:A:715:A:H2'	1:A:716:A:O4'	2.15	0.46
1:A:1172:C:H2'	1:A:1173:G:H8	1.81	0.46
1:A:1440:C:N4	1:A:1461:G:H1	2.14	0.46
3:C:30:ARG:HG2	14:N:37:PHE:C	2.41	0.46
3:C:30:ARG:HG2	14:N:37:PHE:CA	2.46	0.46
4:D:98:GLU:HB3	4:D:189:PRO:CG	2.46	0.46
4:D:173:TRP:CD1	4:D:174:LEU:HG	2.51	0.46
6:F:61:LEU:HD22	6:F:63:TYR:CE1	2.50	0.46
20:T:39:LYS:HD3	20:T:55:ILE:HG12	1.97	0.46
1:A:102:G:C2	1:A:103:C:C2	3.04	0.46
1:A:306:G:C2	1:A:307:C:C2	3.04	0.46
1:A:617:G:C2	1:A:618:C:N3	2.84	0.46
1:A:708:C:H2'	1:A:709:G:H8	1.81	0.46
1:A:772:U:H3	1:A:807:A:H61	1.63	0.46
1:A:830:G:N2	1:A:857:C:C2	2.84	0.46
1:A:1459:C:OP1	20:T:28:ALA:HA	2.16	0.46
4:D:147:ALA:HA	4:D:182:LYS:HA	1.97	0.46
8:H:17:THR:HB	8:H:78:GLN:HE22	1.80	0.46
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.98	0.46
20:T:22:ARG:HG3	20:T:25:ARG:HH21	1.81	0.46
1:A:15:G:N1	1:A:921:U:C2	2.84	0.45
1:A:246:A:C3'	17:Q:100:LYS:HA	2.31	0.45
1:A:577:G:N2	1:A:578:C:C2	2.85	0.45
1:A:1017:G:C6	1:A:1018:C:C4	3.04	0.45
1:A:1048:G:H2'	1:A:1050:G:C8	2.51	0.45
1:A:1256:A:N6	1:A:1278:U:C2	2.84	0.45
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.98	0.45
1:A:801:U:H2'	1:A:802:A:O4'	2.15	0.45
1:A:1064:G:H8	1:A:1064:G:OP1	2.00	0.45
1:A:1411:C:H2'	1:A:1412:C:O4'	2.15	0.45
4:D:68:TYR:CD2	4:D:97:LEU:HD22	2.51	0.45
8:H:53:VAL:HB	8:H:58:TYR:CE2	2.52	0.45
1:A:344:A:H4'	1:A:345:C:OP2	2.16	0.45
1:A:416:G:C2	1:A:417:C:C2	3.04	0.45
1:A:456:C:C2	1:A:476:G:C2	3.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:G:N1	1:A:744:C:C2	2.84	0.45
1:A:687:A:H4'	1:A:688:G:O5'	2.15	0.45
1:A:692:U:O2	1:A:695:A:C8	2.69	0.45
1:A:725:G:N1	1:A:726:C:C4	2.84	0.45
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.77	0.45
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.98	0.45
8:H:29:SER:HB3	8:H:32:LYS:HB2	1.98	0.45
13:M:24:GLY:HA3	13:M:66:LEU:HD23	1.99	0.45
23:X:122:PHE:CB	23:X:126:GLU:HG3	2.46	0.45
1:A:130:A:OP1	1:A:130:A:C8	2.69	0.45
1:A:680:C:C2	1:A:711:G:N2	2.85	0.45
1:A:767:A:H2'	1:A:768:A:C8	2.51	0.45
1:A:879:C:H2'	1:A:880:C:C6	2.51	0.45
1:A:949:A:O2'	1:A:971:G:O6	2.32	0.45
1:A:1514:C:H2'	1:A:1515:C:C6	2.52	0.45
1:A:402:G:C2	1:A:403:C:C2	3.05	0.45
1:A:437:U:C4	1:A:438:G:C6	3.05	0.45
1:A:662:G:C6	1:A:744:C:N3	2.84	0.45
1:A:827:U:C2	1:A:872:A:N6	2.83	0.45
1:A:1007:C:C2	1:A:1023:G:N1	2.84	0.45
1:A:1048:G:H2'	1:A:1050:G:H8	1.81	0.45
1:A:1068:G:N2	1:A:1069:C:C2	2.84	0.45
1:A:1270:C:H2'	1:A:1271:G:C8	2.51	0.45
1:A:1512:U:H2'	1:A:1513:A:C8	2.52	0.45
3:C:28:GLN:HA	3:C:31:HIS:HD2	1.81	0.45
4:D:32:ALA:O	4:D:35:ARG:N	2.49	0.45
13:M:80:ARG:O	13:M:84:ILE:HG12	2.17	0.45
15:O:87:ILE:O	15:O:88:ARG:HG3	2.16	0.45
18:R:32:ARG:HA	18:R:69:THR:CG2	2.44	0.45
1:A:229:U:H2'	1:A:230:G:C8	2.51	0.45
1:A:778:G:H2'	1:A:779:C:O4'	2.17	0.45
1:A:827:U:C5	1:A:870:U:N3	2.85	0.45
1:A:1027:C:C2'	1:A:1028:C:H5'	2.46	0.45
1:A:1241:G:C6	1:A:1242:C:N4	2.84	0.45
1:A:1365:G:C5	1:A:1366:C:C4	3.04	0.45
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.98	0.45
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.99	0.45
12:L:24:VAL:HG12	12:L:26:ALA:N	2.31	0.45
13:M:94:ARG:NH1	19:S:80:TYR:HD2	2.14	0.45
18:R:85:LEU:HD23	18:R:88:LYS:HB2	1.98	0.45
1:A:108:G:H5''	1:A:109:A:H2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:G:H2'	1:A:948:C:O4'	2.17	0.45
1:A:1001:A:H2'	1:A:1001(A):G:H8	1.77	0.45
16:P:19:ILE:HG22	16:P:36:ILE:HD11	1.99	0.45
1:A:129(A):G:O2'	1:A:189(F):U:H2'	2.16	0.45
1:A:216:G:H2'	1:A:217:C:C6	2.52	0.45
1:A:516:U:H4'	22:W:2:LYS:HD2	1.98	0.45
1:A:519:C:H4'	22:W:66:ARG:CZ	2.47	0.45
1:A:876:G:H1'	8:H:11:THR:HG21	1.99	0.45
4:D:11:LEU:HD13	4:D:66:ARG:HG2	1.98	0.45
1:A:19:C:C2'	1:A:20:U:H6	2.28	0.45
1:A:19:C:H3'	1:A:20:U:C6	2.52	0.45
1:A:36:C:H2'	1:A:37:U:O4'	2.17	0.45
1:A:309:G:H1'	1:A:608:A:N1	2.32	0.45
1:A:399:G:C2	1:A:400:C:C2	3.04	0.45
1:A:1104:G:H5''	1:A:1104:G:H8	1.80	0.45
3:C:156:ARG:NH1	3:C:193:TYR:O	2.50	0.45
4:D:173:TRP:HB2	4:D:187:ARG:O	2.17	0.45
17:Q:86:GLU:HA	17:Q:89:LEU:HD12	1.99	0.45
1:A:289:G:C6	1:A:290:C:C4	3.05	0.45
1:A:366:C:H1'	1:A:394:G:H22	1.81	0.45
1:A:636:U:H2'	1:A:637:G:H8	1.82	0.45
1:A:676:A:H2'	1:A:677:U:O4'	2.16	0.45
1:A:742:G:H2'	1:A:743:U:O4'	2.16	0.45
2:B:95:GLN:HG3	2:B:147:LYS:HG2	1.98	0.45
5:E:72:GLN:O	5:E:75:THR:HG22	2.17	0.45
12:L:89:ARG:HB3	12:L:89:ARG:HH11	1.82	0.45
1:A:251:G:C2	1:A:266:G:C6	3.05	0.44
1:A:309:G:H2'	1:A:310:G:C8	2.52	0.44
1:A:1007:C:O2	1:A:1023:G:C2	2.69	0.44
1:A:1048:G:C2	1:A:1210:C:N3	2.85	0.44
20:T:67:ALA:CA	20:T:72:LEU:CD2	2.93	0.44
1:A:10:A:N6	1:A:24:U:H3	2.15	0.44
1:A:145:G:C2	1:A:178:C:N3	2.86	0.44
1:A:145:G:N2	1:A:178:C:C2	2.85	0.44
1:A:628:G:H2'	1:A:629:G:C8	2.52	0.44
1:A:666:G:H2'	1:A:667:G:H8	1.82	0.44
1:A:1308:U:H2'	1:A:1309:G:C8	2.52	0.44
1:A:1328:C:H2'	1:A:1329:A:O4'	2.17	0.44
1:A:1438:G:N1	1:A:1439:C:C4	2.85	0.44
3:C:59:ARG:NH1	3:C:64:VAL:HG21	2.33	0.44
12:L:54:LYS:HG2	12:L:75:HIS:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:15:GLU:HB3	22:W:23:ARG:HB2	1.98	0.44
1:A:15:G:C2	1:A:921:U:O2	2.70	0.44
1:A:70:G:C2	1:A:100:C:C2	3.05	0.44
1:A:229:U:H2'	1:A:230:G:H8	1.82	0.44
1:A:312:C:H2'	1:A:313:A:C8	2.52	0.44
1:A:556:C:H2'	1:A:557:G:O4'	2.17	0.44
1:A:922:G:H4'	5:E:20:GLN:HA	1.99	0.44
1:A:937:A:C2	1:A:1379:G:C6	3.05	0.44
1:A:1010:G:H1	1:A:1019:C:H42	1.65	0.44
1:A:1097:C:H2'	1:A:1098:C:C6	2.53	0.44
1:A:1171:G:N2	1:A:1172:C:C2	2.85	0.44
1:A:1443:G:N2	1:A:1444:C:C2	2.85	0.44
8:H:82:HIS:CG	8:H:83:ILE:N	2.86	0.44
10:J:57:LYS:O	10:J:60:ARG:HG3	2.17	0.44
14:N:29:ARG:NH1	14:N:31:ARG:HB3	2.32	0.44
23:X:103:LEU:HA	23:X:106:ILE:HD12	1.98	0.44
1:A:287:U:H2'	1:A:288:A:H8	1.81	0.44
1:A:363:A:OP2	12:L:34:ARG:HG2	2.17	0.44
1:A:551:U:H2'	1:A:552:U:C6	2.52	0.44
1:A:583:A:O2'	17:Q:91:ARG:HG3	2.16	0.44
1:A:613:C:C2	1:A:628:G:N2	2.85	0.44
1:A:769:G:N1	1:A:770:C:C4	2.86	0.44
1:A:1511:G:H2'	1:A:1512:U:C6	2.52	0.44
18:R:40:LEU:HB3	18:R:79:LEU:HD11	2.00	0.44
20:T:16:HIS:O	20:T:20:LEU:HD12	2.17	0.44
1:A:189:G:H2'	1:A:189(A):C:C6	2.52	0.44
1:A:280:C:C2	17:Q:39:SER:HB3	2.52	0.44
1:A:518:C:H5	1:A:529:G:H3'	1.82	0.44
1:A:1056:U:O2	1:A:1056:U:H2'	2.18	0.44
1:A:1512:U:H2'	1:A:1513:A:H8	1.82	0.44
2:B:25:ASN:HA	2:B:26:PRO:HD3	1.74	0.44
4:D:20:TYR:HA	4:D:26:CYS:HB3	1.99	0.44
12:L:94:PRO:C	12:L:96:VAL:H	2.24	0.44
23:X:94:ILE:HG12	23:X:99:TYR:HB2	1.99	0.44
1:A:224:C:OP1	20:T:74:LYS:HD3	2.18	0.44
1:A:581:G:O6	1:A:758:G:C8	2.71	0.44
1:A:1074:G:C6	1:A:1075:C:C4	3.04	0.44
1:A:1126:U:O2	1:A:1126:U:C2'	2.63	0.44
1:A:1143:G:H2'	1:A:1144:G:C8	2.53	0.44
1:A:1464:G:C2	1:A:1465:C:C4	3.05	0.44
10:J:38:ILE:HA	10:J:39:PRO:HD3	1.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:C:N3	1:A:231:G:C2	2.86	0.44
1:A:311:C:H2'	1:A:312:C:H6	1.82	0.44
1:A:333:G:C2	1:A:334:C:C2	3.06	0.44
1:A:1096:C:H2'	1:A:1097:C:H6	1.81	0.44
1:A:132:C:C2	1:A:231:G:N2	2.86	0.44
1:A:187:C:N3	1:A:191:G:C2	2.86	0.44
1:A:439:A:P	1:A:493:G:H1	2.32	0.44
1:A:553:A:H2'	1:A:554:C:C6	2.53	0.44
1:A:628:G:H2'	1:A:629:G:H8	1.82	0.44
1:A:1137:C:H4'	1:A:1138:G:C2	2.53	0.44
1:A:1233:G:C2	1:A:1234:C:N3	2.86	0.44
3:C:155:GLY:HA2	3:C:163:ALA:HB1	2.00	0.44
10:J:71:LEU:HD22	10:J:71:LEU:HA	1.86	0.44
22:W:48:LEU:HD22	23:X:125:ARG:HB2	1.99	0.44
1:A:13:U:H5'	1:A:14:U:C5	2.53	0.44
1:A:122:G:C6	1:A:123:C:N3	2.86	0.44
1:A:138:G:H1	1:A:225:C:H42	1.66	0.44
1:A:695:A:H2'	1:A:696:A:C8	2.53	0.44
1:A:714:G:H2'	1:A:715:A:C8	2.52	0.44
1:A:763:G:C2	1:A:764:C:C2	3.06	0.44
1:A:1207:G:C2	1:A:1208:C:C2	3.06	0.44
2:B:139:LYS:O	2:B:143:GLU:HG2	2.18	0.44
4:D:127:THR:HG23	4:D:131:ARG:C	2.43	0.44
6:F:47:ARG:HB2	6:F:47:ARG:NH1	2.33	0.44
15:O:41:GLU:O	15:O:44:LYS:HB2	2.18	0.44
20:T:67:ALA:N	20:T:72:LEU:HD23	2.27	0.44
1:A:96:U:H2'	1:A:97:G:H8	1.82	0.43
1:A:311:C:H2'	1:A:312:C:C6	2.53	0.43
1:A:671:G:C2	1:A:736:C:C2	3.06	0.43
1:A:861:G:C6	1:A:862:C:C4	3.05	0.43
1:A:962:C:H1'	1:A:1201:A:C6	2.53	0.43
1:A:1147:C:O2'	9:I:5:TYR:OH	2.30	0.43
1:A:1508:G:C6	1:A:1509:C:C4	3.06	0.43
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.53	0.43
2:B:51:LEU:HD21	2:B:214:ILE:HD12	2.00	0.43
3:C:29:TYR:CD1	3:C:29:TYR:O	2.70	0.43
5:E:80:ILE:HD11	5:E:142:LEU:HG	2.00	0.43
17:Q:20:THR:HG23	17:Q:43:LEU:HG	2.00	0.43
17:Q:60:ILE:HD12	17:Q:74:LEU:HD12	2.00	0.43
1:A:31:G:C6	1:A:48:C:O4'	2.70	0.43
1:A:175:C:H2'	1:A:176:C:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:U:H6	1:A:368:U:H2'	1.69	0.43
1:A:790:A:O2'	23:X:87:SER:O	2.32	0.43
1:A:838:G:C2	1:A:849:C:C2	3.06	0.43
1:A:1172:C:H2'	1:A:1173:G:C8	2.53	0.43
1:A:1401:G:H2'	1:A:1402:C:O4'	2.18	0.43
2:B:20:GLU:HB3	2:B:23:ARG:HD2	2.01	0.43
3:C:189:ALA:HB3	3:C:196:LEU:HB2	2.00	0.43
4:D:18:LYS:HA	4:D:33:MET:HG3	2.00	0.43
20:T:72:LEU:O	20:T:76:ALA:HB3	2.18	0.43
1:A:19:C:C3'	1:A:20:U:H6	2.31	0.43
1:A:384:G:C6	1:A:385:C:N4	2.86	0.43
1:A:394:G:C2	1:A:395:C:C2	3.06	0.43
1:A:583:A:H2'	1:A:584:G:O4'	2.18	0.43
1:A:647:C:H2'	1:A:648:A:C8	2.53	0.43
1:A:680:C:C2	1:A:711:G:C2	3.06	0.43
1:A:1074:G:C2	1:A:1075:C:C2	3.06	0.43
1:A:1127:G:N2	1:A:1145:C:C2	2.85	0.43
1:A:1233:G:N2	1:A:1234:C:C2	2.86	0.43
1:A:1253:G:C2	1:A:1254:C:C2	3.06	0.43
4:D:9:CYS:SG	4:D:26:CYS:SG	3.16	0.43
4:D:10:ARG:O	4:D:13:ARG:HB2	2.19	0.43
9:I:96:LEU:HG	9:I:101:PHE:HB2	1.99	0.43
10:J:40:LEU:HB2	10:J:69:ASN:HB3	2.00	0.43
14:N:50:LYS:HB3	14:N:52:GLN:HG3	2.01	0.43
1:A:39:G:C6	1:A:40:C:C4	3.07	0.43
1:A:402:G:C6	1:A:403:C:C4	3.07	0.43
1:A:827:U:C4	1:A:872:A:N6	2.79	0.43
1:A:936:C:H2'	1:A:937:A:O4'	2.19	0.43
1:A:947:G:C2	1:A:948:C:C2	3.06	0.43
1:A:1218:C:H2'	1:A:1219:U:H6	1.80	0.43
1:A:1366:C:C2'	10:J:60:ARG:NH1	2.73	0.43
1:A:1431:C:N4	1:A:1469:G:H1	2.17	0.43
12:L:85:ILE:HG21	12:L:98:TYR:CD2	2.53	0.43
1:A:46:G:H3'	1:A:366:C:H41	1.83	0.43
1:A:236:G:C6	1:A:237:C:C4	3.07	0.43
1:A:416:G:N1	1:A:417:C:C2	2.87	0.43
1:A:505:G:O5'	1:A:505:G:H8	2.01	0.43
1:A:790:A:C4	24:Y:36:A:N6	2.86	0.43
1:A:988:G:C6	1:A:989:C:C4	3.07	0.43
1:A:1096:C:O3'	2:B:140:HIS:CE1	2.72	0.43
2:B:16:HIS:HB3	2:B:44:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:201:GLN:HG2	4:D:205:GLU:OE1	2.17	0.43
5:E:126:ARG:HD3	5:E:126:ARG:HA	1.74	0.43
10:J:48:THR:HG23	10:J:62:HIS:CD2	2.53	0.43
14:N:59:ALA:HB1	14:N:61:TRP:CZ3	2.52	0.43
21:V:3:LYS:O	21:V:11:GLY:HA2	2.18	0.43
1:A:601:C:C2	1:A:638:G:N2	2.87	0.43
1:A:788:U:H2'	1:A:789:U:O4'	2.19	0.43
1:A:1057:G:H2'	1:A:1058:G:O4'	2.19	0.43
1:A:1074:G:N1	1:A:1075:C:C2	2.87	0.43
1:A:1228:C:H2'	1:A:1229:A:C8	2.53	0.43
3:C:28:GLN:CA	3:C:31:HIS:HD2	2.31	0.43
8:H:90:GLY:O	17:Q:34:LYS:HE2	2.19	0.43
13:M:40:ASN:HA	13:M:41:PRO:HD3	1.86	0.43
1:A:324:G:H8	1:A:324:G:OP2	2.01	0.43
1:A:505:G:H2'	1:A:506:G:C8	2.53	0.43
6:F:11:ASN:ND2	6:F:86:ARG:HH12	2.17	0.43
6:F:33:TYR:HD1	6:F:71:ARG:HD2	1.84	0.43
7:G:65:ALA:HB1	7:G:127:ALA:HB3	2.01	0.43
12:L:6:THR:H	12:L:9:GLN:NE2	2.17	0.43
22:W:23:ARG:HE	22:W:33:LEU:HD22	1.60	0.43
1:A:35:G:C6	1:A:36:C:N4	2.87	0.43
1:A:319:G:C2	1:A:320:C:C2	3.06	0.43
1:A:548:G:H8	1:A:548:G:H5''	1.82	0.43
1:A:562:C:N4	1:A:884:U:H2'	2.27	0.43
1:A:600:C:C2	1:A:639:G:C2	3.06	0.43
1:A:734:G:C6	1:A:735:C:N4	2.87	0.43
1:A:1171:G:C2	1:A:1172:C:C2	3.07	0.43
20:T:73:HIS:C	20:T:73:HIS:HD1	2.26	0.43
1:A:90:U:O2'	1:A:91:C:H5'	2.18	0.43
1:A:502:G:H2'	1:A:503:C:O4'	2.19	0.43
1:A:690:G:OP2	11:K:27:ASN:HB3	2.18	0.43
1:A:874:G:C2	1:A:875:C:C2	3.07	0.43
1:A:1189:C:H5''	3:C:5:ILE:HG12	2.01	0.43
1:A:1241:G:N1	1:A:1242:C:C4	2.87	0.43
1:A:1280:A:H3'	1:A:1281:U:H5''	1.99	0.43
3:C:36:ASP:HA	3:C:39:ILE:HD12	2.00	0.43
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.49	0.43
10:J:48:THR:HG23	10:J:62:HIS:HD2	1.83	0.43
10:J:49:VAL:HG11	14:N:44:LEU:HD12	2.01	0.43
13:M:34:LEU:HD13	13:M:41:PRO:HG3	2.01	0.43
1:A:259:G:C2	1:A:268:C:C2	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:G:C6	1:A:307:C:C4	3.07	0.43
1:A:524:G:C2	1:A:525:C:C4	3.06	0.43
1:A:1001(A):G:N1	1:A:1002:G:C6	2.87	0.43
1:A:1308:U:H2'	1:A:1309:G:H8	1.84	0.43
1:A:1404:C:H2'	1:A:1405:G:C8	2.54	0.43
1:A:1457:G:C8	1:A:1457:G:C5'	3.00	0.43
3:C:150:LYS:HD3	3:C:173:VAL:HG11	2.01	0.43
6:F:46:ARG:HB2	6:F:60:PHE:CE1	2.53	0.43
7:G:67:GLU:HA	7:G:70:LYS:HD2	2.00	0.43
17:Q:81:ARG:CZ	17:Q:81:ARG:HB2	2.48	0.43
20:T:54:LYS:HA	20:T:57:ARG:HD3	2.01	0.43
1:A:501:C:H2'	1:A:502:G:H8	1.84	0.42
1:A:604:G:H2'	1:A:605:U:O4'	2.19	0.42
1:A:920:U:C2	1:A:1080:A:N1	2.87	0.42
1:A:1266:G:N2	1:A:1270:C:C2	2.87	0.42
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.82	0.42
5:E:71:LEU:HD21	5:E:115:VAL:HG22	2.01	0.42
18:R:42:ARG:HB3	18:R:42:ARG:HH11	1.84	0.42
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.89	0.42
20:T:26:ASN:HB3	20:T:71:THR:HG23	2.01	0.42
1:A:42:G:C6	1:A:43:C:C4	3.07	0.42
1:A:197:A:H4'	1:A:198:G:O5'	2.19	0.42
1:A:252:U:H2'	1:A:253:U:C5	2.54	0.42
1:A:332:G:C2	1:A:333:G:C8	3.08	0.42
1:A:399:G:C6	1:A:400:C:C4	3.08	0.42
1:A:667:G:H2'	1:A:668:G:H8	1.84	0.42
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.42
1:A:1020:U:H2'	1:A:1021:G:H8	1.83	0.42
1:A:1075:C:H2'	1:A:1076:C:C6	2.55	0.42
2:B:8:LYS:HD2	2:B:9:GLU:H	1.84	0.42
3:C:156:ARG:H	3:C:163:ALA:HA	1.83	0.42
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.78	0.42
1:A:79:G:H2'	1:A:80:G:C8	2.55	0.42
1:A:351:G:H4'	1:A:352:C:OP1	2.19	0.42
1:A:437:U:H2'	1:A:438:G:O4'	2.19	0.42
1:A:651:C:H2'	1:A:652:U:C6	2.55	0.42
1:A:1074:G:C6	1:A:1075:C:N3	2.87	0.42
1:A:1481:U:H2'	1:A:1482:G:O4'	2.19	0.42
23:X:142:GLU:HA	23:X:145:LYS:HE3	2.01	0.42
1:A:461:A:H2'	1:A:470:C:H5''	2.00	0.42
1:A:552:U:H4'	12:L:86:ARG:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:G:N3	8:H:1:MET:HE1	2.34	0.42
1:A:616:G:H2'	1:A:617:G:H8	1.83	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.19	0.42
1:A:823:G:C6	1:A:824:C:N4	2.87	0.42
1:A:1081:G:H3'	1:A:1082:G:C8	2.54	0.42
1:A:1320:C:H5'	19:S:3:ARG:NH1	2.34	0.42
2:B:186:ALA:HB3	2:B:197:VAL:HG11	2.01	0.42
4:D:25:ARG:C	4:D:27:TYR:H	2.28	0.42
6:F:3:ARG:HB2	6:F:3:ARG:HH11	1.83	0.42
18:R:45:SER:N	18:R:49:LYS:O	2.42	0.42
1:A:19:C:H3'	1:A:20:U:H6	1.83	0.42
1:A:105:G:C5	1:A:106:C:C4	3.07	0.42
1:A:533:A:O2'	1:A:535:A:P	2.77	0.42
1:A:681:C:N3	1:A:710:G:C2	2.87	0.42
1:A:926:G:O5'	1:A:926:G:C8	2.59	0.42
1:A:1081:G:C4	1:A:1082:G:C8	3.07	0.42
1:A:1134:G:N2	1:A:1141:C:C2	2.86	0.42
1:A:1253:G:C6	1:A:1254:C:C4	3.07	0.42
1:A:1509:C:H2'	1:A:1510:U:O4'	2.19	0.42
5:E:15:ARG:CZ	5:E:26:PHE:CZ	2.80	0.42
11:K:42:TRP:HZ3	11:K:44:SER:HB3	1.85	0.42
13:M:10:PRO:CB	13:M:18:ALA:HB1	2.42	0.42
16:P:74:LEU:HD13	16:P:80:PHE:CE2	2.53	0.42
1:A:105:G:C6	1:A:106:C:C4	3.07	0.42
1:A:157:G:C2	1:A:165:C:O2	2.72	0.42
1:A:1496:C:H4'	23:X:102:LYS:HE3	2.01	0.42
4:D:36:ARG:CD	4:D:38:TYR:CE2	2.89	0.42
4:D:69:GLY:C	4:D:70:ILE:HG13	2.44	0.42
8:H:101:PRO:HG2	8:H:133:LEU:HD11	1.99	0.42
12:L:89:ARG:HD3	12:L:97:ARG:HG2	2.01	0.42
14:N:49:HIS:HE1	14:N:58:LYS:HE2	1.84	0.42
15:O:87:ILE:HG22	15:O:88:ARG:H	1.84	0.42
20:T:73:HIS:CE1	20:T:75:ASN:N	2.88	0.42
23:X:116:VAL:O	23:X:164:LEU:HA	2.20	0.42
1:A:276:G:C2	1:A:277:C:C2	3.08	0.42
1:A:316:G:H2'	1:A:317:G:H8	1.84	0.42
1:A:441:A:H5''	1:A:441:A:H8	1.85	0.42
1:A:504:C:C2	1:A:542:G:N2	2.87	0.42
1:A:881:G:C2	1:A:882:C:C2	3.07	0.42
1:A:999:C:N3	1:A:1043:C:N3	2.67	0.42
1:A:1008:C:C2	1:A:1022:G:N2	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:C:H2'	1:A:1115:C:H6	1.85	0.42
1:A:1130:A:H2'	1:A:1131:G:C8	2.54	0.42
1:A:1225:A:C4'	19:S:78:ARG:HH11	2.32	0.42
4:D:53:ASP:O	4:D:57:ARG:HD2	2.19	0.42
13:M:113:PRO:HB2	13:M:114:ARG:H	1.68	0.42
19:S:19:VAL:HG11	19:S:44:MET:HG2	2.02	0.42
1:A:39:G:C2	1:A:40:C:C2	3.08	0.42
1:A:502:G:OP1	12:L:118:SER:HB3	2.20	0.42
1:A:636:U:H5'	17:Q:2:PRO:CG	2.48	0.42
1:A:927:G:O3'	1:A:928:G:P	2.78	0.42
1:A:1188:A:H4'	10:J:61:GLU:OE2	2.20	0.42
1:A:1248:A:N3	9:I:70:LYS:HE3	2.35	0.42
1:A:1283:G:N2	1:A:1284:C:C2	2.87	0.42
3:C:29:TYR:HE2	14:N:36:PHE:CE2	2.13	0.42
5:E:51:VAL:HB	5:E:52:PRO:CD	2.50	0.42
6:F:22:GLU:HA	6:F:25:ILE:HD12	2.01	0.42
10:J:63:PHE:HE2	14:N:45:ARG:HG3	1.84	0.42
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.65	0.42
20:T:60:GLU:HG3	20:T:81:LYS:HE3	2.01	0.42
1:A:504:C:N3	1:A:542:G:C2	2.88	0.42
1:A:834:C:O2	1:A:853:G:C2	2.73	0.42
3:C:157:ILE:HD13	3:C:166:GLU:HB2	2.02	0.42
17:Q:12:SER:HA	17:Q:53:LEU:HD11	2.02	0.42
17:Q:46:ASP:HA	17:Q:47:PRO:HD3	1.87	0.42
17:Q:90:ILE:HA	17:Q:93:GLN:HE22	1.80	0.42
18:R:83:GLU:HB3	18:R:84:LYS:H	1.64	0.42
19:S:22:LEU:HD11	19:S:31:ILE:HD11	2.01	0.42
1:A:255:G:H2'	1:A:256:U:C6	2.55	0.42
1:A:542:G:N2	1:A:543:C:C2	2.88	0.42
1:A:837:G:H8	1:A:837:G:O5'	2.02	0.42
1:A:864:A:C2	1:A:865:A:C2	3.08	0.42
1:A:880:C:H2'	1:A:881:G:H8	1.84	0.42
1:A:929:G:C2	1:A:930:C:C2	3.08	0.42
4:D:9:CYS:HB3	4:D:31:CYS:O	2.20	0.42
4:D:29:PRO:O	4:D:30:LYS:HG3	2.20	0.42
7:G:150:ALA:HA	11:K:59:TYR:CB	2.49	0.42
11:K:20:TYR:HD1	11:K:85:ARG:HE	1.67	0.42
18:R:44:LEU:HD22	18:R:79:LEU:HD22	2.01	0.42
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.55	0.42
1:A:197:A:N6	1:A:221:C:H4'	2.35	0.41
1:A:299:G:C6	1:A:300:A:C6	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:C:N3	1:A:492:G:C2	2.88	0.41
1:A:500:G:C2	1:A:501:C:C2	3.08	0.41
1:A:539:A:H2'	1:A:540:G:C8	2.55	0.41
1:A:772:U:H2'	1:A:773:G:C8	2.55	0.41
1:A:975:A:H4'	1:A:976:G:C5'	2.50	0.41
1:A:1086:U:O5'	1:A:1086:U:H6	2.03	0.41
4:D:11:LEU:HD22	4:D:66:ARG:CZ	2.50	0.41
4:D:25:ARG:CZ	4:D:30:LYS:HB3	2.49	0.41
5:E:51:VAL:HB	5:E:52:PRO:HD3	2.02	0.41
6:F:49:ALA:HB1	18:R:80:PRO:HA	2.00	0.41
14:N:23:ARG:CZ	14:N:30:ALA:HB2	2.49	0.41
15:O:15:PHE:CE2	15:O:84:LYS:HD3	2.55	0.41
17:Q:72:ARG:HE	17:Q:72:ARG:HB2	1.68	0.41
20:T:97:ALA:HA	20:T:98:PRO:HD2	1.83	0.41
1:A:342:C:C2	1:A:348:G:N2	2.89	0.41
1:A:407:G:H2'	1:A:408:A:H8	1.85	0.41
1:A:577:G:C6	1:A:578:C:C4	3.07	0.41
1:A:664:G:H5'	18:R:64:ARG:NH1	2.36	0.41
1:A:689:C:H2'	1:A:690:G:O4'	2.20	0.41
1:A:821:G:C2	1:A:822:C:C2	3.08	0.41
1:A:1207:G:C6	1:A:1208:C:C4	3.09	0.41
1:A:1356:G:C2	1:A:1367:C:C2	3.08	0.41
1:A:1461:G:H2'	1:A:1462:G:C8	2.55	0.41
1:A:1464:G:C6	1:A:1465:C:N4	2.88	0.41
2:B:90:MET:HA	2:B:91:PRO:HD2	1.83	0.41
5:E:87:SER:HB3	5:E:131:ILE:HD13	2.01	0.41
7:G:148:ASN:C	7:G:150:ALA:H	2.26	0.41
10:J:6:ILE:HA	10:J:97:GLU:O	2.20	0.41
1:A:18:C:H2'	1:A:19:C:C6	2.55	0.41
1:A:245:C:C2	1:A:284:G:C2	3.08	0.41
1:A:590:C:C2	1:A:650:G:N2	2.88	0.41
1:A:731:G:C6	1:A:732:C:C4	3.09	0.41
1:A:823:G:N1	1:A:824:C:C4	2.88	0.41
1:A:903:G:C2	1:A:904:C:C2	3.08	0.41
1:A:1003:G:N2	1:A:1038:C:O2	2.54	0.41
1:A:1310:G:N2	1:A:1328:C:C2	2.89	0.41
1:A:1423:G:C2	1:A:1424:C:C2	3.09	0.41
1:A:1508:G:H2'	1:A:1509:C:O4'	2.20	0.41
3:C:30:ARG:HG2	14:N:37:PHE:HA	2.02	0.41
5:E:31:LEU:HD23	5:E:45:PHE:HB2	2.02	0.41
8:H:53:VAL:HB	8:H:58:TYR:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:113:LYS:H	9:I:119:ALA:HA	1.85	0.41
10:J:52:GLY:HA2	10:J:53:PRO:HD2	1.79	0.41
23:X:17:ARG:NH2	23:X:19:VAL:HG22	2.35	0.41
1:A:246:A:C4	1:A:279:A:C6	3.08	0.41
1:A:382:A:H2'	1:A:383:A:O4'	2.21	0.41
1:A:503:C:H2'	1:A:504:C:O4'	2.19	0.41
1:A:626:U:H2'	1:A:627:G:C8	2.55	0.41
1:A:768:A:C5	1:A:769:G:C8	3.08	0.41
1:A:1124:G:H1	1:A:1149:C:H42	1.69	0.41
3:C:150:LYS:HE3	3:C:167:TRP:CZ2	2.55	0.41
4:D:21:LEU:HD12	4:D:21:LEU:HA	1.94	0.41
5:E:58:ALA:HA	5:E:61:TYR:HD2	1.85	0.41
9:I:17:VAL:HG13	9:I:63:ILE:HG12	2.02	0.41
1:A:15:G:C3'	1:A:16:A:H8	2.32	0.41
1:A:42:G:C2	1:A:43:C:C2	3.09	0.41
1:A:280:C:N3	17:Q:39:SER:HB3	2.35	0.41
1:A:444:C:H2'	1:A:445:G:H8	1.85	0.41
1:A:446:G:N2	1:A:489:C:C2	2.88	0.41
1:A:542:G:H5'	4:D:41:GLY:HA3	2.02	0.41
1:A:568:G:C2	1:A:569:C:C2	3.09	0.41
1:A:734:G:C6	1:A:735:C:C4	3.08	0.41
1:A:1343:G:C5	1:A:1344:C:C4	3.09	0.41
1:A:1350:A:H2'	1:A:1351:U:C6	2.55	0.41
4:D:173:TRP:HD1	4:D:185:PHE:CE1	2.38	0.41
16:P:71:ARG:O	16:P:74:LEU:HB2	2.21	0.41
23:X:64:LYS:O	23:X:68:GLU:HG2	2.20	0.41
1:A:96:U:H2'	1:A:97:G:C8	2.56	0.41
1:A:679:C:H2'	1:A:680:C:C6	2.54	0.41
1:A:701:C:C4	23:X:67:TYR:HB2	2.55	0.41
1:A:754:C:P	15:O:72:ARG:HH22	2.43	0.41
1:A:763:G:C6	1:A:764:C:C4	3.08	0.41
1:A:810:C:H2'	1:A:811:C:O4'	2.21	0.41
1:A:1407:C:H2'	1:A:1408:A:H8	1.84	0.41
8:H:6:ILE:HG13	8:H:31:PHE:CE2	2.55	0.41
12:L:79:GLU:C	12:L:81:SER:H	2.28	0.41
12:L:88:GLY:O	12:L:99:HIS:ND1	2.53	0.41
1:A:28:G:O2'	1:A:296:U:OP1	2.38	0.41
1:A:333:G:C6	1:A:334:C:N4	2.88	0.41
1:A:548:G:C6	1:A:549:C:C4	3.09	0.41
1:A:671:G:C6	1:A:736:C:N4	2.88	0.41
1:A:855:G:C6	1:A:856:C:C4	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:ILE:H	3:C:14:ILE:HG12	1.73	0.41
1:A:276:G:H2'	1:A:277:C:C6	2.56	0.41
1:A:372:C:H4'	1:A:373:A:O5'	2.19	0.41
1:A:824:C:H42	1:A:876:G:H1	1.69	0.41
1:A:985:C:H2'	1:A:986:A:C8	2.56	0.41
1:A:1258:G:C6	1:A:1259:C:N4	2.89	0.41
2:B:105:PHE:O	2:B:109:SER:HB2	2.20	0.41
8:H:45:ILE:HG22	8:H:63:LEU:HD13	2.01	0.41
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.56	0.41
20:T:73:HIS:HE1	20:T:75:ASN:C	2.23	0.41
1:A:18:C:C6	1:A:19:C:C5	3.09	0.41
1:A:127:G:C2	1:A:235:C:N3	2.89	0.41
1:A:319:G:C6	1:A:320:C:C4	3.09	0.41
1:A:362:G:H5''	12:L:61:THR:HB	2.03	0.41
1:A:425:G:H2'	1:A:426:G:O4'	2.21	0.41
1:A:427:U:O2'	1:A:541:G:OP1	2.37	0.41
1:A:612:C:H2'	1:A:613:C:H6	1.84	0.41
1:A:625:G:H2'	1:A:626:U:C6	2.56	0.41
1:A:725:G:C2	1:A:726:C:C2	3.09	0.41
1:A:922:G:C2	1:A:923:A:C4	3.09	0.41
1:A:1080:A:H5''	5:E:16:THR:HG23	2.03	0.41
1:A:1128:C:H1'	1:A:1146:A:N6	2.35	0.41
1:A:1243:C:H2'	1:A:1244:C:O4'	2.21	0.41
1:A:1489:G:C2	1:A:1490:C:C2	3.08	0.41
3:C:19:GLU:HB3	14:N:52:GLN:HA	2.03	0.41
3:C:23:TYR:HA	10:J:11:PHE:CE2	2.56	0.41
4:D:13:ARG:NH2	4:D:36:ARG:HG2	2.34	0.41
4:D:30:LYS:C	4:D:32:ALA:H	2.29	0.41
9:I:55:ALA:HB1	9:I:58:HIS:HB3	2.02	0.41
16:P:65:GLN:HA	16:P:66:PRO:HD3	1.98	0.41
17:Q:98:LEU:H	17:Q:98:LEU:HG	1.63	0.41
19:S:53:ASN:ND2	19:S:75:ALA:HB1	2.35	0.41
20:T:53:LEU:HD23	20:T:100:ILE:HG22	2.03	0.41
1:A:147:G:C2	1:A:176:C:C2	3.08	0.41
1:A:254:G:H1	1:A:272:C:H42	1.68	0.41
1:A:376:G:O2'	1:A:377:G:H5'	2.21	0.41
1:A:377:G:H1	1:A:386:C:N4	2.19	0.41
1:A:394:G:C6	1:A:395:C:C4	3.09	0.41
1:A:667:G:H2'	1:A:668:G:C8	2.56	0.41
1:A:891:U:H2'	1:A:892:A:H8	1.86	0.41
1:A:1111:A:H5'	2:B:133:LYS:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:U:H2'	1:A:1149:C:O4'	2.21	0.41
1:A:1226:C:OP2	13:M:91:ARG:NH1	2.54	0.41
7:G:16:LEU:HD22	9:I:45:ALA:HB2	2.02	0.41
14:N:14:PRO:HB2	14:N:16:PHE:O	2.21	0.41
20:T:56:MET:HG2	20:T:84:LEU:HD21	2.02	0.41
1:A:35:G:H2'	1:A:36:C:C6	2.55	0.40
1:A:54:C:H41	1:A:352:C:H2'	1.85	0.40
1:A:76:C:C2'	1:A:77:G:H5'	2.51	0.40
1:A:174:C:H2'	1:A:175:C:C6	2.56	0.40
1:A:354:G:N1	1:A:355:C:C4	2.89	0.40
1:A:424:G:H8	1:A:424:G:O5'	2.05	0.40
1:A:521:G:C2	1:A:522:C:C4	3.09	0.40
1:A:1064:G:N2	1:A:1190:G:H2'	2.36	0.40
1:A:1241:G:C2	1:A:1242:C:C4	3.09	0.40
1:A:1511:G:H2'	1:A:1512:U:O4'	2.22	0.40
2:B:211:ILE:H	2:B:211:ILE:HG13	1.74	0.40
3:C:29:TYR:CD1	3:C:29:TYR:C	2.99	0.40
17:Q:48:GLU:HB2	17:Q:50:LYS:HB2	2.03	0.40
1:A:6:G:H4'	1:A:298:A:H4'	2.04	0.40
1:A:108:G:H5''	1:A:109:A:C2	2.56	0.40
1:A:115:G:O2'	1:A:289:G:H5''	2.22	0.40
1:A:137:C:C2	1:A:227:G:N2	2.89	0.40
1:A:502:G:C6	1:A:503:C:C4	3.09	0.40
1:A:559:A:H1'	1:A:561:U:H2'	2.02	0.40
1:A:662:G:C2	1:A:744:C:C2	3.09	0.40
1:A:688:G:H5'	11:K:46:GLY:C	2.46	0.40
1:A:722:A:H2'	1:A:724:G:C8	2.56	0.40
1:A:903:G:C6	1:A:904:C:N4	2.89	0.40
1:A:939:G:H1'	1:A:1375:A:H2	1.86	0.40
1:A:1064:G:O6	1:A:1192:C:N4	2.54	0.40
1:A:1188:A:H5''	10:J:61:GLU:OE2	2.21	0.40
1:A:1201:A:H4'	1:A:1202:G:O5'	2.22	0.40
1:A:1462:G:N2	1:A:1463:C:C2	2.89	0.40
3:C:153:VAL:HG22	3:C:198:VAL:HG22	2.03	0.40
5:E:10:MET:HA	5:E:32:VAL:HG23	2.04	0.40
5:E:44:GLY:HA3	5:E:58:ALA:O	2.22	0.40
22:W:53:VAL:HB	22:W:67:ILE:HG23	2.04	0.40
1:A:7:G:C2	1:A:298:A:C6	3.10	0.40
1:A:77:G:H3'	1:A:77:G:C8	2.57	0.40
1:A:262:A:H2'	1:A:263:A:C8	2.56	0.40
1:A:570:G:N3	1:A:570:G:H2'	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:G:O2'	17:Q:98:LEU:HD22	2.22	0.40
1:A:874:G:C6	1:A:875:C:C4	3.09	0.40
1:A:881:G:C6	1:A:882:C:C4	3.10	0.40
1:A:1162:C:N3	1:A:1175:G:C2	2.90	0.40
1:A:1423:G:C6	1:A:1424:C:C4	3.09	0.40
2:B:215:LEU:O	2:B:219:VAL:HG23	2.21	0.40
8:H:51:VAL:HB	8:H:52:ASP:H	1.65	0.40
8:H:96:GLY:HA2	8:H:130:GLY:HA3	2.04	0.40
11:K:56:GLY:O	11:K:89:ALA:HB3	2.21	0.40
1:A:83:U:H2'	1:A:84:U:O4'	2.22	0.40
1:A:113:G:H1'	1:A:354:G:H5'	2.03	0.40
1:A:267:C:H2'	1:A:268:C:C6	2.56	0.40
1:A:441:A:H3'	1:A:442:C:H6	1.86	0.40
1:A:502:G:C2	1:A:503:C:C2	3.10	0.40
1:A:910:C:H2'	1:A:911:U:O4'	2.21	0.40
1:A:1072:G:N2	2:B:107:THR:HG21	2.36	0.40
1:A:1144:G:N2	1:A:1146:A:H62	2.20	0.40
1:A:1158:C:H5'	2:B:132:LYS:CG	2.47	0.40
1:A:1431:C:C2	1:A:1470:G:N2	2.90	0.40
2:B:163:PHE:C	2:B:163:PHE:CD1	3.00	0.40
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.20	0.40
10:J:16:LEU:HD23	10:J:70:ARG:CG	2.40	0.40
10:J:64:GLU:HG2	14:N:59:ALA:HA	2.04	0.40
22:W:61:ASP:HA	22:W:62:PRO:HD3	1.91	0.40
1:A:103:C:H1'	1:A:151:A:C2	2.57	0.40
1:A:430:A:OP1	4:D:9:CYS:N	2.54	0.40
1:A:629:G:H2'	1:A:630:G:C8	2.56	0.40
1:A:821:G:C6	1:A:822:C:C4	3.09	0.40
1:A:1235:U:O3'	21:V:3:LYS:HB2	2.20	0.40
1:A:1361:G:C2	1:A:1362:C:O2	2.75	0.40
4:D:97:LEU:O	4:D:100:ARG:HB2	2.21	0.40
12:L:110:VAL:HG12	12:L:113:ARG:HG3	2.04	0.40
22:W:32:ILE:HD13	22:W:32:ILE:N	2.35	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	B	232/256 (91%)	182 (78%)	36 (16%)	14 (6%)	1	12
3	C	204/239 (85%)	181 (89%)	21 (10%)	2 (1%)	12	47
4	D	206/209 (99%)	182 (88%)	21 (10%)	3 (2%)	8	38
5	E	148/162 (91%)	127 (86%)	20 (14%)	1 (1%)	18	55
6	F	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	47
7	G	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	9	40
8	H	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	18	55
9	I	125/128 (98%)	98 (78%)	19 (15%)	8 (6%)	1	12
10	J	96/105 (91%)	79 (82%)	13 (14%)	4 (4%)	2	17
11	K	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	7	34
12	L	122/132 (92%)	97 (80%)	21 (17%)	4 (3%)	3	20
13	M	115/126 (91%)	100 (87%)	13 (11%)	2 (2%)	7	34
14	N	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	10
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
17	Q	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	5	28
18	R	71/88 (81%)	63 (89%)	4 (6%)	4 (6%)	1	13
19	S	78/93 (84%)	64 (82%)	10 (13%)	4 (5%)	1	14
20	T	97/106 (92%)	85 (88%)	8 (8%)	4 (4%)	2	17
21	V	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	16
22	W	69/72 (96%)	63 (91%)	5 (7%)	1 (1%)	9	38
23	X	166/171 (97%)	143 (86%)	18 (11%)	5 (3%)	3	22
All	All	2578/2781 (93%)	2218 (86%)	291 (11%)	69 (3%)	6	24

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	16	HIS
2	B	24	TRP
2	B	229	VAL
7	G	55	GLY
9	I	11	LYS
9	I	56	LEU
12	L	27	LEU
13	M	113	PRO
14	N	22	THR
23	X	54	PRO
23	X	55	PRO
2	B	17	PHE
2	B	131	PRO
2	B	207	ALA
4	D	37	PRO
9	I	23	ASN
10	J	55	LYS
12	L	45	PRO
18	R	18	ARG
18	R	48	GLY
19	S	6	LYS
23	X	23	GLY
23	X	81	LYS
2	B	21	ARG
2	B	100	GLY
2	B	228	GLY
12	L	89	ARG
14	N	23	ARG
17	Q	67	LYS
17	Q	97	SER
18	R	17	SER
22	W	2	LYS
23	X	8	ASN
2	B	233	SER
4	D	5	ILE
5	E	17	ALA
7	G	7	ALA
8	H	5	PRO
9	I	42	ARG
9	I	119	ALA
10	J	34	VAL
10	J	54	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	S	71	LEU
20	T	9	ASN
20	T	97	ALA
20	T	98	PRO
21	V	5	ASP
2	B	99	GLY
2	B	125	PRO
2	B	130	ARG
3	C	108	ASN
4	D	69	GLY
6	F	15	ASP
11	K	13	GLN
11	K	104	GLN
14	N	26	ARG
18	R	87	ARG
19	S	30	LEU
9	I	44	VAL
9	I	54	ASP
9	I	55	ALA
14	N	14	PRO
19	S	8	GLY
13	M	100	GLY
20	T	96	GLY
10	J	37	PRO
3	C	77	ILE
12	L	88	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	150 (74%)	52 (26%)	0	4
3	C	160/188 (85%)	136 (85%)	24 (15%)	3	13
4	D	180/181 (99%)	136 (76%)	44 (24%)	1	4
5	E	115/123 (94%)	86 (75%)	29 (25%)	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	90/90 (100%)	74 (82%)	16 (18%)	2	10
7	G	126/127 (99%)	115 (91%)	11 (9%)	9	29
8	H	119/119 (100%)	97 (82%)	22 (18%)	1	9
9	I	98/99 (99%)	84 (86%)	14 (14%)	3	14
10	J	87/92 (95%)	76 (87%)	11 (13%)	4	16
11	K	90/99 (91%)	71 (79%)	19 (21%)	1	6
12	L	104/109 (95%)	84 (81%)	20 (19%)	1	8
13	M	94/101 (93%)	84 (89%)	10 (11%)	6	21
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	23
15	O	79/80 (99%)	57 (72%)	22 (28%)	0	3
16	P	72/74 (97%)	61 (85%)	11 (15%)	3	12
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1	6
18	R	64/77 (83%)	50 (78%)	14 (22%)	1	6
19	S	71/80 (89%)	59 (83%)	12 (17%)	2	11
20	T	76/82 (93%)	55 (72%)	21 (28%)	0	3
21	V	19/22 (86%)	18 (95%)	1 (5%)	20	40
22	W	62/63 (98%)	51 (82%)	11 (18%)	2	10
23	X	145/150 (97%)	119 (82%)	26 (18%)	2	10
All	All	2196/2323 (94%)	1781 (81%)	415 (19%)	3	9

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	12	GLU
2	B	15	VAL
2	B	16	HIS
2	B	21	ARG
2	B	23	ARG
2	B	25	ASN
2	B	30	ARG
2	B	40	HIS
2	B	44	LEU
2	B	51	LEU
2	B	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	64	ARG
2	B	73	THR
2	B	75	LYS
2	B	80	ILE
2	B	83	MET
2	B	87	ARG
2	B	101	MET
2	B	107	THR
2	B	109	SER
2	B	112	VAL
2	B	113	HIS
2	B	117	GLU
2	B	122	PHE
2	B	134	GLU
2	B	137	ARG
2	B	142	LEU
2	B	144	ARG
2	B	145	LEU
2	B	155	LEU
2	B	160	ASP
2	B	168	THR
2	B	172	ILE
2	B	175	ARG
2	B	178	ARG
2	B	184	VAL
2	B	187	LEU
2	B	191	ASP
2	B	196	LEU
2	B	200	ILE
2	B	205	ASP
2	B	206	ASP
2	B	211	ILE
2	B	216	SER
2	B	220	ASP
2	B	221	LEU
2	B	222	ILE
2	B	229	VAL
2	B	233	SER
2	B	240	GLN
3	C	3	ASN
3	C	11	ARG
3	C	14	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	17	ASP
3	C	21	ARG
3	C	27	LYS
3	C	33	LEU
3	C	42	LEU
3	C	64	VAL
3	C	72	LYS
3	C	82	GLU
3	C	87	LEU
3	C	90	GLU
3	C	94	LEU
3	C	97	LYS
3	C	98	ASN
3	C	101	LEU
3	C	115	LEU
3	C	119	ARG
3	C	162	GLN
3	C	170	GLN
3	C	188	LEU
3	C	190	ARG
3	C	191	THR
4	D	5	ILE
4	D	8	VAL
4	D	12	CYS
4	D	15	GLU
4	D	25	ARG
4	D	27	TYR
4	D	34	GLU
4	D	35	ARG
4	D	36	ARG
4	D	42	GLN
4	D	45	GLN
4	D	47	ARG
4	D	58	LEU
4	D	59	ARG
4	D	61	LYS
4	D	62	GLN
4	D	64	LEU
4	D	65	ARG
4	D	70	ILE
4	D	78	LEU
4	D	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	96	LEU
4	D	97	LEU
4	D	112	VAL
4	D	118	ARG
4	D	121	VAL
4	D	122	ARG
4	D	131	ARG
4	D	135	LEU
4	D	139	ARG
4	D	140	VAL
4	D	141	ARG
4	D	144	ASP
4	D	146	ILE
4	D	158	ILE
4	D	162	LEU
4	D	174	LEU
4	D	176	LEU
4	D	177	ASP
4	D	186	LEU
4	D	187	ARG
4	D	194	LEU
4	D	196	LEU
4	D	209	ARG
5	E	7	GLU
5	E	8	GLU
5	E	11	ILE
5	E	12	LEU
5	E	14	ARG
5	E	16	THR
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	25	ARG
5	E	27	ARG
5	E	32	VAL
5	E	36	ASP
5	E	38	GLN
5	E	41	VAL
5	E	51	VAL
5	E	55	VAL
5	E	68	GLU
5	E	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	87	SER
5	E	98	THR
5	E	118	ILE
5	E	122	GLU
5	E	123	LEU
5	E	144	THR
5	E	147	ASP
6	F	1	MET
6	F	3	ARG
6	F	9	VAL
6	F	10	LEU
6	F	18	GLN
6	F	36	ARG
6	F	37	VAL
6	F	40	VAL
6	F	47	ARG
6	F	55	ASP
6	F	75	LEU
6	F	77	ARG
6	F	82	ARG
6	F	83	ASP
6	F	92	LYS
6	F	98	LEU
7	G	6	ARG
7	G	16	LEU
7	G	22	LEU
7	G	57	GLU
7	G	72	ARG
7	G	74	GLU
7	G	91	VAL
7	G	94	ARG
7	G	126	ASP
7	G	136	LYS
7	G	142	GLU
8	H	9	MET
8	H	18	ARG
8	H	34	GLU
8	H	38	ILE
8	H	39	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	41	ARG
8	H	45	ILE
8	H	50	ARG
8	H	54	ASP
8	H	59	LEU
8	H	77	GLU
8	H	85	ARG
8	H	93	VAL
8	H	95	VAL
8	H	100	ILE
8	H	104	ARG
8	H	109	ILE
8	H	112	LEU
8	H	122	ARG
8	H	126	LYS
8	H	127	LEU
8	H	133	LEU
9	I	12	GLU
9	I	14	VAL
9	I	26	VAL
9	I	40	LEU
9	I	48	GLU
9	I	56	LEU
9	I	78	LYS
9	I	79	LEU
9	I	85	LEU
9	I	87	GLN
9	I	102	LEU
9	I	111	ARG
9	I	112	LYS
9	I	127	LYS
10	J	7	LYS
10	J	16	LEU
10	J	23	ILE
10	J	49	VAL
10	J	51	ARG
10	J	57	LYS
10	J	62	HIS
10	J	71	LEU
10	J	74	ILE
10	J	88	LEU
10	J	96	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	13	GLN
11	K	25	TYR
11	K	34	ASP
11	K	40	ILE
11	K	44	SER
11	K	48	ILE
11	K	54	ARG
11	K	55	LYS
11	K	57	THR
11	K	66	LEU
11	K	77	MET
11	K	84	VAL
11	K	91	ARG
11	K	92	GLU
11	K	96	ARG
11	K	103	LEU
11	K	105	VAL
11	K	123	LYS
11	K	126	ARG
12	L	7	ILE
12	L	15	ARG
12	L	17	LYS
12	L	18	VAL
12	L	19	ARG
12	L	28	LYS
12	L	39	VAL
12	L	41	ARG
12	L	53	ARG
12	L	55	VAL
12	L	59	ARG
12	L	65	GLU
12	L	70	ILE
12	L	77	LEU
12	L	81	SER
12	L	83	VAL
12	L	89	ARG
12	L	90	VAL
12	L	110	VAL
12	L	113	ARG
13	M	32	GLU
13	M	45	VAL
13	M	49	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	56	LEU
13	M	73	GLU
13	M	77	ASN
13	M	87	TYR
13	M	90	LEU
13	M	115	LYS
13	M	116	THR
14	N	7	ILE
14	N	12	ARG
14	N	43	CYS
14	N	44	LEU
14	N	50	LYS
15	O	3	ILE
15	O	9	GLN
15	O	10	LYS
15	O	13	GLN
15	O	17	ARG
15	O	25	THR
15	O	27	VAL
15	O	28	GLN
15	O	29	VAL
15	O	31	LEU
15	O	32	LEU
15	O	41	GLU
15	O	44	LYS
15	O	48	LYS
15	O	49	ASP
15	O	54	ARG
15	O	56	LEU
15	O	58	MET
15	O	70	LEU
15	O	71	GLN
15	O	81	LEU
15	O	87	ILE
16	P	4	ILE
16	P	20	VAL
16	P	23	ASP
16	P	28	ARG
16	P	29	ASP
16	P	44	THR
16	P	49	LEU
16	P	53	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	62	VAL
16	P	67	THR
16	P	71	ARG
17	Q	5	VAL
17	Q	18	THR
17	Q	20	THR
17	Q	34	LYS
17	Q	38	ARG
17	Q	39	SER
17	Q	53	LEU
17	Q	57	VAL
17	Q	63	ARG
17	Q	68	ARG
17	Q	70	ARG
17	Q	76	LEU
17	Q	81	ARG
17	Q	82	MET
17	Q	84	LEU
17	Q	92	ARG
17	Q	93	GLN
17	Q	98	LEU
17	Q	99	SER
17	Q	100	LYS
18	R	22	VAL
18	R	32	ARG
18	R	39	VAL
18	R	40	LEU
18	R	41	LYS
18	R	42	ARG
18	R	44	LEU
18	R	45	SER
18	R	54	ARG
18	R	55	ARG
18	R	66	LEU
18	R	75	ILE
18	R	76	LEU
18	R	81	PHE
19	S	7	LYS
19	S	13	ASP
19	S	15	LEU
19	S	18	LYS
19	S	19	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	S	25	LYS
19	S	29	ARG
19	S	30	LEU
19	S	37	ARG
19	S	39	THR
19	S	43	GLU
19	S	63	THR
20	T	9	ASN
20	T	10	LEU
20	T	15	ARG
20	T	19	SER
20	T	20	LEU
20	T	21	LYS
20	T	23	ARG
20	T	24	LEU
20	T	25	ARG
20	T	36	LEU
20	T	53	LEU
20	T	55	ILE
20	T	62	LEU
20	T	68	LYS
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	80	ARG
20	T	84	LEU
20	T	85	MET
20	T	104	LEU
21	V	3	LYS
22	W	7	ILE
22	W	19	ASN
22	W	21	THR
22	W	23	ARG
22	W	32	ILE
22	W	33	LEU
22	W	47	ILE
22	W	48	LEU
22	W	58	THR
22	W	69	TYR
22	W	70	ARG
23	X	4	GLU
23	X	19	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	X	26	LEU
23	X	30	ASP
23	X	35	LEU
23	X	37	LEU
23	X	41	MET
23	X	69	GLN
23	X	83	THR
23	X	87	SER
23	X	91	ARG
23	X	100	GLN
23	X	120	ILE
23	X	121	MET
23	X	123	ARG
23	X	132	LEU
23	X	134	GLU
23	X	135	ARG
23	X	144	LEU
23	X	147	LEU
23	X	156	MET
23	X	157	LEU
23	X	159	ARG
23	X	162	ASN
23	X	164	LEU
23	X	168	VAL

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

Mol	Chain	Res	Type
2	B	94	ASN
2	B	95	GLN
2	B	140	HIS
2	B	212	GLN
2	B	224	GLN
3	C	31	HIS
3	C	108	ASN
3	C	123	GLN
3	C	170	GLN
4	D	116	GLN
4	D	123	HIS
4	D	129	ASN
4	D	154	ASN
4	D	201	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	11	ASN
6	F	64	GLN
6	F	100	ASN
7	G	28	ASN
7	G	68	ASN
7	G	84	ASN
8	H	82	HIS
10	J	68	HIS
10	J	76	ASN
11	K	27	ASN
11	K	62	GLN
11	K	99	GLN
11	K	104	GLN
11	K	116	HIS
12	L	8	ASN
12	L	75	HIS
13	M	106	ASN
15	O	28	GLN
15	O	37	ASN
15	O	62	GLN
17	Q	16	GLN
17	Q	93	GLN
17	Q	94	ASN
18	R	36	ASN
19	S	14	HIS
19	S	23	ASN
19	S	53	ASN
20	T	16	HIS
20	T	18	GLN
20	T	45	GLN
20	T	73	HIS
23	X	15	GLN
23	X	69	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	446 (29%)	103 (6%)
24	Y	19/39 (48%)	11 (57%)	3 (15%)
All	All	1526/1561 (97%)	457 (29%)	106 (6%)

All (457) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	18	C
1	A	20	U
1	A	22	G
1	A	31	G
1	A	32	A
1	A	35	G
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	54	C
1	A	60	A
1	A	61	G
1	A	66	G
1	A	73	G
1	A	76	C
1	A	77	G
1	A	78	G
1	A	79	G
1	A	81	U
1	A	83	U
1	A	91	C
1	A	97	G
1	A	108	G
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	134	A
1	A	142	G
1	A	151	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	157	G
1	A	163	C
1	A	173	U
1	A	181	G
1	A	182	U
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	197	A
1	A	198	G
1	A	199	G
1	A	201	C
1	A	203	U
1	A	204	U
1	A	217	C
1	A	220	G
1	A	225	C
1	A	243	A
1	A	244	U
1	A	247	G
1	A	251	G
1	A	253	U
1	A	262	A
1	A	266	G
1	A	267	C
1	A	276	G
1	A	279	A
1	A	280	C
1	A	281	G
1	A	282	A
1	A	283	C
1	A	288	A
1	A	289	G
1	A	290	C
1	A	291	C
1	A	298	A
1	A	299	G
1	A	301	G
1	A	306	G
1	A	313	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	315	A
1	A	316	G
1	A	321	A
1	A	324	G
1	A	325	A
1	A	327	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	342	C
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	366	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	375	U
1	A	378	G
1	A	383	A
1	A	384	G
1	A	388	G
1	A	392	G
1	A	397	A
1	A	398	C
1	A	399	G
1	A	406	G
1	A	412	A
1	A	413	G
1	A	419	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	441	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	446	G
1	A	452	A
1	A	454	C
1	A	455	C
1	A	470	C
1	A	481	G
1	A	483	C
1	A	484	G
1	A	485	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	503	C
1	A	508	C
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	521	G
1	A	524	G
1	A	527	G
1	A	528	C
1	A	529	G
1	A	531	U
1	A	532	A
1	A	534	U
1	A	535	A
1	A	537	G
1	A	543	C
1	A	545	C
1	A	547	A
1	A	548	G
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	568	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	572	A
1	A	573	A
1	A	574	A
1	A	576	G
1	A	577	G
1	A	580	U
1	A	596	C
1	A	619	U
1	A	641	U
1	A	642	A
1	A	644	G
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	690	G
1	A	693	G
1	A	695	A
1	A	697	U
1	A	698	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	704	A
1	A	713	G
1	A	716	A
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	748	C
1	A	749	C
1	A	755	G
1	A	760	G
1	A	763	G
1	A	777	A
1	A	785	G
1	A	787	A
1	A	792	A
1	A	793	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	794	A
1	A	796	C
1	A	799	G
1	A	802	A
1	A	812	C
1	A	815	A
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	821	G
1	A	828	A
1	A	831	U
1	A	835	U
1	A	836	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	851	G
1	A	853	G
1	A	855	G
1	A	871	U
1	A	872	A
1	A	873	A
1	A	876	G
1	A	884	U
1	A	885	G
1	A	889	A
1	A	891	U
1	A	900	A
1	A	902	G
1	A	911	U
1	A	920	U
1	A	927	G
1	A	931	C
1	A	932	C
1	A	933	G
1	A	934	C
1	A	935	A
1	A	943	U
1	A	945	G
1	A	950	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	998	G
1	A	1000	U
1	A	1001	A
1	A	1001(A)	G
1	A	1002	G
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1030(C)	G
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1056	U
1	A	1060	C
1	A	1065	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1066	C
1	A	1067	A
1	A	1070	U
1	A	1074	G
1	A	1075	C
1	A	1078	U
1	A	1081	G
1	A	1083	U
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1100	C
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1108	G
1	A	1112	C
1	A	1113	C
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1144	G
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1169	A
1	A	1171	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1183	A
1	A	1184	G
1	A	1187	G
1	A	1188	A
1	A	1190	G
1	A	1191	A
1	A	1195	C
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1234	C
1	A	1236	A
1	A	1238	A
1	A	1240	U
1	A	1249	C
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1275	A
1	A	1279	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1295	G
1	A	1299	A
1	A	1300	G
1	A	1301	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1312	G
1	A	1315	U
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1332	A
1	A	1336	C
1	A	1338	G
1	A	1342	C
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1349	A
1	A	1353	G
1	A	1357	A
1	A	1362	C
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
1	A	1365	G
1	A	1367	C
1	A	1370	G
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1387	G
1	A	1394	A
1	A	1398	A
1	A	1400	C
1	A	1412	C
1	A	1423	G
1	A	1440	C
1	A	1442	G
1	A	1443	G
1	A	1447	A
1	A	1452	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1456	G
1	A	1457	G
1	A	1484	C
1	A	1485	U
1	A	1488	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1532	U
1	A	1535	C
1	A	1536	C
1	A	1541	U
24	Y	21	G
24	Y	28	A
24	Y	30	G
24	Y	32	A
24	Y	33	A
24	Y	34	A
24	Y	35	A
24	Y	36	A
24	Y	37	U
24	Y	38	G
24	Y	39	U

All (106) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	13	U
1	A	19	C
1	A	30	U
1	A	31	G
1	A	48	C
1	A	51	A
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	173	U
1	A	181	G
1	A	189(F)	U
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	274	A
1	A	279	A
1	A	281	G
1	A	289	G
1	A	315	A
1	A	327	A
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	372	C
1	A	412	A
1	A	421	U
1	A	428	G
1	A	429	U
1	A	484	G
1	A	495	A
1	A	496	A
1	A	508	C
1	A	509	A
1	A	518	C
1	A	535	A
1	A	559	A
1	A	560	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	562	C
1	A	575	G
1	A	576	G
1	A	595	G
1	A	641	U
1	A	687	A
1	A	701	C
1	A	703	G
1	A	748	C
1	A	777	A
1	A	792	A
1	A	835	U
1	A	840	C
1	A	864	A
1	A	872	A
1	A	884	U
1	A	932	C
1	A	934	C
1	A	960	U
1	A	965	A
1	A	968	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1064	G
1	A	1065	U
1	A	1101	A
1	A	1125	U
1	A	1128	C
1	A	1145	C
1	A	1182	G
1	A	1187	G
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1226	C
1	A	1239	A
1	A	1257	U
1	A	1279	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1285	A
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1322	C
1	A	1331	G
1	A	1336	C
1	A	1346	A
1	A	1364	U
1	A	1380	U
1	A	1442(B)	A
1	A	1447	A
1	A	1452	C
1	A	1493	A
1	A	1498	U
1	A	1504	G
1	A	1534	A
24	Y	31	U
24	Y	33	A
24	Y	34	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 110 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	84:U	O3'	88:A	P	5.54
1	A	93:G	O3'	96:U	P	5.11
1	A	204:U	O3'	216:G	P	4.54
1	A	1442(A):G	O3'	1442(B):A	P	3.89
1	A	841:U	O3'	848:C	P	3.88
1	A	1387:G	O3'	1388:C	P	3.26
1	A	927:G	O3'	928:G	P	2.78

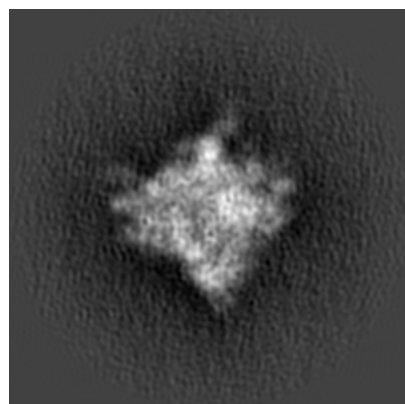
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4075. These allow visual inspection of the internal detail of the map and identification of artifacts.

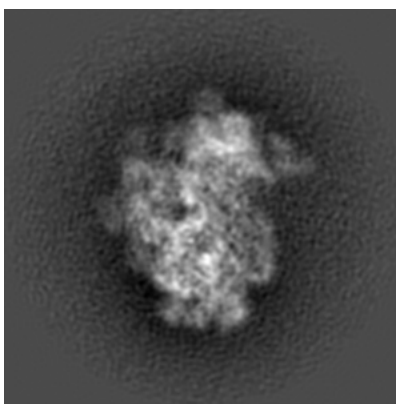
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

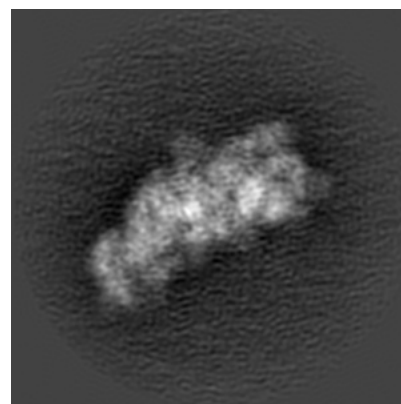
6.1.1 Primary map



X

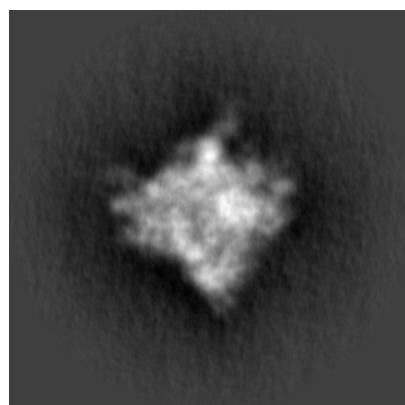


Y

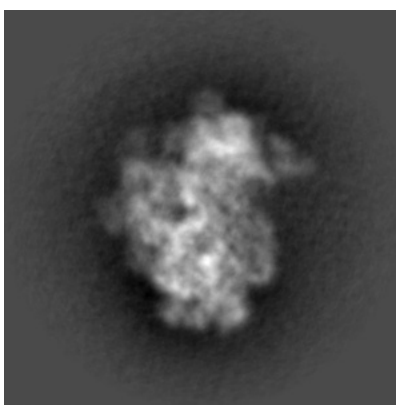


Z

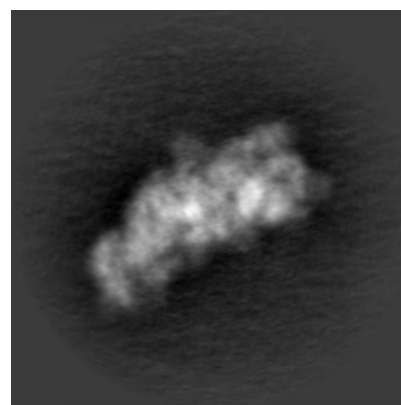
6.1.2 Raw map



X



Y

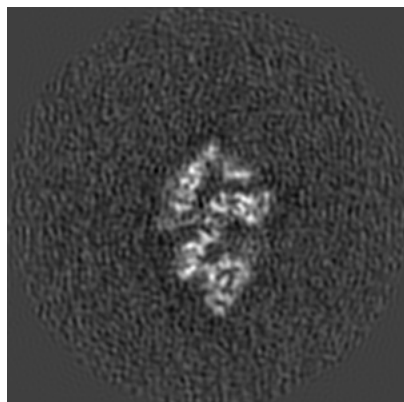


Z

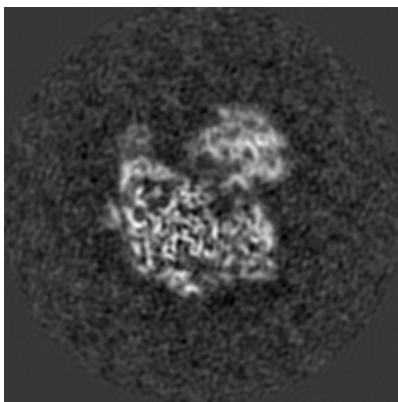
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

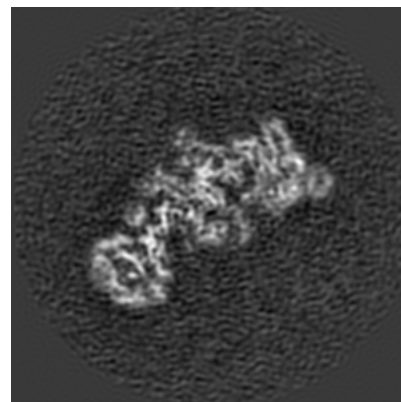
6.2.1 Primary map



X Index: 130

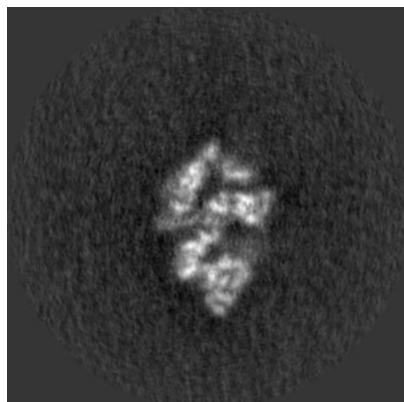


Y Index: 130

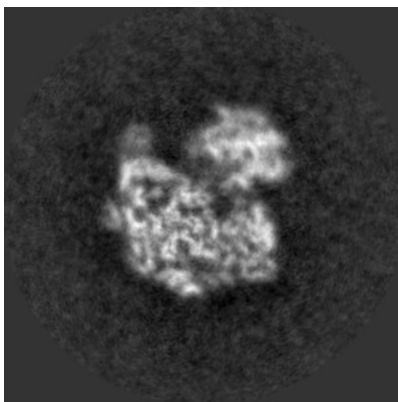


Z Index: 130

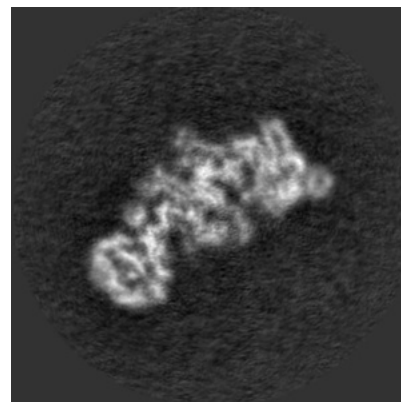
6.2.2 Raw map



X Index: 130



Y Index: 130

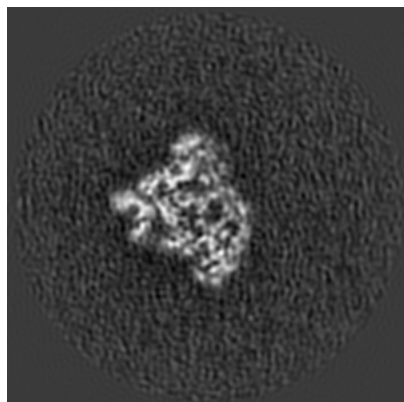


Z Index: 130

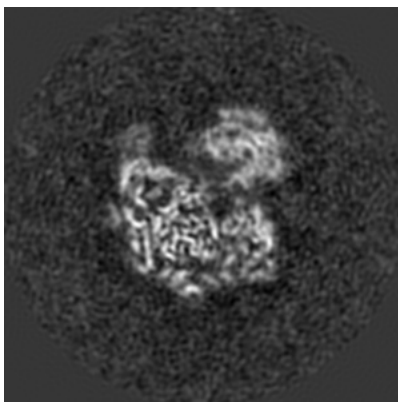
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

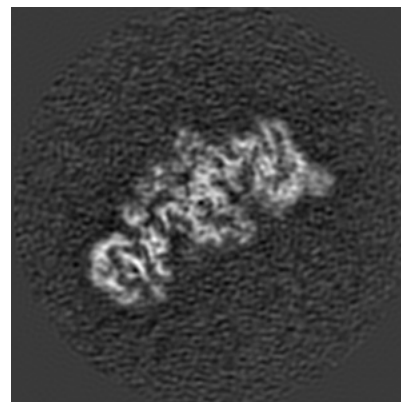
6.3.1 Primary map



X Index: 96

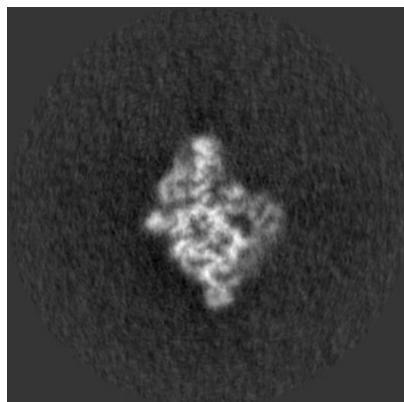


Y Index: 129

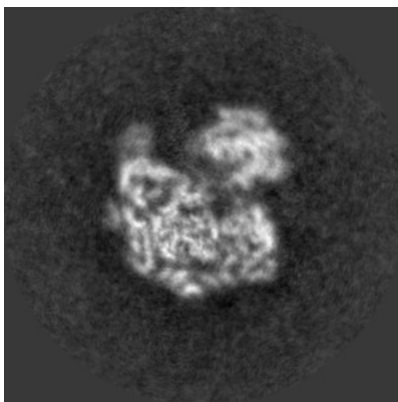


Z Index: 128

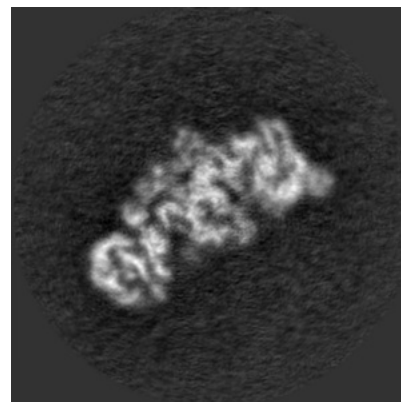
6.3.2 Raw map



X Index: 118



Y Index: 129

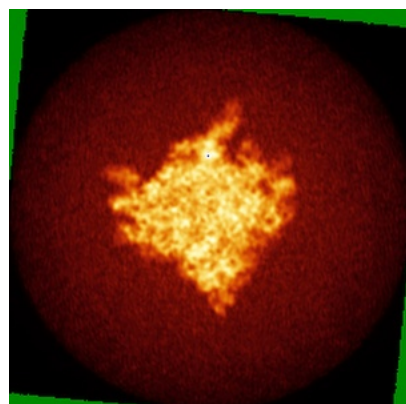


Z Index: 128

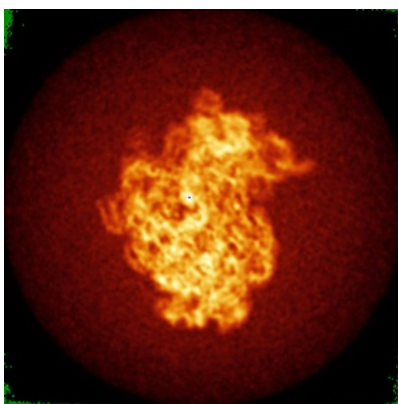
The images above show the largest variance slices of the map in three orthogonal directions.

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

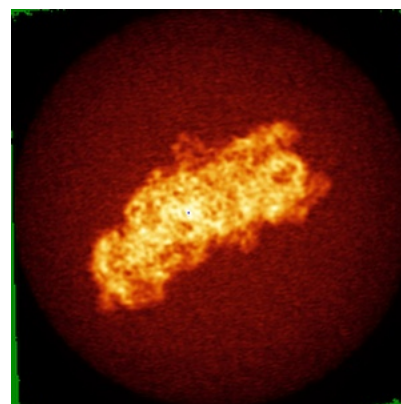
6.4.1 Primary map



X

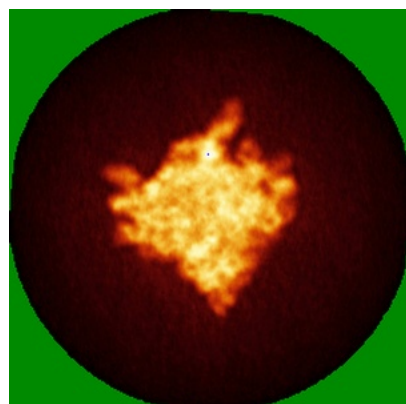


Y

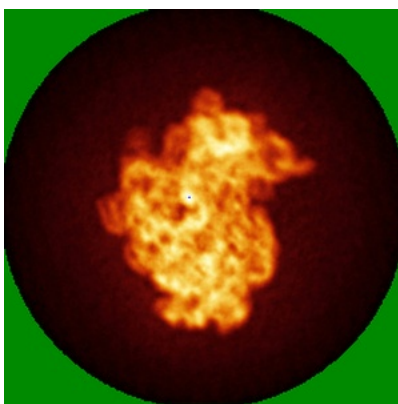


Z

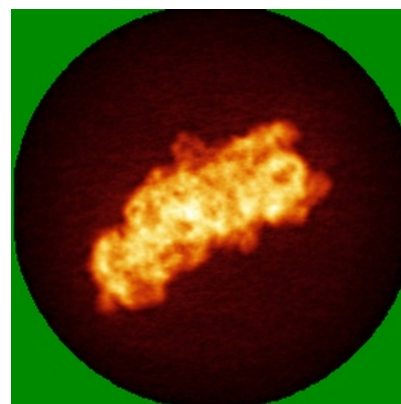
6.4.2 Raw map



X



Y

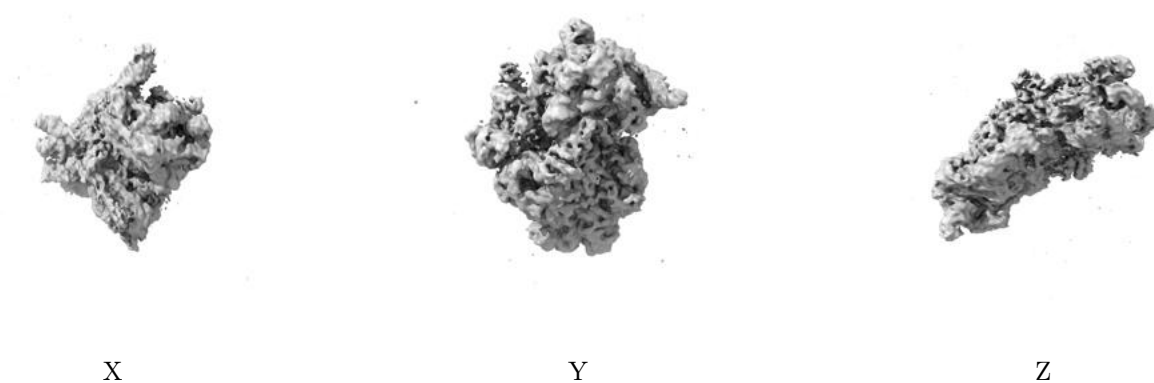


Z

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.

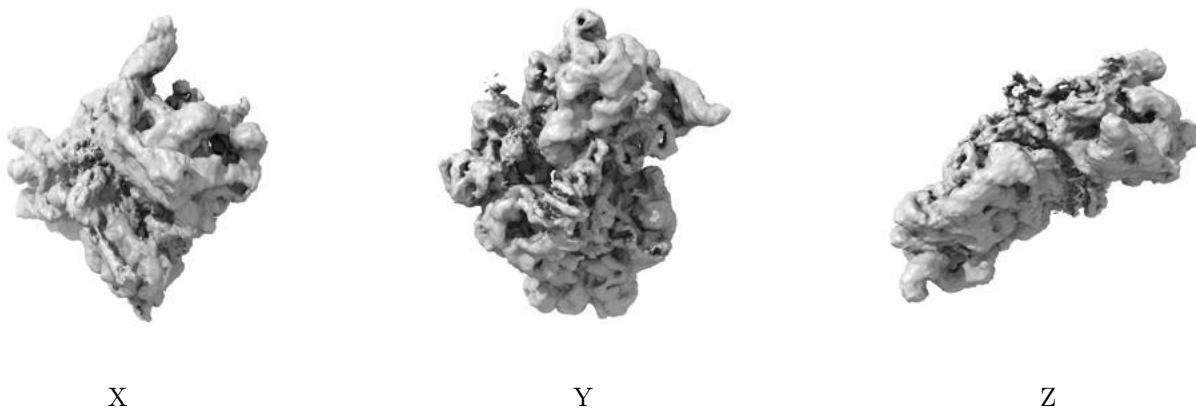
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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



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.

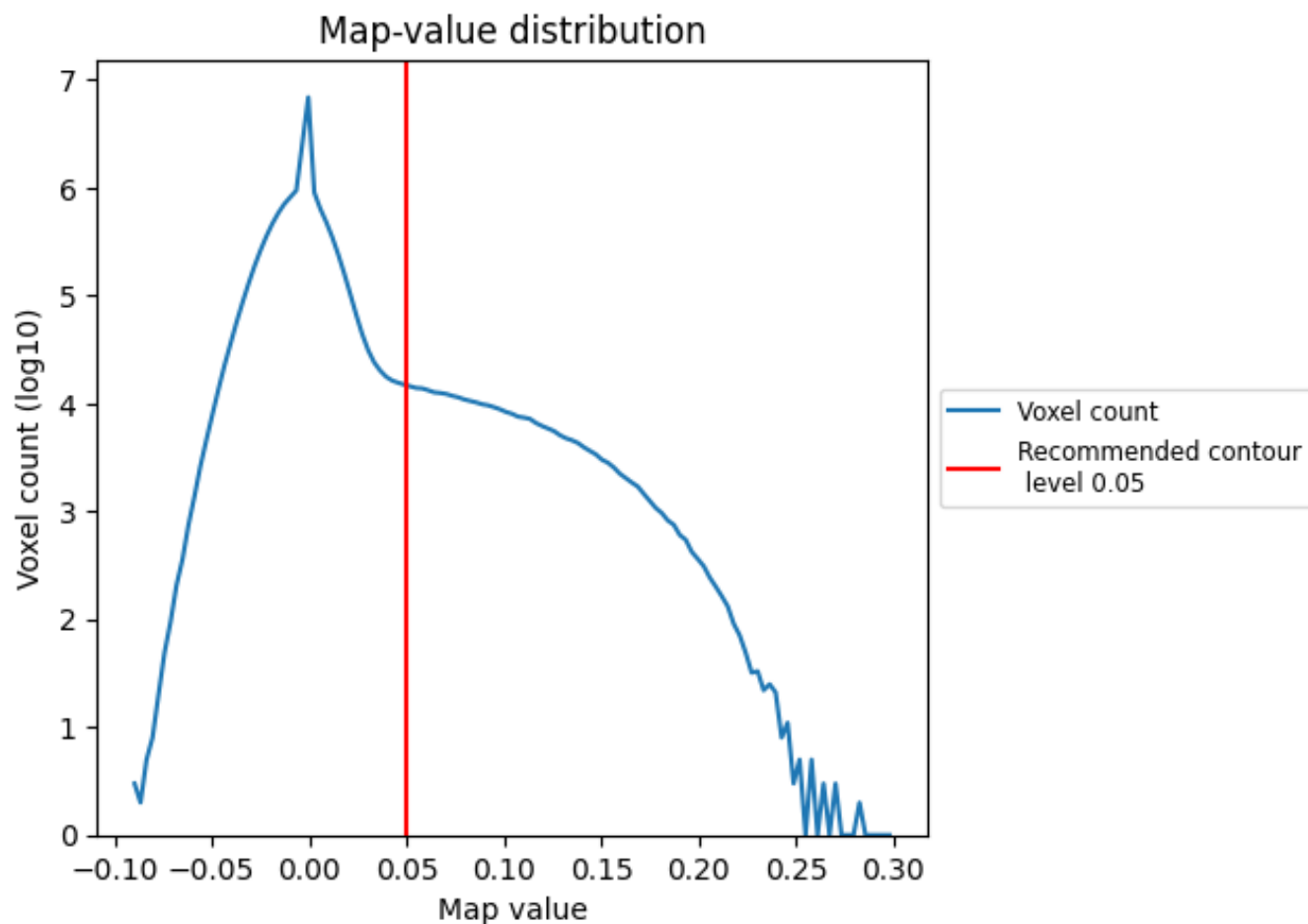
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

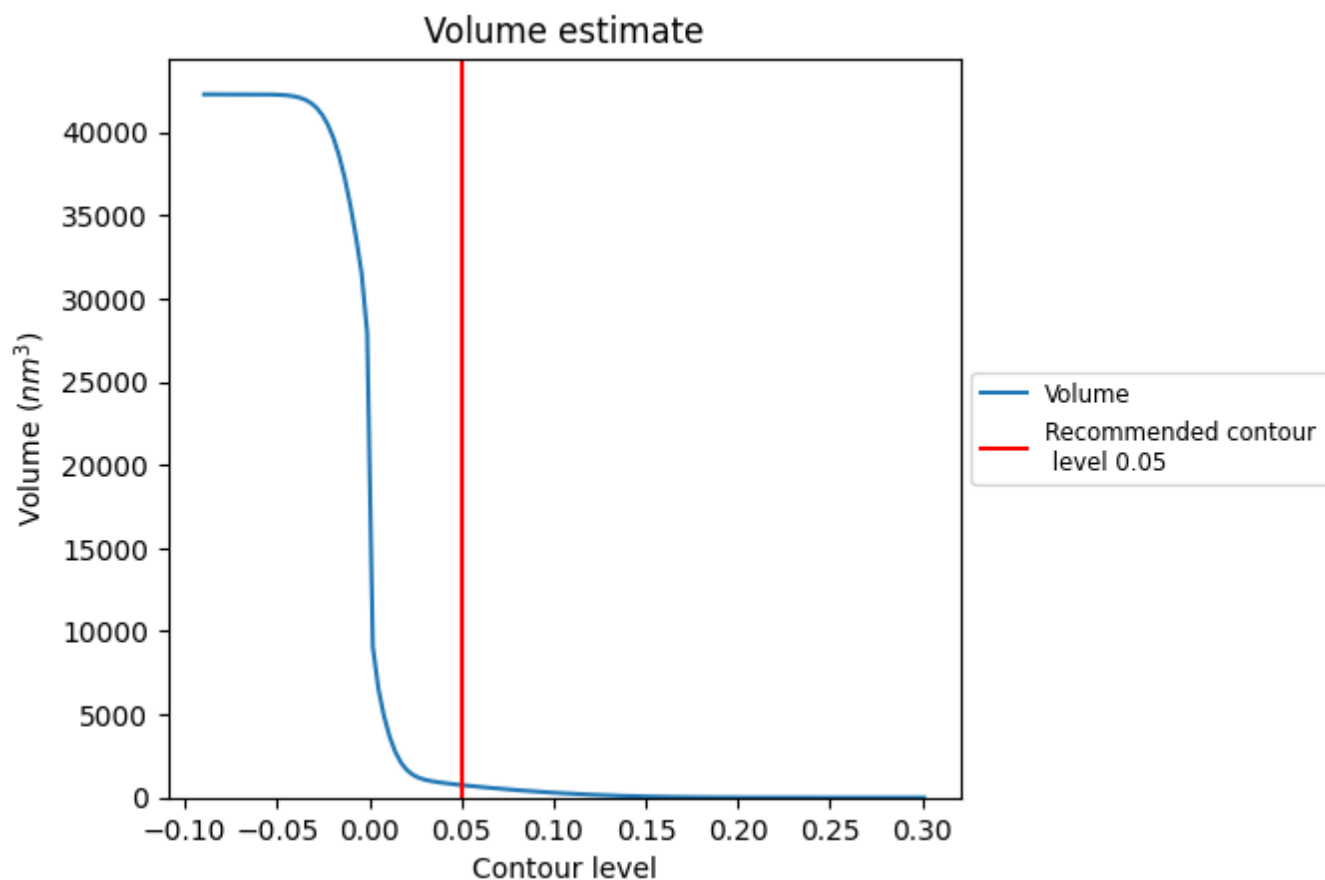
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

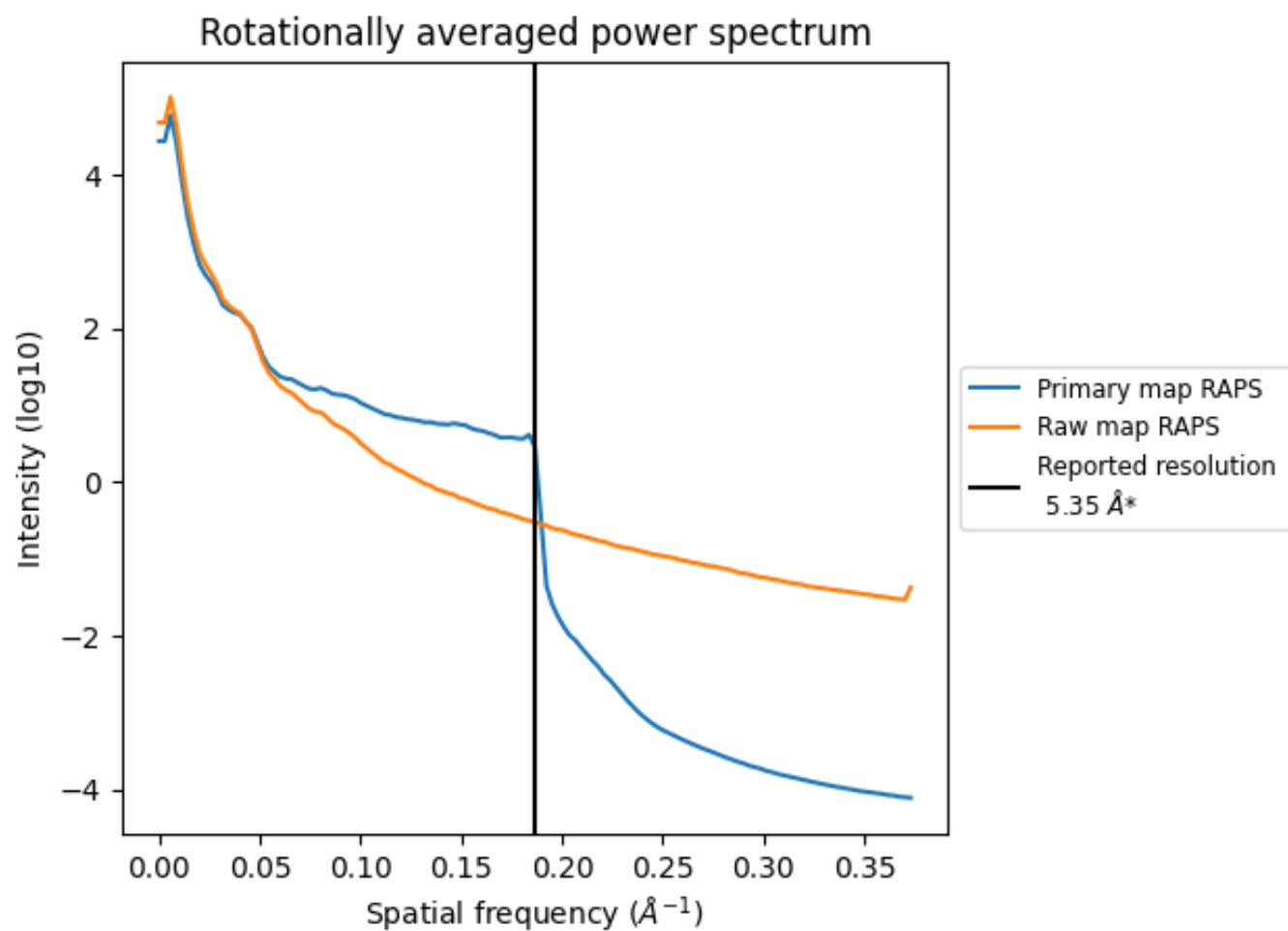
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 753 nm^3 ; this corresponds to an approximate mass of 680 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 ⓘ

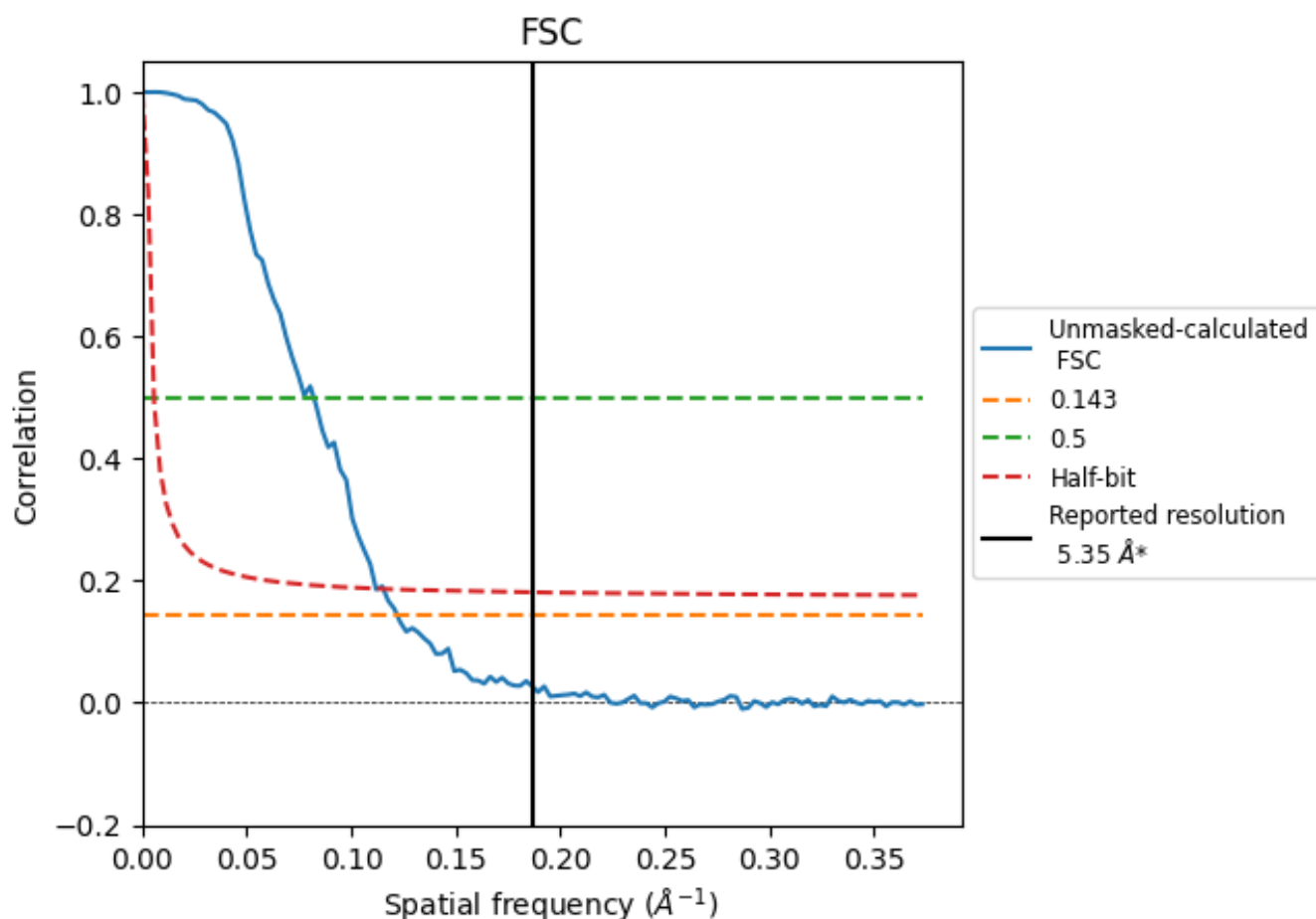


*Reported resolution corresponds to spatial frequency of 0.187 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.187 Å⁻¹

8.2 Resolution estimates [i](#)

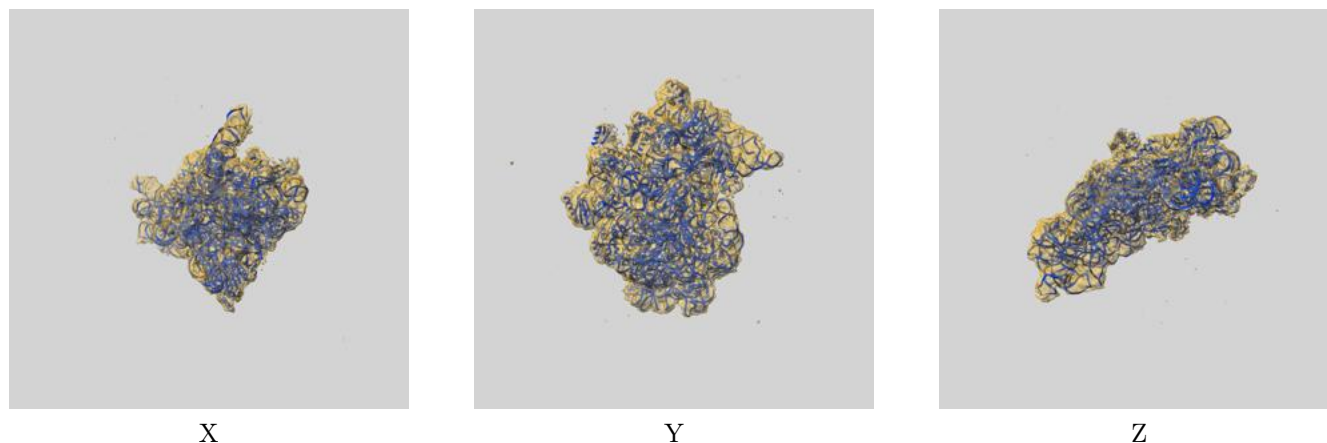
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.20	12.20	8.94

*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 8.20 differs from the reported value 5.35 by more than 10 %

9 Map-model fit [i](#)

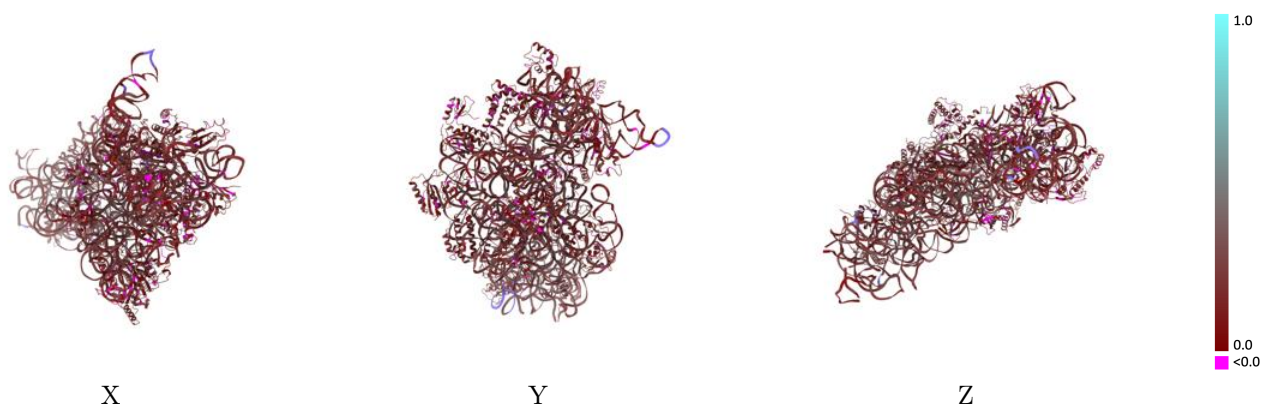
This section contains information regarding the fit between EMDB map EMD-4075 and PDB model 5LMP. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



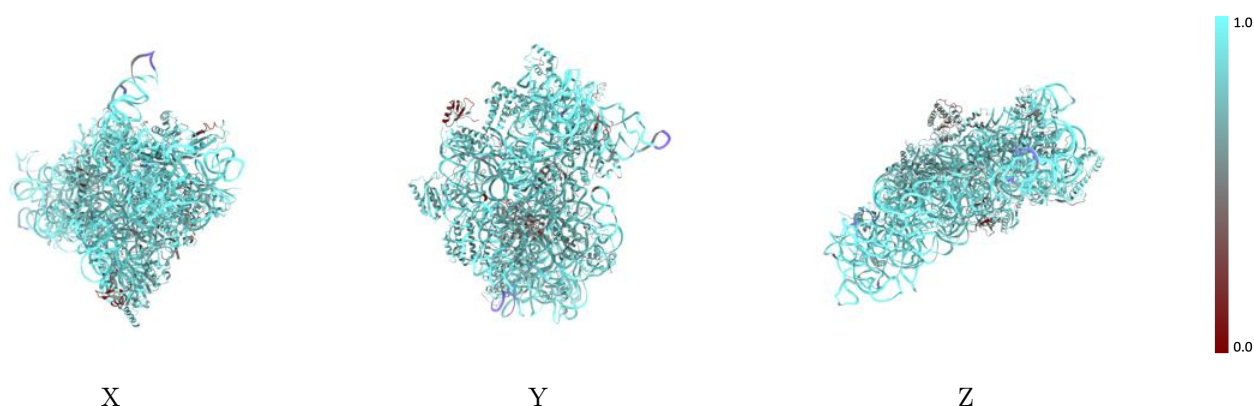
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



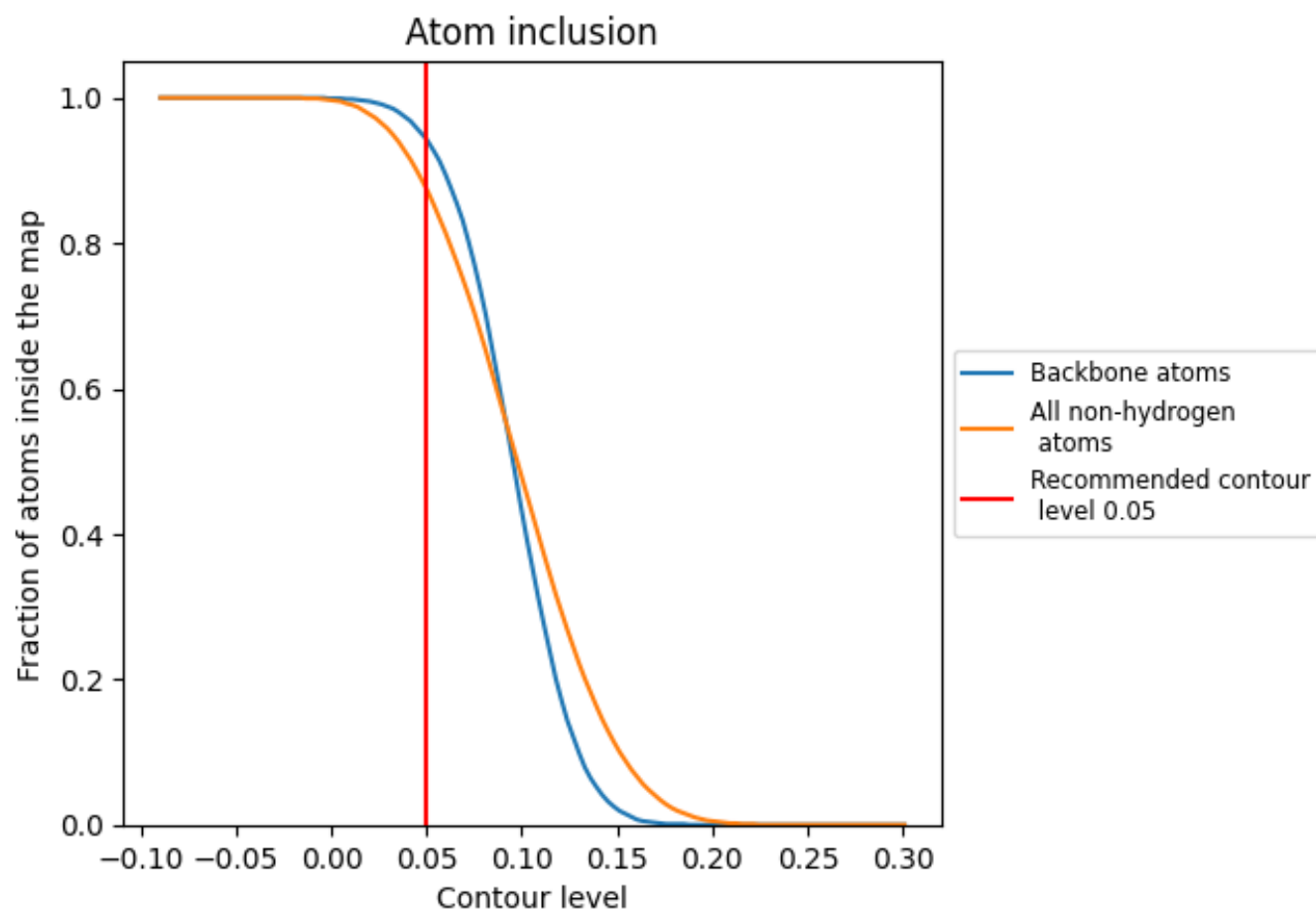
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.2130
A	 0.9610	 0.2380
B	 0.5610	 0.1520
C	 0.7940	 0.1940
D	 0.7440	 0.1880
E	 0.7550	 0.2110
F	 0.8010	 0.1950
G	 0.7810	 0.1650
H	 0.7900	 0.1930
I	 0.8100	 0.1690
J	 0.6710	 0.1510
K	 0.8080	 0.1820
L	 0.7610	 0.2140
M	 0.8020	 0.1300
N	 0.8230	 0.1800
O	 0.7970	 0.1920
P	 0.8140	 0.2020
Q	 0.7960	 0.2000
R	 0.7300	 0.1490
S	 0.7800	 0.1210
T	 0.7560	 0.1700
V	 0.8530	 0.1380
W	 0.5440	 0.1510
X	 0.6160	 0.1540
Y	 0.6900	 0.1760

