



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:16 AM UTC

PDB ID : 6ZXF / pdb_00006zxf
EMDB ID : EMD-11519
Title : Cryo-EM structure of a late human pre-40S ribosomal subunit - State G
Authors : Ameismeier, M.; Zemp, I.; van den Heuvel, J.; Thoms, M.; Berninghausen, O.;
Kutay, U.; Beckmann, R.
Deposited on : 2020-07-29
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

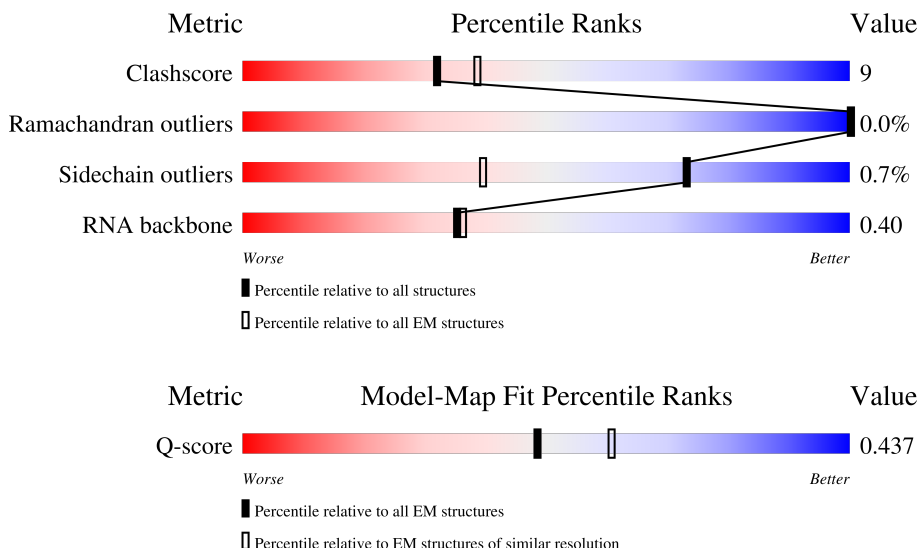
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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.



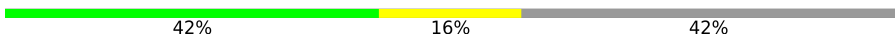
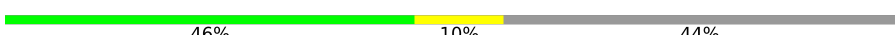
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1874	
2	A	295	
3	B	264	

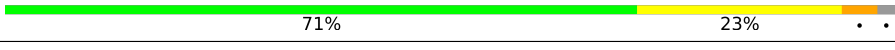
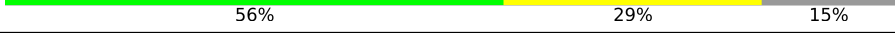
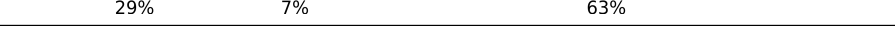
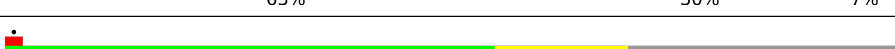
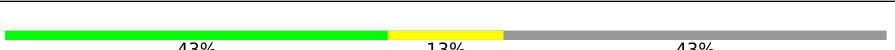
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	293	
5	E	263	
6	D	243	
7	G	249	
8	H	194	
9	I	208	
10	J	194	
11	F	204	
12	L	158	
13	K	165	
14	N	151	
15	O	151	
16	M	132	
17	P	145	
18	R	135	
19	Q	146	
20	S	152	
21	T	145	
22	V	83	
23	W	130	
24	X	143	
25	Y	133	
26	U	119	
27	Z	125	
28	b	84	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	c	69	
30	d	56	
31	e	59	
32	f	156	
33	g	317	
34	j	165	
35	z	568	
36	y	412	
37	k	583	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 80133 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 pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1656	Total	C	N	O	P	0	0
			35367	15787	6366	11558	1656		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	216	Total	C	N	O	S	0	0
			1674	1085	287	292	10		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	255	Total	C	N	O	S	0	0
			2031	1299	377	347	8		

- Molecule 6 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	223	Total	C	N	O	S	0	0
			1802	1128	358	309	7		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	179	Total	C	N	O	S	0	0
			1446	927	264	254	1		

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	199	Total	C	N	O	S	0	0
			1638	1027	322	284	5		

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	176	Total	C	N	O	S	0	0
			1465	934	295	234	2		

- Molecule 11 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	136	Total	C	N	O	S	0	0
			1127	719	212	190	6		

- Molecule 13 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	126	Total	C	N	O	S	0	0
			947	580	188	173	6		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	108	Total	C	N	O	S	0	0
			837	530	147	153	7		

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 18 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	121	Total	C	N	O	S	0	0
			983	617	183	180	3		

- Molecule 19 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	141	Total	C	N	O	S	0	0
			1162	731	232	198	1		

- Molecule 21 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 23 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 24 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 25 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	122	Total	C	N	O	S	0	0
			987	624	193	165	5		

- Molecule 26 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	98	Total	C	N	O	S	0	0
			774	486	145	139	4		

- Molecule 27 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	70	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 28 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	77	Total	C	N	O	S	0	0
			611	386	113	107	5		

- Molecule 29 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 30 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 31 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	50	Total	C	N	O	S	0	0
			398	244	90	63	1		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	295	Total	C	N	O	S	0	0
			2306	1460	403	431	12		

- Molecule 34 is a protein called Probable RNA-binding protein EIF1AD.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	115	Total	C	N	O	S	0	0
			928	590	166	170	2		

- Molecule 35 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	373	Total	C	N	O	S	0	0
			3041	1911	553	555	22		

- Molecule 36 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	233	Total	C	N	O	S	0	0
			1838	1167	335	327	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	10	ASN	ASP	conflict	UNP Q9ULX3

- Molecule 37 is a protein called Leucine-rich repeat-containing protein 47.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	430	Total	C	N	O	0	0
			2117	1257	430	430		

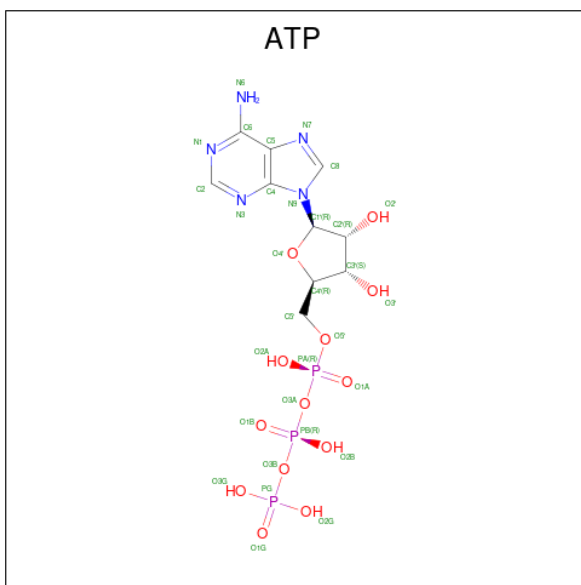
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	d	1	Total	Zn	0
			1	1	
38	f	1	Total	Zn	0
			1	1	
38	y	1	Total	Zn	0
			1	1	

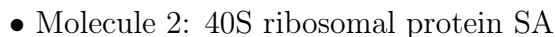
- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	z	2	Total	Mg	0
			2	2	

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

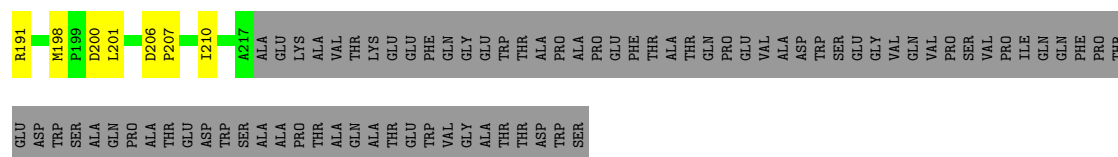


Mol	Chain	Residues	Atoms					AltConf
40	z	1	Total	C	N	O	P	0
			31	10	5	13	3	

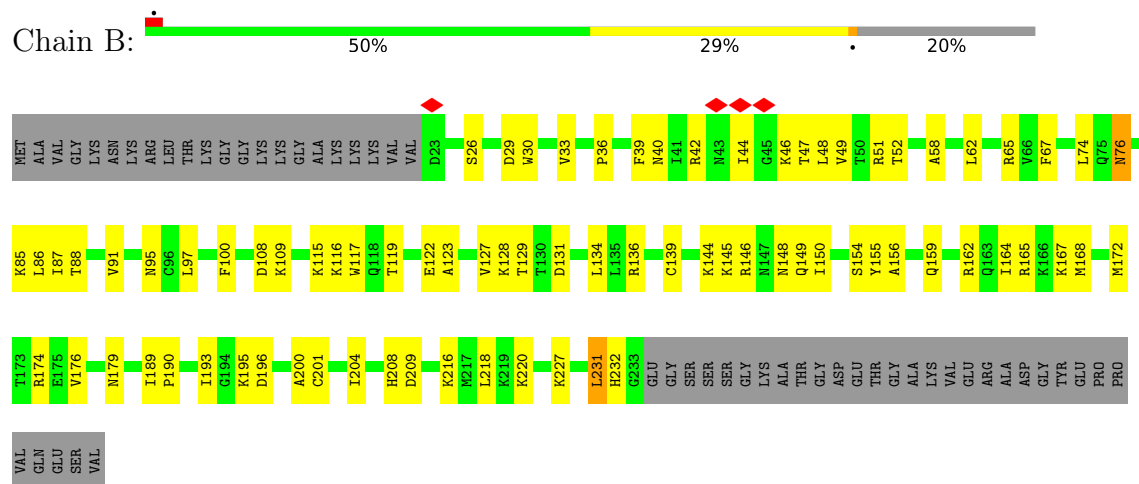


Response	Percentage
Yes	59%
No	14%
Don't know	27%

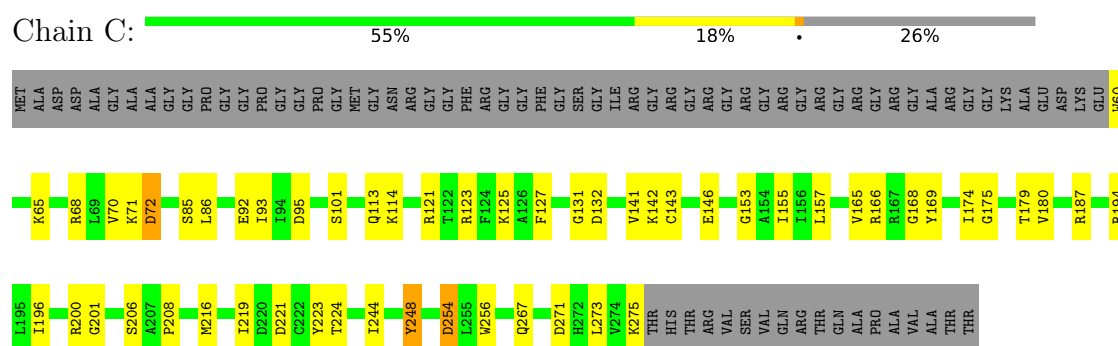




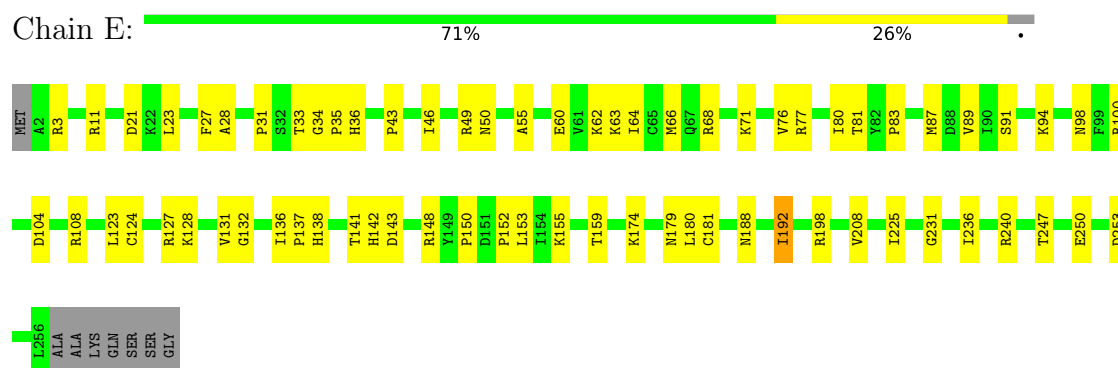
• Molecule 3: 40S ribosomal protein S3a



• Molecule 4: 40S ribosomal protein S2

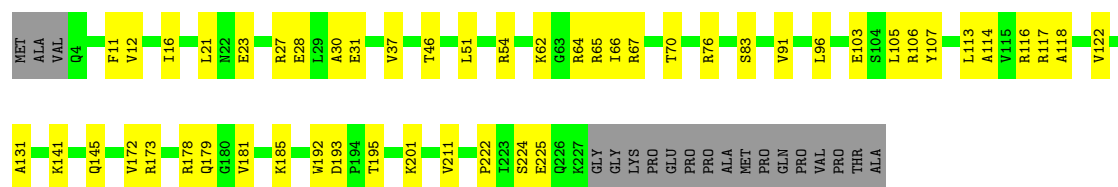


• Molecule 5: 40S ribosomal protein S4, X isoform



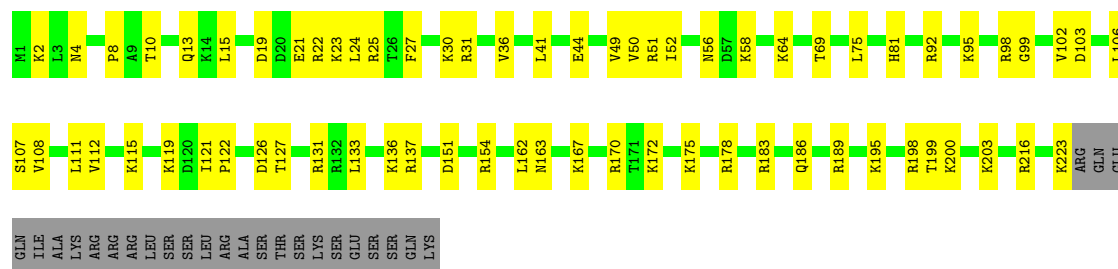
• Molecule 6: 40S ribosomal protein S3

Chain D:  72% 21% 8%



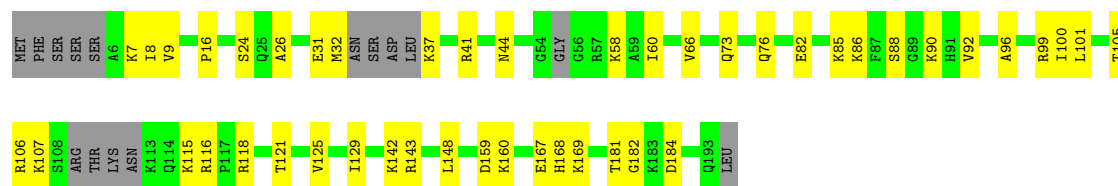
• Molecule 7: 40S ribosomal protein S6

Chain G:  62% 27% 10%



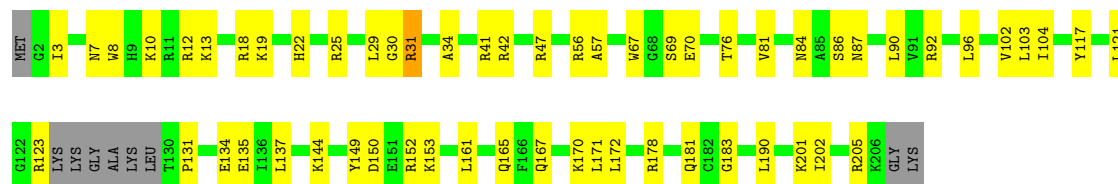
• Molecule 8: 40S ribosomal protein S7

Chain H:  69% 24% 8%



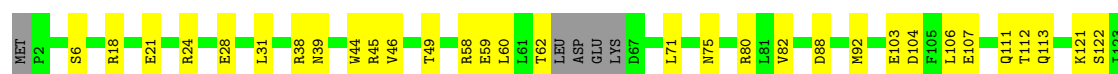
• Molecule 9: 40S ribosomal protein S8

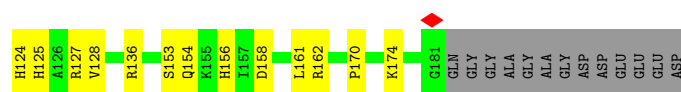
Chain I:  68% 27% 5%



• Molecule 10: 40S ribosomal protein S9

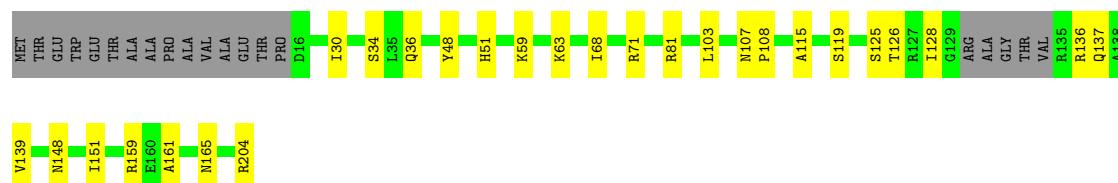
Chain J:  68% 23% 9%





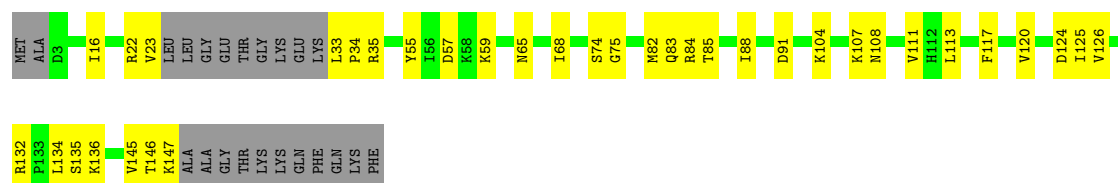
- Molecule 11: 40S ribosomal protein S5

Chain F: 77% 13% 10%



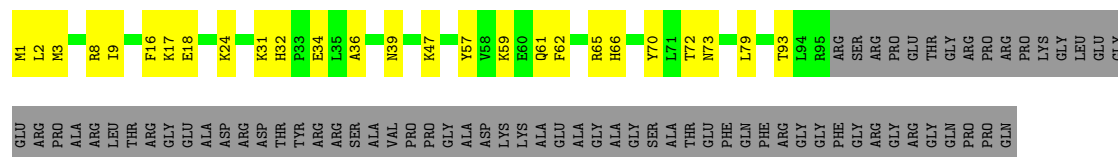
- Molecule 12: 40S ribosomal protein S11

Chain L: 63% 23% 14%



- Molecule 13: 40S ribosomal protein S10

Chain K: 42% 16% 42%



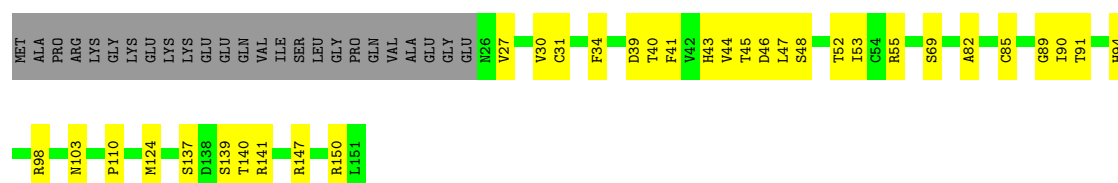
- Molecule 14: 40S ribosomal protein S13

Chain N: 85% 13% 2%



- Molecule 15: 40S ribosomal protein S14

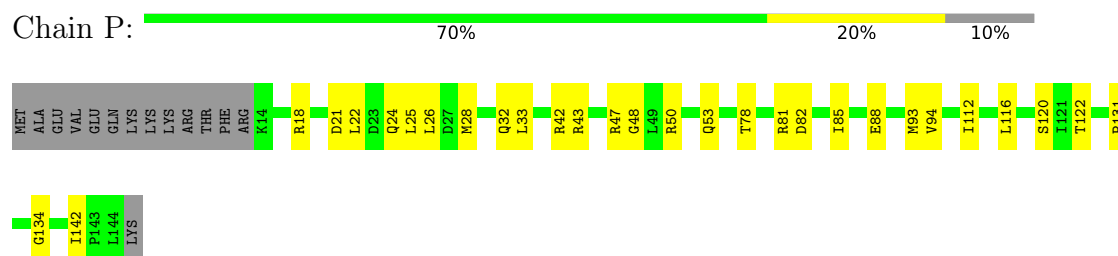
Chain O: 62% 22% 17%



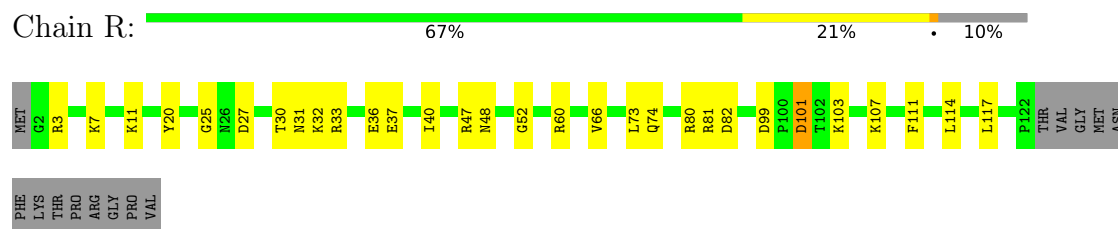
- Molecule 16: 40S ribosomal protein S12



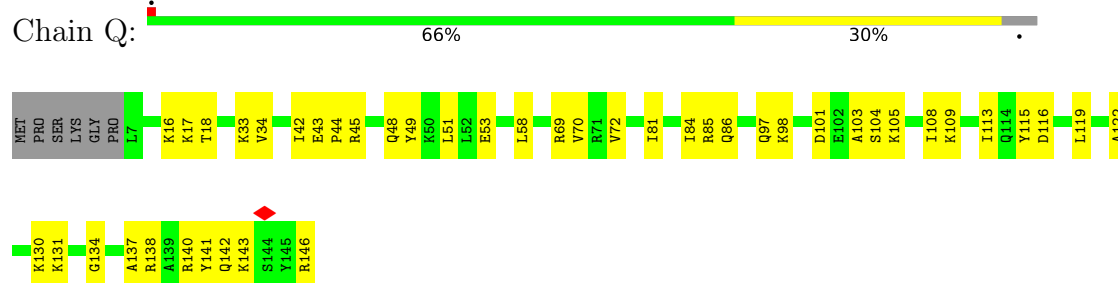
- Molecule 17: 40S ribosomal protein S15



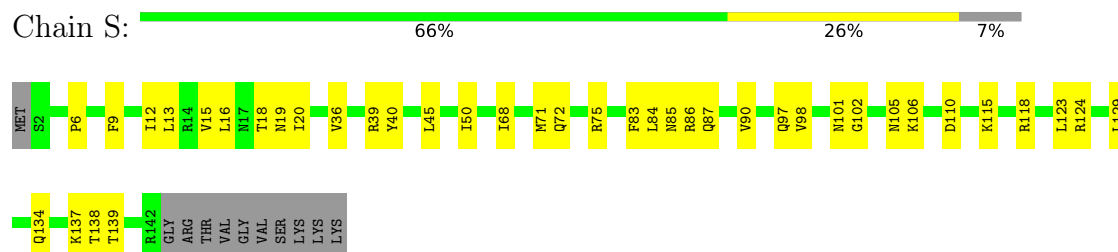
- Molecule 18: 40S ribosomal protein S17



- Molecule 19: 40S ribosomal protein S16

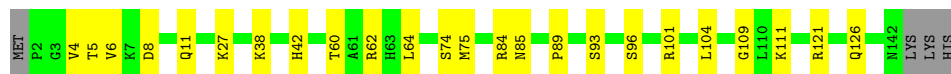


- Molecule 20: 40S ribosomal protein S18



- Molecule 21: 40S ribosomal protein S19

Chain T:  81% 17%



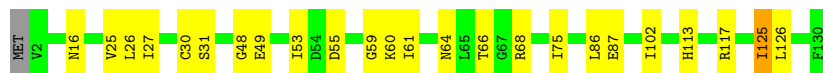
- Molecule 22: 40S ribosomal protein S21

Chain V:  86% 14%



- Molecule 23: 40S ribosomal protein S15a

Chain W:  81% 18%



- Molecule 24: 40S ribosomal protein S23

Chain X:  78% 20%



- Molecule 25: 40S ribosomal protein S24

Chain Y:  72% 20% 8%



PRO
LYS
GLU

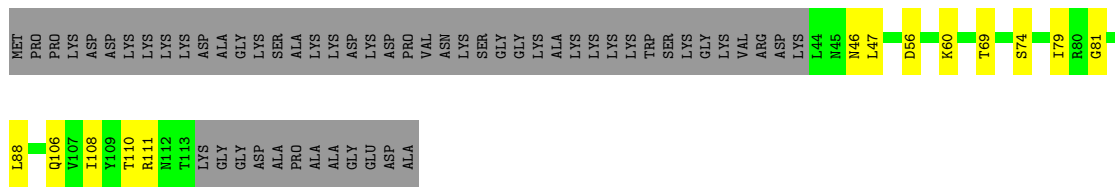
- Molecule 26: 40S ribosomal protein S20

Chain U:  63% 19% 18%



ASP
ALA

- Molecule 27: 40S ribosomal protein S25



- Molecule 28: 40S ribosomal protein S27



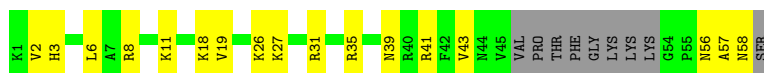
- Molecule 29: 40S ribosomal protein S28



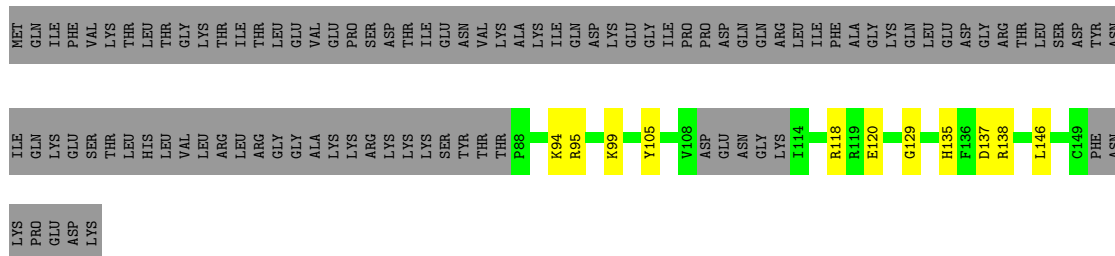
- Molecule 30: 40S ribosomal protein S29



- Molecule 31: 40S ribosomal protein S30

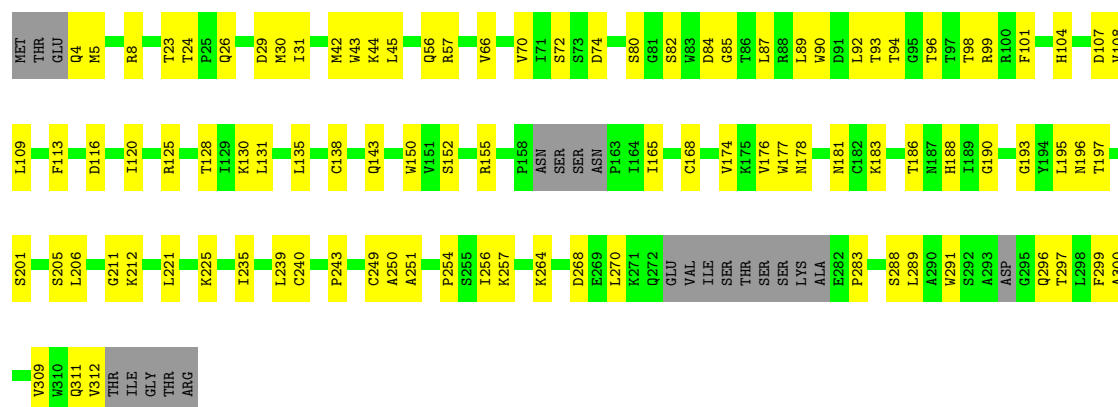


- Molecule 32: Ubiquitin-40S ribosomal protein S27a



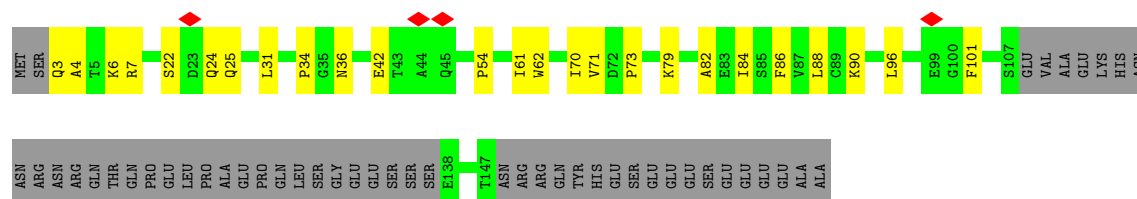
- Molecule 33: Receptor of activated protein C kinase 1

Chain g:  63% 30% 7%



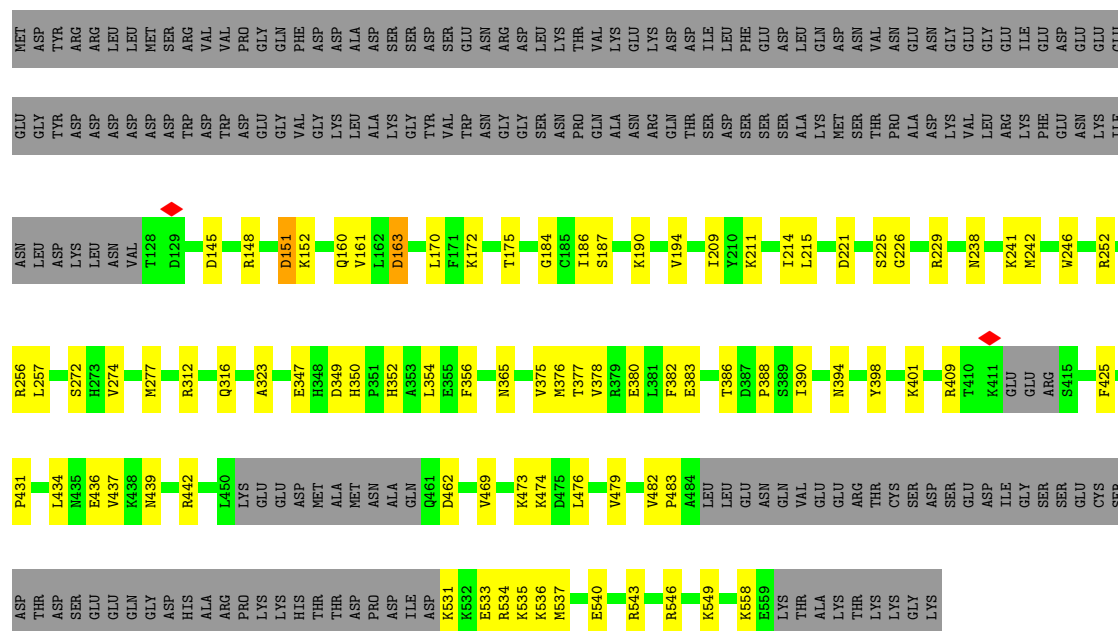
• Molecule 34: Probable RNA-binding protein EIF1AD

Chain j:  55% 15% 30%



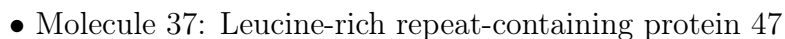
• Molecule 35: Serine/threonine-protein kinase RIO1

Chain z:  51% 14% 34%



• Molecule 36: RNA-binding protein NOB1

Satisfaction Level	Percentage
Very satisfied	43%
Satisfied	13%
Dissatisfied	43%



Response	Percentage
Doing a good job	18%
Not doing a good job	71%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.340	Depositor
Minimum map value	-0.135	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.53	0/39549	0.49	1/61629 (0.0%)
2	A	0.51	0/1742	0.52	0/2367
3	B	0.44	0/1742	0.60	0/2330
4	C	0.55	0/1710	0.58	0/2310
5	E	0.43	0/2073	0.51	0/2791
6	D	0.41	0/1773	0.53	0/2387
7	G	0.33	0/1825	0.52	0/2431
8	H	0.35	0/1466	0.51	0/1959
9	I	0.43	0/1666	0.55	0/2223
10	J	0.41	0/1489	0.55	0/1987
11	F	0.43	0/1481	0.54	0/1988
12	L	0.53	0/1147	0.51	0/1535
13	K	0.40	0/823	0.51	0/1111
14	N	0.43	0/1226	0.48	0/1649
15	O	0.42	0/959	0.58	0/1286
16	M	0.26	0/845	0.49	0/1134
17	P	0.38	0/1094	0.55	0/1464
18	R	0.41	0/995	0.53	0/1335
19	Q	0.46	0/1133	0.58	0/1517
20	S	0.38	0/1180	0.53	0/1582
21	T	0.41	0/1113	0.49	0/1493
22	V	0.46	0/643	0.52	0/860
23	W	0.54	0/1051	0.59	0/1406
24	X	0.48	0/1097	0.54	0/1464
25	Y	0.35	0/1004	0.50	0/1337
26	U	0.44	0/783	0.54	0/1052
27	Z	0.30	0/563	0.53	0/758
28	b	0.43	0/623	0.51	0/834
29	c	0.41	0/481	0.62	0/643
30	d	0.56	0/469	0.76	0/623
31	e	0.36	0/401	0.51	0/526
32	f	0.30	0/474	0.54	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.37	0/2360	0.55	0/3207
34	j	0.31	0/946	0.54	0/1274
35	z	0.44	0/3088	0.58	0/4134
36	y	0.42	0/1874	0.57	0/2531
37	k	0.21	0/2111	0.51	0/2926
All	All	0.47	0/84999	0.52	1/122709 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	Q	0	1
35	z	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1060	A	P-O3'-C3'	5.28	128.12	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	Q	103	ALA	Peptide
35	z	272	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	35367	0	17861	469	0
2	A	1705	0	1706	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1715	0	1785	60	0
4	C	1674	0	1764	42	0
5	E	2031	0	2133	47	0
6	D	1745	0	1839	36	0
7	G	1802	0	1954	58	0
8	H	1446	0	1540	27	0
9	I	1638	0	1710	45	0
10	J	1465	0	1583	41	0
11	F	1461	0	1511	22	0
12	L	1127	0	1190	24	0
13	K	799	0	823	19	0
14	N	1202	0	1289	18	0
15	O	947	0	976	25	0
16	M	837	0	870	21	0
17	P	1072	0	1121	23	0
18	R	983	0	1030	24	0
19	Q	1116	0	1185	29	0
20	S	1162	0	1215	30	0
21	T	1094	0	1120	19	0
22	V	636	0	637	10	0
23	W	1034	0	1080	17	0
24	X	1080	0	1147	20	0
25	Y	987	0	1038	18	0
26	U	774	0	839	14	0
27	Z	557	0	610	11	0
28	b	611	0	637	8	0
29	c	479	0	507	10	0
30	d	458	0	448	13	0
31	e	398	0	439	14	0
32	f	465	0	483	10	0
33	g	2306	0	2266	59	0
34	j	928	0	923	20	0
35	z	3041	0	3106	55	0
36	y	1838	0	1860	40	0
37	k	2117	0	957	7	0
38	d	1	0	0	0	0
38	f	1	0	0	0	0
38	y	1	0	0	0	0
39	z	2	0	0	0	0
40	z	31	0	12	3	0
All	All	80133	0	63194	1200	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 9.

All (1200) 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)
1:2:878:G:H1	1:2:908:A:N6	1.63	0.95
1:2:878:G:H1	1:2:908:A:H61	0.97	0.94
1:2:880:G:H1	1:2:906:U:H3	1.12	0.93
9:I:31:ARG:HH11	9:I:31:ARG:HG3	1.33	0.92
1:2:1748:G:H1	1:2:1786:U:H3	0.93	0.89
1:2:1033:G:H1	1:2:1080:A:HO2'	1.19	0.87
12:L:125:ILE:HB	12:L:146:THR:O	1.76	0.86
9:I:31:ARG:HG3	9:I:31:ARG:NH1	1.96	0.78
1:2:185:G:H1	1:2:214:U:H3	1.28	0.77
1:2:1351:G:H1	1:2:1360:U:H3	1.34	0.75
3:B:227:LYS:O	3:B:231:LEU:HB2	1.86	0.75
34:j:25:GLN:HA	34:j:71:VAL:O	1.87	0.74
1:2:1310:U:OP2	16:M:36:ARG:NH2	2.21	0.74
1:2:925:G:H1	1:2:1017:U:H3	1.34	0.73
21:T:42:HIS:HD1	21:T:93:SER:HG	1.36	0.73
20:S:36:VAL:HG11	20:S:71:MET:HE1	1.72	0.72
1:2:1611:G:H21	20:S:87:GLN:HE22	1.36	0.71
1:2:1396:A:N7	1:2:1449:G:O6	2.22	0.71
1:2:1518:C:H5''	1:2:1519:U:H5''	1.72	0.71
8:H:8:ILE:HG21	8:H:16:PRO:HG3	1.73	0.70
4:C:125:LYS:HG2	4:C:143:CYS:HB3	1.74	0.70
2:A:147:LEU:O	2:A:165:ASN:ND2	2.25	0.69
1:2:332:G:N7	7:G:189:ARG:NH1	2.41	0.69
1:2:1143:A:OP2	4:C:187:ARG:NH2	2.25	0.69
1:2:351:G:OP1	9:I:7:ASN:ND2	2.26	0.69
1:2:205:G:N7	9:I:144:LYS:NZ	2.41	0.68
1:2:1247:C:OP1	35:z:152:LYS:NZ	2.27	0.68
1:2:1648:G:N2	1:2:1675:A:OP2	2.26	0.68
3:B:67:PHE:O	3:B:85:LYS:HA	1.93	0.68
17:P:21:ASP:H	17:P:24:GLN:HE21	1.41	0.68
20:S:39:ARG:HH12	21:T:38:LYS:HB3	1.60	0.67
18:R:103:LYS:HZ2	18:R:117:LEU:HB2	1.59	0.67
1:2:1513:C:H2'	1:2:1514:G:H8	1.58	0.67
1:2:1622:U:H3	17:P:122:THR:HG22	1.60	0.67
8:H:66:VAL:HG22	8:H:96:ALA:HB1	1.77	0.67
36:y:75:ASP:OD2	36:y:243:ASN:ND2	2.27	0.67
35:z:312:ARG:NH2	35:z:390:ILE:O	2.28	0.66
1:2:1533:A:O2'	11:F:81:ARG:NH1	2.27	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:35:ARG:NH2	12:L:55:TYR:O	2.28	0.66
24:X:59:ALA:HB2	24:X:67:ARG:HE	1.59	0.66
1:2:916:A:H1'	14:N:73:ARG:HH21	1.61	0.66
1:2:643:A:OP1	10:J:39:ASN:ND2	2.29	0.66
1:2:988:C:H5''	3:B:116:LYS:HG2	1.78	0.66
13:K:61:GLN:HE21	13:K:62:PHE:H	1.43	0.66
33:g:130:LYS:NZ	33:g:138:CYS:SG	2.69	0.66
4:C:248:TYR:OH	22:V:10:ASP:OD1	2.14	0.65
1:2:4:C:O2'	10:J:18:ARG:NH2	2.30	0.65
15:O:82:ALA:HB1	15:O:124:MET:HE3	1.77	0.65
1:2:830:A:OP2	1:2:846:G:N2	2.30	0.65
5:E:35:PRO:HD2	5:E:83:PRO:HG2	1.79	0.65
1:2:878:G:N2	1:2:908:A:N1	2.41	0.64
2:A:198:MET:HG2	2:A:200:ASP:H	1.62	0.64
11:F:71:ARG:NH2	11:F:148:ASN:OD1	2.27	0.64
25:Y:110:ARG:NH1	25:Y:114:MET:SD	2.70	0.64
14:N:63:VAL:HG21	14:N:71:ILE:HG13	1.79	0.64
2:A:84:GLN:HG3	2:A:100:ALA:HB1	1.79	0.64
33:g:251:ALA:HB2	33:g:289:LEU:HD11	1.80	0.64
1:2:1122:A:N3	3:B:146:ARG:NH1	2.45	0.64
1:2:1252:C:N4	19:Q:146:ARG:O	2.31	0.64
2:A:29:ASN:HB2	2:A:151:ASP:HB3	1.79	0.64
1:2:203:G:N2	1:2:204:G:O6	2.29	0.64
1:2:1718:G:O2'	1:2:1815:A:N6	2.30	0.64
1:2:627:U:O4	34:j:6:LYS:NZ	2.30	0.64
1:2:495:U:O2'	5:E:27:PHE:O	2.16	0.64
4:C:146:GLU:OE2	6:D:116:ARG:NH2	2.29	0.63
2:A:89:LYS:NZ	2:A:201:LEU:O	2.32	0.63
6:D:64:ARG:NH2	13:K:73:ASN:OD1	2.31	0.63
1:2:1309:C:OP1	32:f:118:ARG:NH1	2.31	0.63
6:D:76:ARG:O	6:D:76:ARG:NH1	2.29	0.63
1:2:159:A:N6	1:2:467:G:O2'	2.31	0.63
1:2:388:U:H2'	1:2:389:A:H8	1.63	0.63
9:I:13:LYS:NZ	12:L:108:ASN:O	2.31	0.63
10:J:111:GLN:OE1	10:J:127:ARG:NH2	2.32	0.63
1:2:1314:U:O2'	13:K:8:ARG:NH2	2.32	0.63
1:2:185:G:O6	1:2:214:U:O4	2.17	0.63
1:2:527:C:O2'	10:J:121:LYS:NZ	2.32	0.62
17:P:94:VAL:HG11	17:P:116:LEU:HD21	1.81	0.62
1:2:1452:A:OP2	18:R:32:LYS:NZ	2.32	0.62
1:2:1599:U:OP2	27:Z:46:ASN:ND2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:170:PRO:HB3	10:J:174:LYS:HD2	1.80	0.62
9:I:29:LEU:HD23	9:I:29:LEU:O	1.99	0.62
24:X:67:ARG:NH2	24:X:114:ASP:OD2	2.31	0.62
1:2:818:A:OP1	10:J:80:ARG:NH2	2.32	0.62
12:L:104:LYS:O	24:X:11:ARG:NH2	2.32	0.62
1:2:919:A:OP2	14:N:64:ARG:NH1	2.33	0.62
10:J:107:GLU:HA	10:J:112:THR:HG21	1.81	0.62
33:g:181:ASN:O	33:g:183:LYS:NZ	2.30	0.62
34:j:70:ILE:HB	34:j:86:PHE:HB3	1.81	0.62
1:2:1605:G:OP1	21:T:84:ARG:NH2	2.32	0.62
23:W:30:CYS:SG	23:W:31:SER:N	2.73	0.62
32:f:137:ASP:OD1	32:f:138:ARG:NH1	2.32	0.62
1:2:975:G:OP1	15:O:98:ARG:NH1	2.33	0.61
1:2:1470:C:OP2	11:F:59:LYS:NZ	2.33	0.61
12:L:135:SER:OG	12:L:136:LYS:N	2.33	0.61
1:2:1015:U:OP2	28:b:20:LYS:NZ	2.33	0.61
36:y:288:CYS:SG	36:y:289:GLY:N	2.74	0.61
1:2:526:A:OP1	31:e:35:ARG:NH1	2.33	0.61
1:2:1362:U:H5''	1:2:1363:C:H5	1.65	0.61
7:G:44:GLU:HG3	7:G:119:LYS:HG3	1.82	0.61
33:g:250:ALA:HB3	33:g:257:LYS:O	2.01	0.61
1:2:1869:A:H2'	1:2:1870:A:O4'	1.99	0.61
3:B:129:THR:HG23	3:B:131:ASP:H	1.64	0.61
33:g:44:LYS:HG2	33:g:56:GLN:HB2	1.83	0.61
33:g:174:VAL:HB	33:g:188:HIS:HB2	1.80	0.61
9:I:81:VAL:HG12	9:I:102:VAL:HG12	1.81	0.61
17:P:81:ARG:NH1	17:P:120:SER:OG	2.34	0.61
24:X:107:ARG:HB2	24:X:112:VAL:HG22	1.83	0.61
13:K:3:MET:HB2	13:K:8:ARG:HH21	1.66	0.61
35:z:375:VAL:O	35:z:409:ARG:NH2	2.34	0.61
1:2:615:C:O2	31:e:11:LYS:NZ	2.33	0.60
1:2:583:A:OP1	10:J:162:ARG:NH2	2.34	0.60
35:z:365:ASN:ND2	35:z:376:MET:O	2.34	0.60
9:I:67:TRP:HD1	9:I:70:GLU:H	1.48	0.60
7:G:8:PRO:O	7:G:131:ARG:NH2	2.35	0.60
1:2:156:G:OP1	7:G:2:LYS:NZ	2.35	0.60
1:2:1588:A:H2'	1:2:1589:A:C8	2.36	0.60
10:J:46:VAL:O	10:J:49:THR:OG1	2.18	0.60
12:L:91:ASP:OD1	12:L:91:ASP:N	2.32	0.60
3:B:40:ASN:O	3:B:42:ARG:NH1	2.34	0.60
29:c:17:VAL:HA	29:c:30:VAL:HG23	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:196:ILE:HB	4:C:223:TYR:HB2	1.84	0.60
11:F:125:SER:HB2	11:F:136:ARG:HB3	1.83	0.60
20:S:12:ILE:HD11	20:S:19:ASN:HB3	1.84	0.60
33:g:201:SER:HB3	33:g:206:LEU:HB2	1.83	0.60
33:g:296:GLN:HG2	33:g:297:THR:HG23	1.84	0.60
1:2:526:A:O2'	10:J:125:HIS:ND1	2.35	0.60
2:A:206:ASP:OD1	2:A:206:ASP:N	2.33	0.60
1:2:677:G:N1	1:2:1027:A:OP2	2.26	0.60
1:2:973:C:O2	15:O:55:ARG:NH2	2.34	0.60
1:2:1695:A:N6	1:2:1832:A:O2'	2.35	0.60
4:C:221:ASP:OD1	4:C:221:ASP:N	2.30	0.59
7:G:98:ARG:NH2	7:G:103:ASP:OD2	2.35	0.59
21:T:85:ASN:ND2	21:T:89:PRO:O	2.34	0.59
26:U:61:LEU:O	26:U:81:GLN:HA	2.02	0.59
33:g:99:ARG:NH1	33:g:135:LEU:O	2.31	0.59
3:B:87:ILE:HG21	3:B:220:LYS:HZ1	1.67	0.59
5:E:11:ARG:HA	5:E:28:ALA:HB2	1.83	0.59
19:Q:101:ASP:O	19:Q:104:SER:OG	2.19	0.59
20:S:138:THR:HG23	20:S:139:THR:HG23	1.83	0.59
4:C:174:ILE:O	4:C:200:ARG:NH2	2.35	0.59
19:Q:98:LYS:O	33:g:57:ARG:NH2	2.36	0.59
1:2:186:C:H2'	1:2:187:G:C8	2.36	0.59
1:2:186:C:H2'	1:2:187:G:H8	1.68	0.59
21:T:60:THR:HG23	21:T:75:MET:HE2	1.84	0.59
1:2:201:C:OP1	1:2:202:G:N2	2.36	0.59
1:2:1258:A:H62	1:2:1659:U:H2'	1.68	0.59
3:B:145:LYS:NZ	3:B:149:GLN:O	2.34	0.59
23:W:49:GLU:O	23:W:64:ASN:ND2	2.34	0.59
33:g:176:VAL:HB	33:g:186:THR:HB	1.85	0.59
5:E:137:PRO:HG2	5:E:150:PRO:HD2	1.85	0.59
15:O:139:SER:OG	15:O:140:THR:N	2.32	0.59
16:M:14:VAL:HG23	16:M:123:VAL:HG22	1.84	0.59
35:z:163:ASP:OD1	35:z:163:ASP:N	2.32	0.59
1:2:3:C:O2	10:J:18:ARG:NH2	2.35	0.59
1:2:527:C:H2'	1:2:528:A:H8	1.68	0.59
6:D:192:TRP:NE1	6:D:201:LYS:O	2.31	0.59
35:z:439:ASN:HB3	35:z:442:ARG:HD2	1.84	0.59
1:2:16:G:H21	1:2:1195:A:H62	1.50	0.59
2:A:132:GLN:NE2	2:A:136:GLU:OE2	2.36	0.59
1:2:658:U:O2	24:X:17:ARG:NH1	2.35	0.59
33:g:128:THR:OG1	33:g:143:GLN:NE2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:y:238:ASP:HB3	36:y:241:MET:HG2	1.85	0.59
1:2:1056:U:O2'	35:z:229:ARG:NH2	2.36	0.58
36:y:68:GLU:O	36:y:72:LYS:NZ	2.30	0.58
1:2:1535:U:O4	11:F:159:ARG:NH1	2.36	0.58
1:2:1711:U:OP1	34:j:79:LYS:NZ	2.34	0.58
7:G:2:LYS:HB2	7:G:108:VAL:HG22	1.84	0.58
14:N:87:ASP:N	14:N:87:ASP:OD1	2.35	0.58
15:O:34:PHE:HB3	15:O:41:PHE:HB2	1.86	0.58
18:R:27:ASP:OD1	18:R:30:THR:N	2.36	0.58
18:R:101:ASP:OD1	18:R:101:ASP:N	2.31	0.58
1:2:71:G:O6	7:G:170:ARG:NH1	2.37	0.58
1:2:354:U:OP2	12:L:107:LYS:NZ	2.36	0.58
1:2:844:U:OP1	5:E:240:ARG:NH2	2.34	0.58
33:g:297:THR:HG22	33:g:311:GLN:HG2	1.86	0.58
1:2:1154:U:OP1	1:2:1155:U:O2'	2.21	0.58
7:G:19:ASP:OD1	7:G:19:ASP:N	2.34	0.58
10:J:71:LEU:O	10:J:75:ASN:ND2	2.32	0.58
12:L:120:VAL:HG22	12:L:145:VAL:HG11	1.85	0.58
35:z:187:SER:HB2	40:z:603:ATP:H4'	1.86	0.58
1:2:507:G:O6	25:Y:105:LYS:NZ	2.37	0.58
1:2:628:A:O2'	6:D:145:GLN:NE2	2.37	0.58
16:M:93:LYS:HE2	16:M:101:ARG:HE	1.68	0.58
21:T:109:GLY:O	21:T:111:LYS:NZ	2.37	0.58
3:B:129:THR:OG1	3:B:179:ASN:O	2.21	0.58
36:y:8:VAL:HG21	36:y:90:THR:HB	1.85	0.58
1:2:1203:G:H2'	1:2:1204:A:C8	2.39	0.57
1:2:1677:U:OP2	11:F:63:LYS:NZ	2.28	0.57
1:2:523:A:OP2	10:J:38:ARG:NH1	2.37	0.57
7:G:64:LYS:HZ1	7:G:81:HIS:HB3	1.68	0.57
26:U:26:SER:OG	26:U:27:ARG:N	2.37	0.57
1:2:942:G:OP1	3:B:216:LYS:NZ	2.38	0.57
1:2:996:A:H2'	1:2:997:A:C8	2.40	0.57
3:B:46:LYS:HB2	15:O:27:VAL:HG22	1.87	0.57
6:D:28:GLU:OE1	6:D:65:ARG:NH2	2.36	0.57
6:D:31:GLU:O	6:D:54:ARG:NH2	2.37	0.57
8:H:60:ILE:HB	8:H:92:VAL:HG12	1.85	0.57
26:U:56:MET:HB2	26:U:86:LYS:HB3	1.84	0.57
1:2:1410:C:H2'	1:2:1411:G:H8	1.68	0.57
1:2:454:U:H2'	1:2:455:A:H8	1.70	0.57
1:2:874:G:H2'	1:2:875:A:H8	1.69	0.57
1:2:1182:A:O2'	35:z:549:LYS:NZ	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:6:LEU:HA	30:d:9:SER:HB3	1.86	0.57
35:z:383:GLU:OE1	35:z:398:TYR:OH	2.23	0.57
7:G:21:GLU:O	7:G:25:ARG:NH1	2.37	0.57
1:2:1829:G:O2'	1:2:1850:A:N6	2.37	0.57
4:C:267:GLN:NE2	22:V:35:ASN:OD1	2.38	0.57
15:O:27:VAL:HB	15:O:91:THR:H	1.69	0.57
1:2:1562:C:H2'	1:2:1563:G:H8	1.70	0.57
27:Z:74:SER:OG	27:Z:79:ILE:O	2.22	0.57
5:E:23:LEU:HD21	10:J:6:SER:HB2	1.86	0.57
9:I:172:LEU:HB3	9:I:190:LEU:HD12	1.86	0.57
27:Z:47:LEU:H	27:Z:79:ILE:HA	1.70	0.57
34:j:70:ILE:HG13	34:j:88:LEU:HD21	1.87	0.57
35:z:151:ASP:OD1	35:z:151:ASP:N	2.35	0.57
1:2:986:G:OP1	1:2:1001:A:O2'	2.22	0.57
1:2:1677:U:O4	1:2:1678:A:N6	2.38	0.57
5:E:127:ARG:HD2	5:E:142:HIS:HA	1.87	0.57
26:U:49:LYS:HB3	26:U:92:HIS:HB2	1.87	0.57
35:z:238:ASN:HD22	35:z:241:LYS:HD2	1.69	0.57
1:2:64:A:N7	1:2:84:A:N6	2.52	0.56
1:2:1854:U:OP2	15:O:147:ARG:NH1	2.38	0.56
2:A:85:ARG:NH2	18:R:82:ASP:O	2.34	0.56
1:2:752:G:N2	1:2:791:C:O2'	2.37	0.56
2:A:157:VAL:O	22:V:65:SER:OG	2.23	0.56
35:z:161:VAL:HG12	35:z:211:LYS:HA	1.87	0.56
1:2:1753:C:N4	1:2:1754:G:O6	2.38	0.56
8:H:73:GLN:HA	8:H:76:GLN:HB2	1.86	0.56
13:K:17:LYS:NZ	13:K:18:GLU:OE1	2.36	0.56
33:g:107:ASP:OD2	33:g:125:ARG:NH1	2.39	0.56
35:z:145:ASP:O	35:z:148:ARG:NH2	2.36	0.56
2:A:34:MET:HE1	2:A:162:PRO:HB3	1.87	0.56
1:2:810:A:N6	1:2:851:C:N3	2.54	0.56
9:I:165:GLN:HB3	9:I:171:LEU:HD23	1.88	0.56
12:L:74:SER:OG	12:L:75:GLY:N	2.35	0.56
27:Z:69:THR:HG22	27:Z:108:ILE:HA	1.87	0.56
1:2:1873:G:O2'	36:y:309:HIS:O	2.23	0.56
1:2:1874:A:N7	36:y:264:ARG:NE	2.54	0.56
25:Y:62:THR:HA	25:Y:69:THR:HG22	1.87	0.56
33:g:87:LEU:HB2	33:g:101:PHE:HB2	1.87	0.56
25:Y:37:LYS:HA	25:Y:40:ILE:HD12	1.88	0.56
1:2:1451:G:OP1	18:R:33:ARG:NH2	2.39	0.56
20:S:13:LEU:HB2	20:S:20:ILE:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1019:C:OP2	14:N:70:LYS:NZ	2.37	0.56
1:2:1629:C:H2'	1:2:1630:A:H8	1.71	0.56
1:2:1722:G:H3'	1:2:1723:G:H8	1.70	0.56
1:2:969:U:OP1	1:2:970:G:O2'	2.20	0.55
1:2:1024:A:OP2	14:N:124:ARG:NH2	2.38	0.55
1:2:1332:A:N3	6:D:141:LYS:NZ	2.43	0.55
3:B:172:MET:HE1	3:B:193:ILE:HD12	1.88	0.55
26:U:64:THR:HG22	26:U:79:ARG:HG3	1.88	0.55
29:c:38:THR:HG22	29:c:40:ARG:H	1.70	0.55
35:z:277:MET:HE3	40:z:603:ATP:HN61	1.70	0.55
1:2:600:G:H2'	1:2:601:G:H8	1.71	0.55
1:2:1869:A:H1'	36:y:11:ALA:O	2.06	0.55
1:2:1873:G:H1'	36:y:311:SER:HB2	1.88	0.55
33:g:165:ILE:HG13	33:g:177:TRP:HB2	1.89	0.55
1:2:606:G:O4'	31:e:56:ASN:ND2	2.39	0.55
2:A:207:PRO:HA	2:A:210:ILE:HG22	1.88	0.55
3:B:76:ASN:OD1	3:B:76:ASN:N	2.37	0.55
33:g:288:SER:O	33:g:300:ALA:HA	2.06	0.55
1:2:800:U:O4	8:H:106:ARG:NH1	2.39	0.55
33:g:197:THR:HG21	33:g:239:LEU:H	1.71	0.55
1:2:33:G:O2'	1:2:564:A:O2'	2.23	0.55
2:A:184:ARG:NH1	2:A:191:ARG:O	2.40	0.55
1:2:168:C:O2'	7:G:133:LEU:O	2.23	0.55
33:g:85:GLY:HA2	33:g:108:VAL:HG23	1.88	0.55
2:A:30:LEU:O	36:y:323:ARG:NH1	2.34	0.55
4:C:208:PRO:HD3	10:J:18:ARG:HH12	1.72	0.55
25:Y:7:ILE:HD13	25:Y:43:LYS:HB3	1.88	0.55
1:2:107:A:H2'	1:2:108:G:C8	2.42	0.55
1:2:1401:A:N6	1:2:1441:U:O2'	2.40	0.55
3:B:65:ARG:H	3:B:88:THR:HG22	1.72	0.55
7:G:2:LYS:HD3	7:G:15:LEU:HD21	1.89	0.55
8:H:7:LYS:N	8:H:24:SER:OG	2.38	0.55
27:Z:56:ASP:N	27:Z:56:ASP:OD1	2.40	0.55
1:2:864:A:H2'	1:2:865:A:H8	1.71	0.55
37:k:378:HIS:O	37:k:480:PHE:CB	2.55	0.55
1:2:10:G:O2'	4:C:113:GLN:NE2	2.40	0.54
18:R:80:ARG:HE	18:R:81:ARG:HH21	1.54	0.54
1:2:388:U:H2'	1:2:389:A:C8	2.41	0.54
1:2:527:C:H4'	10:J:121:LYS:HG3	1.89	0.54
6:D:106:ARG:NH2	6:D:107:TYR:OH	2.40	0.54
33:g:23:THR:HG22	33:g:31:ILE:HD12	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:162:C:O3'	7:G:95:LYS:NZ	2.38	0.54
1:2:1410:C:H2'	1:2:1411:G:C8	2.43	0.54
3:B:30:TRP:HA	3:B:48:LEU:HD12	1.90	0.54
3:B:127:VAL:HG11	3:B:176:VAL:HG11	1.88	0.54
10:J:46:VAL:HG21	10:J:106:LEU:HD21	1.89	0.54
10:J:59:GLU:O	10:J:62:THR:OG1	2.26	0.54
12:L:57:ASP:OD1	12:L:84:ARG:NH1	2.40	0.54
33:g:70:VAL:HG21	33:g:113:PHE:HB2	1.89	0.54
2:A:40:LYS:NZ	2:A:41:ARG:O	2.40	0.54
11:F:137:GLN:HE22	29:c:63:ARG:HH12	1.55	0.54
20:S:97:GLN:NE2	20:S:98:VAL:O	2.41	0.54
37:k:22:ARG:O	37:k:53:HIS:N	2.40	0.54
1:2:616:A:OP1	31:e:8:ARG:NH2	2.38	0.54
3:B:117:TRP:O	3:B:154:SER:OG	2.25	0.54
5:E:63:LYS:NZ	25:Y:84:LYS:O	2.39	0.54
1:2:386:C:H5''	9:I:10:LYS:HZ2	1.73	0.54
1:2:525:A:H2'	1:2:526:A:H8	1.71	0.54
1:2:1461:G:N1	1:2:1464:C:OP2	2.34	0.54
6:D:193:ASP:OD2	6:D:195:THR:OG1	2.24	0.54
1:2:367:U:O2'	1:2:371:A:N7	2.37	0.54
1:2:1748:G:O6	1:2:1786:U:O4	2.26	0.54
6:D:105:LEU:HD22	6:D:122:VAL:HG21	1.89	0.54
10:J:136:ARG:NE	10:J:158:ASP:OD2	2.41	0.54
16:M:81:ASP:HB3	16:M:84:LYS:HG2	1.87	0.54
20:S:15:VAL:O	20:S:18:THR:HB	2.08	0.54
4:C:168:GLY:N	4:C:179:THR:O	2.41	0.54
7:G:30:LYS:HD3	7:G:36:VAL:HG11	1.89	0.54
8:H:148:LEU:HD21	23:W:48:GLY:HA2	1.90	0.54
1:2:1232:U:H2'	1:2:1233:G:H8	1.73	0.54
2:A:81:ASN:HA	2:A:84:GLN:HB2	1.90	0.54
3:B:164:ILE:HD12	3:B:201:CYS:HB3	1.90	0.54
21:T:42:HIS:ND1	21:T:93:SER:OG	2.30	0.54
1:2:1253:A:OP2	1:2:1526:G:N2	2.40	0.53
1:2:1825:A:N6	34:j:61:ILE:O	2.39	0.53
5:E:64:ILE:HD11	25:Y:18:LEU:HD22	1.91	0.53
35:z:540:GLU:OE2	35:z:543:ARG:NH1	2.42	0.53
1:2:1213:C:H2'	1:2:1214:A:C8	2.43	0.53
1:2:1298:G:H4'	17:P:78:THR:HA	1.89	0.53
1:2:1839:U:H2'	1:2:1840:U:C6	2.43	0.53
6:D:16:ILE:HD11	30:d:36:LEU:HD23	1.89	0.53
16:M:17:ALA:HB3	16:M:123:VAL:HG11	1.88	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:45:LEU:HD22	20:S:50:ILE:HD11	1.89	0.53
1:2:1554:C:OP2	1:2:1555:U:O2'	2.21	0.53
4:C:165:VAL:HG12	4:C:244:ILE:HG23	1.90	0.53
5:E:180:LEU:HD21	5:E:192:ILE:HD11	1.90	0.53
1:2:1275:G:N2	1:2:1506:A:OP2	2.31	0.53
4:C:68:ARG:NH1	4:C:275:LYS:O	2.41	0.53
1:2:1736:G:H2'	1:2:1737:G:C8	2.43	0.53
3:B:26:SER:O	3:B:51:ARG:NH2	2.41	0.53
5:E:46:ILE:HA	5:E:50:ASN:HD22	1.73	0.53
6:D:114:ALA:HB3	6:D:117:ARG:HG3	1.89	0.53
7:G:136:LYS:NZ	7:G:175:LYS:O	2.32	0.53
16:M:87:GLU:HA	16:M:92:CYS:HB2	1.90	0.53
33:g:152:SER:OG	33:g:168:CYS:SG	2.67	0.53
36:y:20:LEU:HD11	36:y:235:LEU:HG	1.90	0.53
1:2:1171:G:O2'	1:2:1187:G:O6	2.25	0.53
8:H:105:THR:HG23	8:H:107:LYS:H	1.72	0.53
19:Q:34:VAL:HG22	19:Q:70:VAL:HB	1.90	0.53
19:Q:86:GLN:HE22	19:Q:122:ALA:HB2	1.72	0.53
23:W:55:ASP:HB3	28:b:25:VAL:HG12	1.91	0.53
26:U:51:LYS:HB2	26:U:90:ASP:HB2	1.90	0.53
1:2:563:G:H2'	1:2:564:A:H8	1.72	0.53
1:2:961:G:N2	35:z:349:ASP:OD2	2.37	0.53
1:2:1010:G:H2'	1:2:1011:A:H8	1.74	0.53
1:2:1736:G:H2'	1:2:1737:G:H8	1.74	0.53
6:D:51:LEU:HB3	6:D:91:VAL:HG12	1.91	0.53
17:P:48:GLY:O	17:P:50:ARG:NH1	2.41	0.53
20:S:115:LYS:O	20:S:118:ARG:NH1	2.42	0.53
36:y:40:LYS:HA	36:y:43:ARG:HG2	1.90	0.53
1:2:677:G:OP1	14:N:124:ARG:NH1	2.38	0.53
1:2:1232:U:H2'	1:2:1233:G:C8	2.43	0.53
1:2:1848:U:O3'	1:2:1849:G:N2	2.23	0.53
4:C:179:THR:OG1	4:C:180:VAL:N	2.39	0.53
6:D:12:VAL:HG21	30:d:34:TYR:HB3	1.90	0.53
6:D:178:ARG:NH2	6:D:179:GLN:OE1	2.41	0.53
17:P:131:PRO:HG2	35:z:184:GLY:HA3	1.91	0.53
1:2:1396:A:N7	1:2:1449:G:C6	2.76	0.53
4:C:166:ARG:NH2	4:C:254:ASP:OD2	2.42	0.53
19:Q:53:GLU:OE1	19:Q:85:ARG:NH2	2.35	0.53
1:2:482:G:N1	1:2:485:A:OP2	2.41	0.52
1:2:562:U:H2'	1:2:563:G:C8	2.44	0.52
1:2:1406:G:H2'	1:2:1407:U:C6	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:150:ILE:HD12	36:y:318:ASN:HD21	1.73	0.52
36:y:104:LYS:NZ	36:y:106:GLU:O	2.32	0.52
1:2:160:U:O2'	1:2:162:C:OP2	2.27	0.52
1:2:913:A:OP2	8:H:99:ARG:NH2	2.42	0.52
1:2:640:A:H2'	1:2:641:A:C8	2.44	0.52
1:2:795:A:H2'	1:2:796:G:H8	1.72	0.52
36:y:270:CYS:SG	36:y:292:THR:OG1	2.67	0.52
1:2:1659:U:O2	1:2:1664:A:N7	2.41	0.52
1:2:1709:G:N2	34:j:34:PRO:O	2.43	0.52
1:2:1748:G:N2	1:2:1786:U:O2	2.36	0.52
9:I:131:PRO:O	9:I:135:GLU:HB2	2.09	0.52
1:2:1071:G:OP2	35:z:535:LYS:NZ	2.42	0.52
1:2:1373:C:OP1	18:R:7:LYS:NZ	2.32	0.52
1:2:1609:C:OP2	20:S:134:GLN:NE2	2.32	0.52
8:H:101:LEU:O	8:H:116:ARG:NH1	2.42	0.52
1:2:1204:A:O2'	1:2:1700:C:OP2	2.26	0.52
2:A:190:SER:OG	2:A:191:ARG:N	2.42	0.52
3:B:164:ILE:HD11	3:B:204:ILE:HB	1.92	0.52
8:H:8:ILE:HG12	8:H:24:SER:HB2	1.92	0.52
30:d:21:CYS:SG	30:d:22:ARG:N	2.82	0.52
1:2:960:U:O2'	1:2:962:A:N7	2.35	0.52
3:B:174:ARG:NH2	3:B:196:ASP:OD2	2.39	0.52
24:X:140:ARG:O	24:X:140:ARG:NH1	2.36	0.52
1:2:156:G:H1'	7:G:56:ASN:HD22	1.75	0.52
1:2:1058:A:H2'	1:2:1059:G:C4	2.45	0.52
1:2:1413:G:H2'	1:2:1414:A:H8	1.75	0.52
24:X:67:ARG:HG3	24:X:115:ILE:HG23	1.92	0.52
1:2:492:C:N4	1:2:507:G:OP2	2.32	0.52
1:2:942:G:OP1	3:B:136:ARG:NH1	2.43	0.52
4:C:201:GLY:O	10:J:58:ARG:NH2	2.43	0.52
8:H:26:ALA:O	8:H:86:LYS:NZ	2.43	0.52
37:k:364:GLU:O	37:k:369:LYS:N	2.41	0.52
1:2:1217:A:H2'	1:2:1218:C:C6	2.44	0.51
8:H:9:VAL:HG11	8:H:44:ASN:HD22	1.74	0.51
16:M:80:ASP:OD1	16:M:80:ASP:N	2.42	0.51
28:b:2:PRO:HA	28:b:5:LYS:HE2	1.92	0.51
35:z:401:LYS:NZ	35:z:483:PRO:O	2.35	0.51
1:2:306:C:OP2	9:I:41:ARG:NH2	2.43	0.51
1:2:345:U:O2	5:E:33:THR:OG1	2.24	0.51
1:2:1532:C:OP1	1:2:1604:G:O2'	2.29	0.51
1:2:1856:C:H2'	1:2:1857:G:C8	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:32:HIS:NE2	13:K:34:GLU:OE1	2.43	0.51
15:O:30:VAL:HG22	15:O:94:HIS:HB2	1.91	0.51
23:W:102:ILE:HB	23:W:113:HIS:HB3	1.92	0.51
28:b:6:ASP:N	28:b:6:ASP:OD1	2.43	0.51
1:2:153:G:N3	7:G:13:GLN:NE2	2.57	0.51
1:2:521:A:OP1	10:J:45:ARG:NH1	2.39	0.51
5:E:174:LYS:O	5:E:179:ASN:ND2	2.42	0.51
14:N:83:ASP:OD1	14:N:83:ASP:N	2.43	0.51
1:2:1283:C:H42	16:M:102:LYS:HD3	1.74	0.51
7:G:126:ASP:OD1	7:G:126:ASP:N	2.41	0.51
10:J:18:ARG:O	10:J:24:ARG:NH1	2.43	0.51
5:E:131:VAL:HA	5:E:137:PRO:HA	1.93	0.51
15:O:85:CYS:O	15:O:89:GLY:N	2.44	0.51
1:2:1570:G:O2'	1:2:1614:A:O2'	2.28	0.51
2:A:33:GLN:NE2	22:V:63:GLY:O	2.44	0.51
5:E:132:GLY:N	5:E:136:ILE:O	2.43	0.51
3:B:148:ASN:OD1	3:B:148:ASN:N	2.41	0.51
14:N:119:GLU:O	14:N:123:HIS:ND1	2.43	0.51
16:M:89:VAL:HG23	16:M:91:LEU:H	1.76	0.51
35:z:252:ARG:HD2	35:z:256:ARG:HD3	1.93	0.51
1:2:1010:G:H2'	1:2:1011:A:C8	2.46	0.51
1:2:1563:G:OP1	21:T:121:ARG:NH1	2.44	0.51
9:I:67:TRP:CD1	9:I:70:GLU:H	2.27	0.51
9:I:134:GLU:HA	9:I:137:LEU:HB3	1.91	0.51
24:X:49:GLY:O	24:X:99:GLU:HA	2.11	0.51
1:2:1714:U:H2'	1:2:1715:A:C8	2.45	0.51
1:2:1823:A:N3	34:j:36:ASN:ND2	2.59	0.51
11:F:137:GLN:HG3	29:c:68:LEU:HD21	1.93	0.51
33:g:243:PRO:HD3	33:g:291:TRP:HE1	1.76	0.51
1:2:106:C:H2'	1:2:107:A:H8	1.75	0.50
6:D:21:LEU:HD22	6:D:37:VAL:HG21	1.93	0.50
19:Q:97:GLN:HB2	19:Q:105:LYS:HD3	1.93	0.50
24:X:54:LYS:NZ	24:X:91:LEU:O	2.44	0.50
33:g:84:ASP:OD1	33:g:84:ASP:N	2.44	0.50
1:2:145:G:O6	7:G:178:ARG:NH2	2.45	0.50
36:y:62:TYR:HA	36:y:65:LEU:HD12	1.94	0.50
1:2:71:G:H2'	1:2:72:C:H4'	1.93	0.50
1:2:1236:G:O6	20:S:137:LYS:NZ	2.44	0.50
1:2:1844:U:H2'	1:2:1845:A:C8	2.46	0.50
3:B:29:ASP:HB2	3:B:49:VAL:HG12	1.93	0.50
31:e:18:LYS:NZ	31:e:19:VAL:O	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1155:U:OP2	4:C:194:ARG:NE	2.41	0.50
1:2:1550:G:H3'	1:2:1579:A:H61	1.77	0.50
10:J:113:GLN:NE2	10:J:154:GLN:OE1	2.44	0.50
4:C:169:TYR:OH	4:C:175:GLY:O	2.30	0.50
8:H:88:SER:O	8:H:88:SER:OG	2.30	0.50
9:I:31:ARG:NH1	9:I:31:ARG:CG	2.69	0.50
12:L:59:LYS:NZ	12:L:134:LEU:O	2.42	0.50
33:g:66:VAL:HA	33:g:82:SER:HA	1.93	0.50
1:2:530:U:H2'	1:2:531:A:H8	1.76	0.50
4:C:70:VAL:HG11	4:C:93:ILE:HG12	1.93	0.50
5:E:247:THR:HG23	5:E:250:GLU:H	1.76	0.50
24:X:60:LYS:HE3	24:X:116:PRO:HB3	1.93	0.50
33:g:24:THR:OG1	33:g:26:GLN:OE1	2.29	0.50
1:2:316:G:O5'	7:G:183:ARG:NH1	2.45	0.50
3:B:46:LYS:H	15:O:27:VAL:HA	1.76	0.50
3:B:119:THR:HG21	3:B:156:ALA:H	1.77	0.50
5:E:153:LEU:HD13	7:G:216:ARG:HE	1.76	0.50
28:b:14:GLU:OE2	28:b:17:ARG:NH2	2.45	0.50
1:2:1138:C:O2	22:V:61:ARG:NH1	2.45	0.50
1:2:1674:G:OP1	11:F:51:HIS:NE2	2.44	0.50
9:I:29:LEU:CD2	9:I:29:LEU:H	2.24	0.50
18:R:25:GLY:H	18:R:31:ASN:HD21	1.60	0.50
35:z:386:THR:HG21	35:z:469:VAL:HG22	1.94	0.50
1:2:953:C:H2'	1:2:954:U:C2	2.47	0.50
1:2:1521:C:OP1	20:S:124:ARG:NH2	2.44	0.50
6:D:172:VAL:HG22	6:D:185:LYS:HG2	1.94	0.50
23:W:87:GLU:OE2	23:W:117:ARG:NH2	2.45	0.50
1:2:551:U:H2'	1:2:552:G:C8	2.47	0.49
5:E:123:LEU:HD12	5:E:159:THR:HG22	1.94	0.49
8:H:32:MET:SD	8:H:37:LYS:N	2.85	0.49
13:K:65:ARG:NH1	30:d:20:SER:OG	2.45	0.49
36:y:245:LEU:HD22	36:y:250:LEU:HD22	1.94	0.49
1:2:15:U:O2'	1:2:669:A:N6	2.44	0.49
1:2:1511:U:H2'	1:2:1512:C:C6	2.47	0.49
3:B:36:PRO:HA	3:B:232:HIS:HA	1.93	0.49
3:B:97:LEU:HA	3:B:232:HIS:CE1	2.47	0.49
8:H:167:GLU:OE2	8:H:168:HIS:ND1	2.38	0.49
16:M:31:LEU:HB2	16:M:109:VAL:HG13	1.93	0.49
17:P:50:ARG:H	17:P:53:GLN:HE21	1.59	0.49
1:2:527:C:H2'	1:2:528:A:C8	2.47	0.49
1:2:1856:C:H2'	1:2:1857:G:H8	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:57:ALA:HB2	9:I:183:GLY:HA2	1.94	0.49
24:X:73:GLN:HA	24:X:80:LYS:HA	1.94	0.49
26:U:61:LEU:HD12	26:U:82:MET:HB3	1.93	0.49
1:2:925:G:N2	1:2:1017:U:O2	2.39	0.49
1:2:1228:A:H2'	1:2:1229:G:C8	2.48	0.49
1:2:1236:G:H21	1:2:1522:A:H62	1.60	0.49
21:T:4:VAL:HG23	21:T:8:ASP:HB2	1.93	0.49
22:V:53:TYR:OH	22:V:76:ASP:OD2	2.25	0.49
1:2:5:U:H2'	1:2:6:G:H8	1.76	0.49
1:2:817:G:H21	1:2:847:A:H62	1.61	0.49
1:2:923:G:OP1	14:N:2:GLY:N	2.46	0.49
1:2:1568:C:OP1	21:T:96:SER:OG	2.29	0.49
4:C:206:SER:HG	4:C:224:THR:HG1	1.61	0.49
20:S:101:ASN:O	20:S:105:ASN:ND2	2.45	0.49
35:z:534:ARG:HA	35:z:537:MET:HE2	1.95	0.49
1:2:67:C:O2	7:G:167:LYS:NZ	2.44	0.49
1:2:1576:G:H2'	1:2:1577:G:C8	2.48	0.49
1:2:70:G:N7	7:G:167:LYS:NZ	2.47	0.49
1:2:85:A:H2'	1:2:86:C:H6	1.77	0.49
7:G:162:LEU:HD11	7:G:172:LYS:HE3	1.93	0.49
1:2:831:G:H2'	1:2:832:G:H8	1.77	0.49
20:S:16:LEU:HD21	20:S:72:GLN:HE22	1.76	0.49
1:2:1498:A:P	6:D:27:ARG:HH22	2.35	0.49
36:y:290:ASN:HB2	36:y:292:THR:HG23	1.94	0.49
1:2:155:G:H2'	1:2:156:G:H8	1.77	0.49
1:2:1221:G:H2'	1:2:1222:G:C8	2.48	0.49
16:M:20:GLU:HB3	16:M:120:ALA:HB2	1.94	0.49
1:2:383:G:O3'	12:L:132:ARG:NH1	2.45	0.48
25:Y:78:SER:HG	25:Y:81:TYR:H	1.57	0.48
35:z:474:LYS:HB3	35:z:476:LEU:HG	1.95	0.48
28:b:11:SER:OG	28:b:13:GLU:OE1	2.31	0.48
1:2:1628:C:H2'	1:2:1629:C:C6	2.49	0.48
13:K:16:PHE:HB2	13:K:79:LEU:HD13	1.95	0.48
1:2:624:C:N4	24:X:63:ASN:OD1	2.46	0.48
3:B:190:PRO:O	3:B:195:LYS:NZ	2.46	0.48
35:z:323:ALA:HA	35:z:356:PHE:HB3	1.94	0.48
35:z:347:GLU:N	35:z:347:GLU:OE1	2.46	0.48
1:2:455:A:H2'	1:2:456:C:C6	2.48	0.48
19:Q:43:GLU:O	19:Q:45:ARG:N	2.46	0.48
27:Z:47:LEU:HB2	27:Z:79:ILE:HG22	1.94	0.48
32:f:120:GLU:OE2	32:f:129:GLY:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:j:22:SER:OG	34:j:24:GLN:OE1	2.30	0.48
36:y:56:LYS:HD2	36:y:56:LYS:HA	1.69	0.48
1:2:1099:G:H5'	36:y:323:ARG:HD2	1.96	0.48
1:2:1454:A:H5''	18:R:3:ARG:HD3	1.94	0.48
1:2:1639:G:H2'	1:2:1640:A:C8	2.49	0.48
3:B:116:LYS:HB2	3:B:117:TRP:CE3	2.48	0.48
19:Q:51:LEU:HD11	19:Q:81:ILE:HD12	1.95	0.48
22:V:60:ARG:HG2	22:V:65:SER:HB3	1.95	0.48
33:g:30:MET:HA	33:g:43:TRP:O	2.14	0.48
1:2:454:U:H2'	1:2:455:A:C8	2.49	0.48
1:2:463:C:H2'	1:2:465:A:C5	2.49	0.48
1:2:864:A:H2'	1:2:865:A:C8	2.48	0.48
1:2:1152:U:H1'	23:W:16:ASN:HD21	1.78	0.48
19:Q:109:LYS:O	19:Q:113:ILE:HB	2.14	0.48
26:U:67:LYS:HG2	26:U:78:ASP:HB2	1.95	0.48
1:2:145:G:H2'	1:2:146:G:C8	2.49	0.48
21:T:111:LYS:HB2	21:T:126:GLN:HE22	1.78	0.48
34:j:4:ALA:HB2	34:j:7:ARG:HH21	1.78	0.48
1:2:1170:A:N6	1:2:1189:A:OP2	2.44	0.48
5:E:180:LEU:N	5:E:231:GLY:O	2.46	0.48
11:F:161:ALA:O	11:F:165:ASN:ND2	2.45	0.48
14:N:46:THR:HG23	14:N:49:GLN:H	1.78	0.48
33:g:116:ASP:N	33:g:116:ASP:OD1	2.47	0.48
1:2:384:U:O2'	1:2:386:C:OP1	2.27	0.48
1:2:639:C:OP1	31:e:41:ARG:NH2	2.47	0.48
1:2:809:A:H2'	1:2:810:A:O4'	2.14	0.48
20:S:85:ASN:HD22	20:S:98:VAL:HG22	1.79	0.48
35:z:473:LYS:HB3	35:z:479:VAL:HG11	1.96	0.48
1:2:155:G:H2'	1:2:156:G:C8	2.49	0.47
1:2:172:U:OP1	1:2:314:U:O2'	2.27	0.47
1:2:196:C:H2'	1:2:197:U:H5	1.79	0.47
1:2:527:C:OP1	10:J:122:SER:OG	2.28	0.47
14:N:25:TRP:CH2	28:b:45:THR:HG21	2.49	0.47
19:Q:138:ARG:O	19:Q:140:ARG:NH1	2.47	0.47
21:T:5:THR:HG22	21:T:6:VAL:H	1.78	0.47
33:g:42:MET:HG2	33:g:56:GLN:HB3	1.96	0.47
33:g:80:SER:OG	33:g:90:TRP:NE1	2.46	0.47
1:2:384:U:H2'	1:2:386:C:H5	1.79	0.47
1:2:472:C:O2'	1:2:474:G:OP1	2.25	0.47
1:2:563:G:N7	1:2:586:G:N2	2.62	0.47
1:2:750:C:H2'	1:2:751:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1202:U:H2'	1:2:1203:G:H8	1.79	0.47
2:A:141:ASN:ND2	4:C:85:SER:O	2.46	0.47
8:H:142:LYS:O	8:H:143:ARG:NH1	2.37	0.47
10:J:31:LEU:HD21	10:J:103:GLU:HG3	1.94	0.47
12:L:22:ARG:HG2	12:L:23:VAL:HG13	1.95	0.47
16:M:19:GLN:HG2	16:M:88:TRP:CD2	2.48	0.47
19:Q:72:VAL:HG11	19:Q:84:ILE:HD11	1.95	0.47
1:2:64:A:OP1	7:G:136:LYS:NZ	2.35	0.47
1:2:580:U:O2'	25:Y:63:HIS:O	2.33	0.47
1:2:642:U:H5''	10:J:39:ASN:HD22	1.79	0.47
1:2:1280:G:OP2	16:M:101:ARG:NH1	2.45	0.47
9:I:12:ARG:HA	9:I:18:ARG:HH21	1.79	0.47
9:I:67:TRP:NE1	9:I:69:SER:OG	2.48	0.47
20:S:84:LEU:O	20:S:87:GLN:NE2	2.48	0.47
33:g:94:THR:HG23	33:g:96:THR:HG22	1.96	0.47
1:2:1340:U:OP2	1:2:1341:C:O2'	2.26	0.47
17:P:82:ASP:OD1	17:P:82:ASP:N	2.33	0.47
24:X:24:ASP:OD1	24:X:26:GLN:N	2.47	0.47
33:g:120:ILE:O	33:g:131:LEU:HA	2.13	0.47
1:2:1309:C:OP2	32:f:105:TYR:OH	2.29	0.47
1:2:1595:U:H2'	1:2:1596:U:C6	2.49	0.47
1:2:1648:G:O2'	1:2:1674:G:O6	2.23	0.47
2:A:57:LYS:HZ3	22:V:70:LEU:HD13	1.80	0.47
3:B:208:HIS:ND1	3:B:209:ASP:OD1	2.47	0.47
1:2:795:A:H2'	1:2:796:G:C8	2.49	0.47
1:2:1706:G:H2'	1:2:1707:U:C6	2.49	0.47
6:D:201:LYS:HE3	6:D:201:LYS:HB2	1.75	0.47
10:J:127:ARG:HD3	31:e:31:ARG:HH11	1.80	0.47
17:P:142:ILE:HG12	34:j:62:TRP:CD1	2.49	0.47
1:2:107:A:H2'	1:2:108:G:H8	1.78	0.47
1:2:290:U:N3	1:2:293:C:OP2	2.48	0.47
1:2:920:A:O2'	1:2:922:A:OP1	2.30	0.47
1:2:942:G:H21	15:O:137:SER:HB3	1.79	0.47
1:2:1013:U:OP1	1:2:1129:G:O2'	2.32	0.47
1:2:1213:C:H2'	1:2:1214:A:H8	1.80	0.47
1:2:1453:C:H2'	1:2:1454:A:H4'	1.95	0.47
1:2:1466:G:H2'	1:2:1467:C:C6	2.50	0.47
1:2:1492:U:O2'	1:2:1495:G:OP1	2.32	0.47
1:2:1536:G:H2'	1:2:1537:A:C8	2.50	0.47
5:E:71:LYS:HB2	5:E:91:SER:HB2	1.96	0.47
26:U:20:ILE:HB	26:U:91:LEU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:j:54:PRO:HD3	34:j:84:ILE:HB	1.95	0.47
36:y:13:ALA:HB1	36:y:20:LEU:HD21	1.97	0.47
1:2:126:G:H8	7:G:199:THR:HG21	1.80	0.47
1:2:1308:U:H5'	32:f:135:HIS:HD2	1.79	0.47
15:O:45:THR:HA	15:O:52:THR:HA	1.97	0.47
16:M:61:TYR:HA	16:M:64:LEU:HB3	1.97	0.47
35:z:354:LEU:HD13	35:z:382:PHE:HZ	1.80	0.47
1:2:291:G:N2	12:L:68:ILE:O	2.34	0.47
19:Q:16:LYS:HG3	19:Q:17:LYS:H	1.80	0.47
19:Q:138:ARG:HA	19:Q:138:ARG:HD3	1.70	0.47
1:2:600:G:H2'	1:2:601:G:C8	2.50	0.47
1:2:1738:C:OP1	7:G:92:ARG:NH1	2.48	0.47
7:G:23:LYS:HD2	7:G:41:LEU:HA	1.96	0.47
25:Y:103:SER:OG	25:Y:104:ARG:N	2.47	0.47
34:j:4:ALA:HA	34:j:7:ARG:HB3	1.97	0.47
34:j:31:LEU:HD11	34:j:42:GLU:HB3	1.96	0.47
36:y:276:THR:O	36:y:276:THR:OG1	2.32	0.47
1:2:641:A:H2'	1:2:642:U:O4'	2.15	0.46
1:2:1673:U:OP2	19:Q:17:LYS:NZ	2.35	0.46
1:2:1872:G:O2'	1:2:1873:G:OP1	2.31	0.46
4:C:179:THR:HA	4:C:219:ILE:HG23	1.98	0.46
6:D:46:THR:N	6:D:83:SER:O	2.48	0.46
10:J:88:ASP:OD1	10:J:88:ASP:N	2.48	0.46
10:J:125:HIS:HA	10:J:128:VAL:HG12	1.97	0.46
19:Q:131:LYS:NZ	19:Q:137:ALA:O	2.48	0.46
31:e:39:ASN:HA	31:e:43:VAL:HB	1.97	0.46
1:2:1018:U:H2'	1:2:1019:C:H6	1.80	0.46
1:2:1556:A:H61	30:d:18:SER:HB2	1.80	0.46
11:F:128:ILE:HG12	29:c:68:LEU:HD22	1.97	0.46
1:2:154:U:O2	7:G:4:ASN:ND2	2.44	0.46
8:H:31:GLU:OE2	8:H:41:ARG:NE	2.48	0.46
25:Y:55:ILE:HG12	25:Y:75:ILE:HG12	1.97	0.46
33:g:72:SER:OG	33:g:74:ASP:OD1	2.28	0.46
33:g:196:ASN:H	33:g:211:GLY:HA2	1.80	0.46
35:z:172:LYS:HA	35:z:175:THR:HG22	1.98	0.46
1:2:118:C:H2'	1:2:119:U:O4'	2.16	0.46
1:2:185:G:O6	1:2:214:U:C4	2.68	0.46
1:2:530:U:H2'	1:2:531:A:C8	2.51	0.46
1:2:1329:U:H3	1:2:1500:G:H1	1.62	0.46
1:2:1413:G:H2'	1:2:1414:A:C8	2.51	0.46
3:B:123:ALA:HB2	3:B:165:ARG:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:113:LEU:HD23	6:D:118:ALA:HB2	1.97	0.46
6:D:172:VAL:O	6:D:173:ARG:NH1	2.48	0.46
6:D:224:SER:OG	6:D:225:GLU:N	2.47	0.46
8:H:82:GLU:HA	8:H:85:LYS:HD2	1.97	0.46
10:J:153:SER:HA	10:J:156:HIS:CD2	2.50	0.46
11:F:30:ILE:HG21	11:F:36:GLN:HA	1.98	0.46
35:z:229:ARG:HD3	35:z:252:ARG:HH12	1.81	0.46
35:z:312:ARG:NH2	35:z:316:GLN:HE21	2.13	0.46
1:2:199:C:H2'	1:2:200:G:N7	2.30	0.46
1:2:1395:C:H2'	1:2:1396:A:N3	2.31	0.46
20:S:124:ARG:HH21	20:S:129:LEU:HB3	1.81	0.46
21:T:11:GLN:OE1	21:T:62:ARG:NH1	2.42	0.46
1:2:434:G:OP2	9:I:25:ARG:NH2	2.44	0.46
1:2:1633:A:H2'	1:2:1634:A:C8	2.50	0.46
1:2:1726:G:O6	1:2:1808:U:O2	2.34	0.46
4:C:142:LYS:HE2	4:C:153:GLY:HA3	1.97	0.46
7:G:58:LYS:HA	7:G:107:SER:HB2	1.98	0.46
10:J:21:GLU:HG3	10:J:24:ARG:H	1.80	0.46
10:J:82:VAL:HG21	10:J:92:MET:HE2	1.97	0.46
18:R:36:GLU:HB2	18:R:47:ARG:HD2	1.97	0.46
1:2:804:U:H2'	1:2:805:U:C6	2.51	0.46
1:2:1048:G:N1	1:2:1069:U:OP2	2.39	0.46
1:2:1356:G:H2'	1:2:1357:A:C8	2.51	0.46
1:2:1780:G:N2	1:2:1781:A:N7	2.64	0.46
9:I:76:THR:HG21	9:I:104:ILE:HD12	1.98	0.46
9:I:150:ASP:HA	9:I:153:LYS:HE3	1.98	0.46
13:K:57:TYR:O	13:K:72:THR:OG1	2.28	0.46
19:Q:141:TYR:O	19:Q:143:LYS:N	2.48	0.46
27:Z:110:THR:OG1	27:Z:111:ARG:N	2.49	0.46
1:2:155:G:H21	7:G:56:ASN:ND2	2.14	0.46
1:2:506:G:OP1	25:Y:108:LYS:NZ	2.49	0.46
2:A:52:LYS:O	2:A:56:GLU:HG2	2.15	0.46
7:G:151:ASP:OD1	7:G:151:ASP:N	2.48	0.46
9:I:8:TRP:NE1	9:I:22:HIS:HE1	2.14	0.46
1:2:649:U:H2'	1:2:650:A:C8	2.50	0.46
1:2:965:U:H5''	1:2:966:U:H5	1.81	0.46
12:L:113:LEU:HD11	12:L:117:PHE:HB2	1.98	0.46
33:g:205:SER:O	33:g:221:LEU:N	2.40	0.46
35:z:257:LEU:HD23	35:z:257:LEU:HA	1.76	0.46
1:2:445:A:H5''	9:I:47:ARG:HH21	1.81	0.46
1:2:674:C:H2'	1:2:675:U:C6	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:946:U:H2'	1:2:947:G:C8	2.51	0.46
1:2:1669:G:OP1	26:U:79:ARG:NH1	2.48	0.46
8:H:118:ARG:O	8:H:121:THR:OG1	2.23	0.46
13:K:31:LYS:HE2	13:K:39:ASN:HA	1.98	0.46
20:S:102:GLY:HA2	20:S:105:ASN:HD22	1.81	0.46
36:y:236:THR:OG1	36:y:237:THR:N	2.46	0.46
1:2:126:G:H5'	7:G:195:LYS:HE3	1.99	0.45
1:2:1322:G:H2'	1:2:1323:U:C6	2.52	0.45
1:2:1814:G:O2'	1:2:1815:A:OP1	2.28	0.45
12:L:75:GLY:HA3	12:L:88:ILE:HD12	1.98	0.45
19:Q:116:ASP:HB3	19:Q:119:LEU:HD12	1.97	0.45
37:k:362:LEU:O	37:k:366:LEU:CB	2.64	0.45
37:k:401:PRO:HA	37:k:467:SER:HA	1.99	0.45
1:2:15:U:H2'	1:2:16:G:O4'	2.16	0.45
1:2:441:C:H2'	1:2:442:C:C6	2.51	0.45
1:2:449:A:O3'	5:E:3:ARG:NH1	2.49	0.45
1:2:747:U:O2'	1:2:748:C:O4'	2.32	0.45
3:B:97:LEU:HD22	3:B:232:HIS:ND1	2.31	0.45
5:E:87:MET:SD	5:E:100:ARG:NH1	2.89	0.45
6:D:103:GLU:HA	6:D:106:ARG:HG2	1.98	0.45
8:H:168:HIS:CD2	8:H:169:LYS:HG3	2.51	0.45
24:X:74:LEU:HD12	24:X:79:LYS:HB2	1.97	0.45
35:z:242:MET:HE3	35:z:242:MET:HB3	1.74	0.45
1:2:1065:G:H2'	1:2:1066:U:C6	2.52	0.45
1:2:1667:U:H2'	1:2:1668:U:C6	2.51	0.45
1:2:1723:G:H2'	1:2:1724:A:H8	1.81	0.45
16:M:32:ALA:HB1	16:M:37:GLU:HB3	1.98	0.45
16:M:48:HIS:ND1	16:M:112:LYS:O	2.50	0.45
20:S:39:ARG:HG2	20:S:83:PHE:HZ	1.81	0.45
1:2:675:U:H2'	1:2:676:C:H6	1.82	0.45
1:2:1398:G:H22	1:2:1448:A:H2	1.64	0.45
1:2:1857:G:P	15:O:141:ARG:HH22	2.40	0.45
4:C:123:ARG:HE	4:C:143:CYS:HB2	1.81	0.45
5:E:124:CYS:HB3	5:E:141:THR:HB	1.97	0.45
9:I:3:ILE:HB	9:I:30:GLY:O	2.16	0.45
19:Q:42:ILE:HG22	19:Q:44:PRO:HD2	1.98	0.45
31:e:2:VAL:HG12	31:e:3:HIS:CD2	2.52	0.45
33:g:178:ASN:N	33:g:183:LYS:O	2.44	0.45
35:z:378:VAL:HG12	35:z:425:PHE:HE2	1.81	0.45
1:2:989:C:OP2	3:B:155:TYR:OH	2.27	0.45
1:2:1415:C:H2'	1:2:1416:C:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:58:ALA:O	3:B:62:LEU:HG	2.15	0.45
4:C:101:SER:HB3	4:C:132:ASP:HB2	1.98	0.45
7:G:22:ARG:HA	7:G:25:ARG:HG2	1.98	0.45
10:J:39:ASN:N	10:J:39:ASN:OD1	2.49	0.45
14:N:135:LEU:HD23	14:N:135:LEU:HA	1.84	0.45
32:f:99:LYS:HE3	32:f:99:LYS:HB3	1.71	0.45
1:2:554:A:H4'	1:2:555:A:C5	2.51	0.45
1:2:1513:C:P	30:d:12:ARG:HH12	2.39	0.45
1:2:1867:U:O2	1:2:1867:U:O5'	2.35	0.45
1:2:380:G:O6	9:I:178:ARG:NH1	2.45	0.45
1:2:544:G:H2'	1:2:545:A:C8	2.52	0.45
1:2:569:A:H2'	1:2:570:C:H6	1.81	0.45
1:2:752:G:N2	1:2:791:C:HO2'	2.13	0.45
1:2:831:G:H2'	1:2:832:G:C8	2.52	0.45
1:2:1337:C:H2'	1:2:1338:G:H8	1.81	0.45
1:2:1746:U:H2'	1:2:1747:C:C6	2.51	0.45
5:E:77:ARG:HA	5:E:77:ARG:HD3	1.68	0.45
30:d:54:LYS:HE2	30:d:54:LYS:HB2	1.66	0.45
36:y:30:ILE:HG12	36:y:33:VAL:HG23	1.98	0.45
36:y:80:SER:OG	36:y:83:ASP:OD2	2.30	0.45
1:2:1281:G:H3'	1:2:1282:A:C8	2.52	0.45
3:B:39:PHE:HB3	3:B:74:LEU:HB3	1.98	0.45
12:L:124:ASP:HB3	12:L:147:LYS:HA	1.99	0.45
16:M:60:MET:SD	16:M:60:MET:N	2.90	0.45
33:g:5:MET:HA	33:g:312:VAL:HA	1.98	0.45
35:z:209:ILE:HG12	35:z:274:VAL:HG13	1.99	0.45
36:y:10:ASN:OD1	36:y:10:ASN:N	2.49	0.45
1:2:343:A:O3'	5:E:128:LYS:NZ	2.47	0.45
1:2:649:U:H2'	1:2:650:A:H8	1.82	0.45
1:2:817:G:H2'	1:2:818:A:H8	1.82	0.45
1:2:952:G:O2'	1:2:953:C:O4'	2.29	0.45
1:2:1016:U:H5'	14:N:15:ALA:H	1.82	0.45
1:2:1565:C:OP2	21:T:101:ARG:NE	2.40	0.45
1:2:1821:U:H2'	1:2:1822:A:H8	1.81	0.45
4:C:254:ASP:OD1	4:C:254:ASP:N	2.30	0.45
11:F:48:TYR:HD2	19:Q:53:GLU:HG2	1.80	0.45
23:W:126:LEU:HD23	23:W:126:LEU:HA	1.84	0.45
1:2:434:G:H2'	1:2:435:A:C8	2.52	0.45
1:2:928:G:H2'	1:2:929:G:C8	2.52	0.45
1:2:1737:G:H1	1:2:1797:U:H3	1.64	0.45
17:P:18:ARG:HH11	20:S:90:VAL:HA	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:135:HIS:HB2	32:f:138:ARG:HG2	1.98	0.45
33:g:8:ARG:HB2	33:g:309:VAL:HG23	1.98	0.45
36:y:317:LEU:HD23	36:y:317:LEU:HA	1.86	0.45
1:2:520:A:O2'	1:2:825:A:N3	2.45	0.44
1:2:659:G:O2'	1:2:662:G:O2'	2.22	0.44
33:g:240:CYS:HB3	33:g:249:CYS:HB2	1.34	0.44
1:2:1560:U:H2'	1:2:1561:A:H8	1.80	0.44
1:2:1711:U:H5''	34:j:79:LYS:HG3	1.99	0.44
1:2:1862:G:H2'	1:2:1863:A:O4'	2.17	0.44
4:C:131:GLY:HA3	4:C:216:MET:HB3	1.99	0.44
5:E:80:ILE:HG13	5:E:81:THR:HG23	1.98	0.44
5:E:198:ARG:HB2	5:E:208:VAL:HG12	1.98	0.44
15:O:44:VAL:HG13	15:O:53:ILE:HB	2.00	0.44
21:T:27:LYS:HA	21:T:27:LYS:HD2	1.79	0.44
34:j:6:LYS:HD2	34:j:6:LYS:HA	1.71	0.44
1:2:1854:U:OP1	15:O:150:ARG:NH2	2.50	0.44
5:E:68:ARG:HH21	5:E:76:VAL:HG21	1.82	0.44
20:S:106:LYS:HD3	20:S:106:LYS:HA	1.84	0.44
31:e:57:ALA:O	31:e:58:ASN:ND2	2.50	0.44
1:2:976:G:H2'	1:2:977:C:C6	2.53	0.44
1:2:1351:G:O2'	1:2:1378:A:N1	2.44	0.44
13:K:47:LYS:HA	13:K:47:LYS:HD3	1.69	0.44
19:Q:53:GLU:OE2	19:Q:115:TYR:OH	2.26	0.44
1:2:223:C:H2'	1:2:224:A:C8	2.52	0.44
1:2:1189:A:H2'	1:2:1190:A:C8	2.53	0.44
1:2:1401:A:H2'	1:2:1402:A:C8	2.53	0.44
3:B:128:LYS:HE3	3:B:128:LYS:HB2	1.76	0.44
9:I:117:TYR:CE1	9:I:152:ARG:HG2	2.52	0.44
36:y:7:VAL:HG11	36:y:235:LEU:HD23	1.99	0.44
1:2:591:U:OP2	31:e:26:LYS:NZ	2.43	0.44
1:2:642:U:P	10:J:39:ASN:HB2	2.58	0.44
1:2:1236:G:H5'	17:P:134:GLY:HA2	1.99	0.44
1:2:1845:A:H2'	1:2:1846:G:C8	2.53	0.44
3:B:52:THR:HB	3:B:58:ALA:HB3	1.99	0.44
7:G:121:ILE:HA	7:G:122:PRO:HD3	1.89	0.44
7:G:223:LYS:HA	7:G:223:LYS:HD3	1.85	0.44
9:I:165:GLN:HE21	9:I:172:LEU:H	1.66	0.44
23:W:27:ILE:HG13	23:W:61:ILE:HB	1.99	0.44
33:g:193:GLY:HA3	33:g:212:LYS:HG2	2.00	0.44
36:y:266:TYR:HA	36:y:296:VAL:O	2.18	0.44
1:2:294:U:C4	12:L:65:ASN:HB2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:317:C:H2'	1:2:318:A:C8	2.53	0.44
1:2:1741:U:OP1	9:I:42:ARG:NH1	2.50	0.44
1:2:1845:A:H2'	1:2:1846:G:H8	1.83	0.44
3:B:62:LEU:HD13	3:B:91:VAL:HG11	1.99	0.44
6:D:96:LEU:HD22	6:D:131:ALA:HB2	1.99	0.44
9:I:3:ILE:O	9:I:30:GLY:N	2.49	0.44
17:P:26:LEU:HD22	17:P:88:GLU:HA	2.00	0.44
17:P:28:MET:HG2	17:P:33:LEU:HG	1.99	0.44
27:Z:88:LEU:HD23	27:Z:88:LEU:HA	1.72	0.44
36:y:64:ARG:HA	36:y:67:THR:HG22	2.00	0.44
1:2:902:G:H2'	1:2:903:A:C8	2.53	0.44
1:2:912:C:C2	1:2:914:U:H1'	2.53	0.44
1:2:1613:G:OP1	17:P:42:ARG:NH2	2.40	0.44
3:B:67:PHE:CZ	15:O:48:SER:HB3	2.53	0.44
5:E:55:ALA:HB1	5:E:60:GLU:HB2	1.99	0.44
15:O:46:ASP:OD2	15:O:48:SER:OG	2.35	0.44
17:P:28:MET:HG3	17:P:32:GLN:HB2	1.99	0.44
19:Q:130:LYS:NZ	19:Q:134:GLY:O	2.42	0.44
24:X:133:LEU:HD23	24:X:133:LEU:HA	1.86	0.44
35:z:160:GLN:HA	35:z:214:ILE:HD12	2.00	0.44
35:z:350:HIS:HD1	35:z:352:HIS:H	1.66	0.44
35:z:390:ILE:HG12	35:z:482:VAL:HG11	1.99	0.44
1:2:184:G:H2'	1:2:185:G:H8	1.83	0.44
1:2:190:G:OP1	9:I:149:TYR:OH	2.24	0.44
1:2:1013:U:P	14:N:11:LEU:H	2.40	0.44
19:Q:33:LYS:HB2	19:Q:69:ARG:HG3	2.00	0.44
26:U:28:ASN:OD1	26:U:28:ASN:N	2.49	0.44
33:g:212:LYS:HA	33:g:235:ILE:HG13	2.00	0.44
35:z:316:GLN:HE22	35:z:388:PRO:HA	1.83	0.44
1:2:914:U:H2'	1:2:915:G:H8	1.83	0.43
1:2:1228:A:H2'	1:2:1229:G:H8	1.83	0.43
3:B:91:VAL:HG23	3:B:95:ASN:C	2.43	0.43
8:H:58:LYS:HB2	8:H:90:LYS:HG2	2.00	0.43
10:J:124:HIS:CD2	31:e:35:ARG:HD2	2.53	0.43
13:K:2:LEU:HD12	13:K:2:LEU:HA	1.89	0.43
18:R:37:GLU:OE2	33:g:150:TRP:NE1	2.51	0.43
26:U:97:ILE:O	26:U:101:ILE:HG12	2.19	0.43
1:2:290:U:O2'	1:2:292:A:N7	2.46	0.43
1:2:914:U:H2'	1:2:915:G:C8	2.53	0.43
1:2:1735:A:H3'	1:2:1736:G:H8	1.83	0.43
3:B:136:ARG:HB2	3:B:218:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:100:ILE:HG12	8:H:125:VAL:HG21	2.00	0.43
10:J:60:LEU:HA	10:J:60:LEU:HD23	1.76	0.43
17:P:22:LEU:HA	17:P:25:LEU:HB2	2.00	0.43
23:W:26:LEU:HD11	23:W:60:LYS:HD2	1.99	0.43
34:j:73:PRO:HA	34:j:82:ALA:HA	2.00	0.43
1:2:552:G:H2'	1:2:553:U:C6	2.54	0.43
1:2:1259:A:N6	1:2:1519:U:O4'	2.48	0.43
1:2:1452:A:H5''	18:R:48:ASN:ND2	2.32	0.43
1:2:1868:U:C2'	1:2:1869:A:H5'	2.48	0.43
7:G:25:ARG:HA	7:G:25:ARG:HD3	1.85	0.43
9:I:86:SER:OG	9:I:87:ASN:N	2.50	0.43
13:K:59:LYS:HG3	13:K:70:TYR:HD2	1.83	0.43
35:z:194:VAL:HG11	40:z:603:ATP:C8	2.53	0.43
35:z:225:SER:OG	35:z:226:GLY:N	2.52	0.43
1:2:984:C:H2'	1:2:985:G:C8	2.54	0.43
1:2:1038:U:OP1	35:z:546:ARG:NH2	2.52	0.43
4:C:60:TRP:O	4:C:71:LYS:NZ	2.42	0.43
4:C:256:TRP:CD1	23:W:68:ARG:HD3	2.53	0.43
6:D:222:PRO:HA	33:g:190:GLY:HA3	2.00	0.43
7:G:102:VAL:HG13	7:G:106:LEU:HD21	2.00	0.43
11:F:34:SER:HA	29:c:55:VAL:HB	2.00	0.43
30:d:55:LEU:O	30:d:56:ASP:C	2.62	0.43
1:2:1100:A:OP1	36:y:320:ARG:NH1	2.41	0.43
7:G:200:LYS:HE3	7:G:200:LYS:HB3	1.85	0.43
9:I:103:LEU:HD22	9:I:170:LYS:HE2	2.01	0.43
11:F:103:LEU:HD23	11:F:103:LEU:HA	1.86	0.43
20:S:86:ARG:HD3	20:S:86:ARG:HA	1.69	0.43
31:e:27:LYS:HE2	31:e:27:LYS:HB2	1.87	0.43
36:y:282:ARG:NE	36:y:286:SER:OG	2.52	0.43
1:2:1061:U:H5	1:2:1850:A:H2'	1.82	0.43
1:2:1652:G:H1	1:2:1672:U:H3	1.65	0.43
2:A:120:ARG:HH22	4:C:267:GLN:HG3	1.84	0.43
4:C:65:LYS:HB3	4:C:273:LEU:HD21	2.00	0.43
4:C:72:ASP:OD1	4:C:72:ASP:N	2.50	0.43
5:E:36:HIS:NE2	5:E:143:ASP:OD1	2.52	0.43
5:E:62:LYS:HE2	5:E:62:LYS:HB3	1.74	0.43
5:E:94:LYS:HG3	25:Y:16:ARG:HG3	2.00	0.43
13:K:24:LYS:HG3	13:K:66:HIS:NE2	2.33	0.43
19:Q:49:TYR:HD1	19:Q:49:TYR:HA	1.72	0.43
23:W:66:THR:O	23:W:68:ARG:N	2.46	0.43
1:2:659:G:H21	24:X:17:ARG:HH22	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:874:G:H2'	1:2:875:A:C8	2.51	0.43
1:2:1157:G:H8	24:X:5:ARG:HD3	1.84	0.43
2:A:57:LYS:HA	2:A:57:LYS:HD3	1.77	0.43
4:C:86:LEU:HD23	4:C:86:LEU:HA	1.74	0.43
6:D:211:VAL:O	18:R:20:TYR:OH	2.28	0.43
9:I:34:ALA:HB2	9:I:56:ARG:HH11	1.82	0.43
9:I:202:ILE:HG23	9:I:205:ARG:HH21	1.83	0.43
1:2:89:C:H2'	1:2:90:G:H8	1.83	0.43
1:2:870:A:H62	1:2:915:G:H2'	1.83	0.43
5:E:89:VAL:HG12	5:E:98:ASN:HD21	1.83	0.43
8:H:159:ASP:OD1	8:H:160:LYS:N	2.52	0.43
11:F:115:ALA:O	11:F:119:SER:OG	2.33	0.43
15:O:31:CYS:HA	15:O:44:VAL:HA	2.00	0.43
16:M:26:LEU:HD22	16:M:90:GLY:HA3	2.01	0.43
19:Q:45:ARG:O	19:Q:48:GLN:HB2	2.19	0.43
22:V:24:ILE:HG12	22:V:56:CYS:HB3	2.00	0.43
28:b:81:ARG:HE	28:b:81:ARG:HB3	1.69	0.43
1:2:1226:G:N1	1:2:1639:G:OP2	2.33	0.43
1:2:1290:G:O6	32:f:95:ARG:NH2	2.42	0.43
1:2:1715:A:H2'	1:2:1716:C:C6	2.54	0.43
2:A:104:THR:HA	2:A:105:PRO:HD3	1.92	0.43
8:H:181:THR:OG1	8:H:182:GLY:N	2.51	0.43
9:I:29:LEU:HD23	9:I:29:LEU:H	1.83	0.43
17:P:93:MET:HE3	17:P:93:MET:HB3	1.82	0.43
33:g:29:ASP:HA	33:g:45:LEU:HD23	2.01	0.43
1:2:678:U:H2'	1:2:679:A:H8	1.83	0.43
1:2:1453:C:O2'	18:R:52:GLY:HA3	2.19	0.43
9:I:201:LYS:HA	9:I:201:LYS:HD3	1.82	0.43
10:J:104:ASP:O	10:J:107:GLU:HG2	2.19	0.43
20:S:40:TYR:HA	20:S:83:PHE:HE2	1.84	0.43
24:X:77:ASN:OD1	24:X:77:ASN:N	2.52	0.43
25:Y:35:VAL:HG13	25:Y:40:ILE:HD11	2.01	0.43
33:g:93:THR:OG1	33:g:94:THR:N	2.52	0.43
35:z:558:LYS:HE3	35:z:558:LYS:HB3	1.91	0.43
1:2:67:C:O5'	7:G:172:LYS:NZ	2.52	0.42
1:2:831:G:O6	25:Y:11:LYS:NZ	2.46	0.42
1:2:946:U:H2'	1:2:947:G:H8	1.83	0.42
1:2:952:G:H2'	1:2:953:C:C2	2.54	0.42
1:2:1548:G:H2'	1:2:1549:U:C6	2.54	0.42
3:B:134:LEU:HB3	3:B:218:LEU:HB2	2.00	0.42
5:E:138:HIS:ND1	5:E:148:ARG:HG2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:62:LYS:HE3	6:D:62:LYS:HB2	1.80	0.42
7:G:203:LYS:HD3	7:G:203:LYS:HA	1.82	0.42
10:J:38:ARG:HH12	10:J:127:ARG:HH11	1.66	0.42
12:L:16:ILE:HD12	12:L:16:ILE:HA	1.91	0.42
20:S:68:ILE:O	20:S:72:GLN:HG2	2.19	0.42
36:y:8:VAL:HG12	36:y:28:TYR:HB2	2.00	0.42
1:2:455:A:O2'	1:2:1735:A:N3	2.50	0.42
1:2:931:C:H2'	1:2:932:G:C8	2.55	0.42
6:D:62:LYS:O	6:D:67:ARG:NH2	2.34	0.42
9:I:19:LYS:HB2	9:I:19:LYS:HE3	1.86	0.42
27:Z:56:ASP:O	27:Z:60:LYS:HB3	2.18	0.42
1:2:564:A:H3'	1:2:565:G:H8	1.83	0.42
1:2:626:G:N1	34:j:3:GLN:OE1	2.53	0.42
7:G:24:LEU:HA	7:G:27:PHE:HD2	1.84	0.42
9:I:84:ASN:HD22	9:I:90:LEU:HB2	1.84	0.42
14:N:114:ARG:HA	14:N:114:ARG:HD3	1.83	0.42
35:z:377:THR:HG23	35:z:380:GLU:H	1.84	0.42
1:2:453:C:H2'	1:2:454:U:C6	2.55	0.42
3:B:33:VAL:HG21	15:O:47:LEU:HD23	2.01	0.42
3:B:39:PHE:HE1	3:B:189:ILE:HD11	1.84	0.42
6:D:67:ARG:NE	13:K:93:THR:O	2.44	0.42
7:G:51:ARG:HB3	7:G:112:VAL:HG13	2.02	0.42
11:F:126:THR:HB	29:c:26:GLN:HE21	1.84	0.42
16:M:48:HIS:HB3	16:M:49:LEU:HD12	2.02	0.42
33:g:256:ILE:HB	33:g:270:LEU:HB2	2.01	0.42
35:z:394:ASN:OD1	35:z:394:ASN:N	2.50	0.42
1:2:902:G:H2'	1:2:903:A:H8	1.85	0.42
1:2:1124:C:H5''	3:B:150:ILE:HG12	2.02	0.42
1:2:1692:U:H2'	1:2:1693:G:C8	2.54	0.42
4:C:125:LYS:HE2	4:C:125:LYS:HB3	1.72	0.42
7:G:69:THR:O	7:G:98:ARG:NH1	2.48	0.42
33:g:42:MET:HE3	33:g:92:LEU:HD12	2.00	0.42
33:g:299:PHE:HD1	33:g:309:VAL:HG12	1.83	0.42
1:2:373:G:N2	12:L:83:GLN:OE1	2.32	0.42
1:2:942:G:H2'	1:2:943:U:C6	2.54	0.42
1:2:1412:C:H2'	1:2:1413:G:H8	1.84	0.42
1:2:1593:C:H4'	19:Q:45:ARG:HH12	1.83	0.42
1:2:1610:G:O2'	20:S:110:ASP:OD2	2.25	0.42
2:A:56:GLU:HG3	22:V:83:PHE:HD2	1.84	0.42
6:D:30:ALA:HB1	6:D:107:TYR:HE2	1.85	0.42
12:L:82:MET:HE3	12:L:85:THR:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:85:ILE:HB	17:P:112:ILE:HA	2.02	0.42
1:2:120:U:H6	5:E:34:GLY:HA2	1.84	0.42
1:2:196:C:H2'	1:2:197:U:C5	2.54	0.42
1:2:380:G:C2	1:2:382:C:H5''	2.54	0.42
1:2:868:G:C4	8:H:115:LYS:HB2	2.54	0.42
1:2:1064:C:H2'	1:2:1065:G:H8	1.84	0.42
1:2:1358:U:H5'	4:C:114:LYS:HD2	2.00	0.42
1:2:1798:C:H2'	1:2:1799:G:O4'	2.20	0.42
5:E:31:PRO:HG3	5:E:43:PRO:HG3	2.01	0.42
5:E:181:CYS:HB2	5:E:225:ILE:HG23	2.02	0.42
6:D:224:SER:HB3	33:g:225:LYS:HD2	2.01	0.42
17:P:47:ARG:O	17:P:50:ARG:NH1	2.41	0.42
1:2:30:C:H5''	24:X:132:ALA:HB2	2.02	0.42
1:2:442:C:H2'	1:2:443:U:C6	2.55	0.42
1:2:556:U:H2'	1:2:557:U:C6	2.54	0.42
1:2:683:G:O2'	1:2:684:G:H5'	2.20	0.42
1:2:1284:A:H61	1:2:1313:A:H2'	1.85	0.42
4:C:92:GLU:HA	4:C:95:ASP:HB2	2.02	0.42
4:C:121:ARG:HH12	4:C:123:ARG:HH11	1.68	0.42
6:D:23:GLU:OE2	6:D:27:ARG:NE	2.53	0.42
7:G:98:ARG:NH1	7:G:99:GLY:O	2.52	0.42
11:F:204:ARG:HH11	29:c:60:GLU:HB2	1.84	0.42
18:R:80:ARG:NE	18:R:81:ARG:HH21	2.17	0.42
21:T:64:LEU:HD23	21:T:64:LEU:HA	1.88	0.42
33:g:4:GLN:NE2	33:g:268:ASP:OD2	2.53	0.42
1:2:1036:A:O2'	1:2:1855:G:N2	2.49	0.42
1:2:1360:U:O2'	1:2:1379:A:OP2	2.37	0.42
1:2:1430:C:H2'	1:2:1431:G:C8	2.55	0.42
1:2:1612:G:OP1	17:P:18:ARG:NH2	2.53	0.42
9:I:96:LEU:HD23	9:I:96:LEU:HA	1.86	0.42
9:I:123:ARG:N	9:I:167:GLN:OE1	2.53	0.42
13:K:9:ILE:HD13	13:K:9:ILE:HA	1.86	0.42
18:R:27:ASP:HB3	18:R:30:THR:HG22	2.01	0.42
25:Y:9:THR:HG23	25:Y:23:MET:HB2	2.02	0.42
32:f:146:LEU:HD23	32:f:146:LEU:HA	1.86	0.42
37:k:156:GLN:HA	37:k:181:LEU:HA	2.02	0.42
1:2:85:A:H2'	1:2:86:C:C6	2.55	0.42
1:2:106:C:H2'	1:2:107:A:C8	2.55	0.42
3:B:33:VAL:HG12	3:B:44:ILE:HD12	2.01	0.42
3:B:139:CYS:HB2	3:B:168:MET:SD	2.60	0.42
3:B:167:LYS:NZ	3:B:200:ALA:O	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:271:ASP:OD1	4:C:271:ASP:N	2.52	0.42
5:E:64:ILE:HD13	5:E:64:ILE:HA	1.83	0.42
7:G:31:ARG:H	7:G:31:ARG:HG2	1.60	0.42
7:G:52:ILE:HA	7:G:111:LEU:HD23	2.02	0.42
33:g:89:LEU:O	33:g:98:THR:OG1	2.34	0.42
34:j:90:LYS:HE2	34:j:90:LYS:HB2	1.91	0.42
1:2:1489:A:H5''	35:z:148:ARG:HG3	2.01	0.41
4:C:157:LEU:HD23	4:C:157:LEU:HA	1.88	0.41
5:E:87:MET:HG2	5:E:123:LEU:HB2	2.02	0.41
5:E:250:GLU:HA	5:E:253:ASP:HB3	2.01	0.41
7:G:49:VAL:HG12	7:G:115:LYS:HB3	2.01	0.41
15:O:103:ASN:OD1	15:O:103:ASN:N	2.53	0.41
23:W:86:LEU:HD12	23:W:86:LEU:HA	1.90	0.41
37:k:108:GLY:HA2	37:k:138:GLY:HA3	2.02	0.41
1:2:496:C:OP1	5:E:49:ARG:NH2	2.40	0.41
1:2:1362:U:H5''	1:2:1363:C:C5	2.52	0.41
1:2:1423:C:H2'	1:2:1424:G:O4'	2.20	0.41
2:A:137:ALA:HB1	2:A:142:LEU:HB3	2.02	0.41
11:F:107:ASN:HA	11:F:108:PRO:HD3	1.93	0.41
13:K:31:LYS:NZ	13:K:36:ALA:O	2.42	0.41
19:Q:58:LEU:HD22	19:Q:108:ILE:HD12	2.02	0.41
35:z:462:ASP:N	35:z:462:ASP:OD1	2.51	0.41
1:2:673:G:H2'	1:2:674:C:C6	2.55	0.41
1:2:903:A:H2'	1:2:904:A:C8	2.55	0.41
1:2:976:G:H2'	1:2:977:C:H6	1.85	0.41
1:2:1387:G:H2'	1:2:1388:A:O4'	2.20	0.41
2:A:34:MET:HE3	2:A:34:MET:HB3	1.85	0.41
3:B:144:LYS:HB3	3:B:208:HIS:CD2	2.56	0.41
8:H:129:ILE:HD13	8:H:129:ILE:HA	1.93	0.41
36:y:61:GLU:O	36:y:64:ARG:HG2	2.21	0.41
1:2:16:G:N2	1:2:1195:A:H62	2.16	0.41
1:2:196:C:C5	1:2:198:U:H1'	2.55	0.41
1:2:543:C:C4	1:2:544:G:H1'	2.55	0.41
1:2:1295:A:H62	1:2:1304:U:H3	1.68	0.41
2:A:58:LEU:HA	2:A:58:LEU:HD23	1.80	0.41
10:J:28:GLU:OE2	10:J:44:TRP:NE1	2.33	0.41
11:F:165:ASN:OD1	11:F:165:ASN:N	2.52	0.41
14:N:125:LEU:HD12	14:N:125:LEU:HA	1.90	0.41
20:S:6:PRO:HD2	20:S:9:PHE:HB2	2.02	0.41
33:g:254:PRO:HB3	33:g:283:PRO:HB2	2.02	0.41
33:g:264:LYS:HA	33:g:264:LYS:HD3	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:z:431:PRO:HB3	35:z:436:GLU:HG2	2.02	0.41
36:y:61:GLU:OE2	36:y:61:GLU:N	2.43	0.41
1:2:77:A:C8	7:G:154:ARG:HB2	2.55	0.41
1:2:222:U:H2'	1:2:223:C:C6	2.56	0.41
1:2:936:G:H2'	1:2:937:C:C6	2.56	0.41
1:2:997:A:H2'	1:2:998:A:H8	1.86	0.41
1:2:1263:U:H5''	30:d:27:ARG:HH21	1.86	0.41
1:2:1391:C:O3'	26:U:83:ARG:NH2	2.52	0.41
1:2:1616:U:OP2	17:P:43:ARG:NH2	2.53	0.41
3:B:49:VAL:HG21	3:B:62:LEU:HD21	2.02	0.41
7:G:50:VAL:HB	7:G:111:LEU:HD22	2.03	0.41
7:G:137:ARG:HD3	7:G:178:ARG:HD2	2.02	0.41
18:R:107:LYS:HB3	18:R:107:LYS:HE2	1.78	0.41
18:R:114:LEU:HD12	18:R:117:LEU:HD11	2.01	0.41
33:g:30:MET:HE3	33:g:30:MET:HB3	1.90	0.41
36:y:30:ILE:HG13	36:y:32:GLU:H	1.86	0.41
1:2:1686:G:H2'	1:2:1687:C:C6	2.56	0.41
3:B:108:ASP:OD1	3:B:109:LYS:N	2.54	0.41
5:E:225:ILE:HD13	5:E:225:ILE:HA	1.79	0.41
7:G:195:LYS:O	7:G:199:THR:HG23	2.20	0.41
10:J:136:ARG:HD3	10:J:161:LEU:HG	2.03	0.41
15:O:69:SER:O	15:O:110:PRO:HG2	2.21	0.41
23:W:53:ILE:O	23:W:59:GLY:HA2	2.21	0.41
24:X:56:GLY:HA3	31:e:6:LEU:HD11	2.02	0.41
35:z:186:ILE:HD13	35:z:186:ILE:HA	1.81	0.41
1:2:566:U:H2'	1:2:567:C:O4'	2.20	0.41
1:2:1513:C:OP2	30:d:12:ARG:NH1	2.52	0.41
1:2:1533:A:H62	1:2:1602:U:H3	1.69	0.41
2:A:42:LYS:NZ	18:R:99:ASP:OD2	2.33	0.41
7:G:163:ASN:OD1	7:G:163:ASN:N	2.51	0.41
35:z:170:LEU:HD23	35:z:170:LEU:HA	1.92	0.41
35:z:434:LEU:HD12	35:z:437:VAL:HG21	2.03	0.41
1:2:2:A:O2'	4:C:224:THR:O	2.35	0.41
1:2:379:C:P	9:I:181:GLN:HE21	2.44	0.41
1:2:433:A:H5''	9:I:22:HIS:HB3	2.03	0.41
1:2:554:A:H2'	1:2:556:U:C5	2.56	0.41
1:2:1689:C:H2'	1:2:1690:U:H6	1.84	0.41
2:A:177:MET:HE2	2:A:177:MET:HB2	1.83	0.41
3:B:193:ILE:H	3:B:193:ILE:HG12	1.62	0.41
5:E:152:PRO:O	5:E:155:LYS:NZ	2.30	0.41
7:G:75:LEU:HD23	7:G:75:LEU:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:132:LYS:HA	14:N:132:LYS:HD3	1.81	0.41
15:O:39:ASP:OD1	15:O:40:THR:N	2.50	0.41
15:O:43:HIS:CD2	15:O:55:ARG:HB3	2.54	0.41
23:W:102:ILE:H	23:W:113:HIS:CD2	2.38	0.41
32:f:94:LYS:HA	32:f:94:LYS:HD2	1.83	0.41
35:z:536:LYS:HD2	35:z:536:LYS:HA	1.89	0.41
36:y:269:ARG:HG3	36:y:276:THR:HG22	2.02	0.41
1:2:490:C:O2'	1:2:574:A:N6	2.53	0.41
1:2:750:C:H2'	1:2:751:G:H8	1.86	0.41
1:2:876:C:H2'	1:2:877:C:C6	2.55	0.41
1:2:880:G:N2	1:2:906:U:O2	2.37	0.41
1:2:1058:A:H2'	1:2:1059:G:C5	2.56	0.41
1:2:1337:C:H2'	1:2:1338:G:C8	2.55	0.41
1:2:1348:G:C8	1:2:1349:G:C8	3.08	0.41
3:B:86:LEU:HD13	3:B:100:PHE:HA	2.02	0.41
3:B:122:GLU:O	3:B:165:ARG:NE	2.53	0.41
6:D:11:PHE:HE2	26:U:84:ILE:HG23	1.84	0.41
6:D:66:ILE:O	6:D:70:THR:HG23	2.21	0.41
7:G:162:LEU:HA	7:G:162:LEU:HD23	1.84	0.41
12:L:85:THR:OG1	12:L:111:VAL:O	2.24	0.41
16:M:23:LYS:O	16:M:27:ILE:HG12	2.21	0.41
18:R:60:ARG:NH2	18:R:66:VAL:HG13	2.36	0.41
18:R:73:LEU:HD12	18:R:74:GLN:HG2	2.03	0.41
19:Q:101:ASP:OD1	33:g:56:GLN:NE2	2.53	0.41
20:S:39:ARG:HH22	21:T:38:LYS:N	2.18	0.41
21:T:104:LEU:HA	21:T:104:LEU:HD23	1.82	0.41
29:c:20:ARG:HA	29:c:20:ARG:HD2	1.87	0.41
33:g:195:LEU:HA	33:g:195:LEU:HD23	1.84	0.41
33:g:299:PHE:CD1	33:g:309:VAL:HG12	2.55	0.41
35:z:215:LEU:HD23	35:z:215:LEU:HA	1.90	0.41
36:y:348:GLN:HG2	36:y:350:ARG:HG2	2.03	0.41
1:2:164:A:H2'	1:2:165:G:O4'	2.21	0.41
1:2:656:G:H5'	1:2:662:G:N2	2.36	0.41
1:2:851:C:O3'	1:2:852:G:N2	2.41	0.41
1:2:1640:A:C2	35:z:190:LYS:HD3	2.56	0.41
1:2:1844:U:H2'	1:2:1845:A:H8	1.84	0.41
5:E:104:ASP:OD1	5:E:108:ARG:N	2.43	0.41
9:I:92:ARG:HD2	9:I:92:ARG:HA	1.79	0.41
20:S:123:LEU:HD23	20:S:123:LEU:HA	1.86	0.41
25:Y:37:LYS:HD2	25:Y:57:VAL:HG23	2.03	0.41
30:d:56:ASP:OD1	30:d:56:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:z:531:LYS:HE2	35:z:533:GLU:HB3	2.02	0.41
1:2:12:U:H2'	1:2:13:C:C6	2.56	0.40
1:2:652:U:H2'	1:2:653:A:H8	1.86	0.40
1:2:844:U:H2'	1:2:845:G:C8	2.55	0.40
2:A:135:THR:O	2:A:138:SER:OG	2.28	0.40
11:F:139:VAL:HB	29:c:45:ASN:O	2.21	0.40
25:Y:49:LYS:HE2	25:Y:49:LYS:HB2	1.94	0.40
33:g:109:LEU:HD23	33:g:109:LEU:HA	1.89	0.40
36:y:245:LEU:HA	36:y:245:LEU:HD23	1.89	0.40
1:2:126:G:OP2	7:G:198:ARG:NH1	2.32	0.40
1:2:1113:A:H2'	1:2:1114:U:C6	2.56	0.40
1:2:1221:G:H2'	1:2:1222:G:H8	1.85	0.40
1:2:1286:G:N1	16:M:37:GLU:OE2	2.41	0.40
1:2:1587:G:N2	21:T:74:SER:OG	2.54	0.40
1:2:1868:U:O4	3:B:115:LYS:NZ	2.54	0.40
2:A:12:GLU:HG3	18:R:111:PHE:HE1	1.87	0.40
3:B:33:VAL:HG23	3:B:47:THR:HG21	2.02	0.40
13:K:65:ARG:HD3	30:d:25:SER:HB2	2.03	0.40
19:Q:142:GLN:H	19:Q:142:GLN:HG2	1.75	0.40
27:Z:69:THR:HB	27:Z:106:GLN:HE22	1.86	0.40
1:2:319:C:N4	7:G:186:GLN:OE1	2.54	0.40
1:2:611:G:H2'	1:2:612:U:C6	2.56	0.40
1:2:799:U:H3	1:2:866:U:H3	1.69	0.40
1:2:808:A:H5'	5:E:188:ASN:HD21	1.86	0.40
1:2:910:G:H2'	1:2:911:C:O4'	2.21	0.40
1:2:1299:A:O2'	1:2:1301:A:OP1	2.32	0.40
1:2:1470:C:H2'	1:2:1471:C:C6	2.56	0.40
1:2:1598:G:O2'	27:Z:81:GLY:N	2.51	0.40
1:2:1621:U:O2'	1:2:1622:U:H2'	2.22	0.40
3:B:164:ILE:HD13	3:B:164:ILE:HA	1.85	0.40
4:C:127:PHE:HD2	4:C:141:VAL:HG22	1.86	0.40
5:E:62:LYS:O	5:E:66:MET:HG2	2.21	0.40
7:G:10:THR:OG1	7:G:127:THR:O	2.35	0.40
11:F:68:ILE:HD11	11:F:151:ILE:HD11	2.02	0.40
12:L:33:LEU:HD12	12:L:34:PRO:HD2	2.03	0.40
17:P:120:SER:OG	17:P:120:SER:O	2.40	0.40
1:2:1101:U:H2'	1:2:1102:G:H8	1.86	0.40
3:B:159:GLN:OE1	3:B:162:ARG:NH1	2.49	0.40
5:E:208:VAL:HG21	5:E:225:ILE:HG13	2.02	0.40
10:J:111:GLN:NE2	10:J:127:ARG:HB2	2.36	0.40
13:K:1:MET:HB3	13:K:3:MET:HE2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:27:VAL:HG11	15:O:90:ILE:HA	2.02	0.40
18:R:7:LYS:O	18:R:11:LYS:HB2	2.20	0.40
23:W:75:ILE:HG13	23:W:125:ILE:HD11	2.02	0.40
23:W:102:ILE:H	23:W:113:HIS:HD2	1.67	0.40
33:g:155:ARG:HA	33:g:155:ARG:HD3	1.98	0.40
1:2:1059:G:H2'	1:2:1060:A:C8	2.56	0.40
1:2:1339:U:H2'	1:2:1340:U:C6	2.57	0.40
1:2:1653:U:H3	1:2:1671:G:H1	1.69	0.40
1:2:1870:A:H4'	1:2:1870:A:OP1	2.21	0.40
4:C:114:LYS:HD3	4:C:121:ARG:NH2	2.37	0.40
12:L:88:ILE:HG21	12:L:126:VAL:HG21	2.03	0.40
20:S:75:ARG:H	20:S:75:ARG:HG3	1.73	0.40
34:j:96:LEU:HD22	34:j:101:PHE:HB2	2.04	0.40
36:y:92:GLN:O	36:y:96:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	214/295 (72%)	199 (93%)	15 (7%)	0	100	100
3	B	209/264 (79%)	194 (93%)	15 (7%)	0	100	100
4	C	214/293 (73%)	198 (92%)	16 (8%)	0	100	100
5	E	253/263 (96%)	232 (92%)	21 (8%)	0	100	100
6	D	222/243 (91%)	211 (95%)	11 (5%)	0	100	100
7	G	221/249 (89%)	203 (92%)	18 (8%)	0	100	100
8	H	171/194 (88%)	165 (96%)	6 (4%)	0	100	100
9	I	195/208 (94%)	181 (93%)	14 (7%)	0	100	100
10	J	172/194 (89%)	159 (92%)	13 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	F	180/204 (88%)	170 (94%)	10 (6%)	0	100	100
12	L	132/158 (84%)	128 (97%)	4 (3%)	0	100	100
13	K	93/165 (56%)	92 (99%)	1 (1%)	0	100	100
14	N	147/151 (97%)	140 (95%)	7 (5%)	0	100	100
15	O	124/151 (82%)	113 (91%)	11 (9%)	0	100	100
16	M	102/132 (77%)	97 (95%)	5 (5%)	0	100	100
17	P	129/145 (89%)	117 (91%)	12 (9%)	0	100	100
18	R	119/135 (88%)	110 (92%)	9 (8%)	0	100	100
19	Q	138/146 (94%)	124 (90%)	14 (10%)	0	100	100
20	S	139/152 (91%)	128 (92%)	11 (8%)	0	100	100
21	T	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
22	V	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
23	W	127/130 (98%)	114 (90%)	13 (10%)	0	100	100
24	X	137/143 (96%)	128 (93%)	8 (6%)	1 (1%)	18	50
25	Y	120/133 (90%)	113 (94%)	7 (6%)	0	100	100
26	U	96/119 (81%)	90 (94%)	6 (6%)	0	100	100
27	Z	68/125 (54%)	63 (93%)	5 (7%)	0	100	100
28	b	73/84 (87%)	67 (92%)	6 (8%)	0	100	100
29	c	59/69 (86%)	53 (90%)	6 (10%)	0	100	100
30	d	53/56 (95%)	44 (83%)	9 (17%)	0	100	100
31	e	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
32	f	53/156 (34%)	46 (87%)	7 (13%)	0	100	100
33	g	287/317 (90%)	256 (89%)	31 (11%)	0	100	100
34	j	111/165 (67%)	98 (88%)	13 (12%)	0	100	100
35	z	365/568 (64%)	318 (87%)	47 (13%)	0	100	100
36	y	225/412 (55%)	187 (83%)	37 (16%)	1 (0%)	30	60
37	k	418/583 (72%)	359 (86%)	59 (14%)	0	100	100
All	All	5632/7089 (79%)	5152 (92%)	478 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	y	40	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	X	86	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/243 (74%)	180 (100%)	0	100	100
3	B	192/231 (83%)	190 (99%)	2 (1%)	68	74
4	C	182/225 (81%)	178 (98%)	4 (2%)	45	63
5	E	220/225 (98%)	217 (99%)	3 (1%)	59	70
6	D	188/202 (93%)	187 (100%)	1 (0%)	81	80
7	G	194/218 (89%)	194 (100%)	0	100	100
8	H	160/174 (92%)	159 (99%)	1 (1%)	78	79
9	I	174/180 (97%)	171 (98%)	3 (2%)	53	67
10	J	156/168 (93%)	156 (100%)	0	100	100
11	F	156/170 (92%)	156 (100%)	0	100	100
12	L	126/142 (89%)	126 (100%)	0	100	100
13	K	86/136 (63%)	86 (100%)	0	100	100
14	N	130/131 (99%)	130 (100%)	0	100	100
15	O	99/119 (83%)	99 (100%)	0	100	100
16	M	91/108 (84%)	91 (100%)	0	100	100
17	P	117/130 (90%)	117 (100%)	0	100	100
18	R	109/122 (89%)	107 (98%)	2 (2%)	51	67
19	Q	116/121 (96%)	115 (99%)	1 (1%)	70	75
20	S	122/132 (92%)	122 (100%)	0	100	100
21	T	111/115 (96%)	111 (100%)	0	100	100
22	V	67/67 (100%)	67 (100%)	0	100	100
23	W	112/113 (99%)	110 (98%)	2 (2%)	51	67
24	X	111/115 (96%)	111 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Y	103/115 (90%)	103 (100%)	0	100	100
26	U	90/107 (84%)	89 (99%)	1 (1%)	65	73
27	Z	62/103 (60%)	62 (100%)	0	100	100
28	b	70/76 (92%)	70 (100%)	0	100	100
29	c	54/62 (87%)	53 (98%)	1 (2%)	50	65
30	d	48/49 (98%)	45 (94%)	3 (6%)	16	43
31	e	40/48 (83%)	40 (100%)	0	100	100
32	f	51/140 (36%)	51 (100%)	0	100	100
33	g	255/275 (93%)	254 (100%)	1 (0%)	84	81
34	j	102/150 (68%)	102 (100%)	0	100	100
35	z	336/512 (66%)	332 (99%)	4 (1%)	63	72
36	y	201/367 (55%)	200 (100%)	1 (0%)	81	80
All	All	4611/5591 (82%)	4581 (99%)	30 (1%)	73	77

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	76	ASN
3	B	231	LEU
4	C	72	ASP
4	C	155	ILE
4	C	248	TYR
4	C	254	ASP
5	E	21	ASP
5	E	192	ILE
5	E	236	ILE
6	D	181	VAL
8	H	184	ASP
9	I	31	ARG
9	I	121	LEU
9	I	161	LEU
18	R	40	ILE
18	R	101	ASP
19	Q	18	THR
23	W	25	VAL
23	W	125	ILE
26	U	60	THR
29	c	32	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	d	23	VAL
30	d	54	LYS
30	d	56	ASP
33	g	104	HIS
35	z	151	ASP
35	z	163	ASP
35	z	221	ASP
35	z	246	TRP
36	y	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	33	GLN
2	A	169	HIS
3	B	163	GLN
3	B	179	ASN
4	C	113	GLN
4	C	267	GLN
5	E	8	HIS
5	E	50	ASN
5	E	98	ASN
5	E	188	ASN
6	D	145	GLN
7	G	56	ASN
7	G	65	GLN
7	G	155	GLN
7	G	177	GLN
7	G	187	HIS
8	H	73	GLN
8	H	163	GLN
8	H	165	ASN
9	I	64	ASN
9	I	84	ASN
9	I	155	ASN
10	J	113	GLN
10	J	154	GLN
11	F	29	GLN
11	F	65	GLN
11	F	83	ASN
11	F	107	ASN
11	F	114	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	F	137	GLN
12	L	11	GLN
12	L	13	GLN
12	L	141	ASN
13	K	39	ASN
13	K	44	HIS
13	K	61	GLN
13	K	77	GLN
14	N	36	GLN
14	N	58	HIS
15	O	113	GLN
17	P	24	GLN
17	P	41	GLN
17	P	53	GLN
17	P	104	GLN
18	R	31	ASN
18	R	83	ASN
19	Q	24	HIS
20	S	72	GLN
20	S	87	GLN
20	S	105	ASN
21	T	126	GLN
22	V	35	ASN
23	W	16	ASN
23	W	70	ASN
23	W	98	GLN
24	X	46	HIS
24	X	61	GLN
24	X	92	ASN
24	X	127	ASN
27	Z	89	GLN
30	d	5	GLN
30	d	45	GLN
31	e	15	GLN
31	e	58	ASN
33	g	4	GLN
33	g	14	HIS
33	g	56	GLN
33	g	143	GLN
33	g	188	HIS
33	g	196	ASN
33	g	222	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	g	285	GLN
33	g	305	ASN
35	z	232	HIS
35	z	273	HIS
35	z	309	GLN
35	z	316	GLN
35	z	363	ASN
35	z	365	ASN
35	z	463	ASN
36	y	26	ASN
36	y	102	HIS
36	y	318	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1645/1874 (87%)	428 (26%)	19 (1%)

All (428) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	11	A
1	2	14	C
1	2	17	C
1	2	25	A
1	2	33	G
1	2	37	C
1	2	41	G
1	2	46	A
1	2	49	C
1	2	56	G
1	2	58	C
1	2	59	U
1	2	62	G
1	2	65	C
1	2	67	C
1	2	68	A
1	2	72	C
1	2	80	G
1	2	96	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	101	U
1	2	103	A
1	2	113	G
1	2	115	U
1	2	118	C
1	2	120	U
1	2	126	G
1	2	127	C
1	2	129	C
1	2	130	G
1	2	142	C
1	2	143	U
1	2	147	A
1	2	149	A
1	2	155	G
1	2	160	U
1	2	163	U
1	2	168	C
1	2	172	U
1	2	176	U
1	2	178	C
1	2	179	C
1	2	182	C
1	2	183	G
1	2	184	G
1	2	194	C
1	2	195	C
1	2	196	C
1	2	197	U
1	2	198	U
1	2	199	C
1	2	201	C
1	2	202	G
1	2	203	G
1	2	204	G
1	2	205	G
1	2	214	U
1	2	220	U
1	2	291	G
1	2	292	A
1	2	293	C
1	2	305	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	306	C
1	2	307	G
1	2	308	G
1	2	310	C
1	2	312	G
1	2	319	C
1	2	320	G
1	2	331	C
1	2	332	G
1	2	333	G
1	2	335	G
1	2	347	G
1	2	362	C
1	2	364	A
1	2	368	U
1	2	370	G
1	2	381	C
1	2	382	C
1	2	385	G
1	2	386	C
1	2	398	A
1	2	400	C
1	2	407	G
1	2	409	C
1	2	418	A
1	2	428	U
1	2	435	A
1	2	448	A
1	2	449	A
1	2	450	C
1	2	464	A
1	2	465	A
1	2	470	G
1	2	471	G
1	2	472	C
1	2	474	G
1	2	476	A
1	2	482	G
1	2	483	C
1	2	487	U
1	2	488	U
1	2	489	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	492	C
1	2	493	A
1	2	496	C
1	2	508	A
1	2	510	G
1	2	512	A
1	2	516	A
1	2	517	C
1	2	525	A
1	2	529	A
1	2	539	C
1	2	540	U
1	2	541	U
1	2	542	U
1	2	544	G
1	2	545	A
1	2	547	G
1	2	548	C
1	2	549	C
1	2	550	C
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	561	A
1	2	564	A
1	2	574	A
1	2	575	A
1	2	576	A
1	2	577	U
1	2	583	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	595	U
1	2	597	G
1	2	598	G
1	2	606	G
1	2	607	U
1	2	608	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	614	C
1	2	623	G
1	2	626	G
1	2	628	A
1	2	629	A
1	2	634	A
1	2	637	U
1	2	639	C
1	2	640	A
1	2	642	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	658	U
1	2	660	C
1	2	662	G
1	2	663	C
1	2	664	A
1	2	668	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	682	U
1	2	684	G
1	2	687	C
1	2	749	U
1	2	792	C
1	2	796	G
1	2	798	G
1	2	801	U
1	2	809	A
1	2	810	A
1	2	811	A
1	2	812	A
1	2	821	G
1	2	822	U
1	2	827	A
1	2	830	A
1	2	831	G
1	2	847	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	853	C
1	2	862	A
1	2	869	A
1	2	870	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	879	C
1	2	882	U
1	2	884	C
1	2	901	G
1	2	902	G
1	2	903	A
1	2	914	U
1	2	916	A
1	2	917	U
1	2	920	A
1	2	922	A
1	2	933	G
1	2	938	A
1	2	939	U
1	2	949	G
1	2	950	C
1	2	952	G
1	2	961	G
1	2	963	A
1	2	966	U
1	2	969	U
1	2	970	G
1	2	971	G
1	2	972	A
1	2	980	A
1	2	982	G
1	2	983	A
1	2	989	C
1	2	990	A
1	2	992	A
1	2	997	A
1	2	1001	A
1	2	1002	U
1	2	1008	A
1	2	1017	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1023	A
1	2	1026	C
1	2	1027	A
1	2	1028	A
1	2	1036	A
1	2	1041	G
1	2	1045	U
1	2	1049	A
1	2	1052	A
1	2	1054	G
1	2	1055	A
1	2	1056	U
1	2	1057	C
1	2	1061	U
1	2	1062	A
1	2	1064	C
1	2	1066	U
1	2	1069	U
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1087	A
1	2	1096	G
1	2	1108	G
1	2	1110	G
1	2	1120	U
1	2	1133	A
1	2	1138	C
1	2	1139	C
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1170	A
1	2	1171	G
1	2	1188	A
1	2	1195	A
1	2	1215	C
1	2	1221	G
1	2	1242	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1243	U
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1258	A
1	2	1263	U
1	2	1264	C
1	2	1271	C
1	2	1274	G
1	2	1275	G
1	2	1276	A
1	2	1281	G
1	2	1282	A
1	2	1286	G
1	2	1291	A
1	2	1295	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1306	U
1	2	1307	U
1	2	1313	A
1	2	1316	C
1	2	1318	G
1	2	1320	G
1	2	1322	G
1	2	1341	C
1	2	1348	G
1	2	1354	G
1	2	1368	U
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1382	A
1	2	1398	G
1	2	1404	U
1	2	1406	G
1	2	1418	C
1	2	1428	G
1	2	1429	G
1	2	1430	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1438	A
1	2	1440	C
1	2	1441	U
1	2	1446	A
1	2	1449	G
1	2	1454	A
1	2	1455	A
1	2	1462	U
1	2	1463	U
1	2	1466	G
1	2	1477	U
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1493	C
1	2	1494	U
1	2	1495	G
1	2	1497	G
1	2	1498	A
1	2	1508	A
1	2	1518	C
1	2	1521	C
1	2	1526	G
1	2	1533	A
1	2	1534	C
1	2	1544	C
1	2	1552	G
1	2	1553	C
1	2	1556	A
1	2	1558	C
1	2	1559	C
1	2	1560	U
1	2	1569	A
1	2	1570	G
1	2	1578	U
1	2	1580	A
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1594	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1598	G
1	2	1606	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1641	A
1	2	1646	C
1	2	1648	G
1	2	1649	U
1	2	1654	G
1	2	1659	U
1	2	1660	C
1	2	1661	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1680	G
1	2	1683	C
1	2	1693	G
1	2	1695	A
1	2	1699	A
1	2	1702	G
1	2	1720	U
1	2	1722	G
1	2	1724	A
1	2	1726	G
1	2	1742	C
1	2	1744	G
1	2	1746	U
1	2	1748	G
1	2	1755	C
1	2	1756	C
1	2	1757	G
1	2	1759	G
1	2	1761	U
1	2	1775	U
1	2	1780	G
1	2	1783	C
1	2	1784	G
1	2	1785	C
1	2	1786	U
1	2	1800	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1805	G
1	2	1806	A
1	2	1812	U
1	2	1813	A
1	2	1814	G
1	2	1815	A
1	2	1817	G
1	2	1819	A
1	2	1824	A
1	2	1825	A
1	2	1826	G
1	2	1829	G
1	2	1834	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1841	C
1	2	1849	G
1	2	1850	A
1	2	1851	A
1	2	1852	C
1	2	1861	G
1	2	1862	G
1	2	1867	U
1	2	1869	A
1	2	1870	A
1	2	1872	G
1	2	1873	G
1	2	1874	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	119	U
1	2	291	G
1	2	381	C
1	2	509	G
1	2	563	G
1	2	576	A
1	2	681	U
1	2	809	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1060	A
1	2	1065	G
1	2	1119	A
1	2	1367	U
1	2	1440	C
1	2	1605	G
1	2	1679	A
1	2	1692	U
1	2	1814	G
1	2	1850	A
1	2	1872	G

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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
40	ATP	z	603	39	32,33,33	1.32	5 (15%)	48,52,52	1.66	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	ATP	z	603	39	-	1/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	z	603	ATP	C5-C4	4.14	1.46	1.39
40	z	603	ATP	C5-N7	-2.81	1.33	1.39
40	z	603	ATP	C4-N9	-2.52	1.32	1.37
40	z	603	ATP	C5-C6	2.16	1.47	1.41
40	z	603	ATP	C8-N7	2.10	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	z	603	ATP	C5-C4-N3	-5.55	119.08	126.72
40	z	603	ATP	N3-C4-N9	4.34	134.54	127.17
40	z	603	ATP	C2-N3-C4	3.36	120.03	111.83
40	z	603	ATP	C4-C5-N7	-3.10	107.04	110.58
40	z	603	ATP	N3-C2-N1	-2.78	124.38	128.58
40	z	603	ATP	C4-N9-C8	2.51	108.38	105.74
40	z	603	ATP	C3'-C2'-C1'	2.28	105.78	101.46
40	z	603	ATP	C5-N7-C8	2.14	106.82	103.45

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	z	603	ATP	C5'-O5'-PA-O3A

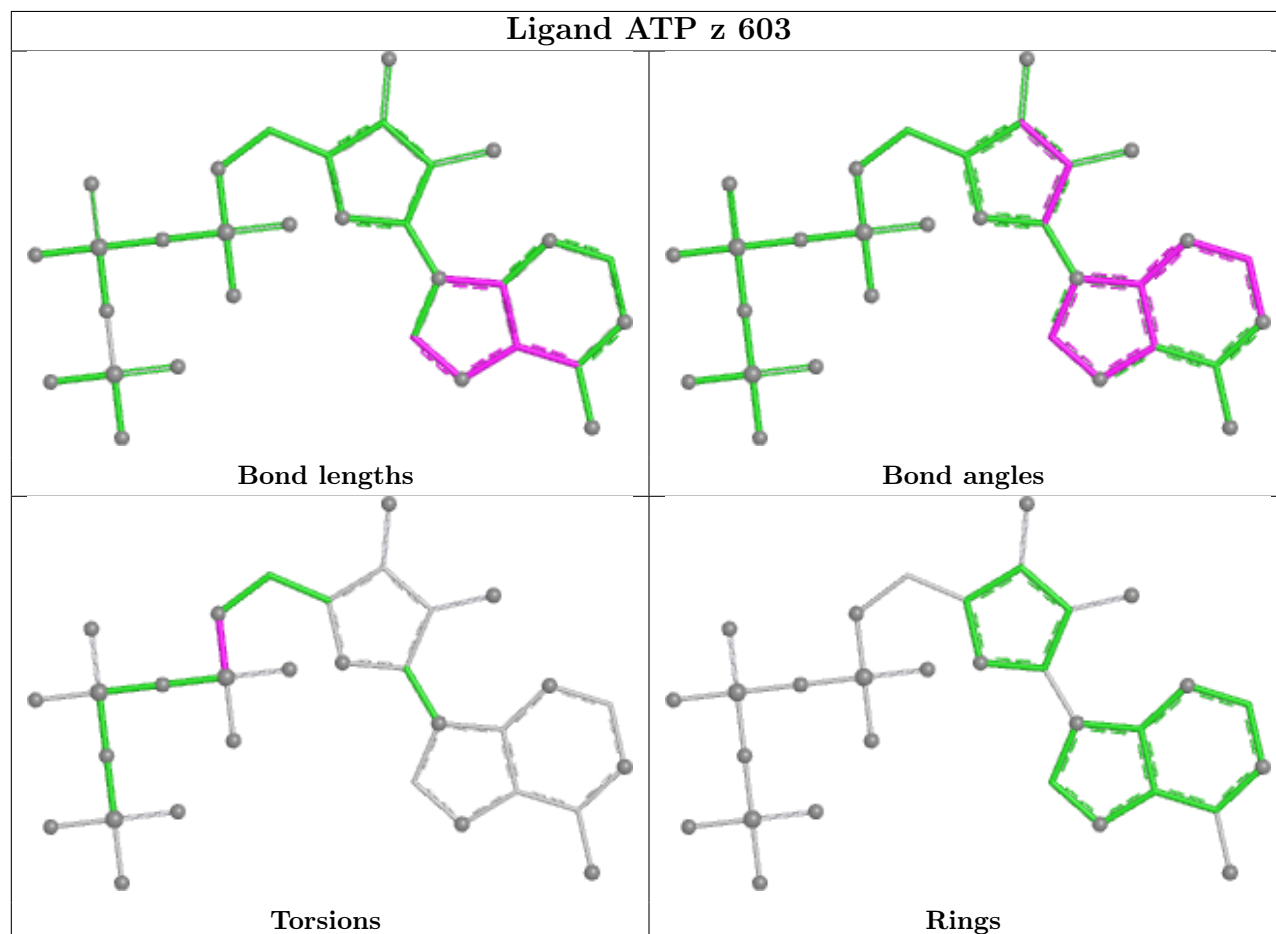
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	z	603	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

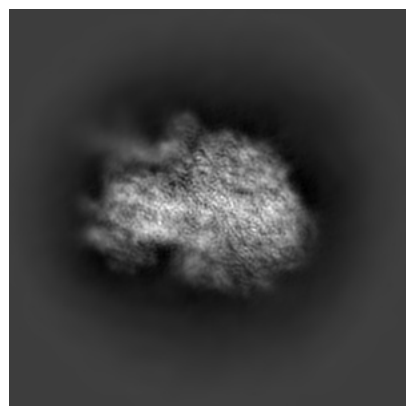
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11519. These allow visual inspection of the internal detail of the map and identification of artifacts.

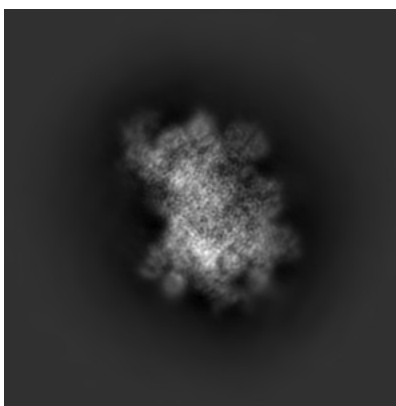
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

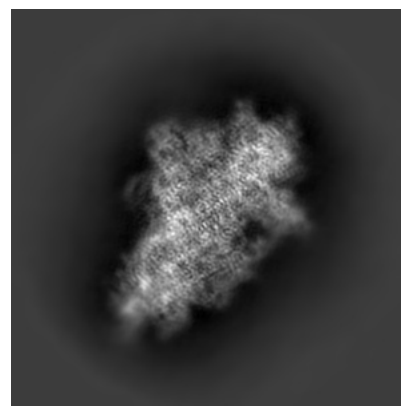
6.1.1 Primary map



X

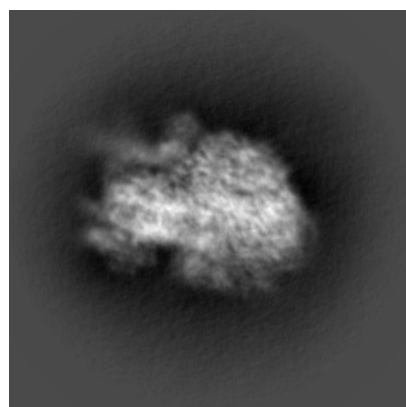


Y

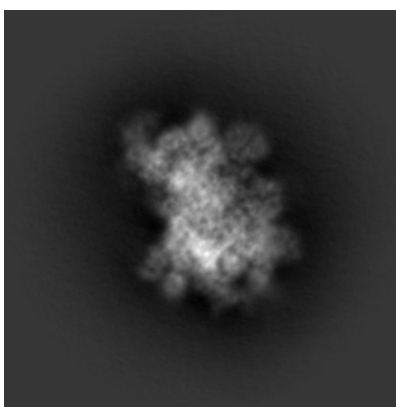


Z

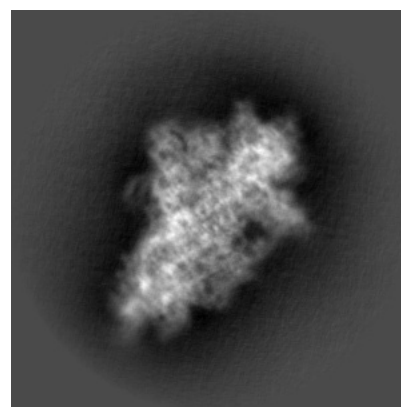
6.1.2 Raw map



X



Y

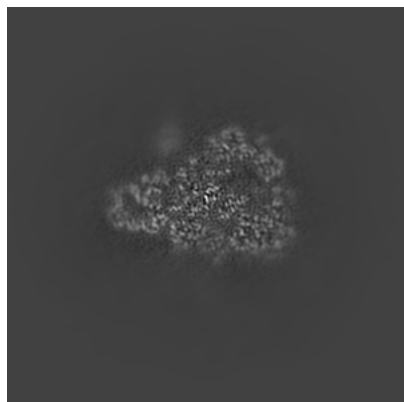


Z

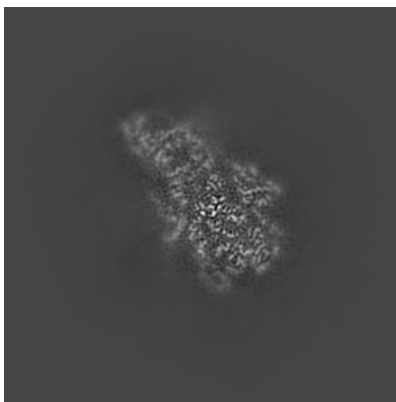
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

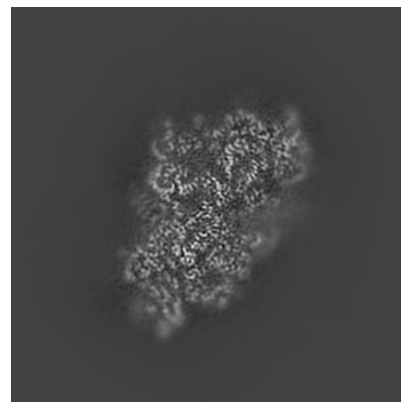
6.2.1 Primary map



X Index: 180

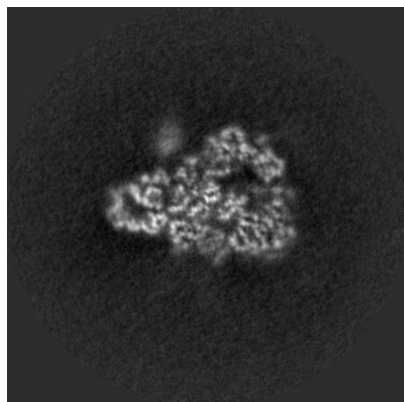


Y Index: 180

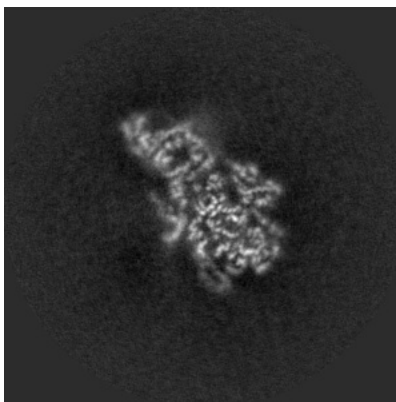


Z Index: 180

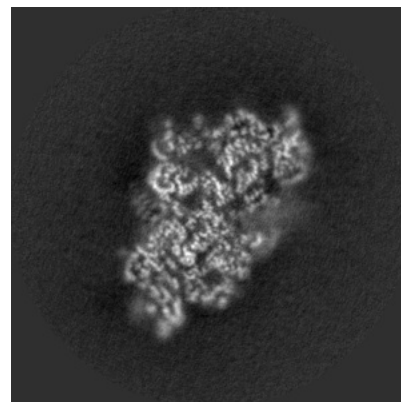
6.2.2 Raw map



X Index: 180



Y Index: 180

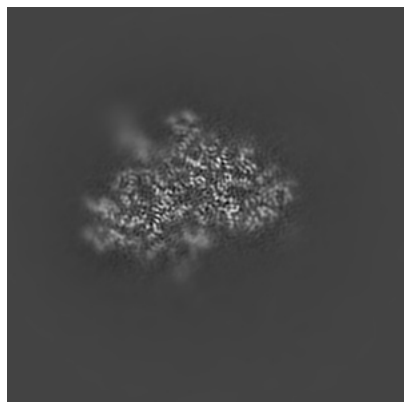


Z Index: 180

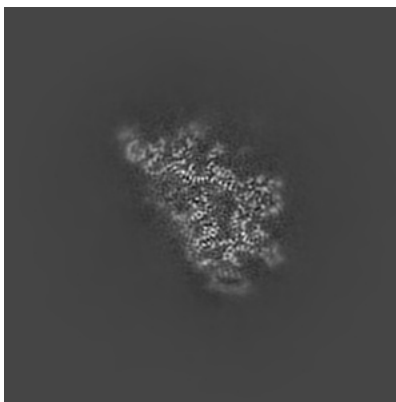
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

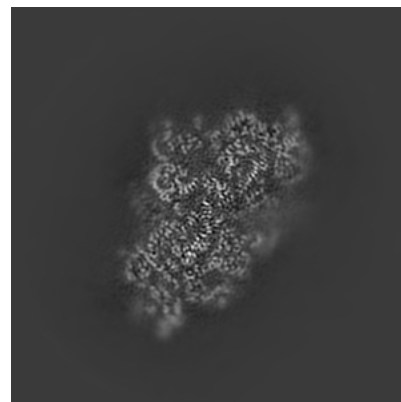
6.3.1 Primary map



X Index: 150

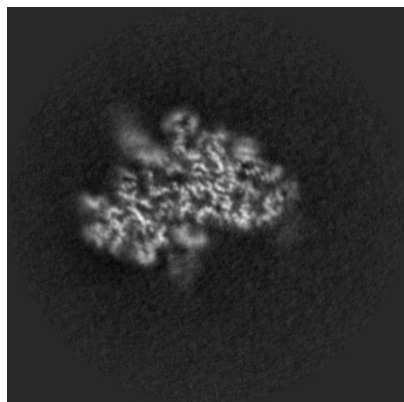


Y Index: 198

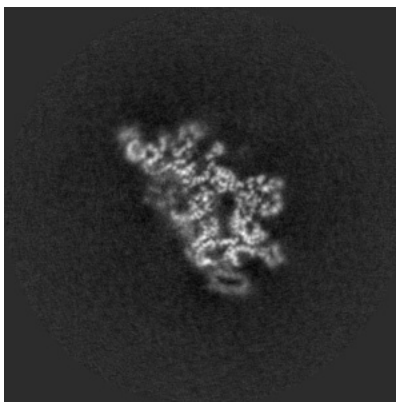


Z Index: 181

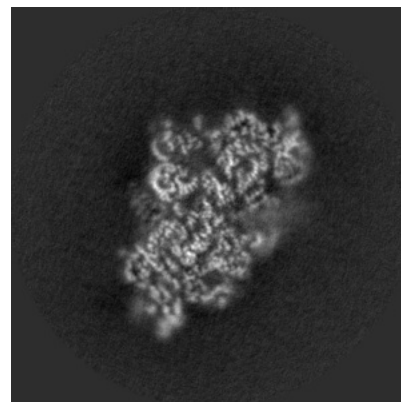
6.3.2 Raw map



X Index: 145



Y Index: 197

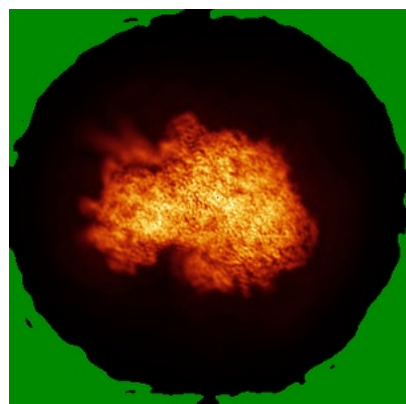


Z Index: 181

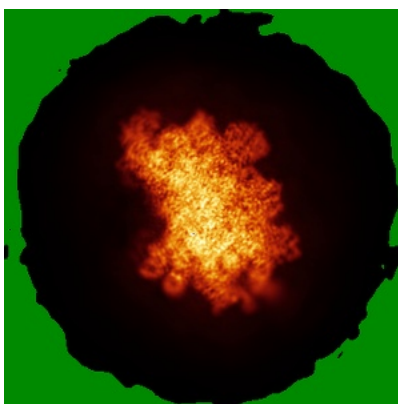
The images above show the largest variance slices of the map in three orthogonal directions.

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

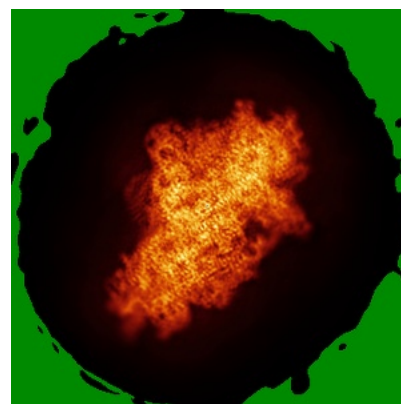
6.4.1 Primary map



X

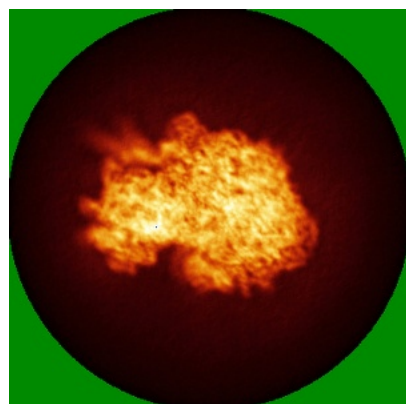


Y

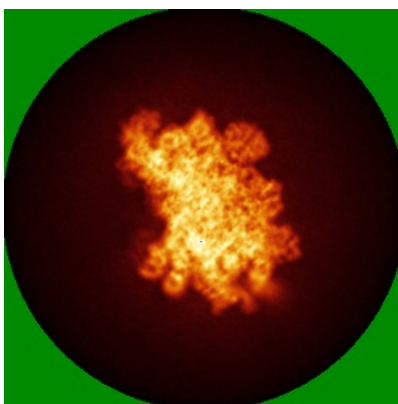


Z

6.4.2 Raw map



X



Y

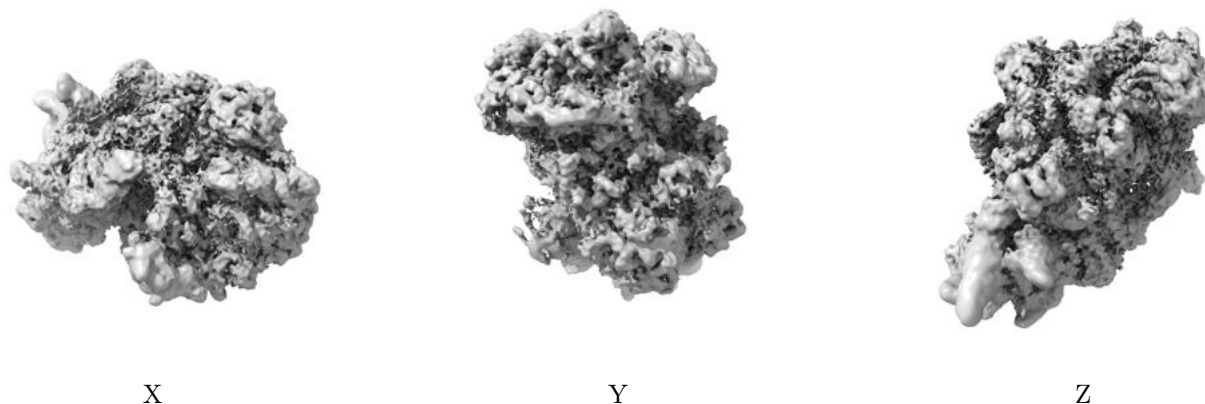


Z

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.

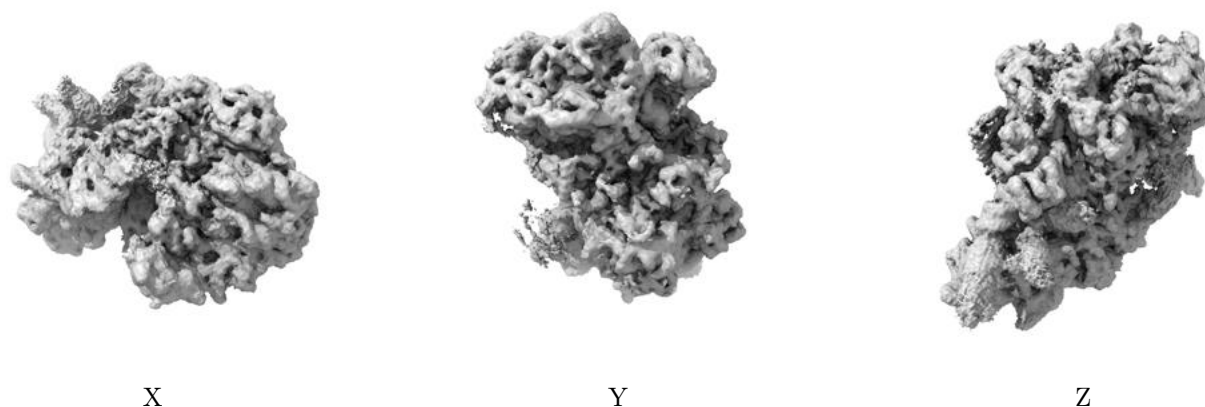
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

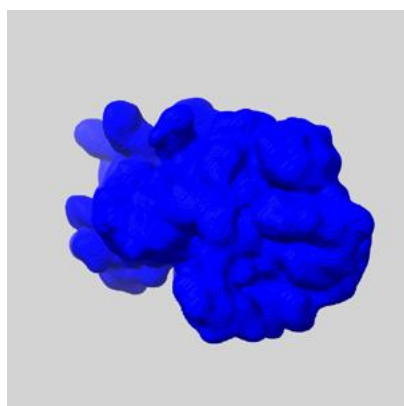
6.6 Mask visualisation [i](#)

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

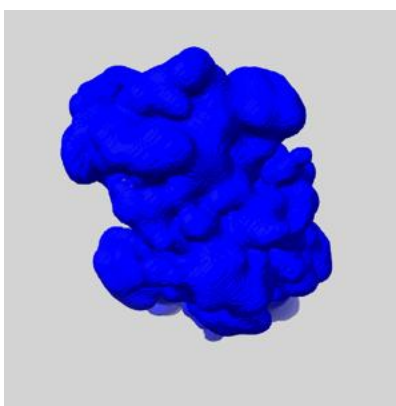
A mask typically either:

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

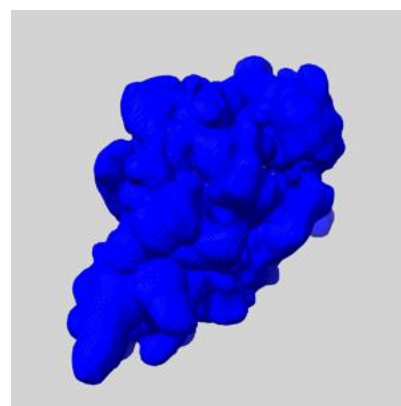
6.6.1 emd_11519_msk_1.map [i](#)



X



Y

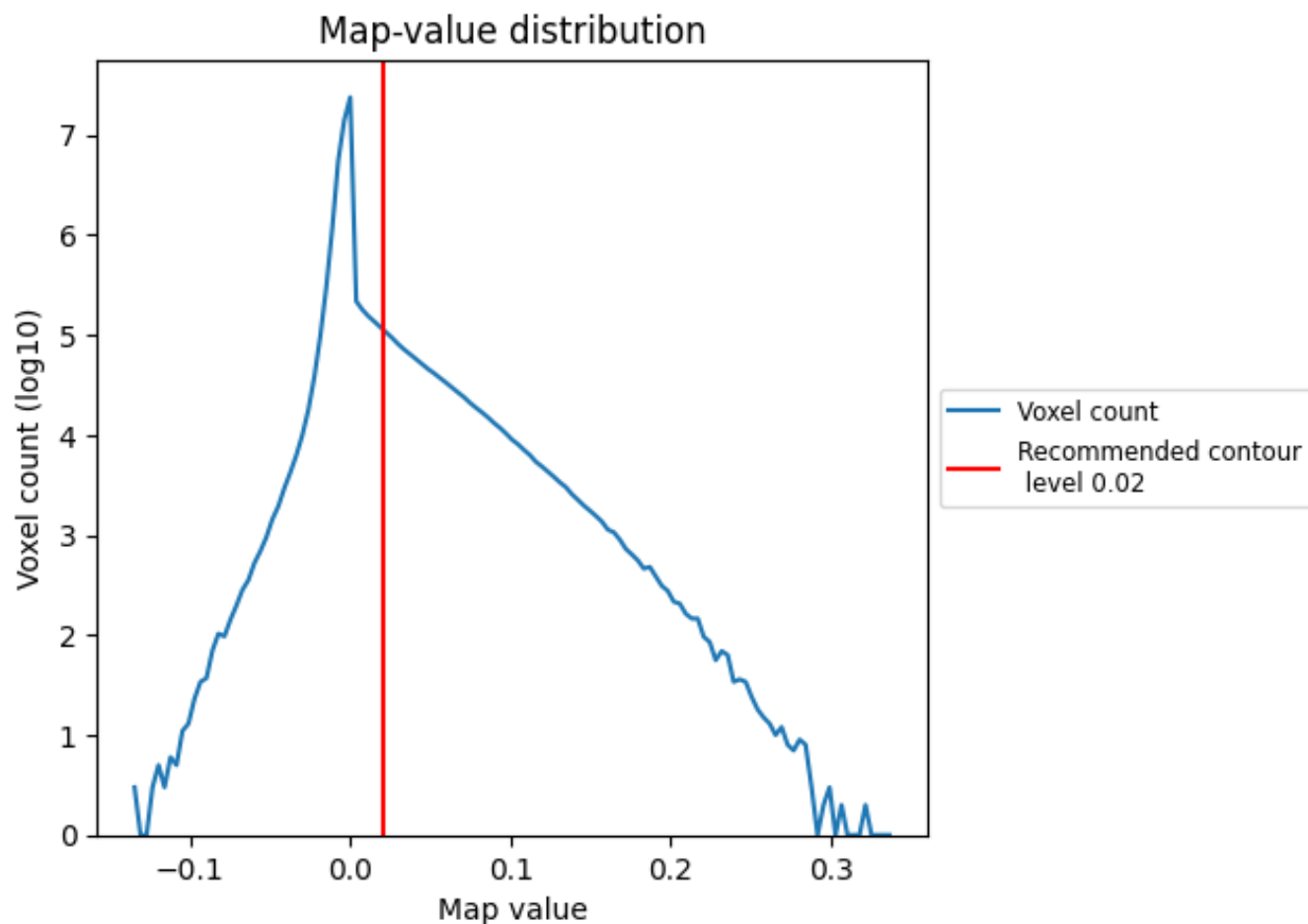


Z

7 Map analysis [i](#)

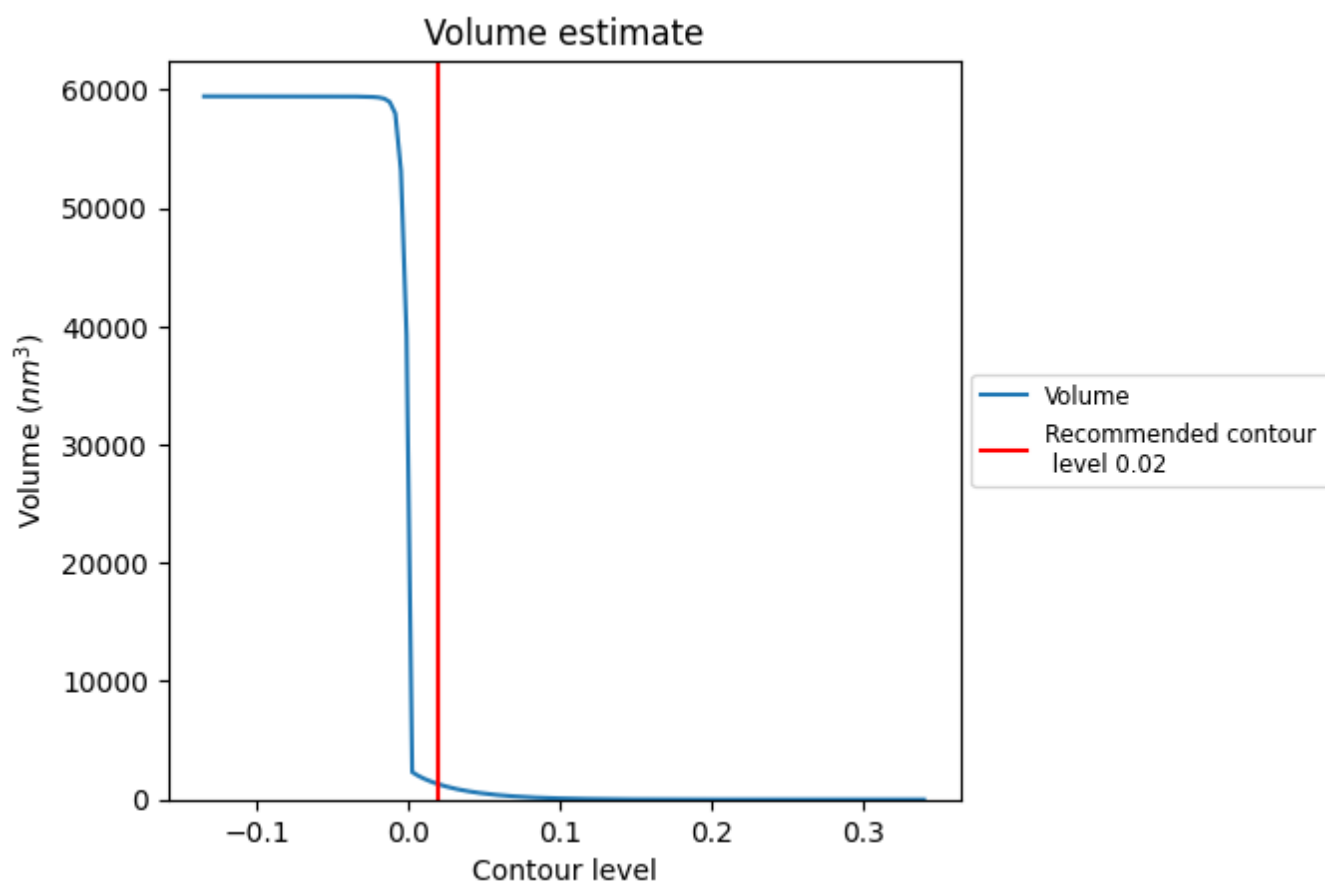
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

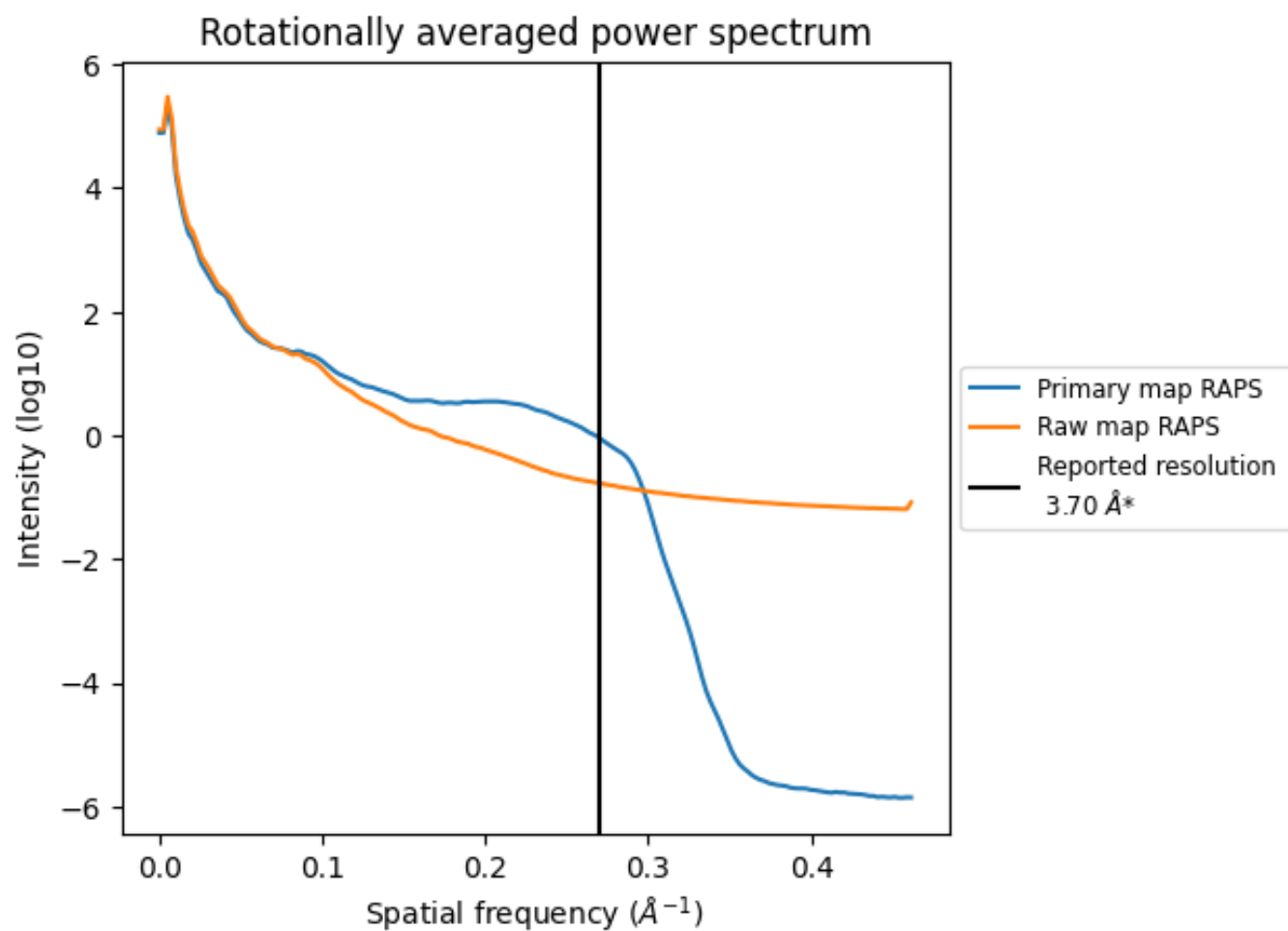
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1298 nm^3 ; this corresponds to an approximate mass of 1173 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 ⓘ

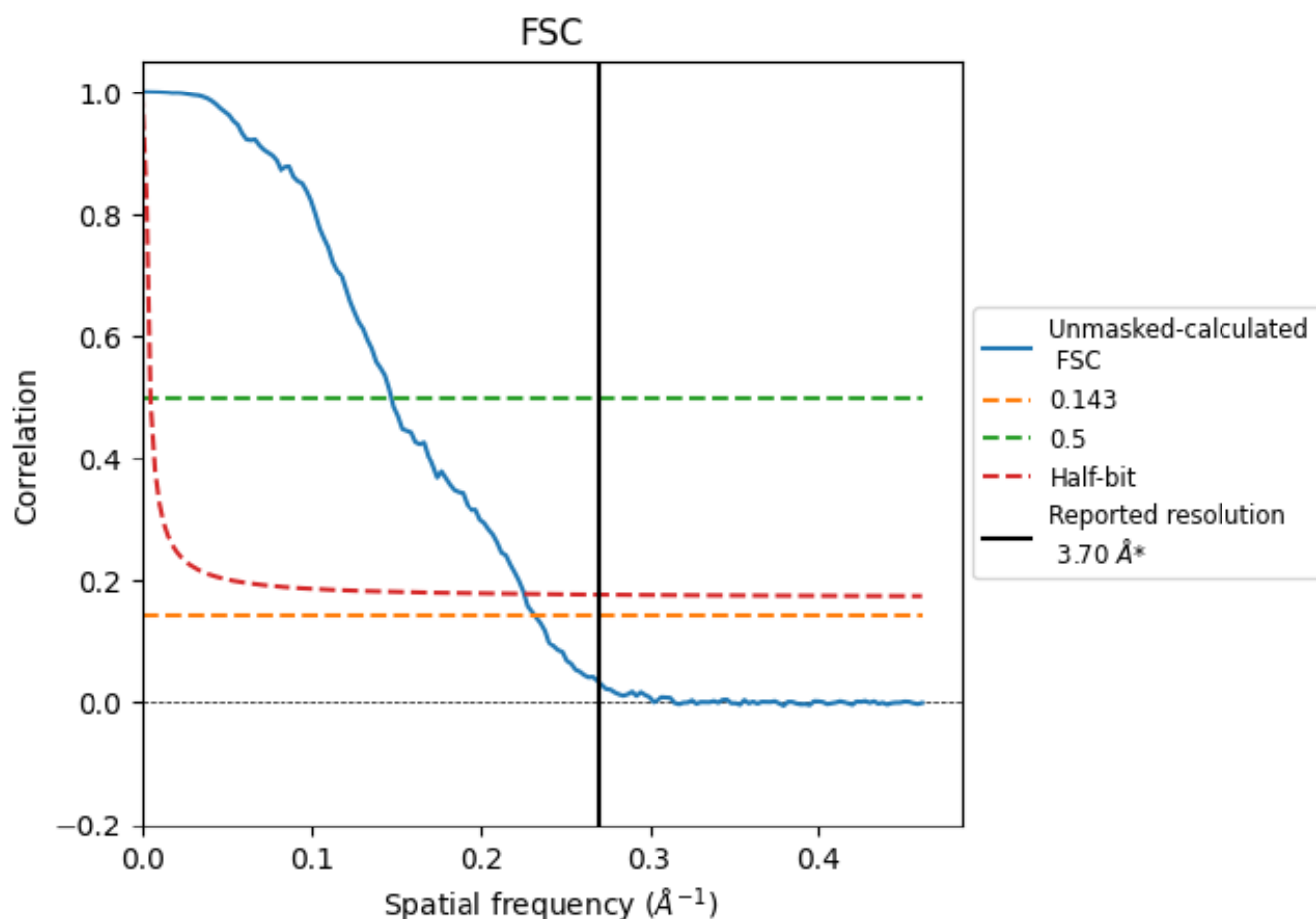


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

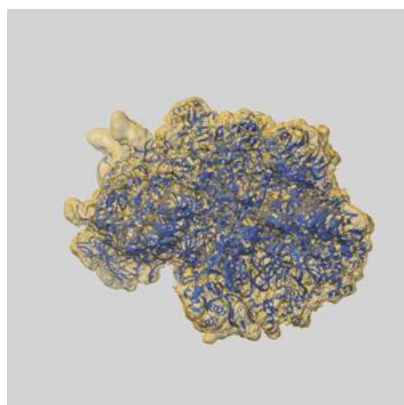
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	6.79	4.42

*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 4.30 differs from the reported value 3.7 by more than 10 %

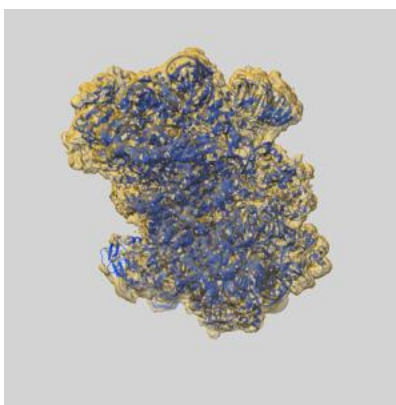
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11519 and PDB model 6ZXF. Per-residue inclusion information can be found in section [3](#) on page [12](#).

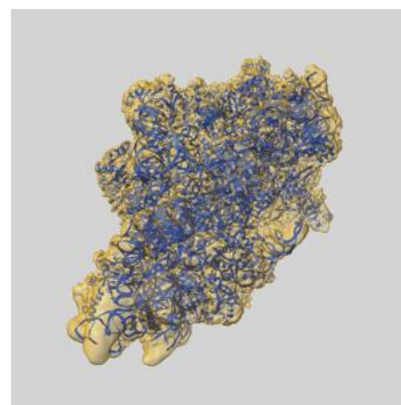
9.1 Map-model overlay [i](#)



X



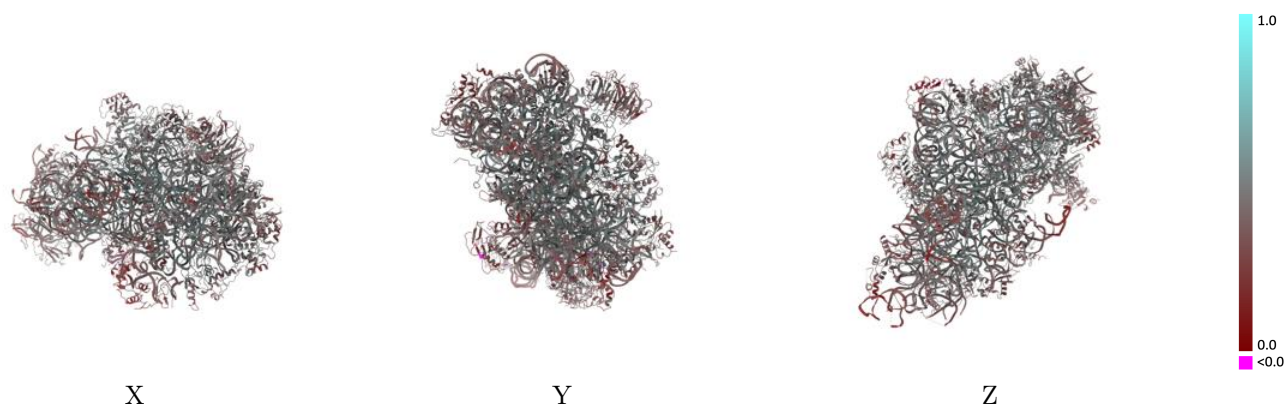
Y



Z

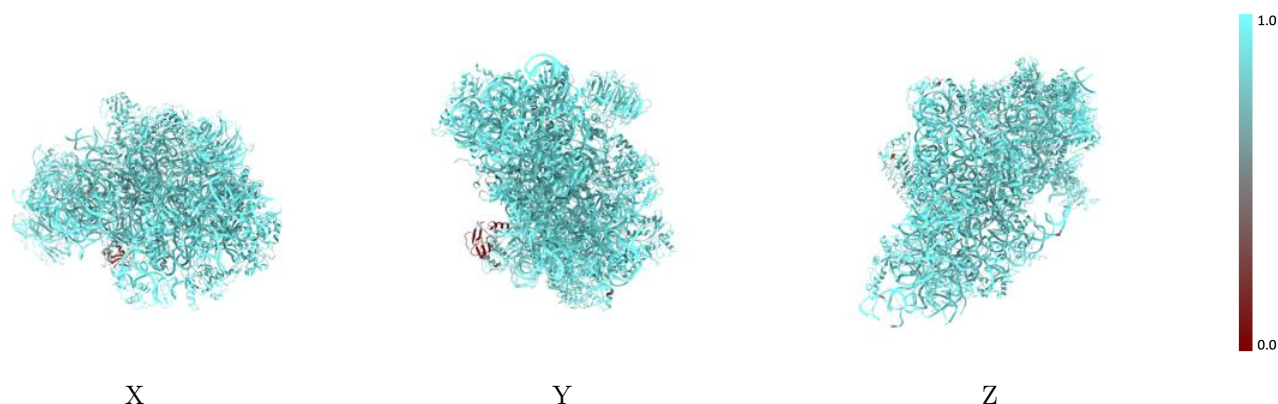
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



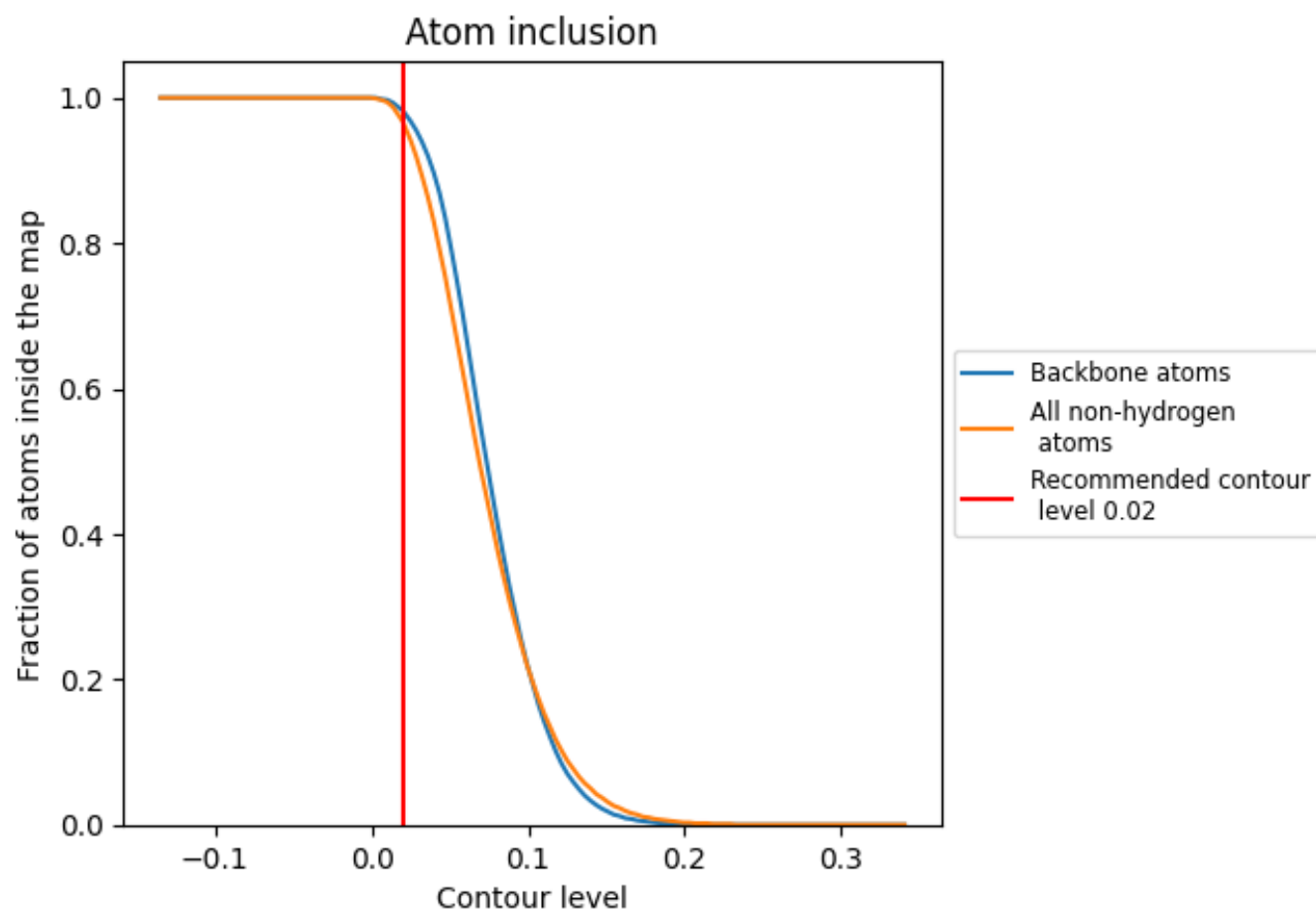
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9670	 0.4370
2	 0.9940	 0.4450
A	 0.9660	 0.4650
B	 0.9340	 0.3750
C	 0.9510	 0.4750
D	 0.9610	 0.4460
E	 0.9580	 0.4510
F	 0.9610	 0.4670
G	 0.9630	 0.3710
H	 0.9580	 0.3880
I	 0.9640	 0.4110
J	 0.9520	 0.4090
K	 0.9730	 0.4240
L	 0.9600	 0.4910
M	 0.9580	 0.2680
N	 0.9610	 0.4650
O	 0.9560	 0.4470
P	 0.9720	 0.4350
Q	 0.9590	 0.4700
R	 0.9560	 0.4430
S	 0.9550	 0.4160
T	 0.9660	 0.4600
U	 0.9630	 0.4410
V	 0.9610	 0.4700
W	 0.9660	 0.5000
X	 0.9780	 0.4980
Y	 0.9780	 0.4030
Z	 0.9450	 0.3820
b	 0.9750	 0.4740
c	 0.9330	 0.4620
d	 0.9820	 0.5090
e	 0.9790	 0.4410
f	 0.9870	 0.3310
g	 0.9690	 0.3990
j	 0.8450	 0.4290



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.7000	 0.3540
y	 0.9580	 0.4540
z	 0.9310	 0.4480