



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:03 AM UTC

PDB ID : 9P38 / pdb_00009p38
EMDB ID : EMD-71238
Title : YsxC-GMPPNP treated 44.5SYsxC particles. Class 1.
Authors : Ortega, J.; Seffouh, A.
Deposited on : 2025-06-13
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

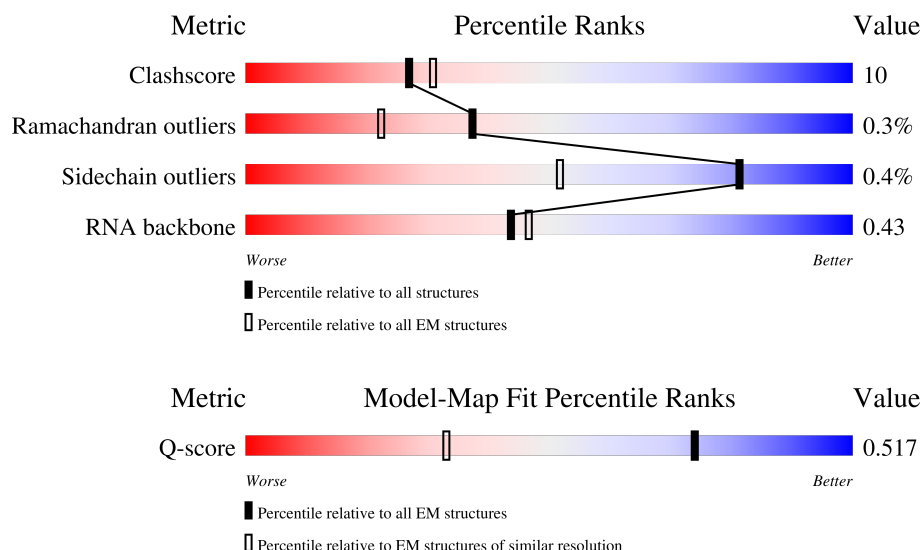
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



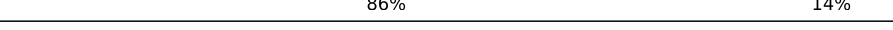
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	A	2927	
2	D	209	
3	E	207	

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Mol	Chain	Length	Quality of chain
4	J	145	 86% 12% .
5	K	122	 77% 23%
6	L	146	 49% 30% . 19%
7	N	120	 82% 18% .
8	P	115	 69% 30% ..
9	Q	118	 74% 25% .
10	R	102	 74% 24% ...
11	S	113	 79% 13% . .
12	T	95	 77% 21% .
13	U	103	 71% 26% .
14	Z	59	 63% 36% .
15	b	59	 49% 19% 8% 24%
16	Y	66	 65% 32% . .
17	d	44	 5% 86% 14%
18	B	195	 83% 17%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 60495 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2116	Total	C	N	O	P	0	0
			45478	20291	8433	14638	2116		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	C	U	conflict	GB 2210155072
A	1558	C	G	conflict	GB 2210155072

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	177	Total	C	N	O	S	0	0
			1341	846	238	254	3		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	201	Total	C	N	O	S	0	0
			1535	966	282	285	2		

- Molecule 4 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 5 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 6 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	118	Total	C	N	O	S	0	0
			871	542	162	166	1		

- Molecule 7 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 8 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	114	Total	C	N	O	0	0
			936	595	184	157		

- Molecule 9 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 10 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	101	Total	C	N	O	0	0
			786	501	139	146		

- Molecule 11 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 12 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	93	Total	C	N	O	S	0	0
			752	472	137	139	4		

- Molecule 13 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	100	Total	C	N	O	S	0	0
			754	473	141	137	3		

- Molecule 14 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 15 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	45	Total	C	N	O	S	0	0
			359	222	74	56	7		

- Molecule 16 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 17 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

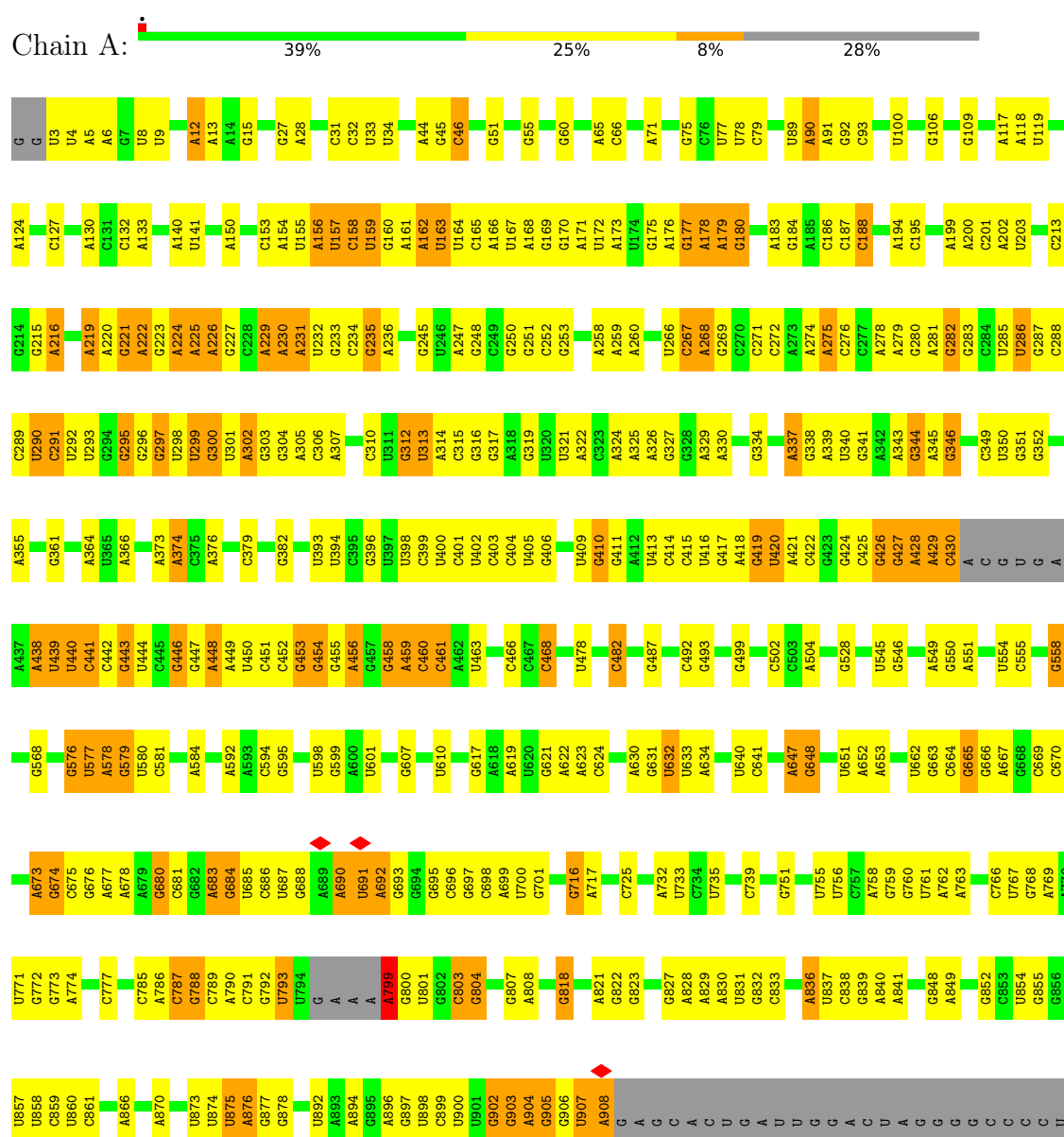
- Molecule 18 is a protein called Probable GTP-binding protein EngB.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	195	Total	C	N	O	S	0	0
			1553	992	267	290	4		

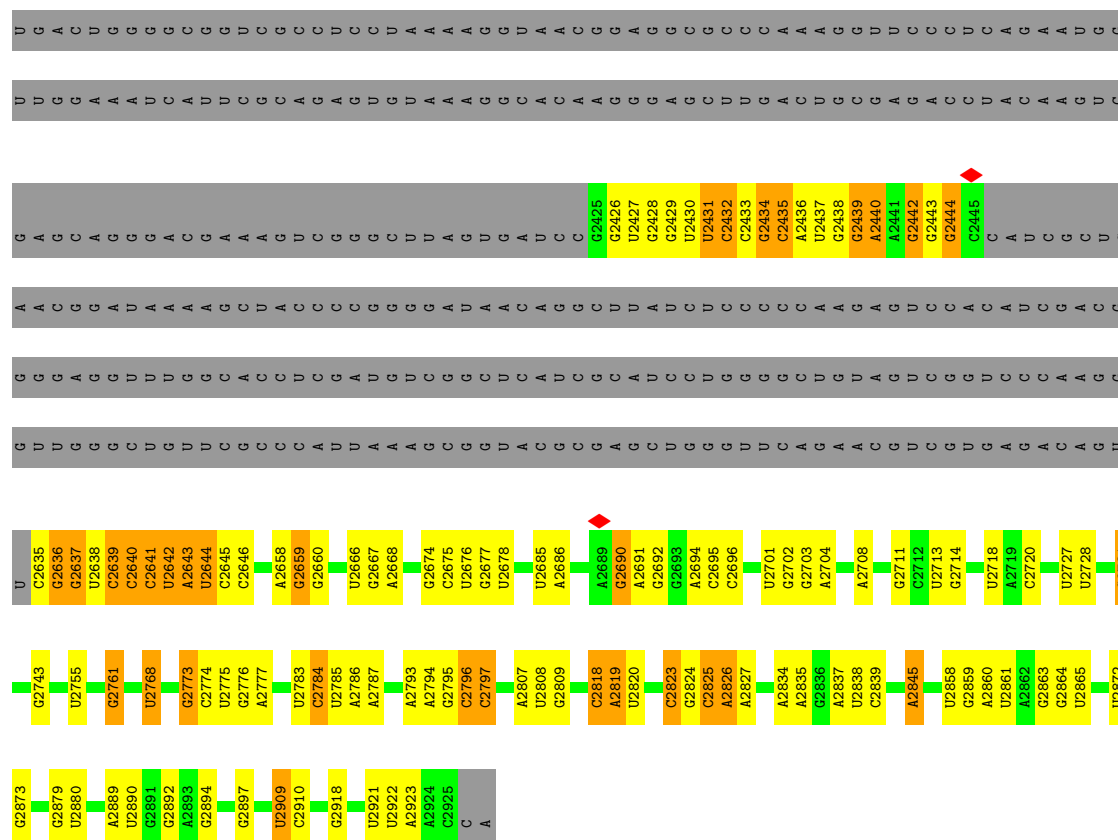
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S rRNA

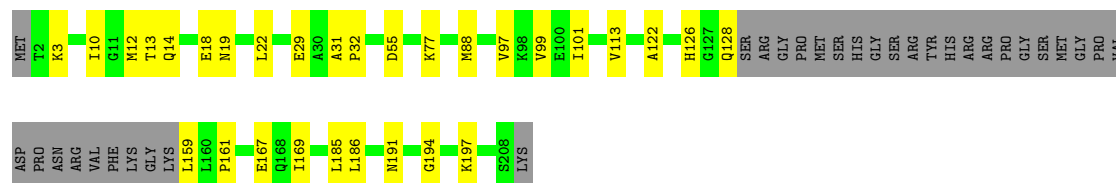






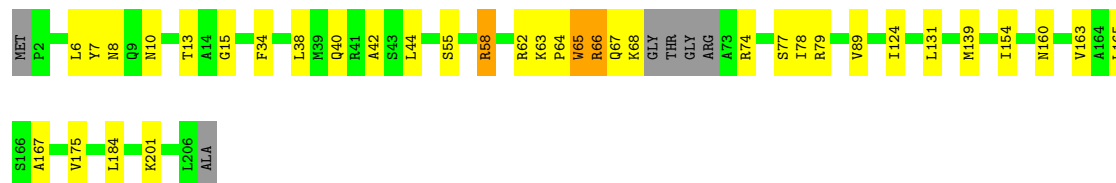
• Molecule 2: 50S ribosomal protein L3

Chain D: 70% 14% 15%



• Molecule 3: 50S ribosomal protein L4

Chain E: 80% 16% 4%



• Molecule 4: 50S ribosomal protein L13

Chain J: 86% 12% 2%



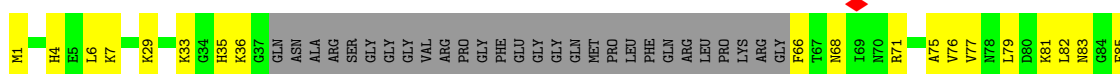
- Molecule 5: 50S ribosomal protein L14

Chain K: 77% 23%



- Molecule 6: 50S ribosomal protein L15

Chain L: 49% 30% 19%



- Molecule 7: 50S ribosomal protein L17

Chain N: 82% 18%



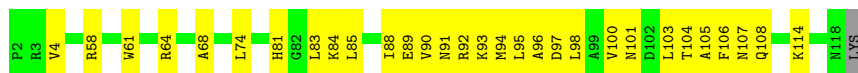
- Molecule 8: 50S ribosomal protein L19

Chain P: 69% 30% 1%



- Molecule 9: 50S ribosomal protein L20

Chain Q: 74% 25%



- Molecule 10: 50S ribosomal protein L21

Chain R: 74% 24% 2%



- Molecule 11: 50S ribosomal protein L22

Chain S:  79% 13% . .



- Molecule 12: 50S ribosomal protein L23

Chain T:  77% 21% .



- Molecule 13: 50S ribosomal protein L24

Chain U:  71% 26% .



- Molecule 14: 50S ribosomal protein L30

Chain Z:  63% 36% .



- Molecule 15: 50S ribosomal protein L32

Chain b:  49% 19% 8% 24%



- Molecule 16: 50S ribosomal protein L29

Chain Y:  65% 32% . .

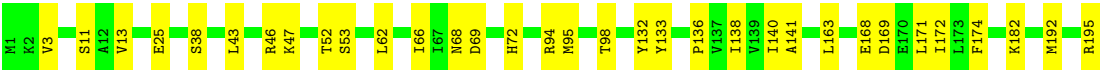
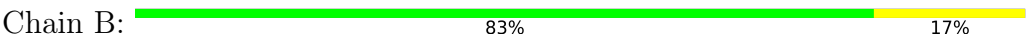


- Molecule 17: 50S ribosomal protein L34

Chain d:  5% 86% 14%



● Molecule 18: Probable GTP-binding protein EngB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	873768	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.066	Depositor
Minimum map value	-0.518	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	359.1, 359.1, 359.1	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/50949	0.41	2/79475 (0.0%)
2	D	0.40	0/1354	0.57	0/1814
3	E	0.43	0/1553	0.63	0/2095
4	J	0.31	0/1146	0.52	0/1542
5	K	0.30	0/927	0.60	0/1245
6	L	0.65	0/877	0.88	1/1168 (0.1%)
7	N	0.31	0/960	0.43	0/1284
8	P	0.32	0/949	0.58	0/1269
9	Q	0.46	0/952	0.71	1/1266 (0.1%)
10	R	0.58	0/797	0.85	1/1070 (0.1%)
11	S	0.69	0/851	0.92	2/1146 (0.2%)
12	T	0.46	0/759	0.65	0/1011
13	U	0.54	0/764	0.71	0/1022
14	Z	0.24	0/457	0.49	0/613
15	b	0.64	0/365	1.10	2/483 (0.4%)
16	Y	0.84	0/531	1.15	0/707
17	d	0.28	0/370	0.32	0/483
18	B	0.33	0/1583	0.51	0/2133
All	All	0.35	0/66144	0.48	9/99826 (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
3	E	0	3
8	P	0	1
11	S	0	6
12	T	0	1
13	U	0	1
15	b	0	1
16	Y	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	B	0	1
All	All	0	20

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	44	LYS	N-CA-C	-8.57	102.02	111.36
11	S	85	PHE	CA-C-N	-6.17	115.56	123.16
11	S	85	PHE	C-N-CA	-6.17	115.56	123.16
6	L	115	GLY	CA-C-O	-5.96	118.02	122.37
10	R	51	PRO	CB-CA-C	5.58	120.77	111.56
9	Q	105	ALA	N-CA-C	-5.53	106.56	113.15
1	A	799	A	C2'-C3'-O3'	5.35	117.52	109.50
15	b	32	SER	CA-C-O	-5.28	115.40	121.47
1	A	1362	G	C2'-C3'-O3'	5.27	121.60	113.70

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	B	195	ARG	Sidechain
3	E	58	ARG	Sidechain
3	E	62	ARG	Sidechain
3	E	66	ARG	Sidechain
8	P	30	ARG	Sidechain
11	S	41	ARG	Sidechain
11	S	8	ARG	Sidechain
11	S	84	ARG	Sidechain
11	S	86	ARG	Sidechain
11	S	88	ARG	Sidechain
11	S	92	ARG	Sidechain
12	T	68	ARG	Sidechain
13	U	92	ARG	Sidechain
16	Y	29	ARG	Sidechain
16	Y	42	ARG	Sidechain
16	Y	47	ARG	Sidechain
16	Y	58	ARG	Sidechain
16	Y	60	ARG	Sidechain
16	Y	7	ARG	Sidechain
15	b	41	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	45478	0	22875	578	0
2	D	1341	0	1409	34	0
3	E	1535	0	1620	43	0
4	J	1123	0	1162	18	0
5	K	920	0	977	25	0
6	L	871	0	920	78	0
7	N	953	0	983	16	0
8	P	936	0	1008	38	0
9	Q	940	0	1005	49	0
10	R	786	0	826	27	0
11	S	842	0	899	23	0
12	T	752	0	802	16	0
13	U	754	0	809	24	0
14	Z	455	0	491	16	0
15	b	359	0	381	20	0
16	Y	530	0	568	13	0
17	d	367	0	410	8	0
18	B	1553	0	1597	20	0
All	All	60495	0	38742	971	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 10.

All (971) 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)
6:L:121:LEU:CD1	6:L:122:THR:O	1.75	1.34
9:Q:84:LYS:CB	9:Q:89:GLU:OE2	1.77	1.32
1:A:1491:A:N6	1:A:1512:G:H1	1.30	1.30
9:Q:84:LYS:HB2	9:Q:89:GLU:OE2	1.10	1.25
2:D:97:VAL:HG13	2:D:101:ILE:CD1	1.73	1.19
1:A:818:G:OP1	17:d:14:LYS:NZ	1.76	1.17
1:A:1660:C:H2'	11:S:92:ARG:HH21	1.03	1.14
6:L:121:LEU:HD13	6:L:122:THR:O	1.38	1.13
3:E:66:ARG:H	3:E:74:ARG:HD2	0.96	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:81:HIS:O	9:Q:85:LEU:HD13	1.46	1.12
5:K:107:ARG:HD3	5:K:112:MET:SD	1.90	1.11
2:D:97:VAL:HG13	2:D:101:ILE:HD11	1.34	1.07
6:L:97:LEU:HD22	6:L:105:LEU:HD13	1.33	1.05
6:L:91:VAL:HG23	6:L:121:LEU:HD11	1.39	1.03
6:L:97:LEU:HB2	6:L:105:LEU:HD11	1.40	1.02
8:P:49:VAL:HG21	8:P:114:LYS:HE2	1.37	1.02
6:L:91:VAL:HG12	6:L:96:LEU:HD21	1.41	0.99
6:L:97:LEU:HD22	6:L:105:LEU:CD1	1.90	0.99
3:E:66:ARG:N	3:E:74:ARG:HD2	1.75	0.98
1:A:1660:C:H2'	11:S:92:ARG:NH2	1.79	0.98
1:A:1491:A:N7	1:A:1512:G:N2	2.12	0.97
1:A:275:A:H62	1:A:296:G:N2	1.62	0.97
1:A:281:A:HO2'	1:A:282:G:H8	1.06	0.97
1:A:275:A:H62	1:A:296:G:H21	1.02	0.96
1:A:1660:C:C6	11:S:92:ARG:HD3	2.02	0.94
17:d:10:ARG:HG2	17:d:14:LYS:HE2	1.49	0.94
3:E:34:PHE:CE2	3:E:38:LEU:HD11	2.03	0.94
3:E:66:ARG:H	3:E:74:ARG:CD	1.81	0.93
6:L:85:PHE:HZ	6:L:96:LEU:HD13	1.30	0.93
6:L:121:LEU:HD11	6:L:122:THR:O	1.66	0.93
2:D:3:LYS:HD2	2:D:101:ILE:HG22	1.51	0.92
1:A:2777:A:H62	1:A:2783:U:H3	1.12	0.91
1:A:275:A:N6	1:A:296:G:H21	1.68	0.91
9:Q:92:ARG:HH12	10:R:11:GLN:H	1.18	0.91
6:L:118:GLU:O	6:L:119:LYS:HG2	1.69	0.90
1:A:1513:U:H3	1:A:1572:G:H1	1.15	0.90
1:A:1497:G:H1	1:A:1505:U:H3	0.90	0.90
6:L:91:VAL:CG1	6:L:96:LEU:HD21	2.00	0.90
9:Q:81:HIS:CD2	9:Q:85:LEU:HD11	2.07	0.90
1:A:1660:C:O2'	11:S:92:ARG:NE	2.06	0.89
8:P:49:VAL:HG21	8:P:114:LYS:CE	2.02	0.89
1:A:343:A:OP2	13:U:95:LYS:NZ	2.05	0.88
6:L:121:LEU:HD13	6:L:122:THR:N	1.87	0.88
8:P:30:ARG:HD2	8:P:90:VAL:HG21	1.56	0.88
1:A:421:A:H62	1:A:447:G:H21	1.18	0.87
9:Q:92:ARG:NH1	10:R:11:GLN:H	1.72	0.87
8:P:36:VAL:HG22	8:P:41:GLU:OE2	1.75	0.86
1:A:421:A:H62	1:A:447:G:N2	1.73	0.86
15:b:44:LYS:C	15:b:46:CYS:H	1.83	0.86
6:L:97:LEU:CB	6:L:105:LEU:HD11	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:GLU:OE1	2:D:185:LEU:HD21	1.74	0.86
2:D:128:GLN:OE1	2:D:159:LEU:HD13	1.74	0.85
1:A:904:A:H61	1:A:967:G:H1	1.22	0.85
2:D:97:VAL:HG13	2:D:101:ILE:HD12	1.56	0.85
6:L:88:GLY:O	6:L:121:LEU:HD21	1.77	0.84
9:Q:81:HIS:O	9:Q:85:LEU:CD1	2.26	0.84
7:N:102:MET:HB3	15:b:42:VAL:HG11	1.59	0.84
2:D:29:GLU:OE1	2:D:185:LEU:CD2	2.25	0.84
1:A:421:A:N6	1:A:447:G:H21	1.75	0.83
2:D:97:VAL:CG1	2:D:101:ILE:CD1	2.56	0.83
6:L:85:PHE:CZ	6:L:96:LEU:HD13	2.13	0.83
11:S:35:ILE:O	11:S:39:THR:HG23	1.79	0.83
2:D:97:VAL:CG1	2:D:101:ILE:HD12	2.09	0.82
12:T:90:ILE:HG13	12:T:92:ILE:HG13	1.62	0.82
1:A:998:G:H3'	1:A:999:A:C8	2.16	0.81
6:L:121:LEU:HD13	6:L:121:LEU:C	2.06	0.81
9:Q:64:ARG:HD2	9:Q:97:ASP:OD2	1.81	0.80
6:L:96:LEU:HB3	6:L:102:ILE:HG22	1.63	0.80
6:L:92:THR:O	6:L:96:LEU:HD23	1.82	0.80
6:L:83:ASN:HA	6:L:117:LEU:HA	1.63	0.79
3:E:66:ARG:N	3:E:74:ARG:CD	2.44	0.79
12:T:92:ILE:O	12:T:92:ILE:HG22	1.80	0.79
14:Z:9:LYS:HD3	14:Z:55:SER:HB3	1.63	0.78
1:A:732:A:H8	1:A:735:U:H3	1.28	0.78
6:L:89:THR:O	6:L:121:LEU:CD2	2.32	0.78
6:L:90:GLU:O	6:L:95:LEU:HD12	1.84	0.78
12:T:72:MET:HB2	17:d:1:MET:HG2	1.66	0.78
1:A:630:A:H62	1:A:1291:A:H2	1.31	0.78
1:A:904:A:N6	1:A:967:G:H1	1.81	0.78
3:E:139:MET:HG2	3:E:167:ALA:HB2	1.65	0.78
1:A:894:A:H62	1:A:979:U:H3	1.32	0.77
1:A:2685:U:O2	1:A:2694:A:N7	2.17	0.77
1:A:2090:G:H21	1:A:2636:G:H1	1.33	0.77
8:P:36:VAL:HG12	8:P:36:VAL:O	1.85	0.77
3:E:34:PHE:CZ	3:E:38:LEU:HD11	2.20	0.76
6:L:75:ALA:HB1	6:L:102:ILE:HD11	1.67	0.76
5:K:107:ARG:HH12	8:P:37:GLU:HB2	1.51	0.76
9:Q:103:LEU:HD22	10:R:2:TYR:OH	1.85	0.76
1:A:305:A:H62	1:A:411:G:N2	1.83	0.76
1:A:319:G:N2	1:A:326:A:C2	2.53	0.76
1:A:159:U:H3'	1:A:160:G:H8	1.48	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:77:VAL:HA	6:L:81:LYS:HD3	1.68	0.75
1:A:430:C:H1'	1:A:438:A:H61	1.52	0.75
13:U:73:PRO:HG2	13:U:99:GLN:OE1	1.86	0.75
1:A:324:A:H61	1:A:403:C:H4'	1.52	0.74
6:L:117:LEU:O	6:L:117:LEU:HD12	1.87	0.74
1:A:1726:G:H5''	1:A:1727:A:H5'	1.68	0.74
6:L:96:LEU:HB3	6:L:102:ILE:CG2	2.16	0.74
1:A:213:C:OP1	17:d:25:LYS:NZ	2.18	0.74
9:Q:103:LEU:CD2	10:R:2:TYR:OH	2.36	0.74
9:Q:84:LYS:CG	9:Q:89:GLU:OE2	2.36	0.73
1:A:89:U:H3'	1:A:90:A:H2'	1.69	0.73
1:A:2777:A:N6	1:A:2783:U:H3	1.87	0.73
10:R:25:LEU:HG	10:R:25:LEU:O	1.87	0.73
9:Q:84:LYS:CA	9:Q:89:GLU:OE2	2.36	0.72
6:L:89:THR:HA	6:L:121:LEU:CD2	2.19	0.72
6:L:118:GLU:O	6:L:119:LYS:CG	2.37	0.72
1:A:1799:G:H1	1:A:2011:U:H3	0.77	0.72
13:U:8:LYS:HG3	13:U:71:LEU:HD12	1.71	0.72
6:L:89:THR:HA	6:L:121:LEU:HD22	1.70	0.71
6:L:89:THR:O	6:L:121:LEU:HD22	1.89	0.71
9:Q:68:ALA:HB2	9:Q:100:VAL:HG13	1.73	0.71
1:A:1497:G:N2	1:A:1505:U:O2	2.22	0.71
1:A:2777:A:N7	1:A:2783:U:O4	2.23	0.71
1:A:268:A:H2'	1:A:269:G:H4'	1.72	0.71
1:A:677:A:H1'	1:A:2444:G:H1'	1.73	0.71
9:Q:84:LYS:HA	9:Q:89:GLU:HB2	1.73	0.71
18:B:66:ILE:HG21	18:B:69:ASP:OD1	1.91	0.70
1:A:1587:U:H2'	1:A:1588:A:H8	1.55	0.70
1:A:1087:U:O2	1:A:1160:G:O6	2.09	0.70
1:A:836:A:N7	3:E:68:LYS:O	2.25	0.70
9:Q:68:ALA:CB	9:Q:100:VAL:HG13	2.21	0.70
1:A:1745:A:H4'	1:A:1746:A:H5'	1.72	0.70
1:A:499:G:N7	3:E:58:ARG:NH2	2.40	0.69
8:P:30:ARG:HD2	8:P:90:VAL:CG2	2.22	0.69
5:K:107:ARG:CD	5:K:112:MET:SD	2.75	0.69
6:L:85:PHE:HE1	6:L:101:VAL:HG11	1.57	0.69
11:S:86:ARG:C	11:S:88:ARG:H	2.00	0.69
1:A:905:G:H22	1:A:966:U:H3	1.39	0.69
1:A:305:A:N6	1:A:411:G:H21	1.91	0.69
1:A:1004:U:H3'	1:A:1005:A:H5''	1.73	0.69
5:K:87:ILE:HD11	5:K:91:LYS:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:G:O6	1:A:1507:U:O4	2.11	0.69
1:A:229:A:H2'	1:A:230:A:C8	2.27	0.69
12:T:49:VAL:HG12	12:T:87:SER:OG	1.92	0.69
6:L:97:LEU:HB2	6:L:105:LEU:CD1	2.21	0.68
4:J:46:THR:HG22	9:Q:64:ARG:NH2	2.08	0.68
9:Q:68:ALA:HB2	9:Q:100:VAL:CG1	2.22	0.68
4:J:46:THR:HG22	9:Q:64:ARG:HH21	1.58	0.68
1:A:1345:U:H3	1:A:1667:A:H61	1.42	0.68
6:L:96:LEU:C	6:L:102:ILE:HG22	2.18	0.68
6:L:121:LEU:HD13	6:L:122:THR:C	2.16	0.68
1:A:279:A:H2'	1:A:280:G:C8	2.29	0.68
1:A:1516:A:H62	1:A:1568:G:H8	1.42	0.68
1:A:2825:C:H3'	1:A:2826:A:H8	1.59	0.68
1:A:165:C:H3'	1:A:166:A:H8	1.59	0.67
1:A:343:A:P	13:U:95:LYS:NZ	2.67	0.67
3:E:34:PHE:CE2	3:E:38:LEU:CD1	2.75	0.67
13:U:22:THR:HB	13:U:36:GLU:OE2	1.93	0.67
1:A:177:G:O2'	1:A:178:A:H5'	1.94	0.67
3:E:63:LYS:O	3:E:74:ARG:NE	2.27	0.67
1:A:1660:C:C2'	11:S:92:ARG:HH21	1.94	0.66
1:A:1008:A:H3'	1:A:1009:U:H6	1.60	0.66
1:A:1661:A:C8	11:S:88:ARG:NH2	2.63	0.66
6:L:85:PHE:CZ	6:L:96:LEU:CD1	2.79	0.66
1:A:150:A:H61	1:A:179:A:H2	1.42	0.66
1:A:1444:C:H2'	1:A:1445:A:H8	1.61	0.66
2:D:3:LYS:HD2	2:D:101:ILE:CG2	2.25	0.66
14:Z:6:ILE:HG23	14:Z:54:VAL:HG21	1.76	0.66
1:A:647:A:H4'	1:A:648:G:O5'	1.94	0.66
5:K:63:VAL:HG12	5:K:64:ARG:HG3	1.77	0.65
1:A:1359:G:H1	1:A:1370:C:H41	1.43	0.65
1:A:278:A:H2'	1:A:279:A:H8	1.60	0.65
9:Q:81:HIS:CD2	9:Q:85:LEU:CD1	2.77	0.65
8:P:109:LYS:H	8:P:109:LYS:HD2	1.62	0.65
9:Q:81:HIS:NE2	9:Q:85:LEU:HD11	2.12	0.65
8:P:49:VAL:HG21	8:P:114:LYS:NZ	2.12	0.65
12:T:52:ASP:HB2	12:T:84:THR:HG22	1.78	0.65
16:Y:9:LEU:N	16:Y:9:LEU:HD12	2.12	0.65
9:Q:96:ALA:O	9:Q:100:VAL:HG23	1.97	0.65
1:A:1244:A:H8	6:L:4:HIS:HB3	1.62	0.64
1:A:760:G:H2'	1:A:761:U:C6	2.32	0.64
1:A:1100:A:H2'	1:A:1101:G:C8	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:42:ARG:HH11	16:Y:46:VAL:HG22	1.62	0.64
1:A:1042:A:H4'	9:Q:92:ARG:HD2	1.79	0.64
1:A:167:U:H2'	1:A:168:A:C8	2.33	0.63
1:A:683:A:H4'	1:A:684:G:O5'	1.98	0.63
1:A:224:A:H1'	1:A:236:A:H1'	1.79	0.63
15:b:27:MET:HG3	15:b:36:MET:CE	2.28	0.63
7:N:24:LEU:HD23	7:N:44:VAL:HG21	1.80	0.63
8:P:109:LYS:HA	8:P:112:ARG:HG2	1.78	0.63
10:R:6:LYS:HD2	10:R:39:LEU:HD21	1.80	0.63
1:A:1125:C:H2'	1:A:1126:A:C8	2.33	0.63
1:A:1359:G:H22	1:A:1370:C:N4	1.96	0.63
1:A:1799:G:N2	1:A:2011:U:O2	2.27	0.63
3:E:65:TRP:HB3	3:E:74:ARG:HA	1.81	0.63
1:A:2082:G:C5	1:A:2083:A:H1'	2.34	0.63
18:B:168:GLU:OE2	18:B:169:ASP:OD1	2.17	0.63
3:E:66:ARG:HA	3:E:74:ARG:HD3	1.80	0.62
1:A:427:G:C2	1:A:428:A:H1'	2.34	0.62
1:A:1527:C:H3'	1:A:1528:U:H3'	1.80	0.62
8:P:55:GLY:HA3	8:P:60:GLU:HA	1.79	0.62
1:A:275:A:N6	1:A:296:G:N2	2.38	0.62
1:A:1444:C:H2'	1:A:1445:A:C8	2.34	0.62
1:A:440:U:H2'	1:A:441:C:C6	2.35	0.62
1:A:1515:C:H2'	1:A:1516:A:C8	2.35	0.62
1:A:1799:G:O6	1:A:2011:U:O4	2.18	0.62
1:A:1660:C:N1	11:S:92:ARG:HD3	2.14	0.62
1:A:1096:A:H3'	1:A:1097:A:H8	1.65	0.62
5:K:2:ILE:HG12	5:K:8:LEU:HD21	1.81	0.62
16:Y:28:LEU:HD11	16:Y:42:ARG:HG3	1.82	0.62
13:U:88:GLY:O	13:U:89:LYS:HD2	2.00	0.61
1:A:305:A:N6	1:A:411:G:N2	2.46	0.61
1:A:429:A:H8	1:A:430:C:H5''	1.65	0.61
1:A:499:G:C8	3:E:58:ARG:HG3	2.35	0.61
1:A:1491:A:N6	1:A:1512:G:N1	2.08	0.61
1:A:1497:G:O6	1:A:1505:U:O4	2.18	0.61
1:A:2825:C:H3'	1:A:2826:A:C8	2.35	0.61
9:Q:83:LEU:HD23	9:Q:88:ILE:HD11	1.81	0.61
1:A:1117:G:H1	1:A:1138:C:H41	1.46	0.61
4:J:43:PRO:HB3	9:Q:100:VAL:HG12	1.83	0.61
1:A:968:C:H2'	1:A:969:C:C6	2.35	0.61
1:A:969:C:H2'	1:A:970:A:C8	2.35	0.61
1:A:1000:G:H5'	1:A:1003:A:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:81:LYS:HE3	6:L:101:VAL:CG1	2.30	0.61
3:E:66:ARG:CA	3:E:74:ARG:HD3	2.31	0.61
6:L:121:LEU:CD1	6:L:121:LEU:C	2.73	0.61
11:S:88:ARG:HH22	11:S:92:ARG:HA	1.65	0.61
2:D:18:GLU:HG2	2:D:19:ASN:N	2.15	0.60
5:K:53:LYS:N	5:K:53:LYS:HE2	2.17	0.60
8:P:30:ARG:CD	8:P:90:VAL:CG2	2.78	0.60
1:A:319:G:H21	1:A:326:A:H2	1.42	0.60
14:Z:37:HIS:HB3	14:Z:43:ILE:HD13	1.83	0.60
1:A:1008:A:H3'	1:A:1009:U:C6	2.35	0.60
8:P:95:VAL:HG12	8:P:97:ARG:H	1.67	0.60
6:L:68:ASN:HD21	6:L:71:ARG:HB2	1.67	0.60
1:A:324:A:N6	1:A:403:C:H4'	2.17	0.60
1:A:1551:C:H2'	1:A:1552:C:C6	2.37	0.60
13:U:84:LYS:HE2	13:U:100:VAL:HG12	1.84	0.60
1:A:1478:G:H2'	1:A:1479:G:C8	2.37	0.59
1:A:1046:A:H2'	1:A:1047:A:C8	2.38	0.59
1:A:1527:C:C3'	1:A:1528:U:H3'	2.32	0.59
5:K:106:LEU:HD13	5:K:114:ILE:HD11	1.84	0.59
1:A:793:U:H1'	1:A:799:A:H61	1.66	0.59
10:R:50:ASN:O	10:R:51:PRO:C	2.45	0.59
10:R:50:ASN:O	10:R:52:THR:N	2.35	0.59
1:A:278:A:H2'	1:A:279:A:C8	2.37	0.59
1:A:1214:U:H2'	1:A:1215:U:C6	2.37	0.59
1:A:426:G:H2'	1:A:427:G:C8	2.38	0.59
1:A:578:A:H4'	1:A:579:G:C8	2.38	0.59
1:A:220:A:H2'	1:A:221:G:H8	1.67	0.59
2:D:29:GLU:OE1	2:D:185:LEU:HD23	2.02	0.59
8:P:30:ARG:CD	8:P:90:VAL:HG21	2.32	0.59
4:J:24:LYS:HD2	4:J:143:LEU:HD12	1.84	0.59
6:L:97:LEU:HD22	6:L:105:LEU:HD11	1.82	0.58
1:A:904:A:N1	1:A:967:G:N2	2.50	0.58
1:A:1125:C:H2'	1:A:1126:A:H8	1.67	0.58
1:A:2090:G:H3'	1:A:2091:A:H2'	1.84	0.58
18:B:13:VAL:HA	18:B:95:MET:SD	2.43	0.58
1:A:416:U:H5''	1:A:417:G:H5'	1.83	0.58
15:b:44:LYS:C	15:b:46:CYS:N	2.51	0.58
1:A:167:U:H2'	1:A:168:A:H8	1.68	0.58
1:A:343:A:P	13:U:95:LYS:HZ1	2.26	0.58
1:A:1179:A:H4'	1:A:1180:C:OP1	2.03	0.58
5:K:4:GLN:HG2	5:K:5:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2685:U:C2	1:A:2694:A:N7	2.71	0.58
6:L:82:LEU:HA	6:L:85:PHE:HB2	1.86	0.58
1:A:1387:G:H2'	1:A:1388:A:H5''	1.86	0.58
1:A:2685:U:H2'	1:A:2686:A:C8	2.39	0.58
1:A:349:C:H2'	1:A:350:U:C6	2.39	0.57
1:A:187:C:HO2'	1:A:188:C:H6	1.52	0.57
1:A:1220:G:H2'	1:A:1221:A:H8	1.69	0.57
1:A:2872:U:H2'	1:A:2873:G:O4'	2.03	0.57
3:E:131:LEU:HD11	3:E:139:MET:HE3	1.84	0.57
10:R:26:ALA:O	10:R:65:GLN:NE2	2.37	0.57
1:A:2826:A:H2'	1:A:2827:A:C8	2.39	0.57
15:b:30:CYS:O	15:b:30:CYS:SG	2.61	0.57
1:A:1347:A:H62	1:A:1651:G:H8	1.50	0.57
1:A:1580:A:H62	1:A:1586:G:H21	1.51	0.57
18:B:25:GLU:HG2	18:B:72:HIS:HB2	1.85	0.57
1:A:1220:G:H2'	1:A:1221:A:C8	2.39	0.57
2:D:167:GLU:HG3	2:D:169:ILE:HD11	1.87	0.57
1:A:1619:A:H2'	1:A:1620:A:C8	2.39	0.56
11:S:87:PRO:HG3	11:S:96:ILE:HG12	1.87	0.56
1:A:698:C:H3'	1:A:699:A:H8	1.70	0.56
1:A:1219:C:H3'	1:A:1220:G:O4'	2.05	0.56
6:L:89:THR:O	6:L:121:LEU:HD21	2.06	0.56
8:P:78:PRO:HG2	8:P:81:THR:HB	1.87	0.56
2:D:126:HIS:ND1	2:D:159:LEU:HA	2.20	0.56
6:L:86:ALA:O	6:L:87:GLU:C	2.48	0.56
1:A:1586:G:H2'	1:A:1587:U:C6	2.40	0.56
16:Y:1:MET:HG2	16:Y:5:GLU:OE1	2.04	0.56
1:A:1008:A:H5''	1:A:1009:U:H5	1.71	0.56
6:L:97:LEU:CD2	6:L:105:LEU:CD1	2.76	0.56
1:A:1726:G:O2'	1:A:1792:G:H5''	2.05	0.56
1:A:2012:C:H2'	1:A:2013:U:C6	2.41	0.56
1:A:287:G:H3'	1:A:288:C:H6	1.71	0.56
1:A:2768:U:H3	1:A:2793:A:H62	1.54	0.56
1:A:169:G:H2'	1:A:170:G:C8	2.39	0.56
1:A:2085:G:H3'	1:A:2086:G:H8	1.70	0.56
11:S:21:MET:HG3	11:S:76:VAL:HG23	1.87	0.56
11:S:35:ILE:HG12	15:b:27:MET:HE1	1.87	0.56
1:A:1042:A:O3'	9:Q:92:ARG:HD2	2.05	0.56
1:A:1618:A:H2'	1:A:1619:A:C8	2.41	0.56
1:A:2838:U:H2'	1:A:2839:C:H6	1.71	0.56
1:A:2434:G:H2'	1:A:2440:A:H61	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:G:H1'	1:A:337:A:H8	1.71	0.55
1:A:1002:G:H2'	1:A:1008:A:H62	1.70	0.55
1:A:2435:C:H5'	1:A:2437:U:C5	2.41	0.55
12:T:3:ASP:OD1	12:T:4:PRO:HD2	2.06	0.55
13:U:74:LYS:HG3	13:U:75:THR:HG23	1.88	0.55
1:A:1496:G:H1	1:A:1507:U:H3	0.71	0.55
1:A:1723:A:H2'	1:A:1724:A:C8	2.41	0.55
3:E:77:SER:C	3:E:79:ARG:H	2.14	0.55
1:A:259:A:H2'	1:A:260:A:H8	1.70	0.55
1:A:439:U:H2'	1:A:440:U:C6	2.42	0.55
1:A:896:A:H2'	1:A:897:G:H8	1.72	0.55
3:E:63:LYS:O	3:E:74:ARG:NH1	2.40	0.55
3:E:66:ARG:CG	3:E:74:ARG:HD3	2.36	0.55
4:J:115:LEU:HG	4:J:119:MET:HE3	1.89	0.55
15:b:30:CYS:SG	15:b:32:SER:O	2.65	0.55
1:A:319:G:H1'	1:A:326:A:H61	1.72	0.55
1:A:1534:A:H2'	1:A:1535:U:H6	1.72	0.55
6:L:91:VAL:CG2	6:L:121:LEU:HD11	2.24	0.55
1:A:159:U:H3	1:A:169:G:H1	1.55	0.55
1:A:279:A:H2'	1:A:280:G:H8	1.72	0.55
1:A:442:C:H2'	1:A:443:G:C8	2.41	0.55
9:Q:89:GLU:O	9:Q:90:VAL:C	2.49	0.55
1:A:1433:U:H2'	1:A:1434:A:H5''	1.88	0.55
2:D:3:LYS:HB2	2:D:101:ILE:HG21	1.89	0.54
2:D:14:GLN:HB3	2:D:22:LEU:HD22	1.89	0.54
18:B:138:ILE:HD11	18:B:192:MET:HG3	1.89	0.54
1:A:169:G:H2'	1:A:170:G:H8	1.72	0.54
1:A:1092:A:H5''	1:A:1093:G:C8	2.43	0.54
1:A:1174:A:H1'	1:A:1175:A:C8	2.42	0.54
1:A:419:G:H4'	1:A:420:U:C6	2.43	0.54
3:E:6:LEU:HD22	3:E:13:THR:HG21	1.89	0.54
6:L:89:THR:CA	6:L:121:LEU:CD2	2.86	0.54
9:Q:64:ARG:HD2	9:Q:97:ASP:CG	2.32	0.54
1:A:2090:G:H2'	1:A:2091:A:C8	2.43	0.54
1:A:1722:A:H2'	1:A:1723:A:H8	1.73	0.54
10:R:50:ASN:HB3	10:R:51:PRO:HD2	1.90	0.54
1:A:1726:G:H4'	1:A:1792:G:N7	2.22	0.54
1:A:1280:G:H2'	1:A:1281:C:O2	2.07	0.54
1:A:27:G:H22	1:A:558:G:H2'	1.74	0.53
1:A:170:G:H2'	1:A:171:A:C8	2.43	0.53
1:A:319:G:N2	1:A:326:A:H2	2.01	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:C:H2'	1:A:416:U:C6	2.43	0.53
1:A:2685:U:H2'	1:A:2686:A:H8	1.73	0.53
5:K:3:GLN:HG2	5:K:4:GLN:H	1.72	0.53
12:T:72:MET:SD	17:d:1:MET:HA	2.48	0.53
1:A:458:G:H4'	1:A:459:A:H5'	1.90	0.53
3:E:13:THR:HG22	3:E:15:GLY:H	1.73	0.53
9:Q:90:VAL:HG12	10:R:39:LEU:HD13	1.91	0.53
1:A:1581:A:O3'	1:A:1582:U:H3'	2.09	0.53
9:Q:84:LYS:HG3	9:Q:89:GLU:OE2	2.09	0.53
9:Q:98:LEU:C	9:Q:100:VAL:H	2.16	0.53
8:P:37:GLU:CD	8:P:38:GLY:H	2.16	0.53
16:Y:9:LEU:N	16:Y:9:LEU:CD1	2.71	0.53
1:A:630:A:H5'	3:E:89:VAL:HG21	1.91	0.53
1:A:836:A:C8	3:E:68:LYS:O	2.62	0.53
1:A:1405:A:H2'	1:A:1406:A:C8	2.44	0.53
1:A:1491:A:N6	1:A:1512:G:C6	2.77	0.53
1:A:1513:U:C5	1:A:1594:G:H2'	2.43	0.53
1:A:1520:A:H61	1:A:1564:C:H42	1.56	0.53
1:A:45:G:H5'	1:A:46:C:OP1	2.08	0.53
1:A:65:A:OP1	17:d:1:MET:SD	2.67	0.53
1:A:2082:G:H3'	1:A:2083:A:H4'	1.90	0.53
1:A:274:A:H3'	1:A:275:A:H8	1.74	0.53
6:L:76:VAL:HG13	6:L:112:LEU:HD13	1.91	0.53
6:L:103:SER:O	6:L:105:LEU:HD12	2.09	0.53
10:R:12:ILE:HG13	10:R:14:VAL:HG13	1.91	0.53
13:U:22:THR:H	13:U:36:GLU:HG2	1.73	0.53
1:A:1326:A:H5'	7:N:107:ARG:HD2	1.91	0.53
1:A:1520:A:H61	1:A:1564:C:N4	2.07	0.53
1:A:1547:U:H2'	1:A:1548:U:C6	2.44	0.53
1:A:1792:G:H2'	1:A:1793:G:H5'	1.90	0.53
10:R:23:GLU:O	10:R:24:LYS:C	2.52	0.53
1:A:403:C:H2'	1:A:404:C:C6	2.45	0.52
1:A:1041:C:N3	4:J:5:PRO:HD2	2.24	0.52
1:A:1279:C:H2'	1:A:1280:G:C8	2.44	0.52
6:L:85:PHE:O	6:L:86:ALA:C	2.52	0.52
9:Q:68:ALA:CB	9:Q:100:VAL:CG1	2.85	0.52
1:A:680:G:H2'	1:A:681:C:C6	2.44	0.52
1:A:1722:A:H2'	1:A:1723:A:C8	2.44	0.52
1:A:1130:A:H4'	1:A:1131:A:OP1	2.09	0.52
9:Q:95:LEU:HD11	10:R:13:LYS:HB2	1.91	0.52
1:A:1014:A:H4'	14:Z:16:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:6:LYS:HG2	10:R:37:ASP:HB2	1.90	0.52
15:b:44:LYS:O	15:b:46:CYS:N	2.42	0.52
1:A:1768:A:H2'	1:A:1769:G:O4'	2.10	0.52
1:A:1525:G:H2'	1:A:1526:G:C8	2.45	0.52
5:K:88:ARG:HD3	5:K:94:ARG:HG2	1.92	0.52
8:P:40:ARG:HH22	8:P:42:ARG:HD3	1.74	0.52
1:A:688:G:N2	1:A:690:A:H3'	2.25	0.52
2:D:122:ALA:HB2	2:D:161:PRO:HD3	1.92	0.52
1:A:873:U:H2'	1:A:875:U:H5'	1.91	0.52
1:A:226:A:H8	1:A:454:G:H21	1.58	0.52
1:A:598:U:H2'	1:A:599:G:O4'	2.10	0.52
13:U:84:LYS:HG2	13:U:93:VAL:CG2	2.40	0.52
5:K:3:GLN:HG2	5:K:4:GLN:N	2.25	0.52
6:L:91:VAL:HG13	6:L:96:LEU:HD21	1.89	0.52
1:A:259:A:H2'	1:A:260:A:C8	2.45	0.51
1:A:898:U:H2'	1:A:899:C:C6	2.45	0.51
1:A:1101:G:H2'	1:A:1102:G:O4'	2.10	0.51
1:A:2427:U:H3'	1:A:2428:G:H8	1.75	0.51
7:N:26:ILE:HD12	7:N:71:ALA:HA	1.92	0.51
12:T:1:MET:SD	12:T:38:GLU:HG2	2.50	0.51
13:U:69:MET:HE3	13:U:78:VAL:HB	1.93	0.51
5:K:107:ARG:NH1	8:P:37:GLU:HB2	2.23	0.51
1:A:168:A:C2	1:A:169:G:H1'	2.45	0.51
1:A:266:U:H2'	1:A:267:C:O4'	2.10	0.51
1:A:631:G:N2	6:L:33:LYS:HE2	2.26	0.51
1:A:793:U:H5''	1:A:1660:C:H5	1.75	0.51
1:A:2432:C:H2'	1:A:2433:C:C6	2.46	0.51
3:E:160:ASN:HD21	3:E:163:VAL:HG23	1.75	0.51
1:A:221:G:N3	1:A:221:G:H2'	2.25	0.51
1:A:420:U:H2'	1:A:421:A:H8	1.75	0.51
1:A:1187:U:H4'	1:A:1188:A:O4'	2.10	0.51
1:A:1493:C:H2'	1:A:1494:G:C8	2.45	0.51
4:J:46:THR:OG1	4:J:49:VAL:HG12	2.10	0.51
5:K:88:ARG:HB3	5:K:94:ARG:HD2	1.92	0.51
6:L:90:GLU:O	6:L:95:LEU:CD1	2.57	0.51
1:A:446:G:H3'	1:A:447:G:H8	1.75	0.51
14:Z:19:GLN:O	14:Z:23:VAL:HG13	2.11	0.51
1:A:399:C:H2'	1:A:400:U:O4'	2.11	0.51
1:A:677:A:HO2'	6:L:66:PHE:N	2.07	0.51
1:A:1000:G:H2'	1:A:1000:G:N3	2.26	0.51
1:A:1426:A:H5'	1:A:1515:C:H1'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:104:THR:HG22	9:Q:104:THR:O	2.11	0.51
14:Z:28:LEU:CD2	14:Z:35:VAL:HG23	2.41	0.51
1:A:1476:C:H2'	1:A:1477:A:C8	2.46	0.51
1:A:2677:G:H2'	1:A:2678:U:C6	2.46	0.51
6:L:79:LEU:O	6:L:83:ASN:N	2.44	0.51
1:A:1220:G:O5'	1:A:1220:G:H8	1.94	0.51
1:A:1250:G:C8	1:A:1250:G:H5'	2.46	0.51
1:A:1360:A:H3'	1:A:1361:A:H8	1.75	0.51
1:A:2659:G:H2'	1:A:2660:G:H8	1.76	0.51
11:S:86:ARG:C	11:S:88:ARG:N	2.67	0.50
1:A:337:A:N3	1:A:337:A:H2'	2.25	0.50
1:A:739:C:H5''	18:B:53:SER:HB2	1.92	0.50
1:A:1065:U:H3	1:A:1188:A:H62	1.59	0.50
1:A:2644:U:C2	15:b:4:PRO:HA	2.46	0.50
6:L:85:PHE:CE1	6:L:101:VAL:HG11	2.43	0.50
1:A:163:U:H2'	1:A:166:A:N6	2.26	0.50
1:A:1250:G:H5'	1:A:1250:G:H8	1.77	0.50
1:A:692:A:H2'	1:A:693:G:O4'	2.10	0.50
18:B:38:SER:HB3	18:B:52:THR:HG21	1.94	0.50
1:A:2823:C:H3'	1:A:2824:G:H8	1.77	0.50
8:P:40:ARG:HH12	8:P:42:ARG:HD3	1.75	0.50
1:A:1073:A:H62	1:A:1173:A:H8	1.58	0.50
1:A:1567:U:H5	1:A:1568:G:C6	2.29	0.50
1:A:2085:G:H8	1:A:2085:G:OP1	1.95	0.50
3:E:154:ILE:HB	3:E:175:VAL:HG22	1.94	0.50
4:J:7:ALA:HA	4:J:46:THR:HG21	1.92	0.50
1:A:225:A:C2	1:A:236:A:H5''	2.47	0.50
6:L:97:LEU:HA	6:L:102:ILE:O	2.12	0.50
8:P:49:VAL:CG2	8:P:114:LYS:NZ	2.75	0.50
6:L:97:LEU:CD2	6:L:105:LEU:HD11	2.41	0.50
9:Q:89:GLU:C	9:Q:91:ASN:N	2.68	0.50
14:Z:17:GLU:O	14:Z:21:VAL:HG23	2.11	0.50
1:A:5:A:H2'	1:A:6:A:C8	2.47	0.49
1:A:1072:A:O2'	1:A:1073:A:H5'	2.12	0.49
1:A:1117:G:H1	1:A:1138:C:N4	2.09	0.49
1:A:2773:G:H2'	1:A:2774:C:H6	1.77	0.49
1:A:993:A:H2'	1:A:994:C:C6	2.47	0.49
1:A:1531:G:H2'	1:A:1532:A:H8	1.77	0.49
1:A:27:G:N2	1:A:558:G:H2'	2.26	0.49
1:A:177:G:O2'	1:A:178:A:C8	2.62	0.49
1:A:343:A:P	13:U:95:LYS:HZ3	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:G:H2'	1:A:456:A:C8	2.47	0.49
1:A:1172:A:H5'	1:A:1173:A:C4	2.47	0.49
2:D:13:THR:HG21	8:P:8:ILE:CG2	2.42	0.49
3:E:66:ARG:CA	3:E:74:ARG:CD	2.89	0.49
11:S:85:PHE:HA	11:S:95:GLN:HA	1.93	0.49
1:A:441:C:H2'	1:A:442:C:C6	2.48	0.49
1:A:286:U:H3'	1:A:287:G:H8	1.77	0.49
1:A:632:U:H2'	1:A:633:U:C6	2.48	0.49
1:A:2703:G:H2'	1:A:2704:A:C8	2.48	0.49
4:J:5:PRO:HD3	9:Q:94:MET:HE3	1.94	0.49
9:Q:90:VAL:HG11	10:R:39:LEU:HD22	1.95	0.49
11:S:6:VAL:HG11	11:S:8:ARG:HH21	1.78	0.49
1:A:373:A:N6	13:U:15:LYS:H	2.10	0.49
1:A:1552:C:H2'	1:A:1553:A:O4'	2.11	0.49
2:D:13:THR:HG21	8:P:8:ILE:HG23	1.94	0.49
8:P:88:GLU:N	8:P:88:GLU:OE1	2.46	0.49
1:A:222:A:H2'	1:A:223:G:N3	2.27	0.49
1:A:1015:G:H2'	1:A:1016:U:C6	2.47	0.49
1:A:2677:G:H2'	1:A:2678:U:H6	1.77	0.49
2:D:126:HIS:HB3	2:D:159:LEU:HD22	1.93	0.49
9:Q:106:PHE:C	9:Q:108:GLN:N	2.70	0.49
1:A:302:A:H2'	1:A:303:G:C8	2.48	0.49
1:A:807:G:H2'	1:A:808:A:O4'	2.13	0.49
1:A:2643:A:H4'	1:A:2644:U:C5	2.48	0.49
1:A:2773:G:H2'	1:A:2774:C:C6	2.48	0.49
13:U:8:LYS:CG	13:U:71:LEU:HD12	2.42	0.49
1:A:194:A:H2'	1:A:195:C:C6	2.47	0.49
1:A:312:G:H2'	1:A:313:U:O4'	2.13	0.49
1:A:755:U:H2'	1:A:756:U:C6	2.48	0.49
1:A:1214:U:H2'	1:A:1215:U:H6	1.77	0.49
1:A:2879:G:H2'	1:A:2880:U:C6	2.48	0.49
3:E:77:SER:C	3:E:79:ARG:N	2.70	0.49
1:A:194:A:H2'	1:A:195:C:H6	1.78	0.48
1:A:1067:A:H62	1:A:1187:U:H3	1.61	0.48
1:A:1491:A:H62	1:A:1512:G:H1	0.58	0.48
1:A:1727:A:H5''	1:A:1791:A:C2	2.48	0.48
1:A:1759:U:H2'	1:A:1760:A:H8	1.78	0.48
15:b:30:CYS:SG	15:b:33:CYS:C	2.95	0.48
1:A:326:A:C2	1:A:402:U:H1'	2.48	0.48
1:A:676:G:H4'	1:A:686:C:O2'	2.13	0.48
1:A:2727:U:H2'	1:A:2728:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:ILE:HD11	2:D:29:GLU:HB2	1.94	0.48
6:L:81:LYS:HE3	6:L:101:VAL:HG12	1.94	0.48
7:N:41:ARG:O	7:N:45:GLU:HG3	2.13	0.48
12:T:92:ILE:O	12:T:92:ILE:CG2	2.52	0.48
1:A:459:A:N3	1:A:459:A:H2'	2.28	0.48
1:A:2677:G:H1	1:A:2701:U:H3	1.61	0.48
3:E:7:TYR:HD2	3:E:124:ILE:HG23	1.77	0.48
5:K:81:GLU:N	5:K:81:GLU:OE2	2.46	0.48
9:Q:90:VAL:HG21	10:R:51:PRO:HA	1.94	0.48
15:b:30:CYS:O	15:b:31:PRO:C	2.56	0.48
1:A:580:U:H2'	1:A:581:C:C6	2.49	0.48
7:N:26:ILE:HD11	7:N:79:ALA:HB2	1.95	0.48
1:A:1531:G:H2'	1:A:1532:A:C8	2.48	0.48
1:A:691:U:H5''	1:A:692:A:H5'	1.95	0.48
1:A:818:G:OP1	17:d:14:LYS:CE	2.60	0.48
1:A:2013:U:H2'	1:A:2014:G:O4'	2.14	0.48
1:A:2879:G:H2'	1:A:2880:U:H6	1.77	0.48
6:L:92:THR:C	6:L:96:LEU:HD23	2.39	0.48
11:S:21:MET:SD	11:S:74:ALA:HB1	2.54	0.48
14:Z:6:ILE:HG22	14:Z:28:LEU:HD11	1.95	0.48
1:A:761:U:H2'	1:A:763:A:N7	2.28	0.48
1:A:2643:A:H4'	1:A:2644:U:H5	1.79	0.48
4:J:43:PRO:O	9:Q:101:ASN:OD1	2.31	0.48
1:A:292:U:H2'	1:A:293:U:C6	2.49	0.48
1:A:319:G:N3	1:A:326:A:N1	2.62	0.48
1:A:329:A:H2'	1:A:330:A:H8	1.79	0.48
1:A:1566:G:H2'	1:A:1567:U:O4'	2.13	0.48
1:A:1715:C:H2'	1:A:1716:U:O4'	2.14	0.48
1:A:2708:A:H2	2:D:191:ASN:HD22	1.62	0.48
2:D:126:HIS:CB	2:D:159:LEU:HD22	2.44	0.48
14:Z:35:VAL:HG12	14:Z:36:VAL:N	2.29	0.48
1:A:1660:C:C2'	11:S:92:ARG:NH2	2.64	0.48
1:A:291:C:H2'	1:A:292:U:C6	2.49	0.47
1:A:1727:A:H2'	1:A:1728:C:C6	2.49	0.47
6:L:1:MET:HE2	6:L:6:LEU:HA	1.96	0.47
6:L:89:THR:CA	6:L:121:LEU:HD22	2.41	0.47
1:A:285:U:H2'	1:A:286:U:C6	2.49	0.47
1:A:316:G:H2'	1:A:317:G:H8	1.79	0.47
1:A:793:U:H1'	1:A:799:A:N6	2.28	0.47
1:A:1160:G:H2'	1:A:1161:A:C8	2.48	0.47
1:A:1425:C:H2'	1:A:1426:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:28:LEU:HD23	14:Z:35:VAL:CG2	2.44	0.47
1:A:685:U:H2'	1:A:686:C:C6	2.49	0.47
1:A:696:C:H2'	1:A:697:G:H8	1.79	0.47
1:A:1103:A:C8	1:A:1132:A:H2'	2.48	0.47
1:A:1660:C:H6	11:S:92:ARG:HH21	1.62	0.47
1:A:2690:G:H3'	1:A:2691:A:C8	2.50	0.47
4:J:6:MET:HE2	4:J:6:MET:H	1.79	0.47
1:A:179:A:O3'	1:A:180:G:H8	1.98	0.47
1:A:787:C:H2'	1:A:788:G:C8	2.50	0.47
7:N:103:LYS:HB2	15:b:41:ARG:HD2	1.95	0.47
8:P:117:ARG:HB2	8:P:117:ARG:NH1	2.29	0.47
18:B:132:TYR:HD2	18:B:133:TYR:CD1	2.31	0.47
1:A:286:U:H3'	1:A:287:G:C8	2.49	0.47
1:A:767:U:H2'	1:A:768:G:C8	2.50	0.47
1:A:1088:G:N1	1:A:1159:U:N3	2.62	0.47
1:A:1580:A:H62	1:A:1586:G:N2	2.12	0.47
1:A:2090:G:N2	1:A:2636:G:H22	2.12	0.47
8:P:30:ARG:NH1	8:P:88:GLU:OE2	2.47	0.47
1:A:662:U:H2'	1:A:663:G:H8	1.79	0.47
1:A:860:U:H2'	1:A:861:C:C6	2.49	0.47
1:A:2703:G:H2'	1:A:2704:A:H8	1.80	0.47
3:E:42:ALA:C	3:E:44:LEU:H	2.23	0.47
7:N:22:THR:O	7:N:26:ILE:HG12	2.15	0.47
11:S:10:VAL:HG11	11:S:46:ILE:HG21	1.97	0.47
12:T:5:ARG:HD3	16:Y:26:PHE:HB2	1.96	0.47
1:A:215:G:H2'	1:A:216:A:O4'	2.14	0.47
1:A:282:G:HO2'	1:A:283:G:H8	1.61	0.47
1:A:286:U:H2'	1:A:287:G:O4'	2.15	0.47
1:A:971:A:H2'	1:A:972:U:N3	2.29	0.47
1:A:2639:C:H2'	1:A:2640:C:C2	2.49	0.47
4:J:25:THR:HB	4:J:28:ARG:HG3	1.97	0.47
5:K:18:GLU:OE1	5:K:44:LYS:HB2	2.15	0.47
14:Z:28:LEU:HD23	14:Z:35:VAL:HG23	1.95	0.47
1:A:287:G:H3'	1:A:288:C:C6	2.48	0.47
1:A:971:A:H2'	1:A:972:U:C4	2.49	0.47
1:A:1019:A:OP1	1:A:1019:A:H8	1.98	0.47
1:A:1349:G:H1'	1:A:1656:C:H5''	1.97	0.47
1:A:268:A:H2'	1:A:269:G:C4'	2.44	0.47
10:R:25:LEU:O	10:R:25:LEU:CG	2.58	0.47
12:T:40:LYS:O	12:T:44:GLU:HG2	2.14	0.47
1:A:183:A:H5''	1:A:482:C:H1'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:A:N6	6:L:112:LEU:HD23	2.30	0.47
1:A:275:A:H2	1:A:305:A:H4'	1.79	0.46
1:A:350:U:H2'	1:A:351:G:O4'	2.16	0.46
1:A:982:U:H2'	1:A:983:U:C6	2.50	0.46
1:A:1541:A:H2'	1:A:1542:A:C8	2.51	0.46
9:Q:103:LEU:HD23	10:R:2:TYR:OH	2.13	0.46
18:B:141:ALA:HB2	18:B:171:LEU:HD11	1.95	0.46
1:A:316:G:H2'	1:A:317:G:C8	2.50	0.46
1:A:610:U:H5''	6:L:29:LYS:HD2	1.95	0.46
1:A:1673:G:H2'	1:A:1674:G:H8	1.80	0.46
13:U:24:LEU:HD11	13:U:36:GLU:HB3	1.98	0.46
1:A:379:C:H4'	13:U:69:MET:SD	2.55	0.46
1:A:1523:U:H5''	1:A:1524:A:C8	2.51	0.46
1:A:2431:U:H4'	1:A:2432:C:H5	1.80	0.46
10:R:2:TYR:CD1	10:R:13:LYS:HE2	2.51	0.46
1:A:403:C:H2'	1:A:404:C:H6	1.80	0.46
1:A:576:G:N3	1:A:576:G:H2'	2.31	0.46
1:A:617:G:N2	1:A:2060:A:H5''	2.31	0.46
1:A:1795:C:H2'	1:A:1796:C:C6	2.50	0.46
1:A:2031:G:H2'	1:A:2032:A:H8	1.81	0.46
5:K:52:VAL:C	5:K:53:LYS:HE2	2.40	0.46
13:U:40:MET:HE3	13:U:40:MET:HB3	1.83	0.46
1:A:282:G:O2'	1:A:283:G:H8	1.98	0.46
1:A:664:C:O2'	1:A:665:G:C8	2.66	0.46
6:L:118:GLU:C	6:L:119:LYS:HG2	2.38	0.46
7:N:100:ARG:HG2	7:N:120:VAL:HG12	1.98	0.46
1:A:351:G:H21	1:A:374:A:H62	1.64	0.46
1:A:1087:U:O2	1:A:1160:G:C6	2.68	0.46
1:A:296:G:H2'	1:A:297:G:C4	2.51	0.46
1:A:1503:G:O6	1:A:2731:G:O6	2.33	0.46
1:A:1558:C:H2'	1:A:1559:C:C6	2.51	0.46
1:A:2666:U:H2'	1:A:2667:G:O4'	2.15	0.46
16:Y:2:LYS:HE3	16:Y:2:LYS:HB3	1.74	0.46
13:U:9:VAL:HB	13:U:68:VAL:HG22	1.97	0.46
1:A:78:U:H2'	1:A:79:C:C6	2.51	0.46
1:A:1392:A:H2'	1:A:1393:A:C8	2.51	0.46
1:A:1555:A:C4	1:A:1556:A:C8	3.04	0.46
16:Y:9:LEU:CD1	16:Y:9:LEU:H	2.29	0.46
1:A:229:A:H1'	1:A:231:A:H61	1.80	0.45
1:A:621:G:H2'	1:A:622:A:C8	2.51	0.45
1:A:1553:A:N3	1:A:1553:A:H2'	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:90:VAL:HG12	8:P:91:ARG:HG3	1.99	0.45
10:R:5:ILE:HD11	10:R:58:VAL:HG21	1.98	0.45
15:b:43:CYS:O	15:b:46:CYS:HB2	2.16	0.45
1:A:427:G:H8	1:A:427:G:OP2	2.00	0.45
1:A:848:G:H8	3:E:55:SER:HB3	1.81	0.45
1:A:1002:G:H2'	1:A:1008:A:N6	2.32	0.45
1:A:1453:A:H2'	1:A:1454:C:C6	2.50	0.45
1:A:2796:C:H2'	1:A:2797:C:H6	1.81	0.45
1:A:306:C:H2'	1:A:307:A:C8	2.51	0.45
1:A:340:U:H2'	1:A:341:G:O4'	2.16	0.45
1:A:971:A:H2'	1:A:972:U:C2	2.51	0.45
1:A:2090:G:H21	1:A:2636:G:H22	1.64	0.45
5:K:56:GLU:OE1	5:K:56:GLU:N	2.48	0.45
10:R:101:ASN:O	10:R:102:ALA:C	2.59	0.45
1:A:352:G:O2'	13:U:15:LYS:HE3	2.17	0.45
1:A:688:G:H22	1:A:691:U:P	2.38	0.45
1:A:848:G:C8	3:E:55:SER:HB3	2.51	0.45
8:P:47:GLU:OE2	8:P:47:GLU:N	2.49	0.45
7:N:102:MET:HB3	15:b:42:VAL:CG1	2.37	0.45
1:A:686:C:H2'	1:A:687:U:C6	2.52	0.45
1:A:803:C:H2'	1:A:804:G:C8	2.52	0.45
1:A:854:U:H2'	1:A:855:G:C8	2.52	0.45
8:P:39:ASN:OD1	8:P:40:ARG:N	2.50	0.45
8:P:46:PHE:CZ	8:P:66:LYS:HG2	2.52	0.45
1:A:1767:A:H2'	1:A:1768:A:C8	2.51	0.45
1:A:2641:C:H3'	1:A:2642:U:C4'	2.45	0.45
5:K:63:VAL:HG22	5:K:106:LEU:HD11	1.98	0.45
7:N:22:THR:HG21	7:N:67:ARG:HB2	1.98	0.45
1:A:275:A:N6	1:A:296:G:C2	2.84	0.45
1:A:306:C:H2'	1:A:307:A:H8	1.81	0.45
1:A:430:C:H1'	1:A:438:A:N6	2.27	0.45
1:A:751:G:H1'	1:A:774:A:H61	1.82	0.45
1:A:966:U:H2'	1:A:967:G:O4'	2.16	0.45
3:E:40:GLN:NE2	3:E:184:LEU:HB2	2.32	0.45
1:A:3:U:H2'	1:A:4:U:C6	2.52	0.45
1:A:154:A:H2'	1:A:155:U:C6	2.52	0.45
1:A:428:A:O5'	1:A:428:A:H8	1.99	0.45
1:A:1681:U:H2'	1:A:1682:C:C6	2.52	0.45
7:N:29:ARG:O	7:N:30:ILE:HD13	2.17	0.45
14:Z:31:THR:HG22	14:Z:32:ASN:OD1	2.17	0.45
1:A:225:A:H61	1:A:235:G:H1'	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:A:H3'	1:A:763:A:C8	2.52	0.45
10:R:16:GLU:HG2	10:R:100:ILE:HG12	1.98	0.45
16:Y:16:GLN:HA	16:Y:19:LYS:HE2	1.99	0.45
1:A:200:A:H3'	1:A:201:C:C6	2.52	0.44
1:A:446:G:H3'	1:A:447:G:C8	2.52	0.44
1:A:545:U:H2'	1:A:546:G:O4'	2.17	0.44
1:A:898:U:O2	14:Z:42:ALA:HB1	2.17	0.44
1:A:1002:G:N2	1:A:1006:A:H62	2.15	0.44
1:A:1008:A:C8	1:A:1009:U:C5	3.06	0.44
1:A:2442:G:N3	1:A:2442:G:H2'	2.31	0.44
12:T:15:GLU:OE2	12:T:15:GLU:N	2.50	0.44
1:A:662:U:H2'	1:A:663:G:C8	2.52	0.44
1:A:1094:A:H1'	1:A:1158:G:H21	1.81	0.44
1:A:1240:U:H1'	9:Q:4:VAL:HG22	1.98	0.44
1:A:1331:C:H2'	1:A:1332:U:C6	2.52	0.44
1:A:2863:G:C4	1:A:2864:G:C8	3.06	0.44
1:A:2921:U:H2'	1:A:2922:U:C6	2.52	0.44
12:T:83:LEU:HD11	12:T:89:GLU:HG3	1.98	0.44
1:A:32:C:O2'	1:A:33:U:H5'	2.17	0.44
1:A:1222:A:H2'	1:A:1223:C:C6	2.52	0.44
1:A:1754:U:H2'	1:A:1755:C:C6	2.52	0.44
1:A:2426:G:H2'	1:A:2427:U:O4'	2.18	0.44
5:K:19:VAL:HB	5:K:41:CYS:HB3	1.98	0.44
5:K:105:GLU:OE2	5:K:105:GLU:N	2.50	0.44
1:A:275:A:C2	1:A:305:A:H4'	2.52	0.44
1:A:640:U:H2'	1:A:641:C:C6	2.53	0.44
1:A:902:G:C2	1:A:970:A:C2	3.05	0.44
1:A:1111:U:H2'	1:A:1112:U:C6	2.52	0.44
1:A:1513:U:H2'	1:A:1514:C:C6	2.52	0.44
6:L:118:GLU:O	6:L:119:LYS:CD	2.66	0.44
1:A:247:A:H2'	1:A:248:G:O4'	2.17	0.44
1:A:296:G:H2'	1:A:297:G:C5	2.52	0.44
1:A:690:A:H2'	1:A:692:A:C8	2.53	0.44
1:A:1530:G:H2'	1:A:1531:G:H8	1.82	0.44
4:J:6:MET:SD	4:J:6:MET:N	2.91	0.44
13:U:87:ASP:O	13:U:89:LYS:HG2	2.18	0.44
1:A:162:A:N6	1:A:167:U:H1'	2.32	0.44
1:A:576:G:H4'	1:A:577:U:OP2	2.18	0.44
1:A:1009:U:H2'	1:A:1010:C:C6	2.53	0.44
1:A:1106:U:H1'	1:A:1134:A:C8	2.53	0.44
1:A:1128:U:H2'	1:A:1129:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1327:U:H2'	1:A:1327:U:O2	2.17	0.44
1:A:2080:A:N6	1:A:2642:U:O2'	2.51	0.44
1:A:224:A:Cl'	1:A:236:A:H1'	2.46	0.44
1:A:896:A:H2'	1:A:897:G:C8	2.50	0.44
1:A:907:U:H2'	1:A:908:A:H4'	1.98	0.44
1:A:1328:C:H2'	1:A:1329:C:H6	1.83	0.44
3:E:64:PRO:O	3:E:65:TRP:HB2	2.17	0.44
13:U:12:ILE:HD11	13:U:78:VAL:HG11	1.98	0.44
15:b:36:MET:HE3	15:b:36:MET:HB3	1.93	0.44
1:A:427:G:N2	1:A:428:A:H1'	2.32	0.44
1:A:873:U:C4	1:A:875:U:H1'	2.53	0.44
1:A:1160:G:H2'	1:A:1161:A:H8	1.81	0.44
1:A:2640:C:H2'	1:A:2641:C:C6	2.52	0.44
6:L:89:THR:C	6:L:121:LEU:CD2	2.90	0.44
6:L:96:LEU:HB3	6:L:102:ILE:HG21	1.98	0.44
6:L:113:GLY:HA3	6:L:131:SER:HB2	1.99	0.44
1:A:677:A:H2'	1:A:678:A:O4'	2.18	0.44
1:A:1013:U:H2'	1:A:1014:A:C8	2.52	0.44
1:A:1213:G:H2'	1:A:1214:U:C6	2.52	0.44
1:A:1537:G:C6	1:A:1546:G:C6	3.05	0.44
1:A:1774:A:H3'	1:A:1775:G:H8	1.83	0.44
1:A:2704:A:H61	1:A:2761:G:H1	1.64	0.44
10:R:93:THR:HG22	10:R:95:VAL:HG23	2.00	0.44
16:Y:1:MET:HE3	16:Y:53:MET:HE1	1.99	0.44
1:A:1496:G:N2	1:A:1507:U:O2	2.26	0.43
6:L:121:LEU:HD13	6:L:122:THR:CA	2.48	0.43
8:P:83:LYS:HE3	8:P:83:LYS:HB3	1.70	0.43
1:A:771:U:H2'	1:A:772:G:O4'	2.18	0.43
8:P:61:THR:HG22	8:P:78:PRO:HA	2.00	0.43
12:T:5:ARG:HG3	12:T:5:ARG:HH11	1.84	0.43
1:A:178:A:O2'	1:A:179:A:C8	2.67	0.43
1:A:2825:C:H5''	1:A:2826:A:N7	2.34	0.43
5:K:44:LYS:HB3	5:K:45:GLN:OE1	2.18	0.43
15:b:43:CYS:HB3	15:b:46:CYS:HB2	1.54	0.43
1:A:968:C:H2'	1:A:969:C:H6	1.83	0.43
1:A:1131:A:H2'	1:A:1132:A:C8	2.54	0.43
1:A:1199:C:H2'	1:A:1200:G:O4'	2.18	0.43
1:A:1513:U:H5	1:A:1594:G:H2'	1.83	0.43
9:Q:74:LEU:HD11	9:Q:114:LYS:HG3	2.00	0.43
1:A:1081:U:H2'	1:A:1082:G:H8	1.84	0.43
1:A:1112:U:H3'	1:A:1113:A:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1349:G:N2	1:A:1352:U:C4	2.87	0.43
15:b:30:CYS:SG	15:b:35:GLU:N	2.91	0.43
1:A:499:G:C5	3:E:58:ARG:NH2	2.86	0.43
1:A:1018:G:H3'	1:A:1019:A:H5''	2.01	0.43
1:A:2845:A:C6	2:D:197:LYS:HD2	2.53	0.43
2:D:22:LEU:HD23	2:D:22:LEU:HA	1.76	0.43
3:E:139:MET:HA	3:E:139:MET:HE2	2.01	0.43
9:Q:81:HIS:C	9:Q:85:LEU:HD13	2.33	0.43
9:Q:81:HIS:CE1	9:Q:85:LEU:HD21	2.53	0.43
1:A:12:A:OP2	1:A:12:A:H8	2.02	0.43
1:A:1244:A:C8	6:L:4:HIS:HB3	2.50	0.43
1:A:1685:A:H2'	1:A:1686:A:H8	1.84	0.43
1:A:2039:G:H5''	11:S:42:ALA:HB2	1.99	0.43
4:J:29:LEU:HD13	4:J:143:LEU:HD11	2.01	0.43
6:L:126:ASN:OD1	6:L:126:ASN:C	2.62	0.43
12:T:21:MET:HE3	12:T:21:MET:HB2	1.73	0.43
1:A:106:G:H1'	1:A:337:A:C8	2.51	0.43
1:A:304:G:H2'	1:A:305:A:O4'	2.19	0.43
1:A:398:U:H2'	1:A:399:C:C6	2.54	0.43
1:A:441:C:H2'	1:A:442:C:O4'	2.18	0.43
1:A:1106:U:H1'	1:A:1134:A:H8	1.83	0.43
14:Z:2:ALA:HA	14:Z:39:ASP:HB2	2.00	0.43
18:B:66:ILE:CG2	18:B:69:ASP:OD1	2.62	0.43
1:A:875:U:H2'	1:A:876:A:N3	2.34	0.43
1:A:970:A:H2'	1:A:971:A:C8	2.54	0.43
1:A:972:U:O2'	1:A:973:G:H5''	2.18	0.43
1:A:1345:U:O2'	1:A:1346:A:H5''	2.19	0.43
1:A:1409:C:H2'	1:A:1410:G:O4'	2.19	0.43
1:A:1695:A:H2'	1:A:1696:G:H5'	2.01	0.43
1:A:2439:G:H2'	1:A:2439:G:N3	2.33	0.43
1:A:2643:A:H5'	15:b:2:ALA:HB1	2.00	0.43
8:P:6:LYS:HA	8:P:9:GLU:HG2	2.01	0.43
18:B:94:ARG:O	18:B:98:THR:HG23	2.18	0.43
1:A:2909:U:H2'	1:A:2910:C:O4'	2.18	0.43
3:E:66:ARG:HG3	3:E:74:ARG:CZ	2.49	0.43
5:K:90:ASP:OD1	5:K:90:ASP:C	2.62	0.43
8:P:29:LEU:CD2	8:P:89:VAL:HG22	2.49	0.43
18:B:163:LEU:HD23	18:B:163:LEU:HA	1.87	0.43
1:A:326:A:H2	1:A:402:U:H1'	1.84	0.42
1:A:1000:G:N2	1:A:1011:C:H1'	2.34	0.42
1:A:1080:G:H2'	1:A:1081:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:A:H2'	1:A:1312:A:N3	2.34	0.42
3:E:6:LEU:CD2	3:E:13:THR:HG21	2.49	0.42
1:A:77:U:H2'	1:A:78:U:C6	2.54	0.42
1:A:89:U:H2'	1:A:90:A:C8	2.53	0.42
1:A:140:A:H2'	1:A:141:U:H6	1.83	0.42
1:A:156:A:H2'	1:A:157:U:C6	2.54	0.42
1:A:623:A:H2'	1:A:624:C:C6	2.54	0.42
1:A:1097:A:HO2'	1:A:1098:C:H6	1.64	0.42
1:A:1542:A:H2'	1:A:1544:C:C5	2.54	0.42
1:A:2889:A:H2'	1:A:2890:U:C6	2.54	0.42
3:E:8:ASN:HB3	3:E:10:ASN:OD1	2.19	0.42
8:P:36:VAL:O	8:P:36:VAL:CG1	2.57	0.42
1:A:65:A:H2'	1:A:66:C:H6	1.85	0.42
1:A:409:U:C2	1:A:410:G:C8	3.07	0.42
1:A:450:U:H5''	1:A:453:G:H4'	2.01	0.42
1:A:972:U:C2	1:A:973:G:C8	3.07	0.42
1:A:1547:U:H2'	1:A:1548:U:H6	1.84	0.42
1:A:1799:G:N3	1:A:1799:G:H2'	2.34	0.42
1:A:2773:G:H5''	1:A:2784:C:H41	1.84	0.42
3:E:201:LYS:HE3	3:E:201:LYS:HB2	1.91	0.42
10:R:15:GLU:OE1	10:R:16:GLU:HG3	2.19	0.42
1:A:1004:U:C3'	1:A:1005:A:H5''	2.46	0.42
1:A:1146:C:H2'	1:A:1147:U:O4'	2.19	0.42
1:A:1173:A:O2'	1:A:1174:A:H5'	2.19	0.42
1:A:1477:A:H2'	1:A:1478:G:C8	2.54	0.42
1:A:1797:A:H2'	1:A:1798:G:C8	2.54	0.42
7:N:44:VAL:O	7:N:48:ILE:HG13	2.19	0.42
9:Q:58:ARG:NH2	9:Q:93:LYS:HE2	2.33	0.42
1:A:1457:U:H3'	1:A:1459:U:C5	2.54	0.42
1:A:2641:C:H3'	1:A:2642:U:O4'	2.20	0.42
7:N:103:LYS:O	15:b:42:VAL:HG22	2.20	0.42
9:Q:92:ARG:HG2	9:Q:93:LYS:H	1.85	0.42
12:T:19:ASP:OD2	12:T:19:ASP:C	2.62	0.42
1:A:77:U:H2'	1:A:78:U:H6	1.84	0.42
1:A:78:U:H2'	1:A:79:C:H6	1.83	0.42
1:A:132:C:H2'	1:A:133:A:H8	1.84	0.42
1:A:695:G:H2'	1:A:696:C:C6	2.55	0.42
1:A:1178:U:OP2	1:A:1179:A:H2'	2.19	0.42
3:E:78:ILE:HG13	3:E:79:ARG:HG2	2.02	0.42
13:U:46:LYS:HD2	13:U:47:PRO:HD2	2.00	0.42
1:A:187:C:O2'	1:A:188:C:H6	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:C:H2'	1:A:982:U:H6	1.85	0.42
1:A:1410:G:OP1	18:B:47:LYS:HG2	2.19	0.42
1:A:1721:A:C6	1:A:1722:A:C6	3.07	0.42
1:A:1798:G:H5'	1:A:1799:G:OP2	2.20	0.42
1:A:2864:G:C5	1:A:2865:U:C5	3.07	0.42
3:E:63:LYS:O	3:E:74:ARG:CZ	2.67	0.42
6:L:94:GLU:HG2	6:L:98:GLU:CG	2.49	0.42
11:S:95:GLN:HG2	11:S:95:GLN:O	2.19	0.42
1:A:157:U:H2'	1:A:158:C:C6	2.55	0.42
1:A:159:U:H3'	1:A:160:G:C8	2.39	0.42
1:A:285:U:H2'	1:A:286:U:C5	2.55	0.42
1:A:300:G:H2'	1:A:468:C:OP2	2.19	0.42
2:D:88:MET:HA	2:D:88:MET:HE2	2.02	0.42
6:L:94:GLU:O	6:L:95:LEU:C	2.62	0.42
6:L:131:SER:HA	6:L:134:GLU:HG3	2.02	0.42
15:b:33:CYS:SG	15:b:34:GLY:N	2.92	0.42
1:A:159:U:H5'	1:A:160:G:OP2	2.20	0.42
1:A:676:G:O2'	1:A:686:C:H4'	2.20	0.42
1:A:755:U:H2'	1:A:756:U:H6	1.83	0.42
1:A:1177:G:H4'	4:J:85:LEU:HD22	2.02	0.42
3:E:66:ARG:HG2	3:E:74:ARG:HD3	2.02	0.42
1:A:219:A:N7	1:A:478:U:H5	2.17	0.42
1:A:290:U:C6	1:A:291:C:H5	2.38	0.42
6:L:1:MET:HE2	6:L:7:LYS:H	1.85	0.42
9:Q:58:ARG:HA	9:Q:61:TRP:CE3	2.55	0.42
13:U:88:GLY:O	13:U:89:LYS:CD	2.66	0.42
1:A:329:A:H2'	1:A:330:A:C8	2.54	0.41
1:A:669:C:H2'	1:A:670:C:C6	2.55	0.41
1:A:1721:A:H2'	1:A:1722:A:C8	2.55	0.41
1:A:1726:G:H5''	1:A:1727:A:C5'	2.45	0.41
1:A:2659:G:H2'	1:A:2660:G:C8	2.54	0.41
8:P:40:ARG:HG3	8:P:40:ARG:O	2.20	0.41
1:A:281:A:O2'	1:A:282:G:H8	1.83	0.41
1:A:652:A:H2'	1:A:653:A:C8	2.54	0.41
1:A:2088:A:H1'	1:A:2637:G:H1	1.84	0.41
2:D:12:MET:O	2:D:13:THR:CG2	2.68	0.41
7:N:8:ARG:HB3	7:N:12:GLN:HB2	2.02	0.41
1:A:171:A:H2'	1:A:172:U:C6	2.55	0.41
1:A:448:A:H2'	1:A:449:A:O4'	2.20	0.41
1:A:716:G:N3	1:A:716:G:H2'	2.35	0.41
1:A:1161:A:H2'	1:A:1162:C:C6	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2089:A:H1'	1:A:2090:G:C8	2.55	0.41
1:A:2727:U:H2'	1:A:2728:U:H6	1.85	0.41
2:D:31:ALA:O	2:D:32:PRO:C	2.62	0.41
2:D:113:VAL:O	2:D:194:GLY:HA2	2.20	0.41
4:J:20:ASP:OD1	4:J:20:ASP:C	2.64	0.41
6:L:35:HIS:ND1	6:L:36:LYS:HG3	2.36	0.41
16:Y:15:GLU:H	16:Y:15:GLU:HG2	1.72	0.41
1:A:153:C:H2'	1:A:154:A:H8	1.85	0.41
1:A:1061:A:H2'	1:A:1062:C:C6	2.56	0.41
1:A:2695:C:H2'	1:A:2696:C:O4'	2.19	0.41
4:J:102:LEU:HD23	4:J:102:LEU:HA	1.94	0.41
17:d:35:ARG:HG3	17:d:42:LEU:HD21	2.03	0.41
18:B:140:ILE:HD13	18:B:172:ILE:HB	2.00	0.41
1:A:186:C:H2'	1:A:187:C:H5'	2.03	0.41
1:A:1180:C:H6	1:A:1180:C:H2'	1.72	0.41
1:A:2635:C:H1'	1:A:2636:G:C4	2.56	0.41
1:A:2922:U:H2'	1:A:2923:A:C8	2.56	0.41
5:K:18:GLU:OE1	5:K:18:GLU:C	2.64	0.41
10:R:22:ILE:HG22	10:R:23:GLU:H	1.85	0.41
18:B:174:PHE:HE1	18:B:182:LYS:HA	1.85	0.41
1:A:160:G:C2	1:A:167:U:C5	3.09	0.41
1:A:401:C:H2'	1:A:402:U:C6	2.56	0.41
1:A:460:C:C2	1:A:461:C:C5	3.08	0.41
1:A:1511:C:H2'	1:A:1512:G:O4'	2.20	0.41
1:A:1685:A:H2'	1:A:1686:A:C8	2.55	0.41
1:A:1747:G:H2'	1:A:1748:G:C8	2.56	0.41
6:L:79:LEU:HD22	6:L:117:LEU:CD2	2.51	0.41
8:P:51:ILE:HD11	8:P:103:LEU:HD11	2.03	0.41
8:P:109:LYS:H	8:P:109:LYS:CD	2.31	0.41
18:B:3:VAL:HA	18:B:68:ASN:ND2	2.36	0.41
18:B:136:PRO:HB2	18:B:192:MET:SD	2.60	0.41
1:A:793:U:H5''	1:A:1660:C:C5	2.54	0.41
1:A:2645:C:H2'	1:A:2646:C:H6	1.86	0.41
2:D:12:MET:O	2:D:13:THR:HG23	2.20	0.41
1:A:200:A:H3'	1:A:201:C:H6	1.85	0.41
1:A:299:U:OP1	1:A:299:U:H4'	2.19	0.41
1:A:492:C:H2'	1:A:493:G:O4'	2.21	0.41
1:A:688:G:H22	1:A:690:A:H3'	1.85	0.41
1:A:897:G:H2'	1:A:898:U:C6	2.55	0.41
1:A:970:A:H2'	1:A:971:A:O4'	2.20	0.41
1:A:2054:C:H2'	1:A:2055:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2774:C:H2'	1:A:2775:U:C6	2.56	0.41
1:A:2774:C:H2'	1:A:2775:U:H6	1.86	0.41
5:K:22:ILE:HG22	5:K:23:LYS:HG3	2.02	0.41
18:B:46:ARG:HA	18:B:46:ARG:HD2	1.92	0.41
1:A:295:G:C6	1:A:296:G:C5	3.08	0.41
1:A:364:A:H4'	1:A:366:A:N7	2.36	0.41
1:A:398:U:H2'	1:A:399:C:H6	1.86	0.41
1:A:902:G:C2	1:A:903:G:C4	3.09	0.41
1:A:981:C:H2'	1:A:982:U:C6	2.56	0.41
1:A:1312:A:H1'	1:A:1663:A:N6	2.36	0.41
1:A:1530:G:H2'	1:A:1531:G:C8	2.56	0.41
1:A:2796:C:H2'	1:A:2797:C:C6	2.55	0.41
1:A:2834:A:H2'	1:A:2835:A:C8	2.56	0.41
2:D:55:ASP:HA	2:D:77:LYS:HA	2.03	0.41
8:P:95:VAL:HG11	8:P:100:LEU:HD21	2.02	0.41
9:Q:84:LYS:HA	9:Q:89:GLU:OE2	2.19	0.41
18:B:43:LEU:HD23	18:B:43:LEU:HA	1.84	0.41
1:A:982:U:H2'	1:A:983:U:H6	1.86	0.41
1:A:1475:G:H2'	1:A:1476:C:C6	2.56	0.41
1:A:1723:A:C6	1:A:1724:A:C6	3.09	0.41
1:A:1759:U:H2'	1:A:1760:A:C8	2.55	0.41
1:A:1784:A:O2'	1:A:1785:G:H5'	2.21	0.41
10:R:25:LEU:O	10:R:26:ALA:C	2.64	0.41
14:Z:50:VAL:O	14:Z:54:VAL:HG12	2.21	0.41
1:A:224:A:H5''	1:A:225:A:OP1	2.21	0.40
1:A:275:A:N3	1:A:275:A:H2'	2.35	0.40
1:A:449:A:H2'	1:A:450:U:O4'	2.21	0.40
1:A:633:U:H2'	1:A:634:A:H8	1.86	0.40
1:A:1359:G:H22	1:A:1370:C:H42	1.66	0.40
1:A:1754:U:H2'	1:A:1755:C:H6	1.86	0.40
2:D:126:HIS:CD2	2:D:126:HIS:N	2.90	0.40
7:N:104:LEU:HD11	7:N:116:ILE:HG12	2.02	0.40
9:Q:106:PHE:O	9:Q:107:ASN:C	2.64	0.40
11:S:21:MET:HE3	11:S:103:ILE:HG23	2.03	0.40
1:A:339:A:H2'	1:A:340:U:C6	2.56	0.40
1:A:344:G:C2	1:A:346:G:C8	3.09	0.40
1:A:579:G:H2'	1:A:580:U:C6	2.56	0.40
1:A:1320:G:H2'	1:A:1321:U:C6	2.56	0.40
1:A:1617:A:H2'	1:A:1618:A:C8	2.56	0.40
1:A:1662:C:H2'	1:A:1663:A:H3'	2.03	0.40
6:L:82:LEU:HA	6:L:85:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:14:ILE:O	16:Y:15:GLU:C	2.64	0.40
18:B:11:SER:HA	18:B:62:LEU:O	2.21	0.40
1:A:685:U:H2'	1:A:686:C:H6	1.87	0.40
1:A:1355:U:H2'	1:A:1356:G:H8	1.87	0.40
1:A:1504:A:H4'	1:A:1505:U:O4'	2.21	0.40
16:Y:3:ALA:O	16:Y:4:ASN:C	2.62	0.40
1:A:558:G:OP1	1:A:1275:G:H5'	2.21	0.40
1:A:2676:U:H3	1:A:2702:G:H1	1.69	0.40
1:A:2818:C:H4'	1:A:2819:A:OP1	2.21	0.40
2:D:99:VAL:HG13	2:D:186:LEU:HG	2.04	0.40
3:E:165:LEU:HD23	3:E:165:LEU:HA	1.81	0.40
14:Z:42:ALA:O	14:Z:46:MET:HG2	2.21	0.40
1:A:674:G:H2'	1:A:675:C:C6	2.57	0.40
1:A:1549:U:H2'	1:A:1550:C:C6	2.55	0.40
1:A:1673:G:H2'	1:A:1674:G:C8	2.56	0.40
1:A:2691:A:H2'	1:A:2692:G:O4'	2.21	0.40
2:D:12:MET:C	2:D:13:THR:HG23	2.47	0.40
4:J:22:ALA:HA	4:J:62:LYS:HB2	2.03	0.40
6:L:89:THR:C	6:L:121:LEU:HD22	2.47	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	D	173/209 (83%)	165 (95%)	8 (5%)	0	100	100
3	E	197/207 (95%)	184 (93%)	12 (6%)	1 (0%)	24	43
4	J	140/145 (97%)	130 (93%)	10 (7%)	0	100	100
5	K	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
6	L	114/146 (78%)	95 (83%)	18 (16%)	1 (1%)	14	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	N	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
8	P	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
9	Q	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
10	R	99/102 (97%)	84 (85%)	13 (13%)	2 (2%)	6	10
11	S	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
12	T	91/95 (96%)	85 (93%)	6 (7%)	0	100	100
13	U	98/103 (95%)	92 (94%)	5 (5%)	1 (1%)	12	24
14	Z	56/59 (95%)	56 (100%)	0	0	100	100
15	b	43/59 (73%)	37 (86%)	5 (12%)	1 (2%)	5	8
16	Y	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
17	d	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	B	193/195 (99%)	183 (95%)	10 (5%)	0	100	100
All	All	1880/2018 (93%)	1744 (93%)	130 (7%)	6 (0%)	37	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	65	TRP
6	L	87	GLU
10	R	51	PRO
15	b	45	ALA
10	R	100	ILE
13	U	86	GLU

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	D	143/170 (84%)	143 (100%)	0	100	100
3	E	167/170 (98%)	166 (99%)	1 (1%)	78	91
4	J	120/123 (98%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	K	101/101 (100%)	101 (100%)	0	100	100
6	L	90/110 (82%)	89 (99%)	1 (1%)	65	84
7	N	99/100 (99%)	99 (100%)	0	100	100
8	P	99/100 (99%)	99 (100%)	0	100	100
9	Q	96/97 (99%)	96 (100%)	0	100	100
10	R	83/84 (99%)	82 (99%)	1 (1%)	63	83
11	S	90/93 (97%)	90 (100%)	0	100	100
12	T	84/85 (99%)	84 (100%)	0	100	100
13	U	84/87 (97%)	84 (100%)	0	100	100
14	Z	52/53 (98%)	52 (100%)	0	100	100
15	b	41/53 (77%)	39 (95%)	2 (5%)	22	45
16	Y	56/57 (98%)	54 (96%)	2 (4%)	31	58
17	d	39/39 (100%)	39 (100%)	0	100	100
18	B	170/170 (100%)	170 (100%)	0	100	100
All	All	1614/1692 (95%)	1607 (100%)	7 (0%)	81	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	67	GLN
6	L	121	LEU
10	R	51	PRO
15	b	33	CYS
15	b	43	CYS
16	Y	61	GLU
16	Y	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	191	ASN
4	J	8	ASN
6	L	27	ASN
6	L	68	ASN
7	N	27	ASN
8	P	15	GLN

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Mol	Chain	Res	Type
9	Q	81	HIS
10	R	81	ASN
10	R	88	HIS
14	Z	19	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2109/2927 (72%)	579 (27%)	49 (2%)

All (579) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	12	A
1	A	13	A
1	A	15	G
1	A	28	A
1	A	31	C
1	A	34	U
1	A	44	A
1	A	46	C
1	A	51	G
1	A	55	G
1	A	60	G
1	A	71	A
1	A	75	G
1	A	90	A
1	A	91	A
1	A	92	G
1	A	93	C
1	A	100	U
1	A	109	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	124	A
1	A	127	C
1	A	130	A
1	A	156	A

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Mol	Chain	Res	Type
1	A	157	U
1	A	158	C
1	A	159	U
1	A	161	A
1	A	162	A
1	A	163	U
1	A	164	U
1	A	173	A
1	A	175	G
1	A	176	A
1	A	177	G
1	A	178	A
1	A	179	A
1	A	180	G
1	A	184	G
1	A	188	C
1	A	199	A
1	A	202	A
1	A	203	U
1	A	216	A
1	A	219	A
1	A	221	G
1	A	222	A
1	A	224	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	230	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	234	C
1	A	235	G
1	A	245	G
1	A	250	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	258	A
1	A	267	C
1	A	268	A
1	A	272	C

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Mol	Chain	Res	Type
1	A	275	A
1	A	276	C
1	A	282	G
1	A	286	U
1	A	289	C
1	A	290	U
1	A	291	C
1	A	295	G
1	A	297	G
1	A	298	U
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	310	C
1	A	312	G
1	A	313	U
1	A	314	A
1	A	315	C
1	A	321	U
1	A	322	A
1	A	325	A
1	A	327	G
1	A	334	G
1	A	337	A
1	A	338	G
1	A	344	G
1	A	345	A
1	A	346	G
1	A	355	A
1	A	361	G
1	A	374	A
1	A	376	A
1	A	382	G
1	A	393	U
1	A	394	U
1	A	396	G
1	A	405	U
1	A	406	G
1	A	410	G
1	A	413	U
1	A	414	C

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Mol	Chain	Res	Type
1	A	418	A
1	A	419	G
1	A	420	U
1	A	422	C
1	A	424	G
1	A	425	C
1	A	426	G
1	A	427	G
1	A	428	A
1	A	429	A
1	A	430	C
1	A	438	A
1	A	439	U
1	A	440	U
1	A	441	C
1	A	443	G
1	A	444	U
1	A	446	G
1	A	448	A
1	A	451	C
1	A	452	C
1	A	453	G
1	A	454	G
1	A	456	A
1	A	458	G
1	A	459	A
1	A	460	C
1	A	461	C
1	A	463	U
1	A	466	C
1	A	468	C
1	A	482	C
1	A	487	G
1	A	502	C
1	A	504	A
1	A	528	G
1	A	550	G
1	A	551	A
1	A	554	U
1	A	555	C
1	A	558	G
1	A	568	G

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Mol	Chain	Res	Type
1	A	576	G
1	A	577	U
1	A	578	A
1	A	579	G
1	A	584	A
1	A	592	A
1	A	594	C
1	A	595	G
1	A	601	U
1	A	607	G
1	A	619	A
1	A	632	U
1	A	647	A
1	A	648	G
1	A	651	U
1	A	665	G
1	A	666	G
1	A	667	A
1	A	673	A
1	A	674	G
1	A	680	G
1	A	683	A
1	A	684	G
1	A	690	A
1	A	691	U
1	A	692	A
1	A	700	U
1	A	701	G
1	A	716	G
1	A	717	A
1	A	725	C
1	A	733	U
1	A	758	A
1	A	759	G
1	A	766	C
1	A	769	A
1	A	773	G
1	A	777	C
1	A	786	A
1	A	787	C
1	A	788	G
1	A	789	C

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Mol	Chain	Res	Type
1	A	790	A
1	A	791	C
1	A	792	G
1	A	793	U
1	A	800	G
1	A	801	U
1	A	803	C
1	A	804	G
1	A	818	G
1	A	821	A
1	A	822	G
1	A	823	G
1	A	827	G
1	A	828	A
1	A	829	A
1	A	830	A
1	A	831	U
1	A	832	G
1	A	833	C
1	A	836	A
1	A	837	U
1	A	838	C
1	A	839	G
1	A	840	A
1	A	841	A
1	A	849	A
1	A	852	G
1	A	857	U
1	A	858	U
1	A	859	C
1	A	866	A
1	A	870	A
1	A	874	U
1	A	875	U
1	A	876	A
1	A	877	G
1	A	878	G
1	A	892	U
1	A	900	U
1	A	902	G
1	A	903	G
1	A	904	A

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Mol	Chain	Res	Type
1	A	905	G
1	A	906	G
1	A	907	U
1	A	908	A
1	A	968	C
1	A	972	U
1	A	974	A
1	A	975	C
1	A	977	U
1	A	978	A
1	A	979	U
1	A	981	C
1	A	987	A
1	A	988	G
1	A	991	A
1	A	992	G
1	A	998	G
1	A	999	A
1	A	1000	G
1	A	1001	U
1	A	1002	G
1	A	1003	A
1	A	1004	U
1	A	1005	A
1	A	1006	A
1	A	1008	A
1	A	1009	U
1	A	1010	C
1	A	1012	G
1	A	1013	U
1	A	1019	A
1	A	1020	A
1	A	1037	C
1	A	1042	A
1	A	1045	U
1	A	1058	U
1	A	1059	A
1	A	1063	G
1	A	1068	G
1	A	1072	A
1	A	1073	A
1	A	1074	A

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Mol	Chain	Res	Type
1	A	1079	U
1	A	1091	U
1	A	1092	A
1	A	1093	G
1	A	1098	C
1	A	1100	A
1	A	1103	A
1	A	1104	U
1	A	1106	U
1	A	1107	U
1	A	1108	G
1	A	1111	U
1	A	1113	A
1	A	1114	G
1	A	1115	A
1	A	1116	A
1	A	1117	G
1	A	1118	C
1	A	1120	G
1	A	1121	C
1	A	1122	C
1	A	1123	A
1	A	1124	C
1	A	1125	C
1	A	1126	A
1	A	1128	U
1	A	1129	U
1	A	1130	A
1	A	1131	A
1	A	1133	G
1	A	1135	G
1	A	1136	U
1	A	1139	G
1	A	1141	A
1	A	1142	A
1	A	1150	C
1	A	1152	G
1	A	1158	G
1	A	1173	A
1	A	1174	A
1	A	1176	U
1	A	1178	U

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Mol	Chain	Res	Type
1	A	1179	A
1	A	1180	C
1	A	1181	C
1	A	1182	G
1	A	1185	G
1	A	1188	A
1	A	1201	A
1	A	1202	A
1	A	1218	U
1	A	1219	C
1	A	1220	G
1	A	1222	A
1	A	1247	G
1	A	1248	C
1	A	1252	G
1	A	1269	A
1	A	1271	U
1	A	1276	G
1	A	1278	G
1	A	1287	A
1	A	1289	U
1	A	1293	A
1	A	1296	G
1	A	1311	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G
1	A	1339	A
1	A	1340	A
1	A	1345	U
1	A	1346	A
1	A	1359	G
1	A	1362	G
1	A	1363	G
1	A	1364	C
1	A	1372	C
1	A	1375	A
1	A	1376	G
1	A	1377	G
1	A	1384	C
1	A	1388	A

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Mol	Chain	Res	Type
1	A	1391	U
1	A	1397	G
1	A	1403	G
1	A	1404	A
1	A	1405	A
1	A	1417	A
1	A	1418	U
1	A	1423	A
1	A	1424	A
1	A	1425	C
1	A	1434	A
1	A	1435	U
1	A	1436	U
1	A	1449	C
1	A	1450	C
1	A	1456	A
1	A	1458	U
1	A	1459	U
1	A	1460	G
1	A	1464	A
1	A	1465	A
1	A	1472	G
1	A	1473	A
1	A	1474	C
1	A	1483	A
1	A	1490	A
1	A	1496	G
1	A	1497	G
1	A	1498	U
1	A	1499	A
1	A	1501	U
1	A	1507	U
1	A	1513	U
1	A	1519	C
1	A	1520	A
1	A	1521	G
1	A	1524	A
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1533	A

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Mol	Chain	Res	Type
1	A	1534	A
1	A	1535	U
1	A	1536	A
1	A	1538	G
1	A	1539	C
1	A	1540	A
1	A	1546	G
1	A	1547	U
1	A	1549	U
1	A	1551	C
1	A	1553	A
1	A	1554	U
1	A	1555	A
1	A	1556	A
1	A	1558	C
1	A	1561	G
1	A	1562	A
1	A	1563	G
1	A	1571	G
1	A	1581	A
1	A	1582	U
1	A	1583	A
1	A	1586	G
1	A	1596	U
1	A	1606	A
1	A	1607	C
1	A	1608	A
1	A	1614	A
1	A	1617	A
1	A	1623	C
1	A	1626	U
1	A	1631	A
1	A	1632	G
1	A	1637	G
1	A	1653	A
1	A	1654	A
1	A	1655	A
1	A	1656	C
1	A	1659	A
1	A	1660	C
1	A	1661	A
1	A	1662	C

Continued on next page...

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Mol	Chain	Res	Type
1	A	1663	A
1	A	1664	G
1	A	1667	A
1	A	1668	G
1	A	1677	A
1	A	1679	A
1	A	1691	A
1	A	1692	U
1	A	1693	C
1	A	1697	A
1	A	1712	G
1	A	1718	G
1	A	1719	G
1	A	1720	C
1	A	1721	A
1	A	1722	A
1	A	1726	G
1	A	1727	A
1	A	1728	C
1	A	1731	C
1	A	1733	U
1	A	1735	A
1	A	1745	A
1	A	1746	A
1	A	1747	G
1	A	1750	G
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1767	A
1	A	1771	C
1	A	1774	A
1	A	1779	G
1	A	1780	C
1	A	1781	C
1	A	1782	G
1	A	1785	G
1	A	1792	G
1	A	1793	G
1	A	1797	A
1	A	1798	G
1	A	1799	G

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Mol	Chain	Res	Type
1	A	1800	C
1	A	2014	G
1	A	2020	U
1	A	2022	U
1	A	2024	U
1	A	2026	A
1	A	2052	A
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2064	G
1	A	2065	C
1	A	2068	G
1	A	2072	C
1	A	2081	G
1	A	2083	A
1	A	2084	C
1	A	2085	G
1	A	2086	G
1	A	2089	A
1	A	2091	A
1	A	2429	G
1	A	2430	U
1	A	2431	U
1	A	2432	C
1	A	2434	G
1	A	2435	C
1	A	2436	A
1	A	2438	G
1	A	2439	G
1	A	2440	A
1	A	2442	G
1	A	2443	G
1	A	2444	G
1	A	2636	G
1	A	2637	G
1	A	2638	U
1	A	2639	C
1	A	2640	C
1	A	2641	C
1	A	2642	U

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Mol	Chain	Res	Type
1	A	2643	A
1	A	2644	U
1	A	2658	A
1	A	2659	G
1	A	2668	A
1	A	2674	G
1	A	2675	C
1	A	2690	G
1	A	2711	G
1	A	2713	U
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2731	G
1	A	2743	G
1	A	2755	U
1	A	2761	G
1	A	2768	U
1	A	2773	G
1	A	2776	G
1	A	2784	C
1	A	2785	U
1	A	2786	A
1	A	2787	A
1	A	2794	A
1	A	2795	G
1	A	2797	C
1	A	2807	A
1	A	2808	U
1	A	2809	G
1	A	2818	C
1	A	2819	A
1	A	2820	U
1	A	2823	C
1	A	2825	C
1	A	2826	A
1	A	2837	A
1	A	2845	A
1	A	2858	U
1	A	2859	G
1	A	2860	A
1	A	2861	U

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Mol	Chain	Res	Type
1	A	2892	G
1	A	2894	G
1	A	2897	G
1	A	2909	U
1	A	2918	G

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	163	U
1	A	175	G
1	A	179	A
1	A	229	A
1	A	271	C
1	A	405	U
1	A	549	A
1	A	576	G
1	A	647	A
1	A	683	A
1	A	700	U
1	A	785	C
1	A	799	A
1	A	828	A
1	A	829	A
1	A	831	U
1	A	840	A
1	A	874	U
1	A	1103	A
1	A	1107	U
1	A	1130	A
1	A	1313	A
1	A	1314	A
1	A	1362	G
1	A	1363	G
1	A	1434	A
1	A	1455	C
1	A	1518	G
1	A	1555	A
1	A	1595	U
1	A	1653	A
1	A	1654	A
1	A	1659	A

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Mol	Chain	Res	Type
1	A	1660	C
1	A	1661	A
1	A	1663	A
1	A	1779	G
1	A	1784	A
1	A	2059	A
1	A	2060	A
1	A	2064	G
1	A	2083	A
1	A	2639	C
1	A	2642	U
1	A	2643	A
1	A	2784	C
1	A	2785	U
1	A	2796	C
1	A	2818	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

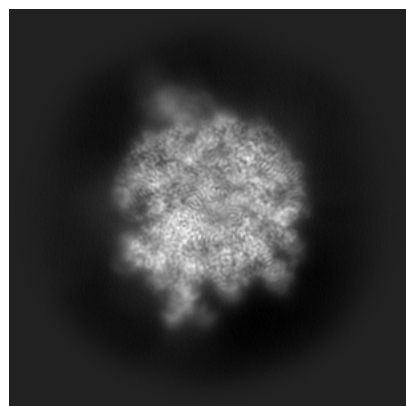
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71238. These allow visual inspection of the internal detail of the map and identification of artifacts.

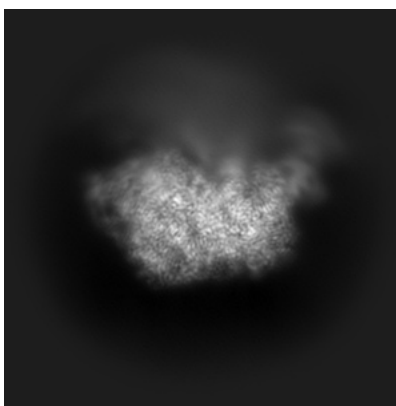
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

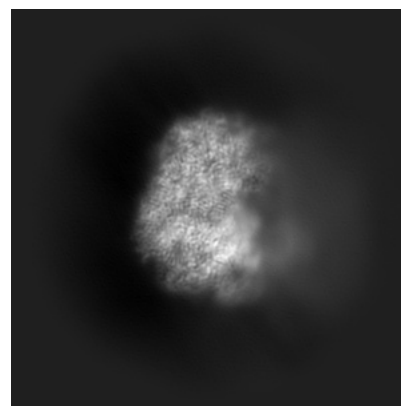
6.1.1 Primary map



X

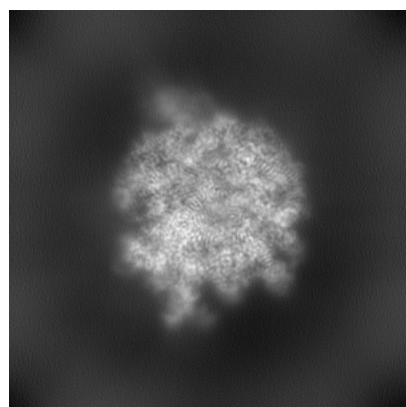


Y

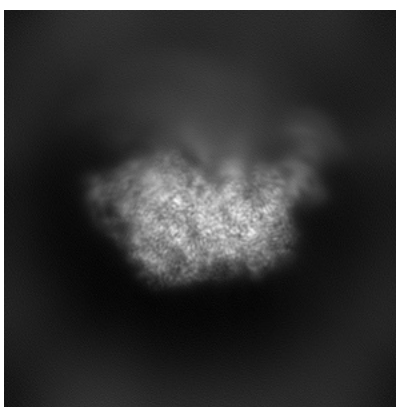


Z

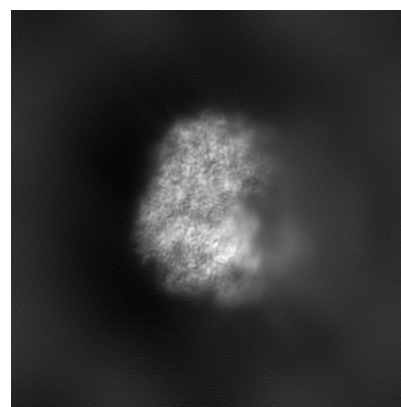
6.1.2 Raw map



X



Y

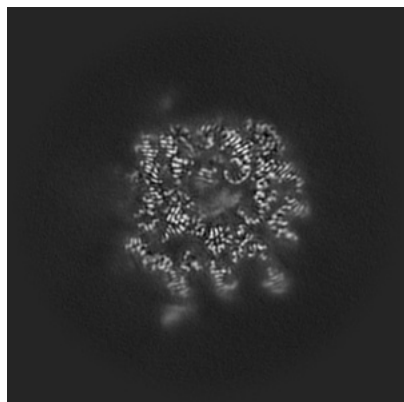


Z

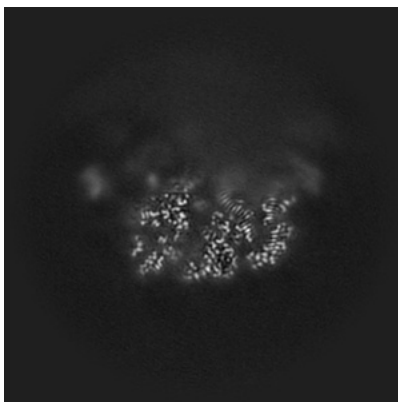
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

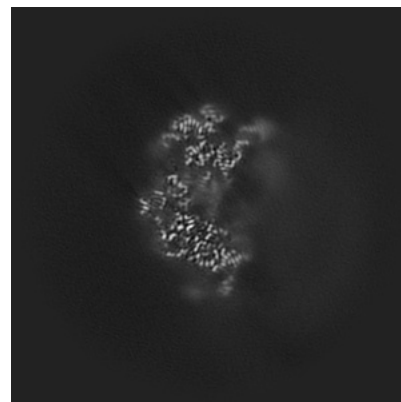
6.2.1 Primary map



X Index: 210

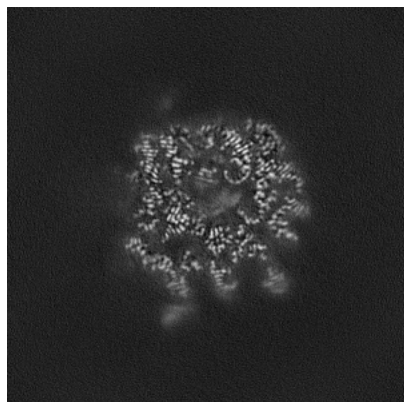


Y Index: 210

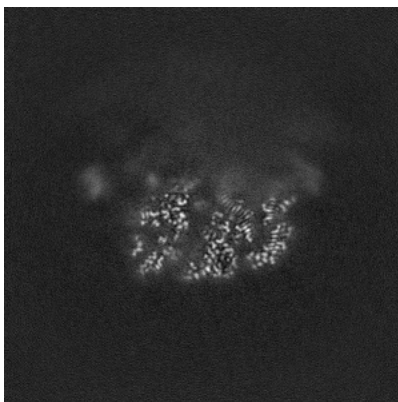


Z Index: 210

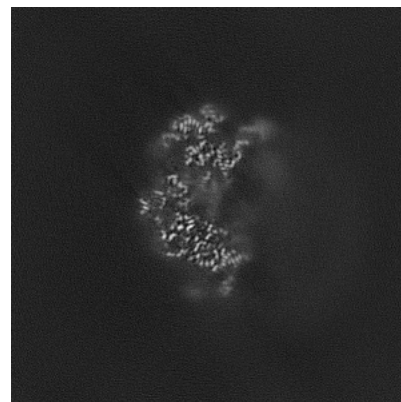
6.2.2 Raw map



X Index: 210



Y Index: 210

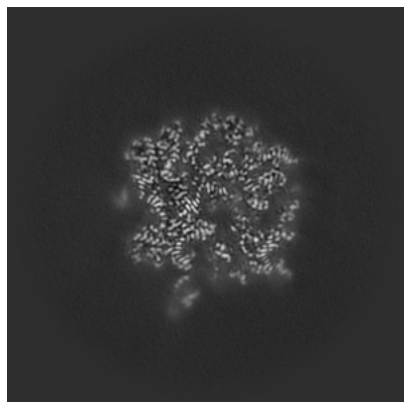


Z Index: 210

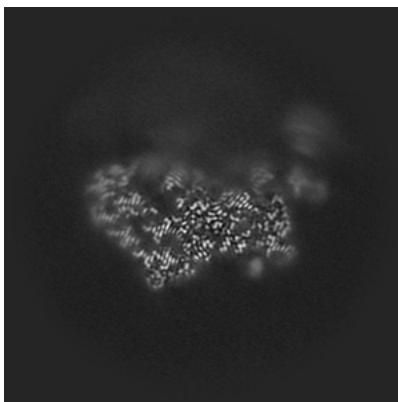
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

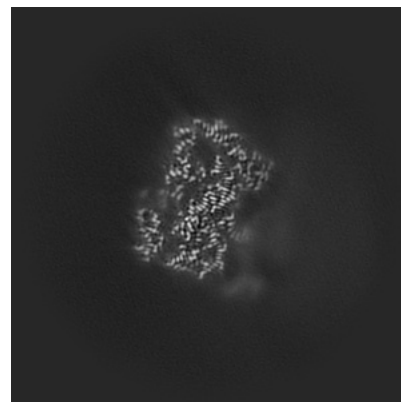
6.3.1 Primary map



X Index: 188

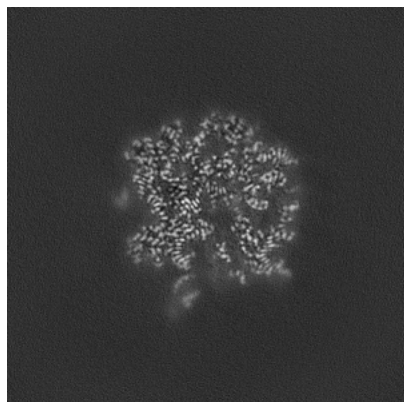


Y Index: 180

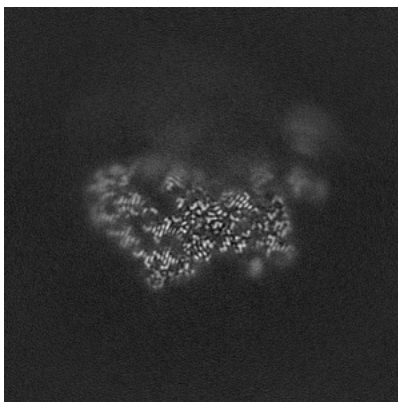


Z Index: 185

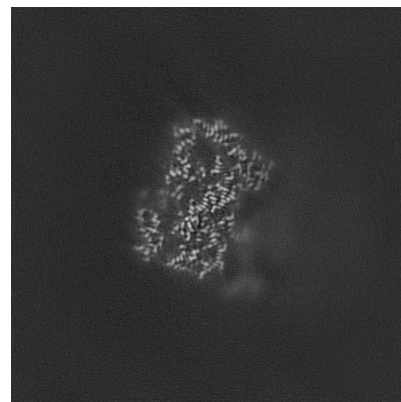
6.3.2 Raw map



X Index: 187



Y Index: 180

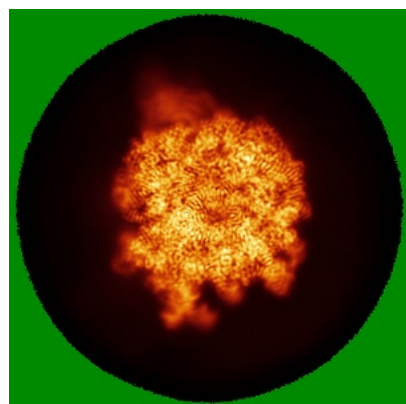


Z Index: 185

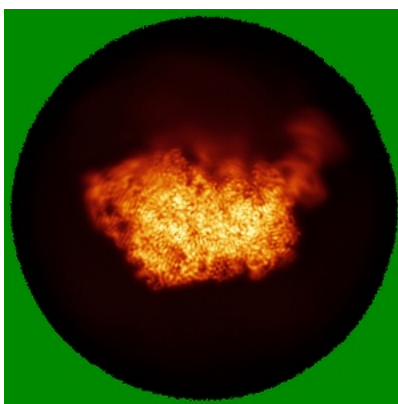
The images above show the largest variance slices of the map in three orthogonal directions.

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

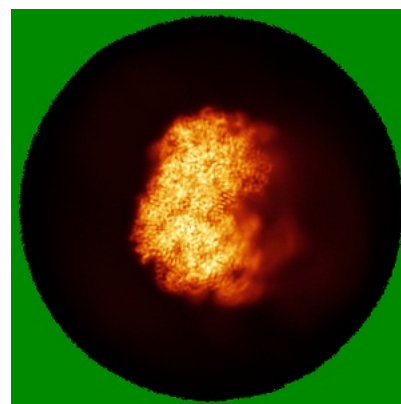
6.4.1 Primary map



X

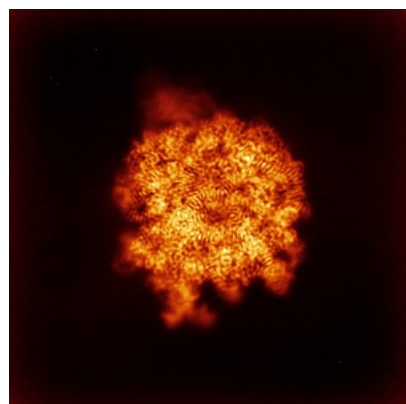


Y

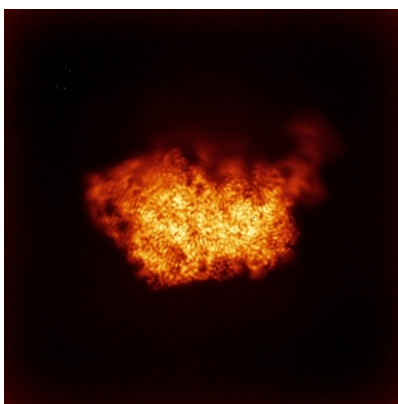


Z

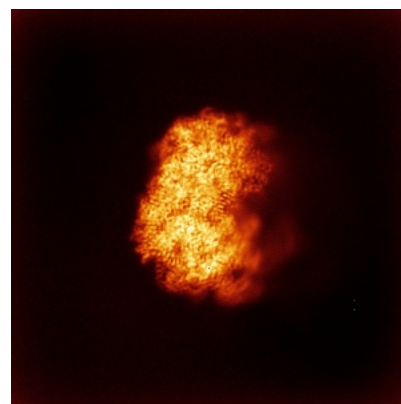
6.4.2 Raw map



X



Y

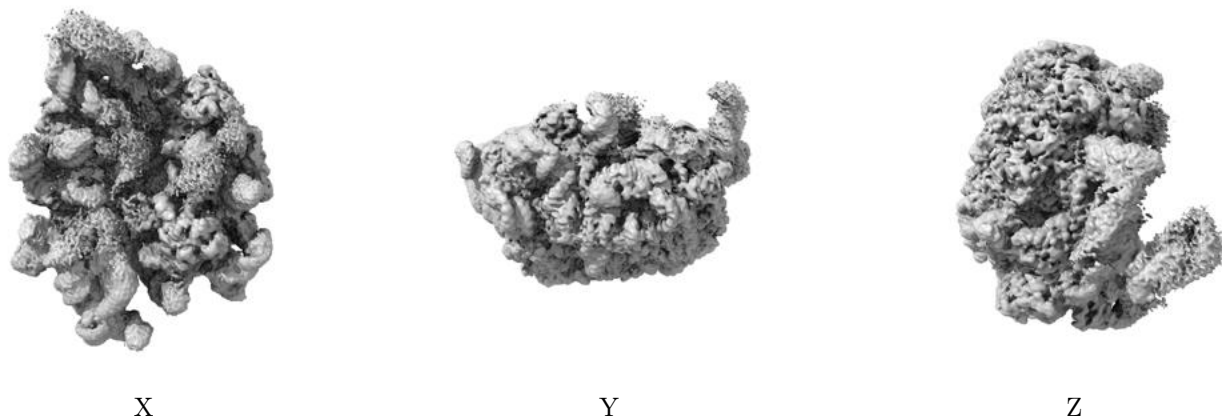


Z

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.

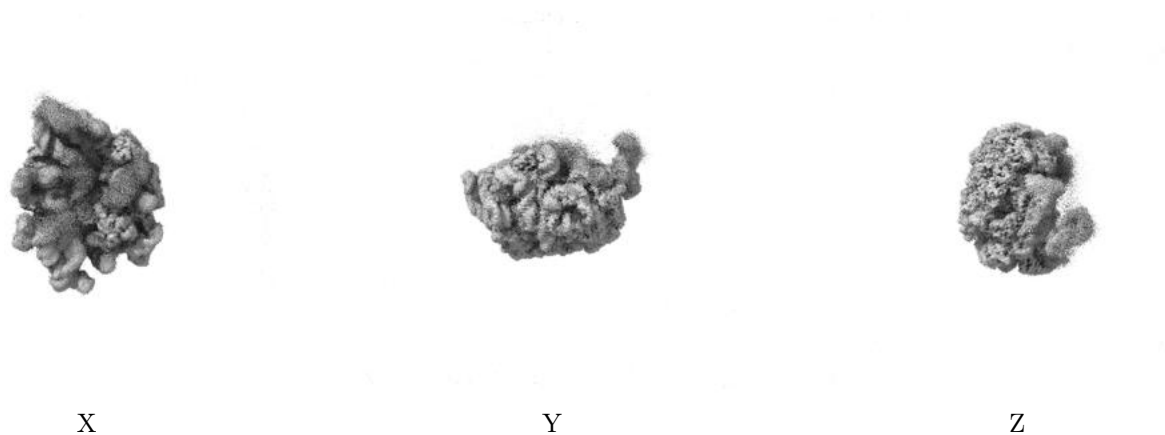
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

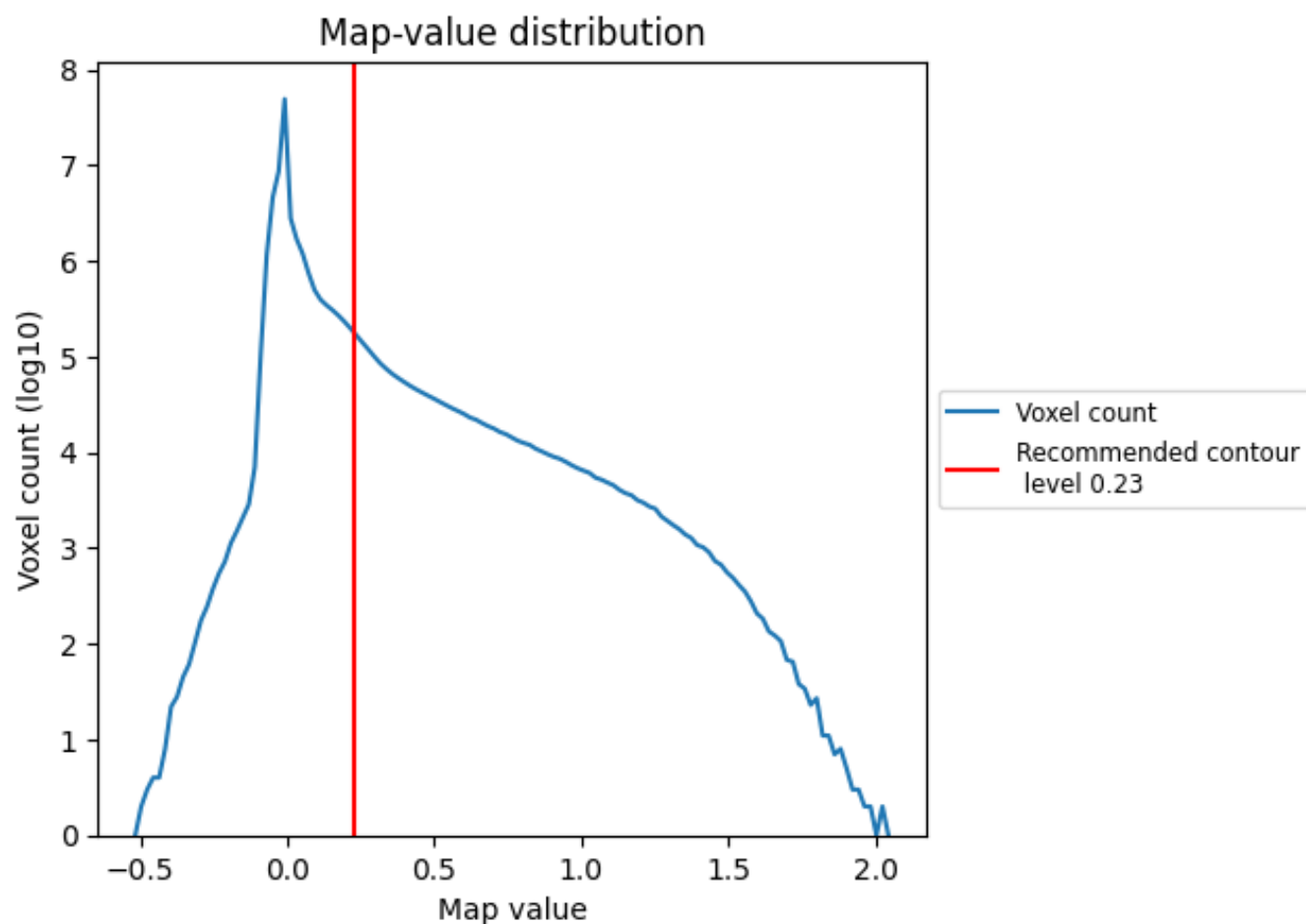
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

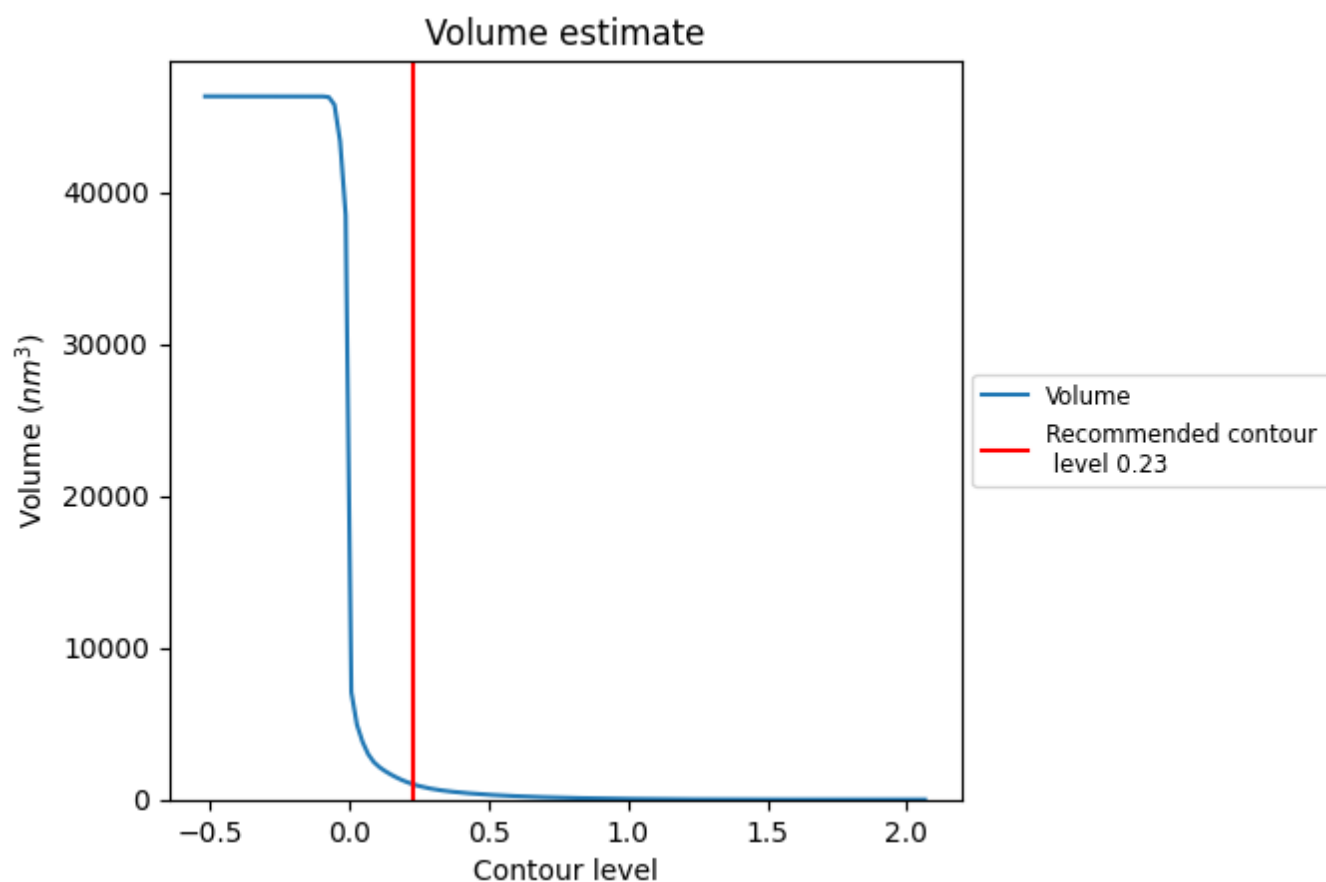
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

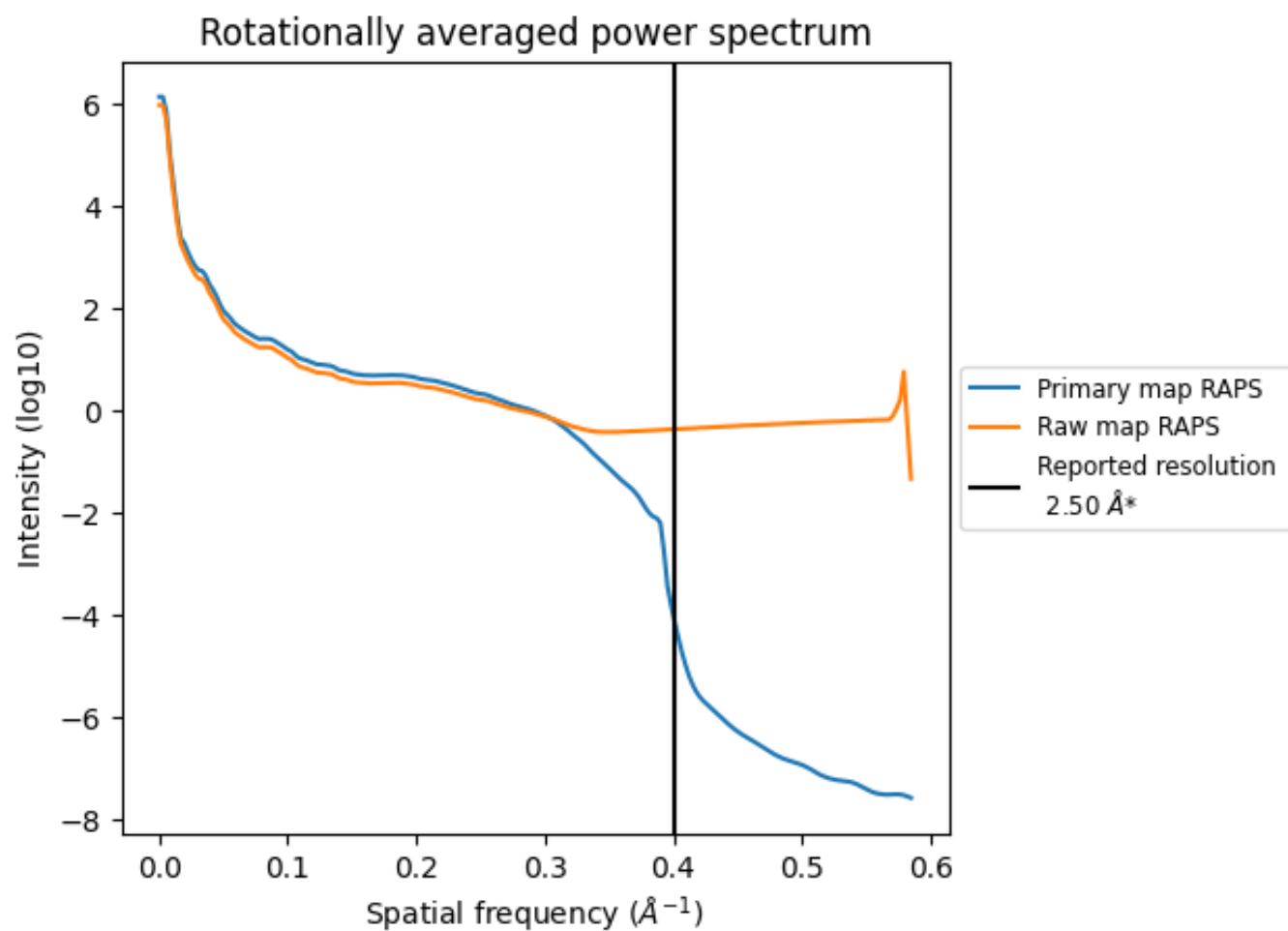
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 999 nm^3 ; this corresponds to an approximate mass of 903 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 ⓘ

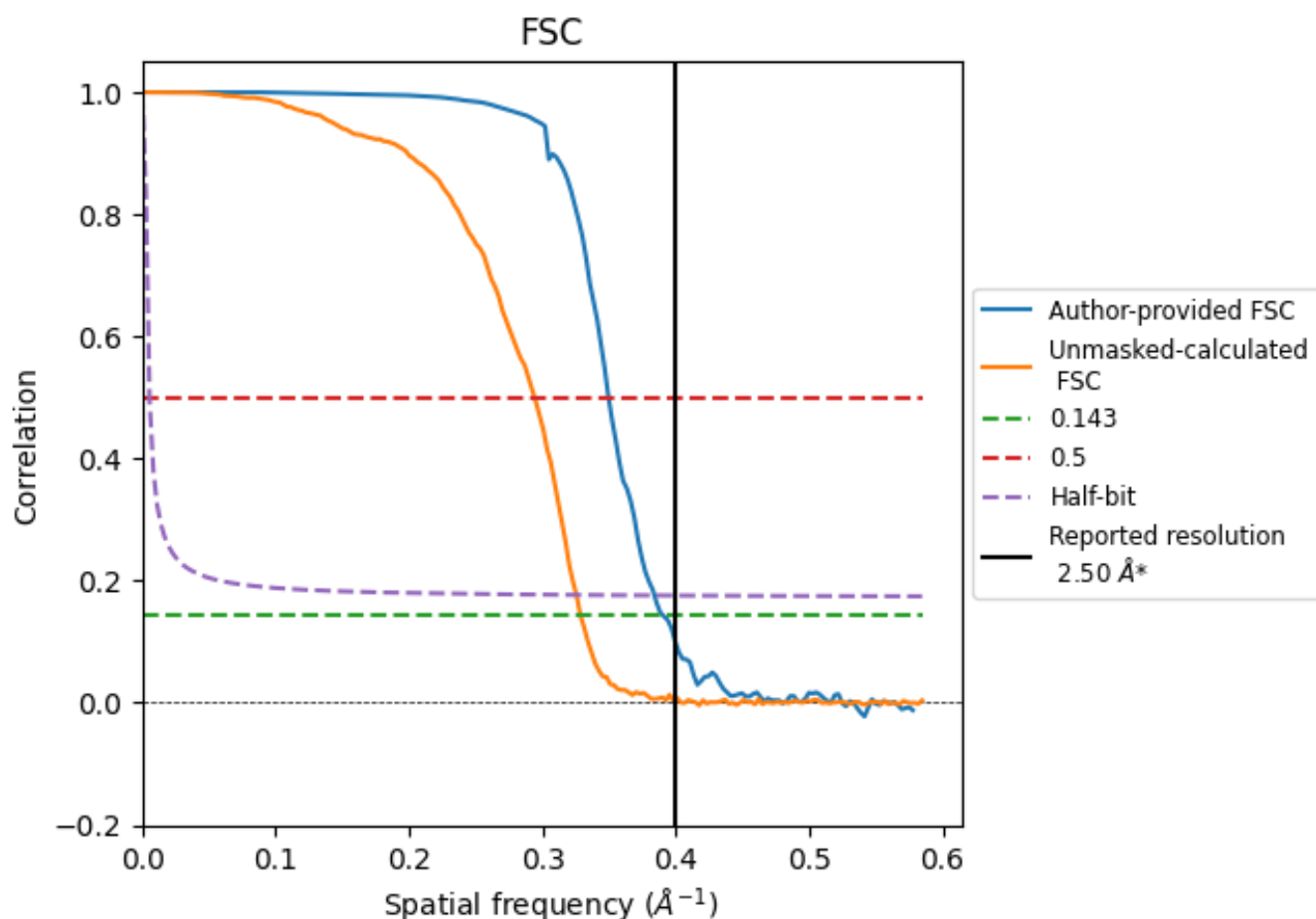


*Reported resolution corresponds to spatial frequency of $0.400 \text{ \AA}^{-1}$

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 $0.400 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

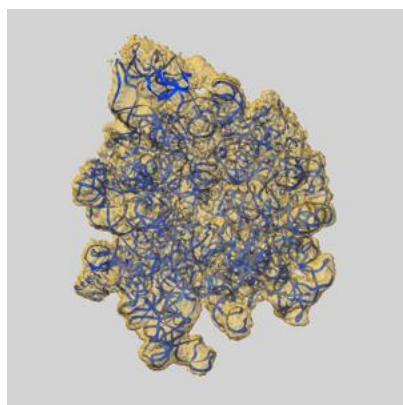
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.56	2.86	2.60
Unmasked-calculated*	3.04	3.40	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.04 differs from the reported value 2.5 by more than 10 %

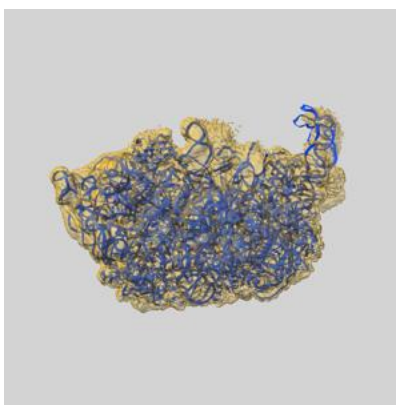
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71238 and PDB model 9P38. Per-residue inclusion information can be found in section 3 on page 7.

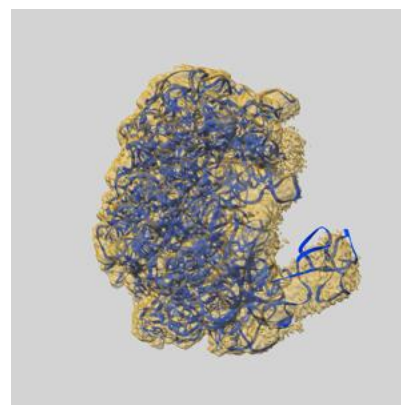
9.1 Map-model overlay [i](#)



X



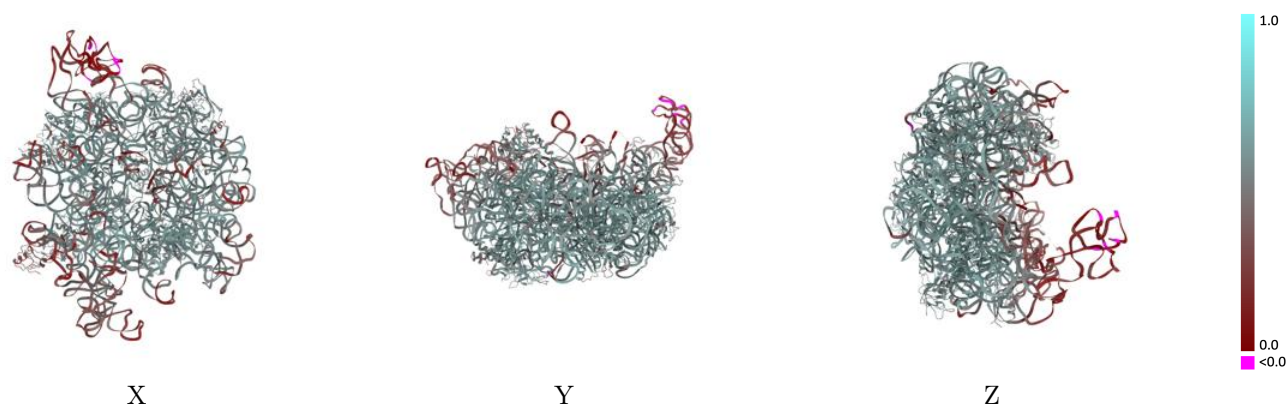
Y



Z

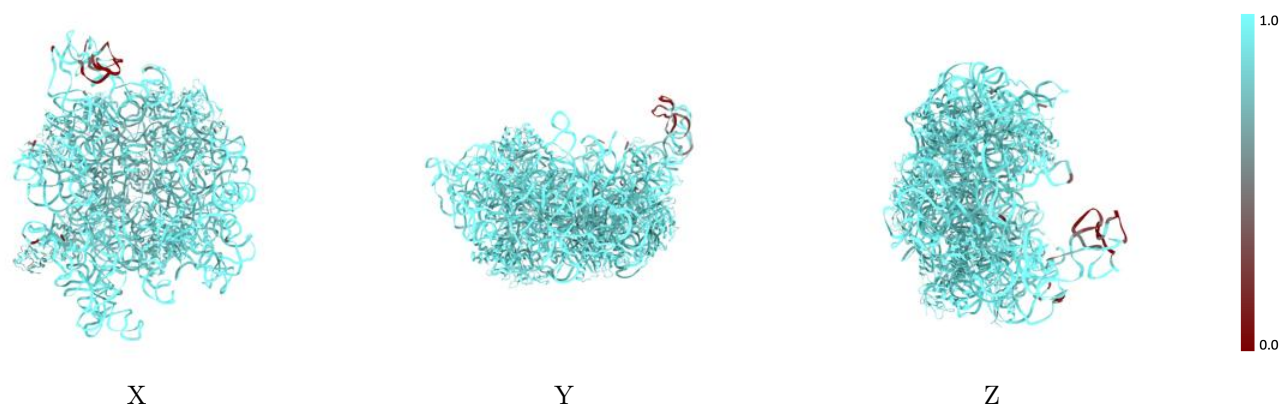
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



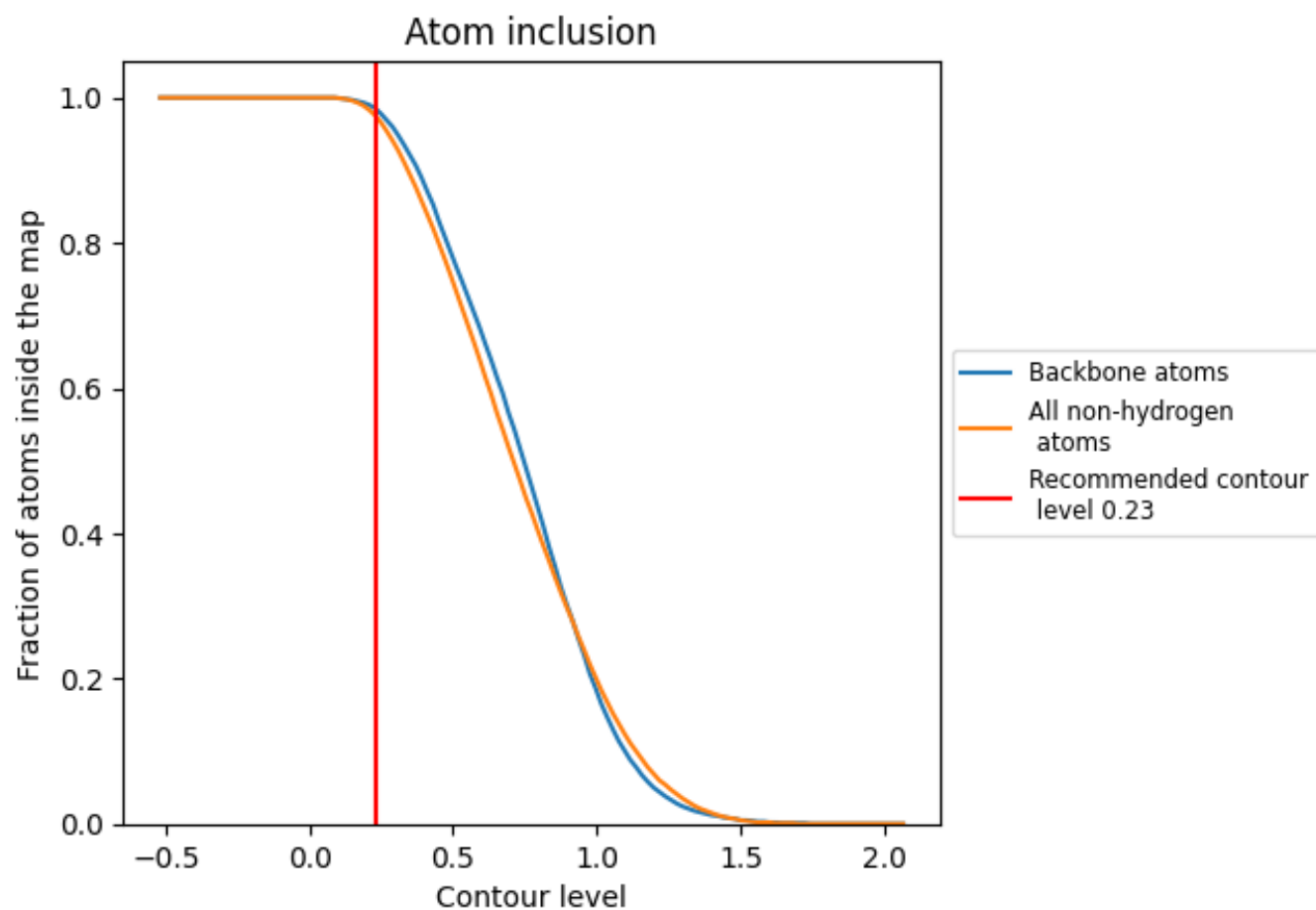
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.5170
A	 0.9780	 0.5070
B	 0.9720	 0.5430
D	 0.9800	 0.5700
E	 0.9710	 0.5460
J	 0.9920	 0.5770
K	 0.9650	 0.5220
L	 0.8350	 0.4080
N	 0.9830	 0.5860
P	 0.9740	 0.5260
Q	 0.9890	 0.5770
R	 0.9640	 0.5610
S	 0.9830	 0.5640
T	 0.9810	 0.5750
U	 0.9670	 0.5590
Y	 0.9610	 0.5250
Z	 0.9510	 0.5220
b	 0.9940	 0.5570
d	 0.9390	 0.5920

