



Full wwPDB EM Validation Report ⓘ

May 5, 2025 – 05:00 pm BST

PDB ID : 9QT5 / pdb_00009qt5
EMDB ID : EMD-53347
Title : Structure of the 50S ribosomal subunit from the antibiotic-producing bacterium *Streptomyces fradiae*
Authors : Ekemezie, C.L.; Melnikov, S.V.
Deposited on : 2025-04-07
Resolution : 3.13 Å(reported)
Based on initial model : .

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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

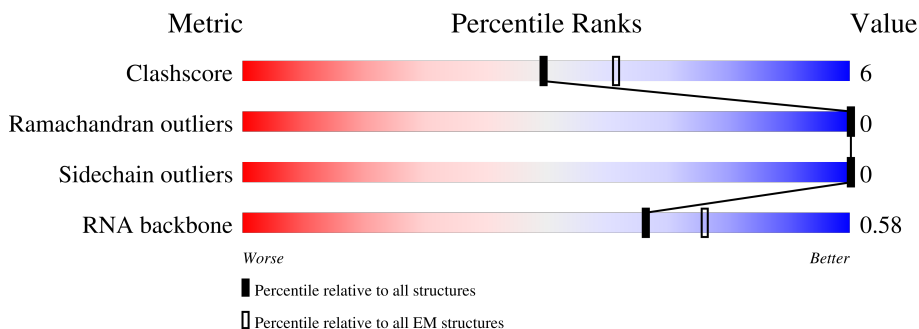
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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.













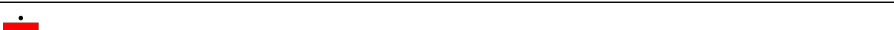

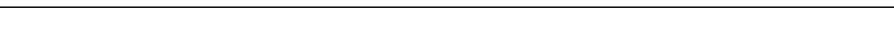
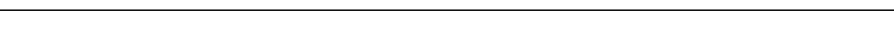
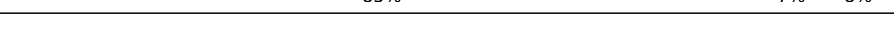








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	M	139	 84% 14% .
2	2	117	 63% 31% . .
3	B	278	 86% 12% .
4	C	214	 83% 16% .
5	D	216	 82% 11% 7% .
6	E	185	 15% 62% 30% 9%
7	F	179	 10% 77% 18% . .

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Mol	Chain	Length	Quality of chain
8	G	148	
9	J	147	
10	K	122	
11	O	127	
12	L	151	
13	P	116	
14	Q	128	
15	R	106	
16	S	115	
17	T	107	
18	U	107	
19	V	195	
20	W	84	
21	X	61	
22	Y	74	
23	Z	60	
24	3	57	
25	4	54	
26	5	45	
27	6	64	
28	7	37	
29	N	164	
30	1	3119	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 81897 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	137	Total	C	N	O	S	0	0
			1095	690	219	179	7		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	114	Total	C	N	O	P	0	0
			2448	1090	450	794	114		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	271	Total	C	N	O	S	0	0
			2082	1279	433	366	4		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	212	Total	C	N	O	S	0	0
			1577	981	303	287	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	201	Total	C	N	O	S	0	0
			1519	949	287	282	1		

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	169	Total	C	N	O	S	0	0
			1342	847	248	242	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	171	Total	C	N	O	S	0	0
			1293	819	235	238	1		

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	48	Total	C	N	O	S	0	0
			364	232	65	66	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	146	Total	C	N	O	S	0	0
			1137	718	213	202	4		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	122	Total	C	N	O	S	0	0
			941	587	181	170	3		

- Molecule 11 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	126	Total	C	N	O		0	0
			929	572	189	168			

- Molecule 12 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	148	Total	C	N	O	S	0	0
			1102	691	205	204	2		

- Molecule 13 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	115	Total	C	N	O	S	0	0
			919	577	180	161	1		

- Molecule 14 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Q	124	Total	C	N	O	0	0
			992	619	203	170		

- Molecule 15 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	103	Total	C	N	O	S	0
			796	500	148	147	1	0

- Molecule 16 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	S	111	Total	C	N	O	S	0
			870	542	171	154	3	0

- Molecule 17 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	T	97	Total	C	N	O		0
			770	484	144	142		0

- Molecule 18 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	U	99	Total	C	N	O	S	0
			763	477	146	139	1	0

- Molecule 19 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	175	Total	C	N	O	S	0
			1301	824	226	249	2	0

- Molecule 20 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	W	72	Total	C	N	O	0	0
			541	333	114	94		

- Molecule 21 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	56	Total	C	N	O	S	0	0
			432	260	96	72	4		

- Molecule 22 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	62	Total	C	N	O	S	0	0
			506	314	97	94	1		

- Molecule 23 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	58	Total	C	N	O	S	0	0
			472	291	92	88	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	24	Total	C	N	O	S	0	0
			199	121	47	30	1		

- Molecule 25 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4	48	Total	C	N	O	S	0	0
			399	240	86	68	5		

- Molecule 26 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	44	Total	C	N	O	S	0	0
			363	216	91	55	1		

- Molecule 27 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	61	Total	C	N	O	S	0	0
			471	290	99	80	2		

- Molecule 28 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	7	37	Total	C	N	O	S	0	0
			303	186	66	46	5		

- Molecule 29 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	116	Total	C	N	O	S	0	0
			901	565	178	157	1		

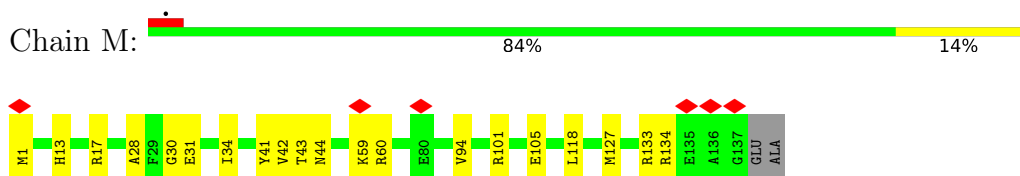
- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1	2562	Total	C	N	O	P	0	0
			55070	24535	10147	17826	2562		

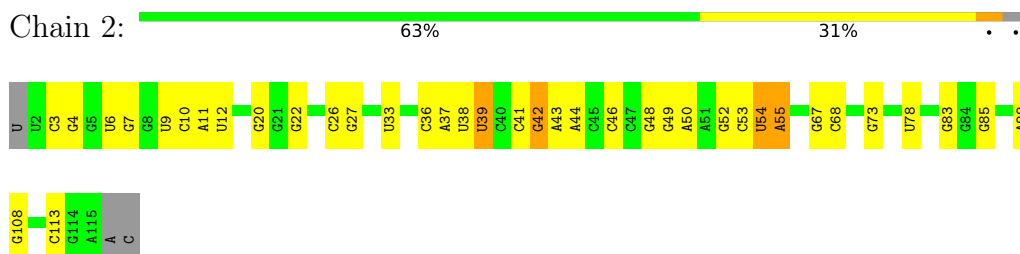
3 Residue-property plots [i](#)

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.

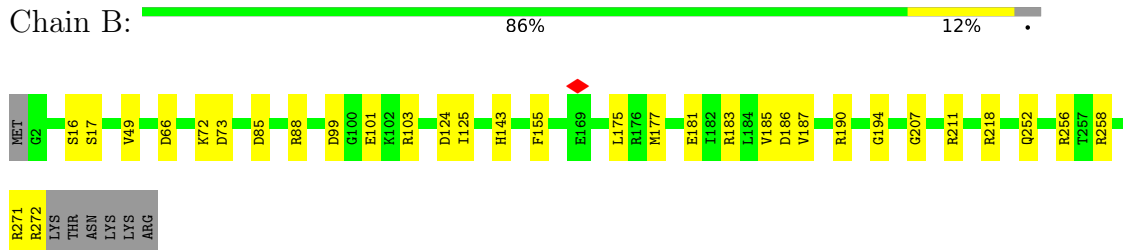
- Molecule 1: Large ribosomal subunit protein uL16



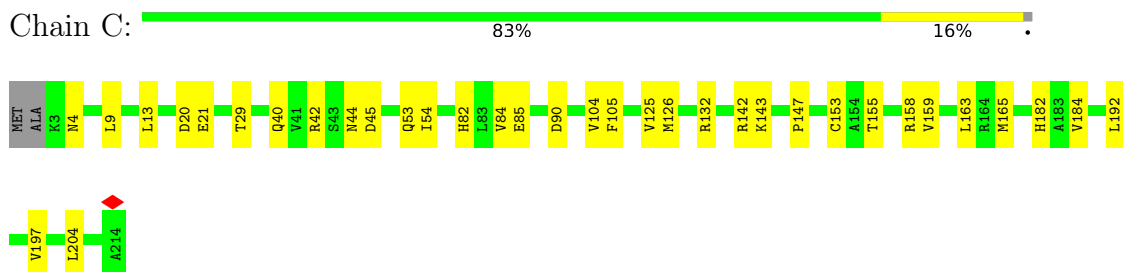
- Molecule 2: 5S rRNA




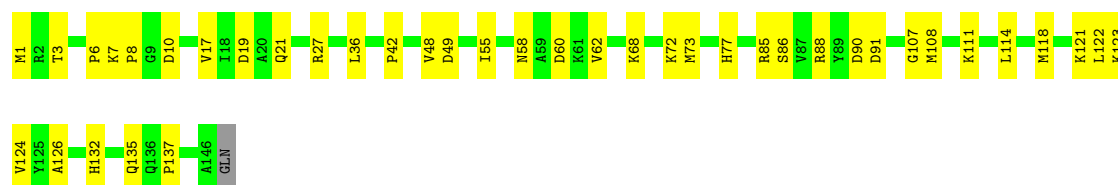
- Molecule 3: Large ribosomal subunit protein uL2




- Molecule 4: Large ribosomal subunit protein uL3

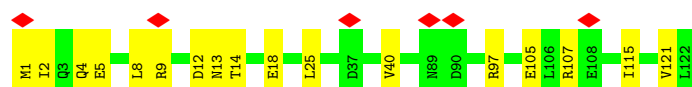


Chain J:  72% 27% .




- Molecule 10: Large ribosomal subunit protein uL14

Chain K:  5% 86% 14%




- Molecule 11: Large ribosomal subunit protein uL18

Chain O:  77% 22% .




- Molecule 12: Large ribosomal subunit protein uL15

Chain L:  84% 14% .




- Molecule 13: Large ribosomal subunit protein bL19

Chain P:  9% 78% 21%




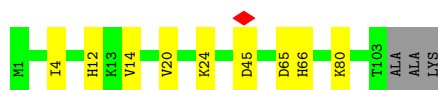
- Molecule 14: Large ribosomal subunit protein bL20

Chain Q:  77% 20% .

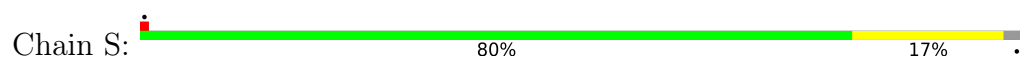


- Molecule 15: Large ribosomal subunit protein bL21

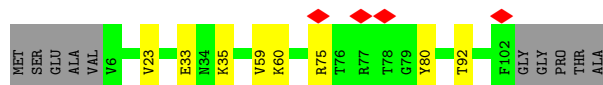
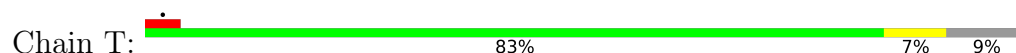
Chain R:  89% 8% .



- Molecule 16: Large ribosomal subunit protein uL22



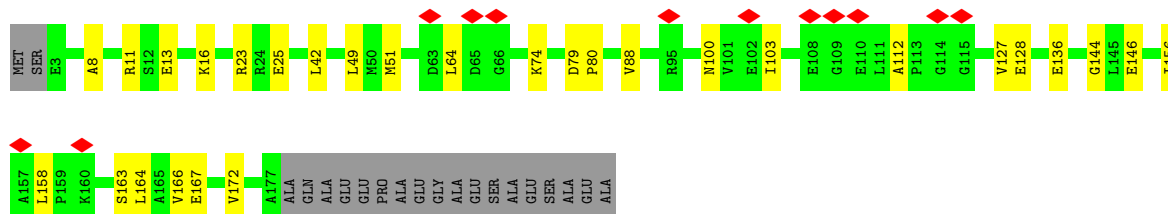
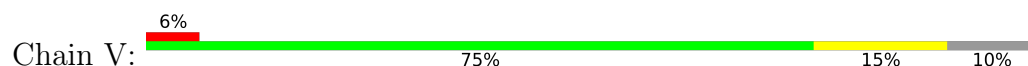
- Molecule 17: Large ribosomal subunit protein uL23



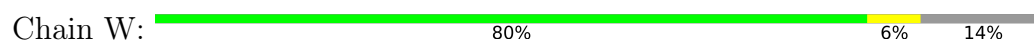
- Molecule 18: Large ribosomal subunit protein uL24



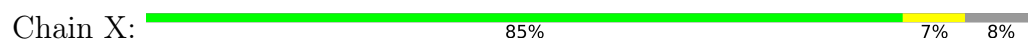
- Molecule 19: Large ribosomal subunit protein bL25



- Molecule 20: Large ribosomal subunit protein bL27



- Molecule 21: Large ribosomal subunit protein bL28





- Molecule 22: Large ribosomal subunit protein uL29

Chain Y: 69% 15% 16%



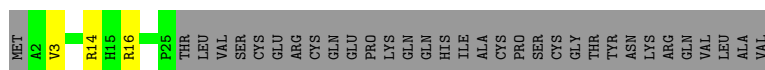
- Molecule 23: Large ribosomal subunit protein uL30

Chain Z: 82% 15% .



- Molecule 24: Large ribosomal subunit protein bL32

Chain 3: 37% 5% 58%



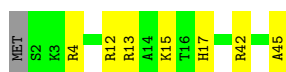
- Molecule 25: Large ribosomal subunit protein bL33

Chain 4: 76% 13% 11%



- Molecule 26: Large ribosomal subunit protein bL34

Chain 5: 82% 16% .



- Molecule 27: Large ribosomal subunit protein bL35

Chain 6: 73% 22% 5%

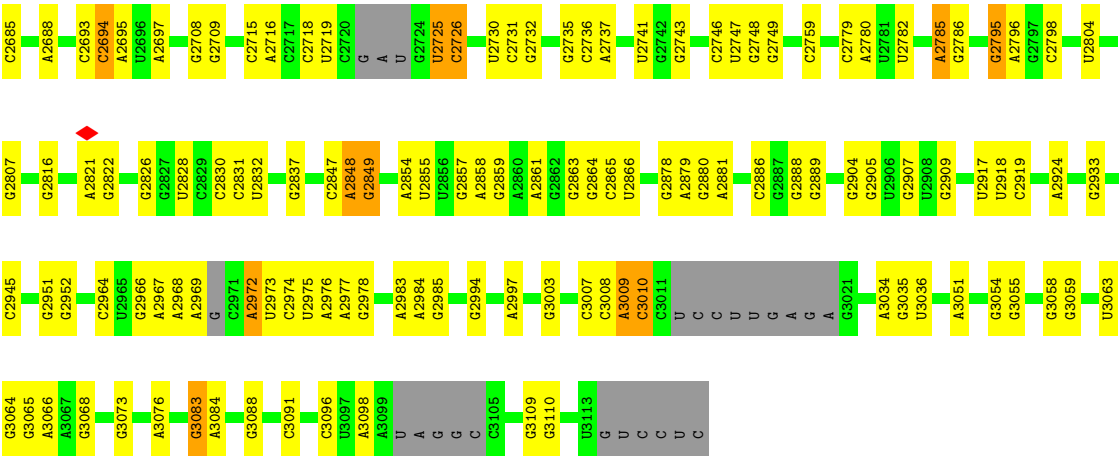


- Molecule 28: Large ribosomal subunit protein bL36

Chain 7: 43% 89% 11%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	250126	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.175	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0769	Depositor
Map size (Å)	478.208, 478.208, 478.208	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.934, 0.934, 0.934	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	M	0.20	0/1121	0.36	0/1505
2	2	0.16	0/2739	0.25	0/4272
3	B	0.20	0/2125	0.33	0/2859
4	C	0.19	0/1601	0.36	0/2154
5	D	0.19	0/1544	0.32	0/2085
6	E	0.19	0/1364	0.39	0/1833
7	F	0.19	0/1312	0.39	1/1769 (0.1%)
8	G	0.19	0/370	0.36	0/498
9	J	0.22	0/1163	0.35	0/1575
10	K	0.20	0/949	0.33	0/1269
11	O	0.20	0/936	0.40	0/1249
12	L	0.20	0/1117	0.39	0/1501
13	P	0.19	0/933	0.34	0/1252
14	Q	0.25	0/1005	0.37	0/1348
15	R	0.20	0/807	0.34	0/1091
16	S	0.22	0/884	0.36	0/1192
17	T	0.17	0/779	0.33	0/1049
18	U	0.19	0/768	0.33	0/1024
19	V	0.15	0/1319	0.31	0/1794
20	W	0.21	0/549	0.34	0/735
21	X	0.20	0/439	0.35	0/589
22	Y	0.16	0/509	0.32	0/677
23	Z	0.19	0/477	0.29	0/638
24	3	0.27	0/203	0.38	0/270
25	4	0.20	0/405	0.39	0/541
26	5	0.22	0/366	0.41	0/480
27	6	0.20	0/475	0.38	0/623
28	7	0.18	0/305	0.31	0/399
29	N	0.19	0/914	0.34	0/1228
30	1	0.21	0/61648	0.28	0/96153
All	All	0.20	0/89126	0.30	1/133652 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	129	PRO	CA-N-CD	-5.82	103.85	112.00

There are no chirality outliers.

There are no planarity outliers.

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	M	1095	0	1147	12	0
2	2	2448	0	1235	23	0
3	B	2082	0	2122	24	0
4	C	1577	0	1629	25	0
5	D	1519	0	1560	21	0
6	E	1342	0	1376	47	0
7	F	1293	0	1367	26	0
8	G	364	0	372	9	0
9	J	1137	0	1162	36	0
10	K	941	0	1002	13	0
11	O	929	0	981	34	0
12	L	1102	0	1163	18	0
13	P	919	0	961	17	0
14	Q	992	0	1033	27	0
15	R	796	0	829	7	0
16	S	870	0	901	17	0
17	T	770	0	812	6	0
18	U	763	0	818	19	0
19	V	1301	0	1358	22	0
20	W	541	0	542	3	0
21	X	432	0	444	4	0
22	Y	506	0	523	8	0
23	Z	472	0	489	6	0
24	3	199	0	212	5	0
25	4	399	0	411	5	0
26	5	363	0	394	6	0
27	6	471	0	518	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	7	303	0	342	5	0
29	N	901	0	962	11	0
30	1	55070	0	27712	393	0
All	All	81897	0	54377	736	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 6.

All (736) 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)
30:1:270:G:N2	30:1:514:C:C2	2.29	0.99
18:U:4:LYS:NZ	30:1:84:A:OP2	1.99	0.96
30:1:270:G:C2	30:1:514:C:C2	2.57	0.93
11:O:127:PHE:OXT	30:1:2596:A:O2'	1.90	0.90
1:M:17:ARG:NH1	1:M:41:TYR:OH	2.06	0.89
6:E:65:ILE:O	6:E:107:ARG:NH2	2.06	0.88
28:7:19:ARG:NE	30:1:2975:U:OP2	2.05	0.88
30:1:80:G:N2	30:1:106:C:O2	2.06	0.88
30:1:2795:G:O2'	30:1:2798:C:OP2	1.94	0.85
30:1:270:G:N2	30:1:514:C:O2	2.10	0.84
3:B:124:ASP:OD2	3:B:125:ILE:N	2.10	0.83
14:Q:48:ASN:OD1	30:1:1256:A:N6	2.12	0.82
29:N:96:ARG:NH1	30:1:3098:A:OP1	2.13	0.81
27:6:62:LEU:HD23	27:6:62:LEU:O	1.81	0.81
6:E:42:ASN:ND2	30:1:2532:C:O4'	2.14	0.81
8:G:23:ASP:OD2	8:G:24:GLY:N	2.13	0.81
11:O:104:ARG:NH1	30:1:2512:C:OP1	2.14	0.80
30:1:270:G:C2	30:1:514:C:O2	2.34	0.80
29:N:64:ARG:NH1	30:1:1669:U:O2	2.15	0.80
10:K:25:LEU:HD11	10:K:40:VAL:HG23	1.64	0.79
19:V:158:LEU:HD11	19:V:164:LEU:HD12	1.63	0.79
9:J:85:ARG:NH2	30:1:2861:A:OP2	2.16	0.79
30:1:11:A:N6	30:1:2847:C:OP1	2.15	0.78
10:K:105:GLU:N	10:K:105:GLU:OE1	2.17	0.77
30:1:1651:G:HO2'	30:1:1732:G:HO2'	1.21	0.77
3:B:88:ARG:NH2	30:1:2027:G:OP1	2.18	0.77
30:1:2200:G:O2'	30:1:2202:C:OP2	2.03	0.76
29:N:73:LYS:NZ	30:1:1669:U:O4	2.19	0.76
2:2:6:U:O2'	11:O:37:ARG:NH2	2.18	0.76
30:1:270:G:N1	30:1:514:C:N3	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:2477:U:O2'	30:1:2646:C:OP2	2.02	0.75
30:1:269:G:N2	30:1:515:U:O2	2.19	0.75
30:1:270:G:C2	30:1:514:C:N3	2.55	0.74
9:J:3:THR:HG21	14:Q:61:TRP:HE1	1.51	0.74
12:L:108:ARG:NH2	30:1:724:G:N7	2.35	0.74
19:V:136:GLU:OE1	19:V:136:GLU:N	2.20	0.74
4:C:4:ASN:ND2	4:C:90:ASP:OD2	2.21	0.73
30:1:2069:A:N6	30:1:2103:G:O2'	2.21	0.73
7:F:35:HIS:HB2	7:F:76:MET:HE1	1.71	0.73
16:S:4:ARG:NH1	30:1:581:G:OP1	2.20	0.73
14:Q:26:GLY:O	14:Q:30:ARG:NH1	2.20	0.73
3:B:155:PHE:CD1	3:B:177:MET:HE1	2.24	0.72
4:C:44:ASN:OD1	4:C:45:ASP:N	2.22	0.72
12:L:108:ARG:NH1	30:1:724:G:O6	2.22	0.72
3:B:101:GLU:OE2	3:B:103:ARG:NE	2.21	0.72
3:B:85:ASP:OD2	3:B:88:ARG:NH1	2.21	0.72
18:U:12:ILE:O	18:U:17:LYS:NZ	2.22	0.72
28:7:15:LYS:NZ	30:1:2972:A:N3	2.38	0.71
6:E:43:MET:HE2	6:E:58:ALA:HB1	1.73	0.71
30:1:846:U:O2'	30:1:2830:C:O2'	2.05	0.71
30:1:106:C:O2'	30:1:376:A:O2'	2.07	0.70
30:1:744:U:O2'	30:1:745:A:OP1	2.09	0.70
30:1:117:G:OP2	30:1:119:A:O2'	2.09	0.70
6:E:123:SER:O	6:E:133:TYR:OH	2.08	0.70
25:4:7:ARG:NH1	30:1:2504:C:OP2	2.25	0.69
24:3:16:ARG:NH2	30:1:1376:G:OP1	2.20	0.69
12:L:24:ARG:NH2	30:1:1362:G:N7	2.39	0.69
30:1:550:G:N2	30:1:553:A:OP2	2.23	0.69
30:1:391:G:O2'	30:1:392:A:O5'	2.11	0.68
30:1:675:A:OP1	30:1:1367:U:O2'	2.11	0.68
29:N:117:GLU:OE2	29:N:117:GLU:N	2.27	0.68
1:M:101:ARG:NH2	30:1:1006:C:O2'	2.26	0.68
27:6:12:LYS:NZ	30:1:252:C:O2	2.27	0.67
3:B:66:ASP:OD2	3:B:103:ARG:NH1	2.27	0.67
10:K:2:ILE:HD13	10:K:8:LEU:HD21	1.75	0.67
4:C:21:GLU:N	4:C:21:GLU:OE1	2.27	0.67
1:M:1:MET:HE3	1:M:44:ASN:ND2	2.10	0.66
3:B:155:PHE:CG	3:B:177:MET:HE1	2.31	0.66
25:4:19:GLU:OE1	25:4:43:ARG:NH2	2.29	0.66
30:1:674:G:O2'	30:1:1366:A:OP1	2.14	0.66
9:J:90:ASP:OD1	9:J:91:ASP:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:75:G:H22	30:1:111:G:H1	1.41	0.65
7:F:68:LEU:HD12	30:1:2976:A:N1	2.11	0.65
12:L:84:ASP:OD1	12:L:85:LYS:N	2.30	0.65
30:1:200:A:N6	30:1:2649:A:O2'	2.30	0.64
30:1:2469:G:O2'	30:1:2715:C:OP1	2.04	0.64
1:M:42:VAL:CG1	1:M:127:MET:HE1	2.27	0.64
5:D:40:GLN:NE2	30:1:714:U:O2'	2.29	0.64
8:G:6:THR:OG1	8:G:34:GLY:O	2.14	0.64
23:Z:39:ASP:OD1	23:Z:44:ARG:NH2	2.31	0.64
13:P:87:VAL:HG12	13:P:88:THR:HG23	1.80	0.64
19:V:8:ALA:HB1	19:V:42:LEU:HD12	1.79	0.63
20:W:42:GLY:N	20:W:57:ASP:OD2	2.32	0.63
12:L:132:VAL:HG11	12:L:147:VAL:HG11	1.79	0.63
13:P:21:ARG:NH2	30:1:3065:G:O6	2.28	0.63
16:S:93:ARG:O	30:1:1826:A:N6	2.27	0.63
30:1:3008:C:O2'	30:1:3009:A:OP2	2.14	0.63
30:1:586:G:N1	30:1:589:A:OP2	2.31	0.63
7:F:22:ARG:NH1	7:F:37:VAL:O	2.32	0.62
4:C:158:ARG:NH2	30:1:1229:U:O2	2.32	0.62
30:1:1075:G:HO2'	30:1:1255:A:HO2'	1.45	0.62
28:7:30:LEU:HD13	30:1:2746:C:OP1	2.00	0.62
2:2:12:U:OP2	2:2:68:C:O2'	2.17	0.62
7:F:32:THR:C	7:F:33:LEU:HD22	2.24	0.62
27:6:42:ARG:NH1	30:1:2570:G:N7	2.47	0.62
17:T:75:ARG:NH2	30:1:1445:C:OP1	2.33	0.62
6:E:42:ASN:OD1	6:E:43:MET:N	2.33	0.61
30:1:499:G:OP2	30:1:2625:U:O2'	2.11	0.61
30:1:2510:U:O2'	30:1:2593:C:O2	2.18	0.61
10:K:9:ARG:NH1	10:K:18:GLU:OE1	2.33	0.61
8:G:41:LYS:HE3	8:G:41:LYS:HA	1.82	0.61
14:Q:27:GLN:HG2	14:Q:31:LEU:HD12	1.80	0.61
14:Q:25:ARG:NH1	30:1:17:G:O2'	2.34	0.61
5:D:156:VAL:HG12	5:D:195:THR:OG1	2.01	0.60
30:1:1387:C:OP2	30:1:1857:G:O2'	2.19	0.60
30:1:2161:C:N4	30:1:2185:C:O4'	2.34	0.60
30:1:59:U:O2'	30:1:74:G:OP2	2.19	0.60
30:1:968:U:O2'	30:1:969:G:O5'	2.18	0.60
6:E:169:ASP:OD1	6:E:170:GLU:N	2.34	0.60
1:M:31:GLU:OE2	1:M:133:ARG:NH2	2.35	0.60
13:P:96:LYS:NZ	30:1:3063:U:OP1	2.28	0.60
18:U:91:ASP:OD1	18:U:92:GLU:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:221:G:H22	30:1:238:U:H4'	1.66	0.60
30:1:269:G:C2	30:1:515:U:O2	2.54	0.60
30:1:804:G:N2	30:1:826:G:O2'	2.35	0.60
4:C:163:LEU:HD23	4:C:165:MET:HE2	1.83	0.59
5:D:63:LYS:NZ	30:1:775:A:OP1	2.32	0.59
14:Q:88:VAL:HG22	14:Q:88:VAL:O	2.01	0.59
1:M:13:HIS:ND1	30:1:1053:G:H5''	2.17	0.59
4:C:29:THR:HG21	4:C:197:VAL:HG13	1.85	0.59
9:J:73:MET:HE3	9:J:86:SER:HB2	1.83	0.59
5:D:174:HIS:NE2	30:1:713:G:O6	2.35	0.59
6:E:99:ASP:OD1	6:E:100:ARG:N	2.35	0.59
18:U:102:ARG:NH2	30:1:384:G:OP1	2.35	0.59
30:1:2011:G:H3'	30:1:2012:A:H5'	1.85	0.59
9:J:17:VAL:HG23	9:J:137:PRO:HB2	1.85	0.59
16:S:23:LEU:O	16:S:27:MET:HE2	2.01	0.59
30:1:2024:G:OP2	30:1:2025:A:O2'	2.16	0.59
30:1:2621:G:N2	30:1:2622:G:O6	2.36	0.59
13:P:46:VAL:HG21	13:P:110:ILE:HD13	1.85	0.58
27:6:28:GLY:O	27:6:36:LYS:NZ	2.34	0.58
12:L:58:MET:HE2	30:1:2611:A:C2	2.38	0.58
15:R:65:ASP:OD1	15:R:66:HIS:N	2.36	0.58
30:1:2857:G:O2'	30:1:2994:G:N2	2.34	0.58
22:Y:52:LYS:NZ	30:1:75:G:O2'	2.37	0.58
4:C:42:ARG:NH2	4:C:85:GLU:OE2	2.36	0.58
14:Q:36:LYS:NZ	30:1:1364:G:N7	2.50	0.58
18:U:13:THR:O	18:U:13:THR:HG23	2.04	0.57
30:1:1690:G:O2'	30:1:1730:G:O6	2.22	0.57
3:B:72:LYS:NZ	3:B:99:ASP:OD2	2.35	0.57
30:1:230:A:O2'	30:1:231:C:OP2	2.18	0.57
30:1:1079:A:O2'	30:1:1080:A:O5'	2.14	0.57
30:1:2848:A:O2'	30:1:2849:G:OP2	2.20	0.57
30:1:914:C:O2'	30:1:1335:G:N2	2.35	0.57
30:1:1057:U:O2'	30:1:1058:A:P	2.63	0.57
9:J:7:LYS:N	9:J:10:ASP:OD2	2.36	0.57
15:R:80:LYS:HE3	30:1:668:A:O2'	2.05	0.56
6:E:164:THR:HG22	6:E:164:THR:O	2.04	0.56
13:P:95:ALA:N	30:1:3064:G:OP2	2.38	0.56
19:V:112:ALA:HB3	19:V:146:GLU:OE1	2.04	0.56
27:6:33:LEU:HD13	30:1:2638:U:OP2	2.05	0.56
7:F:33:LEU:HD21	7:F:137:ILE:HD12	1.87	0.56
9:J:1:MET:HE1	15:R:12:HIS:ND1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:75:ARG:NH1	17:T:80:TYR:OH	2.38	0.56
8:G:14:ALA:N	8:G:17:ASP:OD2	2.37	0.56
30:1:1875:U:O2'	30:1:2905:G:H4'	2.05	0.56
2:2:9:U:OP2	2:2:10:C:N4	2.37	0.56
5:D:180:GLN:OE1	30:1:712:U:N3	2.34	0.56
6:E:43:MET:CE	6:E:58:ALA:HB1	2.35	0.56
24:3:14:ARG:HG3	24:3:14:ARG:HH11	1.70	0.56
12:L:62:MET:HE2	30:1:253:G:H4'	1.87	0.55
4:C:9:LEU:HD11	4:C:84:VAL:HG22	1.88	0.55
13:P:71:GLU:OE1	13:P:101:ARG:NH1	2.39	0.55
14:Q:102:ASP:OD2	14:Q:105:ALA:N	2.29	0.55
26:5:4:ARG:HA	26:5:4:ARG:NE	2.21	0.55
30:1:1234:C:O2'	30:1:1235:G:OP1	2.18	0.55
30:1:1075:G:O2'	30:1:1255:A:O2'	2.22	0.55
4:C:143:LYS:NZ	30:1:2271:A:OP1	2.40	0.55
6:E:56:GLU:OE2	6:E:60:ARG:NH2	2.40	0.55
11:O:53:ASP:O	11:O:57:GLY:N	2.34	0.55
11:O:5:VAL:HG22	11:O:6:LYS:H	1.72	0.55
12:L:52:ARG:O	12:L:52:ARG:HG2	2.07	0.55
23:Z:18:ASN:OD1	23:Z:19:HIS:N	2.40	0.55
16:S:79:GLU:O	30:1:24:G:O2'	2.24	0.55
30:1:905:G:N2	30:1:929:A:OP1	2.40	0.55
5:D:182:ASN:ND2	5:D:185:ASP:OD2	2.36	0.54
30:1:2017:G:N2	30:1:2020:A:OP2	2.39	0.54
2:2:48:G:OP1	11:O:78:SER:OG	2.18	0.54
16:S:45:VAL:HB	16:S:46:PRO:HD3	1.90	0.54
7:F:57:ASN:O	7:F:62:ASN:ND2	2.40	0.54
9:J:108:MET:HE2	30:1:1237:G:N3	2.22	0.54
12:L:135:SER:OG	30:1:736:A:OP1	2.19	0.54
14:Q:78:ARG:NE	14:Q:121:VAL:HG11	2.23	0.54
18:U:15:LYS:HA	30:1:392:A:H5'	1.90	0.54
11:O:40:VAL:HG13	11:O:40:VAL:O	2.07	0.54
27:6:24:ARG:NH1	30:1:2580:G:OP1	2.40	0.54
30:1:1658:A:H2'	30:1:1660:C:C5	2.43	0.54
30:1:1850:C:O2	30:1:2917:U:O2'	2.26	0.54
18:U:73:LEU:HD23	18:U:107:ILE:HD13	1.89	0.54
11:O:7:ILE:HG22	11:O:8:ALA:H	1.73	0.53
22:Y:20:GLY:O	22:Y:23:ARG:N	2.41	0.53
7:F:128:SER:OG	7:F:129:PRO:CD	2.56	0.53
8:G:39:TRP:CD1	8:G:40:THR:N	2.77	0.53
14:Q:31:LEU:HD22	30:1:678:C:H5'	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:49:LEU:HD21	19:V:88:VAL:HG21	1.91	0.53
9:J:17:VAL:HG22	9:J:55:ILE:HB	1.91	0.53
9:J:19:ASP:OD1	9:J:58:ASN:ND2	2.37	0.53
14:Q:27:GLN:OE1	30:1:2239:C:H5''	2.09	0.53
4:C:40:GLN:NE2	4:C:53:GLN:OE1	2.40	0.53
5:D:152:LEU:HD11	5:D:193:VAL:HG23	1.90	0.53
30:1:884:G:H5'	30:1:885:G:OP1	2.09	0.52
6:E:78:SER:OG	6:E:86:GLU:N	2.39	0.52
2:2:41:C:O2	6:E:97:ARG:NE	2.42	0.52
16:S:1:MET:HE3	16:S:1:MET:O	2.09	0.52
30:1:275:A:H2	30:1:324:A:HO2'	1.57	0.52
30:1:389:G:H3'	30:1:390:C:C6	2.45	0.52
2:2:7:G:OP1	11:O:37:ARG:NH1	2.41	0.52
27:6:10:ALA:HB2	27:6:61:MET:HE3	1.91	0.52
30:1:683:A:N1	30:1:909:G:O2'	2.37	0.52
27:6:24:ARG:HD3	27:6:50:MET:SD	2.50	0.52
29:N:51:LEU:HD13	29:N:70:ILE:HD11	1.91	0.52
30:1:1989:U:OP2	30:1:1994:A:N6	2.36	0.52
14:Q:83:LEU:HD22	14:Q:88:VAL:HG13	1.92	0.52
3:B:17:SER:O	3:B:211:ARG:NH2	2.43	0.52
13:P:49:ARG:NH2	30:1:2904:G:OP1	2.36	0.52
9:J:42:PRO:O	14:Q:64:ARG:HG2	2.10	0.51
11:O:101:VAL:HG13	11:O:101:VAL:O	2.11	0.51
22:Y:28:GLU:O	22:Y:32:LEU:HD23	2.10	0.51
7:F:90:ILE:HD11	7:F:132:PHE:CE2	2.46	0.51
14:Q:74:ILE:HG21	14:Q:110:VAL:HG23	1.92	0.51
24:3:3:VAL:CG1	30:1:2236:U:H1'	2.40	0.51
30:1:195:G:O2'	30:1:902:A:N3	2.43	0.51
30:1:892:A:C8	30:1:2659:C:O2	2.64	0.51
6:E:108:THR:HG23	6:E:109:LEU:N	2.26	0.51
9:J:73:MET:SD	9:J:88:ARG:HG3	2.51	0.51
18:U:67:HIS:CD2	30:1:411:U:H4'	2.45	0.51
30:1:2796:A:O4'	30:1:2831:C:N4	2.43	0.51
6:E:47:ASP:O	6:E:47:ASP:OD2	2.29	0.51
30:1:934:C:C2	30:1:935:A:C8	2.98	0.51
14:Q:6:ARG:NH1	30:1:682:G:OP2	2.43	0.51
30:1:3073:G:N2	30:1:3076:A:OP2	2.32	0.51
27:6:30:ARG:NH1	30:1:2613:C:OP2	2.44	0.51
2:2:9:U:C5	2:2:10:C:N3	2.79	0.51
9:J:114:LEU:HG	9:J:118:MET:HE3	1.93	0.51
16:S:93:ARG:NH2	30:1:847:U:O2'	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:800:G:O2'	30:1:1844:A:N3	2.39	0.51
3:B:218:ARG:NH2	30:1:881:A:OP1	2.44	0.50
10:K:4:GLN:HG2	10:K:5:GLU:OE1	2.10	0.50
18:U:34:LEU:HD23	18:U:65:PRO:HA	1.91	0.50
30:1:389:G:O3'	30:1:390:C:O4'	2.29	0.50
1:M:59:LYS:O	1:M:60:ARG:HG2	2.11	0.50
30:1:1399:A:O2'	30:1:1438:G:N2	2.42	0.50
11:O:7:ILE:HG22	11:O:8:ALA:N	2.26	0.50
30:1:498:G:O2'	30:1:2626:G:OP2	2.28	0.50
13:P:27:ASN:ND2	13:P:42:GLN:OE1	2.44	0.50
14:Q:121:VAL:HG12	14:Q:121:VAL:O	2.12	0.50
6:E:37:VAL:HG12	6:E:38:LYS:HG2	1.93	0.50
7:F:108:LEU:HD13	7:F:153:ARG:HB3	1.94	0.50
11:O:5:VAL:HG22	11:O:6:LYS:N	2.27	0.50
23:Z:47:VAL:HG11	23:Z:56:VAL:HG11	1.93	0.50
27:6:43:ARG:NH2	30:1:2582:U:OP2	2.33	0.50
2:2:10:C:N3	11:O:3:TYR:HE1	2.10	0.50
2:2:49:G:OP1	11:O:76:ASP:HA	2.11	0.50
30:1:2253:A:O2'	30:1:2255:G:OP2	2.23	0.50
4:C:184:VAL:HG13	4:C:184:VAL:O	2.12	0.50
11:O:42:ARG:HD3	11:O:112:ARG:HH21	1.77	0.50
19:V:156:ILE:HD11	19:V:172:VAL:HG11	1.93	0.50
18:U:15:LYS:NZ	30:1:587:A:OP1	2.37	0.50
2:2:37:A:C2	2:2:42:G:C2	2.99	0.49
9:J:107:GLY:O	9:J:111:LYS:NZ	2.45	0.49
7:F:2:SER:OG	7:F:66:HIS:ND1	2.45	0.49
4:C:159:VAL:HG21	30:1:2837:G:H21	1.77	0.49
10:K:115:ILE:HG23	10:K:121:VAL:HG21	1.94	0.49
29:N:43:ARG:HA	29:N:43:ARG:NE	2.27	0.49
30:1:2462:U:H2'	30:1:2463:U:C6	2.47	0.49
7:F:30:LYS:NZ	7:F:82:GLN:O	2.38	0.49
7:F:128:SER:OG	7:F:129:PRO:HD3	2.13	0.49
30:1:1858:U:H4'	30:1:1859:U:OP1	2.12	0.49
6:E:11:THR:O	6:E:15:GLU:OE1	2.30	0.49
30:1:360:C:O2'	30:1:362:G:N2	2.39	0.49
30:1:389:G:H2'	30:1:390:C:N1	2.27	0.49
30:1:2747:U:O2'	30:1:2749:G:OP1	2.25	0.49
6:E:140:GLN:O	6:E:140:GLN:NE2	2.46	0.49
30:1:2505:A:H4'	30:1:2506:A:O4'	2.12	0.49
30:1:2649:A:N3	30:1:2649:A:H2'	2.28	0.49
9:J:49:ASP:OD2	9:J:121:LYS:NZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:73:LEU:HD21	18:U:98:ARG:NH1	2.28	0.49
30:1:1642:C:O2'	30:1:1783:A:OP2	2.19	0.49
30:1:2049:G:C2	30:1:2050:G:C8	3.01	0.49
1:M:34:ILE:HD11	1:M:118:LEU:HB3	1.94	0.48
3:B:175:LEU:HD12	3:B:185:VAL:HG21	1.95	0.48
27:6:40:LEU:O	27:6:40:LEU:HD23	2.12	0.48
30:1:390:C:O2'	30:1:391:G:C8	2.63	0.48
5:D:58:ARG:HD3	30:1:540:G:C8	2.48	0.48
6:E:11:THR:O	6:E:14:ARG:N	2.46	0.48
9:J:132:HIS:ND1	30:1:7:G:H5'	2.28	0.48
30:1:161:G:O2'	30:1:162:A:P	2.70	0.48
30:1:2623:C:H2'	30:1:2624:U:H5''	1.94	0.48
2:2:73:G:O2'	19:V:11:ARG:NH2	2.46	0.48
7:F:32:THR:O	7:F:33:LEU:HD22	2.13	0.48
7:F:140:GLN:NE2	30:1:2964:C:O2	2.47	0.48
4:C:82:HIS:CG	4:C:204:LEU:HD22	2.48	0.48
15:R:14:VAL:HG12	15:R:20:VAL:HG11	1.96	0.48
3:B:256:ARG:CZ	3:B:271:ARG:NH2	2.77	0.48
14:Q:6:ARG:NH2	30:1:682:G:N7	2.61	0.48
30:1:968:U:O2'	30:1:969:G:P	2.72	0.48
3:B:181:GLU:OE2	30:1:2009:G:O2'	2.19	0.48
5:D:18:GLU:HA	5:D:18:GLU:OE2	2.13	0.48
9:J:3:THR:HG21	14:Q:61:TRP:NE1	2.25	0.48
12:L:35:THR:OG1	30:1:1302:G:OP1	2.31	0.48
1:M:13:HIS:CD2	30:1:1009:A:C5	3.02	0.47
2:2:22:G:N7	2:2:54:U:H2'	2.29	0.47
3:B:272:ARG:HH11	3:B:272:ARG:HG2	1.79	0.47
30:1:31:C:O2'	30:1:1350:C:OP1	2.32	0.47
30:1:222:A:N3	30:1:237:U:O2'	2.36	0.47
30:1:2666:G:O2'	30:1:2719:U:OP2	2.30	0.47
2:2:102:U:O3'	19:V:74:LYS:NZ	2.45	0.47
3:B:183:ARG:NH2	30:1:2010:C:OP2	2.45	0.47
30:1:666:U:O2'	30:1:1082:A:N1	2.42	0.47
30:1:738:U:H2'	30:1:739:C:C6	2.49	0.47
11:O:103:ASP:C	11:O:103:ASP:OD1	2.55	0.47
30:1:1111:C:O2'	30:1:1112:G:OP1	2.28	0.47
16:S:85:ARG:HG2	16:S:85:ARG:HH11	1.79	0.47
19:V:103:ILE:HD12	19:V:127:VAL:CG2	2.44	0.47
23:Z:40:ARG:HH11	23:Z:40:ARG:HG2	1.80	0.47
5:D:111:ARG:HG3	5:D:111:ARG:HH11	1.80	0.47
14:Q:21:ALA:HA	14:Q:24:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:162:A:OP2	30:1:167:A:N6	2.48	0.47
30:1:740:C:O2'	30:1:2569:U:OP1	2.27	0.47
30:1:2972:A:H2'	30:1:2973:U:O4'	2.14	0.47
2:2:85:G:N2	2:2:88:A:OP2	2.40	0.47
5:D:137:LYS:NZ	30:1:403:G:OP2	2.44	0.47
6:E:116:ILE:CG1	6:E:142:MET:HE3	2.44	0.47
9:J:7:LYS:HB3	9:J:8:PRO:CD	2.44	0.47
20:W:16:SER:OG	30:1:2481:U:OP2	2.26	0.47
30:1:1080:A:OP2	30:1:1081:C:N4	2.47	0.47
19:V:158:LEU:HD11	19:V:164:LEU:CD1	2.39	0.47
23:Z:4:LEU:HD21	23:Z:44:ARG:NH2	2.30	0.47
30:1:95:G:H2'	30:1:96:A:O4'	2.15	0.47
30:1:117:G:P	30:1:119:A:HO2'	2.36	0.47
30:1:162:A:C8	30:1:169:A:C6	3.03	0.47
30:1:843:G:O2'	30:1:1871:U:OP1	2.32	0.47
30:1:1497:C:H2'	30:1:1498:C:C6	2.50	0.47
30:1:1932:A:H2'	30:1:1933:U:O4'	2.15	0.47
19:V:128:GLU:OE2	19:V:163:SER:OG	2.26	0.47
30:1:1127:A:N6	30:1:1224:G:H2'	2.30	0.47
30:1:2000:C:H2'	30:1:2001:A:C8	2.50	0.47
30:1:2858:A:H2'	30:1:2859:G:O4'	2.15	0.47
30:1:2907:G:O2'	30:1:2909:G:N7	2.48	0.47
3:B:211:ARG:NH1	30:1:1780:G:OP1	2.47	0.47
30:1:606:G:H2'	30:1:607:U:O4'	2.15	0.47
30:1:959:G:O2'	30:1:1015:G:O6	2.19	0.47
30:1:2743:G:O6	30:1:2759:C:N4	2.48	0.47
1:M:30:GLY:N	1:M:105:GLU:OE1	2.34	0.46
6:E:11:THR:O	6:E:12:LYS:C	2.58	0.46
6:E:62:LEU:O	6:E:66:THR:HG22	2.15	0.46
7:F:68:LEU:C	7:F:68:LEU:HD23	2.40	0.46
9:J:60:ASP:OD2	9:J:60:ASP:N	2.48	0.46
11:O:32:THR:OG1	11:O:35:ARG:O	2.30	0.46
11:O:47:ILE:HG23	11:O:47:ILE:O	2.14	0.46
30:1:469:G:O2'	30:1:470:G:H5'	2.15	0.46
30:1:2725:U:O2'	30:1:2726:C:O5'	2.29	0.46
2:2:38:U:N3	2:2:42:G:OP2	2.48	0.46
3:B:143:HIS:ND1	3:B:194:GLY:O	2.37	0.46
30:1:2924:A:O2'	30:1:3068:G:OP1	2.29	0.46
21:X:22:HIS:O	21:X:22:HIS:ND1	2.42	0.46
30:1:618:C:N4	30:1:2240:A:N3	2.61	0.46
6:E:164:THR:O	6:E:164:THR:CG2	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:46:VAL:O	13:P:61:VAL:HA	2.16	0.46
23:Z:25:SER:O	30:1:1027:G:O2'	2.32	0.46
30:1:893:A:OP2	30:1:2290:A:O2'	2.33	0.46
30:1:1672:U:H5'	30:1:1673:U:OP1	2.14	0.46
5:D:172:GLN:OE1	5:D:172:GLN:HA	2.15	0.46
6:E:42:ASN:HD22	30:1:2532:C:C1'	2.29	0.46
13:P:2:SER:OG	13:P:5:LEU:HB3	2.15	0.46
14:Q:89:GLU:O	14:Q:89:GLU:HG2	2.15	0.46
22:Y:7:ALA:N	22:Y:9:GLU:OE2	2.49	0.46
6:E:28:GLU:CD	6:E:28:GLU:H	2.24	0.46
30:1:745:A:H2'	30:1:746:G:C8	2.50	0.46
30:1:1421:G:N2	30:1:1424:U:C4	2.84	0.46
30:1:2538:U:O2	30:1:2538:U:O4'	2.33	0.46
11:O:6:LYS:CD	30:1:2538:U:C5	2.98	0.46
11:O:35:ARG:O	11:O:35:ARG:HG3	2.15	0.46
16:S:65:THR:HG23	16:S:66:ASP:N	2.30	0.46
19:V:51:MET:HE3	19:V:51:MET:HA	1.98	0.46
21:X:28:ARG:NH2	30:1:1476:A:OP1	2.49	0.46
22:Y:23:ARG:HG3	22:Y:23:ARG:HH11	1.80	0.46
3:B:258:ARG:NH1	30:1:2009:G:OP1	2.47	0.46
8:G:18:VAL:HG13	8:G:18:VAL:O	2.15	0.46
18:U:20:GLN:OE1	18:U:20:GLN:N	2.48	0.46
30:1:35:G:H1'	30:1:542:A:C4	2.51	0.46
2:2:39:U:C5	6:E:71:ALA:HB1	2.50	0.46
4:C:125:VAL:HG13	4:C:126:MET:N	2.31	0.46
13:P:46:VAL:HG12	13:P:47:VAL:N	2.31	0.45
3:B:252:GLN:OE1	3:B:252:GLN:HA	2.16	0.45
9:J:114:LEU:N	30:1:655:U:OP1	2.49	0.45
10:K:107:ARG:HG2	10:K:115:ILE:HD13	1.99	0.45
13:P:40:ILE:O	13:P:40:ILE:HG22	2.16	0.45
30:1:226:A:N1	30:1:495:G:O2'	2.45	0.45
30:1:1937:U:C2	30:1:1944:G:N2	2.84	0.45
30:1:1121:G:H1'	30:1:1123:G:O6	2.16	0.45
30:1:1268:G:C6	30:1:1294:G:C6	3.04	0.45
7:F:70:ARG:HH11	7:F:70:ARG:HG2	1.82	0.45
8:G:23:ASP:OD2	8:G:23:ASP:C	2.60	0.45
12:L:67:LEU:HD11	27:6:15:LYS:HB3	1.98	0.45
16:S:51:LEU:CD1	16:S:72:ILE:HD11	2.46	0.45
30:1:607:U:H2'	30:1:608:G:C8	2.52	0.45
30:1:928:U:H2'	30:1:929:A:C8	2.52	0.45
30:1:2665:G:N2	30:1:2668:U:O2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:2708:G:O2'	30:1:2709:G:H5'	2.17	0.45
6:E:43:MET:HE2	6:E:58:ALA:CB	2.44	0.45
6:E:84:LEU:HD12	6:E:88:GLN:HE21	1.82	0.45
6:E:116:ILE:HG12	6:E:142:MET:HE3	1.99	0.45
6:E:117:ARG:HH11	6:E:117:ARG:HG2	1.81	0.45
10:K:2:ILE:HD13	10:K:8:LEU:CD2	2.43	0.45
18:U:15:LYS:HG3	30:1:392:A:OP1	2.16	0.45
30:1:469:G:C2	30:1:482:C:C2	3.05	0.45
30:1:1452:A:OP1	30:1:1508:U:N3	2.43	0.45
30:1:2485:A:H4'	30:1:2486:A:N3	2.31	0.45
9:J:3:THR:HG23	30:1:1094:C:O2	2.16	0.45
19:V:100:ASN:OD1	19:V:100:ASN:O	2.35	0.45
30:1:219:A:C8	30:1:520:A:N6	2.85	0.45
30:1:465:A:N6	30:1:486:G:O6	2.50	0.45
30:1:932:U:H2'	30:1:933:G:H8	1.82	0.45
30:1:1692:A:N6	30:1:1730:G:O2'	2.44	0.45
30:1:2485:A:H4'	30:1:2486:A:O5'	2.16	0.45
30:1:2725:U:O2'	30:1:2726:C:O4'	2.34	0.45
6:E:10:LYS:HD3	6:E:102:TRP:NE1	2.32	0.45
6:E:137:LEU:HD22	6:E:142:MET:HE1	1.99	0.45
9:J:77:HIS:CE1	30:1:1230:G:C5	3.05	0.45
11:O:77:LYS:HB2	11:O:112:ARG:HD3	1.99	0.45
12:L:121:VAL:HG21	12:L:125:LEU:HD13	1.99	0.45
30:1:451:G:N2	30:1:452:A:H1'	2.32	0.45
30:1:1820:A:H1'	30:1:1822:A:OP2	2.17	0.45
12:L:119:GLY:O	12:L:139:LYS:NZ	2.41	0.45
18:U:76:GLU:OE1	18:U:76:GLU:HA	2.16	0.45
30:1:250:G:OP2	30:1:252:C:N4	2.50	0.45
2:2:11:A:N1	2:2:67:G:O2'	2.37	0.45
7:F:36:THR:HG23	7:F:36:THR:O	2.17	0.45
12:L:38:ARG:CZ	30:1:684:G:H22	2.30	0.45
12:L:86:LEU:O	12:L:86:LEU:HD12	2.17	0.45
27:6:40:LEU:HD23	27:6:40:LEU:C	2.42	0.45
30:1:324:A:C4	30:1:325:U:C6	3.05	0.45
30:1:563:G:N1	30:1:566:A:OP2	2.48	0.45
30:1:2510:U:OP1	30:1:2599:U:O2'	2.35	0.45
5:D:148:GLU:CD	5:D:148:GLU:H	2.25	0.44
16:S:1:MET:O	16:S:1:MET:SD	2.75	0.44
19:V:166:VAL:HG22	19:V:167:GLU:N	2.32	0.44
24:3:16:ARG:HH22	30:1:1376:G:P	2.37	0.44
26:5:17:HIS:HB2	26:5:45:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:585:U:H2'	30:1:586:G:O4'	2.17	0.44
16:S:6:GLN:OE1	16:S:105:THR:OG1	2.34	0.44
30:1:272:C:N4	30:1:317:U:O2	2.50	0.44
30:1:369:U:H2'	30:1:370:U:O4'	2.17	0.44
30:1:1110:G:C4	30:1:1112:G:C8	3.05	0.44
6:E:30:VAL:O	6:E:33:VAL:HG23	2.17	0.44
11:O:83:GLN:O	11:O:87:LEU:HG	2.18	0.44
11:O:103:ASP:OD1	11:O:103:ASP:O	2.35	0.44
13:P:2:SER:HB3	30:1:3091:C:H4'	1.98	0.44
17:T:33:GLU:OE2	17:T:33:GLU:HA	2.17	0.44
19:V:23:ARG:HG3	19:V:23:ARG:HH11	1.82	0.44
26:5:42:ARG:O	26:5:42:ARG:HG3	2.17	0.44
30:1:487:U:H2'	30:1:488:G:O4'	2.18	0.44
30:1:920:A:H4'	30:1:936:G:N2	2.33	0.44
30:1:2056:G:H2'	30:1:2057:A:O4'	2.18	0.44
30:1:2283:C:H2'	30:1:2283:C:O2	2.16	0.44
9:J:72:LYS:NZ	30:1:1238:G:OP2	2.46	0.44
20:W:63:GLN:O	20:W:80:ILE:HG21	2.18	0.44
30:1:325:U:C2	30:1:326:C:C5	3.05	0.44
30:1:429:A:C4	30:1:430:A:C8	3.05	0.44
30:1:3065:G:N7	30:1:3083:G:N2	2.63	0.44
4:C:142:ARG:HG3	4:C:142:ARG:HH11	1.82	0.44
5:D:150:LYS:O	5:D:172:GLN:HB3	2.18	0.44
26:5:15:LYS:NZ	30:1:871:G:OP1	2.40	0.44
5:D:49:HIS:ND1	5:D:92:PRO:HB2	2.33	0.44
17:T:35:LYS:NZ	17:T:92:THR:OG1	2.49	0.44
26:5:13:ARG:O	26:5:13:ARG:HG2	2.17	0.44
30:1:1065:A:O4'	30:1:2486:A:N6	2.50	0.44
30:1:2517:A:N6	30:1:2537:G:O2'	2.51	0.44
6:E:60:ARG:HG3	6:E:60:ARG:HH11	1.83	0.44
11:O:70:ILE:HD11	11:O:87:LEU:HD11	2.00	0.44
16:S:29:ALA:HB1	16:S:55:ILE:HD11	1.99	0.44
17:T:23:VAL:HG13	17:T:23:VAL:O	2.17	0.44
30:1:719:A:H4'	30:1:720:A:C5'	2.48	0.44
30:1:1778:U:H2'	30:1:1779:C:C6	2.53	0.44
30:1:3034:A:O2'	30:1:3035:G:H5'	2.18	0.44
5:D:46:GLN:HG2	5:D:48:THR:HG23	2.00	0.44
30:1:324:A:C5	30:1:325:U:C5	3.05	0.44
30:1:2779:C:N4	30:1:2780:A:H62	2.16	0.44
9:J:7:LYS:HB3	9:J:8:PRO:HD2	2.00	0.44
30:1:429:A:C5	30:1:430:A:C8	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:2546:A:H2'	30:1:2547:A:C8	2.52	0.44
30:1:3054:G:C4	30:1:3055:G:C8	3.06	0.44
2:2:26:C:H2'	2:2:27:G:O4'	2.18	0.43
4:C:40:GLN:HB3	4:C:53:GLN:OE1	2.18	0.43
11:O:7:ILE:HD13	11:O:20:ARG:HD2	2.00	0.43
21:X:35:ARG:NH1	21:X:35:ARG:HB3	2.33	0.43
29:N:103:ARG:HG2	29:N:104:ARG:O	2.18	0.43
30:1:1894:C:H2'	30:1:1895:C:C6	2.53	0.43
30:1:2673:G:C6	30:1:2718:C:N4	2.86	0.43
1:M:28:ALA:O	1:M:134:ARG:NH2	2.51	0.43
5:D:180:GLN:NE2	30:1:711:G:O2'	2.50	0.43
11:O:70:ILE:CD1	11:O:87:LEU:HD11	2.47	0.43
28:7:30:LEU:CD1	30:1:2746:C:OP1	2.66	0.43
30:1:578:A:H2'	30:1:579:G:O4'	2.19	0.43
30:1:745:A:H2'	30:1:746:G:O4'	2.18	0.43
30:1:1932:A:C6	30:1:1949:A:C8	3.06	0.43
30:1:2693:C:H2'	30:1:2694:C:O5'	2.18	0.43
30:1:3009:A:H4'	30:1:3010:C:H5''	1.99	0.43
4:C:9:LEU:HD12	4:C:54:ILE:CD1	2.48	0.43
30:1:223:G:C5	30:1:515:U:H5	2.36	0.43
30:1:913:U:O2'	30:1:1336:A:H1'	2.18	0.43
4:C:132:ARG:HG3	4:C:132:ARG:HH11	1.83	0.43
7:F:90:ILE:HD11	7:F:132:PHE:CD2	2.54	0.43
30:1:266:U:H2'	30:1:267:G:O4'	2.18	0.43
30:1:319:G:N2	30:1:321:G:C8	2.87	0.43
30:1:368:G:H2'	30:1:369:U:C6	2.53	0.43
30:1:920:A:H4'	30:1:936:G:H22	1.83	0.43
30:1:1496:A:H1'	30:1:1497:C:C6	2.54	0.43
30:1:2012:A:H2'	30:1:2013:A:C8	2.53	0.43
30:1:2293:U:O2'	30:1:2816:G:H1'	2.19	0.43
30:1:2547:A:H2'	30:1:2548:G:C8	2.53	0.43
6:E:116:ILE:HB	6:E:119:PHE:HB2	2.00	0.43
14:Q:74:ILE:HG23	14:Q:74:ILE:O	2.18	0.43
30:1:1675:U:H4'	30:1:1676:C:OP2	2.18	0.43
30:1:1982:G:N2	30:1:1984:C:H5''	2.33	0.43
30:1:2478:G:C8	30:1:2646:C:C4	3.07	0.43
30:1:2863:G:O2'	30:1:2864:G:H5'	2.19	0.43
25:4:26:LYS:O	25:4:26:LYS:HG3	2.19	0.43
30:1:208:G:HO2'	30:1:209:U:P	2.41	0.43
30:1:244:A:O4'	30:1:246:U:C6	2.72	0.43
30:1:520:A:C6	30:1:521:U:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:685:U:H2'	30:1:686:U:C6	2.52	0.43
30:1:2464:U:H5''	30:1:2465:A:H5'	2.01	0.43
2:2:46:C:P	11:O:42:ARG:HH12	2.41	0.43
5:D:45:ARG:HD2	30:1:531:A:C5	2.54	0.43
30:1:61:G:O2'	30:1:62:G:H5'	2.18	0.43
3:B:49:VAL:HG23	3:B:49:VAL:O	2.18	0.43
12:L:27:ARG:NH1	30:1:911:U:C4	2.87	0.43
24:3:3:VAL:HG11	30:1:2236:U:O4'	2.18	0.43
28:7:6:SER:HB2	30:1:2685:C:H5''	2.00	0.43
30:1:1046:A:H2'	30:1:1047:C:C6	2.53	0.43
25:4:37:MET:HE1	30:1:2505:A:C2	2.54	0.43
30:1:325:U:N3	30:1:326:C:C5	2.86	0.43
30:1:2865:C:OP2	30:1:2951:G:O2'	2.36	0.43
30:1:2880:G:H2'	30:1:2881:A:O4'	2.19	0.43
30:1:3083:G:O2'	30:1:3084:A:OP2	2.32	0.43
1:M:43:THR:HG22	1:M:94:VAL:HG12	2.01	0.43
7:F:19:ILE:HD12	7:F:19:ILE:N	2.34	0.43
9:J:6:PRO:HG2	9:J:48:VAL:HG21	1.99	0.43
15:R:45:ASP:OD1	15:R:45:ASP:O	2.37	0.43
21:X:40:VAL:HG23	21:X:40:VAL:O	2.19	0.43
25:4:22:TYR:OH	25:4:40:HIS:O	2.36	0.43
30:1:968:U:H2'	30:1:969:G:O4'	2.19	0.43
30:1:1719:A:H2'	30:1:1720:C:O4'	2.19	0.43
30:1:2540:G:H5'	30:1:2541:A:OP2	2.19	0.43
6:E:127:PHE:CZ	6:E:175:LEU:HD12	2.53	0.42
11:O:40:VAL:O	11:O:40:VAL:CG1	2.67	0.42
13:P:48:ILE:HD11	13:P:60:THR:HG21	2.01	0.42
14:Q:94:ILE:CD1	15:R:4:ILE:HG21	2.49	0.42
17:T:59:VAL:HG22	17:T:60:LYS:N	2.34	0.42
4:C:104:VAL:HG13	4:C:105:PHE:CD2	2.54	0.42
5:D:156:VAL:HG23	5:D:164:TRP:NE1	2.34	0.42
6:E:20:LYS:HD3	6:E:177:HIS:CD2	2.54	0.42
7:F:53:VAL:HG11	7:F:70:ARG:HB2	2.01	0.42
18:U:73:LEU:HD22	18:U:86:VAL:HG21	2.01	0.42
30:1:23:G:C6	30:1:604:G:C6	3.07	0.42
30:1:407:A:N6	30:1:422:U:O4'	2.52	0.42
30:1:719:A:H2'	30:1:719:A:N3	2.34	0.42
30:1:2290:A:H2'	30:1:2291:C:C6	2.54	0.42
4:C:13:LEU:HD22	13:P:1:MET:O	2.18	0.42
22:Y:9:GLU:HG2	22:Y:10:LEU:HD22	2.01	0.42
26:5:12:ARG:O	26:5:12:ARG:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:389:G:H2'	30:1:390:C:C1'	2.48	0.42
30:1:1434:A:O2'	30:1:1435:G:H5'	2.19	0.42
30:1:1671:G:C2'	30:1:1672:U:O5'	2.67	0.42
30:1:2681:U:H2'	30:1:2682:U:C6	2.54	0.42
3:B:73:ASP:OD1	3:B:190:ARG:NH2	2.52	0.42
16:S:4:ARG:HB3	16:S:107:VAL:HG22	2.00	0.42
19:V:25:GLU:O	19:V:25:GLU:HG2	2.19	0.42
30:1:735:G:O2'	30:1:737:G:O2'	2.34	0.42
30:1:2464:U:O2'	30:1:2655:G:OP2	2.32	0.42
30:1:2917:U:H2'	30:1:2918:U:C6	2.54	0.42
30:1:222:A:C6	30:1:223:G:C6	3.07	0.42
3:B:16:SER:HB3	3:B:207:GLY:HA3	2.02	0.42
6:E:84:LEU:HD11	6:E:90:ILE:HG21	2.02	0.42
9:J:123:LYS:N	9:J:123:LYS:HD2	2.35	0.42
29:N:35:THR:O	29:N:35:THR:HG23	2.20	0.42
30:1:319:G:C2	30:1:509:U:H5	2.38	0.42
30:1:2052:G:H2'	30:1:2053:C:H6	1.84	0.42
30:1:2731:C:H2'	30:1:2732:G:O4'	2.20	0.42
30:1:2968:A:OP2	30:1:2969:A:O2'	2.35	0.42
12:L:31:SER:OG	12:L:32:LYS:N	2.53	0.42
14:Q:83:LEU:HD22	14:Q:88:VAL:CG1	2.49	0.42
29:N:59:ASP:OD1	29:N:62:ASN:ND2	2.51	0.42
30:1:503:A:H2'	30:1:504:C:C6	2.55	0.42
30:1:1433:A:N1	30:1:1444:C:O2'	2.46	0.42
3:B:124:ASP:OD2	3:B:124:ASP:C	2.61	0.42
6:E:66:THR:OG1	6:E:96:LEU:HD21	2.20	0.42
6:E:175:LEU:O	6:E:180:PHE:HD1	2.02	0.42
7:F:84:TYR:CE2	7:F:139:LYS:HB2	2.54	0.42
11:O:77:LYS:CB	11:O:112:ARG:HD3	2.49	0.42
13:P:31:ARG:NH2	13:P:82:GLU:OE2	2.44	0.42
30:1:390:C:H2'	30:1:391:G:H8	1.85	0.42
30:1:474:G:H4'	30:1:475:A:OP2	2.19	0.42
30:1:1496:A:C6	30:1:1514:A:C6	3.08	0.42
30:1:2854:A:C2	30:1:3003:G:C6	3.08	0.42
6:E:175:LEU:HD22	6:E:180:PHE:CE1	2.54	0.42
9:J:132:HIS:CE1	30:1:7:G:H5'	2.55	0.42
29:N:97:ILE:O	29:N:97:ILE:HG23	2.20	0.42
30:1:677:C:H2'	30:1:678:C:C6	2.54	0.42
30:1:1880:A:H4'	30:1:1881:A:O5'	2.20	0.42
30:1:2741:U:O2'	30:1:2866:U:OP1	2.28	0.42
11:O:6:LYS:HD3	30:1:2538:U:C5	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:53:ARG:HA	14:Q:56:ASP:HB3	2.00	0.42
30:1:154:C:H2'	30:1:155:A:H8	1.85	0.42
30:1:391:G:OP1	30:1:587:A:H4'	2.19	0.42
30:1:465:A:C6	30:1:486:G:C6	3.07	0.42
30:1:913:U:H2'	30:1:914:C:C6	2.55	0.42
30:1:1083:G:N3	30:1:1083:G:H2'	2.35	0.42
30:1:1470:A:OP2	30:1:1482:G:N2	2.46	0.42
30:1:1472:G:H2'	30:1:1473:C:C6	2.55	0.42
30:1:1984:C:O2	30:1:1984:C:H2'	2.20	0.42
30:1:2284:C:H2'	30:1:2285:C:C6	2.55	0.42
30:1:2465:A:H2'	30:1:2466:A:C8	2.55	0.42
6:E:13:TYR:HA	6:E:17:ILE:HB	2.02	0.41
30:1:31:C:C4	30:1:32:C:C5	3.08	0.41
30:1:268:A:H4'	30:1:269:G:OP1	2.19	0.41
30:1:316:G:C2	30:1:317:U:O4	2.73	0.41
30:1:2918:U:H2'	30:1:2919:C:C6	2.55	0.41
2:2:52:G:N2	6:E:31:MET:SD	2.93	0.41
3:B:186:ASP:OD2	3:B:187:VAL:N	2.53	0.41
4:C:153:CYS:O	4:C:155:THR:N	2.54	0.41
5:D:100:ARG:O	30:1:759:G:H4'	2.20	0.41
18:U:88:TYR:CD2	30:1:379:C:OP1	2.74	0.41
19:V:23:ARG:HG3	19:V:23:ARG:NH1	2.35	0.41
30:1:112:U:H2'	30:1:113:G:O4'	2.21	0.41
30:1:742:A:N1	30:1:2588:A:O2'	2.47	0.41
30:1:1430:G:H2'	30:1:1431:U:C6	2.55	0.41
30:1:1496:A:C6	30:1:1514:A:C5	3.08	0.41
30:1:1876:A:H1'	30:1:2904:G:O2'	2.21	0.41
30:1:2295:U:OP2	30:1:2457:G:N2	2.41	0.41
2:2:43:A:C4	2:2:44:A:C8	3.08	0.41
9:J:122:LEU:CD2	9:J:124:VAL:HG13	2.49	0.41
9:J:135:GLN:NE2	30:1:7:G:H1'	2.36	0.41
10:K:12:ASP:OD2	10:K:14:THR:HG23	2.21	0.41
19:V:13:GLU:HA	19:V:13:GLU:OE2	2.20	0.41
30:1:44:A:H2'	30:1:45:A:O4'	2.20	0.41
30:1:320:U:OP2	30:1:508:C:OP2	2.38	0.41
30:1:672:A:C2	30:1:673:U:C5	3.08	0.41
30:1:1505:U:H2'	30:1:1506:A:O4'	2.20	0.41
4:C:132:ARG:HG3	4:C:132:ARG:NH1	2.34	0.41
5:D:45:ARG:NH2	30:1:532:C:OP1	2.45	0.41
11:O:37:ARG:HG2	11:O:39:VAL:HG23	2.02	0.41
14:Q:78:ARG:CD	14:Q:121:VAL:HG11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:2548:G:H2'	30:1:2549:U:C6	2.55	0.41
4:C:20:ASP:OD1	4:C:20:ASP:N	2.52	0.41
15:R:24:LYS:NZ	30:1:1263:U:OP1	2.54	0.41
22:Y:20:GLY:O	22:Y:24:GLU:OE1	2.38	0.41
30:1:521:U:O2'	30:1:522:U:H5'	2.21	0.41
30:1:1057:U:HO2'	30:1:1058:A:P	2.44	0.41
30:1:1646:G:H2'	30:1:1647:G:C8	2.55	0.41
30:1:1689:U:O2'	30:1:1690:G:H5'	2.21	0.41
30:1:1821:A:H4'	30:1:1822:A:OP1	2.20	0.41
30:1:2878:G:N2	30:1:2881:A:OP2	2.50	0.41
6:E:45:VAL:O	6:E:45:VAL:HG13	2.21	0.41
9:J:21:GLN:OE1	9:J:21:GLN:HA	2.20	0.41
9:J:36:LEU:HD11	9:J:122:LEU:HB2	2.03	0.41
9:J:62:VAL:O	9:J:62:VAL:HG23	2.21	0.41
11:O:78:SER:HA	11:O:112:ARG:HG2	2.03	0.41
30:1:224:A:C4	30:1:269:G:N7	2.88	0.41
30:1:2074:U:OP1	30:1:2629:G:O2'	2.33	0.41
30:1:2888:G:C2'	30:1:2889:G:O5'	2.69	0.41
30:1:2975:U:H4'	30:1:2976:A:OP1	2.21	0.41
4:C:147:PRO:O	30:1:2730:U:O2'	2.38	0.41
7:F:71:THR:HG21	30:1:2966:G:O3'	2.21	0.41
7:F:111:SER:OG	30:1:2886:C:O2	2.35	0.41
10:K:1:MET:HE1	30:1:1876:A:H2	1.86	0.41
9:J:68:LYS:NZ	30:1:1239:C:OP2	2.47	0.41
18:U:40:ARG:HA	18:U:63:GLU:HA	2.03	0.41
22:Y:11:ARG:O	22:Y:64:ARG:NH2	2.53	0.41
30:1:502:C:H2'	30:1:503:A:C8	2.56	0.41
30:1:2693:C:C2'	30:1:2694:C:O5'	2.69	0.41
30:1:2735:G:O2'	30:1:2736:C:H5'	2.21	0.41
30:1:3007:C:N4	30:1:3008:C:N4	2.69	0.41
2:2:78:U:O4	19:V:16:LYS:NZ	2.53	0.41
4:C:182:HIS:N	4:C:192:LEU:O	2.51	0.41
6:E:8:ARG:O	6:E:11:THR:OG1	2.38	0.41
6:E:43:MET:SD	6:E:43:MET:C	3.04	0.41
8:G:20:ASP:OD2	8:G:20:ASP:C	2.64	0.41
9:J:27:ARG:NH1	30:1:1111:C:O2	2.54	0.41
10:K:13:ASN:ND2	10:K:97:ARG:HB3	2.36	0.41
10:K:107:ARG:NH1	10:K:107:ARG:HB3	2.35	0.41
18:U:62:VAL:HG12	18:U:63:GLU:N	2.35	0.41
19:V:79:ASP:OD1	19:V:80:PRO:HD2	2.21	0.41
19:V:112:ALA:HB2	19:V:144:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:81:G:H2'	30:1:82:G:O4'	2.21	0.41
30:1:539:C:N4	30:1:542:A:OP2	2.36	0.41
30:1:1489:A:O2'	30:1:1490:U:OP2	2.28	0.41
30:1:1917:G:O2'	30:1:1918:G:H5'	2.21	0.41
30:1:2212:G:N2	30:1:2216:C:O2'	2.54	0.41
30:1:2622:G:N2	30:1:2634:G:H1'	2.36	0.41
30:1:2674:G:C4	30:1:2675:C:C5	3.09	0.41
30:1:2782:U:O2	30:1:2785:A:C5	2.74	0.41
30:1:2807:G:O6	30:1:2826:G:C6	2.73	0.41
6:E:5:THR:O	6:E:5:THR:HG23	2.21	0.41
7:F:97:VAL:HG13	7:F:97:VAL:O	2.21	0.41
14:Q:61:TRP:CZ2	14:Q:93:LYS:HG3	2.56	0.41
30:1:1124:G:H4'	30:1:1125:G:OP2	2.21	0.41
30:1:1699:G:H2'	30:1:1700:U:C6	2.56	0.41
30:1:2239:C:O2'	30:1:2240:A:H5'	2.21	0.41
30:1:2674:G:H2'	30:1:2675:C:H6	1.86	0.41
30:1:2854:A:H2'	30:1:2855:U:O4'	2.21	0.41
18:U:34:LEU:HD23	18:U:65:PRO:CA	2.51	0.40
19:V:42:LEU:HD11	19:V:64:LEU:HD12	2.02	0.40
30:1:1237:G:O6	30:1:1238:G:N2	2.54	0.40
30:1:2051:U:C2	30:1:2052:G:C8	3.09	0.40
8:G:8:GLU:OE2	8:G:8:GLU:C	2.64	0.40
11:O:38:LEU:O	11:O:38:LEU:HG	2.22	0.40
14:Q:75:THR:OG1	30:1:1110:G:OP1	2.38	0.40
30:1:1126:A:H61	30:1:1226:C:H5	1.69	0.40
2:2:53:C:O2'	2:2:55:A:N7	2.54	0.40
11:O:125:LEU:HD12	11:O:125:LEU:N	2.36	0.40
16:S:1:MET:O	16:S:1:MET:CE	2.69	0.40
16:S:64:HIS:O	16:S:64:HIS:ND1	2.54	0.40
29:N:51:LEU:CD1	29:N:70:ILE:HD11	2.50	0.40
30:1:1099:A:H2'	30:1:1100:A:C8	2.56	0.40
30:1:1111:C:H3'	30:1:1112:G:H5''	2.02	0.40
30:1:2669:A:OP1	30:1:2716:A:O2'	2.36	0.40
7:F:27:LYS:HD3	7:F:27:LYS:C	2.46	0.40
7:F:165:TYR:HB2	7:F:168:GLU:HB2	2.04	0.40
9:J:77:HIS:ND1	30:1:1230:G:C5	2.89	0.40
12:L:38:ARG:HD2	30:1:684:G:H1	1.86	0.40
30:1:131:G:C2	30:1:132:G:C8	3.10	0.40
30:1:744:U:HO2'	30:1:745:A:P	2.39	0.40
30:1:1231:U:H3'	30:1:1232:A:H5''	2.04	0.40
30:1:2966:G:O6	30:1:2974:C:H5''	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:10:LYS:HD3	6:E:102:TRP:CD1	2.57	0.40
9:J:60:ASP:OD2	9:J:126:ALA:O	2.39	0.40
10:K:107:ARG:CG	10:K:115:ILE:HD13	2.51	0.40
13:P:24:ASP:OD1	13:P:90:GLY:N	2.54	0.40
16:S:51:LEU:HD13	16:S:72:ILE:HD11	2.02	0.40
27:6:61:MET:O	27:6:61:MET:HG2	2.22	0.40
30:1:259:A:H2'	30:1:260:A:C8	2.57	0.40
30:1:323:G:C2	30:1:324:A:C8	3.09	0.40
30:1:1667:G:H2'	30:1:1672:U:O4	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	135/139 (97%)	130 (96%)	5 (4%)	0	100	100
3	B	269/278 (97%)	262 (97%)	7 (3%)	0	100	100
4	C	210/214 (98%)	196 (93%)	14 (7%)	0	100	100
5	D	197/216 (91%)	195 (99%)	2 (1%)	0	100	100
6	E	165/185 (89%)	154 (93%)	11 (7%)	0	100	100
7	F	167/179 (93%)	160 (96%)	7 (4%)	0	100	100
8	G	46/148 (31%)	46 (100%)	0	0	100	100
9	J	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
10	K	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
11	O	124/127 (98%)	113 (91%)	11 (9%)	0	100	100
12	L	146/151 (97%)	136 (93%)	10 (7%)	0	100	100
13	P	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
14	Q	122/128 (95%)	117 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	R	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
16	S	109/115 (95%)	102 (94%)	7 (6%)	0	100	100
17	T	95/107 (89%)	93 (98%)	2 (2%)	0	100	100
18	U	95/107 (89%)	90 (95%)	5 (5%)	0	100	100
19	V	173/195 (89%)	171 (99%)	2 (1%)	0	100	100
20	W	70/84 (83%)	68 (97%)	2 (3%)	0	100	100
21	X	54/61 (88%)	53 (98%)	1 (2%)	0	100	100
22	Y	60/74 (81%)	59 (98%)	1 (2%)	0	100	100
23	Z	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
24	3	22/57 (39%)	22 (100%)	0	0	100	100
25	4	46/54 (85%)	46 (100%)	0	0	100	100
26	5	42/45 (93%)	41 (98%)	1 (2%)	0	100	100
27	6	59/64 (92%)	57 (97%)	2 (3%)	0	100	100
28	7	35/37 (95%)	35 (100%)	0	0	100	100
29	N	114/164 (70%)	111 (97%)	3 (3%)	0	100	100
All	All	3089/3480 (89%)	2975 (96%)	114 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	112/113 (99%)	112 (100%)	0	100	100
3	B	212/219 (97%)	212 (100%)	0	100	100
4	C	163/164 (99%)	163 (100%)	0	100	100
5	D	160/171 (94%)	160 (100%)	0	100	100
6	E	143/158 (90%)	143 (100%)	0	100	100
7	F	139/144 (96%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	36/114 (32%)	36 (100%)	0	100	100
9	J	120/121 (99%)	120 (100%)	0	100	100
10	K	99/99 (100%)	99 (100%)	0	100	100
11	O	86/87 (99%)	86 (100%)	0	100	100
12	L	115/117 (98%)	115 (100%)	0	100	100
13	P	100/101 (99%)	100 (100%)	0	100	100
14	Q	97/99 (98%)	97 (100%)	0	100	100
15	R	85/86 (99%)	85 (100%)	0	100	100
16	S	90/93 (97%)	90 (100%)	0	100	100
17	T	85/91 (93%)	85 (100%)	0	100	100
18	U	82/88 (93%)	82 (100%)	0	100	100
19	V	142/154 (92%)	142 (100%)	0	100	100
20	W	53/61 (87%)	53 (100%)	0	100	100
21	X	48/51 (94%)	48 (100%)	0	100	100
22	Y	52/61 (85%)	52 (100%)	0	100	100
23	Z	54/55 (98%)	54 (100%)	0	100	100
24	3	21/51 (41%)	21 (100%)	0	100	100
25	4	45/49 (92%)	45 (100%)	0	100	100
26	5	35/36 (97%)	35 (100%)	0	100	100
27	6	49/52 (94%)	49 (100%)	0	100	100
28	7	35/35 (100%)	35 (100%)	0	100	100
29	N	92/122 (75%)	92 (100%)	0	100	100
All	All	2550/2792 (91%)	2550 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	81	HIS
3	B	113	GLN
3	B	245	HIS
5	D	180	GLN
6	E	88	GLN

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Mol	Chain	Res	Type
6	E	93	HIS
7	F	75	ASN
9	J	144	GLN
11	O	22	HIS
11	O	58	HIS
12	L	4	ASN
13	P	9	ASN
13	P	29	HIS
17	T	51	GLN
18	U	80	ASN
20	W	17	ASN
23	Z	8	GLN
25	4	21	ASN
25	4	47	HIS
26	5	7	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	113/117 (96%)	14 (12%)	0
30	1	2539/3119 (81%)	286 (11%)	11 (0%)
All	All	2652/3236 (81%)	300 (11%)	11 (0%)

All (300) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	3	C
2	2	4	G
2	2	20	G
2	2	33	U
2	2	36	C
2	2	39	U
2	2	42	G
2	2	50	A
2	2	54	U
2	2	55	A
2	2	83	G
2	2	104	G
2	2	108	G
2	2	113	C
30	1	13	A

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Mol	Chain	Res	Type
30	1	34	U
30	1	39	C
30	1	46	C
30	1	71	A
30	1	74	G
30	1	75	G
30	1	118	A
30	1	120	U
30	1	151	A
30	1	162	A
30	1	165	A
30	1	175	U
30	1	178	G
30	1	199	A
30	1	202	A
30	1	218	G
30	1	219	A
30	1	224	A
30	1	225	A
30	1	231	C
30	1	232	C
30	1	236	A
30	1	251	G
30	1	269	G
30	1	319	G
30	1	320	U
30	1	321	G
30	1	356	G
30	1	359	U
30	1	363	A
30	1	391	G
30	1	392	A
30	1	394	A
30	1	399	C
30	1	400	G
30	1	405	A
30	1	412	A
30	1	413	A
30	1	414	G
30	1	446	U
30	1	452	A
30	1	460	G

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Mol	Chain	Res	Type
30	1	474	G
30	1	486	G
30	1	494	G
30	1	499	G
30	1	517	A
30	1	543	U
30	1	544	A
30	1	568	G
30	1	587	A
30	1	590	U
30	1	591	A
30	1	594	A
30	1	595	C
30	1	616	G
30	1	617	C
30	1	618	C
30	1	660	G
30	1	670	G
30	1	671	A
30	1	672	A
30	1	683	A
30	1	685	U
30	1	690	G
30	1	701	A
30	1	712	U
30	1	713	G
30	1	719	A
30	1	726	A
30	1	736	A
30	1	743	A
30	1	745	A
30	1	747	G
30	1	750	G
30	1	769	G
30	1	786	U
30	1	830	A
30	1	847	U
30	1	850	A
30	1	857	G
30	1	875	G
30	1	876	G
30	1	882	A

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Mol	Chain	Res	Type
30	1	884	G
30	1	885	G
30	1	904	A
30	1	905	G
30	1	912	C
30	1	927	U
30	1	928	U
30	1	959	G
30	1	968	U
30	1	969	G
30	1	1009	A
30	1	1013	C
30	1	1037	G
30	1	1040	A
30	1	1045	G
30	1	1052	G
30	1	1058	A
30	1	1060	G
30	1	1073	G
30	1	1079	A
30	1	1080	A
30	1	1082	A
30	1	1095	G
30	1	1112	G
30	1	1125	G
30	1	1232	A
30	1	1233	G
30	1	1234	C
30	1	1241	C
30	1	1242	A
30	1	1243	A
30	1	1322	U
30	1	1323	G
30	1	1329	G
30	1	1341	A
30	1	1342	G
30	1	1350	C
30	1	1362	G
30	1	1365	A
30	1	1367	U
30	1	1368	G
30	1	1383	G

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Mol	Chain	Res	Type
30	1	1384	A
30	1	1385	U
30	1	1386	A
30	1	1400	C
30	1	1411	A
30	1	1412	U
30	1	1436	C
30	1	1463	U
30	1	1470	A
30	1	1476	A
30	1	1479	G
30	1	1489	A
30	1	1490	U
30	1	1495	A
30	1	1506	A
30	1	1507	U
30	1	1634	U
30	1	1635	G
30	1	1642	C
30	1	1659	G
30	1	1664	G
30	1	1667	G
30	1	1675	U
30	1	1676	C
30	1	1682	G
30	1	1697	G
30	1	1704	A
30	1	1731	A
30	1	1783	A
30	1	1792	U
30	1	1819	U
30	1	1820	A
30	1	1821	A
30	1	1828	U
30	1	1858	U
30	1	1859	U
30	1	1860	C
30	1	1865	G
30	1	1866	A
30	1	1886	G
30	1	1908	G
30	1	1935	A

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Mol	Chain	Res	Type
30	1	1938	C
30	1	1940	U
30	1	1941	G
30	1	1943	A
30	1	1946	G
30	1	1953	G
30	1	1970	C
30	1	1974	C
30	1	1983	A
30	1	1996	A
30	1	1997	A
30	1	2001	A
30	1	2010	C
30	1	2011	G
30	1	2026	U
30	1	2030	U
30	1	2039	A
30	1	2057	A
30	1	2149	G
30	1	2150	G
30	1	2158	A
30	1	2160	U
30	1	2175	U
30	1	2187	C
30	1	2190	A
30	1	2191	U
30	1	2192	G
30	1	2202	C
30	1	2211	U
30	1	2213	U
30	1	2217	A
30	1	2240	A
30	1	2241	C
30	1	2242	U
30	1	2243	A
30	1	2251	A
30	1	2252	G
30	1	2253	A
30	1	2263	C
30	1	2275	C
30	1	2276	G
30	1	2312	G

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Mol	Chain	Res	Type
30	1	2422	G
30	1	2423	G
30	1	2430	G
30	1	2444	A
30	1	2457	G
30	1	2458	G
30	1	2498	G
30	1	2502	C
30	1	2506	A
30	1	2507	A
30	1	2539	U
30	1	2540	G
30	1	2544	G
30	1	2546	A
30	1	2553	C
30	1	2554	A
30	1	2555	A
30	1	2566	C
30	1	2569	U
30	1	2602	G
30	1	2604	A
30	1	2622	G
30	1	2624	U
30	1	2625	U
30	1	2644	A
30	1	2645	A
30	1	2648	G
30	1	2649	A
30	1	2653	A
30	1	2654	A
30	1	2660	C
30	1	2667	A
30	1	2683	C
30	1	2688	A
30	1	2694	C
30	1	2695	A
30	1	2697	A
30	1	2725	U
30	1	2726	C
30	1	2737	A
30	1	2748	G
30	1	2785	A

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Mol	Chain	Res	Type
30	1	2786	G
30	1	2795	G
30	1	2804	U
30	1	2821	A
30	1	2822	G
30	1	2828	U
30	1	2832	U
30	1	2848	A
30	1	2849	G
30	1	2879	A
30	1	2933	G
30	1	2945	C
30	1	2952	G
30	1	2967	A
30	1	2972	A
30	1	2977	A
30	1	2978	G
30	1	2983	A
30	1	2984	A
30	1	2985	G
30	1	2997	A
30	1	3009	A
30	1	3010	C
30	1	3036	U
30	1	3051	A
30	1	3058	G
30	1	3059	G
30	1	3066	A
30	1	3083	G
30	1	3088	G
30	1	3096	C
30	1	3109	G
30	1	3110	G

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	1	161	G
30	1	744	U
30	1	884	G
30	1	968	U
30	1	1057	U

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Mol	Chain	Res	Type
30	1	1469	G
30	1	1634	U
30	1	1858	U
30	1	2029	A
30	1	2644	A
30	1	2666	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](#)

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.

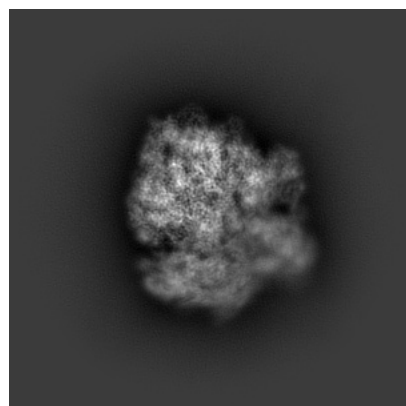
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53347. These allow visual inspection of the internal detail of the map and identification of artifacts.

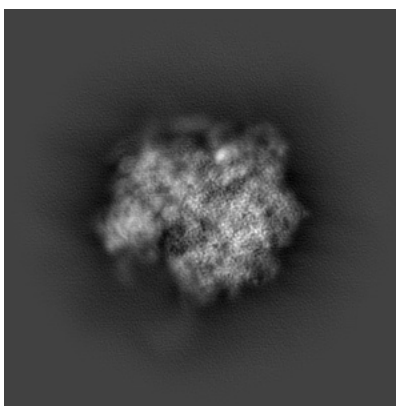
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

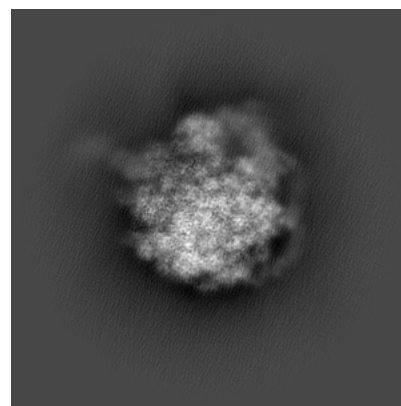
6.1.1 Primary map



X

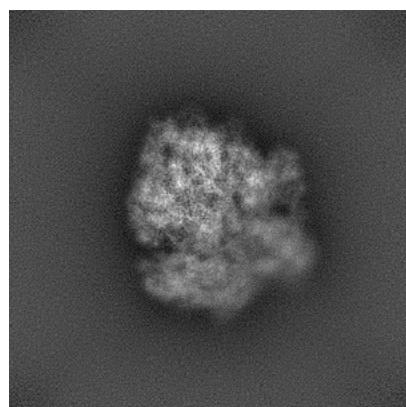


Y

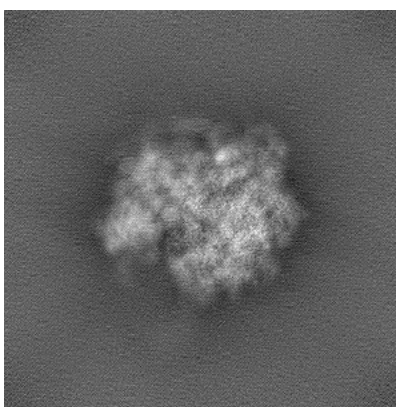


Z

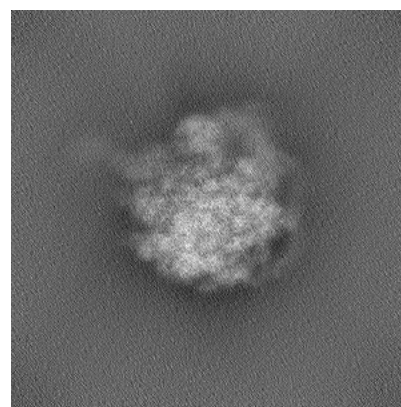
6.1.2 Raw map



X



Y

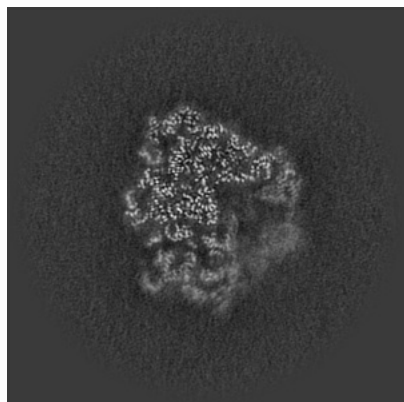


Z

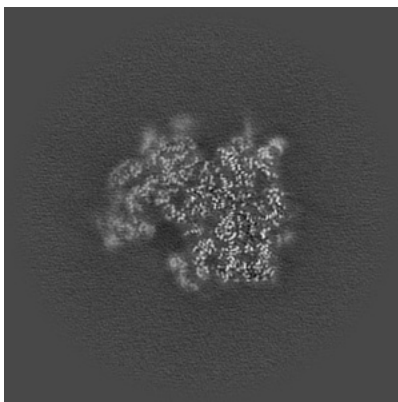
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

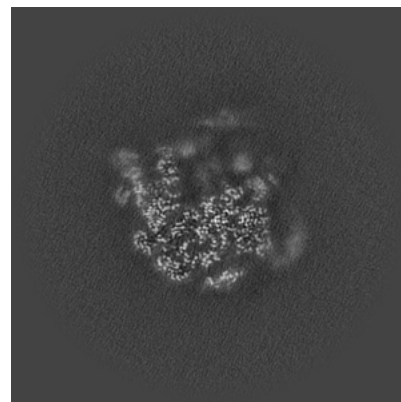
6.2.1 Primary map



X Index: 256

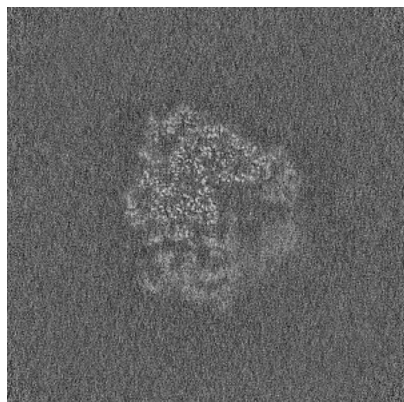


Y Index: 256

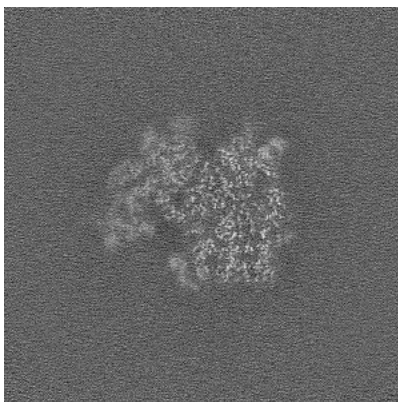


Z Index: 256

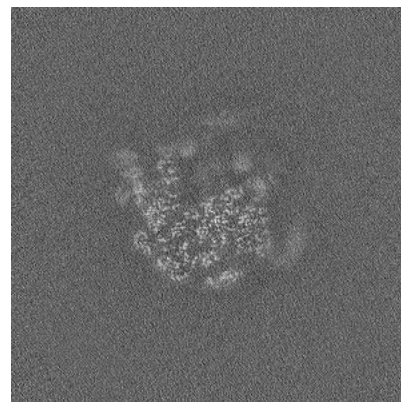
6.2.2 Raw map



X Index: 256



Y Index: 256

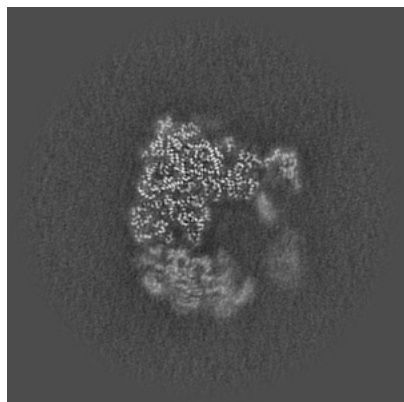


Z Index: 256

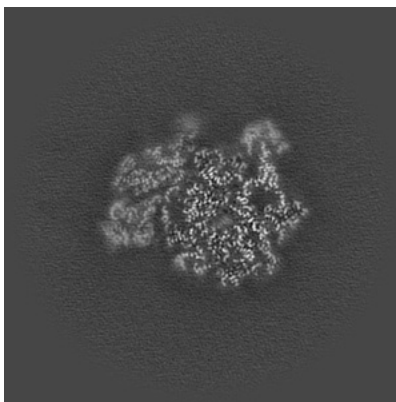
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

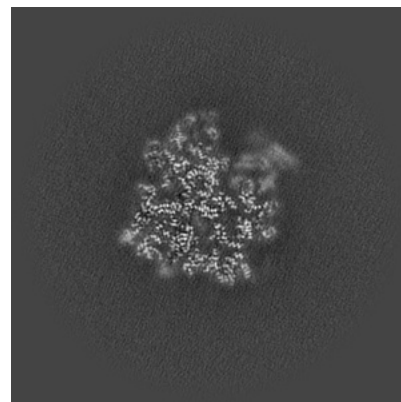
6.3.1 Primary map



X Index: 226

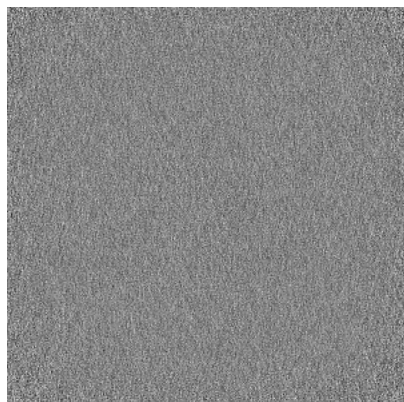


Y Index: 241

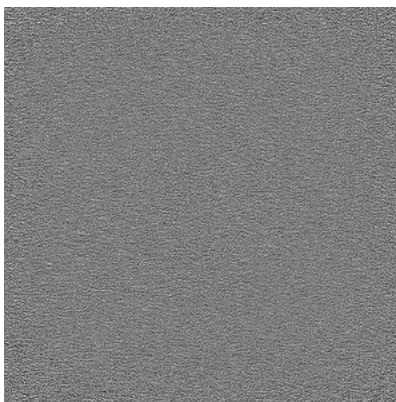


Z Index: 291

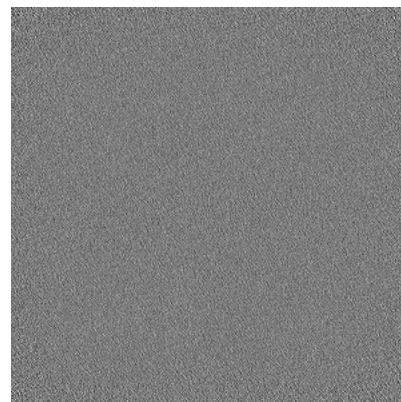
6.3.2 Raw map



X Index: 0



Y Index: 0

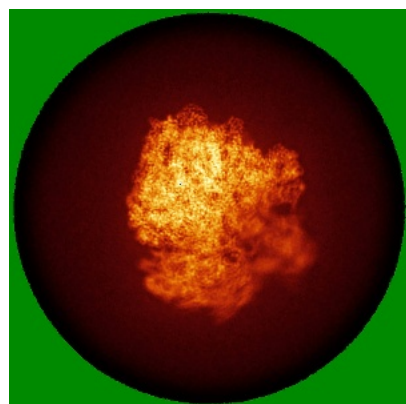


Z Index: 0

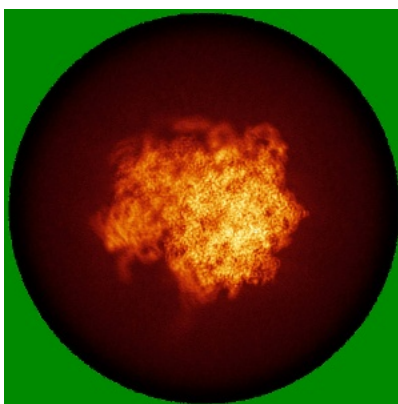
The images above show the largest variance slices of the map in three orthogonal directions.

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

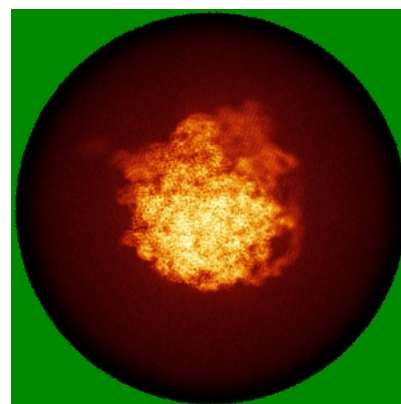
6.4.1 Primary map



X

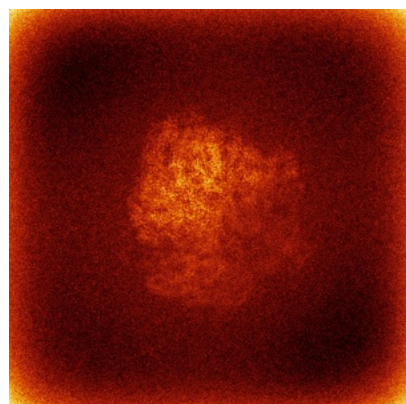


Y

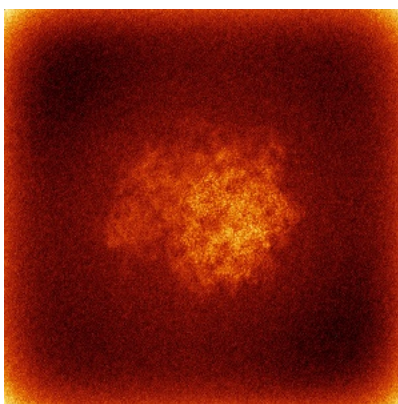


Z

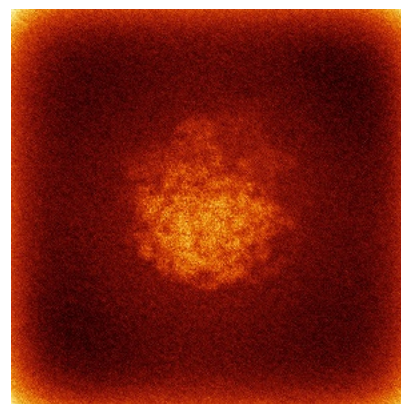
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

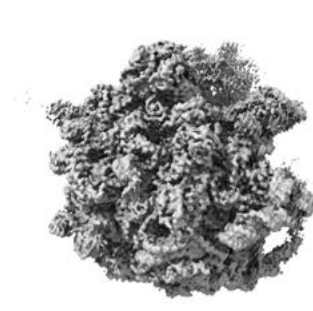
6.5.1 Primary map



X



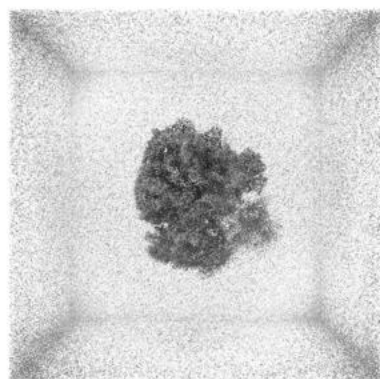
Y



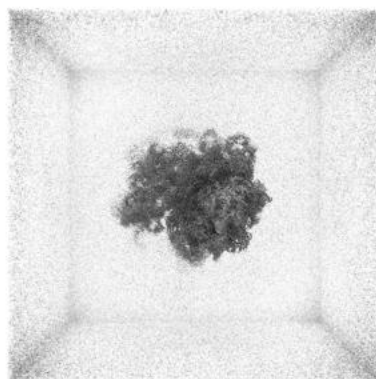
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0769. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

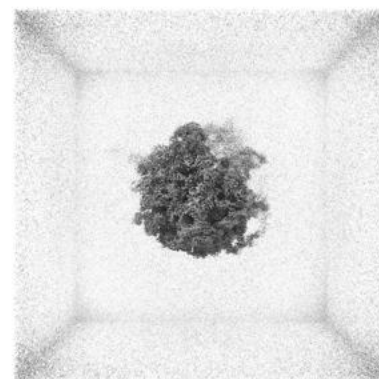
6.5.2 Raw map



X



Y



Z

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

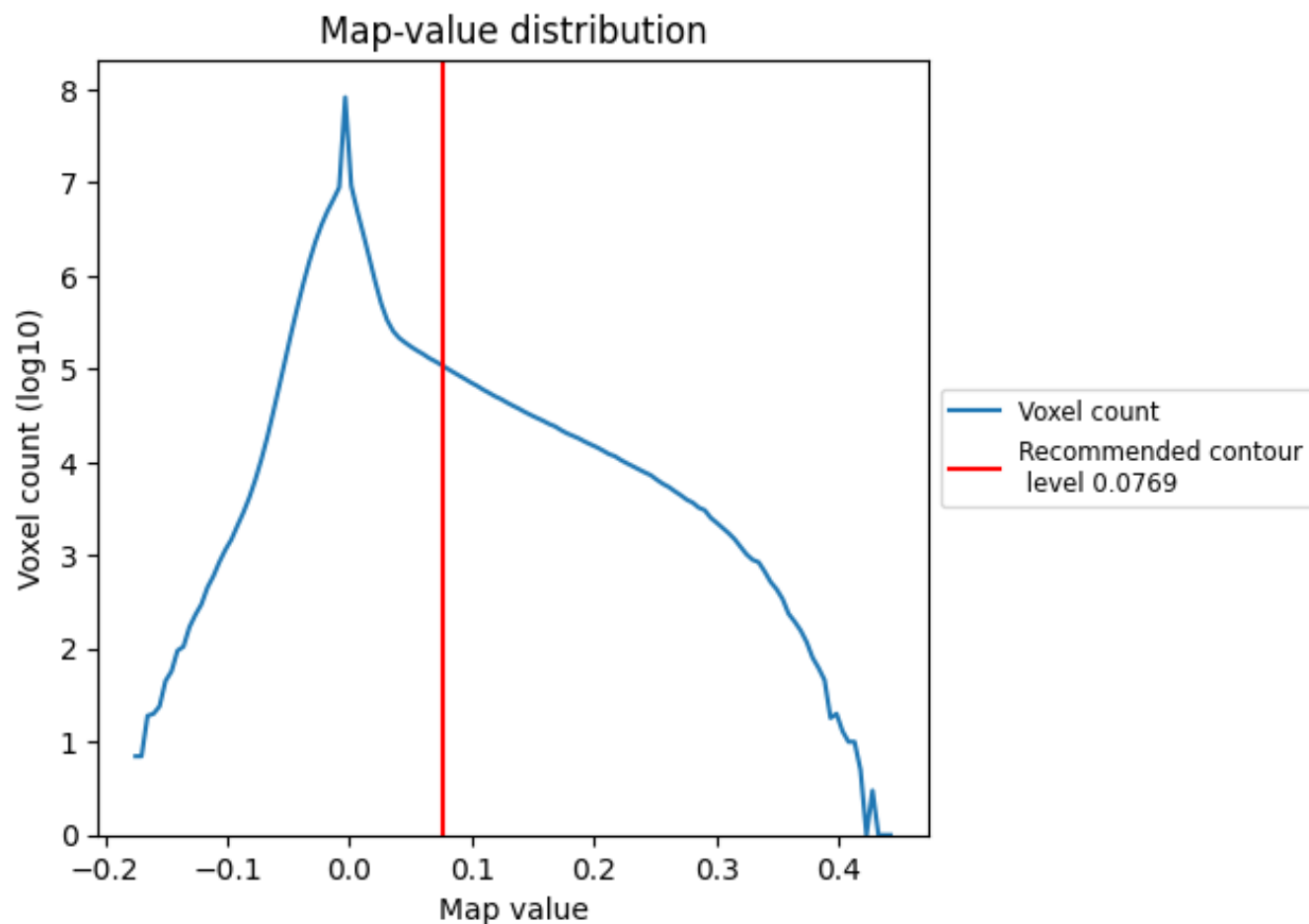
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

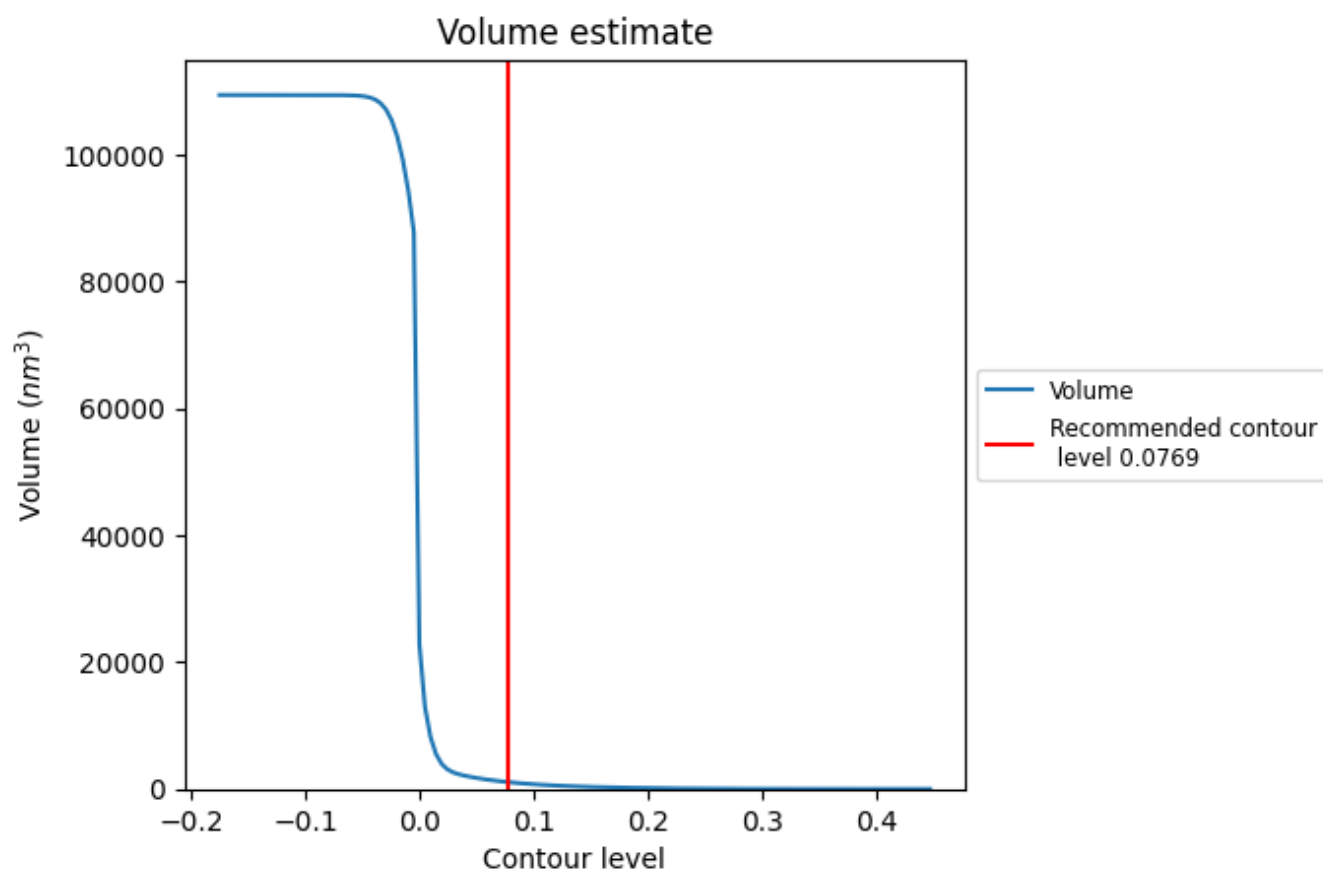
This section contains the results of statistical analysis of the map.

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.

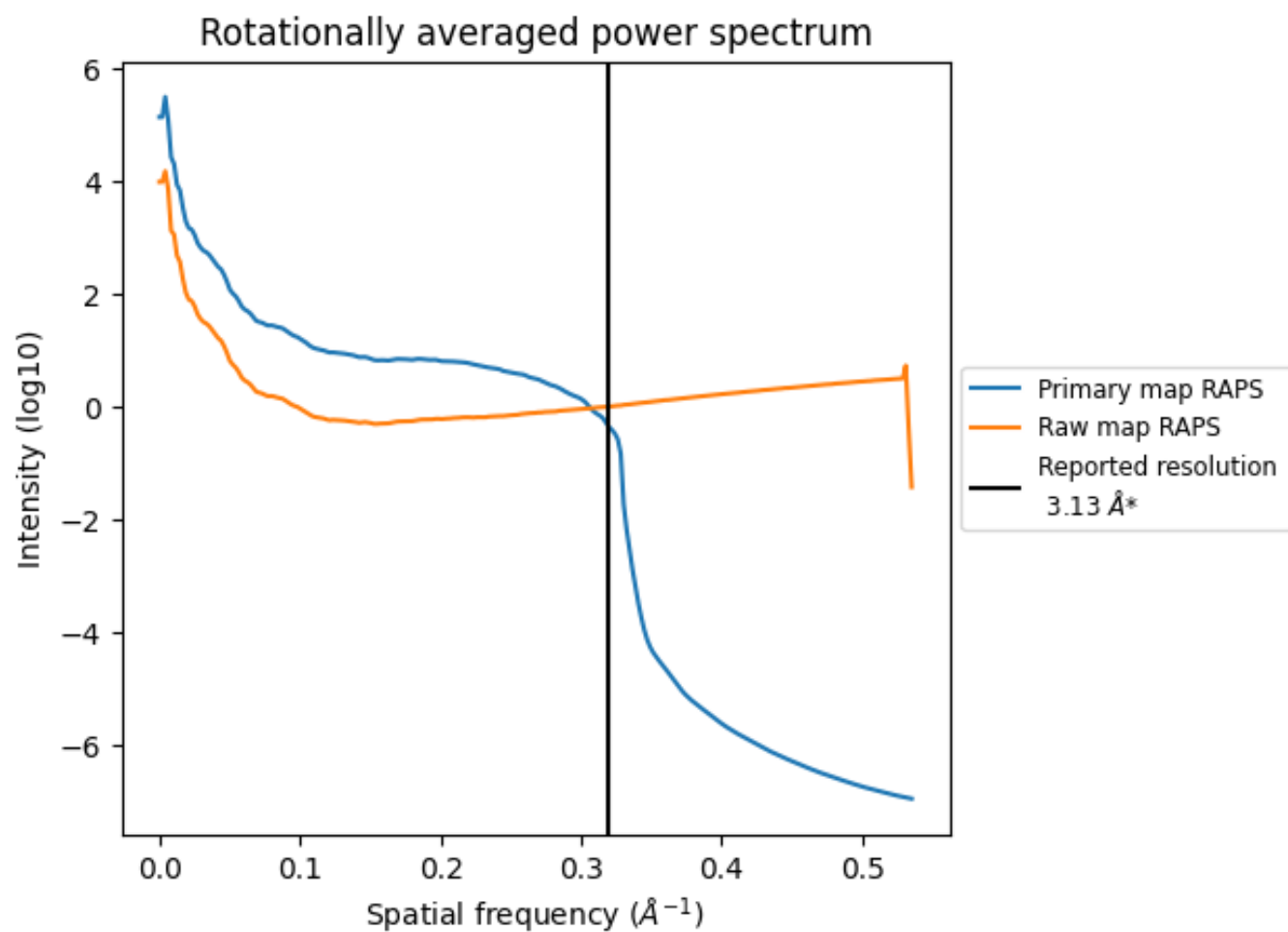
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1093 nm^3 ; this corresponds to an approximate mass of 988 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 ⓘ

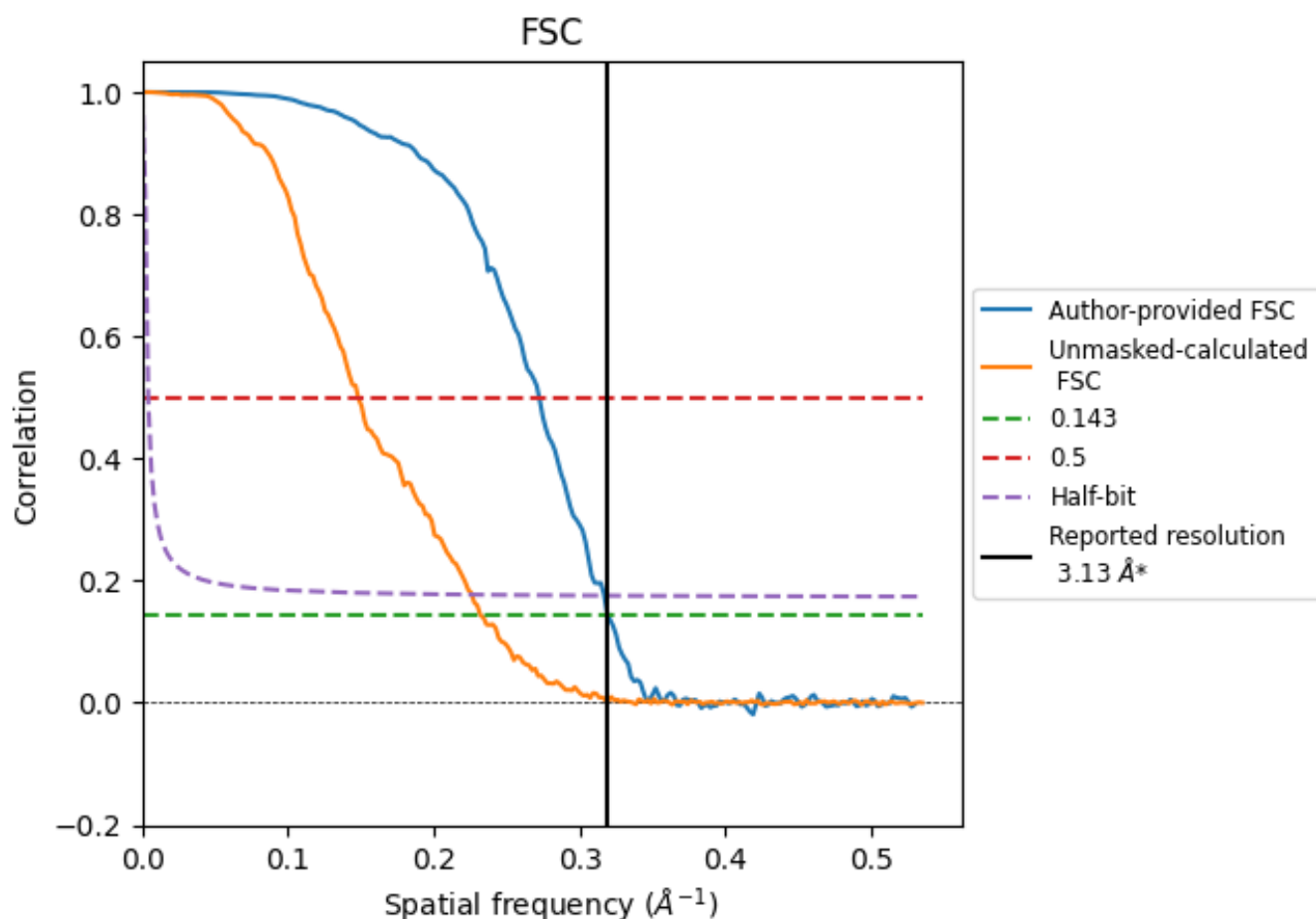


*Reported resolution corresponds to spatial frequency of 0.319 \AA^{-1}

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 0.319 \AA^{-1}

8.2 Resolution estimates [i](#)

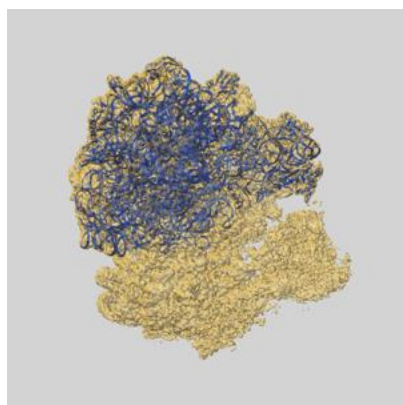
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.67	3.15
Unmasked-calculated*	4.31	6.74	4.42

*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 4.31 differs from the reported value 3.13 by more than 10 %

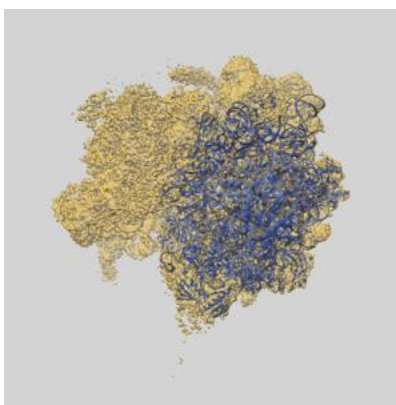
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53347 and PDB model 9QT5. Per-residue inclusion information can be found in section [3](#) on page [9](#).

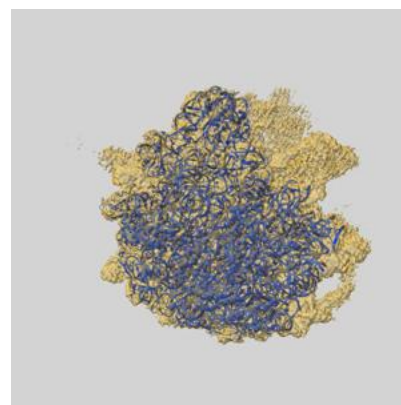
9.1 Map-model overlay [i](#)



X



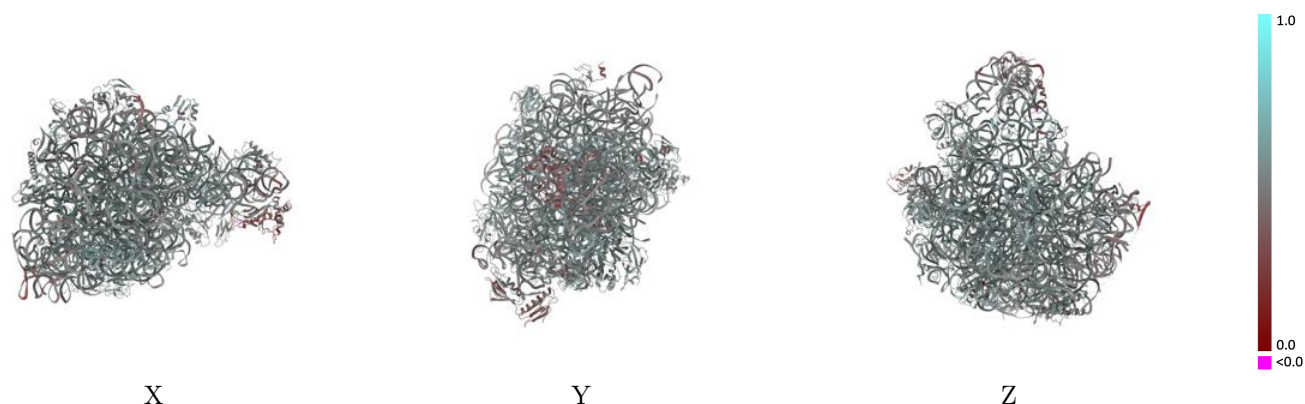
Y



Z

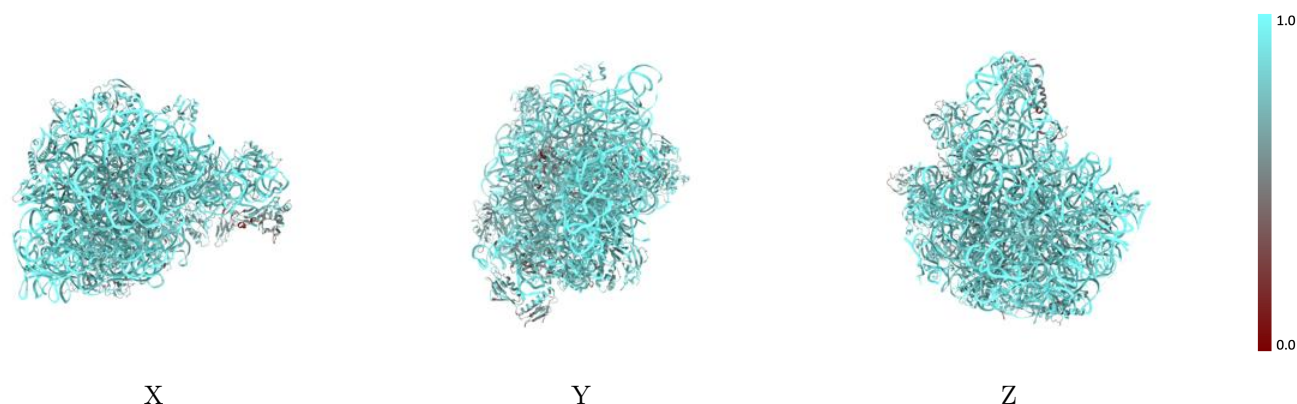
The images above show the 3D surface view of the map at the recommended contour level 0.0769 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



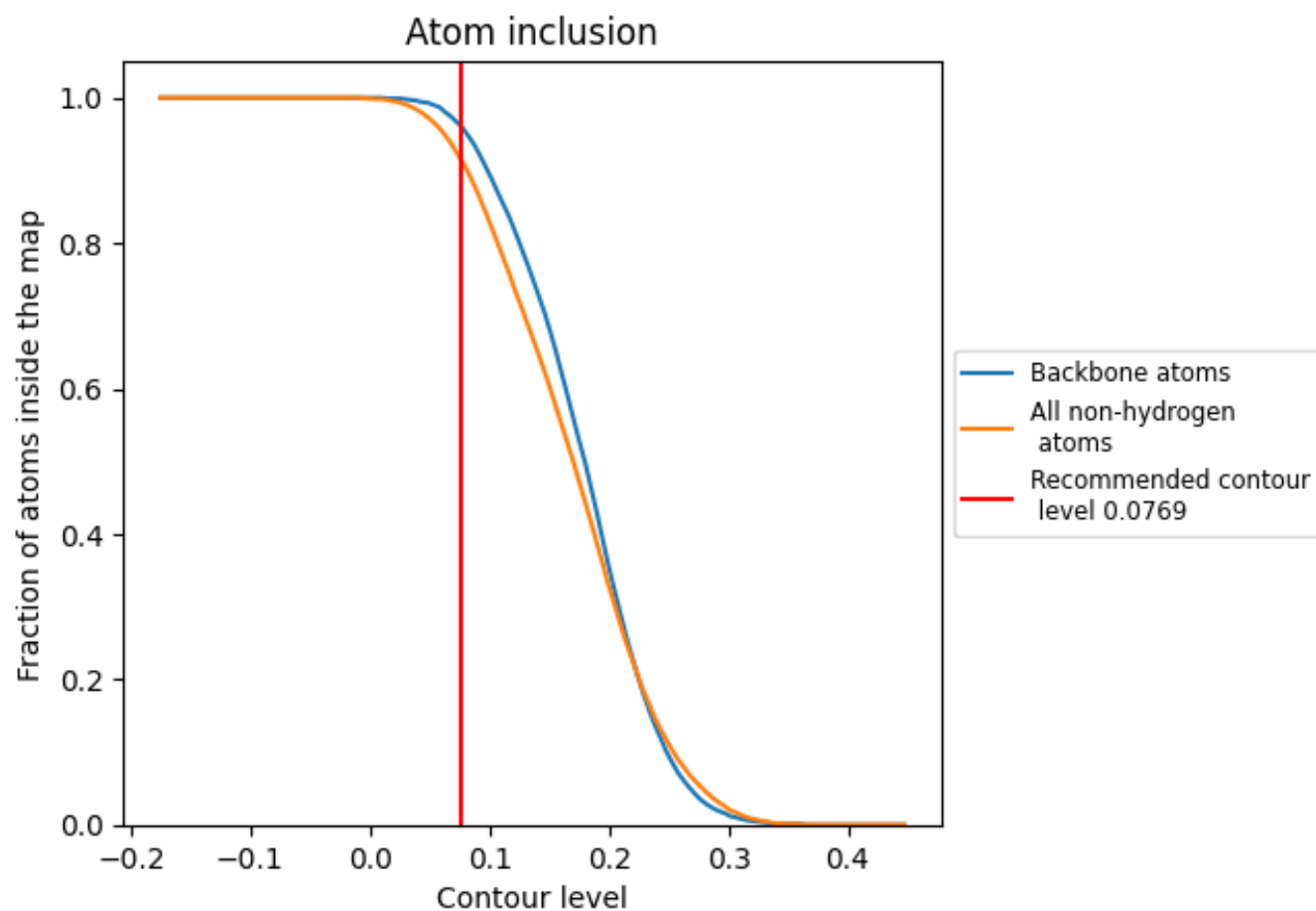
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0769).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.0769) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.5170
1	 0.9630	 0.5210
2	 0.9680	 0.4890
3	 0.8990	 0.5670
4	 0.7530	 0.5080
5	 0.9170	 0.5580
6	 0.8130	 0.5450
7	 0.4740	 0.4800
B	 0.8360	 0.5520
C	 0.8370	 0.5430
D	 0.8220	 0.5290
E	 0.6140	 0.3650
F	 0.6770	 0.3960
G	 0.8510	 0.4630
J	 0.8630	 0.5390
K	 0.7110	 0.5320
L	 0.8430	 0.5310
M	 0.7950	 0.5260
N	 0.8430	 0.5390
O	 0.8000	 0.4880
P	 0.7630	 0.5170
Q	 0.8640	 0.5390
R	 0.8580	 0.5380
S	 0.8420	 0.5450
T	 0.7800	 0.5100
U	 0.7850	 0.5020
V	 0.7150	 0.4850
W	 0.8790	 0.5560
X	 0.8120	 0.5350
Y	 0.8200	 0.4920
Z	 0.8190	 0.5400

