



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:42 AM UTC

PDB ID : 9ZCD / pdb_00009zcd
EMDB ID : EMD-74034
Title : Flavobacterium johnsoniae 30S ribosomal subunit.
Authors : Ortega, J.; Arpin, D.
Deposited on : 2025-11-23
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

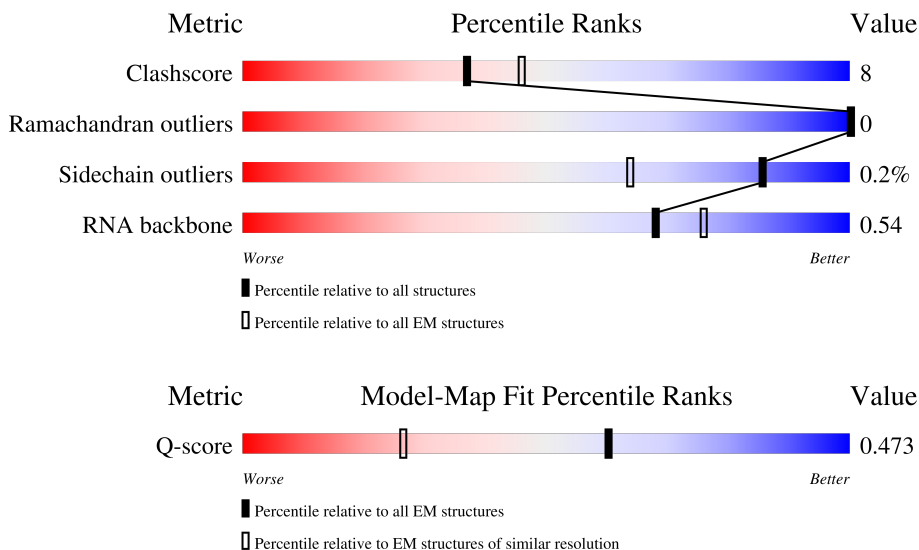
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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















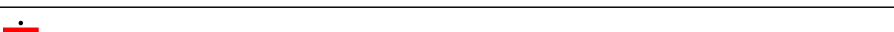

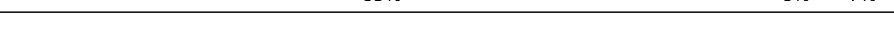




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	A	591	<div> <div>5%</div> <div>94%</div> </div>
2	H	254	<div> <div>66%</div> <div>20%</div> <div>14%</div> </div>
3	h	252	<div> <div>38%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	i	201	
5	j	173	
6	k	113	
7	l	158	
8	m	132	
9	n	128	
10	o	101	
11	p	127	
12	q	127	
13	r	124	
14	s	89	
15	t	88	
16	u	188	
17	v	86	
18	w	98	
19	x	92	
20	y	83	
21	z	64	
22	2	1520	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 49917 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 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	37	Total	C	N	O	0	0
			281	178	47	56		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	219	Total	C	N	O	S	0	0
			1641	1045	288	300	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	h	215	Total	C	N	O	S	0	0
			1592	1009	288	289	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	i	200	Total	C	N	O	S	0	0
			1561	988	289	281	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	j	169	Total	C	N	O	S	0	0
			1160	732	226	201	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	107	Total	C	N	O	S	0	0
			807	528	147	130	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	132	Total	C	N	O	S	0	0
			1034	654	200	175	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	131	Total	C	N	O	S	0	0
			961	623	167	169	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	125	Total	C	N	O	S	0	0
			972	612	188	168	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	o	98	Total	C	N	O	S	0	0
			701	450	123	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	p	117	Total	C	N	O	S	0	0
			811	506	157	143	5		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	121	Total	C	N	O	S	0	0
			918	564	194	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	r	53	Total	C	N	O	S	0	0
			388	244	74	68	2		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	115	THR	-	expression tag	UNP P0A7T1
r	116	VAL	-	expression tag	UNP P0A7T1
r	117	ALA	-	expression tag	UNP P0A7T1
r	118	ASN	-	expression tag	UNP P0A7T1
r	119	LYS	-	expression tag	UNP P0A7T1
r	120	LYS	-	expression tag	UNP P0A7T1
r	121	LYS	-	expression tag	UNP P0A7T1
r	122	ALA	-	expression tag	UNP P0A7T1
r	123	THR	-	expression tag	UNP P0A7T1
r	124	LYS	-	expression tag	UNP P0A7T1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	s	88	Total	C	N	O	S	0	0
			665	416	136	110	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	t	87	Total	C	N	O	0	0
			679	434	131	114		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	71	ARG	LYS	conflict	UNP A0A1M6QTP8

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	u	151	Total	C	N	O	0	0
			1100	693	205	202		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	v	80	Total	C	N	O	S	0	0
			638	404	124	107	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	65	Total	C	N	O	S	0	0
			517	339	95	81	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	83	Total	C	N	O	S	0	0
			632	404	118	108	2		

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

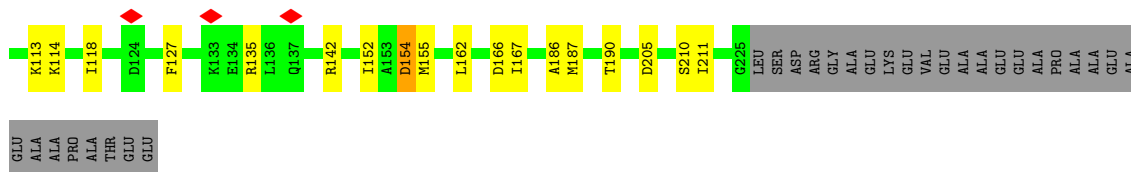
Mol	Chain	Residues	Atoms					AltConf	Trace
20	y	79	Total	C	N	O	S	0	0
			609	378	126	104	1		

- Molecule 21 is a protein called 30S ribosomal protein S21.

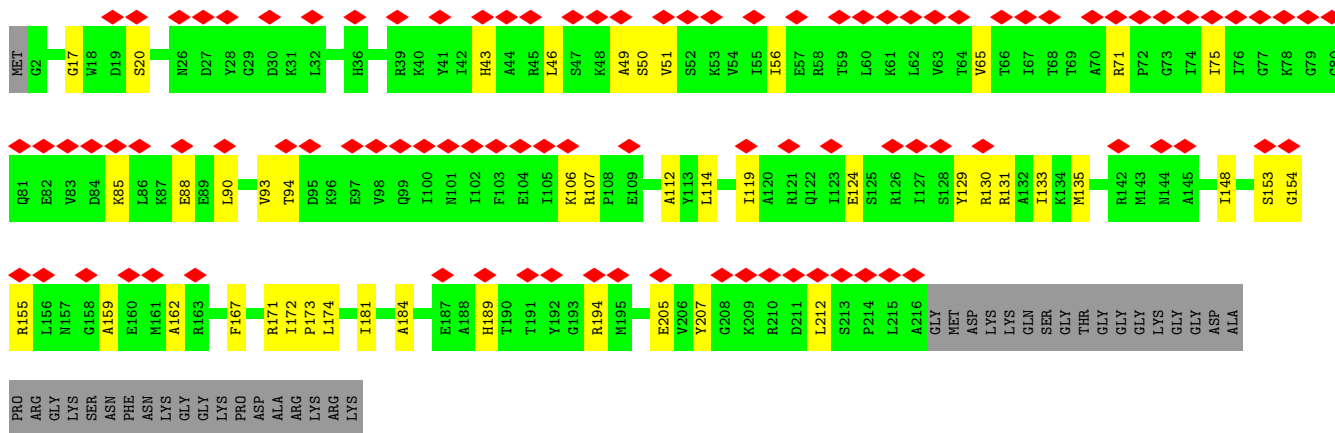
Mol	Chain	Residues	Atoms					AltConf	Trace
21	z	64	Total	C	N	O	S	0	0
			522	331	99	91	1		

- Molecule 22 is a RNA chain called 16S rRNA.

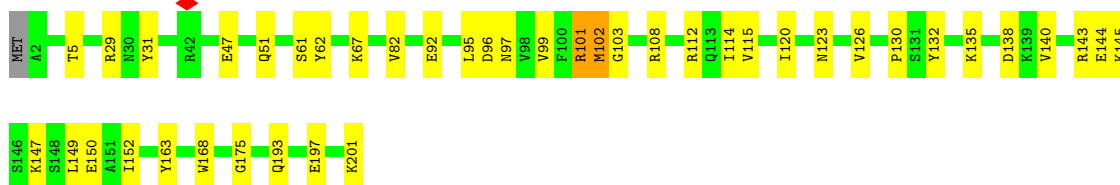
Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	1481	Total	C	N	O	P	0	0
			31728	14167	5801	10279	1481		



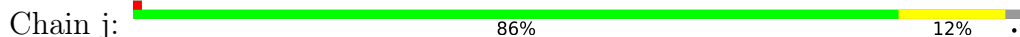
• Molecule 3: 30S ribosomal protein S3



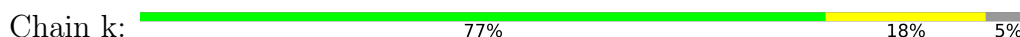
• Molecule 4: 30S ribosomal protein S4



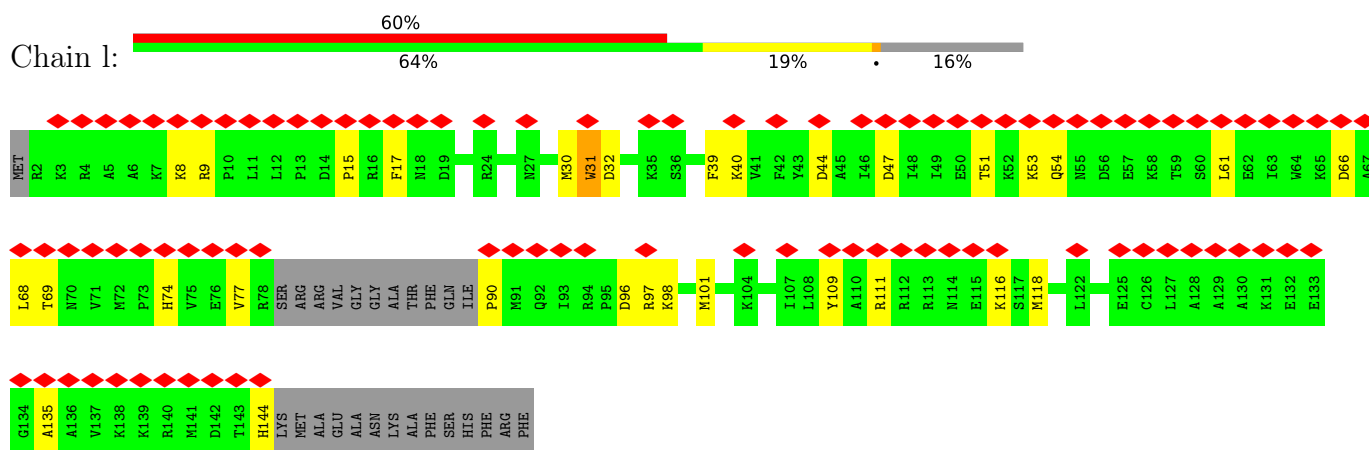
• Molecule 5: 30S ribosomal protein S5



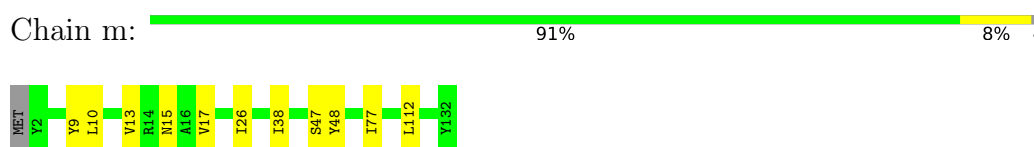
• Molecule 6: 30S ribosomal protein S6



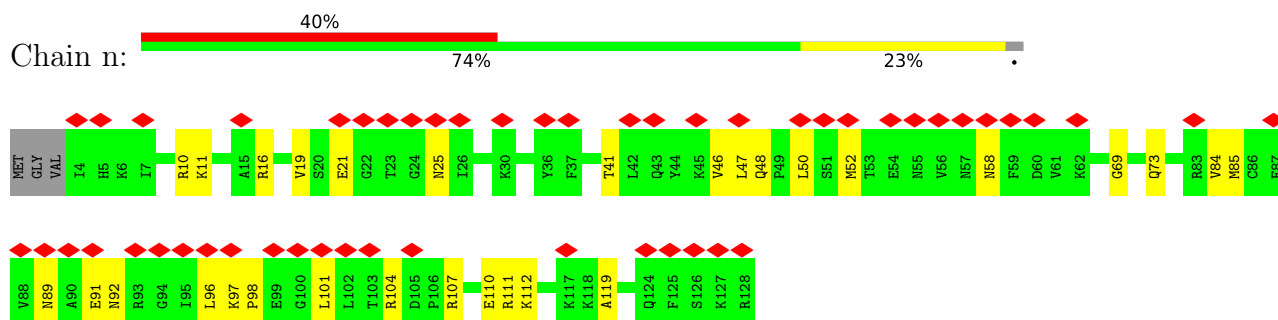
• Molecule 7: 30S ribosomal protein S7



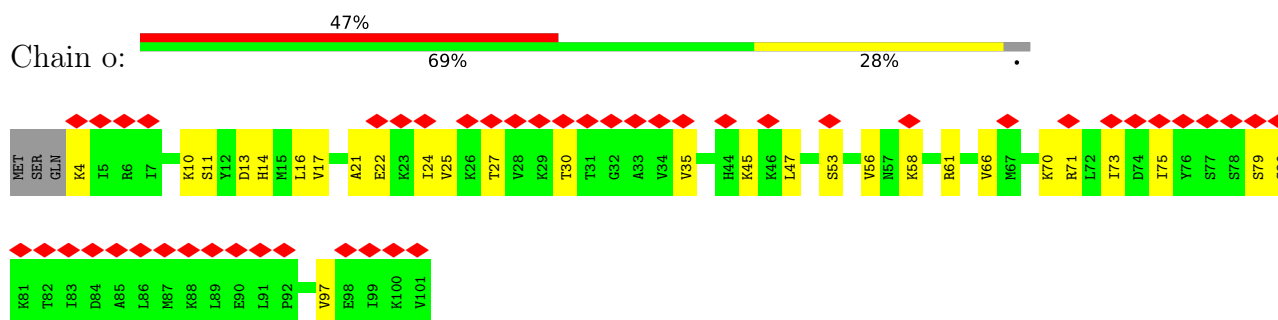
• Molecule 8: 30S ribosomal protein S8



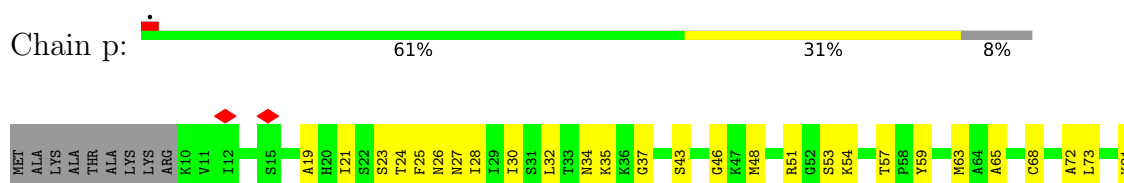
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11





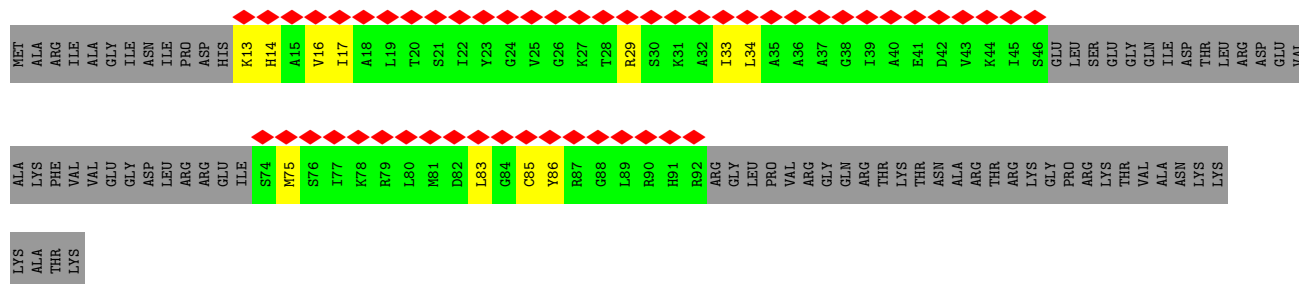
- Molecule 12: Small ribosomal subunit protein uS12

Chain q: 83% 12% 5%



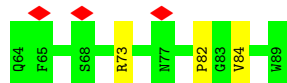
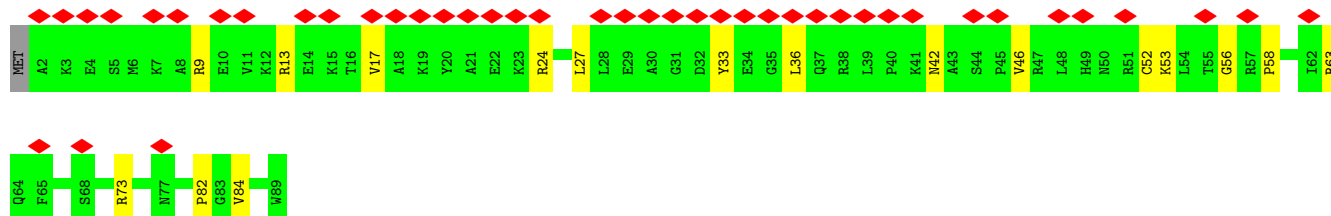
- Molecule 13: 30S ribosomal protein S13

Chain r: 43% 34% 9% 57%



- Molecule 14: 30S ribosomal protein S14

Chain s: 48% 80% 19%



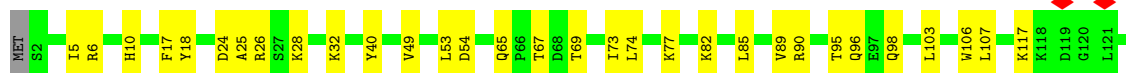
- Molecule 15: 30S ribosomal protein S15

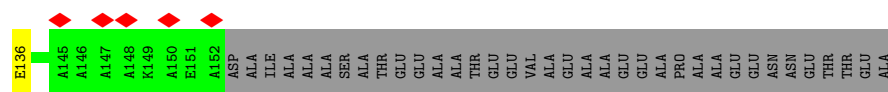
Chain t: 80% 19%



- Molecule 16: Small ribosomal subunit protein bS16

Chain u: 63% 17% 20%





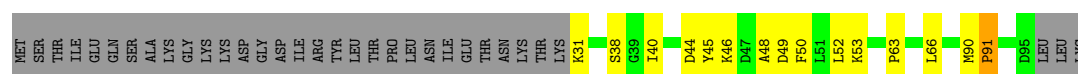
- Molecule 17: 30S ribosomal protein S17

Chain v: 85% 8% 7%



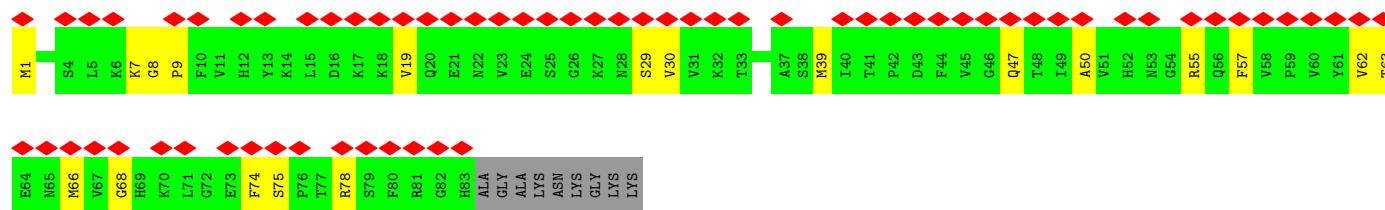
- Molecule 18: 30S ribosomal protein S18

Chain w: 51% 14% 34%



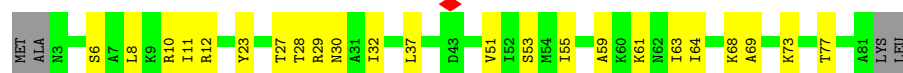
- Molecule 19: 30S ribosomal protein S19

Chain x: 73% 70% 21% 10%



- Molecule 20: 30S ribosomal protein S20

Chain y: 67% 28% 5%



- Molecule 21: 30S ribosomal protein S21

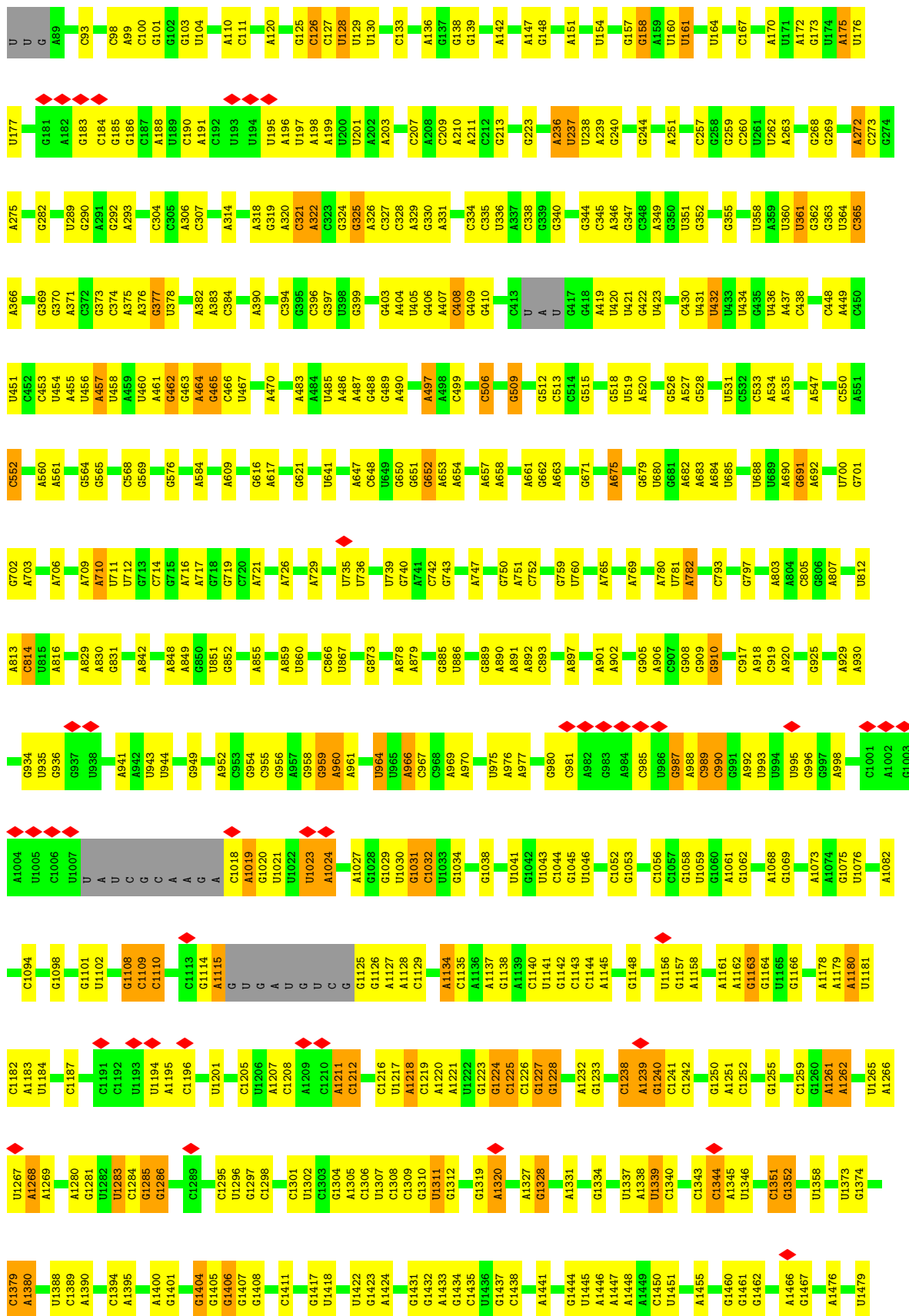
Chain z: 11% 83% 17%



- Molecule 22: 16S rRNA

Chain 2: 58% 34% 6%





A1486	C1487
G1490	A1491
A1492	G1493
C1497	G1498
G1502	G1503
A1504	U1510
C1511	C1512
U1513	U1514
U1515	C1516
U1517	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	431185	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 ($e^-/\text{\AA}^2$)	50	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	0.240	Depositor
Minimum map value	-0.111	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0328	Depositor
Map size (Å)	342.0, 342.0, 342.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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	A	0.14	0/287	0.47	0/390
2	H	0.16	0/1667	0.42	1/2258 (0.0%)
3	h	0.19	0/1615	0.38	0/2182
4	i	0.23	1/1591 (0.1%)	0.42	3/2139 (0.1%)
5	j	0.15	0/1175	0.28	0/1589
6	k	0.15	0/826	0.34	0/1121
7	l	0.17	0/1052	0.40	0/1414
8	m	0.15	0/976	0.27	0/1324
9	n	0.20	0/986	0.43	0/1322
10	o	0.20	0/712	0.39	0/973
11	p	0.17	0/825	0.47	1/1122 (0.1%)
12	q	0.14	0/931	0.28	0/1254
13	r	0.13	0/390	0.43	0/519
14	s	0.36	1/676 (0.1%)	0.51	1/906 (0.1%)
15	t	0.19	0/689	0.56	2/928 (0.2%)
16	u	0.17	0/1118	0.37	0/1511
17	v	0.14	0/646	0.40	0/866
18	w	0.38	1/527 (0.2%)	0.53	1/706 (0.1%)
19	x	0.16	0/648	0.37	0/876
20	y	0.27	0/613	0.49	0/818
21	z	0.17	0/527	0.42	0/701
22	2	0.17	0/35523	0.29	0/55388
All	All	0.18	3/54000 (0.0%)	0.33	9/80307 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	w	91	PRO	N-CD	-7.84	1.36	1.47
14	s	58	PRO	N-CD	7.16	1.57	1.47
4	i	102	MET	CA-C	5.20	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	i	103	GLY	N-CA-C	-7.90	103.63	115.32
15	t	70	LYS	N-CA-C	7.20	119.13	111.28
4	i	101	ARG	N-CA-C	-6.50	104.28	111.36
4	i	102	MET	N-CA-C	6.43	119.11	111.71
14	s	42	ASN	N-CA-C	6.30	121.11	113.17
11	p	46	GLY	N-CA-C	6.08	121.20	113.24
15	t	72	LYS	N-CA-CB	6.00	119.63	110.39
18	w	91	PRO	N-CA-CB	-5.94	96.42	102.72
2	H	154	ASP	N-CA-C	5.92	117.40	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	281	0	222	3	0
2	H	1641	0	1651	34	0
3	h	1592	0	1582	25	0
4	i	1561	0	1562	29	0
5	j	1160	0	1164	18	0
6	k	807	0	758	17	0
7	l	1034	0	1046	20	0
8	m	961	0	978	7	0
9	n	972	0	1005	27	0
10	o	701	0	694	21	0
11	p	811	0	787	33	0
12	q	918	0	962	13	0
13	r	388	0	409	9	0
14	s	665	0	669	12	0
15	t	679	0	679	11	0
16	u	1100	0	1098	23	0
17	v	638	0	684	4	0
18	w	517	0	542	12	0
19	x	632	0	624	16	0
20	y	609	0	661	18	0
21	z	522	0	573	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	2	31728	0	15978	328	0
All	All	49917	0	34328	621	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 8.

All (621) 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)
11:p:43:SER:HB3	11:p:68:CYS:SG	1.92	1.09
10:o:10:LYS:O	10:o:97:VAL:HG12	1.74	0.88
9:n:96:LEU:HD22	9:n:101:LEU:HD22	1.57	0.87
10:o:56:VAL:HG23	22:2:955:C:O2'	1.75	0.87
2:H:152:ILE:HG23	2:H:155:MET:HE2	1.59	0.85
9:n:10:ARG:HG3	9:n:11:LYS:H	1.44	0.81
2:H:36:ARG:O	2:H:39:ILE:HG22	1.81	0.80
11:p:51:ARG:NH1	11:p:51:ARG:HA	1.99	0.78
22:2:1163:G:O2'	22:2:1164:G:N7	2.16	0.76
19:x:1:MET:N	19:x:8:GLY:O	2.19	0.75
11:p:43:SER:CB	11:p:68:CYS:SG	2.73	0.75
2:H:118:ILE:HD11	2:H:142:ARG:HD3	1.70	0.74
22:2:930:A:H61	22:2:1216:C:H42	1.37	0.72
4:i:102:MET:HE1	4:i:140:VAL:HB	1.73	0.71
22:2:654:A:H5'	22:2:714:C:H1'	1.73	0.71
22:2:661:A:H2'	22:2:662:G:C8	2.26	0.70
18:w:49:ASP:HA	18:w:52:LEU:HD13	1.74	0.70
4:i:123:ASN:ND2	4:i:138:ASP:OD1	2.24	0.70
13:r:29:ARG:O	13:r:33:ILE:HD12	1.91	0.70
22:2:1286:G:N2	22:2:1312:G:O2'	2.17	0.70
11:p:51:ARG:HA	11:p:51:ARG:HH11	1.55	0.69
9:n:21:GLU:OE2	9:n:21:GLU:N	2.21	0.69
5:j:121:LEU:HD13	5:j:129:VAL:HG21	1.74	0.69
22:2:373:G:N2	22:2:376:A:OP2	2.25	0.69
22:2:1400:A:N6	22:2:1455:A:O2'	2.26	0.68
4:i:102:MET:HE2	4:i:175:GLY:HA3	1.75	0.68
22:2:1337:U:H2'	22:2:1338:A:C8	2.29	0.68
2:H:167:ILE:HD11	2:H:186:ALA:HB1	1.76	0.67
9:n:91:GLU:N	9:n:91:GLU:OE2	2.27	0.67
4:i:126:VAL:HG21	4:i:143:ARG:HH11	1.57	0.67
15:t:32:THR:HG22	15:t:62:ARG:HH11	1.59	0.67
18:w:44:ASP:OD1	18:w:45:TYR:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:n:96:LEU:HD22	9:n:101:LEU:CD2	2.24	0.66
22:2:355:G:N2	22:2:358:U:OP2	2.25	0.66
11:p:34:ASN:OD1	11:p:35:LYS:N	2.29	0.66
22:2:62:U:OP1	22:2:378:U:O2'	2.14	0.66
22:2:959:G:OP2	22:2:1339:U:O2'	2.13	0.66
14:s:52:CYS:HB3	14:s:56:GLY:H	1.60	0.65
11:p:19:ALA:HA	11:p:32:LEU:HA	1.79	0.65
11:p:109:ILE:HD12	21:z:3:ILE:HD13	1.79	0.65
2:H:73:THR:O	2:H:73:THR:HG22	1.95	0.65
3:h:131:ARG:O	3:h:135:MET:HG3	1.97	0.65
9:n:16:ARG:NH1	22:2:1129:C:O2	2.28	0.65
5:j:49:ASN:OD1	5:j:50:GLY:N	2.30	0.64
22:2:453:C:N3	22:2:462:G:N2	2.45	0.64
22:2:410:G:H22	22:2:419:A:H2	1.45	0.64
3:h:124:GLU:OE2	3:h:189:HIS:N	2.30	0.64
4:i:144:GLU:HG2	4:i:147:LYS:HE3	1.80	0.64
19:x:62:VAL:HA	19:x:66:MET:HE3	1.80	0.64
22:2:489:G:H2'	22:2:490:A:C8	2.32	0.64
22:2:1268:A:H2'	22:2:1269:A:C8	2.32	0.64
2:H:80:ILE:HD11	2:H:211:ILE:HG22	1.80	0.64
9:n:16:ARG:NH2	22:2:1110:C:OP1	2.30	0.64
22:2:1503:G:H2'	22:2:1504:A:H8	1.63	0.63
22:2:489:G:H2'	22:2:490:A:H8	1.64	0.63
4:i:102:MET:CE	4:i:175:GLY:HA3	2.29	0.63
3:h:93:VAL:HG12	3:h:94:THR:HG23	1.81	0.62
13:r:75:MET:HA	13:r:75:MET:HE3	1.80	0.62
5:j:85:GLN:OE1	5:j:125:GLY:O	2.16	0.62
22:2:710:A:O2'	22:2:712:U:OP2	2.16	0.62
11:p:23:SER:OG	11:p:87:PRO:O	2.16	0.62
7:l:77:VAL:HA	7:l:90:PRO:HA	1.81	0.62
20:y:73:LYS:O	20:y:77:THR:HG22	1.99	0.61
5:j:58:LYS:NZ	22:2:1062:G:N7	2.48	0.61
8:m:10:LEU:HD22	8:m:77:ILE:HD11	1.81	0.61
22:2:138:G:H2'	22:2:139:G:C8	2.35	0.61
20:y:6:SER:OG	22:2:61:G:N7	2.33	0.61
4:i:145:LYS:HB3	16:u:136:GLU:HG2	1.81	0.61
10:o:45:LYS:NZ	10:o:47:LEU:HD21	2.16	0.61
22:2:272:A:H5''	22:2:273:C:H3'	1.82	0.61
22:2:662:G:H2'	22:2:663:A:H8	1.66	0.61
3:h:46:LEU:HD13	3:h:75:ILE:HG12	1.82	0.61
22:2:370:G:H2'	22:2:371:A:H8	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:1407:G:H1	22:2:1448:A:H61	1.48	0.61
16:u:95:THR:HG22	16:u:96:GLN:H	1.66	0.61
18:w:44:ASP:OD1	18:w:46:LYS:N	2.25	0.61
22:2:1404:G:O6	22:2:1451:U:O4	2.19	0.60
11:p:54:LYS:O	11:p:57:THR:OG1	2.20	0.60
2:H:69:LEU:HD21	2:H:162:LEU:HG	1.84	0.60
2:H:72:ALA:HB3	2:H:81:VAL:HG11	1.84	0.60
12:q:39:THR:HG21	12:q:49:MET:HG3	1.82	0.60
18:w:31:LYS:N	22:2:1514:U:O4	2.34	0.60
18:w:38:SER:OG	22:2:1516:C:OP2	2.17	0.60
22:2:421:U:OP2	22:2:422:G:O2'	2.19	0.60
22:2:432:U:O2'	22:2:434:U:O4	2.20	0.60
14:s:9:ARG:NH1	22:2:964:U:OP1	2.35	0.60
17:v:28:GLU:O	17:v:44:THR:HG23	2.02	0.60
22:2:1405:G:H2'	22:2:1406:G:C8	2.37	0.60
6:k:5:GLU:OE2	6:k:93:LEU:HD21	2.02	0.59
7:l:9:ARG:NH2	22:2:1358:U:O4	2.35	0.59
2:H:205:ASP:HA	2:H:211:ILE:HD11	1.84	0.59
11:p:27:ASN:OD1	11:p:28:ILE:N	2.32	0.59
11:p:83:TYR:HD1	11:p:109:ILE:HB	1.67	0.58
7:l:30:MET:HG2	7:l:31:TRP:N	2.18	0.58
22:2:716:A:H2'	22:2:717:A:C8	2.39	0.58
5:j:58:LYS:O	5:j:68:LYS:NZ	2.36	0.58
22:2:1337:U:H2'	22:2:1338:A:H8	1.69	0.58
12:q:50:ARG:HD2	12:q:90:LEU:HD11	1.86	0.58
13:r:13:LYS:NZ	22:2:1283:U:OP1	2.36	0.58
15:t:1:MET:N	22:2:729:A:OP1	2.37	0.58
22:2:397:G:O2'	22:2:486:A:N1	2.35	0.58
6:k:107:LYS:NZ	22:2:1516:C:O2'	2.33	0.58
11:p:37:GLY:O	22:2:671:G:N2	2.37	0.58
19:x:1:MET:H3	19:x:7:LYS:HB2	1.69	0.58
17:v:22:LYS:H	17:v:54:ASN:HD21	1.52	0.57
22:2:488:G:H2'	22:2:489:G:H8	1.69	0.57
7:l:47:ASP:O	7:l:51:THR:HG23	2.05	0.57
22:2:1114:G:H3'	22:2:1115:A:C8	2.39	0.57
10:o:71:ARG:NH2	22:2:1134:A:OP1	2.38	0.57
11:p:73:LEU:HD11	11:p:102:GLY:HA3	1.85	0.57
13:r:85:CYS:SG	13:r:86:TYR:N	2.77	0.57
4:i:99:VAL:HG11	4:i:120:ILE:HD13	1.87	0.57
11:p:30:ILE:HD11	11:p:65:ALA:HA	1.86	0.57
22:2:17:U:H2'	22:2:18:C:C6	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:1404:G:N1	22:2:1451:U:N3	2.53	0.57
10:o:58:LYS:HE3	10:o:61:ARG:HH22	1.68	0.57
14:s:73:ARG:NH2	22:2:1041:U:OP1	2.38	0.57
2:H:15:VAL:HG12	2:H:210:SER:HB2	1.86	0.56
20:y:8:LEU:O	20:y:12:ARG:NH1	2.37	0.56
22:2:987:G:C2	22:2:1019:A:H1'	2.40	0.56
22:2:1446:A:H2'	22:2:1447:A:C8	2.39	0.56
11:p:21:ILE:HG23	11:p:30:ILE:HG22	1.87	0.56
22:2:1307:U:H2'	22:2:1308:C:H6	1.71	0.56
22:2:185:G:H2'	22:2:186:G:H8	1.70	0.56
22:2:1238:C:O2'	22:2:1239:A:OP2	2.19	0.56
2:H:98:PRO:HG2	2:H:101:MET:HE1	1.88	0.56
22:2:960:A:H2'	22:2:961:A:H5''	1.88	0.56
5:j:59:SER:OG	5:j:60:LYS:N	2.39	0.56
10:o:56:VAL:O	10:o:56:VAL:HG13	2.05	0.56
13:r:29:ARG:NH1	22:2:1309:C:O2'	2.39	0.55
6:k:9:ILE:HD13	6:k:87:ARG:HB3	1.88	0.55
16:u:6:ARG:NH2	16:u:28:LYS:O	2.39	0.55
22:2:142:A:H62	22:2:161:U:H3	1.54	0.55
22:2:812:U:H2'	22:2:813:A:H8	1.72	0.55
18:w:40:ILE:H	18:w:40:ILE:HD12	1.71	0.55
22:2:464:A:H2'	22:2:465:G:C8	2.41	0.55
22:2:995:U:H2'	22:2:996:G:H8	1.72	0.55
22:2:488:G:H2'	22:2:489:G:C8	2.42	0.54
22:2:958:G:H4'	22:2:959:G:H5''	1.89	0.54
11:p:32:LEU:HD23	11:p:32:LEU:H	1.71	0.54
22:2:195:U:H2'	22:2:196:A:H8	1.71	0.54
16:u:5:ILE:N	16:u:65:GLN:O	2.32	0.54
22:2:349:A:N3	22:2:361:U:O2'	2.33	0.54
22:2:290:G:N2	22:2:293:A:OP2	2.34	0.54
7:l:116:LYS:O	22:2:1221:A:O2'	2.24	0.54
22:2:184:C:H42	22:2:191:A:H61	1.55	0.54
22:2:292:G:H2'	22:2:293:A:C8	2.42	0.54
22:2:1304:G:H2'	22:2:1305:A:C8	2.43	0.54
7:l:111:ARG:HG2	7:l:118:MET:HE1	1.90	0.54
9:n:89:ASN:ND2	9:n:92:ASN:OD1	2.32	0.54
18:w:63:PRO:HD2	18:w:66:LEU:HD22	1.89	0.54
10:o:11:SER:HB3	10:o:17:VAL:HG22	1.89	0.53
19:x:39:MET:HE1	19:x:68:GLY:HA2	1.90	0.53
18:w:90:MET:HB3	18:w:91:PRO:HD2	1.89	0.53
2:H:106:VAL:O	2:H:110:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:85:GLN:HG3	5:j:85:GLN:O	2.07	0.53
22:2:812:U:H2'	22:2:813:A:C8	2.44	0.53
22:2:1240:G:H2'	22:2:1241:C:C6	2.43	0.53
10:o:13:ASP:OD1	10:o:16:LEU:HG	2.07	0.53
12:q:18:LYS:NZ	22:2:893:C:OP2	2.42	0.53
11:p:19:ALA:N	11:p:81:LYS:O	2.29	0.53
11:p:115:PRO:HG2	21:z:35:ARG:NH1	2.23	0.53
22:2:394:C:O2'	22:2:609:A:N3	2.39	0.53
22:2:1503:G:H2'	22:2:1504:A:C8	2.42	0.53
22:2:1250:G:H2'	22:2:1251:A:C8	2.44	0.53
4:i:101:ARG:HD2	4:i:163:TYR:CE2	2.44	0.53
11:p:83:TYR:CD1	11:p:109:ILE:HB	2.44	0.53
4:i:61:SER:O	4:i:108:ARG:NH1	2.41	0.52
4:i:95:LEU:O	4:i:99:VAL:HG13	2.09	0.52
22:2:1417:G:H2'	22:2:1418:U:C6	2.43	0.52
20:y:51:VAL:O	20:y:55:ILE:HG13	2.08	0.52
22:2:1446:A:H2'	22:2:1447:A:H8	1.72	0.52
22:2:1486:A:H2'	22:2:1487:C:C6	2.44	0.52
4:i:150:GLU:N	4:i:150:GLU:OE1	2.41	0.52
21:z:13:ASP:O	21:z:17:LYS:HG2	2.10	0.52
22:2:1101:G:H2'	22:2:1102:U:C6	2.44	0.52
9:n:89:ASN:HB3	9:n:92:ASN:ND2	2.24	0.52
3:h:50:SER:HB2	3:h:114:LEU:HD22	1.92	0.52
4:i:114:ILE:HD11	4:i:152:ILE:HD11	1.92	0.52
16:u:106:TRP:HE3	16:u:107:LEU:HD23	1.74	0.51
19:x:75:SER:O	19:x:75:SER:OG	2.25	0.51
22:2:326:A:H2'	22:2:327:C:C6	2.45	0.51
10:o:4:LYS:N	10:o:75:ILE:O	2.44	0.51
22:2:198:A:H2'	22:2:199:A:C8	2.45	0.51
7:l:30:MET:CG	7:l:31:TRP:N	2.74	0.51
22:2:236:A:H4'	22:2:237:U:O5'	2.10	0.51
16:u:103:LEU:O	16:u:107:LEU:HG	2.11	0.51
22:2:363:G:O2'	22:2:470:A:O2'	2.27	0.51
9:n:48:GLN:O	9:n:52:MET:HG3	2.11	0.51
20:y:63:ILE:HG22	20:y:64:ILE:HG23	1.93	0.51
22:2:506:C:H2'	22:2:518:G:C8	2.45	0.51
3:h:119:ILE:HD13	3:h:133:ILE:HD13	1.93	0.51
9:n:25:ASN:OD1	9:n:25:ASN:N	2.43	0.51
5:j:144:LYS:NZ	22:2:1059:U:O2'	2.43	0.51
7:l:32:ASP:OD1	22:2:1331:A:O2'	2.24	0.51
22:2:262:U:H2'	22:2:263:A:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:326:A:H2'	22:2:327:C:H6	1.75	0.51
22:2:1109:C:O2'	22:2:1110:C:OP1	2.27	0.51
22:2:448:C:C2	22:2:449:A:C8	2.99	0.50
22:2:1043:U:H2'	22:2:1044:C:C6	2.46	0.50
22:2:1394:C:H2'	22:2:1395:A:C8	2.46	0.50
13:r:16:VAL:HG13	13:r:17:ILE:HG13	1.93	0.50
19:x:29:SER:OG	19:x:30:VAL:N	2.44	0.50
22:2:377:G:H2'	22:2:378:U:C6	2.46	0.50
20:y:12:ARG:HH21	22:2:93:C:P	2.34	0.50
22:2:710:A:H2	22:2:721:A:H61	1.59	0.50
22:2:1295:C:H2'	22:2:1296:U:C6	2.46	0.50
22:2:1461:G:H2'	22:2:1462:G:C8	2.47	0.50
10:o:58:LYS:NZ	22:2:956:G:OP1	2.38	0.50
17:v:69:PRO:O	22:2:257:C:O2'	2.25	0.50
22:2:172:A:H2'	22:2:173:G:C2	2.47	0.50
22:2:1126:G:N2	22:2:1128:A:H62	2.08	0.50
22:2:1240:G:H2'	22:2:1241:C:H6	1.77	0.50
22:2:1307:U:H2'	22:2:1308:C:C6	2.47	0.50
22:2:1388:U:H2'	22:2:1389:C:C6	2.47	0.50
3:h:85:LYS:O	3:h:88:GLU:HG3	2.12	0.50
22:2:430:C:H2'	22:2:431:U:C6	2.46	0.50
6:k:100:TRP:HA	6:k:103:ARG:NH1	2.27	0.50
22:2:1491:A:H2'	22:2:1492:A:C8	2.46	0.50
5:j:111:VAL:O	5:j:118:ARG:NH2	2.44	0.50
21:z:13:ASP:O	21:z:17:LYS:HE3	2.12	0.50
22:2:702:G:H2'	22:2:703:A:C8	2.47	0.50
22:2:1218:A:H2'	22:2:1219:C:C6	2.47	0.50
22:2:1432:G:H2'	22:2:1433:A:H8	1.77	0.50
2:H:10:LEU:HB2	2:H:15:VAL:HG22	1.94	0.49
10:o:70:LYS:O	10:o:71:ARG:NH1	2.35	0.49
5:j:132:LYS:NZ	22:2:9:G:OP2	2.38	0.49
6:k:100:TRP:HA	6:k:103:ARG:HH12	1.76	0.49
22:2:60:A:OP1	22:2:324:G:N1	2.29	0.49
22:2:929:A:H2'	22:2:930:A:C8	2.47	0.49
22:2:1142:G:C2	22:2:1143:C:C6	3.00	0.49
22:2:1319:G:H2'	22:2:1320:A:C8	2.47	0.49
1:A:32:LEU:HA	1:A:35:PHE:CD2	2.47	0.49
22:2:28:G:O2'	22:2:289:U:OP1	2.30	0.49
22:2:512:G:H2'	22:2:513:C:C6	2.47	0.49
22:2:409:G:H3'	22:2:410:G:H8	1.77	0.49
22:2:1058:G:N2	22:2:1061:A:OP2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:94:ASP:O	6:k:98:ILE:HD12	2.12	0.49
22:2:383:A:H2'	22:2:384:C:C6	2.47	0.49
11:p:53:SER:OG	22:2:682:A:OP1	2.31	0.49
11:p:59:TYR:O	11:p:63:MET:HG2	2.12	0.49
12:q:39:THR:CG2	12:q:49:MET:HG3	2.42	0.49
19:x:1:MET:N	19:x:7:LYS:HB2	2.27	0.49
22:2:1295:C:H2'	22:2:1296:U:H6	1.77	0.49
9:n:89:ASN:HB3	9:n:92:ASN:HD21	1.76	0.49
19:x:50:ALA:HB1	19:x:57:PHE:HB3	1.94	0.49
21:z:20:LYS:NZ	21:z:24:ASP:OD2	2.40	0.49
6:k:94:ASP:O	6:k:97:ALA:N	2.46	0.49
7:l:74:HIS:HB2	7:l:144:HIS:CE1	2.48	0.49
3:h:20:SER:O	14:s:82:PRO:HB3	2.13	0.49
20:y:29:ARG:O	20:y:32:ILE:HD12	2.13	0.49
22:2:700:U:H2'	22:2:701:G:C8	2.48	0.49
22:2:1388:U:O2'	22:2:1490:G:N2	2.45	0.49
22:2:321:C:H4'	22:2:322:A:H5'	1.95	0.48
22:2:998:A:C2	22:2:1201:U:H1'	2.48	0.48
22:2:1265:U:H2'	22:2:1266:A:C8	2.47	0.48
10:o:14:HIS:NE2	22:2:1134:A:H4'	2.27	0.48
14:s:63:ARG:NH2	22:2:1340:C:O2	2.45	0.48
15:t:38:LEU:HD22	15:t:51:THR:CG2	2.43	0.48
22:2:919:C:C2	22:2:920:A:C8	3.01	0.48
22:2:1232:A:H2'	22:2:1233:G:C8	2.48	0.48
3:h:174:LEU:HD23	3:h:181:ILE:HD12	1.95	0.48
7:l:53:LYS:O	7:l:54:GLN:HG3	2.14	0.48
6:k:4:TYR:OH	22:2:726:A:OP1	2.13	0.48
9:n:47:LEU:HA	9:n:50:LEU:HD13	1.96	0.48
16:u:117:LYS:HA	16:u:117:LYS:HE2	1.95	0.48
16:u:24:ASP:OD1	16:u:25:ALA:N	2.47	0.48
20:y:10:ARG:HD2	22:2:98:C:H42	1.78	0.48
4:i:47:GLU:O	4:i:51:GLN:HG3	2.13	0.48
5:j:43:VAL:HG11	5:j:70:VAL:HG22	1.95	0.48
5:j:106:SER:OG	22:2:6:G:O6	2.31	0.48
22:2:56:U:H2'	22:2:57:G:C8	2.48	0.48
22:2:408:C:N4	22:2:421:U:H3	2.11	0.48
22:2:1126:G:H21	22:2:1128:A:H62	1.62	0.48
22:2:1395:A:H2	22:2:1460:G:H22	1.61	0.48
2:H:113:LYS:HA	2:H:113:LYS:HD3	1.59	0.48
4:i:96:ASP:OD1	4:i:97:ASN:N	2.47	0.48
2:H:32:ILE:HD11	2:H:190:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:u:98:GLN:H	16:u:98:GLN:CD	2.17	0.48
22:2:1261:A:H2'	22:2:1261:A:N3	2.29	0.48
5:j:168:GLU:N	5:j:168:GLU:OE2	2.47	0.48
7:l:109:TYR:HB3	7:l:135:ALA:HB3	1.96	0.48
10:o:21:ALA:O	10:o:25:VAL:HG12	2.14	0.48
18:w:50:PHE:O	18:w:53:LYS:NZ	2.45	0.48
22:2:1404:G:O6	22:2:1451:U:C4	2.66	0.48
2:H:152:ILE:HG23	2:H:155:MET:CE	2.37	0.47
3:h:56:ILE:HG12	3:h:65:VAL:HG22	1.96	0.47
6:k:9:ILE:HA	6:k:59:PHE:O	2.15	0.47
22:2:127:C:O2'	22:2:128:U:H6	1.97	0.47
4:i:149:LEU:HB2	4:i:152:ILE:HD13	1.96	0.47
8:m:9:TYR:HD2	8:m:26:ILE:HG21	1.79	0.47
20:y:61:LYS:NZ	22:2:167:C:OP1	2.45	0.47
22:2:151:A:OP1	22:2:151:A:H8	1.97	0.47
22:2:873:G:O2'	22:2:889:G:O6	2.27	0.47
2:H:73:THR:O	2:H:73:THR:CG2	2.62	0.47
22:2:750:G:H2'	22:2:751:A:C8	2.49	0.47
22:2:1143:C:C2	22:2:1144:C:C5	3.02	0.47
22:2:1450:C:H2'	22:2:1451:U:C6	2.49	0.47
16:u:69:THR:O	16:u:73:ILE:HG23	2.15	0.47
18:w:48:ALA:O	18:w:52:LEU:CD1	2.62	0.47
22:2:848:A:H2'	22:2:849:A:C8	2.49	0.47
22:2:1445:U:H2'	22:2:1446:A:H8	1.79	0.47
15:t:32:THR:HG22	15:t:62:ARG:NH1	2.28	0.47
22:2:41:G:H2'	22:2:42:G:C8	2.50	0.47
22:2:41:G:H2'	22:2:42:G:H8	1.79	0.47
22:2:998:A:H2	22:2:1201:U:H1'	1.78	0.47
2:H:75:LYS:HA	2:H:78:LYS:HE3	1.96	0.47
22:2:569:G:N1	22:2:747:A:OP2	2.40	0.47
22:2:1108:G:H1'	22:2:1262:A:C6	2.49	0.47
22:2:1211:A:H2'	22:2:1212:C:C6	2.49	0.47
22:2:1422:U:H2'	22:2:1423:G:O4'	2.15	0.47
2:H:88:ALA:O	2:H:90:MET:HG2	2.15	0.47
4:i:193:GLN:NE2	4:i:197:GLU:OE2	2.48	0.47
9:n:58:ASN:O	9:n:58:ASN:ND2	2.47	0.47
22:2:891:A:H2'	22:2:892:A:H8	1.79	0.47
22:2:437:A:H2'	22:2:438:C:C6	2.49	0.47
22:2:662:G:H2'	22:2:663:A:C8	2.49	0.47
16:u:85:LEU:O	16:u:89:VAL:HG23	2.15	0.47
22:2:197:U:H2'	22:2:198:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:987:G:N2	22:2:1019:A:O3'	2.48	0.47
22:2:183:G:H2'	22:2:184:C:C6	2.50	0.46
22:2:1408:G:H1	22:2:1447:A:H61	1.63	0.46
10:o:79:SER:OG	10:o:80:SER:N	2.48	0.46
22:2:377:G:H2'	22:2:378:U:H6	1.79	0.46
22:2:651:G:H2'	22:2:652:G:C8	2.51	0.46
22:2:1018:C:H2'	22:2:1019:A:C4	2.51	0.46
22:2:1110:C:O2'	22:2:1125:G:N2	2.48	0.46
10:o:24:ILE:HD11	10:o:73:ILE:HD13	1.97	0.46
21:z:22:LYS:O	21:z:26:THR:HG23	2.15	0.46
22:2:328:C:H2'	22:2:329:A:H8	1.80	0.46
22:2:980:G:H2'	22:2:981:C:C6	2.51	0.46
8:m:13:VAL:O	8:m:17:VAL:HG23	2.15	0.46
10:o:22:GLU:HA	10:o:25:VAL:HG12	1.97	0.46
11:p:108:ILE:O	11:p:109:ILE:HD13	2.16	0.46
22:2:683:A:H2'	22:2:684:A:C8	2.50	0.46
22:2:334:C:H2'	22:2:335:C:H6	1.80	0.46
3:h:171:ARG:HH21	3:h:173:PRO:HG3	1.80	0.46
11:p:65:ALA:HB1	11:p:98:ILE:HG13	1.98	0.46
12:q:53:ALA:HB2	12:q:67:ILE:HD11	1.96	0.46
11:p:26:ASN:ND2	22:2:680:U:OP2	2.48	0.46
12:q:51:LYS:NZ	22:2:509:G:OP1	2.49	0.46
22:2:1023:U:O2'	22:2:1024:A:OP1	2.28	0.46
22:2:1310:G:H2'	22:2:1311:U:H5'	1.97	0.46
22:2:1343:C:O2'	22:2:1344:C:H5'	2.16	0.46
22:2:1497:C:H2'	22:2:1498:G:C8	2.51	0.46
1:A:33:GLN:HA	1:A:36:GLU:OE1	2.16	0.46
9:n:97:LYS:HB3	9:n:98:PRO:HD3	1.98	0.46
12:q:30:ARG:NH2	12:q:58:THR:OG1	2.45	0.46
22:2:969:A:H2'	22:2:970:A:C8	2.51	0.46
22:2:1461:G:H2'	22:2:1462:G:H8	1.80	0.46
6:k:9:ILE:CD1	6:k:87:ARG:HB3	2.46	0.46
10:o:27:THR:O	10:o:30:THR:OG1	2.29	0.46
20:y:64:ILE:HB	20:y:68:LYS:HD2	1.98	0.46
22:2:1373:U:H2'	22:2:1374:G:C8	2.51	0.46
9:n:107:ARG:HB3	22:2:1328:G:H5''	1.97	0.46
16:u:73:ILE:HG13	16:u:74:LEU:N	2.30	0.46
2:H:127:PHE:CZ	2:H:135:ARG:HG3	2.51	0.45
3:h:112:ALA:O	3:h:184:ALA:HB3	2.16	0.45
3:h:133:ILE:HG21	3:h:167:PHE:CD1	2.52	0.45
8:m:38:ILE:HD12	8:m:112:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:w:40:ILE:HD12	18:w:40:ILE:N	2.31	0.45
22:2:239:A:C2	22:2:275:A:C5	3.03	0.45
22:2:759:G:H2'	22:2:760:U:C6	2.51	0.45
22:2:175:A:H2'	22:2:176:U:C6	2.51	0.45
22:2:351:U:H2'	22:2:352:G:H8	1.82	0.45
22:2:703:A:OP1	22:2:793:C:O2'	2.30	0.45
22:2:739:U:H2'	22:2:740:G:O4'	2.16	0.45
22:2:1486:A:H2'	22:2:1487:C:H6	1.81	0.45
5:j:126:ILE:CG2	5:j:129:VAL:HG13	2.47	0.45
12:q:56:ARG:HH11	12:q:56:ARG:HG2	1.81	0.45
20:y:53:SER:OG	22:2:201:U:OP1	2.34	0.45
22:2:183:G:H2'	22:2:184:C:H6	1.80	0.45
22:2:382:A:H3'	22:2:383:A:H8	1.80	0.45
22:2:842:A:OP2	22:2:852:G:N1	2.38	0.45
4:i:82:VAL:HG13	5:j:108:GLY:HA3	1.98	0.45
15:t:77:TYR:O	15:t:81:ILE:HG23	2.17	0.45
15:t:28:ILE:O	15:t:32:THR:HG23	2.17	0.45
22:2:463:G:N7	22:2:464:A:C8	2.85	0.45
22:2:1018:C:H2'	22:2:1019:A:C2	2.52	0.45
22:2:1052:C:H2'	22:2:1053:G:H8	1.82	0.45
22:2:1407:G:H1	22:2:1448:A:N6	2.14	0.45
3:h:106:LYS:C	3:h:107:ARG:HG2	2.40	0.45
4:i:67:LYS:HG3	22:2:534:A:OP1	2.17	0.45
11:p:94:ALA:O	11:p:98:ILE:HD12	2.17	0.45
16:u:32:LYS:NZ	22:2:304:C:OP1	2.33	0.45
19:x:55:ARG:HB3	22:2:941:A:C2	2.52	0.45
22:2:173:G:OP2	22:2:173:G:N2	2.30	0.45
22:2:527:A:H2'	22:2:528:G:C8	2.51	0.45
22:2:1031:G:O2'	22:2:1032:C:OP1	2.28	0.45
12:q:26:SER:O	12:q:26:SER:OG	2.32	0.45
22:2:751:A:H2'	22:2:752:C:C6	2.52	0.45
21:z:32:LEU:HD12	21:z:32:LEU:HA	1.86	0.45
22:2:908:G:C2	22:2:910:G:C8	3.05	0.45
22:2:935:U:H2'	22:2:936:G:H8	1.82	0.45
6:k:12:PRO:HA	6:k:59:PHE:CE2	2.51	0.45
11:p:32:LEU:HD11	11:p:72:ALA:HB2	1.99	0.45
22:2:99:A:C6	22:2:319:G:C6	3.05	0.45
22:2:684:A:H2'	22:2:685:U:C6	2.51	0.45
9:n:10:ARG:HG3	9:n:11:LYS:N	2.21	0.45
3:h:205:GLU:HB2	3:h:207:TYR:CE1	2.52	0.44
8:m:15:ASN:ND2	22:2:814:C:O2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:p:84:VAL:HG21	11:p:91:ARG:HB3	1.98	0.44
5:j:126:ILE:HG21	5:j:129:VAL:CG1	2.47	0.44
19:x:78:ARG:NH2	22:2:1205:C:OP2	2.33	0.44
22:2:262:U:H2'	22:2:263:A:C8	2.52	0.44
22:2:1516:C:H1'	22:2:1517:U:H5	1.82	0.44
3:h:148:ILE:N	3:h:172:ILE:HD11	2.32	0.44
12:q:12:ARG:HH21	22:2:552:C:P	2.40	0.44
14:s:46:VAL:HG21	22:2:1297:G:H4'	1.99	0.44
2:H:187:MET:HE1	2:H:211:ILE:HD13	1.98	0.44
4:i:112:ARG:HA	4:i:115:VAL:HG12	1.99	0.44
9:n:69:GLY:O	9:n:73:GLN:HG3	2.17	0.44
22:2:185:G:H2'	22:2:186:G:C8	2.51	0.44
22:2:462:G:C2	22:2:463:G:N7	2.86	0.44
10:o:35:VAL:HG12	10:o:75:ILE:HG23	1.99	0.44
16:u:18:TYR:O	16:u:40:TYR:N	2.46	0.44
3:h:154:GLY:HA3	3:h:162:ALA:HB1	2.00	0.44
9:n:110:GLU:HG2	9:n:119:ALA:HB1	1.99	0.44
11:p:21:ILE:HG12	11:p:30:ILE:HG22	1.99	0.44
22:2:859:A:H2'	22:2:860:U:C6	2.53	0.44
22:2:878:A:H2'	22:2:879:A:C8	2.53	0.44
22:2:901:A:H2'	22:2:902:A:C8	2.53	0.44
22:2:1031:G:HO2'	22:2:1032:C:P	2.40	0.44
4:i:130:PRO:HD2	22:2:396:C:H5''	1.99	0.44
16:u:49:VAL:HG12	16:u:77:LYS:HD2	2.00	0.44
22:2:0:U:H4'	22:2:1:A:H5'	1.98	0.44
10:o:58:LYS:HE3	10:o:61:ARG:NH2	2.31	0.44
12:q:114:ARG:NH2	22:2:489:G:OP1	2.44	0.44
16:u:54:ASP:OD1	16:u:82:LYS:NZ	2.45	0.44
6:k:93:LEU:HD22	6:k:97:ALA:HB1	1.99	0.44
15:t:71:ARG:O	15:t:71:ARG:HG2	2.17	0.44
22:2:21:G:H2'	22:2:22:G:C8	2.52	0.44
4:i:5:THR:O	4:i:5:THR:OG1	2.34	0.43
9:n:19:VAL:HG21	9:n:84:VAL:HG11	1.99	0.43
22:2:930:A:H61	22:2:1216:C:N4	2.11	0.43
22:2:989:C:H4'	22:2:990:C:OP1	2.17	0.43
22:2:1068:A:H2'	22:2:1069:G:H8	1.82	0.43
22:2:1126:G:H2'	22:2:1127:A:C8	2.52	0.43
16:u:5:ILE:O	16:u:67:THR:HG23	2.18	0.43
22:2:-1:A:H1'	22:2:0:U:C5	2.53	0.43
22:2:1259:C:O2'	22:2:1261:A:C8	2.69	0.43
2:H:68:ILE:H	2:H:90:MET:CE	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:ARG:HG2	2:H:109:ARG:HH11	1.82	0.43
3:h:17:GLY:HA3	3:h:212:LEU:O	2.18	0.43
3:h:155:ARG:NE	3:h:159:ALA:O	2.52	0.43
13:r:83:LEU:HG	19:x:74:PHE:HE1	1.83	0.43
19:x:63:THR:H	19:x:66:MET:HE3	1.83	0.43
22:2:157:G:H2'	22:2:158:G:C8	2.52	0.43
22:2:197:U:H2'	22:2:198:A:C8	2.53	0.43
22:2:370:G:H2'	22:2:371:A:C8	2.50	0.43
22:2:1161:A:H2'	22:2:1162:A:O4'	2.18	0.43
8:m:47:SER:OG	8:m:48:TYR:N	2.51	0.43
14:s:13:ARG:O	14:s:17:VAL:HG23	2.18	0.43
22:2:125:G:C6	22:2:318:A:N1	2.86	0.43
22:2:526:G:H2'	22:2:527:A:H8	1.84	0.43
22:2:568:C:H2'	22:2:569:G:O4'	2.18	0.43
11:p:23:SER:OG	11:p:24:THR:N	2.51	0.43
16:u:90:ARG:NH2	22:2:130:U:OP1	2.51	0.43
4:i:95:LEU:HB2	4:i:132:TYR:HB3	2.01	0.43
7:l:8:LYS:HE2	7:l:96:ASP:OD2	2.18	0.43
17:v:72:LYS:HG2	17:v:73:THR:OG1	2.18	0.43
22:2:-1:A:H1'	22:2:0:U:H5	1.84	0.43
22:2:125:G:O2'	22:2:126:C:O5'	2.37	0.43
22:2:905:G:H2'	22:2:906:A:C8	2.53	0.43
22:2:966:A:H5''	22:2:967:C:OP2	2.19	0.43
22:2:1068:A:H2'	22:2:1069:G:C8	2.54	0.43
5:j:150:LEU:HD12	5:j:150:LEU:HA	1.91	0.43
7:l:17:PHE:HB3	7:l:61:LEU:HD21	2.01	0.43
20:y:30:ASN:ND2	22:2:1431:G:OP1	2.24	0.43
21:z:7:LYS:HG3	21:z:10:GLU:OE1	2.18	0.43
22:2:45:G:H2'	22:2:46:G:C8	2.53	0.43
22:2:1101:G:H2'	22:2:1102:U:H6	1.83	0.43
16:u:53:LEU:HD23	16:u:53:LEU:HA	1.88	0.43
22:2:103:G:H2'	22:2:104:U:C6	2.53	0.43
2:H:109:ARG:HG2	2:H:109:ARG:NH1	2.34	0.43
7:l:40:LYS:HB3	7:l:40:LYS:HE3	1.71	0.43
22:2:328:C:C2	22:2:329:A:C8	3.07	0.43
22:2:456:U:O2'	22:2:457:A:O4'	2.37	0.43
22:2:533:C:H2'	22:2:534:A:O4'	2.19	0.43
22:2:647:A:H2'	22:2:648:C:C6	2.53	0.43
22:2:675:A:C2	22:2:692:A:C5	3.06	0.43
22:2:1401:G:N1	22:2:1455:A:H1'	2.34	0.43
22:2:1434:G:H2'	22:2:1435:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:t:23:LYS:HD3	15:t:25:GLU:HB2	2.01	0.43
16:u:6:ARG:HB2	22:2:369:G:H5''	2.01	0.43
22:2:198:A:H2'	22:2:199:A:H8	1.83	0.43
22:2:934:G:H2'	22:2:935:U:C6	2.53	0.43
22:2:1285:G:O2'	22:2:1286:G:OP1	2.32	0.43
9:n:84:VAL:HG12	9:n:85:MET:HE2	2.01	0.42
22:2:128:U:H2'	22:2:129:U:C6	2.54	0.42
22:2:437:A:H2'	22:2:438:C:H6	1.84	0.42
22:2:851:U:H2'	22:2:852:G:O4'	2.19	0.42
2:H:114:LYS:O	2:H:118:ILE:HG23	2.20	0.42
3:h:194:ARG:HH11	22:2:1187:C:H4'	1.84	0.42
19:x:9:PRO:HB3	19:x:39:MET:HG2	2.01	0.42
22:2:321:C:H1'	22:2:322:A:OP2	2.19	0.42
22:2:497:A:N3	22:2:531:U:O2'	2.48	0.42
22:2:1180:A:H2'	22:2:1181:U:C6	2.54	0.42
22:2:1513:U:H1'	22:2:1514:U:C6	2.54	0.42
11:p:48:MET:N	11:p:48:MET:SD	2.92	0.42
22:2:885:G:H2'	22:2:886:U:H6	1.85	0.42
22:2:1227:G:HO2'	22:2:1228:G:P	2.40	0.42
22:2:1405:G:H2'	22:2:1406:G:H8	1.84	0.42
6:k:12:PRO:HA	6:k:59:PHE:HE2	1.84	0.42
7:l:44:ASP:OD1	7:l:44:ASP:N	2.52	0.42
15:t:42:LEU:HD21	15:t:52:GLU:HG2	2.02	0.42
19:x:78:ARG:NH1	22:2:1302:U:O2'	2.53	0.42
22:2:866:C:O2'	22:2:867:U:H5'	2.20	0.42
22:2:891:A:H2'	22:2:892:A:C8	2.54	0.42
22:2:1306:C:H2'	22:2:1307:U:H6	1.84	0.42
22:2:1437:G:H2'	22:2:1438:C:H6	1.84	0.42
2:H:31:TYR:CD2	2:H:31:TYR:N	2.87	0.42
2:H:74:LYS:HD2	2:H:166:ASP:HB2	2.01	0.42
3:h:153:SER:HB2	22:2:1038:G:H5''	2.02	0.42
9:n:104:ARG:HH21	22:2:1098:G:H5''	1.83	0.42
20:y:37:LEU:HD23	20:y:37:LEU:HA	1.84	0.42
22:2:1126:G:O5'	22:2:1126:G:H8	2.02	0.42
2:H:54:ALA:O	2:H:58:LEU:HG	2.19	0.42
2:H:85:ALA:O	2:H:89:ASN:N	2.53	0.42
6:k:30:LEU:HD23	6:k:30:LEU:HA	1.76	0.42
10:o:53:SER:HB2	22:2:1041:U:O2'	2.19	0.42
12:q:30:ARG:HD2	12:q:30:ARG:HA	1.82	0.42
13:r:14:HIS:HB3	13:r:16:VAL:HG12	2.01	0.42
15:t:71:ARG:NH2	22:2:742:C:OP1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:w:44:ASP:OD1	18:w:44:ASP:C	2.62	0.42
22:2:690:A:H5''	22:2:691:G:N7	2.34	0.42
22:2:878:A:H2'	22:2:879:A:H8	1.83	0.42
22:2:1417:G:H2'	22:2:1418:U:H6	1.81	0.42
13:r:34:LEU:HD23	13:r:34:LEU:HA	1.86	0.42
22:2:196:A:H2'	22:2:197:U:H6	1.84	0.42
22:2:420:U:H2'	22:2:421:U:C6	2.54	0.42
11:p:30:ILE:CD1	11:p:65:ALA:HA	2.49	0.42
14:s:33:TYR:CE2	19:x:7:LYS:HB3	2.55	0.42
20:y:29:ARG:HA	20:y:32:ILE:HD11	2.00	0.42
22:2:306:A:H2'	22:2:307:C:C6	2.55	0.42
22:2:1134:A:H2'	22:2:1135:C:O4'	2.20	0.42
20:y:11:ILE:HD11	22:2:325:G:O2'	2.20	0.42
4:i:29:ARG:HA	4:i:31:TYR:CE1	2.55	0.42
4:i:168:TRP:HA	4:i:168:TRP:CE3	2.55	0.42
16:u:40:TYR:HD1	16:u:49:VAL:HG22	1.85	0.42
19:x:19:VAL:CG2	19:x:47:GLN:HE21	2.33	0.42
22:2:209:C:C2	22:2:210:A:C8	3.08	0.42
22:2:616:G:H2'	22:2:617:A:C8	2.55	0.42
3:h:43:HIS:CE1	3:h:51:VAL:HG23	2.55	0.41
22:2:463:G:C6	22:2:464:A:C4	3.08	0.41
22:2:1351:C:H2'	22:2:1352:G:C8	2.55	0.41
6:k:28:GLU:HA	6:k:31:THR:HG22	2.02	0.41
9:n:111:ARG:NE	9:n:112:LYS:O	2.48	0.41
22:2:647:A:H2'	22:2:648:C:H6	1.85	0.41
22:2:1029:G:H5'	22:2:1030:U:OP1	2.21	0.41
22:2:1144:C:C2	22:2:1145:A:C8	3.09	0.41
22:2:1379:C:H4'	22:2:1380:A:OP2	2.21	0.41
2:H:43:ASN:O	2:H:47:THR:OG1	2.36	0.41
7:l:68:LEU:HD12	7:l:68:LEU:HA	1.87	0.41
8:m:9:TYR:CD2	8:m:26:ILE:HG21	2.56	0.41
21:z:7:LYS:HE2	21:z:7:LYS:HB2	1.86	0.41
22:2:268:G:C2	22:2:269:G:C8	3.09	0.41
22:2:463:G:O6	22:2:464:A:C6	2.74	0.41
4:i:197:GLU:O	22:2:8:A:N6	2.52	0.41
7:l:15:PRO:HG2	9:n:41:THR:HG22	2.01	0.41
22:2:1114:G:N3	22:2:1114:G:H2'	2.35	0.41
22:2:1497:C:H2'	22:2:1498:G:H8	1.85	0.41
22:2:321:C:H4'	22:2:322:A:C5'	2.50	0.41
22:2:374:C:H2'	22:2:375:A:O4'	2.20	0.41
22:2:436:U:O4	22:2:437:A:N6	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:HB2	2:H:33:TYR:OH	2.20	0.41
2:H:21:THR:HG22	2:H:40:HIS:NE2	2.35	0.41
9:n:46:VAL:O	9:n:47:LEU:HG	2.19	0.41
20:y:28:THR:O	20:y:32:ILE:HG13	2.21	0.41
22:2:330:G:H2'	22:2:331:A:C8	2.55	0.41
22:2:679:G:H2'	22:2:680:U:C6	2.55	0.41
7:l:74:HIS:ND1	7:l:98:LYS:HD3	2.34	0.41
14:s:27:LEU:HB3	14:s:36:LEU:HD13	2.03	0.41
22:2:780:A:H1'	22:2:782:A:N7	2.36	0.41
22:2:1137:A:H2'	22:2:1138:G:O4'	2.21	0.41
22:2:1233:G:O2'	22:2:1351:C:O2'	2.36	0.41
5:j:60:LYS:NZ	5:j:60:LYS:HB2	2.36	0.41
12:q:17:LYS:HD3	12:q:17:LYS:HA	1.92	0.41
16:u:26:ARG:NH2	22:2:223:G:O2'	2.53	0.41
20:y:23:TYR:O	20:y:27:THR:HG22	2.21	0.41
22:2:336:U:H2'	22:2:338:C:C5	2.55	0.41
22:2:364:U:H2'	22:2:365:C:O4'	2.21	0.41
3:h:129:TYR:CE1	3:h:130:ARG:HG2	2.55	0.41
6:k:46:LYS:HE3	6:k:46:LYS:HB2	1.84	0.41
14:s:52:CYS:O	14:s:53:LYS:HB3	2.20	0.41
22:2:1445:U:H2'	22:2:1446:A:C8	2.56	0.41
2:H:16:HIS:HB3	2:H:44:LEU:HD21	2.03	0.41
11:p:24:THR:HG22	11:p:25:PHE:N	2.36	0.41
22:2:100:C:C2	22:2:101:G:C8	3.09	0.41
22:2:157:G:C2	22:2:158:G:C5	3.09	0.41
22:2:408:C:C2	22:2:409:G:C8	3.08	0.41
3:h:90:LEU:HD23	3:h:90:LEU:HA	1.91	0.40
4:i:135:LYS:HE2	4:i:135:LYS:HB2	1.85	0.40
4:i:201:LYS:HB2	22:2:8:A:N6	2.35	0.40
6:k:6:THR:O	6:k:62:LEU:HA	2.22	0.40
11:p:120:ARG:HA	11:p:121:PRO:HD3	1.94	0.40
15:t:17:ASP:C	15:t:19:LYS:H	2.28	0.40
22:2:930:A:N6	22:2:1216:C:H42	2.12	0.40
22:2:959:G:H5'	22:2:1339:U:O2'	2.22	0.40
22:2:1309:C:H2'	22:2:1310:G:O4'	2.21	0.40
4:i:62:TYR:OH	4:i:92:GLU:OE1	2.38	0.40
10:o:66:VAL:HG22	14:s:84:VAL:HG22	2.04	0.40
14:s:24:ARG:HH21	22:2:1298:C:P	2.44	0.40
20:y:59:ALA:HB2	20:y:69:ALA:HB2	2.03	0.40
22:2:929:A:H2'	22:2:930:A:H8	1.86	0.40
7:l:97:ARG:HG2	7:l:101:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:n:46:VAL:C	9:n:48:GLN:H	2.28	0.40
22:2:175:A:H2'	22:2:176:U:H6	1.86	0.40
22:2:1109:C:HO2'	22:2:1110:C:P	2.42	0.40
3:h:49:ALA:HA	3:h:71:ARG:HH12	1.86	0.40
9:n:104:ARG:HH11	9:n:104:ARG:HG3	1.85	0.40
16:u:10:HIS:O	16:u:17:PHE:N	2.51	0.40
22:2:1:A:H2'	22:2:2:C:C6	2.57	0.40
22:2:750:G:H2'	22:2:751:A:H8	1.86	0.40
22:2:1224:G:HO2'	22:2:1225:C:P	2.44	0.40
22:2:1444:G:H2'	22:2:1445:U:O4'	2.21	0.40
2:H:154:ASP:OD1	2:H:155:MET:N	2.54	0.40
7:l:66:ASP:HA	7:l:69:THR:HG22	2.03	0.40
22:2:657:A:H2'	22:2:658:A:C8	2.56	0.40
22:2:966:A:H2	22:2:967:C:C6	2.40	0.40
22:2:1389:C:H2'	22:2:1390:A:H8	1.86	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	A	35/591 (6%)	34 (97%)	1 (3%)	0	100	100
2	H	217/254 (85%)	213 (98%)	4 (2%)	0	100	100
3	h	213/252 (84%)	197 (92%)	16 (8%)	0	100	100
4	i	198/201 (98%)	193 (98%)	5 (2%)	0	100	100
5	j	167/173 (96%)	158 (95%)	9 (5%)	0	100	100
6	k	105/113 (93%)	102 (97%)	3 (3%)	0	100	100
7	l	128/158 (81%)	123 (96%)	5 (4%)	0	100	100
8	m	129/132 (98%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	n	123/128 (96%)	114 (93%)	9 (7%)	0	100	100
10	o	96/101 (95%)	90 (94%)	6 (6%)	0	100	100
11	p	115/127 (91%)	111 (96%)	4 (4%)	0	100	100
12	q	119/127 (94%)	112 (94%)	7 (6%)	0	100	100
13	r	49/124 (40%)	48 (98%)	1 (2%)	0	100	100
14	s	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	t	85/88 (97%)	83 (98%)	2 (2%)	0	100	100
16	u	149/188 (79%)	145 (97%)	4 (3%)	0	100	100
17	v	78/86 (91%)	74 (95%)	4 (5%)	0	100	100
18	w	63/98 (64%)	62 (98%)	1 (2%)	0	100	100
19	x	81/92 (88%)	75 (93%)	6 (7%)	0	100	100
20	y	77/83 (93%)	74 (96%)	3 (4%)	0	100	100
21	z	62/64 (97%)	62 (100%)	0	0	100	100
All	All	2375/3269 (73%)	2275 (96%)	100 (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	A	25/514 (5%)	25 (100%)	0	100	100
2	H	165/207 (80%)	165 (100%)	0	100	100
3	h	151/201 (75%)	151 (100%)	0	100	100
4	i	159/173 (92%)	159 (100%)	0	100	100
5	j	109/138 (79%)	109 (100%)	0	100	100
6	k	72/101 (71%)	71 (99%)	1 (1%)	59	82
7	l	102/136 (75%)	100 (98%)	2 (2%)	48	76
8	m	93/111 (84%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	n	99/107 (92%)	99 (100%)	0	100	100
10	o	72/94 (77%)	72 (100%)	0	100	100
11	p	77/102 (76%)	77 (100%)	0	100	100
12	q	96/107 (90%)	96 (100%)	0	100	100
13	r	38/100 (38%)	38 (100%)	0	100	100
14	s	61/73 (84%)	61 (100%)	0	100	100
15	t	64/79 (81%)	64 (100%)	0	100	100
16	u	99/135 (73%)	99 (100%)	0	100	100
17	v	71/81 (88%)	71 (100%)	0	100	100
18	w	51/87 (59%)	51 (100%)	0	100	100
19	x	66/78 (85%)	66 (100%)	0	100	100
20	y	64/72 (89%)	64 (100%)	0	100	100
21	z	56/56 (100%)	56 (100%)	0	100	100
All	All	1790/2752 (65%)	1787 (100%)	3 (0%)	85	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	k	79	PHE
7	l	31	TRP
7	l	39	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	8	GLN
4	i	200	ASN
5	j	54	HIS
6	k	96	HIS
10	o	55	HIS
11	p	116	HIS
13	r	14	HIS
16	u	43	ASN
16	u	61	HIS
16	u	62	ASN

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Mol	Chain	Res	Type
16	u	96	GLN
17	v	57	ASN
18	w	74	GLN
19	x	52	HIS
21	z	11	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	2	1476/1520 (97%)	252 (17%)	21 (1%)

All (252) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	2	3	G
22	2	4	A
22	2	9	G
22	2	39	G
22	2	47	C
22	2	48	U
22	2	50	A
22	2	51	A
22	2	54	C
22	2	58	C
22	2	61	G
22	2	69	G
22	2	72	G
22	2	110	A
22	2	111	C
22	2	120	A
22	2	126	C
22	2	128	U
22	2	133	C
22	2	136	A
22	2	147	A
22	2	148	G
22	2	154	U
22	2	158	G
22	2	160	U
22	2	161	U
22	2	164	U

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Mol	Chain	Res	Type
22	2	170	A
22	2	175	A
22	2	177	U
22	2	188	A
22	2	190	C
22	2	203	A
22	2	207	C
22	2	211	A
22	2	213	G
22	2	237	U
22	2	238	U
22	2	240	G
22	2	244	G
22	2	251	A
22	2	259	G
22	2	260	C
22	2	272	A
22	2	282	G
22	2	314	A
22	2	320	A
22	2	321	C
22	2	322	A
22	2	325	G
22	2	340	G
22	2	344	G
22	2	345	C
22	2	346	A
22	2	347	G
22	2	360	U
22	2	361	U
22	2	362	G
22	2	365	C
22	2	366	A
22	2	377	G
22	2	390	A
22	2	399	G
22	2	403	G
22	2	404	A
22	2	405	U
22	2	406	G
22	2	407	A
22	2	408	C

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Mol	Chain	Res	Type
22	2	423	U
22	2	432	U
22	2	451	U
22	2	454	U
22	2	455	A
22	2	457	A
22	2	458	U
22	2	460	U
22	2	461	A
22	2	462	G
22	2	464	A
22	2	465	G
22	2	466	C
22	2	467	U
22	2	483	A
22	2	485	U
22	2	487	A
22	2	497	A
22	2	499	C
22	2	506	C
22	2	509	G
22	2	515	G
22	2	519	U
22	2	520	A
22	2	535	A
22	2	547	A
22	2	550	C
22	2	552	C
22	2	560	A
22	2	561	A
22	2	564	G
22	2	565	G
22	2	576	G
22	2	584	A
22	2	621	G
22	2	641	U
22	2	650	G
22	2	652	G
22	2	653	A
22	2	675	A
22	2	688	U
22	2	691	G

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Mol	Chain	Res	Type
22	2	706	A
22	2	709	A
22	2	710	A
22	2	711	U
22	2	719	G
22	2	735	U
22	2	736	U
22	2	743	G
22	2	765	A
22	2	769	A
22	2	781	U
22	2	782	A
22	2	797	G
22	2	803	A
22	2	805	C
22	2	807	A
22	2	814	C
22	2	816	A
22	2	829	A
22	2	830	A
22	2	831	G
22	2	855	A
22	2	890	A
22	2	897	A
22	2	909	G
22	2	910	G
22	2	917	C
22	2	918	A
22	2	925	G
22	2	943	U
22	2	944	U
22	2	949	G
22	2	952	A
22	2	954	G
22	2	959	G
22	2	960	A
22	2	964	U
22	2	966	A
22	2	975	U
22	2	976	A
22	2	977	A
22	2	985	C

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Mol	Chain	Res	Type
22	2	987	G
22	2	988	A
22	2	989	C
22	2	990	C
22	2	992	A
22	2	993	U
22	2	1019	A
22	2	1020	G
22	2	1021	U
22	2	1023	U
22	2	1024	A
22	2	1027	A
22	2	1032	C
22	2	1034	G
22	2	1045	G
22	2	1046	U
22	2	1056	C
22	2	1073	A
22	2	1075	G
22	2	1076	U
22	2	1082	A
22	2	1094	C
22	2	1108	G
22	2	1110	C
22	2	1115	A
22	2	1134	A
22	2	1140	C
22	2	1141	U
22	2	1148	G
22	2	1156	U
22	2	1157	G
22	2	1158	A
22	2	1163	G
22	2	1166	G
22	2	1178	A
22	2	1179	A
22	2	1180	A
22	2	1182	C
22	2	1183	A
22	2	1184	U
22	2	1194	U
22	2	1195	A

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Mol	Chain	Res	Type
22	2	1196	C
22	2	1207	A
22	2	1208	C
22	2	1212	C
22	2	1218	A
22	2	1220	A
22	2	1223	G
22	2	1225	C
22	2	1226	C
22	2	1227	G
22	2	1228	G
22	2	1239	A
22	2	1240	G
22	2	1242	C
22	2	1252	C
22	2	1255	G
22	2	1261	A
22	2	1262	A
22	2	1267	U
22	2	1268	A
22	2	1280	A
22	2	1281	G
22	2	1283	U
22	2	1284	C
22	2	1286	G
22	2	1301	C
22	2	1311	U
22	2	1320	A
22	2	1327	A
22	2	1328	G
22	2	1334	G
22	2	1339	U
22	2	1344	C
22	2	1345	A
22	2	1346	U
22	2	1352	G
22	2	1380	A
22	2	1404	G
22	2	1406	G
22	2	1411	C
22	2	1424	A
22	2	1441	A

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Mol	Chain	Res	Type
22	2	1466	A
22	2	1467	G
22	2	1476	A
22	2	1479	U
22	2	1493	G
22	2	1502	G
22	2	1503	G
22	2	1504	A
22	2	1510	U
22	2	1512	C
22	2	1513	U
22	2	1514	U
22	2	1515	U
22	2	1516	C
22	2	1517	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	2	2	C
22	2	3	G
22	2	110	A
22	2	236	A
22	2	321	C
22	2	989	C
22	2	1023	U
22	2	1031	G
22	2	1045	G
22	2	1109	C
22	2	1179	A
22	2	1211	A
22	2	1217	U
22	2	1224	G
22	2	1225	C
22	2	1227	G
22	2	1238	C
22	2	1280	A
22	2	1285	G
22	2	1351	C
22	2	1379	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.

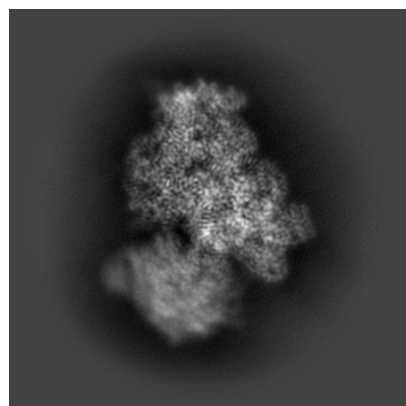
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74034. These allow visual inspection of the internal detail of the map and identification of artifacts.

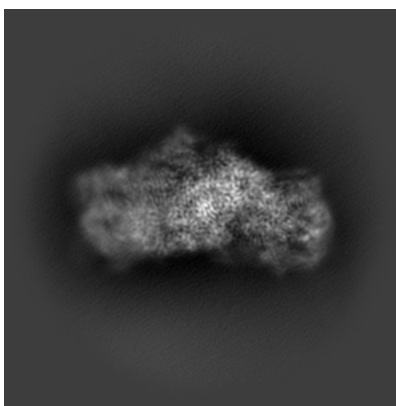
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

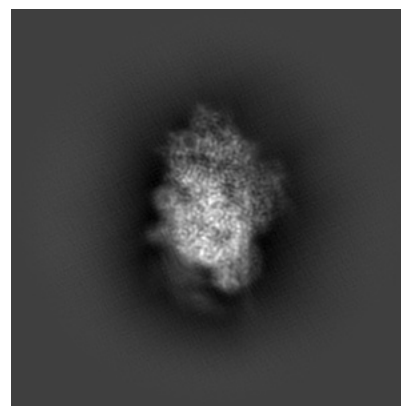
6.1.1 Primary map



X

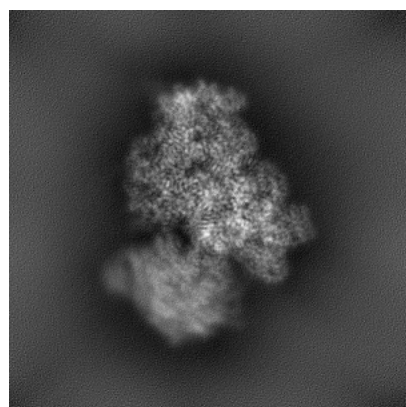


Y

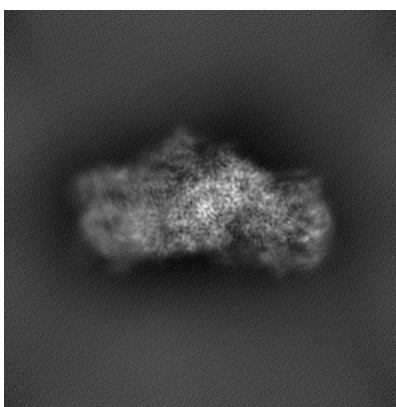


Z

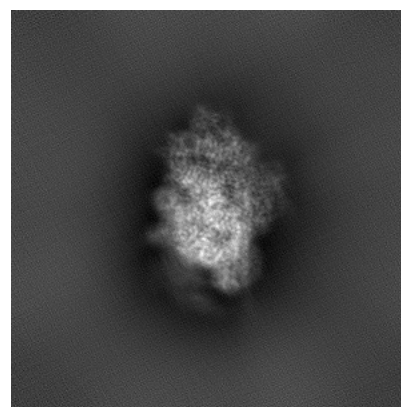
6.1.2 Raw map



X



Y

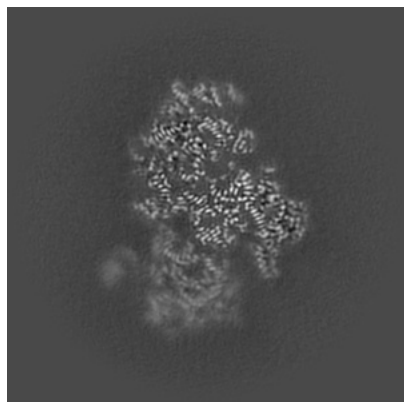


Z

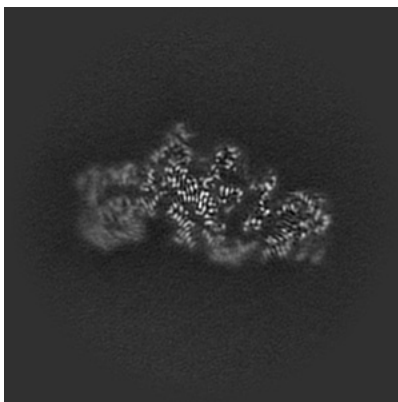
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

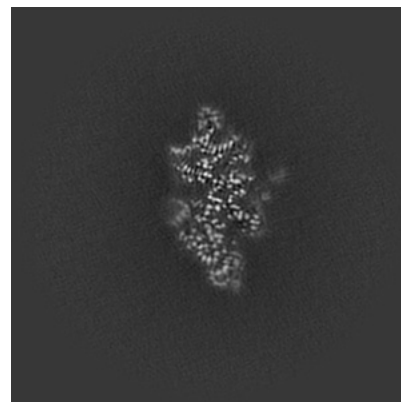
6.2.1 Primary map



X Index: 200

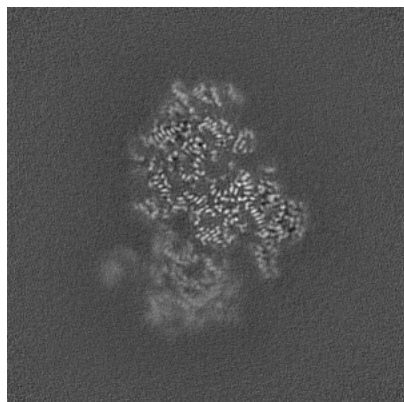


Y Index: 200

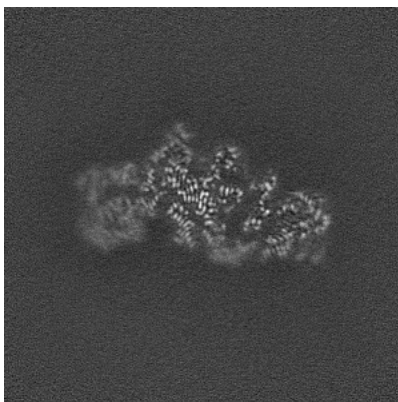


Z Index: 200

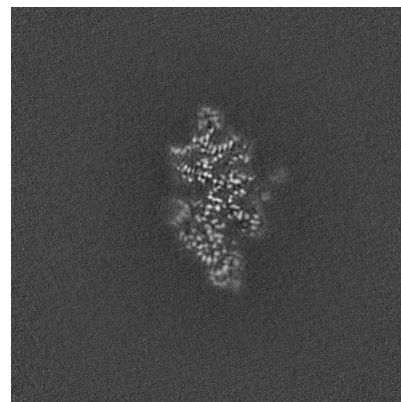
6.2.2 Raw map



X Index: 200



Y Index: 200

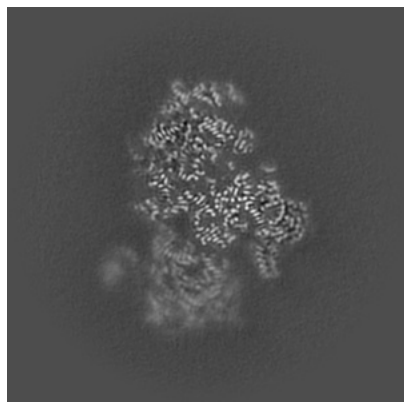


Z Index: 200

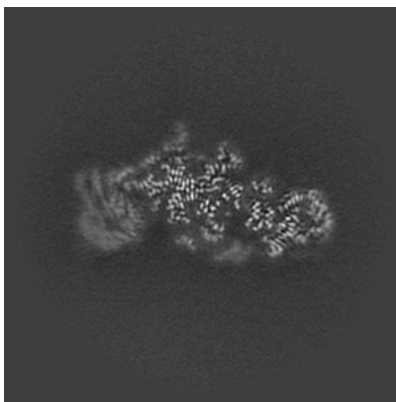
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

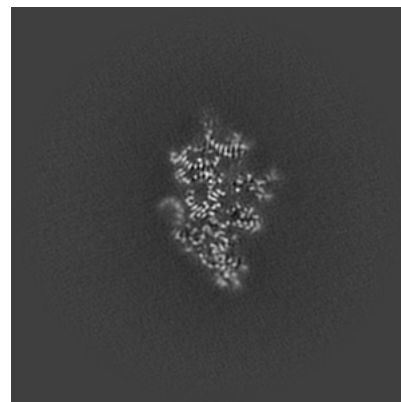
6.3.1 Primary map



X Index: 199

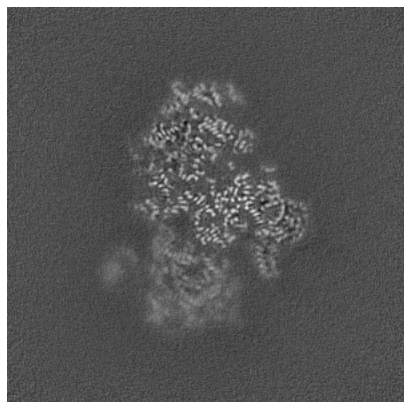


Y Index: 195

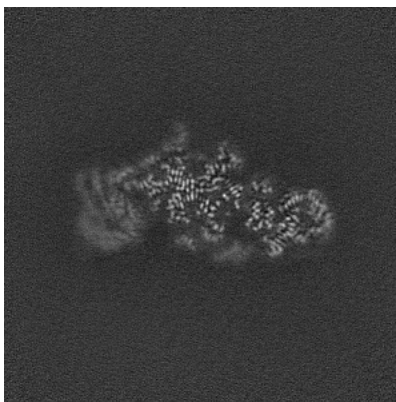


Z Index: 206

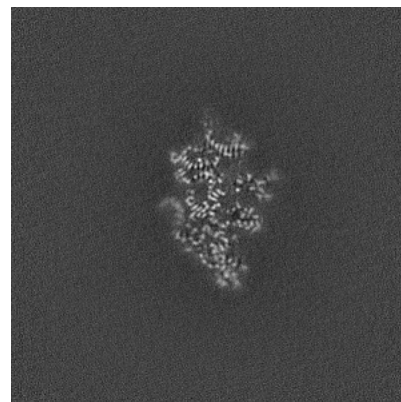
6.3.2 Raw map



X Index: 199



Y Index: 195

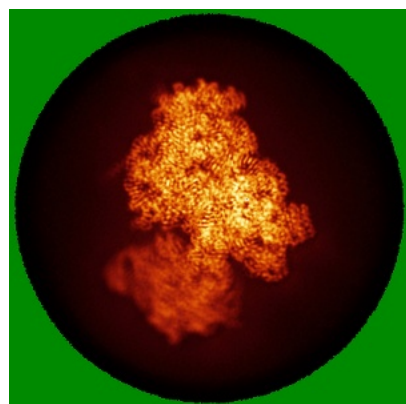


Z Index: 206

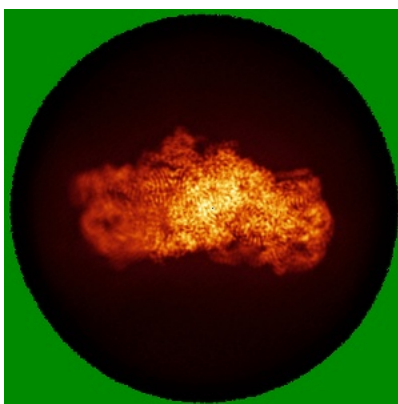
The images above show the largest variance slices of the map in three orthogonal directions.

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

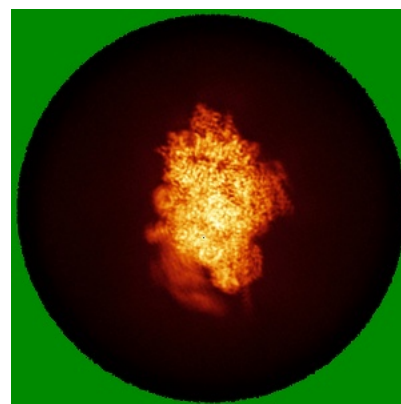
6.4.1 Primary map



X

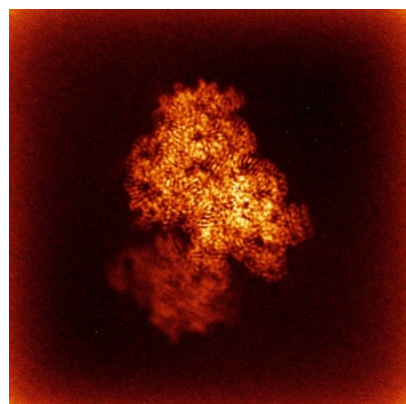


Y

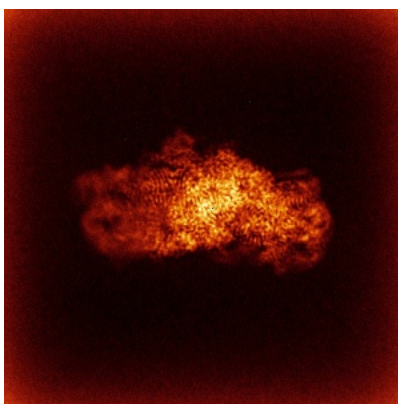


Z

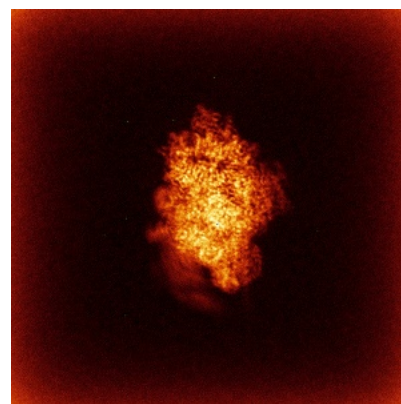
6.4.2 Raw map



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](#)

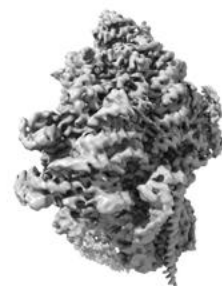
6.5.1 Primary map



X



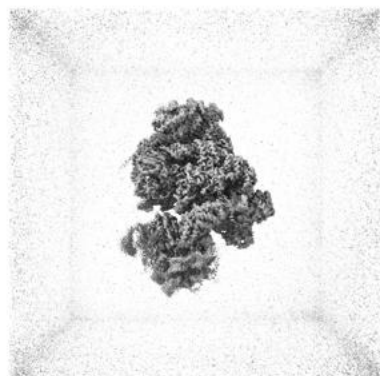
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0328. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

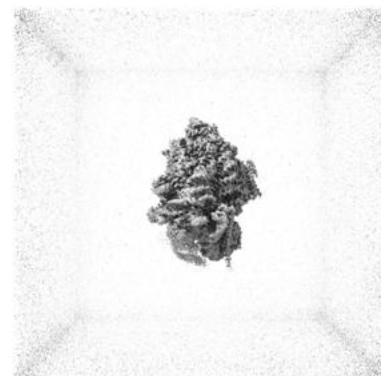
6.5.2 Raw map



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.

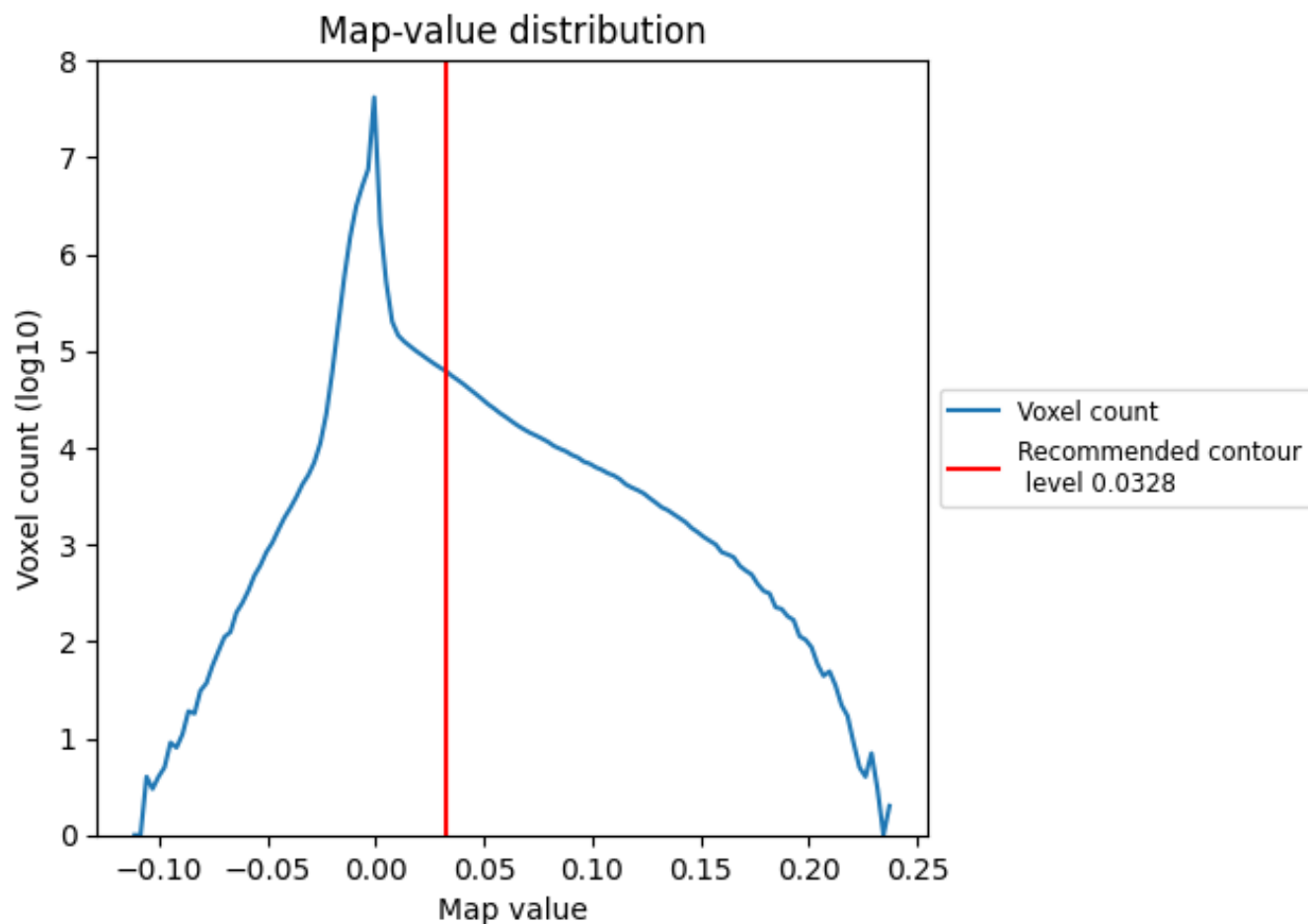
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

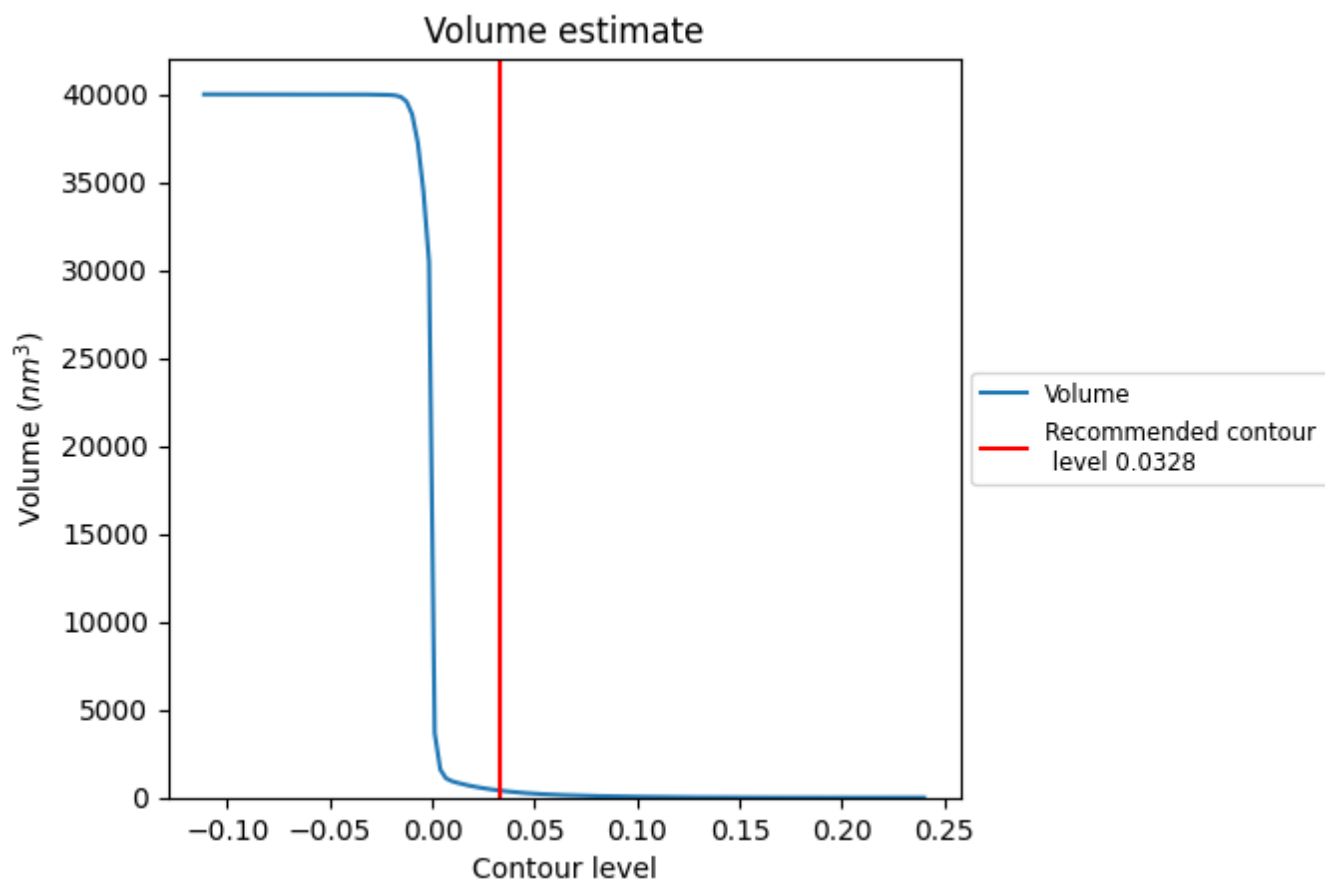
This section contains the results of statistical analysis of the map.

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.

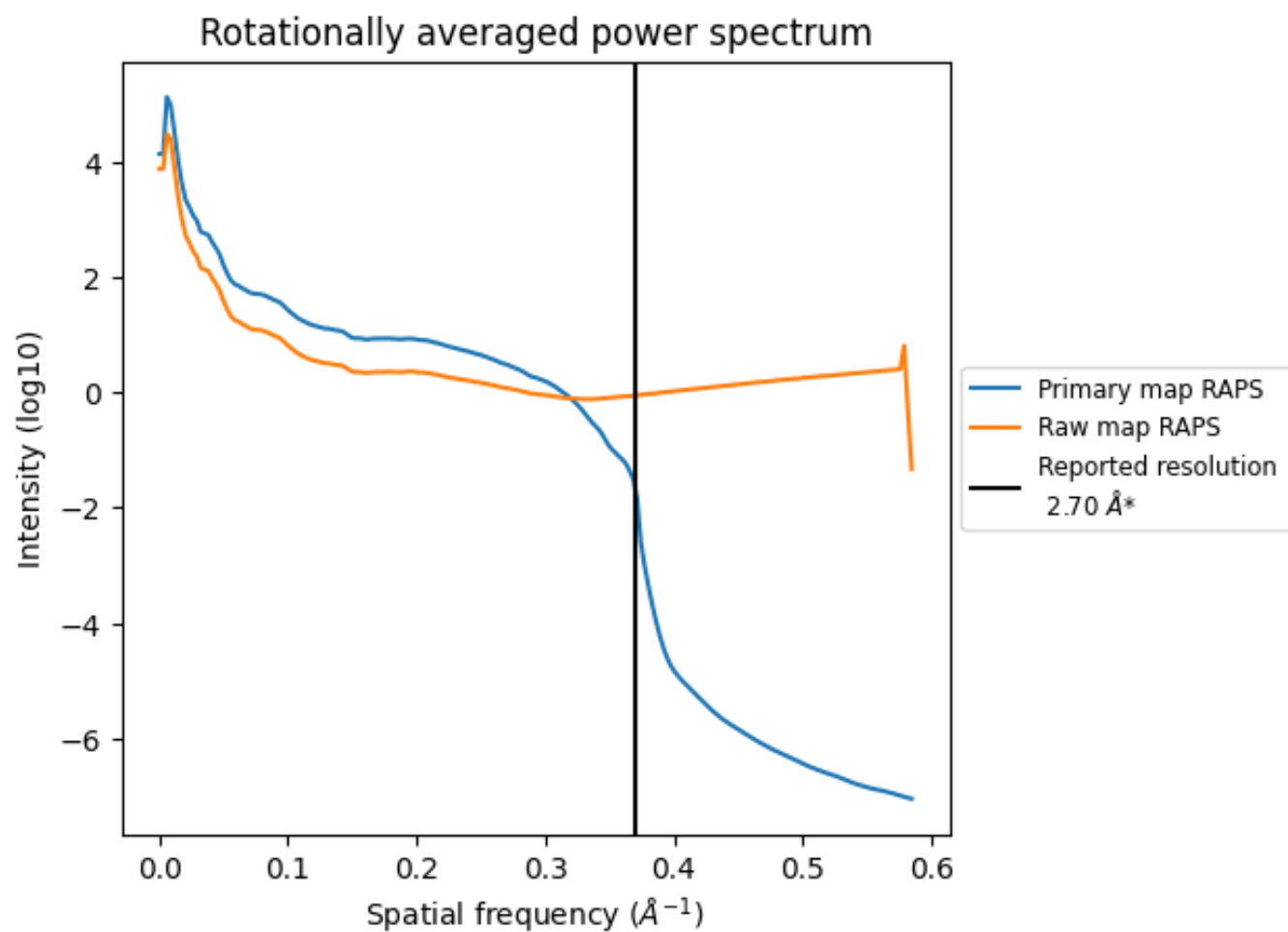
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 402 nm^3 ; this corresponds to an approximate mass of 363 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 ⓘ

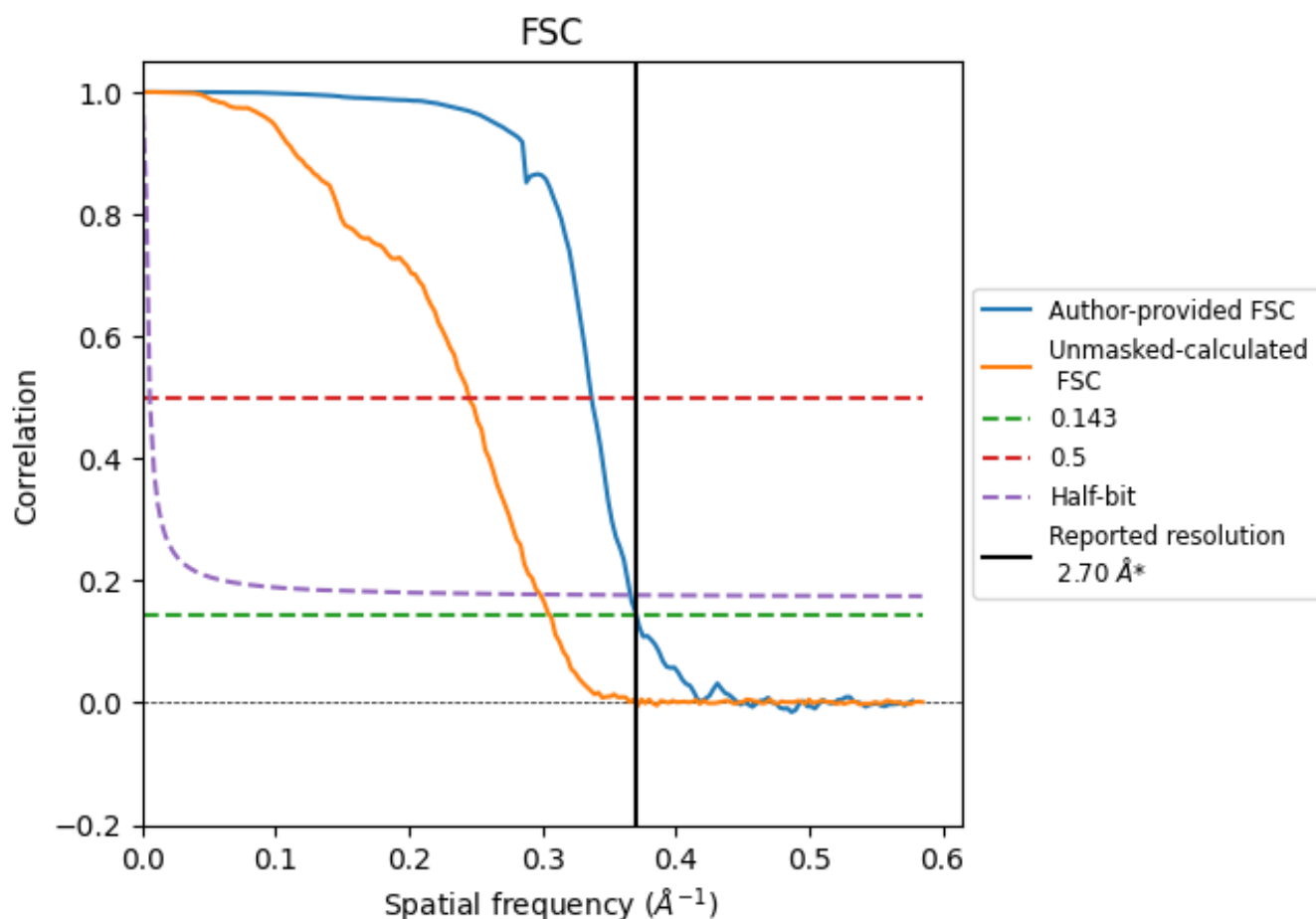


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

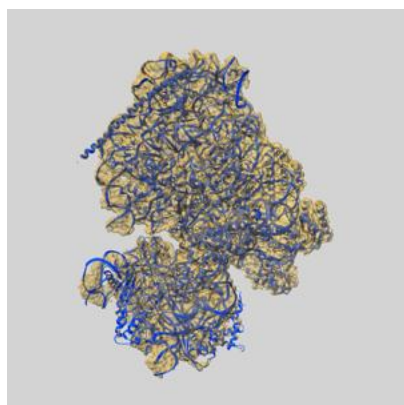
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	2.97	2.73
Unmasked-calculated*	3.27	4.08	3.35

*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 3.27 differs from the reported value 2.7 by more than 10 %

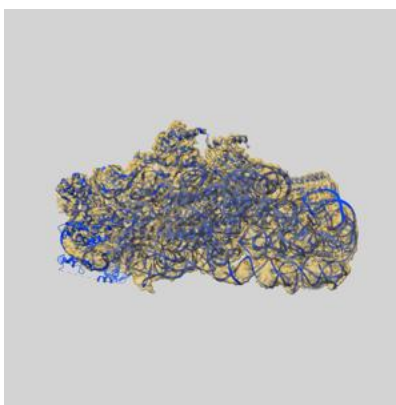
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74034 and PDB model 9ZCD. Per-residue inclusion information can be found in section [3](#) on page [8](#).

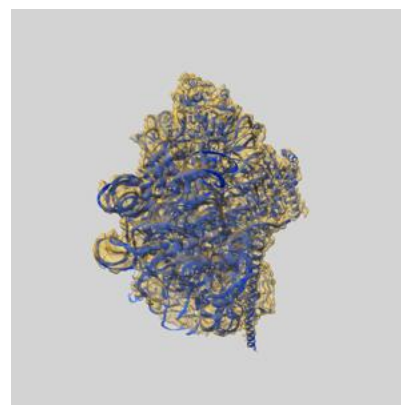
9.1 Map-model overlay [i](#)



X



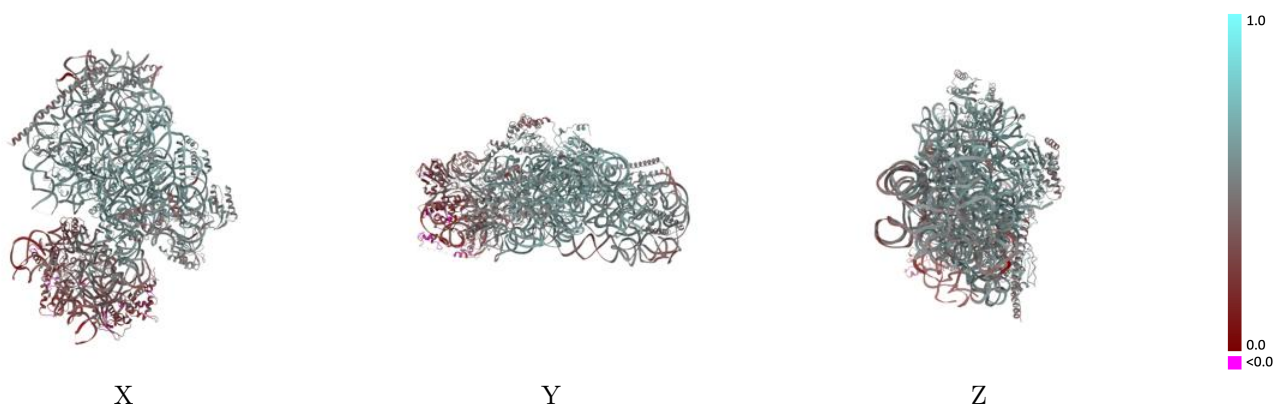
Y



Z

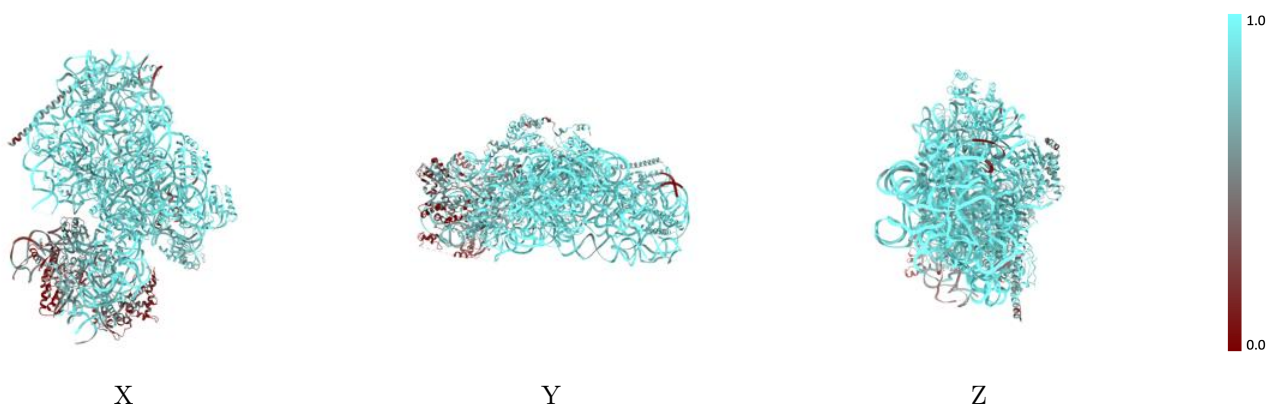
The images above show the 3D surface view of the map at the recommended contour level 0.0328 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



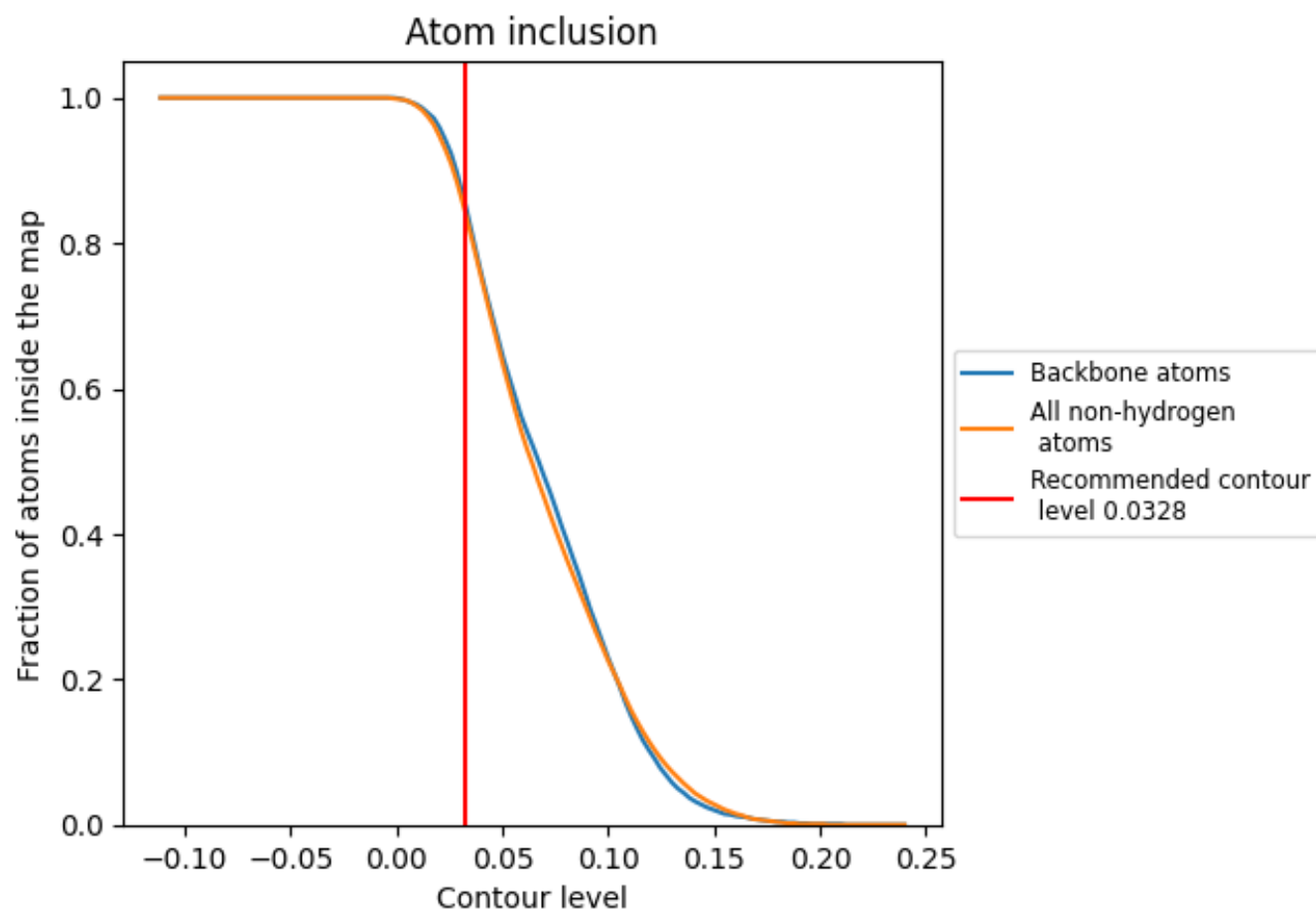
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0328).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.0328) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.4730
2	 0.9090	 0.4850
A	 0.5930	 0.4480
H	 0.8220	 0.4820
h	 0.4490	 0.3580
i	 0.9030	 0.5400
j	 0.9600	 0.5950
k	 0.9190	 0.5130
l	 0.2380	 0.2210
m	 0.9750	 0.6040
n	 0.4610	 0.3100
o	 0.4080	 0.3390
p	 0.8900	 0.5080
q	 0.9340	 0.5800
r	 0.0030	 0.0660
s	 0.4400	 0.2870
t	 0.9640	 0.5720
u	 0.8380	 0.5040
v	 0.9520	 0.5840
w	 0.9700	 0.5480
x	 0.1840	 0.1600
y	 0.9010	 0.4920
z	 0.7430	 0.5000

