



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 08:17 PM JST

PDB ID : 9JNS / pdb_00009jns
EMDB ID : EMD-61625
Title : 50S precursor - Erm complex (C-II)
Authors : Sengupta, S.; Mukherjee, R.; Pilsl, M.; Bagale, S.; Adhikary, A.D.; Borkar, A.;
Pradeepkumar, P.I.; Engel, C.; Chowdhury, A.; Kaushal, P.S.; Anand, R.
Deposited on : 2024-09-23
Resolution : 4.70 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

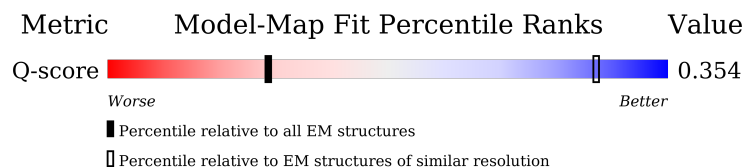
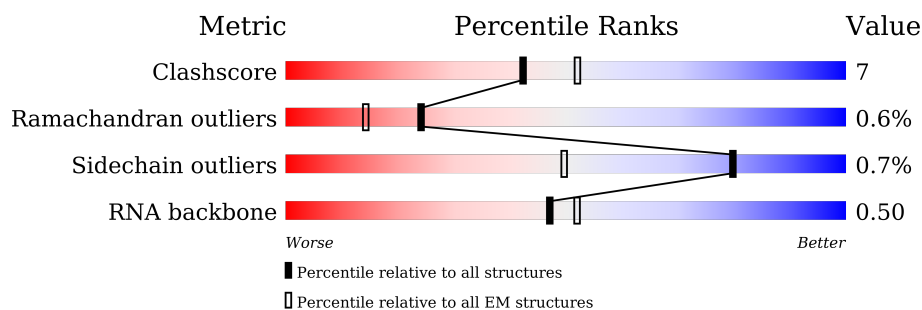
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	0	57	
2	2	46	
3	A	2904	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	244	
5	D	209	
6	E	201	
7	J	142	
8	K	123	
9	L	144	
10	N	127	
11	P	115	
12	Q	118	
13	R	103	
14	S	110	
15	T	100	
16	U	104	
17	Y	63	
18	Z	59	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49329 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 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	41	Total	C	N	O	S	0	0
			331	198	81	51	1		

- Molecule 3 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1601	Total	C	N	O	P	0	0
			34397	15346	6368	11082	1601		

- Molecule 4 is a protein called rRNA adenine N-6-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	235	Total	C	N	O	S	0	0
			1966	1272	339	349	6		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	123	Total	C	N	O	S	0	0
			919	580	162	175	2		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	197	Total	C	N	O	S	0	0
			1526	960	276	285	5		

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	141	Total	C	N	O	S	0	0
			1121	708	211	198	4		

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	121	Total	C	N	O	S	0	0
			932	584	179	163	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	L	107	Total	C	N	O	0	0
			762	474	147	141		

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 11 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	112	Total	C	N	O	S	0	0
			903	567	176	159	1		

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 13 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 14 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 15 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 16 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 17 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		


- Molecule 18 is a protein called 50S ribosomal protein L30.

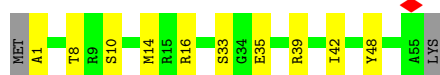
Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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: 50S ribosomal protein L32

Chain 0: 

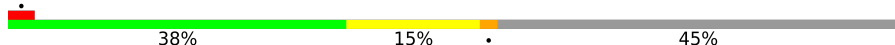


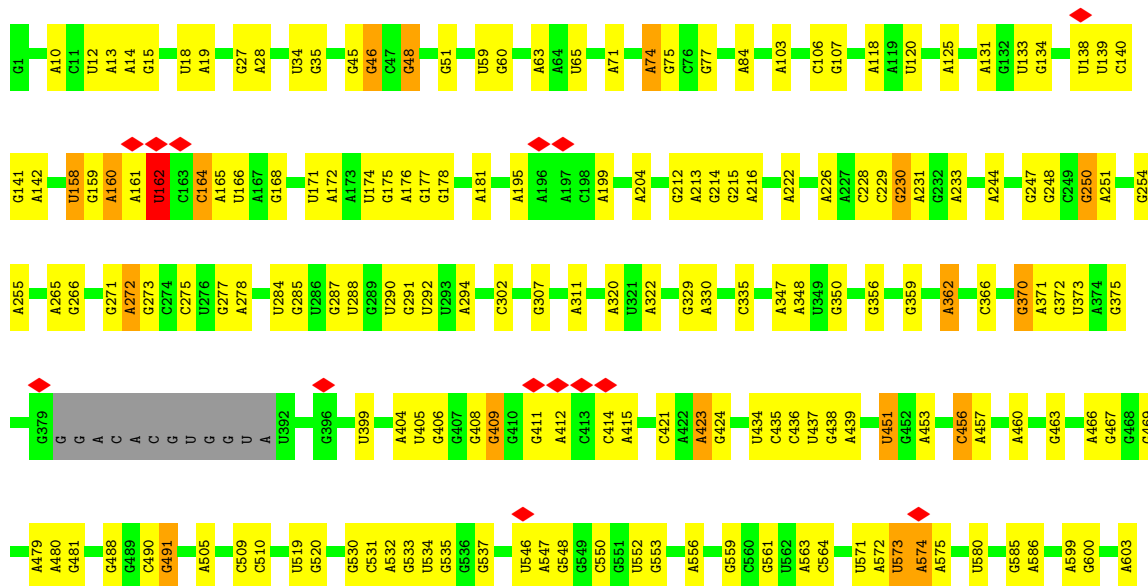
• Molecule 2: 50S ribosomal protein L34

Chain 2: 

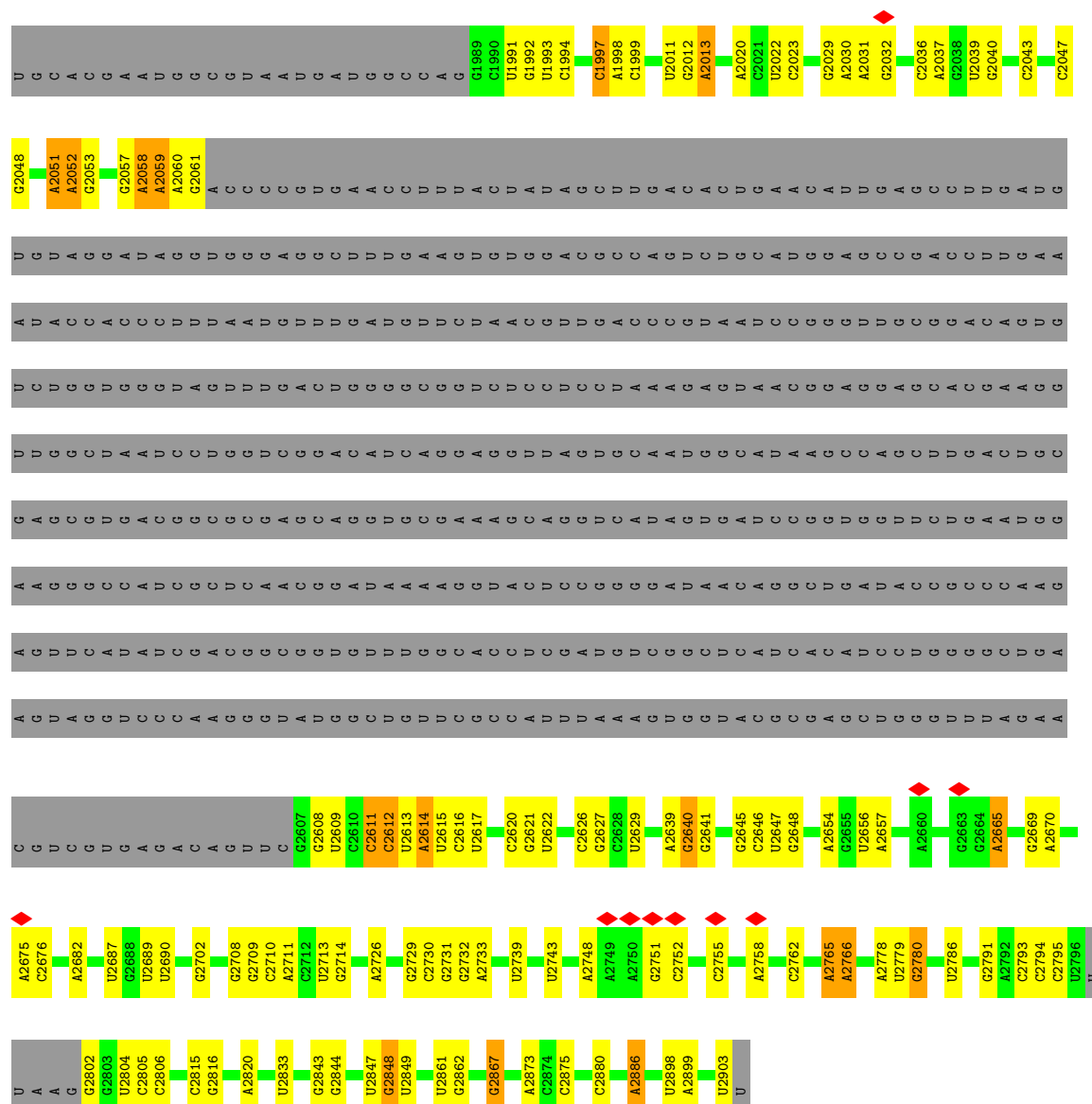


• Molecule 3: 23S ribosomal RNA

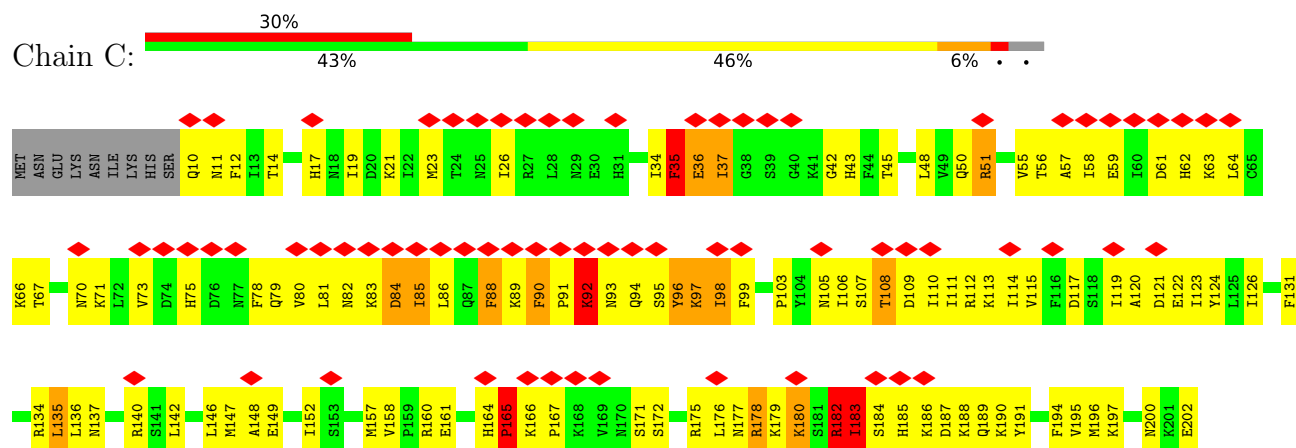
Chain A: 







● Molecule 4: rRNA adenine N-6-methyltransferase





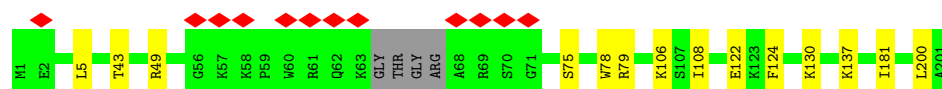
• Molecule 5: 50S ribosomal protein L3

Chain D: 51% 8% 41%



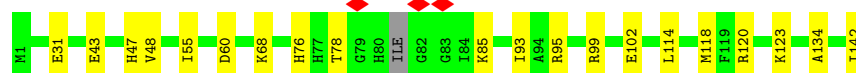
• Molecule 6: 50S ribosomal protein L4

Chain E: 6% 91% 7%



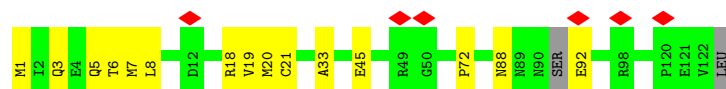
• Molecule 7: 50S ribosomal protein L13

Chain J: 85% 14%



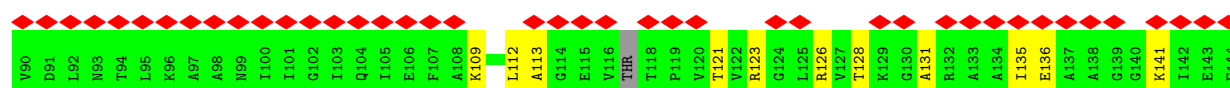
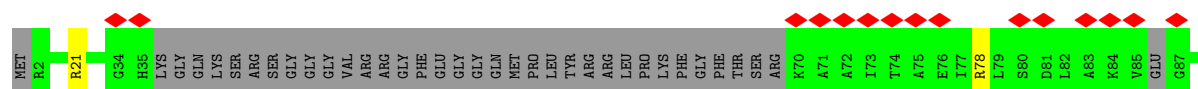
• Molecule 8: 50S ribosomal protein L14

Chain K: 5% 86% 12%

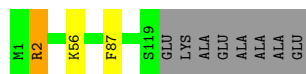


• Molecule 9: 50S ribosomal protein L15


Chain L: 40% 65% 9% 26%



• Molecule 10: 50S ribosomal protein L17

Chain N:  91% .. 6%


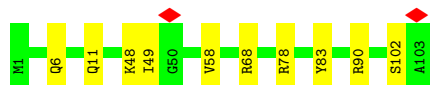
• Molecule 11: 50S ribosomal protein L19

Chain P:  9% 85% 12% .


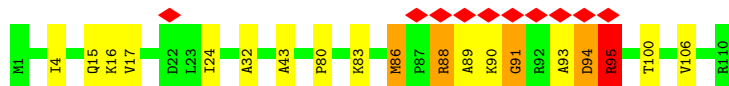
• Molecule 12: 50S ribosomal protein L20

Chain Q:  93% 6% .


• Molecule 13: 50S ribosomal protein L21

Chain R:  90% 10%

• Molecule 14: 50S ribosomal protein L22

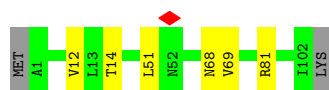
Chain S:  9% 83% 13% . .

• Molecule 15: 50S ribosomal protein L23

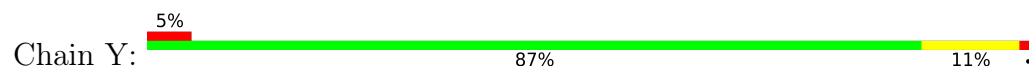
Chain T:  79% 12% . 8%

• Molecule 16: 50S ribosomal protein L24

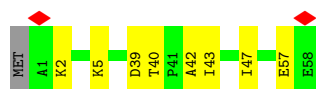
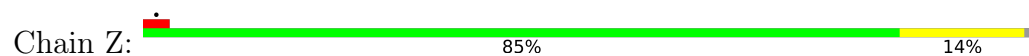
Chain U:  92% 6% .



- Molecule 17: 50S ribosomal protein L29



- Molecule 18: 50S ribosomal protein L30



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55608	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 ($e^-/\text{\AA}^2$)	41.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0136	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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	0	0.20	0/440	0.58	0/588
2	2	0.17	0/333	0.42	0/437
3	A	0.20	0/38523	0.34	4/60073 (0.0%)
4	C	0.52	1/2008 (0.0%)	1.19	30/2697 (1.1%)
5	D	0.20	0/930	0.59	1/1250 (0.1%)
6	E	0.20	0/1544	0.49	0/2076
7	J	0.22	0/1143	0.64	0/1537
8	K	0.25	0/940	0.60	0/1257
9	L	0.17	0/762	0.50	0/1013
10	N	0.23	0/964	0.66	1/1289 (0.1%)
11	P	0.20	0/914	0.58	0/1221
12	Q	0.20	0/960	0.46	0/1278
13	R	0.17	0/829	0.49	0/1107
14	S	0.35	0/864	0.67	0/1156
15	T	0.29	0/736	0.62	0/984
16	U	0.21	0/787	0.57	1/1051 (0.1%)
17	Y	0.21	0/510	1.04	4/677 (0.6%)
18	Z	0.16	0/453	0.41	0/605
All	All	0.22	1/53640 (0.0%)	0.46	41/80296 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	C	0	4
14	S	0	2
15	T	0	1
17	Y	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	180	LYS	N-CA	5.14	1.49	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	183	ILE	N-CA-C	-25.95	76.86	109.30
17	Y	57	LEU	CB-CA-C	17.94	139.44	110.92
4	C	184	SER	N-CA-C	-9.84	89.85	110.80
4	C	90	PHE	N-CA-CB	-9.74	93.04	110.37
4	C	36	GLU	CB-CA-C	-8.80	92.87	113.02
17	Y	57	LEU	CA-C-N	8.71	138.43	121.18
17	Y	57	LEU	C-N-CA	8.71	138.43	121.18
4	C	35	PHE	N-CA-C	-8.55	97.38	109.69
4	C	165	PRO	N-CA-C	-8.53	94.90	112.47
4	C	36	GLU	N-CA-C	8.22	118.81	108.45
4	C	98	ILE	CA-C-N	-8.13	108.81	122.64
4	C	98	ILE	C-N-CA	-8.13	108.81	122.64
4	C	209	LYS	CB-CA-C	8.08	123.22	109.65
4	C	51	ARG	CB-CA-C	-7.82	98.61	110.88
4	C	36	GLU	N-CA-CB	-7.80	96.87	110.76
5	D	119	ALA	N-CA-C	-7.75	95.05	109.32
4	C	36	GLU	CB-CG-CD	7.47	125.31	112.60
4	C	51	ARG	N-CA-CB	7.40	120.74	110.01
3	A	957	C	C2'-C3'-O3'	-6.64	103.74	113.70
3	A	956	G	O3'-P-O5'	-6.33	94.51	104.00
4	C	180	LYS	CB-CA-C	-6.21	108.14	117.07
4	C	209	LYS	N-CA-C	-6.15	105.69	113.43
3	A	957	C	O3'-P-O5'	5.98	112.97	104.00
4	C	182	ARG	CD-NE-CZ	-5.97	116.05	124.40
4	C	88	PHE	N-CA-CB	5.91	118.33	110.29
10	N	2	ARG	N-CA-C	5.88	119.75	111.52
17	Y	57	LEU	N-CA-C	-5.88	103.85	111.02
16	U	51	LEU	CA-CB-CG	5.84	136.76	116.30
4	C	90	PHE	N-CA-C	5.73	122.47	109.81
4	C	63	LYS	CB-CA-C	-5.71	101.85	110.92
4	C	184	SER	N-CA-CB	-5.67	100.91	110.49
4	C	89	LYS	CB-CA-C	-5.67	98.04	110.67
4	C	97	LYS	N-CA-C	-5.58	101.60	109.96
4	C	92	LYS	CA-C-N	-5.56	110.92	121.54
4	C	92	LYS	C-N-CA	-5.56	110.92	121.54
4	C	35	PHE	CA-CB-CG	-5.49	108.31	113.80
4	C	180	LYS	N-CA-C	5.15	113.00	108.78
4	C	209	LYS	CB-CG-CD	5.13	123.11	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	162	U	O3'-P-O5'	-5.06	96.41	104.00
4	C	105	ASN	N-CA-C	-5.04	108.87	114.62
4	C	103	PRO	N-CA-CB	-5.01	97.99	103.25

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	178	ARG	Sidechain
4	C	182	ARG	Sidechain
4	C	35	PHE	Peptide
4	C	51	ARG	Sidechain
14	S	88	ARG	Sidechain
14	S	95	ARG	Sidechain
15	T	3	ARG	Sidechain
17	Y	57	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	434	0	448	10	0
2	2	331	0	364	5	0
3	A	34397	0	17315	218	0
4	C	1966	0	2001	254	0
5	D	919	0	949	11	0
6	E	1526	0	1592	9	0
7	J	1121	0	1150	14	0
8	K	932	0	1006	10	0
9	L	762	0	826	9	0
10	N	951	0	994	3	0
11	P	903	0	953	9	0
12	Q	947	0	1022	7	0
13	R	816	0	839	6	0
14	S	857	0	922	11	0
15	T	730	0	795	6	0
16	U	779	0	834	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Y	509	0	543	5	0
18	Z	449	0	491	5	0
All	All	49329	0	33044	528	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 7.

All (528) 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)
4:C:85:ILE:HG23	4:C:88:PHE:CE2	1.41	1.53
4:C:85:ILE:HA	4:C:88:PHE:CD2	1.48	1.46
4:C:149:GLU:CB	4:C:180:LYS:HG2	1.49	1.41
4:C:149:GLU:HB2	4:C:180:LYS:CG	1.51	1.40
4:C:148:ALA:HB1	4:C:182:ARG:NH1	1.37	1.39
4:C:183:ILE:HA	4:C:187:ASP:OD1	1.19	1.33
4:C:36:GLU:OE1	4:C:58:ILE:CB	1.75	1.32
4:C:106:ILE:HD13	4:C:110:ILE:CD1	1.62	1.30
4:C:106:ILE:CD1	4:C:110:ILE:CD1	2.14	1.24
4:C:36:GLU:CD	4:C:58:ILE:CG2	2.09	1.24
4:C:85:ILE:CG2	4:C:88:PHE:HE2	1.51	1.23
4:C:85:ILE:CG2	4:C:88:PHE:CE2	2.21	1.22
4:C:106:ILE:CD1	4:C:110:ILE:HD12	1.69	1.22
4:C:36:GLU:OE1	4:C:58:ILE:HB	1.34	1.19
4:C:106:ILE:CG2	4:C:109:ASP:HB2	1.73	1.19
4:C:85:ILE:HG23	4:C:88:PHE:CZ	1.79	1.18
3:A:2766:A:H5'	4:C:211:GLN:NE2	1.57	1.17
4:C:106:ILE:HD12	4:C:110:ILE:HD12	1.25	1.15
4:C:183:ILE:HG13	4:C:183:ILE:O	1.38	1.12
3:A:1129:A:H4'	4:C:205:LYS:HZ3	0.98	1.12
3:A:1129:A:O3'	4:C:205:LYS:NZ	1.80	1.12
3:A:2766:A:C5'	4:C:211:GLN:NE2	2.13	1.11
4:C:85:ILE:HA	4:C:88:PHE:CE2	1.83	1.11
4:C:36:GLU:CD	4:C:58:ILE:HB	1.74	1.11
4:C:79:GLN:HE22	4:C:81:LEU:HD12	0.94	1.10
4:C:121:ASP:HB2	4:C:178:ARG:HH12	1.13	1.09
4:C:106:ILE:HG23	4:C:109:ASP:HB2	1.10	1.08
3:A:1129:A:H4'	4:C:205:LYS:NZ	1.68	1.08
4:C:36:GLU:CD	4:C:58:ILE:CB	2.27	1.07
3:A:2766:A:C5'	4:C:211:GLN:HE21	1.65	1.06
4:C:106:ILE:CG2	4:C:110:ILE:H	1.68	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:79:GLN:NE2	4:C:81:LEU:HD12	1.69	1.06
4:C:79:GLN:HE22	4:C:81:LEU:CD1	1.70	1.04
4:C:58:ILE:HD13	4:C:85:ILE:HD13	1.35	1.03
4:C:106:ILE:HG23	4:C:109:ASP:CB	1.87	1.03
4:C:183:ILE:CA	4:C:187:ASP:OD1	2.08	1.01
4:C:85:ILE:CA	4:C:88:PHE:CD2	2.44	1.01
4:C:36:GLU:CG	4:C:58:ILE:HG22	1.92	1.00
4:C:90:PHE:O	4:C:92:LYS:NZ	1.95	0.99
4:C:36:GLU:O	4:C:37:ILE:HG13	1.62	0.99
4:C:36:GLU:CD	4:C:58:ILE:HG22	1.84	0.99
3:A:1129:A:C4'	4:C:205:LYS:HZ3	1.75	0.98
4:C:36:GLU:OE1	4:C:58:ILE:CG2	2.06	0.97
4:C:148:ALA:CB	4:C:182:ARG:NH1	2.28	0.96
3:A:957:C:H42	4:C:84:ASP:H	1.13	0.96
4:C:85:ILE:CB	4:C:88:PHE:HE2	1.78	0.95
3:A:2766:A:H5''	4:C:211:GLN:HE21	1.11	0.95
4:C:106:ILE:HG22	4:C:106:ILE:O	1.64	0.95
4:C:148:ALA:O	4:C:182:ARG:NE	1.99	0.95
4:C:37:ILE:HG22	4:C:37:ILE:O	1.67	0.94
4:C:85:ILE:CD1	4:C:88:PHE:CE2	2.50	0.94
4:C:106:ILE:CD1	4:C:110:ILE:HD11	1.95	0.94
4:C:36:GLU:OE1	4:C:58:ILE:N	2.01	0.94
4:C:134:ARG:O	4:C:135:LEU:HG	1.68	0.93
4:C:85:ILE:CA	4:C:88:PHE:CE2	2.51	0.93
4:C:121:ASP:HB2	4:C:178:ARG:NH1	1.82	0.93
4:C:106:ILE:HD13	4:C:110:ILE:CG1	1.99	0.92
4:C:106:ILE:HD13	4:C:110:ILE:HD11	1.52	0.92
3:A:641:U:H3	3:A:647:G:H1	1.14	0.91
4:C:148:ALA:HB1	4:C:182:ARG:HH11	1.22	0.91
4:C:106:ILE:HG22	4:C:110:ILE:H	1.36	0.90
4:C:36:GLU:CG	4:C:58:ILE:CG2	2.49	0.90
3:A:290:U:H3	3:A:350:G:H1	0.96	0.89
4:C:58:ILE:HD13	4:C:85:ILE:CD1	2.02	0.89
4:C:79:GLN:NE2	4:C:81:LEU:CD1	2.31	0.88
3:A:2766:A:C4'	4:C:211:GLN:NE2	2.36	0.88
4:C:79:GLN:OE1	4:C:81:LEU:HG	1.73	0.87
4:C:85:ILE:HA	4:C:88:PHE:HD2	1.06	0.87
3:A:585:G:H21	3:A:1254:A:H62	1.22	0.86
3:A:585:G:H21	3:A:1254:A:N6	1.72	0.86
4:C:121:ASP:CB	4:C:178:ARG:HH12	1.87	0.86
4:C:106:ILE:CG2	4:C:110:ILE:N	2.39	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:35:PHE:HB2	4:C:98:ILE:HG23	1.56	0.85
4:C:36:GLU:OE1	4:C:58:ILE:CA	2.24	0.84
4:C:106:ILE:HG21	4:C:110:ILE:HG13	1.58	0.84
3:A:957:C:N4	4:C:84:ASP:H	1.75	0.83
4:C:148:ALA:HB1	4:C:182:ARG:CZ	2.07	0.83
4:C:106:ILE:HG21	4:C:110:ILE:H	1.42	0.82
4:C:36:GLU:OE1	4:C:58:ILE:HG22	1.72	0.82
3:A:585:G:N2	3:A:1254:A:H62	1.78	0.82
4:C:94:GLN:HB3	4:C:96:TYR:CE2	2.14	0.82
4:C:35:PHE:O	4:C:99:PHE:O	1.98	0.81
4:C:79:GLN:OE1	4:C:81:LEU:CG	2.29	0.81
3:A:2765:A:H2'	4:C:214:ASN:ND2	1.95	0.81
3:A:2766:A:H4'	4:C:211:GLN:NE2	1.97	0.80
4:C:85:ILE:CB	4:C:88:PHE:CE2	2.62	0.80
4:C:121:ASP:CB	4:C:178:ARG:NH1	2.44	0.80
4:C:182:ARG:HG3	4:C:183:ILE:O	1.81	0.80
1:O:1:ALA:HB1	3:A:2613:U:O2'	1.82	0.79
4:C:36:GLU:CD	4:C:58:ILE:HG21	2.06	0.79
4:C:106:ILE:HD13	4:C:110:ILE:HG13	1.66	0.78
4:C:119:ILE:HG22	4:C:119:ILE:O	1.83	0.78
4:C:85:ILE:HD13	4:C:88:PHE:CE2	2.17	0.78
4:C:85:ILE:HD12	4:C:88:PHE:CE2	2.19	0.77
4:C:135:LEU:CD2	4:C:142:LEU:HD11	2.15	0.77
4:C:106:ILE:HG21	4:C:110:ILE:N	2.00	0.77
4:C:85:ILE:HG23	4:C:88:PHE:HE2	0.95	0.75
4:C:106:ILE:CG2	4:C:109:ASP:CB	2.57	0.74
4:C:182:ARG:HG3	4:C:183:ILE:N	2.02	0.73
1:O:1:ALA:CB	3:A:2613:U:O2'	2.37	0.73
3:A:2765:A:H2'	4:C:214:ASN:HD22	1.52	0.73
3:A:1129:A:C4'	4:C:205:LYS:NZ	2.43	0.71
4:C:91:PRO:HD2	4:C:96:TYR:CE2	2.25	0.71
3:A:1129:A:C3'	4:C:205:LYS:NZ	2.53	0.71
4:C:91:PRO:C	4:C:93:ASN:N	2.46	0.70
4:C:182:ARG:HG3	4:C:183:ILE:H	1.57	0.69
4:C:36:GLU:HG3	4:C:58:ILE:CG2	2.21	0.69
4:C:106:ILE:CG2	4:C:106:ILE:O	2.38	0.69
4:C:91:PRO:HB2	4:C:94:GLN:HB3	1.73	0.69
4:C:108:THR:HA	4:C:111:ILE:HB	1.74	0.69
4:C:134:ARG:O	4:C:135:LEU:CG	2.41	0.69
4:C:23:MET:SD	4:C:26:ILE:HB	2.33	0.68
4:C:79:GLN:CD	4:C:81:LEU:CD1	2.66	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:149:GLU:OE1	4:C:180:LYS:HD3	1.93	0.68
4:C:106:ILE:HG22	4:C:109:ASP:HB2	1.72	0.68
4:C:85:ILE:HD13	4:C:88:PHE:CD2	2.29	0.68
3:A:375:G:H1	3:A:399:U:H3	1.42	0.67
4:C:79:GLN:OE1	4:C:81:LEU:CD1	2.42	0.67
4:C:57:ALA:HB3	4:C:80:VAL:HG12	1.76	0.67
4:C:85:ILE:CA	4:C:88:PHE:HD2	1.97	0.67
4:C:85:ILE:CD1	4:C:88:PHE:HE2	1.99	0.67
6:E:49:ARG:HH21	6:E:75:SER:HB3	1.59	0.66
3:A:244:A:H62	3:A:254:G:H21	1.43	0.66
3:A:957:C:N4	4:C:84:ASP:N	2.44	0.66
4:C:131:PHE:HD1	4:C:135:LEU:HD11	1.60	0.66
4:C:185:HIS:HA	4:C:188:LYS:HD3	1.78	0.65
4:C:34:ILE:CG2	4:C:99:PHE:H	2.09	0.65
3:A:2614:A:O2'	3:A:2615:U:O2	2.14	0.65
4:C:36:GLU:OE2	4:C:58:ILE:HB	1.97	0.65
4:C:36:GLU:HG3	4:C:58:ILE:HG21	1.77	0.65
4:C:91:PRO:C	4:C:93:ASN:H	2.05	0.65
4:C:124:TYR:OH	4:C:175:ARG:NH1	2.31	0.64
4:C:37:ILE:HD13	4:C:110:ILE:HG21	1.80	0.64
4:C:149:GLU:OE1	4:C:180:LYS:CG	2.45	0.63
4:C:183:ILE:HG21	4:C:191:TYR:HB2	1.80	0.63
3:A:1127:A:O2'	4:C:189:GLN:HB2	1.98	0.63
12:Q:23:TYR:HB2	12:Q:28:SER:HB2	1.80	0.63
4:C:148:ALA:C	4:C:182:ARG:HE	2.04	0.63
4:C:37:ILE:O	4:C:37:ILE:CG2	2.39	0.63
9:L:109:LYS:HG3	9:L:126:ARG:HB3	1.81	0.63
3:A:956:G:H1'	3:A:962:G:N1	2.15	0.62
4:C:123:ILE:HB	4:C:176:LEU:HB2	1.81	0.62
4:C:196:MET:O	4:C:200:ASN:ND2	2.33	0.62
3:A:1631:G:N2	3:A:1635:A:H62	1.98	0.61
4:C:79:GLN:OE1	4:C:81:LEU:HD11	1.99	0.61
3:A:158:U:H3	3:A:168:G:H1	1.47	0.61
4:C:83:LYS:O	4:C:84:ASP:C	2.43	0.61
4:C:114:ILE:HB	4:C:123:ILE:HD13	1.82	0.61
6:E:106:LYS:HG3	6:E:200:LEU:HD23	1.83	0.61
4:C:161:GLU:HA	4:C:166:LYS:HG3	1.83	0.61
4:C:34:ILE:HG23	4:C:99:PHE:H	1.66	0.61
1:O:39:ARG:NH2	3:A:2886:A:N1	2.49	0.61
4:C:135:LEU:HD22	4:C:142:LEU:HD11	1.80	0.61
15:T:58:VAL:HG12	15:T:85:VAL:HG12	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:11:ASN:H	4:C:165:PRO:HD2	1.64	0.60
8:K:5:GLN:HG3	8:K:20:MET:HE3	1.83	0.60
3:A:1631:G:H21	3:A:1635:A:N6	2.00	0.60
3:A:2656:U:O2	3:A:2665:A:N7	2.35	0.60
3:A:629:G:N2	3:A:639:U:O2'	2.35	0.60
4:C:99:PHE:CE1	4:C:124:TYR:HB2	2.36	0.60
4:C:99:PHE:CD1	4:C:124:TYR:HB2	2.36	0.60
3:A:1631:G:H21	3:A:1635:A:H62	1.49	0.60
4:C:91:PRO:HB2	4:C:94:GLN:CB	2.32	0.60
3:A:1408:G:H1	3:A:1594:U:H3	1.48	0.60
3:A:1653:G:OP1	10:N:2:ARG:NH1	2.35	0.60
13:R:6:GLN:HB3	13:R:11:GLN:HG2	1.84	0.59
18:Z:5:LYS:HB2	18:Z:57:GLU:HB3	1.84	0.59
3:A:460:A:H62	3:A:469:G:H21	1.50	0.59
7:J:31:GLU:HG2	7:J:142:ILE:HG12	1.84	0.59
4:C:58:ILE:HG21	4:C:85:ILE:HD11	1.85	0.59
4:C:106:ILE:HG21	4:C:110:ILE:CG1	2.31	0.59
3:A:957:C:C4	4:C:83:LYS:HA	2.38	0.59
4:C:91:PRO:O	4:C:93:ASN:N	2.35	0.59
3:A:1666:G:N3	8:K:3:GLN:NE2	2.51	0.59
4:C:64:LEU:HA	4:C:67:THR:HG22	1.85	0.58
4:C:149:GLU:OE1	4:C:180:LYS:CD	2.51	0.58
4:C:106:ILE:HG22	4:C:110:ILE:N	2.12	0.58
3:A:2059:A:H2'	3:A:2060:A:C8	2.37	0.58
1:O:1:ALA:HB2	3:A:2613:U:H1'	1.86	0.58
3:A:957:C:N4	4:C:83:LYS:HA	2.18	0.58
4:C:62:HIS:O	4:C:66:LYS:HG2	2.02	0.58
4:C:149:GLU:CD	4:C:180:LYS:HD3	2.28	0.58
13:R:68:ARG:HB2	13:R:90:ARG:HH21	1.69	0.58
4:C:10:GLN:HB2	4:C:165:PRO:HG2	1.86	0.57
9:L:112:LEU:HD21	9:L:135:ILE:HD11	1.85	0.57
3:A:77:G:OP1	17:Y:52:ARG:NH1	2.36	0.57
4:C:58:ILE:CD1	4:C:85:ILE:HD13	2.22	0.57
3:A:1252:G:N2	12:Q:32:ARG:O	2.38	0.57
3:A:2620:C:H2'	3:A:2621:G:H8	1.68	0.57
14:S:83:LYS:HD3	14:S:95:ARG:HH12	1.69	0.57
18:Z:40:THR:HB	18:Z:43:ILE:HG12	1.84	0.57
3:A:626:A:H2'	9:L:78:ARG:HH12	1.70	0.57
18:Z:2:LYS:NZ	18:Z:39:ASP:OD2	2.38	0.57
1:O:8:THR:HG22	1:O:10:SER:H	1.70	0.57
3:A:2620:C:H2'	3:A:2621:G:C8	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:36:GLU:CB	4:C:58:ILE:HG22	2.34	0.56
5:D:9:VAL:HB	5:D:26:VAL:HG13	1.86	0.56
3:A:580:U:OP1	12:Q:32:ARG:NH1	2.39	0.56
4:C:36:GLU:HA	4:C:99:PHE:O	2.05	0.56
5:D:38:LYS:O	5:D:46:ARG:HA	2.06	0.56
4:C:17:HIS:O	4:C:21:LYS:HG2	2.04	0.56
4:C:36:GLU:CG	4:C:58:ILE:HG21	2.30	0.56
3:A:957:C:H42	4:C:84:ASP:N	1.93	0.56
13:R:58:VAL:H	13:R:102:SER:HB3	1.70	0.56
3:A:2786:U:OP1	5:D:70:LYS:NZ	2.39	0.56
4:C:91:PRO:O	4:C:96:TYR:OH	2.21	0.56
4:C:113:LYS:HA	4:C:117:ASP:HB3	1.87	0.56
11:P:33:GLU:OE1	11:P:38:ARG:NH2	2.39	0.55
4:C:79:GLN:CD	4:C:81:LEU:HD11	2.30	0.55
1:O:33:SER:OG	1:O:35:GLU:OE1	2.22	0.55
3:A:954:G:H1	3:A:963:U:H3	1.55	0.55
3:A:1258:U:O2'	6:E:79:ARG:NH1	2.40	0.55
3:A:2766:A:H5'	4:C:211:GLN:HE21	1.67	0.55
4:C:183:ILE:CB	4:C:187:ASP:OD1	2.55	0.55
3:A:1592:C:H2'	3:A:1593:A:C8	2.42	0.55
4:C:135:LEU:HD21	4:C:142:LEU:HD11	1.86	0.55
3:A:171:U:H2'	3:A:172:A:H8	1.71	0.55
3:A:2611:C:O2'	3:A:2612:C:OP1	2.24	0.55
3:A:1327:A:N6	3:A:1647:U:O2	2.40	0.55
3:A:2743:U:OP2	3:A:2755:C:N4	2.40	0.55
4:C:70:ASN:HA	4:C:73:VAL:HG13	1.89	0.54
4:C:147:MET:HE1	4:C:152:ILE:HG13	1.89	0.54
4:C:58:ILE:CG2	4:C:85:ILE:HD11	2.37	0.54
3:A:1590:A:H3'	3:A:1591:A:H8	1.72	0.54
4:C:14:THR:HA	4:C:43:HIS:CD2	2.42	0.54
3:A:1028:A:H3'	3:A:1126:A:H61	1.73	0.54
3:A:2640:G:OP1	7:J:95:ARG:NH2	2.41	0.54
7:J:55:ILE:HG22	7:J:123:LYS:HB2	1.88	0.54
3:A:552:U:H2'	3:A:553:G:H8	1.73	0.54
3:A:1140:C:OP2	7:J:68:LYS:NZ	2.36	0.54
17:Y:24:GLU:O	17:Y:28:LEU:HB2	2.08	0.54
3:A:2669:G:H2'	3:A:2670:A:H8	1.73	0.53
4:C:80:VAL:O	4:C:81:LEU:HD23	2.08	0.53
14:S:90:LYS:O	14:S:91:GLY:C	2.51	0.53
3:A:1124:G:H2'	3:A:1125:G:O4'	2.08	0.53
3:A:1311:G:H21	3:A:1603:A:H62	1.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1129:A:H4'	4:C:205:LYS:CE	2.36	0.53
14:S:4:ILE:HG12	14:S:106:VAL:HG22	1.88	0.53
3:A:335:C:OP2	16:U:81:ARG:NH2	2.41	0.53
3:A:2766:A:H5''	4:C:211:GLN:HE22	1.61	0.53
3:A:537:G:H21	3:A:556:A:H62	1.57	0.53
4:C:19:ILE:HD11	4:C:43:HIS:HB3	1.90	0.53
4:C:59:GLU:HG3	4:C:61:ASP:H	1.74	0.52
15:T:55:VAL:HA	15:T:87:LEU:HA	1.90	0.52
3:A:414:C:H2'	3:A:415:A:H8	1.73	0.52
4:C:42:GLY:HA2	4:C:45:THR:HG22	1.91	0.52
3:A:177:G:OP2	3:A:177:G:N2	2.36	0.52
3:A:2780:G:OP2	7:J:120:ARG:NE	2.42	0.52
4:C:85:ILE:CG1	4:C:88:PHE:HE2	2.21	0.52
4:C:79:GLN:CD	4:C:81:LEU:HG	2.34	0.52
3:A:571:U:O2'	3:A:573:U:OP2	2.28	0.52
4:C:50:GLN:HE21	4:C:75:HIS:CE1	2.28	0.52
3:A:1154:G:OP2	12:Q:57:ARG:NH1	2.43	0.52
4:C:112:ARG:O	4:C:117:ASP:N	2.43	0.52
3:A:1336:A:OP2	15:T:68:LYS:NZ	2.42	0.52
4:C:188:LYS:HG3	4:C:189:GLN:N	2.24	0.52
3:A:2847:U:OP1	11:P:95:LYS:NZ	2.42	0.52
3:A:1407:G:H2'	3:A:1408:G:H8	1.76	0.51
8:K:18:ARG:HB2	8:K:45:GLU:HB3	1.91	0.51
3:A:1268:A:H62	3:A:2012:G:H21	1.58	0.51
3:A:2051:A:O2'	3:A:2052:A:C8	2.64	0.51
4:C:185:HIS:O	4:C:188:LYS:HE3	2.10	0.51
3:A:1271:G:H22	14:S:89:ALA:HB2	1.76	0.51
3:A:2765:A:N6	4:C:218:HIS:ND1	2.59	0.51
3:A:1631:G:N2	3:A:1634:A:OP2	2.43	0.50
3:A:974:G:O4'	3:A:1186:G:N2	2.45	0.50
3:A:160:A:H5'	3:A:165:A:N6	2.26	0.50
4:C:113:LYS:HD2	4:C:117:ASP:HB3	1.93	0.50
4:C:148:ALA:CB	4:C:182:ARG:CZ	2.83	0.50
3:A:848:C:H2'	3:A:849:A:H8	1.76	0.50
3:A:284:U:O2	3:A:356:G:O6	2.30	0.50
3:A:320:A:OP1	6:E:130:LYS:NZ	2.43	0.50
4:C:85:ILE:CG2	4:C:88:PHE:CZ	2.72	0.50
4:C:202:GLU:O	4:C:202:GLU:HG2	2.11	0.50
8:K:6:THR:HB	8:K:21:CYS:HB3	1.94	0.50
13:R:48:LYS:NZ	13:R:49:ILE:O	2.44	0.50
2:2:39:ARG:NH2	3:A:469:G:O6	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:55:ILE:HA	7:J:123:LYS:O	2.12	0.50
3:A:230:G:H2'	3:A:231:A:H8	1.76	0.50
3:A:1129:A:C3'	4:C:205:LYS:HZ1	2.12	0.50
5:D:118:PHE:O	5:D:119:ALA:C	2.55	0.50
4:C:106:ILE:HD12	4:C:110:ILE:CD1	2.05	0.50
3:A:212:G:H2'	3:A:213:A:C8	2.47	0.49
4:C:183:ILE:O	4:C:183:ILE:CG1	2.30	0.49
11:P:27:VAL:HG11	11:P:73:PHE:HE2	1.77	0.49
3:A:574:A:H61	3:A:2032:G:H2'	1.77	0.49
3:A:957:C:N3	4:C:82:ASN:O	2.44	0.49
3:A:290:U:O2	3:A:350:G:N2	2.38	0.49
3:A:161:A:H62	3:A:164:C:H42	1.59	0.49
6:E:124:PHE:HE1	6:E:137:LYS:HD3	1.76	0.49
7:J:99:ARG:O	7:J:102:GLU:HB3	2.12	0.49
3:A:1409:U:H2'	3:A:1410:G:H8	1.76	0.49
4:C:124:TYR:HE1	4:C:175:ARG:HG3	1.77	0.49
4:C:149:GLU:OE1	4:C:180:LYS:HG3	2.11	0.49
8:K:7:MET:SD	8:K:18:ARG:NH2	2.85	0.49
3:A:13:A:O2'	3:A:15:G:N7	2.44	0.49
3:A:2060:A:H2'	3:A:2061:G:C8	2.48	0.49
3:A:1224:U:H2'	3:A:1225:G:C4	2.48	0.48
3:A:275:C:O2	3:A:362:A:N6	2.46	0.48
3:A:244:A:H62	3:A:254:G:N2	2.10	0.48
4:C:191:TYR:O	4:C:195:VAL:HG23	2.14	0.48
3:A:488:G:H22	3:A:491:G:H5''	1.78	0.48
3:A:1997:C:H2'	3:A:1998:A:H8	1.78	0.48
4:C:35:PHE:CB	4:C:98:ILE:HG23	2.37	0.48
4:C:122:GLU:OE2	4:C:177:ASN:OD1	2.32	0.48
3:A:599:A:H2'	3:A:600:G:H8	1.79	0.48
3:A:974:G:OP1	13:R:78:ARG:NH2	2.47	0.48
4:C:61:ASP:HB3	4:C:64:LEU:HB2	1.96	0.48
4:C:158:VAL:N	4:C:171:SER:O	2.43	0.48
3:A:437:U:H2'	3:A:438:G:H8	1.79	0.48
3:A:585:G:N2	3:A:1254:A:N6	2.46	0.48
3:A:2058:A:H2'	3:A:2059:A:C8	2.48	0.48
4:C:36:GLU:HB2	4:C:58:ILE:HG22	1.96	0.48
17:Y:56:LEU:O	17:Y:57:LEU:C	2.56	0.48
3:A:956:G:H1'	3:A:962:G:H1	1.79	0.47
4:C:188:LYS:HG3	4:C:189:GLN:H	1.79	0.47
5:D:20:VAL:HG12	8:K:72:PRO:HB2	1.95	0.47
3:A:636:G:H5''	9:L:128:THR:HB	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:134:ARG:O	4:C:135:LEU:CB	2.61	0.47
5:D:118:PHE:C	5:D:119:ALA:O	2.55	0.47
9:L:112:LEU:HD23	9:L:131:ALA:HB1	1.95	0.47
3:A:451:U:O2	3:A:453:A:N6	2.48	0.47
3:A:1123:C:H3'	3:A:1124:G:C8	2.49	0.47
4:C:12:PHE:O	4:C:164:HIS:N	2.48	0.47
4:C:45:THR:HA	4:C:48:LEU:HB2	1.95	0.47
5:D:103:ASP:OD1	5:D:103:ASP:N	2.46	0.47
3:A:1028:A:H2'	3:A:1029:A:C8	2.50	0.47
4:C:182:ARG:CG	4:C:183:ILE:H	2.21	0.47
10:N:2:ARG:O	10:N:2:ARG:HD3	2.14	0.47
3:A:247:G:N2	3:A:251:A:OP2	2.40	0.47
4:C:111:ILE:O	4:C:115:VAL:HG12	2.14	0.47
3:A:164:C:H2'	3:A:165:A:O4'	2.14	0.47
12:Q:47:ARG:NH2	12:Q:48:ASP:OD1	2.47	0.47
2:2:24:THR:HG22	2:2:26:ASN:H	1.80	0.47
3:A:630:G:O2'	3:A:640:C:O2'	2.30	0.47
4:C:182:ARG:NH2	4:C:191:TYR:CE2	2.79	0.47
5:D:4:LEU:HD13	5:D:29:VAL:HG11	1.95	0.47
3:A:48:G:N2	3:A:177:G:OP2	2.45	0.47
3:A:59:U:O2'	3:A:74:A:OP2	2.33	0.47
2:2:11:LYS:HB2	2:2:11:LYS:HE2	1.70	0.47
3:A:106:C:H2'	3:A:107:G:H8	1.80	0.47
4:C:164:HIS:CD2	4:C:165:PRO:HD3	2.50	0.47
5:D:34:VAL:HA	5:D:50:VAL:HG12	1.95	0.47
3:A:2848:G:O2'	3:A:2867:G:N2	2.49	0.46
4:C:214:ASN:O	4:C:217:LYS:HG3	2.15	0.46
3:A:559:G:N2	12:Q:48:ASP:OD1	2.41	0.46
3:A:2036:C:H2'	3:A:2037:A:H8	1.80	0.46
4:C:131:PHE:CD1	4:C:135:LEU:HD11	2.47	0.46
4:C:134:ARG:C	4:C:135:LEU:HG	2.39	0.46
11:P:21:PRO:HD3	11:P:49:ILE:HD12	1.98	0.46
4:C:58:ILE:O	4:C:58:ILE:HG23	2.15	0.46
16:U:12:VAL:HA	16:U:69:VAL:HG12	1.98	0.46
4:C:126:ILE:HD12	4:C:158:VAL:HG21	1.97	0.46
3:A:213:A:H2'	3:A:214:G:C8	2.51	0.46
3:A:272:A:H2'	3:A:273:G:H8	1.81	0.46
3:A:1999:C:O2	3:A:2687:U:O2'	2.33	0.46
4:C:36:GLU:HB3	4:C:56:THR:O	2.16	0.46
13:R:78:ARG:HB2	13:R:83:TYR:HD2	1.80	0.46
4:C:91:PRO:O	4:C:94:GLN:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:182:ARG:NH2	4:C:183:ILE:HG12	2.31	0.46
4:C:122:GLU:OE1	4:C:123:ILE:N	2.48	0.46
3:A:463:G:N2	3:A:466:A:OP2	2.43	0.46
4:C:84:ASP:O	4:C:85:ILE:C	2.58	0.46
6:E:5:LEU:HD23	6:E:122:GLU:HB3	1.97	0.46
16:U:14:THR:OG1	16:U:68:ASN:OD1	2.29	0.46
3:A:2641:G:H5''	7:J:78:THR:HG22	1.98	0.46
4:C:149:GLU:O	4:C:179:LYS:N	2.45	0.46
1:O:16:ARG:NH1	14:S:15:GLN:OE1	2.49	0.46
3:A:171:U:H2'	3:A:172:A:C8	2.50	0.46
8:K:88:ASN:HD21	8:K:92:GLU:HB3	1.80	0.46
3:A:2047:C:H2'	3:A:2048:G:C8	2.50	0.45
3:A:2795:C:H1'	3:A:2802:G:N2	2.31	0.45
4:C:206:ILE:HB	4:C:239:TYR:HE2	1.82	0.45
8:K:8:LEU:HB3	8:K:19:VAL:HG13	1.98	0.45
18:Z:40:THR:HG22	18:Z:42:ALA:H	1.80	0.45
4:C:67:THR:HA	4:C:70:ASN:OD1	2.16	0.45
14:S:17:VAL:HG23	14:S:43:ALA:HB1	1.97	0.45
14:S:86:MET:HE3	14:S:86:MET:HB3	1.81	0.45
14:S:93:ALA:O	14:S:94:ASP:C	2.59	0.45
3:A:1608:A:O2'	3:A:1610:A:OP2	2.35	0.45
4:C:120:ALA:HB3	4:C:123:ILE:HD11	1.98	0.45
7:J:114:LEU:O	7:J:118:MET:HB2	2.16	0.45
4:C:119:ILE:O	4:C:119:ILE:CG2	2.55	0.45
3:A:290:U:O4	3:A:350:G:O6	2.35	0.45
4:C:146:LEU:CD2	4:C:152:ILE:HD11	2.47	0.45
3:A:1407:G:H2'	3:A:1408:G:C8	2.52	0.45
4:C:34:ILE:HA	4:C:97:LYS:O	2.16	0.45
3:A:1129:A:HO3'	4:C:205:LYS:NZ	2.08	0.44
3:A:2766:A:H4'	4:C:211:GLN:CD	2.42	0.44
3:A:2656:U:H2'	3:A:2657:A:H8	1.82	0.44
3:A:45:G:H5''	3:A:46:G:H5'	1.99	0.44
3:A:2047:C:H2'	3:A:2048:G:H8	1.83	0.44
3:A:65:U:O2'	3:A:456:C:N3	2.50	0.44
3:A:612:G:H21	3:A:616:A:H62	1.66	0.44
4:C:80:VAL:O	4:C:81:LEU:HG	2.17	0.44
4:C:182:ARG:CZ	4:C:183:ILE:HG12	2.47	0.44
3:A:133:U:H2'	3:A:134:G:H8	1.82	0.44
3:A:1595:C:H2'	3:A:1596:A:H8	1.81	0.44
4:C:34:ILE:HG23	4:C:99:PHE:N	2.32	0.44
4:C:165:PRO:O	4:C:166:LYS:C	2.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:23:ASP:OD1	11:P:23:ASP:N	2.44	0.44
3:A:160:A:H5'	3:A:165:A:H62	1.83	0.44
3:A:434:U:O2	3:A:436:C:N4	2.50	0.44
3:A:926:G:H2'	3:A:927:A:H8	1.83	0.44
3:A:2647:U:H2'	3:A:2648:G:H8	1.82	0.44
10:N:56:LYS:NZ	10:N:87:PHE:O	2.51	0.44
3:A:974:G:O5'	3:A:1186:G:N2	2.51	0.44
3:A:1413:A:H2'	3:A:1414:C:C6	2.53	0.44
4:C:224:LEU:H	4:C:224:LEU:HD23	1.83	0.44
3:A:561:G:O2'	12:Q:44:TYR:OH	2.36	0.44
3:A:1125:G:H3'	3:A:1126:A:H2'	2.00	0.44
3:A:1266:G:N2	3:A:2013:A:OP2	2.51	0.44
4:C:131:PHE:HD1	4:C:135:LEU:CD1	2.30	0.44
9:L:136:GLU:HG2	9:L:141:LYS:HA	1.99	0.44
11:P:30:TRP:NE1	11:P:81:ASP:OD1	2.50	0.44
3:A:174:U:H2'	3:A:175:G:H8	1.83	0.43
3:A:1666:G:H1'	8:K:3:GLN:HE21	1.83	0.43
3:A:2730:C:H2'	3:A:2731:G:C8	2.53	0.43
3:A:2899:A:H1'	7:J:134:ALA:HB1	1.99	0.43
3:A:177:G:H3'	3:A:178:G:H8	1.84	0.43
3:A:375:G:O6	3:A:399:U:O4	2.36	0.43
17:Y:13:GLU:HB3	17:Y:57:LEU:HD21	1.99	0.43
3:A:2626:C:H2'	3:A:2627:G:C8	2.53	0.43
3:A:2708:G:H2'	3:A:2709:G:H8	1.84	0.43
7:J:76:HIS:HB3	7:J:85:LYS:HG2	2.01	0.43
11:P:12:MET:SD	11:P:76:HIS:NE2	2.91	0.43
3:A:2011:U:OP2	14:S:16:LYS:NZ	2.42	0.43
4:C:34:ILE:HG22	4:C:99:PHE:H	1.81	0.43
4:C:84:ASP:O	4:C:86:LEU:N	2.51	0.43
3:A:1414:C:H2'	3:A:1415:U:O4'	2.19	0.43
3:A:2793:C:H2'	3:A:2794:C:C6	2.54	0.43
4:C:157:MET:HA	4:C:172:SER:HA	1.99	0.43
3:A:1412:U:H2'	3:A:1413:A:C8	2.53	0.43
4:C:160:ARG:O	4:C:167:PRO:HD2	2.19	0.43
3:A:175:G:H2'	3:A:176:A:C8	2.54	0.43
3:A:1386:C:H2'	3:A:1387:A:H8	1.83	0.43
3:A:2053:G:H1	3:A:2616:C:H5	1.65	0.43
4:C:216:LEU:HB3	4:C:221:ILE:HB	2.01	0.43
8:K:1:MET:N	8:K:33:ALA:O	2.39	0.43
3:A:347:A:H2'	3:A:348:A:C8	2.54	0.42
3:A:2051:A:O2'	3:A:2052:A:P	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1:ALA:HB2	3:A:2613:U:O2	2.19	0.42
3:A:1257:C:H4'	6:E:78:TRP:CD1	2.54	0.42
3:A:2794:C:H2'	3:A:2795:C:O4'	2.19	0.42
3:A:2861:U:H2'	3:A:2862:G:C8	2.54	0.42
4:C:190:LYS:O	4:C:194:PHE:N	2.51	0.42
9:L:21:ARG:HD3	9:L:21:ARG:HA	1.82	0.42
1:0:42:ILE:HG22	1:0:48:TYR:HB2	2.00	0.42
3:A:607:U:H2'	3:A:608:A:H8	1.83	0.42
3:A:2815:C:H2'	3:A:2816:G:H8	1.84	0.42
6:E:43:THR:O	6:E:43:THR:OG1	2.37	0.42
14:S:80:PRO:O	14:S:100:THR:OG1	2.36	0.42
3:A:285:G:N1	3:A:356:G:N7	2.67	0.42
3:A:1997:C:H2'	3:A:1998:A:C8	2.54	0.42
3:A:2039:U:H2'	3:A:2040:G:C8	2.54	0.42
5:D:84:LEU:HD23	5:D:86:GLU:H	1.85	0.42
5:D:36:GLN:HB3	5:D:49:GLN:HB3	2.02	0.42
3:A:18:U:H2'	3:A:19:A:C8	2.55	0.42
3:A:460:A:H62	3:A:469:G:N2	2.14	0.42
3:A:627:A:H62	9:L:113:ALA:HB2	1.84	0.42
3:A:174:U:H2'	3:A:175:G:C8	2.54	0.42
3:A:1668:A:H1'	3:A:1670:C:H41	1.84	0.42
3:A:2766:A:C4'	4:C:211:GLN:HE22	2.27	0.42
4:C:23:MET:O	4:C:23:MET:HG3	2.19	0.42
4:C:58:ILE:HG21	4:C:85:ILE:CD1	2.49	0.42
3:A:1386:C:H2'	3:A:1387:A:C8	2.55	0.42
4:C:91:PRO:O	4:C:92:LYS:C	2.63	0.42
17:Y:31:GLN:HG2	17:Y:37:LEU:HG	2.01	0.42
3:A:2626:C:H2'	3:A:2627:G:H8	1.85	0.41
3:A:2805:C:H2'	3:A:2806:C:C6	2.55	0.41
7:J:60:ASP:HA	7:J:93:ILE:HD11	2.02	0.41
4:C:35:PHE:CG	4:C:90:PHE:HE1	2.38	0.41
4:C:55:VAL:HB	4:C:78:PHE:HB2	2.01	0.41
4:C:182:ARG:O	4:C:183:ILE:C	2.58	0.41
4:C:197:LYS:HA	4:C:202:GLU:OE2	2.21	0.41
3:A:1316:U:H2'	3:A:1317:G:H8	1.85	0.41
3:A:272:A:H2'	3:A:273:G:C8	2.56	0.41
4:C:56:THR:HG23	4:C:79:GLN:NE2	2.35	0.41
4:C:175:ARG:NE	4:C:177:ASN:HD21	2.19	0.41
3:A:1590:A:H3'	3:A:1591:A:C8	2.55	0.41
3:A:370:G:H5'	3:A:423:A:N7	2.36	0.41
3:A:832:U:H2'	3:A:833:A:H8	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1029:A:N6	3:A:1125:G:H2'	2.35	0.41
7:J:43:GLU:N	7:J:43:GLU:OE1	2.53	0.41
1:O:10:SER:O	1:O:14:MET:HG3	2.21	0.41
2:2:10:LEU:HD12	2:2:10:LEU:HA	1.93	0.41
3:A:195:A:H1'	3:A:250:G:H21	1.85	0.41
3:A:226:A:N6	3:A:409:G:H21	2.18	0.41
3:A:438:G:H2'	3:A:439:A:H8	1.86	0.41
3:A:926:G:H2'	3:A:927:A:C8	2.56	0.41
3:A:1161:C:H2'	3:A:1162:G:H8	1.85	0.41
3:A:1589:U:H2'	3:A:1590:A:C8	2.56	0.41
4:C:137:ASN:OD1	4:C:137:ASN:N	2.53	0.41
6:E:108:ILE:HD11	6:E:181:ILE:HB	2.03	0.41
15:T:6:ARG:NH2	15:T:42:GLU:OE1	2.52	0.41
18:Z:43:ILE:O	18:Z:47:ILE:HG12	2.21	0.41
3:A:1127:A:H1'	4:C:189:GLN:HB2	2.02	0.41
4:C:182:ARG:CG	4:C:183:ILE:O	2.59	0.41
15:T:88:LYS:HG2	15:T:89:GLU:HG2	2.02	0.41
2:2:10:LEU:HG	2:2:14:ARG:HH21	1.87	0.40
3:A:629:G:N2	3:A:639:U:HO2'	2.17	0.40
3:A:946:C:H2'	3:A:947:A:H8	1.85	0.40
3:A:1024:G:OP2	3:A:1025:G:O2'	2.31	0.40
3:A:1190:G:H2'	3:A:1191:G:H8	1.85	0.40
3:A:2898:U:H2'	3:A:2899:A:C8	2.56	0.40
4:C:108:THR:OG1	4:C:112:ARG:HG3	2.22	0.40
15:T:92:ASN:OD1	15:T:93:LEU:N	2.54	0.40
3:A:159:G:C2'	3:A:160:A:H5''	2.51	0.40
3:A:161:A:C8	3:A:162:U:H2'	2.56	0.40
3:A:519:U:H2'	3:A:520:G:C8	2.56	0.40
3:A:1188:U:H2'	3:A:1189:A:H8	1.86	0.40
4:C:111:ILE:H	4:C:111:ILE:HD12	1.86	0.40
4:C:140:ARG:HB3	4:C:142:LEU:HD23	2.03	0.40
14:S:24:ILE:HD11	14:S:32:ALA:HB1	2.04	0.40
3:A:534:U:H2'	3:A:535:G:H8	1.87	0.40
3:A:2710:C:H2'	3:A:2711:A:C8	2.57	0.40
3:A:2875:C:O3'	11:P:1:SER:OG	2.39	0.40
4:C:67:THR:O	4:C:71:LYS:HB2	2.21	0.40
4:C:84:ASP:C	4:C:86:LEU:N	2.77	0.40
7:J:47:HIS:ND1	7:J:48:VAL:HG13	2.37	0.40
3:A:1278:C:H2'	3:A:1279:G:H8	1.86	0.40
3:A:2843:G:H2'	3:A:2844:G:C8	2.56	0.40
4:C:91:PRO:HB2	4:C:96:TYR:HE2	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:121:THR:O	9:L:123:ARG:NH2	2.53	0.40
11:P:14:GLN:OE1	11:P:14:GLN:N	2.54	0.40
3:A:599:A:H2'	3:A:600:G:C8	2.57	0.40
3:A:1278:C:H2'	3:A:1279:G:C8	2.56	0.40
4:C:107:SER:O	4:C:108:THR:HG22	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	53/57 (93%)	48 (91%)	5 (9%)	0	100	100
2	2	39/46 (85%)	36 (92%)	3 (8%)	0	100	100
4	C	233/244 (96%)	205 (88%)	20 (9%)	8 (3%)	3	21
5	D	121/209 (58%)	116 (96%)	5 (4%)	0	100	100
6	E	193/201 (96%)	189 (98%)	4 (2%)	0	100	100
7	J	137/142 (96%)	131 (96%)	6 (4%)	0	100	100
8	K	117/123 (95%)	108 (92%)	9 (8%)	0	100	100
9	L	99/144 (69%)	93 (94%)	6 (6%)	0	100	100
10	N	117/127 (92%)	106 (91%)	11 (9%)	0	100	100
11	P	108/115 (94%)	104 (96%)	4 (4%)	0	100	100
12	Q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
13	R	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
14	S	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	6	32
15	T	90/100 (90%)	84 (93%)	5 (6%)	1 (1%)	12	46
16	U	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
17	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Z	56/59 (95%)	56 (100%)	0	0	100	100
All	All	1848/2065 (90%)	1735 (94%)	102 (6%)	11 (1%)	24	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	37	ILE
4	C	92	LYS
4	C	135	LEU
4	C	182	ARG
14	S	91	GLY
4	C	84	ASP
4	C	208	THR
14	S	94	ASP
15	T	3	ARG
4	C	108	THR
4	C	85	ILE

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	0	46/48 (96%)	46 (100%)	0	100	100
2	2	33/38 (87%)	33 (100%)	0	100	100
4	C	223/232 (96%)	216 (97%)	7 (3%)	35	55
5	D	95/164 (58%)	95 (100%)	0	100	100
6	E	163/165 (99%)	163 (100%)	0	100	100
7	J	115/116 (99%)	115 (100%)	0	100	100
8	K	102/104 (98%)	102 (100%)	0	100	100
9	L	74/103 (72%)	74 (100%)	0	100	100
10	N	99/103 (96%)	99 (100%)	0	100	100
11	P	98/100 (98%)	98 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Q	89/90 (99%)	89 (100%)	0	100	100
13	R	84/84 (100%)	84 (100%)	0	100	100
14	S	93/93 (100%)	90 (97%)	3 (3%)	34	54
15	T	79/84 (94%)	78 (99%)	1 (1%)	65	77
16	U	83/85 (98%)	83 (100%)	0	100	100
17	Y	55/55 (100%)	55 (100%)	0	100	100
18	Z	48/49 (98%)	48 (100%)	0	100	100
All	All	1579/1713 (92%)	1568 (99%)	11 (1%)	80	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	92	LYS
4	C	95	SER
4	C	96	TYR
4	C	136	LEU
4	C	165	PRO
4	C	183	ILE
4	C	186	LYS
14	S	86	MET
14	S	88	ARG
14	S	95	ARG
15	T	4	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	18	HIS
4	C	18	ASN
4	C	43	HIS
4	C	53	ASN
4	C	164	HIS
4	C	177	ASN
4	C	192	ASN
4	C	210	ASN
4	C	211	GLN
4	C	231	GLN
6	E	136	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	J	86	GLN
8	K	3	GLN
8	K	88	ASN
11	P	9	GLN
11	P	55	HIS
13	R	11	GLN
13	R	18	GLN
14	S	9	HIS
14	S	61	ASN
16	U	44	HIS
17	Y	25	GLN
17	Y	36	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	1588/2904 (54%)	293 (18%)	7 (0%)

All (293) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	10	A
3	A	12	U
3	A	14	A
3	A	27	G
3	A	28	A
3	A	34	U
3	A	35	G
3	A	46	G
3	A	48	G
3	A	51	G
3	A	60	G
3	A	63	A
3	A	71	A
3	A	74	A
3	A	75	G
3	A	84	A
3	A	103	A
3	A	118	A
3	A	120	U
3	A	125	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	131	A
3	A	138	U
3	A	139	U
3	A	140	C
3	A	141	G
3	A	142	A
3	A	158	U
3	A	160	A
3	A	162	U
3	A	164	C
3	A	166	U
3	A	181	A
3	A	199	A
3	A	204	A
3	A	215	G
3	A	216	A
3	A	222	A
3	A	228	C
3	A	229	C
3	A	230	G
3	A	233	A
3	A	248	G
3	A	250	G
3	A	255	A
3	A	265	A
3	A	266	G
3	A	271	G
3	A	272	A
3	A	277	G
3	A	278	A
3	A	287	G
3	A	288	U
3	A	291	G
3	A	292	U
3	A	294	A
3	A	302	C
3	A	307	G
3	A	311	A
3	A	322	A
3	A	329	G
3	A	330	A
3	A	359	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	362	A
3	A	366	C
3	A	370	G
3	A	371	A
3	A	372	G
3	A	373	U
3	A	404	A
3	A	405	U
3	A	406	G
3	A	408	G
3	A	409	G
3	A	411	G
3	A	412	A
3	A	421	C
3	A	423	A
3	A	424	G
3	A	435	C
3	A	451	U
3	A	456	C
3	A	457	A
3	A	467	G
3	A	480	A
3	A	481	G
3	A	490	C
3	A	491	G
3	A	505	A
3	A	509	C
3	A	510	C
3	A	530	G
3	A	531	C
3	A	532	A
3	A	533	G
3	A	546	U
3	A	547	A
3	A	548	G
3	A	550	C
3	A	563	A
3	A	564	C
3	A	572	A
3	A	573	U
3	A	574	A
3	A	575	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	621	A
3	A	627	A
3	A	631	A
3	A	634	C
3	A	636	G
3	A	637	A
3	A	646	U
3	A	647	G
3	A	654	A
3	A	668	A
3	A	669	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	793	A
3	A	801	G
3	A	812	C
3	A	819	A
3	A	827	U
3	A	828	U
3	A	829	A
3	A	830	G
3	A	831	G
3	A	845	A
3	A	846	U
3	A	847	U
3	A	858	G
3	A	920	A
3	A	931	U
3	A	934	U
3	A	945	A
3	A	954	G
3	A	957	C
3	A	958	U
3	A	959	A
3	A	960	A
3	A	961	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	962	G
3	A	963	U
3	A	964	C
3	A	974	G
3	A	980	A
3	A	982	C
3	A	983	A
3	A	985	C
3	A	995	C
3	A	996	A
3	A	997	G
3	A	1005	C
3	A	1009	A
3	A	1012	U
3	A	1013	C
3	A	1023	U
3	A	1026	G
3	A	1027	A
3	A	1028	A
3	A	1031	G
3	A	1124	G
3	A	1126	A
3	A	1127	A
3	A	1128	G
3	A	1129	A
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1139	G
3	A	1142	A
3	A	1173	U
3	A	1174	U
3	A	1175	A
3	A	1176	U
3	A	1177	G
3	A	1182	G
3	A	1186	G
3	A	1210	G
3	A	1212	G
3	A	1225	G
3	A	1236	G
3	A	1238	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1247	A
3	A	1251	C
3	A	1252	G
3	A	1253	A
3	A	1256	G
3	A	1266	G
3	A	1271	G
3	A	1272	A
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1314	C
3	A	1341	G
3	A	1345	C
3	A	1376	C
3	A	1378	A
3	A	1379	U
3	A	1380	G
3	A	1383	A
3	A	1386	C
3	A	1395	A
3	A	1412	U
3	A	1416	G
3	A	1591	A
3	A	1592	C
3	A	1593	A
3	A	1595	C
3	A	1596	A
3	A	1598	A
3	A	1607	C
3	A	1633	G
3	A	1634	A
3	A	1646	C
3	A	1647	U
3	A	1648	U
3	A	1654	A
3	A	1663	G
3	A	1667	G
3	A	1669	A
3	A	1674	G
3	A	1991	U
3	A	1992	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1993	U
3	A	1994	C
3	A	1997	C
3	A	2013	A
3	A	2020	A
3	A	2022	U
3	A	2023	C
3	A	2029	G
3	A	2030	A
3	A	2031	A
3	A	2043	C
3	A	2052	A
3	A	2057	G
3	A	2058	A
3	A	2059	A
3	A	2608	G
3	A	2609	U
3	A	2611	C
3	A	2612	C
3	A	2614	A
3	A	2617	U
3	A	2622	U
3	A	2629	U
3	A	2639	A
3	A	2640	G
3	A	2645	G
3	A	2646	C
3	A	2654	A
3	A	2665	A
3	A	2675	A
3	A	2676	C
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2702	G
3	A	2713	U
3	A	2714	G
3	A	2726	A
3	A	2729	G
3	A	2732	G
3	A	2733	A
3	A	2739	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2748	A
3	A	2751	G
3	A	2752	C
3	A	2758	A
3	A	2762	C
3	A	2765	A
3	A	2766	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2791	G
3	A	2804	U
3	A	2820	A
3	A	2833	U
3	A	2848	G
3	A	2849	U
3	A	2867	G
3	A	2873	A
3	A	2880	C
3	A	2886	A
3	A	2903	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	271	G
3	A	287	G
3	A	479	A
3	A	959	A
3	A	1411	U
3	A	2051	A
3	A	2611	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

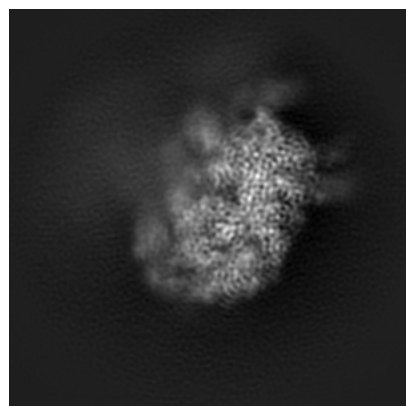
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61625. These allow visual inspection of the internal detail of the map and identification of artifacts.

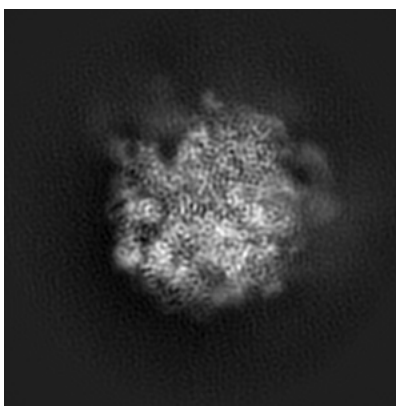
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

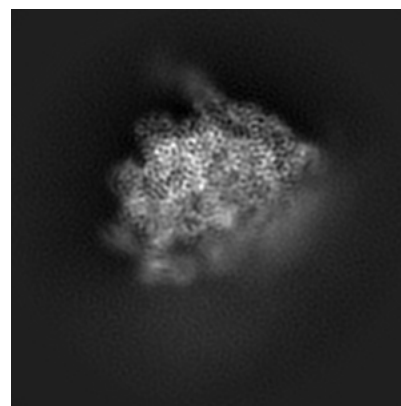
6.1.1 Primary map



X

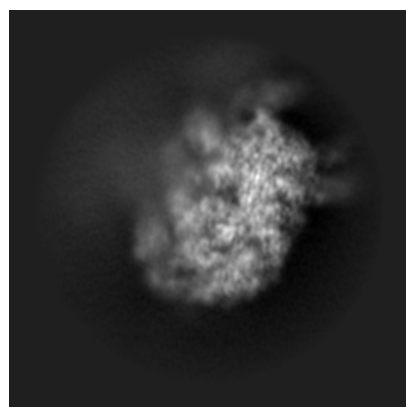


Y

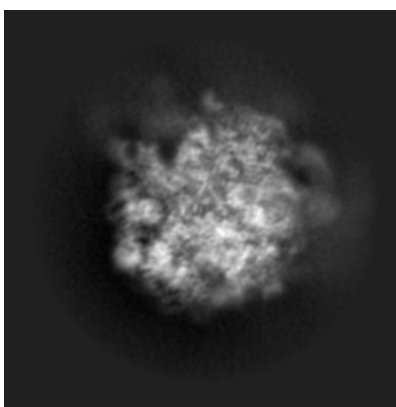


Z

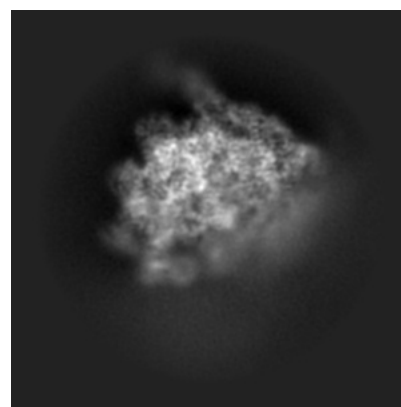
6.1.2 Raw map



X



Y

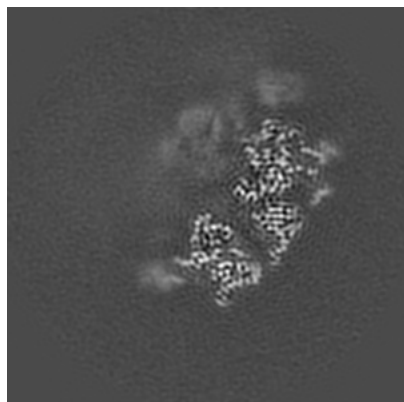


Z

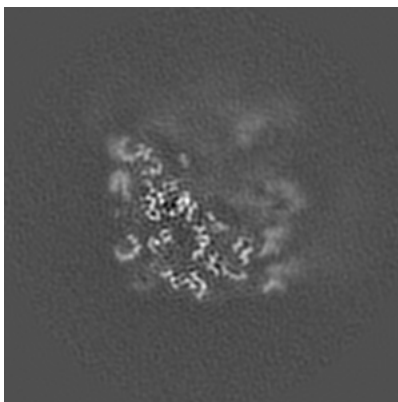
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

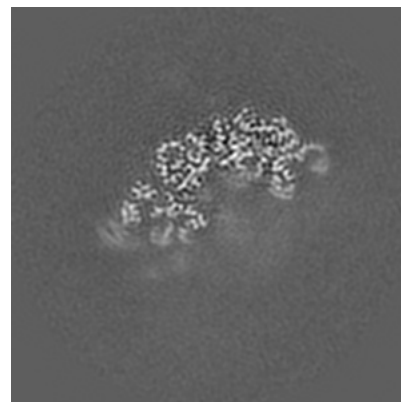
6.2.1 Primary map



X Index: 120

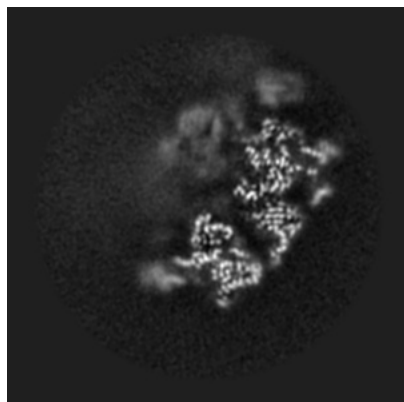


Y Index: 120

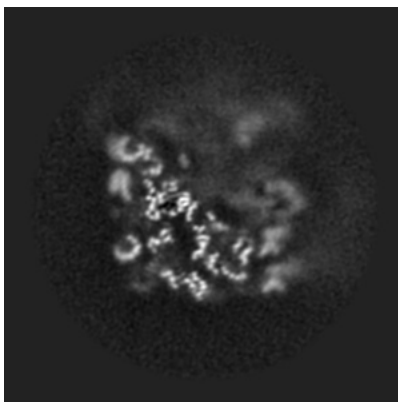


Z Index: 120

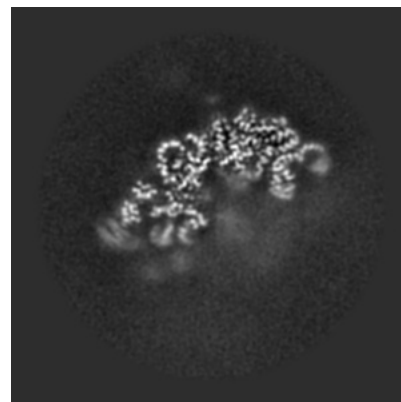
6.2.2 Raw map



X Index: 120



Y Index: 120

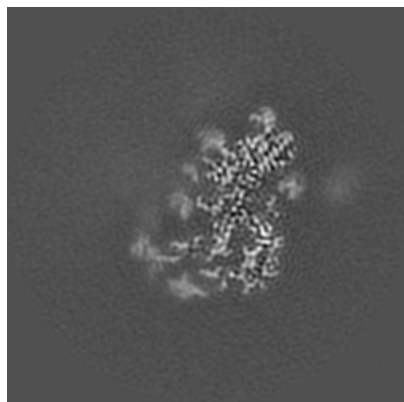


Z Index: 120

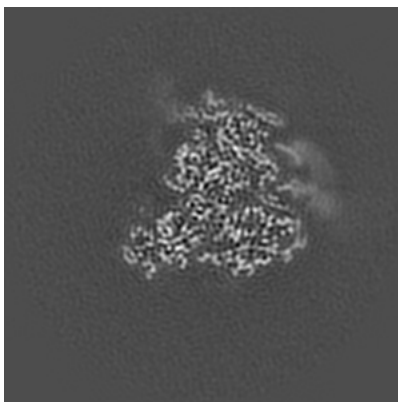
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

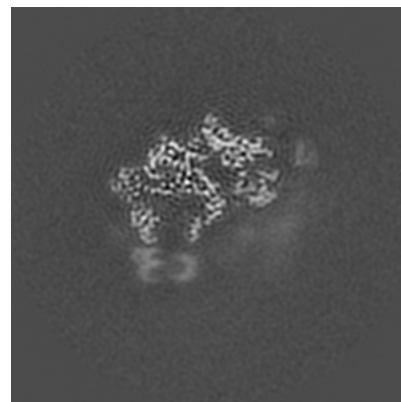
6.3.1 Primary map



X Index: 95

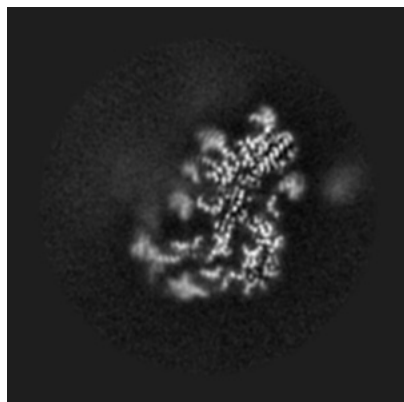


Y Index: 153

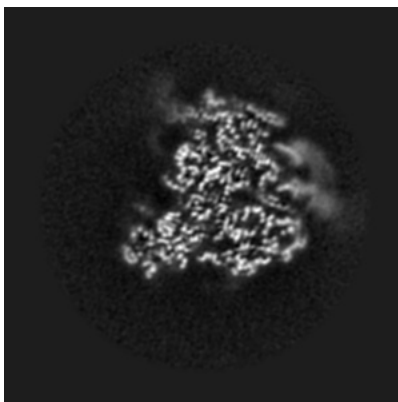


Z Index: 106

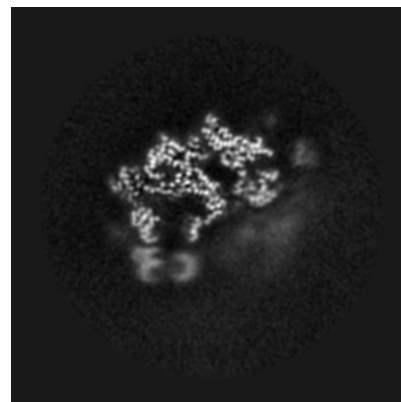
6.3.2 Raw map



X Index: 95



Y Index: 153

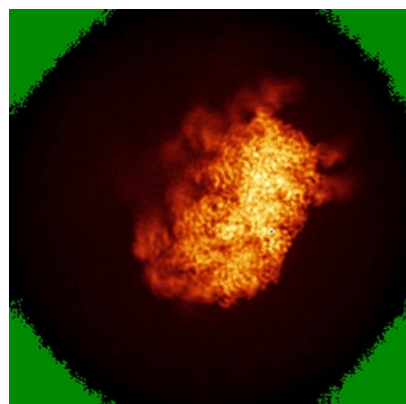


Z Index: 106

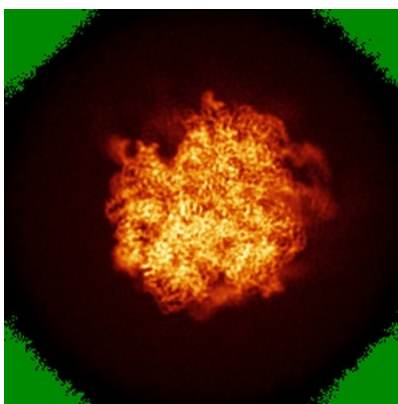
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

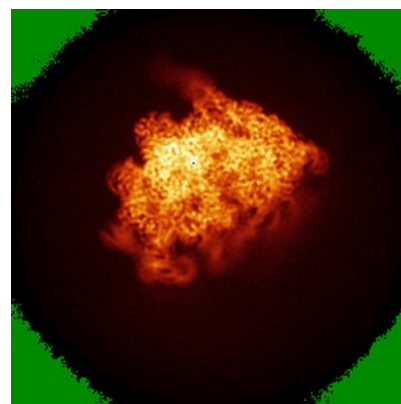
6.4.1 Primary map



X

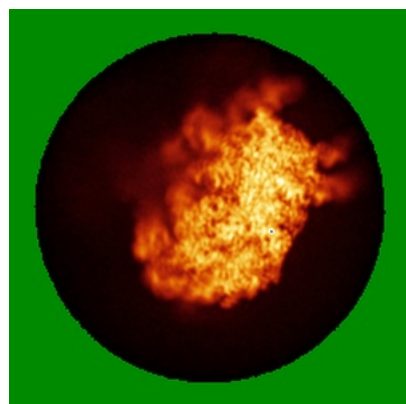


Y

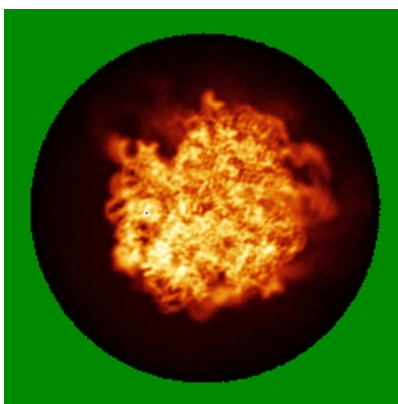


Z

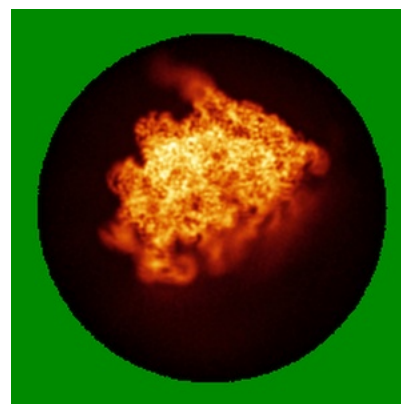
6.4.2 Raw map



X



Y



Z

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

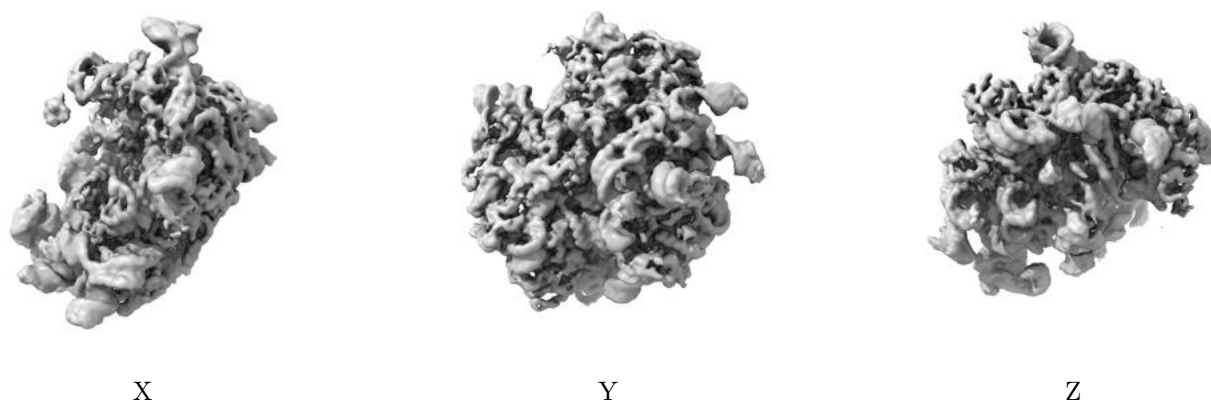
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0136. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

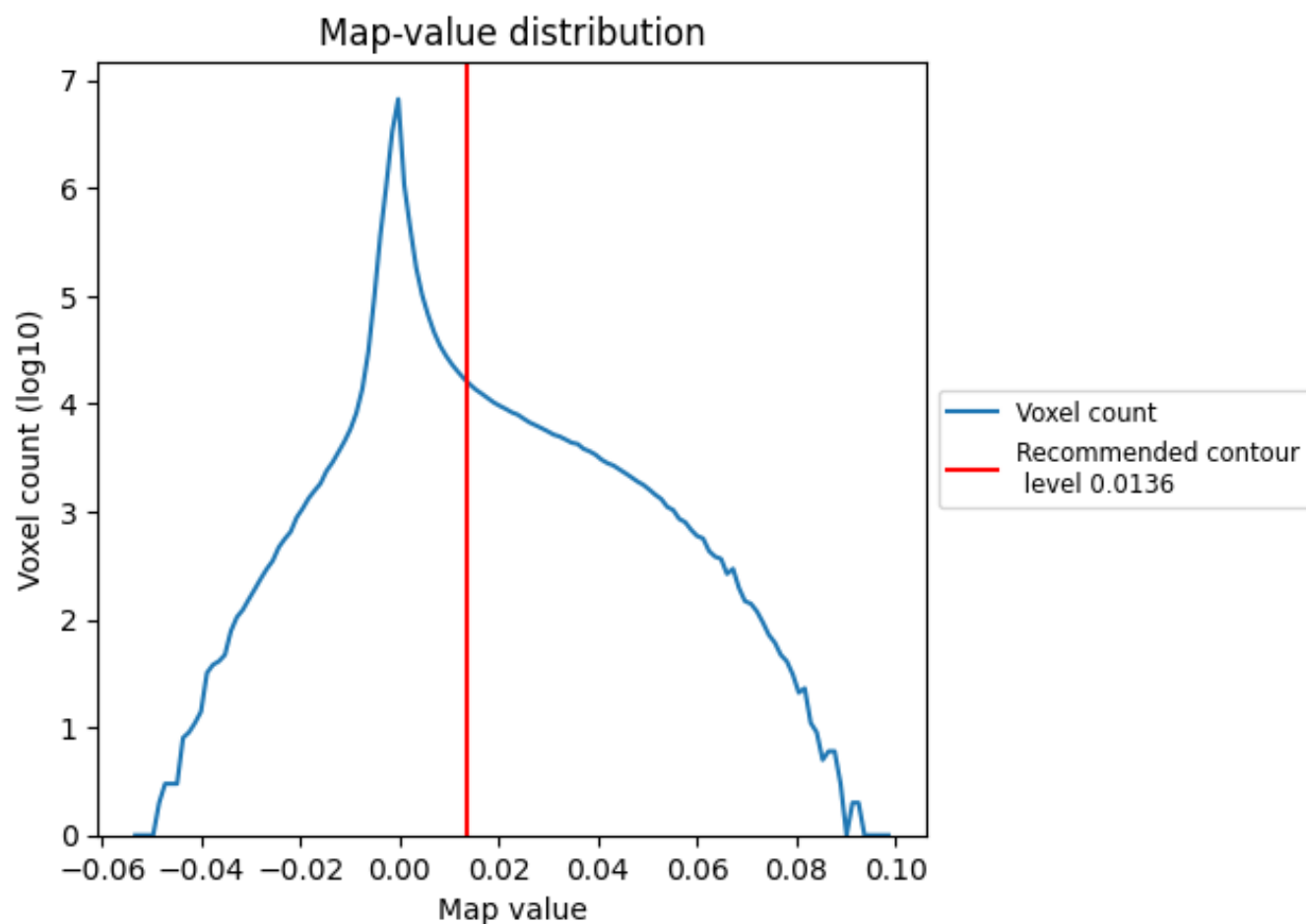
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

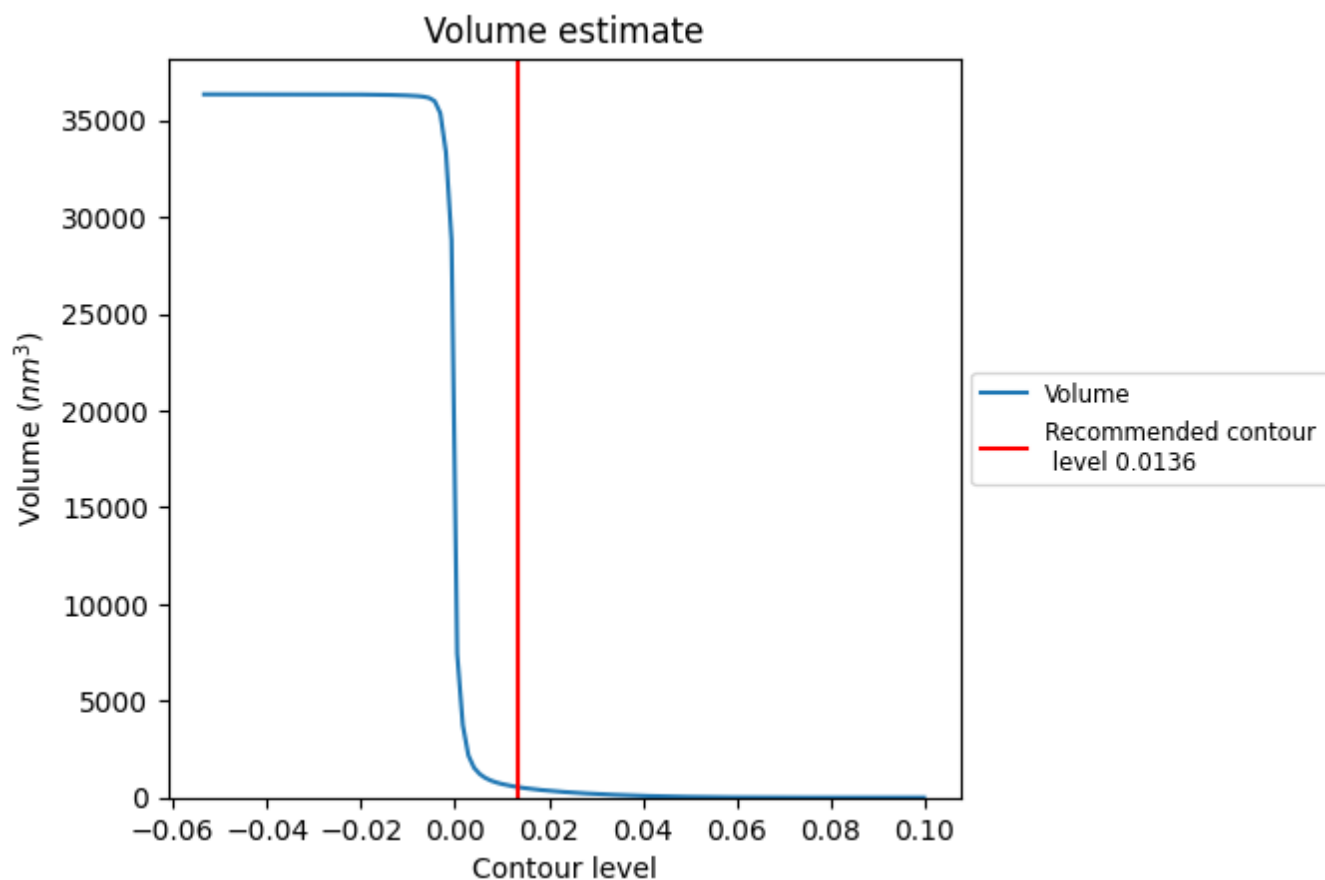
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

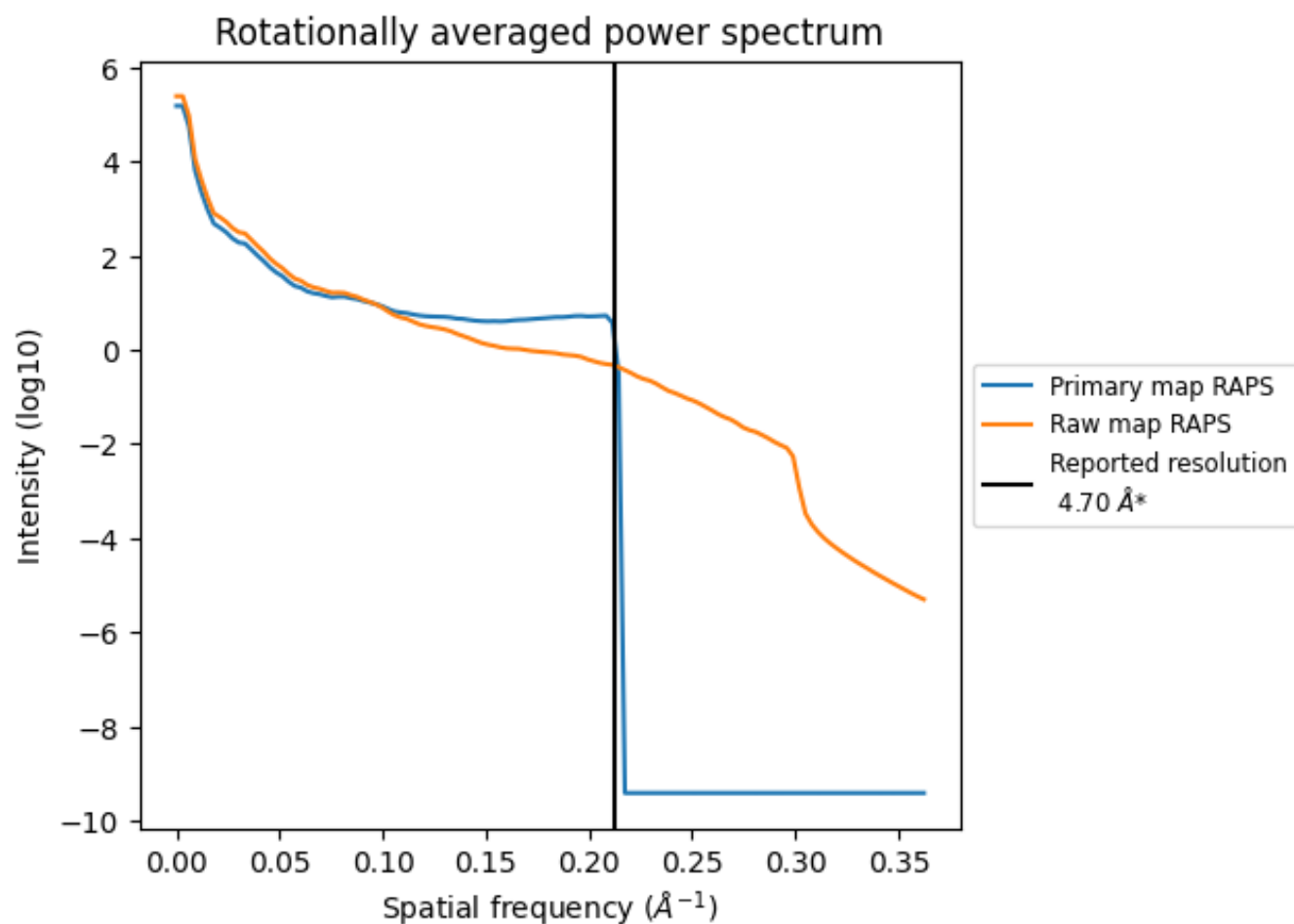
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm^3 ; this corresponds to an approximate mass of 482 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 ⓘ

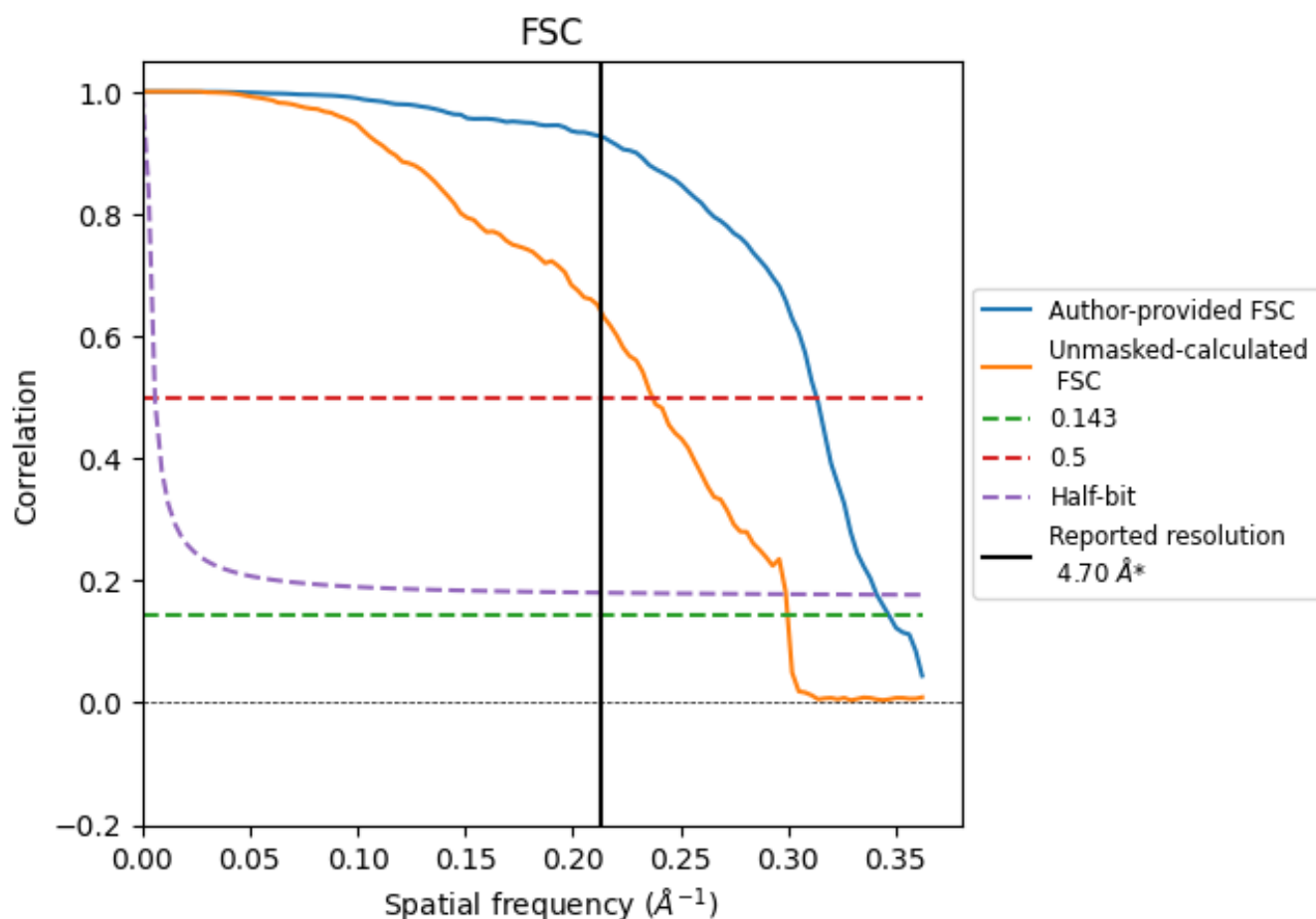


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	2.88	3.19	2.93
Unmasked-calculated*	3.34	4.22	3.34

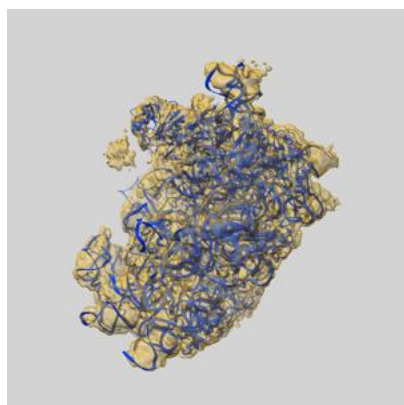
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.88 differs from the reported value 4.7 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.34 differs from the reported value 4.7 by more than 10 %

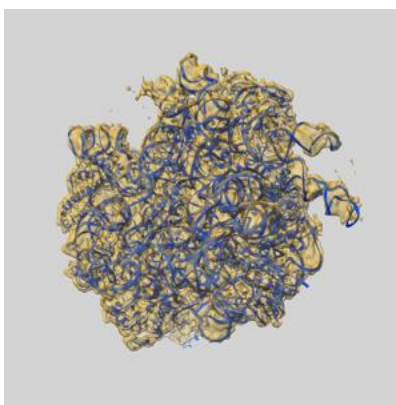
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61625 and PDB model 9JNS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

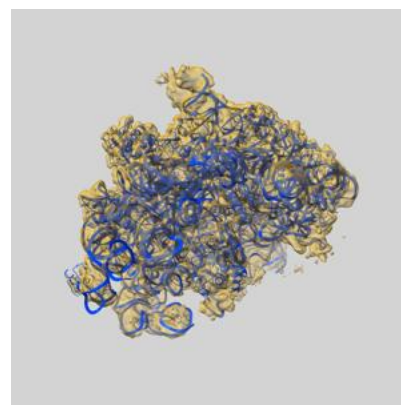
9.1 Map-model overlay [i](#)



X



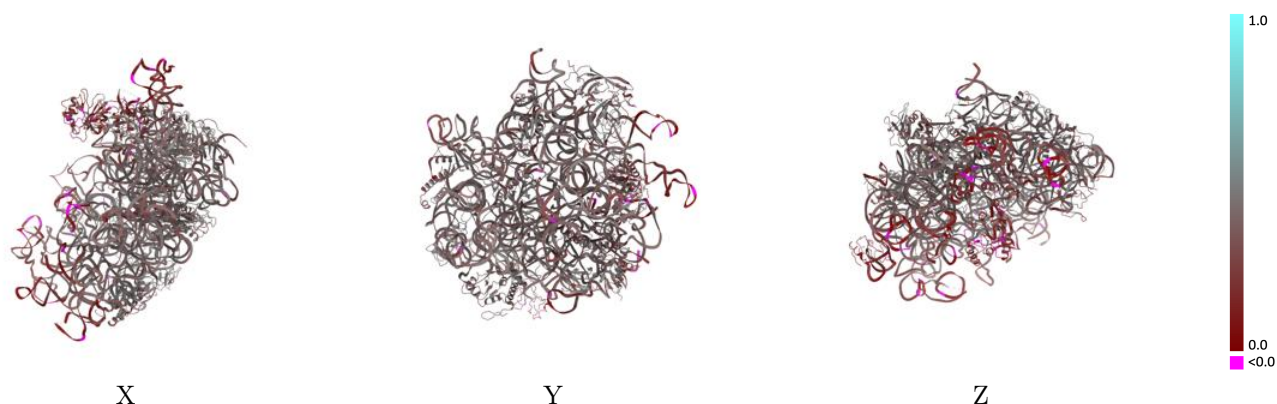
Y



Z

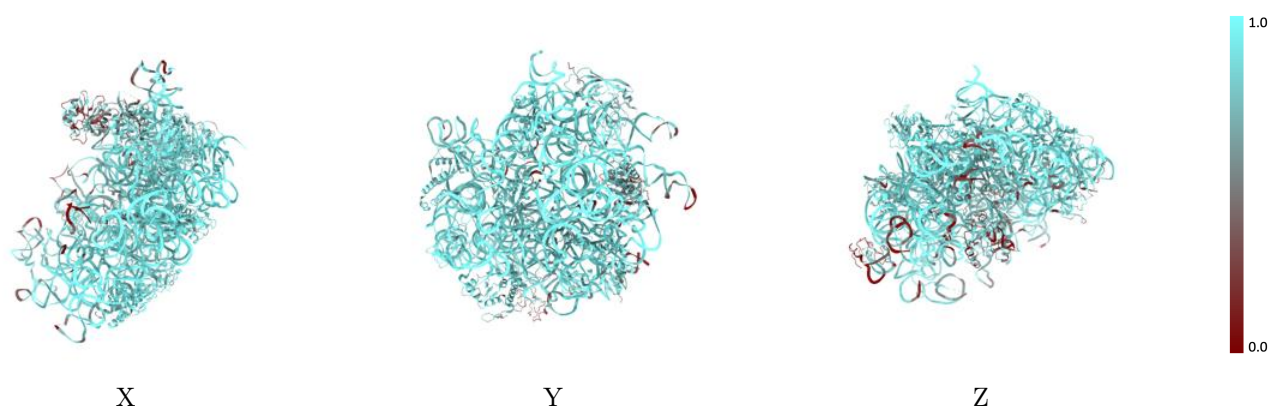
The images above show the 3D surface view of the map at the recommended contour level 0.0136 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



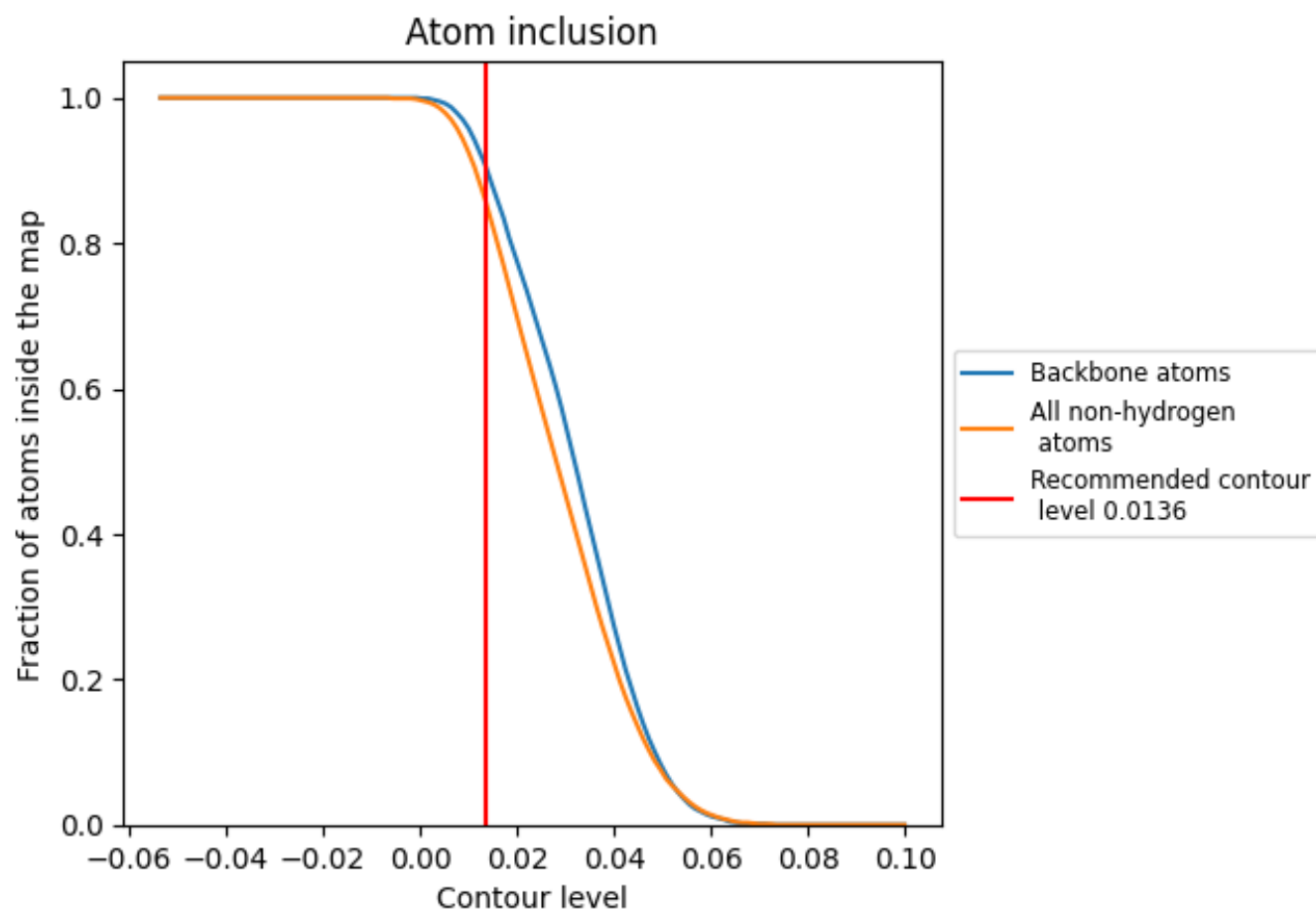
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0136).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.0136) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.3540
0	 0.8900	 0.4130
2	 0.8460	 0.3950
A	 0.8930	 0.3470
C	 0.5230	 0.2170
D	 0.8700	 0.4240
E	 0.7840	 0.3890
J	 0.8430	 0.4130
K	 0.7600	 0.3710
L	 0.3940	 0.2280
N	 0.9100	 0.4210
P	 0.7770	 0.3850
Q	 0.8930	 0.3970
R	 0.8770	 0.4300
S	 0.7910	 0.3950
T	 0.8390	 0.4100
U	 0.8960	 0.4390
Y	 0.8410	 0.3530
Z	 0.7670	 0.4070

