



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:16 PM UTC

PDB ID : 8CDU / pdb_00008cdu
EMDB ID : EMD-16595
Title : Rnase R bound to a 30S degradation intermediate (main state)
Authors : Paternoga, H.; Dimitrova-Paternoga, L.; Wilson, D.N.
Deposited on : 2023-02-01
Resolution : 3.10 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:

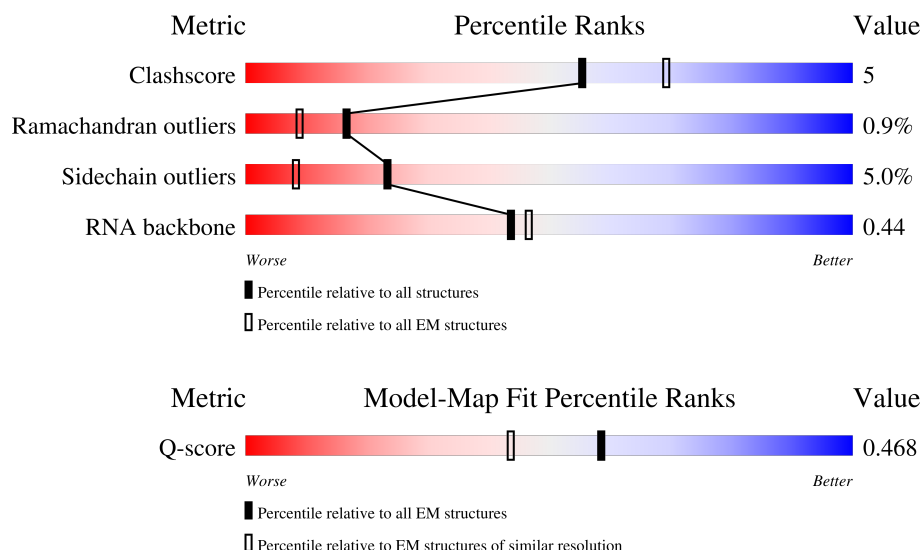
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 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.



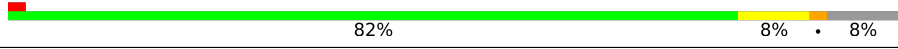
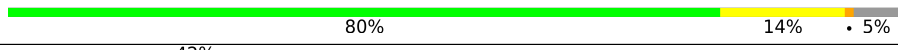
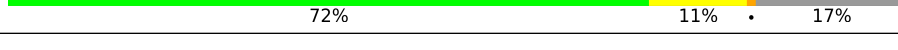
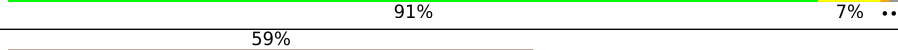
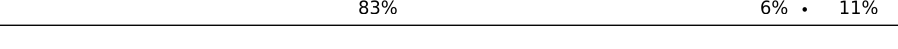
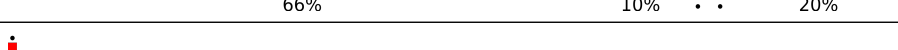
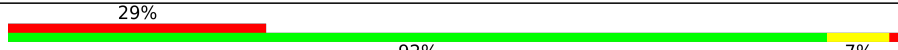
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1554	
2	B	9	
3	C	779	

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Mol	Chain	Length	Quality of chain
4	D	246	
5	E	218	
6	F	200	
7	G	166	
8	H	156	
9	I	132	
10	J	130	
11	L	138	
12	M	121	
13	N	61	
14	O	89	
15	P	90	
16	Q	87	
17	R	92	
18	S	88	
19	T	95	
20	U	79	
21	V	131	
22	K	102	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 51964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1333	Total	C	N	O	P	0	0
			28597	12753	5245	9266	1333		

- Molecule 2 is a RNA chain called RNA Substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	7	Total	C	N	O	P	0	0
			154	70	35	42	7		

- Molecule 3 is a protein called Ribonuclease R.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	708	Total	C	N	O	S	0	0
			5650	3559	962	1102	27		

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	218	Total	C	N	O	S	0	0
			1757	1119	309	323	6		

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	205	Total	C	N	O	S	0	0
			1615	1009	303	300	3		

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	185	Total	C	N	O	S	0	0
			1490	942	276	270	2		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	158	Total	C	N	O	S	0	0
			1170	736	216	216	2		

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 9 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	131	Total	C	N	O	S	0	0
			1036	655	191	187	3		

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	108	Total	C	N	O	S	0	0
			826	510	160	155	1		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	136	Total	C	N	O	S	0	0
			1052	653	211	186	2		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	108	Total	C	N	O	0	0
			868	534	176	158		

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	49	Total	C	N	O	S	0	0
			409	263	79	63	4		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	85	Total	C	N	O	S	0	0
			710	436	144	129	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	88	Total	C	N	O	S	0	0
			695	441	128	124	2		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	84	Total	C	N	O	S	0	0
			691	435	128	126	2		

- Molecule 17 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	78	Total	C	N	O	S	0	0
			633	409	112	110	2		

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

- Molecule 19 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	95	Total	C	N	O	S	0	0
			784	492	138	152	2		

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

- Molecule 21 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	101	Total	C	N	O	S	0	0
			730	450	136	143	1		

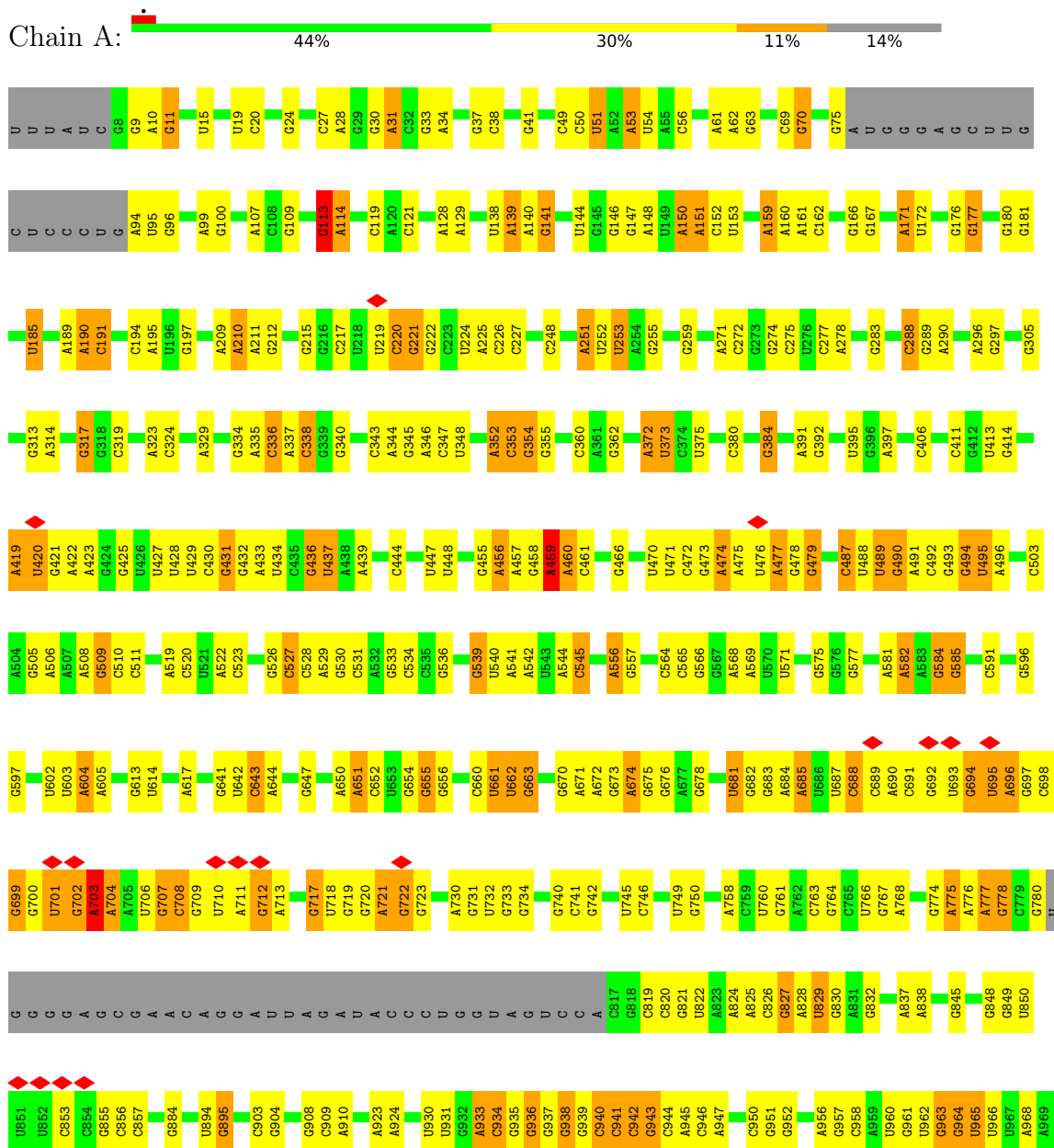
- Molecule 22 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

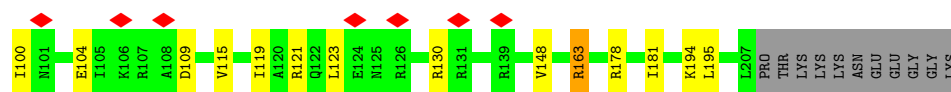
3 Residue-property plots

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

• Molecule 1: 16S rRNA

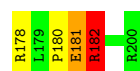






- Molecule 6: 30S ribosomal protein S4

Chain F: 82% 8% 8%



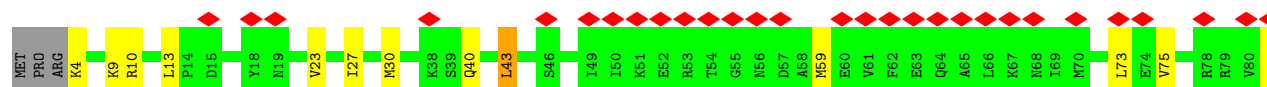
- Molecule 7: 30S ribosomal protein S5

Chain G: 80% 14% 5%



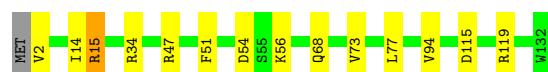
- Molecule 8: 30S ribosomal protein S7

Chain H: 42% 86% 9%



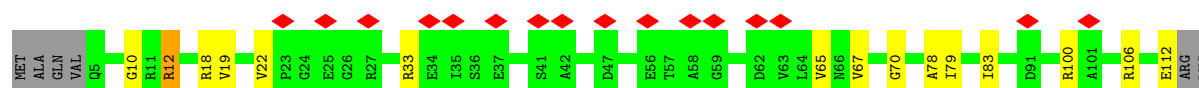
- Molecule 9: 30S ribosomal protein S8

Chain I: 89% 10% 2%



- Molecule 10: 30S ribosomal protein S9

Chain J: 12% 72% 11% 17%



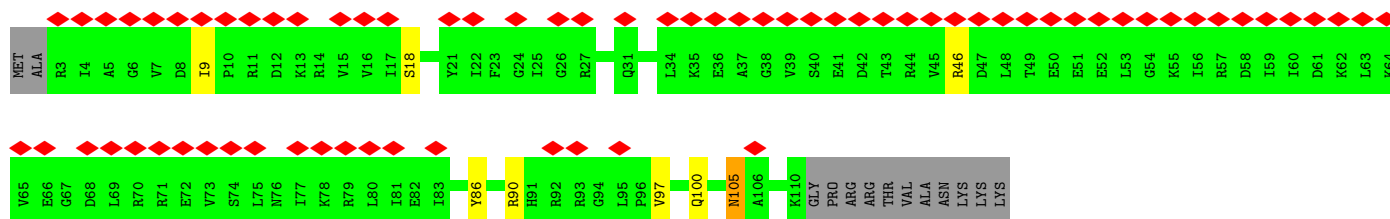
- Molecule 11: 30S ribosomal protein S12

Chain L:  91% 7% ..



- Molecule 12: 30S ribosomal protein S13

Chain M:  59% 83% 6% • 11%



- Molecule 13: 30S ribosomal protein S14

Chain N:  66% 10% • • 20%



- Molecule 14: 30S ribosomal protein S15

Chain O:  91% • • •



- Molecule 15: 30S ribosomal protein S16

Chain P:  86% 11% • •



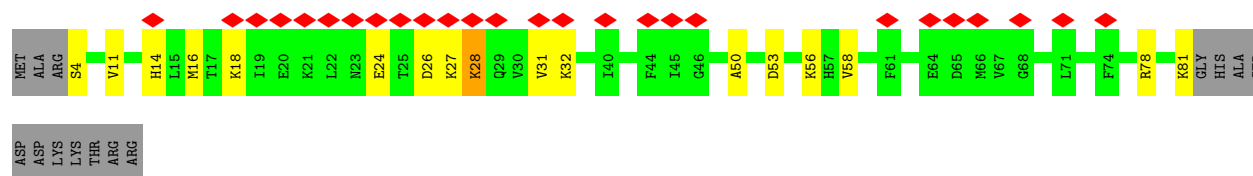
- Molecule 16: 30S ribosomal protein S17

Chain Q:  90% 5% • •

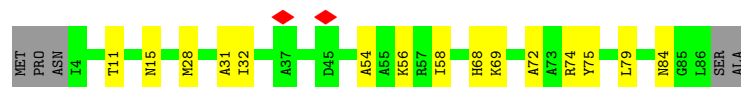
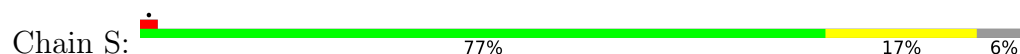


- Molecule 17: 30S ribosomal protein S19

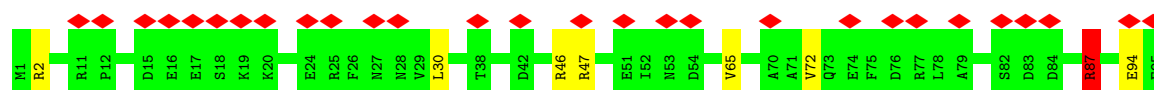
Chain R:  28% 66% 17% • 15%



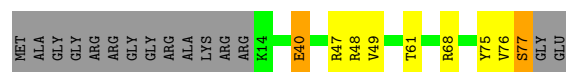
- Molecule 18: 30S ribosomal protein S20



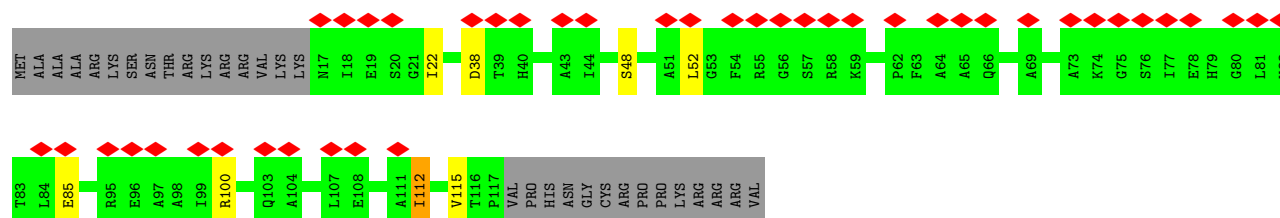
- Molecule 19: 30S ribosomal protein S6



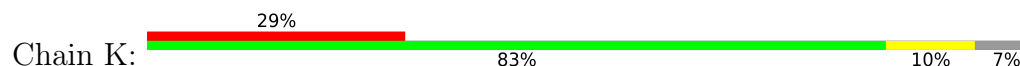
- Molecule 20: 30S ribosomal protein S18



- Molecule 21: 30S ribosomal protein S11



- Molecule 22: 30S ribosomal protein S10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28143	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0178	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	1/32015 (0.0%)	0.92	17/49936 (0.0%)
2	B	0.77	0/174	0.95	0/269
3	C	0.56	0/5748	1.08	6/7760 (0.1%)
4	D	0.54	0/1782	1.19	2/2392 (0.1%)
5	E	0.58	0/1637	1.10	0/2203
6	F	0.58	0/1517	1.17	5/2036 (0.2%)
7	G	0.68	0/1182	1.28	6/1591 (0.4%)
8	H	0.55	0/1196	1.15	0/1604
9	I	0.66	0/1048	1.22	2/1407 (0.1%)
10	J	0.60	0/836	1.08	0/1128
11	L	0.63	0/1069	1.18	3/1435 (0.2%)
12	M	0.58	0/873	1.14	0/1166
13	N	0.55	0/419	1.19	2/558 (0.4%)
14	O	0.61	0/718	1.25	0/960
15	P	0.67	0/708	1.23	1/950 (0.1%)
16	Q	0.57	0/699	1.17	2/933 (0.2%)
17	R	0.56	0/649	1.10	0/872
18	S	0.66	0/639	1.35	1/852 (0.1%)
19	T	0.54	0/795	1.08	1/1067 (0.1%)
20	U	0.54	0/526	1.18	1/705 (0.1%)
21	V	0.59	0/740	1.01	1/1002 (0.1%)
22	K	0.58	0/773	1.09	0/1044
All	All	0.61	1/55743 (0.0%)	1.01	50/81870 (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
3	C	0	2
4	D	0	1
5	E	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	5
7	G	0	4
9	I	0	3
10	J	0	2
11	L	0	2
12	M	0	1
16	Q	0	2
18	S	0	1
19	T	0	2
20	U	0	1
All	All	0	32

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1395	G	O3'-P	6.99	1.71	1.61

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	656	HIS	CA-CB-CG	9.62	123.42	113.80
16	Q	36	TYR	CB-CA-C	7.61	123.57	110.79
7	G	22	ALA	N-CA-C	6.71	119.29	107.61
1	A	980	C	C2'-C3'-O3'	6.49	119.24	109.50
1	A	113	G	C2'-C3'-O3'	6.41	119.11	109.50
1	A	1075	U	C2'-C3'-O3'	6.32	118.98	109.50
7	G	21	VAL	CA-C-O	-6.27	114.58	121.92
20	U	61	THR	CA-CB-OG1	-6.24	100.24	109.60
11	L	22	PRO	N-CA-C	6.20	121.65	114.03
7	G	82	PRO	CB-CA-C	-6.16	103.31	112.55
15	P	69	THR	CA-CB-OG1	-6.11	100.43	109.60
13	N	54	PRO	N-CA-C	5.96	124.74	112.47
1	A	703	A	C2'-C3'-O3'	5.89	118.33	109.50
16	Q	50	ASP	CB-CA-C	5.83	119.42	110.62
6	F	64	ASN	CB-CA-C	5.82	119.46	109.51
6	F	132	LEU	N-CA-CB	-5.68	100.86	110.46
6	F	73	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	459	A	C2'-C3'-O3'	5.58	117.87	109.50
7	G	6	PRO	N-CA-C	5.50	123.81	112.47
9	I	94	VAL	N-CA-CB	5.50	115.19	110.08
1	A	1090	A	O3'-P-O5'	-5.49	95.76	104.00
4	D	188	ASP	CA-CB-CG	5.48	118.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	641	PHE	CA-CB-CG	5.46	119.27	113.80
9	I	115	ASP	CA-CB-CG	5.45	118.05	112.60
19	T	87	ARG	CG-CD-NE	5.43	123.94	112.00
1	A	1153	G	C2'-C3'-O3'	5.41	117.61	109.50
1	A	296	A	P-O5'-C5'	-5.37	112.84	120.90
1	A	661	U	C2'-C3'-O3'	5.33	117.50	109.50
1	A	288	C	C2'-C3'-O3'	5.27	117.41	109.50
6	F	127	ASP	CA-CB-CG	5.25	117.85	112.60
21	V	38	ASP	CA-CB-CG	5.24	117.84	112.60
13	N	30	PRO	N-CA-CB	-5.22	97.76	103.25
3	C	392	LEU	CA-C-N	5.21	123.52	120.24
3	C	392	LEU	C-N-CA	5.21	123.52	120.24
11	L	36	THR	CA-CB-OG1	5.21	117.41	109.60
1	A	487	C	C2'-C3'-O3'	5.18	121.47	113.70
3	C	428	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	171	A	C2'-C3'-O3'	-5.16	105.96	113.70
1	A	317	G	C4'-C3'-C2'	-5.15	97.45	102.60
3	C	266	ASP	CA-CB-CG	5.12	117.72	112.60
7	G	140	THR	CA-CB-OG1	-5.11	101.93	109.60
7	G	41	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	749	U	C4'-C3'-C2'	-5.09	97.50	102.60
1	A	372	A	C2'-C3'-O3'	5.09	121.33	113.70
6	F	68	PHE	CA-CB-CG	5.05	118.85	113.80
18	S	11	THR	CA-CB-OG1	-5.05	102.03	109.60
1	A	151	A	O3'-P-O5'	-5.03	96.46	104.00
1	A	681	U	C4'-C3'-C2'	-5.03	97.57	102.60
11	L	8	ILE	CA-CB-CG1	5.02	118.94	110.40
4	D	130	PRO	CB-CA-C	5.01	119.82	111.56

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	573	ARG	Sidechain
3	C	62	ARG	Sidechain
4	D	21	ARG	Sidechain
5	E	121	ARG	Sidechain
5	E	130	ARG	Sidechain
5	E	16	ARG	Sidechain
5	E	163	ARG	Sidechain
5	E	178	ARG	Sidechain
5	E	58	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	F	13	ARG	Sidechain
6	F	146	ARG	Sidechain
6	F	182	ARG	Sidechain
6	F	3	ARG	Sidechain
6	F	58	ARG	Sidechain
7	G	112	ARG	Sidechain
7	G	14	ARG	Sidechain
7	G	30	ARG	Sidechain
7	G	32	ARG	Sidechain
9	I	119	ARG	Sidechain
9	I	15	ARG	Sidechain
9	I	47	ARG	Sidechain
10	J	18	ARG	Sidechain
10	J	33	ARG	Sidechain
11	L	123	ARG	Sidechain
11	L	96	ARG	Sidechain
12	M	46	ARG	Sidechain
16	Q	67	ARG	Sidechain
16	Q	7	ARG	Sidechain
18	S	74	ARG	Sidechain
19	T	46	ARG	Sidechain
19	T	47	ARG	Sidechain
20	U	47	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28597	0	14401	337	0
2	B	154	0	78	1	0
3	C	5650	0	5619	31	0
4	D	1757	0	1830	21	0
5	E	1615	0	1655	6	0
6	F	1490	0	1518	5	0
7	G	1170	0	1245	6	0
8	H	1181	0	1235	4	0
9	I	1036	0	1095	4	0
10	J	826	0	849	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	1052	0	1112	2	0
12	M	868	0	925	3	0
13	N	409	0	427	4	0
14	O	710	0	735	2	0
15	P	695	0	721	3	0
16	Q	691	0	728	1	0
17	R	633	0	649	8	0
18	S	637	0	696	6	0
19	T	784	0	777	4	0
20	U	518	0	555	3	0
21	V	730	0	735	4	0
22	K	761	0	795	2	0
All	All	51964	0	38380	437	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 5.

All (437) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:G:O2'	1:A:671:A:H5'	1.51	1.10
1:A:663:G:H1	1:A:763:C:H5	1.21	0.84
1:A:458:G:H5'	1:A:459:A:H3'	1.60	0.83
1:A:456:A:H2	1:A:495:U:H3	1.28	0.78
1:A:673:G:H22	1:A:750:G:H1	1.29	0.78
1:A:670:G:C2'	1:A:671:A:H5'	2.13	0.78
1:A:946:C:H2'	1:A:947:A:H8	1.48	0.76
1:A:718:U:H2'	1:A:719:G:H8	1.54	0.73
1:A:420:U:H3	1:A:439:A:H61	1.37	0.71
1:A:1024:A:H2'	1:A:1025:G:C8	2.26	0.71
1:A:1045:G:H3'	1:A:1046:G:H5''	1.73	0.70
1:A:1367:U:H3	1:A:1372:A:H62	1.38	0.70
1:A:11:G:H5'	7:G:108:GLY:HA3	1.75	0.69
1:A:427:U:O2	1:A:433:A:C2	2.47	0.68
3:C:164:ILE:HG21	3:C:182:VAL:HG11	1.75	0.67
1:A:698:C:H3'	1:A:699:G:H5''	1.77	0.66
1:A:1025:G:H2'	1:A:1026:A:C8	2.32	0.65
1:A:1044:G:H2'	1:A:1045:G:C8	2.32	0.65
1:A:495:U:H2'	1:A:496:A:H8	1.62	0.65
1:A:1296:A:H2'	1:A:1297:A:C8	2.31	0.64
1:A:1294:A:H61	1:A:1296:A:H1'	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:G:H2'	1:A:494:G:N2	2.13	0.64
1:A:527:C:H5	1:A:539:G:H5'	1.63	0.63
1:A:1014:A:H2'	1:A:1015:C:C6	2.34	0.63
1:A:1317:C:H2'	1:A:1318:G:H8	1.62	0.63
1:A:1001:U:H1'	1:A:1003:G:H8	1.64	0.62
1:A:1227:C:H2'	1:A:1228:U:C6	2.35	0.62
1:A:166:G:O2'	1:A:167:G:H5'	2.00	0.62
1:A:1003:G:H5''	1:A:1005:C:H41	1.65	0.62
1:A:942:C:HO2'	1:A:943:G:H8	1.46	0.62
10:J:65:VAL:HG11	10:J:79:ILE:HG12	1.82	0.62
1:A:720:G:H2'	1:A:721:A:H8	1.63	0.61
1:A:1248:A:H62	1:A:1308:A:H62	1.48	0.61
1:A:1315:A:N6	1:A:1340:G:H1'	2.15	0.61
4:D:112:LYS:O	4:D:113:ARG:C	2.43	0.61
1:A:503:C:O2'	1:A:505:G:H1'	2.00	0.61
4:D:176:ALA:HB3	4:D:183:ILE:HD11	1.83	0.61
1:A:1048:A:H2'	1:A:1049:G:C8	2.36	0.60
1:A:1111:A:H4'	1:A:1112:A:O5'	2.00	0.60
1:A:1183:G:H2'	1:A:1184:G:H5'	1.84	0.59
1:A:75:G:H1'	1:A:94:A:N6	2.17	0.59
1:A:95:U:H2'	1:A:96:G:C8	2.37	0.59
4:D:114:LEU:HD13	4:D:144:LEU:HB2	1.84	0.59
1:A:696:A:H62	1:A:712:G:H1'	1.67	0.59
4:D:32:PHE:HB2	4:D:42:ASP:HB2	1.84	0.59
1:A:19:U:H2'	1:A:20:C:C6	2.37	0.59
1:A:1325:G:O6	17:R:4:SER:N	2.36	0.59
6:F:68:PHE:CE1	6:F:90:LEU:HD11	2.38	0.59
1:A:1052:U:H2'	1:A:1053:G:C4	2.38	0.58
1:A:224:U:H2'	1:A:225:A:C8	2.38	0.58
1:A:1317:C:H2'	1:A:1318:G:C8	2.37	0.58
1:A:909:C:H2'	1:A:910:A:C8	2.38	0.57
15:P:5:ILE:HG22	15:P:70:VAL:HG11	1.85	0.57
1:A:936:G:H4'	1:A:938:G:N7	2.20	0.57
1:A:1003:G:H21	1:A:1005:C:H42	1.53	0.57
11:L:123:ARG:HD2	11:L:125:GLN:O	2.05	0.57
1:A:691:C:H2'	1:A:692:G:H8	1.70	0.57
12:M:9:ILE:HB	12:M:18:SER:HB3	1.86	0.56
1:A:146:G:H2'	1:A:147:G:C8	2.39	0.56
1:A:700:G:H22	1:A:704:A:H5''	1.70	0.56
16:Q:15:VAL:HG12	16:Q:15:VAL:O	2.05	0.56
1:A:1024:A:H5''	17:R:14:HIS:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:G:HO2'	9:I:2:VAL:N	2.04	0.56
22:K:26:VAL:HG21	22:K:39:PRO:HD3	1.88	0.56
1:A:95:U:H2'	1:A:96:G:H8	1.71	0.56
1:A:1064:C:H5''	1:A:1205:A:H2'	1.88	0.56
1:A:1176:A:H2'	1:A:1178:A:C5	2.41	0.56
1:A:1081:C:H2'	1:A:1082:G:C8	2.41	0.55
1:A:1246:C:H4'	1:A:1309:G:H22	1.71	0.55
1:A:979:A:O2'	1:A:980:C:O2	2.23	0.55
1:A:70:G:H1	1:A:99:A:H62	1.54	0.55
1:A:995:C:H2'	1:A:996:A:C8	2.41	0.55
3:C:28:GLU:HB2	3:C:33:ILE:HB	1.89	0.55
4:D:68:LEU:HB3	4:D:161:LEU:HD22	1.88	0.55
1:A:69:C:H2'	1:A:70:G:C8	2.41	0.55
1:A:1145:U:H4'	1:A:1147:A:H62	1.71	0.55
1:A:1010:U:H2'	1:A:1011:C:C6	2.41	0.55
1:A:1053:G:H2'	1:A:1054:A:C8	2.42	0.55
7:G:115:LEU:HD13	7:G:123:ILE:HG21	1.88	0.55
1:A:460:A:N1	1:A:489:U:H5	2.05	0.55
1:A:1367:U:H3	1:A:1372:A:N6	2.04	0.54
3:C:494:GLY:HA2	21:V:112:ILE:HG21	1.90	0.54
5:E:51:VAL:HG22	5:E:69:THR:HB	1.89	0.54
1:A:1301:U:H2'	1:A:1302:G:O4'	2.08	0.54
1:A:985:A:H2'	1:A:1372:A:H2	1.72	0.54
1:A:1356:G:N7	10:J:12:ARG:NH2	2.56	0.54
1:A:1203:U:H2'	1:A:1204:C:C6	2.43	0.54
1:A:1337:C:H2'	1:A:1338:G:C8	2.43	0.53
1:A:1012:U:O2	1:A:1047:C:N4	2.41	0.53
1:A:923:A:H4'	1:A:924:A:O5'	2.08	0.53
1:A:1167:C:H2'	1:A:1167:C:O2	2.08	0.53
1:A:1315:A:H61	1:A:1340:G:H1'	1.73	0.53
1:A:185:U:O2'	18:S:84:ASN:ND2	2.40	0.53
1:A:1091:G:OP2	7:G:52:LYS:HE3	2.08	0.53
4:D:112:LYS:O	4:D:114:LEU:N	2.41	0.53
1:A:30:G:H2'	1:A:31:A:H5''	1.90	0.53
1:A:531:C:H1'	1:A:545:C:H5''	1.91	0.53
1:A:1044:G:H2'	1:A:1045:G:H8	1.72	0.53
1:A:1275:G:N2	1:A:1277:G:H3'	2.23	0.53
3:C:638:VAL:HG13	3:C:674:MET:HG2	1.91	0.52
1:A:819:C:H2'	1:A:820:C:O4'	2.08	0.52
1:A:1074:G:H8	1:A:1200:A:H62	1.55	0.52
18:S:28:MET:SD	18:S:58:ILE:HA	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338:ARG:O	3:C:362:VAL:HA	2.09	0.52
4:D:42:ASP:HB3	4:D:45:LYS:HD2	1.91	0.52
1:A:427:U:C2	1:A:433:A:C2	2.98	0.52
1:A:699:G:H2'	1:A:700:G:C8	2.45	0.52
6:F:58:ARG:HG2	6:F:58:ARG:HH11	1.74	0.52
18:S:68:HIS:O	18:S:69:LYS:C	2.52	0.52
1:A:1049:G:H2'	1:A:1050:A:C8	2.44	0.52
1:A:458:G:C5'	1:A:459:A:H3'	2.36	0.52
1:A:1026:A:H4'	1:A:1227:C:H4'	1.92	0.52
1:A:70:G:H1	1:A:99:A:N6	2.07	0.52
1:A:696:A:N6	1:A:712:G:H1'	2.25	0.52
1:A:75:G:H1'	1:A:94:A:H61	1.75	0.52
1:A:1024:A:H2	1:A:1228:U:H1'	1.74	0.52
1:A:702:G:H2'	1:A:703:A:C8	2.44	0.51
1:A:1004:A:C4	1:A:1225:A:H4'	2.46	0.51
1:A:1013:G:C6	1:A:1014:A:H1'	2.45	0.51
9:I:14:ILE:O	9:I:15:ARG:C	2.52	0.51
9:I:34:ARG:HG3	9:I:51:PHE:CE1	2.45	0.51
17:R:32:LYS:HA	17:R:50:ALA:HB3	1.91	0.51
1:A:224:U:H4'	1:A:473:G:H4'	1.93	0.51
1:A:718:U:H2'	1:A:719:G:C8	2.42	0.51
1:A:1081:C:H2'	1:A:1082:G:H8	1.74	0.51
3:C:136:ALA:O	3:C:137:ILE:C	2.53	0.51
1:A:1060:G:H1	1:A:1217:C:H42	1.59	0.51
1:A:777:A:H3'	1:A:778:G:H8	1.74	0.51
1:A:277:C:H2'	1:A:278:A:C8	2.45	0.51
1:A:474:A:H2'	1:A:475:A:C8	2.45	0.51
1:A:527:C:C5	1:A:539:G:H5'	2.43	0.51
1:A:661:U:H1'	1:A:662:U:H6	1.76	0.51
1:A:1111:A:H5'	4:D:171:ILE:HD13	1.91	0.51
1:A:1204:C:H2'	1:A:1206:A:O4'	2.10	0.51
1:A:531:C:OP2	11:L:79:TYR:OH	2.24	0.51
1:A:670:G:C2'	1:A:671:A:C5'	2.87	0.51
1:A:1151:G:H2'	1:A:1152:G:O4'	2.11	0.51
21:V:48:SER:O	21:V:52:LEU:HD23	2.11	0.51
1:A:475:A:H8	1:A:475:A:H5''	1.76	0.51
1:A:508:A:H4'	1:A:509:G:O5'	2.10	0.51
1:A:643:C:H2'	1:A:644:A:C8	2.46	0.51
1:A:1183:G:C2'	1:A:1184:G:H5'	2.41	0.51
1:A:456:A:H2	1:A:495:U:N3	2.04	0.50
1:A:1018:U:C2'	1:A:1031:A:H61	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:U:H2'	1:A:761:G:O4'	2.12	0.50
1:A:933:A:H2'	1:A:934:C:N3	2.26	0.50
4:D:69:PHE:HB3	4:D:80:VAL:HG22	1.93	0.50
1:A:159:A:H1'	1:A:352:A:C8	2.46	0.50
1:A:411:C:H5''	6:F:129:PRO:HD2	1.93	0.50
1:A:1015:C:H2'	1:A:1016:A:O4'	2.12	0.50
1:A:1030:G:N2	1:A:1031:A:H62	2.09	0.50
1:A:1045:G:H3'	1:A:1046:G:C5'	2.42	0.50
1:A:190:A:O2'	1:A:191:C:O5'	2.30	0.50
1:A:685:A:H61	1:A:723:G:H1	1.60	0.50
1:A:1265:C:H3'	1:A:1287:C:H42	1.77	0.50
1:A:533:G:H2'	1:A:534:C:C6	2.47	0.49
1:A:950:C:H4'	1:A:1383:A:H2	1.77	0.49
1:A:1093:U:H5''	1:A:1096:U:H3	1.76	0.49
1:A:317:G:H1'	1:A:617:A:C2	2.46	0.49
1:A:353:C:H1'	1:A:354:G:C2	2.48	0.49
1:A:964:G:C8	1:A:964:G:H5''	2.47	0.49
1:A:964:G:H5''	1:A:964:G:H8	1.78	0.49
1:A:1365:G:H2'	1:A:1366:A:C8	2.46	0.49
1:A:1048:A:H2'	1:A:1049:G:H8	1.76	0.49
1:A:470:U:H2'	1:A:471:U:C6	2.47	0.49
1:A:719:G:H3'	1:A:720:G:H8	1.77	0.49
4:D:9:LEU:HB3	4:D:43:LEU:HD22	1.93	0.49
1:A:215:G:H1	1:A:224:U:H3	1.61	0.49
1:A:1023:G:N2	1:A:1025:G:H3'	2.27	0.49
1:A:397:A:N3	1:A:397:A:H2'	2.28	0.49
1:A:1039:U:H3'	1:A:1041:C:O2	2.12	0.49
1:A:1210:A:H4'	1:A:1211:U:H5'	1.94	0.49
5:E:69:THR:O	5:E:104:GLU:HA	2.13	0.49
1:A:698:C:H3'	1:A:699:G:C5'	2.43	0.49
1:A:1314:G:N2	1:A:1340:G:O2'	2.46	0.49
1:A:700:G:N2	1:A:704:A:H8	2.11	0.48
1:A:717:G:H2'	1:A:718:U:C6	2.47	0.48
10:J:10:GLY:HA3	10:J:78:ALA:O	2.12	0.48
1:A:528:C:H2'	1:A:529:A:C8	2.47	0.48
1:A:676:G:H4'	14:O:51:HIS:ND1	2.27	0.48
1:A:419:A:H1'	1:A:420:U:H2'	1.95	0.48
1:A:997:G:H1	1:A:1227:C:H42	1.61	0.48
1:A:1385:U:H2'	1:A:1386:A:C8	2.48	0.48
1:A:643:C:H2'	1:A:644:A:H8	1.78	0.48
1:A:113:G:H4'	1:A:114:A:O5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:A:N3	1:A:777:A:H2'	2.29	0.48
1:A:933:A:H2'	1:A:934:C:C2	2.49	0.48
1:A:1337:C:H2'	1:A:1338:G:H8	1.78	0.48
2:B:9007:A:OP2	3:C:562:ARG:NH1	2.44	0.48
3:C:660:MET:HG2	3:C:707:ILE:HD11	1.96	0.48
1:A:1325:G:H4'	13:N:18:VAL:CG1	2.44	0.48
1:A:478:G:O2'	1:A:479:G:H5''	2.14	0.48
3:C:82:GLY:HA2	3:C:161:THR:HG21	1.95	0.48
5:E:50:SER:HB3	5:E:70:ALA:HB3	1.95	0.48
1:A:958:C:C6	12:M:105:ASN:HB3	2.48	0.48
1:A:1145:U:O2'	1:A:1146:C:H3'	2.14	0.47
1:A:144:U:H3	1:A:176:G:H1	1.61	0.47
1:A:436:G:H4'	1:A:437:U:O5'	2.13	0.47
1:A:1012:U:N3	1:A:1046:G:N7	2.53	0.47
1:A:1020:C:N4	1:A:1029:G:H1	2.11	0.47
17:R:11:VAL:HG11	17:R:16:MET:HE2	1.96	0.47
1:A:602:U:H2'	1:A:603:U:C6	2.50	0.47
1:A:720:G:H2'	1:A:721:A:C8	2.47	0.47
1:A:1022:A:N3	1:A:1022:A:H2'	2.29	0.47
1:A:938:G:H2'	1:A:939:G:C5	2.50	0.47
1:A:1389:U:H4'	1:A:1390:U:O5'	2.14	0.47
1:A:722:G:H4'	1:A:723:G:O5'	2.13	0.47
19:T:87:ARG:HH11	19:T:87:ARG:CG	2.27	0.47
1:A:700:G:O5'	1:A:700:G:H8	1.98	0.47
1:A:973:G:N2	1:A:981:G:OP2	2.47	0.47
1:A:1012:U:H4'	1:A:1012:U:OP1	2.14	0.47
1:A:1079:C:H42	1:A:1116:G:H1	1.63	0.47
1:A:1252:A:H2'	1:A:1253:C:O4'	2.14	0.47
1:A:1278:A:H1'	1:A:1335:U:H1'	1.95	0.47
1:A:1278:A:N1	1:A:1322:U:H5'	2.30	0.47
1:A:1294:A:N6	1:A:1296:A:H1'	2.28	0.47
12:M:86:TYR:O	12:M:90:ARG:HG2	2.14	0.47
15:P:40:TYR:CZ	15:P:42:PRO:HB3	2.50	0.47
17:R:18:LYS:HD2	17:R:31:VAL:HG13	1.97	0.47
1:A:51:U:O4	1:A:373:U:H5	1.98	0.47
1:A:951:G:H2'	1:A:952:G:H8	1.80	0.47
1:A:960:U:H2'	1:A:961:G:C8	2.50	0.47
1:A:1072:U:O2'	1:A:1073:C:O5'	2.24	0.47
1:A:305:G:H4'	1:A:566:G:H4'	1.97	0.47
5:E:109:ASP:HA	5:E:115:VAL:CG2	2.45	0.47
1:A:1046:G:H2'	1:A:1047:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:655:VAL:HG22	3:C:705:PHE:HB2	1.97	0.46
1:A:698:C:N4	1:A:707:G:H1	2.12	0.46
3:C:24:VAL:HG13	3:C:42:LEU:HD21	1.98	0.46
3:C:180:VAL:HG12	3:C:201:ILE:HA	1.97	0.46
4:D:199:VAL:HG12	4:D:201:PRO:HD3	1.97	0.46
1:A:992:U:H4'	1:A:993:A:O5'	2.15	0.46
1:A:1024:A:C2	1:A:1228:U:H1'	2.49	0.46
1:A:1211:U:H2'	1:A:1211:U:O2	2.16	0.46
8:H:23:VAL:CG1	8:H:43:LEU:HD21	2.45	0.46
1:A:741:C:H2'	1:A:742:G:H5''	1.97	0.46
1:A:956:A:H2'	1:A:957:G:C8	2.51	0.46
1:A:1018:U:H2'	1:A:1019:C:C6	2.51	0.46
1:A:1126:U:H3	1:A:1193:G:H1	1.62	0.46
3:C:334:PRO:HB2	3:C:335:LYS:HD2	1.97	0.46
1:A:62:A:H4'	1:A:63:G:O5'	2.16	0.46
1:A:109:G:O6	1:A:338:C:H5	1.98	0.46
1:A:1176:A:H2'	1:A:1178:A:C6	2.50	0.46
1:A:336:C:H2'	1:A:336:C:O2	2.15	0.46
1:A:1390:U:H2'	1:A:1391:C:C6	2.51	0.46
1:A:100:G:N3	1:A:150:A:H2	2.14	0.46
1:A:1045:G:H2'	1:A:1046:G:H4'	1.98	0.46
1:A:1049:G:C6	1:A:1050:A:C6	3.03	0.46
1:A:37:G:H2'	1:A:38:C:C6	2.51	0.46
1:A:661:U:H1'	1:A:662:U:C6	2.51	0.46
1:A:413:U:O4	6:F:2:ALA:HA	2.16	0.46
3:C:69:MET:O	3:C:70:ASN:C	2.59	0.46
4:D:112:LYS:O	4:D:115:LYS:N	2.49	0.46
1:A:707:G:H2'	1:A:708:C:C6	2.51	0.46
1:A:995:C:H2'	1:A:996:A:H8	1.81	0.46
1:A:1039:U:O2'	1:A:1042:G:N1	2.48	0.46
4:D:117:ILE:HG22	4:D:141:LEU:HD12	1.98	0.46
1:A:1385:U:H2'	1:A:1386:A:H8	1.81	0.45
1:A:820:C:H5'	1:A:908:G:H4'	1.97	0.45
1:A:1014:A:H5'	1:A:1034:U:C2	2.51	0.45
1:A:1128:A:H1'	1:A:1188:A:C5	2.52	0.45
1:A:345:G:H2'	1:A:346:A:C8	2.52	0.45
1:A:938:G:H5''	1:A:939:G:C8	2.51	0.45
1:A:1037:C:H2'	1:A:1038:C:C6	2.52	0.45
1:A:1071:G:N3	1:A:1071:G:H2'	2.30	0.45
1:A:1271:A:H2'	1:A:1272:A:C8	2.51	0.45
1:A:1380:G:H5''	10:J:70:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:U:H2'	1:A:961:G:H8	1.81	0.45
1:A:938:G:H2'	1:A:939:G:C4	2.52	0.45
1:A:940:C:H2'	1:A:941:C:C5	2.52	0.45
3:C:111:ILE:HB	3:C:134:GLU:HB3	1.98	0.45
17:R:26:ASP:O	17:R:28:LYS:N	2.49	0.45
1:A:428:U:O2'	1:A:431:G:O6	2.34	0.45
1:A:1068:G:H1	1:A:1208:U:H3	1.65	0.45
3:C:495:TYR:CE1	20:U:40:GLU:HG2	2.52	0.45
18:S:32:ILE:HG23	18:S:79:LEU:HD11	1.98	0.45
1:A:962:U:H2'	1:A:963:G:H5''	2.00	0.45
1:A:1077:A:H5''	1:A:1104:G:N7	2.31	0.44
1:A:1286:C:H2'	1:A:1287:C:H5''	1.99	0.44
1:A:384:G:H8	1:A:384:G:H5''	1.82	0.44
3:C:70:ASN:HA	3:C:116:LEU:HG	1.99	0.44
1:A:251:A:C2	1:A:253:U:H2'	2.52	0.44
1:A:347:C:H2'	1:A:348:U:C6	2.52	0.44
1:A:613:G:H2'	1:A:614:U:O4'	2.17	0.44
1:A:1017:A:H3'	1:A:1018:U:C6	2.53	0.44
10:J:19:VAL:HG11	10:J:83:ILE:HA	2.00	0.44
1:A:510:C:H2'	1:A:511:C:C6	2.52	0.44
6:F:181:GLU:O	6:F:182:ARG:HB3	2.18	0.44
7:G:120:VAL:HG11	7:G:123:ILE:HD12	1.98	0.44
19:T:30:LEU:HD13	19:T:65:VAL:HG11	1.98	0.44
18:S:72:ALA:O	18:S:75:TYR:N	2.51	0.44
1:A:996:A:H2'	1:A:997:G:C8	2.52	0.44
1:A:999:U:H2'	1:A:1000:C:C6	2.52	0.44
1:A:1246:C:O2'	1:A:1344:C:H5'	2.18	0.44
1:A:425:G:H1	1:A:434:U:H3	1.65	0.44
1:A:1247:A:N7	1:A:1308:A:N6	2.66	0.44
1:A:1294:A:N6	1:A:1363:C:H4'	2.32	0.44
1:A:564:C:H2'	1:A:565:C:C6	2.53	0.44
1:A:1175:G:H1'	1:A:1179:A:H61	1.83	0.44
1:A:160:A:H2'	1:A:161:A:C8	2.52	0.43
1:A:271:A:H2'	1:A:272:C:C6	2.53	0.43
4:D:100:THR:HA	4:D:107:ILE:HG13	2.00	0.43
7:G:81:ILE:HD13	7:G:123:ILE:HD11	2.00	0.43
15:P:12:ALA:O	15:P:13:LYS:C	2.61	0.43
1:A:672:A:H5'	1:A:845:G:OP1	2.18	0.43
1:A:1289:A:P	22:K:9:ARG:HH12	2.41	0.43
1:A:774:G:N1	1:A:821:G:H2'	2.33	0.43
1:A:946:C:O2'	1:A:1391:C:N3	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1294:A:H1'	1:A:1295:C:OP2	2.18	0.43
1:A:721:A:OP1	1:A:722:G:H2'	2.18	0.43
8:H:73:LEU:HD23	8:H:90:GLU:HA	1.99	0.43
1:A:141:G:O2'	1:A:210:A:N1	2.50	0.43
1:A:147:G:H2'	1:A:148:A:O4'	2.19	0.43
1:A:603:U:H2'	1:A:604:A:O4'	2.17	0.43
1:A:848:G:H1	1:A:857:C:H42	1.66	0.43
3:C:341:LEU:HD21	3:C:572:ILE:HG21	2.00	0.43
21:V:22:ILE:HA	21:V:85:GLU:O	2.18	0.43
1:A:1195:G:H8	1:A:1195:G:H5''	1.83	0.43
4:D:68:LEU:HD11	4:D:92:VAL:HG23	1.99	0.43
18:S:31:ALA:HB1	18:S:54:ALA:HA	2.01	0.43
3:C:623:MET:HE2	3:C:703:ILE:HD13	2.00	0.43
1:A:180:G:H5''	1:A:180:G:H8	1.83	0.43
1:A:422:A:H2'	1:A:423:A:C8	2.53	0.43
1:A:457:A:H8	1:A:457:A:H5''	1.84	0.43
1:A:663:G:N1	1:A:763:C:H5	2.01	0.43
1:A:1130:C:H2'	1:A:1131:U:C6	2.54	0.43
4:D:173:VAL:HG13	4:D:183:ILE:HD13	2.00	0.43
1:A:690:A:C6	1:A:719:G:C6	3.06	0.43
1:A:1003:G:N2	1:A:1005:C:H42	2.15	0.43
1:A:1220:U:H4'	1:A:1222:A:N3	2.34	0.43
1:A:1287:C:H4'	1:A:1288:A:C4	2.54	0.43
4:D:111:ILE:HD11	4:D:151:ILE:HG13	2.00	0.43
7:G:156:LEU:HD22	9:I:73:VAL:HG22	2.00	0.43
1:A:217:C:H5'	1:A:477:A:O2'	2.19	0.43
1:A:930:U:H2'	1:A:931:U:C6	2.53	0.43
1:A:113:G:H1'	1:A:114:A:N7	2.33	0.42
1:A:1332:G:H2'	1:A:1333:A:C8	2.53	0.42
1:A:27:C:H2'	1:A:28:A:C8	2.55	0.42
1:A:1269:G:H1'	1:A:1284:A:H62	1.83	0.42
1:A:1324:U:O2'	1:A:1369:A:N3	2.45	0.42
3:C:411:MET:HE1	3:C:417:ASP:HB2	2.01	0.42
5:E:54:VAL:HG13	5:E:67:ILE:HG22	2.01	0.42
1:A:582:A:H5'	1:A:582:A:H8	1.84	0.42
1:A:1052:U:O5'	1:A:1052:U:H6	2.01	0.42
4:D:163:ILE:HG23	4:D:169:GLU:HG3	2.01	0.42
13:N:34:ILE:O	13:N:38:LYS:N	2.51	0.42
1:A:903:C:H2'	1:A:904:G:C8	2.54	0.42
1:A:990:C:H1'	13:N:19:GLN:HA	2.02	0.42
1:A:1129:U:H3	1:A:1163:G:H1	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:ARG:HG2	4:D:222:LEU:HD11	2.00	0.42
1:A:1028:A:H2'	1:A:1029:G:C8	2.55	0.42
1:A:1232:C:C5	1:A:1233:U:H5	2.37	0.42
1:A:951:G:H1	1:A:1351:C:H42	1.67	0.42
1:A:1316:U:H2'	1:A:1317:C:C6	2.54	0.42
1:A:225:A:H5''	1:A:472:C:O2'	2.20	0.42
1:A:694:G:H2'	1:A:695:U:C5	2.54	0.42
1:A:700:G:C5	1:A:701:U:H1'	2.54	0.42
1:A:719:G:H3'	1:A:720:G:C8	2.55	0.42
8:H:27:ILE:HD13	8:H:40:GLN:HG2	2.01	0.42
1:A:1035:C:H2'	1:A:1036:C:H5''	2.00	0.42
1:A:1134:G:H1'	1:A:1135:U:H5	1.85	0.42
1:A:176:G:H3'	1:A:177:G:H8	1.85	0.42
3:C:657:VAL:HA	3:C:660:MET:HB2	2.02	0.42
1:A:459:A:H4'	1:A:460:A:O5'	2.20	0.41
3:C:98:ILE:HG21	3:C:129:VAL:HG23	2.02	0.41
19:T:87:ARG:HH11	19:T:87:ARG:HB2	1.85	0.41
1:A:855:G:H2'	1:A:856:C:C6	2.55	0.41
1:A:989:C:H1'	1:A:1326:C:N4	2.35	0.41
3:C:102:GLU:HB3	3:C:128:THR:HG23	2.03	0.41
4:D:30:TYR:HA	4:D:45:LYS:HD3	2.02	0.41
1:A:343:C:H2'	1:A:344:A:C8	2.56	0.41
1:A:490:G:HO2'	1:A:492:C:H41	1.64	0.41
1:A:526:G:O2'	1:A:539:G:H4'	2.18	0.41
1:A:1025:G:H2'	1:A:1026:A:H8	1.85	0.41
3:C:43:VAL:HG21	21:V:52:LEU:CD1	2.51	0.41
3:C:378:LEU:HD21	3:C:396:PHE:HB3	2.02	0.41
13:N:27:CYS:SG	13:N:40:CYS:SG	3.10	0.41
1:A:670:G:H2'	1:A:671:A:H5'	2.00	0.41
1:A:775:A:N1	1:A:776:A:N6	2.68	0.41
1:A:1004:A:H61	1:A:1057:G:H1'	1.85	0.41
1:A:1361:C:H2'	1:A:1362:G:C8	2.55	0.41
3:C:165:PHE:HB3	3:C:195:GLU:HG2	2.02	0.41
1:A:654:G:H2'	1:A:655:G:O4'	2.20	0.41
1:A:1286:C:H1'	1:A:1291:C:O2	2.20	0.41
1:A:1385:U:O4	8:H:10:ARG:NH1	2.53	0.41
3:C:85:PHE:HB3	3:C:95:ASP:HB3	2.01	0.41
3:C:251:LEU:HB2	3:C:363:ILE:HG22	2.02	0.41
19:T:87:ARG:HH11	19:T:87:ARG:HG3	1.84	0.41
20:U:68:ARG:HB3	20:U:75:TYR:CE1	2.55	0.41
1:A:138:U:H2'	1:A:139:A:H5''	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:A:H2'	1:A:523:C:C6	2.56	0.41
1:A:556:A:H4'	1:A:557:G:O5'	2.21	0.41
1:A:1075:U:O2'	1:A:1076:C:OP2	2.34	0.41
1:A:1213:A:H2'	1:A:1214:U:O4'	2.20	0.41
1:A:1231:G:H5''	17:R:78:ARG:HH11	1.86	0.41
1:A:1234:A:H4'	17:R:78:ARG:HE	1.86	0.41
1:A:1254:A:N3	1:A:1254:A:H2'	2.34	0.41
1:A:766:U:H2'	1:A:767:G:O4'	2.21	0.41
1:A:775:A:OP2	1:A:821:G:N2	2.53	0.41
4:D:114:LEU:HD13	4:D:144:LEU:CB	2.49	0.41
1:A:290:A:H2'	1:A:290:A:N3	2.36	0.41
1:A:391:A:C5	1:A:392:G:H1'	2.56	0.41
1:A:660:C:H2'	1:A:661:U:C6	2.56	0.41
1:A:670:G:H2'	1:A:671:A:C5'	2.50	0.41
1:A:674:A:H2'	1:A:734:G:N2	2.36	0.41
1:A:760:U:H1'	14:O:23:GLY:O	2.20	0.41
1:A:849:G:H1	1:A:856:C:H42	1.69	0.41
1:A:939:G:H1'	1:A:940:C:H1'	2.03	0.41
1:A:1014:A:H3'	1:A:1034:U:C2	2.55	0.41
1:A:121:C:OP1	1:A:319:C:O2'	2.38	0.41
1:A:584:G:N2	1:A:585:G:N7	2.65	0.41
1:A:688:C:H2'	1:A:689:C:O4'	2.21	0.41
1:A:1014:A:H3'	1:A:1034:U:O2	2.20	0.41
1:A:1201:C:H3'	1:A:1202:G:H5''	2.02	0.41
1:A:1297:A:H2'	1:A:1298:A:O4'	2.21	0.41
3:C:80:ALA:HA	3:C:159:LYS:HA	2.03	0.41
1:A:53:A:H4'	1:A:54:U:C5'	2.51	0.40
1:A:226:C:H2'	1:A:227:C:C6	2.56	0.40
1:A:651:A:H2'	1:A:652:C:C6	2.57	0.40
1:A:745:U:H2'	1:A:746:C:C6	2.56	0.40
1:A:1153:G:H1'	1:A:1154:C:H2'	2.02	0.40
5:E:119:ILE:O	5:E:123:LEU:HG	2.21	0.40
1:A:827:G:C6	1:A:829:U:H5''	2.57	0.40
1:A:1051:G:H2'	1:A:1052:U:O4'	2.21	0.40
1:A:1175:G:C6	1:A:1177:C:H5'	2.57	0.40
1:A:1063:G:N7	1:A:1208:U:H3'	2.36	0.40
10:J:19:VAL:HG22	10:J:65:VAL:HG22	2.02	0.40
1:A:61:A:H5''	1:A:395:U:H5''	2.03	0.40
1:A:107:A:C6	1:A:334:G:C6	3.09	0.40
1:A:1266:A:H4'	1:A:1267:G:O5'	2.22	0.40
20:U:76:VAL:O	20:U:77:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:G:H4'	1:A:895:G:C8	2.56	0.40
1:A:220:C:H1'	1:A:221:G:C2	2.57	0.40
1:A:964:G:H3'	1:A:965:U:C6	2.57	0.40
1:A:1025:G:C6	1:A:1026:A:C6	3.10	0.40
3:C:92:SER:HA	3:C:481:GLU:OE2	2.22	0.40
3:C:174:ALA:HB2	3:C:180:VAL:HG11	2.04	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	
3	C	706/779 (91%)	657 (93%)	43 (6%)	6 (1%)	16	47
4	D	216/246 (88%)	189 (88%)	23 (11%)	4 (2%)	6	27
5	E	203/218 (93%)	168 (83%)	34 (17%)	1 (0%)	24	57
6	F	179/200 (90%)	170 (95%)	5 (3%)	4 (2%)	5	24
7	G	156/166 (94%)	148 (95%)	6 (4%)	2 (1%)	9	35
8	H	147/156 (94%)	139 (95%)	6 (4%)	2 (1%)	9	34
9	I	129/132 (98%)	122 (95%)	6 (5%)	1 (1%)	16	47
10	J	106/130 (82%)	101 (95%)	5 (5%)	0	100	100
11	L	134/138 (97%)	127 (95%)	7 (5%)	0	100	100
12	M	106/121 (88%)	102 (96%)	4 (4%)	0	100	100
13	N	47/61 (77%)	43 (92%)	3 (6%)	1 (2%)	5	25
14	O	83/89 (93%)	81 (98%)	2 (2%)	0	100	100
15	P	86/90 (96%)	83 (96%)	2 (2%)	1 (1%)	10	37
16	Q	82/87 (94%)	78 (95%)	3 (4%)	1 (1%)	10	37
17	R	76/92 (83%)	72 (95%)	2 (3%)	2 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	S	81/88 (92%)	76 (94%)	5 (6%)	0	100	100
19	T	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
20	U	62/79 (78%)	61 (98%)	1 (2%)	0	100	100
21	V	99/131 (76%)	95 (96%)	4 (4%)	0	100	100
22	K	93/102 (91%)	87 (94%)	6 (6%)	0	100	100
All	All	2884/3200 (90%)	2687 (93%)	172 (6%)	25 (1%)	16	44

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	137	ILE
6	F	24	LYS
6	F	181	GLU
16	Q	3	GLU
17	R	27	LYS
3	C	672	PHE
4	D	113	ARG
4	D	130	PRO
6	F	182	ARG
7	G	90	GLY
8	H	83	ALA
15	P	13	LYS
3	C	365	THR
9	I	56	LYS
3	C	70	ASN
3	C	174	ALA
5	E	60	ALA
13	N	54	PRO
3	C	176	GLU
4	D	112	LYS
7	G	6	PRO
17	R	28	LYS
8	H	81	GLY
6	F	180	PRO
4	D	98	GLY

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	
3	C	628/692 (91%)	601 (96%)	27 (4%)	26	57
4	D	189/212 (89%)	175 (93%)	14 (7%)	13	40
5	E	168/178 (94%)	156 (93%)	12 (7%)	13	41
6	F	159/173 (92%)	154 (97%)	5 (3%)	35	64
7	G	123/130 (95%)	116 (94%)	7 (6%)	18	49
8	H	125/132 (95%)	118 (94%)	7 (6%)	19	49
9	I	111/112 (99%)	108 (97%)	3 (3%)	39	67
10	J	85/102 (83%)	79 (93%)	6 (7%)	13	41
11	L	114/116 (98%)	110 (96%)	4 (4%)	32	62
12	M	94/104 (90%)	91 (97%)	3 (3%)	34	64
13	N	44/54 (82%)	40 (91%)	4 (9%)	9	32
14	O	80/83 (96%)	78 (98%)	2 (2%)	42	69
15	P	74/76 (97%)	70 (95%)	4 (5%)	20	50
16	Q	77/80 (96%)	75 (97%)	2 (3%)	40	68
17	R	70/81 (86%)	65 (93%)	5 (7%)	13	41
18	S	66/70 (94%)	64 (97%)	2 (3%)	36	65
19	T	84/84 (100%)	80 (95%)	4 (5%)	23	54
20	U	56/64 (88%)	52 (93%)	4 (7%)	13	41
21	V	74/100 (74%)	71 (96%)	3 (4%)	27	59
22	K	86/92 (94%)	79 (92%)	7 (8%)	11	36
All	All	2507/2735 (92%)	2382 (95%)	125 (5%)	23	53

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	11	LEU
3	C	41	GLU
3	C	69	MET
3	C	70	ASN
3	C	72	ILE
3	C	96	VAL
3	C	98	ILE

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Mol	Chain	Res	Type
3	C	101	ASN
3	C	103	LEU
3	C	133	LEU
3	C	140	VAL
3	C	195	GLU
3	C	197	GLU
3	C	210	ILE
3	C	266	ASP
3	C	362	VAL
3	C	434	LYS
3	C	521	GLU
3	C	524	VAL
3	C	530	LEU
3	C	634	MET
3	C	643	MET
3	C	656	HIS
3	C	674	MET
3	C	685	ILE
3	C	687	ASP
3	C	710	MET
4	D	10	LEU
4	D	11	GLU
4	D	18	HIS
4	D	60	LEU
4	D	80	VAL
4	D	83	GLU
4	D	111	ILE
4	D	125	THR
4	D	129	LEU
4	D	130	PRO
4	D	132	LYS
4	D	178	LYS
4	D	199	VAL
4	D	204	ASP
5	E	10	LEU
5	E	12	ILE
5	E	30	ASP
5	E	35	ASP
5	E	48	ASP
5	E	75	VAL
5	E	100	ILE
5	E	148	VAL

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Mol	Chain	Res	Type
5	E	163	ARG
5	E	181	ILE
5	E	194	LYS
5	E	195	LEU
6	F	63	VAL
6	F	66	ARG
6	F	71	LEU
6	F	132	LEU
6	F	178	ARG
7	G	8	LYS
7	G	10	GLU
7	G	13	GLU
7	G	39	VAL
7	G	58	GLU
7	G	110	PRO
7	G	125	SER
8	H	4	LYS
8	H	9	LYS
8	H	13	LEU
8	H	30	MET
8	H	43	LEU
8	H	59	MET
8	H	75	VAL
9	I	54	ASP
9	I	68	GLN
9	I	77	LEU
10	J	12	ARG
10	J	22	VAL
10	J	67	VAL
10	J	100	ARG
10	J	106	ARG
10	J	112	GLU
11	L	3	THR
11	L	10	LYS
11	L	58	PRO
11	L	99	ARG
12	M	97	VAL
12	M	100	GLN
12	M	105	ASN
13	N	27	CYS
13	N	30	PRO
13	N	53	ILE

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Mol	Chain	Res	Type
13	N	54	PRO
14	O	47	LYS
14	O	48	LYS
15	P	10	MET
15	P	25	SER
15	P	62	THR
15	P	80	MET
16	Q	7	ARG
16	Q	50	ASP
17	R	24	GLU
17	R	53	ASP
17	R	56	LYS
17	R	58	VAL
17	R	81	LYS
18	S	15	ASN
18	S	56	LYS
19	T	2	ARG
19	T	72	VAL
19	T	87	ARG
19	T	94	GLU
20	U	40	GLU
20	U	48	ARG
20	U	49	VAL
20	U	77	SER
21	V	100	ARG
21	V	112	ILE
21	V	115	VAL
22	K	28	THR
22	K	55	VAL
22	K	57	LYS
22	K	60	ASP
22	K	80	THR
22	K	91	ASP
22	K	98	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	350	GLN
3	C	535	GLN
3	C	541	GLN
4	D	75	GLN

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Mol	Chain	Res	Type
4	D	123	ASN
5	E	136	GLN
6	F	115	ASN
7	G	70	ASN
7	G	131	ASN
8	H	129	ASN
9	I	18	ASN
9	I	57	GLN
10	J	5	GLN
11	L	5	ASN
11	L	29	ASN
12	M	91	HIS
14	O	10	GLN
14	O	46	HIS
14	O	83	ASN
16	Q	54	GLN
18	S	42	ASN
19	T	64	ASN
21	V	17	ASN
21	V	30	ASN
21	V	42	ASN
22	K	56	HIS
22	K	82	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1329/1554 (85%)	342 (25%)	79 (5%)
2	B	6/9 (66%)	2 (33%)	0
All	All	1335/1563 (85%)	344 (25%)	79 (5%)

All (344) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	10	A
1	A	11	G
1	A	15	U
1	A	31	A
1	A	33	G
1	A	34	A

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Mol	Chain	Res	Type
1	A	41	G
1	A	49	C
1	A	50	C
1	A	53	A
1	A	56	C
1	A	70	G
1	A	114	A
1	A	119	C
1	A	128	A
1	A	129	A
1	A	139	A
1	A	140	A
1	A	141	G
1	A	150	A
1	A	151	A
1	A	152	C
1	A	153	U
1	A	159	A
1	A	162	C
1	A	171	A
1	A	172	U
1	A	177	G
1	A	181	G
1	A	185	U
1	A	189	A
1	A	190	A
1	A	191	C
1	A	194	C
1	A	195	A
1	A	197	G
1	A	209	A
1	A	210	A
1	A	211	A
1	A	212	G
1	A	219	U
1	A	220	C
1	A	221	G
1	A	222	G
1	A	248	C
1	A	251	A
1	A	252	U
1	A	253	U

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Mol	Chain	Res	Type
1	A	255	G
1	A	259	G
1	A	274	G
1	A	275	C
1	A	283	G
1	A	288	C
1	A	289	G
1	A	297	G
1	A	313	G
1	A	314	A
1	A	323	A
1	A	324	C
1	A	329	A
1	A	336	C
1	A	337	A
1	A	338	C
1	A	340	G
1	A	352	A
1	A	353	C
1	A	354	G
1	A	355	G
1	A	360	C
1	A	362	G
1	A	373	U
1	A	375	U
1	A	380	C
1	A	384	G
1	A	406	C
1	A	414	G
1	A	419	A
1	A	420	U
1	A	421	G
1	A	429	U
1	A	430	C
1	A	431	G
1	A	432	G
1	A	437	U
1	A	444	C
1	A	447	U
1	A	448	U
1	A	456	A
1	A	459	A

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Mol	Chain	Res	Type
1	A	460	A
1	A	461	C
1	A	466	G
1	A	474	A
1	A	476	U
1	A	477	A
1	A	479	G
1	A	488	U
1	A	489	U
1	A	490	G
1	A	491	A
1	A	493	G
1	A	494	G
1	A	495	U
1	A	506	A
1	A	509	G
1	A	519	A
1	A	520	C
1	A	527	C
1	A	530	G
1	A	536	G
1	A	539	G
1	A	540	U
1	A	541	A
1	A	542	A
1	A	545	C
1	A	556	A
1	A	568	A
1	A	569	A
1	A	571	U
1	A	575	G
1	A	577	G
1	A	581	A
1	A	582	A
1	A	585	G
1	A	591	C
1	A	597	G
1	A	604	A
1	A	605	A
1	A	642	U
1	A	643	C
1	A	647	G

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Mol	Chain	Res	Type
1	A	650	A
1	A	651	A
1	A	655	G
1	A	656	G
1	A	662	U
1	A	663	G
1	A	674	A
1	A	675	G
1	A	678	G
1	A	682	G
1	A	683	G
1	A	684	A
1	A	685	A
1	A	687	U
1	A	688	C
1	A	693	U
1	A	694	G
1	A	695	U
1	A	696	A
1	A	697	G
1	A	699	G
1	A	701	U
1	A	702	G
1	A	703	A
1	A	704	A
1	A	706	U
1	A	707	G
1	A	708	C
1	A	709	G
1	A	710	U
1	A	711	A
1	A	712	G
1	A	713	A
1	A	717	G
1	A	721	A
1	A	722	G
1	A	730	A
1	A	731	G
1	A	732	U
1	A	733	G
1	A	740	G
1	A	758	A

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Mol	Chain	Res	Type
1	A	764	G
1	A	768	A
1	A	775	A
1	A	777	A
1	A	778	G
1	A	780	G
1	A	822	U
1	A	824	A
1	A	825	A
1	A	826	C
1	A	827	G
1	A	828	A
1	A	829	U
1	A	830	G
1	A	837	A
1	A	838	A
1	A	850	U
1	A	853	C
1	A	884	G
1	A	894	U
1	A	895	G
1	A	933	A
1	A	934	C
1	A	935	G
1	A	936	G
1	A	937	G
1	A	938	G
1	A	941	C
1	A	942	C
1	A	943	G
1	A	944	C
1	A	945	A
1	A	963	G
1	A	964	G
1	A	965	U
1	A	966	U
1	A	968	A
1	A	970	U
1	A	971	U
1	A	975	A
1	A	980	C
1	A	981	G

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Mol	Chain	Res	Type
1	A	982	C
1	A	983	G
1	A	985	A
1	A	986	G
1	A	987	A
1	A	996	A
1	A	998	G
1	A	1002	U
1	A	1003	G
1	A	1007	U
1	A	1008	C
1	A	1010	U
1	A	1012	U
1	A	1013	G
1	A	1014	A
1	A	1017	A
1	A	1019	C
1	A	1023	G
1	A	1024	A
1	A	1028	A
1	A	1033	G
1	A	1036	C
1	A	1040	U
1	A	1041	C
1	A	1042	G
1	A	1046	G
1	A	1053	G
1	A	1054	A
1	A	1060	G
1	A	1064	C
1	A	1065	A
1	A	1066	U
1	A	1071	G
1	A	1073	C
1	A	1074	G
1	A	1075	U
1	A	1076	C
1	A	1077	A
1	A	1078	G
1	A	1096	U
1	A	1099	G
1	A	1108	C

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Mol	Chain	Res	Type
1	A	1109	G
1	A	1111	A
1	A	1112	A
1	A	1134	G
1	A	1136	U
1	A	1143	A
1	A	1144	U
1	A	1145	U
1	A	1148	G
1	A	1149	U
1	A	1153	G
1	A	1154	C
1	A	1166	A
1	A	1167	C
1	A	1168	U
1	A	1169	G
1	A	1173	G
1	A	1174	U
1	A	1176	A
1	A	1177	C
1	A	1183	G
1	A	1184	G
1	A	1190	G
1	A	1191	G
1	A	1192	U
1	A	1193	G
1	A	1195	G
1	A	1199	G
1	A	1201	C
1	A	1202	G
1	A	1205	A
1	A	1209	C
1	A	1210	A
1	A	1211	U
1	A	1215	G
1	A	1217	C
1	A	1221	U
1	A	1222	A
1	A	1224	G
1	A	1235	C
1	A	1236	A
1	A	1246	C

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Mol	Chain	Res	Type
1	A	1247	A
1	A	1249	U
1	A	1250	G
1	A	1254	A
1	A	1257	A
1	A	1259	A
1	A	1265	C
1	A	1266	A
1	A	1267	G
1	A	1269	G
1	A	1282	U
1	A	1287	C
1	A	1288	A
1	A	1289	A
1	A	1290	U
1	A	1291	C
1	A	1294	A
1	A	1295	C
1	A	1296	A
1	A	1307	C
1	A	1308	A
1	A	1309	G
1	A	1311	U
1	A	1314	G
1	A	1321	G
1	A	1328	A
1	A	1329	C
1	A	1341	A
1	A	1344	C
1	A	1345	U
1	A	1354	U
1	A	1355	A
1	A	1369	A
1	A	1372	A
1	A	1373	U
1	A	1374	G
1	A	1379	G
1	A	1391	C
1	A	1395	G
1	A	1396	G
1	A	1397	C
2	B	9003	A

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Mol	Chain	Res	Type
2	B	9005	A

All (79) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	15	U
1	A	31	A
1	A	51	U
1	A	113	G
1	A	128	A
1	A	171	A
1	A	189	A
1	A	190	A
1	A	194	C
1	A	209	A
1	A	211	A
1	A	259	G
1	A	313	G
1	A	323	A
1	A	335	A
1	A	336	C
1	A	372	A
1	A	419	A
1	A	420	U
1	A	429	U
1	A	436	G
1	A	459	A
1	A	487	C
1	A	490	G
1	A	540	U
1	A	544	A
1	A	568	A
1	A	584	G
1	A	596	G
1	A	604	A
1	A	641	G
1	A	642	U
1	A	650	A
1	A	655	G
1	A	662	U
1	A	681	U

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Mol	Chain	Res	Type
1	A	687	U
1	A	696	A
1	A	702	G
1	A	707	G
1	A	708	C
1	A	709	G
1	A	710	U
1	A	712	G
1	A	731	G
1	A	824	A
1	A	894	U
1	A	940	C
1	A	941	C
1	A	942	C
1	A	963	G
1	A	965	U
1	A	980	C
1	A	981	G
1	A	1016	A
1	A	1032	C
1	A	1036	C
1	A	1041	C
1	A	1075	U
1	A	1077	A
1	A	1111	A
1	A	1168	U
1	A	1173	G
1	A	1176	A
1	A	1210	A
1	A	1233	U
1	A	1234	A
1	A	1265	C
1	A	1266	A
1	A	1287	C
1	A	1290	U
1	A	1294	A
1	A	1307	C
1	A	1308	A
1	A	1328	A
1	A	1344	C
1	A	1372	A
1	A	1373	U

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.

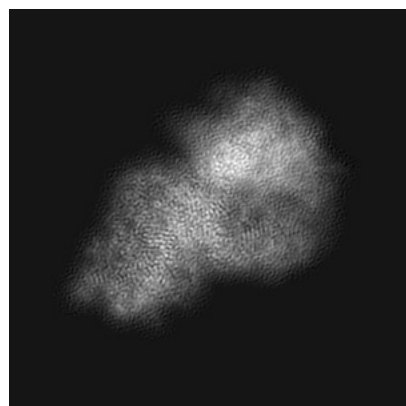
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16595. These allow visual inspection of the internal detail of the map and identification of artifacts.

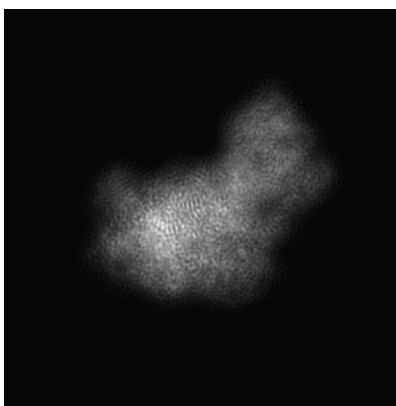
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

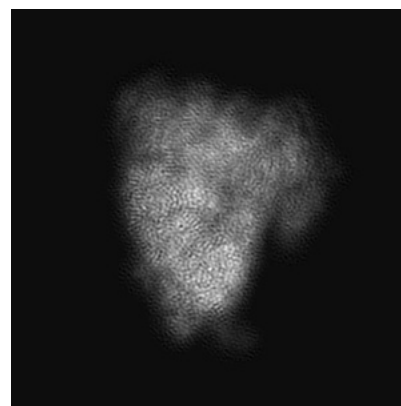
6.1.1 Primary map



X

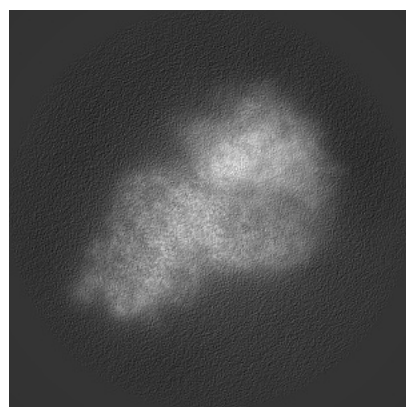


Y

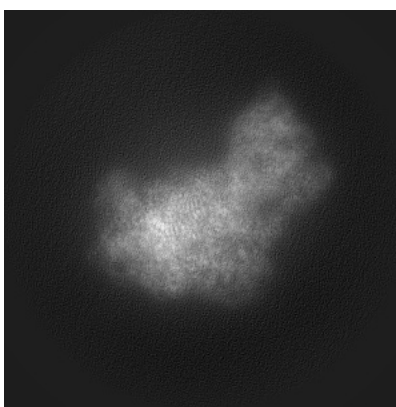


Z

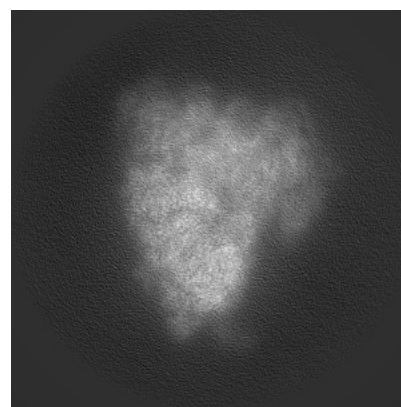
6.1.2 Raw map



X



Y

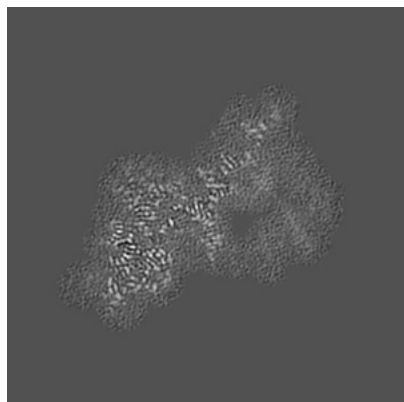


Z

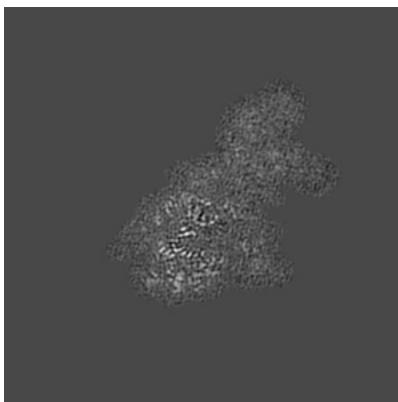
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

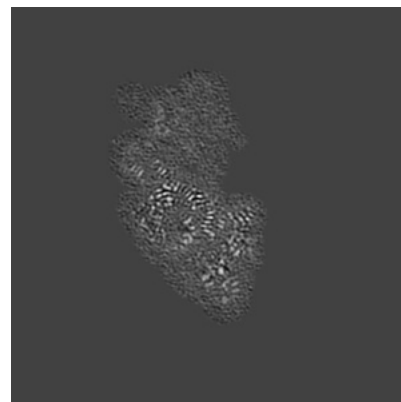
6.2.1 Primary map



X Index: 192

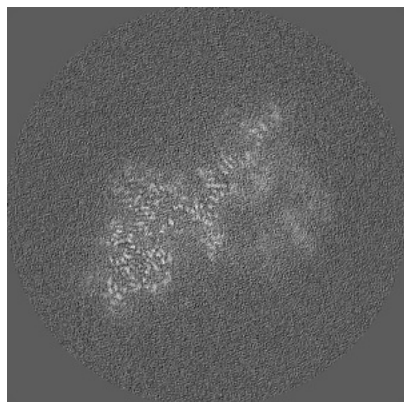


Y Index: 192

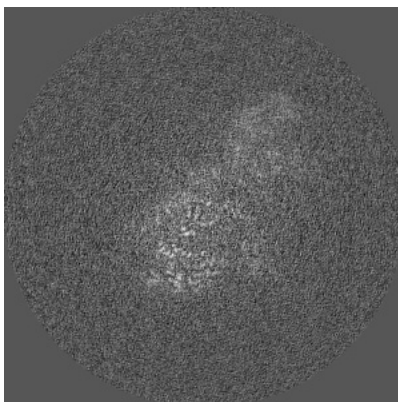


Z Index: 192

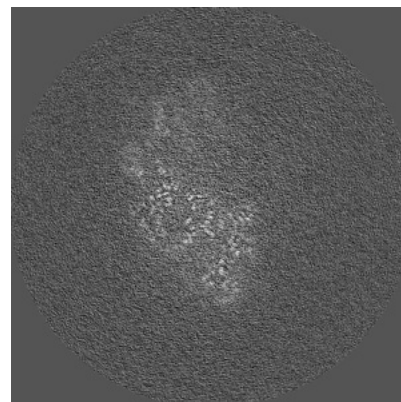
6.2.2 Raw map



X Index: 192



Y Index: 192

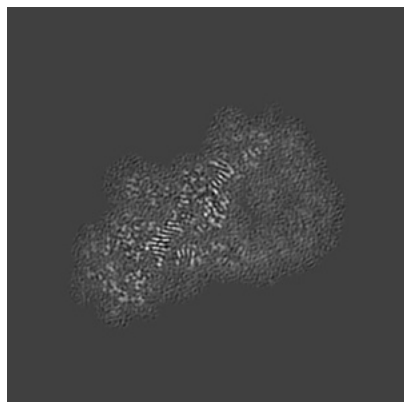


Z Index: 192

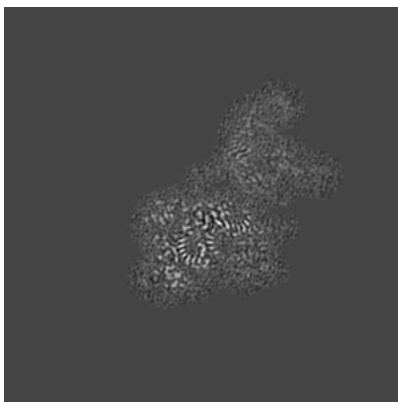
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

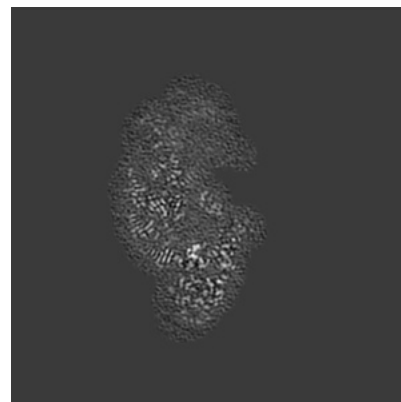
6.3.1 Primary map



X Index: 176

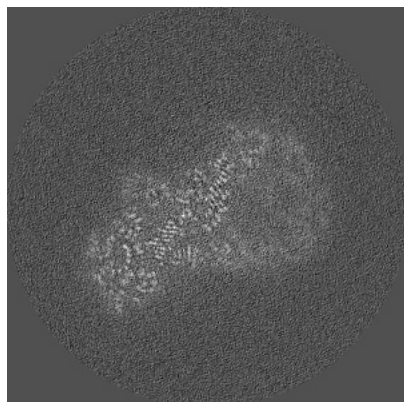


Y Index: 200

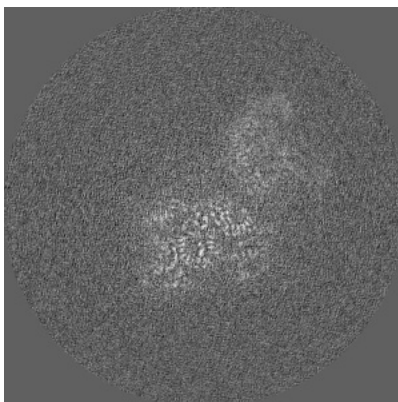


Z Index: 160

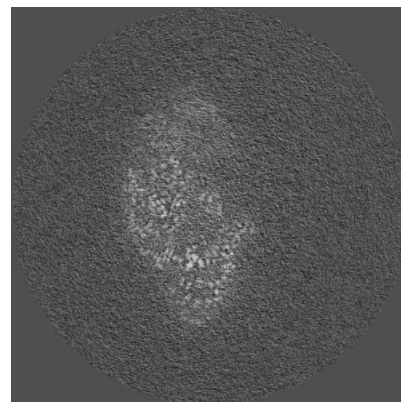
6.3.2 Raw map



X Index: 178



Y Index: 201

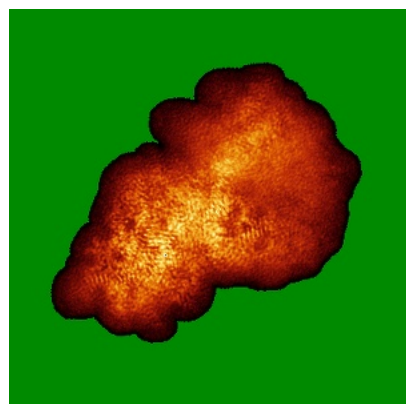


Z Index: 161

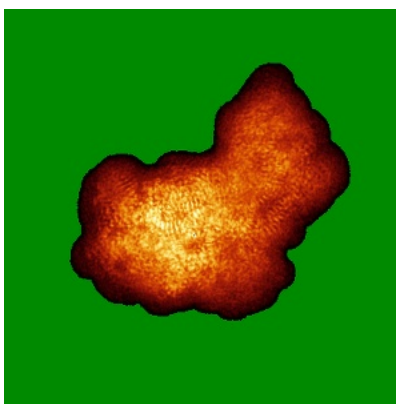
The images above show the largest variance slices of the map in three orthogonal directions.

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

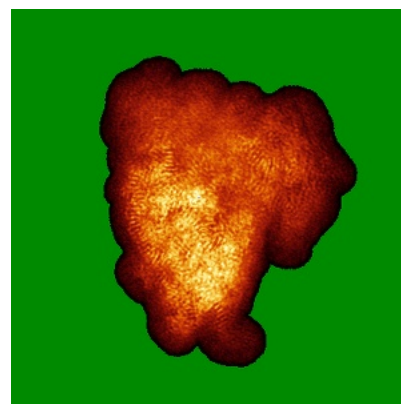
6.4.1 Primary map



X

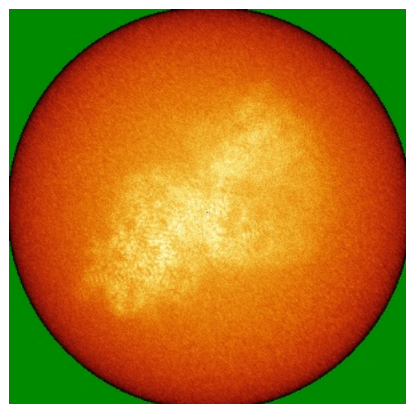


Y

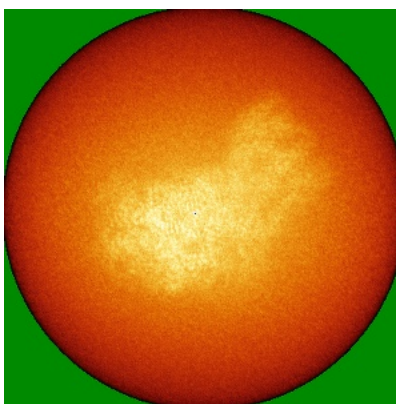


Z

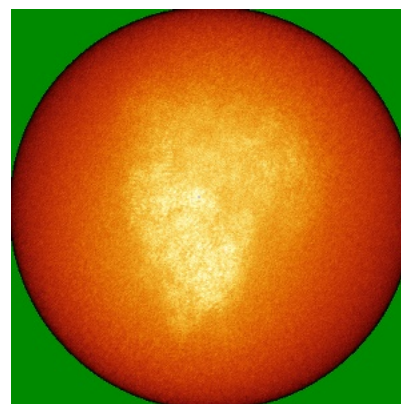
6.4.2 Raw map



X



Y

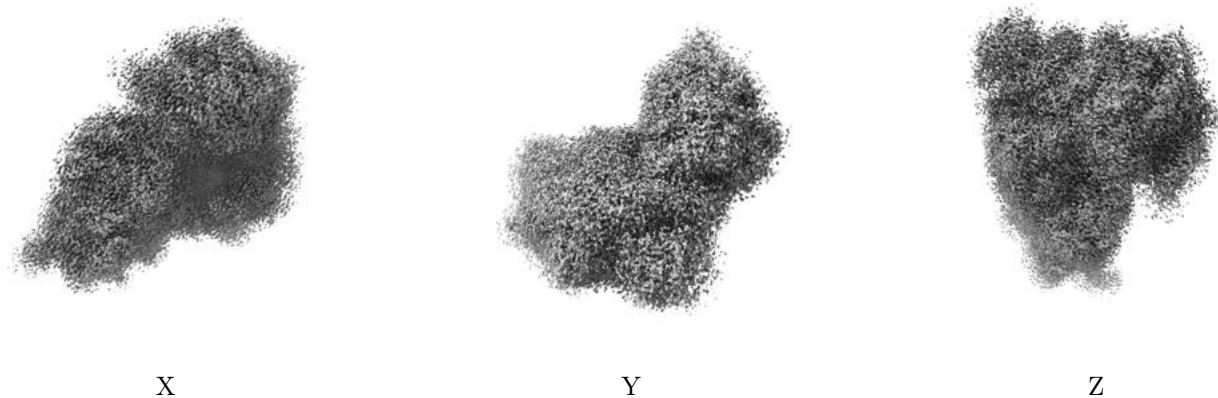


Z

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

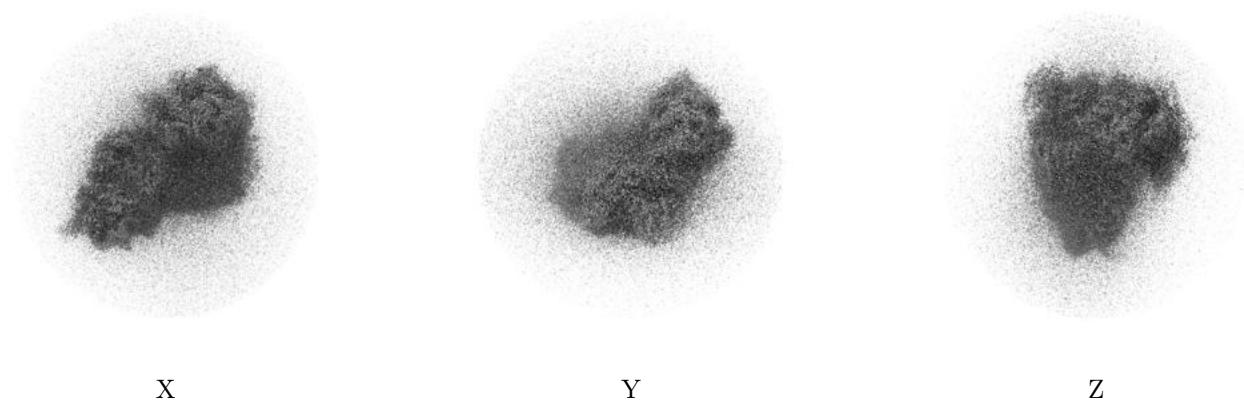
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0178. 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.

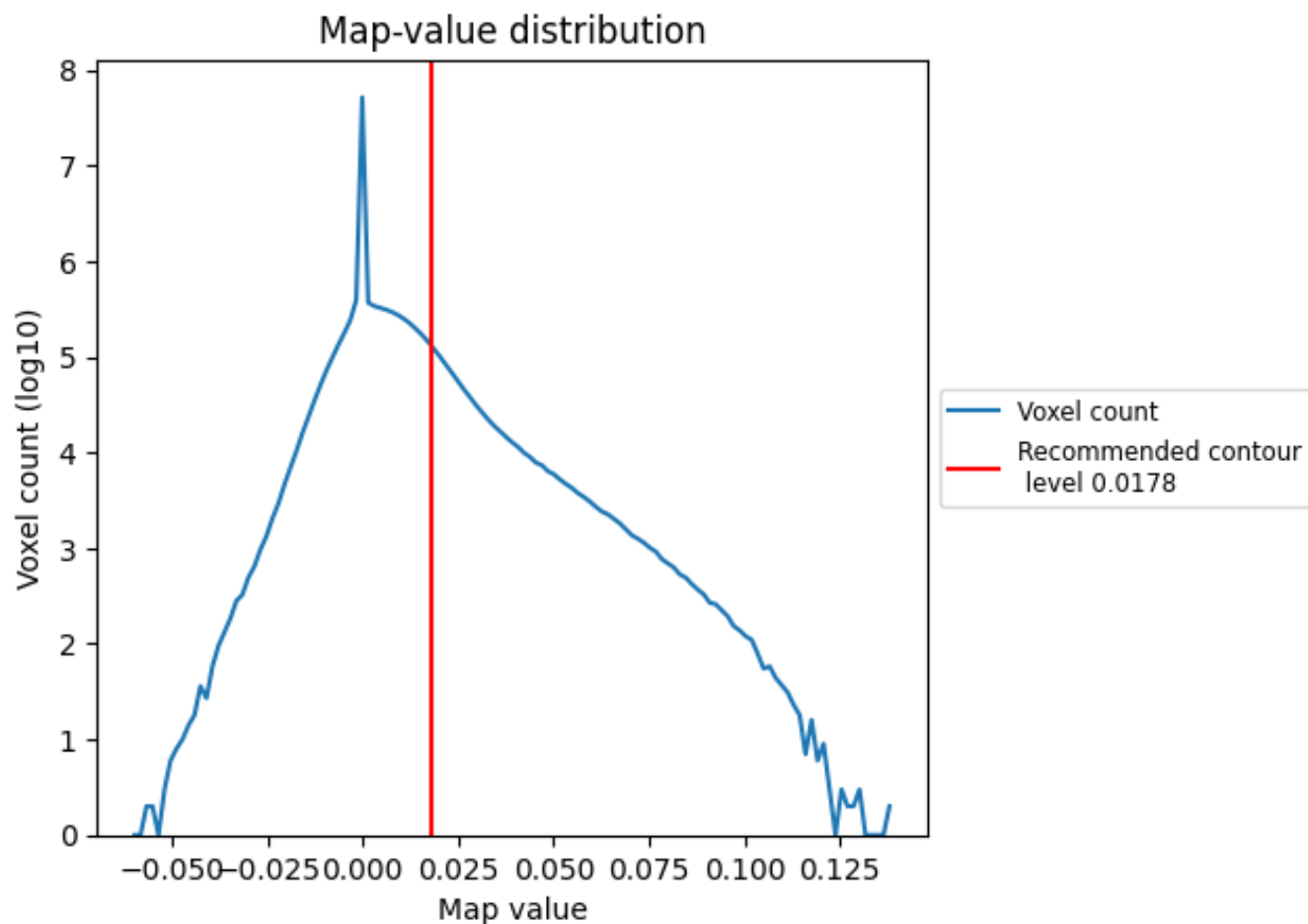
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

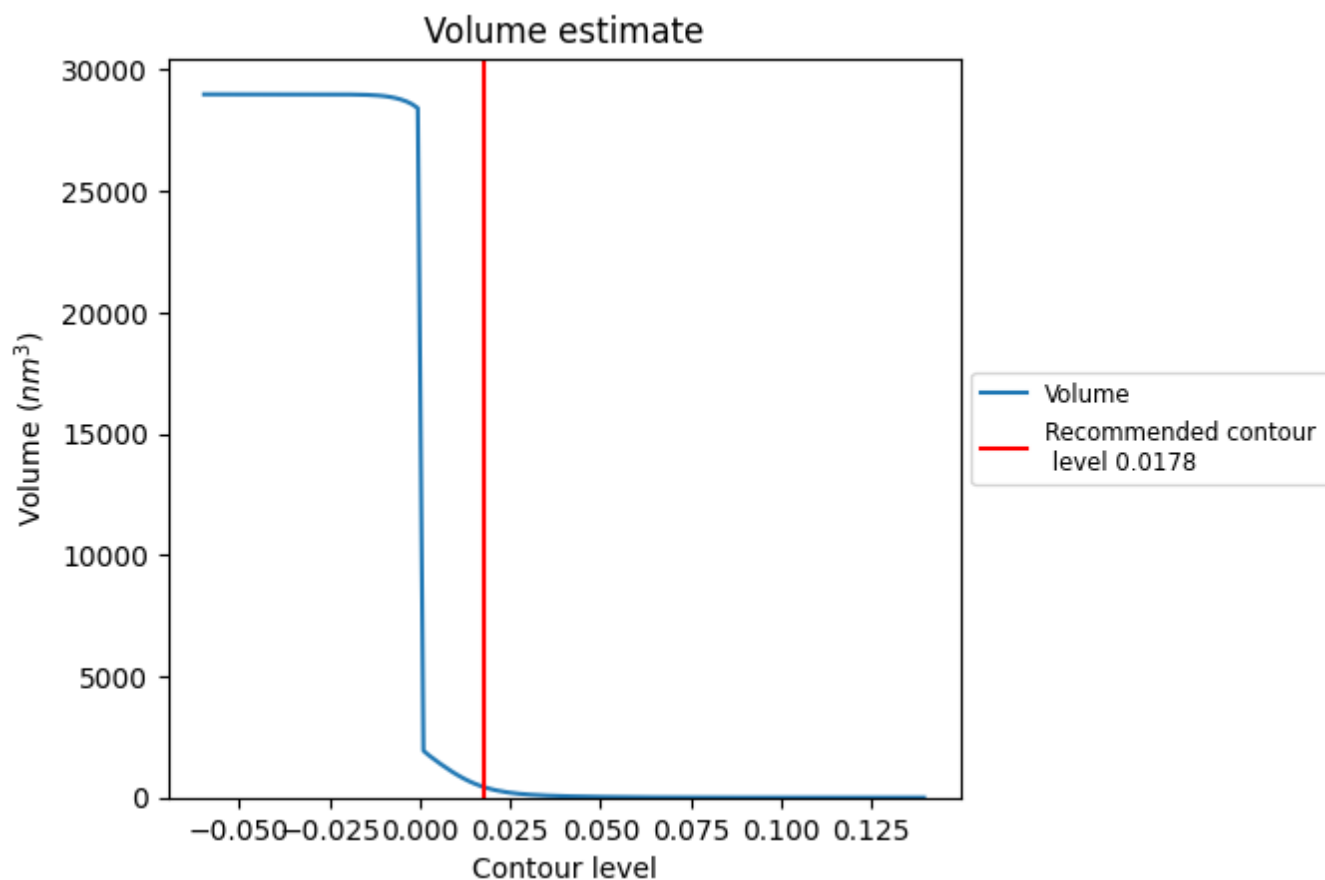
This section contains the results of statistical analysis of the map.

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.

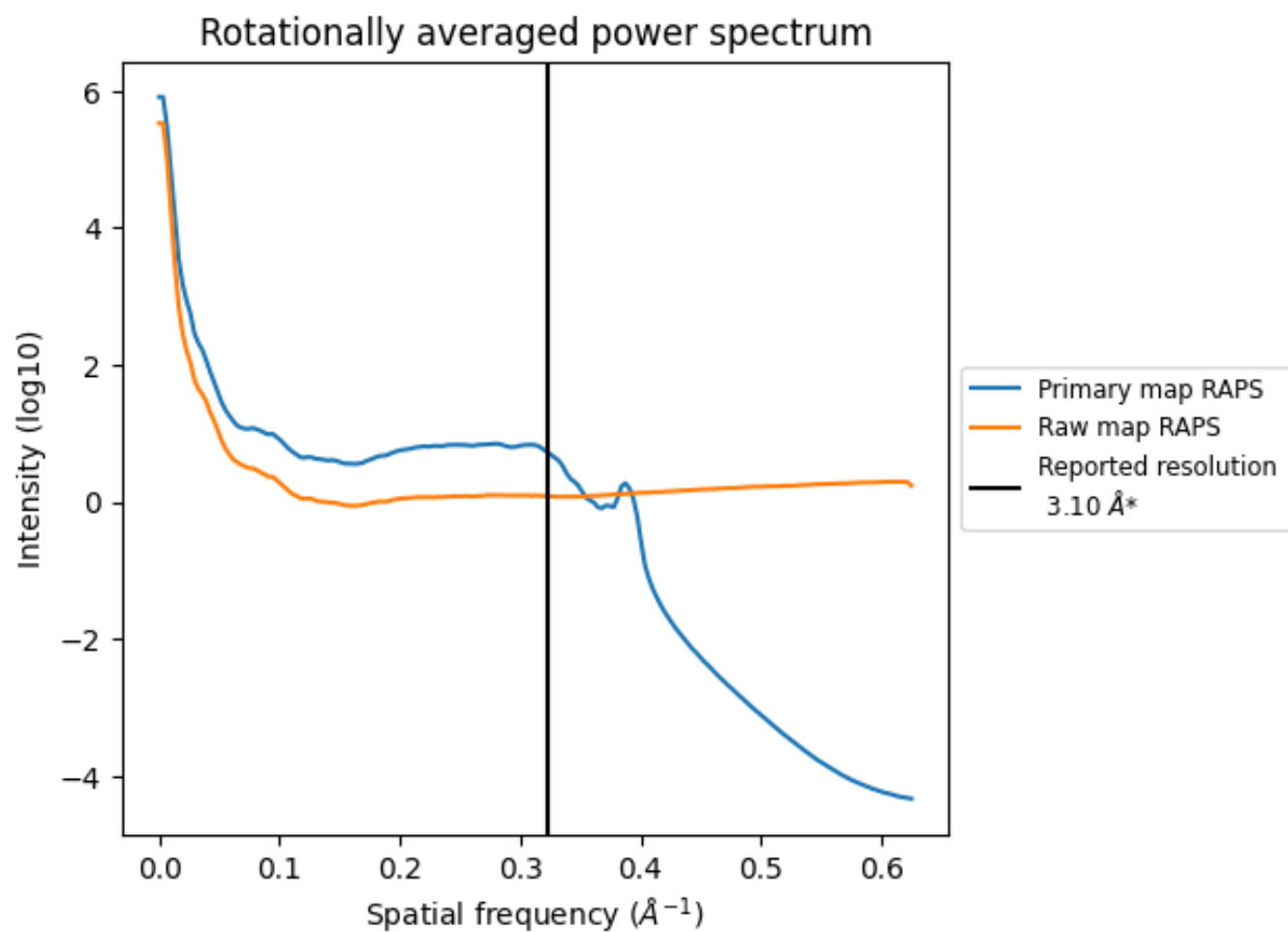
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 430 nm³; this corresponds to an approximate mass of 388 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 ⓘ

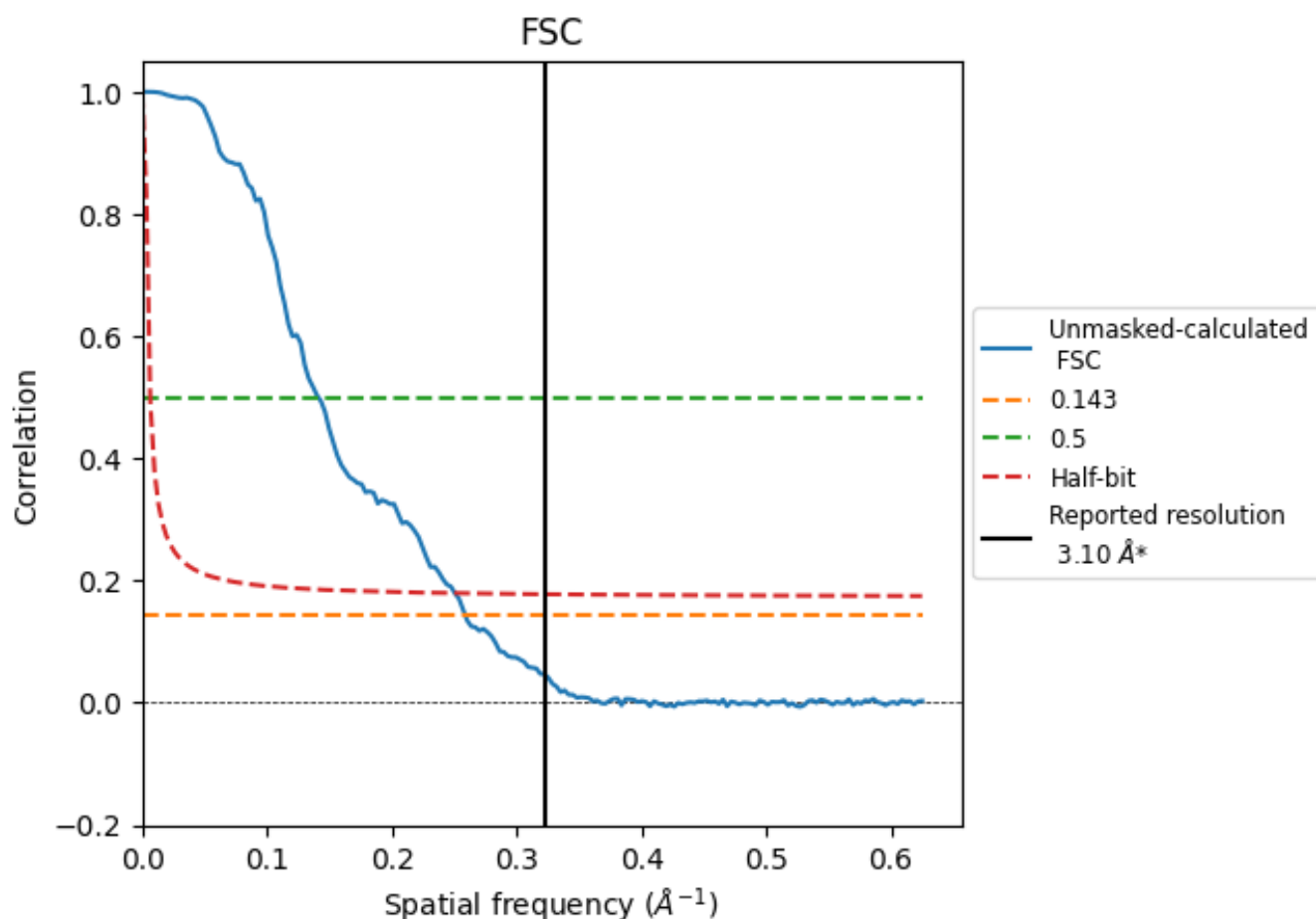


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

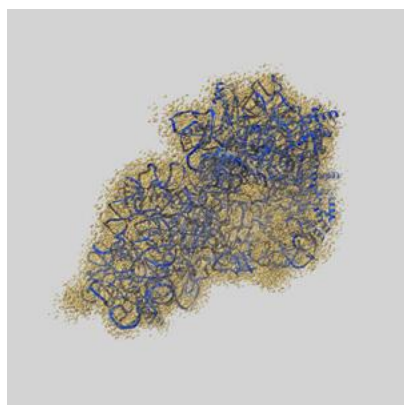
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	7.09	3.99

*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 3.86 differs from the reported value 3.1 by more than 10 %

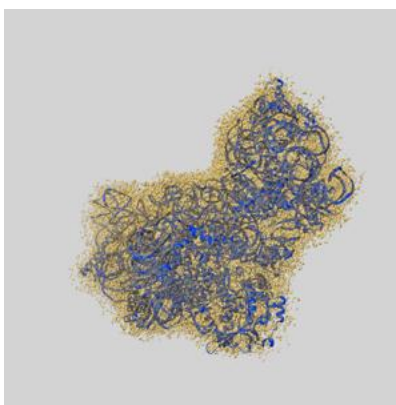
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16595 and PDB model 8CDU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

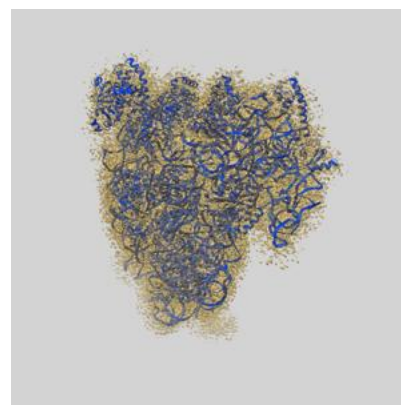
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0178 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](#)



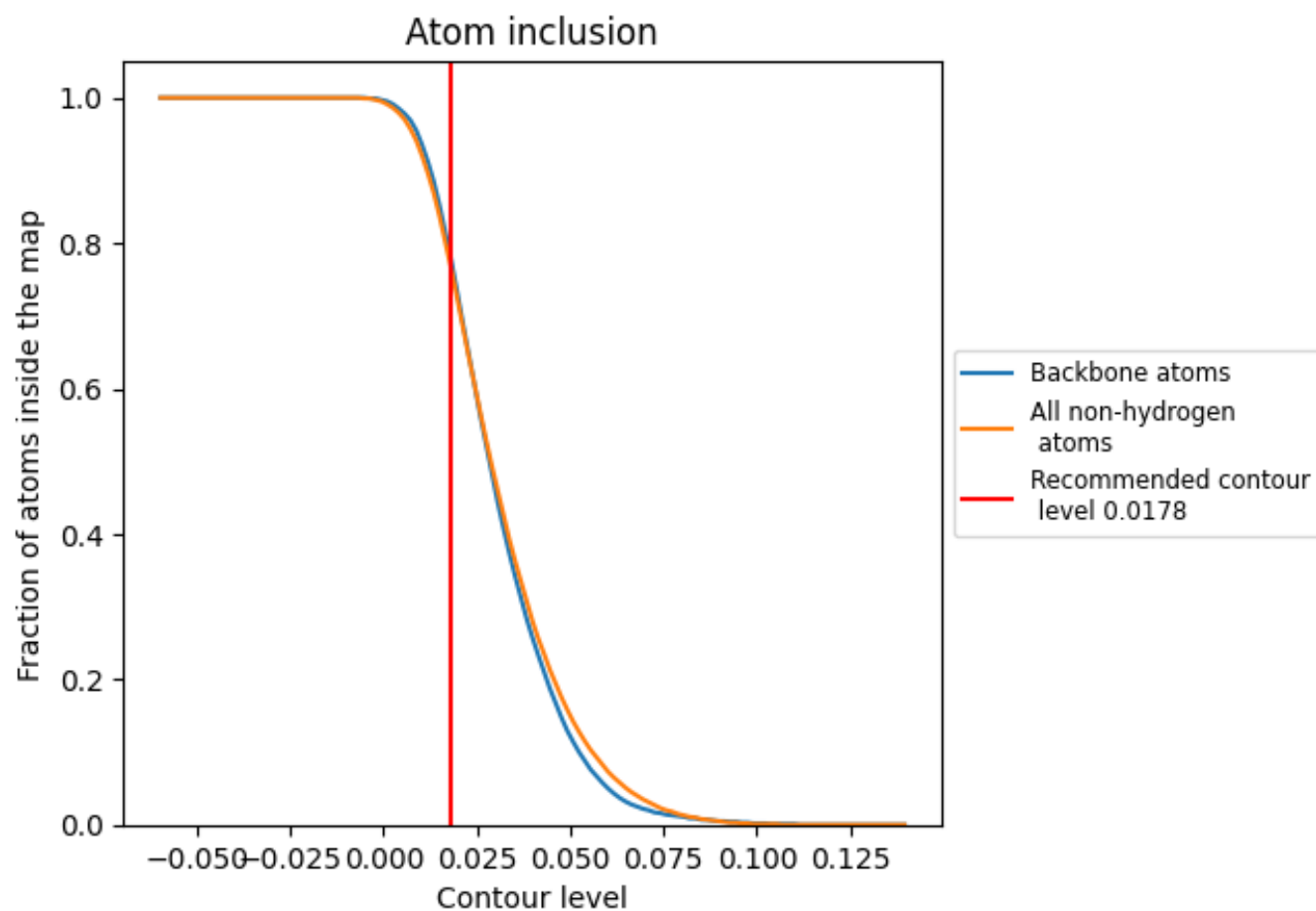
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0178).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.0178) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.4680
A	 0.8750	 0.5160
B	 0.7140	 0.3850
C	 0.3820	 0.2640
D	 0.7520	 0.4960
E	 0.6860	 0.4110
F	 0.8600	 0.5310
G	 0.9220	 0.5780
H	 0.4730	 0.2690
I	 0.9130	 0.5830
J	 0.6740	 0.4010
K	 0.6070	 0.3850
L	 0.9080	 0.5650
M	 0.3470	 0.2630
N	 0.8350	 0.4800
O	 0.8580	 0.5370
P	 0.9010	 0.5800
Q	 0.8750	 0.5530
R	 0.4950	 0.3400
S	 0.8040	 0.5100
T	 0.5410	 0.3630
U	 0.8330	 0.5160
V	 0.4310	 0.2710

