



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:27 PM UTC

PDB ID : 7SYM / pdb_00007sym
EMDB ID : EMD-25533
Title : Structure of the HCV IRES bound to the 40S ribosomal subunit, head opening.
Structure 7(delta dII)
Authors : Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2021-11-25
Resolution : 4.80 Å(reported)
Based on initial models : 5FLX, 6D9J

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

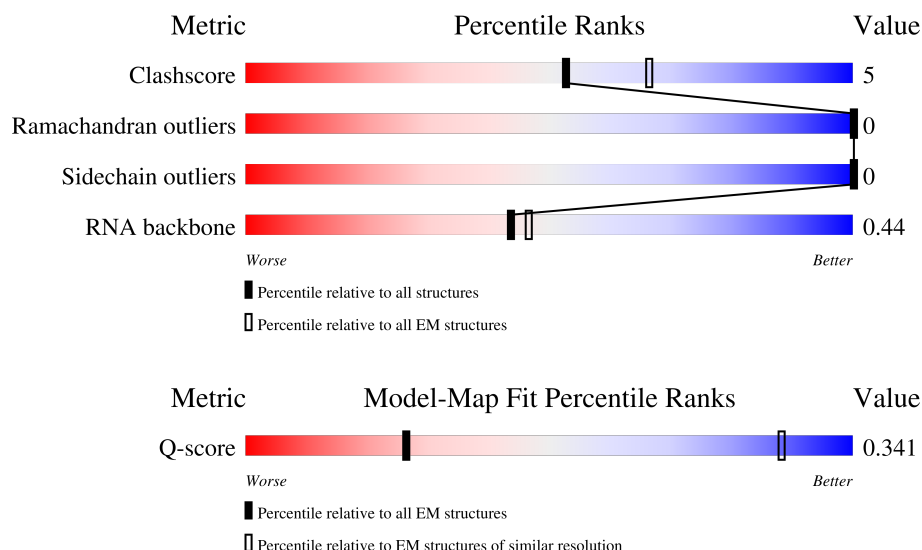
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

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	2	1870	
2	B	295	
3	C	264	

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	281	
6	F	263	
7	G	204	
8	H	249	
9	I	432	
10	J	208	
11	K	194	
12	L	149	
13	M	158	
14	N	132	
15	O	151	
16	P	168	
17	Q	145	
18	R	172	
19	S	135	
20	T	152	
21	U	145	
22	V	119	
23	W	83	
24	X	130	
25	Y	143	
26	Z	131	
27	a	124	
28	b	101	

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Mol	Chain	Length	Quality of chain
29	c	84	
30	d	69	
31	e	56	
32	f	133	
33	g	188	
34	h	317	
35	n	25	
36	z	400	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 78761 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1697	Total	C	N	O	P	0	0
			36227	16170	6504	11857	1696		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	51	ARG	LYS	conflict	UNP G1TK17
F	78	THR	ALA	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 7 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 8 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 11 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 13 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	151	Total	C	N	O	S	0	0
			1233	785	231	211	6		

- Molecule 14 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O	S	0	0
			956	610	176	163	7		

- Molecule 18 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82

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Chain	Residue	Modelled	Actual	Comment	Reference
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 24 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	77	Total	C	N	O	S	0	0
			614	393	114	106	1		

- Molecule 28 is a protein called eS26 (S26).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 30 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	67	Total	C	N	O	S	0	0
			530	321	108	99	2		

- Molecule 31 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 33 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 36 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	162	Total	C	N	O	P	0	0
			3465	1542	621	1140	162		

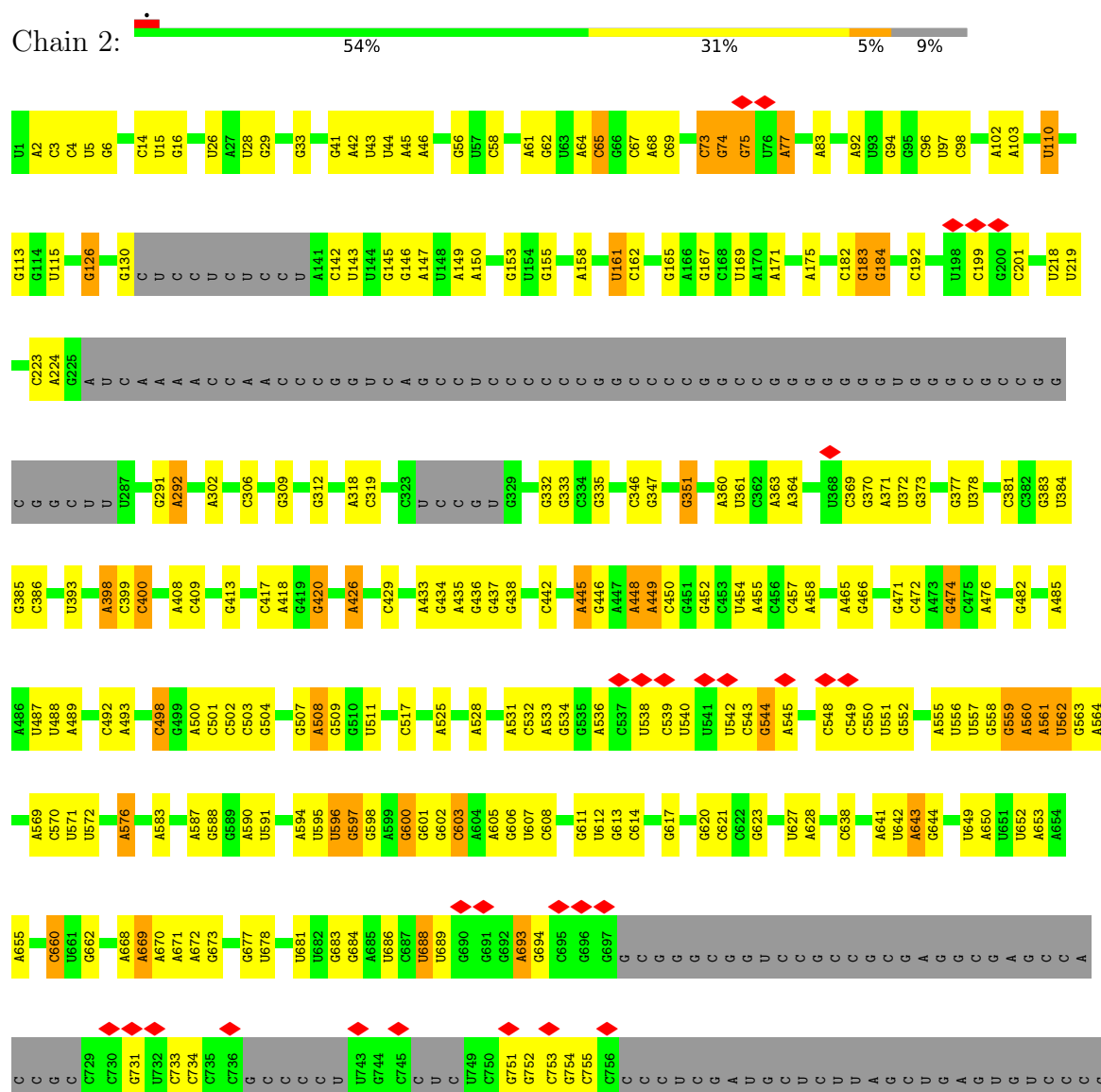
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

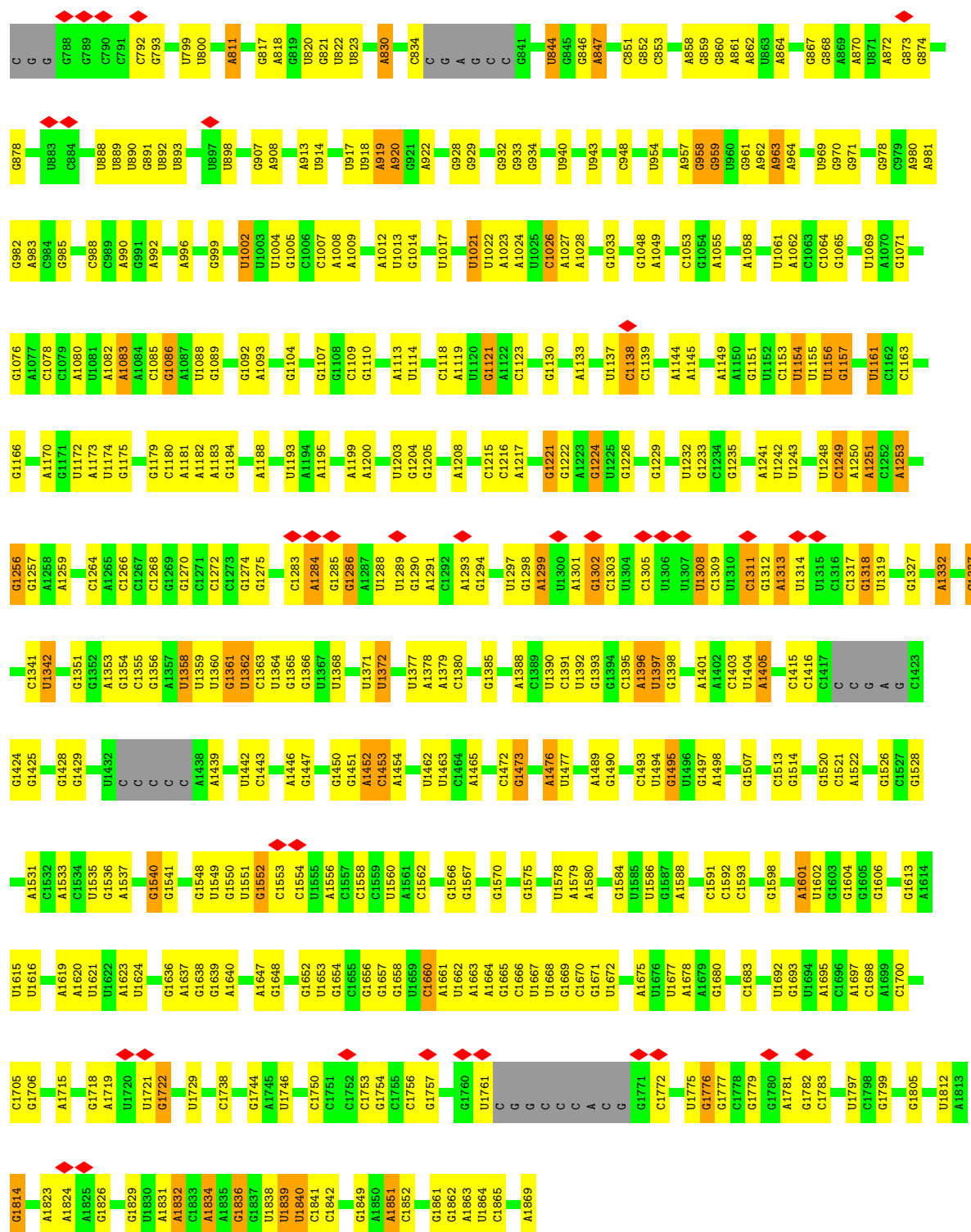
Mol	Chain	Residues	Atoms		AltConf
37	b	1	Total 1	Zn 1	0
37	g	1	Total 1	Zn 1	0

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.

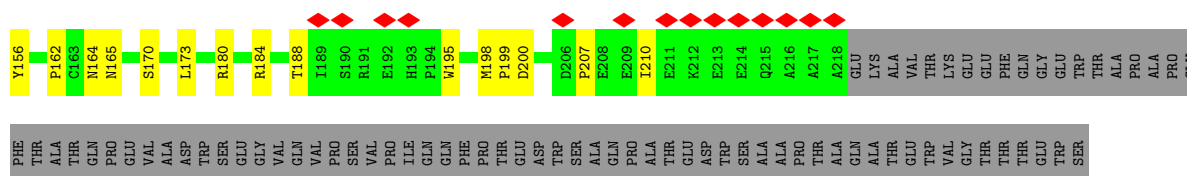
• Molecule 1: 18S rRNA



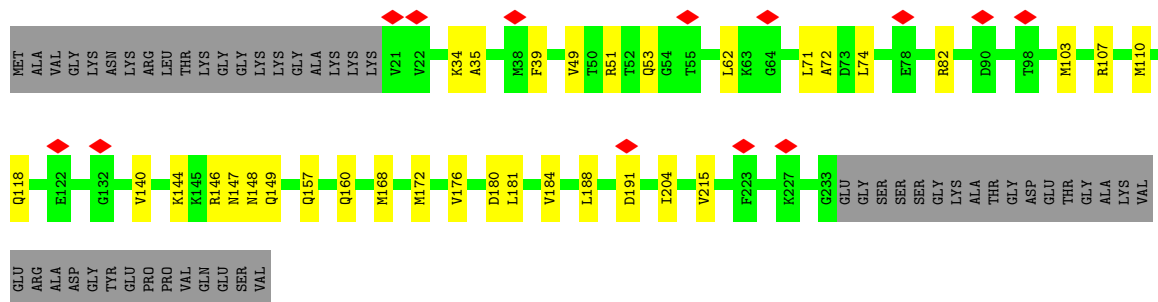


• Molecule 2: 40S ribosomal protein SA

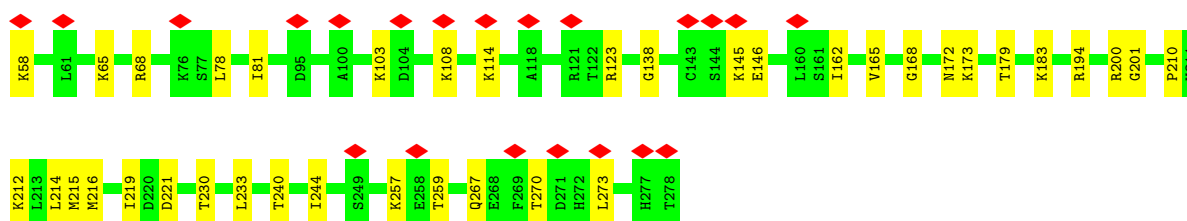
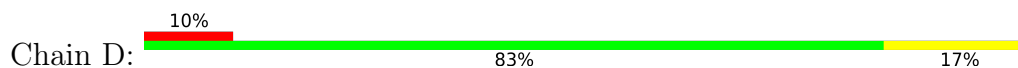




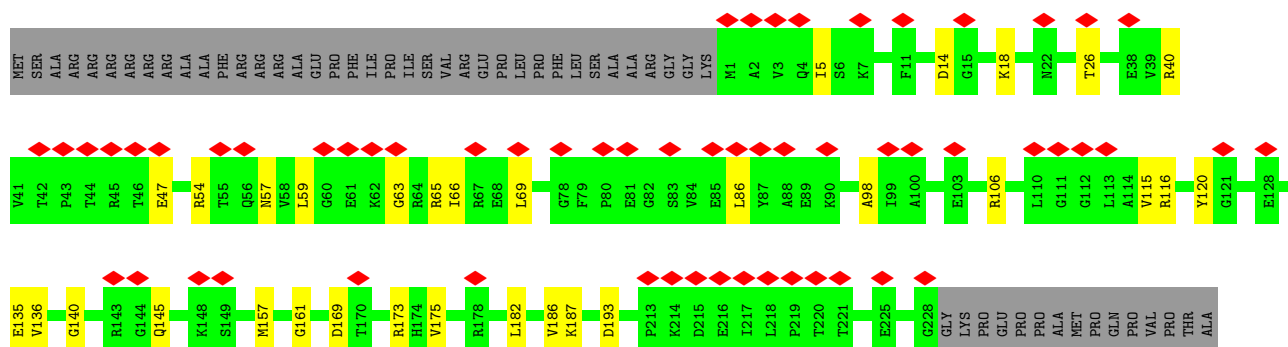
• Molecule 3: 40S ribosomal protein S3a



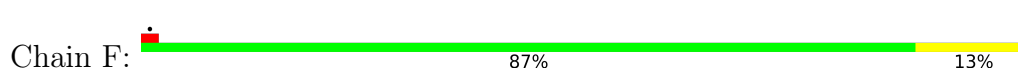
• Molecule 4: 40S ribosomal protein S2

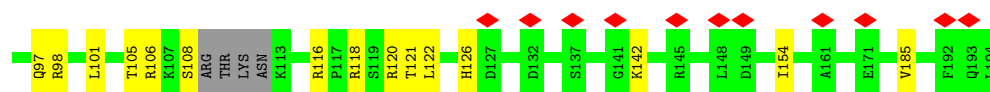


• Molecule 5: uS3

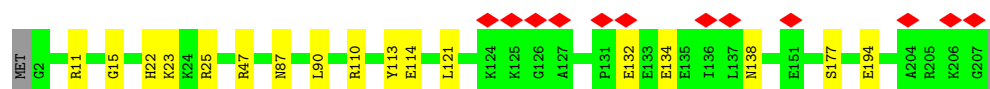


• Molecule 6: 40S ribosomal protein S4

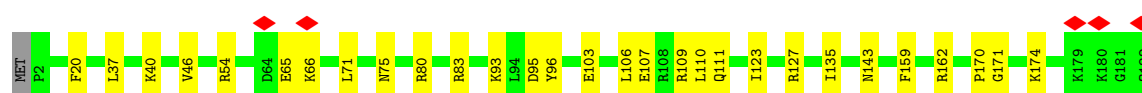
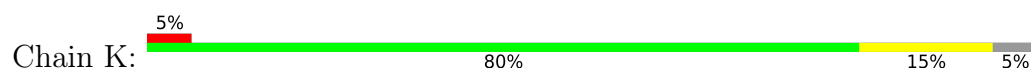




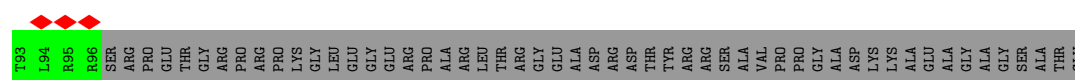
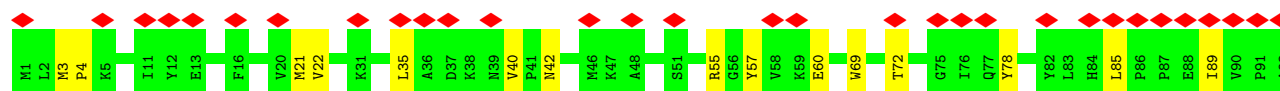
- Molecule 10: eS8



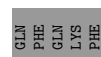
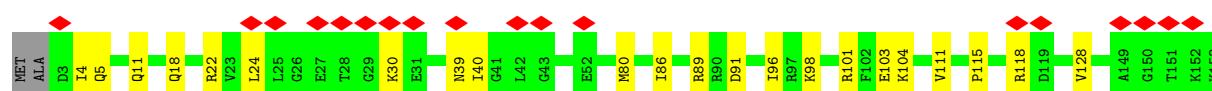
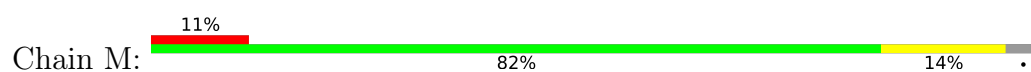
- Molecule 11: uS4



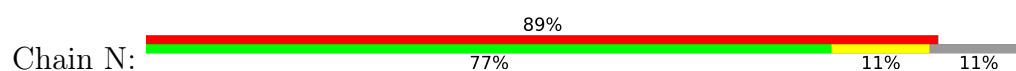
- Molecule 12: eS10

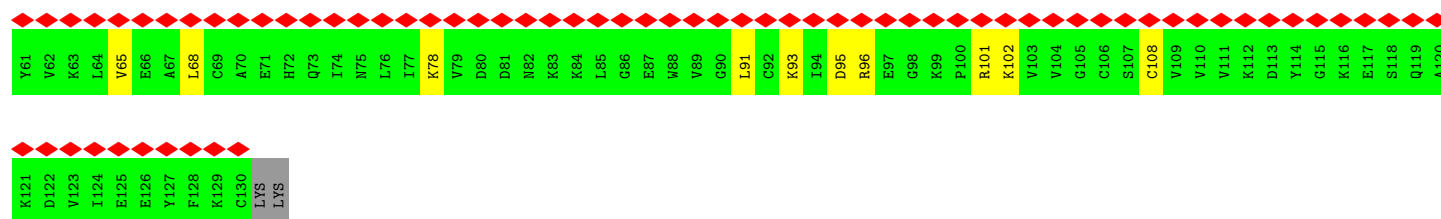


- Molecule 13: uS17

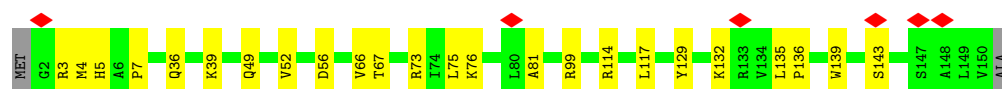
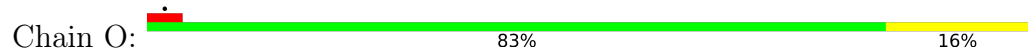


- Molecule 14: eS12

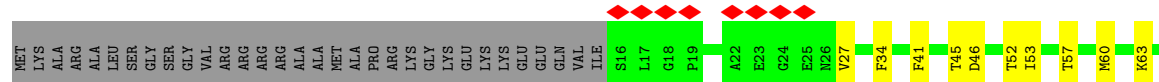




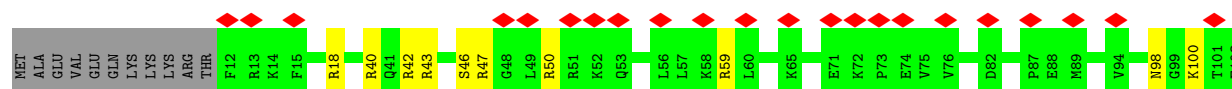
• Molecule 15: uS15



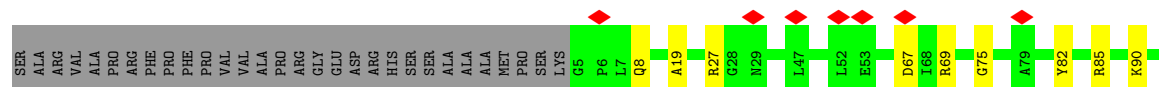
• Molecule 16: uS11



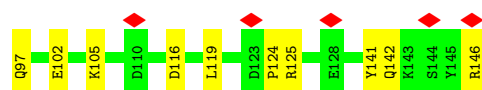
• Molecule 17: uS19

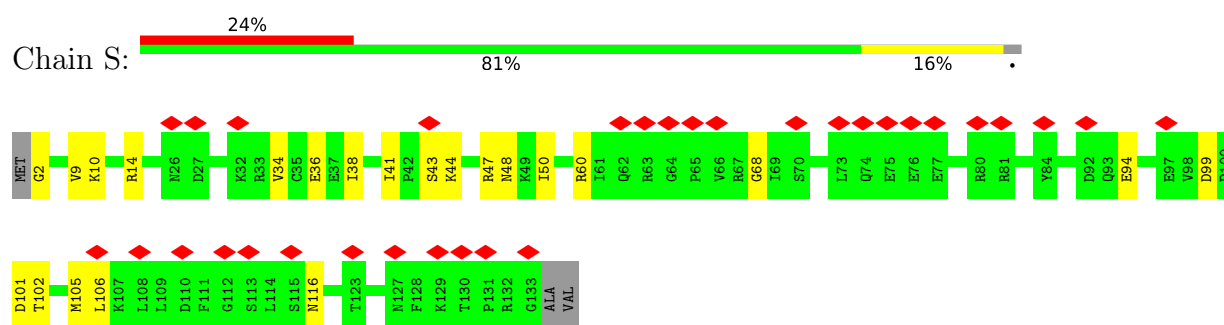


• Molecule 18: uS9

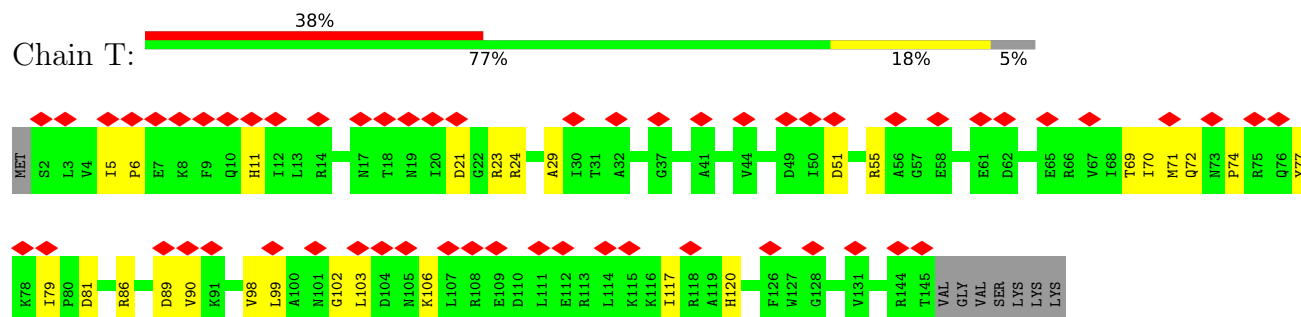


• Molecule 19: eS17

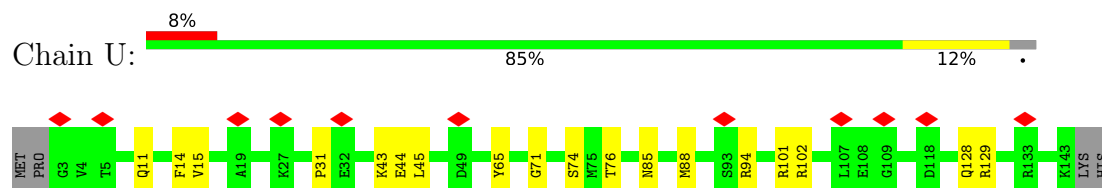




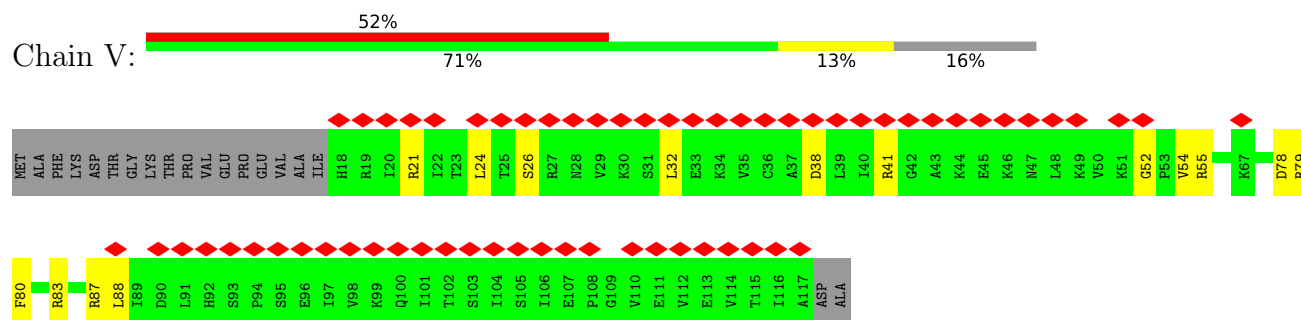
- Molecule 20: uS13



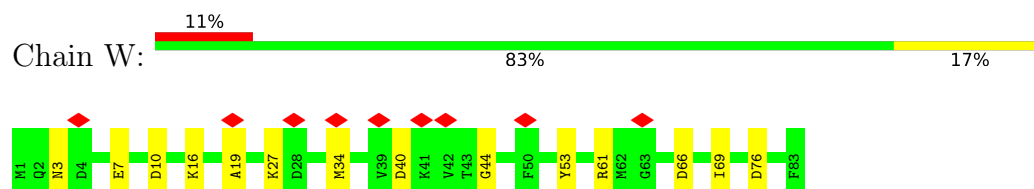
- Molecule 21: eS19



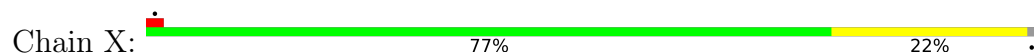
- Molecule 22: uS10

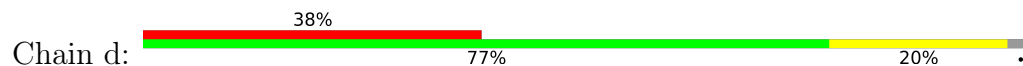


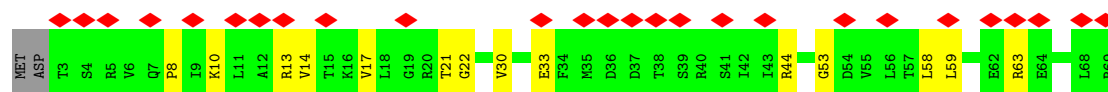
- Molecule 23: 40S ribosomal protein S21



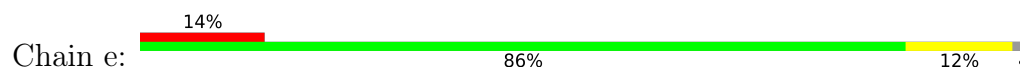
- Molecule 24: uS8



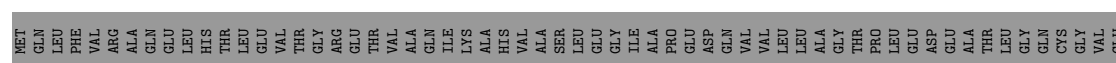
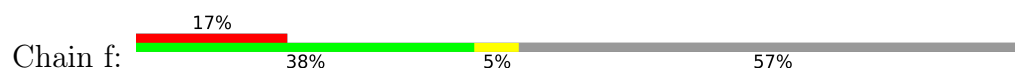




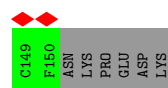
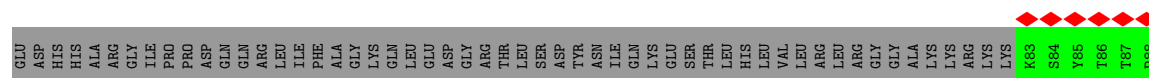
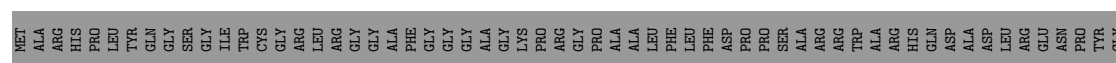
- Molecule 31: eS29



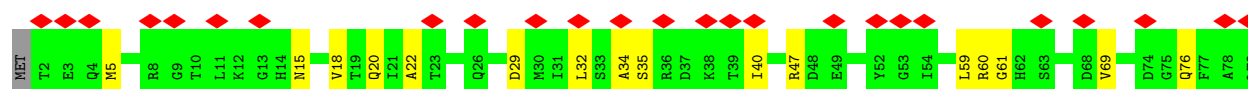
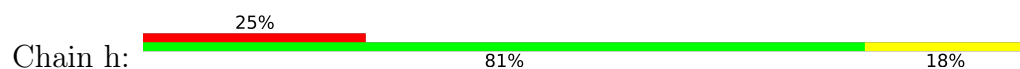
- Molecule 32: eS30

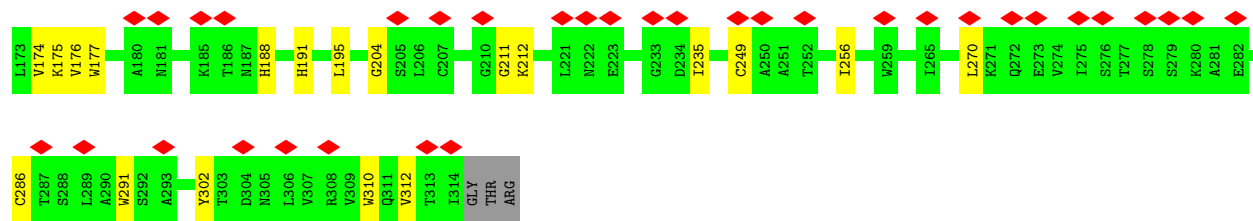


- Molecule 33: 40S ribosomal protein S27a

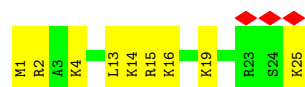


- Molecule 34: RACK1

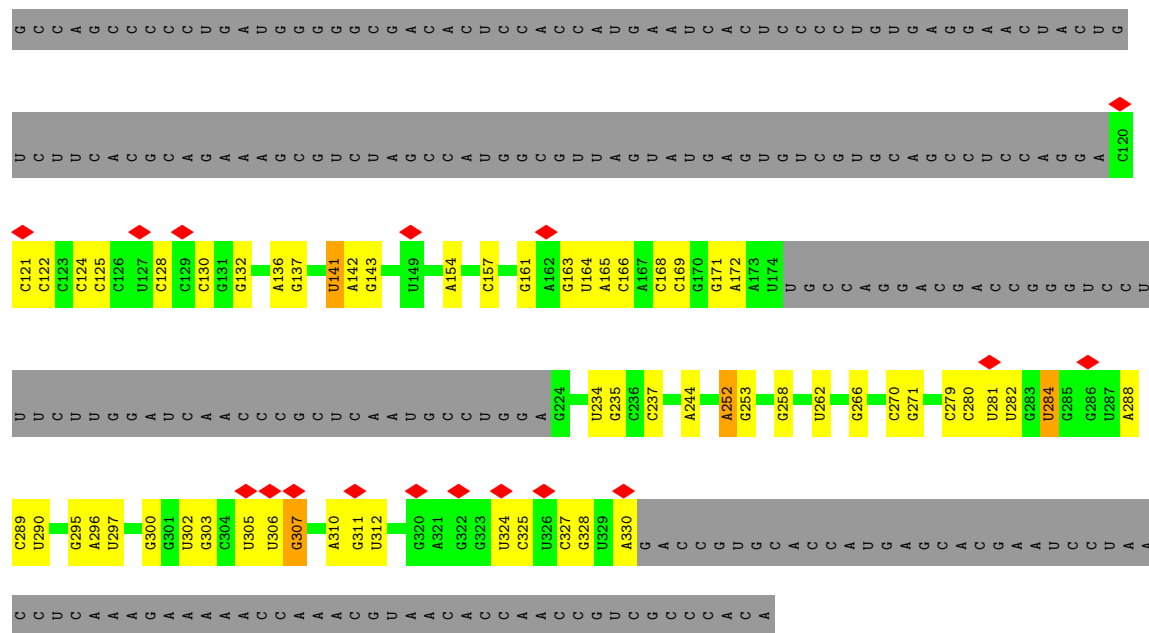




• Molecule 35: 60s ribosomal protein 141



• Molecule 36: HCV IRES



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	59660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	52000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	2	0.15	0/40506	0.34	2/63123 (0.0%)
2	B	0.21	0/1747	0.53	0/2374
3	C	0.18	0/1756	0.46	0/2350
4	D	0.19	0/1753	0.49	0/2369
5	E	0.19	0/1796	0.50	0/2417
6	F	0.20	0/2118	0.51	1/2849 (0.0%)
7	G	0.21	0/1531	0.54	0/2059
8	H	0.20	0/1946	0.51	0/2590
9	I	0.21	0/1510	0.54	0/2022
10	J	0.20	0/1715	0.50	1/2287 (0.0%)
11	K	0.20	0/1550	0.51	0/2069
12	L	0.20	0/834	0.51	0/1125
13	M	0.21	0/1254	0.53	0/1677
14	N	0.20	0/918	0.53	2/1233 (0.2%)
15	O	0.20	0/1226	0.49	0/1649
16	P	0.21	0/1029	0.50	0/1380
17	Q	0.22	0/974	0.59	0/1301
18	R	0.24	0/1146	0.58	1/1534 (0.1%)
19	S	0.26	0/1082	0.67	0/1452
20	T	0.21	0/1208	0.58	0/1618
21	U	0.18	0/1115	0.46	0/1493
22	V	0.19	0/805	0.40	0/1081
23	W	0.18	0/643	0.49	0/860
24	X	0.20	0/1051	0.53	0/1406
25	Y	0.20	0/1116	0.57	1/1490 (0.1%)
26	Z	0.17	0/1028	0.47	0/1366
27	a	0.24	0/620	0.58	0/831
28	b	0.19	0/828	0.45	0/1109
29	c	0.19	0/665	0.56	0/891
30	d	0.19	0/532	0.52	0/712
31	e	0.16	0/470	0.49	0/623
32	f	0.19	0/462	0.49	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.14	0/567	0.39	0/753
34	h	0.18	0/2493	0.51	1/3394 (0.0%)
35	n	0.22	0/240	0.47	0/305
36	z	0.15	0/3871	0.32	0/6034
All	All	0.17	0/84105	0.42	9/122433 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
34	h	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	19	MET	CA-CB-CG	5.47	125.03	114.10
1	2	1753	C	N1-C1'-C2'	5.42	120.12	112.00
25	Y	11	ARG	CA-CB-CG	5.24	124.58	114.10
10	J	132	GLU	CA-CB-CG	5.21	124.52	114.10
1	2	688	U	P-O3'-C3'	5.17	127.95	120.20
18	R	124	PRO	CA-N-CD	-5.15	104.79	112.00
34	h	106	LYS	CB-CA-C	5.14	121.30	111.48
14	N	54	SER	CA-C-N	5.04	129.98	122.82
14	N	54	SER	C-N-CA	5.04	129.98	122.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	h	106	LYS	Peptide

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	2	36227	0	18299	303	0
2	B	1710	0	1708	25	0
3	C	1729	0	1803	22	0
4	D	1716	0	1806	28	0
5	E	1768	0	1866	20	0
6	F	2076	0	2177	20	0
7	G	1509	0	1563	20	0
8	H	1923	0	2089	28	0
9	I	1488	0	1582	19	0
10	J	1686	0	1772	12	0
11	K	1525	0	1640	22	0
12	L	810	0	836	10	0
13	M	1233	0	1310	15	0
14	N	908	0	939	8	0
15	O	1202	0	1289	15	0
16	P	1016	0	1039	14	0
17	Q	956	0	1002	15	0
18	R	1128	0	1195	13	0
19	S	1068	0	1121	15	0
20	T	1190	0	1249	18	0
21	U	1097	0	1130	14	0
22	V	795	0	862	13	0
23	W	636	0	637	14	0
24	X	1034	0	1080	20	0
25	Y	1098	0	1167	16	0
26	Z	1011	0	1083	10	0
27	a	614	0	678	10	0
28	b	814	0	863	8	0
29	c	651	0	672	11	0
30	d	530	0	561	9	0
31	e	459	0	452	8	0
32	f	457	0	502	5	0
33	g	555	0	563	7	0
34	h	2436	0	2393	33	0
35	n	239	0	289	8	0
36	z	3465	0	1751	8	0
37	b	1	0	0	0	0
37	g	1	0	0	0	0
All	All	78761	0	60968	694	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 (694) 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)
1:2:1332:A:H62	1:2:1493:C:N4	1.58	1.00
1:2:1332:A:N6	1:2:1493:C:H42	1.60	0.98
1:2:677:G:N2	1:2:1028:A:H62	1.61	0.98
1:2:677:G:H21	1:2:1028:A:N6	1.68	0.91
1:2:318:A:C2	1:2:333:G:N1	2.39	0.90
1:2:1656:G:H1	1:2:1668:U:H3	1.16	0.90
1:2:16:G:N2	1:2:1195:A:H62	1.70	0.89
1:2:16:G:H21	1:2:1195:A:H62	1.19	0.88
1:2:1533:A:N6	1:2:1602:U:H3	1.71	0.88
1:2:1226:G:H21	1:2:1640:A:H62	1.21	0.87
1:2:677:G:H21	1:2:1028:A:H62	0.89	0.85
1:2:1533:A:H62	1:2:1602:U:H3	0.88	0.85
1:2:16:G:H21	1:2:1195:A:N6	1.76	0.83
1:2:318:A:N1	1:2:333:G:C6	2.47	0.81
1:2:1288:U:H3	1:2:1311:C:H42	1.30	0.76
1:2:1657:G:H1	1:2:1667:U:H3	1.34	0.74
17:Q:42:ARG:O	17:Q:46:SER:HB2	1.88	0.73
1:2:498:C:H42	1:2:504:G:H1	1.38	0.72
1:2:1226:G:N2	1:2:1640:A:H62	1.85	0.72
1:2:1226:G:H21	1:2:1640:A:N6	1.88	0.71
1:2:1361:G:H5'	1:2:1362:U:H5''	1.74	0.69
1:2:1332:A:H62	1:2:1493:C:H42	0.79	0.68
1:2:1396:A:N7	1:2:1450:G:N2	2.43	0.66
15:O:75:LEU:HB3	15:O:81:ALA:HB2	1.77	0.66
3:C:110:MET:HE1	3:C:140:VAL:HG21	1.78	0.66
3:C:103:MET:H	3:C:215:VAL:HB	1.61	0.66
1:2:1110:G:N2	1:2:1123:C:C2	2.64	0.65
1:2:74:G:H22	1:2:77:A:H5''	1.60	0.65
19:S:9:VAL:HG23	19:S:50:ILE:HG13	1.79	0.64
26:Z:7:ILE:HD13	26:Z:40:ILE:HD11	1.79	0.64
1:2:318:A:C2	1:2:333:G:C6	2.84	0.64
3:C:184:VAL:O	3:C:188:LEU:HB2	1.98	0.64
1:2:1166:G:H1	1:2:1193:U:H3	1.42	0.64
1:2:1232:U:H3	1:2:1526:G:H1	1.44	0.64
1:2:1452:A:N6	1:2:1473:G:N2	2.45	0.64
3:C:82:ARG:HH22	3:C:191:ASP:HB3	1.63	0.64
19:S:34:VAL:HG23	19:S:38:ILE:HD13	1.81	0.63
1:2:694:G:H22	1:2:733:C:H1'	1.64	0.62
1:2:940:U:H3	1:2:1002:U:H3	1.47	0.62
1:2:1297:U:H2'	1:2:1298:G:H2'	1.82	0.61
4:D:165:VAL:HG11	4:D:244:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1138:C:H2'	23:W:61:ARG:HH12	1.66	0.61
1:2:1401:A:H4'	22:V:52:GLY:HA3	1.82	0.61
1:2:1653:U:H3	1:2:1671:G:H1	1.49	0.61
1:2:457:C:H2'	1:2:458:A:H8	1.66	0.61
1:2:1776:G:N2	1:2:1777:G:O6	2.34	0.60
9:I:29:GLU:O	9:I:33:ASN:ND2	2.33	0.60
1:2:1562:C:H5''	21:U:71:GLY:HA3	1.83	0.60
2:B:2:SER:HB2	2:B:56:GLU:HG2	1.83	0.60
1:2:153:G:N3	8:H:13:GLN:NE2	2.49	0.60
16:P:70:SER:HB3	16:P:73:ALA:H	1.66	0.60
1:2:1452:A:N6	1:2:1473:G:C2	2.70	0.60
23:W:3:ASN:HD21	23:W:7:GLU:HG2	1.65	0.60
34:h:212:LYS:HA	34:h:235:ILE:HG13	1.84	0.60
25:Y:11:ARG:HA	25:Y:14:ARG:HB3	1.82	0.60
1:2:817:G:H21	1:2:847:A:H62	1.50	0.59
1:2:1729:U:H3	1:2:1805:G:H1	1.50	0.59
12:L:3:MET:HE3	12:L:4:PRO:HD2	1.84	0.59
2:B:54:THR:HG22	2:B:162:PRO:HG2	1.83	0.59
4:D:210:PRO:HB3	4:D:240:THR:HG21	1.83	0.59
1:2:1199:A:H5''	28:b:2:THR:HB	1.85	0.59
5:E:135:GLU:HB3	5:E:187:LYS:HB2	1.85	0.59
30:d:17:VAL:HA	30:d:30:VAL:HG23	1.85	0.59
3:C:146:ARG:H	3:C:149:GLN:HE21	1.50	0.59
16:P:34:PHE:HB3	16:P:41:PHE:HB2	1.85	0.59
1:2:641:A:OP2	32:f:107:ARG:NH1	2.35	0.58
33:g:134:SER:HA	33:g:139:HIS:HA	1.85	0.58
1:2:1156:U:H2'	1:2:1157:G:H21	1.69	0.58
34:h:249:CYS:SG	34:h:291:TRP:NE1	2.76	0.57
1:2:693:A:N1	1:2:734:C:N4	2.51	0.57
1:2:318:A:N1	1:2:333:G:O6	2.37	0.57
1:2:1173:A:OP1	35:n:14:LYS:NZ	2.38	0.57
25:Y:95:GLU:OE2	25:Y:140:ARG:NH2	2.37	0.57
1:2:332:G:N7	8:H:189:ARG:NH2	2.52	0.57
34:h:29:ASP:HA	34:h:47:ARG:HH22	1.69	0.57
24:X:87:GLU:HA	24:X:90:GLN:HG2	1.87	0.57
1:2:934:G:H1	1:2:1008:A:H2	1.48	0.57
1:2:318:A:C2	1:2:333:G:C2	2.92	0.57
1:2:511:U:O2'	1:2:576:A:N6	2.37	0.57
1:2:1472:C:N4	1:2:1476:A:H62	2.03	0.57
8:H:181:THR:HG22	8:H:183:ARG:H	1.69	0.56
1:2:445:A:H5''	10:J:47:ARG:HH22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1405:A:H2	1:2:1443:C:H42	1.53	0.56
12:L:21:MET:HE3	12:L:22:VAL:H	1.70	0.56
12:L:60:GLU:OE1	12:L:69:TRP:NE1	2.37	0.56
30:d:44:ARG:NH1	30:d:63:ARG:O	2.38	0.56
1:2:1205:G:O2'	1:2:1834:A:N6	2.38	0.56
1:2:1669:G:OP1	22:V:79:ARG:NH2	2.39	0.56
11:K:37:LEU:HD11	11:K:106:LEU:HD11	1.86	0.56
15:O:129:TYR:HB3	15:O:135:LEU:HD13	1.86	0.56
21:U:44:GLU:HG2	21:U:45:LEU:HG	1.88	0.56
1:2:1372:U:OP1	1:2:1385:G:N2	2.38	0.56
1:2:1616:U:OP2	17:Q:43:ARG:NH2	2.37	0.56
16:P:45:THR:HA	16:P:52:THR:HA	1.87	0.56
1:2:1302:G:N2	1:2:1305:C:OP2	2.38	0.56
9:I:122:LEU:HG	9:I:126:HIS:CE1	2.41	0.56
19:S:41:ILE:HG22	19:S:43:SER:H	1.70	0.56
8:H:32:MET:HG2	8:H:65:GLN:HG2	1.88	0.56
1:2:563:G:H2'	1:2:564:A:H8	1.71	0.55
1:2:1452:A:H61	1:2:1473:G:N2	2.04	0.55
13:M:22:ARG:HH22	13:M:30:LYS:HZ1	1.53	0.55
34:h:87:LEU:HB2	34:h:101:PHE:HB2	1.88	0.55
22:V:38:ASP:OD1	22:V:41:ARG:NH2	2.39	0.55
1:2:934:G:O6	1:2:1008:A:N1	2.39	0.55
17:Q:98:ASN:ND2	17:Q:121:ILE:O	2.34	0.55
1:2:1332:A:O2'	5:E:145:GLN:O	2.24	0.55
1:2:1658:G:OP2	1:2:1660:C:N4	2.39	0.55
34:h:87:LEU:HD21	34:h:111:VAL:HG11	1.87	0.55
1:2:1706:G:H1	1:2:1829:G:H1	1.55	0.55
1:2:1086:G:OP2	28:b:12:LYS:NZ	2.39	0.55
1:2:1647:A:N6	1:2:1677:U:O4	2.40	0.55
1:2:528:A:H2	1:2:558:G:H1	1.55	0.55
4:D:270:THR:HA	4:D:273:LEU:HG	1.88	0.55
8:H:231:ARG:HH11	8:H:232:ARG:HH12	1.54	0.55
35:n:16:LYS:HA	35:n:19:LYS:HE3	1.89	0.55
1:2:433:A:OP1	10:J:25:ARG:NH2	2.40	0.55
1:2:1337:C:OP1	31:e:44:ARG:NH2	2.39	0.55
24:X:115:GLU:HA	24:X:118:ARG:HG2	1.89	0.55
5:E:98:ALA:HB2	5:E:169:ASP:HB3	1.89	0.54
1:2:603:C:N4	1:2:620:G:O6	2.38	0.54
2:B:120:ARG:HH22	4:D:267:GLN:HB2	1.72	0.54
10:J:194:GLU:OE2	13:M:18:GLN:NE2	2.40	0.54
1:2:1144:A:H5'	1:2:1355:C:H41	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1540:G:OP1	21:U:43:LYS:NZ	2.40	0.54
28:b:20:PRO:HA	28:b:31:PRO:HA	1.88	0.54
34:h:20:GLN:HG2	34:h:69:VAL:H	1.73	0.54
34:h:109:LEU:HD21	34:h:125:ARG:HE	1.72	0.54
1:2:1652:G:H1	1:2:1672:U:H3	1.54	0.54
13:M:101:ARG:NH1	25:Y:6:GLY:O	2.41	0.54
34:h:18:VAL:HA	34:h:35:SER:HA	1.88	0.54
1:2:638:C:H5''	32:f:109:MET:HE1	1.89	0.54
1:2:1615:U:OP2	17:Q:43:ARG:NH1	2.40	0.54
10:J:110:ARG:HG3	10:J:121:LEU:HB3	1.90	0.54
1:2:1398:G:O2'	34:h:88:ARG:NH2	2.40	0.54
2:B:76:VAL:HG12	2:B:123:VAL:HB	1.90	0.54
13:M:5:GLN:HE22	13:M:11:GLN:HB2	1.71	0.54
1:2:65:C:N4	1:2:169:U:O2'	2.41	0.54
1:2:678:U:OP2	1:2:1026:C:N4	2.41	0.54
1:2:851:C:H5''	1:2:852:G:H5'	1.90	0.54
9:I:142:LYS:HB2	24:X:54:ASP:HB3	1.90	0.54
15:O:136:PRO:HG2	15:O:139:TRP:HB2	1.90	0.54
1:2:1738:C:OP1	8:H:92:ARG:NH1	2.41	0.54
6:F:62:LYS:HG2	6:F:80:ILE:HG13	1.90	0.54
1:2:1012:A:OP1	15:O:3:ARG:NH1	2.41	0.53
1:2:1535:U:O2'	7:G:81:ARG:NH2	2.38	0.53
1:2:820:U:OP1	11:K:83:ARG:NH1	2.41	0.53
1:2:1284:A:N6	14:N:91:LEU:O	2.41	0.53
7:G:53:ALA:O	18:R:125:ARG:NH2	2.40	0.53
9:I:105:THR:HG23	9:I:108:SER:H	1.72	0.53
11:K:135:ILE:HA	11:K:159:PHE:HA	1.89	0.53
1:2:158:A:N6	8:H:59:GLN:OE1	2.41	0.53
1:2:1677:U:OP2	7:G:148:ASN:ND2	2.41	0.53
1:2:1841:C:OP2	35:n:2:ARG:NH1	2.40	0.53
2:B:198:MET:HG3	2:B:200:ASP:H	1.73	0.53
24:X:86:LEU:HD21	24:X:113:HIS:HB2	1.89	0.53
30:d:8:PRO:O	30:d:10:LYS:NZ	2.41	0.53
1:2:167:G:O2'	8:H:131:ARG:NH1	2.42	0.53
1:2:662:G:OP2	1:2:1157:G:N2	2.42	0.53
24:X:26:LEU:HD21	24:X:60:LYS:HD3	1.89	0.53
9:I:40:LEU:HG	9:I:43:LEU:HD22	1.91	0.53
20:T:11:HIS:O	20:T:23:ARG:NH1	2.41	0.53
1:2:1182:A:O3'	35:n:15:ARG:NH1	2.42	0.53
8:H:115:LYS:NZ	8:H:116:LYS:O	2.42	0.53
9:I:7:LYS:NZ	9:I:31:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1286:G:N2	1:2:1312:G:O2'	2.38	0.53
1:2:1550:G:H3'	1:2:1579:A:H61	1.74	0.53
1:2:1661:A:OP2	31:e:32:ARG:NH1	2.42	0.53
11:K:71:LEU:O	11:K:75:ASN:ND2	2.41	0.53
2:B:184:ARG:HH21	2:B:188:THR:HB	1.74	0.53
5:E:14:ASP:OD2	5:E:18:LYS:NZ	2.41	0.53
1:2:1289:U:O4	33:g:95:ARG:NH1	2.42	0.53
1:2:1700:C:H5	1:2:1836:G:H1	1.57	0.53
34:h:40:ILE:HB	34:h:59:LEU:HB2	1.90	0.53
3:C:157:GLN:HB2	3:C:160:GLN:HG3	1.91	0.53
4:D:257:LYS:O	23:W:16:LYS:NZ	2.39	0.53
5:E:59:LEU:HB2	5:E:63:GLY:HA2	1.89	0.53
1:2:600:G:H2'	1:2:601:G:H8	1.74	0.52
1:2:1021:U:OP1	15:O:132:LYS:NZ	2.42	0.52
1:2:1613:G:OP1	17:Q:42:ARG:NH2	2.42	0.52
12:L:57:TYR:O	12:L:72:THR:OG1	2.27	0.52
1:2:1283:C:H41	14:N:102:LYS:HG2	1.75	0.52
1:2:161:U:O2	8:H:87:ARG:NH1	2.43	0.52
1:2:1256:G:O4'	31:e:40:ARG:NH1	2.42	0.52
1:2:1289:U:H2'	1:2:1290:G:H8	1.74	0.52
2:B:17:LYS:HB3	2:B:173:LEU:HD11	1.92	0.52
4:D:103:LYS:HB2	4:D:216:MET:HE1	1.92	0.52
35:n:2:ARG:HH21	35:n:4:LYS:HD3	1.74	0.52
1:2:165:G:OP2	1:2:165:G:N2	2.41	0.52
1:2:1119:A:O2'	29:c:72:ARG:NH2	2.38	0.52
17:Q:111:MET:HE1	20:T:117:ILE:HG23	1.92	0.52
4:D:212:LYS:HA	4:D:215:MET:HE2	1.92	0.52
1:2:346:C:O2'	6:F:30:ARG:NH2	2.42	0.52
20:T:24:ARG:HB2	20:T:29:ALA:HB2	1.91	0.52
24:X:41:MET:HG3	24:X:47:ILE:HG12	1.91	0.52
1:2:1552:G:H5'	5:E:5:ILE:HG22	1.92	0.52
2:B:198:MET:HE3	2:B:199:PRO:HD2	1.92	0.52
34:h:286:CYS:HA	34:h:302:TYR:HA	1.91	0.52
14:N:93:LYS:HB3	14:N:96:ARG:HD2	1.92	0.52
1:2:918:U:O2'	1:2:919:A:O4'	2.28	0.51
1:2:1288:U:H3	1:2:1311:C:N4	2.02	0.51
2:B:19:LEU:HD13	2:B:24:HIS:CE1	2.45	0.51
16:P:27:VAL:HG23	16:P:91:THR:H	1.75	0.51
21:U:11:GLN:HA	21:U:14:PHE:HB3	1.92	0.51
1:2:1253:A:HO2'	1:2:1666:C:HO2'	1.57	0.51
6:F:153:LEU:O	6:F:174:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:26:SER:HB3	22:V:32:LEU:HD13	1.91	0.51
22:V:78:ASP:OD2	31:e:44:ARG:NH1	2.39	0.51
1:2:1566:G:N7	21:U:101:ARG:NH2	2.59	0.51
2:B:19:LEU:HD21	19:S:106:LEU:HD21	1.91	0.51
7:G:77:MET:HB3	7:G:89:THR:HG21	1.92	0.51
8:H:54:GLY:O	8:H:110:ASN:ND2	2.43	0.51
15:O:99:ARG:NH2	15:O:143:SER:O	2.44	0.51
1:2:818:A:OP1	11:K:80:ARG:NH1	2.42	0.51
1:2:1705:C:O2	1:2:1851:A:O2'	2.28	0.51
1:2:922:A:OP1	24:X:28:ARG:NH2	2.43	0.51
1:2:1528:G:O2'	1:2:1666:C:OP1	2.29	0.51
8:H:37:ALA:HA	8:H:49:VAL:HA	1.93	0.51
9:I:154:ILE:HB	9:I:185:VAL:HG22	1.92	0.51
34:h:120:ILE:HB	34:h:132:TRP:HB2	1.92	0.51
1:2:1286:G:N2	1:2:1313:A:H62	2.09	0.51
3:C:147:ASN:ND2	36:z:300:G:OP1	2.43	0.51
21:U:65:TYR:HE1	21:U:128:GLN:HE21	1.59	0.51
35:n:13:LEU:HA	35:n:16:LYS:HG2	1.92	0.51
36:z:327:C:N4	36:z:328:G:O6	2.44	0.51
1:2:1161:U:OP1	25:Y:12:LYS:NZ	2.44	0.51
1:2:1226:G:N1	1:2:1639:G:OP2	2.42	0.51
8:H:190:ARG:HH21	8:H:194:LEU:HD21	1.74	0.51
23:W:19:ALA:O	24:X:23:ARG:NH1	2.44	0.51
1:2:1549:U:OP1	31:e:34:TYR:OH	2.26	0.51
1:2:988:C:O2'	3:C:118:GLN:O	2.29	0.50
1:2:1299:A:OP1	17:Q:59:ARG:NH1	2.44	0.50
1:2:1593:C:OP2	7:G:91:ARG:NH1	2.43	0.50
1:2:1677:U:H2'	1:2:1678:A:H8	1.77	0.50
4:D:168:GLY:N	4:D:179:THR:O	2.43	0.50
4:D:201:GLY:N	4:D:221:ASP:OD2	2.44	0.50
21:U:31:PRO:HG3	21:U:102:ARG:HD2	1.93	0.50
34:h:5:MET:HB3	34:h:310:TRP:HB3	1.93	0.50
10:J:134:GLU:OE1	10:J:138:ASN:ND2	2.44	0.50
11:K:170:PRO:HB3	11:K:174:LYS:HD2	1.93	0.50
19:S:14:ARG:HH21	19:S:68:GLY:HA3	1.75	0.50
25:Y:94:ILE:HG13	25:Y:125:VAL:HG21	1.94	0.50
1:2:598:G:O2'	1:2:605:A:N1	2.43	0.50
1:2:1113:A:N6	1:2:1121:G:O6	2.44	0.50
1:2:1121:G:O2'	3:C:204:ILE:O	2.28	0.50
7:G:63:LYS:O	7:G:71:ARG:NH1	2.45	0.50
7:G:125:SER:HA	7:G:138:ALA:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1268:C:H42	1:2:1514:G:H1	1.58	0.50
33:g:141:CYS:SG	33:g:142:GLY:N	2.82	0.50
1:2:928:G:H21	29:c:68:GLY:HA2	1.77	0.50
1:2:1446:A:H1'	22:V:55:ARG:HD2	1.94	0.50
11:K:110:LEU:HD21	11:K:135:ILE:HD11	1.94	0.50
16:P:149:ARG:H	28:b:27:ALA:HB3	1.76	0.50
10:J:87:ASN:HB3	10:J:90:LEU:HD23	1.93	0.50
13:M:103:GLU:OE2	25:Y:11:ARG:NH1	2.45	0.50
20:T:98:VAL:HG13	20:T:103:LEU:HD22	1.93	0.50
36:z:171:G:H3'	36:z:172:A:H8	1.76	0.50
1:2:482:G:O3'	25:Y:76:LYS:NZ	2.44	0.50
1:2:558:G:O6	1:2:559:G:N2	2.44	0.50
1:2:1533:A:N6	1:2:1602:U:N3	2.44	0.50
1:2:346:C:H5'	6:F:38:LEU:HD23	1.93	0.50
1:2:1358:U:OP2	4:D:123:ARG:NH2	2.45	0.50
15:O:114:ARG:HD3	15:O:117:LEU:HD12	1.94	0.50
20:T:98:VAL:HG22	20:T:102:GLY:HA3	1.94	0.50
34:h:191:HIS:HB3	34:h:195:LEU:HD21	1.93	0.50
1:2:686:U:OP1	24:X:32:LYS:N	2.45	0.49
1:2:932:G:H1	1:2:1009:A:H61	1.58	0.49
2:B:50:ASN:HB3	2:B:53:ARG:HD2	1.93	0.49
2:B:207:PRO:HA	2:B:210:ILE:HB	1.94	0.49
16:P:57:THR:H	16:P:60:MET:HE3	1.77	0.49
1:2:1138:C:H3'	23:W:61:ARG:HH22	1.76	0.49
4:D:183:LYS:HD2	4:D:194:ARG:HH12	1.77	0.49
3:C:176:VAL:HG23	3:C:184:VAL:HG11	1.94	0.49
6:F:247:THR:HG22	6:F:250:GLU:HG2	1.94	0.49
20:T:23:ARG:O	20:T:55:ARG:NH1	2.45	0.49
1:2:1601:A:N6	1:2:1636:G:O4'	2.45	0.49
2:B:125:THR:O	2:B:165:ASN:ND2	2.46	0.49
18:R:102:GLU:HB2	18:R:105:LYS:HD3	1.93	0.49
2:B:36:GLN:O	2:B:53:ARG:NH1	2.45	0.49
8:H:2:LYS:HB3	8:H:15:LEU:HD11	1.95	0.49
24:X:15:ASN:C	24:X:15:ASN:HD22	2.21	0.49
1:2:28:U:H2'	1:2:29:G:H8	1.78	0.49
1:2:1670:C:H2'	1:2:1671:G:H8	1.77	0.49
7:G:35:LEU:HD22	7:G:117:ILE:HG22	1.94	0.49
12:L:35:LEU:HD23	12:L:40:VAL:HG21	1.94	0.49
1:2:681:U:OP1	25:Y:8:ARG:NH1	2.42	0.49
7:G:67:PRO:HG2	7:G:70:GLU:HB2	1.95	0.49
18:R:116:ASP:HB2	18:R:119:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:63:PRO:HA	27:a:97:ILE:HD11	1.94	0.49
1:2:126:G:H5''	8:H:195:LYS:HD2	1.95	0.49
3:C:168:MET:O	3:C:172:MET:HB3	2.12	0.49
1:2:751:G:H1	1:2:792:C:H42	1.60	0.49
1:2:1656:G:O6	1:2:1668:U:O4	2.30	0.49
12:L:21:MET:HB3	12:L:69:TRP:HB2	1.93	0.49
1:2:1353:A:H61	1:2:1359:U:H3	1.61	0.49
4:D:172:ASN:ND2	11:K:95:ASP:OD2	2.45	0.48
27:a:98:LYS:NZ	27:a:111:ARG:O	2.42	0.48
1:2:538:U:H3	1:2:545:A:H61	1.60	0.48
1:2:1014:G:N2	29:c:51:GLN:OE1	2.47	0.48
1:2:1082:A:O2'	1:2:1842:C:O2'	2.29	0.48
1:2:1092:G:H2'	1:2:1093:A:H8	1.79	0.48
1:2:1368:U:O3'	19:S:2:GLY:N	2.47	0.48
6:F:32:SER:HB3	6:F:81:THR:HG23	1.95	0.48
24:X:80:ASP:HA	24:X:124:LYS:HA	1.94	0.48
34:h:122:SER:HB3	34:h:132:TRP:HE1	1.77	0.48
36:z:141:U:H2'	36:z:142:A:H8	1.78	0.48
1:2:429:C:O2'	1:2:811:A:N1	2.47	0.48
1:2:982:G:H2'	1:2:983:A:H8	1.78	0.48
1:2:1593:C:OP2	27:a:104:ARG:NH2	2.42	0.48
1:2:1598:G:OP1	27:a:80:ARG:NH2	2.45	0.48
1:2:1692:U:H2'	1:2:1693:G:H8	1.77	0.48
5:E:106:ARG:HG3	5:E:175:VAL:HG22	1.93	0.48
6:F:246:LEU:HD13	6:F:250:GLU:HG3	1.95	0.48
34:h:82:SER:OG	34:h:83:TRP:N	2.46	0.48
15:O:99:ARG:HH22	15:O:143:SER:HB2	1.78	0.48
1:2:398:A:H5''	1:2:400:C:H5'	1.96	0.48
5:E:115:VAL:HG23	5:E:116:ARG:HG3	1.96	0.48
6:F:79:ASP:HB3	6:F:82:TYR:HB2	1.94	0.48
22:V:21:ARG:HH21	22:V:88:LEU:HD13	1.78	0.48
36:z:262:U:O2	36:z:271:G:O6	2.32	0.48
1:2:1130:G:N2	1:2:1130:G:OP2	2.47	0.48
10:J:113:TYR:HD2	10:J:121:LEU:HB2	1.78	0.48
21:U:44:GLU:OE2	21:U:44:GLU:N	2.46	0.48
23:W:10:ASP:N	23:W:10:ASP:OD1	2.43	0.48
29:c:13:GLU:O	29:c:17:ARG:HB2	2.13	0.48
6:F:100:ARG:HB2	6:F:114:ILE:HD13	1.96	0.48
7:G:39:ILE:HG23	7:G:68:ILE:HG13	1.95	0.48
18:R:8:GLN:HB2	18:R:27:ARG:HD2	1.95	0.48
1:2:557:U:H2'	1:2:558:G:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1224:G:H21	18:R:142:GLN:HE22	1.61	0.48
6:F:112:HIS:NE2	6:F:237:SER:O	2.47	0.48
20:T:51:ASP:OD1	20:T:51:ASP:N	2.46	0.48
20:T:86:ARG:HH12	20:T:106:LYS:HE2	1.79	0.48
1:2:641:A:OP1	11:K:40:LYS:NZ	2.46	0.48
1:2:792:C:H2'	1:2:793:G:H8	1.79	0.48
22:V:24:LEU:HG	22:V:32:LEU:HD11	1.95	0.48
25:Y:107:ARG:HD3	25:Y:112:VAL:HG22	1.96	0.48
7:G:39:ILE:HA	7:G:68:ILE:HD11	1.96	0.47
23:W:34:MET:HB2	23:W:53:TYR:HB2	1.96	0.47
1:2:1183:A:H2'	1:2:1184:G:H8	1.78	0.47
2:B:156:TYR:HE1	23:W:61:ARG:HG3	1.78	0.47
4:D:138:GLY:HA3	4:D:162:ILE:HG22	1.97	0.47
4:D:183:LYS:HE3	24:X:95:PRO:HA	1.96	0.47
6:F:11:ARG:NH1	6:F:21:ASP:O	2.42	0.47
15:O:36:GLN:HA	15:O:39:LYS:HG2	1.96	0.47
34:h:149:GLU:CD	34:h:150:TRP:H	2.22	0.47
1:2:1472:C:O2'	34:h:15:ASN:OD1	2.33	0.47
9:I:101:LEU:O	9:I:116:ARG:NH1	2.48	0.47
13:M:24:LEU:HD21	13:M:30:LYS:HE3	1.96	0.47
1:2:844:U:O2'	6:F:255:ARG:NH2	2.46	0.47
1:2:1719:A:OP1	35:n:25:LYS:NZ	2.48	0.47
1:2:1722:G:O6	1:2:1812:U:O2	2.32	0.47
16:P:95:ILE:HB	16:P:129:ILE:HG22	1.97	0.47
18:R:82:TYR:HA	18:R:85:ARG:HG2	1.96	0.47
34:h:156:PHE:HA	34:h:165:ILE:HG22	1.96	0.47
1:2:165:G:H4'	8:H:53:SER:HB2	1.96	0.47
1:2:1216:C:N4	1:2:1342:U:OP1	2.47	0.47
1:2:1541:G:H4'	21:U:15:VAL:HG21	1.97	0.47
1:2:1746:U:H4'	8:H:65:GLN:HE22	1.79	0.47
4:D:173:LYS:HG2	23:W:3:ASN:HA	1.97	0.47
23:W:40:ASP:HB3	23:W:44:GLY:H	1.80	0.47
1:2:15:U:O2'	1:2:669:A:N6	2.48	0.47
1:2:572:U:OP1	26:Z:60:PHE:N	2.45	0.47
19:S:99:ASP:O	19:S:102:THR:OG1	2.32	0.47
27:a:49:LEU:HA	27:a:83:LEU:HD21	1.96	0.47
29:c:67:THR:HG23	29:c:69:GLY:H	1.79	0.47
30:d:13:ARG:N	30:d:33:GLU:O	2.47	0.47
1:2:1251:A:N6	18:R:146:ARG:OXT	2.48	0.47
13:M:89:ARG:NH1	13:M:91:ASP:OD1	2.48	0.47
25:Y:40:PRO:HB3	25:Y:79:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:38:LYS:HE2	28:b:40:VAL:HB	1.97	0.47
1:2:560:A:H5'	11:K:174:LYS:HB2	1.96	0.47
24:X:66:THR:HG23	24:X:68:ARG:H	1.80	0.47
1:2:1397:U:OP1	34:h:60:ARG:NH2	2.48	0.46
1:2:1453:C:OP1	19:S:48:ASN:ND2	2.44	0.46
5:E:193:ASP:N	5:E:193:ASP:OD1	2.46	0.46
1:2:617:G:N7	25:Y:67:ARG:NH2	2.63	0.46
1:2:1616:U:O2'	1:2:1661:A:N3	2.46	0.46
6:F:179:ASN:HA	6:F:231:GLY:H	1.80	0.46
15:O:49:GLN:HA	15:O:52:VAL:HG12	1.97	0.46
1:2:1533:A:N6	1:2:1602:U:C2	2.82	0.46
1:2:1662:U:O4	1:2:1663:A:N6	2.49	0.46
3:C:35:ALA:HB1	3:C:39:PHE:HD2	1.79	0.46
11:K:111:GLN:HE21	11:K:123:ILE:HG13	1.80	0.46
1:2:94:G:HO2'	1:2:508:A:HO2'	1.61	0.46
6:F:61:VAL:HG12	6:F:80:ILE:HD12	1.98	0.46
19:S:94:GLU:HA	19:S:116:ASN:ND2	2.31	0.46
1:2:596:U:H2'	1:2:597:G:C5	2.51	0.46
1:2:602:G:H3'	1:2:603:C:H2'	1.97	0.46
2:B:8:LEU:O	2:B:55:TRP:NE1	2.45	0.46
5:E:136:VAL:HG22	5:E:186:VAL:HG23	1.97	0.46
20:T:81:ASP:OD1	20:T:81:ASP:N	2.46	0.46
23:W:53:TYR:OH	23:W:76:ASP:OD2	2.31	0.46
32:f:78:SER:O	32:f:81:ARG:NH1	2.48	0.46
1:2:1064:C:H2'	1:2:1065:G:H8	1.79	0.46
1:2:1495:G:O2'	31:e:26:ASN:ND2	2.46	0.46
6:F:176:ASP:OD1	6:F:177:THR:N	2.49	0.46
20:T:21:ASP:OD1	20:T:21:ASP:N	2.49	0.46
29:c:34:ASP:HB2	29:c:43:ILE:HD11	1.97	0.46
1:2:291:G:N2	13:M:40:ILE:O	2.42	0.46
1:2:1004:U:H2'	1:2:1005:G:H8	1.80	0.46
1:2:110:U:H3	1:2:351:G:H1	1.64	0.46
1:2:1668:U:OP2	18:R:141:TYR:OH	2.34	0.46
9:I:118:ARG:HA	9:I:121:THR:HG23	1.98	0.46
11:K:162:ARG:HH12	26:Z:30:PRO:HB2	1.81	0.46
14:N:65:VAL:HA	14:N:68:LEU:HG	1.98	0.46
36:z:310:A:H2'	36:z:311:G:H8	1.81	0.46
1:2:97:U:O2	1:2:434:G:N2	2.49	0.46
12:L:42:ASN:OD1	12:L:42:ASN:N	2.49	0.46
1:2:1391:C:H4'	22:V:83:ARG:HH22	1.80	0.46
5:E:26:THR:HG23	5:E:173:ARG:HH12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:18:LYS:HB3	29:c:18:LYS:HE3	1.78	0.46
1:2:570:C:O2'	26:Z:34:THR:O	2.33	0.45
1:2:1620:A:H2'	17:Q:40:ARG:HH21	1.80	0.45
2:B:113:GLN:HG2	2:B:115:ALA:H	1.81	0.45
4:D:78:LEU:HA	4:D:81:ILE:HD12	1.98	0.45
5:E:157:MET:HE3	5:E:187:LYS:HE3	1.97	0.45
1:2:1048:G:N1	1:2:1069:U:OP2	2.45	0.45
1:2:1154:U:H1'	4:D:194:ARG:HE	1.81	0.45
9:I:29:GLU:OE2	9:I:86:LYS:NZ	2.35	0.45
9:I:77:VAL:HG23	9:I:78:ARG:HG2	1.99	0.45
11:K:65:GLU:HG3	11:K:66:LYS:HG3	1.97	0.45
34:h:166:VAL:HG23	34:h:176:VAL:HG22	1.98	0.45
1:2:562:U:H3	1:2:587:A:H62	1.64	0.45
1:2:1360:U:O2'	1:2:1379:A:OP2	2.35	0.45
15:O:56:ASP:OD1	29:c:52:THR:OG1	2.27	0.45
20:T:71:MET:HE1	20:T:99:LEU:HD11	1.97	0.45
1:2:980:A:H2'	1:2:981:A:C8	2.51	0.45
5:E:59:LEU:HA	5:E:66:ILE:HG12	1.98	0.45
8:H:88:ARG:HB2	8:H:91:GLU:HB2	1.99	0.45
18:R:67:ASP:OD2	18:R:69:ARG:NH1	2.49	0.45
1:2:928:G:H2'	1:2:929:G:C8	2.51	0.45
1:2:1174:U:H2'	1:2:1175:G:H8	1.82	0.45
1:2:1472:C:H42	1:2:1476:A:H62	1.64	0.45
1:2:1718:G:N2	1:2:1814:G:O2'	2.49	0.45
5:E:40:ARG:HD3	5:E:47:GLU:HB3	1.99	0.45
7:G:29:GLN:H	7:G:110:GLN:HE22	1.63	0.45
14:N:95:ASP:O	14:N:101:ARG:NH1	2.49	0.45
1:2:683:G:H4'	24:X:4:MET:HB3	1.98	0.45
23:W:27:LYS:HA	23:W:27:LYS:HD2	1.80	0.45
1:2:442:C:H42	1:2:449:A:H62	1.65	0.45
1:2:823:U:H5	11:K:143:ASN:H	1.63	0.45
1:2:996:A:H5'	15:O:7:PRO:HG3	1.99	0.45
1:2:1248:U:H4'	18:R:146:ARG:HA	1.99	0.45
1:2:1365:G:H2'	1:2:1366:G:H8	1.82	0.45
1:2:1392:U:H2'	1:2:1393:G:C8	2.52	0.45
1:2:436:G:H2'	1:2:437:G:C8	2.51	0.45
1:2:681:U:H4'	25:Y:9:THR:HG22	1.99	0.45
1:2:1308:U:O2	33:g:135:HIS:NE2	2.50	0.45
9:I:87:PHE:HB3	9:I:90:LYS:HB2	1.99	0.45
1:2:1048:G:H1'	1:2:1071:G:H22	1.81	0.45
8:H:70:HIS:HB3	8:H:101:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:118:ARG:HB2	33:g:131:PHE:HD2	1.81	0.45
30:d:10:LYS:NZ	30:d:59:LEU:O	2.50	0.45
32:f:79:LEU:HA	32:f:81:ARG:HH11	1.82	0.45
34:h:124:SER:OG	34:h:125:ARG:N	2.50	0.45
1:2:75:G:N2	8:H:155:GLN:O	2.49	0.44
1:2:981:A:H2'	1:2:982:G:C8	2.52	0.44
1:2:1232:U:O2	1:2:1526:G:N2	2.42	0.44
1:2:1562:C:OP1	21:U:74:SER:N	2.49	0.44
2:B:21:ALA:HB2	2:B:173:LEU:HD13	1.99	0.44
10:J:110:ARG:NH1	10:J:114:GLU:OE2	2.49	0.44
26:Z:20:ARG:NH2	26:Z:22:GLN:OE1	2.50	0.44
11:K:93:LYS:HB2	11:K:96:TYR:HD2	1.82	0.44
33:g:141:CYS:HB3	33:g:146:LEU:H	1.82	0.44
34:h:159:ASN:HB2	34:h:204:GLY:HA3	1.99	0.44
1:2:958:G:H2'	1:2:959:G:C4	2.52	0.44
1:2:1007:C:H2'	1:2:1008:A:C8	2.53	0.44
1:2:1864:U:OP2	28:b:5:ARG:NH2	2.50	0.44
20:T:5:ILE:HD12	20:T:6:PRO:HD2	1.99	0.44
1:2:360:A:H4'	1:2:361:U:H3'	1.98	0.44
1:2:1550:G:O2'	1:2:1558:C:O2	2.31	0.44
1:2:1592:C:OP1	7:G:91:ARG:NH2	2.50	0.44
8:H:67:VAL:HG12	8:H:100:CYS:HB3	1.98	0.44
19:S:43:SER:OG	19:S:44:LYS:N	2.51	0.44
22:V:38:ASP:HA	22:V:41:ARG:HH21	1.83	0.44
25:Y:140:ARG:HH21	25:Y:142:ARG:HH11	1.64	0.44
1:2:1536:G:H2'	1:2:1537:A:C8	2.53	0.44
2:B:51:LEU:O	2:B:54:THR:OG1	2.28	0.44
5:E:66:ILE:HD12	5:E:86:LEU:HD22	1.99	0.44
6:F:93:ASP:OD1	6:F:93:ASP:N	2.47	0.44
9:I:101:LEU:HD13	9:I:120:ARG:HG2	1.99	0.44
1:2:64:A:H2	1:2:83:A:H62	1.64	0.44
1:2:420:G:H2'	1:2:660:C:H42	1.83	0.44
1:2:948:C:H42	1:2:978:G:H1	1.64	0.44
1:2:1291:A:N1	1:2:1309:C:N4	2.57	0.44
3:C:51:ARG:HB3	3:C:53:GLN:HE22	1.81	0.44
14:N:35:ILE:HG22	14:N:108:CYS:HB2	2.00	0.44
16:P:45:THR:OG1	16:P:46:ASP:N	2.51	0.44
19:S:10:LYS:O	19:S:14:ARG:HG2	2.18	0.44
1:2:1832:A:H5'	1:2:1840:U:H5'	2.00	0.44
8:H:140:ARG:HA	8:H:143:LYS:HG2	1.99	0.44
13:M:115:PRO:O	13:M:118:ARG:NH1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:70:ILE:HA	20:T:77:TYR:HD2	1.82	0.44
1:2:1620:A:O2'	1:2:1624:U:OP1	2.35	0.43
11:K:109:ARG:HH21	11:K:127:ARG:HH12	1.66	0.43
18:R:97:GLN:HB2	18:R:105:LYS:HD2	1.99	0.43
1:2:1415:C:H4'	21:U:129:ARG:HB2	2.00	0.43
9:I:40:LEU:HA	9:I:43:LEU:HD13	2.00	0.43
24:X:86:LEU:HD23	24:X:117:ARG:HE	1.82	0.43
28:b:12:LYS:HE3	28:b:16:GLY:HA2	2.00	0.43
34:h:5:MET:HE1	34:h:312:VAL:HG22	1.99	0.43
1:2:1123:C:O2'	3:C:148:ASN:O	2.31	0.43
29:c:48:SER:O	29:c:71:ALA:N	2.50	0.43
1:2:94:G:O2'	1:2:508:A:O2'	2.34	0.43
1:2:219:U:O2'	10:J:177:SER:OG	2.35	0.43
1:2:1157:G:O2'	24:X:74:VAL:O	2.34	0.43
12:L:55:ARG:NH1	12:L:78:TYR:OH	2.52	0.43
34:h:195:LEU:HA	34:h:211:GLY:HA3	1.99	0.43
1:2:571:U:OP1	26:Z:37:LYS:NZ	2.51	0.43
4:D:68:ARG:HD2	4:D:68:ARG:HA	1.76	0.43
15:O:4:MET:HG2	15:O:5:HIS:HD2	1.82	0.43
16:P:63:LYS:HA	16:P:63:LYS:HD3	1.76	0.43
34:h:174:VAL:HB	34:h:188:HIS:HB2	2.01	0.43
1:2:5:U:H2'	1:2:6:G:C8	2.53	0.43
1:2:1179:G:O2'	1:2:1181:A:N6	2.41	0.43
34:h:76:GLN:HA	34:h:92:LEU:HD13	2.00	0.43
36:z:307:G:N2	36:z:330:A:O3'	2.51	0.43
1:2:677:G:N1	1:2:1027:A:OP2	2.37	0.43
5:E:140:GLY:HA3	5:E:182:LEU:HG	2.01	0.43
7:G:122:ARG:HD3	30:d:59:LEU:HD21	2.01	0.43
24:X:3:ARG:HD3	24:X:6:VAL:HG12	2.00	0.43
1:2:1172:U:O2	1:2:1188:A:N7	2.52	0.43
1:2:1351:G:H1	1:2:1353:A:H62	1.67	0.43
3:C:180:ASP:OD1	3:C:180:ASP:N	2.47	0.43
17:Q:118:GLU:HG3	20:T:120:HIS:H	1.83	0.43
18:R:19:ALA:HB2	18:R:75:GLY:HA3	1.99	0.43
24:X:41:MET:HE1	24:X:129:PHE:CG	2.54	0.43
25:Y:67:ARG:NH1	25:Y:114:ASP:OD2	2.52	0.43
1:2:149:A:H3'	1:2:150:A:H8	1.83	0.43
1:2:603:C:H5'	11:K:20:PHE:HB3	2.01	0.43
1:2:1013:U:O2'	1:2:1104:G:N3	2.52	0.43
17:Q:100:LYS:HE3	17:Q:100:LYS:HB2	1.85	0.43
21:U:76:THR:HG22	21:U:94:ARG:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:104:LEU:HB3	24:X:125:ILE:HD12	2.01	0.43
1:2:433:A:H2'	1:2:434:G:C8	2.54	0.43
1:2:543:C:H3'	1:2:544:G:H8	1.84	0.43
2:B:10:MET:SD	2:B:10:MET:N	2.91	0.43
2:B:74:VAL:HG13	2:B:121:LEU:HB2	2.00	0.43
3:C:107:ARG:HH22	16:P:135:ILE:H	1.67	0.43
4:D:114:LYS:HB2	4:D:123:ARG:HH12	1.84	0.43
4:D:200:ARG:O	11:K:54:ARG:NH2	2.38	0.43
7:G:127:ARG:NH2	7:G:130:ARG:O	2.43	0.43
13:M:111:VAL:HG11	13:M:128:VAL:HG11	2.00	0.43
22:V:24:LEU:O	22:V:87:ARG:N	2.47	0.43
34:h:256:ILE:HB	34:h:270:LEU:HB3	2.00	0.43
2:B:180:ARG:HG3	2:B:195:TRP:HE1	1.83	0.42
9:I:66:VAL:HG12	9:I:98:ARG:HH21	1.84	0.42
18:R:90:LYS:HE2	18:R:90:LYS:HB3	1.93	0.42
26:Z:56:PHE:HB2	26:Z:74:MET:HB2	2.01	0.42
32:f:101:ARG:HG2	32:f:105:ALA:H	1.83	0.42
34:h:61:GLY:O	34:h:88:ARG:NH2	2.52	0.42
1:2:399:C:N3	13:M:104:LYS:NZ	2.66	0.42
1:2:611:G:H2'	1:2:612:U:H6	1.83	0.42
1:2:1403:C:OP2	1:2:1405:A:N6	2.44	0.42
4:D:146:GLU:OE1	5:E:120:TYR:OH	2.33	0.42
7:G:42:LYS:HG3	7:G:43:GLU:HG2	2.01	0.42
20:T:86:ARG:NE	20:T:89:ASP:OD2	2.52	0.42
36:z:252:A:O2'	36:z:284:U:OP2	2.36	0.42
1:2:16:G:N2	1:2:1195:A:N6	2.45	0.42
1:2:372:U:H2'	1:2:373:G:C8	2.54	0.42
1:2:482:G:N2	1:2:485:A:OP2	2.52	0.42
1:2:1144:A:H2'	1:2:1145:A:C8	2.54	0.42
1:2:1199:A:H2'	1:2:1200:A:C8	2.54	0.42
1:2:1379:A:H2'	1:2:1380:C:C6	2.54	0.42
5:E:54:ARG:NE	5:E:57:ASN:OD1	2.48	0.42
7:G:16:ASP:OD1	7:G:16:ASP:N	2.51	0.42
1:2:830:A:OP2	1:2:846:G:N2	2.51	0.42
7:G:168:THR:HG21	27:a:106:GLN:HB3	2.01	0.42
11:K:162:ARG:NH2	26:Z:30:PRO:O	2.53	0.42
12:L:35:LEU:HD12	12:L:35:LEU:HA	1.87	0.42
19:S:36:GLU:HB2	19:S:47:ARG:HH11	1.84	0.42
33:g:118:ARG:HD3	33:g:133:ALA:HB2	2.01	0.42
1:2:292:A:O2'	13:M:39:ASN:O	2.37	0.42
1:2:800:U:O4	9:I:106:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1619:A:OP1	17:Q:47:ARG:NH1	2.52	0.42
17:Q:47:ARG:HB2	17:Q:50:ARG:HH12	1.83	0.42
1:2:1291:A:H3'	1:2:1302:G:H8	1.84	0.42
1:2:1388:A:H61	5:E:161:GLY:HA2	1.84	0.42
25:Y:77:ASN:HB2	25:Y:79:LYS:HG3	2.01	0.42
29:c:65:GLN:HB3	29:c:72:ARG:HB2	2.02	0.42
1:2:363:A:N6	1:2:400:C:O2	2.53	0.42
1:2:652:U:H2'	1:2:653:A:C8	2.55	0.42
1:2:1465:A:H5'	19:S:60:ARG:HH21	1.83	0.42
3:C:34:LYS:HE3	3:C:34:LYS:HB3	1.91	0.42
4:D:123:ARG:HB2	4:D:145:LYS:HA	2.01	0.42
1:2:448:A:H5''	10:J:25:ARG:HA	2.01	0.42
1:2:1615:U:H3'	17:Q:43:ARG:HH22	1.84	0.42
14:N:52:LEU:HD23	14:N:78:LYS:HE2	2.02	0.42
1:2:649:U:O2	25:Y:45:SER:OG	2.34	0.42
3:C:49:VAL:HG21	3:C:62:LEU:HD13	2.02	0.42
10:J:22:HIS:ND1	10:J:23:LYS:O	2.48	0.42
20:T:69:THR:HA	20:T:72:GLN:HG3	2.02	0.42
1:2:69:C:OP2	8:H:164:LYS:NZ	2.53	0.42
1:2:98:C:OP2	1:2:426:A:O2'	2.32	0.42
1:2:223:C:H2'	1:2:224:A:H8	1.84	0.42
1:2:1395:C:N3	1:2:1451:G:N2	2.67	0.42
1:2:1836:G:OP2	1:2:1839:U:O2'	2.32	0.42
26:Z:86:GLU:OE2	26:Z:90:ARG:NH1	2.52	0.42
29:c:20:LYS:HG3	29:c:21:LYS:HG3	2.01	0.42
1:2:1270:G:N2	1:2:1513:C:O2	2.53	0.41
2:B:164:ASN:O	2:B:170:SER:OG	2.27	0.41
4:D:214:LEU:HD12	4:D:219:ILE:HG21	2.02	0.41
8:H:121:ILE:N	8:H:125:THR:OG1	2.52	0.41
12:L:85:LEU:HB3	12:L:89:ILE:HD11	2.02	0.41
1:2:670:A:HO2'	1:2:1163:C:HO2'	1.52	0.41
1:2:1204:G:H2'	1:2:1205:G:C4	2.55	0.41
1:2:1452:A:C6	1:2:1473:G:N2	2.88	0.41
4:D:108:LYS:HD2	4:D:233:LEU:HD12	2.02	0.41
17:Q:42:ARG:O	17:Q:46:SER:CB	2.64	0.41
19:S:101:ASP:OD2	19:S:101:ASP:N	2.51	0.41
1:2:5:U:OP2	4:D:230:THR:OG1	2.29	0.41
1:2:507:G:OP2	26:Z:104:ARG:NH2	2.53	0.41
6:F:40:GLU:OE2	6:F:40:GLU:N	2.53	0.41
16:P:53:ILE:HG23	16:P:88:LEU:HD13	2.03	0.41
27:a:91:LEU:HB3	27:a:97:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:20:GLN:HB3	34:h:34:ALA:HB3	2.03	0.41
1:2:1232:U:H2'	1:2:1233:G:C8	2.56	0.41
1:2:1653:U:H2'	1:2:1654:G:C8	2.56	0.41
4:D:58:LYS:HA	4:D:58:LYS:HD2	1.89	0.41
8:H:157:VAL:HG11	8:H:176:ILE:HD11	2.02	0.41
21:U:65:TYR:HE1	21:U:128:GLN:NE2	2.18	0.41
21:U:85:ASN:HD22	21:U:88:MET:HB2	1.85	0.41
24:X:83:LEU:HD23	24:X:83:LEU:HA	1.93	0.41
1:2:561:A:H5'	11:K:171:GLY:HA3	2.02	0.41
1:2:183:G:O2'	1:2:184:G:O4'	2.34	0.41
1:2:594:A:O4'	1:2:643:A:N6	2.54	0.41
1:2:1241:A:O2'	1:2:1266:C:O2'	2.29	0.41
1:2:1249:C:H5''	1:2:1250:A:H2'	2.02	0.41
7:G:193:LYS:O	7:G:197:GLU:HG2	2.21	0.41
27:a:94:LYS:HG3	27:a:96:LEU:HD13	2.03	0.41
30:d:14:VAL:HG13	30:d:53:GLY:H	1.84	0.41
34:h:22:ALA:HB3	34:h:32:LEU:HB3	2.02	0.41
34:h:152:SER:H	34:h:169:GLY:HA2	1.84	0.41
1:2:73:C:H2'	1:2:74:G:H4'	2.02	0.41
1:2:1058:A:H61	1:2:1829:G:H5''	1.86	0.41
3:C:72:ALA:HB3	16:P:128:ARG:HH22	1.86	0.41
11:K:46:VAL:HG21	11:K:106:LEU:HD12	2.02	0.41
13:M:96:ILE:HG22	13:M:98:LYS:H	1.85	0.41
1:2:96:C:H1'	1:2:474:G:H5'	2.02	0.41
1:2:907:G:H2'	1:2:908:A:C8	2.55	0.41
1:2:963:A:H2'	1:2:964:A:C8	2.56	0.41
1:2:1317:C:H2'	1:2:1318:G:H8	1.86	0.41
5:E:65:ARG:HG3	5:E:69:LEU:HD23	2.02	0.41
8:H:21:GLU:OE1	8:H:28:TYR:OH	2.32	0.41
9:I:82:GLU:HG2	9:I:83:LEU:HD12	2.03	0.41
13:M:4:ILE:HG13	13:M:5:GLN:HG2	2.02	0.41
22:V:54:VAL:HB	22:V:88:LEU:HB2	2.03	0.41
23:W:66:ASP:HA	23:W:69:ILE:HG22	2.03	0.41
27:a:98:LYS:NZ	27:a:110:THR:OG1	2.42	0.41
30:d:44:ARG:HG3	30:d:58:LEU:HD21	2.03	0.41
34:h:175:LYS:HD3	34:h:177:TRP:HE1	1.86	0.41
1:2:145:G:H2'	1:2:146:G:C8	2.56	0.41
1:2:1424:G:H2'	1:2:1425:G:H8	1.86	0.41
3:C:144:LYS:HA	3:C:144:LYS:HD2	1.87	0.41
8:H:25:ARG:HA	8:H:28:TYR:HD2	1.85	0.41
9:I:60:ILE:HD12	9:I:60:ILE:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:34:PHE:HD2	16:P:98:ARG:HD3	1.86	0.41
31:e:50:ILE:HG23	31:e:52:PHE:H	1.86	0.41
1:2:1033:G:H1	1:2:1080:A:HO2'	1.69	0.40
4:D:259:THR:HB	23:W:16:LYS:HD2	2.02	0.40
6:F:15:PRO:HG2	6:F:18:TRP:CD1	2.56	0.40
15:O:66:VAL:HG13	15:O:67:THR:HG23	2.01	0.40
30:d:21:THR:OG1	30:d:22:GLY:N	2.54	0.40
1:2:454:U:H2'	1:2:455:A:C8	2.57	0.40
2:B:37:TYR:HD2	2:B:162:PRO:HG3	1.86	0.40
10:J:11:ARG:NE	10:J:15:GLY:O	2.43	0.40
13:M:80:MET:HA	13:M:86:ILE:HG22	2.03	0.40
1:2:43:U:OP2	1:2:485:A:N6	2.45	0.40
1:2:919:A:H4'	1:2:920:A:H5''	2.03	0.40
1:2:1083:A:N7	1:2:1841:C:O2'	2.54	0.40
1:2:1221:G:H2'	1:2:1222:G:C8	2.56	0.40
4:D:65:LYS:HD2	4:D:273:LEU:HD13	2.02	0.40
8:H:195:LYS:HB2	8:H:195:LYS:HE3	1.91	0.40
9:I:46:THR:HG21	9:I:97:GLN:HG3	2.03	0.40
27:a:70:PRO:HA	27:a:73:VAL:HG22	2.02	0.40
1:2:557:U:H2'	1:2:558:G:C6	2.56	0.40
1:2:1358:U:H2'	1:2:1359:U:C6	2.56	0.40
1:2:1513:C:H2'	1:2:1514:G:C8	2.57	0.40
2:B:81:ASN:HA	2:B:84:GLN:HB2	2.02	0.40
3:C:71:LEU:HA	3:C:74:LEU:HB3	2.03	0.40
3:C:181:LEU:HA	3:C:184:VAL:HG22	2.03	0.40
6:F:36:HIS:CD2	6:F:85:GLY:HA3	2.57	0.40
6:F:115:THR:HG23	6:F:118:GLU:H	1.85	0.40
7:G:179:ASN:HB3	7:G:186:ASN:HB3	2.03	0.40
15:O:73:ARG:HD3	15:O:76:LYS:HD3	2.03	0.40
16:P:142:ARG:NH2	28:b:26:CYS:O	2.54	0.40
17:Q:18:ARG:HA	20:T:90:VAL:HA	2.04	0.40
19:S:102:THR:HA	19:S:105:MET:HB2	2.03	0.40
22:V:80:PHE:HB3	31:e:52:PHE:HB3	2.03	0.40
1:2:223:C:H2'	1:2:224:A:C8	2.56	0.40
11:K:103:GLU:O	11:K:107:GLU:HB2	2.21	0.40
14:N:26:LEU:HD23	14:N:31:LEU:HD21	2.04	0.40
20:T:74:PRO:HB2	20:T:79:ILE:HB	2.02	0.40
35:n:1:MET:HE2	35:n:1:MET:HB2	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	215/295 (73%)	204 (95%)	11 (5%)	0	100	100
3	C	211/264 (80%)	196 (93%)	15 (7%)	0	100	100
4	D	219/221 (99%)	209 (95%)	10 (5%)	0	100	100
5	E	226/281 (80%)	218 (96%)	8 (4%)	0	100	100
6	F	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
7	G	189/204 (93%)	179 (95%)	10 (5%)	0	100	100
8	H	235/249 (94%)	227 (97%)	8 (3%)	0	100	100
9	I	181/432 (42%)	173 (96%)	8 (4%)	0	100	100
10	J	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
11	K	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
12	L	94/149 (63%)	89 (95%)	5 (5%)	0	100	100
13	M	149/158 (94%)	139 (93%)	10 (7%)	0	100	100
14	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100
15	O	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
16	P	134/168 (80%)	123 (92%)	11 (8%)	0	100	100
17	Q	113/145 (78%)	106 (94%)	7 (6%)	0	100	100
18	R	140/172 (81%)	132 (94%)	8 (6%)	0	100	100
19	S	130/135 (96%)	117 (90%)	13 (10%)	0	100	100
20	T	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
21	U	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
22	V	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
23	W	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
24	X	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
25	Y	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
26	Z	122/131 (93%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	a	75/124 (60%)	72 (96%)	3 (4%)	0	100	100
28	b	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
29	c	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
30	d	65/69 (94%)	57 (88%)	8 (12%)	0	100	100
31	e	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
32	f	55/133 (41%)	50 (91%)	5 (9%)	0	100	100
33	g	66/188 (35%)	61 (92%)	5 (8%)	0	100	100
34	h	311/317 (98%)	291 (94%)	20 (6%)	0	100	100
35	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	4821/5821 (83%)	4567 (95%)	254 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	180/245 (74%)	180 (100%)	0	100	100
3	C	194/231 (84%)	194 (100%)	0	100	100
4	D	187/187 (100%)	187 (100%)	0	100	100
5	E	190/232 (82%)	190 (100%)	0	100	100
6	F	224/225 (100%)	224 (100%)	0	100	100
7	G	161/170 (95%)	161 (100%)	0	100	100
8	H	207/218 (95%)	207 (100%)	0	100	100
9	I	165/360 (46%)	165 (100%)	0	100	100
10	J	178/180 (99%)	178 (100%)	0	100	100
11	K	161/168 (96%)	161 (100%)	0	100	100
12	L	87/125 (70%)	87 (100%)	0	100	100
13	M	136/142 (96%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	99/108 (92%)	99 (100%)	0	100	100
15	O	130/131 (99%)	130 (100%)	0	100	100
16	P	106/130 (82%)	106 (100%)	0	100	100
17	Q	105/130 (81%)	105 (100%)	0	100	100
18	R	117/140 (84%)	117 (100%)	0	100	100
19	S	119/121 (98%)	119 (100%)	0	100	100
20	T	125/132 (95%)	125 (100%)	0	100	100
21	U	111/116 (96%)	111 (100%)	0	100	100
22	V	92/107 (86%)	92 (100%)	0	100	100
23	W	67/67 (100%)	67 (100%)	0	100	100
24	X	112/113 (99%)	112 (100%)	0	100	100
25	Y	113/115 (98%)	113 (100%)	0	100	100
26	Z	107/113 (95%)	107 (100%)	0	100	100
27	a	68/102 (67%)	68 (100%)	0	100	100
28	b	88/88 (100%)	88 (100%)	0	100	100
29	c	75/76 (99%)	75 (100%)	0	100	100
30	d	60/62 (97%)	60 (100%)	0	100	100
31	e	48/49 (98%)	48 (100%)	0	100	100
32	f	47/106 (44%)	47 (100%)	0	100	100
33	g	61/154 (40%)	61 (100%)	0	100	100
34	h	272/275 (99%)	272 (100%)	0	100	100
35	n	24/24 (100%)	24 (100%)	0	100	100
All	All	4216/4942 (85%)	4216 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	164	ASN
3	C	53	GLN
6	F	36	HIS
6	F	142	HIS
6	F	224	ASN

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Mol	Chain	Res	Type
7	G	36	GLN
7	G	79	HIS
7	G	148	ASN
7	G	179	ASN
9	I	162	GLN
10	J	146	GLN
10	J	181	GLN
11	K	111	GLN
11	K	132	GLN
11	K	143	ASN
12	L	7	ASN
14	N	72	HIS
17	Q	41	GLN
18	R	48	GLN
19	S	93	GLN
21	U	11	GLN
21	U	128	GLN
24	X	90	GLN
25	Y	61	GLN
27	a	46	ASN
28	b	72	HIS
30	d	45	ASN
31	e	3	HIS
34	h	4	GLN
34	h	26	GLN
34	h	178	ASN
34	h	188	HIS
34	h	244	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	400 (23%)	8 (0%)
36	z	160/400 (40%)	48 (30%)	0
All	All	1845/2270 (81%)	448 (24%)	8 (0%)

All (448) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C

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Mol	Chain	Res	Type
1	2	4	C
1	2	14	C
1	2	26	U
1	2	33	G
1	2	41	G
1	2	42	A
1	2	44	U
1	2	45	A
1	2	46	A
1	2	56	G
1	2	58	C
1	2	61	A
1	2	62	G
1	2	65	C
1	2	67	C
1	2	68	A
1	2	73	C
1	2	74	G
1	2	75	G
1	2	77	A
1	2	92	A
1	2	102	A
1	2	103	A
1	2	110	U
1	2	113	G
1	2	115	U
1	2	126	G
1	2	130	G
1	2	142	C
1	2	143	U
1	2	147	A
1	2	155	G
1	2	161	U
1	2	162	C
1	2	171	A
1	2	175	A
1	2	182	C
1	2	183	G
1	2	184	G
1	2	192	C
1	2	199	C
1	2	201	C

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Mol	Chain	Res	Type
1	2	218	U
1	2	292	A
1	2	302	A
1	2	306	C
1	2	309	G
1	2	312	G
1	2	319	C
1	2	335	G
1	2	347	G
1	2	351	G
1	2	364	A
1	2	369	C
1	2	370	G
1	2	371	A
1	2	377	G
1	2	378	U
1	2	381	C
1	2	383	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	393	U
1	2	398	A
1	2	400	C
1	2	408	A
1	2	409	C
1	2	413	G
1	2	417	C
1	2	418	A
1	2	420	G
1	2	426	A
1	2	435	A
1	2	438	G
1	2	446	G
1	2	448	A
1	2	449	A
1	2	450	C
1	2	452	G
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C

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Mol	Chain	Res	Type
1	2	474	G
1	2	476	A
1	2	487	U
1	2	488	U
1	2	489	A
1	2	492	C
1	2	493	A
1	2	498	C
1	2	500	A
1	2	501	C
1	2	502	C
1	2	503	C
1	2	508	A
1	2	509	G
1	2	517	C
1	2	525	A
1	2	531	A
1	2	532	C
1	2	533	A
1	2	534	G
1	2	536	A
1	2	539	C
1	2	540	U
1	2	542	U
1	2	544	G
1	2	548	C
1	2	549	C
1	2	550	C
1	2	551	U
1	2	552	G
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	561	A
1	2	562	U
1	2	569	A
1	2	576	A
1	2	583	A
1	2	588	G
1	2	590	A
1	2	591	U

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Mol	Chain	Res	Type
1	2	595	U
1	2	596	U
1	2	597	G
1	2	600	G
1	2	603	C
1	2	606	G
1	2	607	U
1	2	608	C
1	2	613	G
1	2	614	C
1	2	621	C
1	2	623	G
1	2	627	U
1	2	628	A
1	2	642	U
1	2	643	A
1	2	644	G
1	2	650	A
1	2	655	A
1	2	660	C
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	684	G
1	2	688	U
1	2	689	U
1	2	693	A
1	2	731	G
1	2	752	G
1	2	753	C
1	2	754	G
1	2	755	C
1	2	799	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	834	C
1	2	844	U
1	2	847	A

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Mol	Chain	Res	Type
1	2	853	C
1	2	858	A
1	2	859	G
1	2	860	G
1	2	861	A
1	2	862	A
1	2	864	A
1	2	867	G
1	2	868	G
1	2	870	A
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	888	U
1	2	889	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	898	U
1	2	913	A
1	2	914	U
1	2	917	U
1	2	919	A
1	2	920	A
1	2	933	G
1	2	943	U
1	2	954	U
1	2	957	A
1	2	958	G
1	2	959	G
1	2	961	G
1	2	962	A
1	2	963	A
1	2	969	U
1	2	970	G
1	2	971	G
1	2	985	G
1	2	990	A
1	2	992	A
1	2	999	G

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Mol	Chain	Res	Type
1	2	1002	U
1	2	1017	U
1	2	1021	U
1	2	1022	U
1	2	1023	A
1	2	1024	A
1	2	1026	C
1	2	1049	A
1	2	1053	C
1	2	1055	A
1	2	1061	U
1	2	1062	A
1	2	1076	G
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1088	U
1	2	1089	G
1	2	1107	G
1	2	1109	C
1	2	1114	U
1	2	1118	C
1	2	1121	G
1	2	1133	A
1	2	1138	C
1	2	1139	C
1	2	1149	A
1	2	1151	G
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1156	U
1	2	1157	G
1	2	1161	U
1	2	1170	A
1	2	1180	C
1	2	1203	U
1	2	1208	A
1	2	1215	C
1	2	1217	A
1	2	1221	G

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Mol	Chain	Res	Type
1	2	1224	G
1	2	1229	G
1	2	1235	G
1	2	1242	U
1	2	1243	U
1	2	1249	C
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1264	C
1	2	1272	C
1	2	1274	G
1	2	1275	G
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1293	A
1	2	1294	G
1	2	1299	A
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1308	U
1	2	1311	C
1	2	1313	A
1	2	1314	U
1	2	1318	G
1	2	1319	U
1	2	1327	G
1	2	1332	A
1	2	1337	C
1	2	1341	C
1	2	1342	U
1	2	1354	G
1	2	1356	G
1	2	1358	U
1	2	1361	G
1	2	1362	U
1	2	1363	C
1	2	1364	U

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Mol	Chain	Res	Type
1	2	1371	U
1	2	1372	U
1	2	1377	U
1	2	1378	A
1	2	1390	U
1	2	1396	A
1	2	1397	U
1	2	1404	U
1	2	1405	A
1	2	1416	C
1	2	1428	G
1	2	1429	G
1	2	1439	A
1	2	1442	U
1	2	1447	G
1	2	1452	A
1	2	1453	C
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1473	G
1	2	1476	A
1	2	1477	U
1	2	1489	A
1	2	1490	G
1	2	1494	U
1	2	1495	G
1	2	1497	G
1	2	1498	A
1	2	1507	G
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1531	A
1	2	1540	G
1	2	1548	G
1	2	1551	U
1	2	1552	G
1	2	1553	C
1	2	1554	C
1	2	1556	A
1	2	1560	U

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Mol	Chain	Res	Type
1	2	1567	G
1	2	1570	G
1	2	1575	G
1	2	1578	U
1	2	1580	A
1	2	1584	G
1	2	1586	U
1	2	1588	A
1	2	1591	C
1	2	1601	A
1	2	1604	G
1	2	1606	G
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1638	G
1	2	1648	G
1	2	1660	C
1	2	1665	G
1	2	1675	A
1	2	1680	G
1	2	1683	C
1	2	1695	A
1	2	1697	A
1	2	1698	C
1	2	1715	A
1	2	1721	U
1	2	1722	G
1	2	1744	G
1	2	1750	C
1	2	1754	G
1	2	1756	C
1	2	1757	G
1	2	1761	U
1	2	1772	C
1	2	1775	U
1	2	1776	G
1	2	1779	G
1	2	1781	A
1	2	1782	G
1	2	1783	C
1	2	1797	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1799	G
1	2	1814	G
1	2	1823	A
1	2	1824	A
1	2	1826	G
1	2	1831	A
1	2	1832	A
1	2	1834	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1840	U
1	2	1849	G
1	2	1851	A
1	2	1852	C
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1869	A
36	z	121	C
36	z	122	C
36	z	124	C
36	z	125	C
36	z	128	C
36	z	130	C
36	z	132	G
36	z	136	A
36	z	137	G
36	z	141	U
36	z	143	G
36	z	154	A
36	z	157	C
36	z	161	G
36	z	163	G
36	z	164	U
36	z	165	A
36	z	166	C
36	z	168	C
36	z	169	C
36	z	234	U
36	z	235	G

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Continued from previous page...

Mol	Chain	Res	Type
36	z	237	C
36	z	244	A
36	z	252	A
36	z	253	G
36	z	258	G
36	z	266	G
36	z	270	C
36	z	279	C
36	z	280	C
36	z	281	U
36	z	282	U
36	z	284	U
36	z	288	A
36	z	289	C
36	z	290	U
36	z	295	G
36	z	296	A
36	z	297	U
36	z	302	U
36	z	303	G
36	z	305	U
36	z	306	U
36	z	307	G
36	z	312	U
36	z	324	U
36	z	325	C

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	561	A
1	2	627	U
1	2	688	U
1	2	1137	U
1	2	1637	A
1	2	1664	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

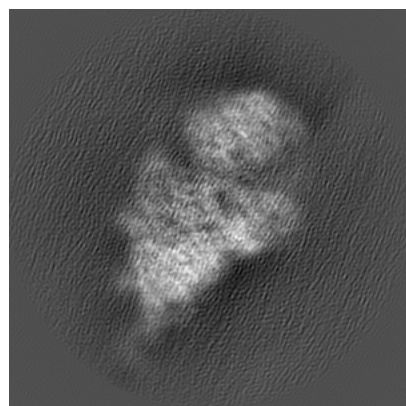
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25533. These allow visual inspection of the internal detail of the map and identification of artifacts.

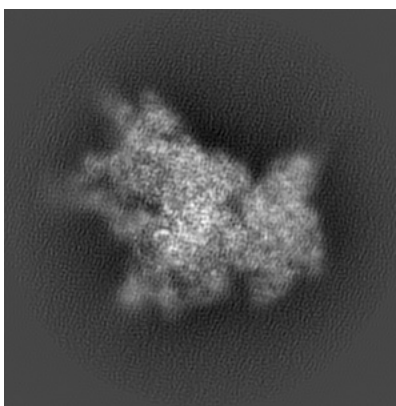
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

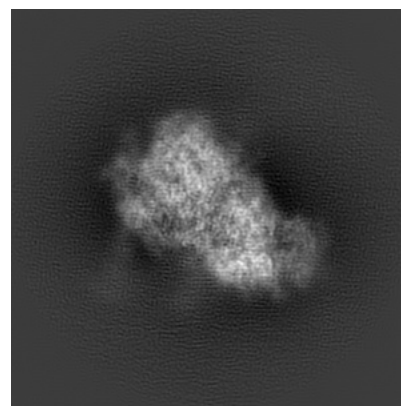
6.1.1 Primary map



X

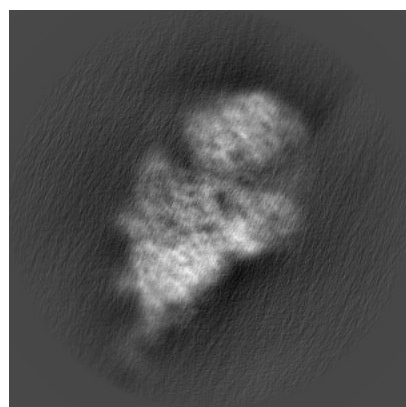


Y

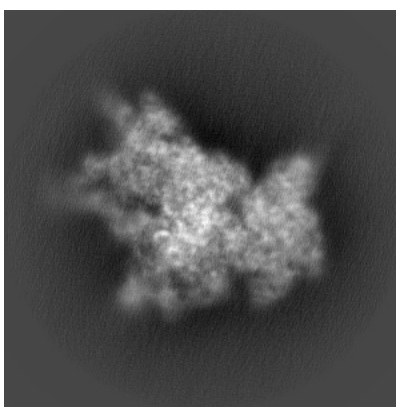


Z

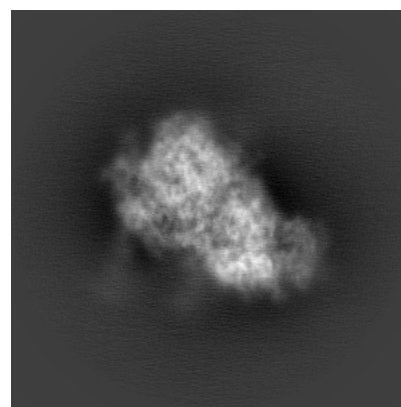
6.1.2 Raw map



X



Y

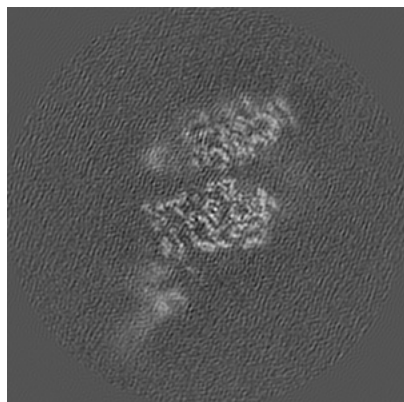


Z

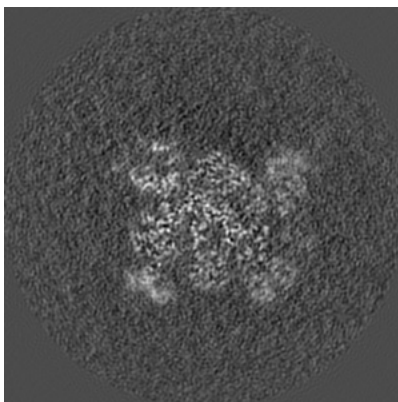
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

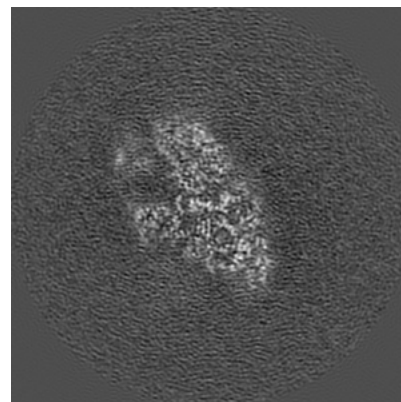
6.2.1 Primary map



X Index: 200

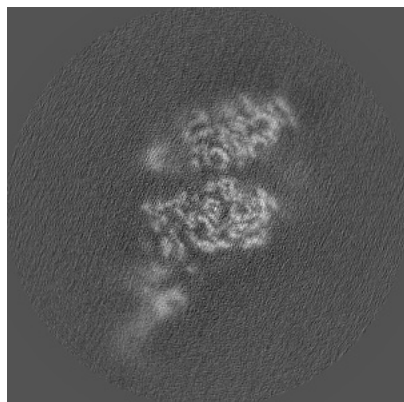


Y Index: 200

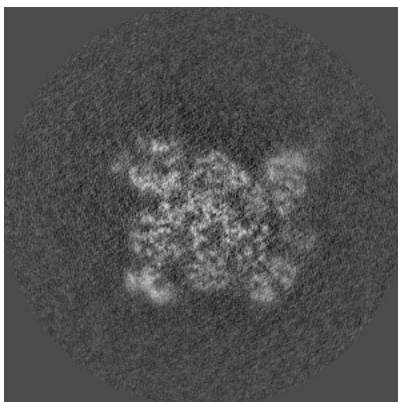


Z Index: 200

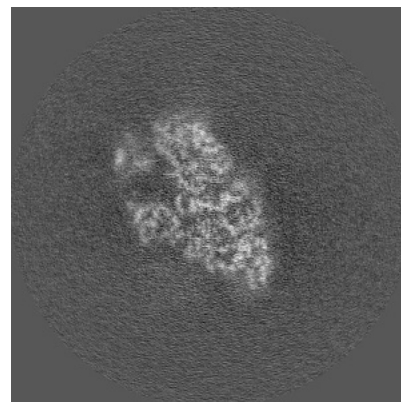
6.2.2 Raw map



X Index: 200



Y Index: 200

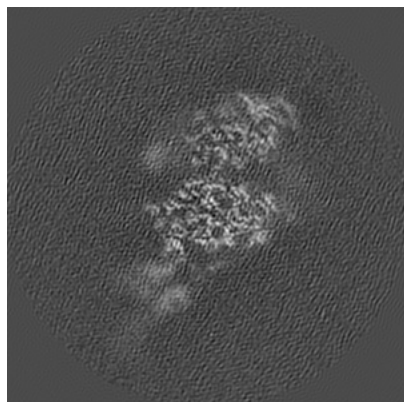


Z Index: 200

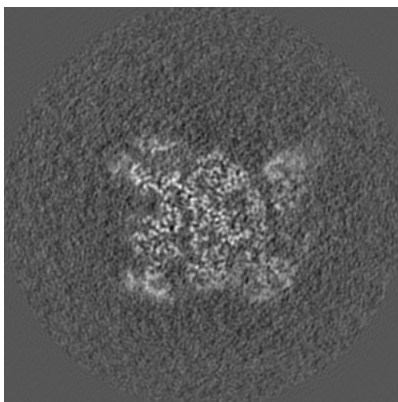
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

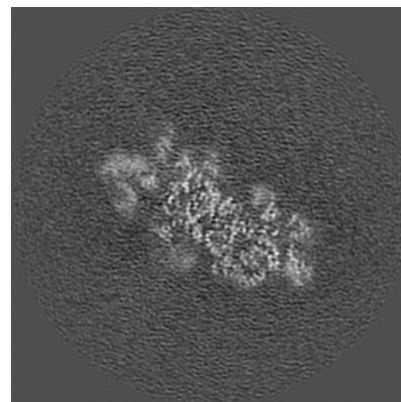
6.3.1 Primary map



X Index: 196

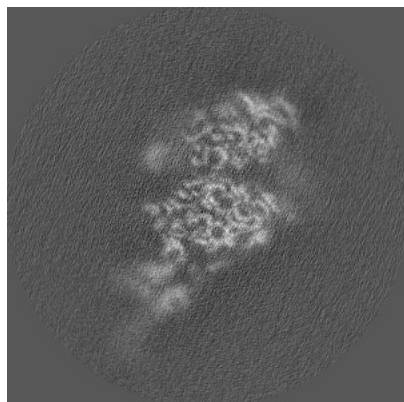


Y Index: 198

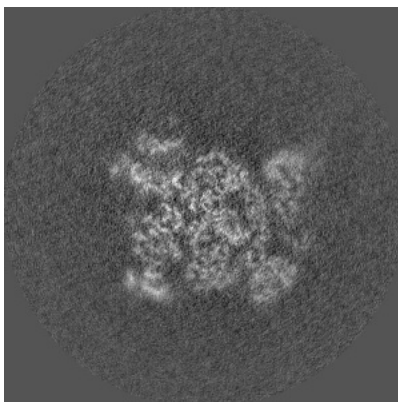


Z Index: 162

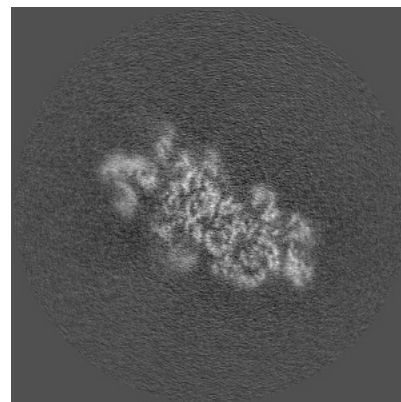
6.3.2 Raw map



X Index: 196



Y Index: 197

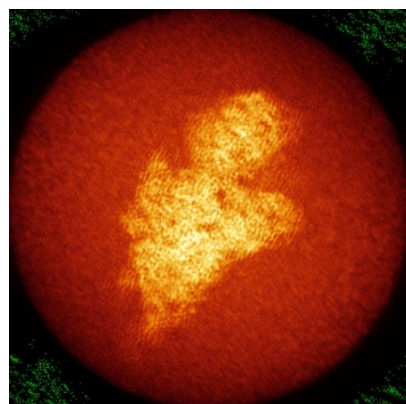


Z Index: 162

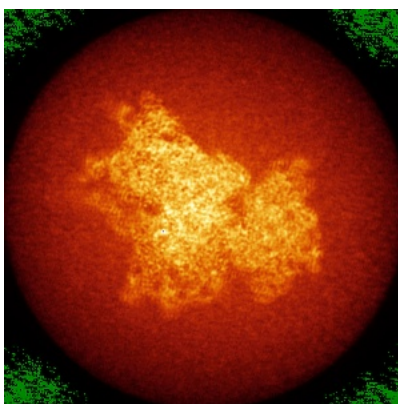
The images above show the largest variance slices of the map in three orthogonal directions.

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

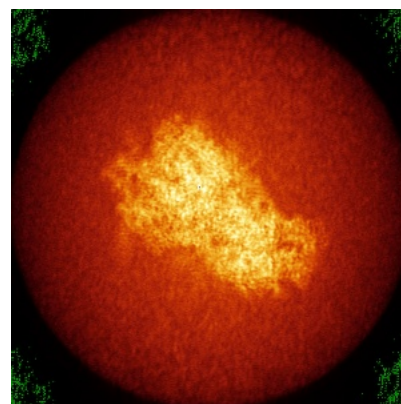
6.4.1 Primary map



X

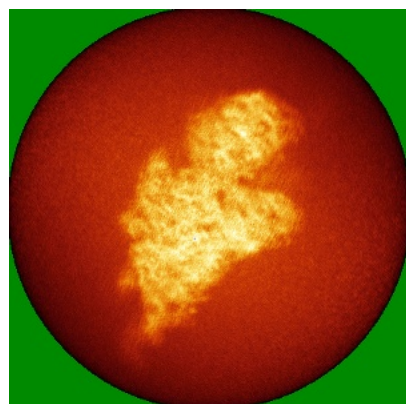


Y

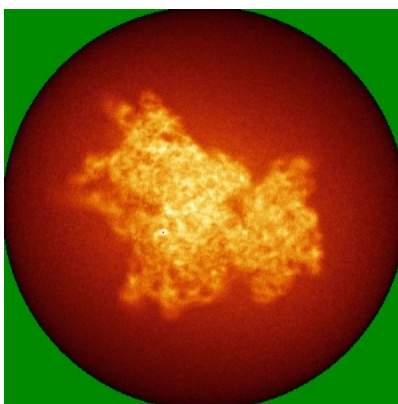


Z

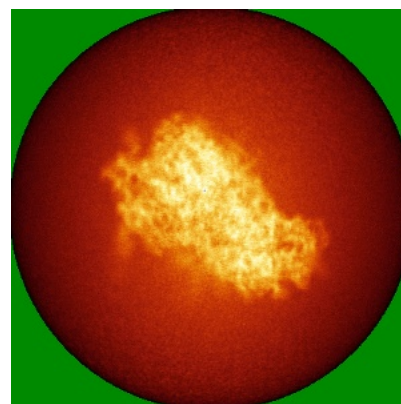
6.4.2 Raw map



X



Y

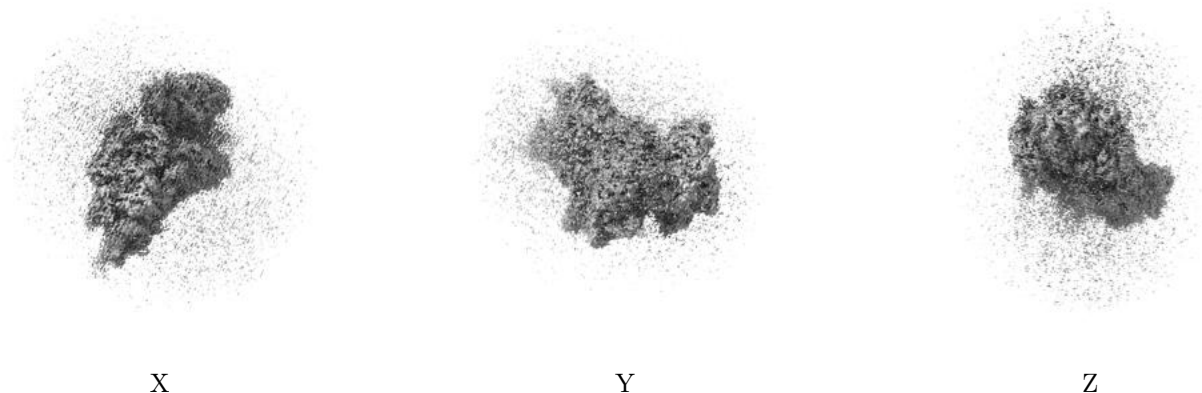


Z

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.

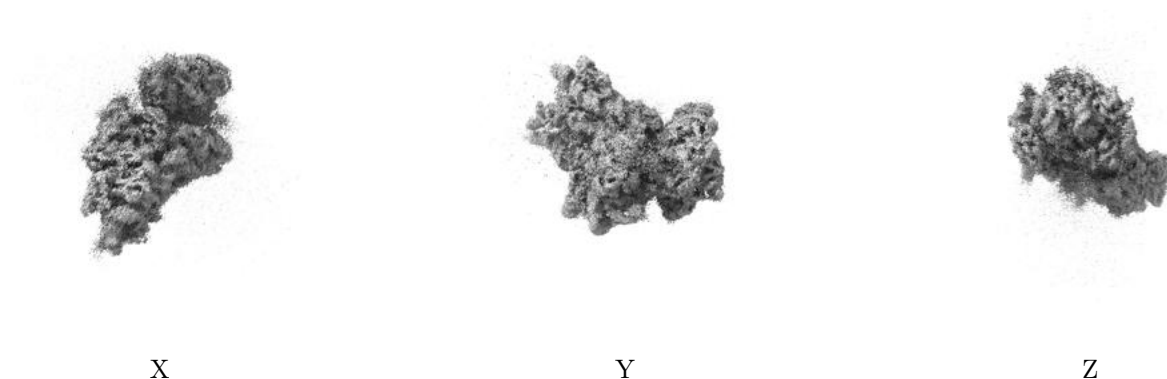
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

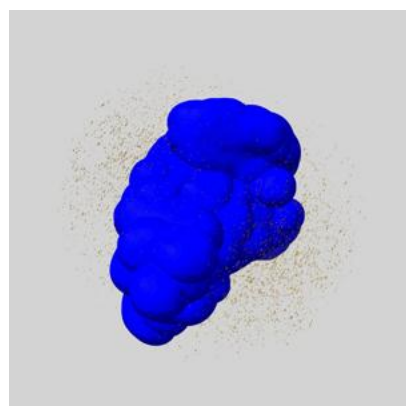
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

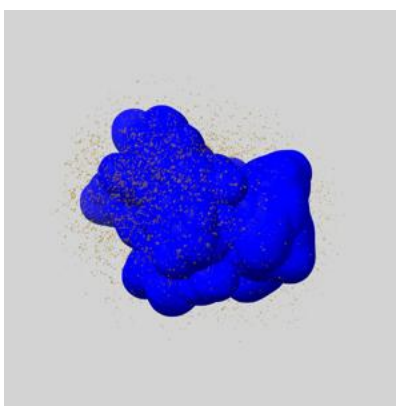
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

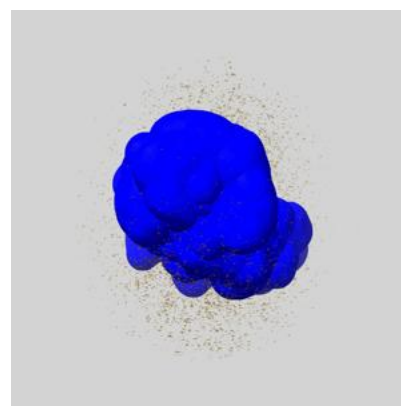
6.6.1 emd_25533_msk_1.map [i](#)



X



Y

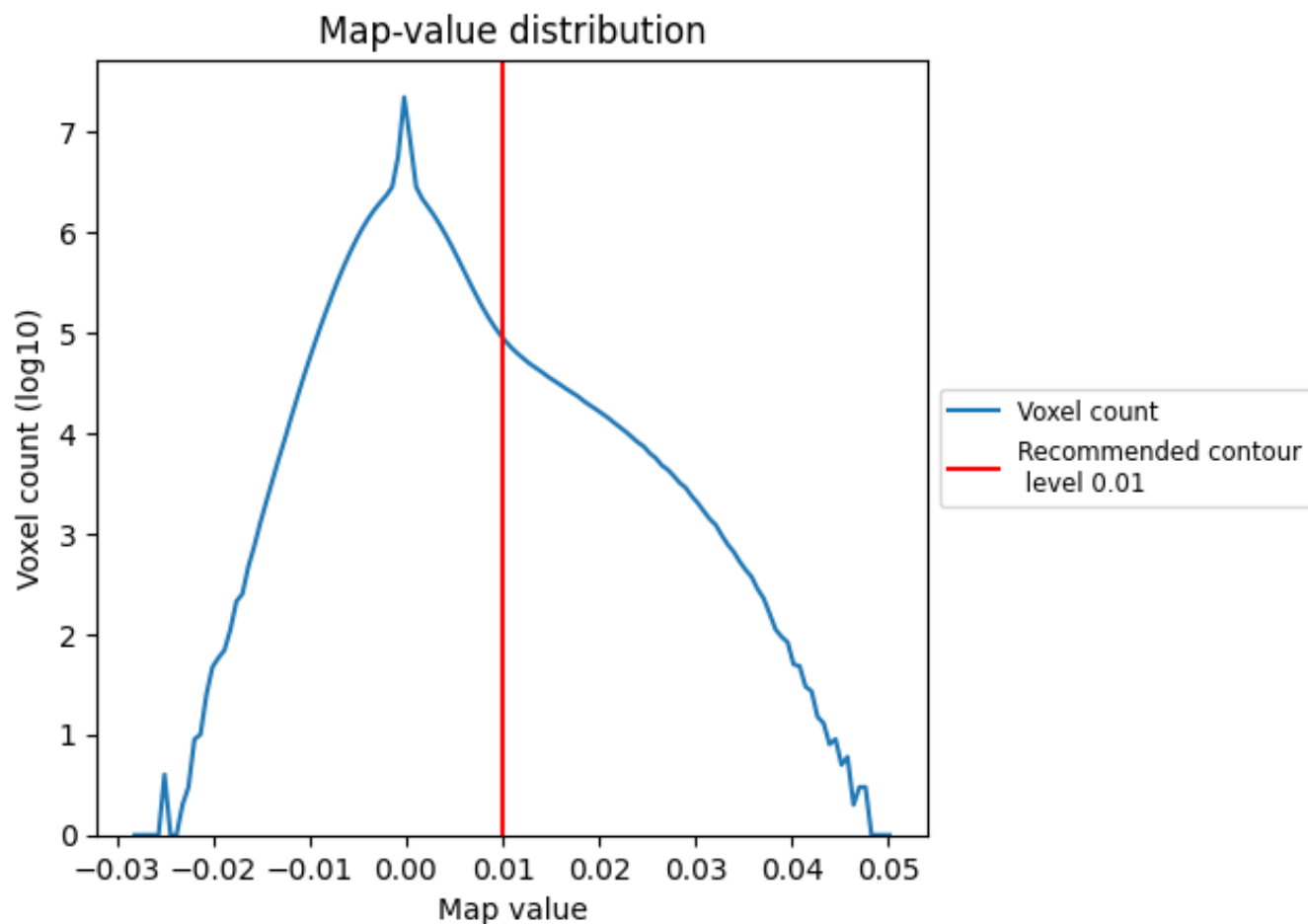


Z

7 Map analysis [i](#)

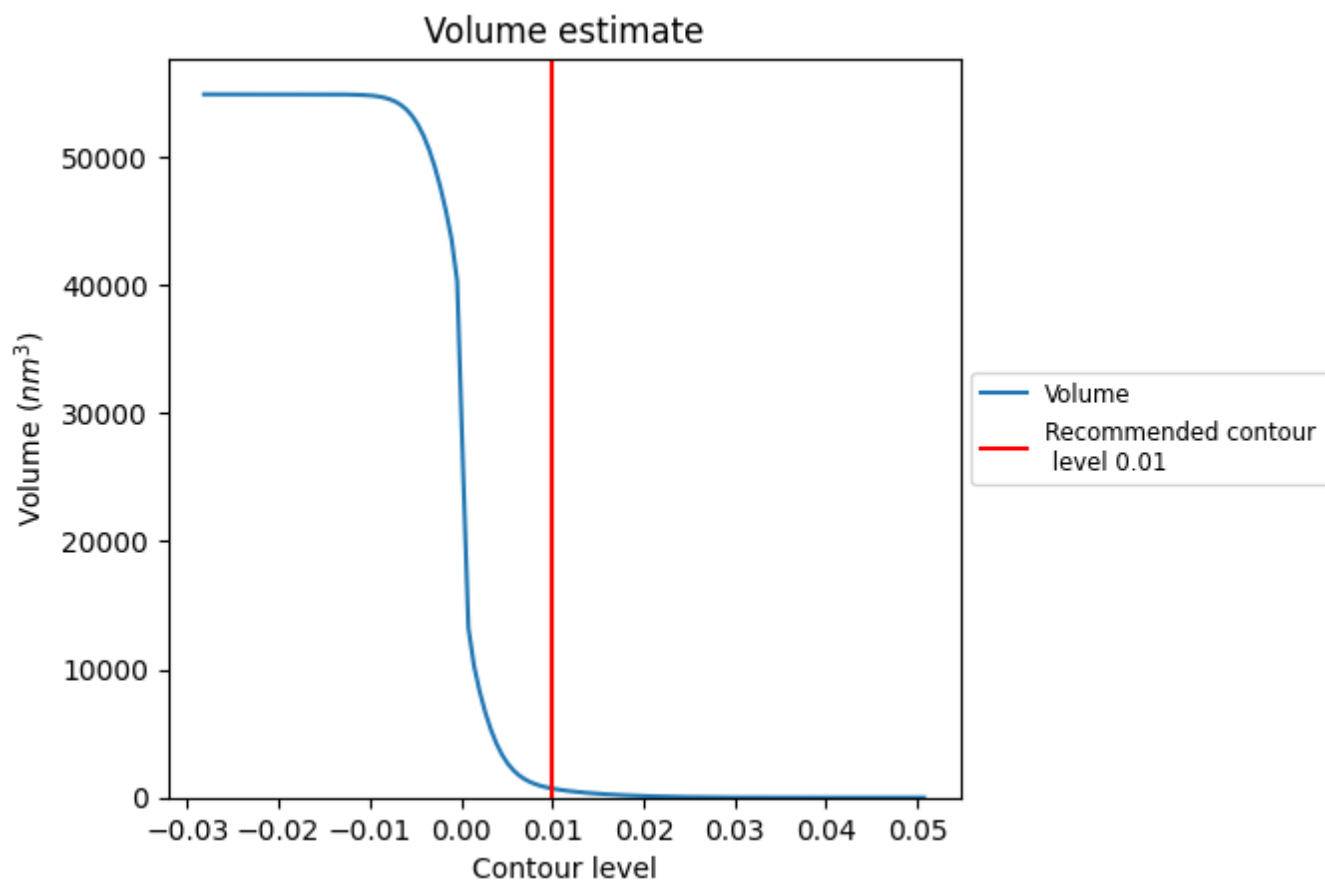
This section contains the results of statistical analysis of the map.

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.

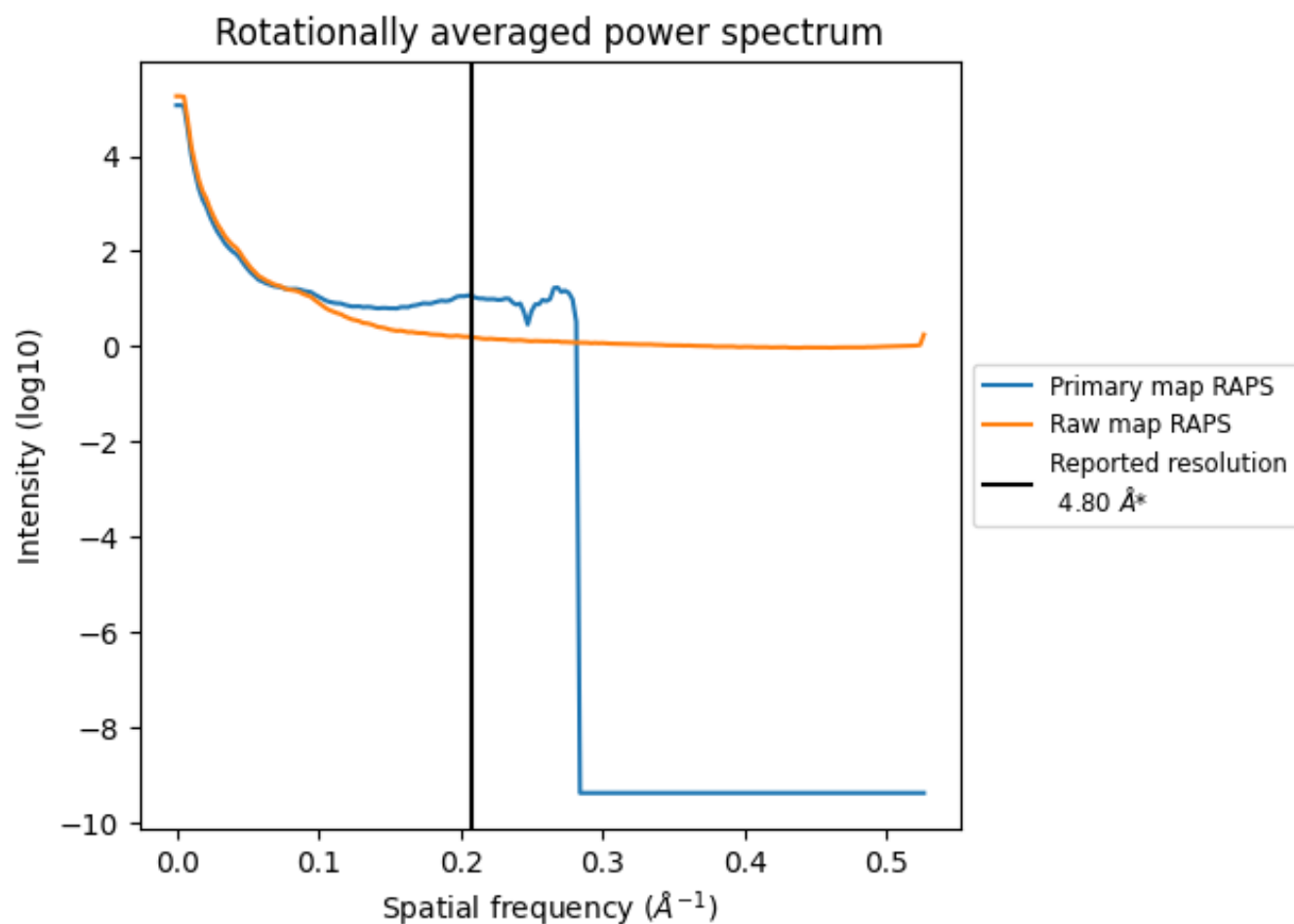
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 706 nm³; this corresponds to an approximate mass of 638 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 ⓘ

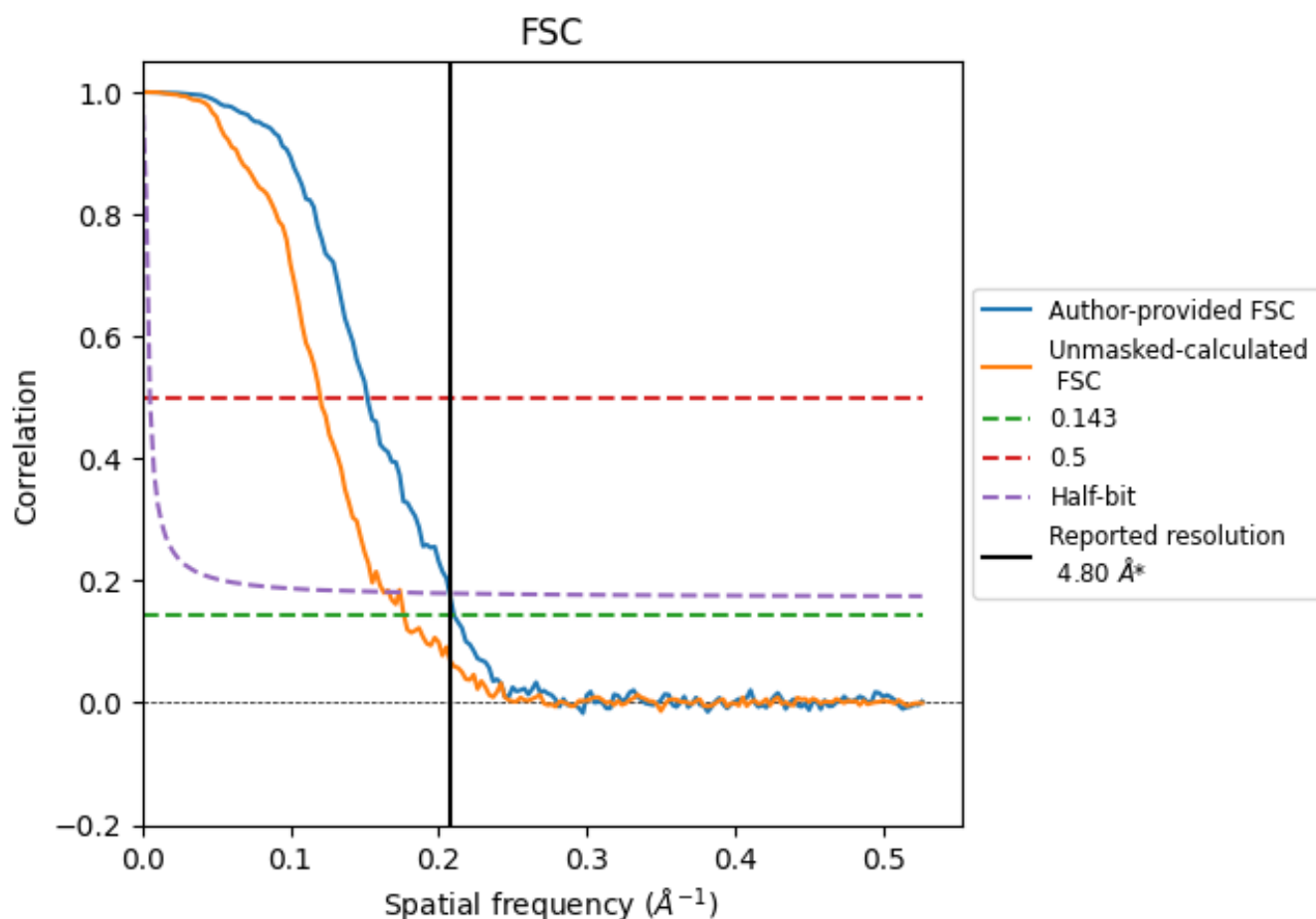


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

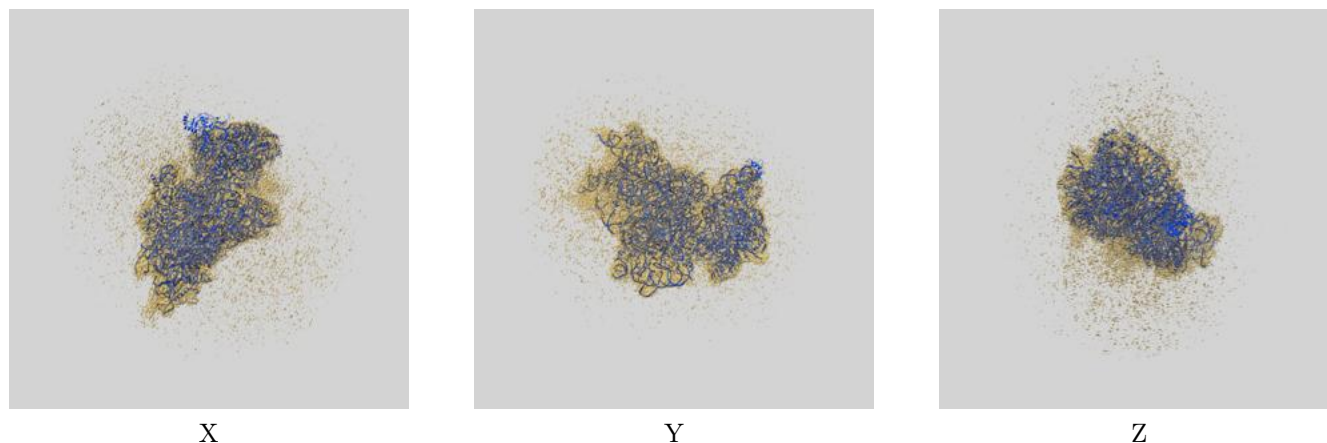
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.75	6.58	4.82
Unmasked-calculated*	5.66	8.33	6.14

*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 5.66 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

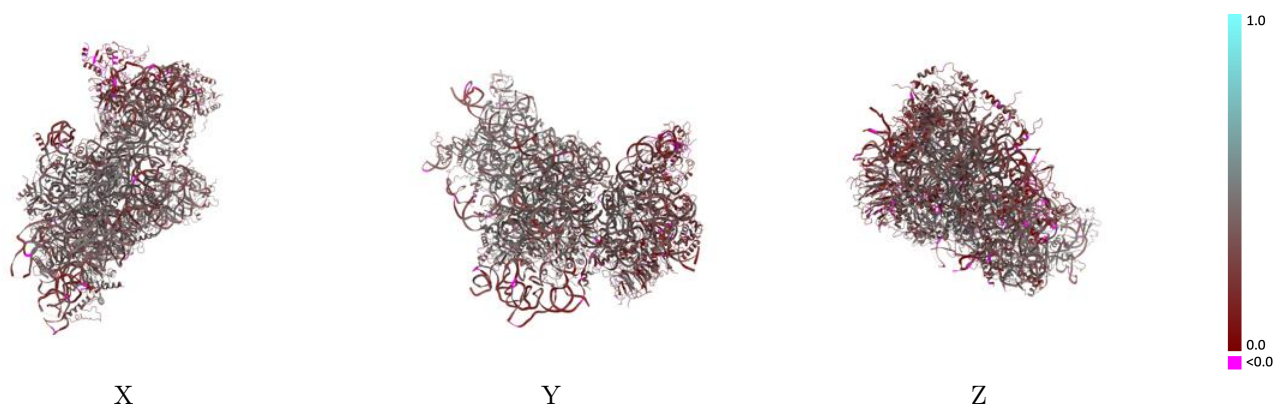
This section contains information regarding the fit between EMDB map EMD-25533 and PDB model 7SYM. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



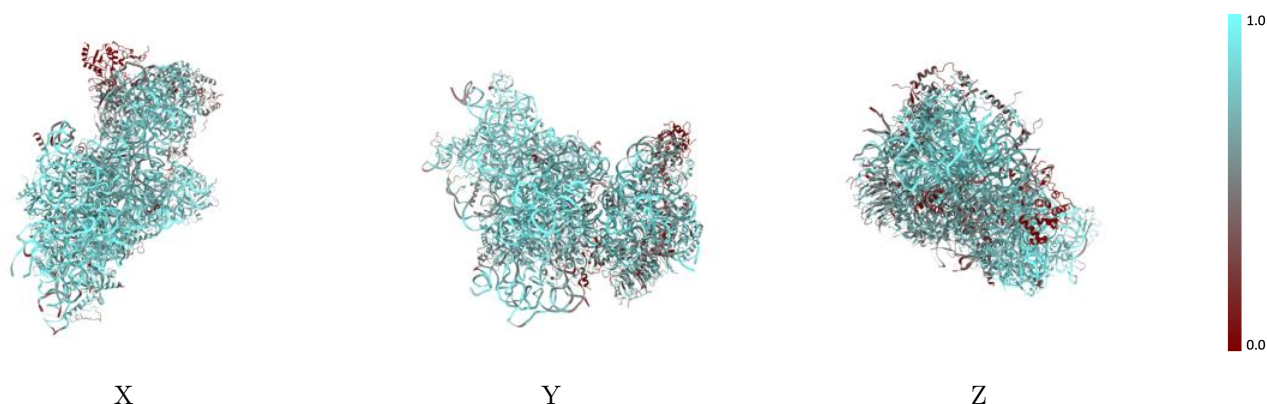
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



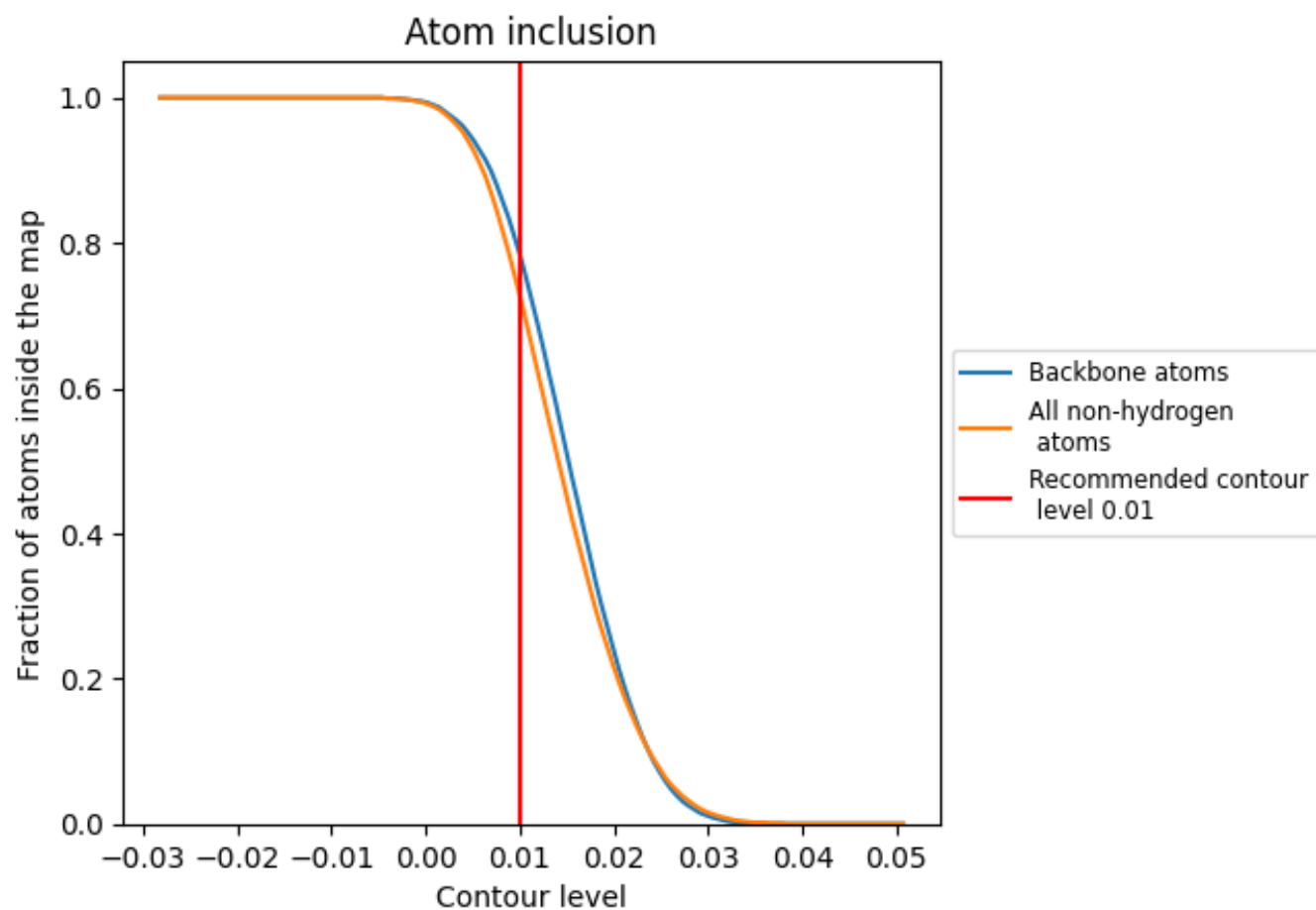
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.3410
2	 0.8400	 0.3440
B	 0.6720	 0.3850
C	 0.7260	 0.3790
D	 0.6730	 0.4000
E	 0.5400	 0.3290
F	 0.7560	 0.4160
G	 0.5970	 0.3090
H	 0.7210	 0.3570
I	 0.6210	 0.3700
J	 0.7500	 0.3940
K	 0.7540	 0.3940
L	 0.5110	 0.2750
M	 0.7140	 0.4200
N	 0.0220	 0.1510
O	 0.7440	 0.4050
P	 0.7240	 0.3700
Q	 0.5430	 0.2550
R	 0.6930	 0.3440
S	 0.5570	 0.3150
T	 0.4900	 0.2730
U	 0.7220	 0.3000
V	 0.3500	 0.2900
W	 0.7060	 0.3890
X	 0.7210	 0.4320
Y	 0.7140	 0.4130
Z	 0.8150	 0.4000
a	 0.3570	 0.2590
b	 0.6980	 0.4110
c	 0.6430	 0.3960
d	 0.4590	 0.3140
e	 0.6100	 0.3490
f	 0.4890	 0.2760
g	 0.0870	 0.1820
h	 0.5610	 0.2880



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Chain	Atom inclusion	Q-score
n	 0.6700	 0.3820
z	 0.6820	 0.2080