Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 12:55 PM EST

PDB ID	:	6P4H
EMDB ID	:	EMD-20249
Title	:	Structure of a mammalian small ribosomal subunit in complex with the Israeli Acute Paralysis Virus IRES (Class 2)
Authors	:	Acosta-Reyes, F.J.; Neupane, R.; Frank, J.; Fernandez, I.S.
Deposited on	:	2019-05-27
Resolution	:	3.20 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:

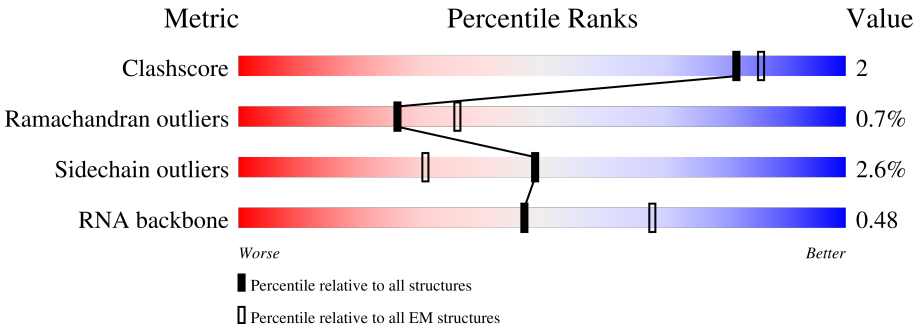
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	1869	6% 64% 24% · 9%
2	B	295	· 65% 8% 26%
3	C	264	· 73% 7% 19%
4	D	255	· 76% 10% · 13%
5	E	281	7% 73% 8% 19%
6	1	253	32% 36% 40% · 20%
7	F	263	· 89% 10%

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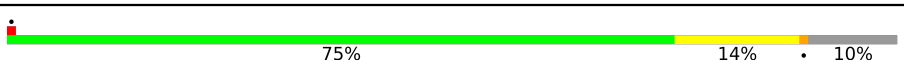
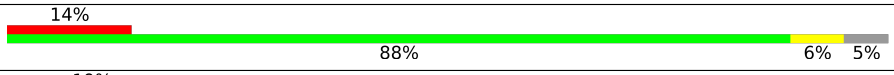
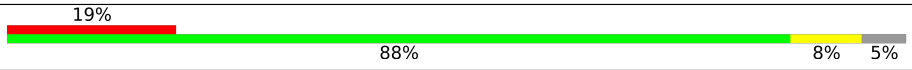
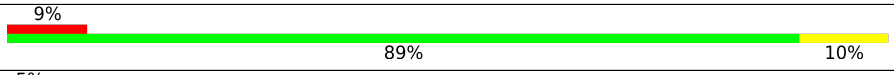
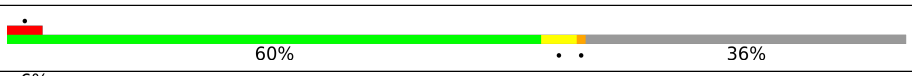
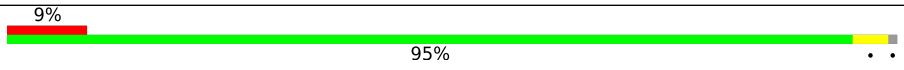
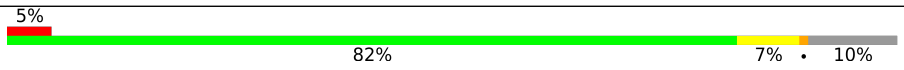
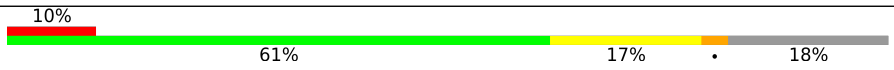
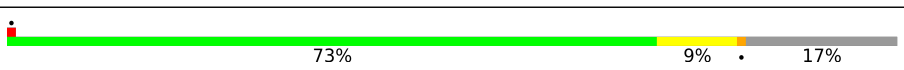
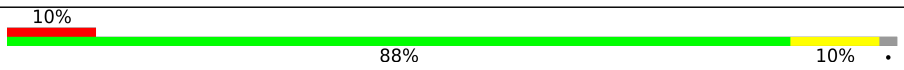
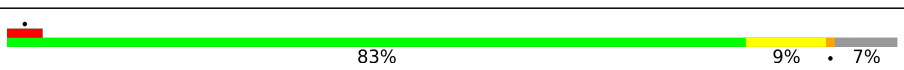
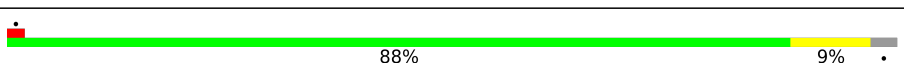
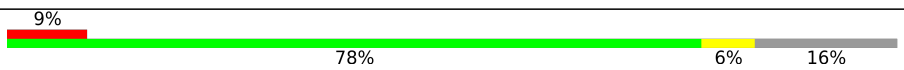
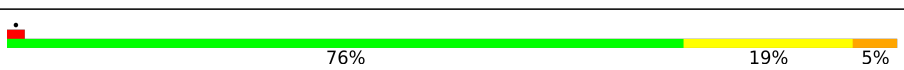
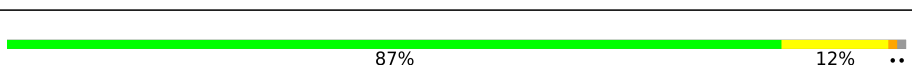
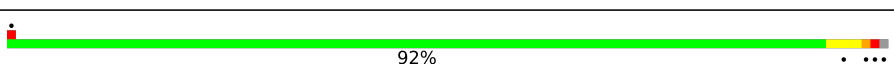
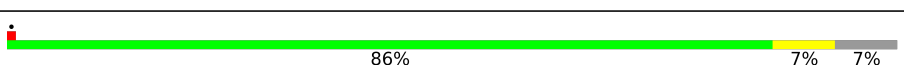
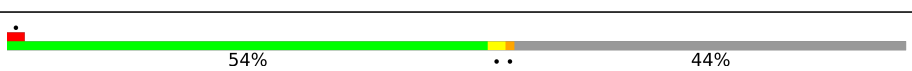
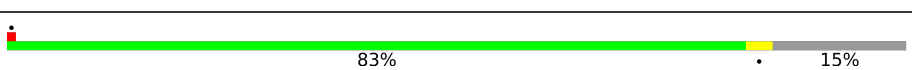
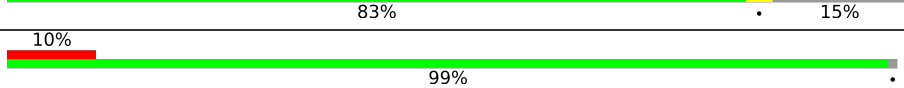
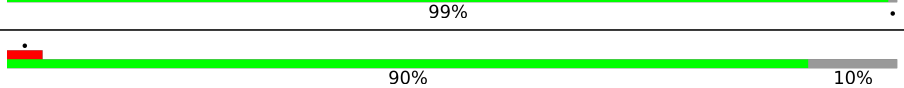
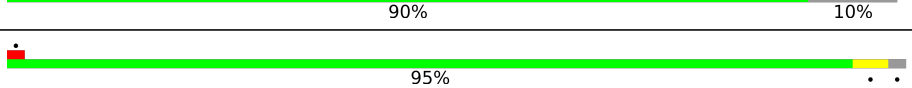
Mol	Chain	Length	Quality of chain
8	G	204	
9	H	249	
10	I	194	
11	J	207	
12	K	194	
13	L	149	
14	M	158	
15	N	132	
16	O	151	
17	P	151	
18	Q	145	
19	R	172	
20	S	135	
21	T	152	
22	U	145	
23	V	119	
24	W	83	
25	X	130	
26	Y	143	
27	Z	134	
28	a	125	
29	b	115	
30	c	84	
31	d	69	
32	e	56	

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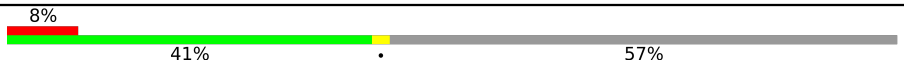
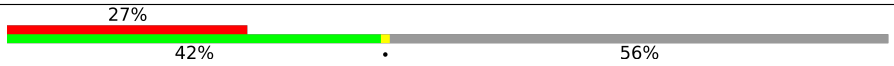
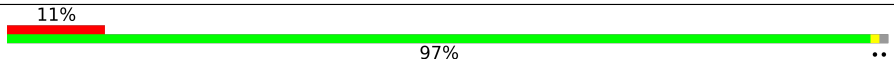
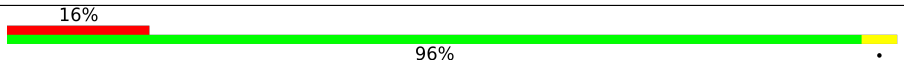
Mol	Chain	Length	Quality of chain
33	f	133	
34	g	156	
35	h	317	
36	n	25	

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 79374 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
			Total	C	N	O	P		
1	2	1697	36229	16171	6507	11855	1696	0	0

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	217	1706	1085	295	317	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	162	PRO	LEU	conflict	UNP G1TWL4

- Molecule 3 is a protein called eS1.

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

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	221	1712	1107	296	299	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	181	PRO	LEU	conflict	UNP G1SWM1
D	191	VAL	-	insertion	UNP G1SWM1

- 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 RNA chain called IAPV-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	203	Total	C	N	O	P	0	0
			4323	1932	767	1421	203		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	6624	G	-	insertion	GB 124494152

- Molecule 7 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	262	Total	C	N	O	S	0	0
			2073	1323	384	357	9		

- Molecule 8 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	184	Total	C	N	O	S	0	0
			1462	915	276	264	7		

- Molecule 9 is a protein called eS6.

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

- Molecule 10 is a protein called eS7.

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

- Molecule 11 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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 12 is a protein called uS4.

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

- Molecule 13 is a protein called eS10.

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

- Molecule 14 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 15 is a protein called eS12.

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

- Molecule 16 is a protein called uS15.

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

- Molecule 17 is a protein called uS11.

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

- Molecule 18 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	119	Total	C	N	O	S	0	0
			990	630	186	167	7		

- Molecule 19 is a protein called uS9.

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

- Molecule 20 is a protein called eS17.

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

- Molecule 21 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	141	Total	C	N	O	S	0	0
			1168	734	235	198	1		

- Molecule 22 is a protein called eS19.

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

- Molecule 23 is a protein called uS10.

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

- Molecule 24 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	83	Total	C	N	O	S	0	0
			630	387	118	120	5		

- Molecule 25 is a protein called uS8.

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

- Molecule 26 is a protein called uS12.

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

- Molecule 27 is a protein called eS24.

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

- Molecule 28 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	70	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 29 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	98	Total	C	N	O	S	0	0
			778	485	158	129	6		

- Molecule 30 is a protein called eS27.

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

- Molecule 31 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 32 is a protein called eS29.

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

- Molecule 33 is a protein called eS30.

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

- Molecule 34 is a protein called eS31.

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

- Molecule 35 is a protein called RACK1.

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

- Molecule 36 is a protein called eL41.

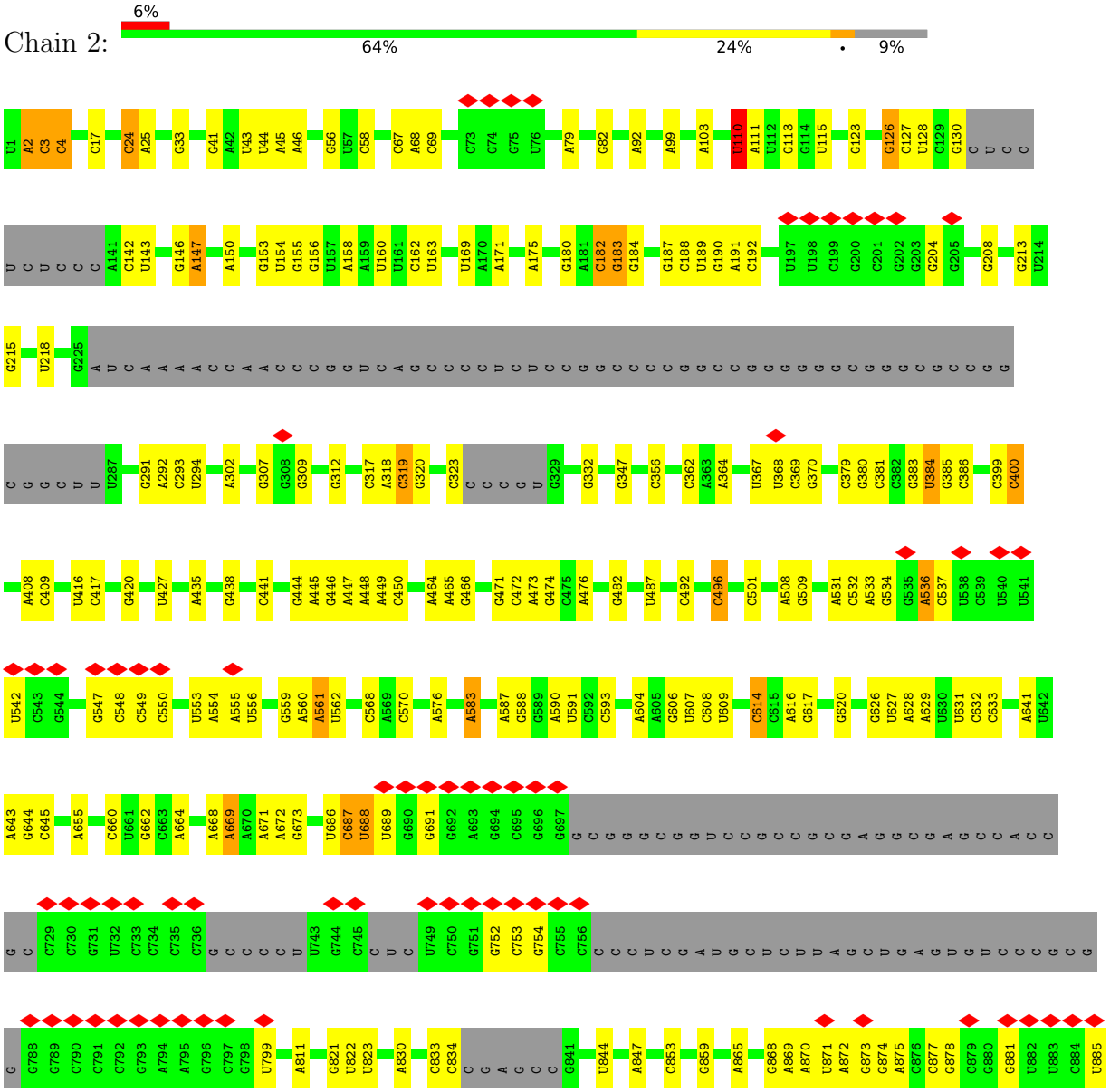
Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

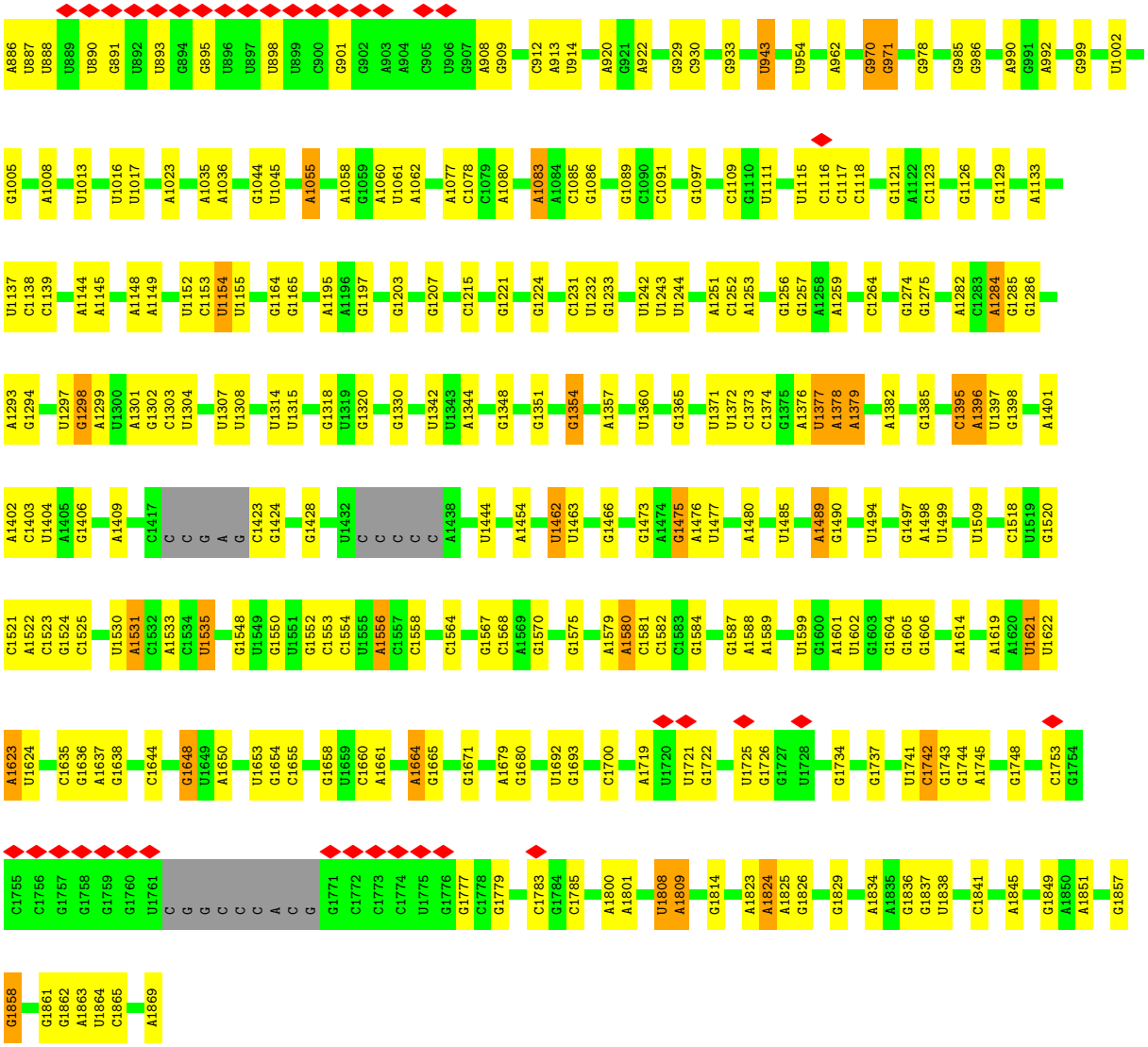
3 Residue-property plots (i)

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

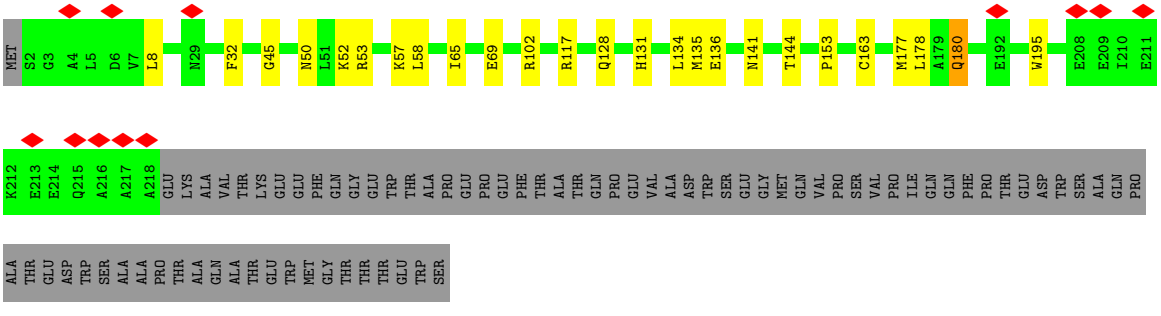
Chain 2:





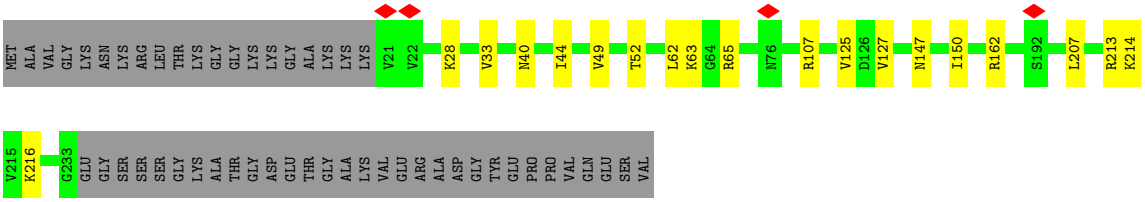
• Molecule 2: uS2

Chain B:



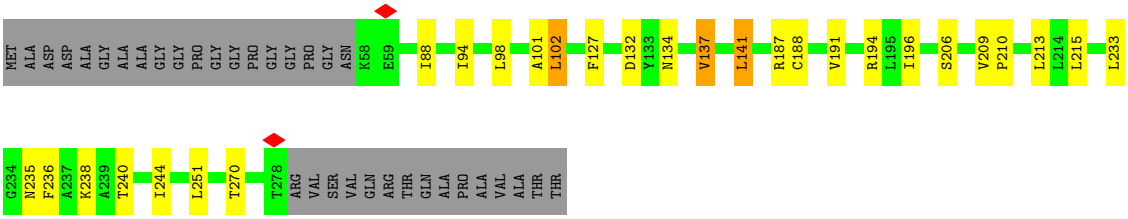
• Molecule 3: eS1

Chain C:



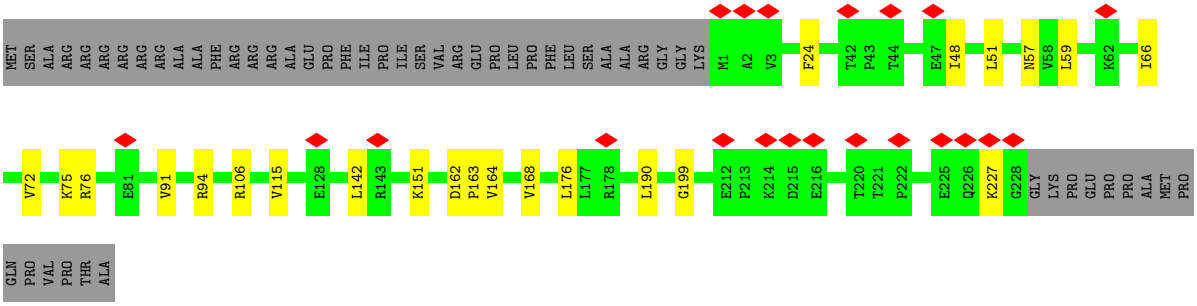
• Molecule 4: uS5

Chain D:



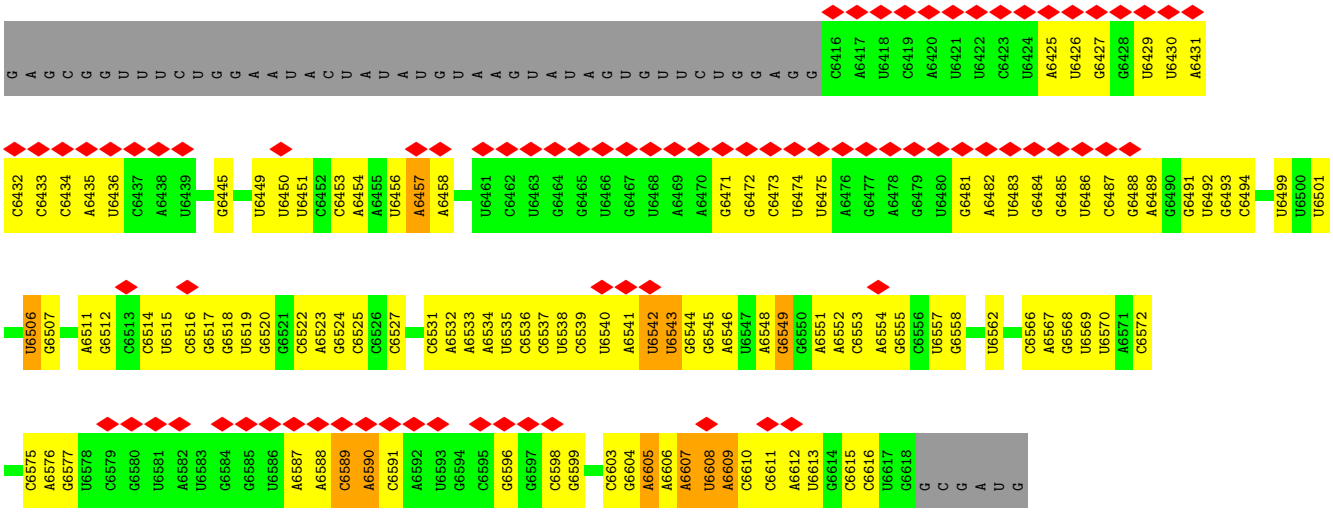
• Molecule 5: uS3

Chain E:



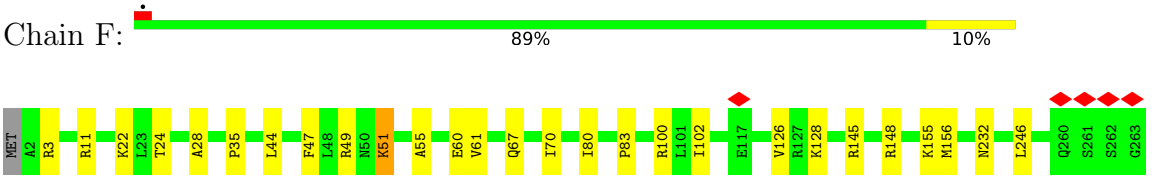
• Molecule 6: IAPV-IRES

Chain 1:



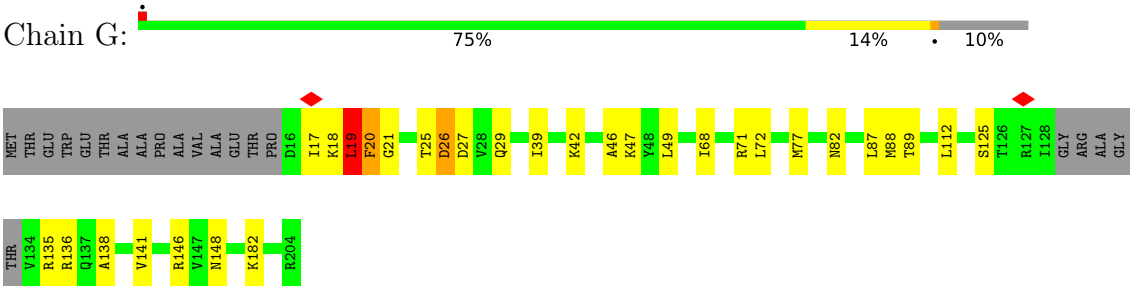
• Molecule 7: eS4

Chain F:



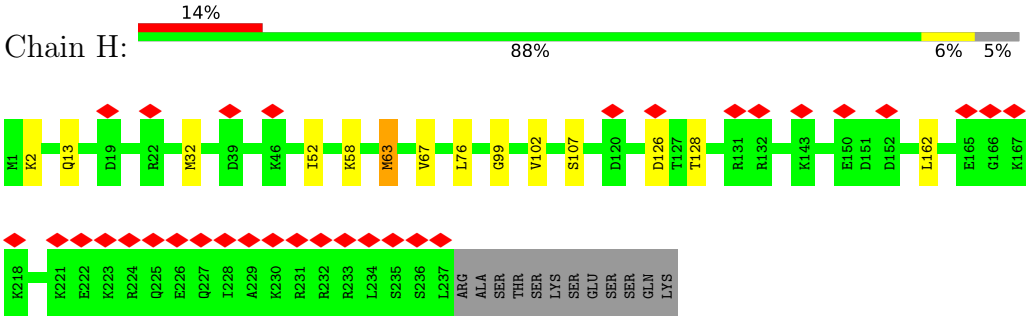
• Molecule 8: uS7

Chain G:



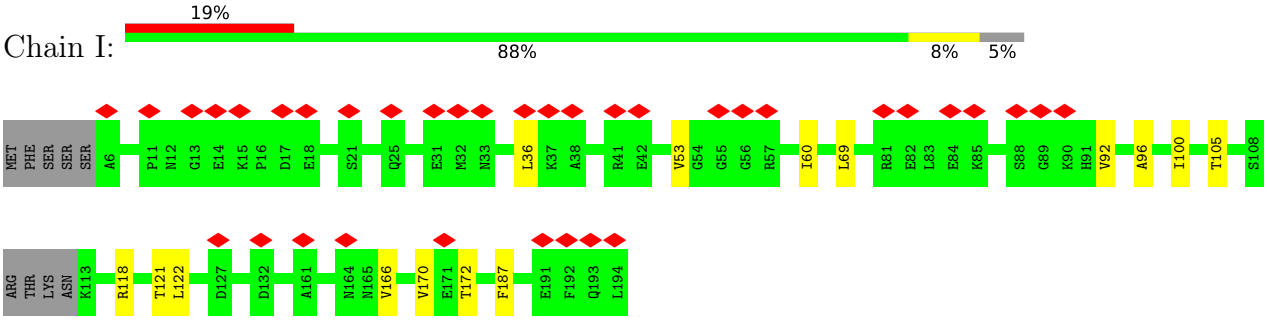
• Molecule 9: eS6

Chain H:



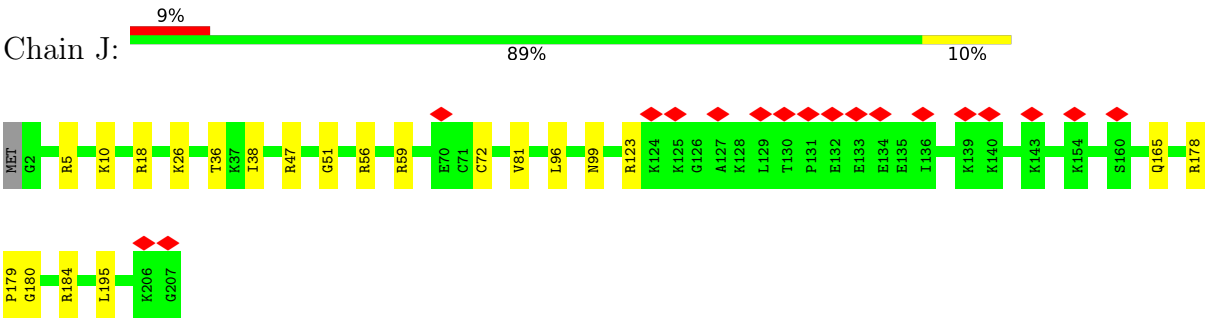
• Molecule 10: eS7

Chain I:



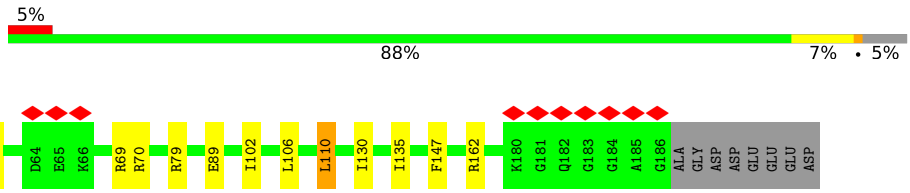
• Molecule 11: eS8

Chain J:



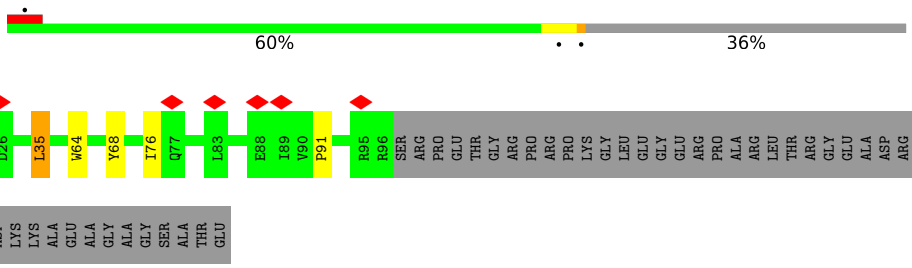
• Molecule 12: uS4

Chain K:



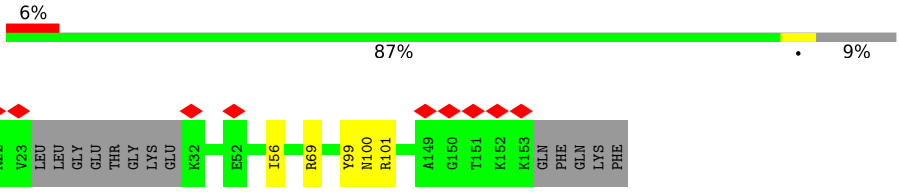
• Molecule 13: eS10

Chain L:



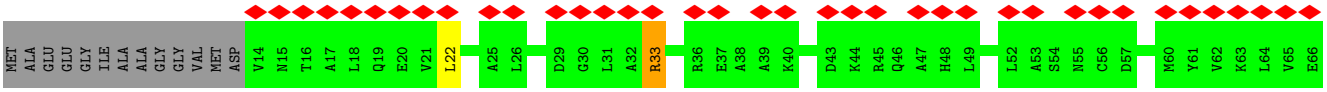
• Molecule 14: uS17

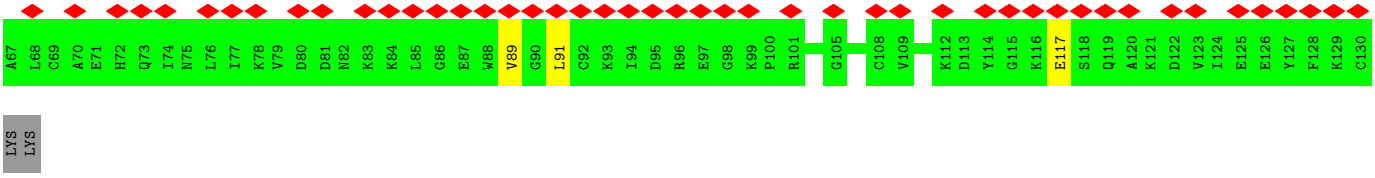
Chain M:



• Molecule 15: eS12

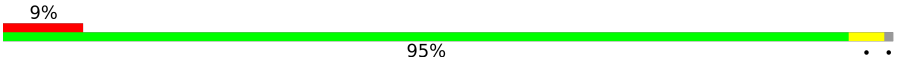
Chain N:

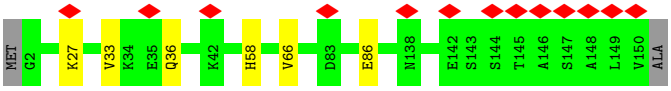




• Molecule 16: uS15

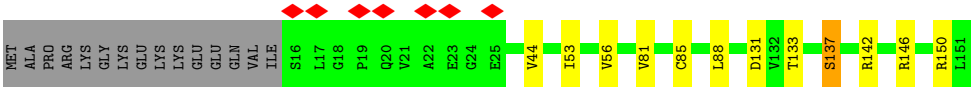
Chain O:



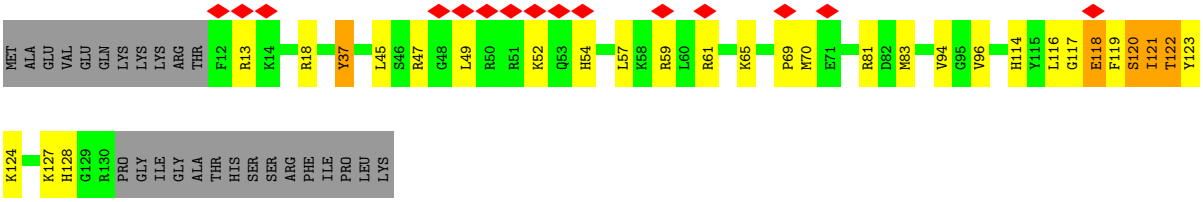


• Molecule 17: uS11

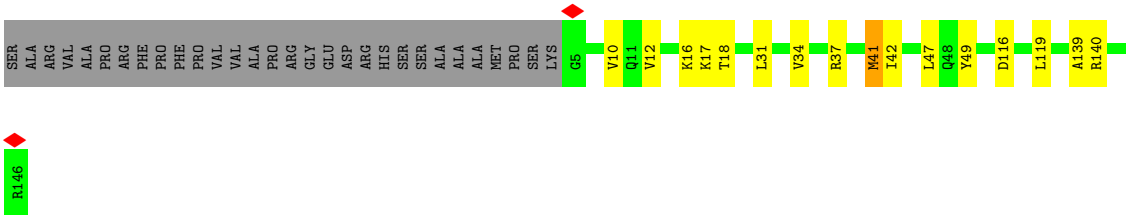
Chain P:



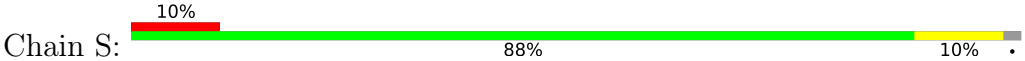
• Molecule 18: uS19

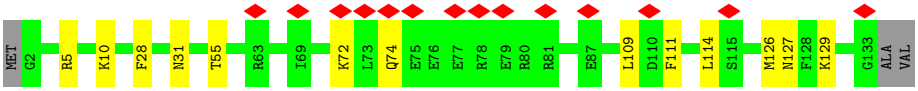


• Molecule 19: uS9

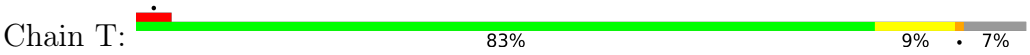


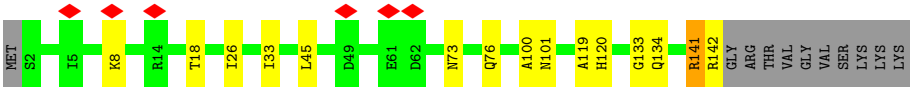
• Molecule 20: eS17



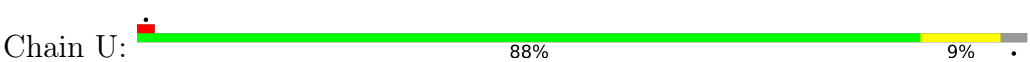


• Molecule 21: uS13

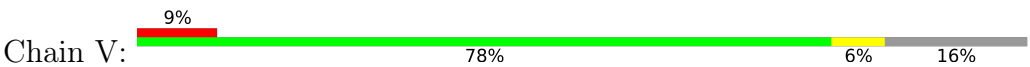


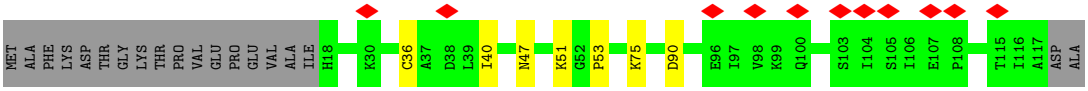


• Molecule 22: eS19



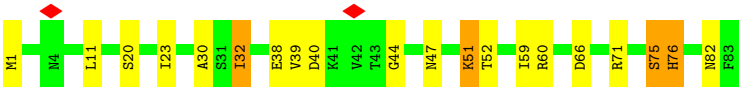
• Molecule 23: uS10





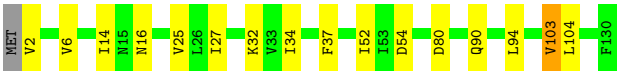
• Molecule 24: eS21

Chain W:



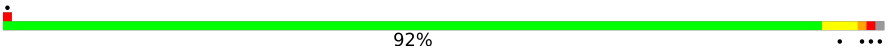
• Molecule 25: uS8

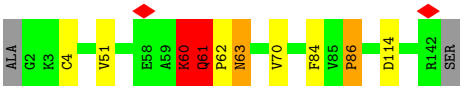
Chain X:



• Molecule 26: uS12

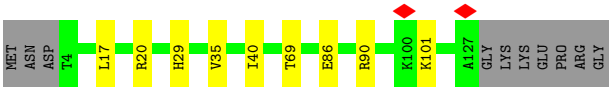
Chain Y:





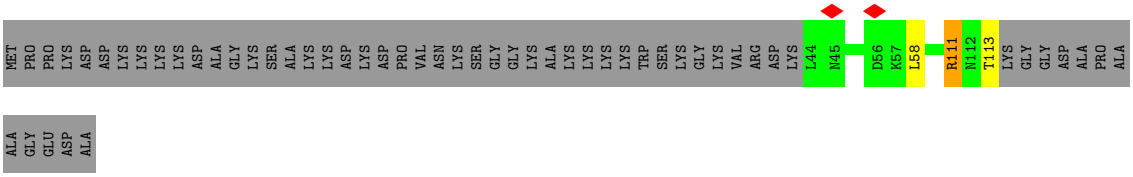
• Molecule 27: eS24

Chain Z:



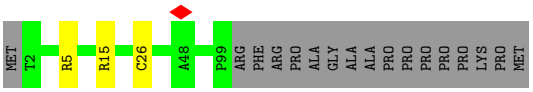
• Molecule 28: eS25

Chain a:



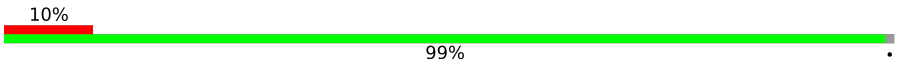
• Molecule 29: eS26

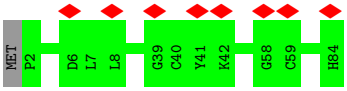
Chain b:



• Molecule 30: eS27

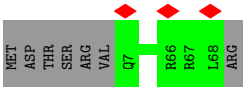
Chain c:





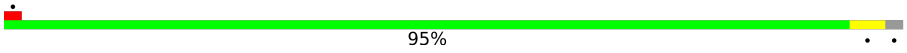
• Molecule 31: eS28

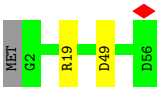
Chain d:



• Molecule 32: eS29

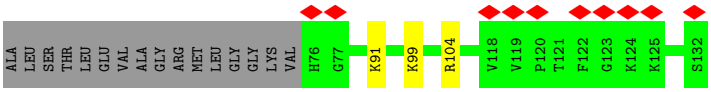
Chain e:





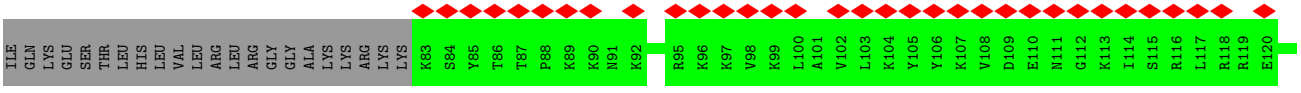
• Molecule 33: eS30

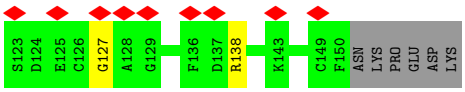
Chain f:



• Molecule 34: eS31

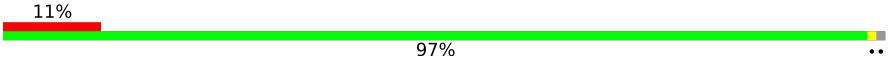
Chain g:

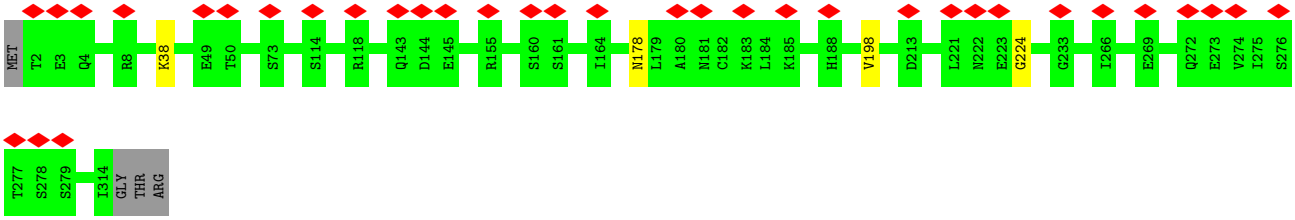




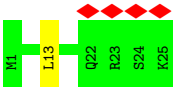
• Molecule 35: RACK1

Chain h:





• Molecule 36: eL41



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96826	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 ($e^-/Å^2$)	42.09	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.213	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	384.696, 384.696, 384.696	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.233, 1.233, 1.233	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	2	0.27	1/40509 (0.0%)	0.69	6/63128 (0.0%)
2	B	0.65	0/1744	0.78	0/2371
3	C	0.65	0/1756	0.79	0/2350
4	D	0.64	0/1748	0.80	0/2362
5	E	0.67	0/1796	0.81	0/2417
6	1	0.23	0/4833	0.71	2/7529 (0.0%)
7	F	0.65	0/2115	0.80	0/2843
8	G	0.67	0/1482	0.82	0/1990
9	H	0.67	0/1946	0.82	0/2590
10	I	0.67	0/1510	0.77	0/2022
11	J	0.65	0/1715	0.80	0/2287
12	K	0.65	0/1550	0.82	0/2069
13	L	0.64	0/834	0.76	0/1125
14	M	0.64	0/1195	0.80	0/1597
15	N	0.71	0/918	0.78	0/1233
16	O	0.67	0/1226	0.78	0/1649
17	P	0.66	0/1029	0.85	0/1380
18	Q	0.65	0/1009	0.83	0/1346
19	R	0.66	0/1146	0.81	0/1534
20	S	0.67	0/1082	0.80	0/1452
21	T	0.66	0/1186	0.82	0/1589
22	U	0.66	0/1115	0.82	0/1493
23	V	0.67	0/805	0.81	0/1081
24	W	0.69	0/638	0.81	0/855
25	X	0.64	0/1051	0.83	0/1406
26	Y	0.65	0/1116	0.82	0/1490
27	Z	0.66	0/1028	0.80	0/1366
28	a	0.68	0/563	0.83	0/758
29	b	0.64	0/791	0.82	0/1062
30	c	0.66	0/665	0.81	0/891
31	d	0.67	0/490	0.83	0/656
32	e	0.65	0/470	0.84	0/623
33	f	0.66	0/462	0.80	0/607
34	g	0.68	0/567	0.82	0/753

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	h	0.68	0/2493	0.79	0/3394
36	n	0.62	0/240	0.85	0/305
All	All	0.49	1/84823 (0.0%)	0.75	8/123603 (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
2	B	0	1
4	D	0	1
7	F	0	1
8	G	0	6
18	Q	0	1
20	S	0	1
25	X	0	2
26	Y	0	2
27	Z	0	1
28	a	0	1
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	885	U	O3'-P	5.86	1.68	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1	6506	U	C2'-C3'-O3'	7.14	125.20	109.50
1	2	24	C	C2'-C3'-O3'	5.91	123.16	113.70
1	2	1664	A	C4'-C3'-O3'	5.84	124.67	113.00
1	2	1489	A	C2'-C3'-O3'	5.74	122.88	113.70
1	2	688	U	C2'-C3'-O3'	5.69	122.80	113.70
6	1	6609	A	C2'-C3'-O3'	5.38	122.31	113.70
1	2	561	A	C2'-C3'-O3'	5.33	122.23	113.70
1	2	110	U	C2'-C3'-O3'	5.30	122.19	113.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	163	CYS	Peptide
4	D	187	ARG	Peptide
7	F	22	LYS	Peptide
8	G	17	ILE	Peptide
8	G	18	LYS	Peptide
8	G	19	LEU	Peptide
8	G	20	PHE	Peptide
8	G	21	GLY	Peptide
8	G	26	ASP	Peptide
18	Q	69	PRO	Peptide
20	S	74	GLN	Peptide
25	X	27	ILE	Peptide
25	X	54	ASP	Peptide
26	Y	60	LYS	Peptide
26	Y	61	GLN	Peptide
27	Z	20	ARG	Peptide
28	a	111	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	36229	0	18300	117	0
2	B	1706	0	1697	12	0
3	C	1729	0	1803	9	0
4	D	1712	0	1808	24	0
5	E	1768	0	1866	12	0
6	1	4323	0	2182	9	0
7	F	2073	0	2173	11	0
8	G	1462	0	1510	11	0
9	H	1923	0	2089	11	0
10	I	1488	0	1582	7	0
11	J	1686	0	1772	14	0
12	K	1525	0	1640	8	0
13	L	810	0	836	4	0
14	M	1175	0	1249	1	0
15	N	908	0	939	3	0
16	O	1202	0	1289	2	0
17	P	1016	0	1039	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Q	990	0	1038	20	0
19	R	1128	0	1195	10	0
20	S	1068	0	1121	6	0
21	T	1168	0	1226	8	0
22	U	1097	0	1130	6	0
23	V	795	0	862	3	0
24	W	630	0	631	11	0
25	X	1034	0	1080	7	0
26	Y	1098	0	1167	6	0
27	Z	1011	0	1083	3	0
28	a	557	0	610	0	0
29	b	778	0	828	0	0
30	c	651	0	672	0	0
31	d	488	0	514	0	0
32	e	459	0	452	0	0
33	f	457	0	502	0	0
34	g	555	0	567	0	0
35	h	2436	0	2393	0	0
36	n	239	0	289	0	0
All	All	79374	0	61134	279	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 2.

All (279) 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)
24:W:32:ILE:HG12	24:W:60:ARG:HD2	1.51	0.89
4:D:101:ALA:O	4:D:132:ASP:CB	2.40	0.70
8:G:19:LEU:HD12	8:G:47:LYS:O	1.91	0.69
1:2:1857:G:H3'	17:P:146:ARG:HH12	1.59	0.68
4:D:101:ALA:O	4:D:132:ASP:HA	1.93	0.67
4:D:141:LEU:HD11	4:D:238:LYS:HE2	1.75	0.67
1:2:1524:G:N7	21:T:141:ARG:NH2	2.43	0.66
4:D:101:ALA:O	4:D:132:ASP:HB3	1.96	0.66
11:J:165:GLN:HE22	11:J:195:LEU:HD11	1.61	0.65
1:2:3:C:O2	12:K:18:ARG:NH2	2.30	0.65
1:2:444:G:O6	11:J:26:LYS:HE2	1.97	0.65
18:Q:54:HIS:O	18:Q:57:LEU:HB2	1.98	0.64
1:2:110:U:H5"	1:2:110:U:H6	1.61	0.64
18:Q:96:VAL:HG11	18:Q:120:SER:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:53:VAL:HG21	10:I:172:THR:HA	1.79	0.63
4:D:141:LEU:CD1	4:D:238:LYS:HE2	2.28	0.63
1:2:501:C:O2	1:2:501:C:H2'	1.99	0.63
1:2:4:C:O2'	12:K:18:ARG:NH1	2.32	0.63
12:K:110:LEU:HD21	12:K:135:ILE:HD11	1.81	0.63
1:2:1473:G:O2'	1:2:1475:G:N2	2.32	0.62
1:2:1742:C:OP2	11:J:59:ARG:NH2	2.32	0.62
20:S:31:ASN:HD21	20:S:55:THR:HG22	1.65	0.62
8:G:72:LEU:HD22	8:G:112:LEU:HD11	1.82	0.61
18:Q:121:ILE:O	18:Q:121:ILE:HD12	2.02	0.60
24:W:1:MET:SD	24:W:1:MET:N	2.74	0.59
3:C:62:LEU:HD12	3:C:65:ARG:HD3	1.83	0.59
18:Q:118:GLU:O	21:T:120:HIS:HB2	2.03	0.59
1:2:379:C:O2	11:J:5:ARG:NH1	2.36	0.58
1:2:1005:G:OP2	3:C:162:ARG:NH1	2.36	0.58
18:Q:83:MET:HB3	18:Q:116:LEU:HD12	1.84	0.58
16:O:33:VAL:HG21	16:O:66:VAL:HG11	1.84	0.58
1:2:191:A:N6	1:2:208:G:O2'	2.36	0.57
17:P:56:VAL:HG23	17:P:81:VAL:HG23	1.86	0.57
1:2:1091:C:HO2'	25:X:2:VAL:N	2.03	0.57
7:F:128:LYS:HA	7:F:156:MET:HG2	1.87	0.56
16:O:36:GLN:HE22	16:O:58:HIS:CG	2.23	0.56
1:2:1568:C:OP1	22:U:96:SER:OG	2.20	0.56
4:D:191:VAL:HG11	4:D:236:PHE:HA	1.86	0.56
8:G:87:LEU:HD22	19:R:47:LEU:HD11	1.86	0.56
20:S:28:PHE:HA	20:S:55:THR:HG21	1.86	0.56
7:F:47:PHE:HA	7:F:51:LYS:HG2	1.87	0.56
2:B:128:GLN:HE21	2:B:153:PRO:HD3	1.70	0.56
2:B:52:LYS:HB2	20:S:109:LEU:HD21	1.88	0.56
25:X:6:VAL:HG12	25:X:34:ILE:HD11	1.88	0.56
1:2:1693:G:N2	1:2:1834:A:H8	2.04	0.56
2:B:180:GLN:HB2	2:B:195:TRP:CE3	2.41	0.55
4:D:101:ALA:O	4:D:132:ASP:CA	2.53	0.55
14:M:99:TYR:O	14:M:101:ARG:N	2.39	0.55
1:2:1858:G:OP2	17:P:146:ARG:NH2	2.35	0.55
18:Q:96:VAL:CG1	18:Q:120:SER:HB3	2.36	0.55
1:2:853:C:O4'	1:2:853:C:O2	2.24	0.55
1:2:1589:A:N3	1:2:1653:U:O2'	2.34	0.55
18:Q:81:ARG:HB3	18:Q:117:GLY:HA3	1.89	0.55
13:L:76:ILE:HD12	13:L:91:PRO:HG2	1.89	0.55
27:Z:35:VAL:HG23	27:Z:40:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:188:CYS:SG	4:D:235:ASN:HA	2.47	0.54
1:2:962:A:N1	1:2:1055:A:O2'	2.40	0.54
26:Y:61:GLN:O	26:Y:63:ASN:N	2.40	0.54
1:2:146:G:O2'	1:2:147:A:O5'	2.23	0.54
1:2:1354:G:N2	1:2:1357:A:OP2	2.38	0.54
5:E:115:VAL:HG11	5:E:142:LEU:HD21	1.90	0.54
1:2:1719:A:N6	1:2:1814:G:O2'	2.41	0.53
27:Z:29:HIS:NE2	27:Z:69:THR:HG23	2.24	0.53
8:G:68:ILE:HD12	8:G:112:LEU:HD22	1.91	0.53
1:2:1623:A:H5"	21:T:133:GLY:HA3	1.91	0.53
1:2:1693:G:H21	1:2:1834:A:H8	1.54	0.53
1:2:583:A:OP1	12:K:162:ARG:NH2	2.41	0.52
1:2:1139:C:O4'	1:2:1139:C:O2	2.27	0.52
1:2:1252:C:OP1	23:V:75:LYS:NZ	2.40	0.52
10:I:36:LEU:HD23	10:I:36:LEU:H	1.75	0.52
1:2:384:U:O4	11:J:5:ARG:NH2	2.43	0.52
1:2:1152:U:O2'	25:X:16:ASN:ND2	2.43	0.52
1:2:319:C:H4'	1:2:319:C:OP1	2.09	0.52
1:2:687:C:N3	10:I:118:ARG:NH2	2.58	0.52
1:2:1499:U:H5"	5:E:176:LEU:HD21	1.90	0.52
18:Q:123:TYR:O	18:Q:123:TYR:CD2	2.63	0.52
5:E:72:VAL:HG13	13:L:68:TYR:CD1	2.46	0.51
1:2:823:U:O4'	1:2:823:U:O2	2.28	0.51
24:W:20:SER:HB3	24:W:59:ILE:HD11	1.93	0.51
2:B:134:LEU:HD23	2:B:144:THR:HG21	1.93	0.51
12:K:46:VAL:HG11	12:K:106:LEU:HD12	1.93	0.51
1:2:614:C:H2'	1:2:626:G:C8	2.46	0.51
10:I:69:LEU:HG	10:I:96:ALA:HB2	1.92	0.51
1:2:626:G:C2'	1:2:626:G:N3	2.74	0.50
1:2:1520:G:N3	1:2:1520:G:H2'	2.26	0.50
11:J:36:THR:HG21	11:J:179:PRO:HB2	1.93	0.50
18:Q:57:LEU:HG	18:Q:83:MET:SD	2.52	0.50
18:Q:119:PHE:CE1	21:T:119:ALA:HB2	2.47	0.50
19:R:34:VAL:HB	19:R:42:ILE:HD11	1.92	0.50
1:2:1377:U:O2'	1:2:1379:A:OP1	2.30	0.50
24:W:38:GLU:OE2	24:W:51:LYS:HG2	2.12	0.50
25:X:37:PHE:CD1	25:X:103:VAL:HG11	2.47	0.50
1:2:1243:U:H2'	1:2:1244:U:O4'	2.12	0.50
4:D:137:VAL:HG21	4:D:244:ILE:HD12	1.93	0.49
1:2:182:C:H4'	1:2:183:G:O5'	2.10	0.49
1:2:1619:A:OP2	18:Q:47:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:40:ASP:N	24:W:47:ASN:HD21	2.10	0.49
1:2:446:G:OP2	11:J:47:ARG:NH1	2.45	0.49
1:2:1365:G:N2	1:2:1462:U:O4	2.45	0.49
12:K:110:LEU:HD23	12:K:130:ILE:HD13	1.94	0.49
1:2:1473:G:C2	1:2:1475:G:H5"	2.48	0.49
1:2:943:U:OP1	3:C:214:LYS:NZ	2.46	0.48
4:D:251:LEU:HD23	24:W:23:ILE:HG23	1.94	0.48
24:W:39:VAL:HG13	24:W:44:GLY:HA2	1.94	0.48
1:2:1658:G:OP2	1:2:1660:C:N4	2.47	0.48
9:H:52:ILE:HD11	9:H:102:VAL:HG21	1.95	0.48
1:2:1737:G:H5"	9:H:76:LEU:HD11	1.95	0.48
24:W:51:LYS:HG3	24:W:76:HIS:CE1	2.48	0.48
1:2:501:C:O2	1:2:501:C:C2'	2.61	0.48
1:2:1315:U:O2	1:2:1315:U:O4'	2.30	0.48
5:E:190:LEU:HD23	5:E:199:GLY:HA2	1.96	0.48
1:2:1522:A:C2	18:Q:128:HIS:CG	3.02	0.48
8:G:49:LEU:CD2	19:R:49:TYR:HB2	2.44	0.48
26:Y:51:VAL:HG22	26:Y:70:VAL:HG11	1.96	0.48
1:2:1824:A:N3	6:1:6616:C:O2'	2.44	0.48
1:2:1518:C:O4'	1:2:1518:C:O2	2.28	0.48
10:I:100:ILE:HD11	10:I:122:LEU:HA	1.96	0.48
1:2:496:C:OP1	7:F:49:ARG:NH1	2.46	0.47
19:R:37:ARG:HB3	22:U:7:LYS:HG2	1.95	0.47
21:T:134:GLN:OE1	21:T:134:GLN:N	2.48	0.47
2:B:131:HIS:O	2:B:135:MET:HG2	2.15	0.47
2:B:58:LEU:HD11	2:B:177:MET:HB3	1.96	0.47
11:J:56:ARG:HD3	11:J:180:GLY:O	2.13	0.47
1:2:1624:U:O2	1:2:1624:U:O4'	2.32	0.47
8:G:125:SER:HA	8:G:138:ALA:HA	1.95	0.47
6:1:6542:U:O4'	6:1:6542:U:O2	2.31	0.47
8:G:71:ARG:NH1	8:G:148:ASN:OD1	2.47	0.47
11:J:38:ILE:HD11	11:J:81:VAL:HG23	1.97	0.47
1:2:318:A:H3'	1:2:319:C:H5"	1.97	0.47
1:2:1621:U:H1'	18:Q:118:GLU:HG2	1.95	0.47
26:Y:84:PHE:CE2	26:Y:86:PRO:HA	2.50	0.47
1:2:150:A:N6	1:2:169:U:O2	2.48	0.46
1:2:1154:U:O3'	4:D:194:ARG:NH1	2.49	0.46
4:D:127:PHE:CD1	4:D:141:LEU:HD23	2.50	0.46
15:N:22:LEU:HD11	15:N:89:VAL:HA	1.97	0.46
5:E:59:LEU:HA	5:E:66:ILE:HG13	1.98	0.46
26:Y:4:CYS:O	26:Y:4:CYS:SG	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:641:A:O2'	1:2:645:C:OP1	2.33	0.46
21:T:18:THR:HG21	21:T:33:ILE:HA	1.98	0.46
1:2:380:G:O6	11:J:178:ARG:NH1	2.46	0.46
1:2:1530:U:H2'	1:2:1531:A:O4'	2.16	0.46
7:F:55:ALA:HB1	7:F:60:GLU:HB2	1.97	0.46
17:P:53:ILE:HG23	17:P:88:LEU:HD22	1.97	0.46
1:2:929:G:H2'	1:2:930:C:O4'	2.16	0.46
1:2:1360:U:O2'	1:2:1379:A:OP2	2.33	0.46
1:2:427:U:O2	1:2:427:U:O4'	2.33	0.45
1:2:1535:U:H2'	1:2:1535:U:O2	2.16	0.45
9:H:126:ASP:O	9:H:128:THR:N	3.50	0.45
18:Q:37:TYR:OH	18:Q:45:LEU:HD12	2.16	0.45
12:K:89:GLU:N	12:K:89:GLU:OE1	2.49	0.45
22:U:42:HIS:HB2	22:U:83:GLN:HA	1.98	0.45
5:E:75:LYS:HE3	13:L:18:GLU:HG2	1.97	0.45
19:R:41:MET:SD	19:R:41:MET:N	2.90	0.45
1:2:1499:U:C5'	5:E:176:LEU:HD21	2.47	0.45
3:C:125:VAL:HG12	3:C:127:VAL:HB	1.98	0.45
1:2:156:G:OP1	9:H:2:LYS:NZ	2.48	0.45
1:2:986:G:C8	17:P:137:SER:O	2.70	0.45
4:D:98:LEU:HB2	4:D:102:LEU:CD2	2.47	0.45
6:1:6481:G:H2'	6:1:6481:G:N3	2.32	0.45
6:1:6549:G:N2	6:1:6605:A:OP1	2.49	0.45
7:F:61:VAL:HG12	7:F:80:ILE:HG22	1.99	0.45
17:P:44:VAL:HG11	17:P:85:CYS:SG	2.57	0.45
1:2:1083:A:N7	1:2:1841:C:O2'	2.41	0.44
1:2:1734:G:O2'	1:2:1800:A:N6	2.49	0.44
8:G:25:THR:CG2	8:G:42:LYS:HA	2.48	0.44
15:N:33:ARG:NH1	15:N:91:LEU:HD21	2.33	0.44
1:2:356:C:O2	1:2:356:C:C2'	2.66	0.44
1:2:417:C:H6	1:2:417:C:O5'	2.00	0.44
1:2:1144:A:H2'	1:2:1145:A:C8	2.51	0.44
9:H:162:LEU:HD22	9:H:170:ARG:HB2	1.98	0.44
23:V:51:LYS:HB2	23:V:90:ASP:HB2	2.00	0.44
1:2:2:A:C2	4:D:196:ILE:HD13	2.53	0.44
20:S:111:PHE:HB3	20:S:114:LEU:HD21	1.99	0.44
1:2:126:G:H2'	9:H:199:THR:HG21	1.99	0.44
1:2:1535:U:O2'	8:G:82:ASN:OD1	2.24	0.44
1:2:1700:C:C2	1:2:1834:A:N6	2.86	0.44
2:B:65:ILE:CD1	2:B:178:LEU:HD21	2.48	0.44
5:E:162:ASP:N	5:E:163:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1303:C:O2	1:2:1303:C:O4'	2.34	0.44
4:D:240:THR:O	4:D:244:ILE:HG12	2.17	0.44
1:2:686:U:OP1	25:X:32:LYS:N	2.51	0.43
1:2:1444:U:O2'	1:2:1580:A:N1	2.42	0.43
1:2:1232:U:H2'	1:2:1233:G:C8	2.54	0.43
8:G:39:ILE:HG23	8:G:68:ILE:HD13	1.99	0.43
22:U:104:LEU:HB3	22:U:121:ARG:HE	1.83	0.43
24:W:71:ARG:O	24:W:75:SER:HB3	2.18	0.43
26:Y:51:VAL:HG13	26:Y:70:VAL:HG13	2.01	0.43
27:Z:86:GLU:OE2	27:Z:90:ARG:HD2	2.19	0.43
1:2:943:U:OP2	3:C:216:LYS:NZ	2.42	0.43
1:2:1351:G:O2'	1:2:1378:A:N1	2.37	0.43
1:2:536:A:N3	1:2:536:A:H2'	2.34	0.43
1:2:1650:A:H5"	19:R:139:ALA:HB2	1.99	0.43
4:D:98:LEU:O	4:D:102:LEU:HD22	2.18	0.43
7:F:35:PRO:HD2	7:F:83:PRO:HG2	2.00	0.43
21:T:73:ASN:HB3	21:T:76:GLN:HE21	1.84	0.43
4:D:88:ILE:HG21	4:D:94:ILE:HD11	2.00	0.43
2:B:53:ARG:O	2:B:57:LYS:HG2	2.19	0.43
7:F:11:ARG:HA	7:F:28:ALA:HB2	2.00	0.43
11:J:10:LYS:O	11:J:18:ARG:NH1	2.52	0.43
18:Q:61:ARG:O	18:Q:65:LYS:HG2	2.18	0.43
4:D:88:ILE:HG21	4:D:94:ILE:CD1	2.49	0.43
13:L:14:LEU:HD22	13:L:35:LEU:HD23	2.00	0.43
25:X:90:GLN:HB2	25:X:94:LEU:HD12	2.00	0.43
1:2:1579:A:O2'	1:2:1581:C:OP2	2.28	0.42
2:B:8:LEU:HD11	24:W:39:VAL:HG21	2.01	0.42
3:C:150:ILE:HD13	20:S:129:LYS:HB2	2.00	0.42
7:F:126:VAL:HG23	7:F:156:MET:HA	2.00	0.42
8:G:141:VAL:HG21	8:G:146:ARG:HG3	2.01	0.42
10:I:170:VAL:HG13	10:I:187:PHE:HB2	2.00	0.42
12:K:47:LYS:HG3	12:K:102:ILE:HD11	2.01	0.42
1:2:970:G:H3'	1:2:971:G:H5'	2.00	0.42
4:D:209:VAL:HG21	4:D:233:LEU:HD11	2.00	0.42
1:2:1648:G:O6	19:R:16:LYS:NZ	2.35	0.42
24:W:30:ALA:O	24:W:60:ARG:HD3	2.20	0.42
1:2:1297:U:O4	18:Q:59:ARG:NH1	2.53	0.42
1:2:1599:U:O2	1:2:1599:U:O4'	2.35	0.42
1:2:1373:C:O2'	20:S:10:LYS:HE3	2.19	0.42
1:2:1644:C:H4'	19:R:140:ARG:HB2	2.00	0.42
18:Q:94:VAL:HG11	18:Q:116:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1423:C:H2'	1:2:1424:G:O4'	2.19	0.42
1:2:1344:A:N1	1:2:1385:G:O2'	2.42	0.42
1:2:1485:U:OP1	5:E:151:LYS:NZ	2.51	0.42
1:2:1550:G:O2'	1:2:1558:C:O2	2.25	0.42
1:2:929:G:N2	1:2:1013:U:O2	2.52	0.42
1:2:1298:G:H2'	1:2:1298:G:N3	2.35	0.42
1:2:669:A:N3	1:2:1164:G:O2'	2.43	0.42
1:2:1808:U:H2'	1:2:1809:A:C8	2.55	0.42
1:2:1013:U:OP1	1:2:1129:G:O2'	2.37	0.42
1:2:1097:G:H4'	2:B:32:PHE:CD1	2.53	0.42
3:C:107:ARG:HD2	17:P:131:ASP:HB2	2.02	0.42
19:R:10:VAL:HG12	19:R:12:VAL:HG23	2.01	0.42
1:2:130:G:H2'	1:2:130:G:N3	2.35	0.41
4:D:209:VAL:HB	4:D:210:PRO:CD	2.50	0.41
6:1:6607:A:H4'	6:1:6608:U:H5'	2.02	0.41
1:2:153:G:N3	9:H:13:GLN:NE2	2.67	0.41
1:2:445:A:H5"	11:J:51:GLY:HA3	2.01	0.41
9:H:32:MET:HE1	9:H:63:MET:HG2	2.02	0.41
10:I:60:ILE:HG23	10:I:92:VAL:HA	2.02	0.41
1:2:399:C:H3'	1:2:400:C:H5'	2.03	0.41
6:1:6589:C:H5"	6:1:6590:A:C4	2.55	0.41
7:F:11:ARG:NH2	7:F:24:THR:OG1	2.53	0.41
1:2:218:U:O2	11:J:184:ARG:NH2	2.54	0.41
4:D:206:SER:OG	4:D:210:PRO:HG2	2.21	0.41
6:1:6457:A:O2'	6:1:6458:A:O4'	2.20	0.41
9:H:58:LYS:HA	9:H:107:SER:HB2	2.02	0.41
5:E:24:PHE:CZ	5:E:72:VAL:HG11	2.56	0.41
9:H:67:VAL:CG1	9:H:99:GLY:HA2	2.50	0.41
25:X:14:ILE:HG22	25:X:25:VAL:HG11	2.02	0.41
1:2:626:G:N3	1:2:626:G:H2'	2.35	0.41
1:2:1622:U:O4	18:Q:122:THR:HB	2.20	0.41
6:1:6453:C:H2'	6:1:6454:A:C8	2.55	0.41
6:1:6542:U:H3'	6:1:6543:U:O4'	2.21	0.41
9:H:67:VAL:HG13	9:H:99:GLY:HA2	2.03	0.41
1:2:1035:A:H2'	1:2:1036:A:O4'	2.21	0.41
3:C:28:LYS:HA	3:C:49:VAL:O	2.21	0.41
1:2:356:C:O2	1:2:356:C:H2'	2.21	0.41
1:2:1284:A:C6	15:N:91:LEU:HD22	2.56	0.41
2:B:69:GLU:HB3	4:D:270:THR:HG21	2.01	0.41
5:E:51:LEU:HG	5:E:91:VAL:HG22	2.03	0.41
7:F:100:ARG:HD2	7:F:102:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:49:LEU:HD13	18:Q:49:LEU:HA	1.98	0.41
22:U:57:ALA:HA	22:U:103:VAL:HG13	2.02	0.41
23:V:40:ILE:HD11	23:V:53:PRO:HG3	2.03	0.41
1:2:1556:A:N3	1:2:1556:A:H2'	2.36	0.41
2:B:134:LEU:CD2	2:B:144:THR:HG21	2.51	0.41
7:F:44:LEU:HD11	7:F:70:ILE:HG21	2.03	0.41
4:D:98:LEU:CB	4:D:102:LEU:HD22	2.50	0.40
26:Y:60:LYS:HB2	26:Y:114:ASP:O	2.21	0.40
1:2:1605:G:OP1	22:U:84:ARG:NH1	2.55	0.40
11:J:36:THR:HG23	11:J:96:LEU:HB2	2.04	0.40
21:T:26:ILE:HG22	21:T:45:LEU:HD11	2.03	0.40
3:C:33:VAL:HG12	3:C:44:ILE:HD12	2.02	0.40
4:D:213:LEU:HD22	4:D:240:THR:HG23	2.04	0.40
19:R:116:ASP:HB3	19:R:119:LEU:HD23	2.02	0.40
1:2:1231:C:H2'	1:2:1232:U:O4'	2.21	0.40
1:2:616:A:N1	1:2:632:C:H1'	2.36	0.40
1:2:1395:C:H4'	1:2:1396:A:OP1	2.21	0.40
1:2:1621:U:C1'	18:Q:118:GLU:HG2	2.52	0.40
5:E:164:VAL:O	5:E:168:VAL:HG22	2.21	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
2	B	215/295 (73%)	202 (94%)	10 (5%)	3 (1%)	11 46
3	C	211/264 (80%)	195 (92%)	15 (7%)	1 (0%)	29 67
4	D	219/255 (86%)	207 (94%)	11 (5%)	1 (0%)	29 67
5	E	226/281 (80%)	211 (93%)	15 (7%)	0	100 100
7	F	260/263 (99%)	249 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	G	180/204 (88%)	159 (88%)	16 (9%)	5 (3%)	5 29
9	H	235/249 (94%)	224 (95%)	11 (5%)	0	100 100
10	I	181/194 (93%)	167 (92%)	14 (8%)	0	100 100
11	J	204/207 (99%)	190 (93%)	13 (6%)	1 (0%)	29 67
12	K	183/194 (94%)	175 (96%)	7 (4%)	1 (0%)	29 67
13	L	94/149 (63%)	86 (92%)	7 (7%)	1 (1%)	14 51
14	M	139/158 (88%)	130 (94%)	8 (6%)	1 (1%)	22 61
15	N	115/132 (87%)	100 (87%)	14 (12%)	1 (1%)	17 56
16	O	147/151 (97%)	137 (93%)	10 (7%)	0	100 100
17	P	134/151 (89%)	121 (90%)	13 (10%)	0	100 100
18	Q	117/145 (81%)	101 (86%)	13 (11%)	3 (3%)	5 31
19	R	140/172 (81%)	131 (94%)	8 (6%)	1 (1%)	22 61
20	S	130/135 (96%)	116 (89%)	13 (10%)	1 (1%)	19 58
21	T	139/152 (91%)	133 (96%)	4 (3%)	2 (1%)	11 46
22	U	139/145 (96%)	126 (91%)	11 (8%)	2 (1%)	11 46
23	V	98/119 (82%)	90 (92%)	8 (8%)	0	100 100
24	W	81/83 (98%)	77 (95%)	4 (5%)	0	100 100
25	X	127/130 (98%)	122 (96%)	5 (4%)	0	100 100
26	Y	139/143 (97%)	132 (95%)	3 (2%)	4 (3%)	4 28
27	Z	122/134 (91%)	116 (95%)	6 (5%)	0	100 100
28	a	68/125 (54%)	65 (96%)	3 (4%)	0	100 100
29	b	96/115 (84%)	88 (92%)	7 (7%)	1 (1%)	15 54
30	c	81/84 (96%)	73 (90%)	8 (10%)	0	100 100
31	d	60/69 (87%)	58 (97%)	2 (3%)	0	100 100
32	e	53/56 (95%)	48 (91%)	5 (9%)	0	100 100
33	f	55/133 (41%)	49 (89%)	5 (9%)	1 (2%)	8 41
34	g	66/156 (42%)	60 (91%)	5 (8%)	1 (2%)	10 44
35	h	311/317 (98%)	281 (90%)	29 (9%)	1 (0%)	41 74
36	n	23/25 (92%)	23 (100%)	0	0	100 100
All	All	4788/5585 (86%)	4442 (93%)	314 (7%)	32 (1%)	26 61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	45	GLY
3	C	52	THR
8	G	19	LEU
8	G	136	ARG
14	M	100	ASN
19	R	17	LYS
21	T	141	ARG
26	Y	61	GLN
8	G	27	ASP
13	L	64	TRP
18	Q	18	ARG
26	Y	60	LYS
35	h	224	GLY
12	K	147	PHE
15	N	117	GLU
18	Q	70	MET
22	U	111	LYS
26	Y	62	PRO
26	Y	86	PRO
33	f	91	LYS
2	B	102	ARG
2	B	141	ASN
4	D	134	ASN
11	J	123	ARG
20	S	126	MET
21	T	100	ALA
34	g	127	GLY
8	G	46	ALA
29	b	26	CYS
8	G	77	MET
18	Q	52	LYS
22	U	86	GLY

5.3.2 Protein sidechains (i)

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%)	176 (98%)	4 (2%)	52 79
3	C	194/231 (84%)	189 (97%)	5 (3%)	46 76
4	D	186/205 (91%)	182 (98%)	4 (2%)	52 79
5	E	190/232 (82%)	184 (97%)	6 (3%)	39 71
7	F	223/225 (99%)	215 (96%)	8 (4%)	35 69
8	G	156/170 (92%)	149 (96%)	7 (4%)	27 63
9	H	207/218 (95%)	205 (99%)	2 (1%)	76 90
10	I	165/174 (95%)	162 (98%)	3 (2%)	59 82
11	J	178/179 (99%)	176 (99%)	2 (1%)	73 88
12	K	161/168 (96%)	157 (98%)	4 (2%)	47 77
13	L	87/125 (70%)	86 (99%)	1 (1%)	73 88
14	M	130/142 (92%)	127 (98%)	3 (2%)	50 78
15	N	99/108 (92%)	98 (99%)	1 (1%)	76 90
16	O	130/131 (99%)	128 (98%)	2 (2%)	65 85
17	P	106/119 (89%)	102 (96%)	4 (4%)	33 67
18	Q	108/130 (83%)	99 (92%)	9 (8%)	11 40
19	R	117/140 (84%)	114 (97%)	3 (3%)	46 76
20	S	119/121 (98%)	116 (98%)	3 (2%)	47 77
21	T	123/132 (93%)	120 (98%)	3 (2%)	49 77
22	U	111/116 (96%)	109 (98%)	2 (2%)	59 82
23	V	92/107 (86%)	90 (98%)	2 (2%)	52 79
24	W	68/68 (100%)	60 (88%)	8 (12%)	5 23
25	X	112/113 (99%)	108 (96%)	4 (4%)	35 69
26	Y	113/114 (99%)	110 (97%)	3 (3%)	44 75
27	Z	107/115 (93%)	105 (98%)	2 (2%)	57 81
28	a	62/103 (60%)	59 (95%)	3 (5%)	25 61
29	b	86/99 (87%)	84 (98%)	2 (2%)	50 78
30	c	75/76 (99%)	75 (100%)	0	100 100
31	d	55/62 (89%)	55 (100%)	0	100 100
32	e	48/49 (98%)	46 (96%)	2 (4%)	30 65
33	f	47/106 (44%)	45 (96%)	2 (4%)	29 64
34	g	61/140 (44%)	60 (98%)	1 (2%)	62 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	h	272/275 (99%)	269 (99%)	3 (1%)	73 88
36	n	24/24 (100%)	23 (96%)	1 (4%)	30 65
All	All	4192/4762 (88%)	4083 (97%)	109 (3%)	49 76

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
2	B	117	ARG
2	B	136	GLU
2	B	180	GLN
3	C	40	ASN
3	C	63	LYS
3	C	147	ASN
3	C	207	LEU
3	C	213	ARG
4	D	102	LEU
4	D	137	VAL
4	D	141	LEU
4	D	215	LEU
5	E	48	ILE
5	E	57	ASN
5	E	76	ARG
5	E	94	ARG
5	E	106	ARG
5	E	227	LYS
7	F	3	ARG
7	F	51	LYS
7	F	67	GLN
7	F	145	ARG
7	F	148	ARG
7	F	155	LYS
7	F	232	ASN
7	F	246	LEU
8	G	20	PHE
8	G	26	ASP
8	G	29	GLN
8	G	88	MET
8	G	89	THR
8	G	135	ARG
8	G	182	LYS

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Mol	Chain	Res	Type
9	H	63	MET
9	H	201	LYS
10	I	105	THR
10	I	121	THR
10	I	166	VAL
11	J	72	CYS
11	J	99	ASN
12	K	69	ARG
12	K	70	ARG
12	K	79	ARG
12	K	110	LEU
13	L	35	LEU
14	M	20	LYS
14	M	56	ILE
14	M	69	ARG
15	N	33	ARG
16	O	27	LYS
16	O	86	GLU
17	P	133	THR
17	P	137	SER
17	P	142	ARG
17	P	150	ARG
18	Q	13	ARG
18	Q	37	TYR
18	Q	114	HIS
18	Q	118	GLU
18	Q	120	SER
18	Q	121	ILE
18	Q	122	THR
18	Q	124	LYS
18	Q	127	LYS
19	R	18	THR
19	R	31	LEU
19	R	41	MET
20	S	5	ARG
20	S	72	LYS
20	S	127	ASN
21	T	8	LYS
21	T	101	ASN
21	T	142	ARG
22	U	62	ARG
22	U	123	LEU

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Mol	Chain	Res	Type
23	V	36	CYS
23	V	47	ASN
24	W	11	LEU
24	W	32	ILE
24	W	51	LYS
24	W	52	THR
24	W	66	ASP
24	W	75	SER
24	W	76	HIS
24	W	82	ASN
25	X	52	ILE
25	X	80	ASP
25	X	103	VAL
25	X	104	LEU
26	Y	60	LYS
26	Y	61	GLN
26	Y	63	ASN
27	Z	17	LEU
27	Z	101	LYS
28	a	58	LEU
28	a	111	ARG
28	a	113	THR
29	b	5	ARG
29	b	15	ARG
32	e	19	ARG
32	e	49	ASP
33	f	99	LYS
33	f	104	ARG
34	g	138	ARG
35	h	38	LYS
35	h	178	ASN
35	h	198	VAL
36	n	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	128	GLN
2	B	141	ASN
2	B	155	HIS
3	C	40	ASN
3	C	147	ASN

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Mol	Chain	Res	Type
3	C	157	GLN
4	D	115	GLN
4	D	120	GLN
4	D	235	ASN
4	D	272	HIS
7	F	138	HIS
8	G	83	ASN
8	G	118	ASN
9	H	110	ASN
9	H	202	ASN
11	J	165	GLN
11	J	168	GLN
14	M	83	GLN
15	N	48	HIS
16	O	36	GLN
18	Q	104	GLN
19	R	86	GLN
19	R	97	GLN
20	S	127	ASN
21	T	76	GLN
21	T	101	ASN
22	U	85	ASN
23	V	47	ASN
24	W	47	ASN
25	X	16	ASN
27	Z	15	ASN
30	c	26	GLN
31	d	26	GLN
35	h	178	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1869 (90%)	378 (22%)	35 (2%)
6	1	202/253 (79%)	104 (51%)	11 (5%)
All	All	1887/2122 (88%)	482 (25%)	46 (2%)

All (482) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A

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Mol	Chain	Res	Type
1	2	3	C
1	2	4	C
1	2	17	C
1	2	25	A
1	2	33	G
1	2	41	G
1	2	44	U
1	2	45	A
1	2	46	A
1	2	56	G
1	2	58	C
1	2	67	C
1	2	68	A
1	2	69	C
1	2	79	A
1	2	82	G
1	2	99	A
1	2	103	A
1	2	110	U
1	2	111	A
1	2	113	G
1	2	115	U
1	2	123	G
1	2	126	G
1	2	127	C
1	2	128	U
1	2	142	C
1	2	143	U
1	2	147	A
1	2	154	U
1	2	155	G
1	2	158	A
1	2	160	U
1	2	162	C
1	2	163	U
1	2	171	A
1	2	175	A
1	2	180	G
1	2	183	G
1	2	184	G
1	2	187	G
1	2	188	C

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Mol	Chain	Res	Type
1	2	189	U
1	2	190	G
1	2	192	C
1	2	204	G
1	2	213	G
1	2	215	G
1	2	291	G
1	2	292	A
1	2	294	U
1	2	302	A
1	2	307	G
1	2	309	G
1	2	312	G
1	2	317	C
1	2	319	C
1	2	320	G
1	2	323	C
1	2	332	G
1	2	347	G
1	2	362	C
1	2	364	A
1	2	367	U
1	2	368	U
1	2	369	C
1	2	370	G
1	2	381	C
1	2	383	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	400	C
1	2	408	A
1	2	409	C
1	2	416	U
1	2	420	G
1	2	435	A
1	2	438	G
1	2	441	C
1	2	447	A
1	2	448	A
1	2	449	A
1	2	450	C

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Mol	Chain	Res	Type
1	2	464	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	487	U
1	2	492	C
1	2	496	C
1	2	508	A
1	2	509	G
1	2	531	A
1	2	532	C
1	2	533	A
1	2	534	G
1	2	536	A
1	2	537	C
1	2	542	U
1	2	547	G
1	2	548	C
1	2	549	C
1	2	550	C
1	2	554	A
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	568	C
1	2	570	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	604	A

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Mol	Chain	Res	Type
1	2	606	G
1	2	607	U
1	2	608	C
1	2	609	U
1	2	614	C
1	2	617	G
1	2	620	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	631	U
1	2	633	C
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	662	G
1	2	664	A
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	687	C
1	2	688	U
1	2	689	U
1	2	691	G
1	2	752	G
1	2	753	C
1	2	754	G
1	2	799	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	833	C
1	2	834	C
1	2	844	U
1	2	847	A
1	2	859	G
1	2	865	A
1	2	868	G

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Mol	Chain	Res	Type
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	875	A
1	2	877	C
1	2	878	G
1	2	881	G
1	2	886	A
1	2	887	U
1	2	888	U
1	2	890	U
1	2	891	G
1	2	893	U
1	2	895	G
1	2	898	U
1	2	901	G
1	2	909	G
1	2	912	C
1	2	913	A
1	2	914	U
1	2	920	A
1	2	922	A
1	2	933	G
1	2	943	U
1	2	954	U
1	2	970	G
1	2	971	G
1	2	978	G
1	2	985	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1002	U
1	2	1008	A
1	2	1017	U
1	2	1023	A
1	2	1044	G
1	2	1045	U
1	2	1055	A
1	2	1058	A

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Mol	Chain	Res	Type
1	2	1060	A
1	2	1061	U
1	2	1062	A
1	2	1077	A
1	2	1078	C
1	2	1080	A
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1089	G
1	2	1109	C
1	2	1111	U
1	2	1115	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1121	G
1	2	1123	C
1	2	1126	G
1	2	1133	A
1	2	1138	C
1	2	1148	A
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1195	A
1	2	1197	G
1	2	1203	G
1	2	1207	G
1	2	1215	C
1	2	1221	G
1	2	1224	G
1	2	1242	U
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	1274	G
1	2	1275	G

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Mol	Chain	Res	Type
1	2	1282	A
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1293	A
1	2	1294	G
1	2	1298	G
1	2	1299	A
1	2	1301	A
1	2	1302	G
1	2	1304	U
1	2	1307	U
1	2	1308	U
1	2	1314	U
1	2	1318	G
1	2	1320	G
1	2	1330	G
1	2	1342	U
1	2	1348	G
1	2	1354	G
1	2	1371	U
1	2	1372	U
1	2	1374	C
1	2	1376	A
1	2	1377	U
1	2	1378	A
1	2	1379	A
1	2	1382	A
1	2	1396	A
1	2	1397	U
1	2	1398	G
1	2	1401	A
1	2	1402	A
1	2	1403	C
1	2	1404	U
1	2	1406	G
1	2	1409	A
1	2	1428	G
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1466	G

Continued on next page...

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Mol	Chain	Res	Type
1	2	1475	G
1	2	1476	A
1	2	1477	U
1	2	1480	A
1	2	1489	A
1	2	1490	G
1	2	1494	U
1	2	1497	G
1	2	1498	A
1	2	1509	U
1	2	1521	C
1	2	1523	C
1	2	1525	C
1	2	1531	A
1	2	1533	A
1	2	1535	U
1	2	1548	G
1	2	1552	G
1	2	1553	C
1	2	1554	C
1	2	1556	A
1	2	1564	C
1	2	1567	G
1	2	1570	G
1	2	1575	G
1	2	1580	A
1	2	1582	C
1	2	1584	G
1	2	1587	G
1	2	1588	A
1	2	1601	A
1	2	1602	U
1	2	1604	G
1	2	1606	G
1	2	1614	A
1	2	1621	U
1	2	1623	A
1	2	1635	C
1	2	1637	A
1	2	1638	G
1	2	1648	G
1	2	1654	G

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Mol	Chain	Res	Type
1	2	1655	C
1	2	1661	A
1	2	1664	A
1	2	1665	G
1	2	1671	G
1	2	1680	G
1	2	1692	U
1	2	1721	U
1	2	1722	G
1	2	1725	U
1	2	1726	G
1	2	1742	C
1	2	1743	G
1	2	1744	G
1	2	1745	A
1	2	1748	G
1	2	1753	C
1	2	1777	G
1	2	1779	G
1	2	1783	C
1	2	1785	C
1	2	1801	A
1	2	1809	A
1	2	1823	A
1	2	1824	A
1	2	1825	A
1	2	1826	G
1	2	1829	G
1	2	1836	G
1	2	1837	G
1	2	1838	U
1	2	1845	A
1	2	1849	G
1	2	1851	A
1	2	1858	G
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1869	A
6	1	6425	A

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Mol	Chain	Res	Type
6	1	6426	U
6	1	6427	G
6	1	6429	U
6	1	6430	U
6	1	6431	A
6	1	6432	C
6	1	6433	C
6	1	6434	C
6	1	6435	A
6	1	6436	U
6	1	6445	G
6	1	6449	U
6	1	6450	U
6	1	6451	U
6	1	6457	A
6	1	6471	G
6	1	6472	G
6	1	6473	C
6	1	6474	U
6	1	6475	U
6	1	6482	A
6	1	6483	U
6	1	6484	G
6	1	6485	G
6	1	6486	U
6	1	6487	C
6	1	6488	G
6	1	6489	A
6	1	6491	G
6	1	6492	U
6	1	6493	G
6	1	6494	C
6	1	6499	U
6	1	6501	U
6	1	6506	U
6	1	6507	G
6	1	6511	A
6	1	6512	G
6	1	6514	C
6	1	6515	U
6	1	6516	C
6	1	6517	G

Continued on next page...

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Mol	Chain	Res	Type
6	1	6518	G
6	1	6519	U
6	1	6520	G
6	1	6522	C
6	1	6523	A
6	1	6524	G
6	1	6525	C
6	1	6527	C
6	1	6531	C
6	1	6532	A
6	1	6533	A
6	1	6534	A
6	1	6535	U
6	1	6536	C
6	1	6537	C
6	1	6539	C
6	1	6540	U
6	1	6541	A
6	1	6542	U
6	1	6543	U
6	1	6544	G
6	1	6545	G
6	1	6546	A
6	1	6548	A
6	1	6549	G
6	1	6551	A
6	1	6552	A
6	1	6553	C
6	1	6555	G
6	1	6557	U
6	1	6558	G
6	1	6562	U
6	1	6566	C
6	1	6567	A
6	1	6568	G
6	1	6569	U
6	1	6570	U
6	1	6572	C
6	1	6575	C
6	1	6576	A
6	1	6577	G
6	1	6587	A

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Mol	Chain	Res	Type
6	1	6588	A
6	1	6589	C
6	1	6590	A
6	1	6591	C
6	1	6596	G
6	1	6598	C
6	1	6599	G
6	1	6603	C
6	1	6604	G
6	1	6605	A
6	1	6606	A
6	1	6607	A
6	1	6608	U
6	1	6609	A
6	1	6610	C
6	1	6611	C
6	1	6612	A
6	1	6613	U
6	1	6615	C

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	24	C
1	2	43	U
1	2	92	A
1	2	110	U
1	2	182	C
1	2	293	C
1	2	465	A
1	2	532	C
1	2	553	U
1	2	554	A
1	2	561	A
1	2	627	U
1	2	668	A
1	2	688	U
1	2	752	G
1	2	869	A
1	2	870	A
1	2	887	U
1	2	908	A

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Mol	Chain	Res	Type
1	2	912	C
1	2	1016	U
1	2	1137	U
1	2	1165	G
1	2	1395	C
1	2	1476	A
1	2	1489	A
1	2	1556	A
1	2	1636	G
1	2	1637	A
1	2	1664	A
1	2	1679	A
1	2	1741	U
1	2	1744	G
1	2	1808	U
1	2	1836	G
6	1	6456	U
6	1	6484	G
6	1	6493	G
6	1	6506	U
6	1	6514	C
6	1	6538	U
6	1	6551	A
6	1	6554	A
6	1	6589	C
6	1	6605	A
6	1	6609	A

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 monosaccharides 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.

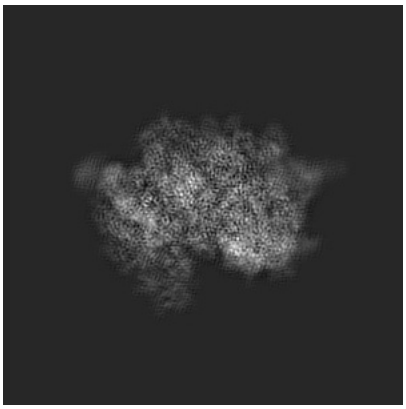
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20249. These allow visual inspection of the internal detail of the map and identification of artifacts.

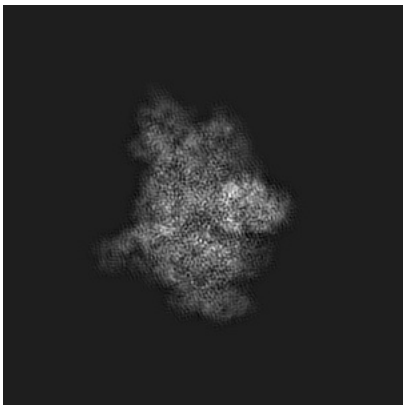
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

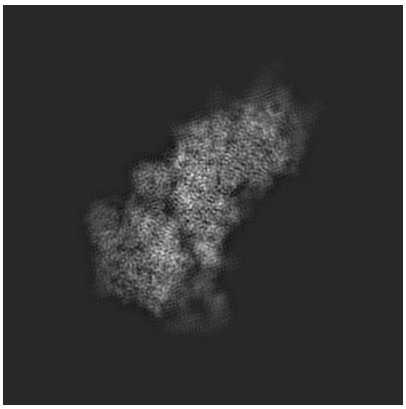
6.1.1 Primary map



X

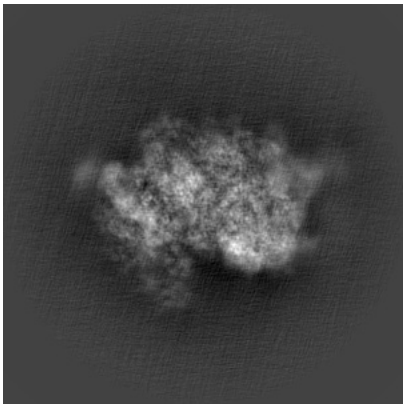


Y

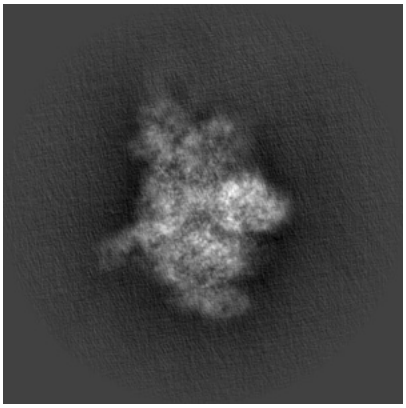


Z

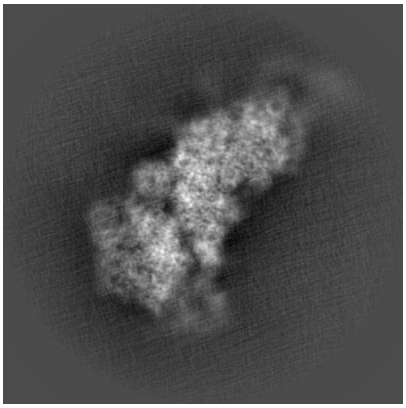
6.1.2 Raw map



X



Y

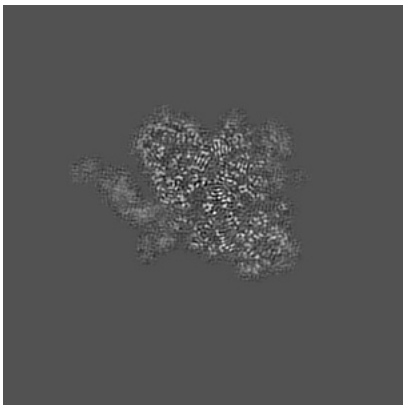


Z

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

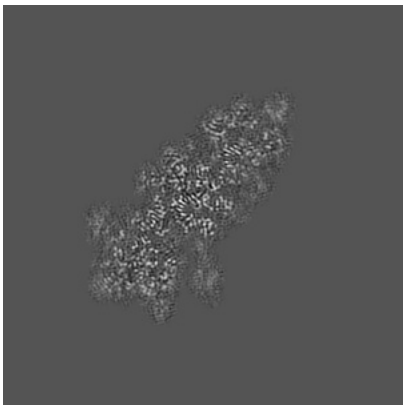
6.2 Central slices (i)

6.2.1 Primary map



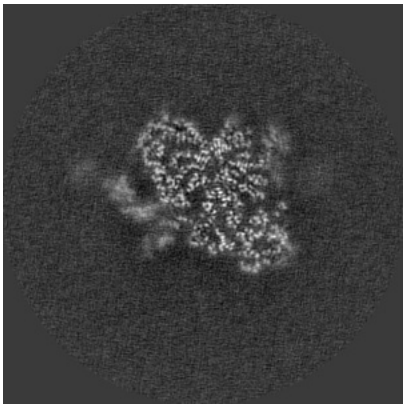
X Index: 156

Y Index: 156

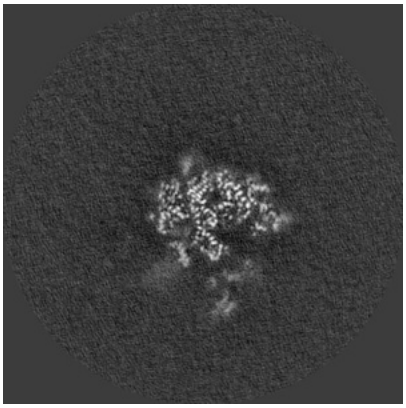


Z Index: 156

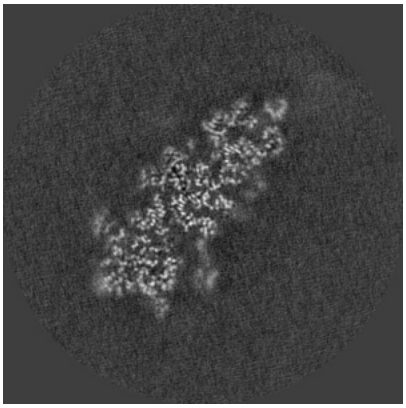
6.2.2 Raw map



X Index: 156



Y Index: 156

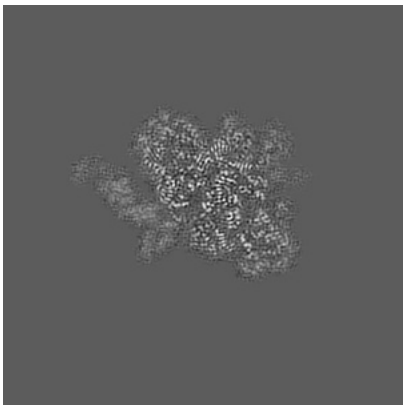


Z Index: 156

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

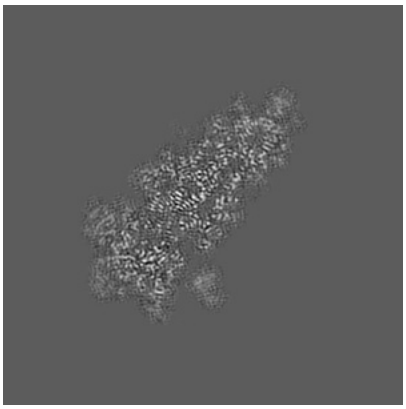
6.3 Largest variance slices (i)

6.3.1 Primary map



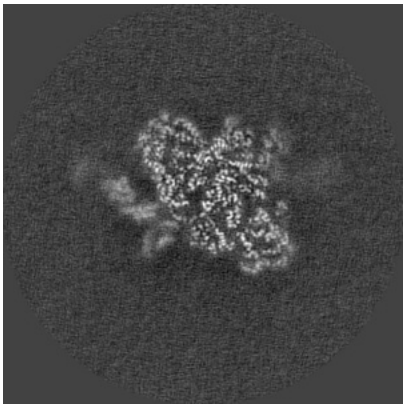
X Index: 157

Y Index: 185

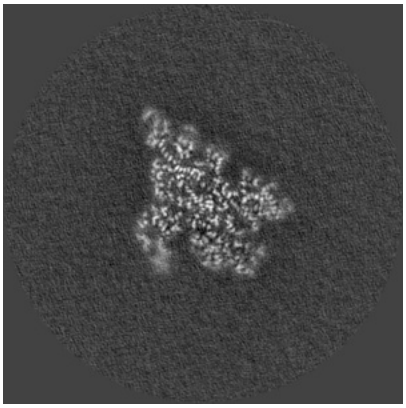


Z Index: 161

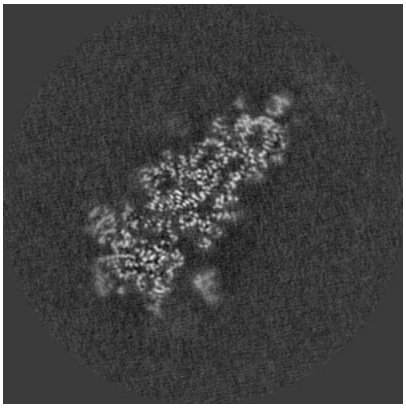
6.3.2 Raw map



X Index: 157



Y Index: 181

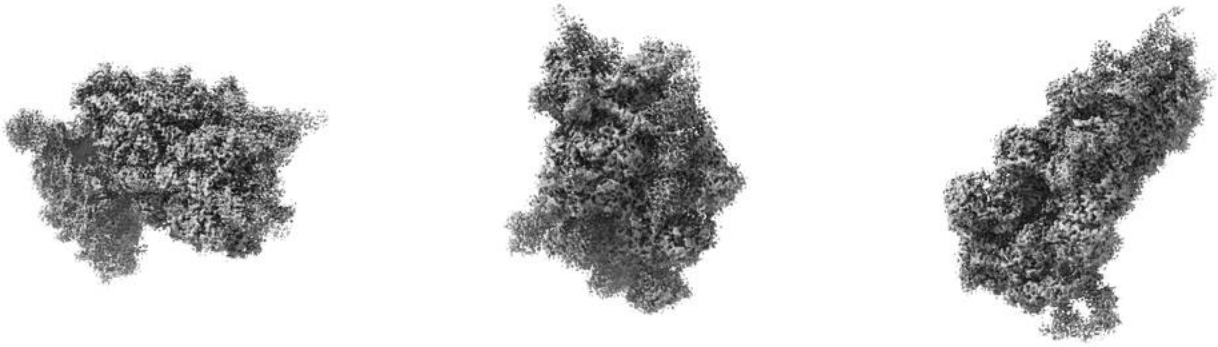


Z Index: 161

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

6.4 Orthogonal surface views (i)

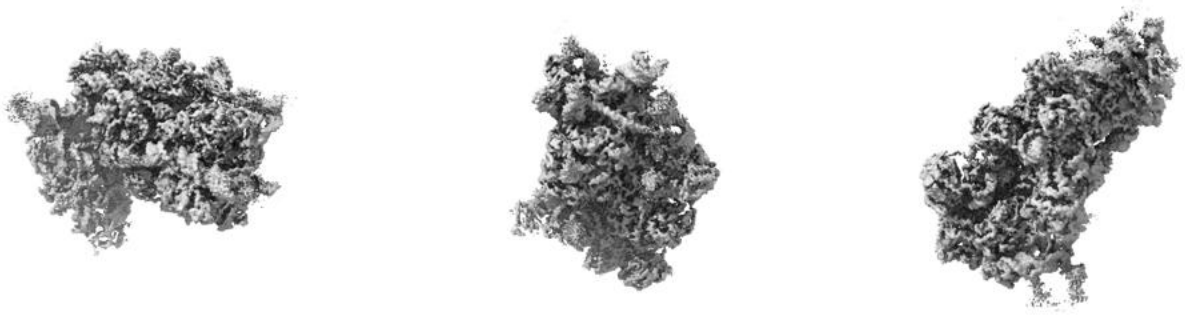
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

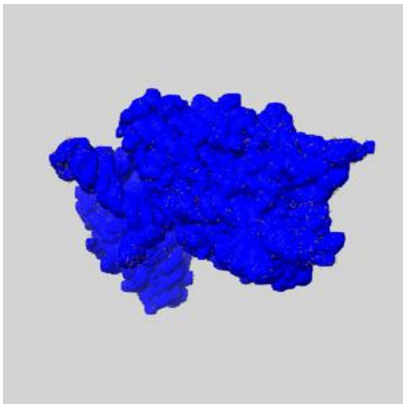
6.5 Mask visualisation

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

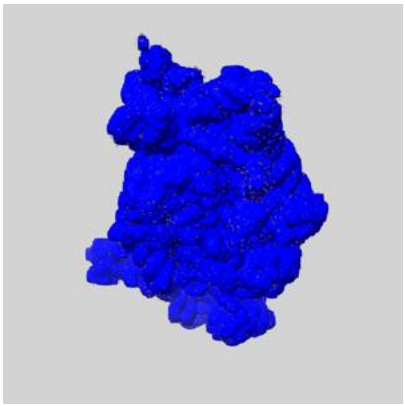
A mask typically either:

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

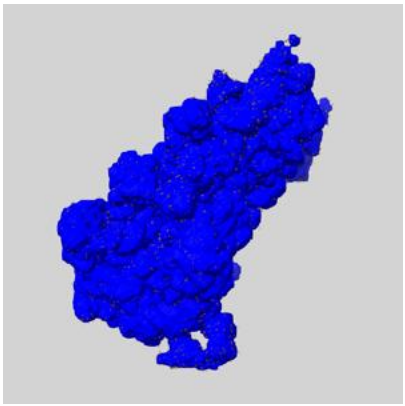
6.5.1 emd_20249_msk_1.map



X



Y

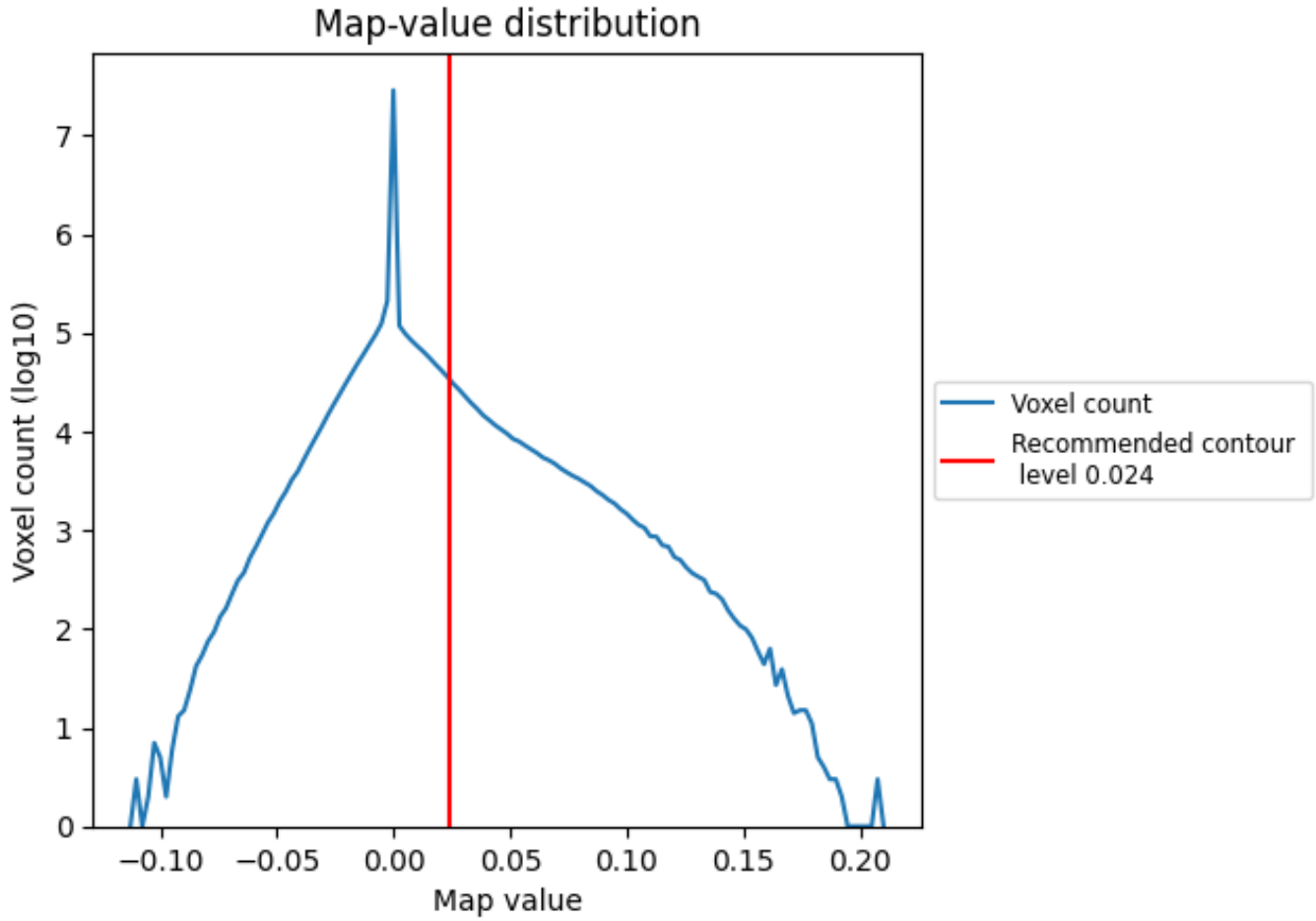


Z

7 Map analysis

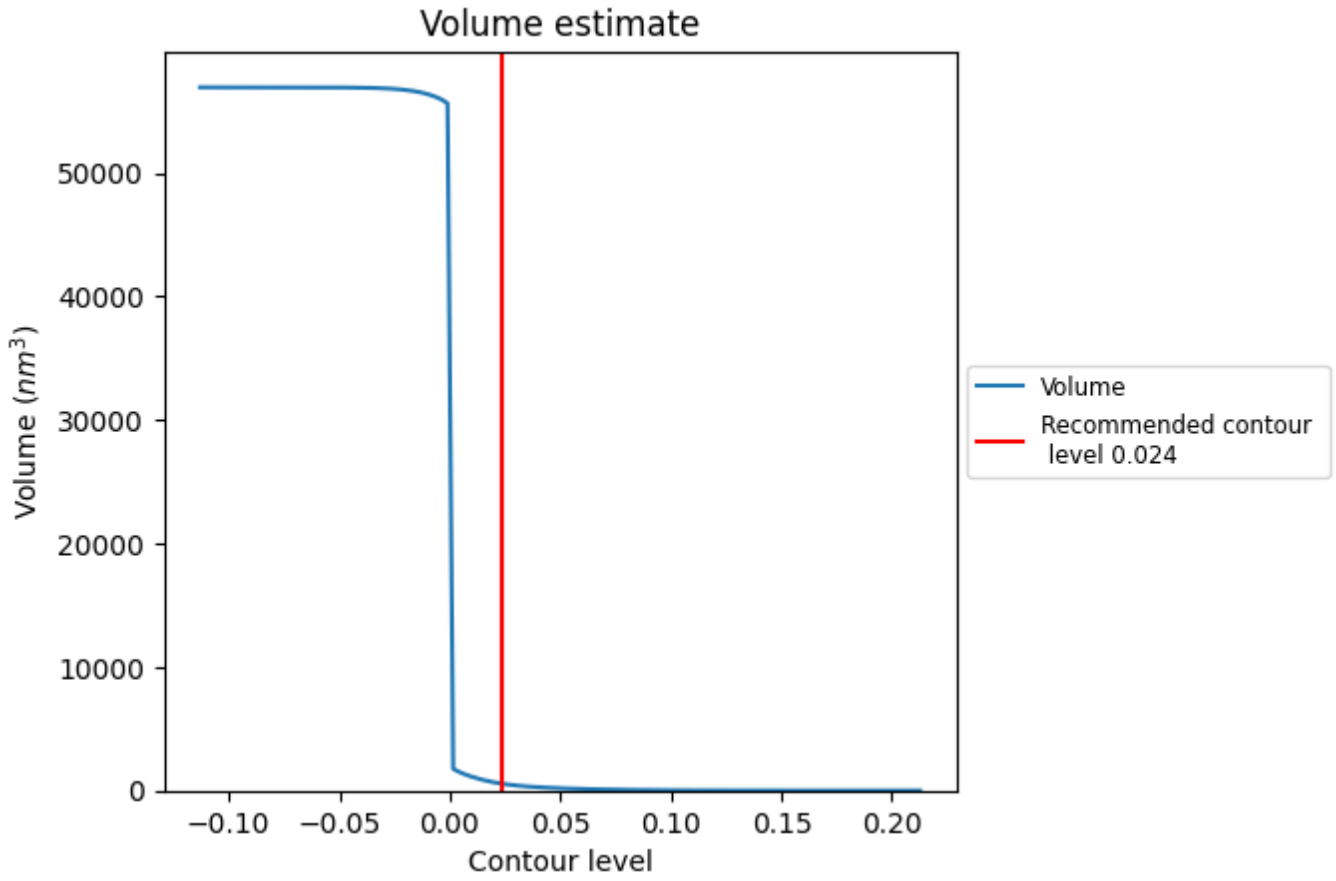
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

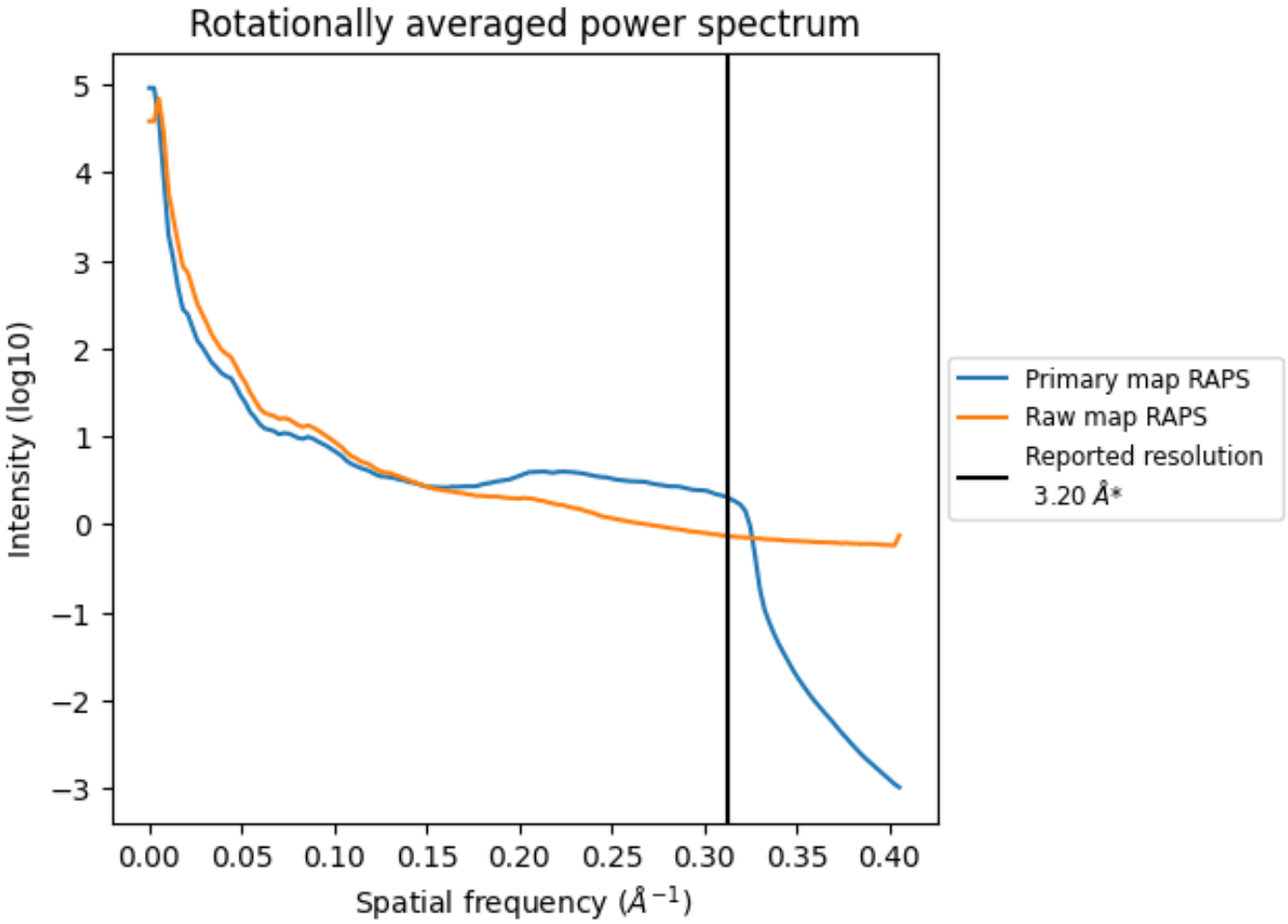
7.2 Volume estimate



The volume at the recommended contour level is 546 nm^3; this corresponds to an approximate mass of 494 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 (i)

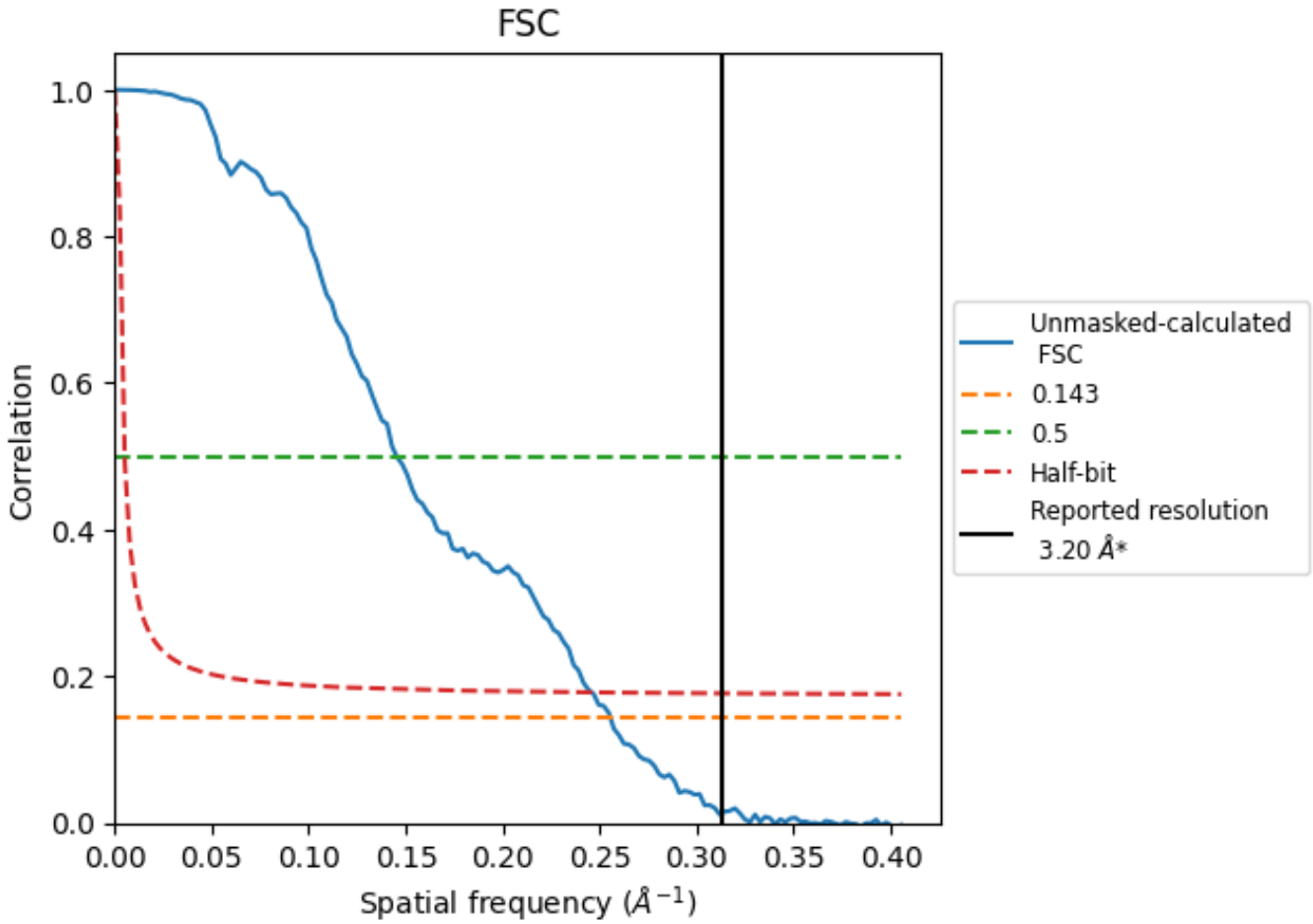


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

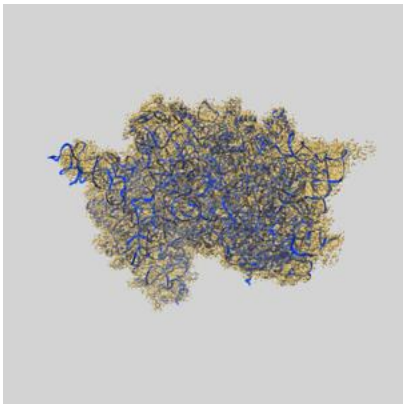
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	6.88	4.07

*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 3.91 differs from the reported value 3.2 by more than 10 %

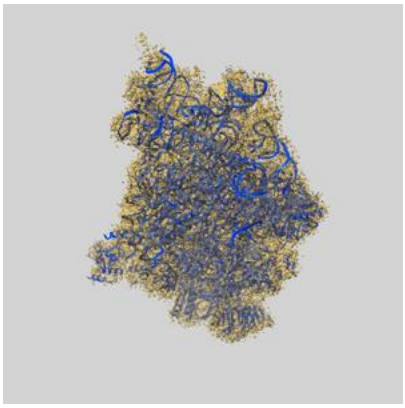
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20249 and PDB model 6P4H. Per-residue inclusion information can be found in section 3 on page 11.

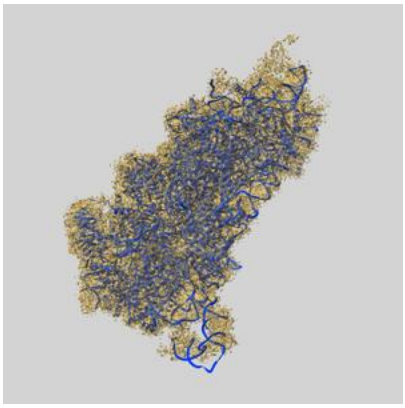
9.1 Map-model overlay



X



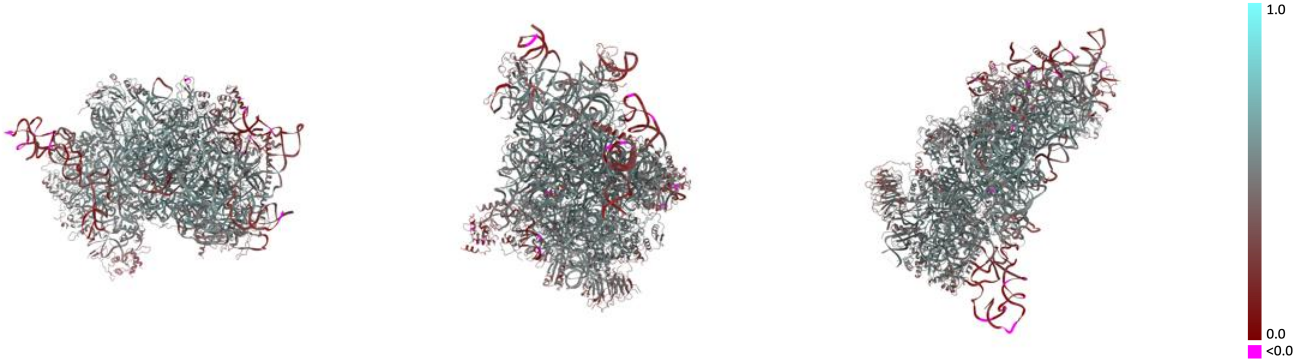
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024 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.

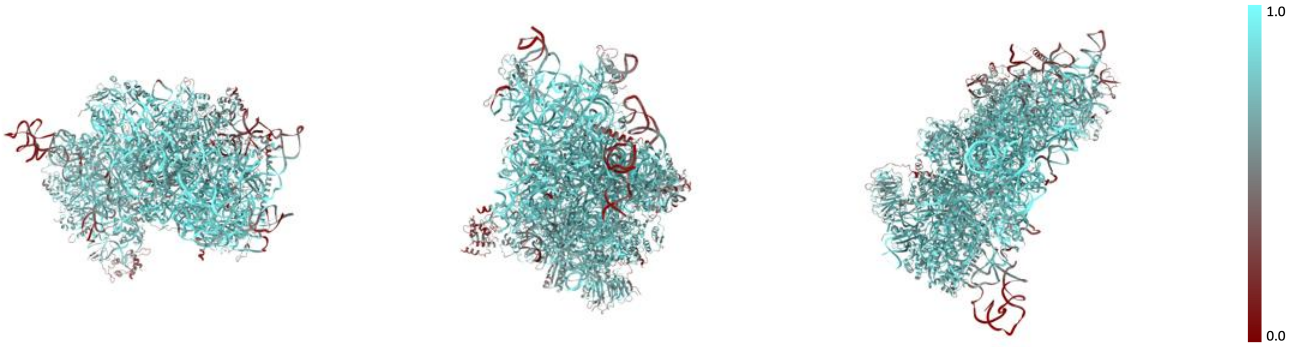
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

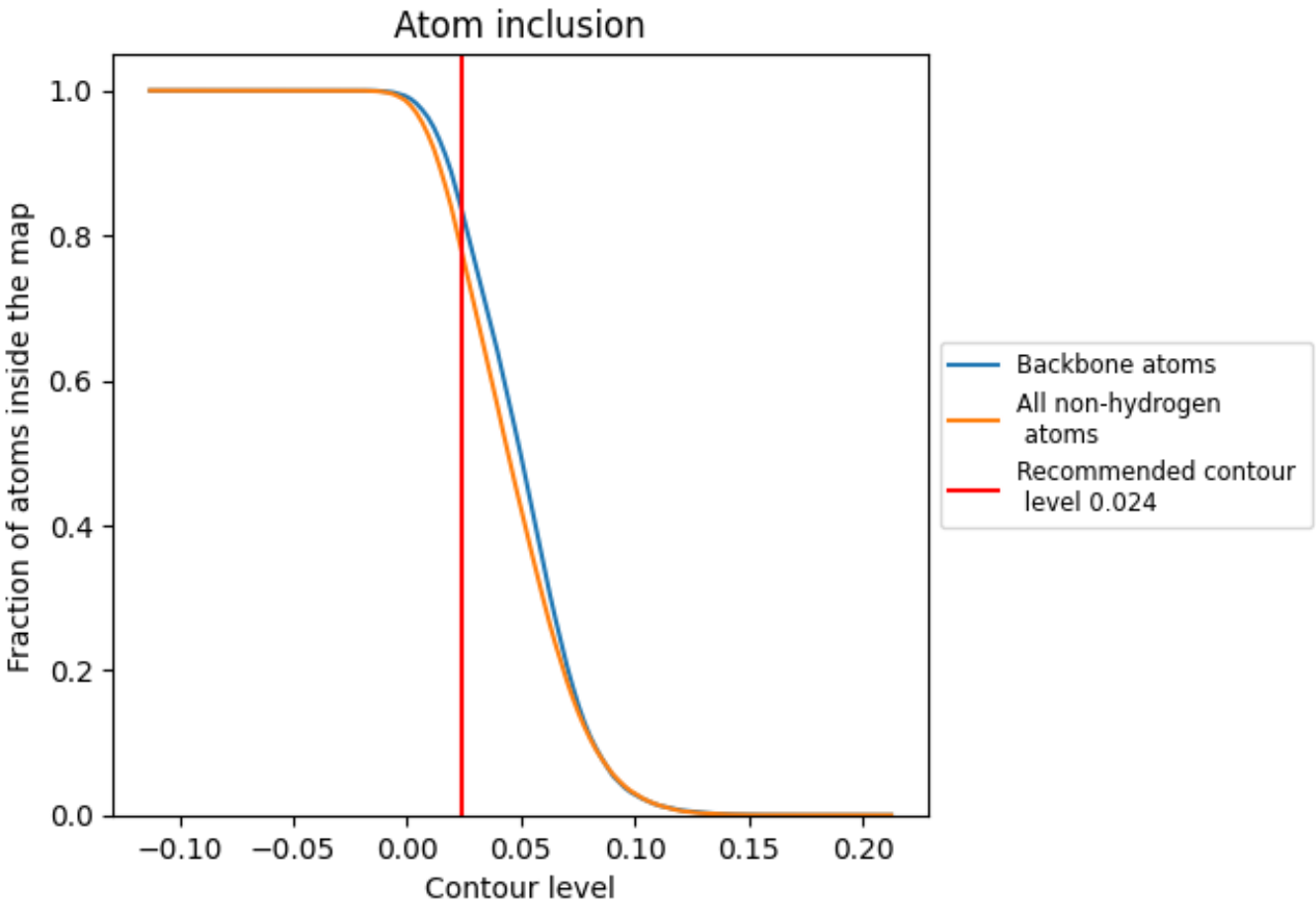
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.024).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7784	0.4690
1	0.4689	0.2280
2	0.8710	0.5060
B	0.7660	0.4970
C	0.7681	0.4790
D	0.8042	0.5200
E	0.6928	0.4550
F	0.7910	0.5010
G	0.7948	0.5090
H	0.6679	0.4090
I	0.5955	0.3870
J	0.7191	0.4500
K	0.7775	0.4940
L	0.7342	0.4560
M	0.7763	0.5060
N	0.2752	0.2130
O	0.7710	0.4780
P	0.7589	0.4970
Q	0.6764	0.3960
R	0.7903	0.5040
S	0.6994	0.4550
T	0.7396	0.4610
U	0.7957	0.4870
V	0.6525	0.4240
W	0.7760	0.5010
X	0.8188	0.5400
Y	0.8123	0.5240
Z	0.7706	0.4820
a	0.7169	0.4700
b	0.7923	0.5220
c	0.7230	0.4600
d	0.7340	0.4750
e	0.8254	0.5290
f	0.6568	0.4500
g	0.3500	0.2680

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Chain	Atom inclusion	Q-score
h	0.6742	0.4090
n	0.6697	0.4550