



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:14 AM UTC

PDB ID : 7SYT / pdb_00007syt
EMDB ID : EMD-25540
Title : Structure of the wt IRES w/o eIF2 48S initiation complex, closed conformation. Structure 13(wt)
Authors : Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2021-11-25
Resolution : 4.40 Å(reported)
Based on initial models : 5FLX, 6D9J, 5K0Y

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

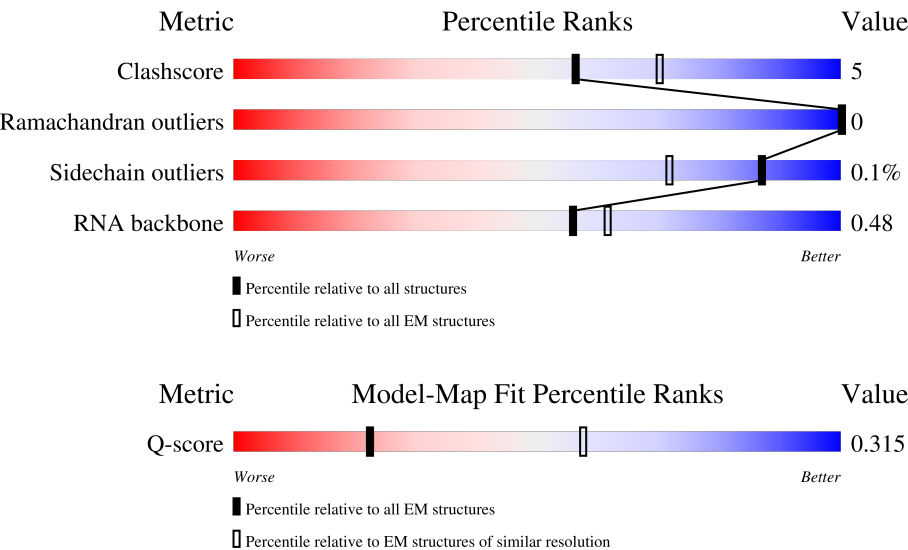
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	i	75	
36	n	25	
37	z	400	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 80962 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 eS1.

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 uS5 (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	1	0
			1691	1061	333	292	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 S10_pectin domain-containing protein.

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	120	Total	C	N	O	S	0	0
			997	635	187	168	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 RNA chain called Met-tRNA-i-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 36 is a protein called 60s ribosomal protein l41.

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

- Molecule 37 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	z	188	Total	C	N	O	P	0	0
			4017	1789	721	1319	188		

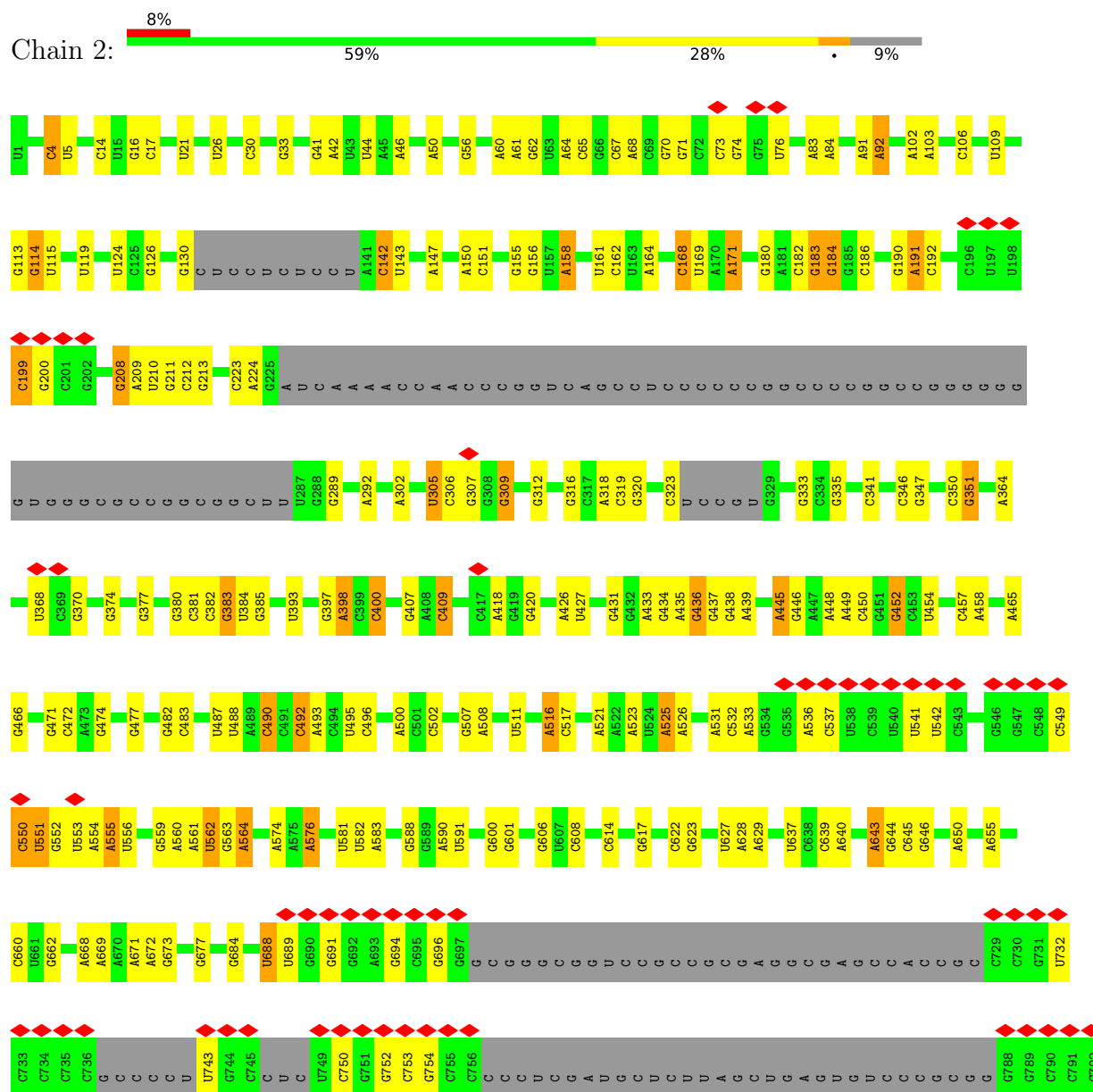
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

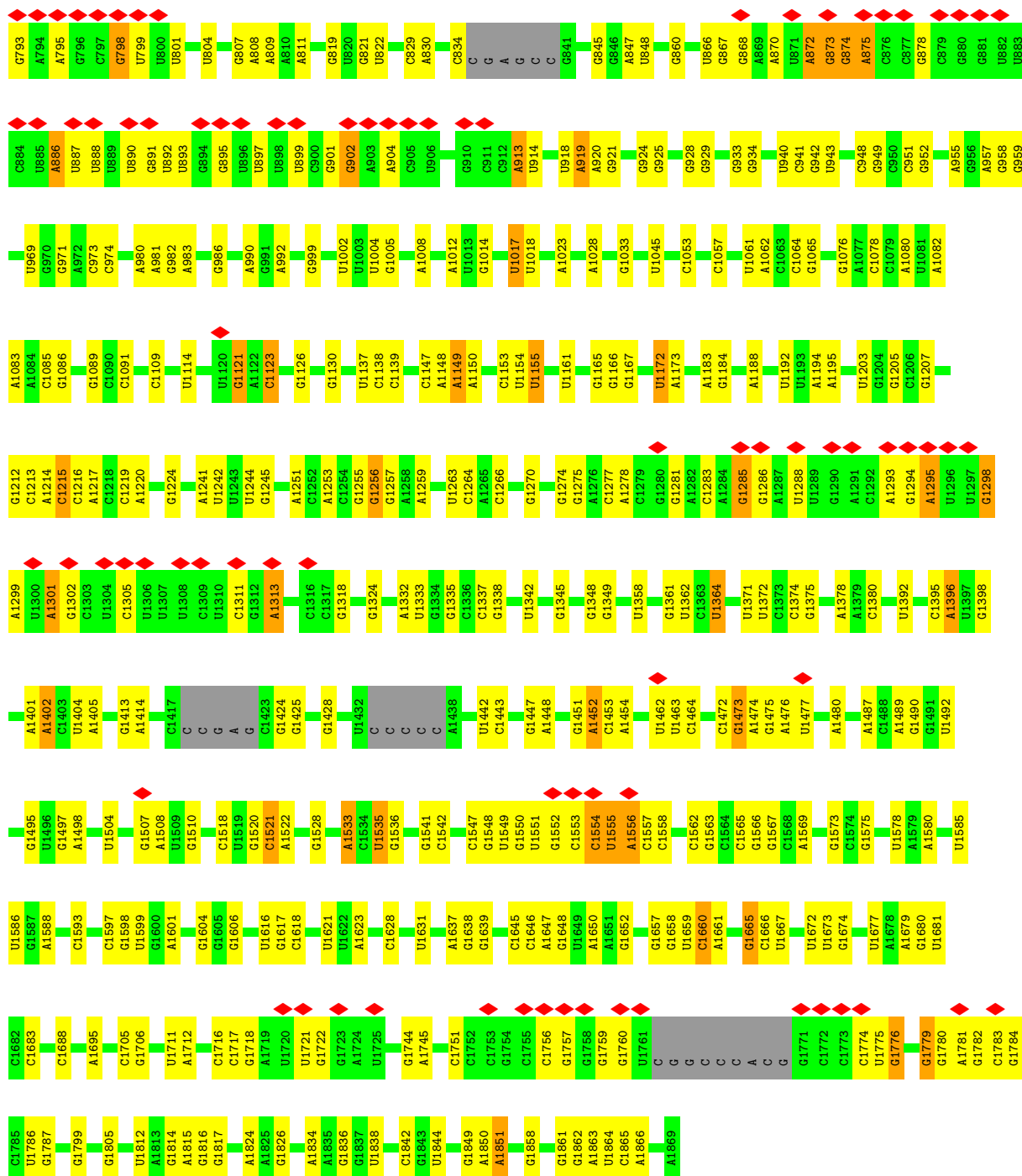
Mol	Chain	Residues	Atoms		AltConf
38	b	1	Total	Zn	0
			1	1	

3 Residue-property plots

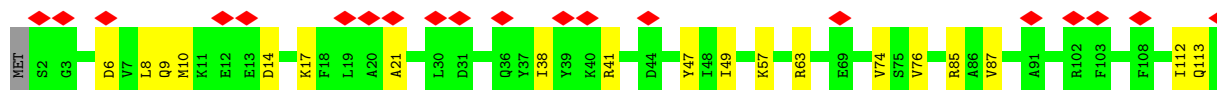
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

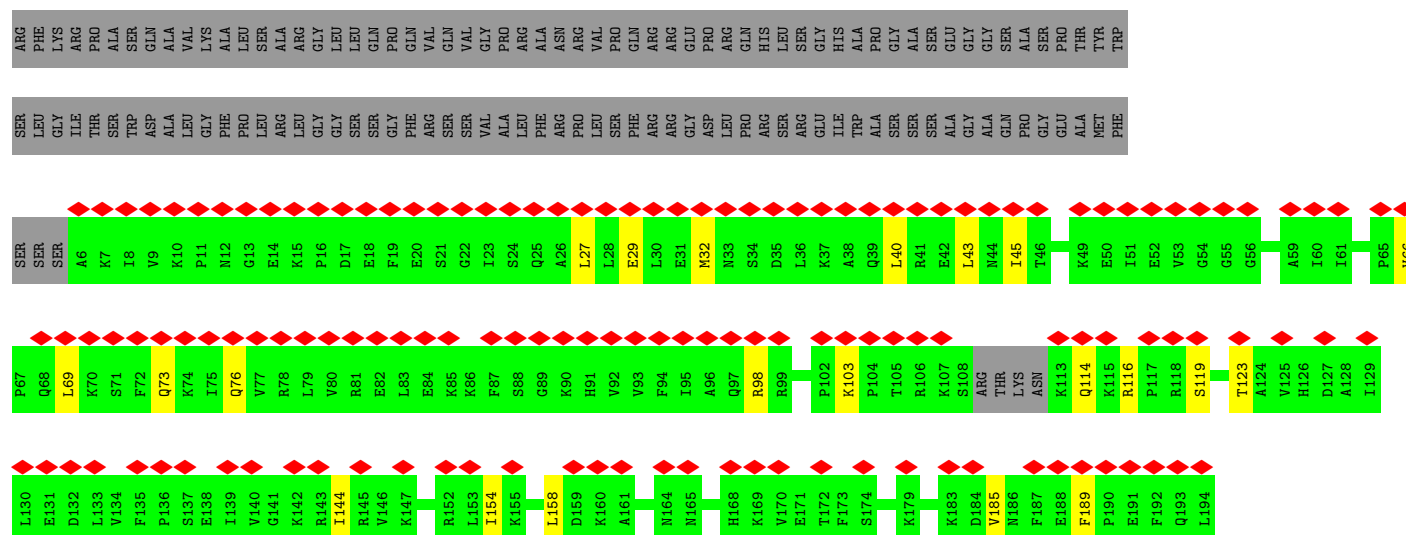
• Molecule 1: 18S rRNA



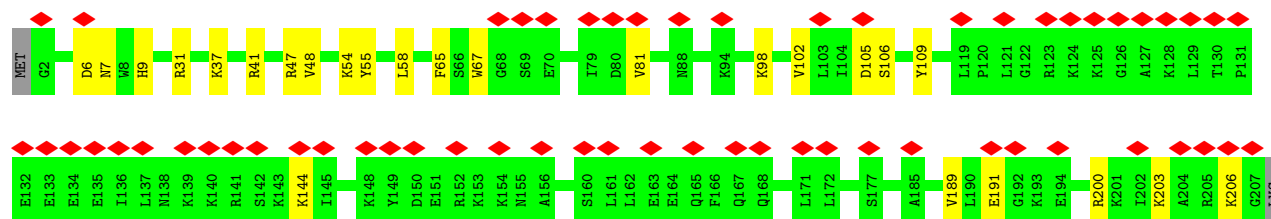
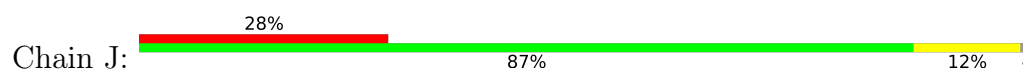


• Molecule 2: 40S ribosomal protein SA

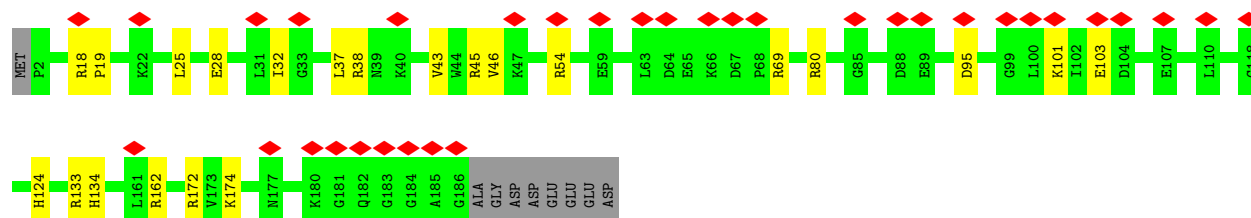
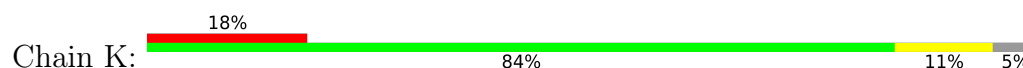




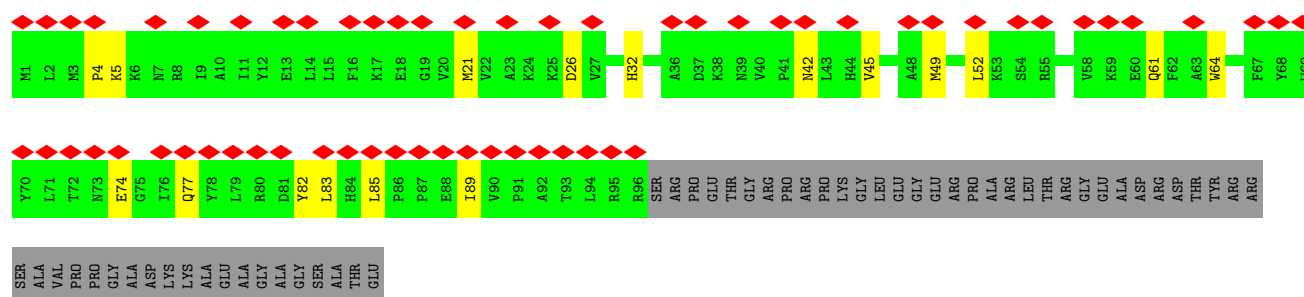
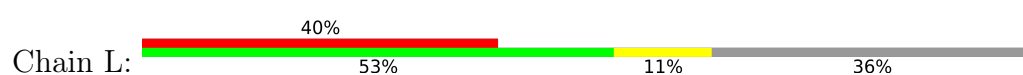
• Molecule 10: eS8



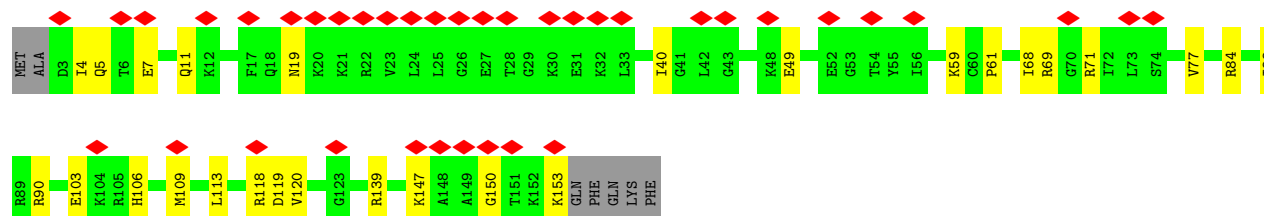
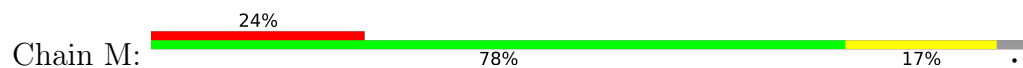
• Molecule 11: uS4



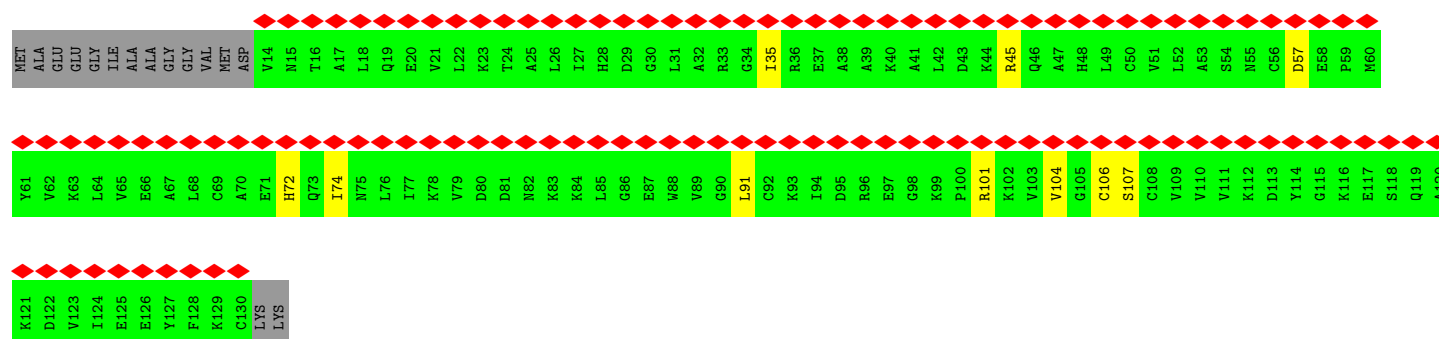
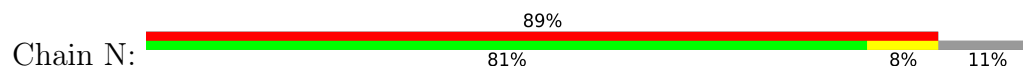
• Molecule 12: S10_pectin domain-containing protein



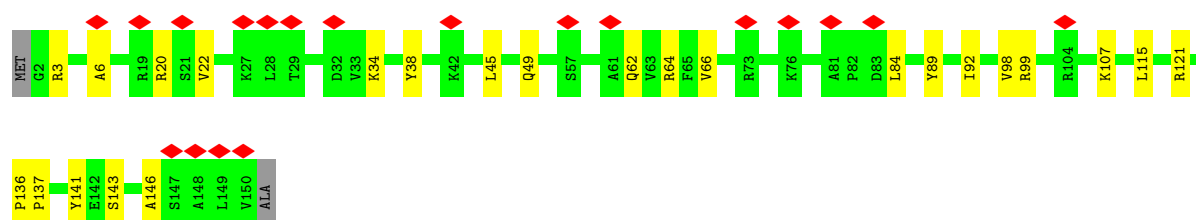
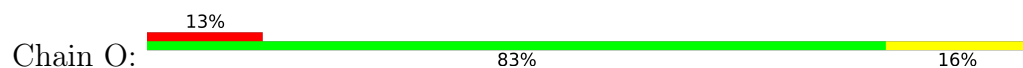
- Molecule 13: uS17



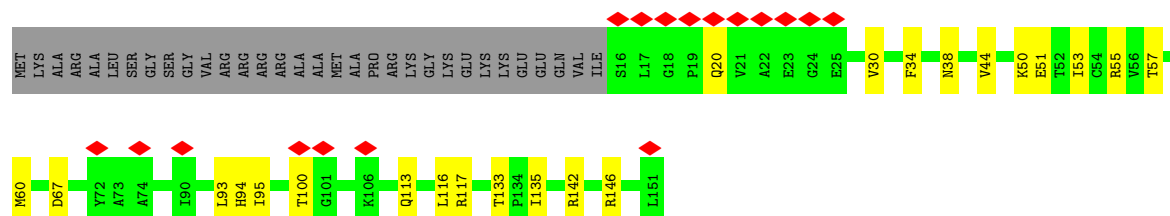
- Molecule 14: eS12



- Molecule 15: uS15

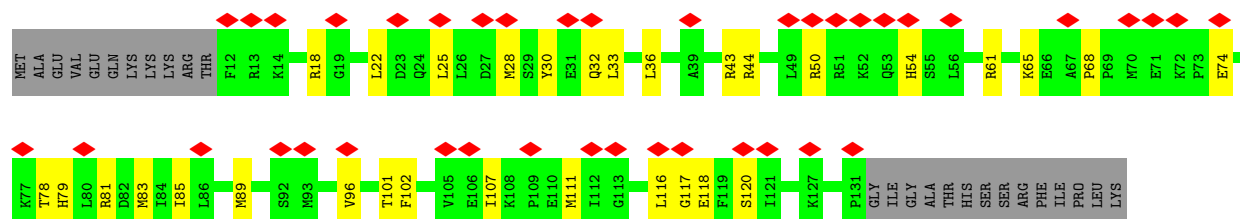


- Molecule 16: uS11

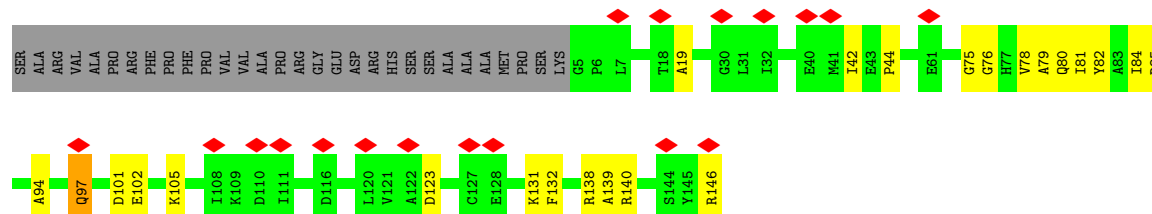


- Molecule 17: uS19

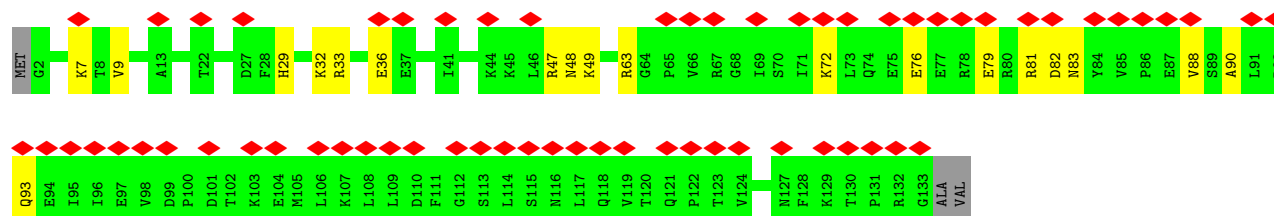
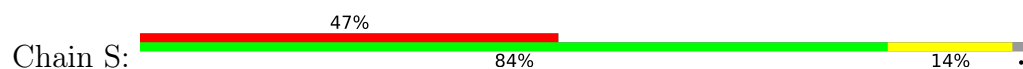




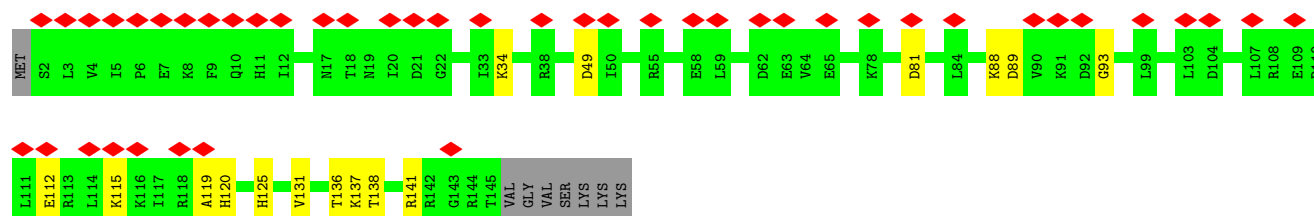
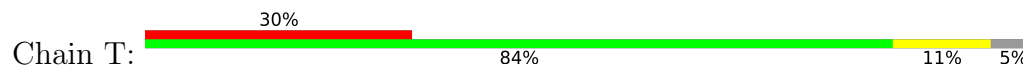
• Molecule 18: uS9



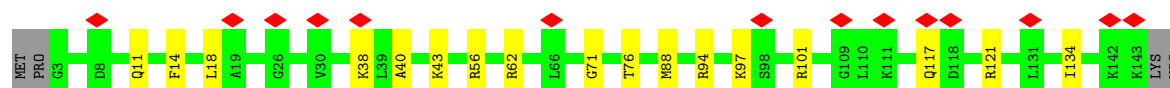
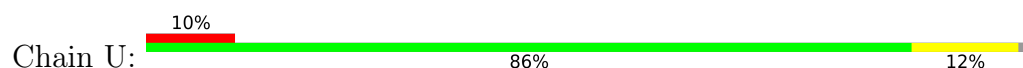
• Molecule 19: eS17



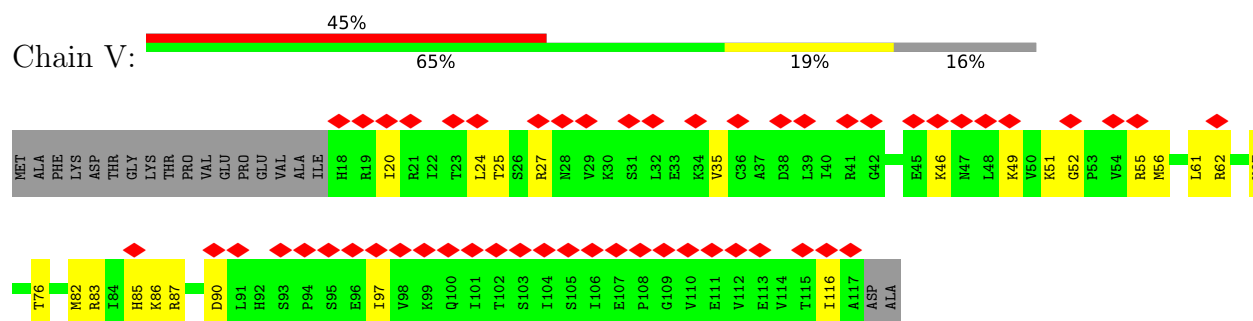
• Molecule 20: uS13



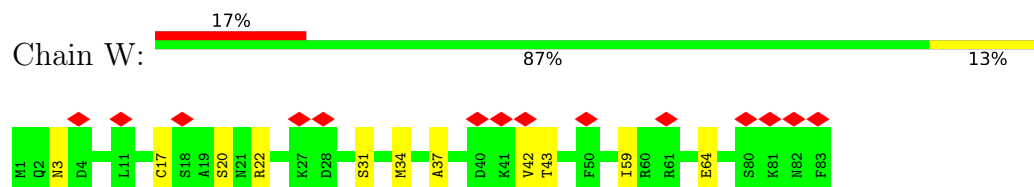
• Molecule 21: eS19



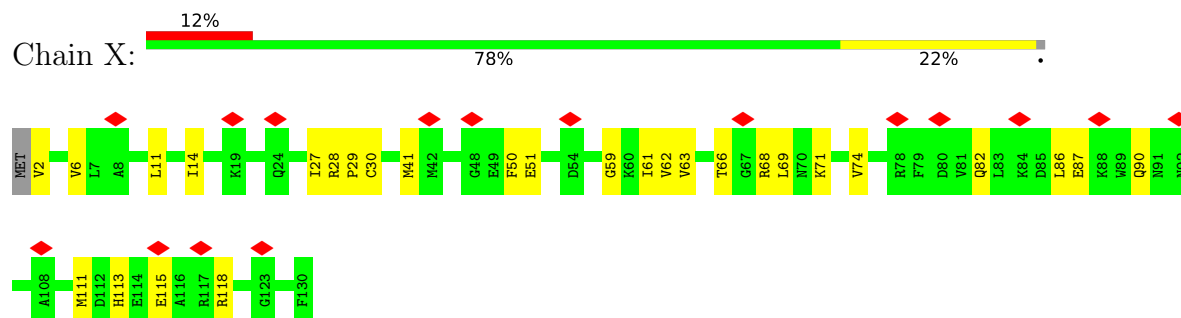
• Molecule 22: uS10



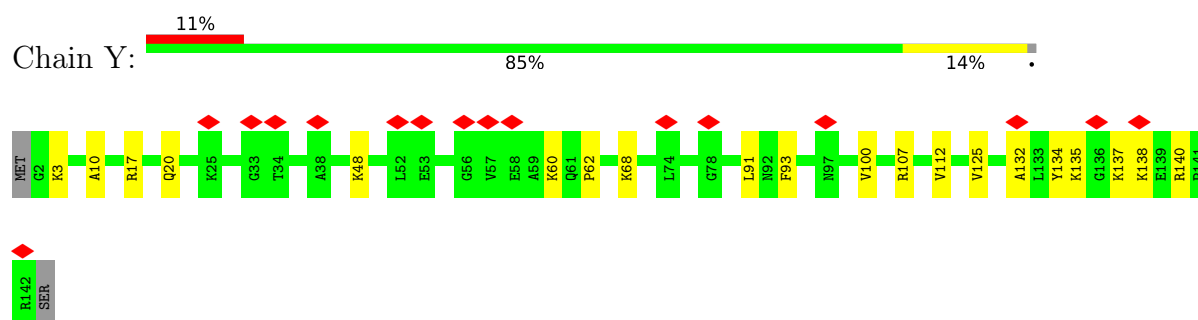
- Molecule 23: 40S ribosomal protein S21



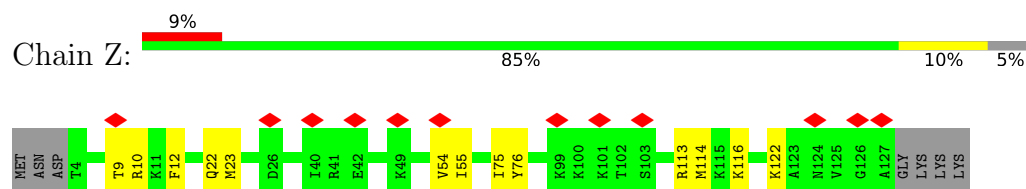
- Molecule 24: uS8



- Molecule 25: uS12

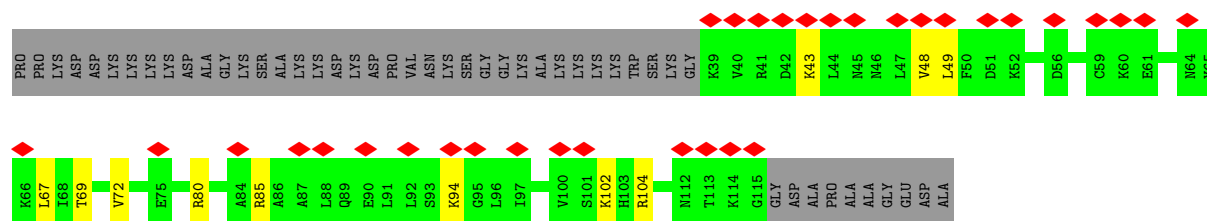


- Molecule 26: 40S ribosomal protein S24

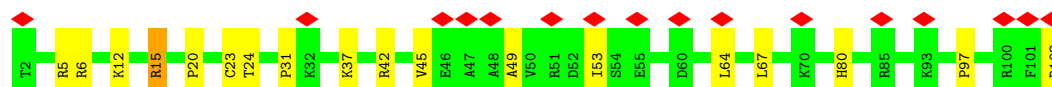
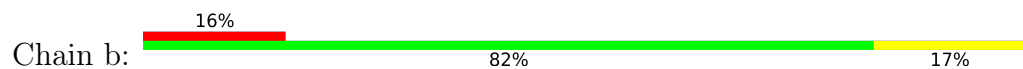


- Molecule 27: 40S ribosomal protein S25

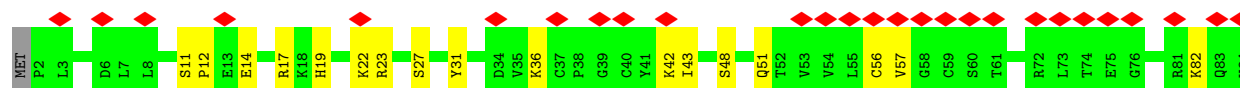
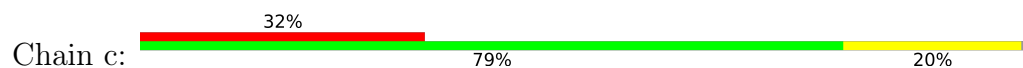




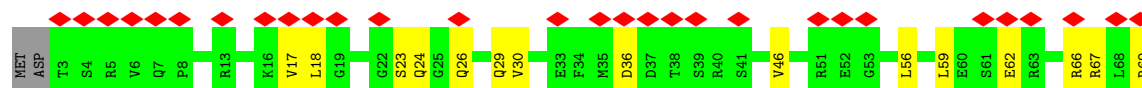
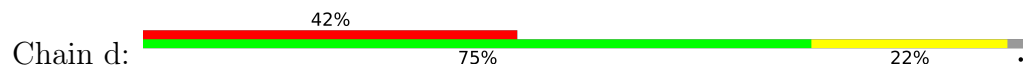
• Molecule 28: eS26 (S26)



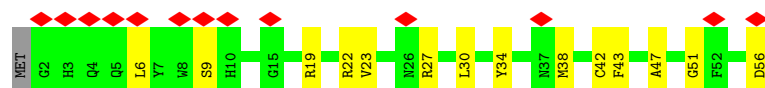
• Molecule 29: eS27



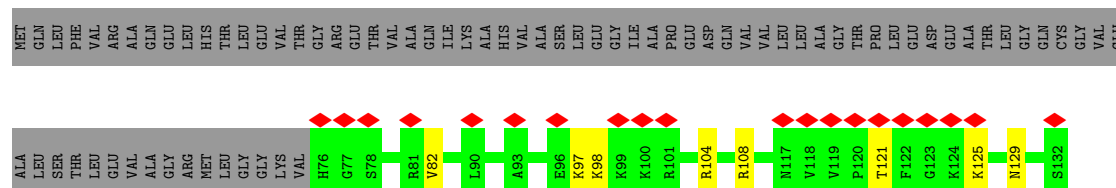
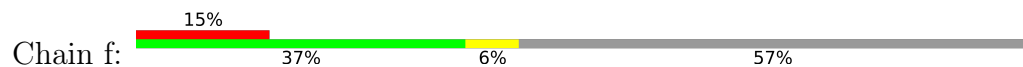
• Molecule 30: eS28



• Molecule 31: eS29



• Molecule 32: eS30



• Molecule 33: 40S ribosomal protein S27a



MET ALA ARG HIS HIS PRO LEU TVR GLN GLY SER GLY ILE TRP CYS GLY ARG LEU ARG LEU ARG GLY GLY GLY ALA ALA GLY LYS PRO ARG GLY ASP GLY ASN LEU PHE LEU PHE LEU ASP PRO PRO VAL SER ALA ARG ARG TRP ALA GLY ARG HIS GLN ASP ALA ASP LYS LEU ARG ARG GLU ASN PRO TYR GLY

GLU ASP HIS HIS ALA ARG GLY PRO SER ASP GLN GLN ARG LEU ILE PHE LEU ALA GLY LYS THR SER ASP TYR ASN ILE ALA GLN LYS LEU PHE LEU PHE THR LEU HIS PRO LEU VAL SER LEU ARG LEU ARG TRP ALA GLY ARG HIS GLN ASP ALA ASP LYS LYS K83 S84 Y85 T86 T87 P88

K89 K90 N91 K92 H93 K94 R95 K96 K97 V98 K99 L100 A101 V102 L103 K104 Y105 Y106 K107 V108 D109 E110 N111 G112 K113 I114 S115 R116 L117 R118 R119 E120 C121 P122 S123 D124 E125 C126 G127 A128 G129 V130 F131 M132 A133 S134 H135 F136 R137 R138 H139 Y140 C141 G142 K143 C144 C145 L146 T147 Y148

C149 F150 ASN LYS PRO GLU ASP LYS

• Molecule 34: RACK1

Chain h: 37% 77% 22%

MET T2 E3 Q4 R6 G9 T10 L11 V18 T19 Q20 P25 D29 K30 T31 L32 S33 A34 S35 R36 D37 K38 T39 I40 T41 M42 W43 K44 L45 T46 R47 D48 E49 T50 G53 I54 P55 Q56 R57 A58 L59 S63 V66 S67 D68 V69 G81 S82 W83 D84 L87 R88 T93 T94 G95 T96 T97 R100 F101 V102 G103 H104 T105 T106 D107 V108 S115 D116 N117 R118 Q119 I120 S122 G123 S124 R125 D126 C207 K127 W132 N133 T134 V137 C138 K139 Y140 Q143 D144 E145 S146 H147 S148 S152 R155 S160 N162 P163 I164 I165 C168 L173 V174 L175 V176 W177 N178 L179 A180 N181 C182 K183 L184 K185 T186 N187 H188 I189 L195 V200 P202 D203 G204 S205 L206 C207 Q208 S209 G210 G211 K212 D213 G214 D220 L221 N222 E223 G224 K225 L230 D231 G232 G233 D234 I235 A238 P243 N244 R245 Y246 V247 L248 T252 T256 K257 T258 W259 D260 L261 E262 G263 K264 T265 T266 L270 K271 Q272 E273 V274 T275 S276 T277 S278 S279 K280 A281 E282 Q285 S288 L289 A290 V291 S292 A293 D294 T297 A300 V307 R308 T313 I314 GLY THR ARG

• Molecule 35: Met-tRNA-i-Met

Chain i: 68% 69% 28%

A1 G2 C3 A4 G5 A6 G7 U8 G9 G10 C11 G12 C13 A14 G15 C16 G17 G18 A19 A20 G21 C22 G23 U24 G25 C32 C40 A43 G44 G45 U46 C47 G48 A49 U50 G51 G52 A53 U54 C55 G56 A57 A58 A59 C60 C61 A62 U63 C64 C65 U66 C67 U68 G69 U71 A72

C73 C74 A75

• Molecule 36: 60s ribosomal protein l41

Chain n: 20% 76% 24%

M1 R11 R12 L13 K16 M20 R21 Q22 R23 S24 K25

Chain z:

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15598	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	0.087	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0175	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 ⓘ

5.1 Standard geometry ⓘ

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	0.14	0/40506	0.32	0/63123
2	B	0.22	0/1747	0.61	2/2374 (0.1%)
3	C	0.20	0/1756	0.53	0/2350
4	D	0.21	0/1753	0.54	0/2369
5	E	0.22	0/1796	0.53	0/2417
6	F	0.18	0/2118	0.49	0/2849
7	G	0.22	0/1531	0.58	2/2059 (0.1%)
8	H	0.22	0/1946	0.53	1/2590 (0.0%)
9	I	0.24	0/1510	0.55	0/2022
10	J	0.21	0/1723	0.59	0/2298
11	K	0.23	0/1550	0.56	0/2069
12	L	0.55	1/834 (0.1%)	0.94	4/1125 (0.4%)
13	M	0.24	0/1254	0.59	2/1677 (0.1%)
14	N	0.23	0/918	0.55	0/1233
15	O	0.22	0/1226	0.53	0/1649
16	P	0.22	0/1029	0.56	0/1380
17	Q	0.24	0/1017	0.63	0/1358
18	R	0.23	0/1146	0.60	3/1534 (0.2%)
19	S	0.29	0/1082	0.65	0/1452
20	T	0.24	0/1208	0.64	0/1618
21	U	0.20	0/1115	0.52	0/1493
22	V	0.23	0/805	0.63	2/1081 (0.2%)
23	W	0.20	0/643	0.56	0/860
24	X	0.24	0/1051	0.54	0/1406
25	Y	0.24	0/1116	0.55	0/1490
26	Z	0.22	0/1028	0.56	0/1366
27	a	0.24	0/620	0.56	0/831
28	b	0.36	1/828 (0.1%)	0.64	3/1109 (0.3%)
29	c	0.21	0/665	0.62	0/891
30	d	0.17	0/532	0.46	0/712
31	e	0.18	0/470	0.50	0/623
32	f	0.21	0/462	0.57	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.16	0/567	0.39	0/753
34	h	0.23	0/2493	0.58	1/3394 (0.0%)
35	i	0.12	0/1795	0.27	0/2798
36	n	0.20	0/240	0.43	0/305
37	z	0.13	0/4488	0.27	0/6995
All	All	0.19	2/86568 (0.0%)	0.44	20/126260 (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
28	b	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	4	PRO	CG-CD	-13.58	1.04	1.50
28	b	97	PRO	CG-CD	-7.62	1.24	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	4	PRO	N-CD-CG	-17.85	76.42	103.20
12	L	4	PRO	CA-CB-CG	-11.50	82.64	104.50
28	b	97	PRO	N-CD-CG	-10.53	87.41	103.20
34	h	25	PRO	CA-N-CD	-10.18	97.75	112.00
12	L	4	PRO	CB-CG-CD	9.02	134.95	106.10
22	V	55	ARG	CA-C-N	7.69	143.38	120.69
22	V	55	ARG	C-N-CA	7.69	143.38	120.69
12	L	4	PRO	CA-N-CD	-7.23	101.87	112.00
28	b	97	PRO	CA-N-CD	-6.63	102.72	112.00
28	b	97	PRO	CA-CB-CG	-6.60	91.96	104.50
2	B	197	VAL	CA-C-N	5.96	136.34	121.80
2	B	197	VAL	C-N-CA	5.96	136.34	121.80
18	R	97	GLN	CA-CB-CG	5.45	125.01	114.10
13	M	150	GLY	CA-C-N	5.25	129.86	122.46
13	M	150	GLY	C-N-CA	5.25	129.86	122.46
18	R	42	ILE	CA-C-N	5.09	128.41	120.68
18	R	42	ILE	C-N-CA	5.09	128.41	120.68
8	H	67	VAL	N-CA-C	-5.02	107.84	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	26	ASP	CA-C-N	5.01	131.12	121.54
7	G	26	ASP	C-N-CA	5.01	131.12	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	b	15	ARG	Sidechain

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	36227	0	18299	269	0
2	B	1710	0	1708	26	0
3	C	1729	0	1803	24	0
4	D	1716	0	1806	22	0
5	E	1768	0	1866	23	0
6	F	2076	0	2177	23	0
7	G	1509	0	1563	25	0
8	H	1923	0	2089	22	0
9	I	1488	0	1582	15	0
10	J	1691	0	1778	20	0
11	K	1525	0	1640	18	0
12	L	810	0	836	11	0
13	M	1233	0	1310	19	0
14	N	908	0	939	7	0
15	O	1202	0	1289	17	0
16	P	1016	0	1039	20	0
17	Q	997	0	1045	24	0
18	R	1128	0	1195	16	0
19	S	1068	0	1121	15	0
20	T	1190	0	1249	12	0
21	U	1097	0	1130	14	0
22	V	795	0	862	15	0
23	W	636	0	637	8	0
24	X	1034	0	1080	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y	1098	0	1167	13	0
26	Z	1011	0	1083	6	0
27	a	614	0	678	9	0
28	b	814	0	863	14	0
29	c	651	0	672	10	0
30	d	530	0	561	12	0
31	e	459	0	452	12	0
32	f	457	0	502	7	0
33	g	555	0	565	6	0
34	h	2436	0	2393	42	0
35	i	1604	0	816	11	0
36	n	239	0	289	5	0
37	z	4017	0	2033	13	0
38	b	1	0	0	0	0
All	All	80962	0	62117	665	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 (665) 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)
1:2:1472:C:N4	1:2:1476:A:H62	1.61	0.97
1:2:1652:G:H1	1:2:1672:U:H3	0.97	0.97
1:2:934:G:H1	1:2:1008:A:H2	1.09	0.95
1:2:1288:U:H3	1:2:1311:C:N4	1.67	0.93
1:2:1657:G:H1	1:2:1667:U:H3	1.16	0.93
1:2:1472:C:H42	1:2:1476:A:N6	1.66	0.92
1:2:16:G:H21	1:2:1195:A:H62	1.12	0.91
1:2:318:A:C2	1:2:333:G:N1	2.43	0.86
1:2:1288:U:H3	1:2:1311:C:H42	0.88	0.86
1:2:1472:C:H42	1:2:1476:A:H62	0.85	0.85
1:2:318:A:N1	1:2:333:G:C6	2.47	0.82
1:2:16:G:N2	1:2:1195:A:H62	1.83	0.76
19:S:79:GLU:O	19:S:83:ASN:HB2	1.85	0.76
1:2:1335:G:H1	1:2:1492:U:H3	1.39	0.71
1:2:934:G:N1	1:2:1008:A:H2	1.88	0.70
1:2:318:A:C2	1:2:333:G:C6	2.79	0.70
1:2:1722:G:H1	1:2:1812:U:H3	1.42	0.67
1:2:934:G:N1	1:2:1008:A:C2	2.52	0.65
3:C:30:TRP:HE3	16:P:20:GLN:HE22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1398:G:H1'	34:h:63:SER:HB3	1.80	0.64
34:h:20:GLN:HG3	34:h:68:ASP:HA	1.80	0.63
2:B:38:ILE:HG12	2:B:49:ILE:HG22	1.80	0.63
17:Q:28:MET:HE3	17:Q:32:GLN:HG3	1.80	0.63
34:h:256:ILE:HB	34:h:270:LEU:HB2	1.80	0.63
34:h:120:ILE:HB	34:h:132:TRP:HB2	1.80	0.62
9:I:66:VAL:HA	9:I:69:LEU:HD23	1.80	0.62
3:C:65:ARG:NH2	16:P:51:GLU:OE2	2.33	0.61
1:2:1402:A:H5'	22:V:51:LYS:HE2	1.82	0.60
34:h:42:MET:HE2	34:h:57:ARG:HG2	1.83	0.60
34:h:107:ASP:HB2	34:h:125:ARG:HG3	1.82	0.60
1:2:1033:G:H1	1:2:1080:A:HO2'	1.49	0.60
1:2:1091:C:HO2'	24:X:2:VAL:N	1.98	0.60
29:c:36:LYS:HE2	29:c:43:ILE:HD12	1.83	0.60
5:E:116:ARG:NH2	5:E:150:MET:SD	2.75	0.60
1:2:1452:A:H61	1:2:1473:G:H21	1.47	0.60
2:B:41:ARG:HH11	2:B:47:TYR:HE2	1.50	0.60
1:2:1298:G:OP1	17:Q:79:HIS:NE2	2.34	0.59
1:2:1616:U:OP2	17:Q:43:ARG:NH2	2.36	0.59
19:S:36:GLU:OE2	19:S:47:ARG:NH1	2.32	0.59
30:d:18:LEU:HB2	30:d:29:GLN:HB2	1.85	0.59
1:2:70:G:N7	8:H:167:LYS:NZ	2.51	0.59
22:V:85:HIS:HB3	22:V:87:ARG:HH22	1.66	0.59
29:c:19:HIS:HB3	29:c:22:LYS:HG2	1.85	0.59
3:C:74:LEU:HD12	3:C:75:GLN:HG2	1.84	0.59
4:D:182:CYS:SG	4:D:183:LYS:N	2.76	0.59
1:2:16:G:H21	1:2:1195:A:N6	1.93	0.58
1:2:934:G:O6	1:2:1008:A:N1	2.36	0.58
1:2:940:U:H3	1:2:1002:U:H3	1.50	0.58
1:2:318:A:C2	1:2:333:G:C2	2.91	0.58
35:i:24:U:H2'	35:i:25:G:H8	1.69	0.58
13:M:4:ILE:HG22	13:M:5:GLN:HG2	1.84	0.58
2:B:17:LYS:HB3	2:B:173:LEU:HD11	1.85	0.58
1:2:1562:C:H5''	21:U:71:GLY:HA3	1.86	0.58
1:2:1349:G:H21	2:B:112:ILE:HD11	1.69	0.57
34:h:234:ASP:OD1	34:h:235:ILE:N	2.36	0.57
1:2:829:C:O2'	1:2:845:G:N2	2.37	0.57
1:2:1563:G:H5''	21:U:121:ARG:HH21	1.68	0.57
1:2:1565:C:OP2	21:U:101:ARG:NH1	2.37	0.57
23:W:20:SER:O	23:W:22:ARG:NH1	2.37	0.57
9:I:29:GLU:HA	9:I:32:MET:HE2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:i:25:G:O6	35:i:43:A:N1	2.38	0.57
1:2:925:G:OP1	15:O:121:ARG:NH2	2.37	0.57
1:2:986:G:H21	16:P:135:ILE:HG12	1.68	0.57
1:2:1593:C:OP2	7:G:91:ARG:NH1	2.38	0.57
15:O:22:VAL:HG22	15:O:66:VAL:HG12	1.87	0.57
30:d:69:ARG:NH2	37:z:337:G:N7	2.52	0.57
1:2:1717:C:O2'	36:n:21:ARG:NH1	2.38	0.56
18:R:94:ALA:HA	18:R:97:GLN:HG2	1.86	0.56
30:d:46:VAL:HG21	30:d:56:LEU:HD11	1.87	0.56
34:h:10:THR:HG22	34:h:308:ARG:HG2	1.88	0.56
16:P:113:GLN:HG3	28:b:45:VAL:HG12	1.87	0.56
2:B:120:ARG:HH11	4:D:266:TYR:HD2	1.51	0.56
16:P:117:ARG:NH2	30:d:62:GLU:O	2.38	0.56
24:X:51:GLU:HB2	24:X:62:VAL:HB	1.87	0.56
30:d:66:ARG:HE	30:d:67:ARG:H	1.52	0.56
1:2:350:C:O2'	1:2:383:G:N1	2.39	0.56
2:B:76:VAL:HG13	2:B:87:VAL:HG13	1.88	0.56
6:F:31:PRO:HG3	6:F:43:PRO:HG3	1.87	0.56
34:h:168:CYS:HB2	34:h:195:LEU:HD11	1.88	0.56
16:P:44:VAL:HG13	16:P:53:ILE:HB	1.88	0.56
31:e:6:LEU:HA	31:e:9:SER:HB2	1.88	0.56
1:2:919:A:OP2	15:O:64:ARG:NH2	2.39	0.56
1:2:1858:G:OP2	16:P:146:ARG:NH2	2.39	0.56
9:I:27:LEU:HD12	9:I:45:ILE:HD11	1.88	0.56
35:i:25:G:N1	35:i:43:A:C2	2.74	0.56
1:2:809:A:H5'	6:F:221:ARG:HE	1.71	0.56
10:J:191:GLU:O	13:M:19:ASN:ND2	2.39	0.55
34:h:177:TRP:HA	34:h:184:LEU:HA	1.86	0.55
1:2:1017:U:OP1	15:O:62:GLN:NE2	2.39	0.55
5:E:137:VAL:HB	5:E:185:LYS:HB2	1.86	0.55
10:J:81:VAL:HG22	10:J:102:VAL:HG12	1.86	0.55
20:T:138:THR:HG23	20:T:141:ARG:HH21	1.71	0.55
25:Y:60:LYS:HG3	25:Y:62:PRO:HD2	1.89	0.55
1:2:848:U:O2'	11:K:69:ARG:NH1	2.39	0.55
1:2:1123:C:O2'	3:C:146:ARG:NH1	2.39	0.55
1:2:1547:C:N4	1:2:1586:U:O4	2.39	0.55
7:G:180:ALA:HA	7:G:190:ILE:HD11	1.88	0.55
34:h:44:LYS:HB2	34:h:56:GLN:HB2	1.87	0.55
35:i:19:A:N7	35:i:59:A:N6	2.47	0.55
1:2:318:A:N1	1:2:333:G:O6	2.39	0.55
1:2:1617:G:O6	17:Q:43:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:11:LEU:HB2	34:h:307:VAL:HB	1.89	0.55
1:2:1183:A:H2'	1:2:1184:G:H8	1.71	0.54
17:Q:107:ILE:HG23	17:Q:111:MET:HG2	1.88	0.54
22:V:61:LEU:HD13	22:V:82:MET:HB2	1.89	0.54
1:2:637:U:O2	32:f:129:ASN:ND2	2.40	0.54
18:R:82:TYR:HA	18:R:85:ARG:HG2	1.89	0.54
25:Y:93:PHE:O	25:Y:140:ARG:NH2	2.40	0.54
28:b:23:CYS:SG	28:b:24:THR:N	2.81	0.54
34:h:168:CYS:HB3	34:h:174:VAL:HG23	1.89	0.54
6:F:174:LYS:HE2	6:F:176:ASP:HB2	1.88	0.54
8:H:64:LYS:HZ3	8:H:82:SER:H	1.54	0.54
1:2:563:G:H2'	1:2:564:A:H8	1.73	0.54
3:C:107:ARG:NH1	16:P:133:THR:O	2.40	0.54
13:M:7:GLU:OE2	13:M:11:GLN:NE2	2.41	0.54
1:2:1464:C:OP1	19:S:63:ARG:NH2	2.41	0.54
1:2:1677:U:OP1	7:G:71:ARG:NH2	2.41	0.54
1:2:1121:G:N2	3:C:202:GLN:O	2.41	0.54
12:L:74:GLU:HA	12:L:77:GLN:HG3	1.90	0.54
16:P:142:ARG:NH1	28:b:23:CYS:O	2.41	0.54
28:b:102:ARG:HH22	37:z:332:A:H5''	1.73	0.54
29:c:56:CYS:SG	29:c:57:VAL:N	2.81	0.54
1:2:1401:A:H4'	22:V:52:GLY:HA3	1.88	0.54
34:h:66:VAL:HA	34:h:82:SER:HA	1.90	0.54
1:2:142:C:H1'	8:H:180:VAL:HG11	1.88	0.53
1:2:1597:C:OP2	27:a:85:ARG:NH2	2.40	0.53
2:B:154:LEU:HD22	2:B:157:VAL:HG21	1.89	0.53
7:G:110:GLN:NE2	7:G:114:ASN:OD1	2.39	0.53
1:2:1219:C:HO2'	30:d:26:GLN:HE21	1.55	0.53
1:2:1844:U:OP1	36:n:11:ARG:NH2	2.42	0.53
13:M:119:ASP:O	13:M:147:LYS:NZ	2.42	0.53
22:V:62:ARG:NH2	31:e:56:ASP:OD2	2.41	0.53
4:D:166:ARG:HB2	4:D:248:TYR:HE1	1.74	0.53
17:Q:83:MET:HB3	17:Q:116:LEU:HD13	1.91	0.53
24:X:30:CYS:SG	24:X:59:GLY:N	2.81	0.53
1:2:1130:G:N2	1:2:1130:G:OP2	2.41	0.53
5:E:69:LEU:HA	5:E:72:VAL:HG22	1.90	0.53
12:L:64:TRP:HD1	31:e:23:VAL:HA	1.73	0.53
16:P:30:VAL:HG12	16:P:94:HIS:HB2	1.90	0.53
17:Q:85:ILE:HG21	17:Q:111:MET:HG3	1.91	0.53
4:D:172:ASN:ND2	11:K:95:ASP:OD2	2.42	0.53
1:2:531:A:H61	1:2:552:G:H1	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ASP:HA	2:B:9:GLN:HE22	1.73	0.53
1:2:156:G:OP1	8:H:2:LYS:NZ	2.41	0.53
2:B:63:ARG:NH1	23:W:37:ALA:O	2.40	0.53
1:2:924:G:H1	1:2:1018:U:H3	1.55	0.53
1:2:1219:C:O2'	30:d:26:GLN:NE2	2.37	0.53
1:2:913:A:N6	9:I:119:SER:O	2.41	0.53
1:2:1241:A:HO2'	1:2:1266:C:HO2'	1.56	0.53
1:2:951:C:O2	16:P:50:LYS:NZ	2.33	0.53
1:2:1452:A:N6	1:2:1473:G:H21	2.06	0.53
24:X:86:LEU:HD21	24:X:113:HIS:HB2	1.91	0.53
26:Z:113:ARG:HH12	26:Z:116:LYS:HD2	1.74	0.53
1:2:1012:A:OP1	15:O:3:ARG:NH1	2.42	0.52
1:2:1864:U:H3'	28:b:5:ARG:HH21	1.75	0.52
3:C:163:GLN:HG2	3:C:204:ILE:HD13	1.90	0.52
16:P:34:PHE:HE1	16:P:100:THR:HA	1.74	0.52
2:B:57:LYS:HB3	2:B:161:ILE:HG12	1.92	0.52
5:E:35:SER:HB3	5:E:51:LEU:HB3	1.91	0.52
34:h:249:CYS:SG	34:h:291:TRP:NE1	2.83	0.52
1:2:305:U:H4'	10:J:41:ARG:HH22	1.73	0.52
1:2:1244:U:H2'	1:2:1245:G:H8	1.74	0.52
7:G:92:ILE:HD13	7:G:169:ILE:HD11	1.91	0.52
1:2:457:C:H2'	1:2:458:A:H8	1.74	0.52
1:2:1661:A:OP2	31:e:19:ARG:NH2	2.42	0.52
25:Y:100:VAL:HG12	25:Y:125:VAL:HG22	1.91	0.52
1:2:523:A:OP2	11:K:38:ARG:NH1	2.43	0.52
1:2:1345:G:OP1	1:2:1688:C:O2'	2.27	0.52
4:D:104:ASP:HB3	4:D:130:ILE:HG22	1.90	0.52
17:Q:81:ARG:NH2	17:Q:117:GLY:O	2.43	0.52
1:2:30:C:O3'	25:Y:137:LYS:NZ	2.40	0.52
1:2:109:U:O2	13:M:71:ARG:NH2	2.42	0.52
1:2:351:G:OP1	10:J:7:ASN:ND2	2.41	0.52
13:M:113:LEU:HD21	13:M:120:VAL:HG21	1.92	0.52
1:2:1533:A:OP2	7:G:164:ARG:NH2	2.43	0.52
3:C:63:LYS:NZ	3:C:90:ASP:OD1	2.42	0.52
13:M:49:GLU:OE1	13:M:118:ARG:NH2	2.42	0.52
17:Q:28:MET:HE1	17:Q:36:LEU:HD12	1.91	0.52
3:C:218:LEU:HB3	3:C:219:LYS:HE2	1.91	0.52
1:2:819:G:OP2	11:K:80:ARG:NH2	2.42	0.51
1:2:1155:U:O2'	24:X:71:LYS:NZ	2.42	0.51
6:F:68:ARG:HD3	6:F:76:VAL:HG11	1.93	0.51
15:O:84:LEU:HD23	15:O:89:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:207:CYS:SG	34:h:208:ALA:N	2.83	0.51
9:I:154:ILE:HB	9:I:185:VAL:HG22	1.92	0.51
18:R:146:ARG:NH2	35:i:32:C:OP2	2.44	0.51
19:S:9:VAL:HG21	19:S:49:LYS:HB3	1.92	0.51
34:h:18:VAL:HA	34:h:35:SER:HA	1.92	0.51
1:2:1658:G:OP2	1:2:1660:C:N4	2.44	0.51
22:V:51:LYS:HB2	22:V:90:ASP:HB2	1.91	0.51
23:W:17:CYS:HB2	23:W:20:SER:HB2	1.93	0.51
34:h:88:ARG:HD2	34:h:97:THR:HG21	1.91	0.51
2:B:205:ARG:NH2	19:S:81:ARG:O	2.43	0.51
1:2:562:U:O4	11:K:172:ARG:NH2	2.44	0.51
12:L:26:ASP:OD1	12:L:42:ASN:ND2	2.43	0.51
25:Y:17:ARG:NH1	25:Y:20:GLN:OE1	2.43	0.51
1:2:398:A:H5''	1:2:400:C:H5'	1.93	0.51
1:2:511:U:O2'	1:2:576:A:N6	2.38	0.51
1:2:1014:G:N2	29:c:51:GLN:OE1	2.43	0.51
3:C:56:LYS:NZ	3:C:57:ILE:O	2.44	0.51
12:L:5:LYS:NZ	12:L:82:TYR:OH	2.43	0.51
21:U:18:LEU:HD13	21:U:134:ILE:HG21	1.91	0.51
1:2:155:G:H2'	1:2:156:G:H8	1.74	0.51
24:X:87:GLU:HA	24:X:90:GLN:HG3	1.93	0.51
3:C:171:ILE:HA	3:C:174:ARG:HG2	1.92	0.51
22:V:46:LYS:HZ3	22:V:97:ILE:HG23	1.75	0.51
24:X:6:VAL:HG13	24:X:29:PRO:HG2	1.91	0.51
1:2:1775:U:N3	1:2:1776:G:O6	2.44	0.50
5:E:116:ARG:HH12	5:E:143:ARG:HH22	1.58	0.50
10:J:37:LYS:N	10:J:58:LEU:O	2.40	0.50
15:O:34:LYS:NZ	15:O:38:TYR:OH	2.44	0.50
1:2:377:G:H5'	10:J:98:LYS:HB3	1.92	0.50
1:2:1277:C:H2'	1:2:1278:A:H8	1.76	0.50
30:d:24:GLN:OE1	30:d:26:GLN:NE2	2.42	0.50
37:z:121:C:H5''	37:z:122:C:H5'	1.93	0.50
1:2:351:G:O3'	13:M:139:ARG:NH1	2.42	0.50
6:F:181:CYS:SG	6:F:182:MET:N	2.84	0.50
34:h:33:SER:HB3	34:h:43:TRP:HE1	1.77	0.50
1:2:918:U:H4'	15:O:20:ARG:HH22	1.76	0.50
18:R:132:PHE:O	18:R:140:ARG:NH1	2.44	0.50
1:2:289:G:OP1	6:F:155:LYS:NZ	2.44	0.50
34:h:212:LYS:HD2	34:h:235:ILE:HG12	1.92	0.50
1:2:346:C:H5''	6:F:38:LEU:HB2	1.93	0.50
1:2:490:C:O2'	1:2:574:A:N1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:TRP:O	4:D:71:LYS:NZ	2.39	0.50
8:H:50:VAL:HG11	8:H:111:LEU:HD23	1.94	0.50
13:M:103:GLU:OE2	25:Y:10:ALA:N	2.39	0.50
27:a:69:THR:HB	27:a:72:VAL:HG12	1.94	0.50
3:C:134:LEU:HD12	3:C:219:LYS:HG2	1.94	0.50
17:Q:61:ARG:HH21	17:Q:65:LYS:HE2	1.77	0.50
1:2:1126:G:OP1	2:B:41:ARG:NH2	2.45	0.49
1:2:1213:C:H2'	1:2:1214:A:H8	1.76	0.49
1:2:1706:G:N3	1:2:1850:A:O2'	2.44	0.49
4:D:189:GLY:HA3	4:D:235:ASN:HD21	1.77	0.49
19:S:29:HIS:HA	19:S:32:LYS:HE2	1.94	0.49
1:2:71:G:O6	8:H:170:ARG:NH1	2.45	0.49
1:2:1147:C:OP1	28:b:6:ARG:NH1	2.45	0.49
1:2:452:G:OP2	8:H:88:ARG:NH2	2.46	0.49
14:N:106:CYS:SG	14:N:107:SER:N	2.86	0.49
25:Y:68:LYS:HE2	32:f:82:VAL:HG22	1.95	0.49
27:a:48:VAL:HG12	27:a:49:LEU:HD12	1.94	0.49
1:2:495:U:OP1	6:F:49:ARG:NH1	2.45	0.49
1:2:1504:U:O3'	33:g:83:LYS:NZ	2.44	0.49
4:D:173:LYS:HE3	23:W:3:ASN:HA	1.95	0.49
7:G:135:ARG:NH1	16:P:67:ASP:OD2	2.45	0.49
17:Q:85:ILE:HD13	17:Q:111:MET:HG3	1.93	0.49
7:G:20:PHE:N	7:G:23:TRP:O	2.44	0.49
17:Q:44:ARG:O	17:Q:50:ARG:NH2	2.46	0.49
33:g:132:MET:HG2	33:g:141:CYS:HA	1.94	0.49
1:2:1161:U:O4	25:Y:3:LYS:NZ	2.46	0.49
5:E:136:VAL:HG22	5:E:186:VAL:HG12	1.95	0.49
18:R:44:PRO:HD2	18:R:81:ILE:HD11	1.95	0.49
26:Z:55:ILE:HG22	26:Z:75:ILE:HA	1.95	0.49
26:Z:114:MET:HE3	26:Z:122:LYS:HB3	1.94	0.49
10:J:191:GLU:HG3	13:M:19:ASN:HD22	1.77	0.49
20:T:49:ASP:OD1	20:T:49:ASP:N	2.46	0.49
24:X:27:ILE:HB	24:X:61:ILE:HB	1.93	0.49
34:h:87:LEU:HB2	34:h:101:PHE:HD2	1.77	0.49
1:2:943:U:O2'	16:P:135:ILE:O	2.29	0.49
28:b:80:HIS:NE2	37:z:338:C:OP2	2.46	0.49
37:z:171:G:H3'	37:z:172:A:H8	1.78	0.49
1:2:439:A:H4'	1:2:1799:G:H4'	1.94	0.49
17:Q:44:ARG:NH1	17:Q:54:HIS:CE1	2.81	0.49
20:T:112:GLU:HA	20:T:115:LYS:HG2	1.95	0.49
1:2:183:G:O2'	1:2:184:G:O4'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1139:C:H41	1:2:1149:A:H62	1.61	0.48
6:F:165:GLU:HG2	6:F:166:THR:HG23	1.94	0.48
8:H:135:PRO:HB3	8:H:140:ARG:HB3	1.94	0.48
19:S:90:ALA:O	19:S:93:GLN:NE2	2.46	0.48
22:V:24:LEU:HD21	22:V:35:VAL:HG13	1.94	0.48
17:Q:30:TYR:HA	17:Q:33:LEU:HB2	1.95	0.48
18:R:19:ALA:HB2	18:R:75:GLY:HA3	1.95	0.48
28:b:42:ARG:HB2	28:b:67:LEU:HB3	1.94	0.48
1:2:1681:U:O2'	30:d:23:SER:O	2.32	0.48
2:B:158:ASP:HB3	23:W:34:MET:HE1	1.96	0.48
19:S:88:VAL:HG22	19:S:90:ALA:H	1.78	0.48
21:U:40:ALA:HB3	21:U:43:LYS:HG2	1.94	0.48
29:c:23:ARG:NH1	29:c:27:SER:O	2.45	0.48
1:2:397:G:OP1	13:M:106:HIS:NE2	2.44	0.48
1:2:1569:A:OP1	21:U:97:LYS:NZ	2.46	0.48
31:e:43:PHE:O	31:e:47:ALA:HB2	2.14	0.48
36:n:13:LEU:HA	36:n:16:LYS:HG2	1.95	0.48
1:2:210:U:H2'	1:2:211:G:H8	1.78	0.48
1:2:381:C:H5''	10:J:54:LYS:HD2	1.94	0.48
1:2:1674:G:H4'	7:G:77:MET:HE1	1.96	0.48
1:2:1705:C:O2	1:2:1851:A:O2'	2.32	0.48
23:W:42:VAL:HG13	23:W:43:THR:HG23	1.95	0.48
4:D:266:TYR:O	4:D:270:THR:HB	2.13	0.48
7:G:55:ARG:NH1	18:R:123:ASP:OD1	2.47	0.48
7:G:97:PHE:HA	7:G:100:ILE:HG22	1.95	0.48
12:L:85:LEU:HD13	12:L:89:ILE:HB	1.96	0.48
17:Q:101:THR:OG1	17:Q:102:PHE:N	2.46	0.48
25:Y:107:ARG:HD3	25:Y:112:VAL:HG22	1.95	0.48
1:2:151:C:O2	8:H:132:ARG:NH1	2.40	0.48
5:E:32:ASP:O	5:E:53:THR:OG1	2.30	0.48
1:2:516:A:N1	1:2:643:A:O2'	2.43	0.48
4:D:200:ARG:O	11:K:54:ARG:NH1	2.43	0.48
1:2:124:U:OP1	8:H:201:LYS:NZ	2.39	0.48
1:2:1424:G:H2'	1:2:1425:G:H8	1.79	0.48
16:P:57:THR:H	16:P:60:MET:HG2	1.79	0.48
30:d:17:VAL:HG12	30:d:30:VAL:HG12	1.95	0.48
1:2:639:C:H2'	1:2:640:A:H8	1.79	0.48
1:2:872:A:O2'	1:2:874:G:OP2	2.32	0.48
4:D:70:VAL:HG11	4:D:93:ILE:HG23	1.94	0.48
5:E:32:ASP:HB3	5:E:54:ARG:HB2	1.95	0.47
6:F:6:LYS:HZ3	6:F:30:ARG:HH12	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:132:GLY:N	6:F:136:ILE:O	2.45	0.47
17:Q:89:MET:HE3	17:Q:89:MET:HB3	1.85	0.47
24:X:50:PHE:HB2	24:X:63:VAL:HG22	1.96	0.47
33:g:108:VAL:HG22	33:g:114:ILE:HG22	1.96	0.47
1:2:582:U:OP1	11:K:162:ARG:NH1	2.48	0.47
17:Q:118:GLU:HG2	20:T:119:ALA:HB1	1.95	0.47
1:2:161:U:O2'	8:H:87:ARG:NH2	2.47	0.47
1:2:1647:A:OP1	18:R:138:ARG:NH2	2.47	0.47
1:2:91:A:H5'	1:2:92:A:H5''	1.94	0.47
5:E:45:ARG:NH2	5:E:85:GLU:OE1	2.45	0.47
15:O:45:LEU:HD23	15:O:49:GLN:HB3	1.95	0.47
1:2:1639:G:H21	35:i:40:C:H1'	1.79	0.47
1:2:168:C:N3	8:H:132:ARG:NH2	2.52	0.47
1:2:874:G:H2'	1:2:875:A:H8	1.79	0.47
14:N:45:ARG:NH2	14:N:72:HIS:O	2.46	0.47
1:2:525:A:H4'	32:f:104:ARG:HH22	1.80	0.47
1:2:1679:A:H2'	7:G:60:ARG:HD2	1.97	0.47
27:a:102:LYS:HE2	27:a:102:LYS:HB3	1.73	0.47
34:h:247:TRP:NE1	34:h:260:ASP:OD2	2.48	0.47
1:2:1148:A:OP1	28:b:6:ARG:NH2	2.48	0.47
1:2:1716:C:H42	1:2:1817:G:H1	1.62	0.47
35:i:10:G:O6	35:i:24:U:O2	2.33	0.47
1:2:496:C:OP1	6:F:49:ARG:NH2	2.47	0.47
1:2:1549:U:OP1	31:e:34:TYR:OH	2.33	0.47
2:B:125:THR:HG22	2:B:175:TRP:HZ2	1.80	0.47
7:G:72:LEU:HD21	7:G:112:LEU:HD11	1.97	0.47
16:P:95:ILE:HD13	16:P:116:LEU:HG	1.96	0.47
1:2:114:G:N7	13:M:69:ARG:NH2	2.63	0.46
1:2:1598:G:N2	1:2:1599:U:O4	2.46	0.46
6:F:11:ARG:NH2	6:F:24:THR:OG1	2.45	0.46
37:z:127:U:OP1	37:z:313:G:O2'	2.30	0.46
1:2:921:G:H3'	24:X:28:ARG:HH22	1.81	0.46
4:D:131:GLY:HA3	4:D:137:VAL:HG12	1.96	0.46
1:2:171:A:OP2	8:H:137:ARG:NH2	2.48	0.46
4:D:167:ARG:HB3	4:D:177:PRO:HB2	1.98	0.46
11:K:25:LEU:HA	11:K:28:GLU:HG2	1.98	0.46
1:2:1281:G:OP2	14:N:101:ARG:NH2	2.48	0.46
1:2:1285:G:N2	14:N:57:ASP:O	2.48	0.46
1:2:1673:U:H5''	18:R:78:VAL:HG12	1.98	0.46
7:G:71:ARG:NH2	7:G:148:ASN:OD1	2.42	0.46
1:2:436:G:H2'	1:2:437:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1082:A:HO2'	1:2:1842:C:HO2'	1.57	0.46
1:2:1337:C:H2'	1:2:1338:G:H8	1.81	0.46
2:B:85:ARG:NH1	2:B:203:PHE:O	2.44	0.46
1:2:1528:G:O2'	1:2:1666:C:OP1	2.28	0.46
3:C:195:LYS:HA	3:C:198:GLU:HG2	1.98	0.46
19:S:72:LYS:NZ	19:S:76:GLU:OE2	2.47	0.46
1:2:64:A:H2	1:2:83:A:H62	1.61	0.46
1:2:886:A:N6	1:2:902:G:N7	2.64	0.46
1:2:1541:G:OP1	21:U:56:ARG:NE	2.47	0.46
3:C:87:ILE:O	3:C:99:ASN:N	2.49	0.46
9:I:40:LEU:HA	9:I:43:LEU:HD22	1.97	0.46
20:T:89:ASP:HB3	20:T:93:GLY:H	1.81	0.46
34:h:40:ILE:HB	34:h:59:LEU:HB2	1.98	0.46
9:I:73:GLN:HA	9:I:76:GLN:HB2	1.98	0.46
29:c:82:LYS:NZ	37:z:233:G:O3'	2.49	0.46
1:2:199:C:H2'	1:2:200:G:H8	1.80	0.46
1:2:1033:G:N1	1:2:1080:A:O2'	2.40	0.46
1:2:1550:G:OP2	5:E:8:LYS:NZ	2.43	0.46
1:2:677:G:H21	1:2:1028:A:H62	1.62	0.45
6:F:103:TYR:HE1	6:F:184:THR:HG23	1.80	0.45
13:M:61:PRO:HB3	13:M:68:ILE:HD11	1.98	0.45
29:c:42:LYS:HD2	29:c:42:LYS:HA	1.75	0.45
1:2:381:C:OP2	10:J:31:ARG:NH1	2.49	0.45
1:2:550:C:O2'	1:2:551:U:O4'	2.33	0.45
1:2:1554:C:H5''	1:2:1555:U:H2'	1.99	0.45
7:G:175:ASP:HA	7:G:178:ILE:HD12	1.99	0.45
1:2:190:G:O2'	1:2:209:A:N6	2.50	0.45
1:2:1064:C:H2'	1:2:1065:G:H8	1.81	0.45
1:2:1452:A:H61	1:2:1473:G:N2	2.12	0.45
1:2:1786:U:H2'	1:2:1787:G:H8	1.82	0.45
3:C:35:ALA:HB1	3:C:39:PHE:HD1	1.81	0.45
6:F:90:ILE:O	6:F:99:PHE:N	2.49	0.45
6:F:130:PHE:O	6:F:138:HIS:N	2.47	0.45
1:2:4:C:O2'	11:K:18:ARG:NH2	2.50	0.45
1:2:973:C:N3	16:P:55:ARG:NH1	2.64	0.45
1:2:1718:G:H21	1:2:1815:A:H62	1.63	0.45
19:S:33:ARG:HH11	19:S:36:GLU:HG3	1.82	0.45
29:c:31:TYR:O	29:c:48:SER:OG	2.32	0.45
1:2:17:C:O2'	1:2:1194:A:N1	2.48	0.45
18:R:102:GLU:HA	18:R:105:LYS:HB3	1.98	0.45
34:h:31:ILE:HG13	34:h:45:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:231:ASP:OD1	34:h:231:ASP:N	2.50	0.45
34:h:294:ASP:OD1	34:h:294:ASP:N	2.49	0.45
1:2:452:G:P	8:H:88:ARG:HH22	2.39	0.45
1:2:350:C:HO2'	1:2:383:G:H1	1.65	0.45
1:2:521:A:OP1	11:K:45:ARG:NH1	2.40	0.45
5:E:23:GLU:HA	5:E:26:THR:HG22	1.98	0.45
34:h:31:ILE:HB	34:h:43:TRP:HB2	1.98	0.45
34:h:122:SER:HB3	34:h:132:TRP:HE1	1.82	0.45
1:2:645:C:H2'	1:2:646:G:H8	1.82	0.45
1:2:919:A:N7	15:O:64:ARG:NH1	2.65	0.45
2:B:21:ALA:HB2	2:B:173:LEU:HD13	1.98	0.45
10:J:65:PHE:O	10:J:109:TYR:OH	2.35	0.45
27:a:43:LYS:HA	27:a:43:LYS:HD2	1.80	0.45
29:c:14:GLU:HA	29:c:17:ARG:HB3	1.98	0.45
1:2:14:C:OP1	4:D:235:ASN:ND2	2.50	0.45
1:2:454:U:O3'	8:H:94:ARG:NH1	2.50	0.45
1:2:1451:G:H21	1:2:1474:A:H61	1.65	0.45
1:2:309:G:OP2	10:J:55:TYR:OH	2.36	0.44
2:B:57:LYS:NZ	2:B:160:ALA:O	2.40	0.44
24:X:11:LEU:HA	24:X:14:ILE:HG22	1.99	0.44
1:2:1294:G:H2'	1:2:1295:A:H8	1.81	0.44
5:E:1:MET:HE3	5:E:4:GLN:HA	1.99	0.44
6:F:118:GLU:OE2	6:F:121:TYR:OH	2.35	0.44
7:G:123:GLU:HB2	30:d:59:LEU:HD13	1.98	0.44
24:X:111:MET:SD	24:X:111:MET:N	2.91	0.44
1:2:873:G:H1	13:M:153:LYS:HZ2	1.64	0.44
1:2:1364:U:H5	1:2:1375:G:H21	1.66	0.44
1:2:1705:C:H2'	1:2:1706:G:H8	1.83	0.44
3:C:122:GLU:OE2	3:C:213:ARG:NH2	2.49	0.44
13:M:40:ILE:HD12	13:M:68:ILE:HD13	1.99	0.44
24:X:66:THR:HG23	24:X:68:ARG:HG3	1.99	0.44
36:n:20:MET:O	36:n:24:SER:HB2	2.16	0.44
1:2:436:G:O6	1:2:458:A:N6	2.50	0.44
1:2:804:U:H5''	24:X:82:GLN:HG2	1.99	0.44
1:2:918:U:O2'	1:2:919:A:O4'	2.32	0.44
1:2:1270:G:O2'	1:2:1301:A:N7	2.51	0.44
2:B:137:ALA:HB1	2:B:142:LEU:HD23	2.00	0.44
26:Z:12:PHE:HA	26:Z:23:MET:HG3	1.99	0.44
30:d:36:ASP:OD1	30:d:36:ASP:N	2.47	0.44
36:n:21:ARG:HA	36:n:21:ARG:HD2	1.81	0.44
1:2:155:G:H4'	8:H:15:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:445:A:H5''	10:J:47:ARG:HH21	1.82	0.44
5:E:7:LYS:HE3	22:V:25:THR:HG21	2.00	0.44
17:Q:44:ARG:HH12	17:Q:54:HIS:CE1	2.36	0.44
21:U:76:THR:HG22	21:U:94:ARG:HB3	1.99	0.44
37:z:262:U:O2	37:z:271:G:O6	2.35	0.44
1:2:84:A:N3	1:2:150:A:O2'	2.49	0.44
1:2:560:A:H5'	11:K:174:LYS:HE3	2.00	0.44
1:2:1374:C:OP1	19:S:7:LYS:NZ	2.51	0.44
8:H:5:ILE:HG22	8:H:111:LEU:HB2	2.00	0.44
15:O:92:ILE:HG12	15:O:141:TYR:HE1	1.83	0.44
34:h:164:ILE:HD11	34:h:221:LEU:HD23	2.00	0.44
1:2:562:U:OP1	11:K:134:HIS:NE2	2.45	0.44
10:J:6:ASP:OD1	10:J:9:HIS:ND1	2.50	0.44
14:N:91:LEU:HD23	14:N:104:VAL:HG23	1.98	0.44
15:O:98:VAL:HG12	15:O:115:LEU:HD12	2.00	0.44
20:T:81:ASP:OD1	20:T:81:ASP:N	2.50	0.44
1:2:436:G:OP2	1:2:471:G:O2'	2.35	0.44
1:2:1392:U:OP1	22:V:83:ARG:NH2	2.51	0.44
3:C:103:MET:HB3	3:C:215:VAL:HG22	1.98	0.44
4:D:194:ARG:HD3	4:D:196:ILE:HD11	1.98	0.44
11:K:101:LYS:HG3	11:K:103:GLU:HG3	2.00	0.44
22:V:20:ILE:HG22	22:V:116:ILE:HG23	1.99	0.44
25:Y:68:LYS:HG2	25:Y:91:LEU:HD22	2.00	0.44
27:a:94:LYS:HB3	27:a:94:LYS:HE3	1.74	0.44
28:b:37:LYS:HE2	28:b:37:LYS:HB2	1.81	0.44
28:b:53:ILE:HG21	28:b:64:LEU:HD21	2.00	0.44
1:2:934:G:C6	1:2:1008:A:N1	2.86	0.44
1:2:1556:A:H5''	1:2:1557:C:H5	1.82	0.44
6:F:125:LYS:HE2	6:F:125:LYS:HB3	1.88	0.44
6:F:128:LYS:HE3	6:F:128:LYS:HB2	1.79	0.44
8:H:116:LYS:HE3	8:H:125:THR:HG21	1.98	0.44
10:J:48:VAL:HG11	10:J:54:LYS:HD3	2.00	0.44
2:B:85:ARG:NH2	19:S:82:ASP:O	2.51	0.43
7:G:112:LEU:HA	7:G:177:LEU:HD23	2.00	0.43
9:I:158:LEU:HB2	9:I:189:PHE:HE1	1.82	0.43
34:h:35:SER:OG	34:h:36:ARG:N	2.51	0.43
1:2:525:A:H2'	1:2:526:A:C8	2.53	0.43
1:2:1283:C:O2'	1:2:1313:A:N1	2.45	0.43
2:B:205:ARG:HH21	19:S:81:ARG:NH2	2.16	0.43
25:Y:134:TYR:HD2	25:Y:135:LYS:HD2	1.83	0.43
28:b:20:PRO:HA	28:b:31:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:i:25:G:C6	35:i:43:A:N1	2.86	0.43
1:2:562:U:H2'	1:2:563:G:C8	2.53	0.43
4:D:253:PRO:HA	4:D:256:TRP:CD1	2.53	0.43
1:2:1215:C:O2'	1:2:1645:C:OP2	2.35	0.43
1:2:1255:G:OP1	1:2:1256:G:O2'	2.31	0.43
3:C:147:ASN:ND2	37:z:300:G:OP1	2.46	0.43
5:E:18:LYS:O	5:E:22:ASN:HB2	2.17	0.43
1:2:65:C:N4	1:2:169:U:O2'	2.48	0.43
4:D:238:LYS:HD3	4:D:238:LYS:HA	1.89	0.43
14:N:35:ILE:HD12	33:g:102:VAL:HG11	2.01	0.43
15:O:99:ARG:HD3	15:O:115:LEU:HD11	1.99	0.43
26:Z:54:VAL:HB	26:Z:76:TYR:HB2	2.00	0.43
1:2:119:U:O2	6:F:33:THR:OG1	2.35	0.43
1:2:191:A:N6	1:2:208:G:O2'	2.52	0.43
1:2:1167:G:H1	1:2:1192:U:H3	1.66	0.43
1:2:1413:G:H2'	1:2:1414:A:H8	1.84	0.43
1:2:1480:A:H5'	18:R:131:LYS:HD2	1.99	0.43
9:I:98:ARG:HA	9:I:98:ARG:HD3	1.72	0.43
10:J:144:LYS:HA	10:J:144:LYS:HD3	1.86	0.43
1:2:1172:U:O2	1:2:1188:A:N7	2.50	0.43
7:G:95:HIS:HA	7:G:98:GLU:HG2	2.01	0.43
12:L:83:LEU:HD12	12:L:85:LEU:HD23	2.01	0.43
15:O:3:ARG:HB2	15:O:6:ALA:HB3	2.01	0.43
17:Q:22:LEU:HA	17:Q:25:LEU:HD12	2.01	0.43
1:2:158:A:N6	1:2:466:G:N7	2.67	0.43
1:2:1172:U:H2'	1:2:1173:A:H8	1.83	0.43
1:2:1337:C:H2'	1:2:1338:G:C8	2.54	0.43
1:2:1447:G:H2'	1:2:1448:A:H8	1.84	0.43
1:2:1566:G:N7	21:U:101:ARG:NH2	2.67	0.43
1:2:1650:A:H5''	18:R:139:ALA:HB2	2.00	0.43
1:2:555:A:H5'	32:f:98:LYS:HE2	2.01	0.43
1:2:1535:U:H6	7:G:88:MET:HE3	1.84	0.43
23:W:59:ILE:HG23	23:W:64:GLU:HG2	2.00	0.43
2:B:141:ASN:ND2	23:W:31:SER:O	2.47	0.43
4:D:271:ASP:OD1	4:D:272:HIS:N	2.52	0.43
11:K:124:HIS:CE1	32:f:108:ARG:HD2	2.54	0.43
25:Y:132:ALA:HB1	25:Y:138:LYS:HB2	2.01	0.43
1:2:483:C:H5''	25:Y:48:LYS:HE2	1.99	0.42
1:2:492:C:N4	1:2:507:G:OP2	2.39	0.42
1:2:867:G:O2'	1:2:868:G:O4'	2.31	0.42
10:J:67:TRP:HA	10:J:189:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1405:A:H2	1:2:1443:C:H42	1.67	0.42
2:B:8:LEU:HD23	2:B:191:ARG:HH21	1.84	0.42
2:B:74:VAL:HG22	2:B:121:LEU:HD12	2.00	0.42
15:O:143:SER:O	15:O:146:ALA:HB3	2.20	0.42
1:2:688:U:OP2	9:I:123:THR:OG1	2.38	0.42
1:2:1076:G:OP2	15:O:107:LYS:NZ	2.49	0.42
1:2:1324:G:O2'	1:2:1510:G:O2'	2.32	0.42
1:2:1487:A:H1'	4:D:118:ALA:HB1	2.00	0.42
34:h:107:ASP:OD2	34:h:125:ARG:NH1	2.50	0.42
8:H:67:VAL:HG12	8:H:69:THR:HG22	2.01	0.42
17:Q:118:GLU:HG2	20:T:120:HIS:H	1.83	0.42
33:g:99:LYS:HD2	33:g:99:LYS:HA	1.76	0.42
34:h:104:HIS:CE1	34:h:124:SER:HB3	2.55	0.42
34:h:289:LEU:HA	34:h:300:ALA:HA	2.00	0.42
37:z:132:G:H2'	37:z:133:G:H8	1.84	0.42
1:2:409:C:N4	1:2:427:U:OP1	2.51	0.42
1:2:1256:G:N2	31:e:30:LEU:O	2.38	0.42
2:B:10:MET:HB2	2:B:14:ASP:HB2	2.01	0.42
7:G:125:SER:OG	7:G:136:ARG:NH1	2.53	0.42
16:P:93:LEU:HD23	16:P:93:LEU:HA	1.90	0.42
17:Q:78:THR:HG23	17:Q:96:VAL:HG23	2.02	0.42
24:X:11:LEU:HD22	24:X:74:VAL:HG23	2.02	0.42
24:X:115:GLU:HG2	24:X:118:ARG:HH22	1.85	0.42
28:b:12:LYS:HG3	28:b:15:ARG:HB2	2.01	0.42
34:h:202:PRO:HG2	34:h:243:PRO:HA	2.01	0.42
35:i:52:G:H2'	35:i:53:A:H8	1.85	0.42
1:2:106:C:OP1	1:2:431:G:O2'	2.37	0.42
1:2:380:G:H5''	10:J:31:ARG:HH11	1.84	0.42
1:2:1652:G:O6	1:2:1672:U:O4	2.37	0.42
3:C:198:GLU:O	3:C:202:GLN:NE2	2.52	0.42
22:V:67:LYS:HB2	22:V:76:THR:HG23	2.01	0.42
37:z:248:U:H2'	37:z:249:G:H8	1.84	0.42
1:2:374:G:O3'	13:M:84:ARG:NH2	2.53	0.42
1:2:600:G:H2'	1:2:601:G:H8	1.85	0.42
1:2:868:G:O2'	9:I:114:GLN:OE1	2.38	0.42
1:2:1220:A:N3	1:2:1677:U:O2'	2.46	0.42
1:2:1665:G:C6	21:U:88:MET:HE1	2.55	0.42
5:E:25:LEU:HA	5:E:25:LEU:HD23	1.81	0.42
5:E:193:ASP:OD2	5:E:195:SER:OG	2.38	0.42
7:G:103:LEU:HD12	27:a:67:LEU:HD22	2.02	0.42
34:h:174:VAL:HG13	34:h:188:HIS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:433:A:H2'	1:2:434:G:C8	2.54	0.42
1:2:1542:C:OP1	21:U:62:ARG:NH2	2.52	0.42
10:J:203:LYS:HA	10:J:206:LYS:HG2	2.02	0.42
12:L:32:HIS:HD2	12:L:42:ASN:HB3	1.85	0.42
34:h:206:LEU:HA	34:h:220:ASP:HA	2.02	0.42
35:i:4:A:H2'	35:i:5:G:C8	2.55	0.42
1:2:982:G:H2'	1:2:983:A:H8	1.84	0.42
7:G:32:ASP:OD2	7:G:34:SER:OG	2.28	0.42
20:T:137:LYS:HA	20:T:137:LYS:HD3	1.90	0.42
37:z:252:A:H4'	37:z:253:G:H5'	2.02	0.42
1:2:959:G:OP2	16:P:38:ASN:ND2	2.35	0.42
1:2:974:C:O2	16:P:55:ARG:NH2	2.52	0.42
10:J:105:ASP:OD1	10:J:106:SER:N	2.53	0.42
18:R:76:GLY:H	18:R:79:ALA:HB3	1.84	0.42
31:e:22:ARG:HG2	31:e:38:MET:HB3	2.01	0.42
1:2:581:U:OP1	11:K:133:ARG:NH2	2.53	0.41
1:2:928:G:H2'	1:2:929:G:C8	2.54	0.41
1:2:1453:C:OP1	19:S:48:ASN:ND2	2.43	0.41
5:E:202:LYS:HB3	5:E:202:LYS:HE3	1.86	0.41
7:G:91:ARG:HH12	27:a:104:ARG:HH21	1.66	0.41
9:I:103:LYS:HD3	9:I:103:LYS:HA	1.81	0.41
18:R:101:ASP:OD1	18:R:102:GLU:N	2.52	0.41
20:T:125:HIS:CD2	20:T:131:VAL:HG11	2.55	0.41
1:2:957:A:H2'	1:2:958:G:H8	1.85	0.41
1:2:1264:C:H42	1:2:1518:C:H41	1.69	0.41
3:C:109:LYS:O	3:C:113:MET:HG3	2.20	0.41
3:C:175:GLU:O	3:C:179:ASN:ND2	2.50	0.41
7:G:177:LEU:HA	7:G:180:ALA:HB3	2.02	0.41
17:Q:18:ARG:NH1	20:T:88:LYS:O	2.53	0.41
24:X:41:MET:HE1	24:X:69:LEU:HD13	2.02	0.41
34:h:225:LYS:HD3	34:h:225:LYS:HA	1.91	0.41
34:h:292:SER:OG	34:h:293:ALA:N	2.52	0.41
1:2:948:C:H2'	1:2:949:G:H8	1.85	0.41
1:2:980:A:H2'	1:2:981:A:C8	2.56	0.41
1:2:1553:C:H41	31:e:22:ARG:NH1	2.19	0.41
3:C:163:GLN:HA	3:C:166:LYS:HG2	2.02	0.41
5:E:175:VAL:HB	5:E:182:LEU:HB3	2.01	0.41
9:I:27:LEU:HD23	9:I:27:LEU:HA	1.88	0.41
9:I:144:ILE:HG12	9:I:154:ILE:HG12	2.02	0.41
14:N:72:HIS:H	14:N:74:ILE:HD12	1.85	0.41
22:V:56:MET:HE2	22:V:86:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:80:ARG:HA	27:a:80:ARG:HD3	1.84	0.41
1:2:60:A:O2'	1:2:316:G:O2'	2.31	0.41
1:2:1711:U:H2'	1:2:1712:A:C8	2.56	0.41
3:C:182:LYS:O	3:C:186:ASN:ND2	2.40	0.41
5:E:28:GLU:OE2	12:L:61:GLN:NE2	2.43	0.41
5:E:32:ASP:HA	5:E:54:ARG:HD2	2.02	0.41
34:h:127:LYS:HD3	34:h:148:SER:HA	2.02	0.41
1:2:1815:A:H3'	1:2:1816:G:H8	1.85	0.41
5:E:1:MET:HG3	5:E:4:GLN:H	1.84	0.41
6:F:94:LYS:HE2	6:F:94:LYS:HB2	1.76	0.41
17:Q:68:PRO:HG2	17:Q:74:GLU:H	1.85	0.41
1:2:212:C:H2'	1:2:213:G:H8	1.86	0.41
1:2:743:U:O2	1:2:798:G:N2	2.53	0.41
1:2:1718:G:H22	1:2:1814:G:H2'	1.86	0.41
11:K:43:VAL:HA	11:K:46:VAL:HG22	2.02	0.41
12:L:21:MET:HE3	12:L:45:VAL:HG11	2.03	0.41
17:Q:81:ARG:NH1	17:Q:120:SER:OG	2.53	0.41
22:V:49:LYS:H	22:V:49:LYS:HG2	1.72	0.41
1:2:21:U:H4'	11:K:19:PRO:HG3	2.03	0.41
1:2:374:G:H5''	13:M:59:LYS:HE3	2.03	0.41
1:2:1779:G:H2'	1:2:1780:G:C8	2.56	0.41
5:E:204:LEU:HD12	5:E:205:PRO:HD2	2.03	0.41
6:F:123:LEU:HD23	6:F:161:GLN:HB3	2.02	0.41
18:R:80:GLN:O	18:R:84:ILE:HG12	2.20	0.41
22:V:27:ARG:HH12	31:e:51:GLY:HA3	1.85	0.41
1:2:1004:U:H2'	1:2:1005:G:H8	1.86	0.41
1:2:1057:C:H5'	37:z:340:C:H4'	2.01	0.41
1:2:1631:U:H5''	20:T:34:LYS:HD2	2.03	0.41
1:2:1745:A:O3'	8:H:31:ARG:NH2	2.54	0.41
2:B:210:ILE:HG23	19:S:81:ARG:HH21	1.85	0.41
4:D:212:LYS:O	4:D:216:MET:HG2	2.21	0.41
15:O:136:PRO:HA	15:O:137:PRO:HD3	1.97	0.41
32:f:121:THR:OG1	32:f:125:LYS:NZ	2.54	0.41
34:h:238:ALA:HB2	34:h:288:SER:HA	2.03	0.41
1:2:1396:A:O2'	1:2:1398:G:N7	2.54	0.41
1:2:1550:G:O2'	1:2:1558:C:O2	2.37	0.41
8:H:197:GLN:HA	8:H:200:LYS:HG2	2.02	0.41
12:L:5:LYS:HD3	12:L:5:LYS:HA	1.96	0.41
32:f:97:LYS:HE3	32:f:97:LYS:HB2	1.87	0.41
1:2:1263:U:H4'	31:e:27:ARG:HH12	1.85	0.40
1:2:1495:G:N2	31:e:42:CYS:SG	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1628:C:OP1	21:U:38:LYS:NZ	2.36	0.40
13:M:77:VAL:HA	13:M:88:ILE:HA	2.02	0.40
1:2:50:A:H62	1:2:477:G:H21	1.69	0.40
1:2:925:G:H1	1:2:1017:U:H3	1.69	0.40
1:2:1521:C:OP2	20:T:136:THR:OG1	2.39	0.40
6:F:127:ARG:HA	6:F:127:ARG:HD2	1.98	0.40
8:H:200:LYS:HA	8:H:203:LYS:HG2	2.03	0.40
9:I:103:LYS:HD3	9:I:116:ARG:HH12	1.86	0.40
10:J:200:ARG:HA	10:J:203:LYS:HG2	2.02	0.40
11:K:32:ILE:HG23	11:K:37:LEU:HB2	2.03	0.40
12:L:49:MET:HG3	12:L:52:LEU:HD23	2.04	0.40
13:M:90:ARG:HD3	13:M:109:MET:HE3	2.03	0.40
21:U:117:GLN:H	21:U:117:GLN:HG3	1.73	0.40
28:b:45:VAL:HB	28:b:49:ALA:HB3	2.02	0.40
34:h:63:SER:OG	34:h:84:ASP:OD2	2.34	0.40
1:2:941:C:H2'	1:2:942:G:C8	2.57	0.40
21:U:11:GLN:HA	21:U:14:PHE:HB3	2.04	0.40
29:c:11:SER:HA	29:c:12:PRO:HD3	1.97	0.40
1:2:223:C:H2'	1:2:224:A:C8	2.57	0.40
4:D:80:GLU:HA	4:D:83:LEU:HB3	2.02	0.40
4:D:209:VAL:HG21	4:D:233:LEU:HD13	2.02	0.40
35:i:4:A:H2'	35:i:5:G:H8	1.87	0.40
1:2:457:C:H2'	1:2:458:A:C8	2.55	0.40
1:2:807:G:H2'	1:2:808:A:C8	2.56	0.40
1:2:1004:U:OP1	3:C:165:ARG:NH2	2.54	0.40
1:2:1380:C:O2'	2:B:113:GLN:OE1	2.39	0.40
5:E:226:GLN:NE2	34:h:185:LYS:O	2.54	0.40
7:G:110:GLN:HA	7:G:113:VAL:HG12	2.03	0.40
18:R:97:GLN:HA	18:R:105:LYS:NZ	2.36	0.40
26:Z:9:THR:O	26:Z:10:ARG:NE	2.55	0.40
33:g:111:ASN:HB2	33:g:113:LYS:HG2	2.04	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%)	200 (93%)	15 (7%)	0	100	100
3	C	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
4	D	219/221 (99%)	211 (96%)	8 (4%)	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%)	229 (97%)	6 (3%)	0	100	100
9	I	181/432 (42%)	170 (94%)	11 (6%)	0	100	100
10	J	205/208 (99%)	194 (95%)	11 (5%)	0	100	100
11	K	183/194 (94%)	172 (94%)	11 (6%)	0	100	100
12	L	94/149 (63%)	88 (94%)	6 (6%)	0	100	100
13	M	149/158 (94%)	135 (91%)	14 (9%)	0	100	100
14	N	115/132 (87%)	107 (93%)	8 (7%)	0	100	100
15	O	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
16	P	134/168 (80%)	124 (92%)	10 (8%)	0	100	100
17	Q	118/145 (81%)	112 (95%)	6 (5%)	0	100	100
18	R	140/172 (81%)	136 (97%)	4 (3%)	0	100	100
19	S	130/135 (96%)	124 (95%)	6 (5%)	0	100	100
20	T	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
21	U	139/145 (96%)	130 (94%)	9 (6%)	0	100	100
22	V	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
23	W	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
24	X	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
25	Y	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
26	Z	122/131 (93%)	120 (98%)	2 (2%)	0	100	100
27	a	75/124 (60%)	73 (97%)	2 (3%)	0	100	100
28	b	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
29	c	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
30	d	65/69 (94%)	64 (98%)	1 (2%)	0	100	100
31	e	53/56 (95%)	53 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	f	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
33	g	66/188 (35%)	65 (98%)	1 (2%)	0	100	100
34	h	311/317 (98%)	287 (92%)	24 (8%)	0	100	100
36	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	4827/5821 (83%)	4588 (95%)	239 (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	42/245 (17%)	42 (100%)	0	100	100
3	C	16/231 (7%)	16 (100%)	0	100	100
4	D	69/187 (37%)	69 (100%)	0	100	100
5	E	147/232 (63%)	147 (100%)	0	100	100
6	F	224/225 (100%)	223 (100%)	1 (0%)	84	82
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	179/180 (99%)	179 (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
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	109/130 (84%)	109 (100%)	0	100	100
18	R	117/140 (84%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	106 (99%)	1 (1%)	70	76
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
36	n	24/24 (100%)	24 (100%)	0	100	100
All	All	3744/4942 (76%)	3742 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	157	ASN
26	Z	22	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	235	ASN
6	F	214	ASN
7	G	107	ASN
7	G	118	ASN
10	J	138	ASN
10	J	165	GLN
10	J	168	GLN

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Mol	Chain	Res	Type
11	K	75	ASN
11	K	124	HIS
11	K	132	GLN
11	K	177	ASN
12	L	50	GLN
13	M	11	GLN
13	M	19	ASN
13	M	39	ASN
15	O	36	GLN
15	O	62	GLN
17	Q	114	HIS
19	S	29	HIS
19	S	116	ASN
21	U	12	GLN
21	U	105	GLN
24	X	56	HIS
26	Z	19	GLN
28	b	19	GLN
31	e	26	ASN
32	f	117	ASN
34	h	143	GLN
34	h	162	ASN
34	h	187	ASN
34	h	222	ASN
34	h	305	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	329 (19%)	10 (0%)
35	i	74/75 (98%)	13 (17%)	0
37	z	186/400 (46%)	55 (29%)	0
All	All	1945/2345 (82%)	397 (20%)	10 (0%)

All (397) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	C
1	2	5	U
1	2	26	U
1	2	33	G

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Mol	Chain	Res	Type
1	2	41	G
1	2	42	A
1	2	44	U
1	2	46	A
1	2	56	G
1	2	61	A
1	2	62	G
1	2	67	C
1	2	68	A
1	2	73	C
1	2	74	G
1	2	76	U
1	2	92	A
1	2	102	A
1	2	103	A
1	2	113	G
1	2	114	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	158	A
1	2	162	C
1	2	164	A
1	2	168	C
1	2	171	A
1	2	180	G
1	2	182	C
1	2	183	G
1	2	184	G
1	2	186	C
1	2	191	A
1	2	192	C
1	2	199	C
1	2	208	G
1	2	292	A
1	2	302	A
1	2	305	U
1	2	306	C
1	2	307	G

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Mol	Chain	Res	Type
1	2	309	G
1	2	312	G
1	2	319	C
1	2	320	G
1	2	323	C
1	2	335	G
1	2	341	C
1	2	347	G
1	2	351	G
1	2	364	A
1	2	368	U
1	2	370	G
1	2	382	C
1	2	383	G
1	2	384	U
1	2	385	G
1	2	393	U
1	2	398	A
1	2	400	C
1	2	407	G
1	2	409	C
1	2	418	A
1	2	420	G
1	2	426	A
1	2	435	A
1	2	436	G
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	472	C
1	2	474	G
1	2	482	G
1	2	487	U
1	2	488	U
1	2	490	C
1	2	492	C
1	2	493	A
1	2	500	A

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Mol	Chain	Res	Type
1	2	502	C
1	2	508	A
1	2	516	A
1	2	517	C
1	2	525	A
1	2	532	C
1	2	533	A
1	2	536	A
1	2	537	C
1	2	541	U
1	2	542	U
1	2	549	C
1	2	550	C
1	2	551	U
1	2	553	U
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	562	U
1	2	564	A
1	2	576	A
1	2	583	A
1	2	588	G
1	2	590	A
1	2	591	U
1	2	606	G
1	2	608	C
1	2	614	C
1	2	617	G
1	2	622	C
1	2	623	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	643	A
1	2	644	G
1	2	650	A
1	2	655	A
1	2	660	C
1	2	662	G
1	2	668	A

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Mol	Chain	Res	Type
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	684	G
1	2	689	U
1	2	691	G
1	2	694	G
1	2	696	G
1	2	732	U
1	2	750	C
1	2	752	G
1	2	753	C
1	2	754	G
1	2	793	G
1	2	795	A
1	2	798	G
1	2	799	U
1	2	801	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	834	C
1	2	847	A
1	2	860	G
1	2	866	U
1	2	870	A
1	2	872	A
1	2	873	G
1	2	875	A
1	2	878	G
1	2	886	A
1	2	887	U
1	2	888	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	895	G
1	2	897	U
1	2	899	U

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Mol	Chain	Res	Type
1	2	901	G
1	2	902	G
1	2	904	A
1	2	913	A
1	2	914	U
1	2	919	A
1	2	920	A
1	2	933	G
1	2	952	G
1	2	955	A
1	2	969	U
1	2	971	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1017	U
1	2	1023	A
1	2	1045	U
1	2	1053	C
1	2	1061	U
1	2	1062	A
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1089	G
1	2	1109	C
1	2	1114	U
1	2	1121	G
1	2	1123	C
1	2	1138	C
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1165	G
1	2	1166	G
1	2	1172	U
1	2	1203	U
1	2	1205	G
1	2	1207	G

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Mol	Chain	Res	Type
1	2	1212	G
1	2	1215	C
1	2	1216	C
1	2	1217	A
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	1274	G
1	2	1275	G
1	2	1285	G
1	2	1286	G
1	2	1293	A
1	2	1295	A
1	2	1298	G
1	2	1299	A
1	2	1301	A
1	2	1302	G
1	2	1305	C
1	2	1313	A
1	2	1318	G
1	2	1332	A
1	2	1333	U
1	2	1342	U
1	2	1348	G
1	2	1358	U
1	2	1361	G
1	2	1362	U
1	2	1364	U
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1396	A
1	2	1402	A
1	2	1404	U
1	2	1428	G
1	2	1442	U
1	2	1452	A
1	2	1454	A

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Mol	Chain	Res	Type
1	2	1462	U
1	2	1463	U
1	2	1473	G
1	2	1475	G
1	2	1477	U
1	2	1489	A
1	2	1490	G
1	2	1497	G
1	2	1498	A
1	2	1507	G
1	2	1508	A
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1548	G
1	2	1551	U
1	2	1552	G
1	2	1554	C
1	2	1555	U
1	2	1556	A
1	2	1567	G
1	2	1573	G
1	2	1575	G
1	2	1578	U
1	2	1580	A
1	2	1585	U
1	2	1588	A
1	2	1601	A
1	2	1604	G
1	2	1606	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1638	G
1	2	1646	C
1	2	1648	G
1	2	1659	U
1	2	1660	C

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Mol	Chain	Res	Type
1	2	1665	G
1	2	1680	G
1	2	1683	C
1	2	1695	A
1	2	1721	U
1	2	1744	G
1	2	1751	C
1	2	1756	C
1	2	1757	G
1	2	1759	G
1	2	1760	G
1	2	1774	C
1	2	1776	G
1	2	1779	G
1	2	1781	A
1	2	1782	G
1	2	1783	C
1	2	1784	G
1	2	1805	G
1	2	1824	A
1	2	1826	G
1	2	1834	A
1	2	1836	G
1	2	1838	U
1	2	1849	G
1	2	1851	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1866	A
35	i	4	A
35	i	16	C
35	i	17	G
35	i	18	G
35	i	20	A
35	i	47	C
35	i	58	A
35	i	59	A
35	i	60	C
35	i	71	U
35	i	73	C

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Mol	Chain	Res	Type
35	i	74	C
35	i	75	A
37	z	122	C
37	z	123	C
37	z	133	G
37	z	136	A
37	z	137	G
37	z	144	U
37	z	154	A
37	z	157	C
37	z	160	U
37	z	161	G
37	z	162	A
37	z	163	G
37	z	165	A
37	z	166	C
37	z	167	A
37	z	168	C
37	z	169	C
37	z	173	A
37	z	229	G
37	z	232	C
37	z	234	U
37	z	237	C
37	z	240	C
37	z	244	A
37	z	253	G
37	z	258	G
37	z	259	U
37	z	265	U
37	z	266	G
37	z	281	U
37	z	282	U
37	z	288	A
37	z	295	G
37	z	296	A
37	z	297	U
37	z	306	U
37	z	324	U
37	z	328	G
37	z	330	A
37	z	331	G

Continued on next page...

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Mol	Chain	Res	Type
37	z	332	A
37	z	333	C
37	z	334	C
37	z	335	G
37	z	337	G
37	z	338	C
37	z	345	A
37	z	346	G
37	z	348	A
37	z	349	C
37	z	351	A
37	z	352	A
37	z	353	U
37	z	355	C
37	z	356	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	561	A
1	2	688	U
1	2	752	G
1	2	874	G
1	2	886	A
1	2	1137	U
1	2	1395	C
1	2	1637	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

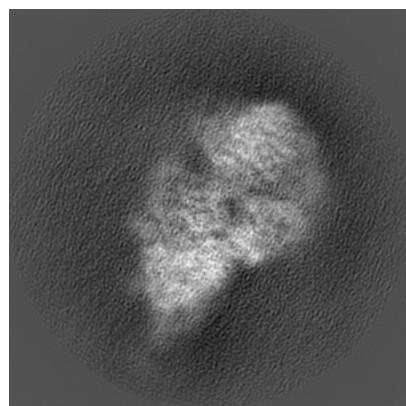
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25540. These allow visual inspection of the internal detail of the map and identification of artifacts.

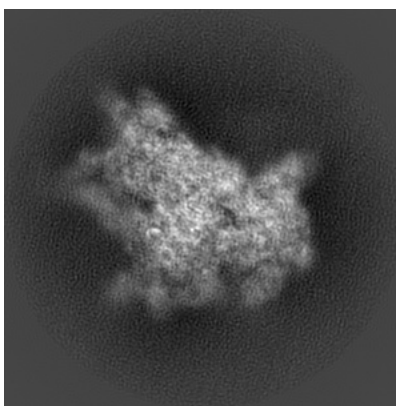
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

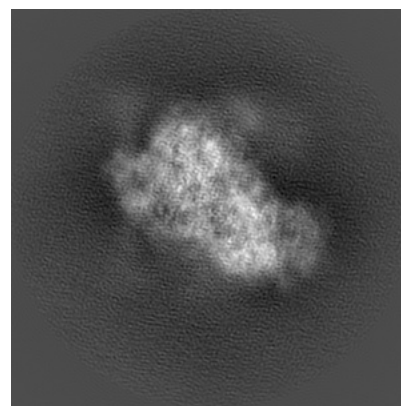
6.1.1 Primary map



X

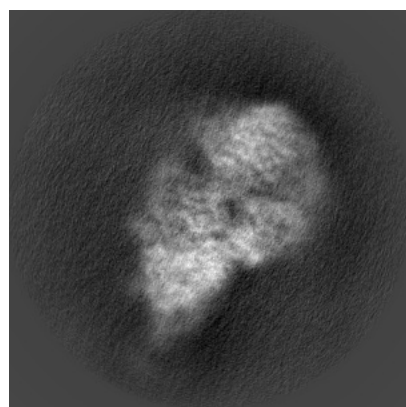


Y

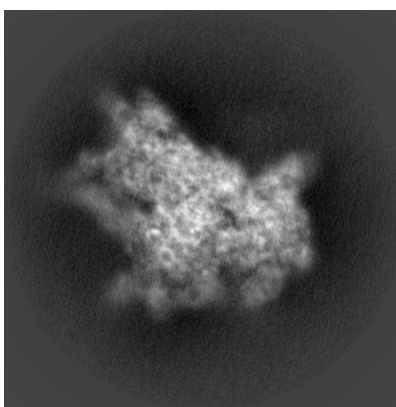


Z

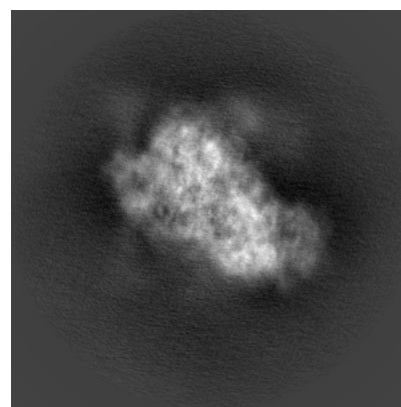
6.1.2 Raw map



X



Y

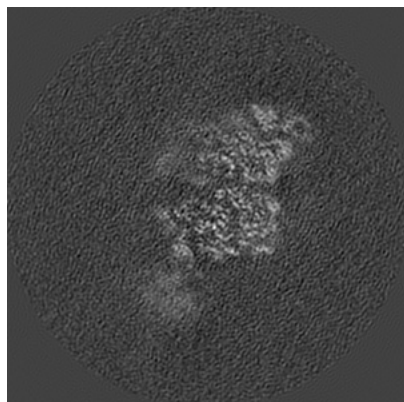


Z

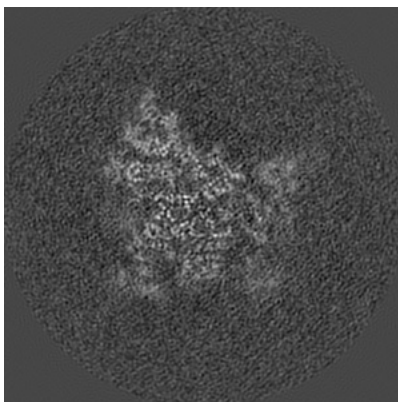
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

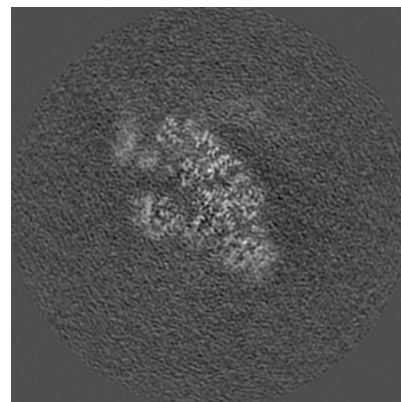
6.2.1 Primary map



X Index: 200

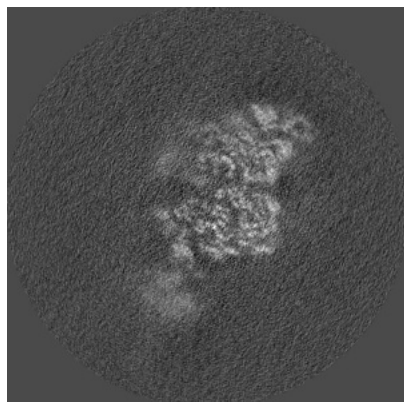


Y Index: 200

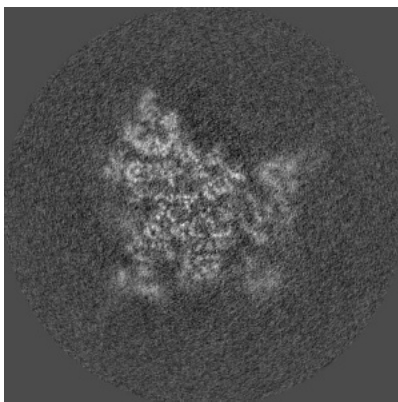


Z Index: 200

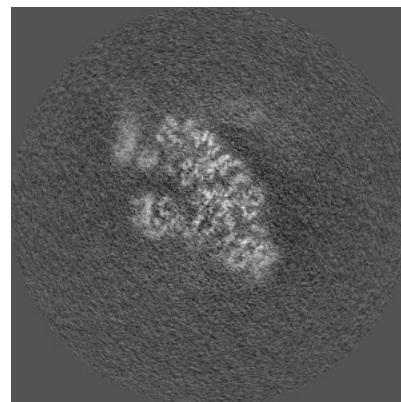
6.2.2 Raw map



X Index: 200



Y Index: 200

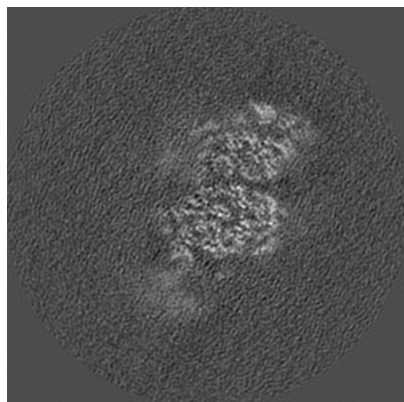


Z Index: 200

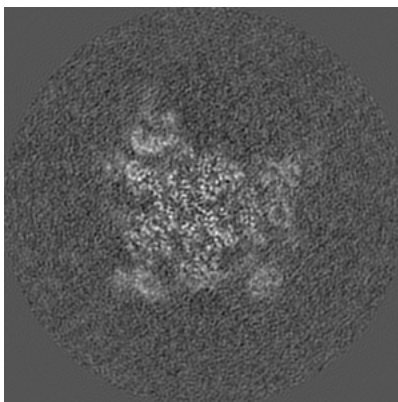
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

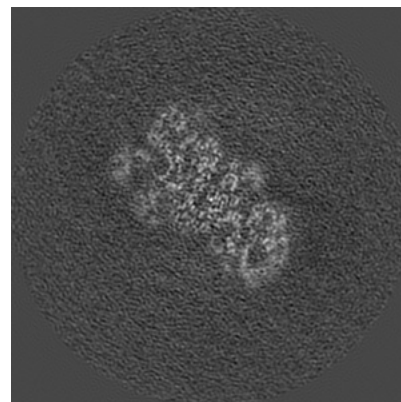
6.3.1 Primary map



X Index: 198

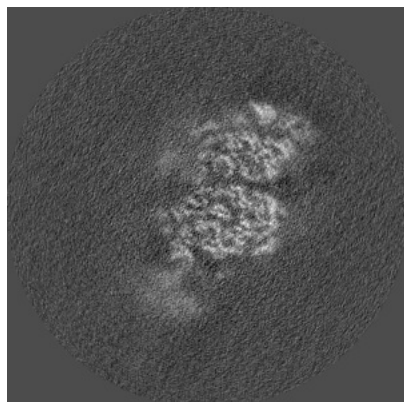


Y Index: 204

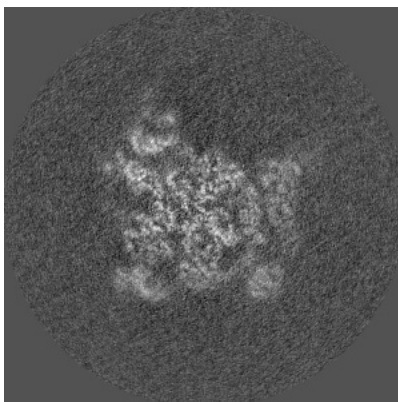


Z Index: 179

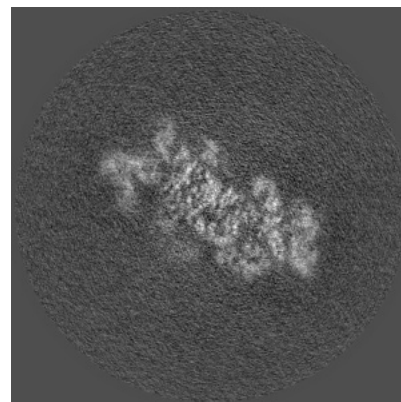
6.3.2 Raw map



X Index: 198



Y Index: 205

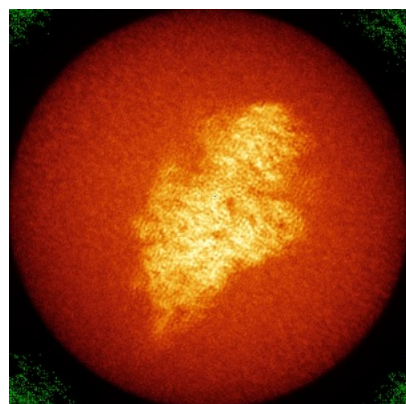


Z Index: 155

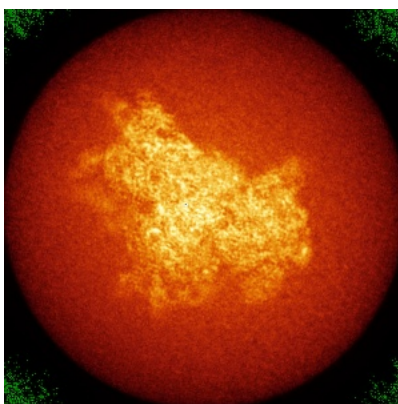
The images above show the largest variance slices of the map in three orthogonal directions.

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

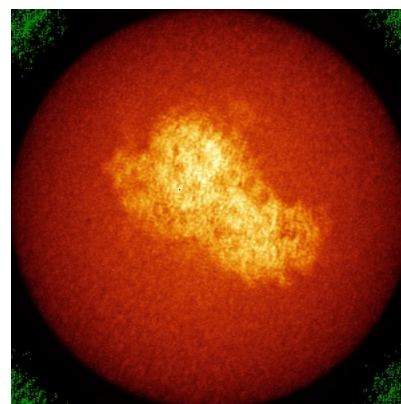
6.4.1 Primary map



X

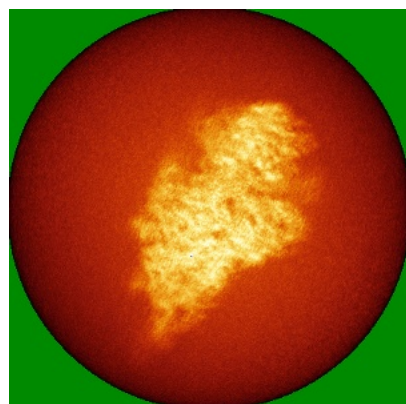


Y

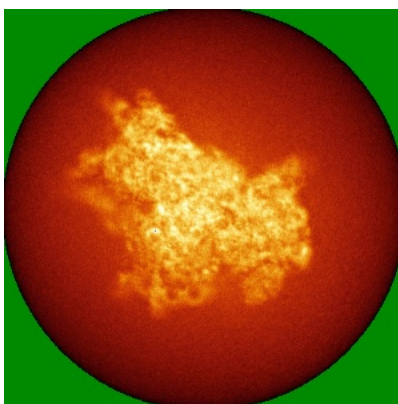


Z

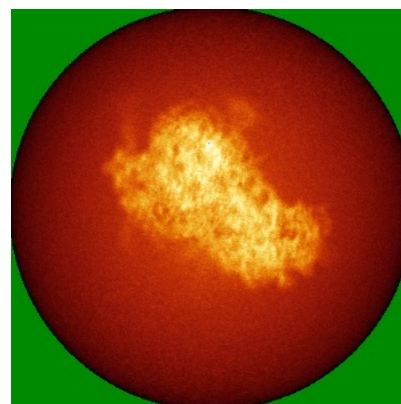
6.4.2 Raw map



X



Y

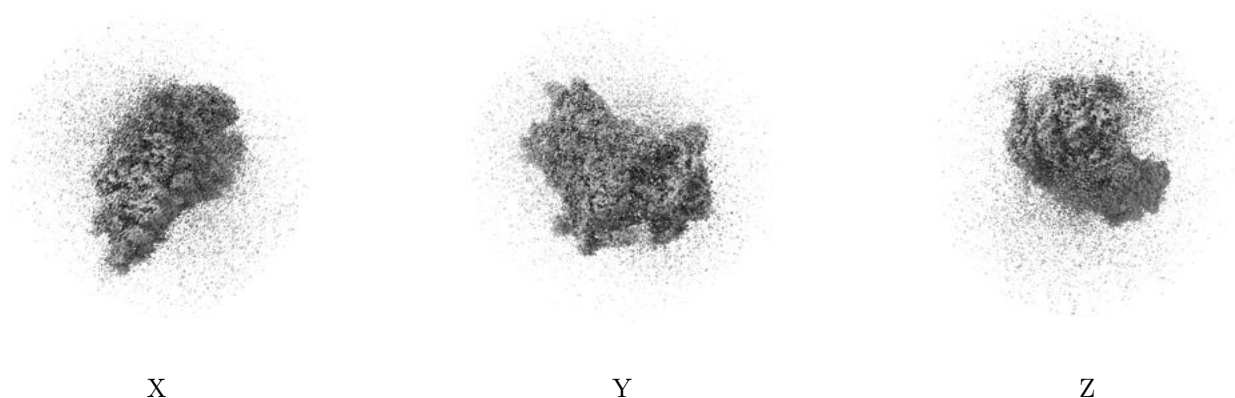


Z

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.

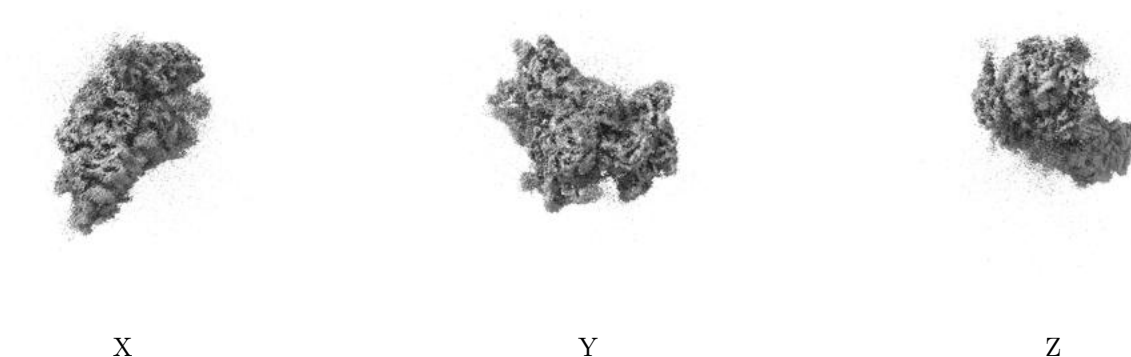
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0175. 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.

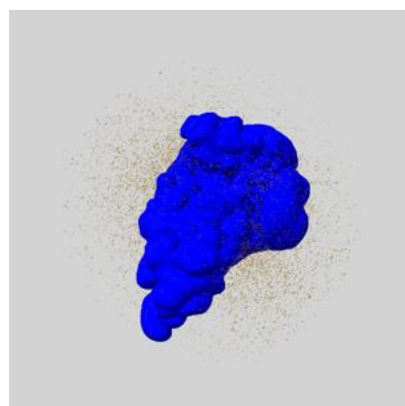
6.6 Mask visualisation [i](#)

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

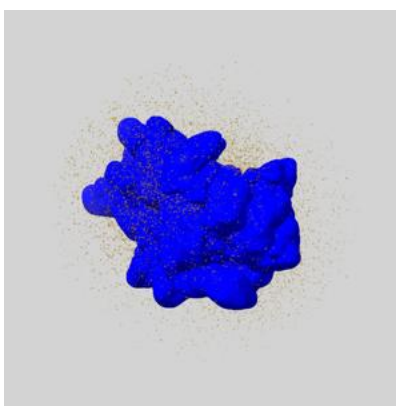
A mask typically either:

- 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_25540_msk_1.map [i](#)



X



Y

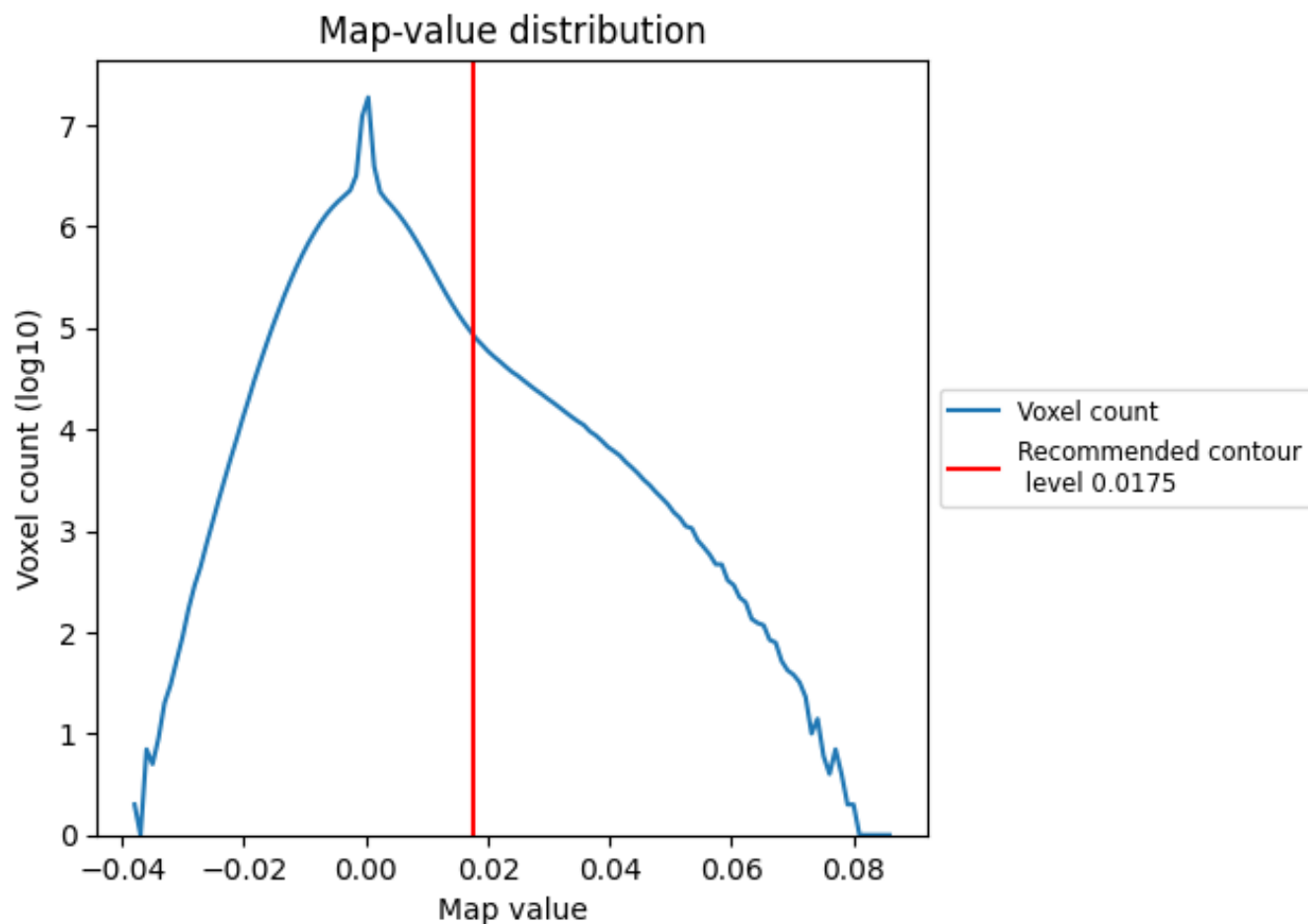


Z

7 Map analysis [i](#)

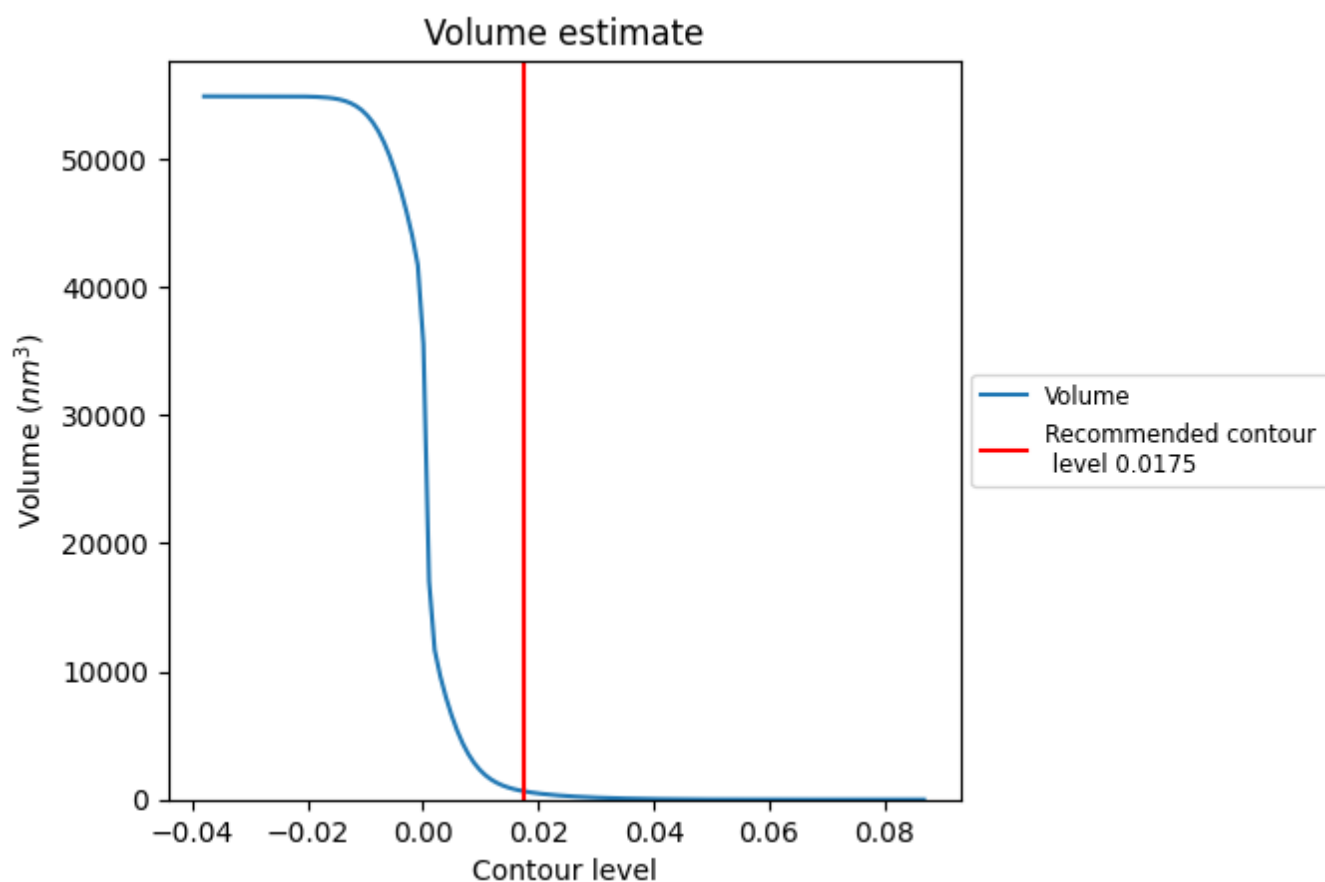
This section contains the results of statistical analysis of the map.

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.

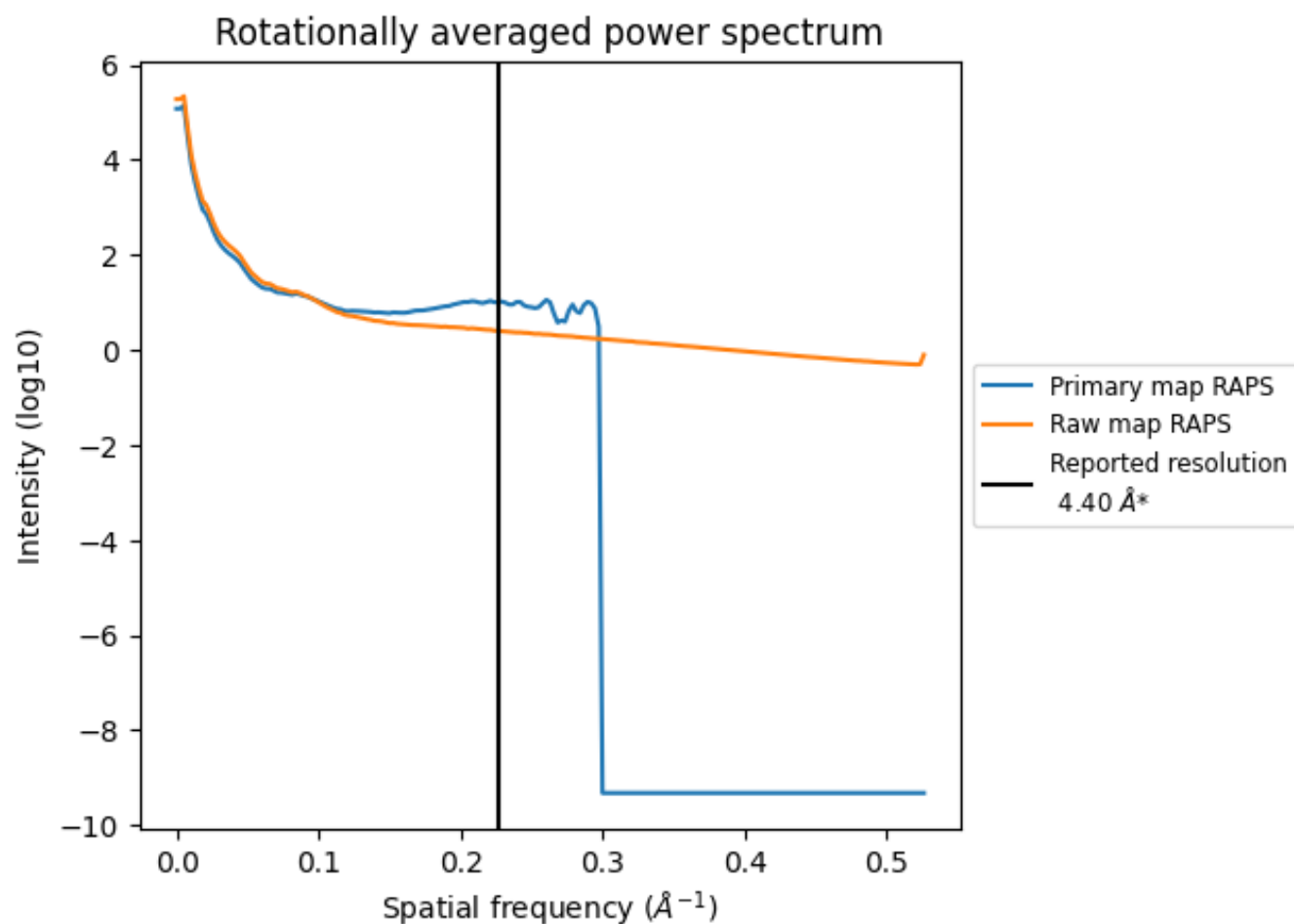
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 649 nm³; this corresponds to an approximate mass of 586 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 ⓘ

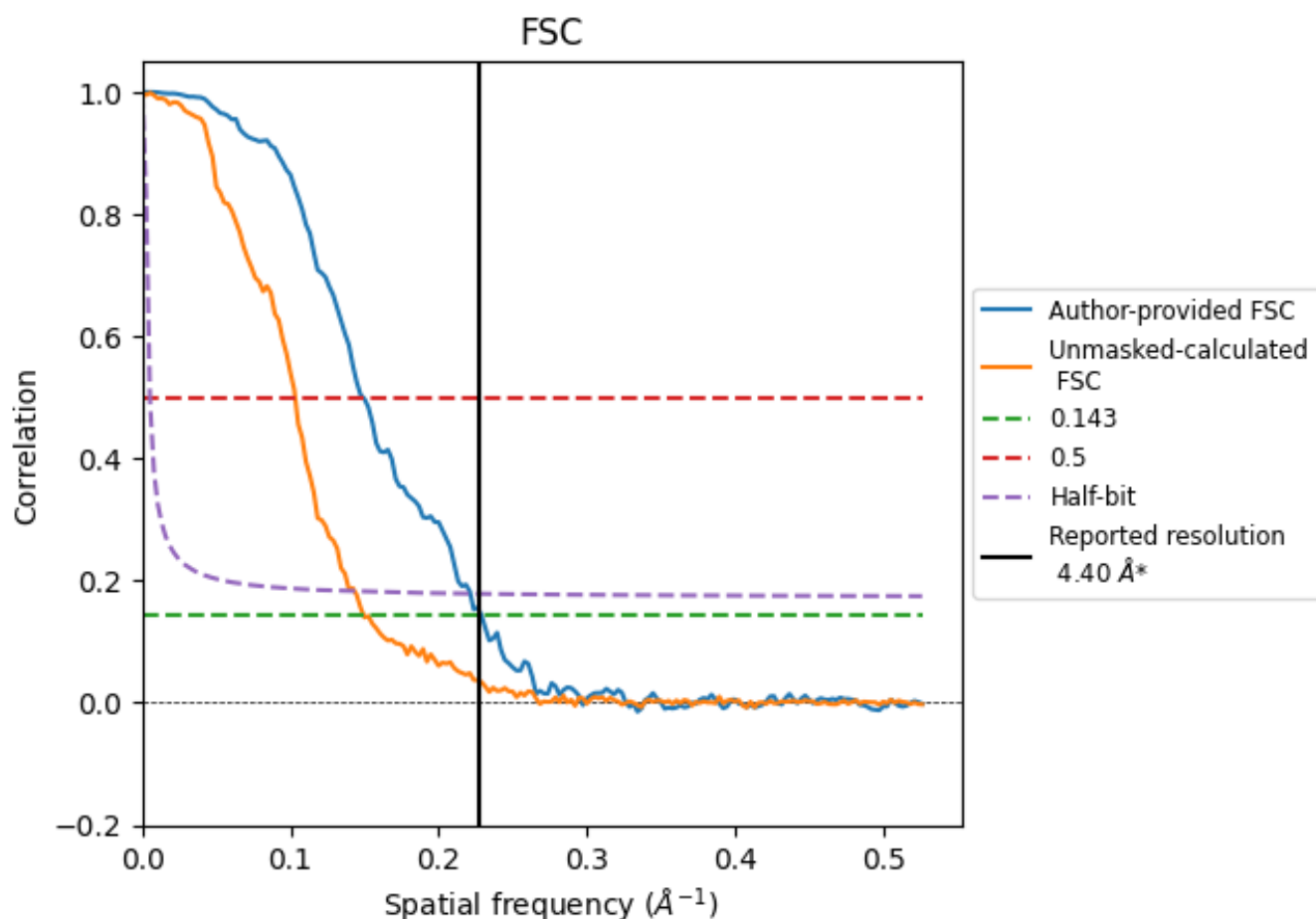


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

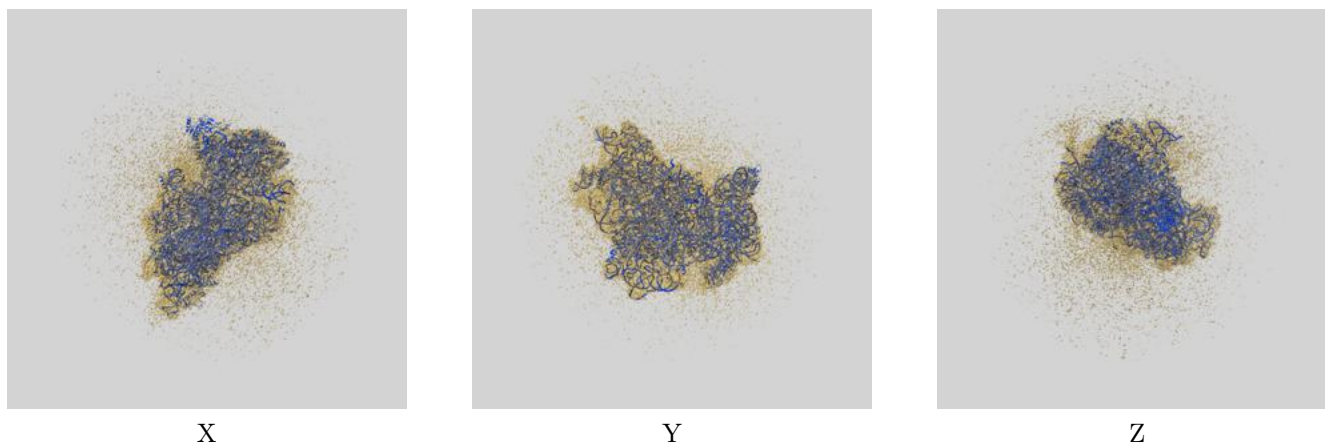
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.37	6.72	4.52
Unmasked-calculated*	6.69	9.69	6.97

*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 6.69 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

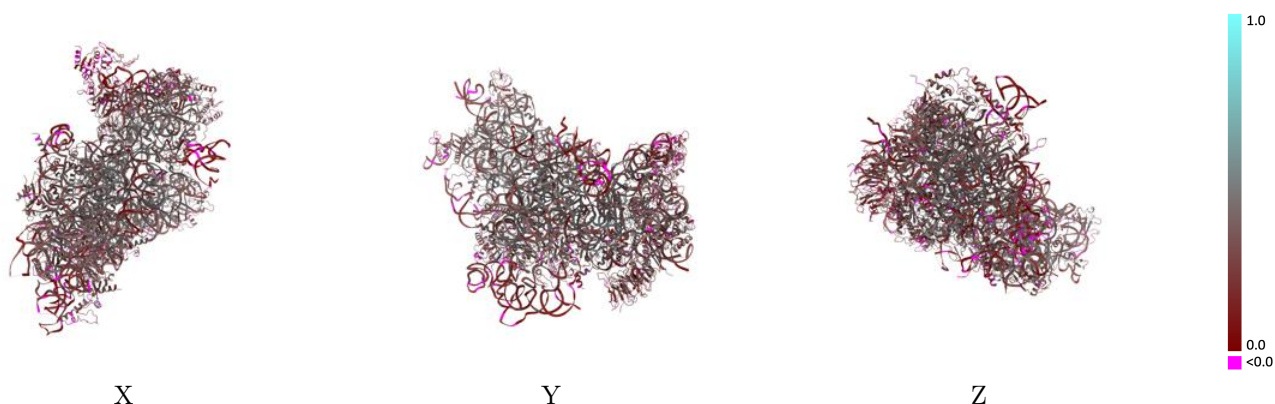
This section contains information regarding the fit between EMDB map EMD-25540 and PDB model 7SYT. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



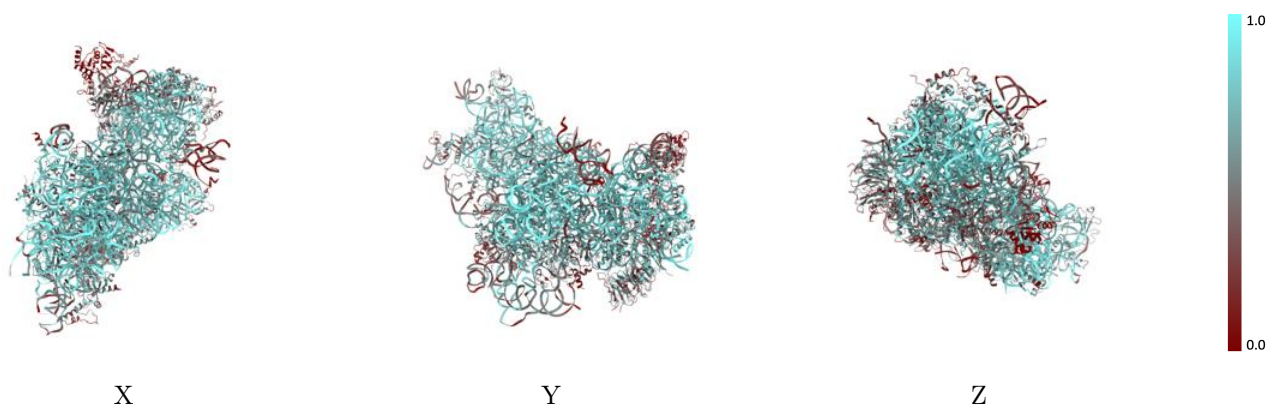
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



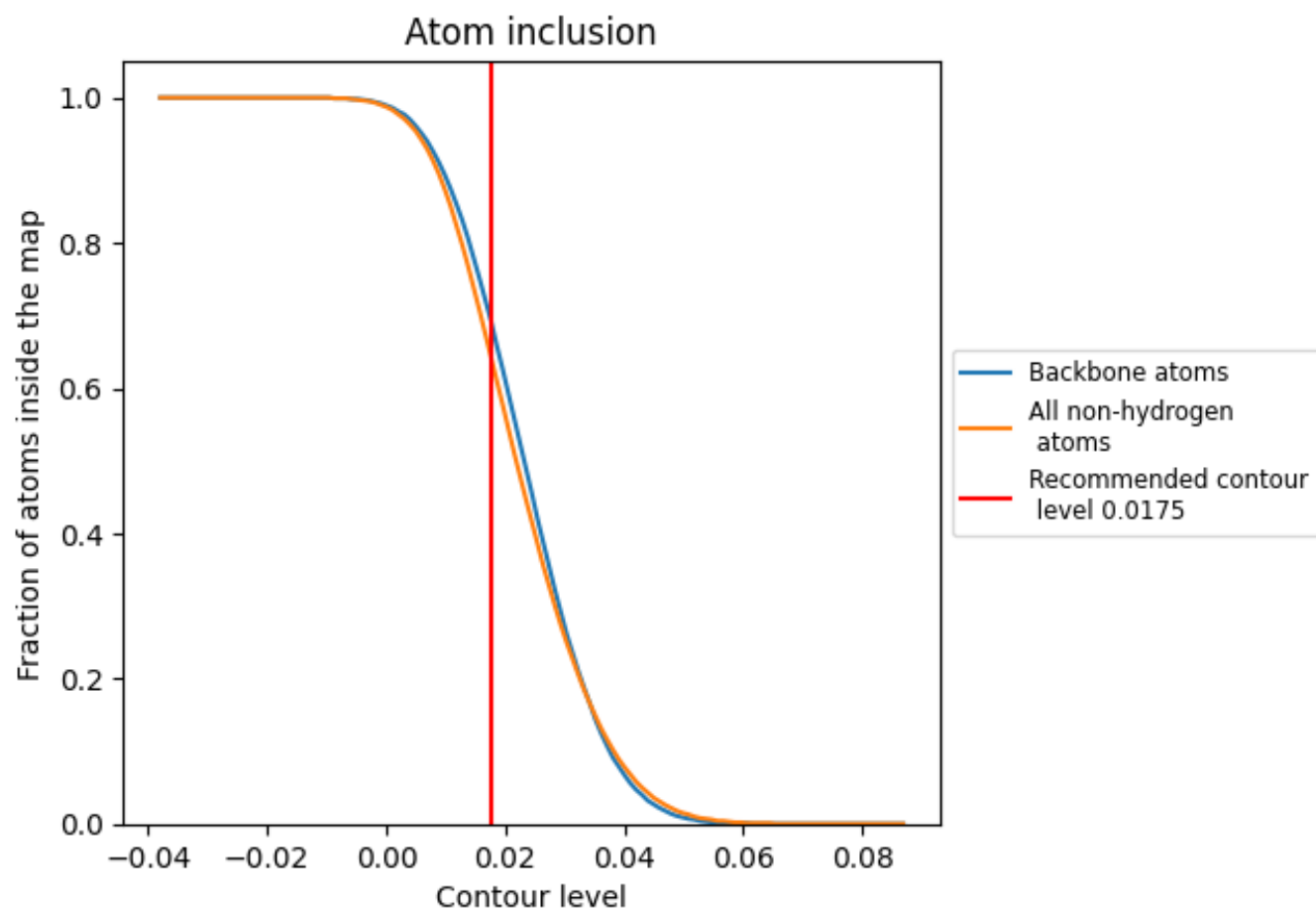
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0175).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 65% 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 (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6480	 0.3150
2	 0.7880	 0.3390
B	 0.5780	 0.3340
C	 0.6330	 0.3500
D	 0.6120	 0.3550
E	 0.4860	 0.2970
F	 0.6800	 0.3660
G	 0.5990	 0.3290
H	 0.5780	 0.2900
I	 0.2610	 0.2420
J	 0.5720	 0.3160
K	 0.6470	 0.3580
L	 0.3650	 0.2440
M	 0.5790	 0.3550
N	 0.0240	 0.1020
O	 0.6570	 0.3700
P	 0.6690	 0.3590
Q	 0.5170	 0.2680
R	 0.6740	 0.3620
S	 0.4580	 0.3140
T	 0.5290	 0.2960
U	 0.6850	 0.3380
V	 0.3860	 0.2490
W	 0.5900	 0.3580
X	 0.6450	 0.4160
Y	 0.6750	 0.4020
Z	 0.6820	 0.3100
a	 0.4360	 0.2910
b	 0.6410	 0.3800
c	 0.4900	 0.3420
d	 0.4530	 0.3120
e	 0.6030	 0.3390
f	 0.4950	 0.3070
g	 0.0690	 0.1130
h	 0.4730	 0.2500



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Chain	Atom inclusion	Q-score
i	 0.3470	 0.1210
n	 0.6740	 0.3710
z	 0.4630	 0.1540