



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 02:03 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 wwPDB EM Validation Summary 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:

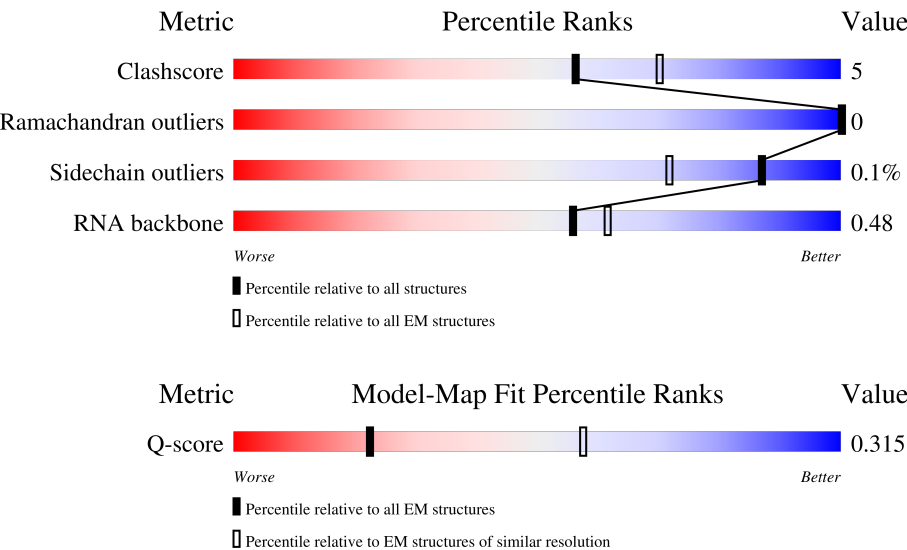
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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	8% 59% 28% • 9%
2	B	295	18% 61% 13% 26%
3	C	264	14% 67% 14% 19%

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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		

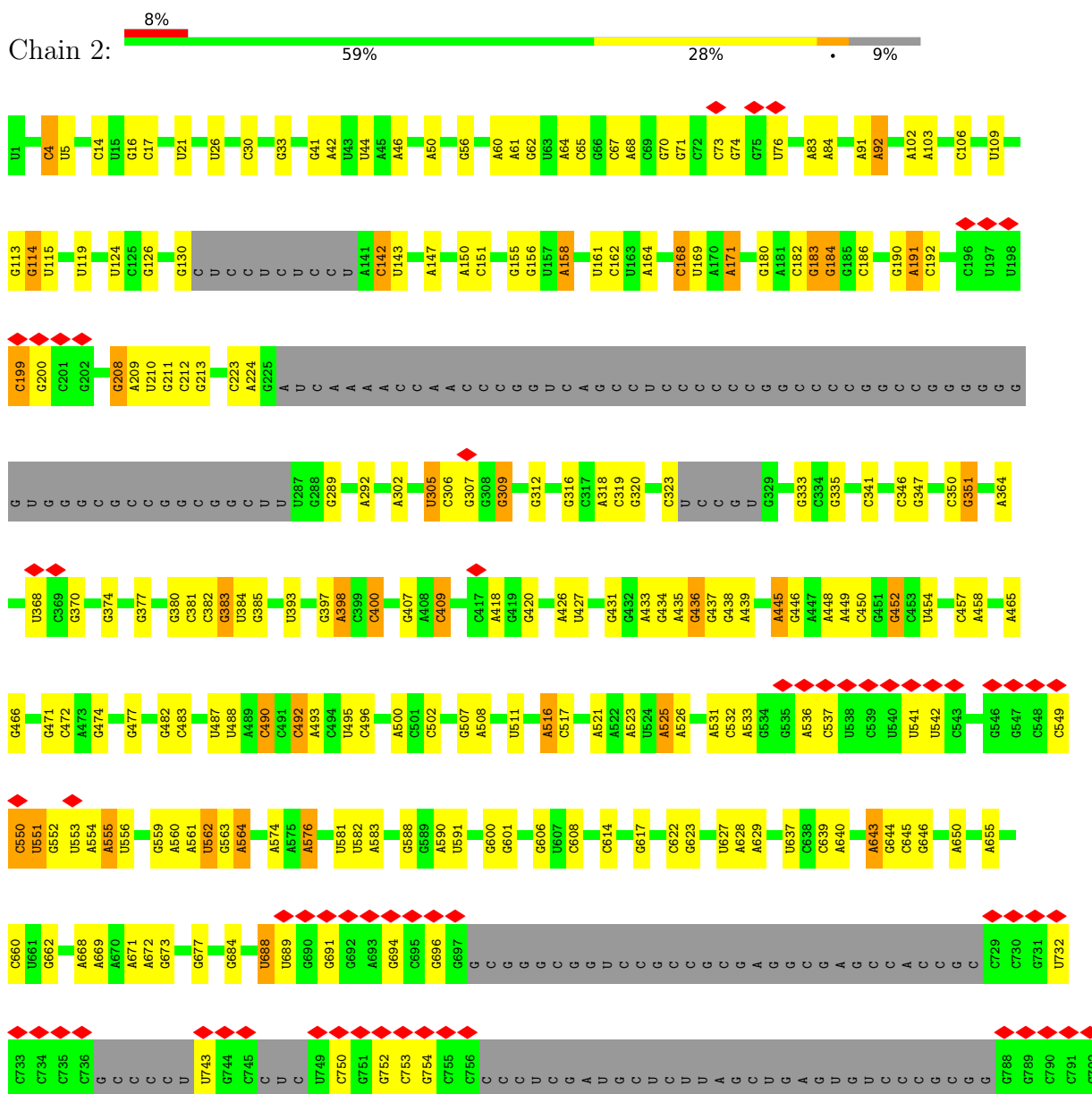
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

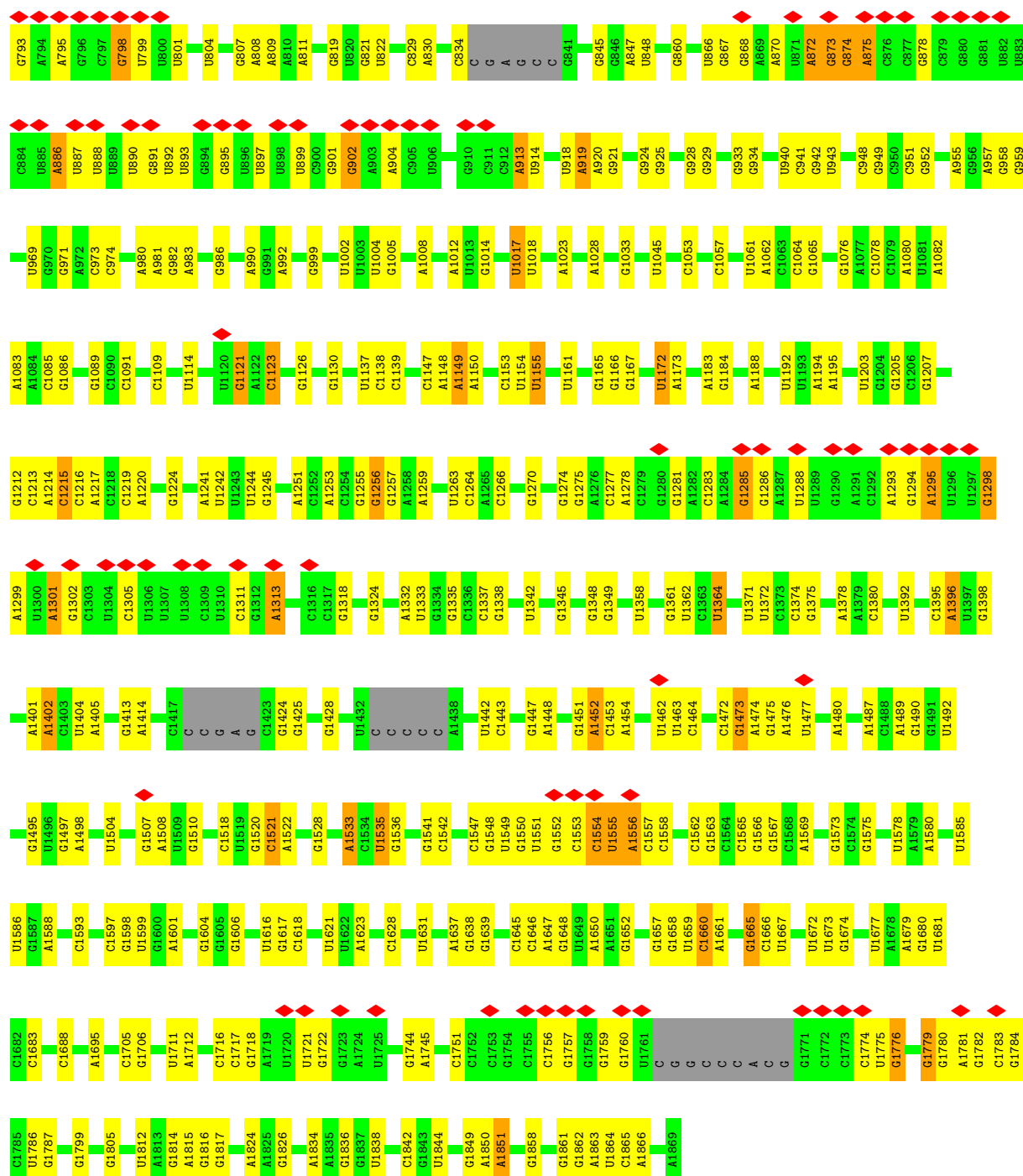
Mol	Chain	Residues	Atoms		AltConf
38	b	1	Total	Zn	0
			1	1	

3 Residue-property plots

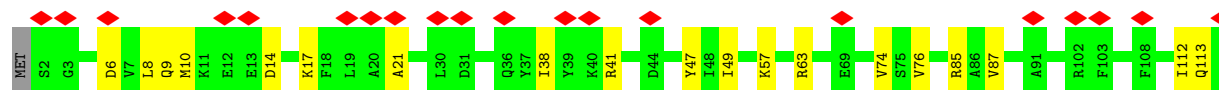
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

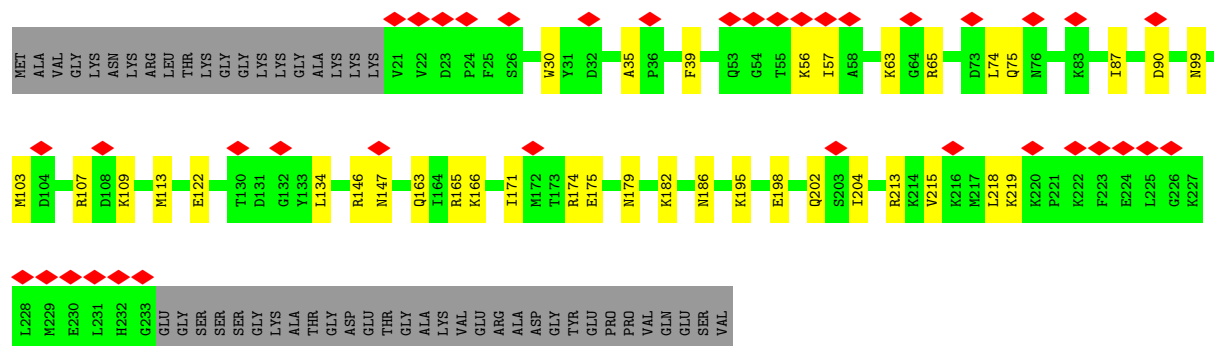




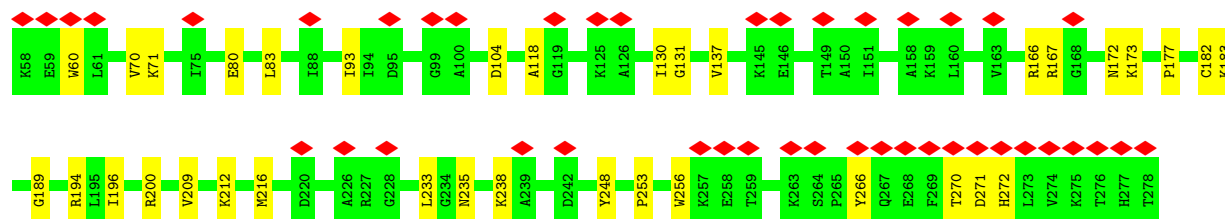
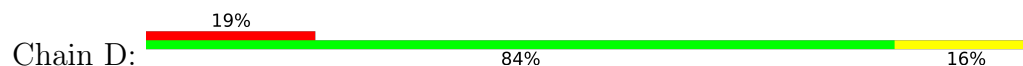
• Molecule 2: 40S ribosomal protein SA



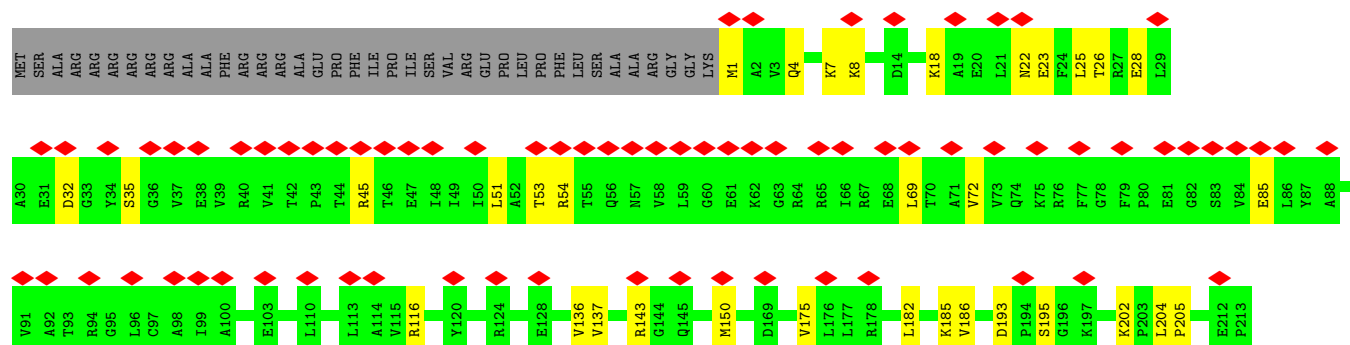
- Molecule 3: eS1

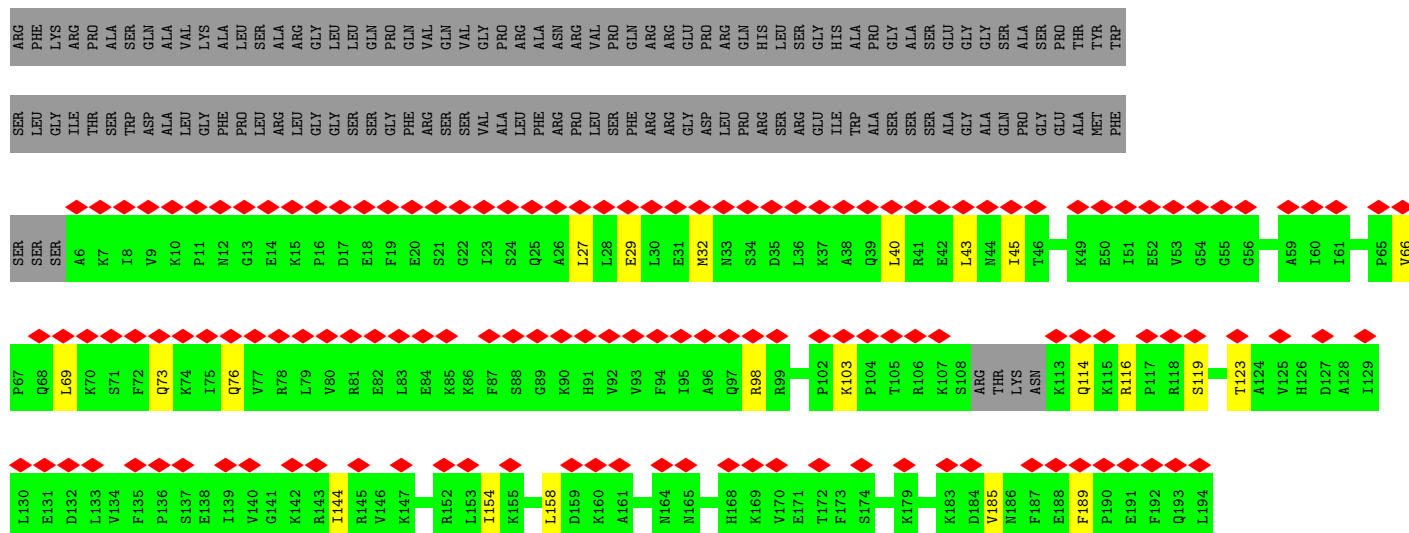


- Molecule 4: uS5 (S2)

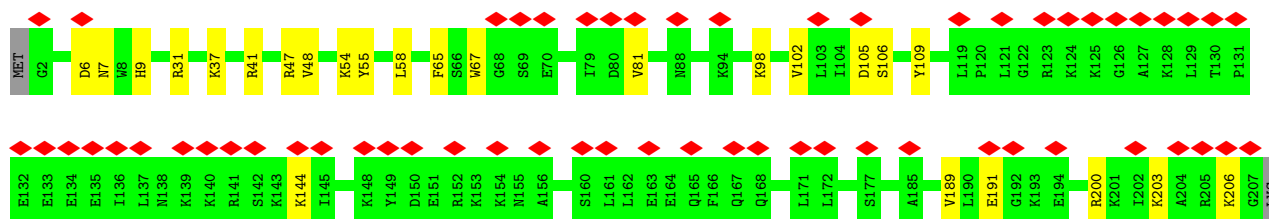
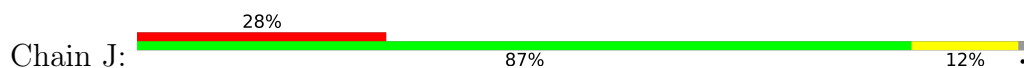


- Molecule 5: uS3

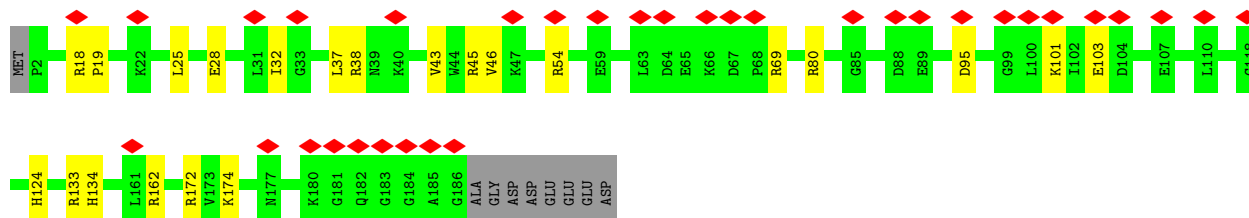
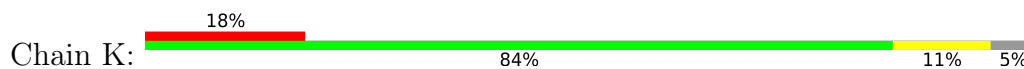




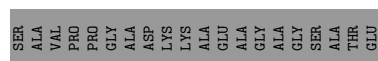
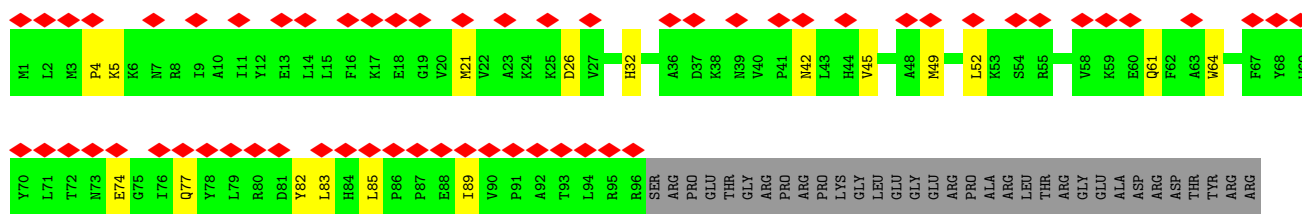
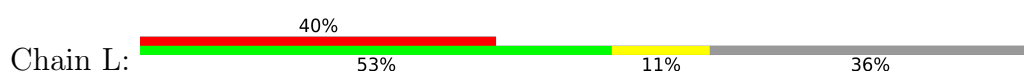
• Molecule 10: eS8



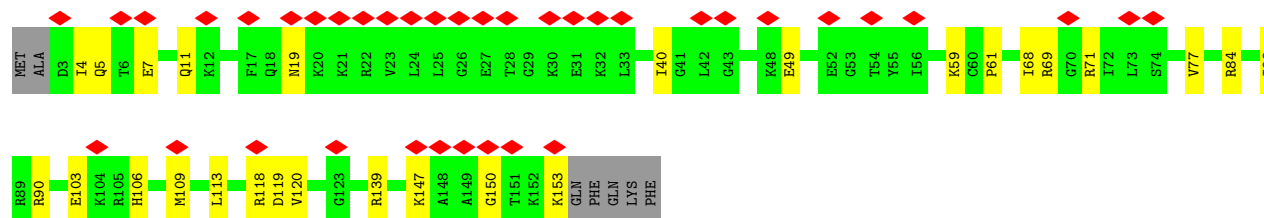
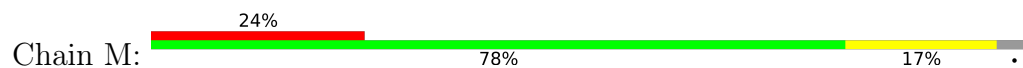
• Molecule 11: uS4



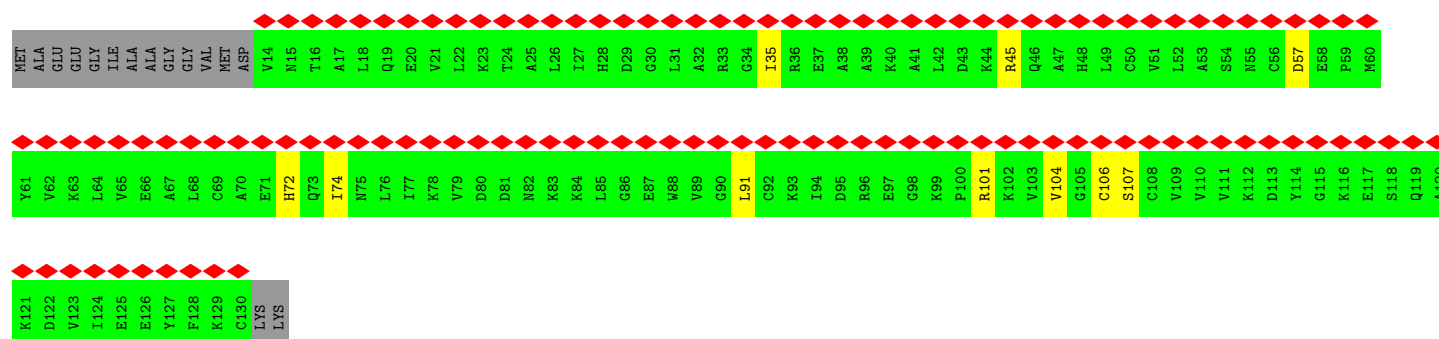
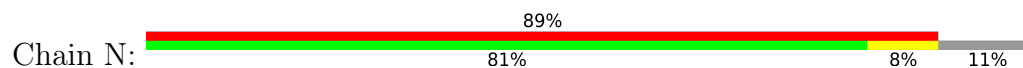
• Molecule 12: S10_pectin domain-containing protein



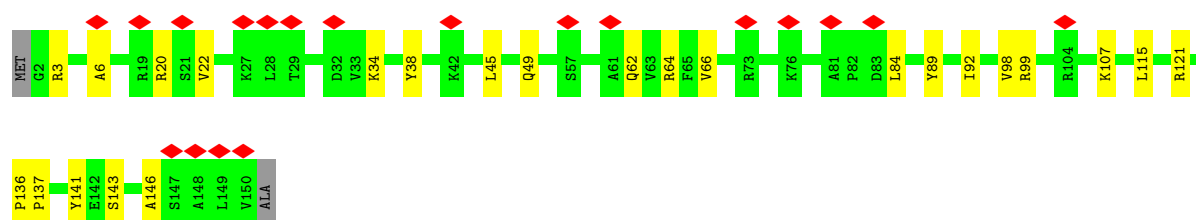
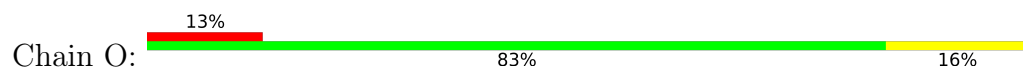
- Molecule 13: uS17



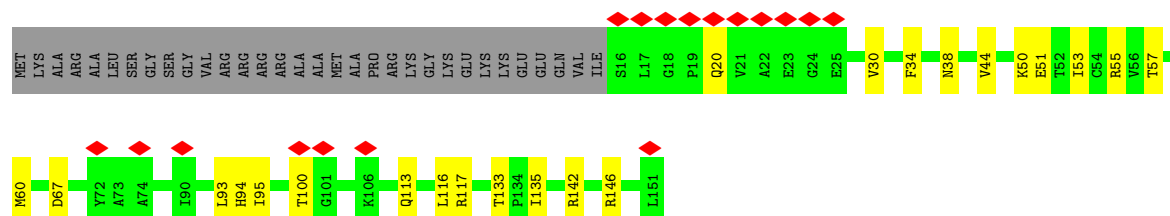
- Molecule 14: eS12



- Molecule 15: uS15

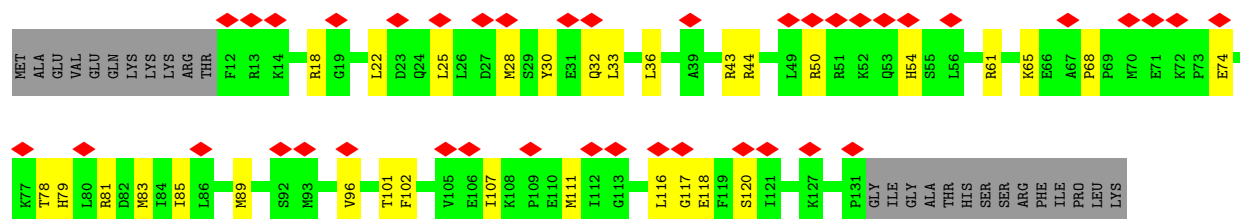


- Molecule 16: uS11

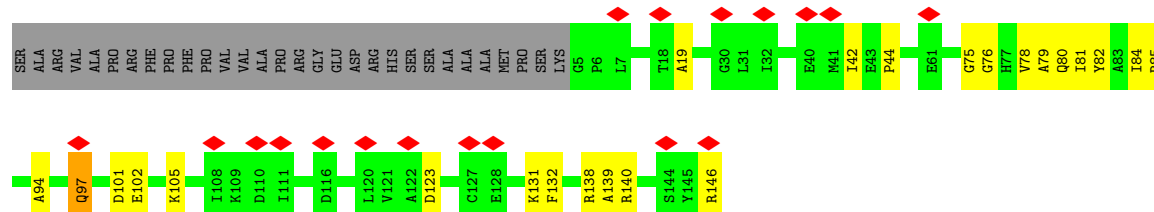


- Molecule 17: uS19

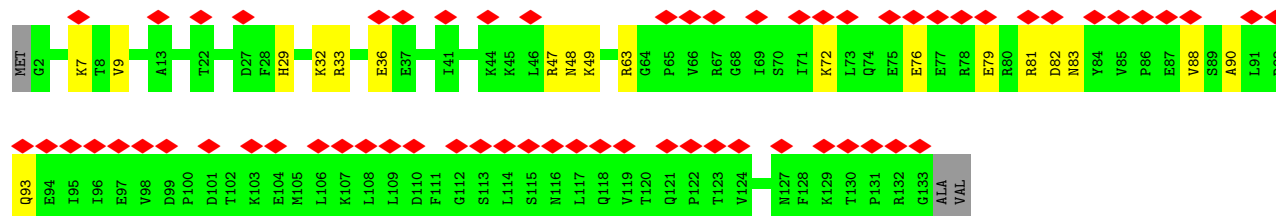
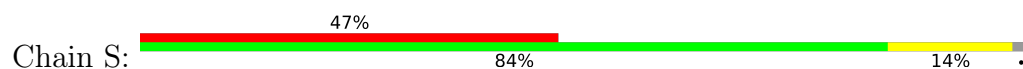




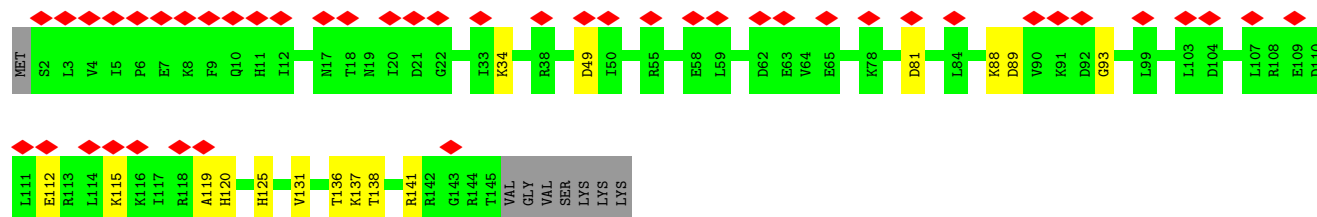
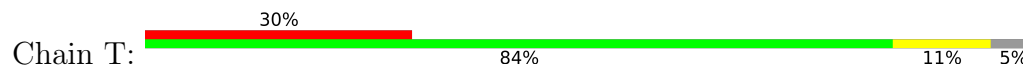
• Molecule 18: uS9



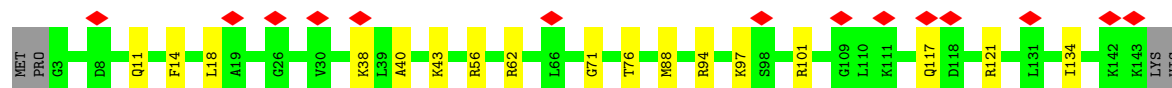
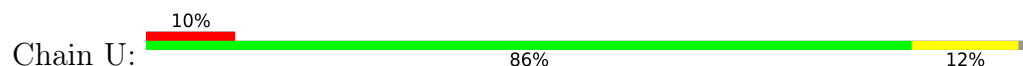
• Molecule 19: eS17



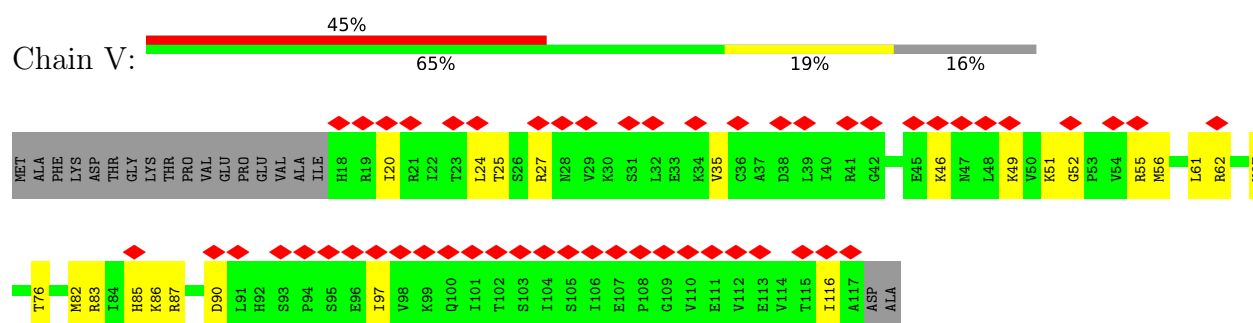
• Molecule 20: uS13



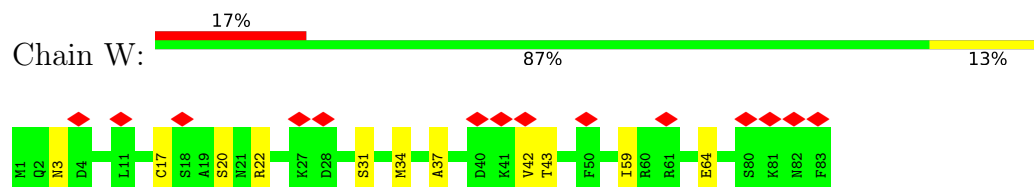
• Molecule 21: eS19



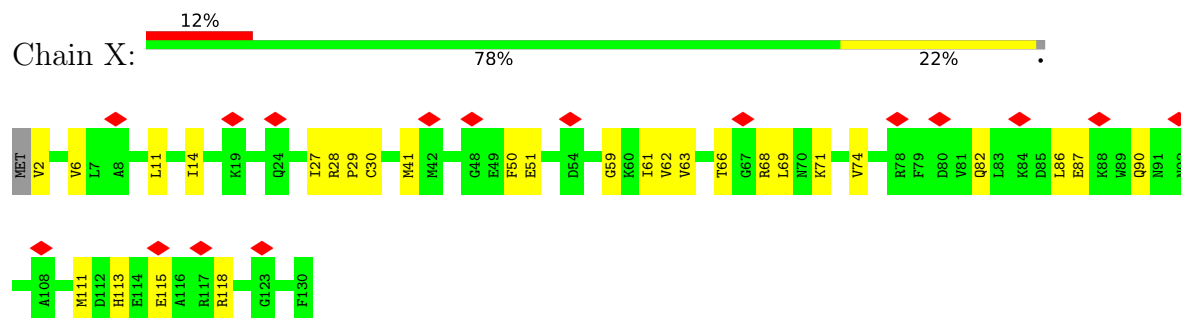
• Molecule 22: uS10



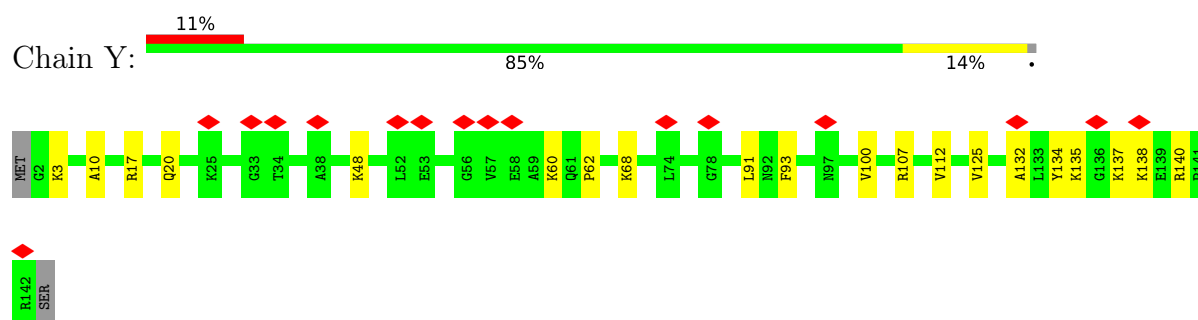
- Molecule 23: 40S ribosomal protein S21



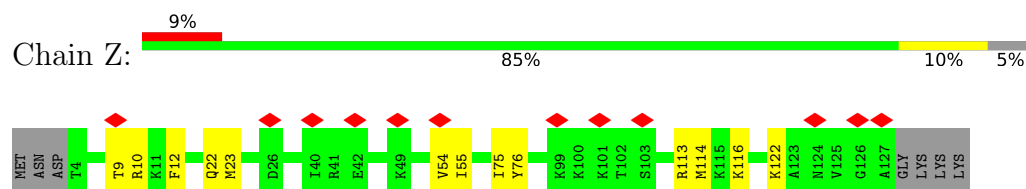
- Molecule 24: uS8



- Molecule 25: uS12

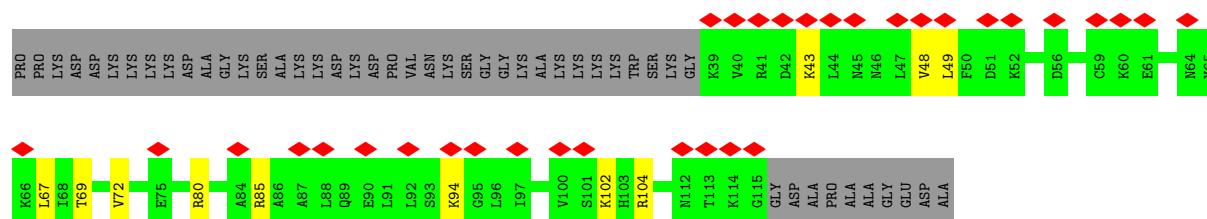


- Molecule 26: 40S ribosomal protein S24

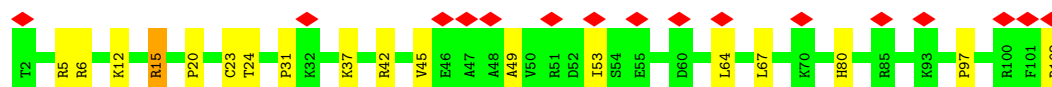
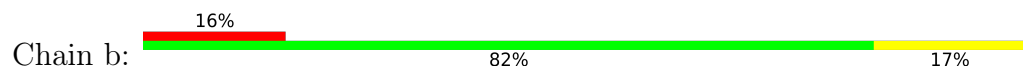


- Molecule 27: 40S ribosomal protein S25

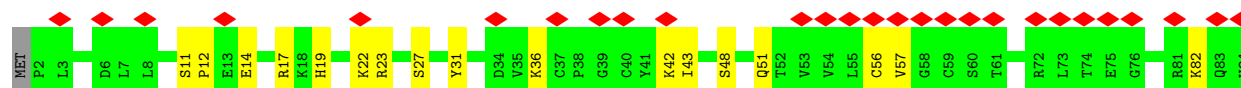
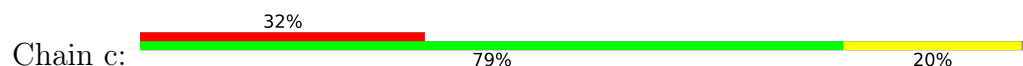




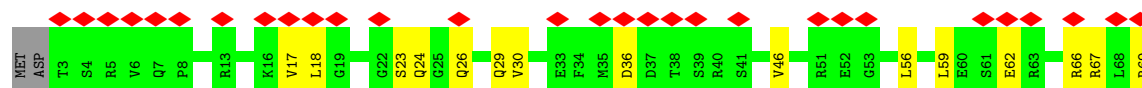
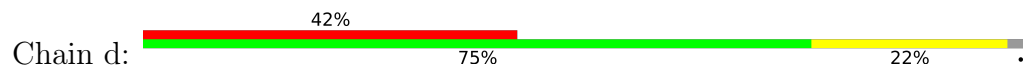
• Molecule 28: eS26 (S26)



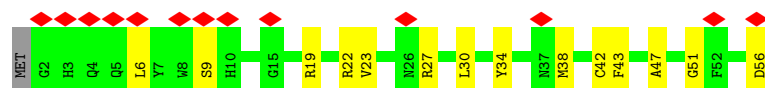
• Molecule 29: eS27



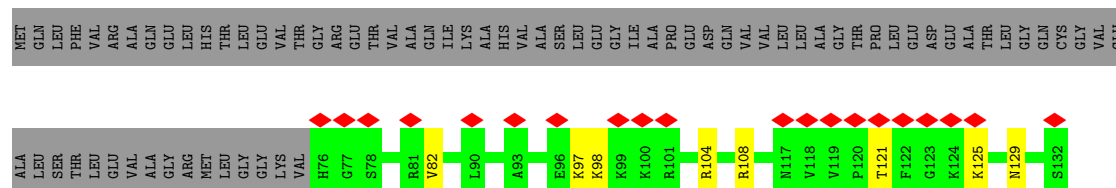
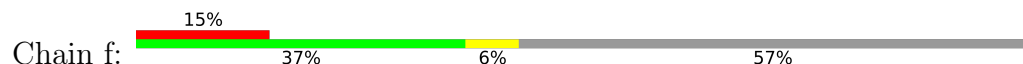
• Molecule 30: eS28



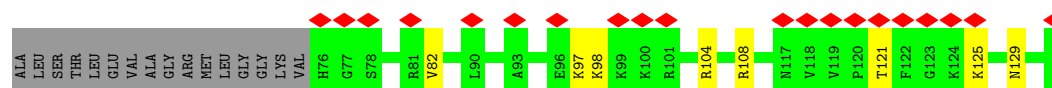
• Molecule 31: eS29



• Molecule 32: eS30



• Molecule 33: 40S ribosomal protein S27a



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

GLU
 ASP
 HIS
 HIS
 ALA
 ARG
 GLY
 ILE
 PRO
 SER
 ASP
 GLN
 ARG
 LEU
 ILE
 PHE
 ALA
 GLY
 LYS
 THR
 SER
 ASP
 TYR
 ASN
 ILE
 GLN
 LYS
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 SER
 THR
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 HIS
 LEU
 VAL
 LEU
 ARG
 LEU
 ARG
 TRP
 ALA
 GLY
 ARG
 HIS
 LYS
 ASP
 ALA
 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:

MET
 T2
 E3
 Q4
 R6
 G9
 T10
 L11
 V18
 T19
 Q20
 P25
 D29
 K30
 T31
 L32
 S33
 A34
 S35
 R36
 D37
 K38
 T39
 T40
 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
 L106
 D107
 V108
 S115
 D116
 N117
 R118
 Q119
 I120
 S122
 G123
 S124
 R125
 D126
 K127
 W132
 N133
 T134
 V137
 C138
 K139
 Y140
 Q143
 D144
 E145
 S146
 H147
 S148
 S152
 R155
 S160
 N161
 N162
 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
 S208
 S209
 G210
 G211
 K212
 D213
 G214
 D220
 L221
 N222
 E223
 G224
 K225
 L230
 D231
 G232
 D233
 D234
 I235
 A238
 P243
 N244
 R245
 Y246
 V247
 L248
 C249
 T252
 I256
 K257
 I258
 W259
 D260
 L261
 E262
 G263
 K264
 L265
 I266
 L270
 K271
 Q272
 E273
 V274
 L275
 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:

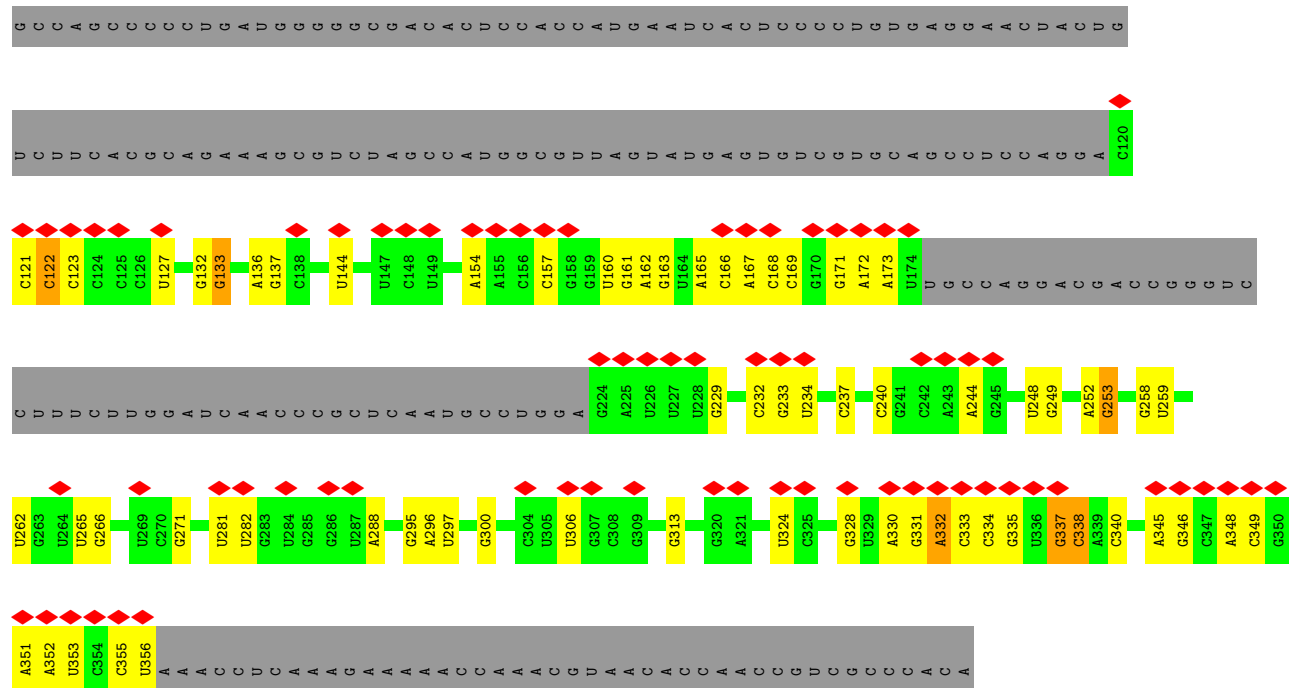
A1
 G2
 C3
 A4
 G5
 A6
 G7
 U8
 G9
 G10
 C11
 G12
 C13
 A14
 G15
 C16
 G17
 G18
 A19
 A20
 G21
 C22
 G23
 U24
 G25
 C32
 C40
 A43
 G44
 G45
 U46
 C47
 G48
 A49
 U50
 G51
 G52
 A53
 U54
 C55
 G56
 A57
 A58
 A59
 C60
 C61
 A62
 U63
 C64
 C65
 U66
 C67
 U68
 G69
 C70
 U71
 A72
 C73
 C74
 A75

• Molecule 36: 60s ribosomal protein l41

Chain n:

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

The worst 5 of 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

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
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.

The worst 5 of 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

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%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
34	h	162	ASN
34	h	187	ASN
13	M	11	GLN
12	L	50	GLN
34	h	222	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%)

5 of 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
1	2	41	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1137	U
1	2	1395	C
1	2	1637	A
1	2	688	U
1	2	752	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

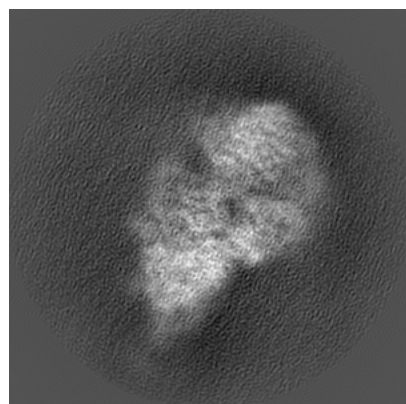
6 Map visualisation [i](#)

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

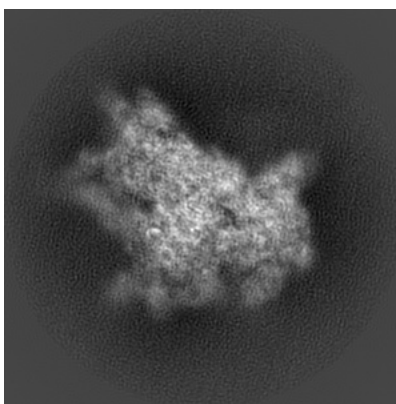
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

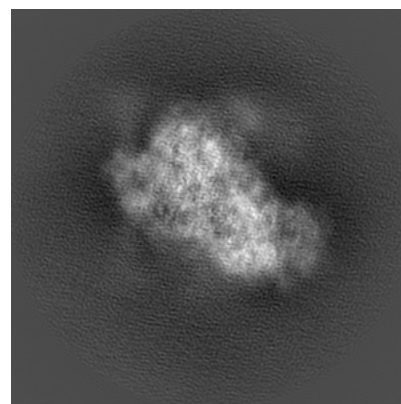
6.1.1 Primary map



X

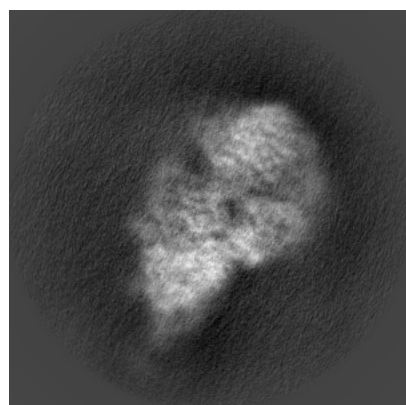


Y

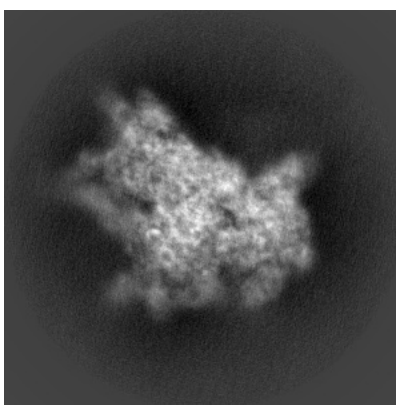


Z

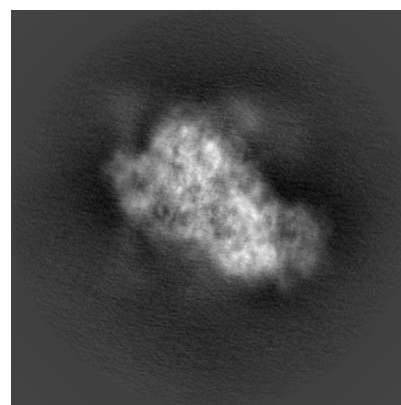
6.1.2 Raw map



X



Y

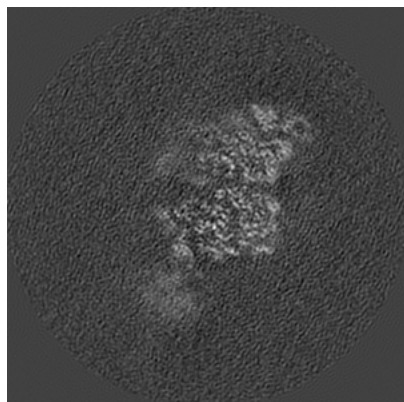


Z

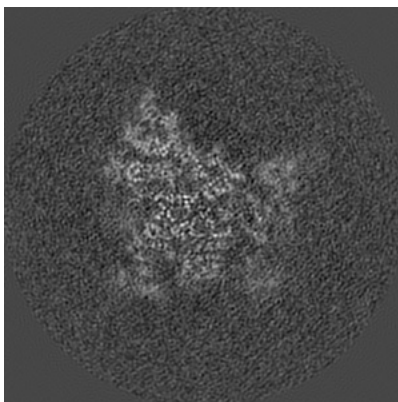
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

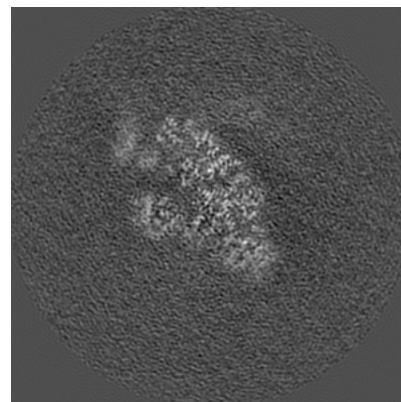
6.2.1 Primary map



X Index: 200

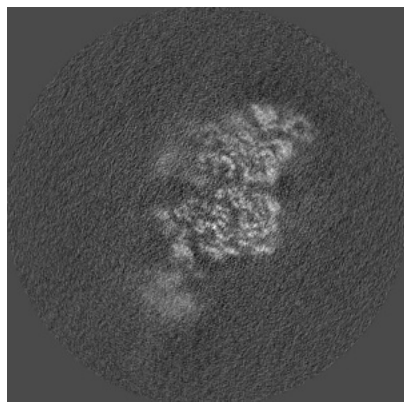


Y Index: 200

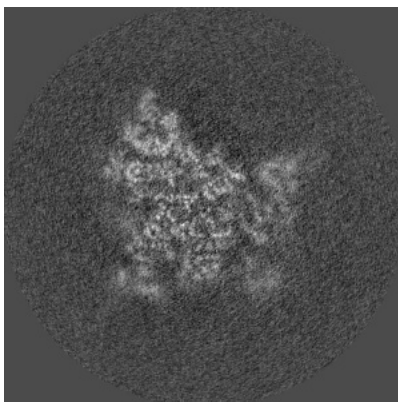


Z Index: 200

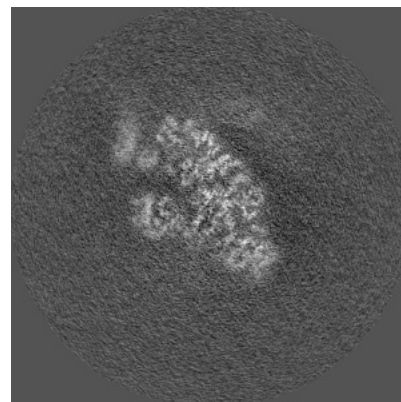
6.2.2 Raw map



X Index: 200



Y Index: 200

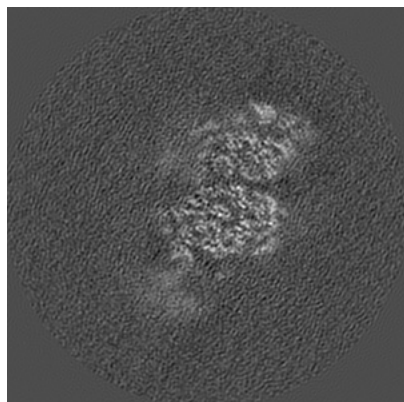


Z Index: 200

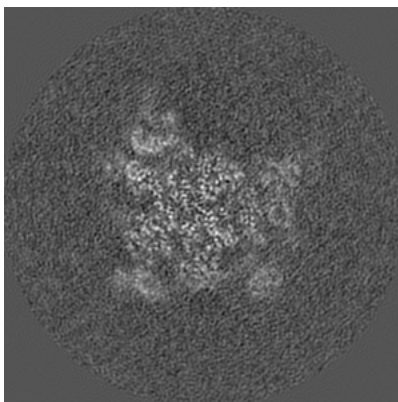
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

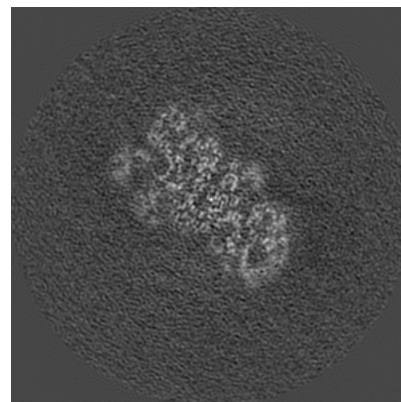
6.3.1 Primary map



X Index: 198

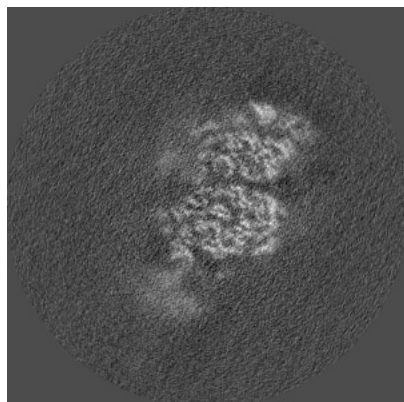


Y Index: 204

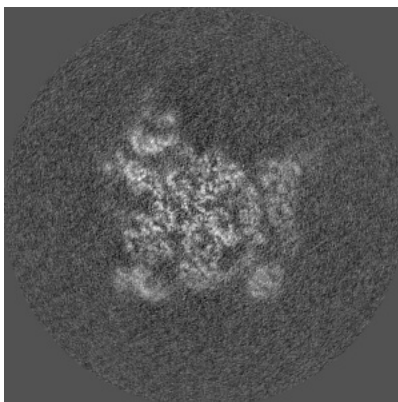


Z Index: 179

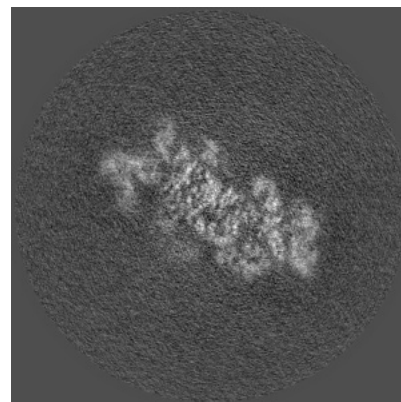
6.3.2 Raw map



X Index: 198



Y Index: 205

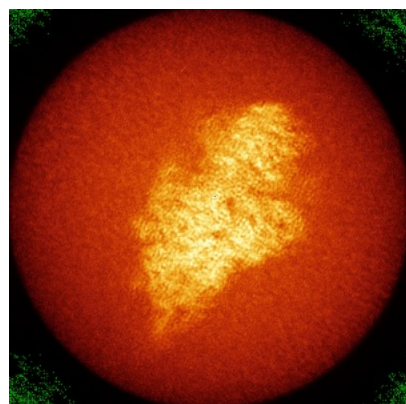


Z Index: 155

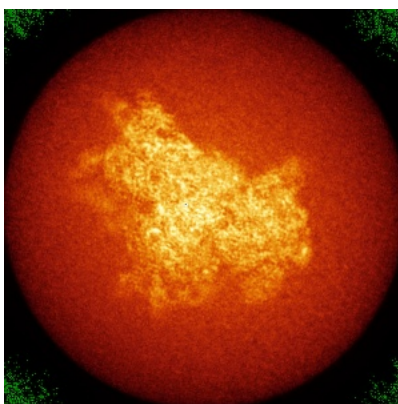
The images above show the largest variance slices of the map in three orthogonal directions.

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

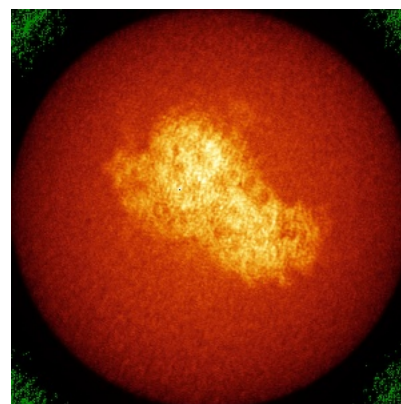
6.4.1 Primary map



X

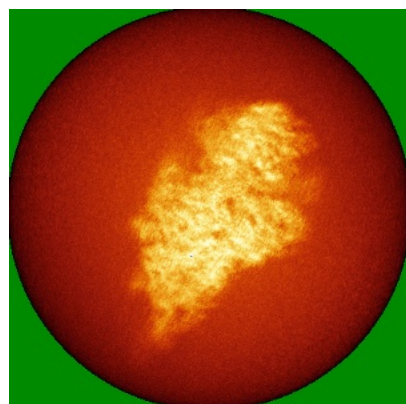


Y

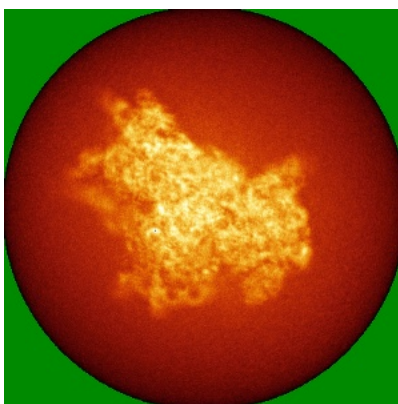


Z

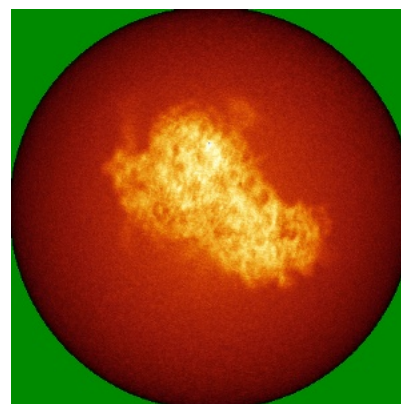
6.4.2 Raw map



X



Y

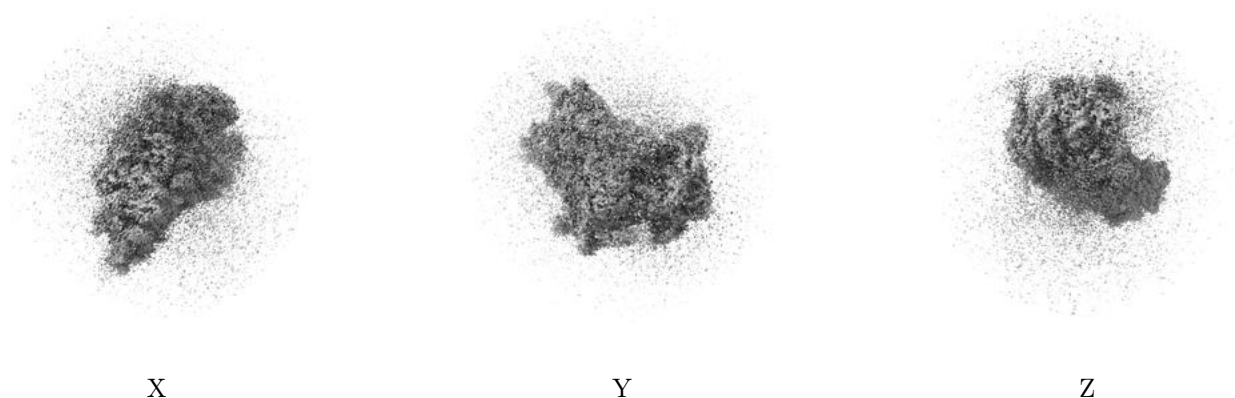


Z

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.

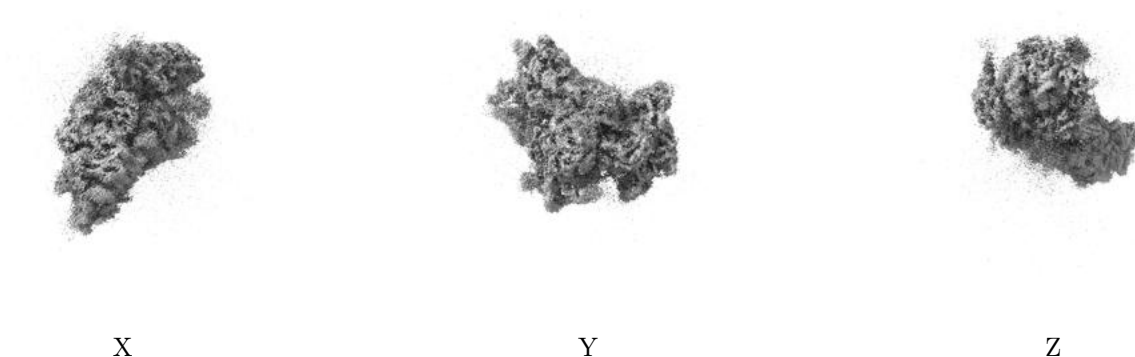
6.5 Orthogonal surface views [i](#)

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.

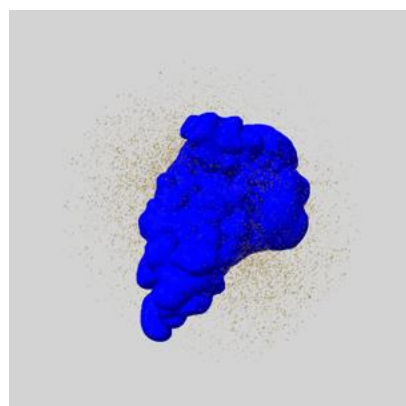
6.6 Mask visualisation [i](#)

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

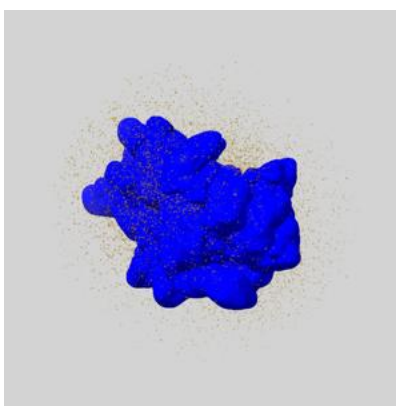
A mask typically either:

- 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

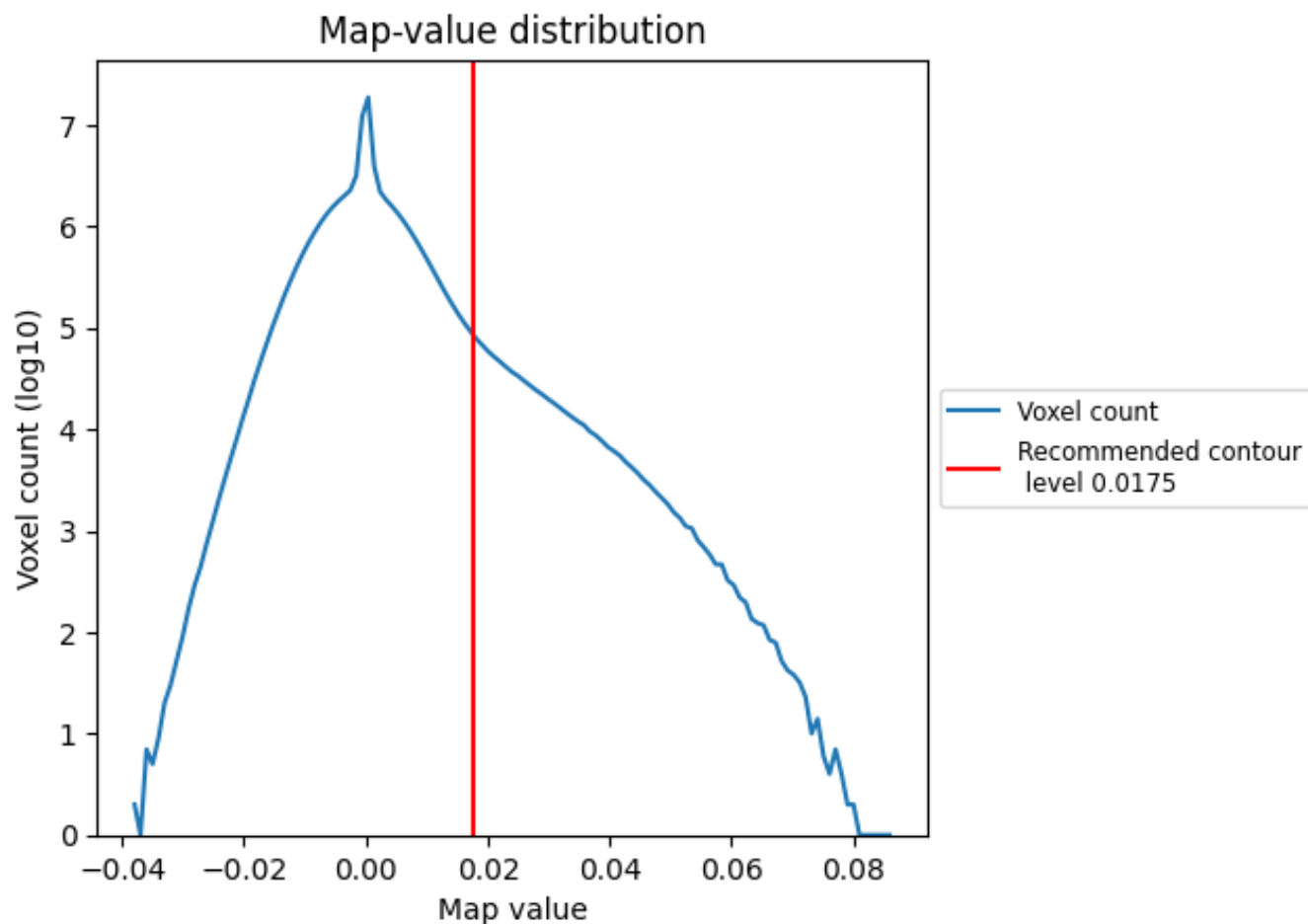


Z

7 Map analysis [i](#)

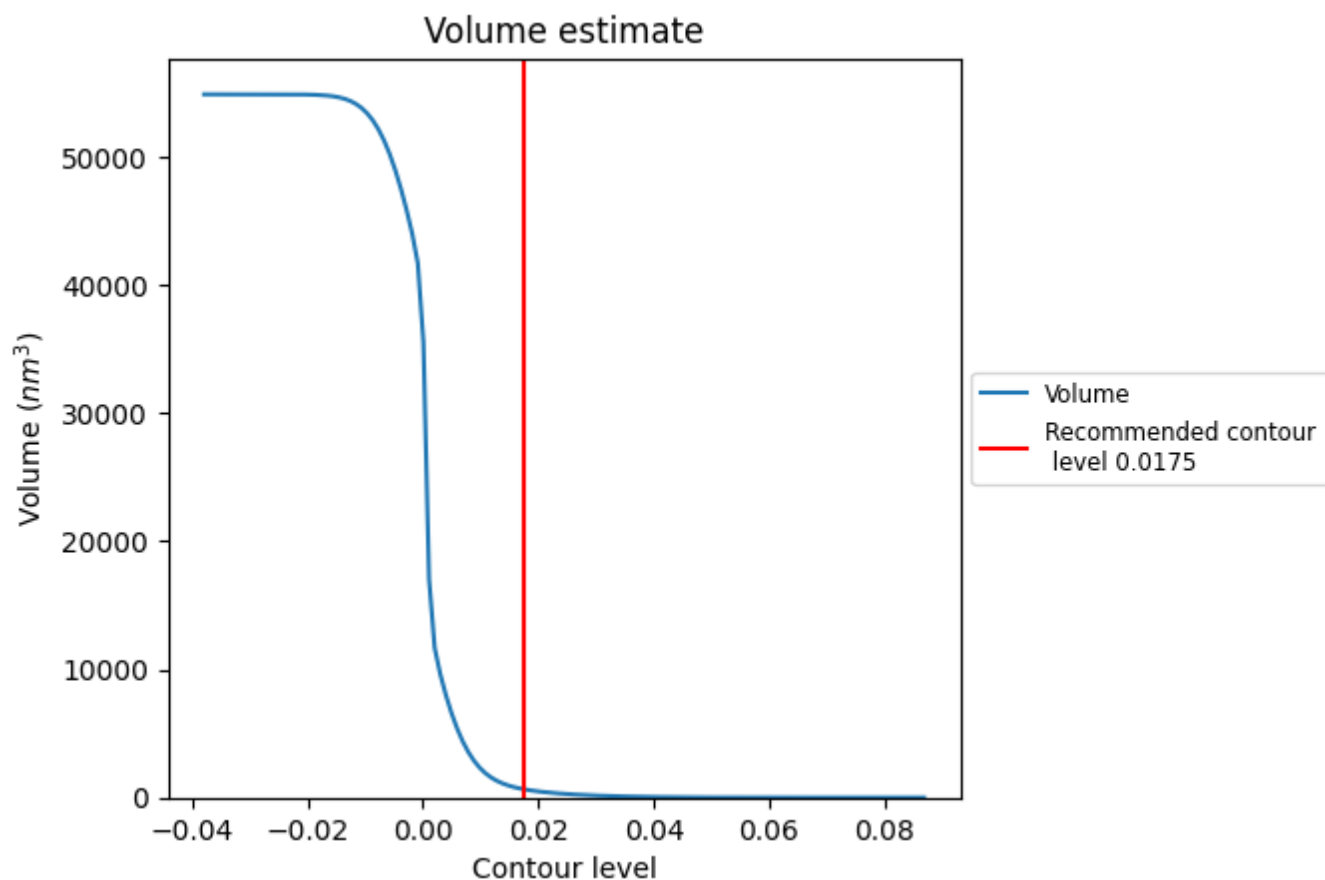
This section contains the results of statistical analysis of the map.

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.

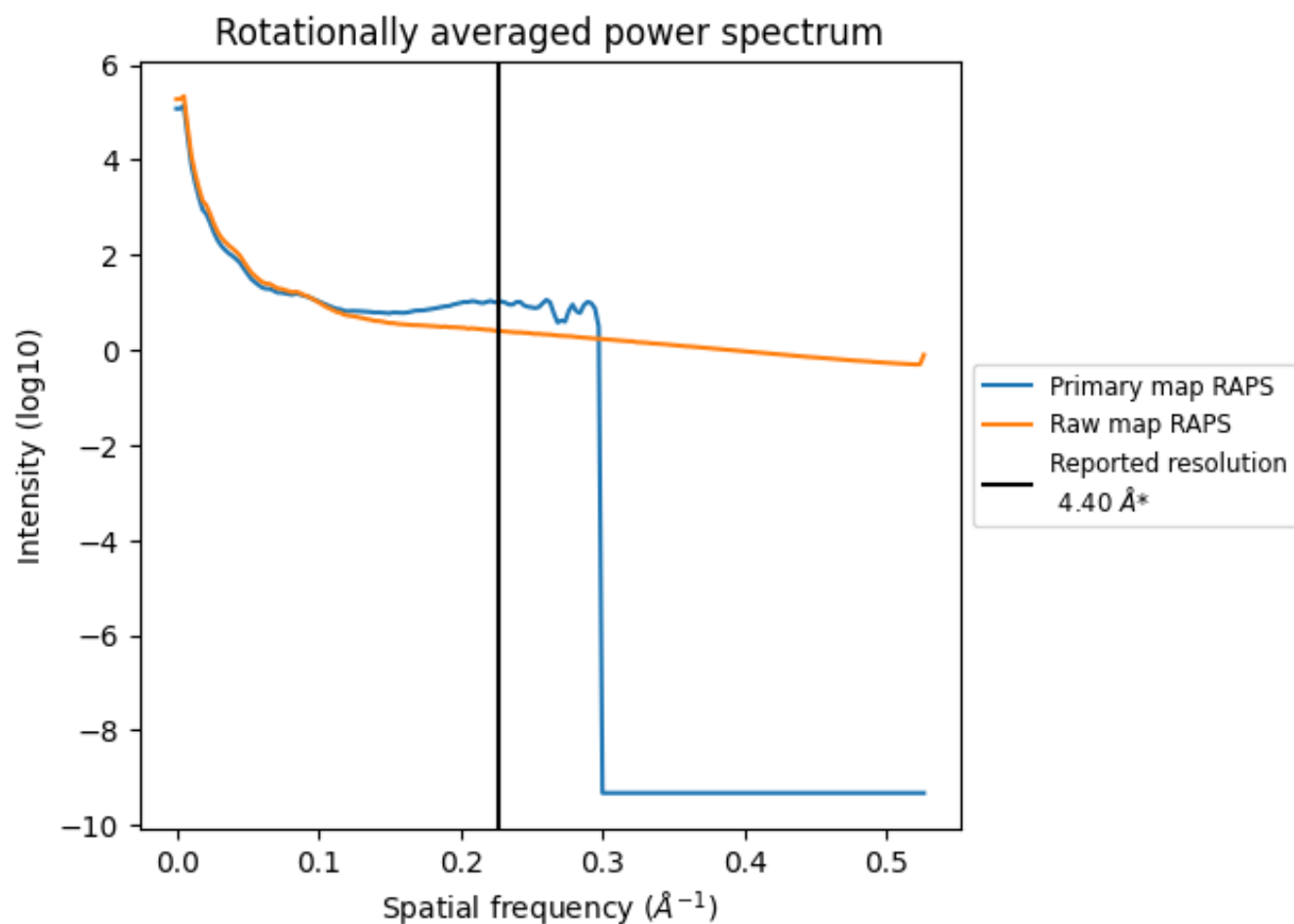
7.2 Volume estimate [i](#)



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 ⓘ

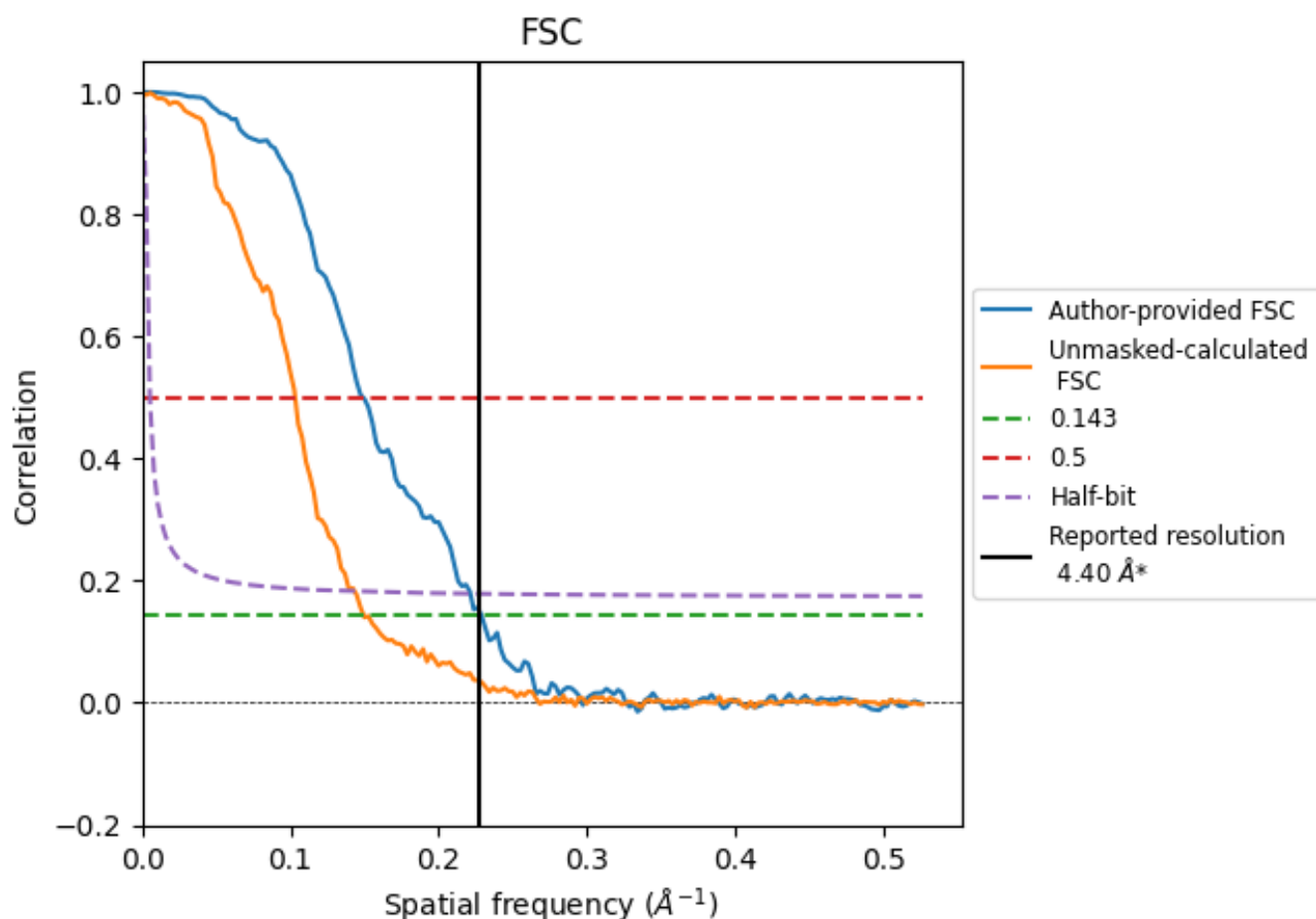


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

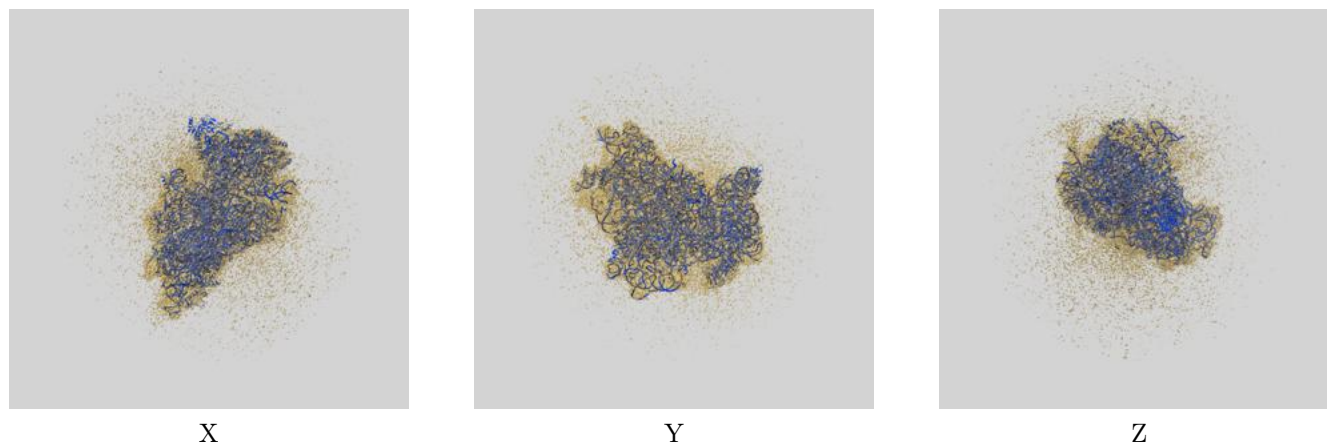
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.37	6.72	4.52
Unmasked-calculated*	6.69	9.69	6.97

*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](#)

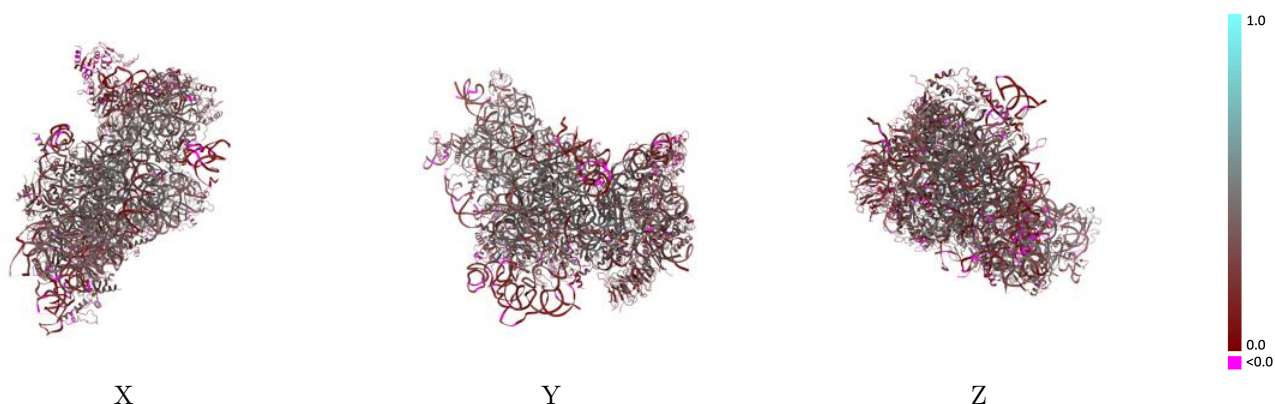
This section contains information regarding the fit between EMDB map EMD-25540 and PDB model 7SYT. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



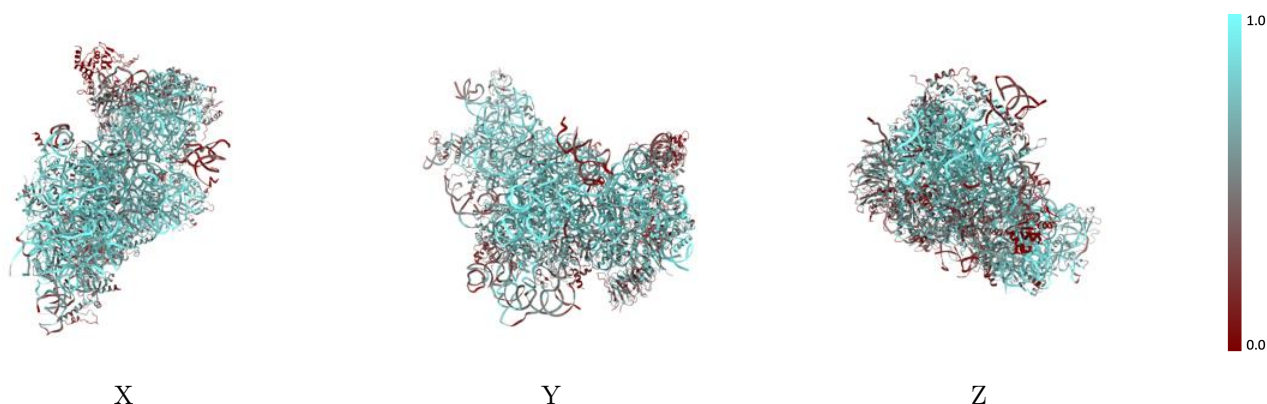
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



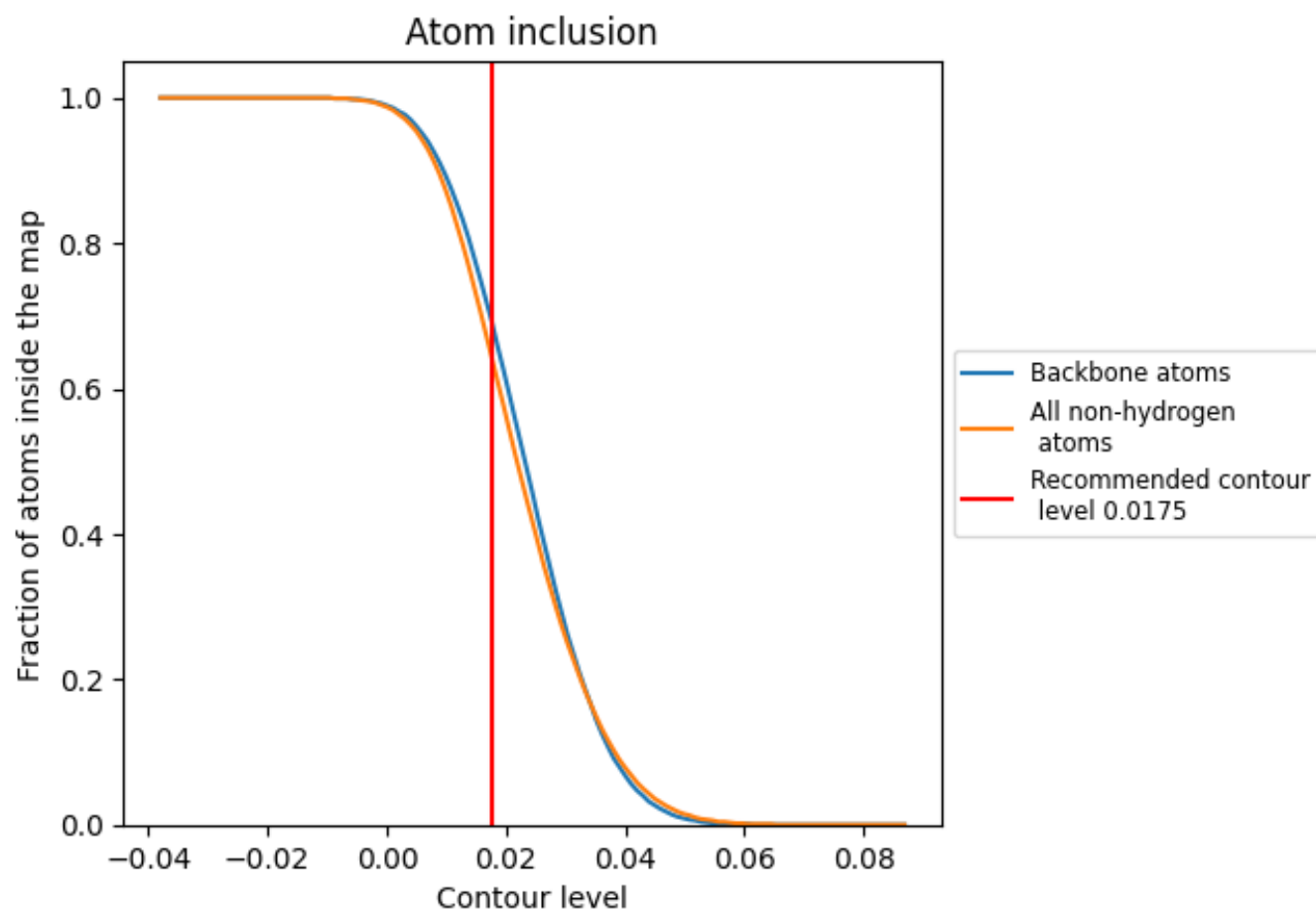
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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