wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 03:24 am BST

PDB ID	:	6SW9
EMDB ID	:	EMD-10320
Title	:	IC2A model of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in P. abyssi
Authors	:	Coureux, P.-D.; Mechulam, Y.; Schmitt, E.
Deposited on	:	2019-09-20
Resolution	:	4.20 Å(reported)

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:

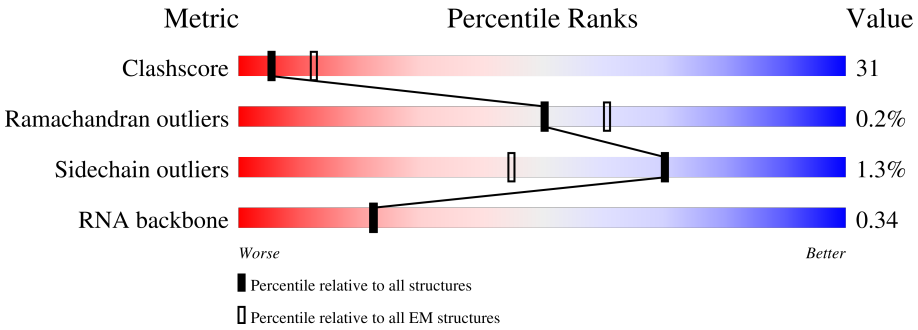
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1497	10% 52% 33% 5%
2	A	199	46% 48% 6%
3	B	202	57% 40%
4	C	63	54% 43%
5	D	180	44% 50%
6	E	243	60% 40%
7	F	236	53% 43%

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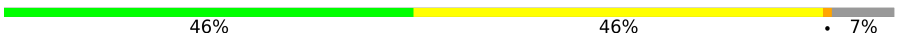
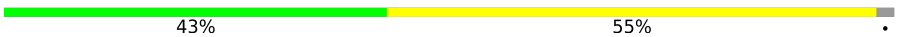
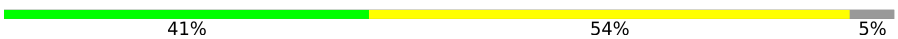
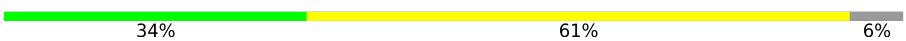
Mol	Chain	Length	Quality of chain
8	G	125	
9	H	215	
10	I	130	
11	J	127	
12	K	135	
13	L	102	
14	M	137	
15	N	147	
16	O	148	
17	P	56	
18	Q	158	
19	R	113	
20	S	67	
21	T	132	
22	U	150	
23	V	99	
24	W	65	
25	X	71	
26	Y	51	
27	Z	210	
28	0	36	
29	3	123	
30	5	20	
31	4	76	
32	6	113	

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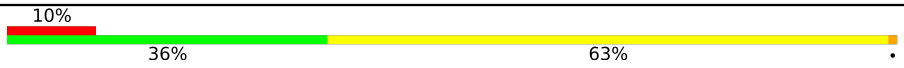
Mol	Chain	Length	Quality of chain
33	7	414	
34	8	129	
35	9	254	

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 70661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1497	32291	14394	5959	10441	1497	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	188	1533	995	268	266	4	0	0

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	196	1571	1017	269	281	4	0	0

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	61	482	304	85	85	8	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	175	1470	924	284	258	4	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	242	1983	1281	358	339	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	213	Total	C	N	O	S	0	0
			1720	1092	322	299	7		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	J	126	Total	C	N	O	0	0
			996	617	206	173		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	134	Total	C	N	O	S	0	0
			1065	668	206	188	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			817	507	158	148	4		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	128	Total	C	N	O	S	0	0
			964	597	192	173	2		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	138	Total	C	N	O	S	0	0
			1116	700	221	190	5		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	152	Total	C	N	O	S	0	0
			1262	804	240	214	4		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	109	Total	C	N	O	S	0	0
			900	572	174	151	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	66	Total	C	N	O	S	0	0
			558	355	106	96	1		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	125	Total	C	N	O	S	0	0
			1018	647	195	169	7		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	149	Total	C	N	O	0	0
			1223	790	221	212		

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	63	Total	C	N	O	S	0	0
			481	303	93	80	5		

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	67	Total	C	N	O	0	0
			536	327	111	98		

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	50	Total	C	N	O	S	0	0
			408	262	77	63	6		

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	197	Total	C	N	O	S	0	0
			1550	989	286	271	4		

- Molecule 28 is a protein called 50S ribosomal protein L41e.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	123	Total	C	N	O	S	0	0
			941	599	157	181	4		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 31 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	76	Total	C	N	O	P	S	0	0
			1622	724	291	530	76	1		

- Molecule 32 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 33 is a protein called Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	414	Total	C	N	O	S	0	0
			3213	2058	548	595	12		

- Molecule 34 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	129	Total	C	N	O	S	0	0
			1032	659	171	192	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	?	-	GLU	deletion	UNP Q97W59
8	?	-	LYS	deletion	UNP Q97W59
8	?	-	GLY	deletion	UNP Q97W59
8	?	-	ARG	deletion	UNP Q97W59
8	?	-	LYS	deletion	UNP Q97W59
8	?	-	GLU	deletion	UNP Q97W59
8	?	-	GLY	deletion	UNP Q97W59
8	?	-	THR	deletion	UNP Q97W59

- Molecule 35 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	253	Total	C	N	O	S	0	0
			2025	1296	345	383	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	?	-	SER	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	TRP	deletion	UNP Q97Z79
9	?	-	VAL	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	HIS	deletion	UNP Q97Z79
9	?	-	ALA	deletion	UNP Q97Z79
9	?	-	GLU	deletion	UNP Q97Z79
9	?	-	GLU	deletion	UNP Q97Z79

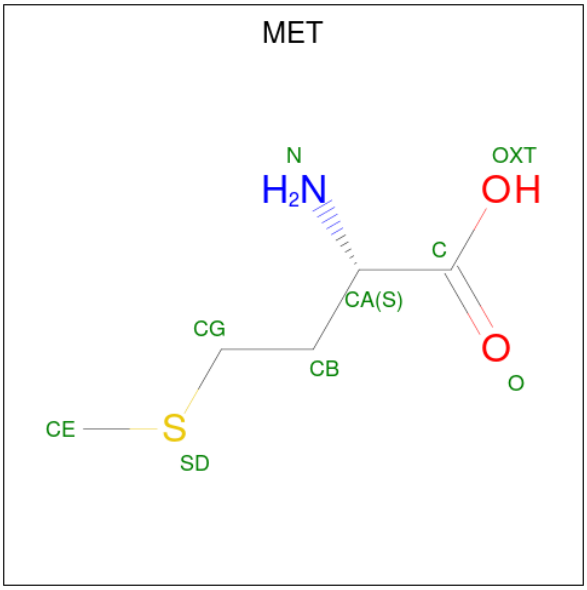
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	31	Total	Mg	0
			31	31	
36	5	1	Total	Mg	0
			1	1	
36	4	1	Total	Mg	0
			1	1	
36	7	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

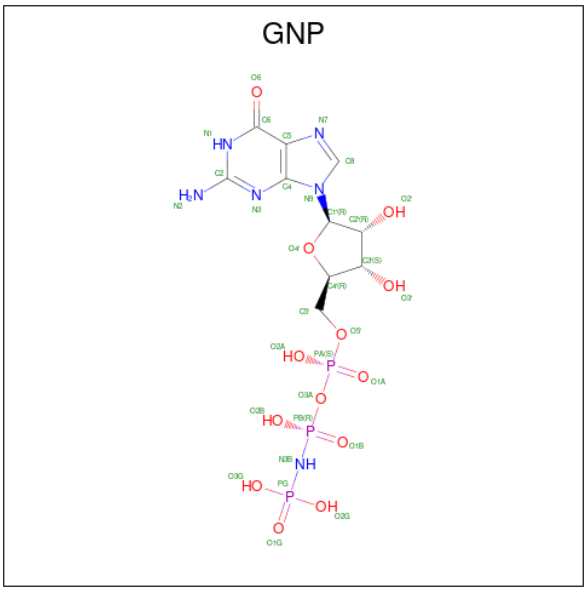
Mol	Chain	Residues	Atoms	AltConf
37	C	2	Total Zn 2 2	0
37	F	1	Total Zn 1 1	0
37	P	1	Total Zn 1 1	0
37	R	1	Total Zn 1 1	0
37	W	1	Total Zn 1 1	0

- Molecule 38 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms	AltConf
38	7	1	Total C N O S 8 5 1 1 1	0

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 40 is water.

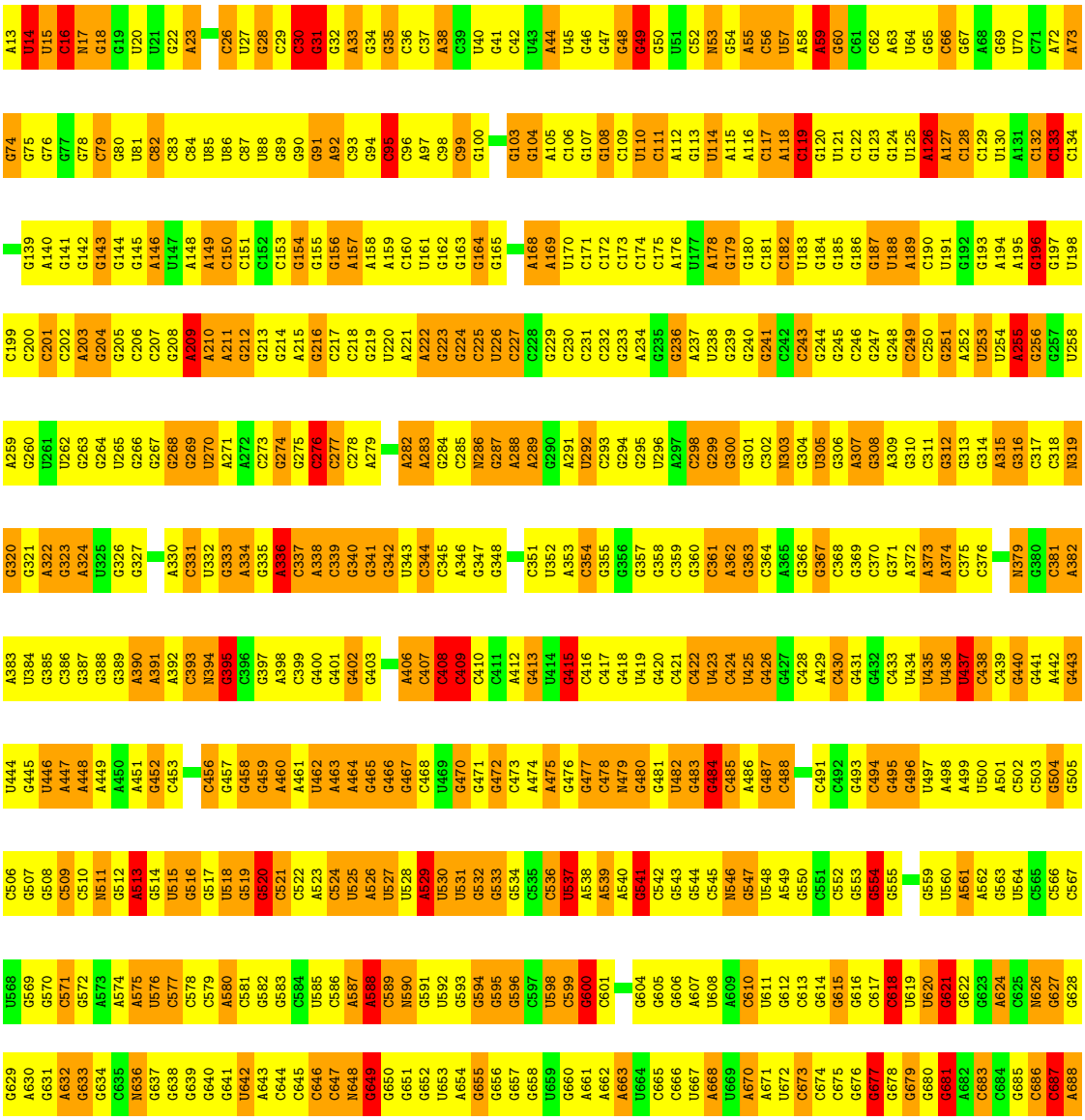
Mol	Chain	Residues	Atoms		AltConf
40	2	40	Total	O	0
			40	40	
40	K	1	Total	O	0
			1	1	
40	Q	1	Total	O	0
			1	1	

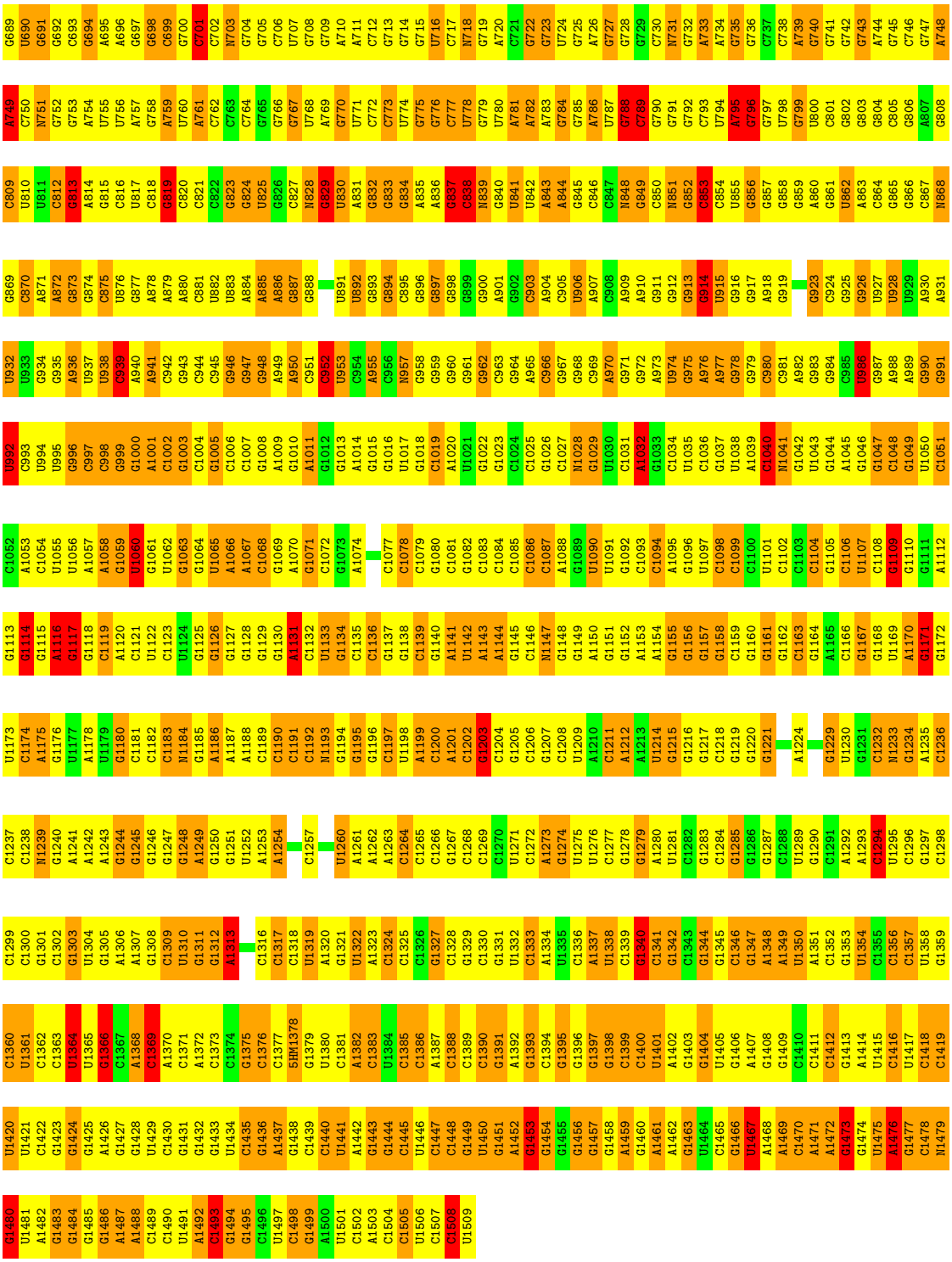
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

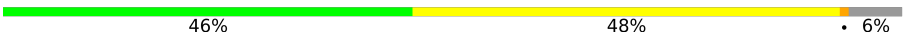
Chain 2: 10% 52% 33% 5%

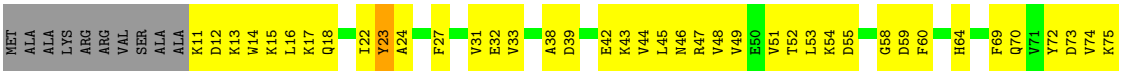


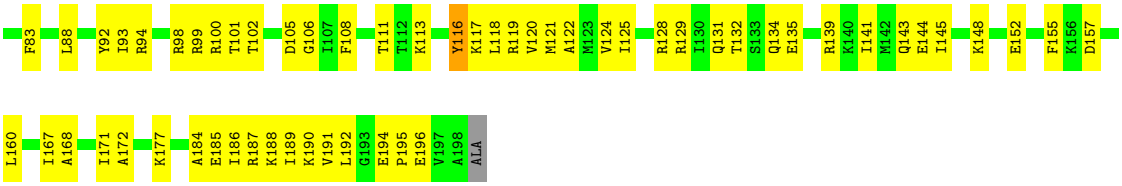


• Molecule 2: 30S ribosomal protein S3Ae

Chain A:

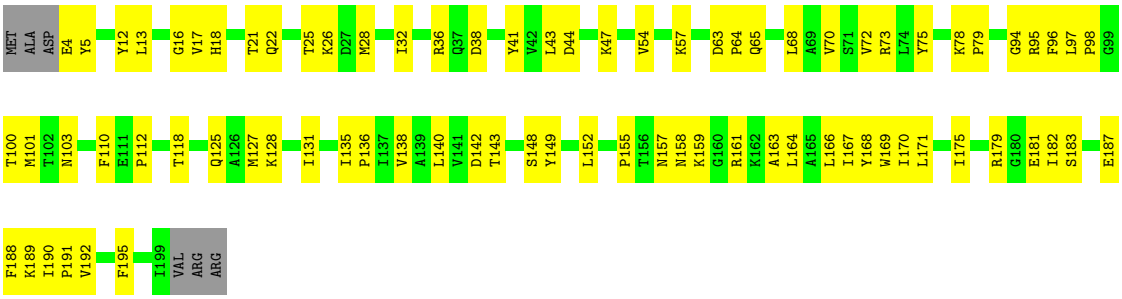






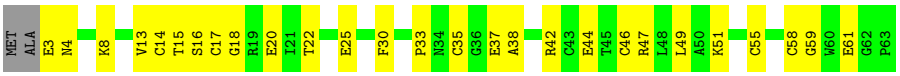
• Molecule 3: 30S ribosomal protein S2

Chain B:



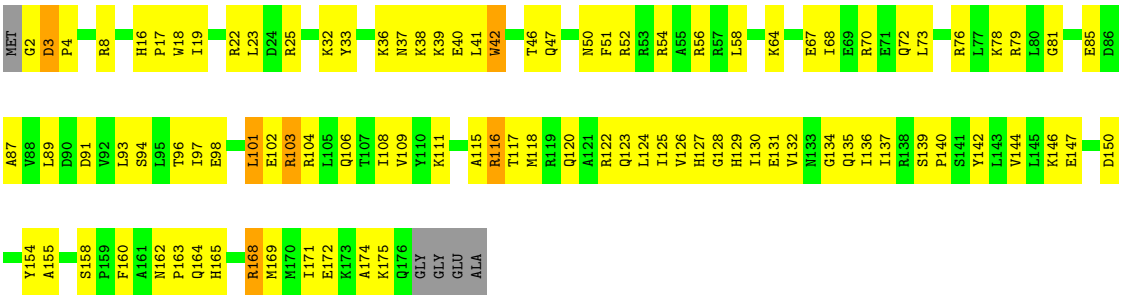
• Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C:



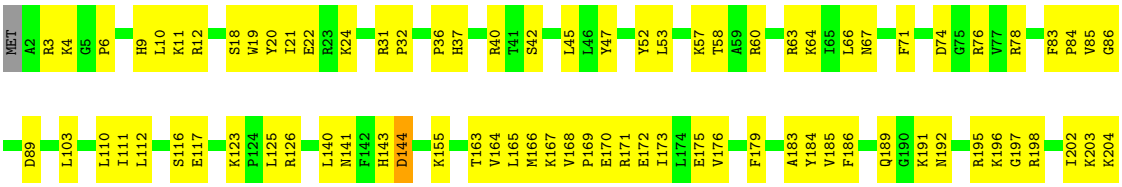
• Molecule 5: 30S ribosomal protein S4

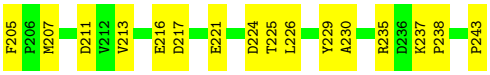
Chain D:



• Molecule 6: 30S ribosomal protein S4e

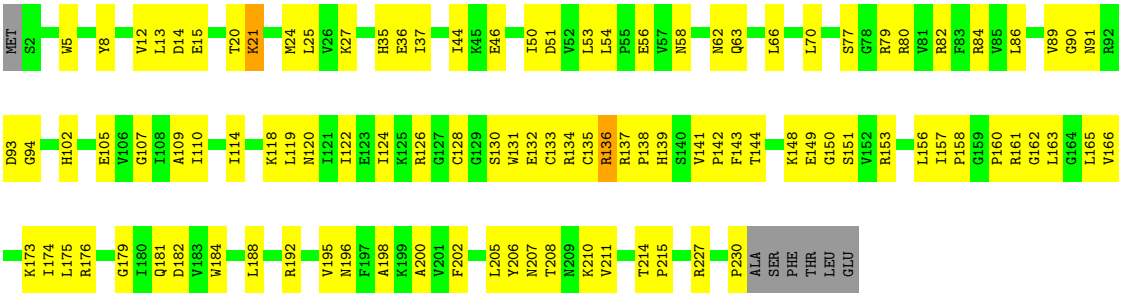
Chain E:





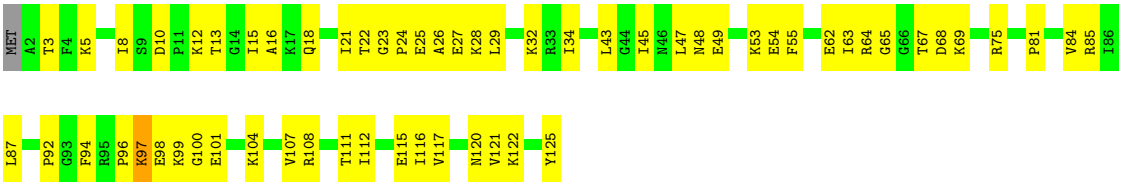
• Molecule 7: 30S ribosomal protein S5

Chain F:



• Molecule 8: 30S ribosomal protein S6e

Chain G:

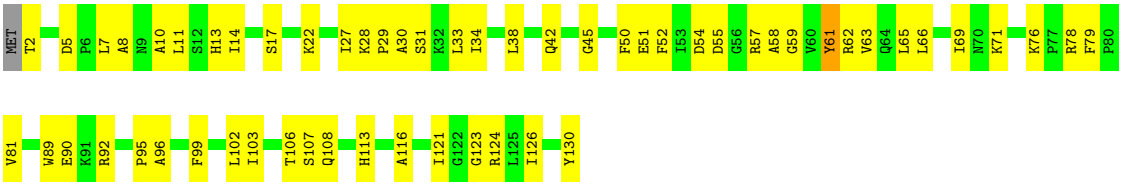


• Molecule 9: 30S ribosomal protein S7

Chain H:

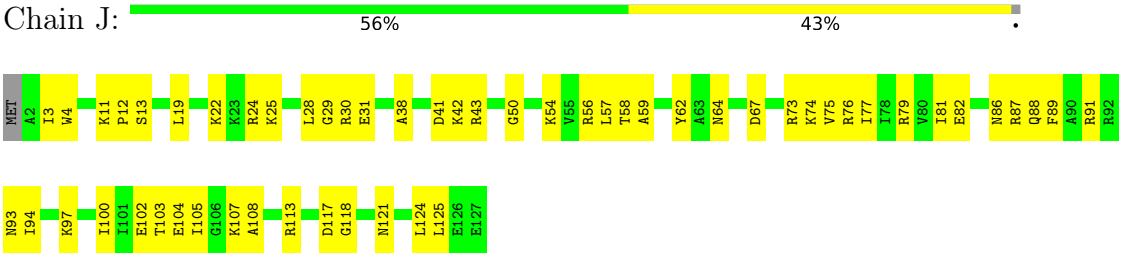
• Molecule 10: 30S ribosomal protein S8

Chain I:



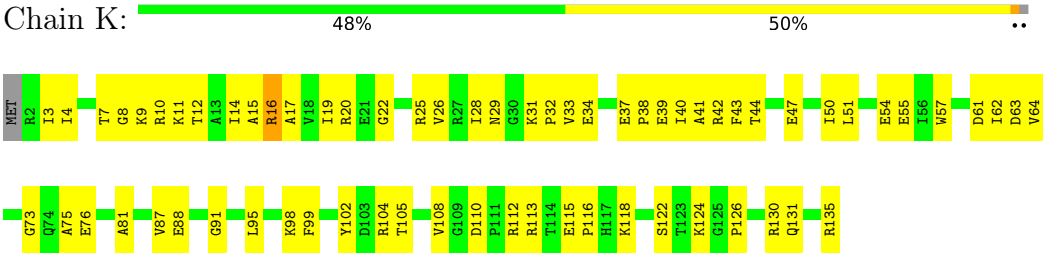
• Molecule 11: 30S ribosomal protein S8e

Chain J:



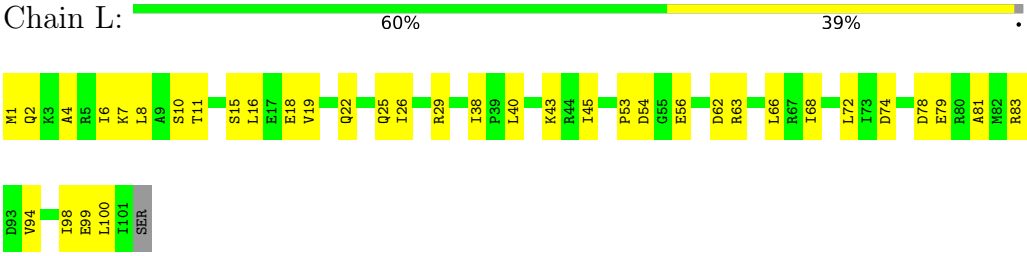
• Molecule 12: 30S ribosomal protein S9

Chain K:



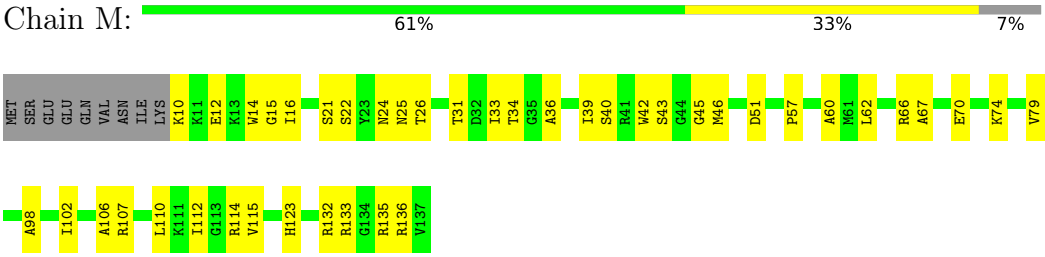
• Molecule 13: 30S ribosomal protein S10

Chain L:



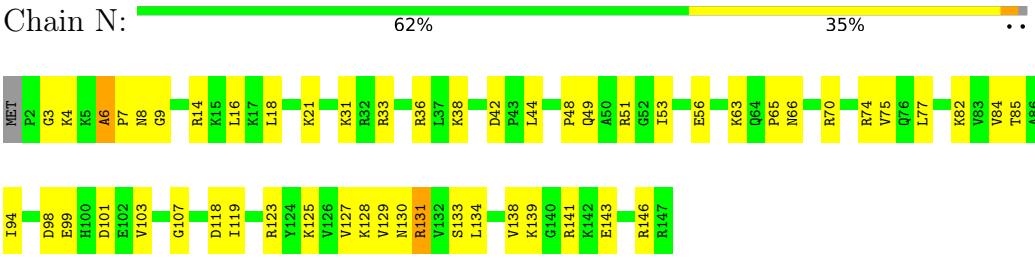
• Molecule 14: 30S ribosomal protein S11

Chain M:



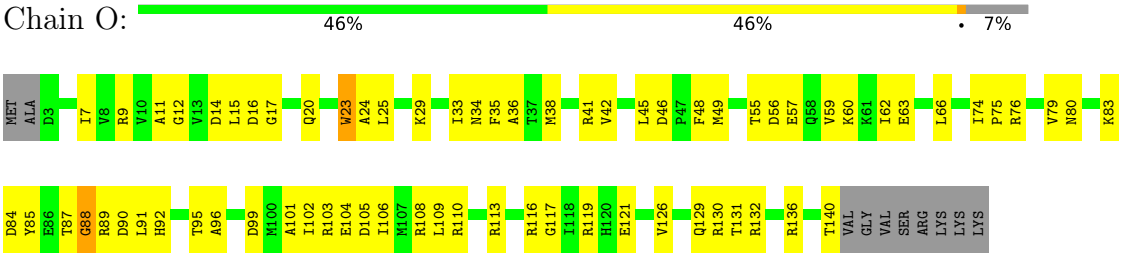
• Molecule 15: 30S ribosomal protein S12

Chain N:



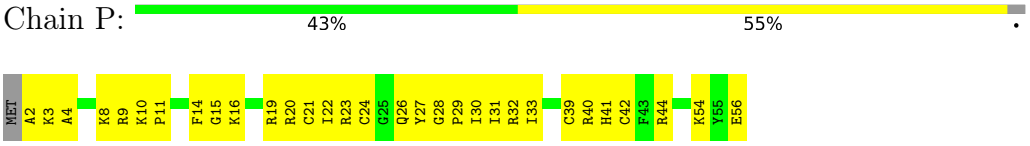
• Molecule 16: 30S ribosomal protein S13

Chain O:



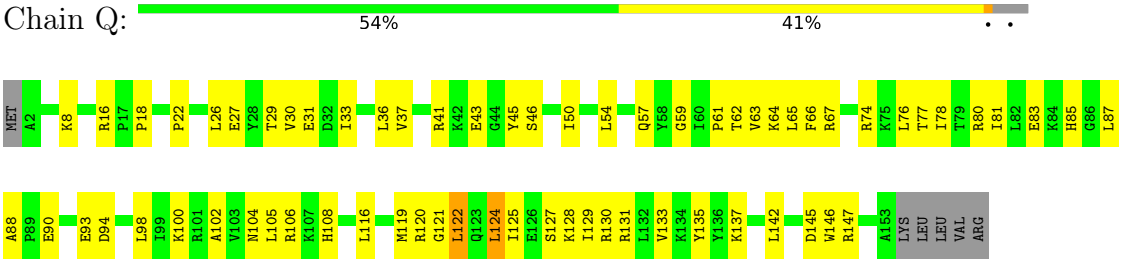
• Molecule 17: 30S ribosomal protein S14 type Z

Chain P:



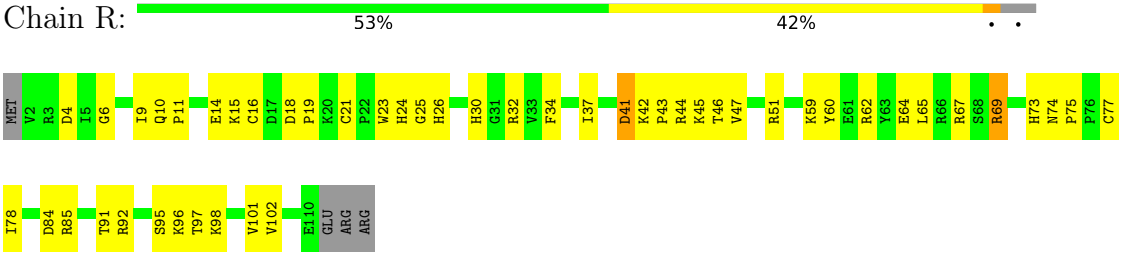
• Molecule 18: 30S ribosomal protein S15

Chain Q:



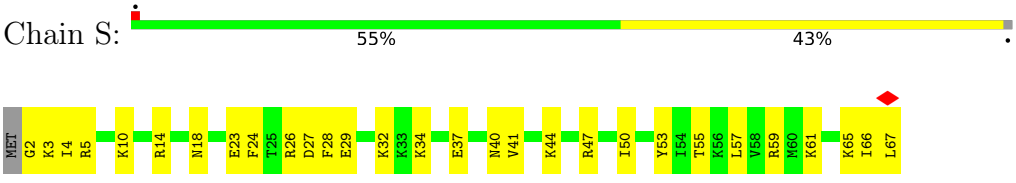
• Molecule 19: 30S ribosomal protein S17

Chain R:



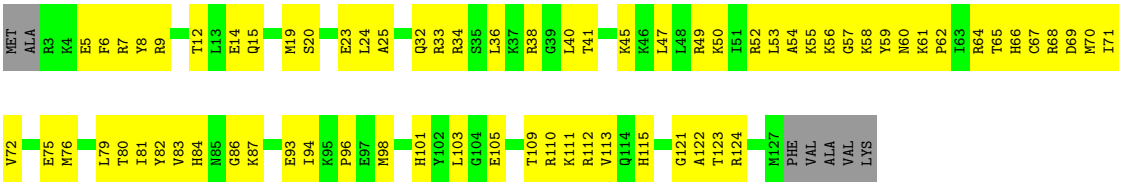
• Molecule 20: 30S ribosomal protein S17e

Chain S:



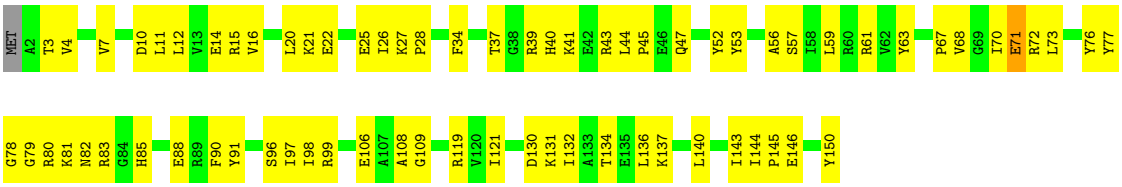
• Molecule 21: 30S ribosomal protein S19

Chain T:



• Molecule 22: 30S ribosomal protein S19e

Chain U:



• Molecule 23: 30S ribosomal protein S24e

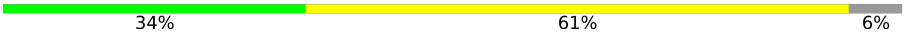
Chain V:

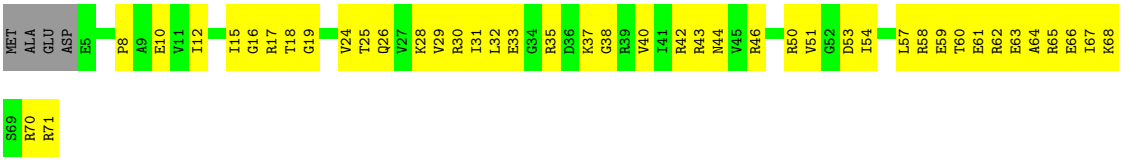
• Molecule 24: 30S ribosomal protein S27e

Chain W:

• Molecule 25: 30S ribosomal protein S28e

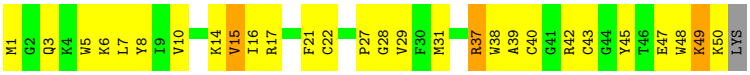
Chain X:





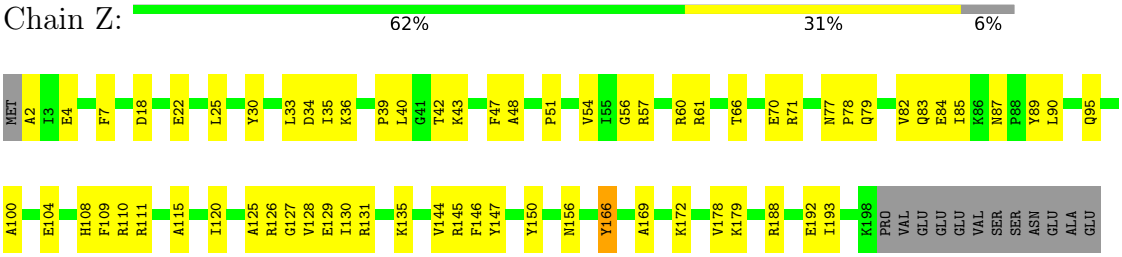
• Molecule 26: 30S ribosomal protein S27ae

Chain Y:



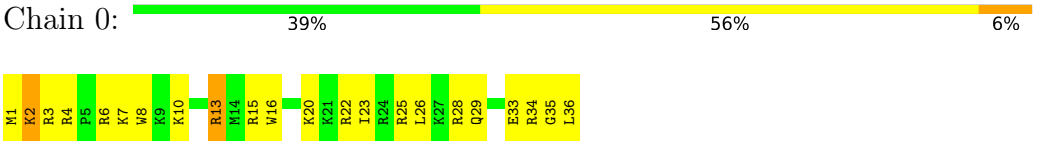
• Molecule 27: 30S ribosomal protein S3

Chain Z:



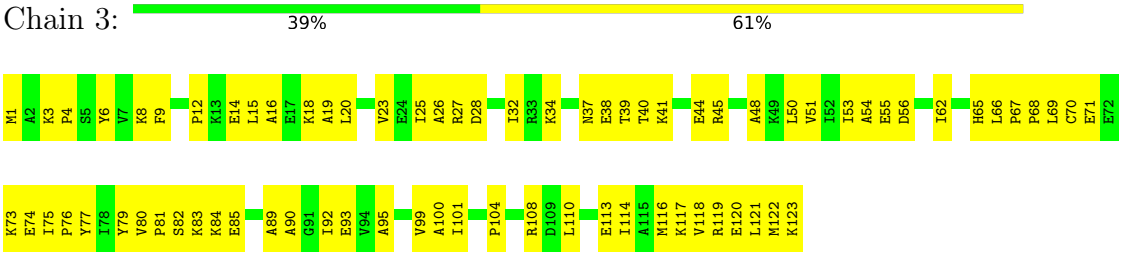
• Molecule 28: 50S ribosomal protein L41e

Chain 0:



• Molecule 29: 50S ribosomal protein L7Ae

Chain 3:

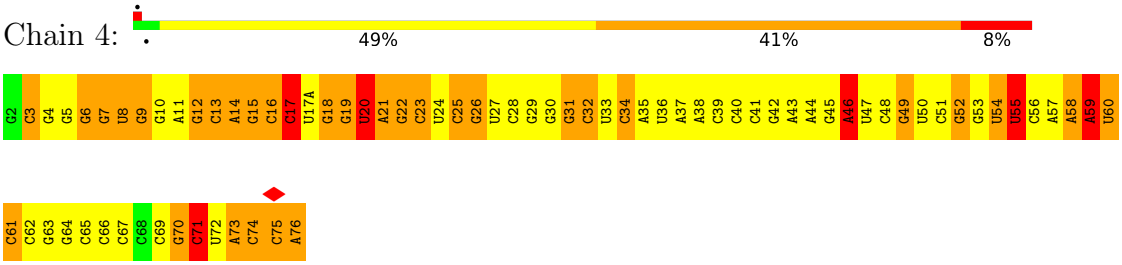


• Molecule 30: mRNA

Chain 5:

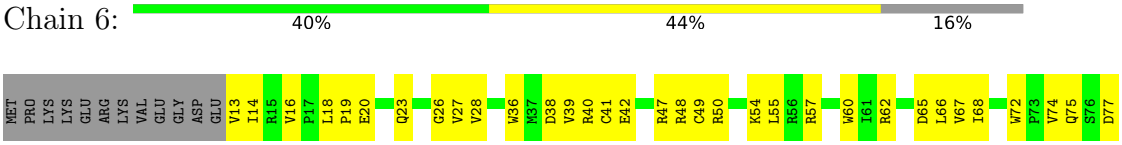
• Molecule 31: initiator Met-tRNA fMet from E. coli (A1U72 variant)

Chain 4:



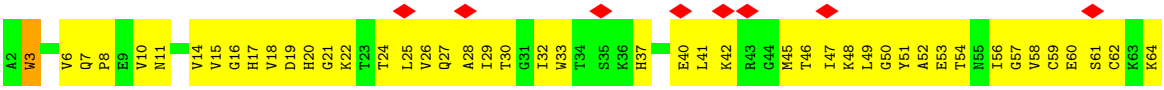
• Molecule 32: Translation initiation factor 1A

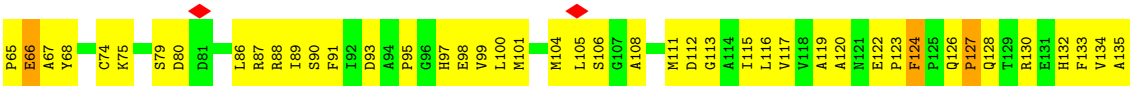
Chain 6:

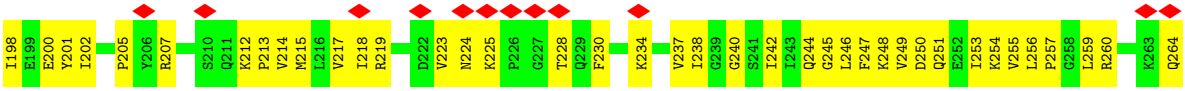


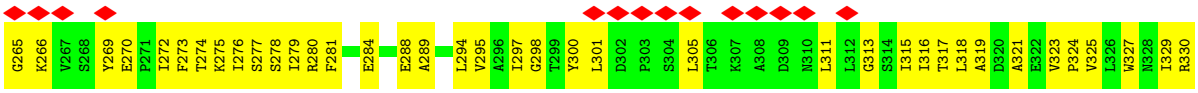
• Molecule 33: Translation initiation factor 2 subunit gamma

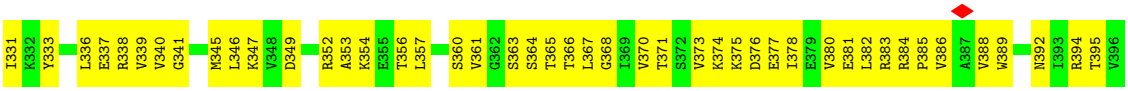
Chain 7:

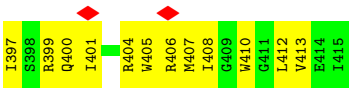






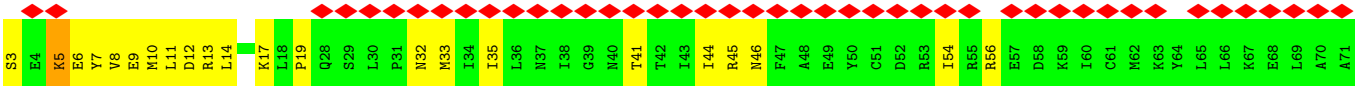


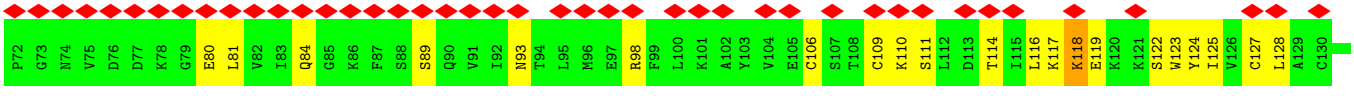


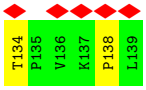


• Molecule 34: Translation initiation factor 2 subunit beta

Chain 8:

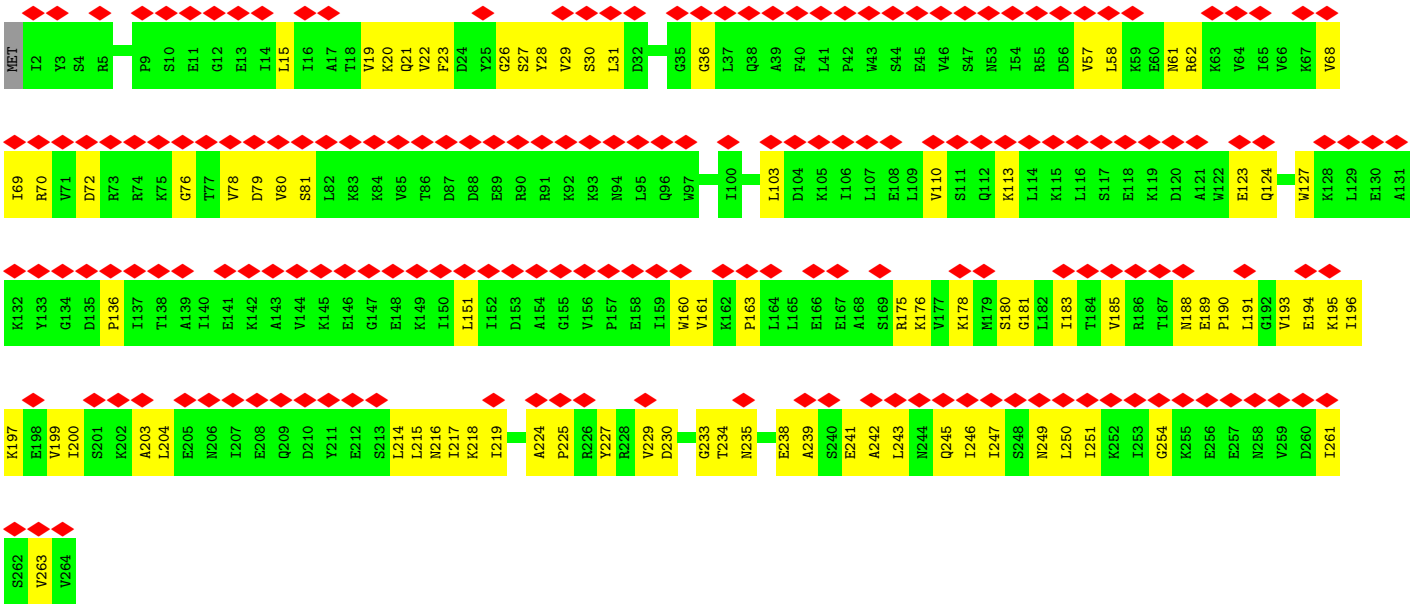






• Molecule 35: Translation initiation factor 2 subunit alpha

Chain 9:


MET I2 Y3 S4 R5 P9 S10 E11 G12 E13 I14 L15 I16 A17 T18 V19 K20 Q21 V22 F23 D24 Y25 G26 S27 Y28 V29 S30 L31 D32 G35 G36 L37 Q38 A39 F40 L41 P42 W43 S44 E45 V46 S47 N53 I54 R55 D56 V57 L58 K59 E60 N61 R62 K63 V64 I65 V66 K67 V68
I69 R70 V71 D72 R73 R74 K75 G76 T77 V78 D79 V80 S81 L82 K83 K84 V85 T86 D87 D88 E89 R90 R91 K92 K93 N94 L95 Q96 W97 I100 L103 D104 K105 I106 L107 E108 L109 V110 S111 Q112 K113 L114 K115 L116 S117 E118 K119 D120 A121 W122 E123 Q124 W127 K128 L129 E130 A131
K132 Y133 G134 D135 P136 I137 T138 A139 I140 E141 K142 A143 V144 K145 E146 G147 E148 K149 I150 L151 I152 D153 A154 G155 V156 P157 E158 I159 W160 V161 K162 P163 L164 L165 E166 E167 A168 S169 R175 K176 V177 K178 M179 S180 G181 L182 I183 T184 V185 R186 T187 N188 E189 P190 L191 G192 V193 E194 K195 I196
K197 E198 V199 I200 S201 K202 A203 L204 E205 N206 I207 E208 Q209 D210 Y211 E212 S213 L214 L215 N216 I217 K218 I219 A224 P225 R226 Y227 R228 V229 D230 G233 T234 N235 E238 A239 S240 E241 A242 L243 N244 Q245 I246 I247 S248 N249 L250 I251 K252 I253 G254 K255 E256 E257 N258 V259 D260 I261
S262 V263 V264

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	379.32, 379.32, 379.32	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LHH, 5MU, H2U, GNP, 4SU, PSU, MA6, A2M, ZN, 6MZ, UR3, MG, OMC, 4AC, B8H, 5HM, 5MC

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	1.32	33/35019 (0.1%)	1.41	329/54586 (0.6%)
2	A	0.61	0/1559	0.63	0/2090
3	B	0.56	0/1602	0.61	0/2165
4	C	0.57	0/496	0.60	0/673
5	D	0.63	1/1494 (0.1%)	0.64	1/2003 (0.0%)
6	E	0.62	0/2032	0.64	0/2742
7	F	0.67	0/1838	0.65	0/2478
8	G	0.46	0/993	0.56	0/1329
9	H	0.52	1/1757 (0.1%)	0.61	1/2359 (0.0%)
10	I	0.69	0/1055	0.72	0/1415
11	J	0.51	0/1005	0.65	0/1339
12	K	0.52	0/1081	0.61	0/1449
13	L	0.45	0/825	0.56	0/1107
14	M	0.51	0/982	0.61	0/1322
15	N	0.62	0/1165	0.67	1/1547 (0.1%)
16	O	0.52	1/1135 (0.1%)	0.60	0/1526
17	P	0.55	0/465	0.58	0/613
18	Q	0.54	0/1290	0.61	1/1734 (0.1%)
19	R	0.68	1/923 (0.1%)	0.64	0/1247
20	S	0.51	0/565	0.56	0/747
21	T	0.50	0/1037	0.63	0/1385
22	U	0.55	0/1253	0.60	0/1689
23	V	0.58	0/808	0.61	0/1086
24	W	0.45	0/488	0.60	0/659
25	X	0.49	0/538	0.62	0/719
26	Y	0.40	0/420	0.63	0/559
27	Z	0.50	0/1572	0.62	0/2110
28	0	0.62	0/349	0.65	0/451
29	3	0.37	0/953	0.59	0/1284
30	5	1.02	0/481	1.29	3/748 (0.4%)
31	4	0.90	1/1699 (0.1%)	1.29	15/2648 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	6	0.43	0/793	0.68	0/1072
33	7	0.37	0/3272	0.62	1/4430 (0.0%)
34	8	0.26	0/1045	0.48	0/1400
35	9	0.26	0/2050	0.44	0/2760
All	All	1.00	38/74039 (0.1%)	1.11	352/107471 (0.3%)

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
7	F	0	1
18	Q	0	1
All	All	0	2

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1453	G	C8-N7	-8.66	1.25	1.30
19	R	41	ASP	CA-CB	-8.15	1.36	1.53
1	2	955	A	N9-C4	-7.73	1.33	1.37
1	2	795	A	N9-C4	-7.69	1.33	1.37
1	2	126	A	N9-C4	-7.46	1.33	1.37

The worst 5 of 352 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	825	U	N3-C2-O2	-9.45	115.58	122.20
1	2	26	C	C6-N1-C2	-9.44	116.52	120.30
1	2	1383	C	C2-N1-C1'	9.44	129.18	118.80
1	2	494	C	N3-C2-O2	-9.26	115.42	121.90
1	2	683	C	N3-C4-N4	8.90	124.23	118.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	F	5	TRP	Peptide
18	Q	106	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	32291	0	16316	2022	0
2	A	1533	0	1627	96	0
3	B	1571	0	1630	68	0
4	C	482	0	461	24	0
5	D	1470	0	1542	90	0
6	E	1983	0	2060	75	0
7	F	1808	0	1879	91	0
8	G	977	0	1037	59	0
9	H	1720	0	1775	87	0
10	I	1034	0	1069	57	0
11	J	996	0	1076	53	0
12	K	1065	0	1121	73	0
13	L	817	0	871	32	0
14	M	964	0	994	43	0
15	N	1148	0	1248	43	0
16	O	1116	0	1152	72	0
17	P	455	0	475	29	0
18	Q	1262	0	1331	53	0
19	R	900	0	921	52	0
20	S	558	0	595	31	0
21	T	1018	0	1086	72	0
22	U	1223	0	1263	64	0
23	V	790	0	806	35	0
24	W	481	0	512	20	0
25	X	536	0	571	43	0
26	Y	408	0	413	33	0
27	Z	1550	0	1637	55	0
28	0	343	0	407	24	0
29	3	941	0	994	86	0
30	5	430	0	215	41	0
31	4	1622	0	830	133	0
32	6	777	0	806	52	0
33	7	3213	0	3331	336	0
34	8	1032	0	1073	39	0
35	9	2025	0	2133	76	0
36	2	31	0	0	0	0
36	4	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5	1	0	0	0	0
36	7	1	0	0	0	0
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	W	1	0	0	0	0
38	7	8	0	8	2	0
39	7	32	0	13	4	0
40	2	40	0	0	18	0
40	K	1	0	0	0	0
40	Q	1	0	0	1	0
All	All	70661	0	55278	3872	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 31.

The worst 5 of 3872 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)
1:2:140:A:N6	1:2:229:G:H1	1.36	1.23
33:7:213:PRO:HA	33:7:244:GLN:O	1.39	1.22
33:7:240:GLY:O	33:7:294:LEU:HA	1.57	1.04
1:2:1300:C:OP1	22:U:39:ARG:NH2	1.96	0.97
1:2:465:G:O6	1:2:512:G:N2	1.99	0.95

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	A	186/199 (94%)	157 (84%)	29 (16%)	0	100	100
3	B	194/202 (96%)	162 (84%)	32 (16%)	0	100	100
4	C	59/63 (94%)	43 (73%)	16 (27%)	0	100	100
5	D	173/180 (96%)	140 (81%)	32 (18%)	1 (1%)	25	64
6	E	240/243 (99%)	179 (75%)	60 (25%)	1 (0%)	34	72
7	F	227/236 (96%)	172 (76%)	55 (24%)	0	100	100
8	G	122/125 (98%)	97 (80%)	25 (20%)	0	100	100
9	H	211/215 (98%)	171 (81%)	40 (19%)	0	100	100
10	I	127/130 (98%)	96 (76%)	31 (24%)	0	100	100
11	J	124/127 (98%)	91 (73%)	33 (27%)	0	100	100
12	K	132/135 (98%)	107 (81%)	25 (19%)	0	100	100
13	L	99/102 (97%)	86 (87%)	13 (13%)	0	100	100
14	M	126/137 (92%)	105 (83%)	21 (17%)	0	100	100
15	N	144/147 (98%)	104 (72%)	39 (27%)	1 (1%)	22	62
16	O	136/148 (92%)	107 (79%)	28 (21%)	1 (1%)	22	62
17	P	53/56 (95%)	40 (76%)	13 (24%)	0	100	100
18	Q	150/158 (95%)	127 (85%)	23 (15%)	0	100	100
19	R	107/113 (95%)	80 (75%)	27 (25%)	0	100	100
20	S	64/67 (96%)	54 (84%)	10 (16%)	0	100	100
21	T	123/132 (93%)	94 (76%)	29 (24%)	0	100	100
22	U	147/150 (98%)	125 (85%)	22 (15%)	0	100	100
23	V	92/99 (93%)	69 (75%)	23 (25%)	0	100	100
24	W	61/65 (94%)	45 (74%)	16 (26%)	0	100	100
25	X	65/71 (92%)	48 (74%)	17 (26%)	0	100	100
26	Y	48/51 (94%)	28 (58%)	20 (42%)	0	100	100
27	Z	195/210 (93%)	152 (78%)	43 (22%)	0	100	100
28	0	34/36 (94%)	22 (65%)	12 (35%)	0	100	100
29	3	121/123 (98%)	96 (79%)	25 (21%)	0	100	100
32	6	93/113 (82%)	78 (84%)	15 (16%)	0	100	100
33	7	412/414 (100%)	363 (88%)	46 (11%)	3 (1%)	22	62
34	8	125/129 (97%)	113 (90%)	12 (10%)	0	100	100
35	9	247/254 (97%)	234 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4437/4630 (96%)	3585 (81%)	845 (19%)	7 (0%)	50 80

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	88	GLY
33	7	66	GLU
5	D	103	ARG
33	7	265	GLY
15	N	6	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	161/167 (96%)	159 (99%)	2 (1%)	71 83
3	B	168/173 (97%)	167 (99%)	1 (1%)	86 92
4	C	54/55 (98%)	53 (98%)	1 (2%)	57 74
5	D	158/160 (99%)	154 (98%)	4 (2%)	47 68
6	E	213/214 (100%)	212 (100%)	1 (0%)	88 93
7	F	192/198 (97%)	187 (97%)	5 (3%)	46 67
8	G	107/108 (99%)	106 (99%)	1 (1%)	78 87
9	H	183/184 (100%)	180 (98%)	3 (2%)	62 79
10	I	106/107 (99%)	105 (99%)	1 (1%)	78 87
11	J	102/103 (99%)	101 (99%)	1 (1%)	76 86
12	K	110/111 (99%)	109 (99%)	1 (1%)	78 87
13	L	90/91 (99%)	89 (99%)	1 (1%)	73 84
14	M	95/104 (91%)	95 (100%)	0	100 100
15	N	120/121 (99%)	118 (98%)	2 (2%)	60 78
16	O	115/123 (94%)	115 (100%)	0	100 100
17	P	45/46 (98%)	44 (98%)	1 (2%)	52 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	Q	137/143 (96%)	135 (98%)	2 (2%)	65 80
19	R	98/102 (96%)	97 (99%)	1 (1%)	76 86
20	S	60/61 (98%)	60 (100%)	0	100 100
21	T	109/114 (96%)	109 (100%)	0	100 100
22	U	126/127 (99%)	124 (98%)	2 (2%)	62 79
23	V	86/90 (96%)	86 (100%)	0	100 100
24	W	54/56 (96%)	54 (100%)	0	100 100
25	X	57/60 (95%)	56 (98%)	1 (2%)	59 76
26	Y	41/42 (98%)	38 (93%)	3 (7%)	14 41
27	Z	156/168 (93%)	154 (99%)	2 (1%)	69 82
28	0	34/34 (100%)	32 (94%)	2 (6%)	19 47
29	3	99/99 (100%)	97 (98%)	2 (2%)	55 73
32	6	83/99 (84%)	83 (100%)	0	100 100
33	7	356/356 (100%)	352 (99%)	4 (1%)	73 84
34	8	117/118 (99%)	113 (97%)	4 (3%)	37 61
35	9	226/228 (99%)	225 (100%)	1 (0%)	91 94
All	All	3858/3962 (97%)	3809 (99%)	49 (1%)	70 82

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	U	71	GLU
27	Z	178	VAL
22	U	85	HIS
26	Y	37	ARG
28	0	13	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	66	ASN
21	T	66	HIS
33	7	224	ASN
16	O	6	HIS
19	R	26	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1458/1497 (97%)	501 (34%)	19 (1%)
30	5	19/20 (95%)	9 (47%)	0
31	4	75/76 (98%)	32 (42%)	1 (1%)
All	All	1552/1593 (97%)	542 (34%)	20 (1%)

5 of 542 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	14	U
1	2	15	U
1	2	16	C
1	2	23	A
1	2	30	C

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1155	G
1	2	1435	C
31	4	73	A
1	2	1448	C
1	2	599	C

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

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	4AC	2	546	1	21,24,25	1.03	2 (9%)	29,34,37	1.44	3 (10%)
1	B8H	2	938	1	19,22,23	0.82	0	22,32,35	1.52	3 (13%)
1	5MC	2	939	1	18,22,23	1.05	2 (11%)	26,32,35	1.25	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	5MU	4	54	31	19,22,23	1.44	6 (31%)	28,32,35	2.05	8 (28%)
1	4AC	2	636	1	21,24,25	1.12	3 (14%)	29,34,37	1.60	4 (13%)
1	6MZ	2	1469	36,1	18,25,26	0.76	1 (5%)	16,36,39	2.10	3 (18%)
1	4AC	2	828	1	21,24,25	1.01	1 (4%)	29,34,37	1.64	4 (13%)
1	5HM	2	1378	1	19,23,24	2.94	7 (36%)	25,33,36	0.64	0
1	4AC	2	751	1	21,24,25	1.13	3 (14%)	29,34,37	1.26	4 (13%)
1	4AC	2	53	1	21,24,25	1.06	2 (9%)	29,34,37	1.48	5 (17%)
1	A2M	2	373	1	18,25,26	1.06	1 (5%)	18,36,39	1.39	4 (22%)
1	4AC	2	1193	1	21,24,25	1.13	2 (9%)	29,34,37	2.00	5 (17%)
1	OMC	2	1376	1	19,22,23	0.90	2 (10%)	26,31,34	0.76	0
31	OMC	4	32	31	19,22,23	0.99	2 (10%)	26,31,34	1.13	2 (7%)
1	MA6	2	1487	1	18,26,27	0.92	1 (5%)	19,38,41	1.28	3 (15%)
1	4AC	2	1233	1	21,24,25	1.09	2 (9%)	29,34,37	1.53	4 (13%)
31	PSU	4	55	31	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
1	4AC	2	511	1	21,24,25	1.15	3 (14%)	29,34,37	1.87	6 (20%)
1	4AC	2	1147	1	21,24,25	1.12	3 (14%)	29,34,37	2.24	6 (20%)
1	MA6	2	1488	1	18,26,27	0.95	1 (5%)	19,38,41	1.18	2 (10%)
1	4AC	2	319	1	21,24,25	1.20	3 (14%)	29,34,37	1.48	4 (13%)
1	4AC	2	590	36,1	21,24,25	1.15	3 (14%)	29,34,37	1.47	4 (13%)
1	4AC	2	648	1	21,24,25	1.20	3 (14%)	29,34,37	1.85	7 (24%)
1	4AC	2	718	1	21,24,25	1.08	2 (9%)	29,34,37	1.18	3 (10%)
31	H2U	4	20	31	18,21,22	1.10	2 (11%)	21,30,33	2.24	1 (4%)
1	4AC	2	703	1	21,24,25	1.07	2 (9%)	29,34,37	1.82	6 (20%)
1	4AC	2	851	1	21,24,25	1.24	3 (14%)	29,34,37	1.57	4 (13%)
1	LHH	2	250	1	22,25,26	2.45	8 (36%)	29,35,38	1.20	2 (6%)
1	4AC	2	1041	1	21,24,25	1.01	2 (9%)	29,34,37	1.98	4 (13%)
1	4AC	2	379	1	21,24,25	1.08	3 (14%)	29,34,37	1.55	5 (17%)
1	4AC	2	394	1	21,24,25	1.02	2 (9%)	29,34,37	1.66	5 (17%)
1	4AC	2	731	1	21,24,25	1.16	3 (14%)	29,34,37	1.37	5 (17%)
1	4AC	2	848	1	21,24,25	1.12	2 (9%)	29,34,37	1.75	4 (13%)
1	5MC	2	1202	1	18,22,23	1.00	1 (5%)	26,32,35	1.21	1 (3%)
1	4AC	2	1028	1	21,24,25	1.05	3 (14%)	29,34,37	1.62	4 (13%)
1	4AC	2	1239	1	21,24,25	1.15	2 (9%)	29,34,37	1.87	4 (13%)
1	4AC	2	839	1	21,24,25	1.13	2 (9%)	29,34,37	1.80	6 (20%)
1	4AC	2	1184	1	21,24,25	1.06	3 (14%)	29,34,37	1.39	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	UR3	2	1467	1	19,22,23	1.10	2 (10%)	26,32,35	1.50	5 (19%)
1	4AC	2	17	1	21,24,25	1.06	2 (9%)	29,34,37	1.77	5 (17%)
1	4AC	2	868	1	21,24,25	1.23	3 (14%)	29,34,37	1.37	4 (13%)
1	4AC	2	957	1	21,24,25	1.12	1 (4%)	29,34,37	2.29	7 (24%)
31	4SU	4	8	31	18,21,22	1.79	5 (27%)	26,30,33	2.15	4 (15%)
1	4AC	2	286	1	21,24,25	1.11	2 (9%)	29,34,37	1.64	7 (24%)
1	4AC	2	1479	1	21,24,25	1.10	3 (14%)	29,34,37	1.50	4 (13%)
1	4AC	2	626	1	21,24,25	1.05	3 (14%)	29,34,37	1.41	4 (13%)
1	4AC	2	303	1	21,24,25	1.16	3 (14%)	29,34,37	1.44	3 (10%)
1	4AC	2	479	1	21,24,25	1.13	3 (14%)	29,34,37	1.59	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	546	1	-	2/11/29/30	0/2/2/2
1	B8H	2	938	1	-	3/7/25/26	0/2/2/2
1	5MC	2	939	1	-	0/7/25/26	0/2/2/2
31	5MU	4	54	31	-	1/7/25/26	0/2/2/2
1	4AC	2	636	1	-	0/11/29/30	0/2/2/2
1	6MZ	2	1469	36,1	-	0/5/27/28	0/3/3/3
1	4AC	2	828	1	-	0/11/29/30	0/2/2/2
1	5HM	2	1378	1	-	2/9/27/28	0/2/2/2
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	A2M	2	373	1	-	1/5/27/28	0/3/3/3
1	4AC	2	1193	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
31	OMC	4	32	31	-	2/9/27/28	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
31	PSU	4	55	31	-	0/7/25/26	0/2/2/2
1	4AC	2	511	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1147	1	-	2/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	0/7/29/30	0/3/3/3
1	4AC	2	319	1	-	4/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	590	36,1	-	2/11/29/30	0/2/2/2
1	4AC	2	648	1	-	2/11/29/30	0/2/2/2
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
31	H2U	4	20	31	-	4/7/38/39	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	4AC	2	851	1	-	4/11/29/30	0/2/2/2
1	LHH	2	250	1	-	1/13/31/32	0/2/2/2
1	4AC	2	1041	1	-	0/11/29/30	0/2/2/2
1	4AC	2	379	1	-	2/11/29/30	0/2/2/2
1	4AC	2	394	1	-	2/11/29/30	0/2/2/2
1	4AC	2	731	1	-	3/11/29/30	0/2/2/2
1	4AC	2	848	1	-	2/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	2/7/25/26	0/2/2/2
1	4AC	2	1028	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1239	1	-	2/11/29/30	0/2/2/2
1	4AC	2	839	1	-	1/11/29/30	0/2/2/2
1	4AC	2	1184	1	-	2/11/29/30	0/2/2/2
1	UR3	2	1467	1	-	6/7/25/26	0/2/2/2
1	4AC	2	17	1	-	0/11/29/30	0/2/2/2
1	4AC	2	868	1	-	2/11/29/30	0/2/2/2
1	4AC	2	957	1	-	1/11/29/30	0/2/2/2
31	4SU	4	8	31	-	5/7/25/26	0/2/2/2
1	4AC	2	286	1	-	5/11/29/30	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	626	1	-	2/11/29/30	0/2/2/2
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	4AC	2	479	1	-	3/11/29/30	0/2/2/2

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1378	5HM	C4-N3	6.29	1.44	1.34
1	2	250	LHH	C4-N4	6.05	1.48	1.39
1	2	250	LHH	C7-N4	5.67	1.47	1.37
1	2	1378	5HM	C2-N3	5.46	1.47	1.36
1	2	1378	5HM	C4-N4	5.36	1.48	1.34

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	20	H2U	C4-N3-C2	-9.61	117.82	125.79
31	4	8	4SU	C4-N3-C2	-6.85	120.68	127.34
1	2	1469	6MZ	C2-N1-C6	6.51	122.17	116.59
1	2	1147	4AC	C5-C4-N4	-6.34	111.91	122.92
1	2	957	4AC	N4-C4-N3	6.19	124.24	113.85

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	250	LHH	C1'-C2'-O2'-C1
1	2	286	4AC	C3'-C4'-C5'-O5'
1	2	373	A2M	C1'-C2'-O2'-CM'
1	2	379	4AC	C3'-C4'-C5'-O5'
1	2	511	4AC	O4'-C4'-C5'-O5'

There are no ring outliers.

47 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	546	4AC	2	0
1	2	938	B8H	1	0
1	2	939	5MC	1	0
31	4	54	5MU	3	0
1	2	636	4AC	2	0
1	2	1469	6MZ	2	0
1	2	828	4AC	3	0
1	2	1378	5HM	4	0
1	2	751	4AC	1	0
1	2	53	4AC	1	0
1	2	373	A2M	7	0
1	2	1193	4AC	3	0
1	2	1376	OMC	2	0
31	4	32	OMC	3	0
1	2	1487	MA6	4	0
1	2	1233	4AC	6	0
31	4	55	PSU	3	0
1	2	511	4AC	1	0
1	2	1147	4AC	5	0
1	2	1488	MA6	3	0
1	2	319	4AC	3	0
1	2	590	4AC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	648	4AC	5	0
1	2	718	4AC	4	0
31	4	20	H2U	1	0
1	2	703	4AC	6	0
1	2	851	4AC	6	0
1	2	1041	4AC	4	0
1	2	379	4AC	2	0
1	2	394	4AC	4	0
1	2	731	4AC	4	0
1	2	848	4AC	2	0
1	2	1202	5MC	3	0
1	2	1028	4AC	2	0
1	2	1239	4AC	5	0
1	2	839	4AC	7	0
1	2	1184	4AC	4	0
1	2	1467	UR3	4	0
1	2	17	4AC	3	0
1	2	868	4AC	3	0
1	2	957	4AC	4	0
31	4	8	4SU	2	0
1	2	286	4AC	1	0
1	2	1479	4AC	5	0
1	2	626	4AC	1	0
1	2	303	4AC	3	0
1	2	479	4AC	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 40 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	MET	7	501	-	6,7,8	0.50	0	2,7,9	0.39	0
39	GNP	7	502	36	29,34,34	1.58	7 (24%)	33,54,54	2.14	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	MET	7	501	-	-	2/5/6/8	-
39	GNP	7	502	36	-	7/14/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	502	GNP	PB-O3A	4.26	1.64	1.59
39	7	502	GNP	PB-O1B	3.18	1.51	1.46
39	7	502	GNP	C6-N1	2.97	1.38	1.33
39	7	502	GNP	PG-N3B	2.80	1.70	1.63
39	7	502	GNP	PG-O1G	2.60	1.50	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	7	502	GNP	C5-C6-N1	-8.34	112.03	123.43
39	7	502	GNP	C2-N1-C6	5.83	125.19	115.93
39	7	502	GNP	PB-O3A-PA	-2.95	122.22	132.62
39	7	502	GNP	N3-C2-N1	-2.85	123.42	127.22
39	7	502	GNP	C4-C5-C6	-2.70	118.22	120.80

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

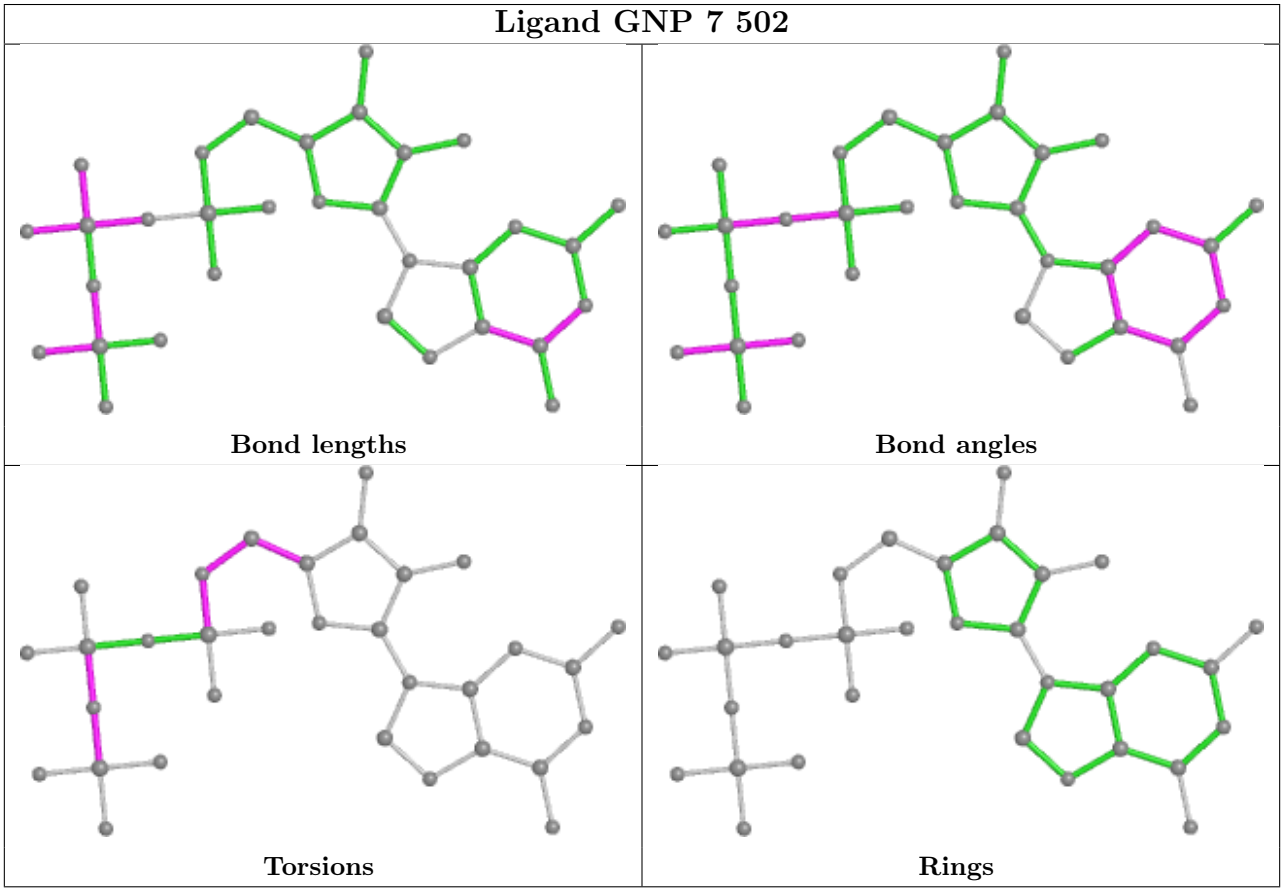
Mol	Chain	Res	Type	Atoms
39	7	502	GNP	PB-N3B-PG-O1G
39	7	502	GNP	PG-N3B-PB-O1B
39	7	502	GNP	C5'-O5'-PA-O3A
39	7	502	GNP	O4'-C4'-C5'-O5'
38	7	501	MET	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	7	501	MET	2	0
39	7	502	GNP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	9	2
34	8	1
9	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	19:PRO	C	28:GLN	N	14.63
1	9	47:SER	C	53:ASN	N	11.57
1	9	169:SER	C	175:ARG	N	8.00
1	H	194:LYS	C	195:ASP	N	1.20

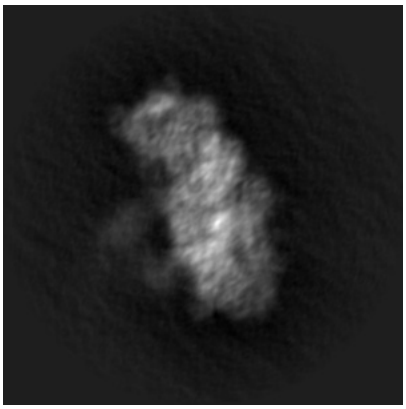
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10320. These allow visual inspection of the internal detail of the map and identification of artifacts.

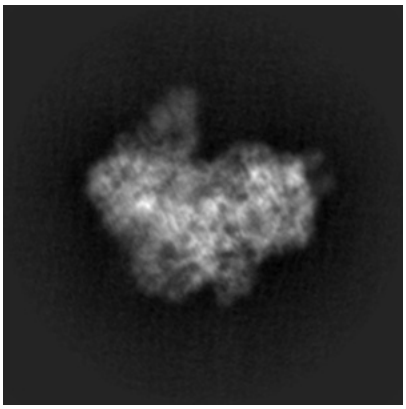
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

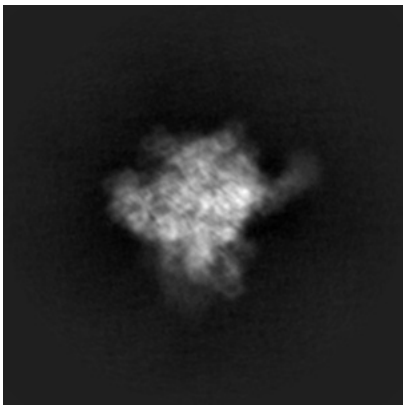
6.1.1 Primary map



X

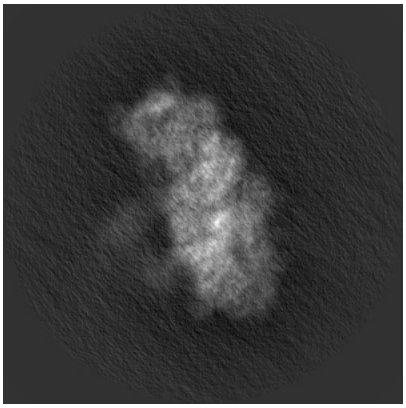


Y

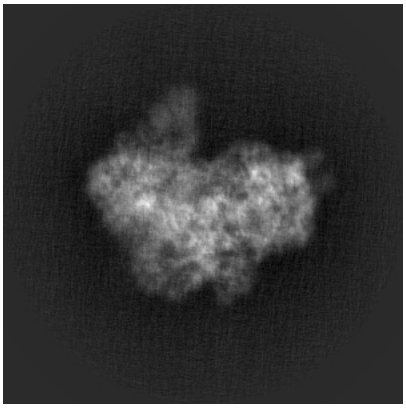


Z

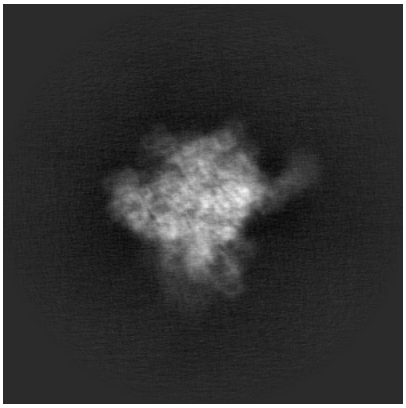
6.1.2 Raw map



X



Y

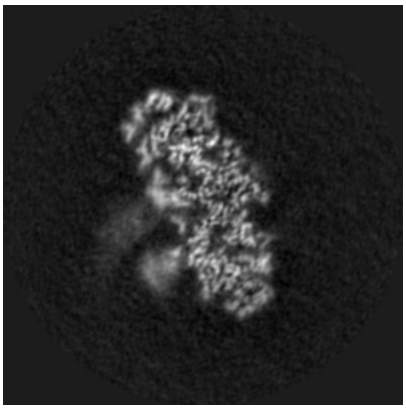


Z

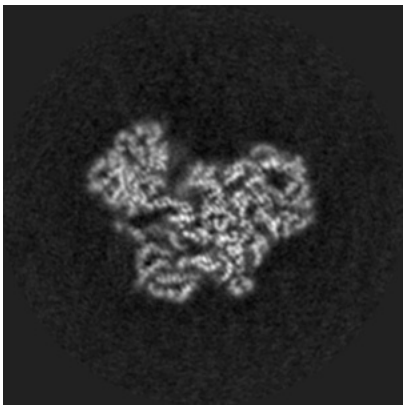
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

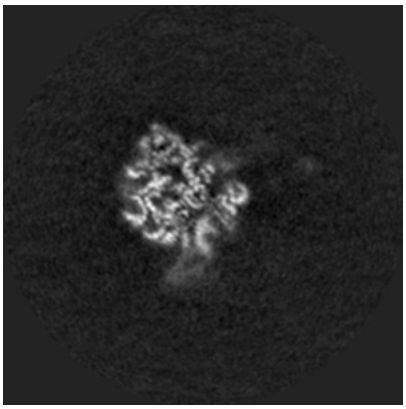
6.2.1 Primary map



X Index: 174

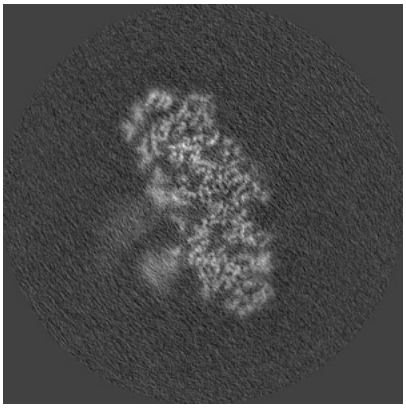


Y Index: 174

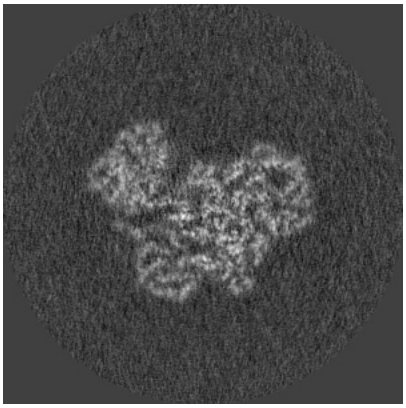


Z Index: 174

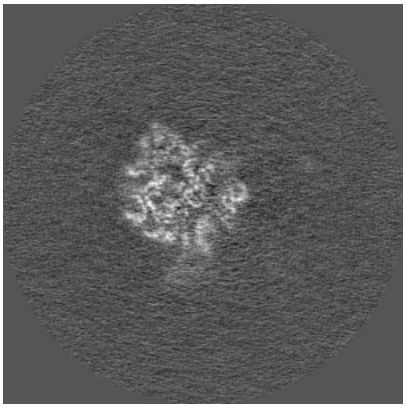
6.2.2 Raw map



X Index: 174



Y Index: 174

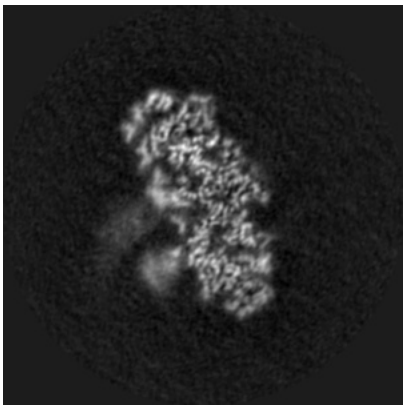


Z Index: 174

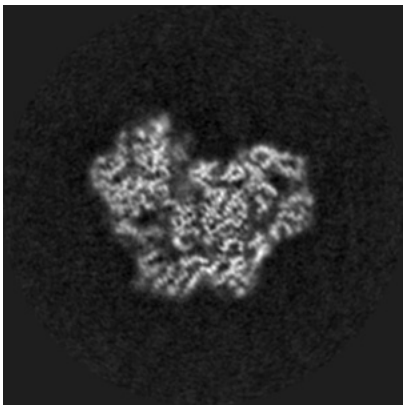
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

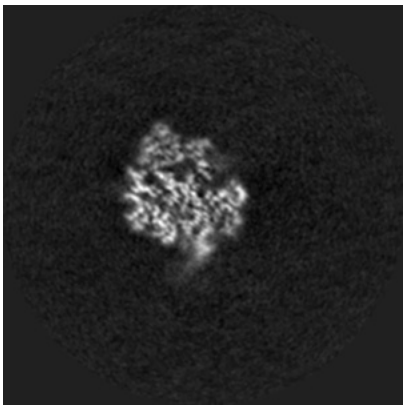
6.3.1 Primary map



X Index: 174

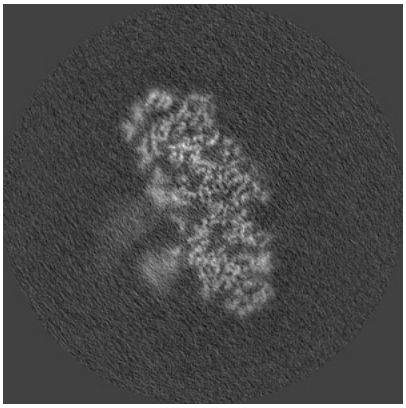


Y Index: 178

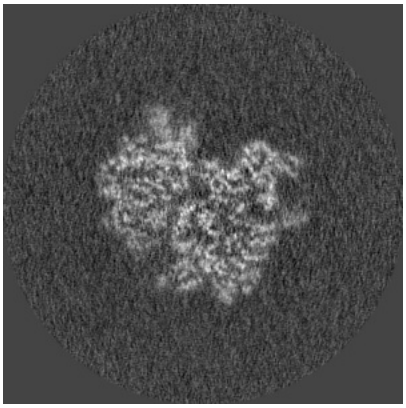


Z Index: 180

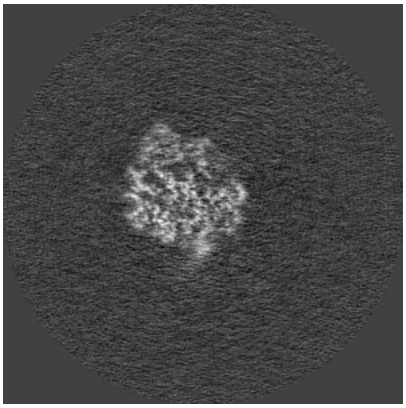
6.3.2 Raw map



X Index: 174



Y Index: 185

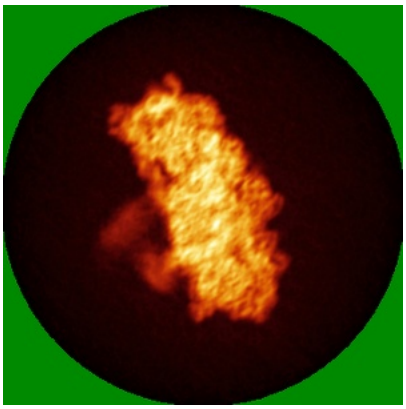


Z Index: 180

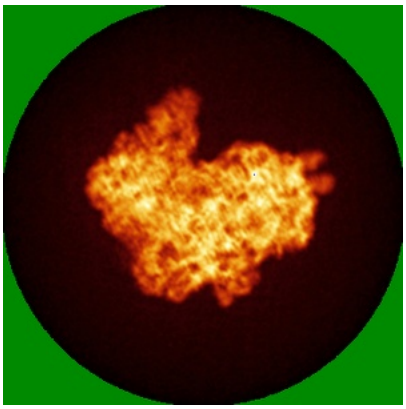
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

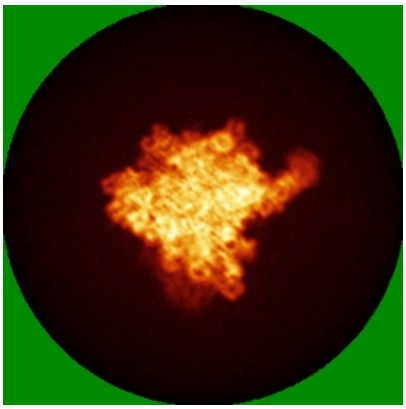
6.4.1 Primary map



X

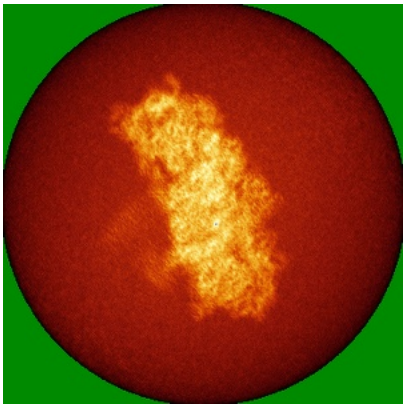


Y

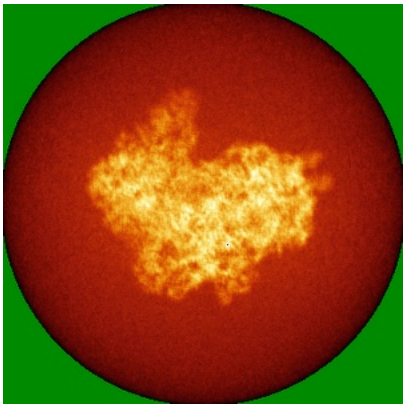


Z

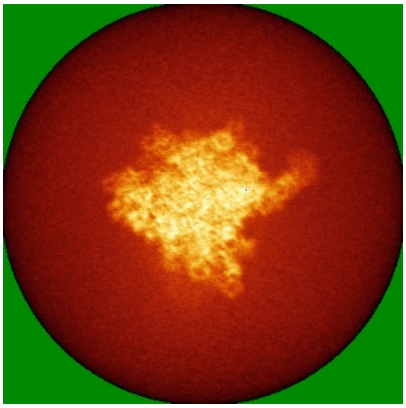
6.4.2 Raw map



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.

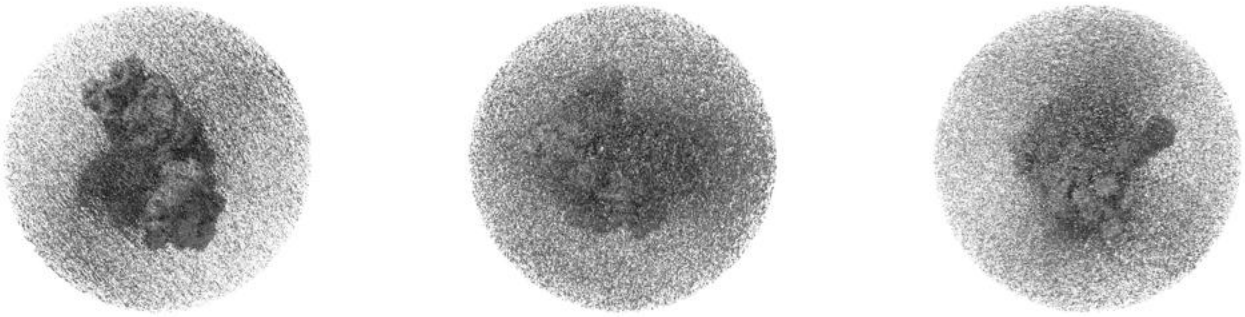
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. 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



X Y Z

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

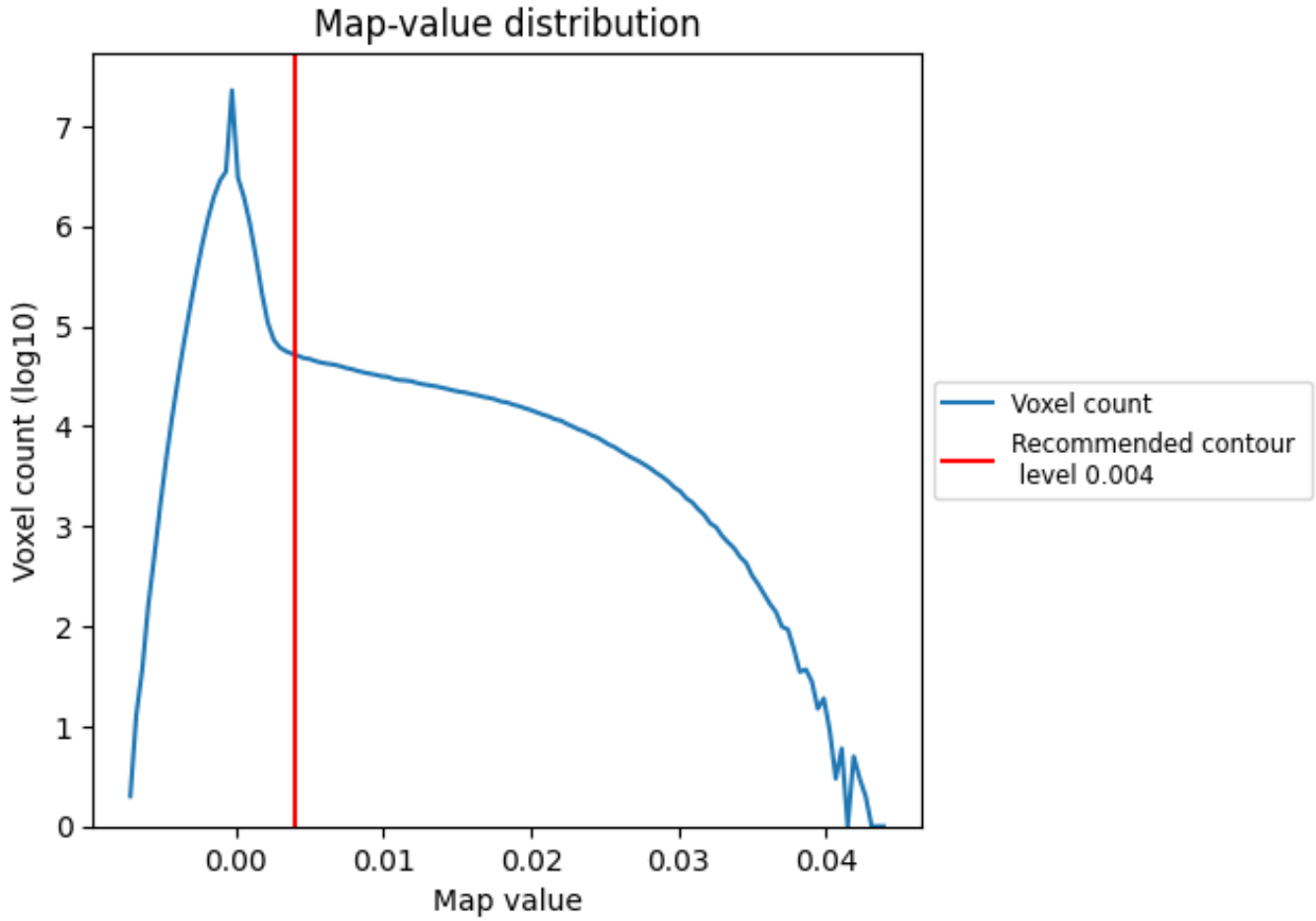
6.6 Mask visualisation (i)

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

7 Map analysis

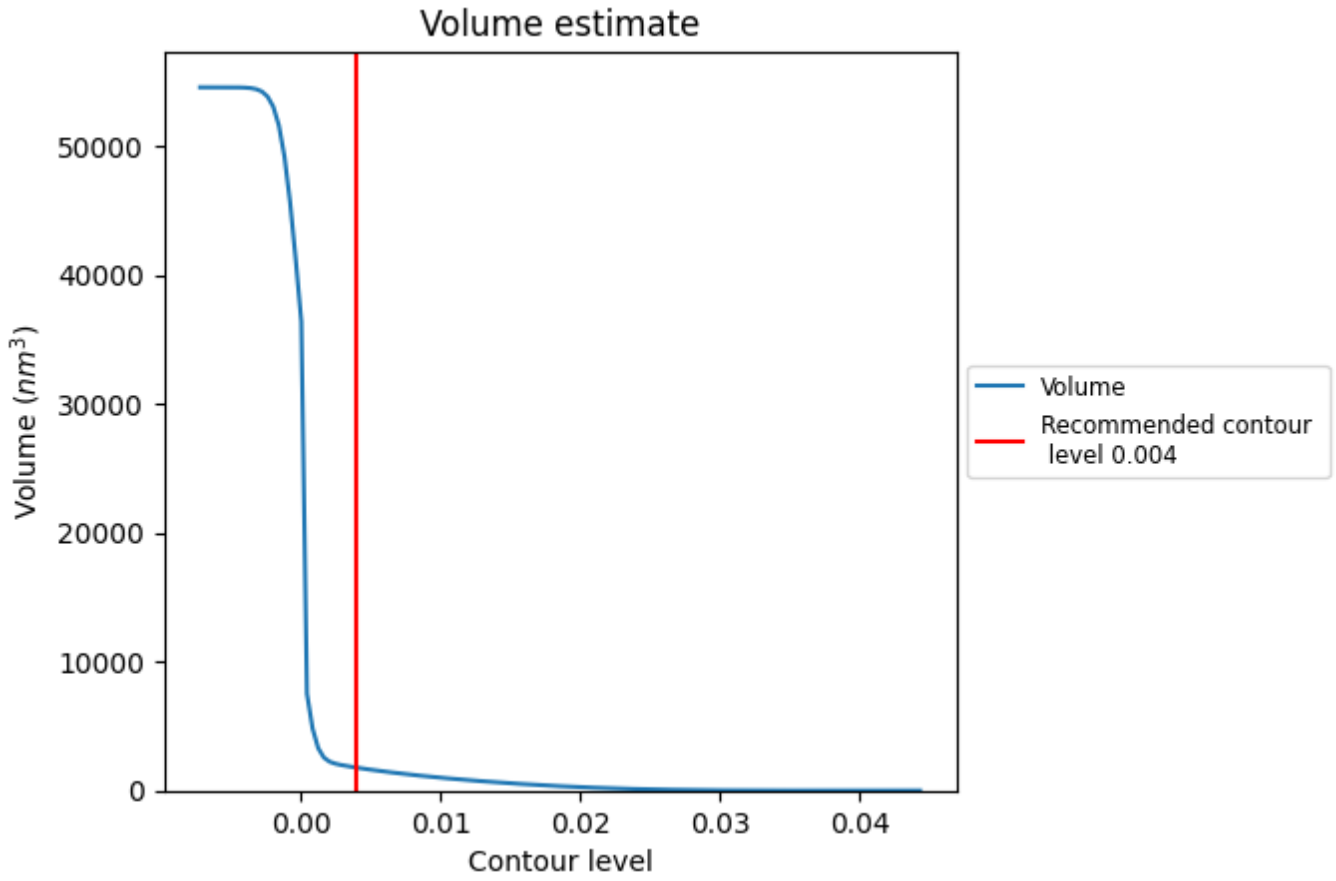
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

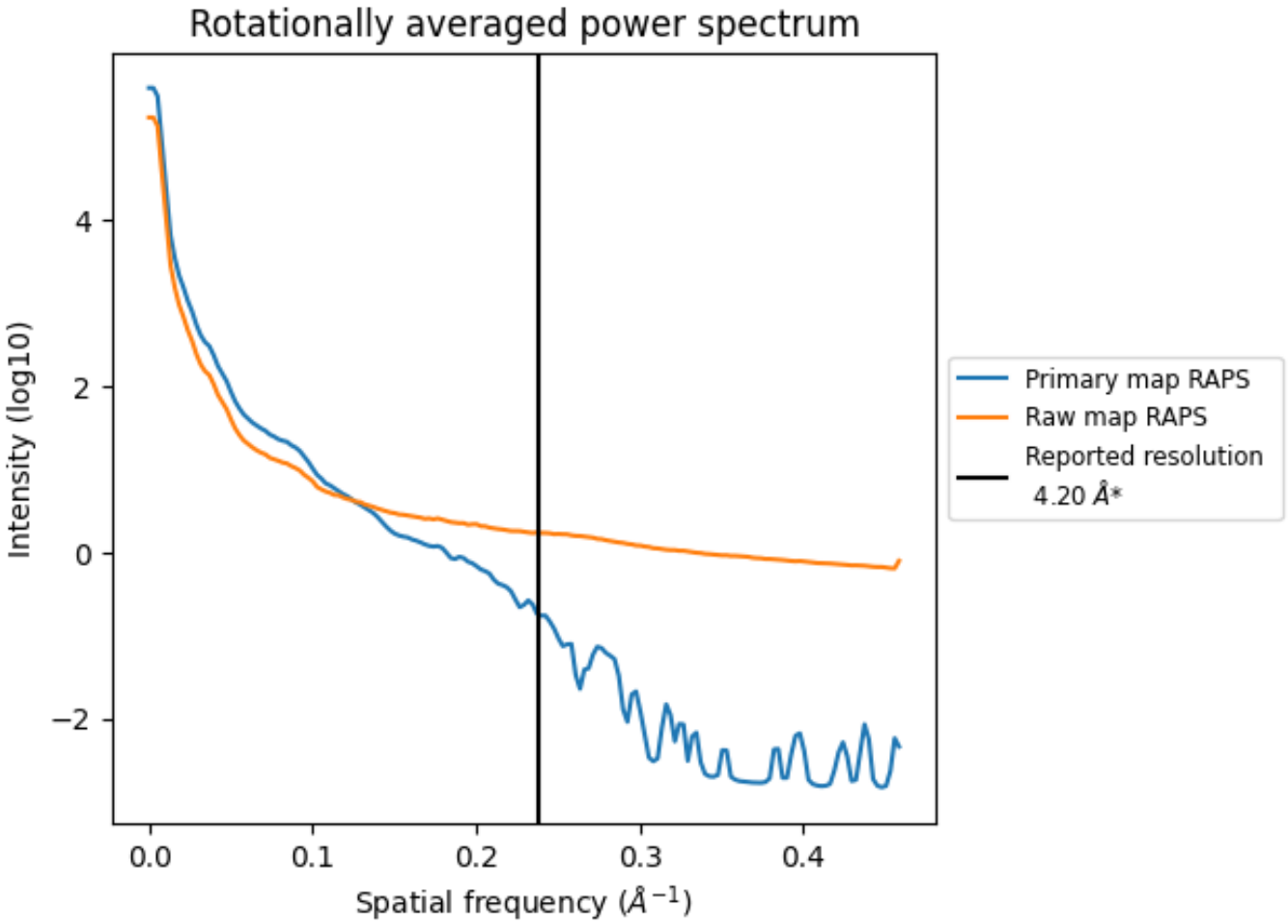
7.2 Volume estimate (i)



The volume at the recommended contour level is 1784 nm^3; this corresponds to an approximate mass of 1611 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

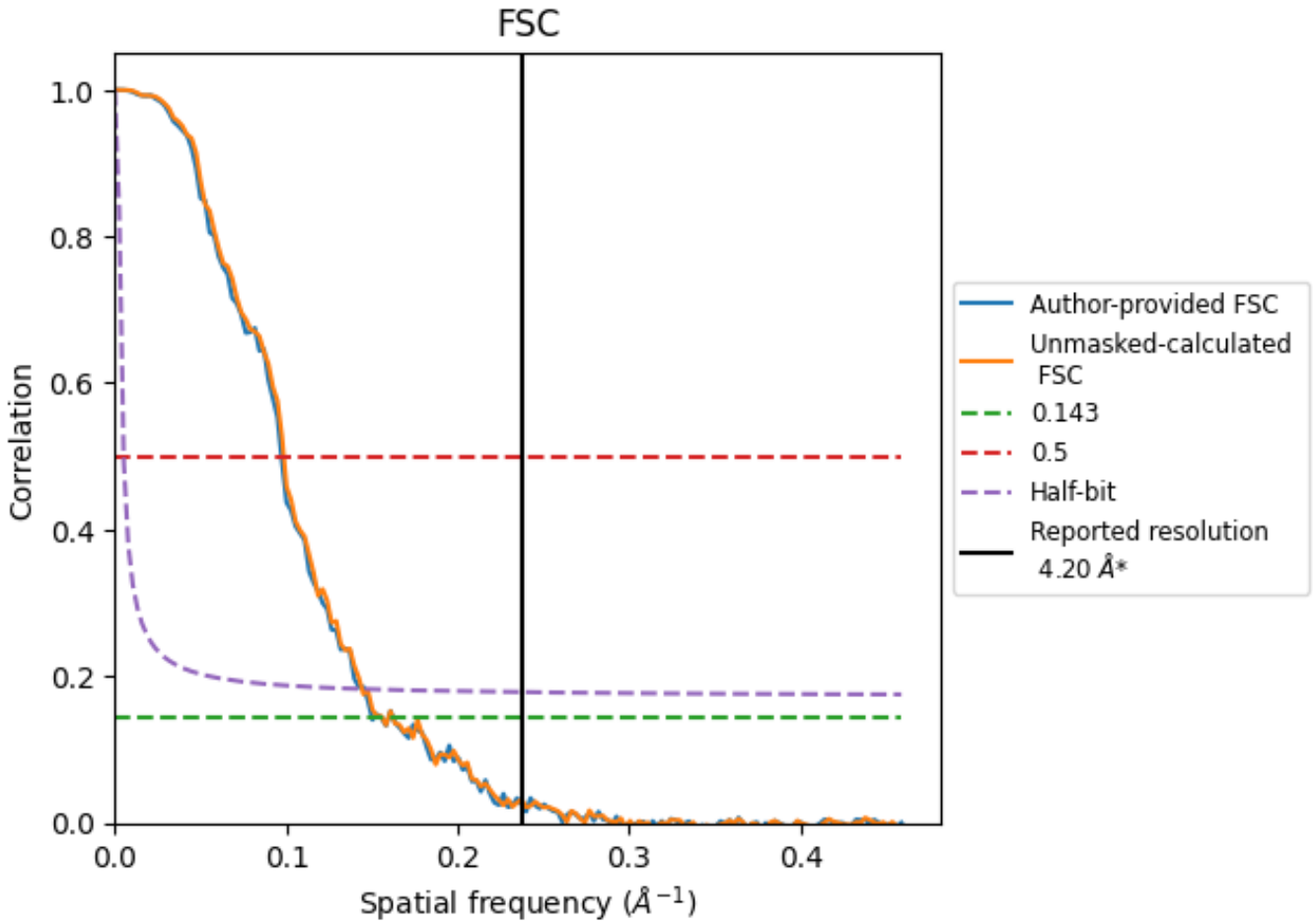


*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	6.67	10.29	6.87
Unmasked-calculated*	6.41	10.14	6.93

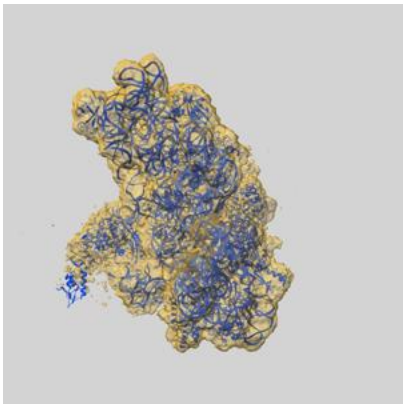
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.67 differs from the reported value 4.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 4.2 by more than 10 %

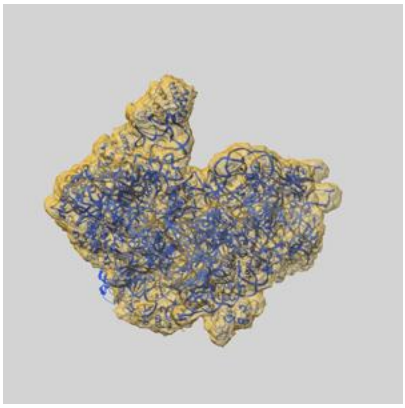
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10320 and PDB model 6SW9. Per-residue inclusion information can be found in section 3 on page 13.

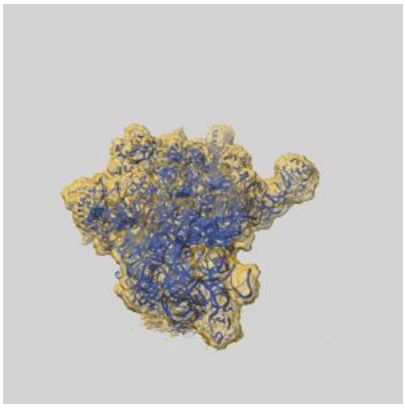
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

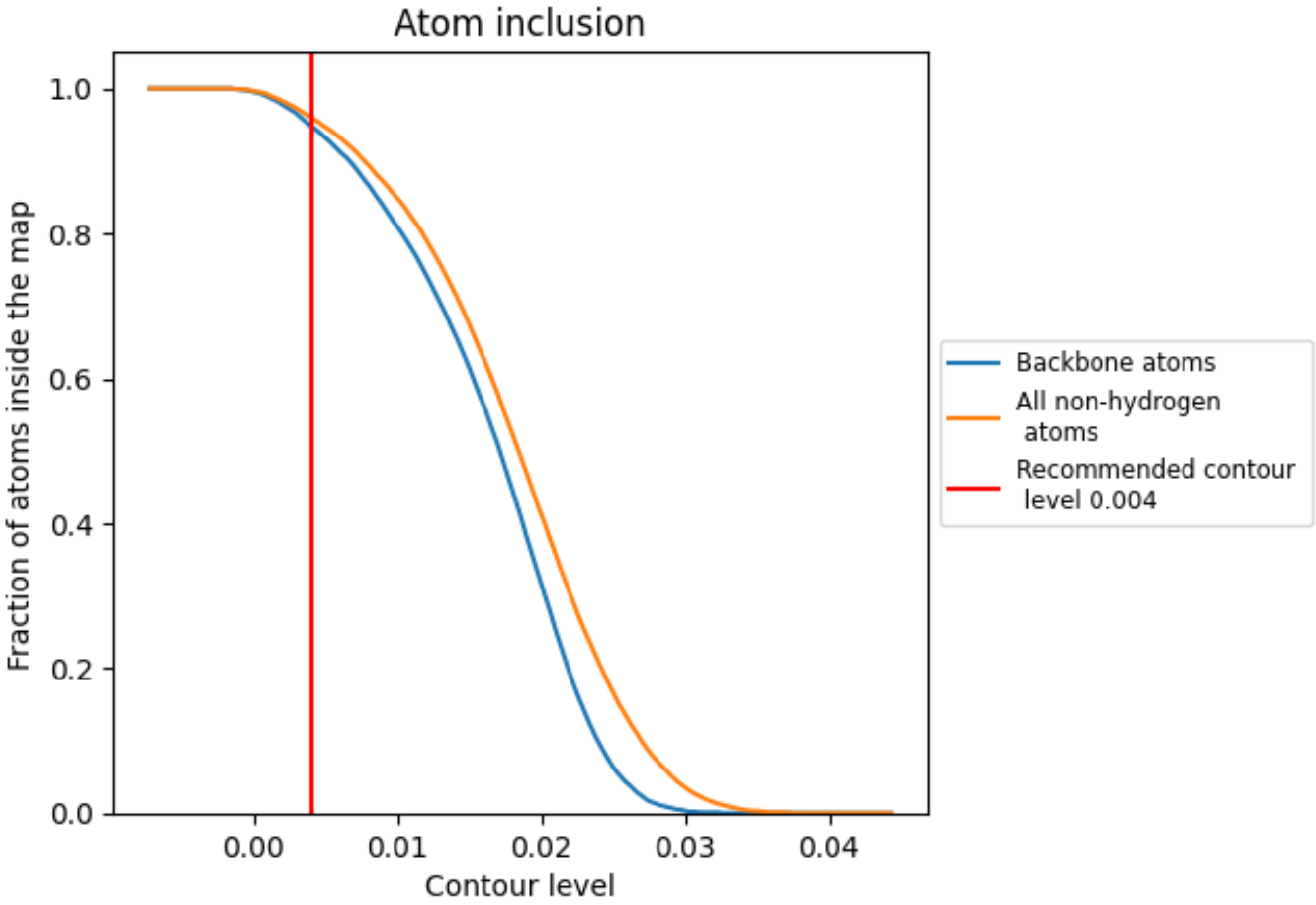
9.2 Q-score mapped to coordinate model

This section was not generated.

9.3 Atom inclusion mapped to coordinate model

This section was not generated.

9.4 Atom inclusion



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.9600
0	0.9970
2	1.0000
3	1.0000
4	0.9870
5	0.9980
6	1.0000
7	0.8600
8	0.2740
9	0.2580
A	0.9960
B	0.9970
C	0.9940
D	1.0000
E	0.9990
F	0.9930
G	0.9980
H	0.9960
I	0.9980
J	0.9980
K	0.9980
L	0.9980
M	1.0000
N	0.9980
O	0.9980
P	1.0000
Q	0.9980
R	0.9990
S	0.9850
T	0.9930
U	0.9980
V	0.9990
W	0.9960
X	1.0000
Y	0.9900
Z	0.9950