wwPDB EM Validation Summary Report

Sep 28, 2024 – 08:35 pm BST

PDB ID	:	5JB3
EMDB ID	:	EMD-8148
Title	:	Cryo-EM structure of a full archaeal ribosomal translation initiation complex in the P-REMOTE conformation
Authors	:	Coureux, P.-D.; Schmitt, E.; Mechulam, Y.
Deposited on	:	2016-04-13
Resolution	:	5.34 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:

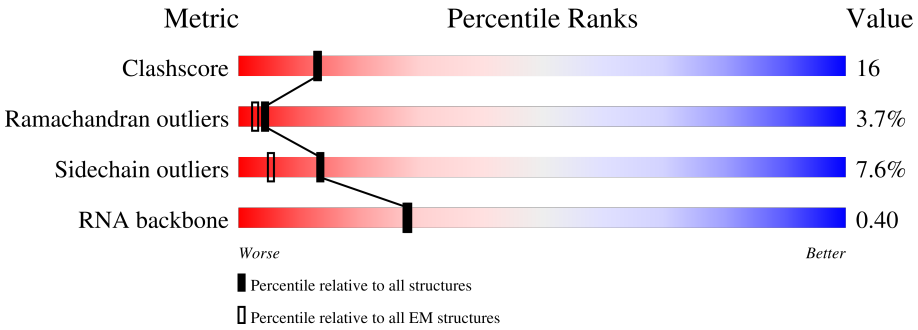
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 5.34 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1519	32% 49% 15%
2	M	137	9% 74% 20%
3	N	147	5% 54% 36% 8%
4	Q	158	8% 75% 19% 6%
5	R	113	5% 77% 22%
6	A	198	5% 71% 22%
7	B	202	76% 22%

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Mol	Chain	Length	Quality of chain
8	V	99	68% 26%
9	W	63	94% 6%
10	Z	210	5% 78% 10% 11%
11	D	180	69% 23%
12	E	243	72% 23%
13	F	236	50% 38% 8%
14	G	125	6% 45% 42% 11%
15	I	130	58% 35% 5%
16	J	127	75% 23%
17	C	57	91% 9%
18	3	123	16% 84% 15%
19	L	102	7% 67% 25% 7%
20	O	148	14% 86% 13%
21	P	56	5% 77% 20%
22	S	67	9% 85% 13%
23	T	132	14% 70% 14% 16%
24	U	150	6% 75% 20%
25	X	71	24% 68% 24% 8%
26	Y	50	14% 90% 8%
27	H	215	15% 55% 31% 12%
28	K	135	8% 79% 20%
29	0	22	5% 50% 45% 5%
30	4	76	9% 24% 49% 26%
31	5	26	15% 23% 31% 31%
32	1	102	55% 23% 19%

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Mol	Chain	Length	Quality of chain
33	6	113	8% 65% 19% 16%
34	7	415	13% 65% 28%
35	8	139	60% 60% 29% 7%
36	9	266	40% 66% 26% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	MET	7	501	-	-	X	-

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 70678 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	1495	32135	14297	5954	10389	1495	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	-3	U	UNK	conflict	GB 5457433
2	227	C	G	conflict	GB 5457433
2	229	G	C	conflict	GB 5457433
2	715	C	G	conflict	GB 5457433
2	718	G	C	conflict	GB 5457433
2	1216	A	U	conflict	GB 5457433
2	1217	C	G	conflict	GB 5457433
2	1224	U	C	conflict	GB 5457433
2	1234	A	G	conflict	GB 5457433
2	1238	G	U	conflict	GB 5457433
2	1316	U	C	conflict	GB 5457433
2	1383	A	G	conflict	GB 5457433
2	1385	U	C	conflict	GB 5457433
2	1387	C	U	conflict	GB 5457433
2	1388	G	A	conflict	GB 5457433
2	1398	U	C	conflict	GB 5457433
2	1417	A	G	conflict	GB 5457433
2	1427	C	U	conflict	GB 5457433
2	1428	G	A	conflict	GB 5457433
2	1463	A	G	conflict	GB 5457433

- Molecule 2 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	133	1004	623	200	179	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	23	PHE	TYR	conflict	UNP P62010

- Molecule 3 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	145	Total	C	N	O	S	0	0
			1140	722	222	193	3		

- Molecule 4 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	158	Total	C	N	O	S	0	0
			1310	834	250	221	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	26	VAL	LEU	conflict	UNP Q9V2K9
Q	32	GLU	ASP	conflict	UNP Q9V2K9
Q	62	SER	THR	conflict	UNP Q9V2K9
Q	67	LYS	ARG	conflict	UNP Q9V2K9
Q	75	ASN	LYS	conflict	UNP Q9V2K9
Q	100	ARG	LYS	conflict	UNP Q9V2K9
Q	145	ASN	ASP	conflict	UNP Q9V2K9
Q	152	THR	GLN	conflict	UNP Q9V2K9

- Molecule 5 is a protein called 30S ribosomal protein S17P.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	113	Total	C	N	O	S	0	0
			934	592	177	160	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	2	MET	VAL	conflict	UNP Q9V1U5
R	9	VAL	ILE	conflict	UNP Q9V1U5
R	26	ASN	HIS	conflict	UNP Q9V1U5
R	55	PHE	HIS	conflict	UNP Q9V1U5
R	58	ASN	LYS	conflict	UNP Q9V1U5
R	69	LYS	ARG	conflict	UNP Q9V1U5
R	85	LYS	ARG	conflict	UNP Q9V1U5

- Molecule 6 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	190	Total	C	N	O	S	0	0
			1559	1007	273	274	5		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	ALA	conflict	UNP Q9V2K7
A	3	ALA	LYS	conflict	UNP Q9V2K7
A	4	LYS	ARG	conflict	UNP Q9V2K7
A	6	ALA	VAL	conflict	UNP Q9V2K7
A	7	THR	SER	conflict	UNP Q9V2K7
A	8	THR	ALA	conflict	UNP Q9V2K7
A	9	THR	ALA	conflict	UNP Q9V2K7
A	10	ARG	LYS	conflict	UNP Q9V2K7
A	20	ILE	VAL	conflict	UNP Q9V2K7
A	55	VAL	ILE	conflict	UNP Q9V2K7
A	60	THR	LEU	conflict	UNP Q9V2K7
A	62	SER	GLY	conflict	UNP Q9V2K7
A	99	LYS	ARG	conflict	UNP Q9V2K7
A	123	ALA	VAL	conflict	UNP Q9V2K7
A	126	MET	ALA	conflict	UNP Q9V2K7
A	161	SER	ALA	conflict	UNP Q9V2K7
A	181	ARG	LYS	conflict	UNP Q9V2K7
A	192	GLU	GLY	conflict	UNP Q9V2K7
A	195	GLN	GLU	conflict	UNP Q9V2K7
A	197	ILE	ALA	conflict	UNP Q9V2K7

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	202	Total	C	N	O	S	0	0
			1623	1046	282	290	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	LYS	ARG	conflict	UNP Q9V191
B	63	GLU	ASP	conflict	UNP Q9V191
B	115	LEU	ILE	conflict	UNP Q9V191
B	117	VAL	ILE	conflict	UNP Q9V191
B	128	ARG	LYS	conflict	UNP Q9V191

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Chain	Residue	Modelled	Actual	Comment	Reference
B	131	VAL	ILE	conflict	UNP Q9V191
B	183	GLN	SER	conflict	UNP Q9V191
B	187	ASP	GLU	conflict	UNP Q9V191

- Molecule 8 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	99	Total	C	N	O	S	0	0
			823	532	134	154	3		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	4	ARG	LYS	conflict	UNP Q9UY20
V	6	LYS	THR	conflict	UNP Q9UY20
V	8	ILE	VAL	conflict	UNP Q9UY20
V	64	ILE	LYS	conflict	UNP Q9UY20
V	71	ALA	TYR	conflict	UNP Q9UY20
V	73	ASP	TYR	conflict	UNP Q9UY20
V	74	SER	ASP	conflict	UNP Q9UY20
V	76	GLU	ASP	conflict	UNP Q9UY20
V	92	LEU	ILE	conflict	UNP Q9UY20

- Molecule 9 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	63	Total	C	N	O	S	0	0
			478	306	85	81	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	1	MET	LEU	conflict	UNP Q9UXZ3
W	2	ALA	PRO	conflict	UNP Q9UXZ3
W	3	LYS	ARG	conflict	UNP Q9UXZ3
W	4	PRO	ASN	conflict	UNP Q9UXZ3
W	5	ILE	VAL	conflict	UNP Q9UXZ3
W	34	LYS	ARG	conflict	UNP Q9UXZ3
W	38	LEU	ASN	conflict	UNP Q9UXZ3
W	39	ILE	VAL	conflict	UNP Q9UXZ3
W	54	VAL	ILE	conflict	UNP Q9UXZ3
W	55	LYS	ARG	conflict	UNP Q9UXZ3

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	186	Total	C	N	O	S	0	0
			1459	933	271	251	4		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	13	ARG	LYS	conflict	UNP Q9V1U1
Z	71	LYS	ARG	conflict	UNP Q9V1U1
Z	81	GLU	ASP	conflict	UNP Q9V1U1
Z	83	GLU	GLN	conflict	UNP Q9V1U1
Z	99	LEU	ILE	conflict	UNP Q9V1U1
Z	117	LEU	MET	conflict	UNP Q9V1U1
Z	122	ASN	SER	conflict	UNP Q9V1U1
Z	132	LEU	ILE	conflict	UNP Q9V1U1
Z	144	ILE	VAL	conflict	UNP Q9V1U1
Z	186	GLY	ASP	conflict	UNP Q9V1U1
Z	205	VAL	SER	conflict	UNP Q9V1U1

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	172	Total	C	N	O	S	0	0
			1434	902	273	255	4		

- Molecule 12 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	241	Total	C	N	O	S	0	0
			1976	1277	355	339	5		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	118	ASP	GLU	conflict	UNP Q9V1U8
E	121	PHE	ASN	conflict	UNP Q9V1U8
E	133	ILE	VAL	conflict	UNP Q9V1U8
E	137	ARG	LYS	conflict	UNP Q9V1U8
E	138	VAL	ILE	conflict	UNP Q9V1U8
E	149	ILE	LEU	conflict	UNP Q9V1U8
E	150	VAL	ILE	conflict	UNP Q9V1U8
E	151	SER	PRO	conflict	UNP Q9V1U8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	152	ILE	LEU	conflict	UNP Q9V1U8
E	153	ALA	SER	conflict	UNP Q9V1U8
E	204	ARG	LYS	conflict	UNP Q9V1U8
E	235	THR	ARG	conflict	UNP Q9V1U8
E	239	LYS	ARG	conflict	UNP Q9V1U8

- Molecule 13 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	217	Total	C	N	O	S	0	0
			1716	1084	319	305	8		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	17	GLU	GLN	conflict	UNP Q9V1V5
F	25	MET	LEU	conflict	UNP Q9V1V5
F	40	ARG	LYS	conflict	UNP Q9V1V5
F	65	VAL	ILE	conflict	UNP Q9V1V5
F	104	LYS	ARG	conflict	UNP Q9V1V5
F	144	ALA	THR	conflict	UNP Q9V1V5
F	155	ARG	LYS	conflict	UNP Q9V1V5
F	180	VAL	ILE	conflict	UNP Q9V1V5
F	188	PHE	LEU	conflict	UNP Q9V1V5
F	210	ARG	LYS	conflict	UNP Q9V1V5
F	212	ALA	VAL	conflict	UNP Q9V1V5
F	213	ILE	VAL	conflict	UNP Q9V1V5
F	214	SER	THR	conflict	UNP Q9V1V5
F	231	THR	ALA	conflict	UNP Q9V1V5
F	232	THR	SER	conflict	UNP Q9V1V5

- Molecule 14 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	125	Total	C	N	O	S	0	0
			984	623	180	179	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	SER	THR	conflict	UNP Q9UYS3
G	19	VAL	ILE	conflict	UNP Q9UYS3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	24	ALA	PRO	conflict	UNP Q9UYS3
G	26	THR	ALA	conflict	UNP Q9UYS3
G	40	ALA	VAL	conflict	UNP Q9UYS3
G	44	ASN	GLY	conflict	UNP Q9UYS3
G	61	LEU	MET	conflict	UNP Q9UYS3
G	86	VAL	ILE	conflict	UNP Q9UYS3

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	68	ARG	LYS	conflict	UNP Q9V1V0
I	83	VAL	ALA	conflict	UNP Q9V1V0
I	84	SER	ARG	conflict	UNP Q9V1V0
I	85	GLU	ASP	conflict	UNP Q9V1V0
I	86	PHE	TYR	conflict	UNP Q9V1V0
I	88	LYS	ARG	conflict	UNP Q9V1V0
I	117	ILE	ARG	conflict	UNP Q9V1V0

- Molecule 16 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	127	Total	C	N	O	S	0	0
			1004	622	207	174	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	10	LYS	ARG	conflict	UNP Q9UZL4
J	53	ARG	LYS	conflict	UNP Q9UZL4

- Molecule 17 is a protein called 30S ribosomal protein SX.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	C	57	Total	C	N	O	0	0
			286	171	57	58		

- Molecule 18 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	123	Total	C	N	O	S	0	0
			939	599	155	181	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	119	LYS	ARG	conflict	UNP P62008

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	102	Total	C	N	O	S	0	0
			822	507	159	152	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	8	ILE	LEU	conflict	UNP Q9V0V6
L	17	ASP	GLU	conflict	UNP Q9V0V6
L	48	THR	VAL	conflict	UNP Q9V0V6
L	68	VAL	ILE	conflict	UNP Q9V0V6

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	148	Total	C	N	O	S	0	0
			1189	746	237	200	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	3	ASN	ASP	conflict	UNP Q9V1A0
O	31	ILE	VAL	conflict	UNP Q9V1A0
O	67	ALA	GLN	conflict	UNP Q9V1A0

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	56	Total	C	N	O	S	0	0
			462	292	95	69	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	34	GLN	HIS	conflict	UNP P62012

- Molecule 22 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	67	Total	C	N	O	S	0	0
			556	353	105	95	3		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	17	VAL	PHE	conflict	UNP Q9V0G0
S	26	THR	ARG	conflict	UNP Q9V0G0
S	36	GLN	GLU	conflict	UNP Q9V0G0
S	54	VAL	ILE	conflict	UNP Q9V0G0
S	62	MET	GLU	conflict	UNP Q9V0G0

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	111	Total	C	N	O	S	0	0
			923	594	173	150	6		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	26	ARG	LYS	conflict	UNP Q9V1T9
T	28	PHE	LEU	conflict	UNP Q9V1T9
T	60	LYS	ASN	conflict	UNP Q9V1T9
T	72	ILE	VAL	conflict	UNP Q9V1T9
T	112	LYS	ARG	conflict	UNP Q9V1T9
T	114	GLU	GLN	conflict	UNP Q9V1T9
T	120	VAL	ILE	conflict	UNP Q9V1T9

- Molecule 24 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	144	Total	C	N	O	S	0	0
			1175	758	212	204	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	89	LYS	ARG	conflict	UNP Q9V0G8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	71	Total	C	N	O	S	0	0
			568	345	115	107	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	51	ILE	VAL	conflict	UNP P61029

- 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
			409	262	75	66	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	9	GLU	ILE	conflict	UNP P61238
Y	10	ILE	VAL	conflict	UNP P61238
Y	42	LYS	ARG	conflict	UNP P61238

- Molecule 27 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	6	ASN	SER	conflict	UNP Q9V109
H	113	GLN	LYS	conflict	UNP Q9V109
H	176	ASN	THR	conflict	UNP Q9V109

- Molecule 28 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	K	135	Total	C	N	O	S	0	0
			1072	671	205	190	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	35	ILE	LEU	conflict	UNP Q9V195
K	36	ILE	VAL	conflict	UNP Q9V195
K	67	GLU	GLN	conflict	UNP Q9V195
K	80	MET	ILE	conflict	UNP Q9V195
K	94	SER	ASN	conflict	UNP Q9V195
K	100	MET	ILE	conflict	UNP Q9V195

- Molecule 29 is a protein called 30S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	0	22	Total	C	N	O	S	0	0
			213	135	52	25	1		

- Molecule 30 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	76	Total	C	N	O	P	0	0
			1622	724	291	531	76		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	18	Total	C	N	O	P	0	0
			388	173	70	127	18		

- Molecule 32 is a protein called Protein translation factor SUI1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	83	Total	C	N	O	S	0	0
			662	418	116	124	4		

- Molecule 33 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	409	Total	C	N	O	S	0	0
			3171	2028	541	590	12		

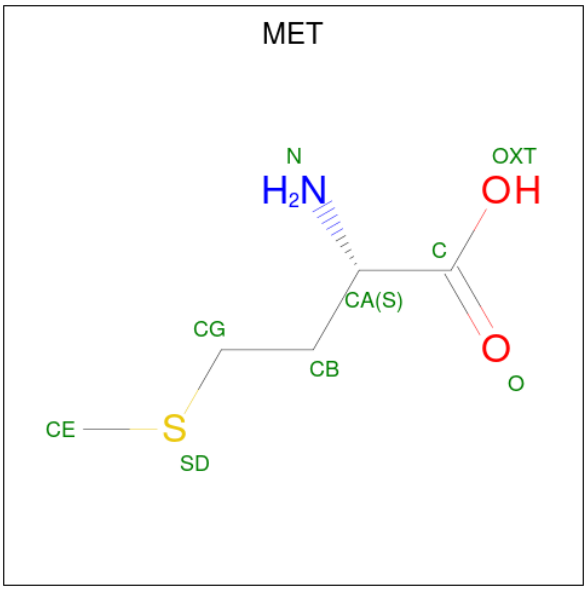
- Molecule 35 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	129	Total	C	N	O	S	0	0
			1034	660	172	192	10		

- Molecule 36 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	254	Total	C	N	O	S	0	0
			2033	1301	346	384	2		

- Molecule 37 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).

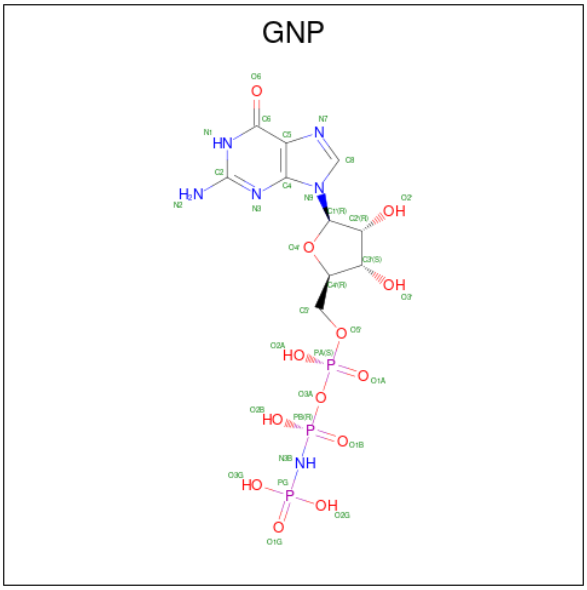


Mol	Chain	Residues	Atoms					AltConf
37	7	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	7	1	Total	Mg	0
			1	1	

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

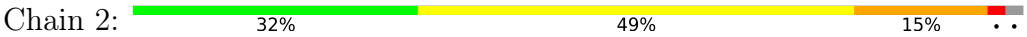
Mol	Chain	Residues	Atoms		AltConf
40	8	1	Total	Zn	0
			1	1	

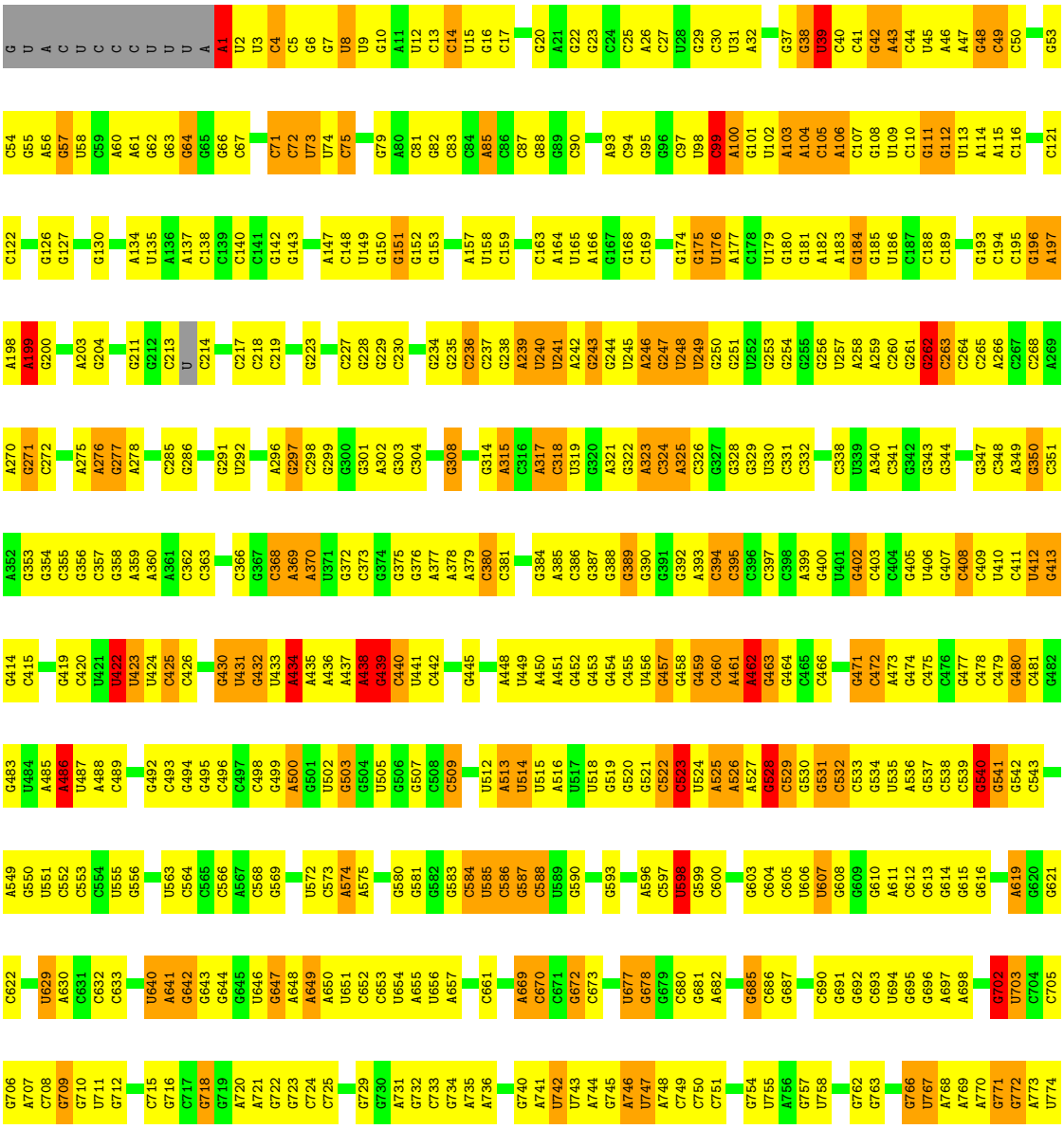
3 Residue-property plots (i)

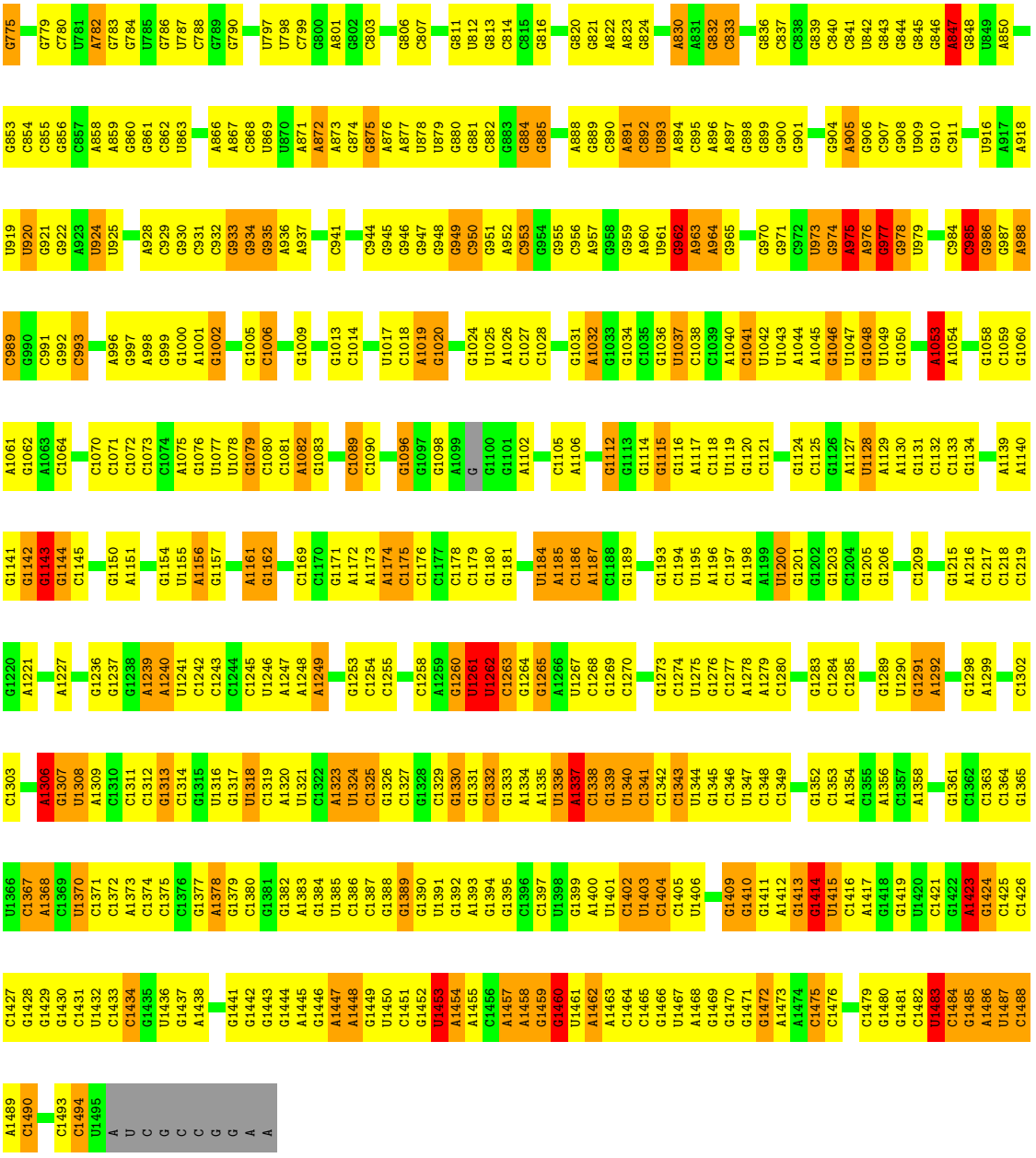
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

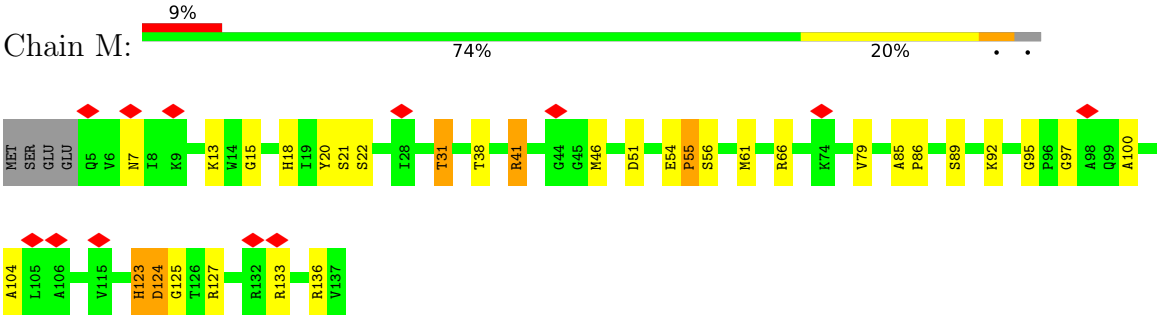






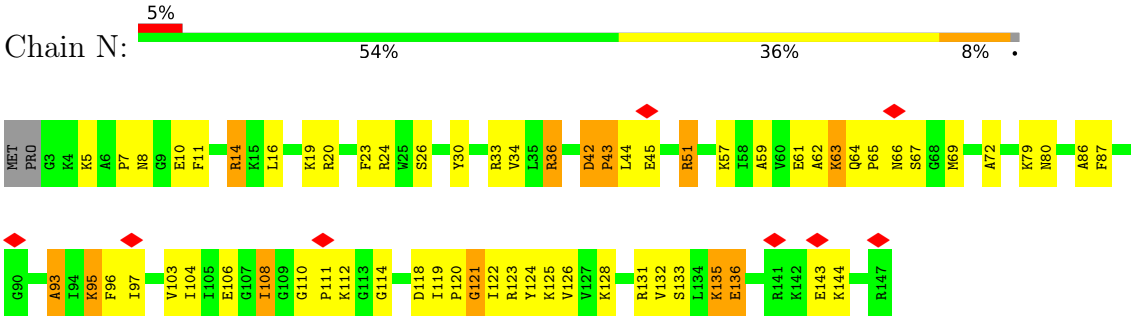
• Molecule 2: 30S ribosomal protein S11

Chain M:



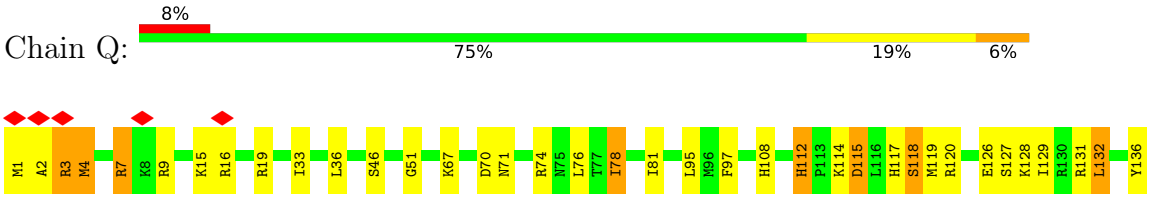
• Molecule 3: 30S ribosomal protein S12

Chain N:



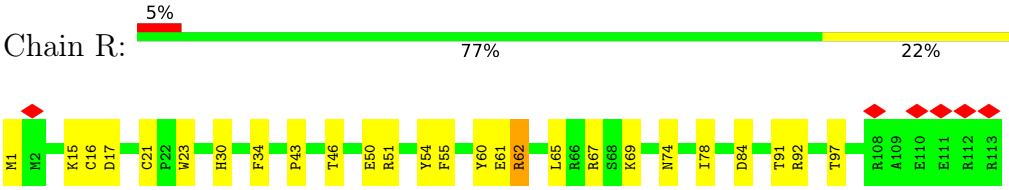
• Molecule 4: 30S ribosomal protein S15

Chain Q:



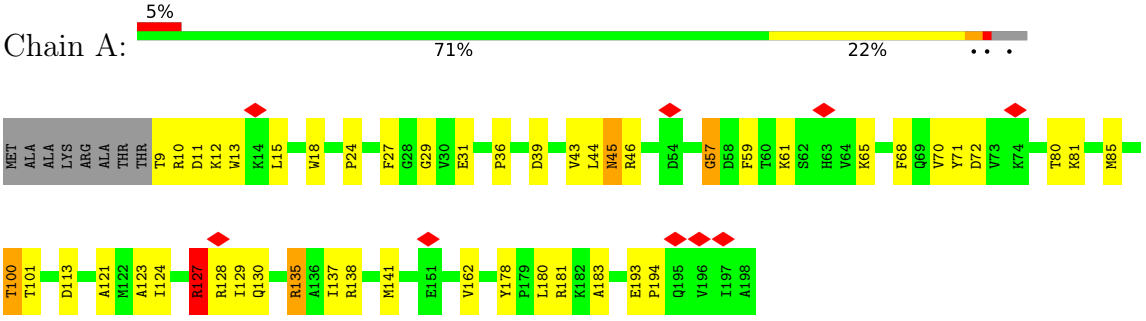
• Molecule 5: 30S ribosomal protein S17P

Chain R:



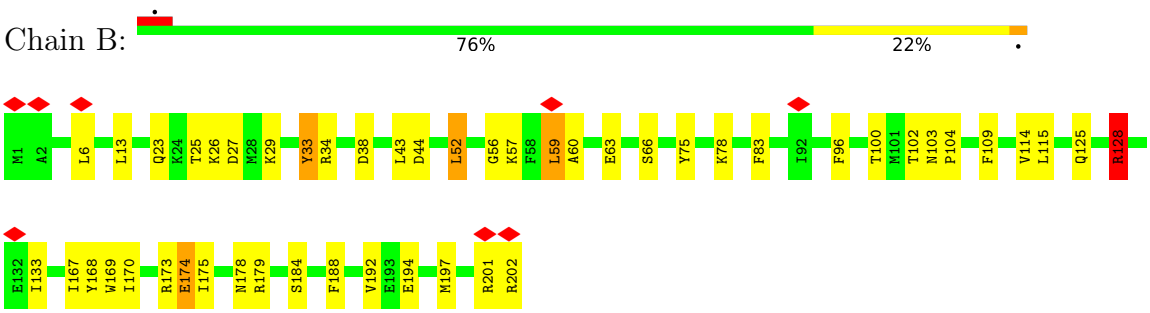
• Molecule 6: 30S ribosomal protein S3Ae

Chain A:



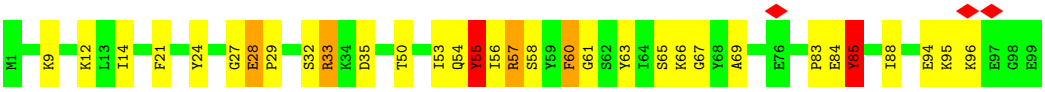
• Molecule 7: 30S ribosomal protein S2

Chain B:



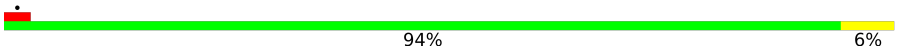
• Molecule 8: 30S ribosomal protein S24e

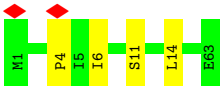
Chain V:



• Molecule 9: 30S ribosomal protein S27e

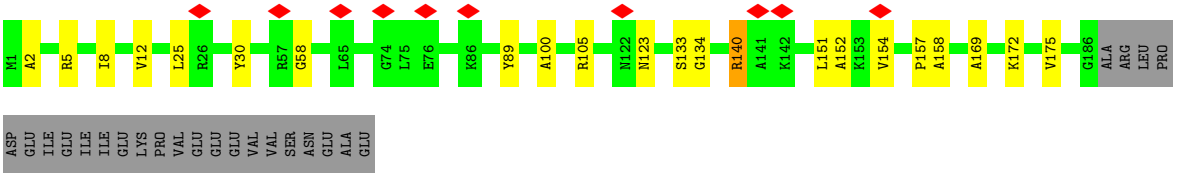
Chain W:





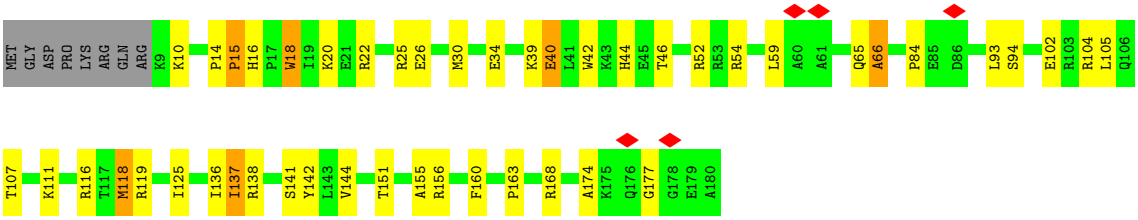
• Molecule 10: 30S ribosomal protein S3

Chain Z:



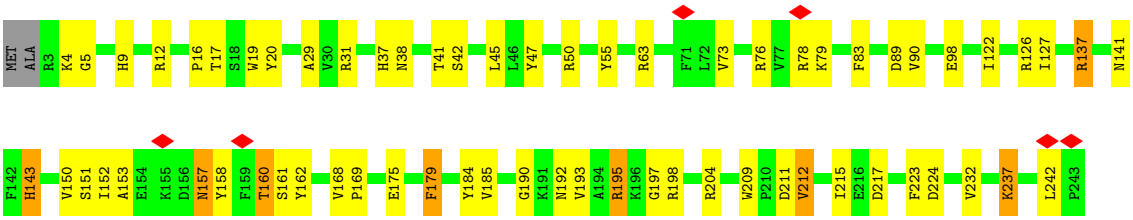
• Molecule 11: 30S ribosomal protein S4

Chain D:

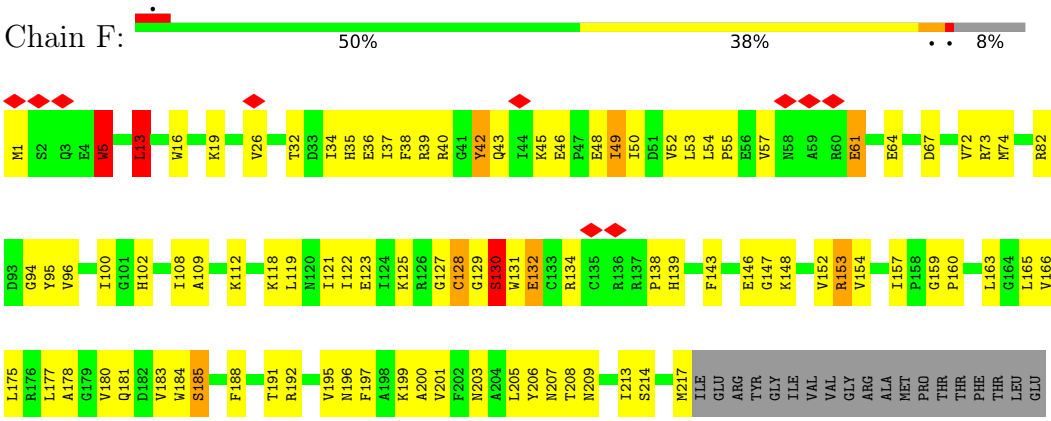


• Molecule 12: 30S ribosomal protein S4e

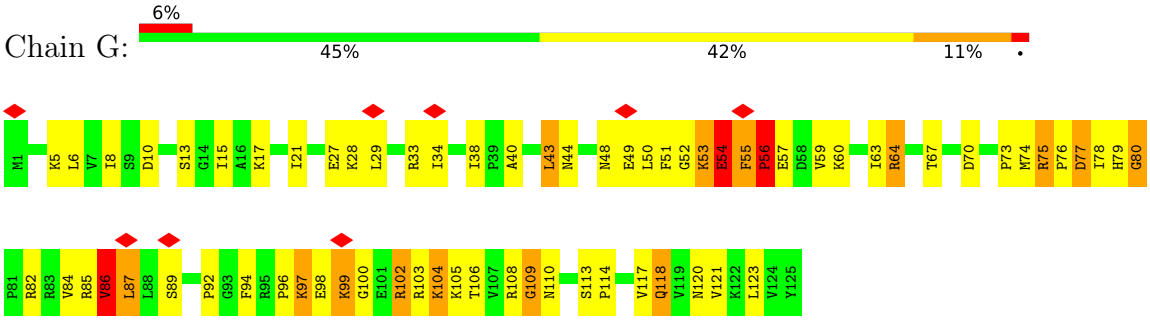
Chain E:



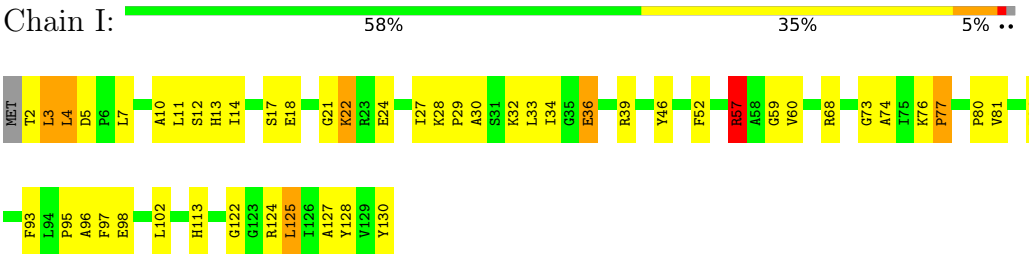
• Molecule 13: 30S ribosomal protein S5



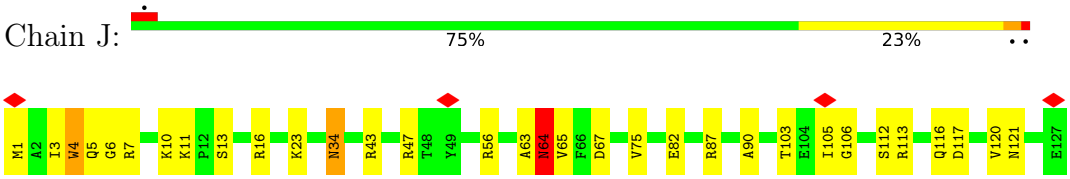
• Molecule 14: 30S ribosomal protein S6e



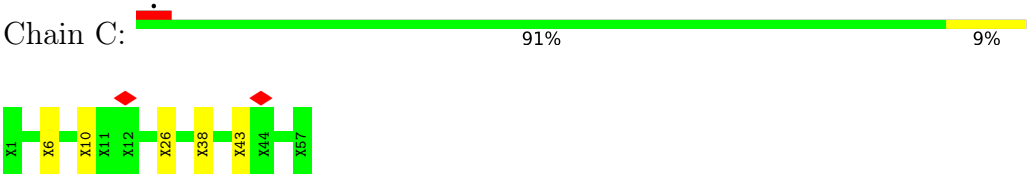
• Molecule 15: 30S ribosomal protein S8



• Molecule 16: 30S ribosomal protein S8e

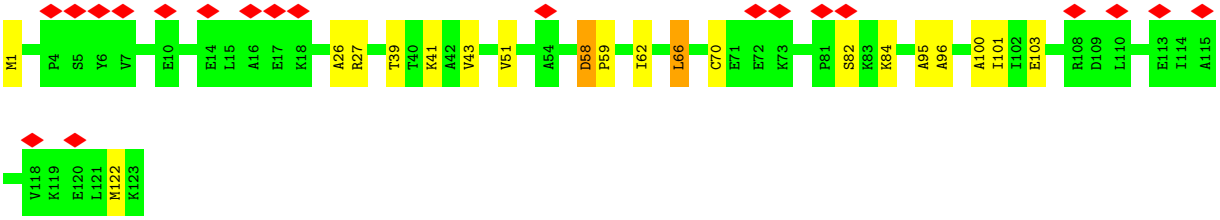


• Molecule 17: 30S ribosomal protein SX



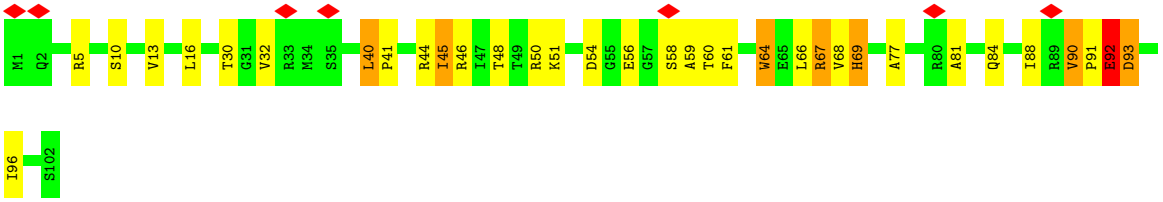
• Molecule 18: 50S ribosomal protein L7Ae

Chain 3:



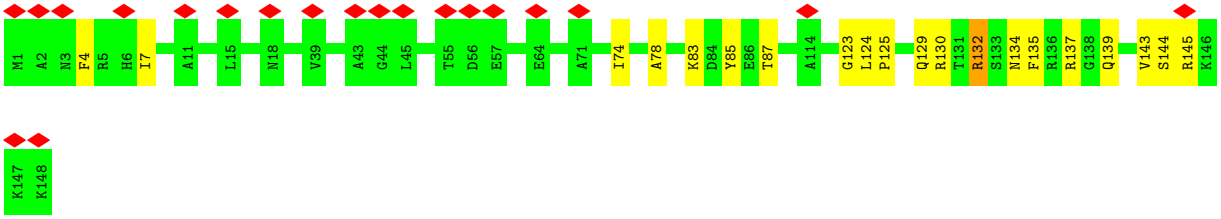
• Molecule 19: 30S ribosomal protein S10

Chain L:



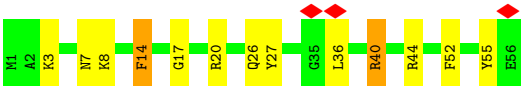
• Molecule 20: 30S ribosomal protein S13

Chain O:



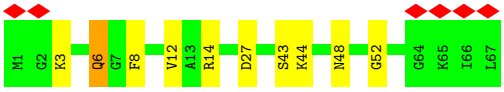
• Molecule 21: 30S ribosomal protein S14 type Z

Chain P:



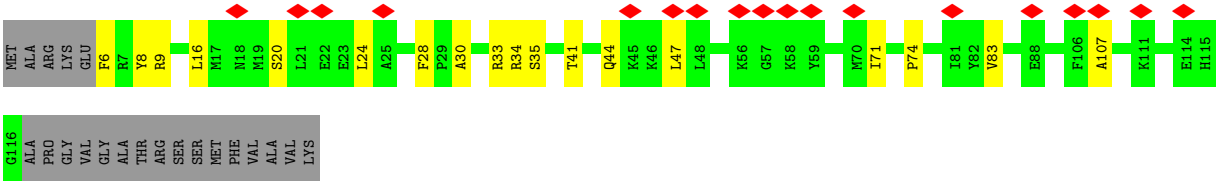
• Molecule 22: 30S ribosomal protein S17e

Chain S:



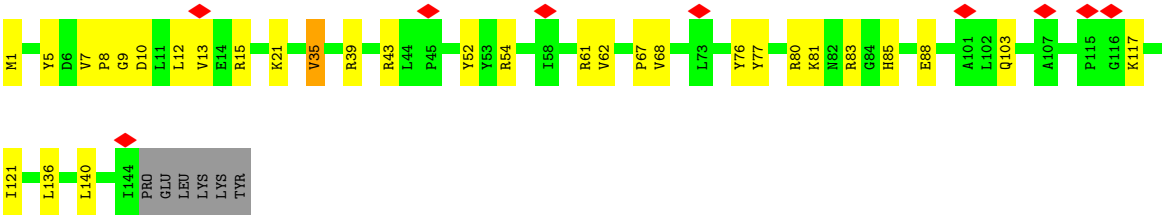
• Molecule 23: 30S ribosomal protein S19

Chain T:



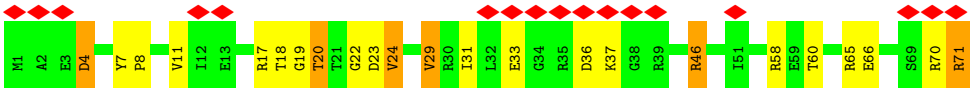
• Molecule 24: 30S ribosomal protein S19e

Chain U:



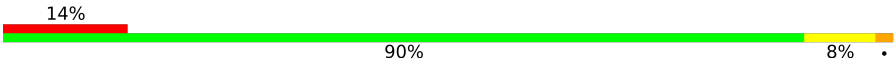
• Molecule 25: 30S ribosomal protein S28e

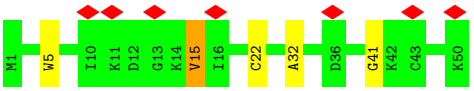
Chain X:



• Molecule 26: 30S ribosomal protein S27ae

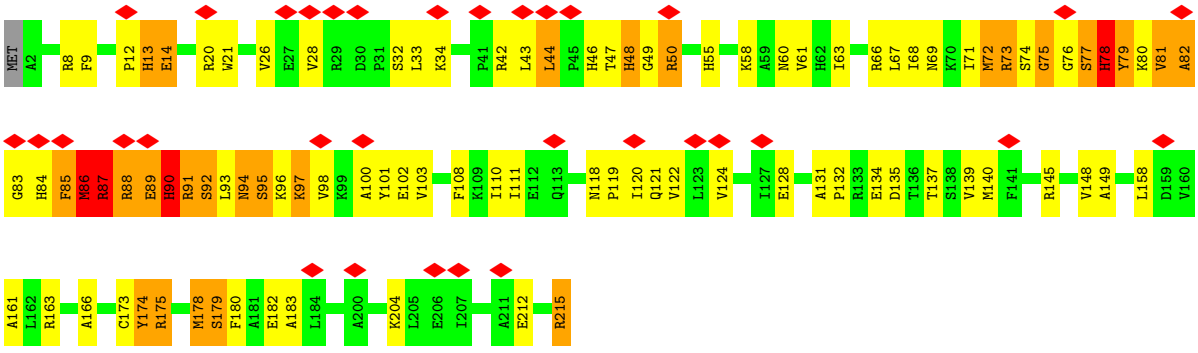
Chain Y:





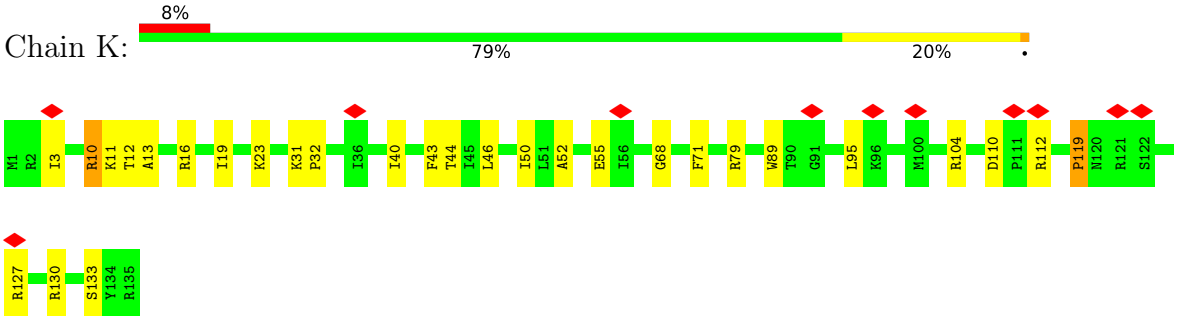
• Molecule 27: 30S ribosomal protein S7

Chain H:



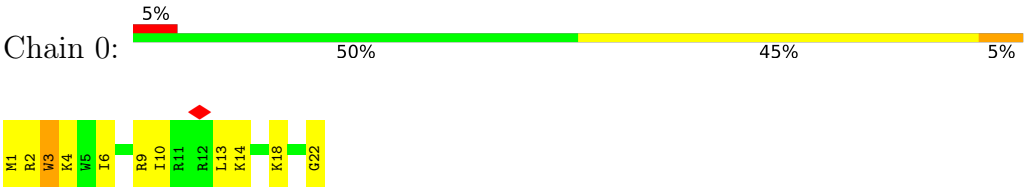
• Molecule 28: 30S ribosomal protein S9

Chain K:



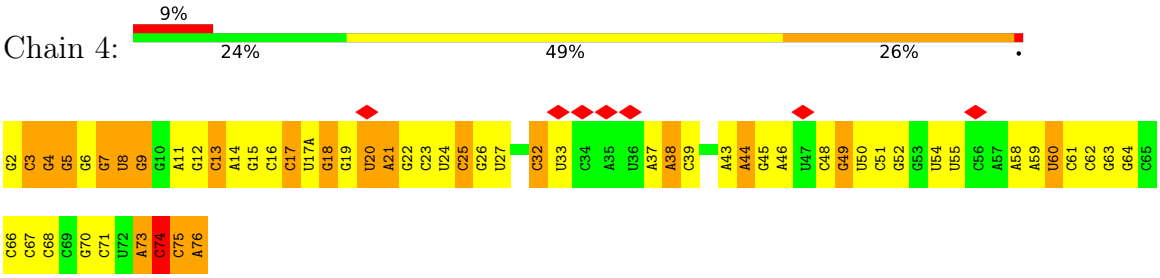
• Molecule 29: 30S ribosomal protein eL41

Chain 0:



• Molecule 30: initiator Met-tRNA fMet from E. coli (A1U72 variant)

Chain 4:

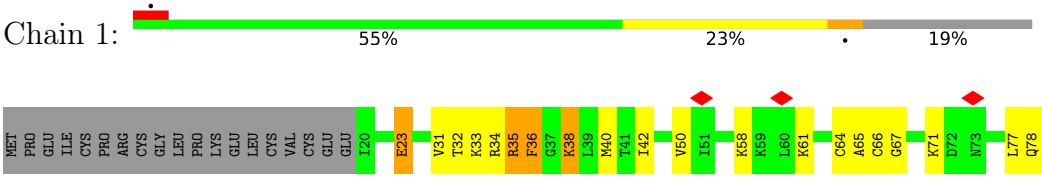


• Molecule 31: mRNA

Chain 5:

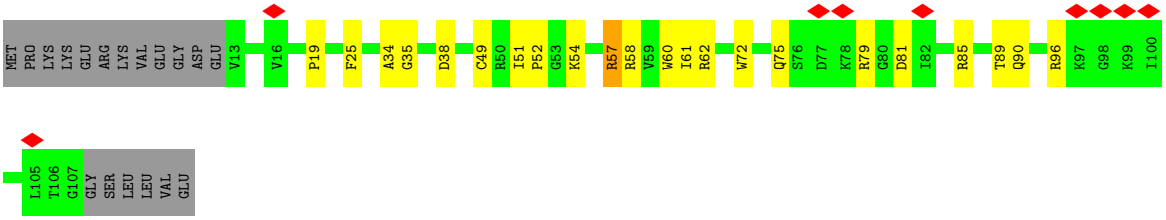
• Molecule 32: Protein translation factor SUI1 homolog

Chain 1:



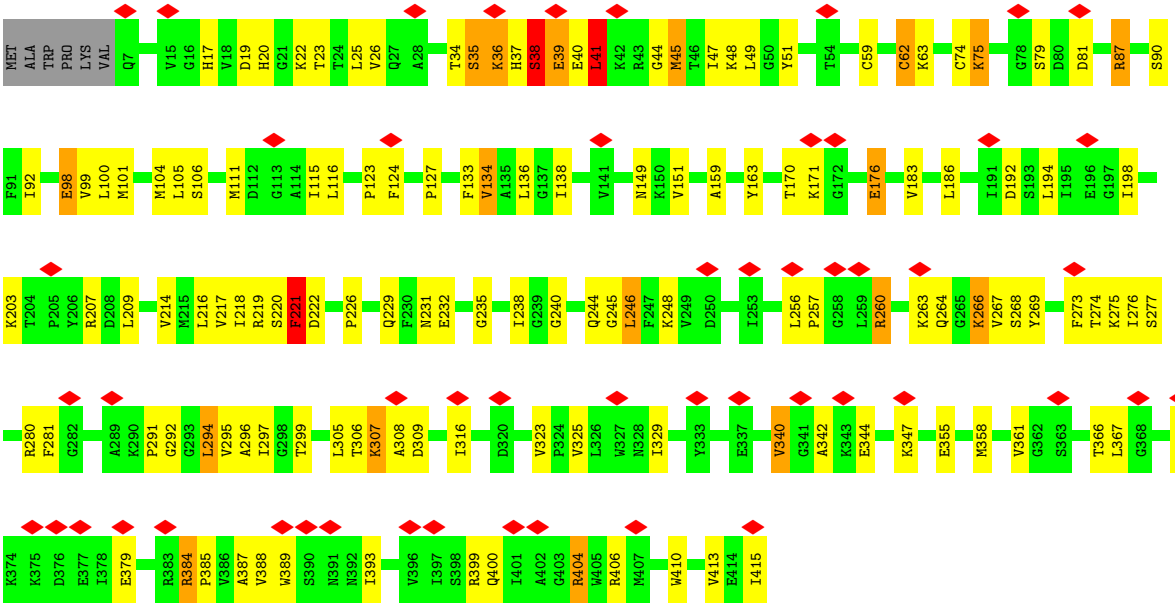
• Molecule 33: Translation initiation factor 1A

Chain 6:



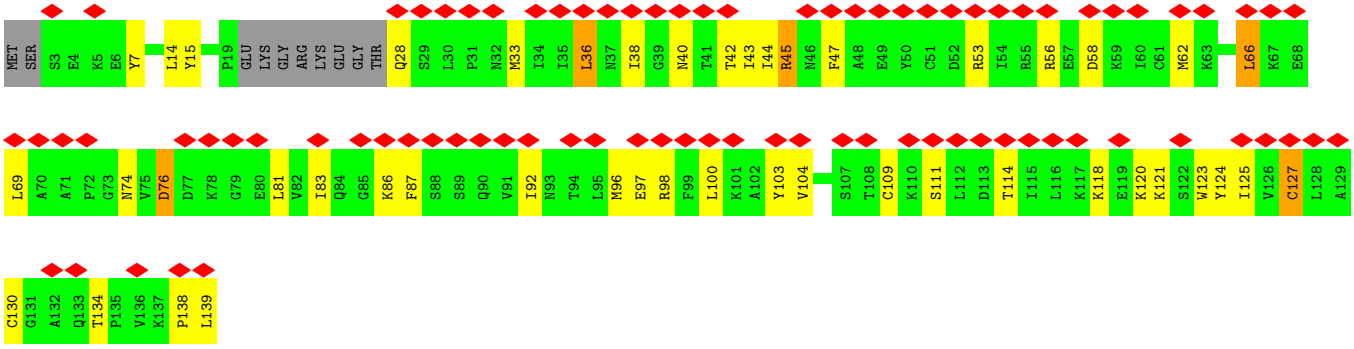
• Molecule 34: Translation initiation factor 2 subunit gamma

Chain 7:



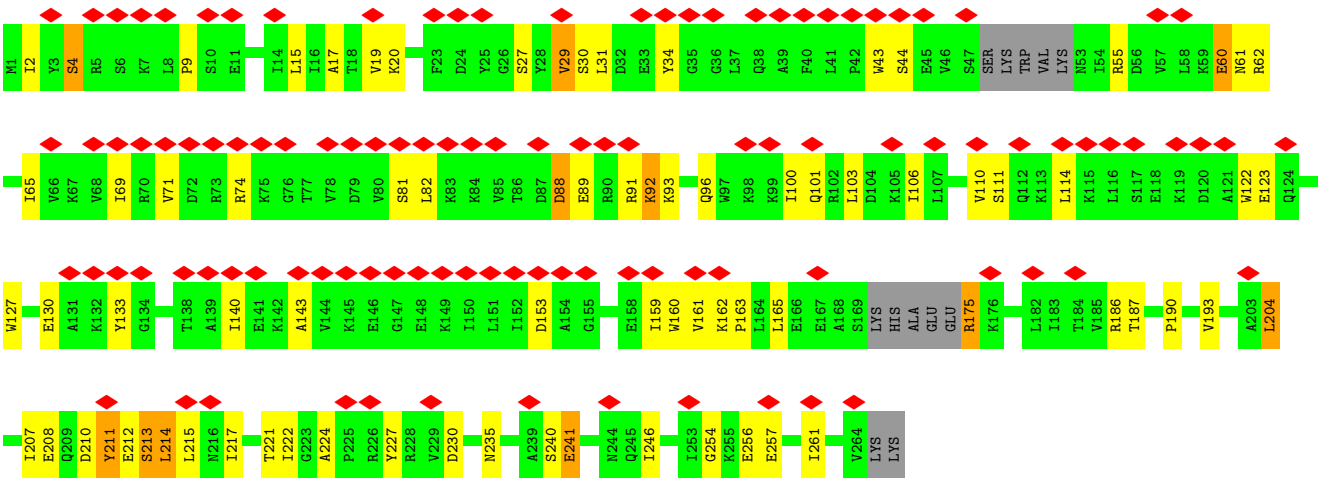
• Molecule 35: Translation initiation factor 2 subunit beta

Chain 8:



• Molecule 36: Translation initiation factor 2 subunit alpha

Chain 9:


M1 I2 Y3 S4 R5 S6 K7 L8 P9 S10 E11 I14 L15 I16 A17 T18 V19 K20 F23 D24 Y25 G26 S27 Y28 V29 S30 L31 D32 E33 Y34 G35 G36 L37 Q38 A39 F40 L41 P42 W43 S44 E45 V46 S47 SER LYS TRP VAL LYS N53 I54 R55 D56 V57 L58 K59 E60 N61 R62
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 Q96 W97 K98 K99 I100 Q101 R102 L103 D104 K105 I106 L107 V110 S111 Q112 K113 L114 K115 L116 S117 E118 K119 D120 A121 W122 E123 Q124
W127 E130 A131 K132 Y133 G134 T138 A139 I140 E141 K142 A143 V144 K145 E146 G147 E148 K149 I150 L151 I152 D153 A154 G155 E158 I159 W160 V161 K162 P163 L164 L165 E166 E167 A168 S169 LYS HIS ALA GLU GLU R175 K176 L182 I183 T184 V185 R186 T187 P190 V193 A203 L204
I207 E208 Q209 D210 Y211 E212 S213 L214 L215 N216 I217 T221 I222 G223 A224 P225 R226 Y227 R228 V229 D230 N235 A239 S240 E241 N244 Q245 I246 I253 G254 K255 E256 E257 I261 V264 LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12600	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 ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	389.76, 389.76, 389.76	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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: H2U, OMC, PSU, 5MU, GNP, MG, 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	0.63	17/35964 (0.0%)	0.90	54/56130 (0.1%)
2	M	0.77	0/1022	0.97	3/1375 (0.2%)
3	N	0.81	0/1156	1.07	3/1535 (0.2%)
4	Q	0.75	0/1338	0.99	5/1797 (0.3%)
5	R	0.72	0/956	0.95	2/1287 (0.2%)
6	A	0.68	0/1585	0.88	2/2124 (0.1%)
7	B	0.75	0/1654	0.99	3/2233 (0.1%)
8	V	0.67	0/839	1.00	3/1122 (0.3%)
9	W	0.65	0/485	0.88	0/651
10	Z	0.69	0/1480	0.87	2/1985 (0.1%)
11	D	0.75	2/1457 (0.1%)	0.94	5/1953 (0.3%)
12	E	0.68	0/2025	0.95	8/2732 (0.3%)
13	F	0.77	1/1745 (0.1%)	1.00	3/2350 (0.1%)
14	G	0.74	0/999	1.09	7/1337 (0.5%)
15	I	0.71	1/1049 (0.1%)	0.96	4/1408 (0.3%)
16	J	0.67	0/1013	0.92	0/1349
18	3	0.86	0/951	0.90	1/1281 (0.1%)
19	L	0.76	1/830 (0.1%)	1.08	3/1113 (0.3%)
20	O	0.82	0/1208	0.96	2/1619 (0.1%)
21	P	0.73	0/471	1.11	1/620 (0.2%)
22	S	0.80	0/562	0.96	1/744 (0.1%)
23	T	0.84	0/942	0.91	0/1257
24	U	0.86	0/1203	0.95	3/1621 (0.2%)
25	X	0.78	0/570	1.07	2/760 (0.3%)
26	Y	0.76	0/421	0.78	0/558
27	H	0.95	1/1765 (0.1%)	1.19	12/2371 (0.5%)
28	K	0.78	0/1088	0.92	3/1455 (0.2%)
29	0	1.17	2/216 (0.9%)	1.10	0/279
30	4	0.62	0/1721	0.91	1/2682 (0.0%)
31	5	0.49	0/434	0.77	0/675
32	1	0.61	0/666	0.82	0/882
33	6	0.70	0/791	0.92	2/1066 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	7	0.72	0/3227	0.84	4/4367 (0.1%)
35	8	0.85	0/1048	0.85	0/1406
36	9	0.84	0/2057	0.88	1/2767 (0.0%)
All	All	0.70	25/74938 (0.0%)	0.93	140/108891 (0.1%)

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
3	N	0	2
4	Q	0	1
5	R	0	1
7	B	0	1
8	V	0	3
10	Z	0	1
12	E	0	1
13	F	0	2
14	G	1	7
15	I	0	1
16	J	0	3
20	O	0	1
25	X	0	3
27	H	4	9
28	K	0	2
34	7	0	2
35	8	0	1
36	9	0	1
All	All	5	42

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1019	A	O3'-P	32.96	2.00	1.61
29	0	3	TRP	CB-CG	-7.21	1.37	1.50
1	2	357	C	O3'-P	-6.99	1.52	1.61
1	2	830	A	O3'-P	-6.54	1.53	1.61
1	2	1471	G	O3'-P	-6.51	1.53	1.61

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1019	A	P-O3'-C3'	21.15	145.09	119.70
1	2	1414	G	O5'-P-OP1	-15.20	92.02	105.70
1	2	962	G	O5'-P-OP1	-13.71	93.36	105.70
1	2	1019	A	O3'-P-O5'	10.24	123.46	104.00
27	H	87	ARG	N-CA-C	9.96	137.90	111.00

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	G	53	LYS	CA
27	H	85	PHE	CA
27	H	86	MET	CA
27	H	87	ARG	CA
27	H	96	LYS	CA

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	B	6	LEU	Peptide
3	N	121	GLY	Peptide
3	N	5	LYS	Peptide
4	Q	2	ALA	Peptide
5	R	34	PHE	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	32135	0	16233	1310	0
2	M	1004	0	1041	15	0
3	N	1140	0	1235	48	0
4	Q	1310	0	1392	21	0
5	R	934	0	960	17	0
6	A	1559	0	1648	32	0
7	B	1623	0	1685	36	0
8	V	823	0	847	26	0
9	W	478	0	524	2	0
10	Z	1459	0	1549	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	1434	0	1498	27	0
12	E	1976	0	2046	36	0
13	F	1716	0	1770	105	0
14	G	984	0	1044	98	0
15	I	1028	0	1065	45	0
16	J	1004	0	1088	16	0
17	C	286	0	61	3	0
18	3	939	0	994	6	0
19	L	822	0	870	26	0
20	O	1189	0	1248	11	0
21	P	462	0	492	7	0
22	S	556	0	604	5	0
23	T	923	0	986	6	0
24	U	1175	0	1216	22	0
25	X	568	0	600	23	0
26	Y	409	0	410	4	0
27	H	1728	0	1775	125	0
28	K	1072	0	1128	14	0
29	0	213	0	250	10	0
30	4	1622	0	830	71	0
31	5	388	0	193	19	0
32	1	662	0	705	22	0
33	6	777	0	804	18	0
34	7	3171	0	3292	111	0
35	8	1034	0	1078	31	0
36	9	2033	0	2144	40	0
37	7	8	0	8	11	0
38	7	1	0	0	0	0
39	7	32	0	13	1	0
40	8	1	0	0	1	0
All	All	70678	0	55326	2020	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 16.

The worst 5 of 2020 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)
35:8:127:CYS:SG	40:8:201:ZN:ZN	1.06	1.41
1:2:8:U:N3	1:2:873:A:N6	1.70	1.36
1:2:1019:A:O3'	1:2:1020:G:P	2.00	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:920:U:H3	1:2:1161:A:N6	1.42	1.16
1:2:516:A:N6	1:2:842:U:H3	1.48	1.11

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	M	131/137 (96%)	116 (88%)	12 (9%)	3 (2%)	5 27
3	N	143/147 (97%)	119 (83%)	12 (8%)	12 (8%)	0 9
4	Q	156/158 (99%)	140 (90%)	12 (8%)	4 (3%)	4 25
5	R	111/113 (98%)	104 (94%)	6 (5%)	1 (1%)	14 51
6	A	188/198 (95%)	163 (87%)	15 (8%)	10 (5%)	1 15
7	B	200/202 (99%)	170 (85%)	28 (14%)	2 (1%)	13 49
8	V	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	1 15
9	W	61/63 (97%)	52 (85%)	8 (13%)	1 (2%)	8 37
10	Z	184/210 (88%)	167 (91%)	15 (8%)	2 (1%)	12 46
11	D	170/180 (94%)	148 (87%)	15 (9%)	7 (4%)	2 17
12	E	239/243 (98%)	209 (87%)	21 (9%)	9 (4%)	2 19
13	F	215/236 (91%)	176 (82%)	32 (15%)	7 (3%)	3 20
14	G	123/125 (98%)	97 (79%)	15 (12%)	11 (9%)	0 8
15	I	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	8 37
16	J	125/127 (98%)	106 (85%)	13 (10%)	6 (5%)	2 16
18	3	121/123 (98%)	102 (84%)	14 (12%)	5 (4%)	2 17
19	L	100/102 (98%)	90 (90%)	3 (3%)	7 (7%)	1 11
20	O	146/148 (99%)	122 (84%)	18 (12%)	6 (4%)	2 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	P	54/56 (96%)	43 (80%)	10 (18%)	1 (2%)	6 31
22	S	65/67 (97%)	63 (97%)	2 (3%)	0	100 100
23	T	109/132 (83%)	97 (89%)	9 (8%)	3 (3%)	4 24
24	U	142/150 (95%)	129 (91%)	10 (7%)	3 (2%)	5 29
25	X	69/71 (97%)	56 (81%)	11 (16%)	2 (3%)	3 23
26	Y	48/50 (96%)	40 (83%)	8 (17%)	0	100 100
27	H	212/215 (99%)	161 (76%)	32 (15%)	19 (9%)	0 8
28	K	133/135 (98%)	117 (88%)	13 (10%)	3 (2%)	5 27
29	0	20/22 (91%)	20 (100%)	0	0	100 100
32	1	81/102 (79%)	71 (88%)	8 (10%)	2 (2%)	4 26
33	6	89/113 (79%)	88 (99%)	1 (1%)	0	100 100
34	7	407/415 (98%)	337 (83%)	50 (12%)	20 (5%)	2 16
35	8	125/139 (90%)	98 (78%)	25 (20%)	2 (2%)	8 37
36	9	247/266 (93%)	204 (83%)	35 (14%)	8 (3%)	3 21
All	All	4438/4674 (95%)	3797 (86%)	478 (11%)	163 (4%)	4 19

5 of 163 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	36	ARG
3	N	42	ASP
3	N	43	PRO
3	N	44	LEU
3	N	63	LYS

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	M	100/104 (96%)	91 (91%)	9 (9%)	8 24
3	N	118/121 (98%)	105 (89%)	13 (11%)	5 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	Q	143/143 (100%)	131 (92%)	12 (8%)	9 28
5	R	102/102 (100%)	99 (97%)	3 (3%)	37 57
6	A	166/171 (97%)	160 (96%)	6 (4%)	30 51
7	B	173/173 (100%)	161 (93%)	12 (7%)	13 33
8	V	89/89 (100%)	81 (91%)	8 (9%)	8 24
9	W	54/54 (100%)	52 (96%)	2 (4%)	29 50
10	Z	145/167 (87%)	142 (98%)	3 (2%)	48 67
11	D	153/160 (96%)	145 (95%)	8 (5%)	19 41
12	E	212/213 (100%)	194 (92%)	18 (8%)	8 27
13	F	181/197 (92%)	173 (96%)	8 (4%)	24 45
14	G	108/108 (100%)	93 (86%)	15 (14%)	3 13
15	I	107/108 (99%)	96 (90%)	11 (10%)	6 20
16	J	103/103 (100%)	99 (96%)	4 (4%)	27 48
18	3	99/99 (100%)	93 (94%)	6 (6%)	15 37
19	L	91/91 (100%)	85 (93%)	6 (7%)	14 35
20	O	122/122 (100%)	118 (97%)	4 (3%)	33 53
21	P	46/46 (100%)	41 (89%)	5 (11%)	5 18
22	S	61/61 (100%)	58 (95%)	3 (5%)	21 42
23	T	99/114 (87%)	95 (96%)	4 (4%)	27 47
24	U	121/127 (95%)	114 (94%)	7 (6%)	17 38
25	X	60/60 (100%)	53 (88%)	7 (12%)	4 16
26	Y	41/41 (100%)	38 (93%)	3 (7%)	11 31
27	H	183/184 (100%)	167 (91%)	16 (9%)	8 25
28	K	111/111 (100%)	102 (92%)	9 (8%)	9 29
29	0	21/21 (100%)	21 (100%)	0	100 100
32	1	73/91 (80%)	66 (90%)	7 (10%)	7 22
33	6	83/99 (84%)	76 (92%)	7 (8%)	9 28
34	7	352/357 (99%)	315 (90%)	37 (10%)	5 19
35	8	118/126 (94%)	106 (90%)	12 (10%)	6 20
36	9	227/239 (95%)	198 (87%)	29 (13%)	3 14
All	All	3862/4002 (96%)	3568 (92%)	294 (8%)	13 30

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	7	134	VAL
36	9	213	SER
34	7	229	GLN
35	8	98	ARG
13	F	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
16	J	52	ASN
27	H	193	ASN
16	J	121	ASN
24	U	103	GLN
34	7	37	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1493/1519 (98%)	335 (22%)	113 (7%)
30	4	75/76 (98%)	28 (37%)	3 (4%)
31	5	17/26 (65%)	10 (58%)	3 (17%)
All	All	1585/1621 (97%)	373 (23%)	119 (7%)

5 of 373 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	4	C
1	2	14	C
1	2	25	C
1	2	38	G

5 of 119 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	919	U
1	2	1460	G
1	2	1017	U
1	2	1459	G

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Mol	Chain	Res	Type
31	5	818	A

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

4 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	$\#\|Z\| > 2$
30	H2U	4	20	30	18,21,22	1.00	1 (5%)	21,30,33	1.90	6 (28%)
30	5MU	4	54	30	19,22,23	1.45	4 (21%)	28,32,35	1.83	8 (28%)
30	PSU	4	55	30	18,21,22	1.47	2 (11%)	22,30,33	2.11	5 (22%)
30	OMC	4	32	30	19,22,23	1.13	1 (5%)	26,31,34	1.31	3 (11%)

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
30	H2U	4	20	30	-	3/7/38/39	0/2/2/2
30	5MU	4	54	30	-	0/7/25/26	0/2/2/2
30	PSU	4	55	30	-	0/7/25/26	0/2/2/2
30	OMC	4	32	30	-	2/9/27/28	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	55	PSU	C6-C5	4.92	1.41	1.35
30	4	54	5MU	C6-C5	3.45	1.40	1.34
30	4	32	OMC	C6-C5	2.65	1.41	1.35
30	4	54	5MU	C4-C5	2.53	1.49	1.44
30	4	54	5MU	C2-N1	2.44	1.42	1.38

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	55	PSU	C6-C5-C4	-5.28	114.51	118.20
30	4	20	H2U	O4'-C1'-N1	4.91	115.98	109.30
30	4	54	5MU	N3-C2-N1	4.70	121.12	114.89
30	4	55	PSU	N1-C2-N3	4.69	120.44	115.13
30	4	20	H2U	C5-C4-N3	3.92	121.05	116.65

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	4	20	H2U	C4'-C5'-O5'-P
30	4	20	H2U	O4'-C1'-N1-C2
30	4	20	H2U	O4'-C1'-N1-C6
30	4	32	OMC	O4'-C4'-C5'-O5'
30	4	32	OMC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
39	GNP	7	503	38	29,34,34	2.66	8 (27%)	33,54,54	2.46	8 (24%)
37	MET	7	501	-	6,7,8	0.95	1 (16%)	2,7,9	0.42	0

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
39	GNP	7	503	38	-	3/14/38/38	0/3/3/3
37	MET	7	501	-	-	4/5/6/8	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	503	GNP	PB-O1B	9.32	1.61	1.46
39	7	503	GNP	C5-C6	5.14	1.50	1.41
39	7	503	GNP	PG-N3B	4.65	1.75	1.63
39	7	503	GNP	PB-N3B	4.59	1.75	1.63
39	7	503	GNP	PB-O2B	-3.17	1.48	1.56

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	7	503	GNP	C2-N3-C4	7.52	123.95	115.36
39	7	503	GNP	PB-O3A-PA	-5.29	114.00	132.62
39	7	503	GNP	C4-C5-C6	-4.86	116.16	120.80
39	7	503	GNP	N3-C2-N1	-4.69	120.97	127.22
39	7	503	GNP	C2-N1-C6	3.97	122.24	115.93

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	7	501	MET	O-C-CA-CB
37	7	501	MET	N-CA-CB-CG
39	7	503	GNP	PB-N3B-PG-O1G
39	7	503	GNP	PG-N3B-PB-O1B
39	7	503	GNP	PG-N3B-PB-O3A

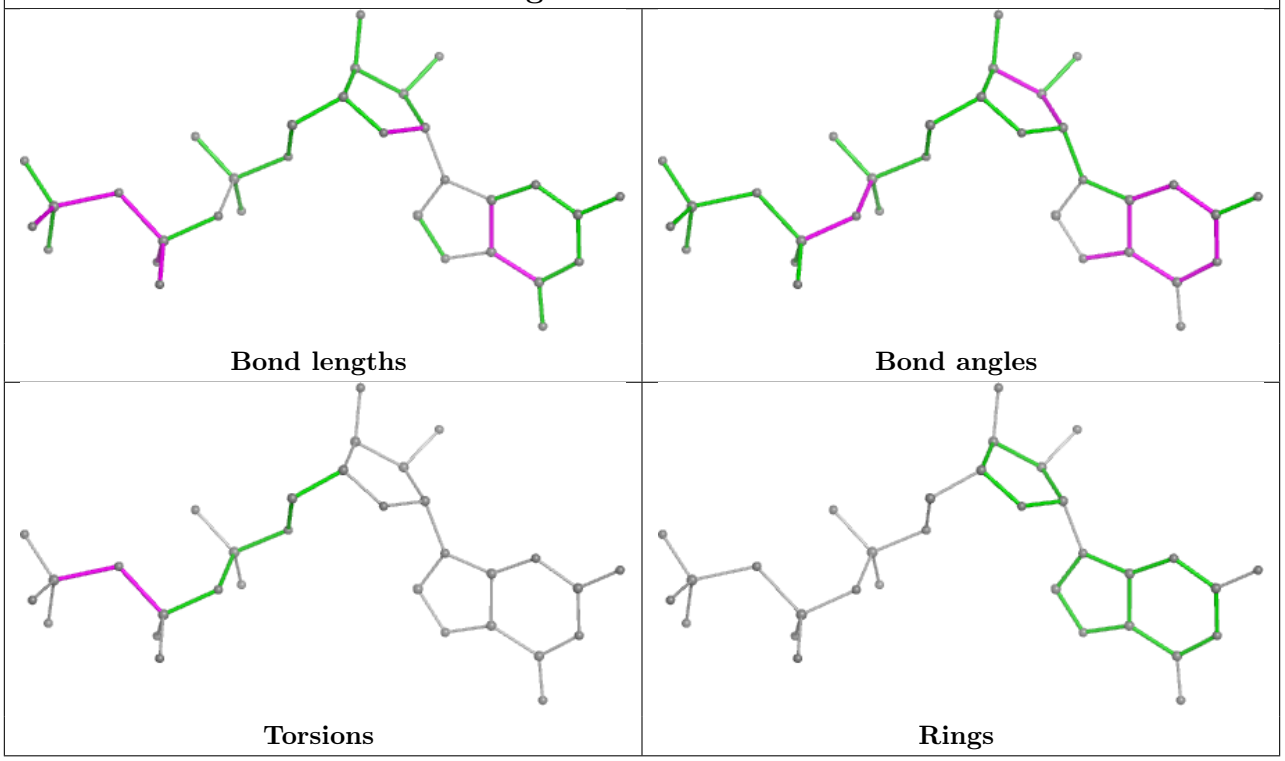
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	7	503	GNP	1	0
37	7	501	MET	11	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.

Ligand GNP 7 503



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
1	2	3

Continued on next page...

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Mol	Chain	Number of breaks
33	6	2
36	9	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1342:C	O3'	1343:C	P	3.20
1	9	1:MET	C	2:ILE	N	3.16
1	6	76:SER	C	77:ASP	N	3.11
1	2	1060:G	O3'	1061:A	P	2.56
1	6	89:THR	C	90:GLN	N	2.54

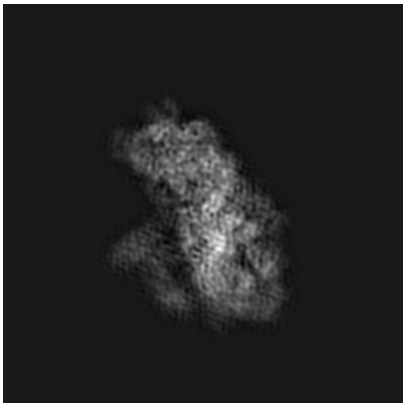
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8148. These allow visual inspection of the internal detail of the map and identification of artifacts.

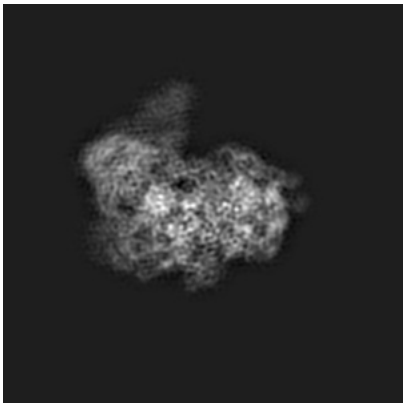
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

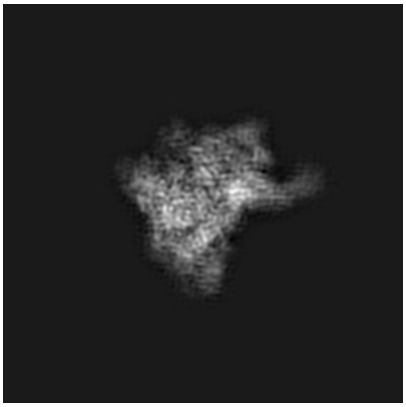
6.1.1 Primary map



X



Y

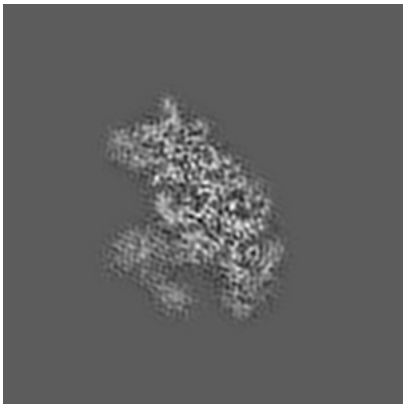


Z

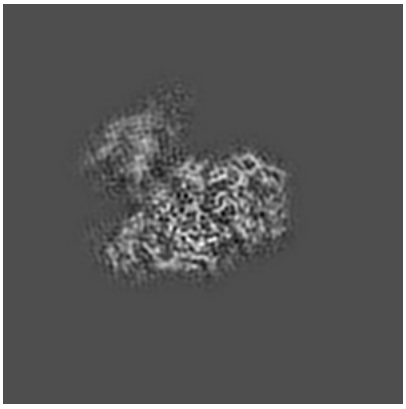
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 174



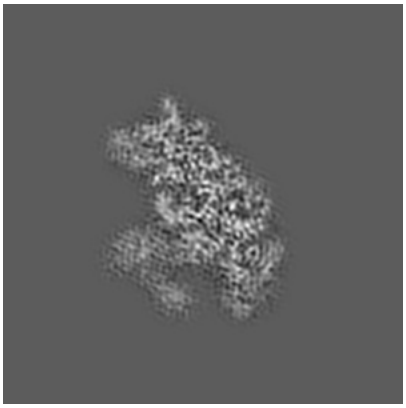
Y Index: 174

Z Index: 174

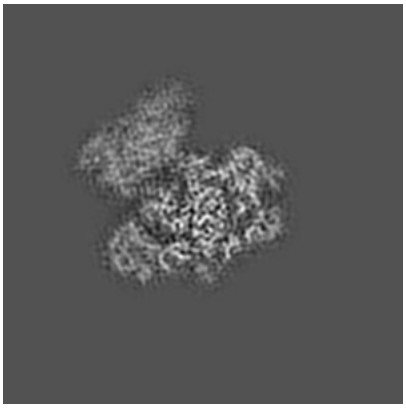
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 174



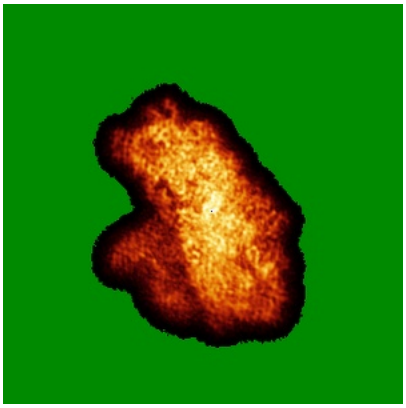
Y Index: 181

Z Index: 203

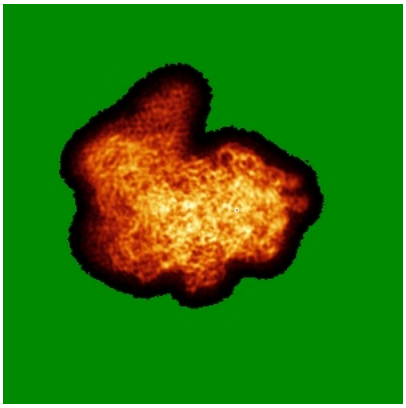
The images above show the largest variance slices of the map in three orthogonal directions.

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

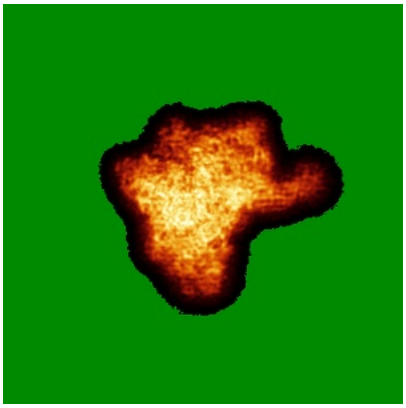
6.4.1 Primary map



X



Y

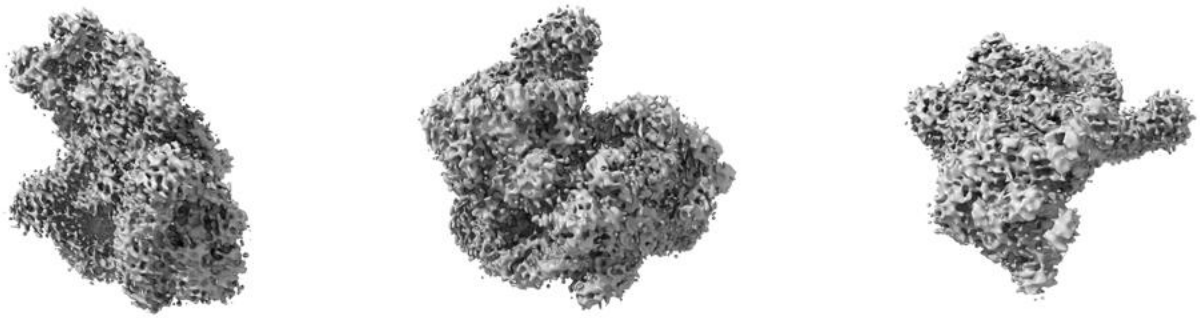


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

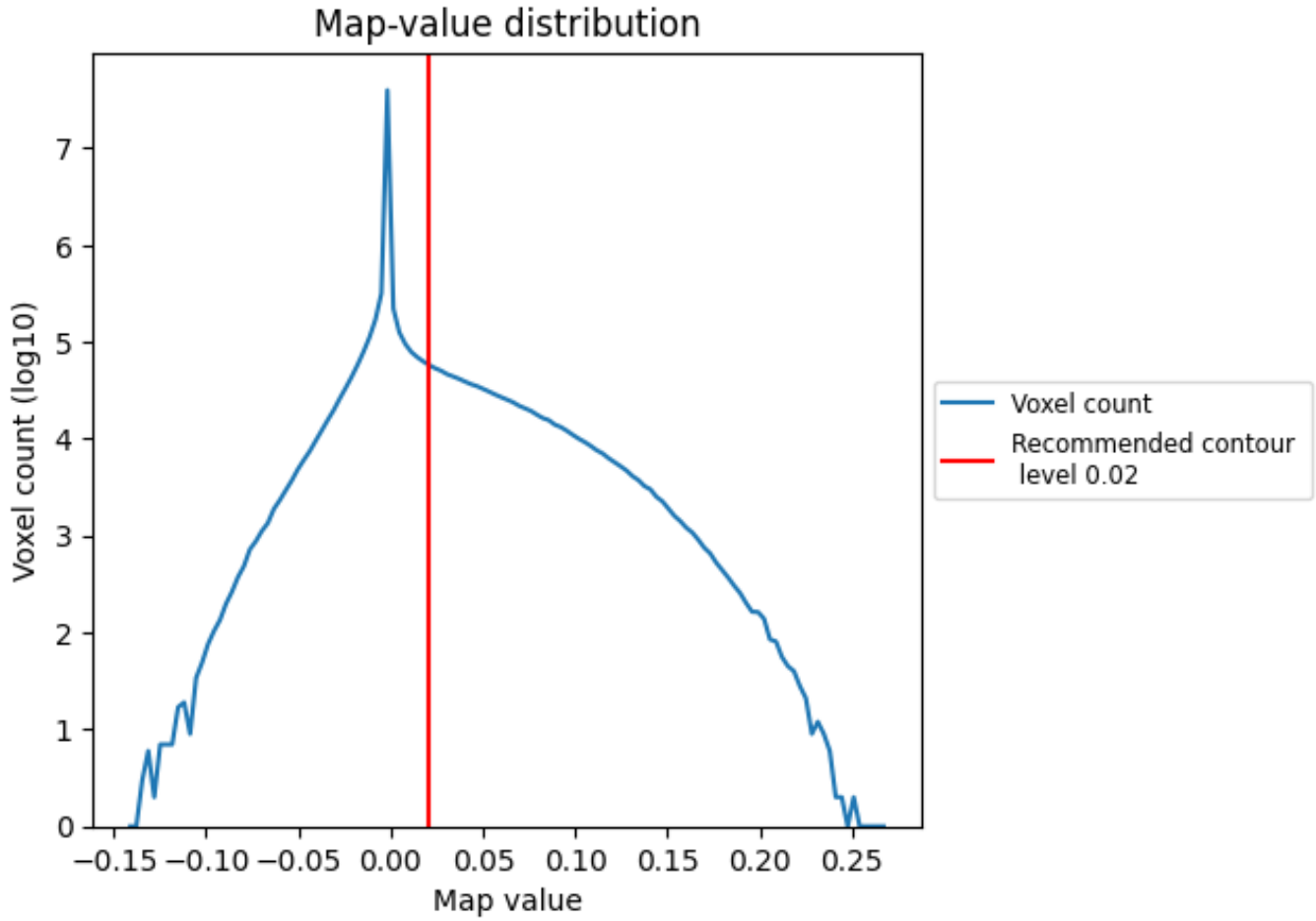
6.6 Mask visualisation (i)

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

7 Map analysis

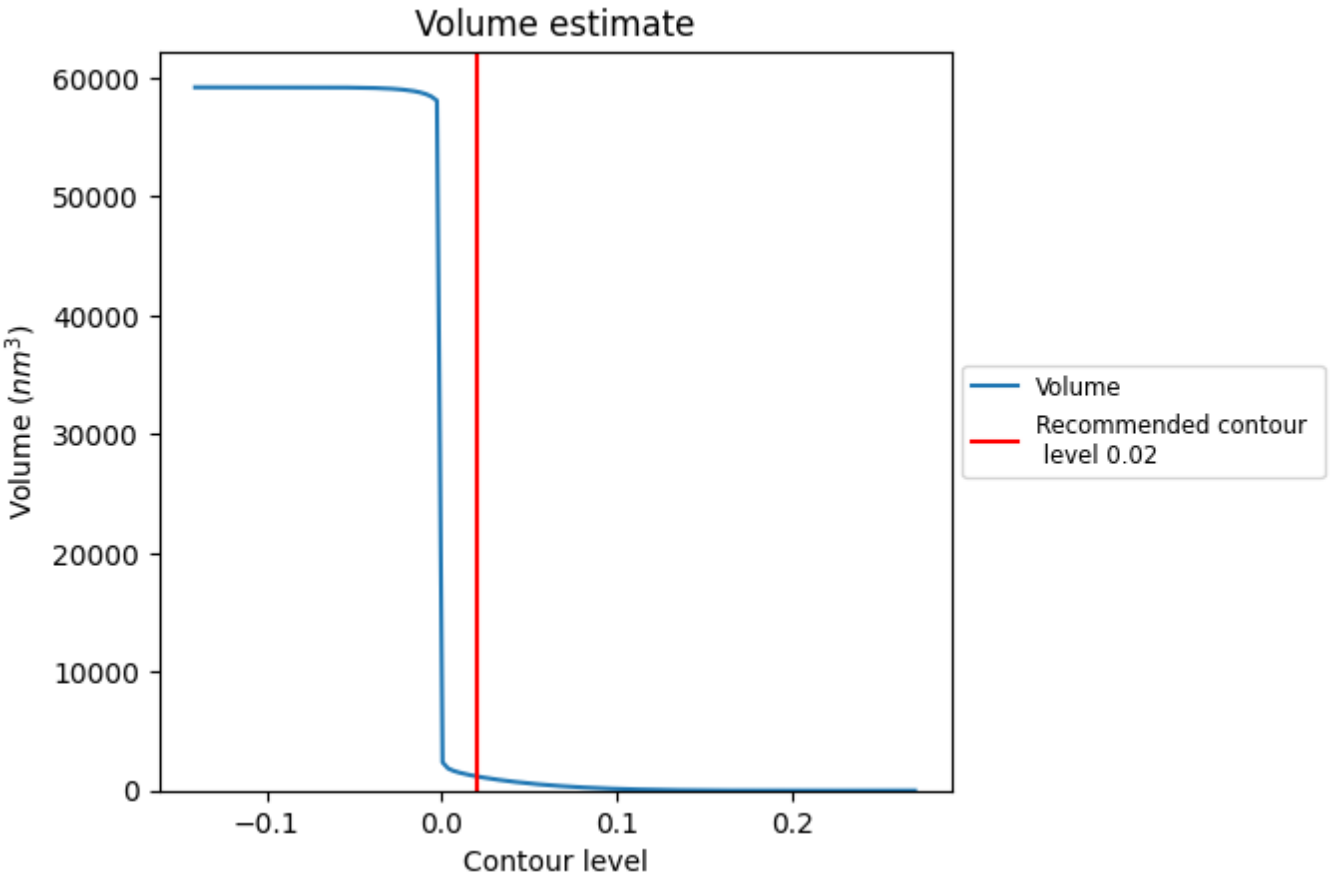
This section contains the results of statistical analysis of the map.

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.

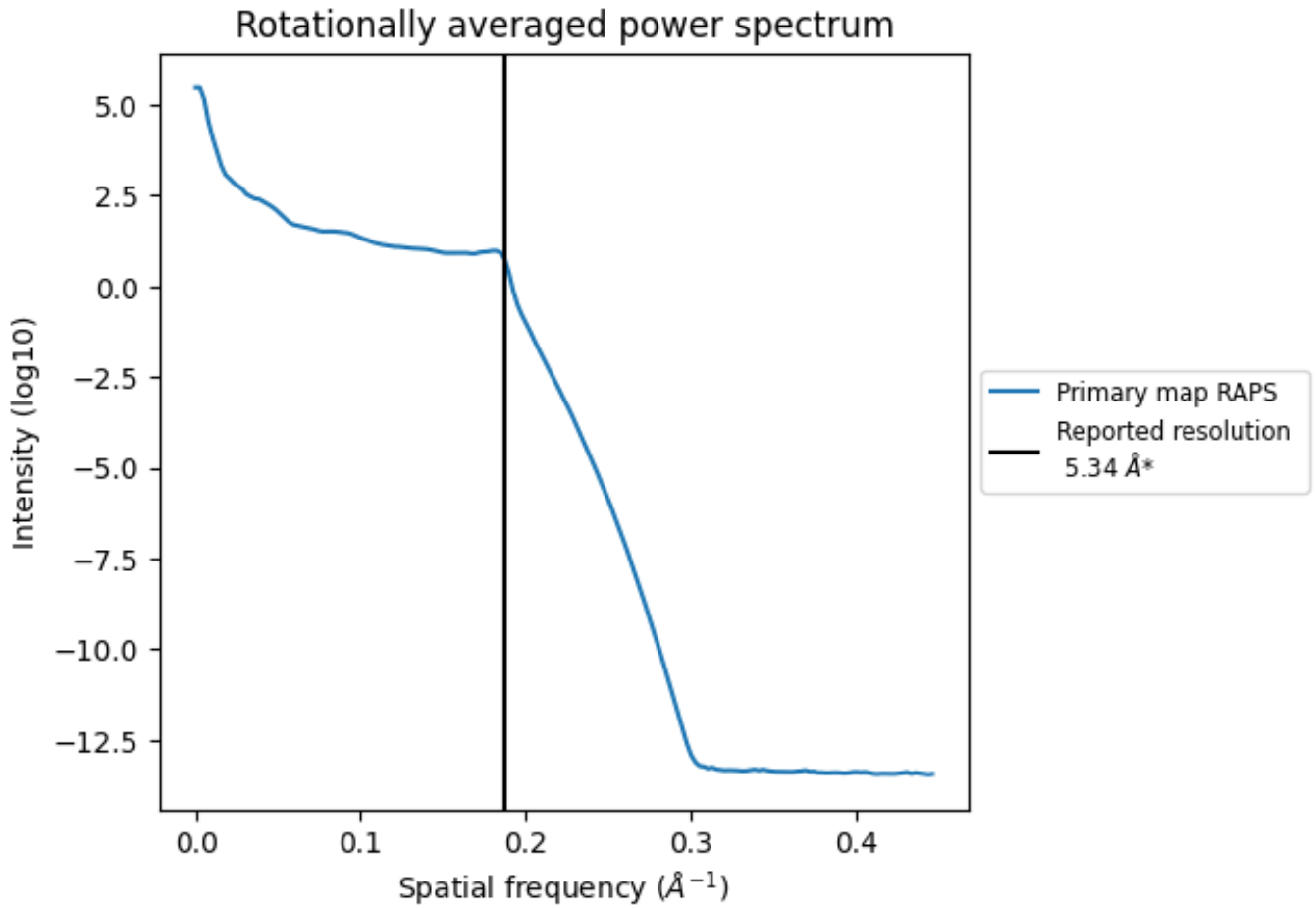
7.2 Volume estimate (i)



The volume at the recommended contour level is 1191 nm^3; this corresponds to an approximate mass of 1076 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)

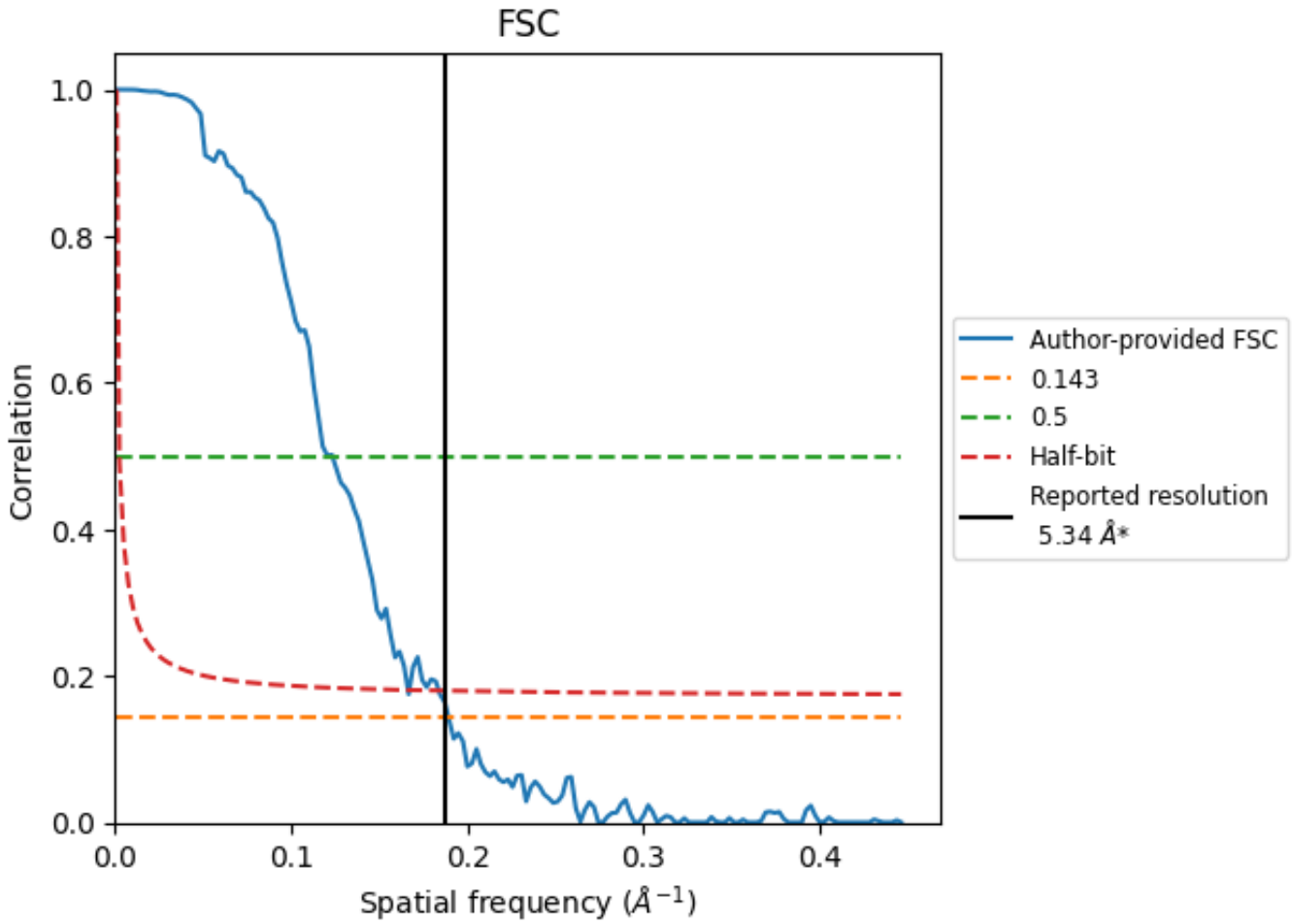


*Reported resolution corresponds to spatial frequency of 0.187 $Å^{-1}$

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 0.187 Å^{-1}

8.2 Resolution estimates (i)

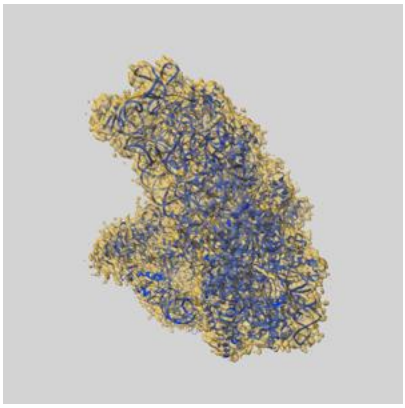
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.34	-	-
Author-provided FSC curve	5.28	8.10	6.01
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

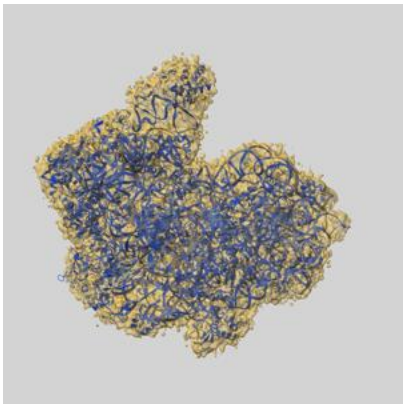
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8148 and PDB model 5JB3. Per-residue inclusion information can be found in section 3 on page 18.

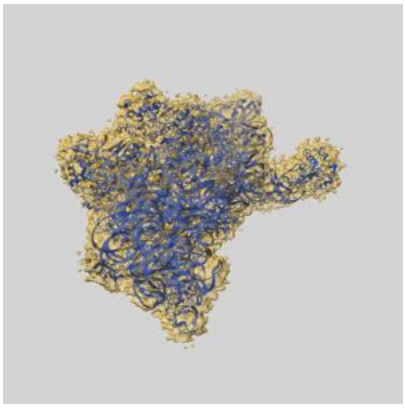
9.1 Map-model overlay



X



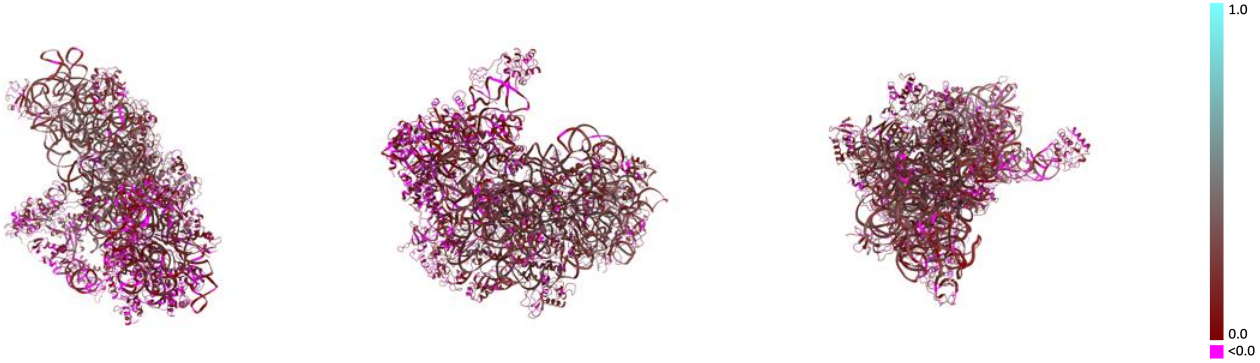
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

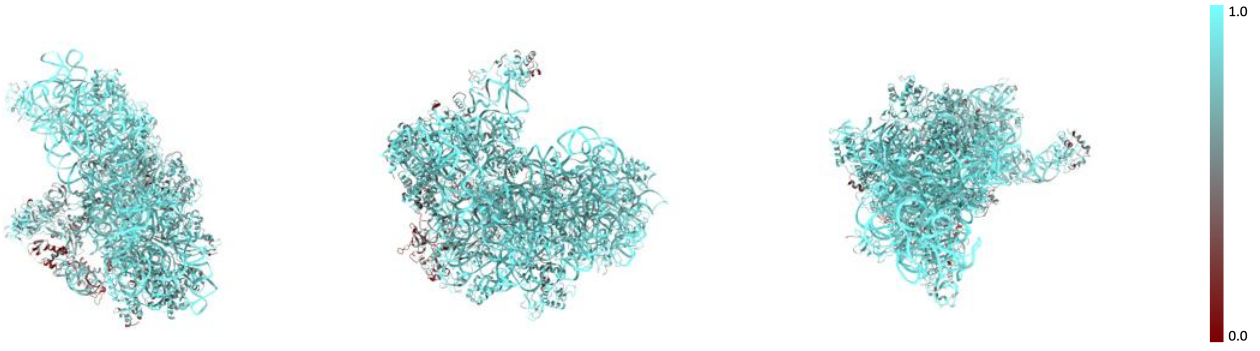
9.2 Q-score mapped to coordinate model



X Y Z

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

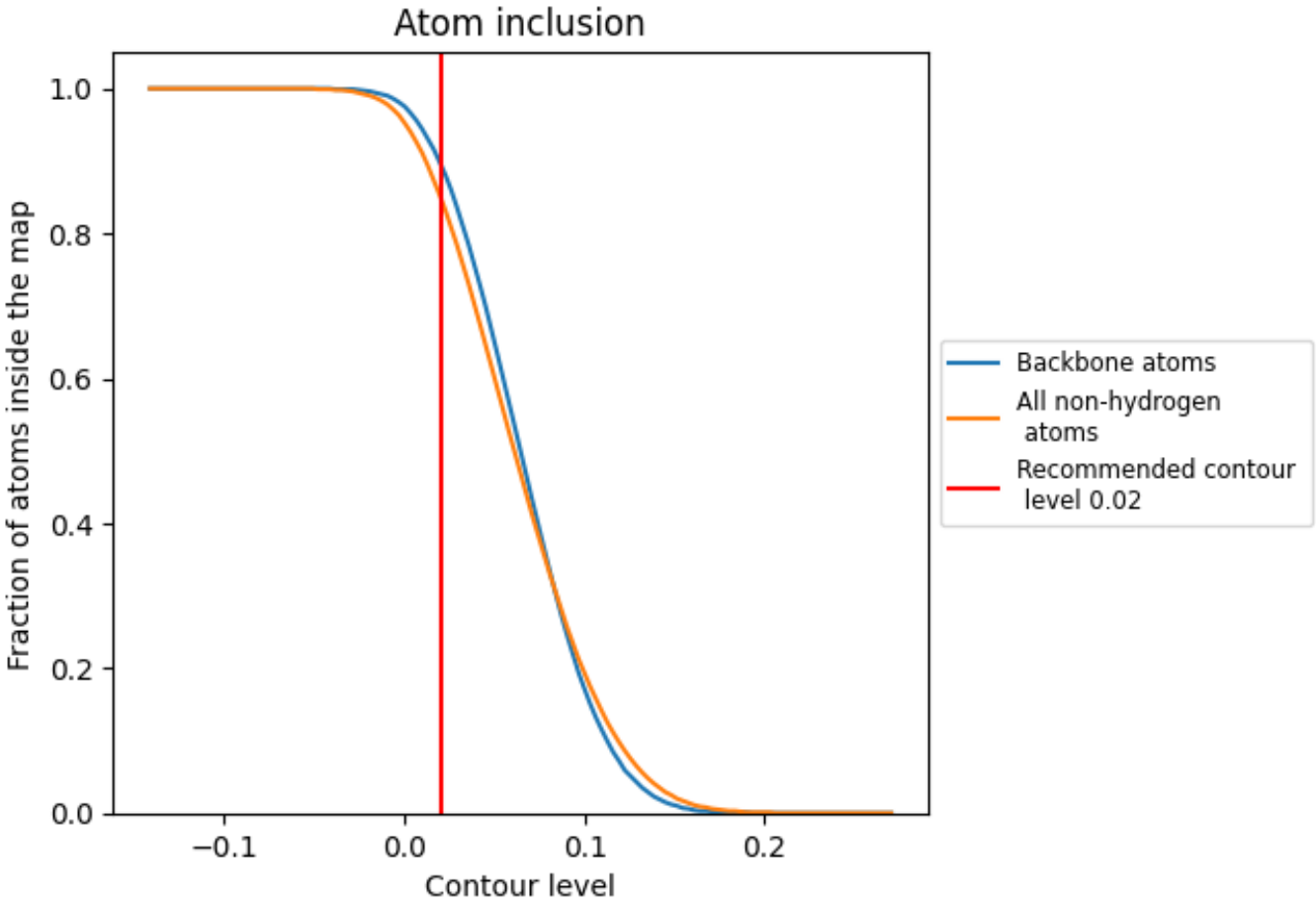
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.1640
0	0.7410	0.1450
1	0.7570	0.1550
2	0.9600	0.2130
3	0.7200	0.0750
4	0.7440	0.0520
5	0.9120	0.2470
6	0.7240	0.1540
7	0.7380	0.1050
8	0.3580	0.0590
9	0.4690	0.0670
A	0.8270	0.1490
B	0.8040	0.1500
C	0.9370	0.2270
D	0.8390	0.1770
E	0.8340	0.1640
F	0.8000	0.1810
G	0.8390	0.1000
H	0.7230	0.0680
I	0.8330	0.1900
J	0.8390	0.1680
K	0.7620	0.1080
L	0.8060	0.1300
M	0.7710	0.1370
N	0.7800	0.1730
O	0.7760	0.0720
P	0.8280	0.1520
Q	0.7920	0.1600
R	0.8440	0.1820
S	0.7600	0.0970
T	0.6990	0.0480
U	0.8100	0.0690
V	0.8140	0.1550
W	0.8470	0.1280
X	0.6490	0.0890

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Chain	Atom inclusion	Q-score
Y	0.7460	0.0750
Z	0.7750	0.1120