wwPDB EM Validation Summary Report (i)

Sep 17, 2026 – 12:12 AM EDT

PDB ID	:	9N2B / pdb_00009n2b
EMDB ID	:	EMD-48830
Title	:	Impacts of ribosomal RNA sequence variation on gene expression and phenotype: Cryo-EM structure of the rrsB ribosome (BBB-70S)
Authors	:	Welfer, G.A.; Brady, R.A.; Natchiar, S.K.; Watson, Z.L.; Rundlet, E.J.; Alejo, J.L.; Singh, A.P.; Mishra, N.K.; Altman, R.B.; Blanchard, S.C.
Deposited on	:	2025-01-28
Resolution	:	2.20 Å(reported)
Based on initial model	:	7N1P

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 (i) 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 (i)) were used in the production of this report:

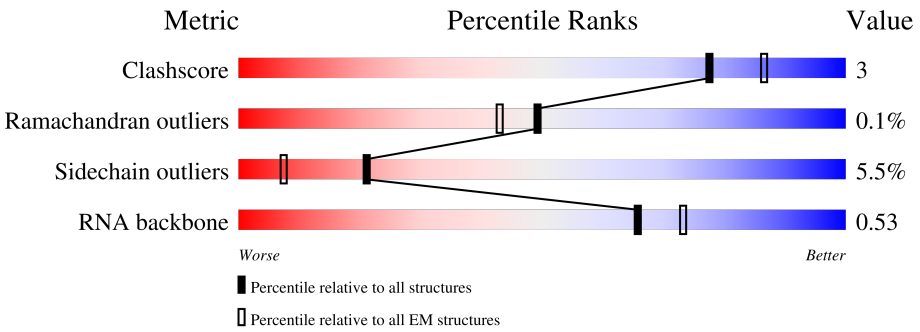
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

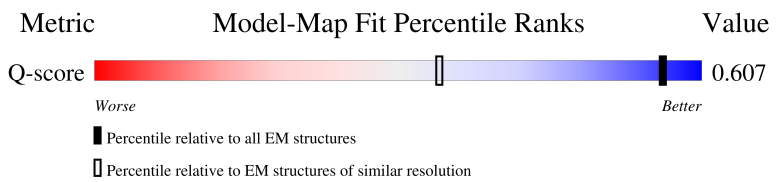
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	16	1542	74% 24% •
2	SB	241	80% 12% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	SC	233	79% 9% 9%
4	SD	206	86% 12%
5	SE	167	81% 11% 5%
6	SF	135	57% 16% 5% 21%
7	SG	179	7% 62% 22% 13%
8	SH	130	91% 8%
9	SI	130	90% 7%
10	SJ	103	6% 67% 23%
11	SK	129	77% 12% 9%
12	SL	124	90% 6%
13	SM	118	80% 15%
14	SN	101	84% 14%
15	SO	89	90% 9%
16	SP	82	78% 18%
17	SQ	84	77% 15% 5%
18	SR	75	73% 13% 11%
19	SS	91	68% 21% 9%
20	ST	87	78% 17%
21	SU	71	11% 76% 17% 6%
22	mR	60	18% 23% 17% 7% 53%
23	23	2904	74% 20% 5%
24	5	120	76% 21%
25	LB	273	88% 11%
26	LC	209	93% 6%
27	LD	201	91% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	LE	179	77% 19%
29	LF	177	85% 11%
30	LI	149	38% 83% 15%
31	LM	142	87% 10%
32	LN	123	84% 15%
33	LO	144	92% 8%
34	LP	136	81% 15%
35	LQ	127	88% 6% 6%
36	LR	117	79% 15%
37	LS	115	83% 17%
38	LT	118	92% 7%
39	LU	103	94% 6%
40	LV	110	84% 14%
41	LW	100	80% 15% 5%
42	LX	104	93% 5%
43	LY	94	86% 10%
44	La	85	9% 80% 12% 7%
45	Lb	78	88% 9%
46	Lc	63	97%
47	Ld	59	86% 10%
48	Le	70	13% 80% 16%
49	Lf	57	93% 5%
50	Lg	55	75% 16% 5%
51	Lh	46	87% 13%
52	Li	65	89% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	Lj	38	68% 24% 8%
54	Pt	77	77% 19%

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 142763 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 (rRNA) from the rrnB operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	16	1542	33092	14767	6064	10719	1542	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	229	1787	1129	320	330	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SC	212	1658	1049	311	294	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SD	205	1643	1026	315	298	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	158	1166	725	220	215	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SF	106	862	545	156	154	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SG	155	1236	772	240	220	4	1	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SH	129	979	616	173	184	6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SI	127	1021	634	206	178	3	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SJ	99	795	498	152	144	1	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SK	118	895	551	178	163	3	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SK	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SL	123	957	591	196	165	5	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SM	115	891	552	179	157	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SN	100	805	499	164	139	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	SO	88	713	439	144	129	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SP	82	649	406	128	114	1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SQ	80	648	411	121	113	3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SR	67	555	351	106	97	1	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	SS	83	663	424	126	111	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	ST	86	669	414	138	114	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	SU	70	589	366	125	97	1	0	0

- Molecule 22 is a RNA chain called Synthetic messenger RNA (mRNA) 60 bp in length.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	mR	28	621	278	113	201	29	1	0

- Molecule 23 is a RNA chain called 23S ribosomal RNA (rRNA) from the rrnB operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	23	2767	59424	26515	10941	19201	2767	0	0

- Molecule 24 is a RNA chain called 5S ribosomal RNA (rRNA) from the B operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	5	120	2572	1145	470	837	120	0	0

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LB	271	2082	1288	423	364	7	0	0

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LC	209	1564	979	288	293	4	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LD	201	1552	974	283	290	5	0	0

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LE	178	1420	905	251	258	6	0	0

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LF	175	1313	826	241	244	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LI	149	1111	699	197	214	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LM	142	1129	714	212	199	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	LN	123	946	593	181	166	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LO	144	1053	654	207	190	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LP	136	1074	686	205	177	6	0	0

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LQ	120	960	593	196	166	5	0	0

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	LR	116	892	552	178	162	0	0

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	LS	114	916	574	179	162	1	0	0

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	LT	117	947	604	192	151	0	0

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LU	103	816	516	153	145	2	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	LV	110	857	532	166	156	3	0	0

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LW	95	757	479	141	135	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	LX	102	779	492	146	141	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	LY	94	753	479	137	134	3	0	0

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	La	84	634	391	129	113	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Lb	77	625	388	129	106	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Lc	62	501	308	98	94	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Ld	58	449	281	87	79	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Le	68	533	330	101	96	6	0	0

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Lf	56	444	269	94	80	1	0	0

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	Lg	52	426	275	78	73	0	0

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Lh	46	377	228	90	57	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Li	64	504	323	105	74	2	0	0

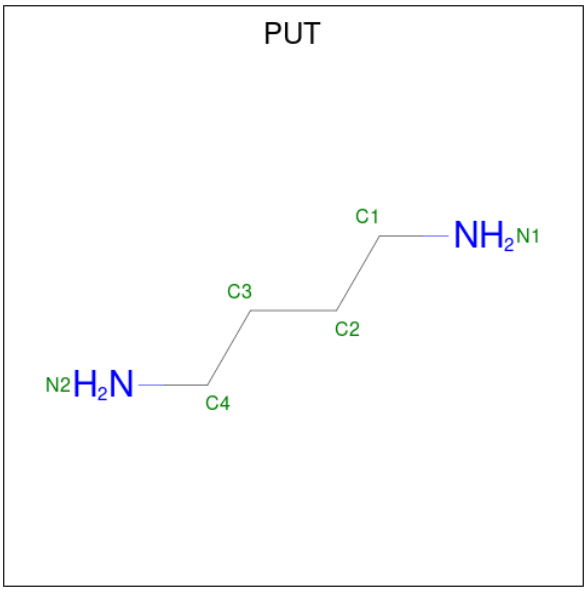
- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Lj	38	302	185	65	48	4	0	0

- Molecule 54 is a RNA chain called N-formyl-methionine initiator tRNA (fMet-tRNAfMet).

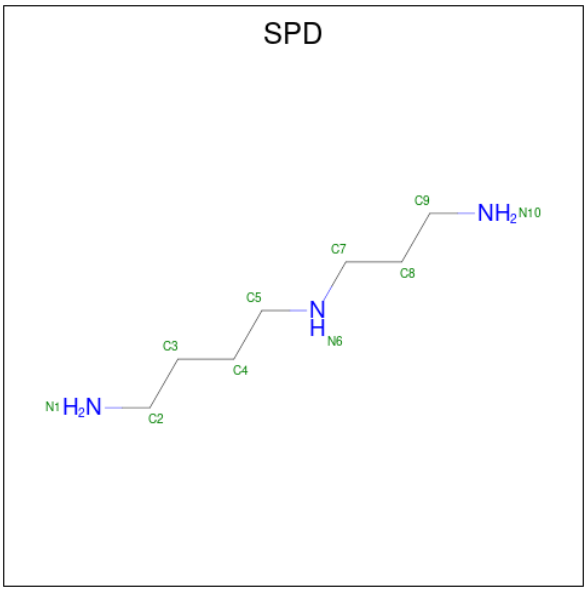
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
54	Pt	77	1646	734	298	536	77	1	0	0

- Molecule 55 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
55	16	1	6	4	2	0
55	23	1	6	4	2	0
55	23	1	6	4	2	0
55	23	1	6	4	2	0
55	23	1	6	4	2	0
55	23	1	6	4	2	0
55	23	1	6	4	2	0
55	23	1	6	4	2	0
55	23	1	6	4	2	0

- Molecule 56 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
56	16	1	10	7	3	0
56	23	1	10	7	3	0
56	23	1	10	7	3	0
56	23	1	10	7	3	0
56	23	1	10	7	3	0

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	16	75	75	75	0
57	mR	3	3	3	0
57	23	185	185	185	0
57	5	6	6	6	0
57	LB	2	2	2	0
57	LC	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	LD	1	1	1	0
57	Lf	1	Total 1	Mg 1	0
57	Pt	2	Total 2	Mg 2	0

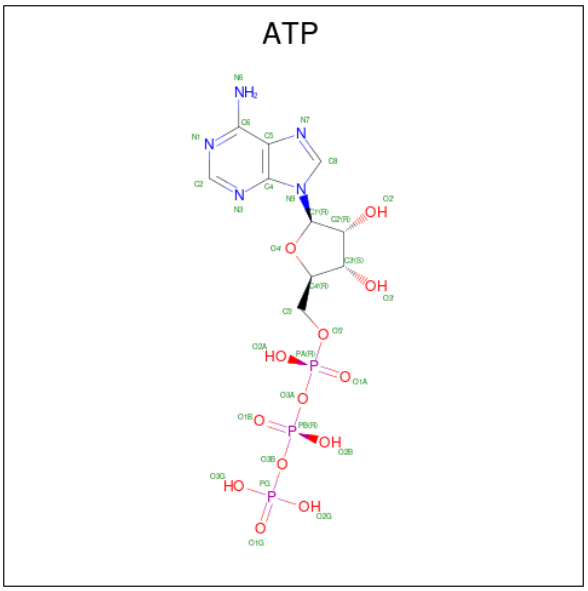
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
58	16	8	8	8	0
58	23	46	Total 46	K 46	0
58	LB	1	Total 1	K 1	0
58	LX	1	Total 1	K 1	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

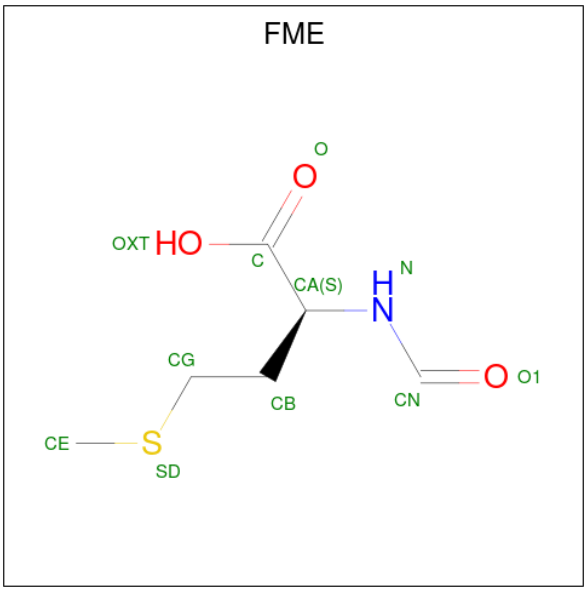
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	SB	1	1	1	0
59	Le	1	Total 1	Zn 1	0
59	Lj	1	Total 1	Zn 1	0

- Molecule 60 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	23	1	31	10	5	13	3	0
			Total	C	N	O	P	
60	23	1	31	10	5	13	3	0

- Molecule 61 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



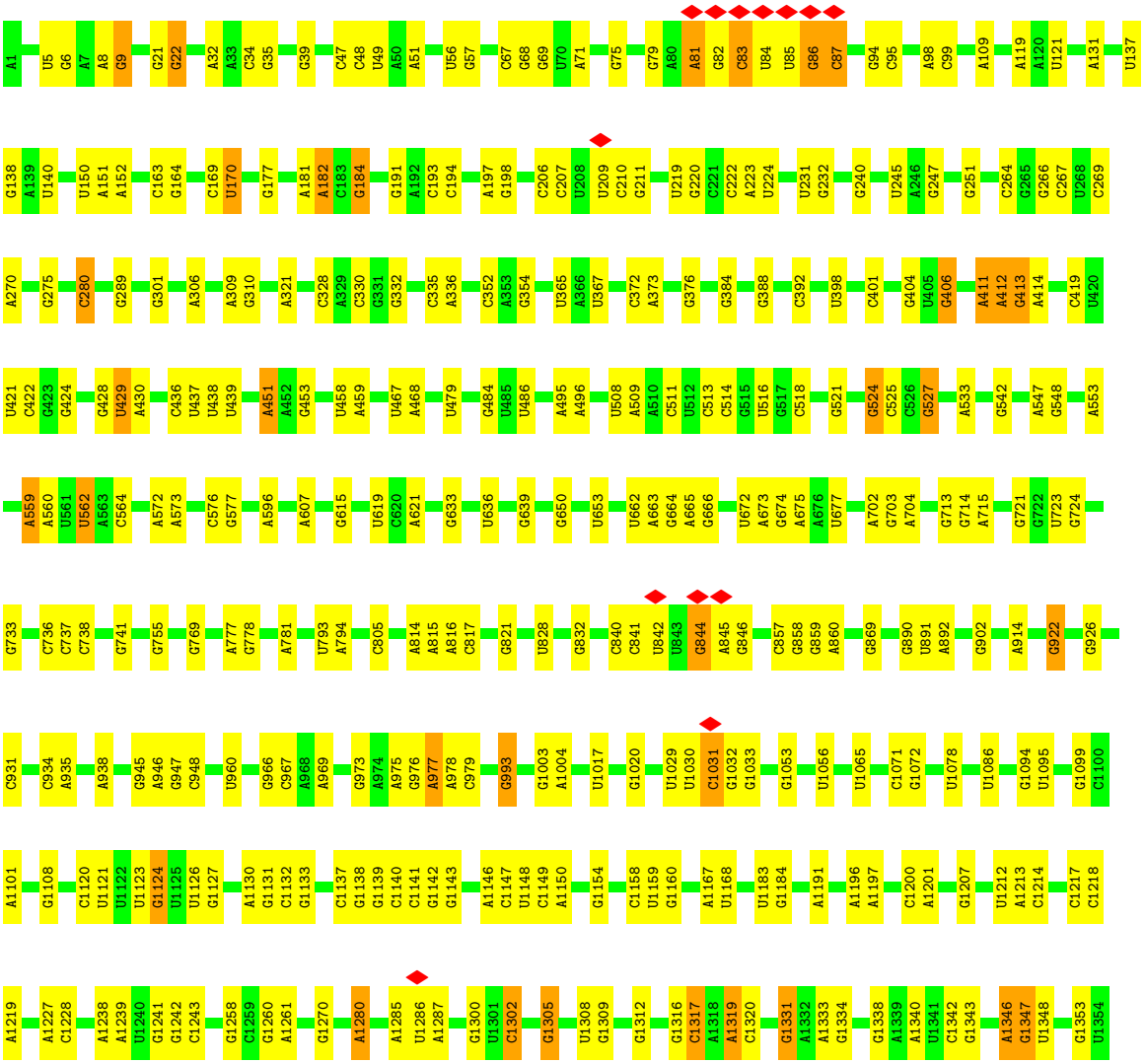
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
61	Pt	1	10	6	1	2	1	0

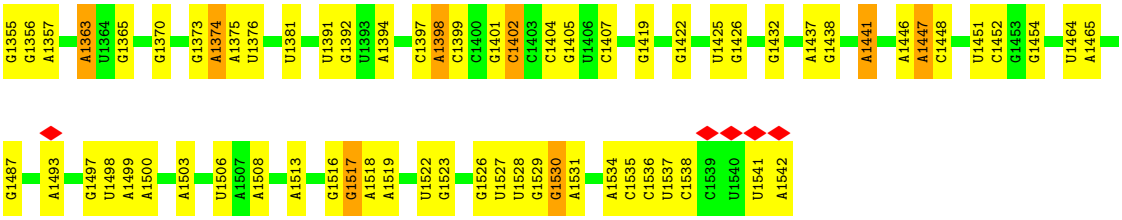
3 Residue-property plots (i)

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 (rRNA) from the rrnB operon

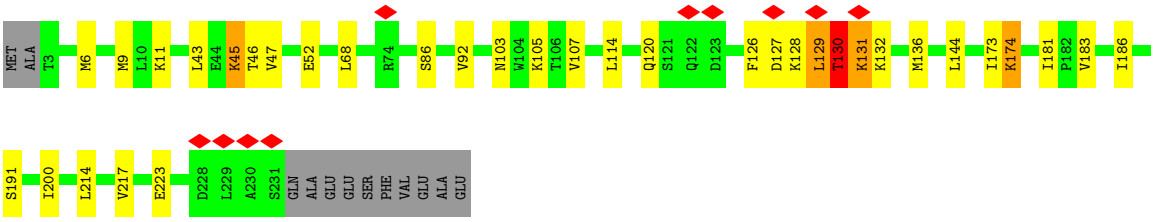
Chain 16:





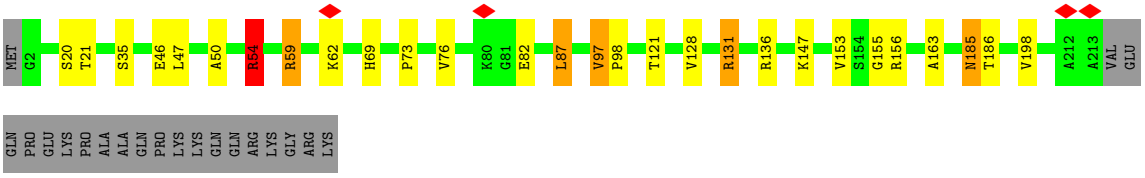
- Molecule 2: 30S ribosomal protein S2

Chain SB:



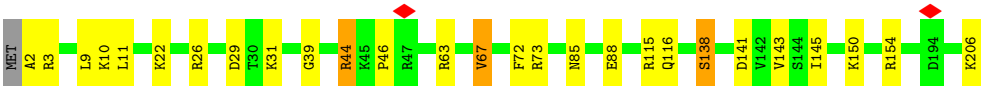
- Molecule 3: 30S ribosomal protein S3

Chain SC:



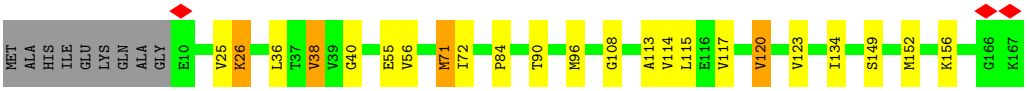
- Molecule 4: 30S ribosomal protein S4

Chain SD:



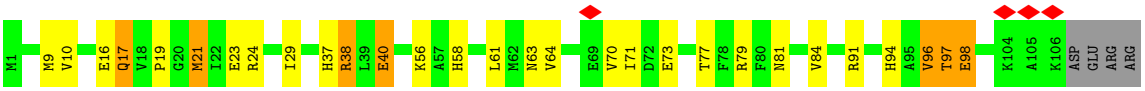
- Molecule 5: 30S ribosomal protein S5

Chain SE:



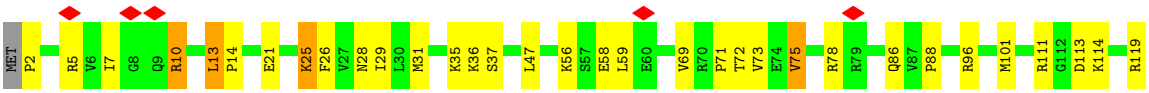
- Molecule 6: 30S ribosomal protein S6

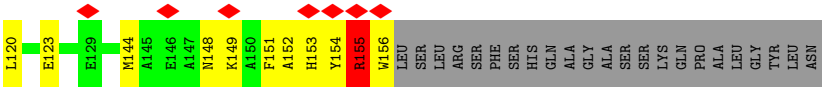
Chain SF:



• Molecule 7: 30S ribosomal protein S7

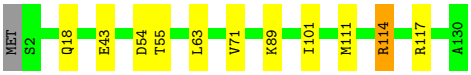
Chain SG:





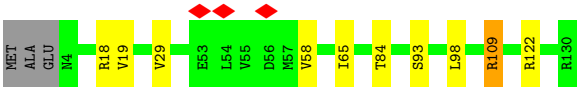
• Molecule 8: 30S ribosomal protein S8

Chain SH:



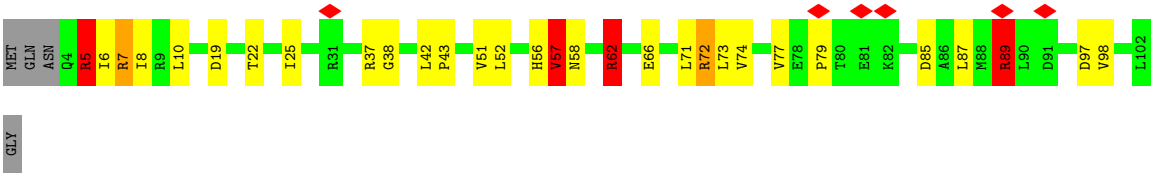
• Molecule 9: 30S ribosomal protein S9

Chain SI:



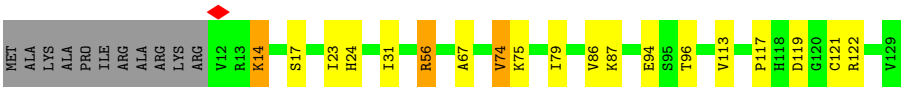
• Molecule 10: 30S ribosomal protein S10

Chain SJ:



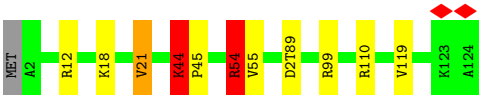
• Molecule 11: Small ribosomal subunit protein uS11

Chain SK:



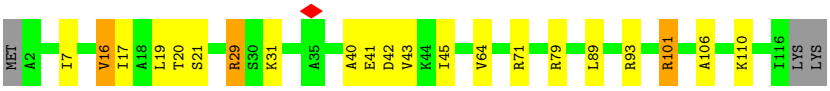
• Molecule 12: Small ribosomal subunit protein uS12

Chain SL:



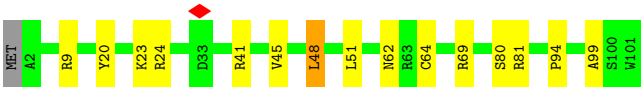
• Molecule 13: 30S ribosomal protein S13

Chain SM:



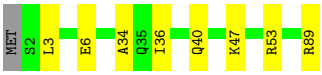
• Molecule 14: 30S ribosomal protein S14

Chain SN:



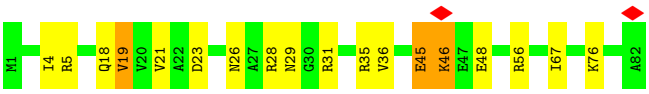
• Molecule 15: 30S ribosomal protein S15

Chain SO:



• Molecule 16: 30S ribosomal protein S16

Chain SP:

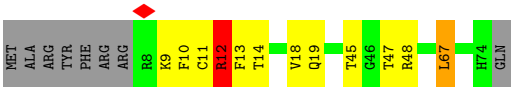


• Molecule 17: 30S ribosomal protein S17

Chain SQ:

• Molecule 18: 30S ribosomal protein S18

Chain SR:

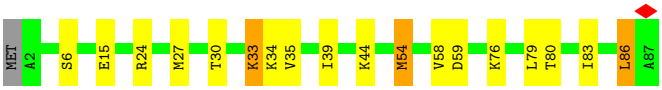


• Molecule 19: Small ribosomal subunit protein uS19

Chain SS:

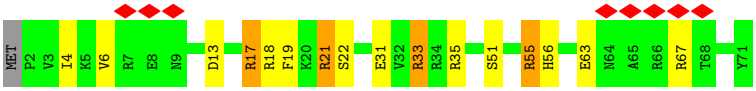
• Molecule 20: 30S ribosomal protein S20

Chain ST:



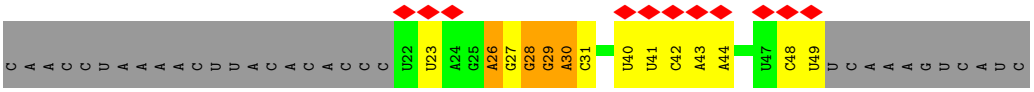
• Molecule 21: 30S ribosomal protein S21

Chain SU:



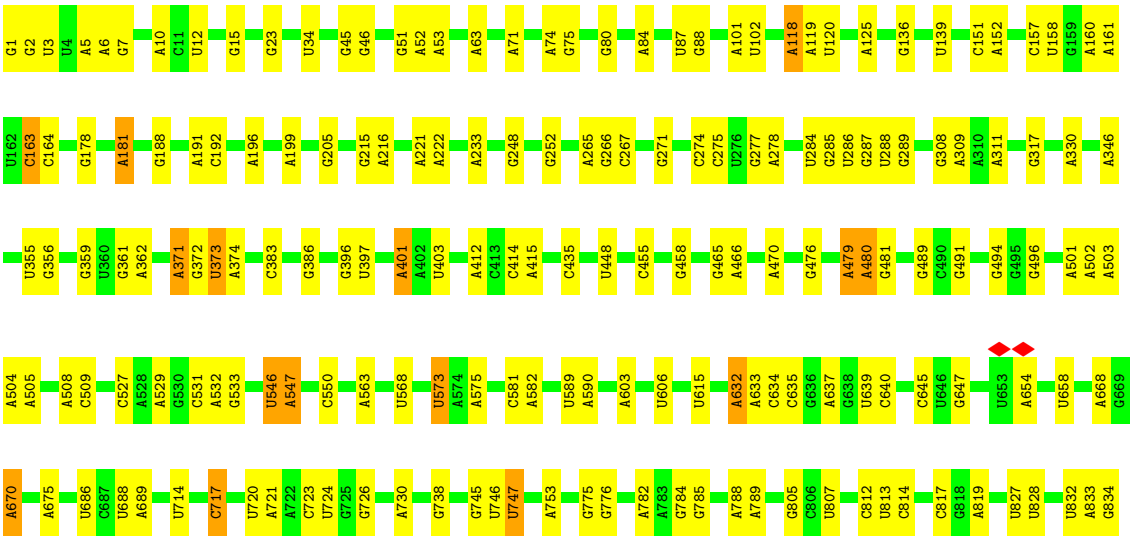
• Molecule 22: Synthetic messenger RNA (mRNA) 60 bp in length

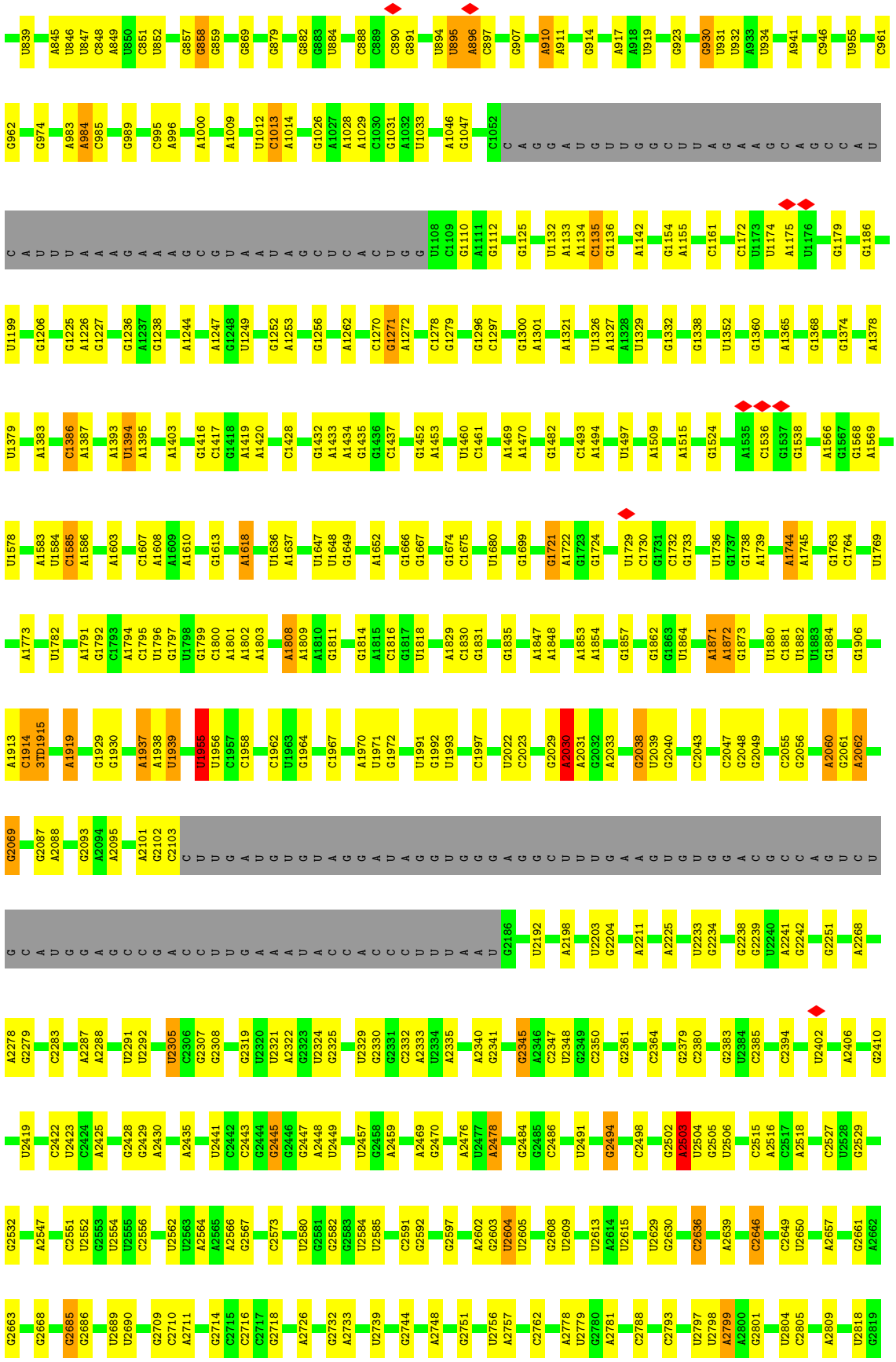
Chain mR:

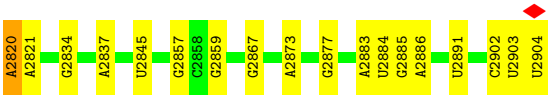


• Molecule 23: 23S ribosomal RNA (rRNA) from the rrnB operon

Chain 23:




U839 A845 U846 U847 C848 A849 U850 C851 U852 G857 G858 G859 G869 G879 G882 G883 U884 C888 C889 C890 G891 U894 U895 A896 C897 G907 A910 A911 G914 A917 A918 U919 G923 G930 U931 U932 A933 U934 A941 C946 U955 C961
G962 G974 A983 A984 C985 G989 C995 A996 A1000 A1009 U1012 C1013 A1014 G1026 A1027 A1028 A1029 C1030 G1031 A1032 U1033 A1046 G1047 C1052 C A G G A U G U U G G C U U A G A A G C A G C C A U
C A U U U A A A G A A A G C G U A A U A G C U G G U1108 C1109 G1110 A1111 G1112 G1125 U1132 A1133 A1134 C1135 G1136 A1142 G1154 A1155 C1161 C1172 U1173 U1174 A1175 U1176 G1179 G1186
U1199 G1206 G1225 A1226 G1227 G1236 A1237 G1238 A1244 A1247 G1248 U1249 G1252 A1253 G1256 A1262 C1270 G1271 A1272 C1278 G1279 G1296 C1297 G1300 A1301 A1321 U1326 A1327 A1328 U1329 G1332 G1338 U1352 G1360 A1365 G1368 G1374 A1378
U1379 A1383 C1386 A1387 A1393 U1394 A1395 A1403 G1416 C1417 G1418 A1419 A1420 C1428 G1432 A1433 A1434 G1435 G1436 C1437 G1452 A1453 U1460 C1461 A1469 A1470 G1482 C1493 A1494 U1497 A1509 A1515 G1524 A1535 C1536 G1537 G1538 A1566 G1567 G1568 A1569
U1578 A1583 U1584 C1585 A1586 A1603 C1607 A1608 A1609 A1610 G1613 A1618 U1636 A1637 U1647 U1648 G1649 A1652 G1666 G1667 G1674 C1675 U1680 G1699 G1721 A1722 G1723 G1724 U1729 C1730 G1731 C1732 G1733 U1736 G1737 G1738 A1739 A1744 A1745 G1763 C1764 U1769
A1773 U1782 A1791 G1792 C1793 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 A1808 A1809 A1810 G1811 G1814 A1815 C1816 G1817 U1818 A1829 C1830 G1831 G1835 A1847 A1848 A1853 A1854 G1857 G1862 G1863 U1864 A1871 A1872 G1873 U1880 C1881 U1882 U1883 G1884 G1906
A1913 C1914 3TD1915 A1919 G1929 G1930 A1937 A1938 U1939 U1955 U1956 C1957 C1958 C1962 U1963 G1964 C1967 A1970 U1971 G1972 U1991 G1992 U1993 C1997 U2022 C2023 G2029 A2030 A2031 G2032 A2033 G2038 U2039 G2040 C2043 C2047 G2048 G2049 C2055 G2056 A2060 G2061 A2062
G2069 G2087 A2088 G2093 A2094 A2095 A2101 G2102 C2103 C U U G A U G U G U A G G A U G G U G G A C U U G C C A A G G C C U U G G A A G U G U G G A C G G C C A G U C U
G C A U G G A G C A C C U U G A A U A A C C A C C A A U G2186 U2192 A2198 U2203 G2204 A2211 A2225 U2233 G2234 G2238 G2239 U2240 A2241 G2242 G2251 A2268
A2278 G2279 C2283 A2287 A2288 U2291 U2292 U2305 C2306 G2307 G2308 G2319 U2320 U2321 A2322 G2323 U2324 G2325 U2329 G2330 G2331 C2332 A2333 U2334 A2335 A2340 G2341 G2345 A2346 C2347 U2348 G2349 C2350 G2361 C2364 G2379 C2380 G2383 U2384 C2385 C2394 U2402 A2406 G2410
U2419 C2422 U2423 C2424 A2425 G2428 G2429 A2430 A2435 U2441 C2442 C2443 G2444 G2445 G2446 G2447 A2448 U2449 U2457 G2458 A2459 A2469 G2470 A2476 U2477 A2478 G2484 G2485 C2486 U2491 G2494 C2498 G2502 A2503 U2504 G2505 U2506 C2515 A2516 C2517 A2518 C2527 U2528 G2529
G2532 A2547 C2551 U2552 G2553 U2554 U2555 C2556 U2562 U2563 A2564 A2565 A2566 G2567 C2573 U2580 G2581 G2582 G2583 U2584 U2585 C2591 G2592 G2597 A2602 G2603 U2604 U2605 G2608 U2609 U2613 A2614 U2615 U2629 G2630 C2636 A2639 C2646 C2649 U2650 A2657 G2661 A2662
G2663 G2668 G2685 G2686 U2689 U2690 G2709 C2710 A2711 G2714 C2715 C2716 C2717 G2718 A2726 G2732 A2733 U2739 G2744 A2748 G2751 U2756 A2757 C2762 A2778 U2779 G2780 A2781 C2788 C2793 U2797 U2798 A2799 A2800 G2801 U2804 C2805 A2809 U2818 G2819

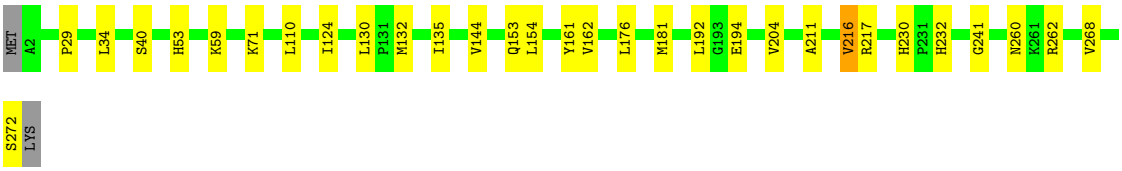


• Molecule 24: 5S ribosomal RNA (rRNA) from the B operon

Chain 5:

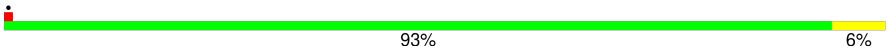
• Molecule 25: 50S ribosomal protein L2

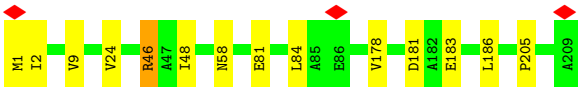
Chain LB:



• Molecule 26: 50S ribosomal protein L3

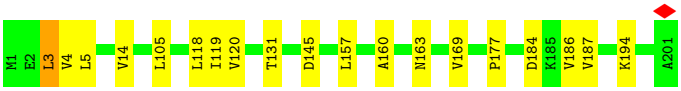
Chain LC:





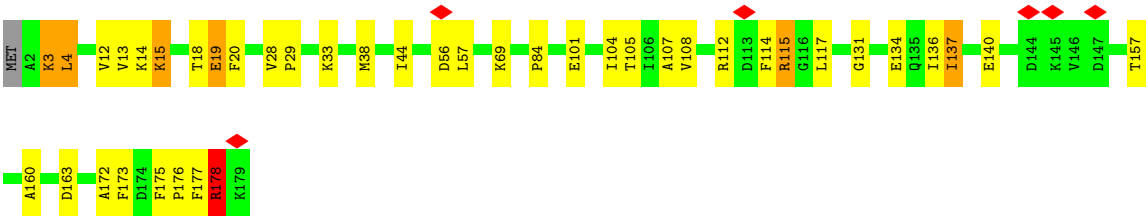
• Molecule 27: Large ribosomal subunit protein uL4

Chain LD:



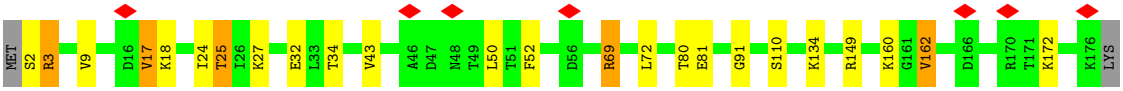
• Molecule 28: 50S ribosomal protein L5

Chain LE:



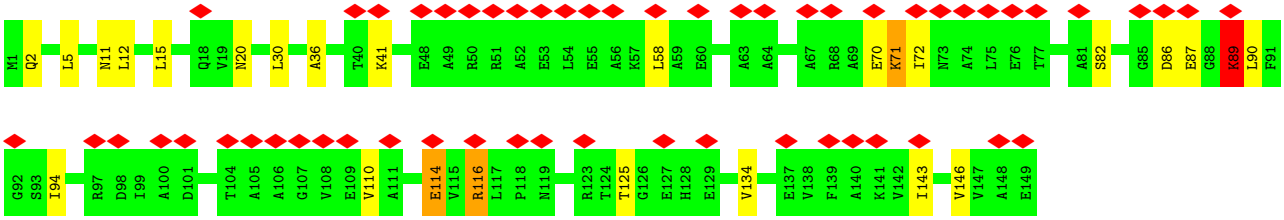
• Molecule 29: 50S ribosomal protein L6

Chain LF:



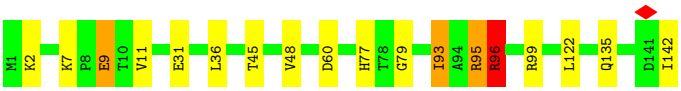
• Molecule 30: 50S ribosomal protein L9

Chain LI:



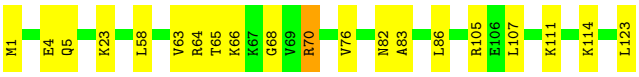
• Molecule 31: 50S ribosomal protein L13

Chain LM:



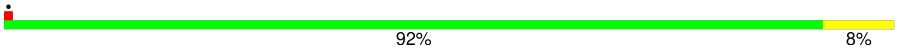
• Molecule 32: 50S ribosomal protein L14

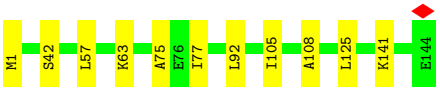
Chain LN:



• Molecule 33: 50S ribosomal protein L15

Chain LO:





• Molecule 34: 50S ribosomal protein L16

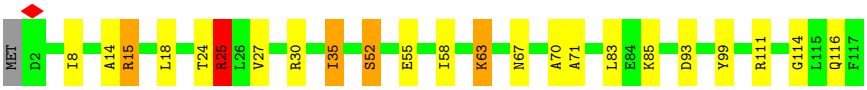
Chain LP:

• Molecule 35: 50S ribosomal protein L17

Chain LQ:

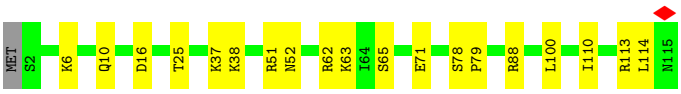
• Molecule 36: 50S ribosomal protein L18

Chain LR:



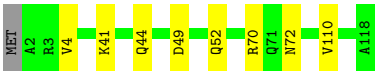
• Molecule 37: 50S ribosomal protein L19

Chain LS:



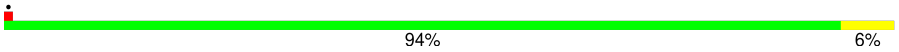
• Molecule 38: 50S ribosomal protein L20

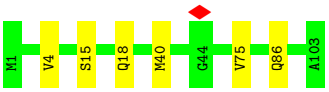
Chain LT:



• Molecule 39: 50S ribosomal protein L21

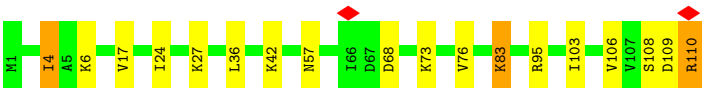
Chain LU:





• Molecule 40: Large ribosomal subunit protein uL22

Chain LV:

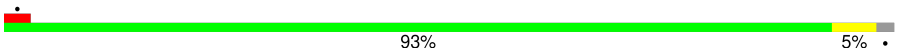


• Molecule 41: 50S ribosomal protein L23

Chain LW:

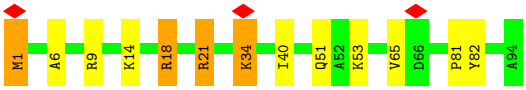
• Molecule 42: 50S ribosomal protein L24

Chain LX:



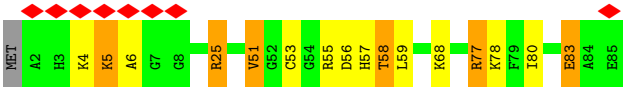
• Molecule 43: 50S ribosomal protein L25

Chain LY:



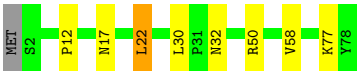
• Molecule 44: 50S ribosomal protein L27

Chain La:



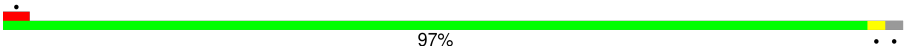
• Molecule 45: 50S ribosomal protein L28

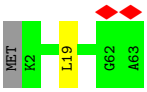
Chain Lb:



• Molecule 46: 50S ribosomal protein L29

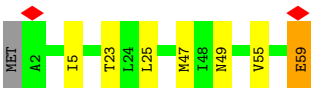
Chain Lc:





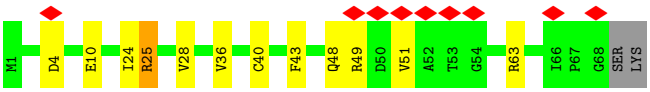
• Molecule 47: 50S ribosomal protein L30

Chain Ld:



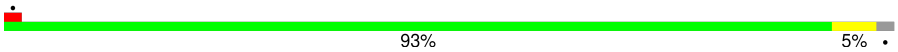
• Molecule 48: 50S ribosomal protein L31

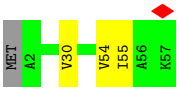
Chain Le:



• Molecule 49: 50S ribosomal protein L32

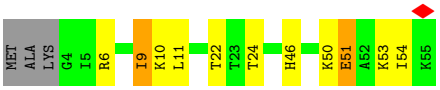
Chain Lf:





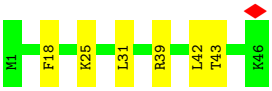
• Molecule 50: 50S ribosomal protein L33

Chain Lg:



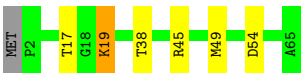
• Molecule 51: 50S ribosomal protein L34

Chain Lh:



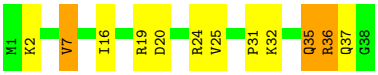
• Molecule 52: 50S ribosomal protein L35

Chain Li:



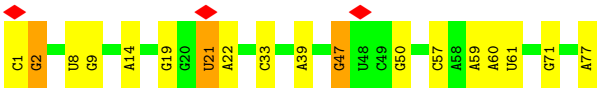
• Molecule 53: 50S ribosomal protein L36

Chain Lj:



• Molecule 54: N-formyl-methionine initiator tRNA (fMet-tRNAfMet)

Chain Pt:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	555112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: 6MZ, FME, PSU, ZN, ATP, H2U, D2T, OMC, MA6, G7M, 4SU, 1MG, 4OC, OMU, IAS, SPD, 5MC, PUT, 2MA, UR3, 2MG, K, 4D4, OMG, 5MU, MG, 3TD

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	16	0.34	1/36772 (0.0%)	0.51	0/57358
2	SB	0.43	0/1818	0.78	2/2450 (0.1%)
3	SC	0.40	0/1685	0.70	0/2270
4	SD	0.46	0/1665	0.74	0/2227
5	SE	0.46	0/1179	0.80	1/1584 (0.1%)
6	SF	0.57	1/881 (0.1%)	0.89	2/1189 (0.2%)
7	SG	0.54	0/1257	0.85	1/1686 (0.1%)
8	SH	0.29	0/989	0.60	0/1326
9	SI	0.38	0/1033	0.70	0/1375
10	SJ	0.55	0/805	0.92	1/1089 (0.1%)
11	SK	0.44	0/902	0.64	1/1215 (0.1%)
12	SL	0.38	0/960	0.71	0/1286
13	SM	0.51	0/900	0.81	0/1204
14	SN	0.35	0/817	0.59	0/1088
15	SO	0.39	0/721	0.64	0/964
16	SP	0.46	0/659	0.74	0/884
17	SQ	0.34	0/657	0.66	0/881
18	SR	0.45	0/564	0.77	1/756 (0.1%)
19	SS	0.42	0/680	0.68	0/915
20	ST	0.52	0/675	0.78	0/895
21	SU	0.40	0/597	0.66	0/792
22	mR	0.47	0/695	0.58	0/1081
23	23	0.33	1/66023 (0.0%)	0.51	2/102992 (0.0%)
24	5	0.36	0/2876	0.50	0/4483
25	LB	0.32	0/2121	0.60	0/2852
26	LC	0.37	0/1585	0.65	0/2134
27	LD	0.29	0/1571	0.59	0/2113
28	LE	0.54	2/1444 (0.1%)	0.81	1/1937 (0.1%)
29	LF	0.40	0/1333	0.68	0/1805
30	LI	0.40	0/1122	0.76	1/1515 (0.1%)
31	LM	0.39	0/1152	0.63	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LN	0.38	0/955	0.68	0/1279
33	LO	0.31	0/1062	0.59	0/1413
34	LP	0.47	0/1080	0.75	0/1443
35	LQ	0.35	0/973	0.69	0/1301
36	LR	0.54	2/902 (0.2%)	0.80	0/1209
37	LS	0.39	0/928	0.64	0/1242
38	LT	0.33	0/960	0.62	0/1278
39	LU	0.32	0/829	0.57	0/1107
40	LV	0.32	0/864	0.65	1/1156 (0.1%)
41	LW	0.38	0/764	0.63	0/1021
42	LX	0.34	0/787	0.59	0/1051
43	LY	0.35	0/766	0.65	0/1025
44	La	0.51	0/642	0.79	0/848
45	Lb	0.47	0/635	0.76	0/848
46	Lc	0.21	0/502	0.44	0/667
47	Ld	0.44	0/453	0.72	0/605
48	Le	0.39	0/543	0.74	0/726
49	Lf	0.26	0/450	0.53	0/599
50	Lg	0.31	0/433	0.65	0/576
51	Lh	0.41	0/380	0.55	0/498
52	Li	0.47	0/513	0.74	0/676
53	Lj	0.60	1/303 (0.3%)	0.71	0/397
54	Pt	0.44	2/1744 (0.1%)	0.56	0/2716
All	All	0.36	10/153606 (0.0%)	0.57	14/229578 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	SC	0	4
6	SF	0	3
7	SG	0	2
8	SH	0	1
9	SI	0	1
10	SJ	0	4
11	SK	0	2
12	SL	0	1
13	SM	0	2
14	SN	0	2
16	SP	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
18	SR	0	2
19	SS	0	2
20	ST	0	1
21	SU	0	4
26	LC	0	1
28	LE	0	2
29	LF	0	2
30	LI	0	1
31	LM	0	2
32	LN	0	1
34	LP	0	1
35	LQ	0	2
36	LR	0	2
37	LS	0	2
38	LT	0	1
40	LV	0	1
43	LY	0	3
44	La	0	2
45	Lb	0	1
48	Le	0	2
51	Lh	0	1
52	Li	0	1
53	Lj	0	1
All	All	0	61

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	LE	178	ARG	C-N	8.06	1.44	1.33
28	LE	177	PHE	C-N	7.37	1.44	1.33
36	LR	14	ALA	C-N	-6.17	1.25	1.33
6	SF	40	GLU	C-N	6.10	1.42	1.33
53	Lj	35	GLN	C-N	5.72	1.41	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	SB	130	THR	N-CA-C	-7.71	103.77	113.02
7	SG	69	VAL	N-CA-C	-6.63	107.03	113.53
11	SK	74	VAL	N-CA-C	-6.17	107.24	113.47
10	SJ	89	ARG	N-CA-C	-6.10	106.16	113.97
6	SF	17	GLN	CA-C-N	-6.04	115.50	120.33

There are no chirality outliers.

5 of 61 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	SC	131	ARG	Sidechain
3	SC	136	ARG	Sidechain
3	SC	54	ARG	Sidechain
3	SC	59	ARG	Sidechain
6	SF	24	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	33092	0	16675	144	0
2	SB	1787	0	1812	20	0
3	SC	1658	0	1732	13	0
4	SD	1643	0	1707	16	0
5	SE	1166	0	1212	14	0
6	SF	862	0	864	14	0
7	SG	1236	0	1290	20	0
8	SH	979	0	1031	5	0
9	SI	1021	0	1070	5	0
10	SJ	795	0	836	17	0
11	SK	895	0	905	8	0
12	SL	957	0	1017	6	0
13	SM	891	0	952	9	0
14	SN	805	0	844	9	0
15	SO	713	0	734	3	0
16	SP	649	0	666	11	0
17	SQ	648	0	691	8	0
18	SR	555	0	578	5	0
19	SS	663	0	688	8	0
20	ST	669	0	719	13	0
21	SU	589	0	629	6	0
22	mR	621	0	312	10	0
23	23	59424	0	29905	170	0
24	5	2572	0	1301	9	0
25	LB	2082	0	2153	20	0
26	LC	1564	0	1616	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	LD	1552	0	1619	10	0
28	LE	1420	0	1457	27	0
29	LF	1313	0	1358	10	0
30	LI	1111	0	1148	14	0
31	LM	1129	0	1162	13	0
32	LN	946	0	1023	9	0
33	LO	1053	0	1128	6	0
34	LP	1074	0	1154	17	0
35	LQ	960	0	1000	3	0
36	LR	892	0	923	9	0
37	LS	916	0	962	9	0
38	LT	947	0	1019	4	0
39	LU	816	0	839	2	0
40	LV	857	0	922	9	0
41	LW	757	0	820	7	0
42	LX	779	0	830	3	0
43	LY	753	0	780	7	0
44	La	634	0	653	12	0
45	Lb	625	0	652	4	0
46	Lc	501	0	531	1	0
47	Ld	449	0	488	3	0
48	Le	533	0	530	3	0
49	Lf	444	0	458	1	0
50	Lg	426	0	464	7	0
51	Lh	377	0	418	2	0
52	Li	504	0	572	4	0
53	Lj	302	0	340	9	0
54	Pt	1646	0	843	2	0
55	16	6	0	12	0	0
55	23	48	0	96	0	0
56	16	10	0	19	0	0
56	23	40	0	76	0	0
57	16	75	0	0	0	0
57	23	185	0	0	0	0
57	5	6	0	0	0	0
57	LB	2	0	0	0	0
57	LC	1	0	0	0	0
57	LD	1	0	0	0	0
57	Lf	1	0	0	0	0
57	Pt	2	0	0	0	0
57	mR	3	0	0	0	0
58	16	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	23	46	0	0	0	0
58	LB	1	0	0	0	0
58	LX	1	0	0	0	0
59	Le	1	0	0	0	0
59	Lj	1	0	0	0	0
59	SB	1	0	0	0	0
60	23	62	0	24	0	0
61	Pt	10	0	10	0	0
All	All	142763	0	96269	691	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 3.

The worst 5 of 691 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)
23:23:2494:G:O2'	34:LP:79:ALA:HA	1.71	0.88
53:Lj:7:VAL:HG22	53:Lj:35:GLN:HG3	1.56	0.87
1:16:1402:4OC:H5	1:16:1500:A:H61	1.44	0.82
1:16:9:G:H5'	5:SE:108:GLY:HA3	1.62	0.81
1:16:406:G:H21	4:SD:116:GLN:HE22	1.30	0.80

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	SB	227/241 (94%)	216 (95%)	11 (5%)	0	100	100
3	SC	210/233 (90%)	202 (96%)	8 (4%)	0	100	100
4	SD	203/206 (98%)	202 (100%)	1 (0%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SE	156/167 (93%)	153 (98%)	3 (2%)	0	100	100
6	SF	104/135 (77%)	103 (99%)	1 (1%)	0	100	100
7	SG	154/179 (86%)	149 (97%)	5 (3%)	0	100	100
8	SH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	SI	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	SJ	97/103 (94%)	91 (94%)	4 (4%)	2 (2%)	5	3
11	SK	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	117 (98%)	2 (2%)	1 (1%)	16	16
13	SM	113/118 (96%)	105 (93%)	8 (7%)	0	100	100
14	SN	98/101 (97%)	98 (100%)	0	0	100	100
15	SO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	SP	80/82 (98%)	76 (95%)	3 (4%)	1 (1%)	9	8
17	SQ	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
18	SR	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
19	SS	81/91 (89%)	80 (99%)	1 (1%)	0	100	100
20	ST	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	SU	68/71 (96%)	68 (100%)	0	0	100	100
25	LB	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
26	LC	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
27	LD	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
28	LE	176/179 (98%)	167 (95%)	9 (5%)	0	100	100
29	LF	173/177 (98%)	163 (94%)	10 (6%)	0	100	100
30	LI	147/149 (99%)	128 (87%)	18 (12%)	1 (1%)	18	19
31	LM	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
32	LN	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
33	LO	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
34	LP	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
35	LQ	118/127 (93%)	114 (97%)	4 (3%)	0	100	100
36	LR	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
37	LS	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
38	LT	115/118 (98%)	114 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	LU	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
40	LV	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	LW	93/100 (93%)	91 (98%)	2 (2%)	0	100	100
42	LX	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
43	LY	92/94 (98%)	92 (100%)	0	0	100	100
44	La	82/85 (96%)	78 (95%)	4 (5%)	0	100	100
45	Lb	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	Lc	60/63 (95%)	60 (100%)	0	0	100	100
47	Ld	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
48	Le	66/70 (94%)	60 (91%)	6 (9%)	0	100	100
49	Lf	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
50	Lg	50/55 (91%)	48 (96%)	2 (4%)	0	100	100
51	Lh	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	Li	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
53	Lj	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
All	All	5636/5912 (95%)	5440 (96%)	191 (3%)	5 (0%)	49	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	SJ	38	GLY
10	SJ	57	VAL
30	LI	89	LYS
12	SL	44	LYS
16	SP	48	GLU

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	SB	190/199 (96%)	177 (93%)	13 (7%)	14	17
3	SC	172/190 (90%)	162 (94%)	10 (6%)	18	22
4	SD	172/173 (99%)	164 (95%)	8 (5%)	23	31
5	SE	120/126 (95%)	114 (95%)	6 (5%)	22	28
6	SF	92/116 (79%)	83 (90%)	9 (10%)	7	8
7	SG	129/147 (88%)	114 (88%)	15 (12%)	5	5
8	SH	104/105 (99%)	100 (96%)	4 (4%)	29	40
9	SI	105/107 (98%)	102 (97%)	3 (3%)	37	51
10	SJ	87/90 (97%)	77 (88%)	10 (12%)	5	5
11	SK	91/98 (93%)	86 (94%)	5 (6%)	19	24
12	SL	102/103 (99%)	96 (94%)	6 (6%)	18	22
13	SM	93/96 (97%)	84 (90%)	9 (10%)	8	8
14	SN	83/84 (99%)	80 (96%)	3 (4%)	31	42
15	SO	76/77 (99%)	74 (97%)	2 (3%)	40	55
16	SP	65/65 (100%)	59 (91%)	6 (9%)	8	9
17	SQ	74/78 (95%)	69 (93%)	5 (7%)	14	17
18	SR	58/65 (89%)	54 (93%)	4 (7%)	14	16
19	SS	72/78 (92%)	60 (83%)	12 (17%)	2	2
20	ST	65/66 (98%)	58 (89%)	7 (11%)	6	6
21	SU	60/61 (98%)	54 (90%)	6 (10%)	7	7
25	LB	216/218 (99%)	212 (98%)	4 (2%)	50	66
26	LC	164/164 (100%)	159 (97%)	5 (3%)	36	49
27	LD	165/165 (100%)	161 (98%)	4 (2%)	43	58
28	LE	149/150 (99%)	139 (93%)	10 (7%)	15	17
29	LF	136/138 (99%)	128 (94%)	8 (6%)	18	22
30	LI	114/114 (100%)	107 (94%)	7 (6%)	17	20
31	LM	116/116 (100%)	112 (97%)	4 (3%)	32	44
32	LN	104/104 (100%)	99 (95%)	5 (5%)	23	30
33	LO	103/103 (100%)	100 (97%)	3 (3%)	37	51
34	LP	108/108 (100%)	100 (93%)	8 (7%)	13	14
35	LQ	100/103 (97%)	99 (99%)	1 (1%)	68	81
36	LR	86/87 (99%)	77 (90%)	9 (10%)	6	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	LS	99/100 (99%)	98 (99%)	1 (1%)	68	81
38	LT	89/90 (99%)	89 (100%)	0	100	100
39	LU	84/84 (100%)	82 (98%)	2 (2%)	43	58
40	LV	93/93 (100%)	87 (94%)	6 (6%)	15	18
41	LW	82/84 (98%)	80 (98%)	2 (2%)	43	58
42	LX	83/85 (98%)	82 (99%)	1 (1%)	63	78
43	LY	78/78 (100%)	73 (94%)	5 (6%)	16	19
44	La	62/63 (98%)	55 (89%)	7 (11%)	5	5
45	Lb	67/68 (98%)	64 (96%)	3 (4%)	24	33
46	Lc	54/55 (98%)	54 (100%)	0	100	100
47	Ld	48/49 (98%)	45 (94%)	3 (6%)	16	19
48	Le	60/62 (97%)	52 (87%)	8 (13%)	4	3
49	Lf	47/48 (98%)	46 (98%)	1 (2%)	47	63
50	Lg	47/49 (96%)	45 (96%)	2 (4%)	26	35
51	Lh	38/38 (100%)	37 (97%)	1 (3%)	40	55
52	Li	51/52 (98%)	50 (98%)	1 (2%)	48	64
53	Lj	34/34 (100%)	30 (88%)	4 (12%)	5	5
All	All	4687/4826 (97%)	4429 (94%)	258 (6%)	21	24

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	La	56	ASP
47	Ld	49	ASN
13	SM	101	ARG
13	SM	42	ASP
48	Le	24	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
28	LE	63	GLN
49	Lf	6	ASN
32	LN	88	ASN
49	Lf	4	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	La	76	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1541/1542 (99%)	241 (15%)	4 (0%)
22	mR	26/60 (43%)	12 (46%)	0
23	23	2764/2904 (95%)	409 (14%)	11 (0%)
24	5	119/120 (99%)	18 (15%)	0
54	Pt	76/77 (98%)	13 (17%)	0
All	All	4526/4703 (96%)	693 (15%)	15 (0%)

5 of 693 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	5	U
1	16	6	G
1	16	9	G
1	16	22	G
1	16	32	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	23	827	U
23	23	2689	U
23	23	858	G
23	23	2756	U
23	23	2324	U

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

40 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	$\#\|Z\| > 2$
23	PSU	23	2457	23	18,21,22	1.39	3 (16%)	21,30,33	2.17	4 (19%)
23	OMU	23	2552	23	19,22,23	1.22	3 (15%)	25,31,34	1.80	6 (24%)
23	PSU	23	955	23	18,21,22	1.44	4 (22%)	21,30,33	2.06	3 (14%)
23	6MZ	23	2030	23	22,25,26	1.49	5 (22%)	29,36,39	2.46	11 (37%)
23	5MU	23	1939	23,58	19,22,23	1.54	4 (21%)	27,32,35	2.34	6 (22%)
54	OMC	Pt	33	54	19,22,23	0.86	0	25,31,34	1.33	3 (12%)
1	5MC	16	967	1	19,22,23	1.57	3 (15%)	26,32,35	1.12	2 (7%)
54	H2U	Pt	21	54	18,21,22	0.96	2 (11%)	19,30,33	0.71	0
54	G7M	Pt	47	54	23,26,27	0.72	1 (4%)	34,39,42	0.62	1 (2%)
23	PSU	23	746	57,23	18,21,22	1.41	3 (16%)	21,30,33	2.04	4 (19%)
1	4OC	16	1402	57,1	20,23,24	0.78	0	25,32,35	2.08	7 (28%)
23	3TD	23	1915	23	19,22,23	1.22	2 (10%)	23,32,35	2.07	3 (13%)
1	MA6	16	1519	1	23,26,27	1.54	5 (21%)	33,38,41	2.20	10 (30%)
12	D2T	SL	89	12	8,9,10	7.08	2 (25%)	6,11,13	2.60	3 (50%)
1	PSU	16	516	57,1	18,21,22	1.36	3 (16%)	21,30,33	2.06	4 (19%)
1	UR3	16	1498	1	19,22,23	0.94	0	26,32,35	1.70	4 (15%)
1	5MC	16	1407	1	19,22,23	1.54	3 (15%)	26,32,35	1.20	3 (11%)
23	OMC	23	2498	57,23	19,22,23	0.83	0	25,31,34	1.05	1 (4%)
23	PSU	23	2604	23	18,21,22	1.68	5 (27%)	21,30,33	2.24	5 (23%)
23	PSU	23	2605	23	18,21,22	1.52	5 (27%)	21,30,33	2.31	4 (19%)
23	2MA	23	2503	57,23,58	22,25,26	1.50	4 (18%)	32,37,40	2.38	8 (25%)
34	4D4	LP	81	34	9,11,12	2.03	2 (22%)	7,13,15	1.78	3 (42%)
1	2MG	16	1516	1	23,26,27	1.24	4 (17%)	33,38,41	2.19	7 (21%)
23	PSU	23	2504	23,58	18,21,22	1.57	4 (22%)	21,30,33	2.15	4 (19%)
1	MA6	16	1518	1	23,26,27	1.55	5 (21%)	33,38,41	2.22	10 (30%)
1	2MG	16	1207	1	23,26,27	1.26	4 (17%)	33,38,41	2.21	6 (18%)
54	4SU	Pt	8	54	18,21,22	1.87	5 (27%)	25,30,33	2.30	5 (20%)
23	G7M	23	2069	23	23,26,27	0.68	1 (4%)	34,39,42	0.63	1 (2%)
23	2MG	23	2445	23	23,26,27	1.25	3 (13%)	33,38,41	2.27	7 (21%)
11	IAS	SK	119	11	6,7,8	1.34	1 (16%)	3,8,10	0.65	0
1	G7M	16	527	1	23,26,27	0.71	1 (4%)	34,39,42	0.68	1 (2%)
23	2MG	23	1835	23	23,26,27	1.27	4 (17%)	33,38,41	2.35	7 (21%)
23	5MC	23	1962	23,58	19,22,23	1.66	3 (15%)	26,32,35	1.08	2 (7%)
1	2MG	16	966	1	23,26,27	1.26	4 (17%)	33,38,41	2.14	6 (18%)
23	6MZ	23	1618	23	22,25,26	1.46	4 (18%)	29,36,39	2.21	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	5MU	23	747	23	19,22,23	1.41	5 (26%)	27,32,35	2.19	9 (33%)
23	1MG	23	745	23	23,26,27	1.19	3 (13%)	33,39,42	1.74	5 (15%)
23	H2U	23	2449	23	18,21,22	1.09	3 (16%)	19,30,33	0.94	1 (5%)
23	PSU	23	2580	23	18,21,22	1.39	3 (16%)	21,30,33	2.12	4 (19%)
23	OMG	23	2251	23,54	23,26,27	1.22	3 (13%)	32,38,41	2.05	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
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	6MZ	23	2030	23	-	2/9/27/28	0/3/3/3
23	5MU	23	1939	23,58	-	0/7/25/26	0/2/2/2
54	OMC	Pt	33	54	-	0/9/27/28	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
54	H2U	Pt	21	54	-	2/7/38/39	0/2/2/2
54	G7M	Pt	47	54	-	2/7/25/26	0/3/3/3
23	PSU	23	746	57,23	-	2/7/25/26	0/2/2/2
1	4OC	16	1402	57,1	-	2/9/29/30	0/2/2/2
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
1	MA6	16	1519	1	-	4/11/29/30	0/3/3/3
12	D2T	SL	89	12	-	4/7/12/14	-
1	PSU	16	516	57,1	-	0/7/25/26	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	57,23	-	0/9/27/28	0/2/2/2
23	PSU	23	2604	23	-	2/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
23	2MA	23	2503	57,23,58	-	2/7/25/26	0/3/3/3
34	4D4	LP	81	34	-	3/11/12/14	-
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
23	PSU	23	2504	23,58	-	2/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	0/11/29/30	0/3/3/3
1	2MG	16	1207	1	-	0/9/27/28	0/3/3/3
54	4SU	Pt	8	54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	G7M	23	2069	23	-	1/7/25/26	0/3/3/3
23	2MG	23	2445	23	-	2/9/27/28	0/3/3/3
11	IAS	SK	119	11	-	0/7/7/8	-
1	G7M	16	527	1	-	3/7/25/26	0/3/3/3
23	2MG	23	1835	23	-	0/9/27/28	0/3/3/3
23	5MC	23	1962	23,58	-	0/7/25/26	0/2/2/2
1	2MG	16	966	1	-	0/9/27/28	0/3/3/3
23	6MZ	23	1618	23	-	2/9/27/28	0/3/3/3
23	5MU	23	747	23	-	1/7/25/26	0/2/2/2
23	1MG	23	745	23	-	0/7/25/26	0/3/3/3
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
23	OMG	23	2251	23,54	-	1/9/27/28	0/3/3/3

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	SL	89	D2T	CB-CA	-19.05	1.48	1.54
23	23	1962	5MC	C5-C4	6.12	1.48	1.44
1	16	967	5MC	C5-C4	5.71	1.48	1.44
1	16	1407	5MC	C5-C4	5.47	1.48	1.44
54	Pt	8	4SU	C4-S4	-5.11	1.59	1.68

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2503	2MA	C5-C4-N3	-8.44	118.29	127.18
23	23	1835	2MG	C2-N3-C4	7.95	121.95	112.00
23	23	2445	2MG	C2-N3-C4	7.65	121.58	112.00
1	16	1207	2MG	C2-N3-C4	7.35	121.19	112.00
23	23	2605	PSU	N1-C2-N3	7.18	122.74	115.17

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	1402	4OC	O4'-C1'-N1-C2
1	16	1402	4OC	O4'-C1'-N1-C6
1	16	1519	MA6	O4'-C4'-C5'-O5'
12	SL	89	D2T	CA-CB-CG-OD1
12	SL	89	D2T	CA-CB-CG-OD2

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	23	2030	6MZ	1	0
23	23	1939	5MU	2	0
1	16	1402	4OC	1	0
23	23	1915	3TD	2	0
23	23	2604	PSU	1	0
23	23	2503	2MA	1	0
34	LP	81	4D4	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 352 ligands modelled in this entry, 335 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
55	PUT	23	3010	-	5,5,5	0.14	0	4,4,4	0.19	0
55	PUT	23	3009	-	5,5,5	0.11	0	4,4,4	0.17	0
56	SPD	16	1602	-	9,9,9	0.16	0	8,8,8	0.20	0
60	ATP	23	3001	-	32,33,33	0.33	0	48,52,52	0.34	0
55	PUT	23	3004	-	5,5,5	0.13	0	4,4,4	0.22	0
56	SPD	23	3013	-	9,9,9	0.27	0	8,8,8	0.28	0
56	SPD	23	3014	-	9,9,9	0.26	0	8,8,8	0.20	0
55	PUT	23	3003	-	5,5,5	0.14	0	4,4,4	0.15	0
55	PUT	23	3008	-	5,5,5	0.14	0	4,4,4	0.20	0
55	PUT	23	3006	-	5,5,5	0.11	0	4,4,4	0.20	0
55	PUT	23	3007	-	5,5,5	0.10	0	4,4,4	0.28	0
56	SPD	23	3011	-	9,9,9	0.27	0	8,8,8	0.27	0
55	PUT	23	3005	-	5,5,5	0.18	0	4,4,4	0.24	0
56	SPD	23	3012	-	9,9,9	0.24	0	8,8,8	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	PUT	16	1601	-	5,5,5	0.13	0	4,4,4	0.23	0
60	ATP	23	3002	-	32,33,33	0.27	0	48,52,52	0.36	0
61	FME	Pt	101	54	8,9,10	0.59	0	8,9,11	1.14	1 (12%)

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
55	PUT	23	3010	-	-	1/3/3/3	-
55	PUT	23	3009	-	-	1/3/3/3	-
56	SPD	16	1602	-	-	3/7/7/7	-
60	ATP	23	3001	-	-	4/22/38/38	0/3/3/3
55	PUT	23	3004	-	-	1/3/3/3	-
56	SPD	23	3013	-	-	2/7/7/7	-
56	SPD	23	3014	-	-	2/7/7/7	-
55	PUT	23	3003	-	-	1/3/3/3	-
55	PUT	23	3008	-	-	0/3/3/3	-
55	PUT	23	3006	-	-	2/3/3/3	-
55	PUT	23	3007	-	-	1/3/3/3	-
56	SPD	23	3011	-	-	2/7/7/7	-
55	PUT	23	3005	-	-	1/3/3/3	-
56	SPD	23	3012	-	-	2/7/7/7	-
55	PUT	16	1601	-	-	2/3/3/3	-
60	ATP	23	3002	-	-	3/22/38/38	0/3/3/3
61	FME	Pt	101	54	-	4/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	Pt	101	FME	O-C-CA	-2.85	117.43	124.77

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	23	3001	ATP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

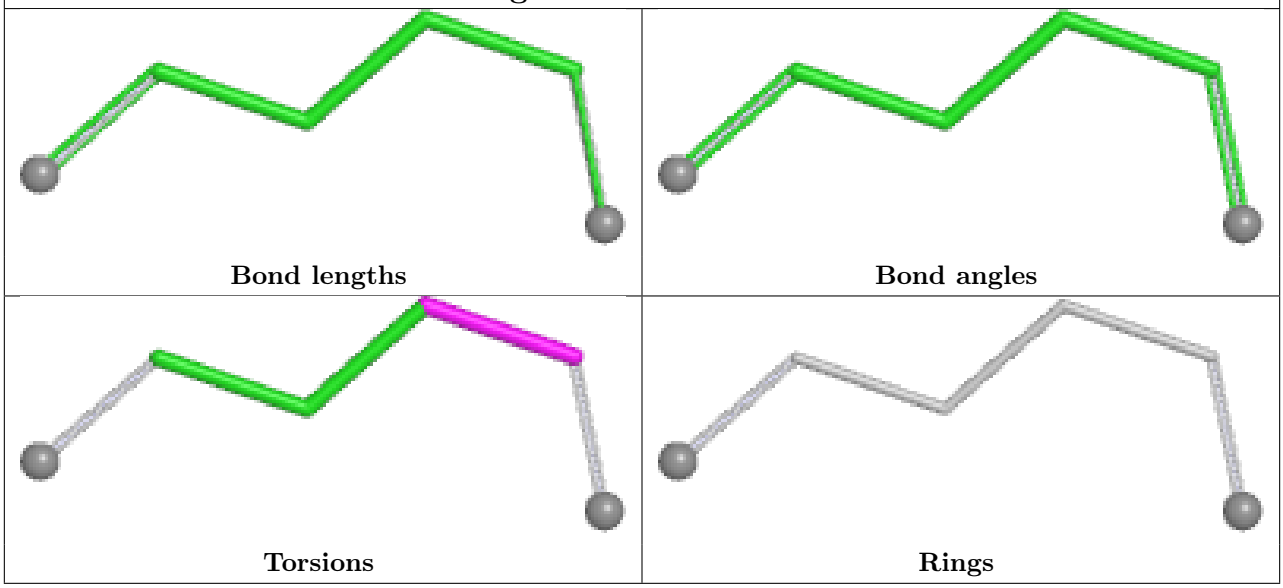
Mol	Chain	Res	Type	Atoms
61	Pt	101	FME	O1-CN-N-CA
61	Pt	101	FME	N-CA-CB-CG
56	16	1602	SPD	N6-C7-C8-C9
55	23	3005	PUT	C1-C2-C3-C4

There are no ring outliers.

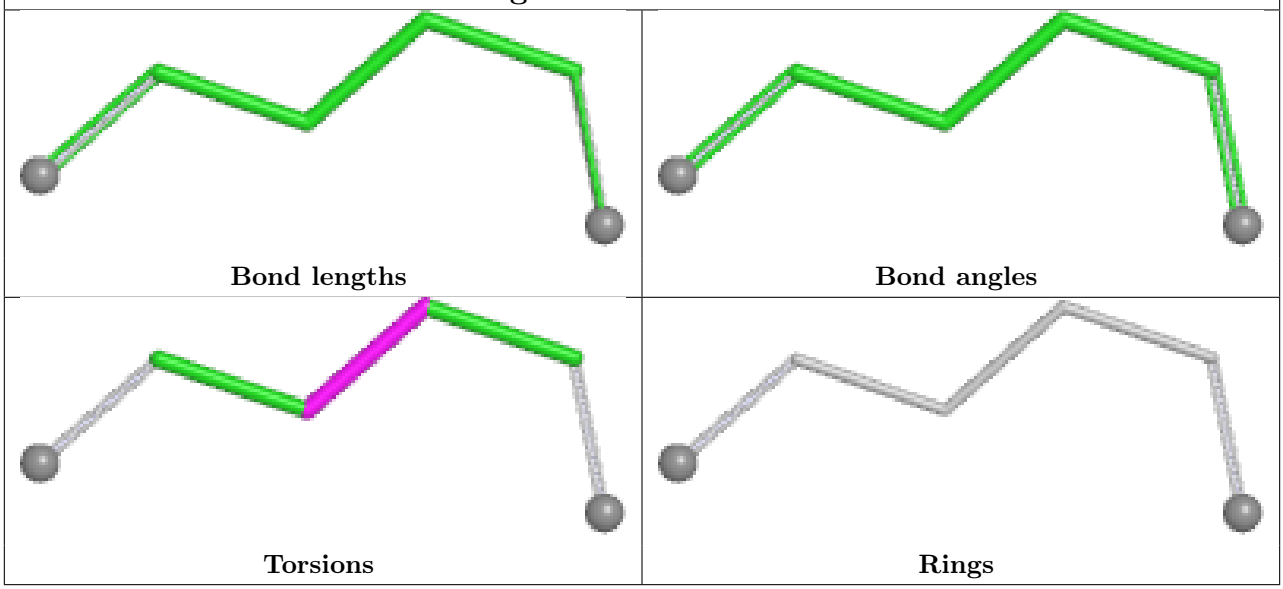
No monomer is involved in short contacts.

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.

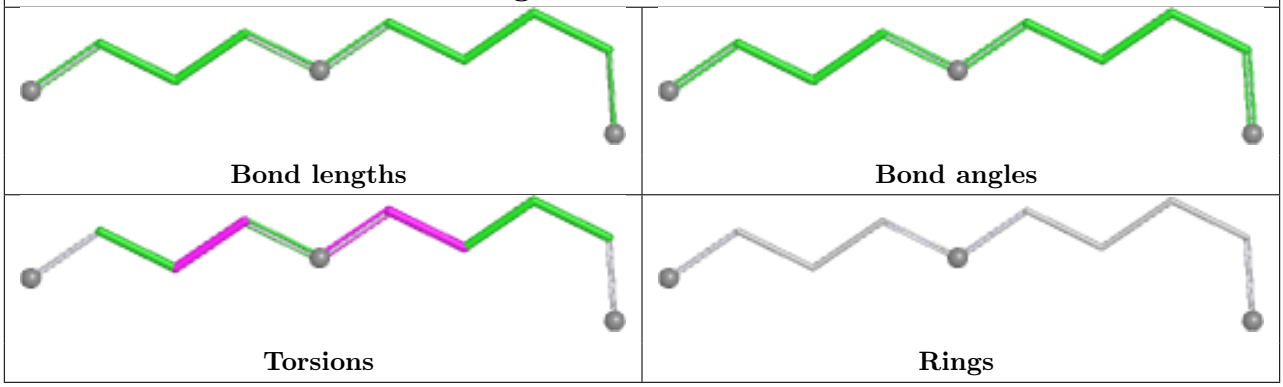
Ligand PUT 23 3010



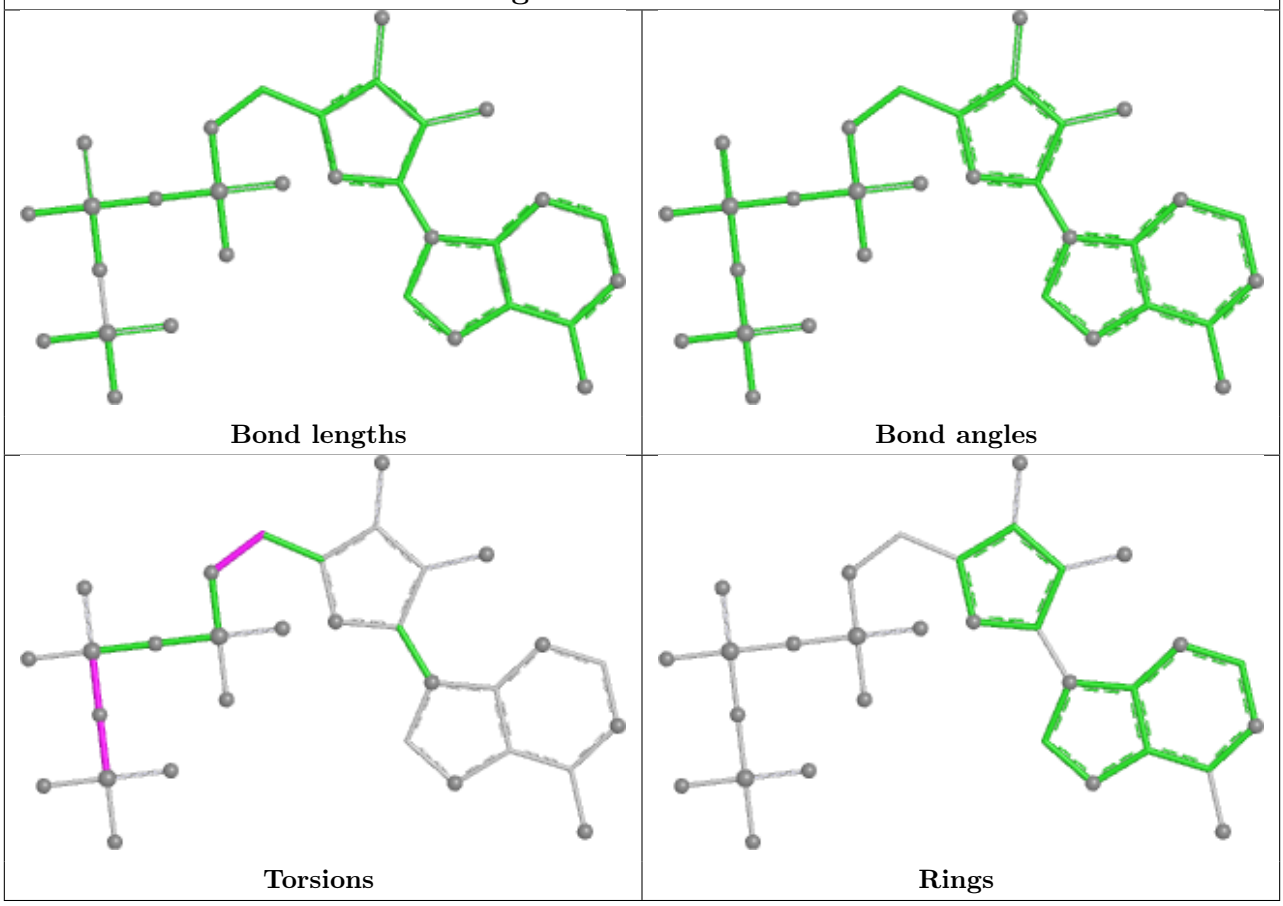
Ligand PUT 23 3009



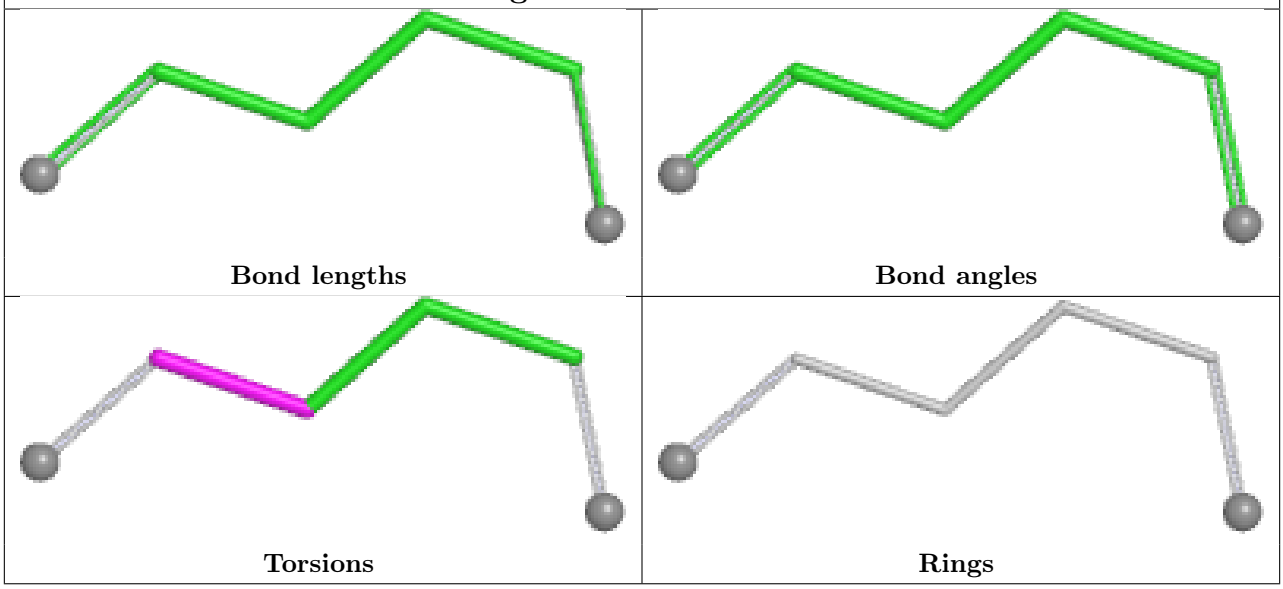
Ligand SPD 16 1602



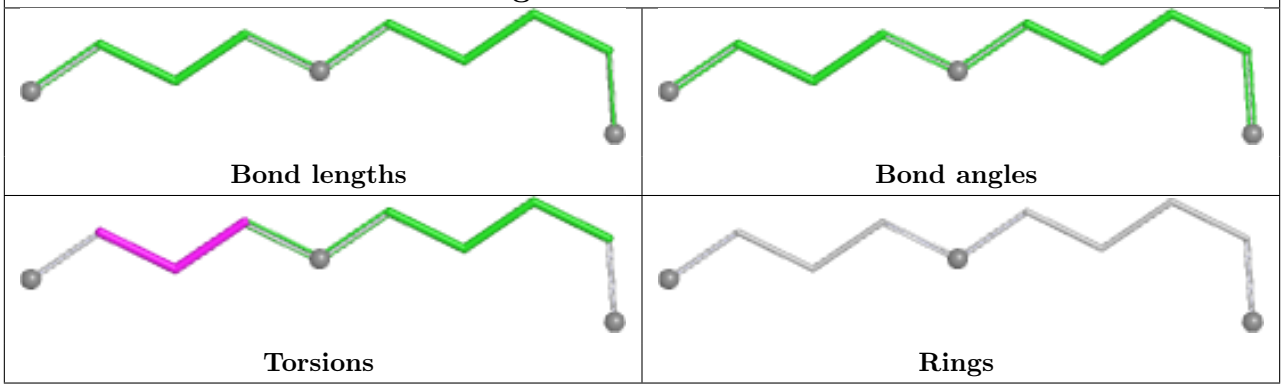
Ligand ATP 23 3001



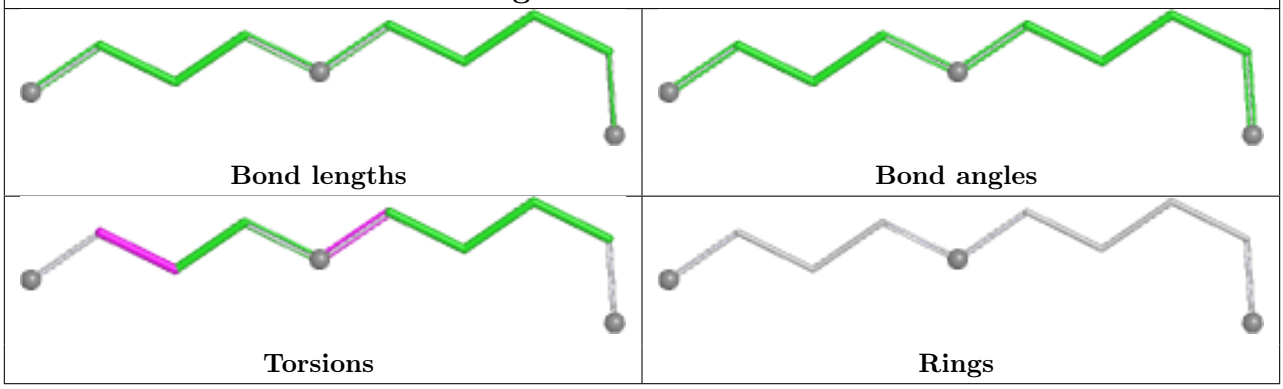
Ligand PUT 23 3004



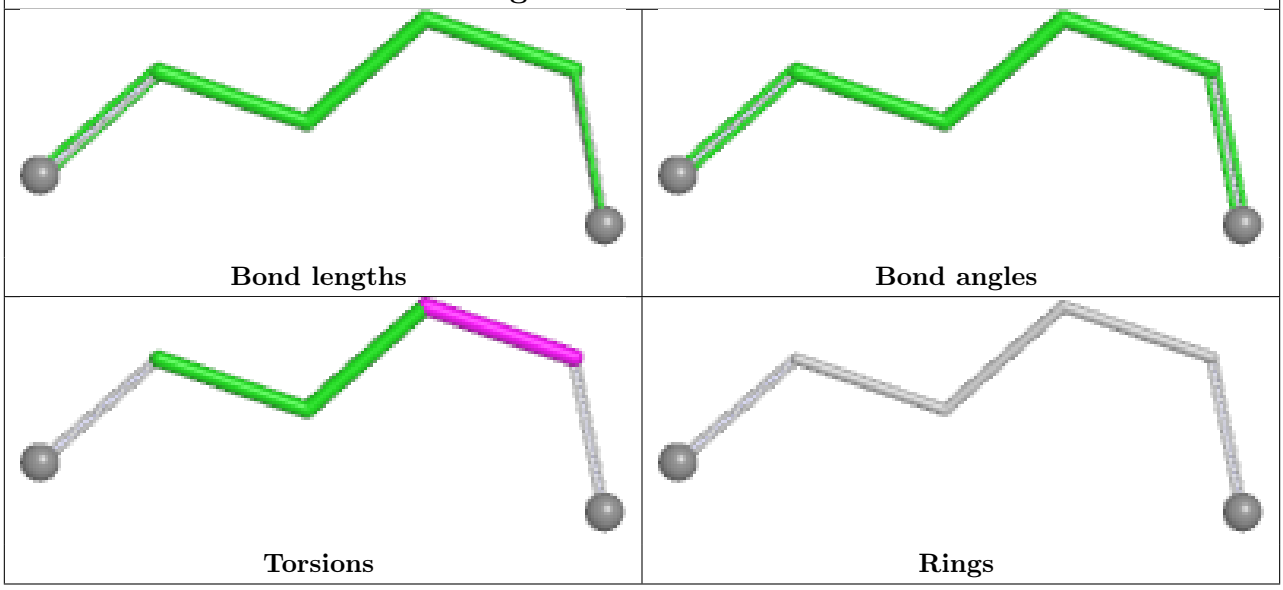
Ligand SPD 23 3013



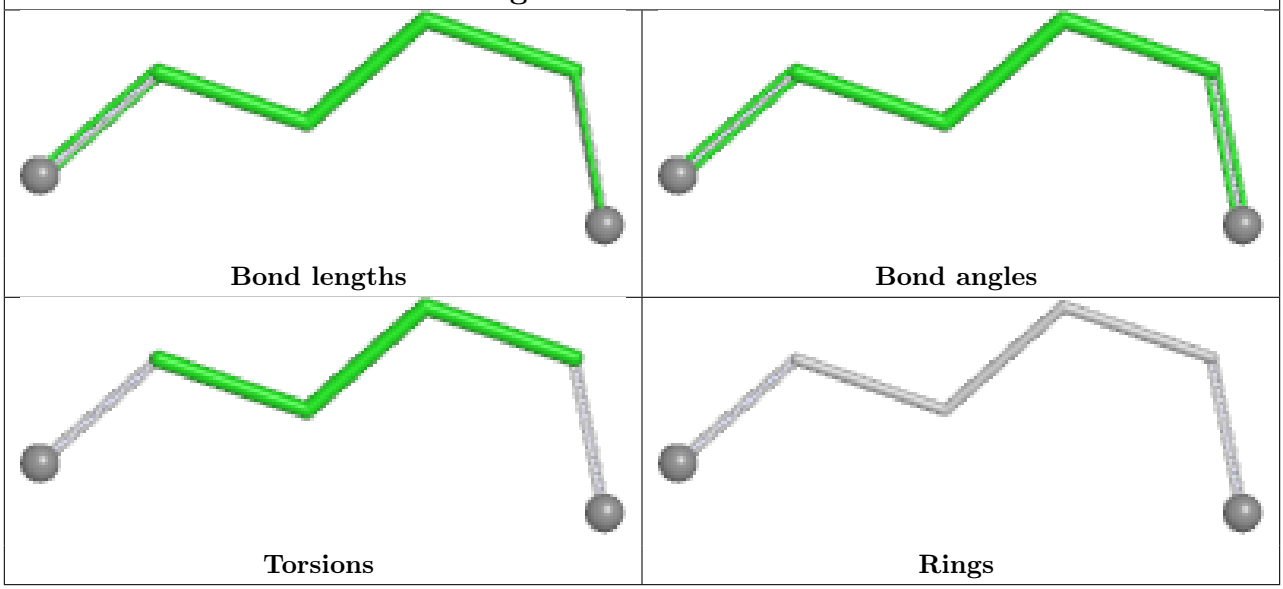
Ligand SPD 23 3014



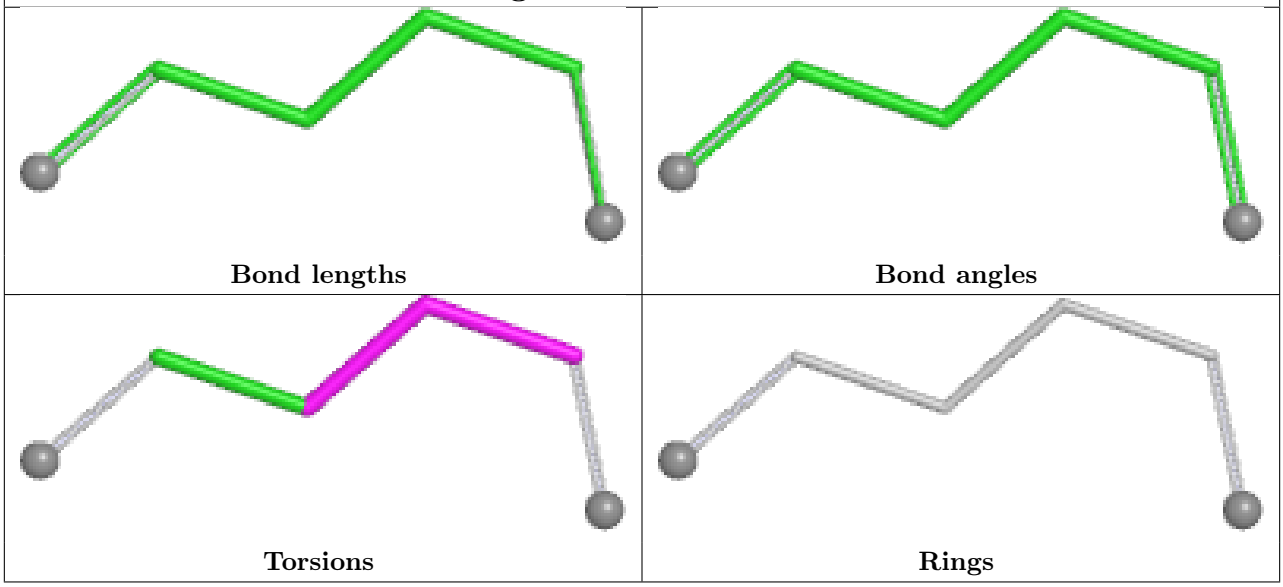
Ligand PUT 23 3003



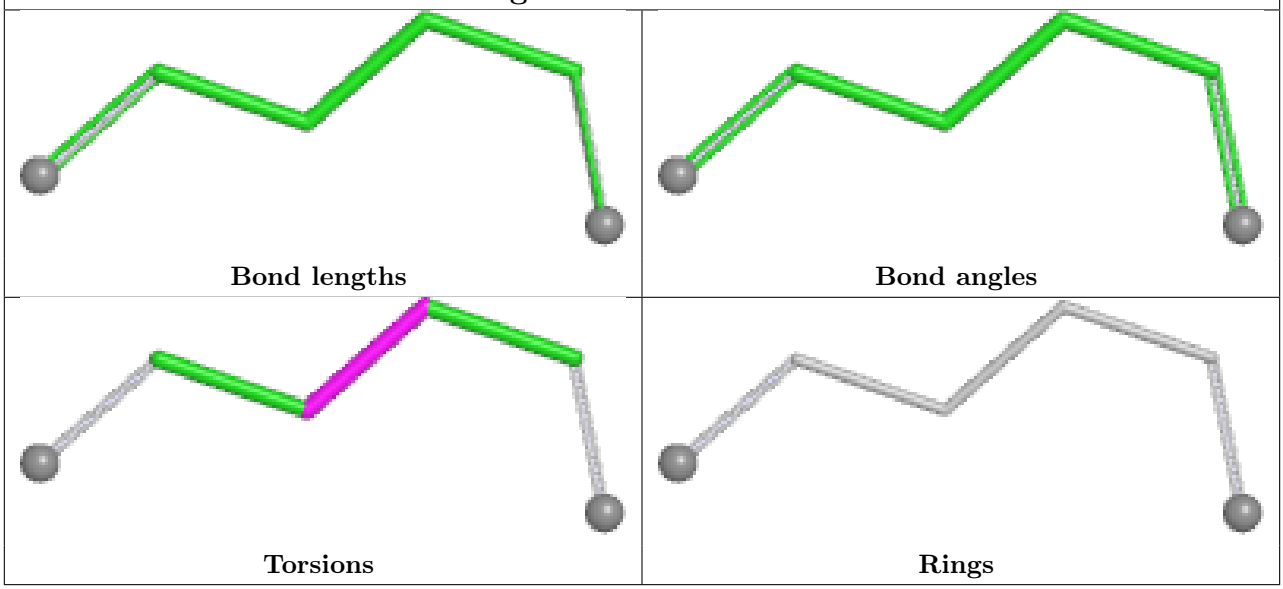
Ligand PUT 23 3008



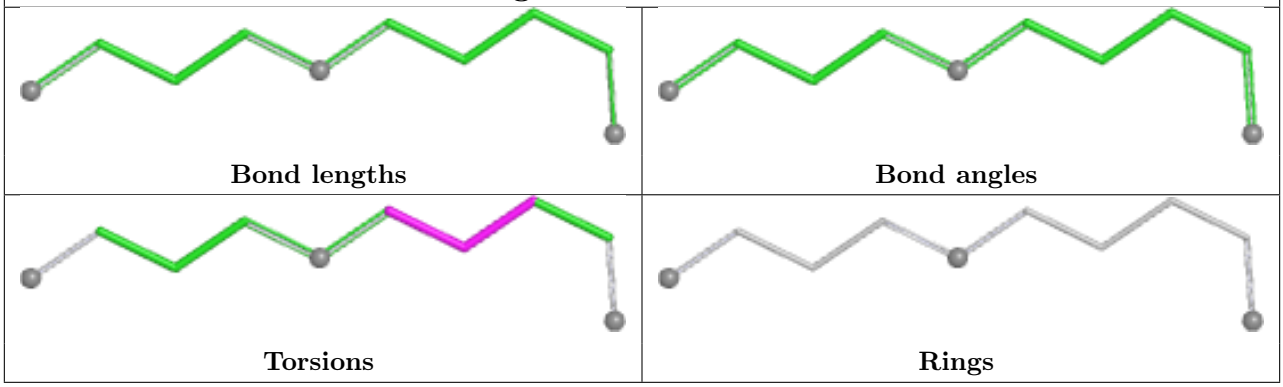
Ligand PUT 23 3006



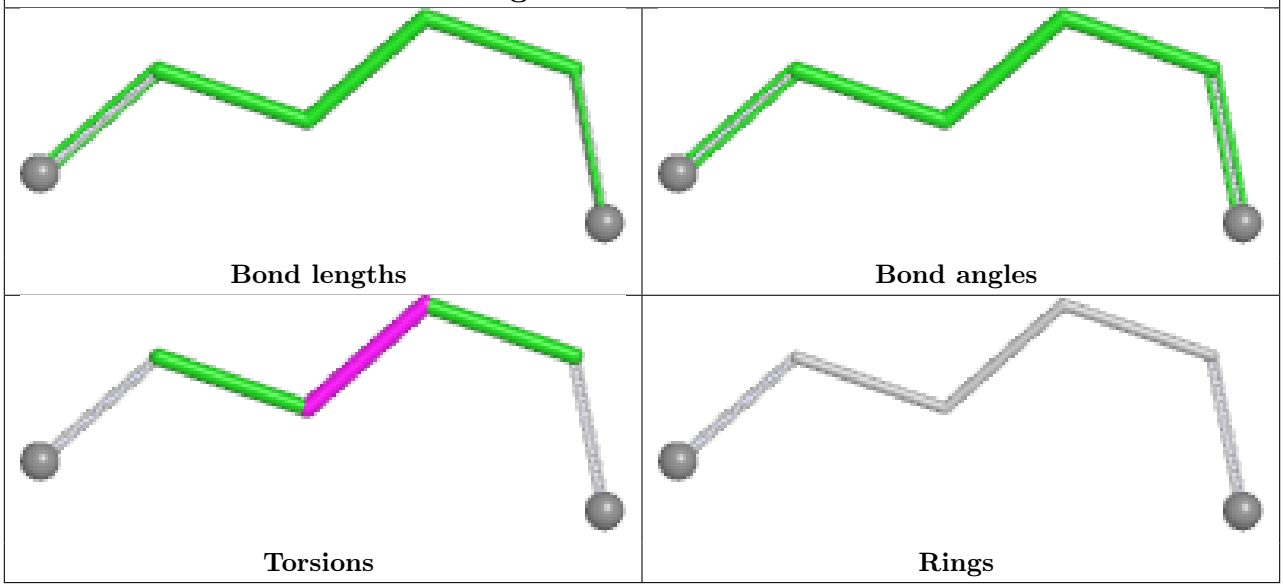
Ligand PUT 23 3007

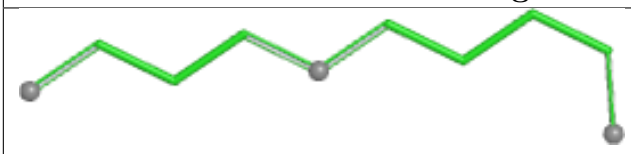
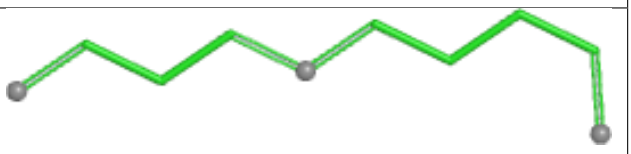
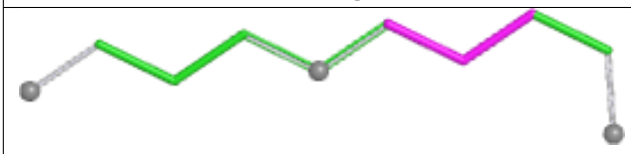
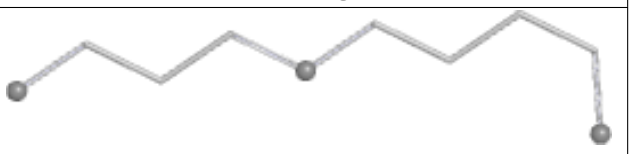


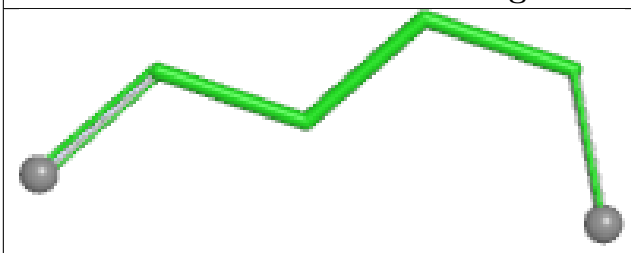
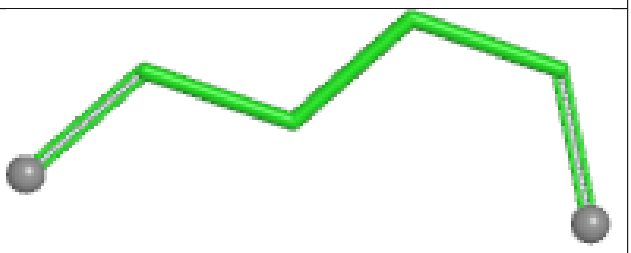
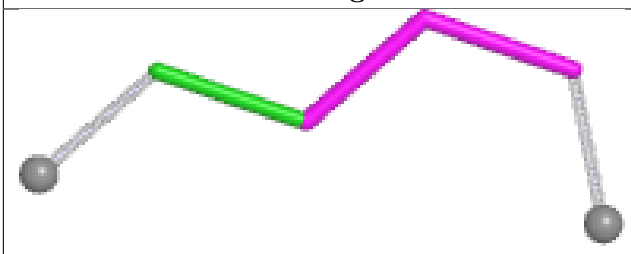
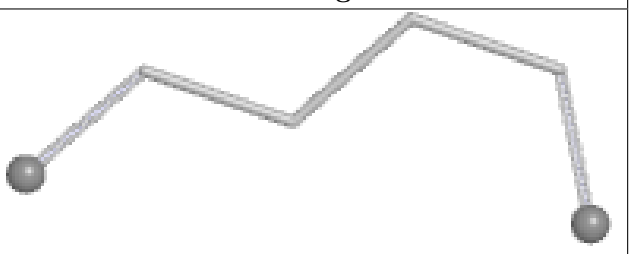
Ligand SPD 23 3011



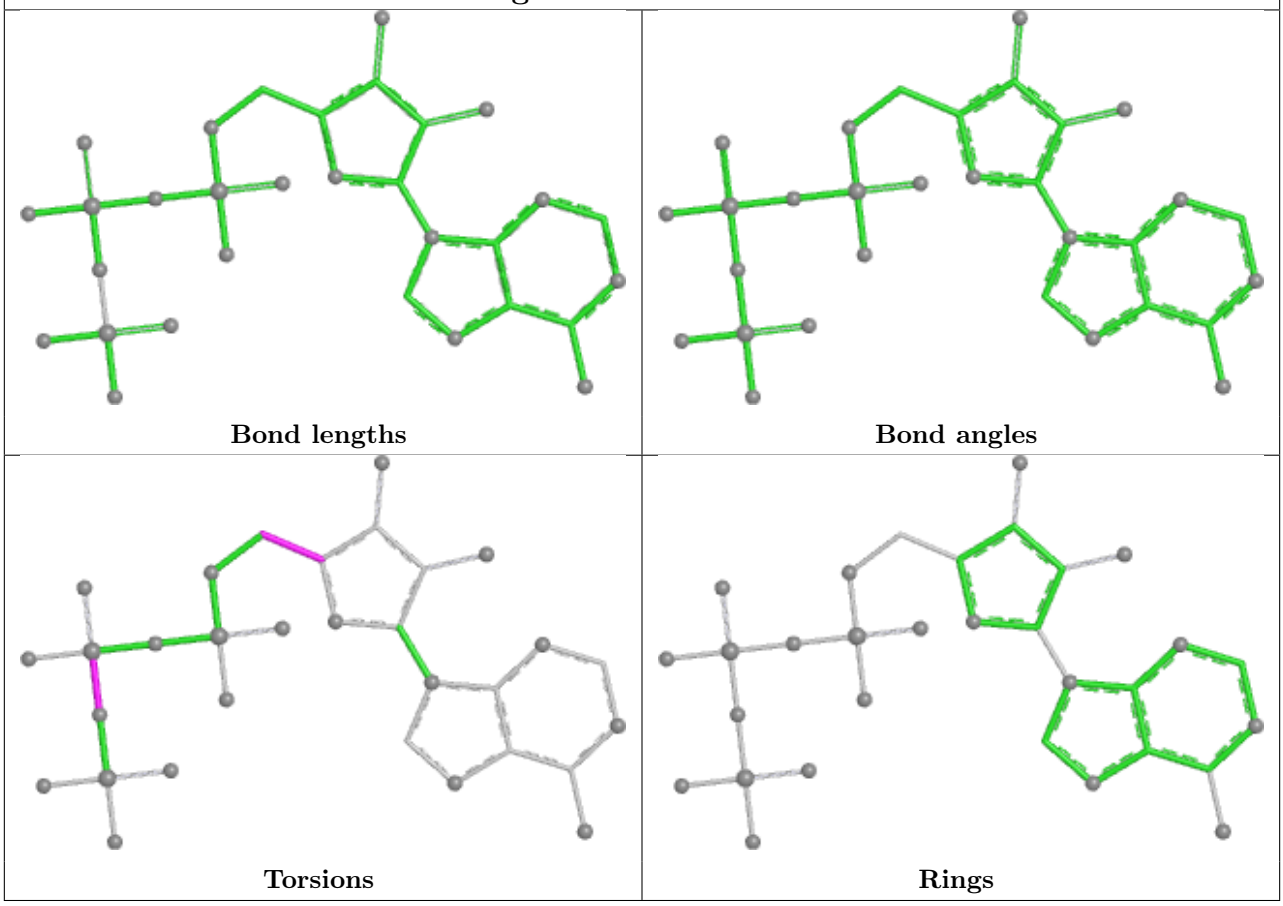
Ligand PUT 23 3005



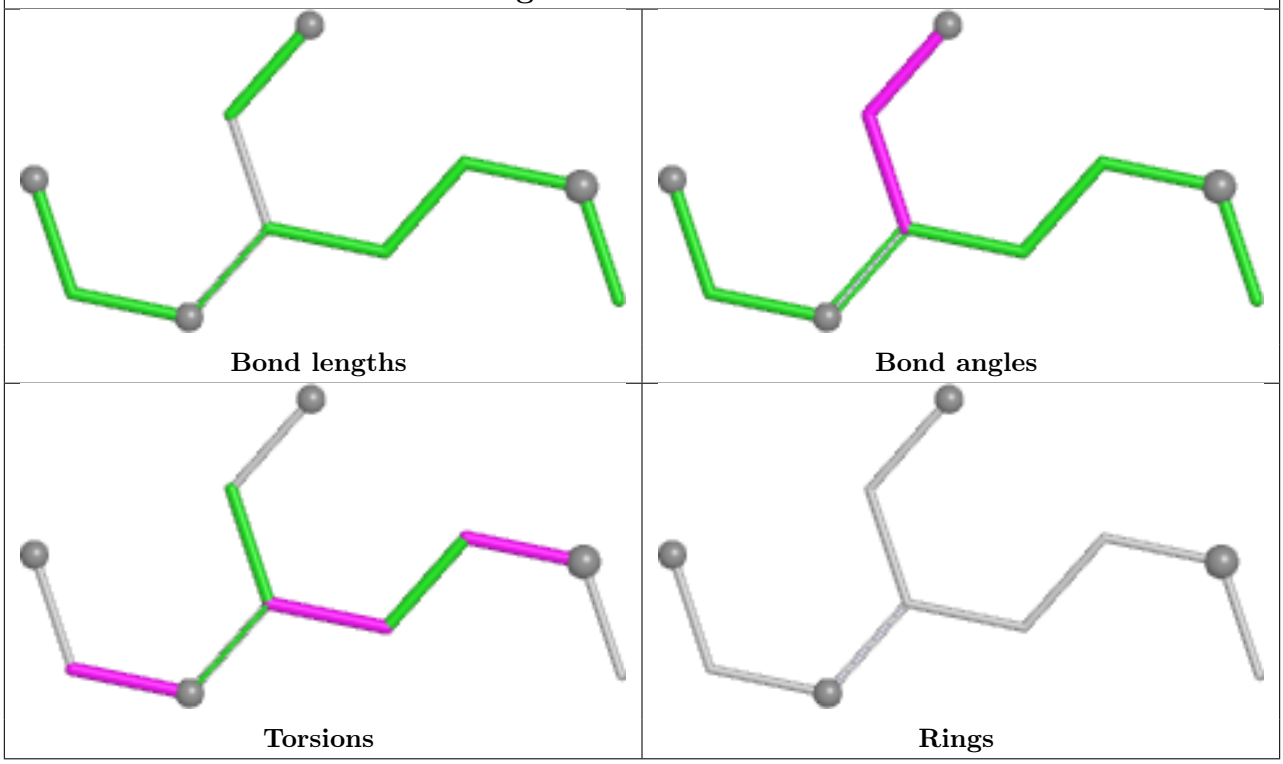
Ligand SPD 23 3012	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PUT 16 1601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP 23 3002



Ligand FME Pt 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

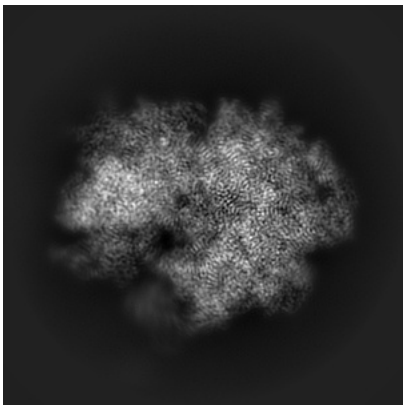
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-48830. These allow visual inspection of the internal detail of the map and identification of artifacts.

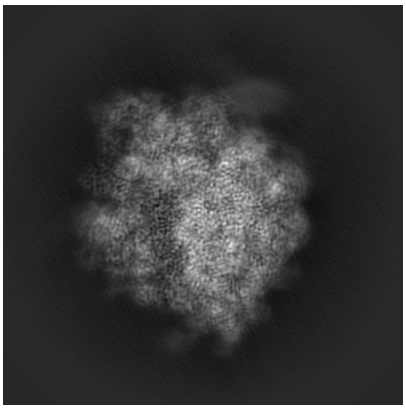
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

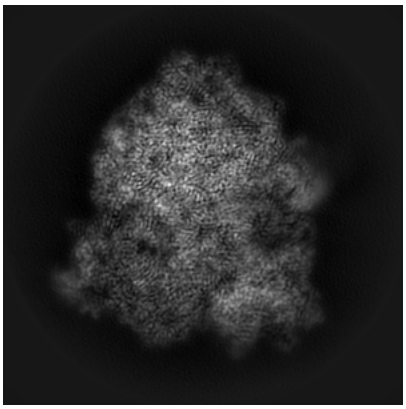
6.1.1 Primary map



X

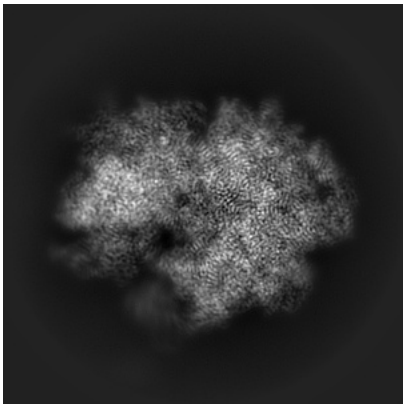


Y

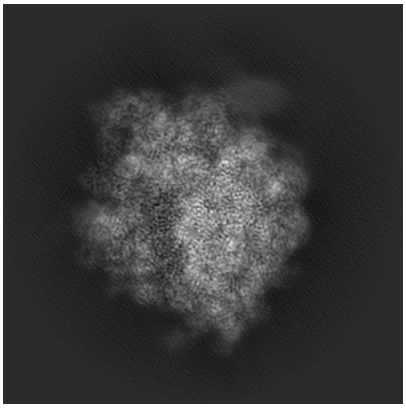


Z

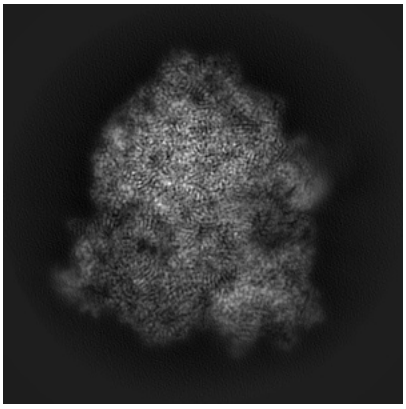
6.1.2 Raw map



X



Y

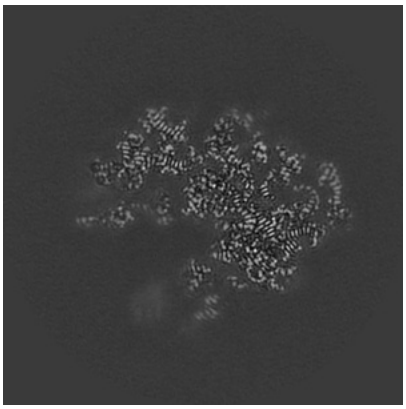


Z

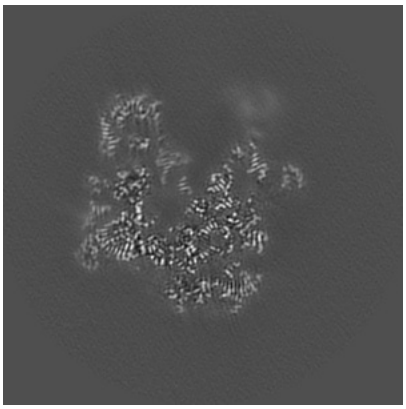
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

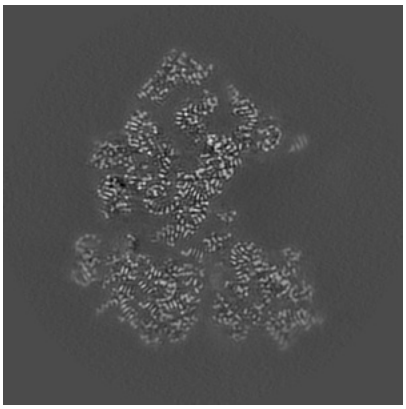
6.2.1 Primary map



X Index: 160

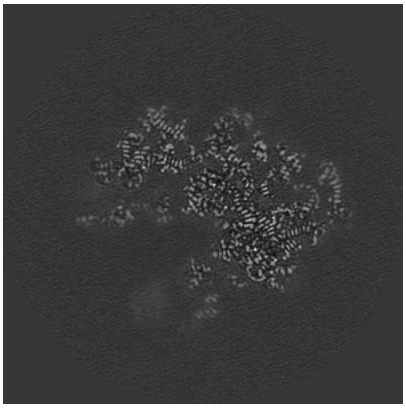


Y Index: 160

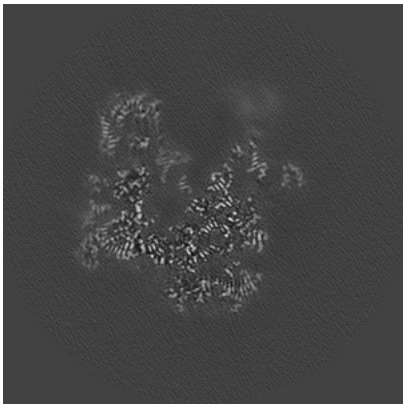


Z Index: 160

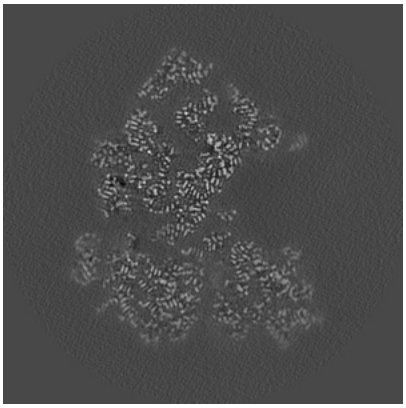
6.2.2 Raw map



X Index: 160



Y Index: 160

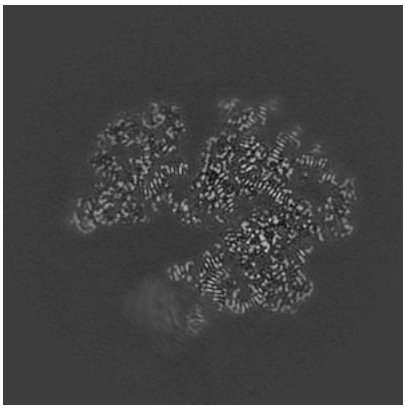


Z Index: 160

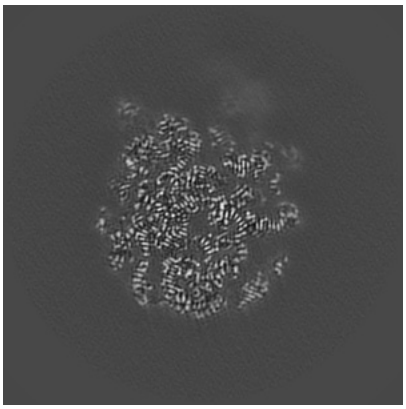
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

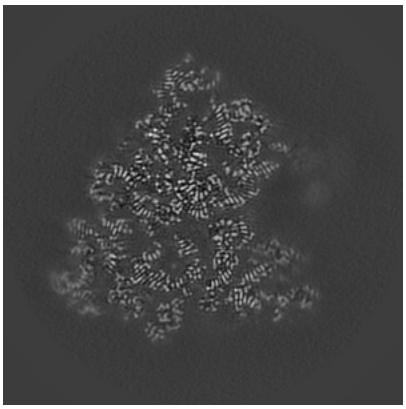
6.3.1 Primary map



X Index: 147

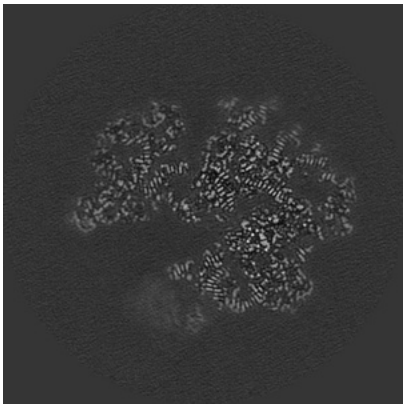


Y Index: 195

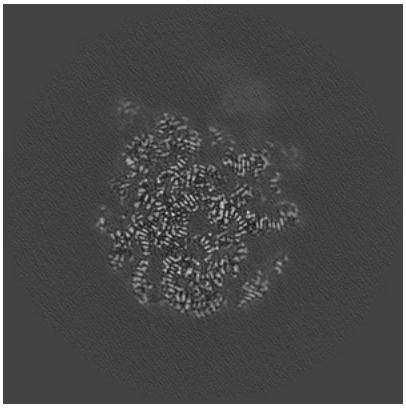


Z Index: 179

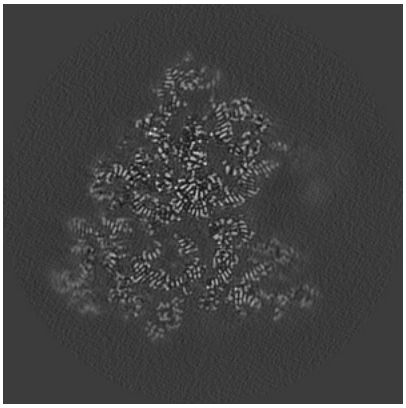
6.3.2 Raw map



X Index: 147



Y Index: 195

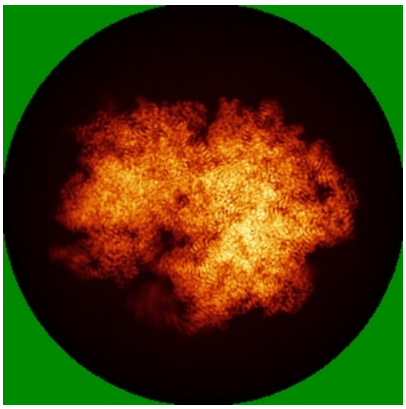


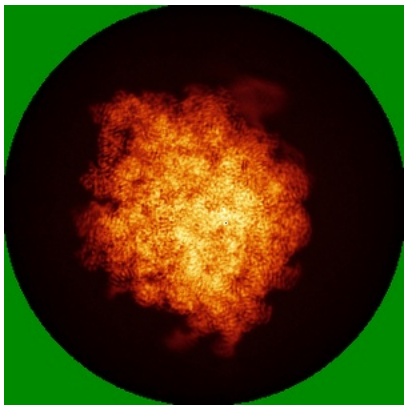
Z Index: 179

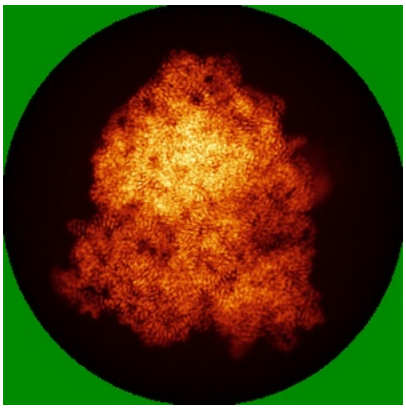
The images above show the largest variance slices of the map in three orthogonal directions.

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

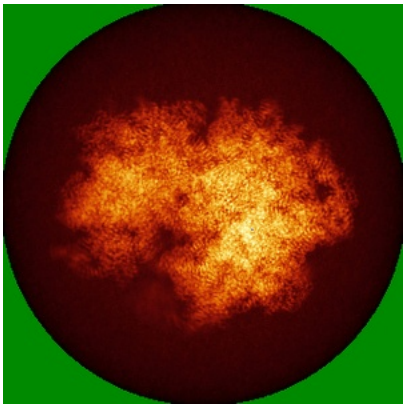
6.4.1 Primary map

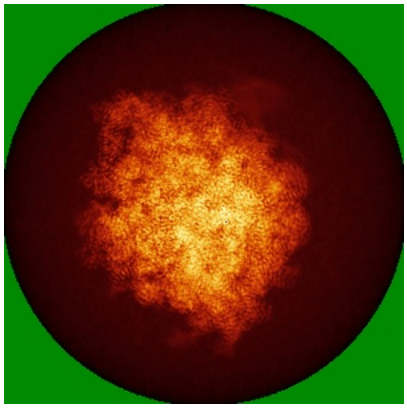

X

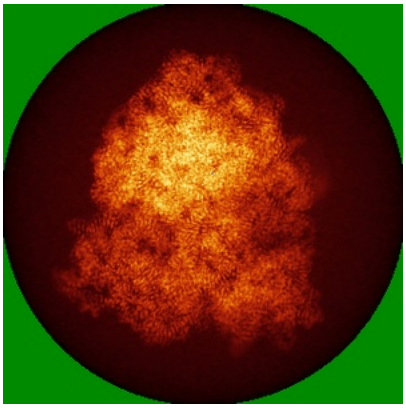

Y


Z

6.4.2 Raw map


X

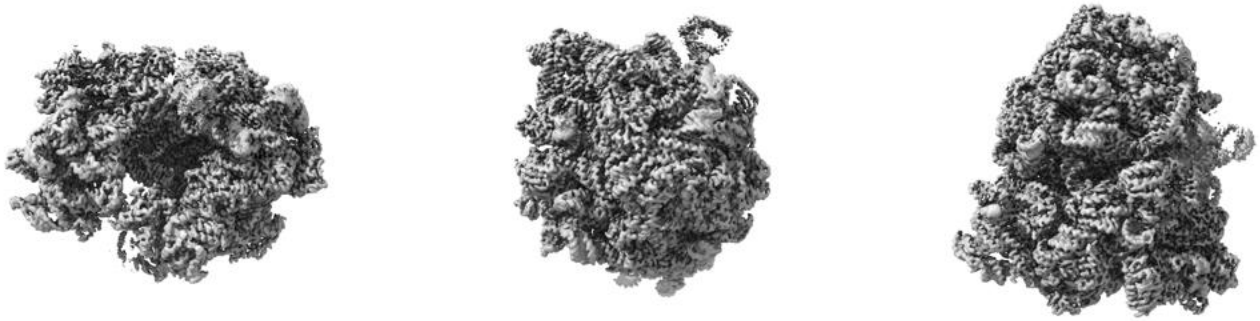

Y


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 0.008. 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.

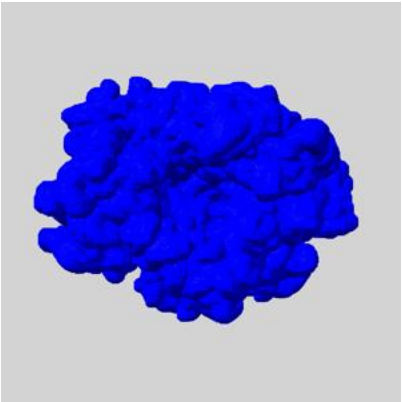
6.6 Mask visualisation (i)

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

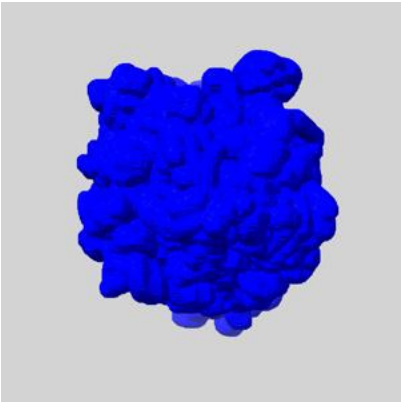
A mask typically either:

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

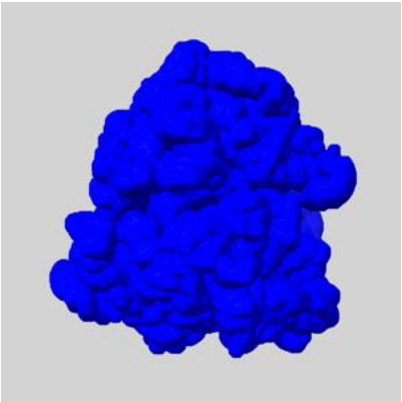
6.6.1 emd_48830_msk_1.map (i)



X



Y

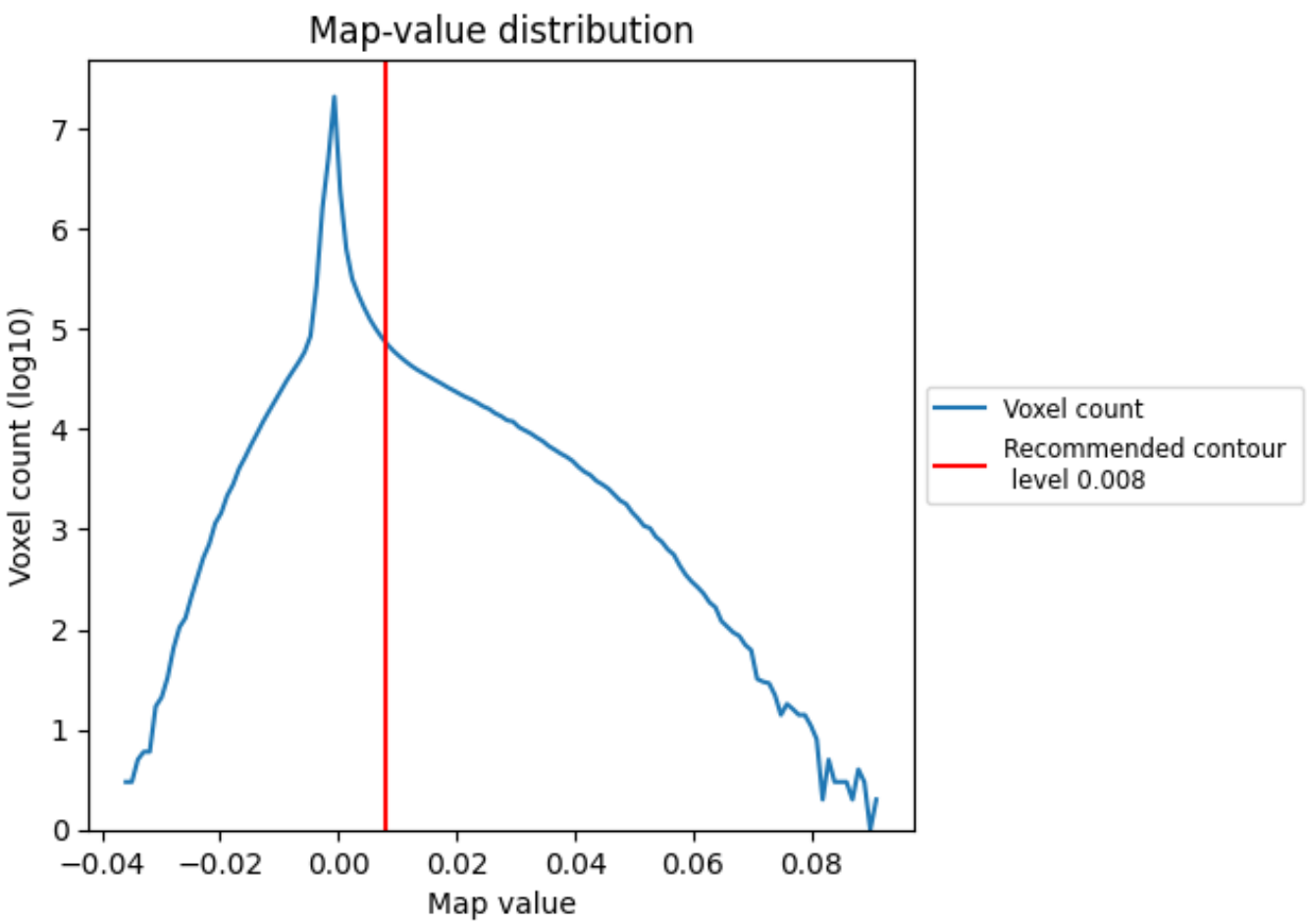


Z

7 Map analysis (i)

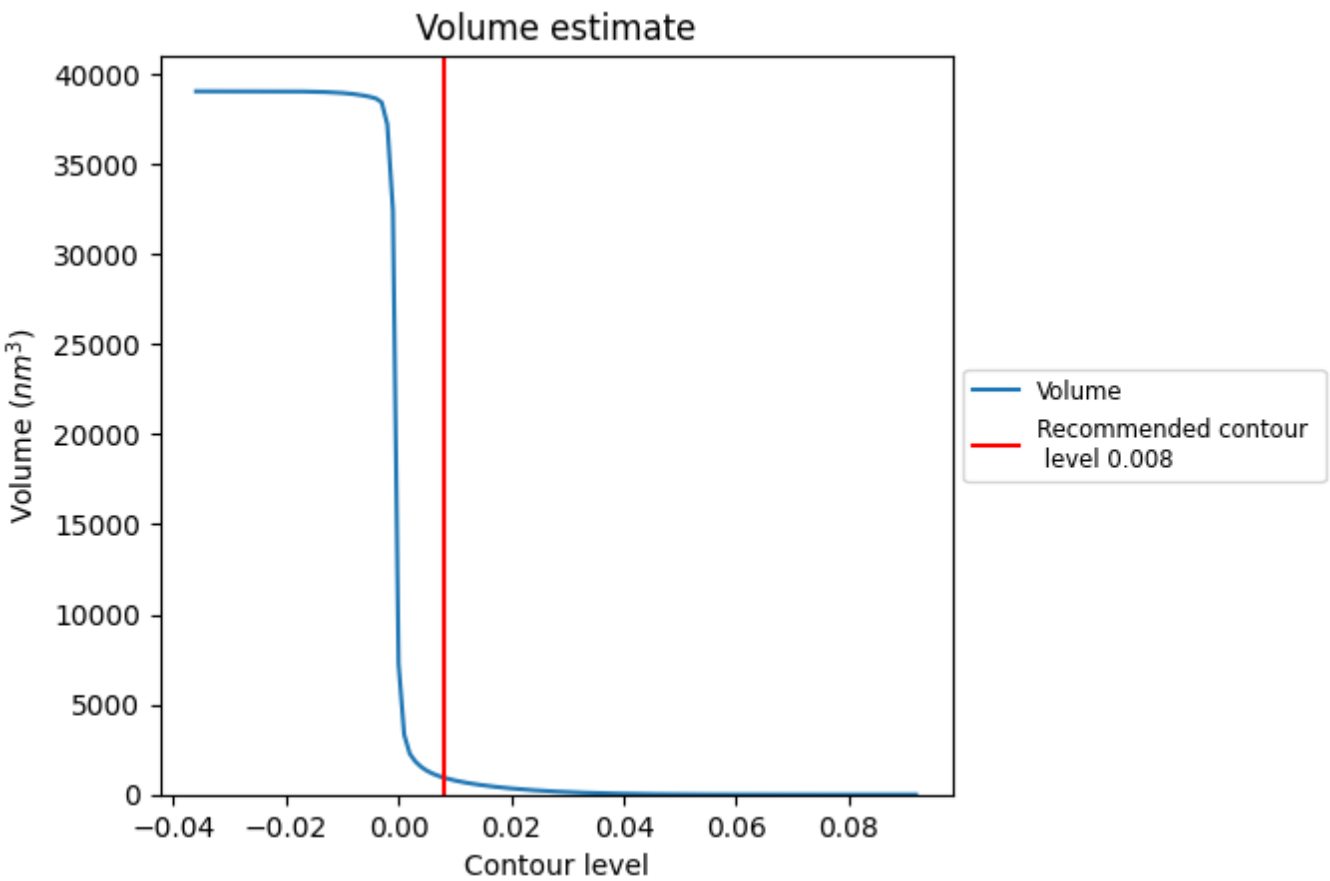
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

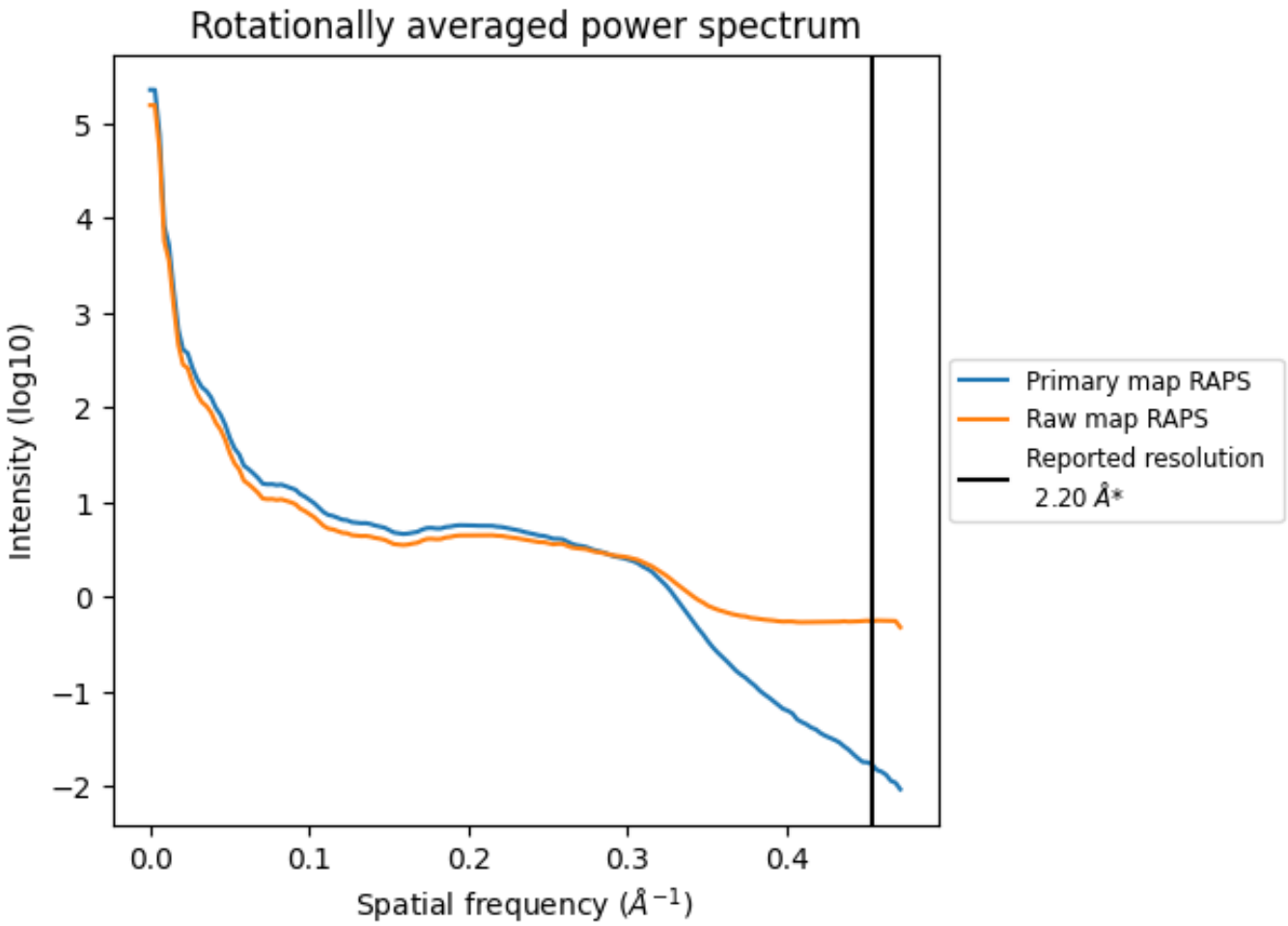
7.2 Volume estimate (i)



The volume at the recommended contour level is 945 nm^3; this corresponds to an approximate mass of 854 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)

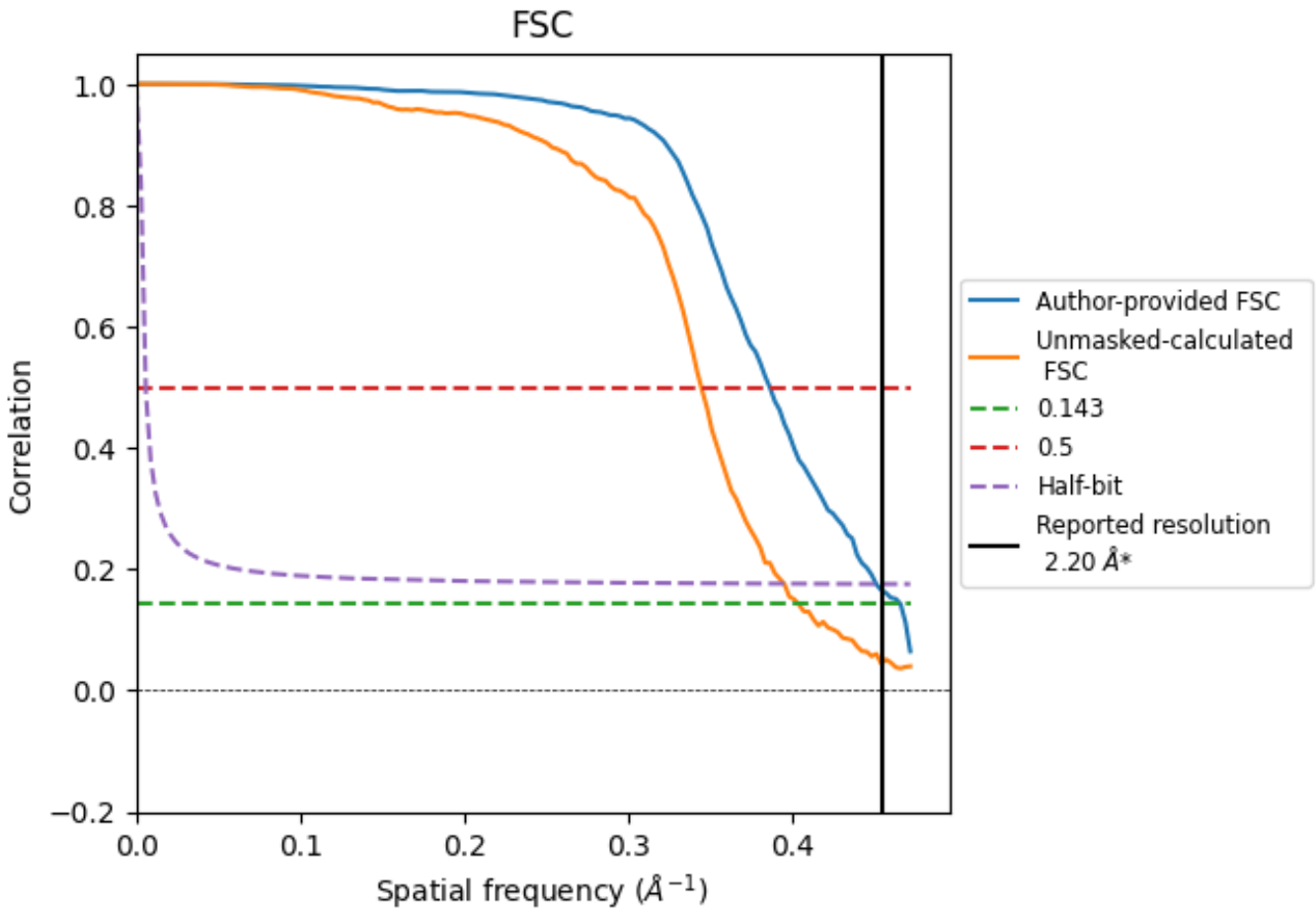


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8.2 Resolution estimates (i)

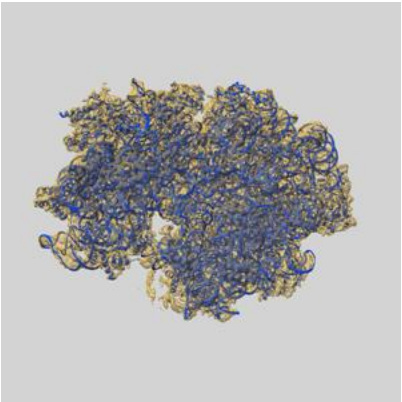
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.15	2.59	2.22
Unmasked-calculated*	2.48	2.90	2.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.48 differs from the reported value 2.2 by more than 10 %

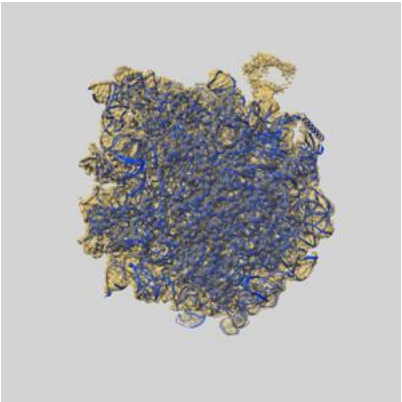
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-48830 and PDB model 9N2B. Per-residue inclusion information can be found in section 3 on page 18.

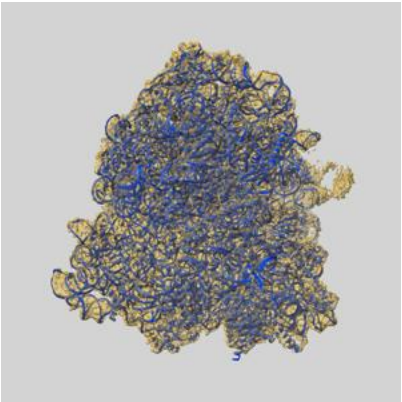
9.1 Map-model overlay (i)



X



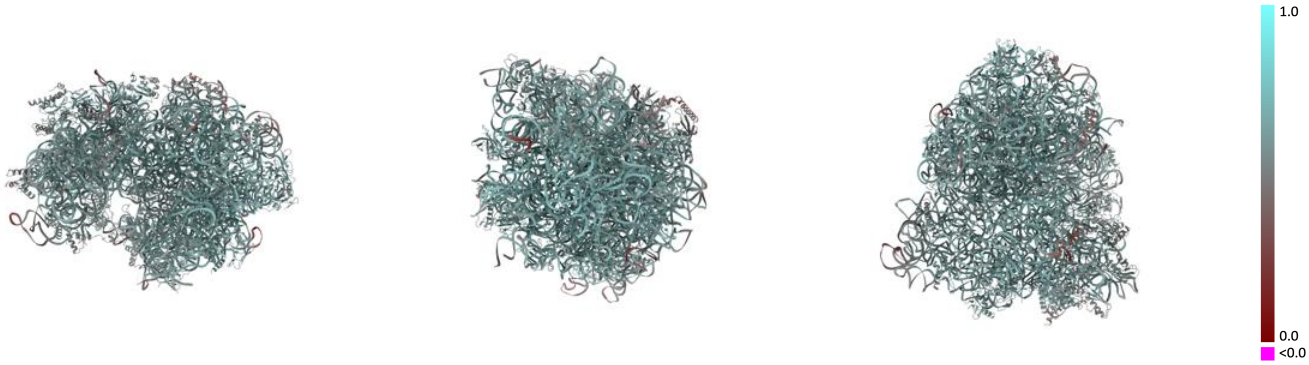
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

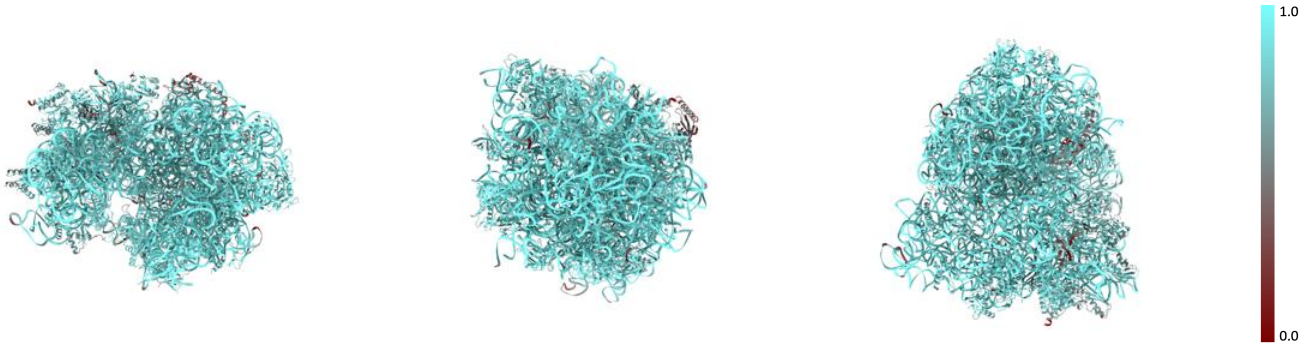
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

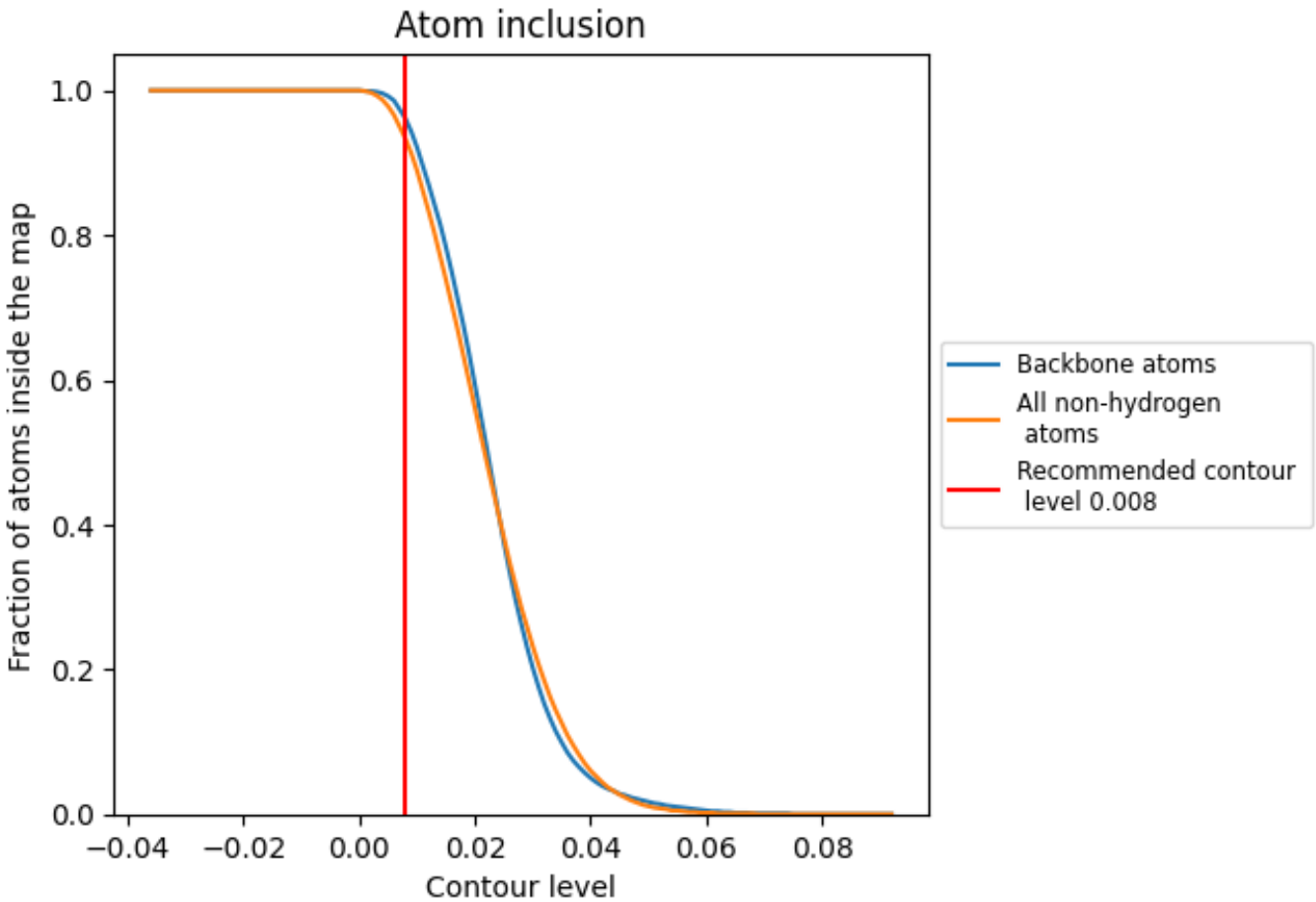
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9340	0.6070
16	0.9630	0.5960
23	0.9770	0.6260
5	0.9650	0.5850
LB	0.9530	0.6530
LC	0.9210	0.6250
LD	0.8940	0.6120
LE	0.7840	0.5360
LF	0.8020	0.5540
LI	0.4980	0.4780
LM	0.9320	0.6330
LN	0.9170	0.6300
LO	0.9140	0.6190
LP	0.9230	0.6350
LQ	0.9390	0.6240
LR	0.8710	0.5640
LS	0.8890	0.6140
LT	0.9620	0.6540
LU	0.9070	0.6250
LV	0.9100	0.6240
LW	0.8680	0.6150
LX	0.8850	0.6130
LY	0.8600	0.5930
La	0.8460	0.6120
Lb	0.9320	0.6280
Lc	0.8590	0.5920
Ld	0.8860	0.6110
Le	0.6830	0.5140
Lf	0.9070	0.6320
Lg	0.8590	0.5930
Lh	0.9410	0.6660
Li	0.9290	0.6400
Lj	0.9520	0.6280
Pt	0.8910	0.5800
SB	0.7910	0.5600

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SC	0.8480	0.5890
SD	0.8610	0.5940
SE	0.9060	0.6200
SF	0.8230	0.5690
SG	0.7270	0.5300
SH	0.8970	0.6170
SI	0.8350	0.5620
SJ	0.7570	0.5320
SK	0.8550	0.5810
SL	0.9090	0.6270
SM	0.8300	0.5670
SN	0.8610	0.5870
SO	0.8900	0.6070
SP	0.8660	0.5830
SQ	0.8340	0.5920
SR	0.8550	0.5990
SS	0.8250	0.5680
ST	0.8500	0.5670
SU	0.7320	0.5430
mR	0.5680	0.4780