wwPDB EM Validation Summary Report (i)

Sep 15, 2026 – 01:03 PM EDT

PDB ID	:	7UG7 / pdb_00007ug7
EMDB ID	:	EMD-26486
Title	:	70S ribosome complex in an intermediate state of translocation bound to EF-G(GDP) stalled by Argyrin B
Authors	:	Rundlet, E.J.; Wieland, M.; Holm, M.; Koller, T.O.; Blanchard, S.C.; Wilson, D.N.
Deposited on	:	2022-03-24
Resolution	:	2.58 Å(reported)
Based on initial model	:	7N2C

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:

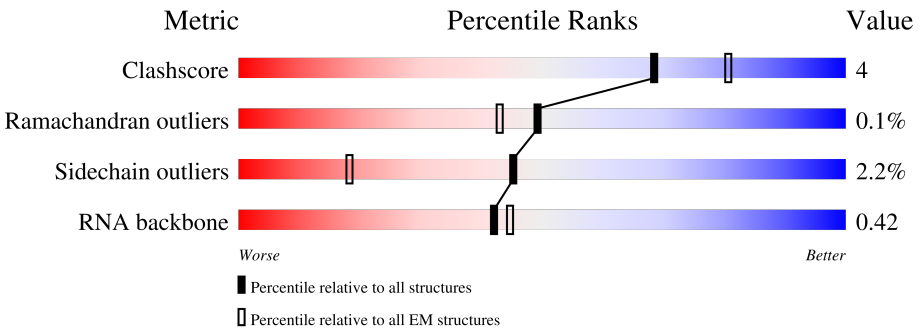
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

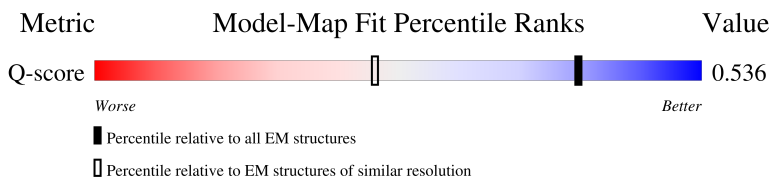
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.58 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	7675 (2.08 - 3.08)

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	1534	60% 36% • •
2	SB	241	11% 84% 10% 6%

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Mol	Chain	Length	Quality of chain
3	SC	233	7% 78% 10% 12%
4	SD	206	84% 14%
5	SE	167	78% 14% 7%
6	SF	135	68% 10% 21%
7	SG	179	40% 77% 11% 13%
8	SH	130	88% 11%
9	SI	130	12% 82% 15%
10	SJ	103	16% 77% 18%
11	SK	129	76% 14% 9%
12	SL	124	86% 11%
13	SM	118	25% 81% 16%
14	SN	101	7% 80% 19%
15	SO	89	97%
16	SP	82	88% 12%
17	SQ	84	88% 7% 5%
18	SR	75	75% 15% 11%
19	SS	92	9% 71% 18% 9%
20	ST	87	91% 8%
21	SU	71	6% 89% 10%
22	23	2904	66% 31%
23	5	120	77% 21%
24	LA	234	44% 48% 9% 43%
25	LB	273	93% 6%
26	LC	209	92% 8%
27	LD	201	94% 6%

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Mol	Chain	Length	Quality of chain
28	LE	179	83% 16%
29	LF	177	86% 12%
30	LI	149	65% 89% 11%
31	LJ	165	65% 66% 12% 22%
32	LK	142	47% 79% 15% 6%
33	LM	142	89% 9%
34	LN	123	88% 11%
35	LO	144	88% 11%
36	LP	136	93% 7%
37	LQ	127	88% 6% 6%
38	LR	117	89% 10%
39	LS	115	93% 6%
40	LT	118	92% 7%
41	LU	103	89% 11%
42	LV	110	93% 7%
43	LW	100	87% 6% 7%
44	LX	104	81% 10% 10%
45	LY	94	91% 9%
46	La	85	87% 6% 7%
47	Lb	78	87% 12%
48	Lc	63	89% 10%
49	Ld	59	92% 7%
50	Le	70	19% 81% 14%
51	Lf	57	81% 16%
52	Lg	55	85% 5% 9%

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Mol	Chain	Length	Quality of chain
53	Lh	46	96%
54	Li	65	88% 9%
55	Lj	38	95% 5%
56	EF	700	75% 19%
57	Dt	77	56% 35% 9%
58	Pt	76	45% 43% 8%
59	mR	60	10% 5% 83%
60	B	8	62% 38%

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
60	SAR	B	8	-	-	X	-
67	PHE	Pt	3002	-	X	-	-

2 Entry composition (i)

There are 67 unique types of molecules in this entry. The entry contains 154353 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	16	1514	32505	14503	5967	10521	1514	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	226	1770	1120	317	325	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	206	1624	1028	305	288	3	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	1642	1026	315	297	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	155	1144	711	216	211	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	156	1236	773	238	221	4	0	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	978	616	173	183	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 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SK	117	876	540	174	159	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

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	804	499	164	138	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 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	SS	84	668	427	127	112	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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	23	2903	62334	27815	11467	20149	2903	0	0

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	5	120	2570	1144	468	838	120	0	0

- Molecule 24 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LA	134	1026	645	186	193	2	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	1565	979	288	294	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L4.

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	177	1410	899	249	256	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	176	1322	832	243	245	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	1110	699	197	213	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LJ	129	974	616	173	180	5	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	LK	134	979	619	169	185	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LM	142	1138	720	215	199	4	1	0

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LO	144	1063	660	211	190	2	1	0

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	LR	116	891	552	178	161	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LU	103	815	516	153	144	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	LV	110	856	532	166	155	3	0	0

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	LW	93	738	466	139	131	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	LX	94	721	454	136	131	0	0

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	LY	94	752	479	137	133	3	0	0

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	La	79	595	367	120	107	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Lb	77	624	388	129	105	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Ld	58	448	281	87	78	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Le	67	529	328	100	95	6	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	Lg	50	409	263	75	71	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Li	64	512	329	107	74	2	1	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	EF	672	5179	3270	894	992	23	0	0

- Molecule 57 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
57	Dt	77	1645	734	298	535	77	1	0	0

- Molecule 58 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
58	Pt	76	1637	733	291	535	76	2	0	0

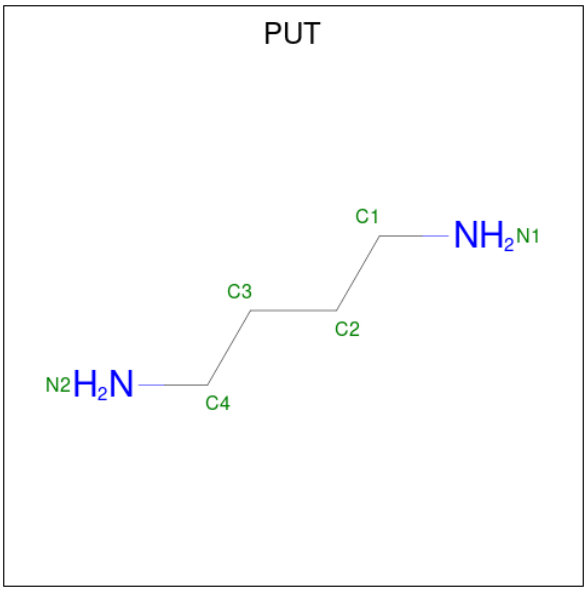
- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
59	mR	10	214	96	39	69	10	0	0

- Molecule 60 is a protein called Argyrin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	B	8	60	41	10	8	1	0	0

- Molecule 61 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
61	16	1	6	4	2	0
			Total	C	N	
61	16	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
62	16	77	77	77	0

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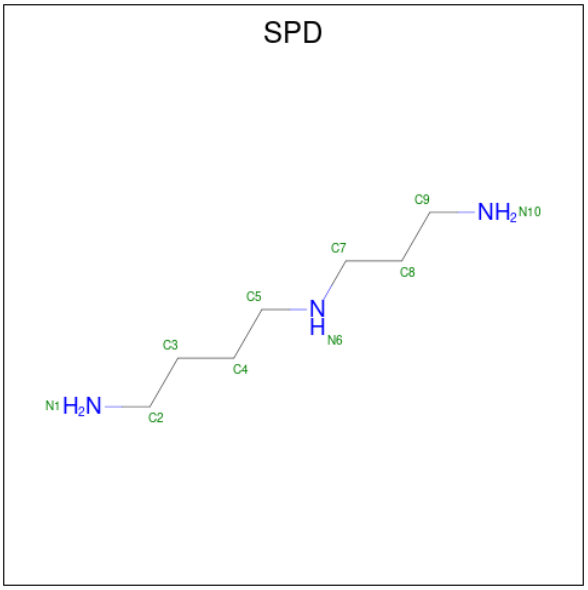
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
62	23	315	315	315	0
			Total	Mg	
62	5	5	5	5	0
			Total	Mg	
62	LB	3	3	3	0
			Total	Mg	
62	LQ	1	1	1	0
			Total	Mg	
62	La	1	1	1	0
			Total	Mg	
62	EF	1	1	1	0
			Total	Mg	
62	Pt	1	1	1	0

- Molecule 63 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).

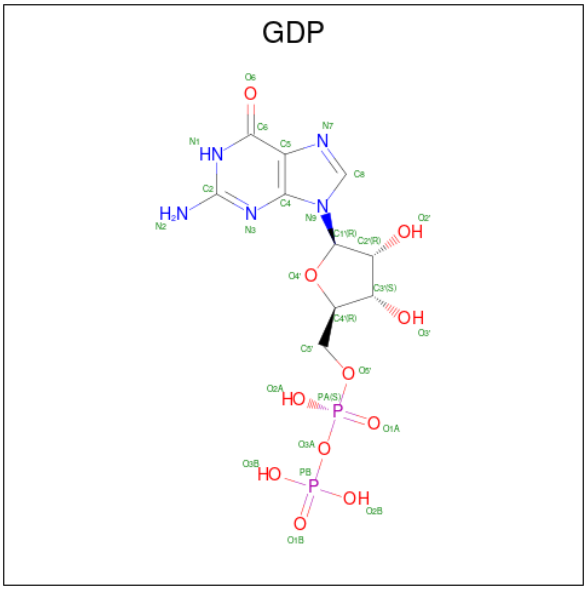


Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
63	23	1	10	7	3	0
			Total	C	N	
63	23	1	10	7	3	0

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

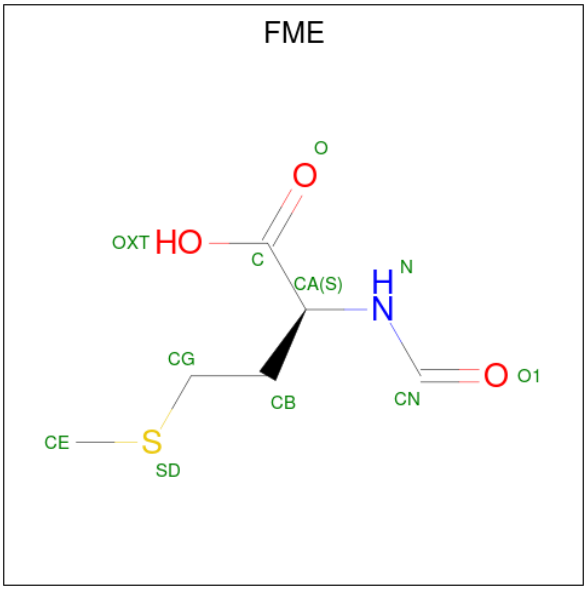
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	Le	1	1	1	0
			Total	Zn	
64	Lj	1	1	1	0

- Molecule 65 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



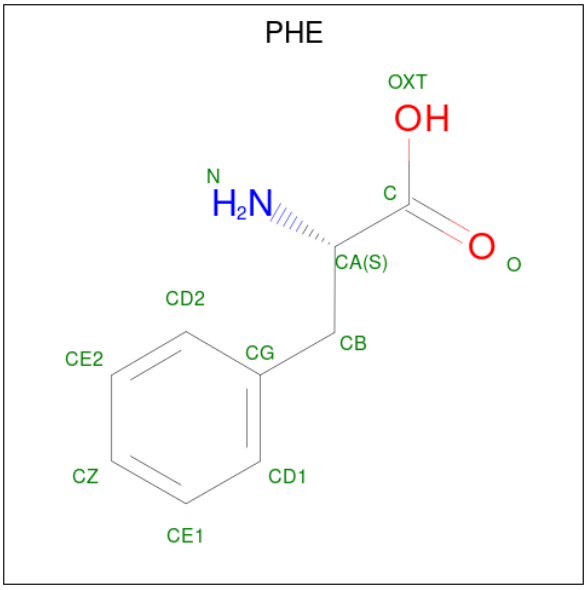
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
65	EF	1	28	10	5	11	2	0

- Molecule 66 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



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

- Molecule 67 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



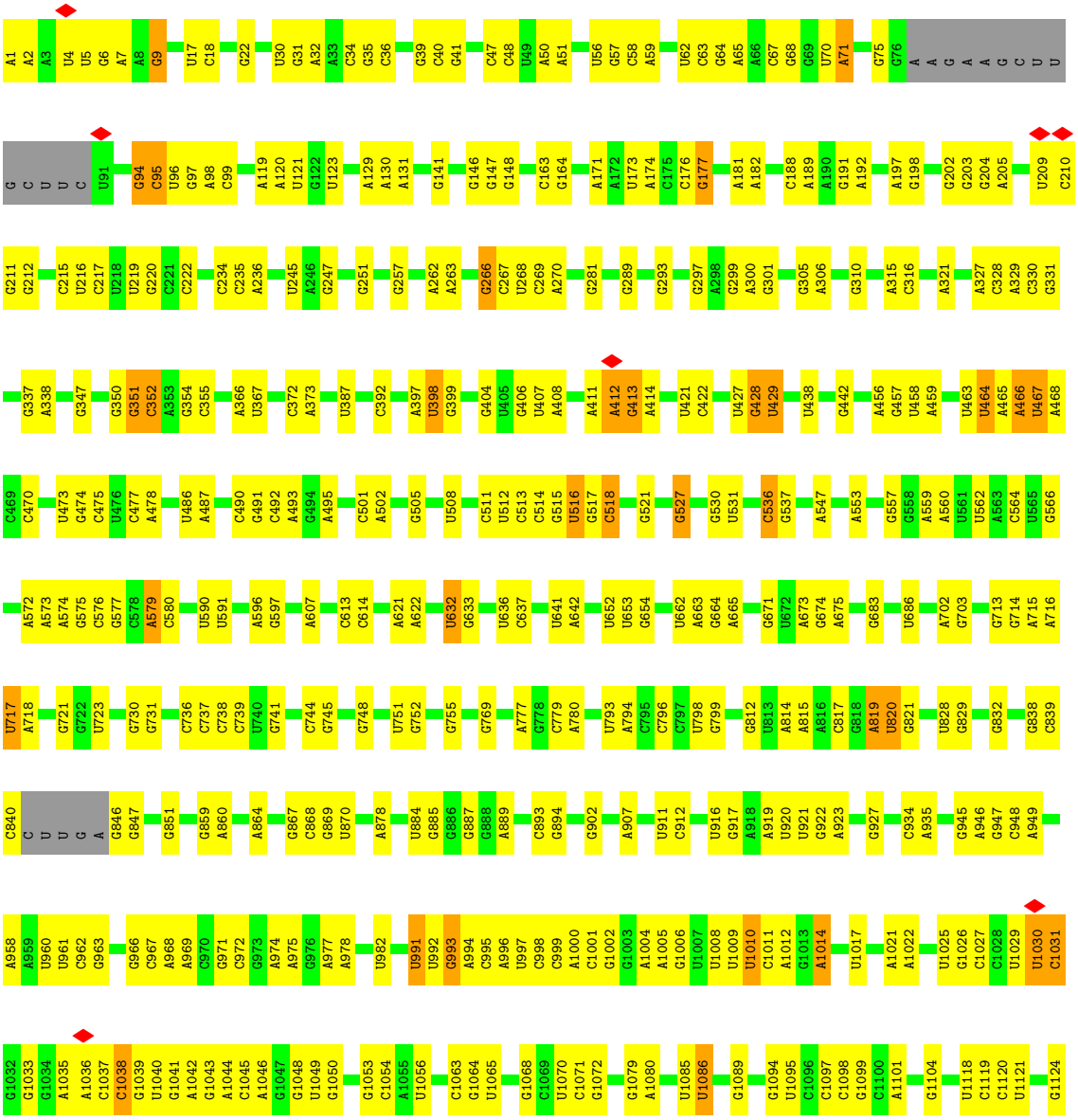
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
67	Pt	1	10	8	1	1	0

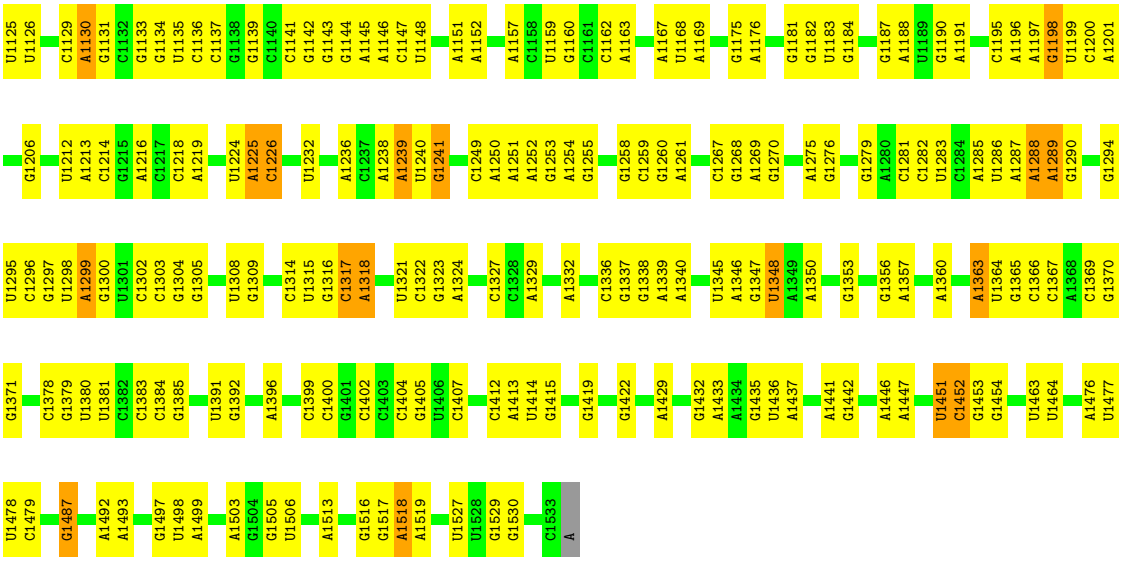
3 Residue-property plots (i)

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 rRNA

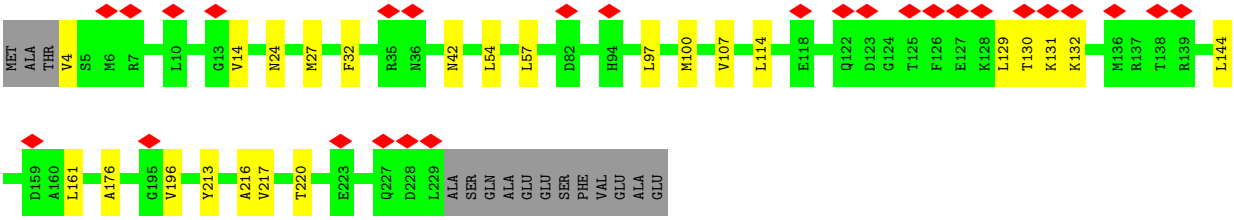
Chain 16: 60% 36%





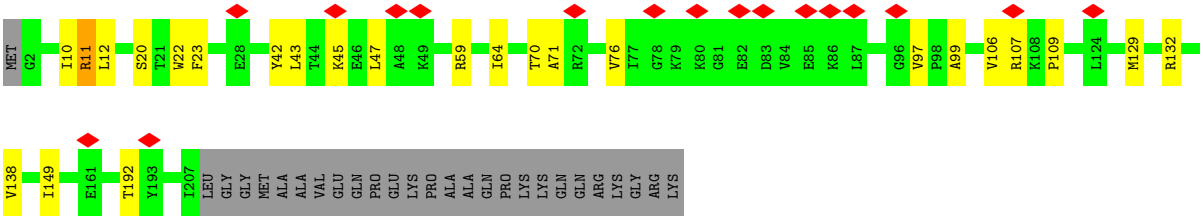
- Molecule 2: 30S ribosomal protein S2

Chain SB:



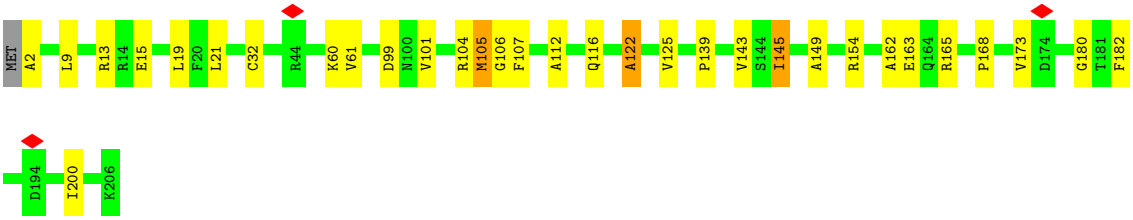
- Molecule 3: 30S ribosomal protein S3

Chain SC:



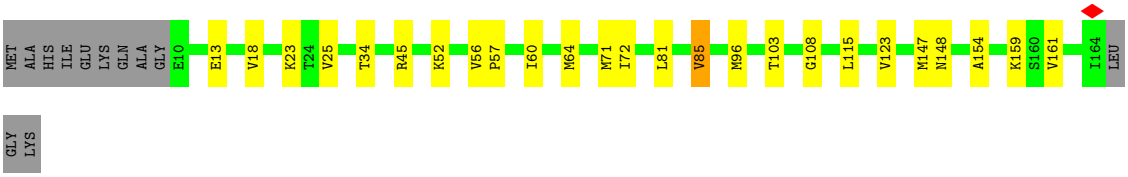
- Molecule 4: 30S ribosomal protein S4

Chain SD:



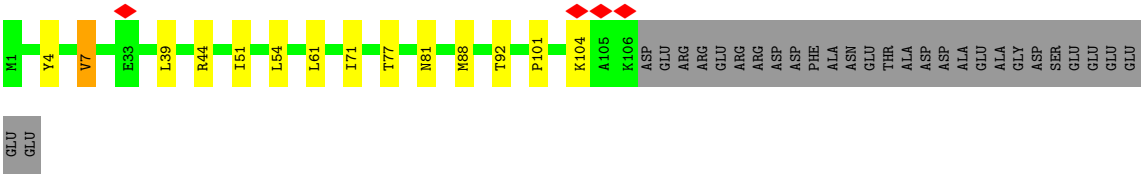
- Molecule 5: 30S ribosomal protein S5

Chain SE:



- Molecule 6: 30S ribosomal protein S6

Chain SF:

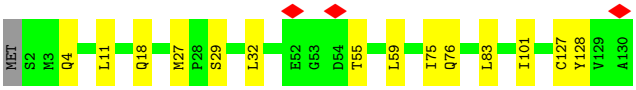


- Molecule 7: 30S ribosomal protein S7

Chain SG:

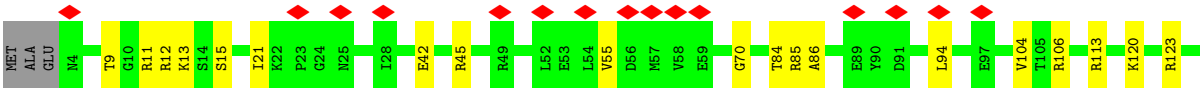
- Molecule 8: 30S ribosomal protein S8

Chain SH:



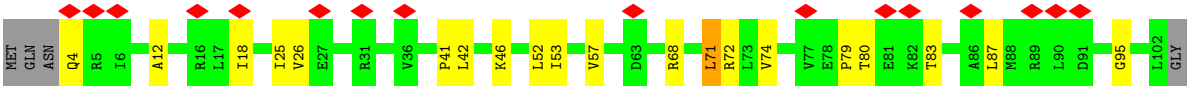
- Molecule 9: 30S ribosomal protein S9

Chain SI:



• Molecule 10: 30S ribosomal protein S10

Chain SJ:

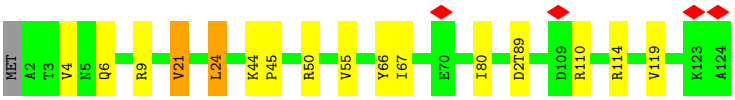


• Molecule 11: 30S ribosomal protein S11

Chain SK:

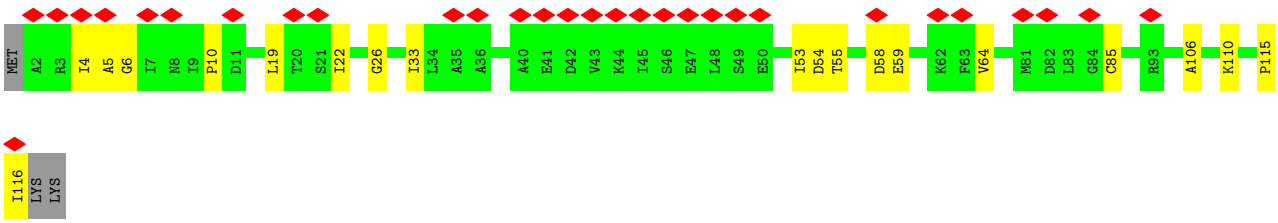
• Molecule 12: 30S ribosomal protein S12

Chain SL:



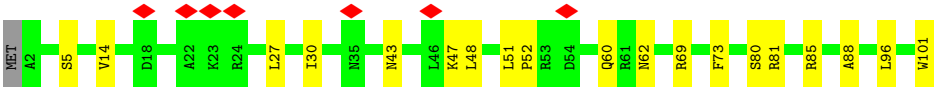
• Molecule 13: 30S ribosomal protein S13

Chain SM:



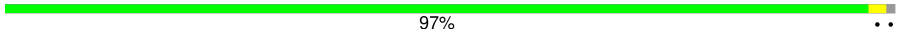
• Molecule 14: 30S ribosomal protein S14

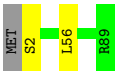
Chain SN:



• Molecule 15: 30S ribosomal protein S15

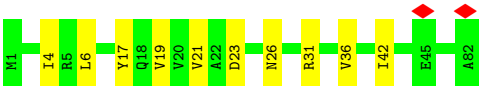
Chain SO:





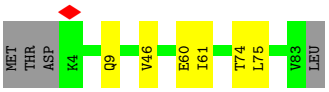
• Molecule 16: 30S ribosomal protein S16

Chain SP:



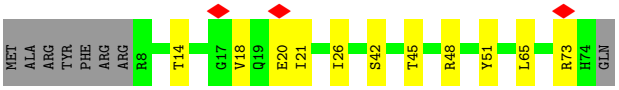
• Molecule 17: 30S ribosomal protein S17

Chain SQ:



• Molecule 18: 30S ribosomal protein S18

Chain SR:

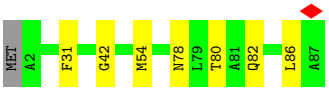


• Molecule 19: 30S ribosomal protein S19

Chain SS:

• Molecule 20: 30S ribosomal protein S20

Chain ST:

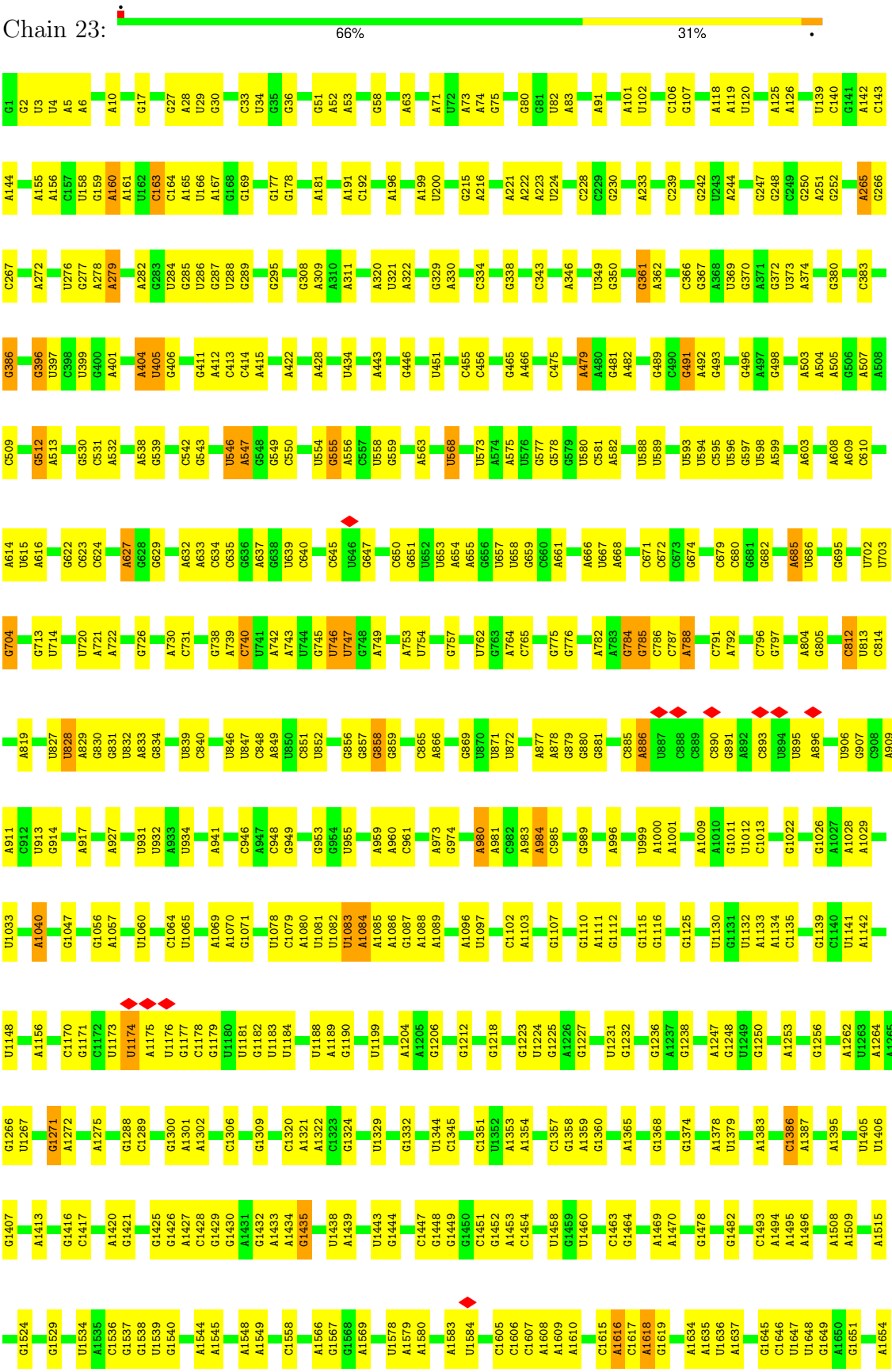


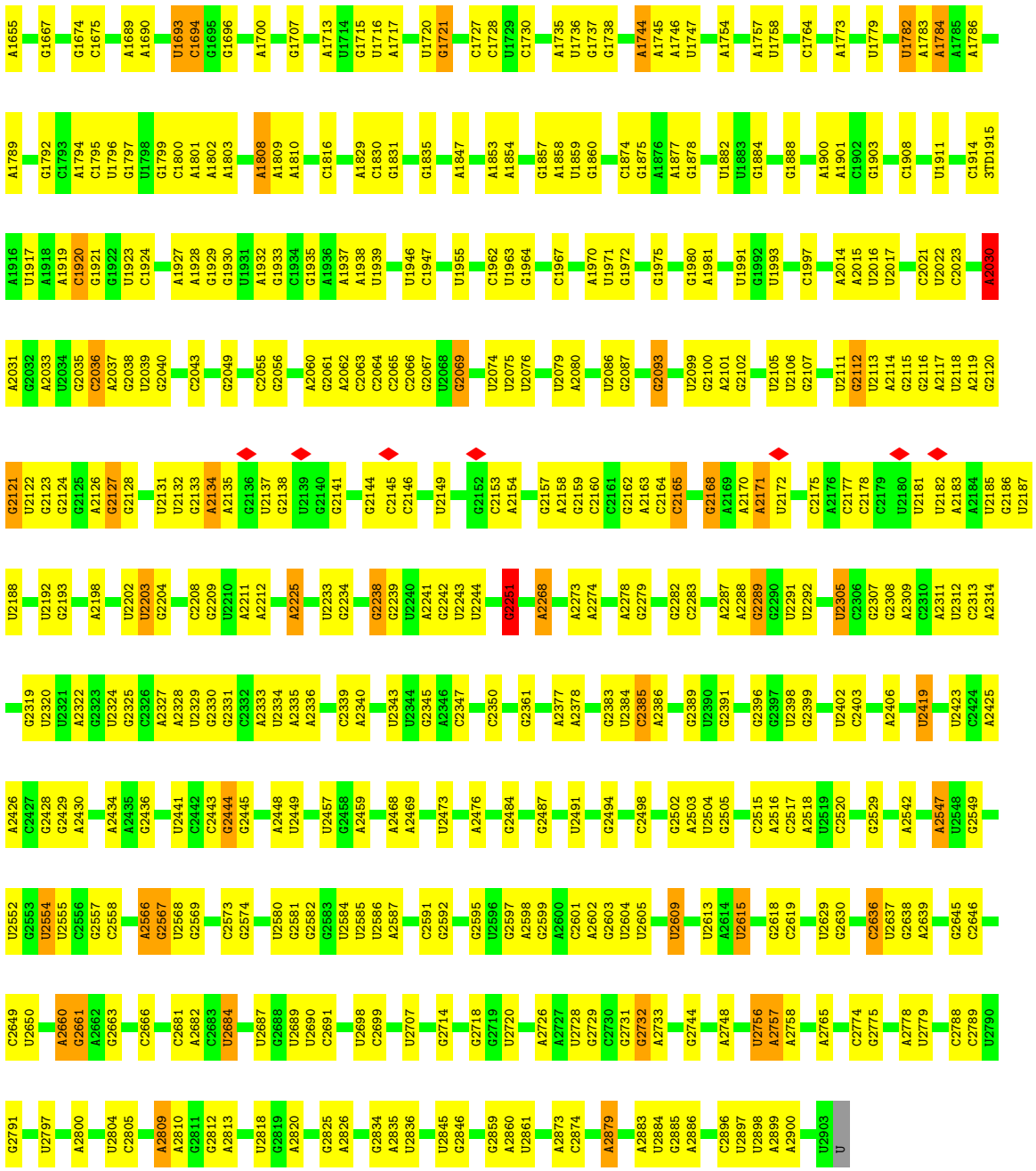
• Molecule 21: 30S ribosomal protein S21

Chain SU:

• Molecule 22: 23S rRNA

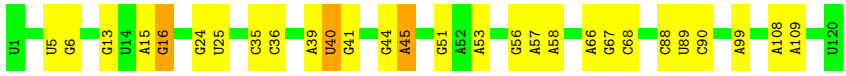
Chain 23:





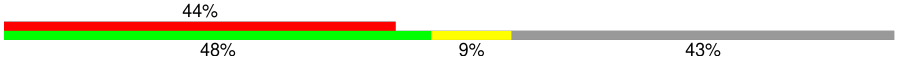
- Molecule 23: 5S rRNA

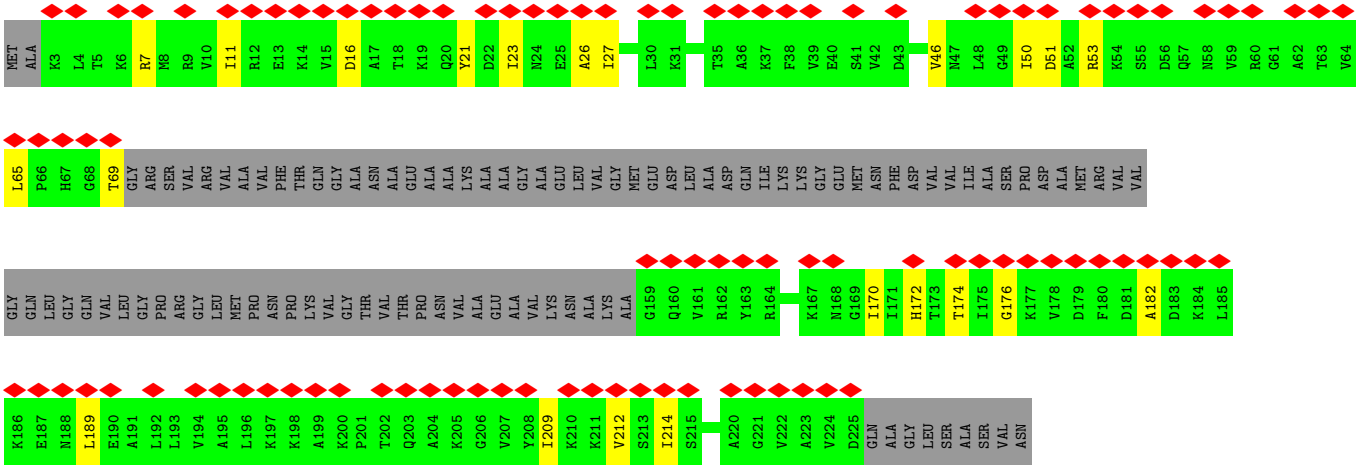
Chain 5:



- Molecule 24: 50S ribosomal protein L1

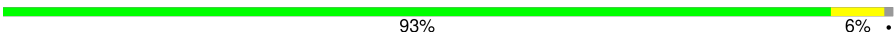
Chain LA:





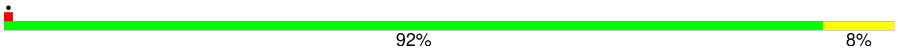
- Molecule 25: 50S ribosomal protein L2

Chain LB:



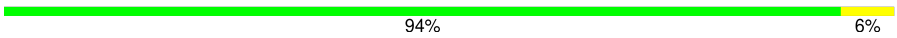
- Molecule 26: 50S ribosomal protein L3

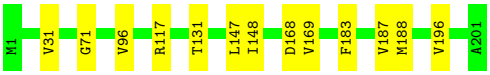
Chain LC:



- Molecule 27: 50S ribosomal protein L4

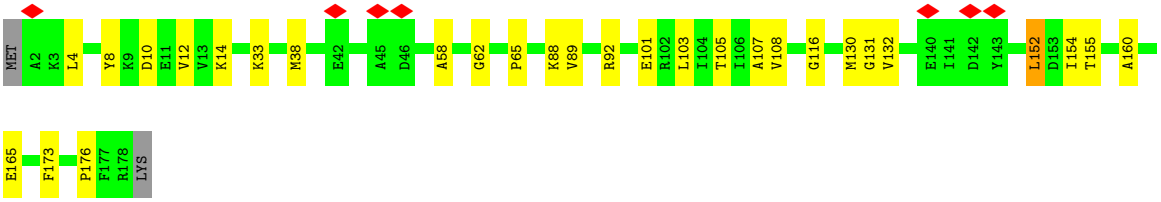
Chain LD:





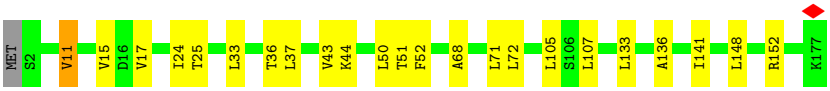
- Molecule 28: 50S ribosomal protein L5

Chain LE:



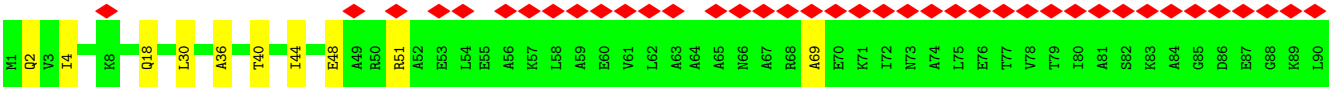
- Molecule 29: 50S ribosomal protein L6

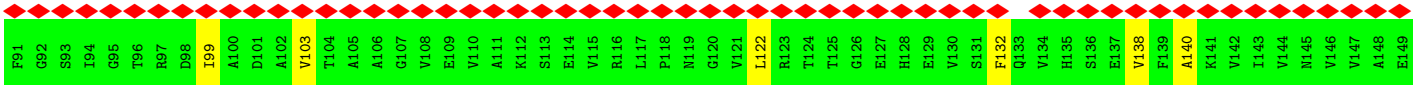
Chain LF:



- Molecule 30: 50S ribosomal protein L9

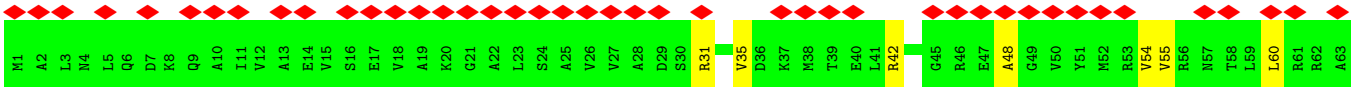
Chain LI:

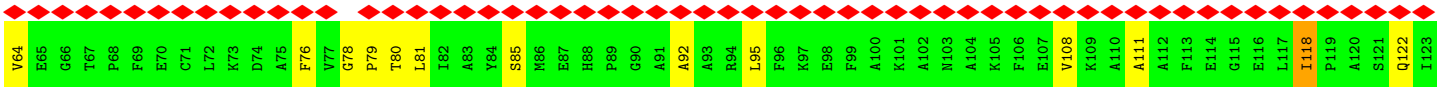


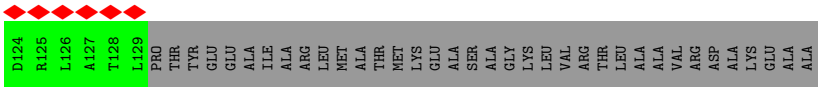


- Molecule 31: 50S ribosomal protein L10

Chain LJ:

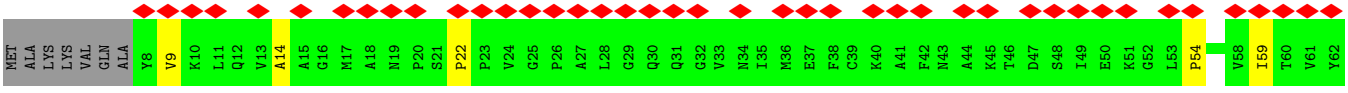


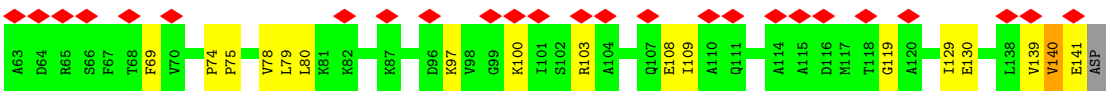




- Molecule 32: 50S ribosomal protein L11

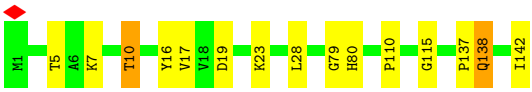
Chain LK:





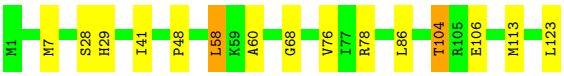
- Molecule 33: 50S ribosomal protein L13

Chain LM:



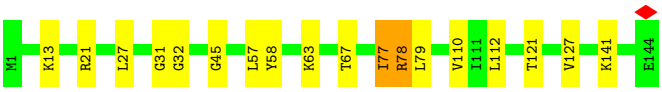
- Molecule 34: 50S ribosomal protein L14

Chain LN: 88% 11%



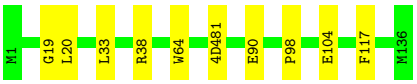
• Molecule 35: 50S ribosomal protein L15

Chain LO: 88% 11%



• Molecule 36: 50S ribosomal protein L16

Chain LP: 93% 7%

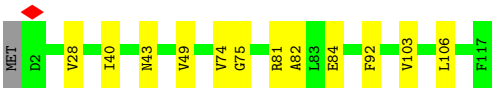


• Molecule 37: 50S ribosomal protein L17

Chain LQ: 88% 6% 6%

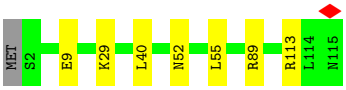
• Molecule 38: 50S ribosomal protein L18

Chain LR: 89% 10%



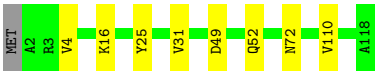
• Molecule 39: 50S ribosomal protein L19

Chain LS: 93% 6%



• Molecule 40: 50S ribosomal protein L20

Chain LT: 92% 7%



• Molecule 41: Ribosomal protein L21

Chain LU: 89% 11%

M1 Q6 Q11 L22 I41 V51 V54 V63 K71 G88 H89 R90 V96 A103

- Molecule 42: 50S ribosomal protein L22

Chain LV: 93% 7%

M1 V20 I24 L36 A44 V45 L46 V50 P87 D109 R110

- Molecule 43: 50S ribosomal protein L23

Chain LW: 87% 6% 7%

M1 Q48 V53 E54 V55 V58 Q72 V85 T86 L87 L93 ASP PHE VAL GLY GLY ALA GLU

- Molecule 44: 50S ribosomal protein L24

Chain LX: 81% 10% 10%

MET A2 I12 G20 V25 K33 V34 K47 PRO VAL PRO ALA LEU ASN GLN PRO G56 A64 I72 F73 N74 A75 A76 I103 LYS

- Molecule 45: 50S ribosomal protein L25

Chain LY: 91% 9%

M1 A6 L42 V60 L61 V72 P81 R93 A94

- Molecule 46: 50S ribosomal protein L27

Chain La: 87% 6% 7%

MET ALA HIS LYS LYS ALA G7 T10 R41 G42 T43 L59 I60 E85

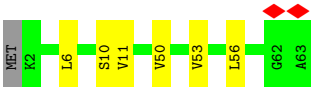
- Molecule 47: 50S ribosomal protein L28

Chain Lb: 87% 12%

MET S2 C5 Q6 V7 S19 F29 N32 L33 L49 I59 Y78

- Molecule 48: 50S ribosomal protein L29

Chain Lc:

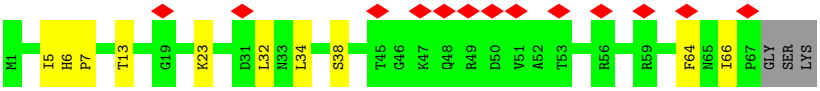


- Molecule 49: 50S ribosomal protein L30

Chain Ld:

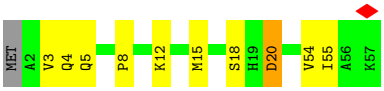
- Molecule 50: 50S ribosomal protein L31

Chain Le:



- Molecule 51: 50S ribosomal protein L32

Chain Lf:

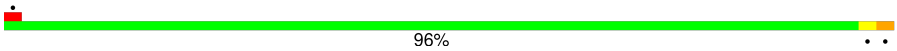


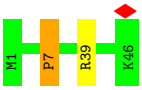
- Molecule 52: 50S ribosomal protein L33

Chain Lg:

- Molecule 53: 50S ribosomal protein L34

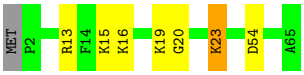
Chain Lh:





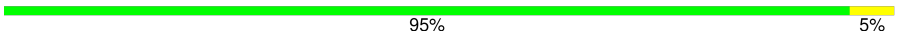
- Molecule 54: 50S ribosomal protein L35

Chain Li:



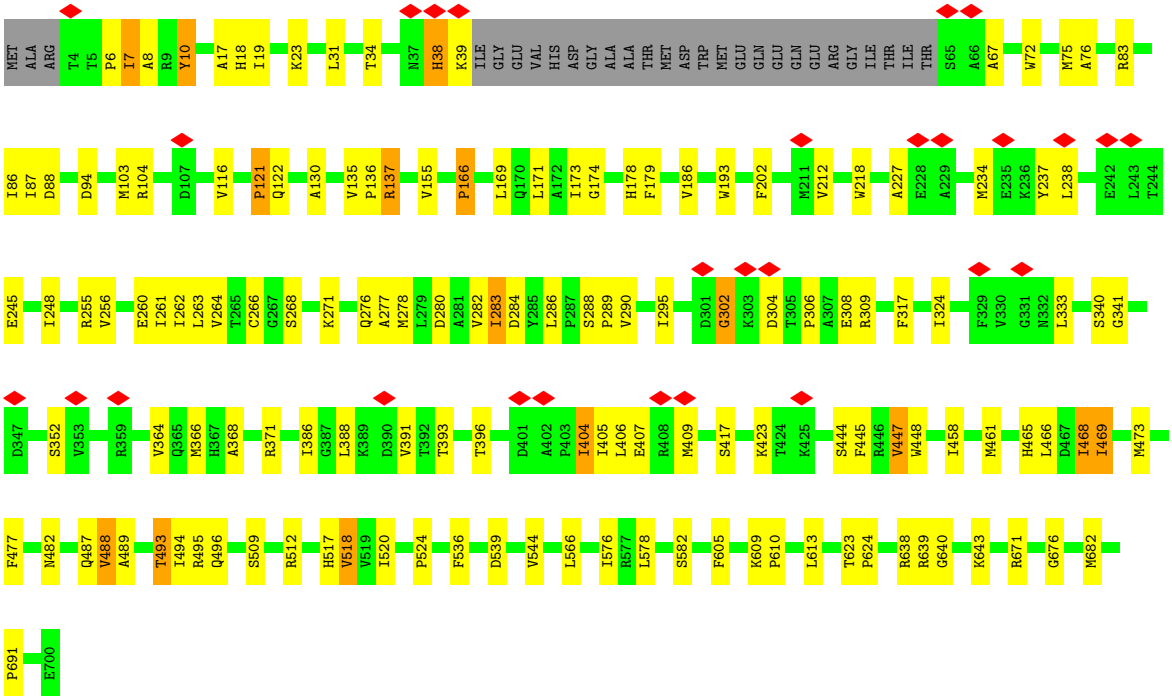
- Molecule 55: 50S ribosomal protein L36

Chain Lj:



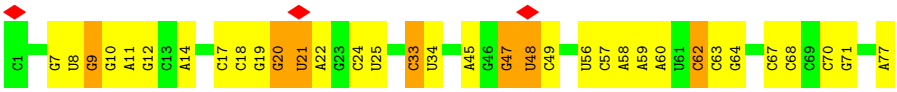
- Molecule 56: Elongation factor G

Chain EF:



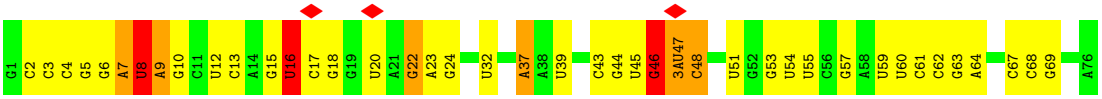
- Molecule 57: tRNA-fMet

Chain Dt:



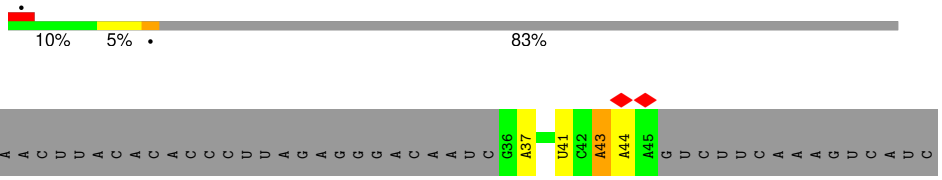
- Molecule 58: tRNA-Phe

Chain Pt:



• Molecule 59: mRNA

Chain mR:



• Molecule 60: Argyrin B

Chain B:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35220	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 ($e^-/Å^2$)	68	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	400.52002, 400.52002, 400.52002	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	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: MA6, 2MA, FME, 1MG, OMU, 3TD, 5MU, PUT, 4SU, 4D4, UR3, PSU, 0UO, 5MC, 6MZ, SPD, BB9, 2MG, OMG, G7M, MG, H2U, MIA, 3AU, DBB, D2T, OMC, DHA, SAR, 4OC, ZN, GDP, DAL

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	0.39	0/36143	0.58	0/56376
2	SB	0.87	0/1801	1.11	0/2426
3	SC	0.83	0/1651	1.07	0/2225
4	SD	0.86	0/1664	1.12	0/2227
5	SE	0.95	0/1157	1.22	0/1557
6	SF	0.94	0/881	1.22	0/1189
7	SG	0.68	0/1254	0.93	0/1683
8	SH	0.98	0/988	1.21	1/1326 (0.1%)
9	SI	0.89	0/1033	1.10	0/1375
10	SJ	0.95	0/805	1.16	0/1089
11	SK	0.93	0/892	1.17	0/1205
12	SL	0.95	0/960	1.14	0/1286
13	SM	0.88	0/900	1.12	0/1204
14	SN	0.82	0/816	1.05	0/1088
15	SO	0.82	0/721	1.14	0/964
16	SP	0.90	0/659	1.11	0/884
17	SQ	0.93	0/657	1.13	0/881
18	SR	0.92	0/564	1.19	1/756 (0.1%)
19	SS	0.95	0/685	1.15	0/922
20	ST	0.88	0/675	1.22	0/895
21	SU	0.76	0/597	1.03	0/792
22	23	0.38	1/69239 (0.0%)	0.58	4/108014 (0.0%)
23	5	0.37	0/2873	0.52	0/4478
24	LA	0.88	0/1033	1.08	0/1387
25	LB	0.88	0/2121	1.14	1/2852 (0.0%)
26	LC	0.85	0/1586	1.09	0/2134
27	LD	0.69	0/1571	0.87	0/2113
28	LE	0.90	0/1434	1.15	1/1926 (0.1%)
29	LF	0.84	0/1342	1.05	0/1816
30	LI	0.81	0/1121	1.02	0/1515

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	LJ	0.92	0/986	1.20	0/1328
32	LK	0.94	0/993	1.13	1/1341 (0.1%)
33	LM	0.83	0/1162	1.10	0/1566
34	LN	0.86	0/955	1.10	0/1279
35	LO	0.91	0/1072	1.21	1/1427 (0.1%)
36	LP	0.85	0/1080	1.08	1/1443 (0.1%)
37	LQ	0.69	0/973	0.95	1/1301 (0.1%)
38	LR	0.83	0/901	1.10	0/1209
39	LS	0.79	0/928	1.02	0/1242
40	LT	0.73	0/960	1.02	0/1278
41	LU	0.84	0/828	1.01	0/1107
42	LV	0.85	0/863	1.10	0/1156
43	LW	0.78	0/744	1.03	0/994
44	LX	0.93	0/725	1.15	0/961
45	LY	0.88	0/765	1.12	0/1025
46	La	0.84	0/602	1.13	0/797
47	Lb	0.85	0/634	1.13	0/848
48	Lc	0.66	0/502	0.95	0/667
49	Ld	0.85	0/452	1.15	0/605
50	Le	0.95	0/539	1.18	0/721
51	Lf	0.88	0/450	1.17	2/599 (0.3%)
52	Lg	0.65	0/416	0.88	0/554
53	Lh	0.82	0/380	1.19	1/498 (0.2%)
54	Li	0.88	0/521	1.19	0/687
55	Lj	0.88	0/303	1.10	0/397
56	EF	0.97	0/5277	1.26	4/7145 (0.1%)
57	Dt	0.42	0/1721	0.59	1/2682 (0.0%)
58	Pt	0.44	0/1625	0.65	0/2523
59	mR	0.38	0/239	0.64	0/370
60	B	1.67	0/18	1.03	0/22
All	All	0.59	1/165437 (0.0%)	0.78	20/246357 (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
12	SL	0	1
33	LM	0	4
35	LO	0	4
41	LU	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	Li	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23	2552	OMU	O3'-P	5.75	1.62	1.56

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	LK	22	PRO	N-CA-C	7.77	120.17	110.70
28	LE	116	GLY	CA-C-O	-6.35	118.09	122.22
56	EF	302	GLY	CA-C-O	-6.31	117.87	122.23
56	EF	524	PRO	CB-CA-C	-6.27	105.69	111.40
36	LP	19	GLY	CA-C-O	-5.97	118.11	122.23

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	LM	79	GLY	Mainchain
33	LM	80[A]	HIS	Mainchain
33	LM	80[B]	HIS	Mainchain
35	LO	77	ILE	Mainchain
12	SL	44	LYS	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	16	32505	0	16376	222	0
2	SB	1770	0	1797	13	0
3	SC	1624	0	1696	15	0
4	SD	1642	0	1707	19	0
5	SE	1144	0	1185	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	SF	862	0	864	5	0
7	SG	1236	0	1288	11	0
8	SH	978	0	1031	6	0
9	SI	1021	0	1070	12	0
10	SJ	795	0	836	13	0
11	SK	876	0	887	12	0
12	SL	957	0	1017	8	0
13	SM	891	0	952	10	0
14	SN	804	0	844	12	0
15	SO	713	0	734	0	0
16	SP	649	0	666	4	0
17	SQ	648	0	691	2	0
18	SR	555	0	578	5	0
19	SS	668	0	693	11	0
20	ST	669	0	719	3	0
21	SU	589	0	629	5	0
22	23	62334	0	31371	317	0
23	5	2570	0	1301	5	0
24	LA	1026	0	1092	9	0
25	LB	2082	0	2154	12	0
26	LC	1565	0	1616	9	0
27	LD	1552	0	1619	8	0
28	LE	1410	0	1444	20	0
29	LF	1322	0	1371	14	0
30	LI	1110	0	1148	7	0
31	LJ	974	0	1011	12	0
32	LK	979	0	1028	15	0
33	LM	1138	0	1168	8	0
34	LN	946	0	1023	13	0
35	LO	1063	0	1141	14	0
36	LP	1074	0	1155	5	0
37	LQ	960	0	1000	4	0
38	LR	891	0	923	7	0
39	LS	916	0	962	4	0
40	LT	947	0	1019	5	0
41	LU	815	0	839	5	0
42	LV	856	0	922	4	0
43	LW	738	0	807	3	0
44	LX	721	0	770	5	0
45	LY	752	0	780	4	0
46	La	595	0	610	3	0
47	Lb	624	0	652	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Lc	501	0	531	3	0
49	Ld	448	0	488	2	0
50	Le	529	0	527	6	0
51	Lf	444	0	458	5	0
52	Lg	409	0	440	2	0
53	Lh	377	0	418	1	0
54	Li	512	0	584	6	0
55	Lj	302	0	340	1	0
56	EF	5179	0	5141	74	0
57	Dt	1645	0	844	9	0
58	Pt	1637	0	843	18	0
59	mR	214	0	108	1	0
60	B	60	0	45	13	0
61	16	12	0	24	1	0
61	23	54	0	108	1	0
62	16	77	0	0	0	0
62	23	315	0	0	0	0
62	5	5	0	0	0	0
62	EF	1	0	0	0	0
62	LB	3	0	0	0	0
62	LQ	1	0	0	0	0
62	La	1	0	0	0	0
62	Pt	1	0	0	0	0
63	23	20	0	38	1	0
64	Le	1	0	0	0	0
64	Lj	1	0	0	0	0
65	EF	28	0	12	0	0
66	Pt	10	0	10	0	0
67	Pt	10	0	6	1	0
All	All	154353	0	106151	965	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 4.

The worst 5 of 965 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)
60:B:7:DHA:HB2	60:B:8:SAR:HN1	1.34	1.10
67:Pt:3002:PHE:CE1	67:Pt:3002:PHE:CE2	2.41	0.99
1:16:1422:G:H5”	34:LN:48:PRO:HB3	1.47	0.95
58:Pt:64:A:C5	58:Pt:64:A:N3	2.44	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EF:639:ARG:HD2	56:EF:691:PRO:HG2	1.67	0.75

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	224/241 (93%)	214 (96%)	10 (4%)	0	100	100
3	SC	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
4	SD	203/206 (98%)	197 (97%)	5 (2%)	1 (0%)	24	44
5	SE	153/167 (92%)	148 (97%)	5 (3%)	0	100	100
6	SF	104/135 (77%)	100 (96%)	4 (4%)	0	100	100
7	SG	154/179 (86%)	145 (94%)	9 (6%)	0	100	100
8	SH	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	32
9	SI	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
10	SJ	97/103 (94%)	93 (96%)	4 (4%)	0	100	100
11	SK	115/129 (89%)	110 (96%)	4 (4%)	1 (1%)	14	29
12	SL	120/124 (97%)	113 (94%)	6 (5%)	1 (1%)	16	32
13	SM	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	SN	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	SO	86/89 (97%)	86 (100%)	0	0	100	100
16	SP	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
17	SQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	SR	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
19	SS	82/92 (89%)	80 (98%)	1 (1%)	1 (1%)	10	22
20	ST	84/87 (97%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	SU	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
24	LA	130/234 (56%)	122 (94%)	8 (6%)	0	100	100
25	LB	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
26	LC	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
27	LD	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
28	LE	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
29	LF	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
30	LI	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
31	LJ	127/165 (77%)	125 (98%)	2 (2%)	0	100	100
32	LK	132/142 (93%)	132 (100%)	0	0	100	100
33	LM	141/142 (99%)	138 (98%)	3 (2%)	0	100	100
34	LN	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
35	LO	143/144 (99%)	138 (96%)	5 (4%)	0	100	100
36	LP	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
37	LQ	118/127 (93%)	114 (97%)	4 (3%)	0	100	100
38	LR	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
39	LS	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
40	LT	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
41	LU	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
42	LV	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	LW	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
44	LX	90/104 (86%)	87 (97%)	3 (3%)	0	100	100
45	LY	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
46	La	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
47	Lb	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
48	Lc	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
49	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	Le	65/70 (93%)	63 (97%)	2 (3%)	0	100	100
51	Lf	54/57 (95%)	54 (100%)	0	0	100	100
52	Lg	48/55 (87%)	48 (100%)	0	0	100	100
53	Lh	44/46 (96%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Li	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
55	Lj	36/38 (95%)	36 (100%)	0	0	100	100
56	EF	668/700 (95%)	642 (96%)	24 (4%)	2 (0%)	36	56
60	B	2/8 (25%)	0	2 (100%)	0	100	100
All	All	6667/7162 (93%)	6448 (97%)	212 (3%)	7 (0%)	49	69

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	SD	122	ALA
19	SS	54	GLY
56	EF	7	ILE
8	SH	55	THR
11	SK	119	ASN

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	188/199 (94%)	187 (100%)	1 (0%)	81	91
3	SC	170/190 (90%)	168 (99%)	2 (1%)	63	82
4	SD	172/173 (99%)	167 (97%)	5 (3%)	37	63
5	SE	118/126 (94%)	112 (95%)	6 (5%)	21	43
6	SF	92/116 (79%)	86 (94%)	6 (6%)	15	33
7	SG	129/147 (88%)	129 (100%)	0	100	100
8	SH	104/105 (99%)	101 (97%)	3 (3%)	37	63
9	SI	105/107 (98%)	105 (100%)	0	100	100
10	SJ	87/90 (97%)	86 (99%)	1 (1%)	65	83
11	SK	90/99 (91%)	89 (99%)	1 (1%)	65	83
12	SL	102/103 (99%)	99 (97%)	3 (3%)	37	63
13	SM	93/96 (97%)	91 (98%)	2 (2%)	45	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	SN	83/84 (99%)	83 (100%)	0	100	100
15	SO	76/77 (99%)	74 (97%)	2 (3%)	40	66
16	SP	65/65 (100%)	62 (95%)	3 (5%)	24	47
17	SQ	74/78 (95%)	72 (97%)	2 (3%)	39	65
18	SR	58/65 (89%)	56 (97%)	2 (3%)	32	58
19	SS	72/79 (91%)	69 (96%)	3 (4%)	26	50
20	ST	65/66 (98%)	64 (98%)	1 (2%)	57	78
21	SU	60/61 (98%)	59 (98%)	1 (2%)	53	76
24	LA	110/181 (61%)	104 (94%)	6 (6%)	19	39
25	LB	216/218 (99%)	214 (99%)	2 (1%)	70	85
26	LC	164/164 (100%)	164 (100%)	0	100	100
27	LD	165/165 (100%)	165 (100%)	0	100	100
28	LE	148/150 (99%)	147 (99%)	1 (1%)	76	88
29	LF	137/138 (99%)	134 (98%)	3 (2%)	45	70
30	LI	114/114 (100%)	111 (97%)	3 (3%)	40	66
31	LJ	98/123 (80%)	95 (97%)	3 (3%)	35	60
32	LK	104/110 (94%)	103 (99%)	1 (1%)	68	84
33	LM	117/116 (101%)	114 (97%)	3 (3%)	40	66
34	LN	104/104 (100%)	101 (97%)	3 (3%)	37	63
35	LO	104/103 (101%)	104 (100%)	0	100	100
36	LP	108/108 (100%)	108 (100%)	0	100	100
37	LQ	100/103 (97%)	100 (100%)	0	100	100
38	LR	86/87 (99%)	84 (98%)	2 (2%)	44	69
39	LS	99/100 (99%)	99 (100%)	0	100	100
40	LT	89/90 (99%)	88 (99%)	1 (1%)	65	83
41	LU	84/84 (100%)	83 (99%)	1 (1%)	63	82
42	LV	93/93 (100%)	92 (99%)	1 (1%)	65	83
43	LW	80/84 (95%)	80 (100%)	0	100	100
44	LX	76/85 (89%)	76 (100%)	0	100	100
45	LY	78/78 (100%)	75 (96%)	3 (4%)	29	54
46	La	59/63 (94%)	58 (98%)	1 (2%)	53	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Lb	67/68 (98%)	67 (100%)	0	100	100
48	Lc	54/55 (98%)	54 (100%)	0	100	100
49	Ld	48/49 (98%)	47 (98%)	1 (2%)	47	71
50	Le	60/62 (97%)	58 (97%)	2 (3%)	33	59
51	Lf	47/48 (98%)	45 (96%)	2 (4%)	26	49
52	Lg	45/49 (92%)	45 (100%)	0	100	100
53	Lh	38/38 (100%)	37 (97%)	1 (3%)	40	66
54	Li	52/52 (100%)	52 (100%)	0	100	100
55	Lj	34/34 (100%)	34 (100%)	0	100	100
56	EF	547/576 (95%)	512 (94%)	35 (6%)	16	33
60	B	1/1 (100%)	1 (100%)	0	100	100
All	All	5529/5819 (95%)	5410 (98%)	119 (2%)	45	70

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	LI	40	THR
56	EF	469	ILE
40	LT	31	VAL
56	EF	468	ILE
56	EF	544	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
30	LI	20	ASN
38	LR	29	HIS
56	EF	465	HIS
30	LI	128	HIS
34	LN	29	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1511/1534 (98%)	304 (20%)	41 (2%)
22	23	2902/2904 (99%)	563 (19%)	68 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	5	119/120 (99%)	24 (20%)	3 (2%)
57	Dt	76/77 (98%)	20 (26%)	0
58	Pt	75/76 (98%)	21 (28%)	0
59	mR	9/60 (15%)	3 (33%)	0
All	All	4692/4771 (98%)	935 (19%)	112 (2%)

5 of 935 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	2	A
1	16	4	U
1	16	5	U
1	16	7	A
1	16	9	G

5 of 112 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	23	685	A
23	5	88	C
22	23	1288	G
23	5	24	G
22	23	2319	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	UR3	16	1498	1	19,22,23	0.96	0	26,32,35	1.84	3 (11%)
22	PSU	23	2504	22	18,21,22	1.48	4 (22%)	21,30,33	2.21	5 (23%)
22	OMU	23	2552	22,62	19,22,23	1.29	3 (15%)	25,31,34	1.99	5 (20%)
58	PSU	Pt	39	58	18,21,22	1.36	2 (11%)	21,30,33	2.07	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MA6	16	1518	1	23,26,27	1.52	5 (21%)	33,38,41	2.15	11 (33%)
58	G7M	Pt	46	58	23,26,27	2.38	5 (21%)	34,39,42	3.20	12 (35%)
22	5MC	23	1962	22,62	19,22,23	1.55	3 (15%)	26,32,35	1.30	2 (7%)
1	4OC	16	1402	1	20,23,24	0.79	0	25,32,35	1.09	1 (4%)
12	D2T	SL	89	12	8,9,10	3.34	2 (25%)	6,11,13	2.06	2 (33%)
60	BB9	B	2	60	2,5,6	3.25	1 (50%)	1,5,7	4.02	1 (100%)
57	PSU	Dt	56	57	18,21,22	1.43	2 (11%)	21,30,33	2.10	3 (14%)
22	PSU	23	1911	22	18,21,22	1.41	3 (16%)	21,30,33	2.05	3 (14%)
1	G7M	16	527	1	23,26,27	2.37	5 (21%)	34,39,42	3.05	11 (32%)
1	PSU	16	516	1	18,21,22	1.42	3 (16%)	21,30,33	2.31	5 (23%)
36	4D4	LP	81	36	9,11,12	3.18	3 (33%)	7,13,15	3.43	3 (42%)
22	PSU	23	1917	22	18,21,22	1.48	3 (16%)	21,30,33	2.09	4 (19%)
22	3TD	23	1915	22	19,22,23	1.26	2 (10%)	23,32,35	2.04	3 (13%)
22	1MG	23	745	22	23,26,27	1.19	3 (13%)	33,39,42	1.72	6 (18%)
22	2MA	23	2503	22,62	22,25,26	1.53	4 (18%)	32,37,40	2.44	8 (25%)
22	OMG	23	2251	22,62,58	23,26,27	1.24	3 (13%)	32,38,41	2.10	7 (21%)
22	PSU	23	2605	22	18,21,22	1.45	4 (22%)	21,30,33	1.99	4 (19%)
58	PSU	Pt	32	58	18,21,22	1.39	3 (16%)	21,30,33	2.10	4 (19%)
58	H2U	Pt	16	58	18,21,22	1.14	3 (16%)	19,30,33	1.18	1 (5%)
1	MA6	16	1519	1	23,26,27	1.50	5 (21%)	33,38,41	2.13	11 (33%)
1	2MG	16	966	1	23,26,27	1.27	3 (13%)	33,38,41	2.25	10 (30%)
60	DHA	B	7	60	3,4,5	4.88	1 (33%)	2,4,6	4.07	2 (100%)
58	4SU	Pt	8	58	18,21,22	1.91	5 (27%)	25,30,33	2.34	5 (20%)
60	0UO	B	4	60	16,17,18	1.53	5 (31%)	17,23,25	1.73	5 (29%)
58	3AU	Pt	47	58	24,28,29	1.05	1 (4%)	30,40,43	1.41	4 (13%)
57	4SU	Dt	8	57	18,21,22	1.88	5 (27%)	25,30,33	2.22	5 (20%)
22	5MU	23	747	22	19,22,23	1.48	6 (31%)	27,32,35	2.15	7 (25%)
58	MIA	Pt	37	58	28,31,32	2.30	7 (25%)	38,44,47	2.85	15 (39%)
22	PSU	23	2604	22	18,21,22	1.52	3 (16%)	21,30,33	2.20	5 (23%)
22	PSU	23	2457	22	18,21,22	1.57	4 (22%)	21,30,33	2.20	6 (28%)
22	6MZ	23	2030	22	22,25,26	1.48	5 (22%)	29,36,39	2.56	11 (37%)
60	DBB	B	6	60	4,5,6	0.51	0	1,5,7	0.41	0
57	G7M	Dt	47	57	23,26,27	2.36	5 (21%)	34,39,42	3.10	11 (32%)
22	5MU	23	1939	22,62	19,22,23	1.44	5 (26%)	27,32,35	2.21	6 (22%)
57	OMC	Dt	33	57	19,22,23	0.85	0	25,31,34	0.88	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	SAR	B	8	60	3,4,5	1.04	0	1,3,5	1.88	0
1	2MG	16	1516	1	23,26,27	1.25	4 (17%)	33,38,41	2.33	9 (27%)
1	5MC	16	1407	1	19,22,23	1.53	3 (15%)	26,32,35	1.26	3 (11%)
22	PSU	23	746	22,62	18,21,22	1.43	3 (16%)	21,30,33	1.97	3 (14%)
22	OMC	23	2498	22,62	19,22,23	0.85	0	25,31,34	0.82	0
22	PSU	23	2580	22	18,21,22	1.52	4 (22%)	21,30,33	2.17	5 (23%)
22	G7M	23	2069	22	23,26,27	2.38	5 (21%)	34,39,42	3.11	12 (35%)
22	6MZ	23	1618	22	22,25,26	1.47	5 (22%)	29,36,39	2.20	10 (34%)
22	PSU	23	955	22	18,21,22	1.48	4 (22%)	21,30,33	2.20	3 (14%)
1	5MC	16	967	1	19,22,23	1.62	3 (15%)	26,32,35	1.75	7 (26%)
57	H2U	Dt	21	57	18,21,22	1.06	3 (16%)	19,30,33	1.52	5 (26%)
22	H2U	23	2449	22	18,21,22	1.16	3 (16%)	19,30,33	1.11	1 (5%)
22	2MG	23	1835	22	23,26,27	1.26	3 (13%)	33,38,41	2.36	10 (30%)
58	PSU	Pt	55	58	18,21,22	1.39	2 (11%)	21,30,33	2.07	3 (14%)
22	2MG	23	2445	22,62	23,26,27	1.27	4 (17%)	33,38,41	2.29	10 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
22	PSU	23	2504	22	-	0/7/25/26	0/2/2/2
22	OMU	23	2552	22,62	-	0/9/27/28	0/2/2/2
58	PSU	Pt	39	58	-	0/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	0/11/29/30	0/3/3/3
58	G7M	Pt	46	58	-	0/7/25/26	0/3/3/3
22	5MC	23	1962	22,62	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	1	-	1/9/29/30	0/2/2/2
12	D2T	SL	89	12	-	2/7/12/14	-
60	BB9	B	2	60	-	0/0/4/6	-
57	PSU	Dt	56	57	-	0/7/25/26	0/2/2/2
22	PSU	23	1911	22	-	0/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/7/25/26	0/3/3/3
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
36	4D4	LP	81	36	-	3/11/12/14	-
22	PSU	23	1917	22	-	0/7/25/26	0/2/2/2
22	3TD	23	1915	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	23	745	22	-	0/7/25/26	0/3/3/3
22	2MA	23	2503	22,62	-	2/7/25/26	0/3/3/3
22	OMG	23	2251	22,62,58	-	3/9/27/28	0/3/3/3
22	PSU	23	2605	22	-	0/7/25/26	0/2/2/2
58	PSU	Pt	32	58	-	0/7/25/26	0/2/2/2
58	H2U	Pt	16	58	-	0/7/38/39	0/2/2/2
1	MA6	16	1519	1	-	0/11/29/30	0/3/3/3
1	2MG	16	966	1	-	1/9/27/28	0/3/3/3
60	DHA	B	7	60	-	0/0/2/4	-
58	4SU	Pt	8	58	-	3/7/25/26	0/2/2/2
60	0UO	B	4	60	-	2/7/8/10	0/2/2/2
58	3AU	Pt	47	58	-	6/16/34/35	0/2/2/2
57	4SU	Dt	8	57	-	0/7/25/26	0/2/2/2
22	5MU	23	747	22	-	2/7/25/26	0/2/2/2
58	MIA	Pt	37	58	-	3/15/33/34	0/3/3/3
22	PSU	23	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	23	2457	22	-	0/7/25/26	0/2/2/2
22	6MZ	23	2030	22	-	1/9/27/28	0/3/3/3
60	DBB	B	6	60	-	1/3/4/6	-
57	G7M	Dt	47	57	-	0/7/25/26	0/3/3/3
22	5MU	23	1939	22,62	-	0/7/25/26	0/2/2/2
57	OMC	Dt	33	57	-	1/9/27/28	0/2/2/2
60	SAR	B	8	60	-	1/1/2/3	-
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	23	746	22,62	-	1/7/25/26	0/2/2/2
22	OMC	23	2498	22,62	-	2/9/27/28	0/2/2/2
22	PSU	23	2580	22	-	0/7/25/26	0/2/2/2
22	G7M	23	2069	22	-	2/7/25/26	0/3/3/3
22	6MZ	23	1618	22	-	0/9/27/28	0/3/3/3
22	PSU	23	955	22	-	0/7/25/26	0/2/2/2
1	5MC	16	967	1	-	2/7/25/26	0/2/2/2
57	H2U	Dt	21	57	-	1/7/38/39	0/2/2/2
22	H2U	23	2449	22	-	0/7/38/39	0/2/2/2
22	2MG	23	1835	22	-	0/9/27/28	0/3/3/3
58	PSU	Pt	55	58	-	0/7/25/26	0/2/2/2
22	2MG	23	2445	22,62	-	1/9/27/28	0/3/3/3

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	B	7	DHA	C-CA	8.30	1.59	1.45
58	Pt	46	G7M	C8-N7	8.00	1.46	1.33
22	23	2069	G7M	C8-N7	7.74	1.46	1.33
57	Dt	47	G7M	C8-N7	7.69	1.46	1.33
1	16	527	G7M	C8-N7	7.68	1.46	1.33

The worst 5 of 293 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	Pt	37	MIA	C12-C13-C14	-9.13	110.62	127.01
22	23	2503	2MA	C5-C4-N3	-8.89	117.82	127.18
22	23	2069	G7M	CN7-N7-C8	-8.43	112.03	124.79
58	Pt	46	G7M	CN7-N7-C8	-8.38	112.09	124.79
57	Dt	47	G7M	CN7-N7-C8	-8.37	112.12	124.79

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	LP	81	4D4	NE-CD-CG-CB
36	LP	81	4D4	NH1-CZ-NE-CD
1	16	527	G7M	O4'-C4'-C5'-O5'
1	16	967	5MC	O4'-C1'-N1-C2
1	16	967	5MC	O4'-C1'-N1-C6

There are no ring outliers.

15 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	16	1518	MA6	2	0
58	Pt	46	G7M	1	0
60	B	2	BB9	1	0
1	16	516	PSU	1	0
22	23	2251	OMG	1	0
58	Pt	16	H2U	1	0
60	B	7	DHA	3	0
58	Pt	8	4SU	2	0
60	B	4	0UO	2	0
58	Pt	37	MIA	1	0
22	23	2030	6MZ	1	0
60	B	6	DBB	2	0
57	Dt	47	G7M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	Dt	33	OMC	1	0
60	B	8	SAR	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 422 ligands modelled in this entry, 406 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
61	PUT	23	3009	-	5,5,5	0.15	0	4,4,4	0.21	0
66	FME	Pt	3001	67	8,9,10	0.55	0	8,9,11	1.52	2 (25%)
61	PUT	23	3001	-	5,5,5	0.15	0	4,4,4	0.26	0
67	PHE	Pt	3002	66,58	8,9,12	3.35	3 (37%)	3,10,15	4.30	3 (100%)
61	PUT	16	1602	-	5,5,5	0.14	0	4,4,4	0.20	0
61	PUT	23	3004	-	5,5,5	0.15	0	4,4,4	0.27	0
61	PUT	23	3007	-	5,5,5	0.15	0	4,4,4	0.22	0
61	PUT	23	3008	-	5,5,5	0.15	0	4,4,4	0.20	0
63	SPD	23	3010	-	9,9,9	0.15	0	8,8,8	0.18	0
61	PUT	23	3002	-	5,5,5	0.15	0	4,4,4	0.28	0
63	SPD	23	3011	-	9,9,9	0.15	0	8,8,8	0.25	0
61	PUT	23	3006	-	5,5,5	0.15	0	4,4,4	0.20	0
61	PUT	23	3005	-	5,5,5	0.15	0	4,4,4	0.23	0
61	PUT	23	3003	-	5,5,5	0.14	0	4,4,4	0.23	0
61	PUT	16	1601	-	5,5,5	0.14	0	4,4,4	0.21	0
65	GDP	EF	801	-	29,30,30	1.15	4 (13%)	45,47,47	1.76	5 (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
61	PUT	23	3009	-	-	0/3/3/3	-
66	FME	Pt	3001	67	-	5/7/9/11	-
61	PUT	23	3001	-	-	0/3/3/3	-
67	PHE	Pt	3002	66,58	-	4/8/6/8	-
61	PUT	16	1602	-	-	0/3/3/3	-
61	PUT	23	3004	-	-	0/3/3/3	-
61	PUT	23	3007	-	-	0/3/3/3	-
61	PUT	23	3008	-	-	0/3/3/3	-
63	SPD	23	3010	-	-	1/7/7/7	-
61	PUT	23	3002	-	-	1/3/3/3	-
63	SPD	23	3011	-	-	0/7/7/7	-
61	PUT	23	3006	-	-	0/3/3/3	-
61	PUT	23	3005	-	-	1/3/3/3	-
61	PUT	23	3003	-	-	0/3/3/3	-
61	PUT	16	1601	-	-	0/3/3/3	-
65	GDP	EF	801	-	-	0/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	Pt	3002	PHE	CD1-CG	7.85	1.39	1.33
67	Pt	3002	PHE	CD2-CG	-3.76	1.39	1.47
65	EF	801	GDP	C5-C4	2.97	1.46	1.38
67	Pt	3002	PHE	CE1-CD1	-2.82	1.39	1.49
65	EF	801	GDP	C6-N1	-2.63	1.33	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
65	EF	801	GDP	C5-C4-N3	-5.73	119.27	128.39
65	EF	801	GDP	C2-N3-C4	4.90	120.73	112.30
67	Pt	3002	PHE	CB-CG-CD1	-4.66	119.27	126.41
67	Pt	3002	PHE	CE1-CD1-CG	-4.45	119.59	126.98
65	EF	801	GDP	N9-C4-N3	4.14	134.23	125.95

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
66	Pt	3001	FME	N-CA-CB-CG

Continued on next page...

Continued from previous page...

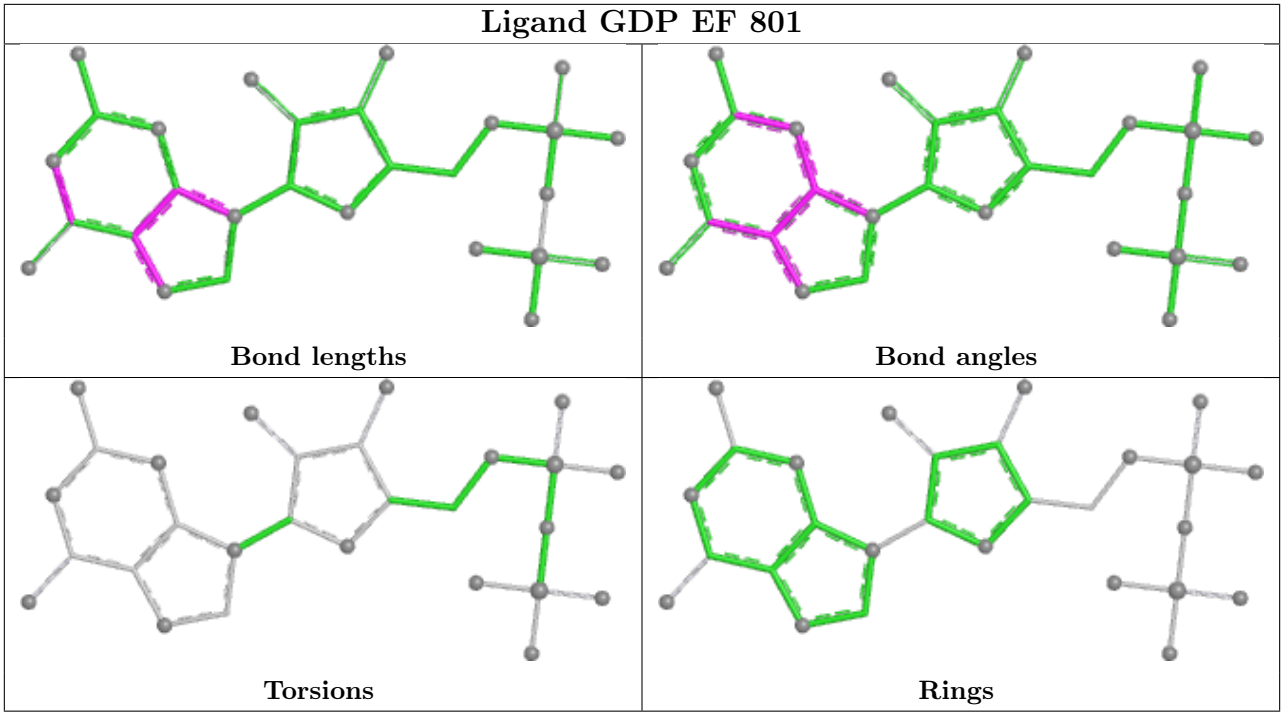
Mol	Chain	Res	Type	Atoms
67	Pt	3002	PHE	C-CA-CB-CG
67	Pt	3002	PHE	CE2-CD2-CG-CD1
63	23	3010	SPD	C3-C4-C5-N6
66	Pt	3001	FME	O1-CN-N-CA

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	Pt	3002	PHE	1	0
61	23	3004	PUT	1	0
63	23	3011	SPD	1	0
61	16	1601	PUT	1	0

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

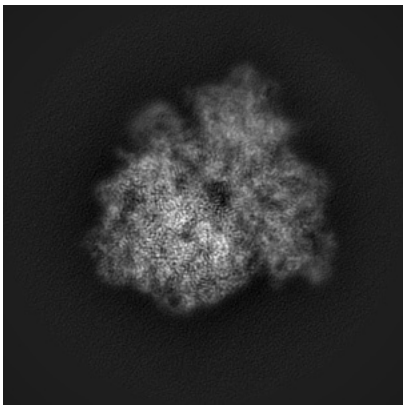
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26486. These allow visual inspection of the internal detail of the map and identification of artifacts.

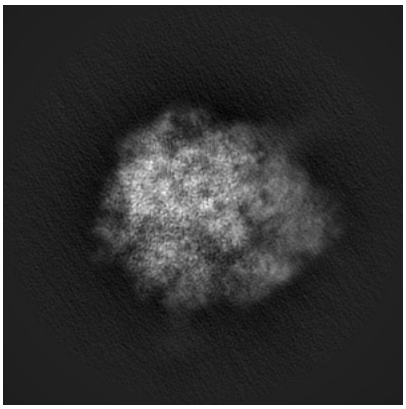
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

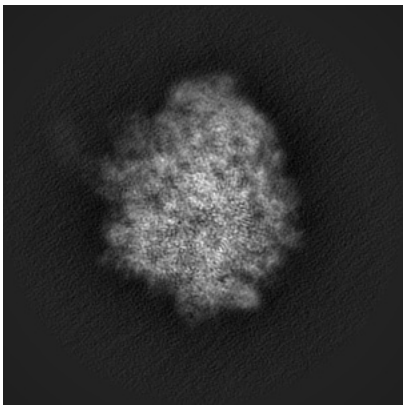
6.1.1 Primary map



X

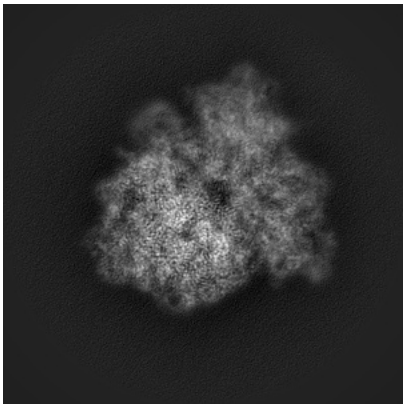


Y

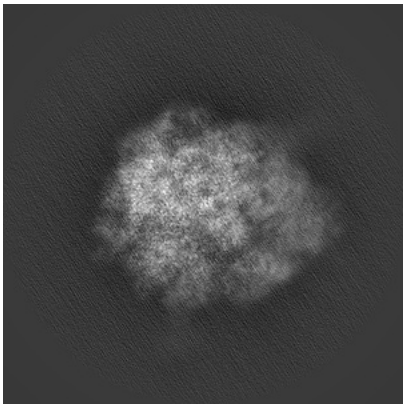


Z

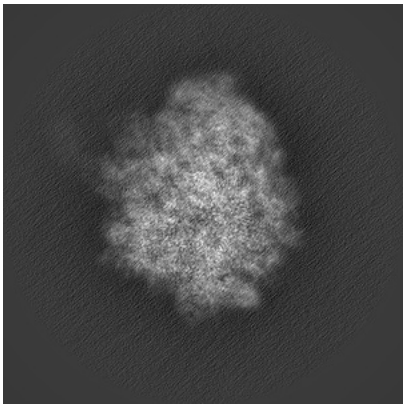
6.1.2 Raw map



X



Y

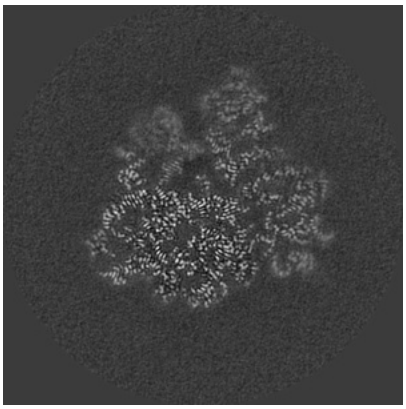


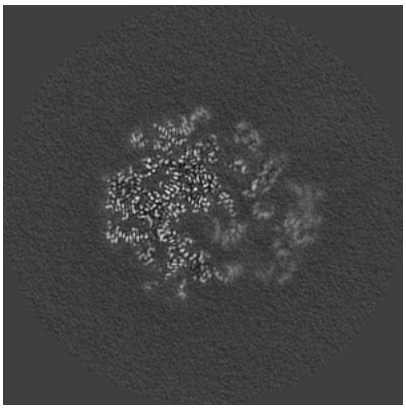
Z

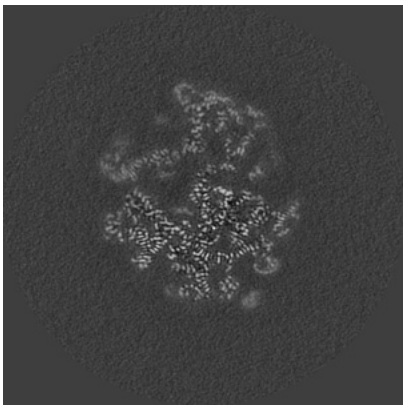
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

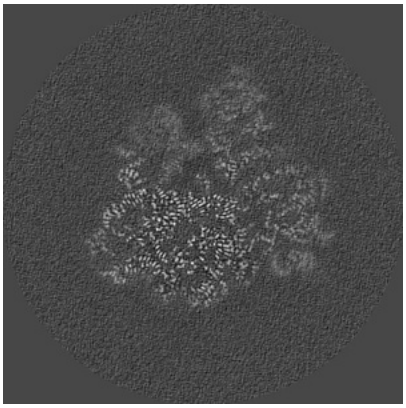
6.2.1 Primary map

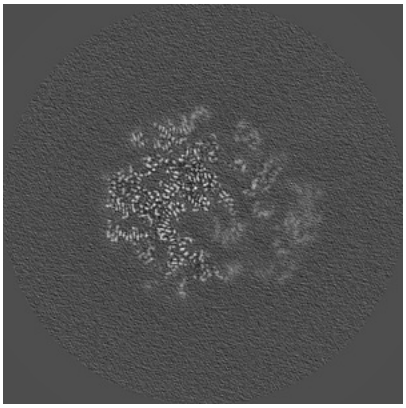

X Index: 190

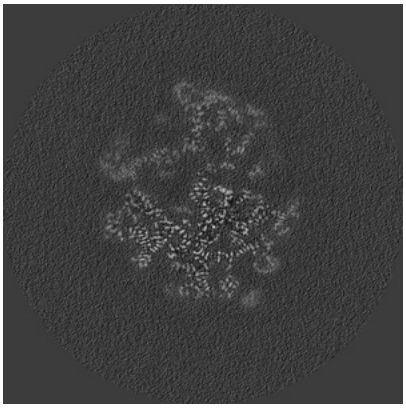

Y Index: 190


Z Index: 190

6.2.2 Raw map


X Index: 190

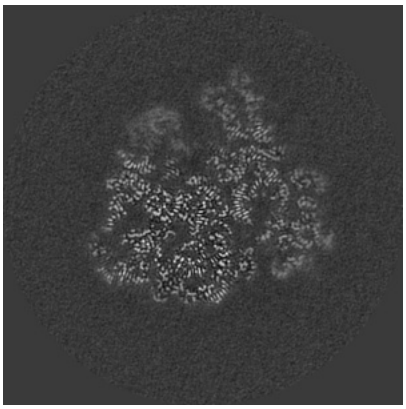

Y Index: 190


Z Index: 190

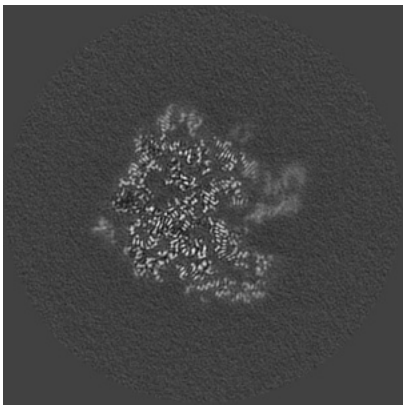
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

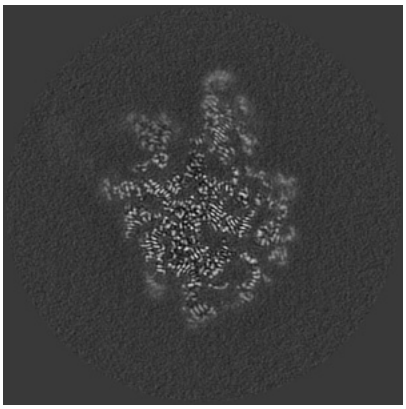
6.3.1 Primary map



X Index: 195

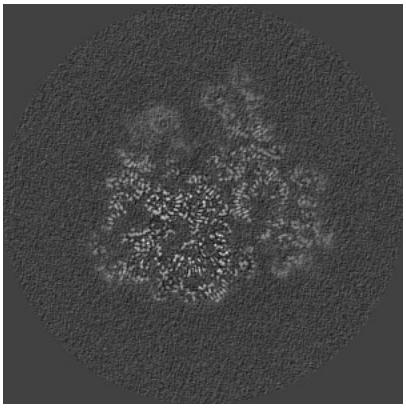


Y Index: 157

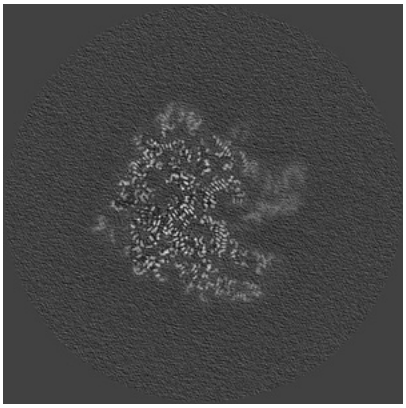


Z Index: 153

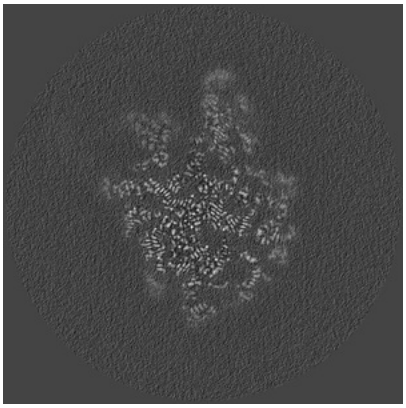
6.3.2 Raw map



X Index: 195



Y Index: 158

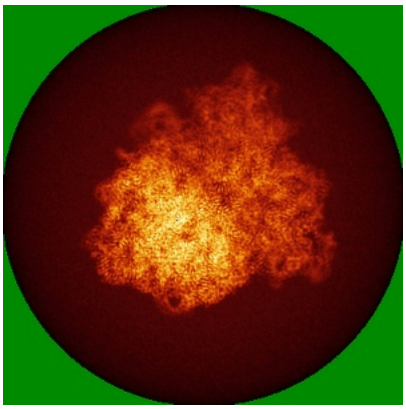


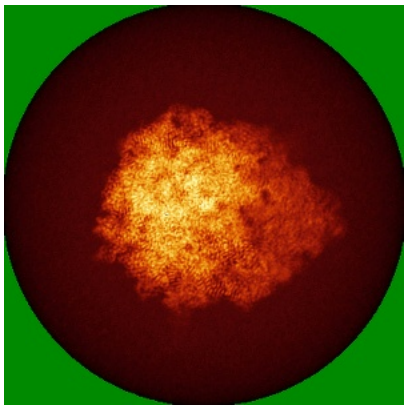
Z Index: 153

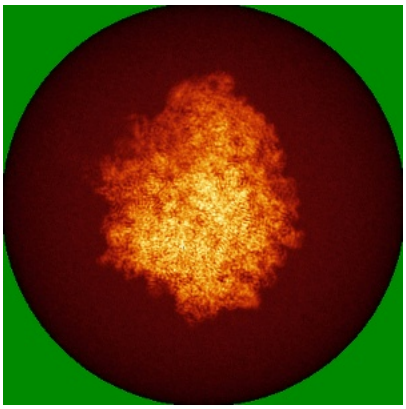
The images above show the largest variance slices of the map in three orthogonal directions.

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

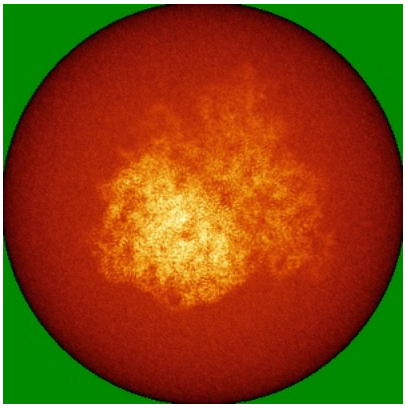
6.4.1 Primary map

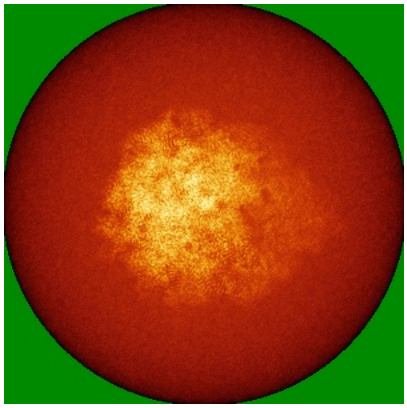

X

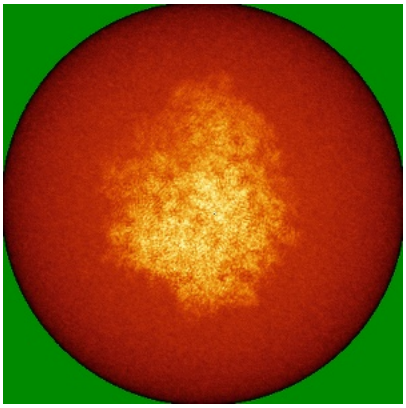

Y


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

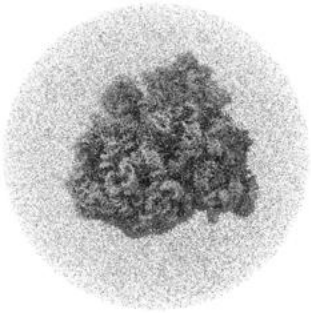
X

Y

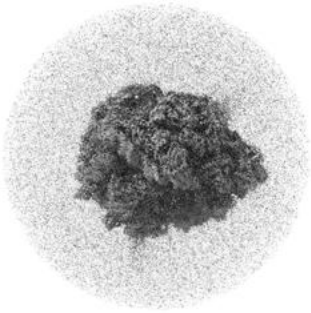
Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

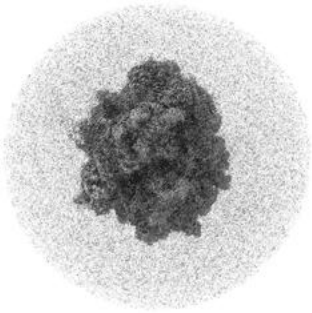
6.5.2 Raw map



X



Y



Z

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

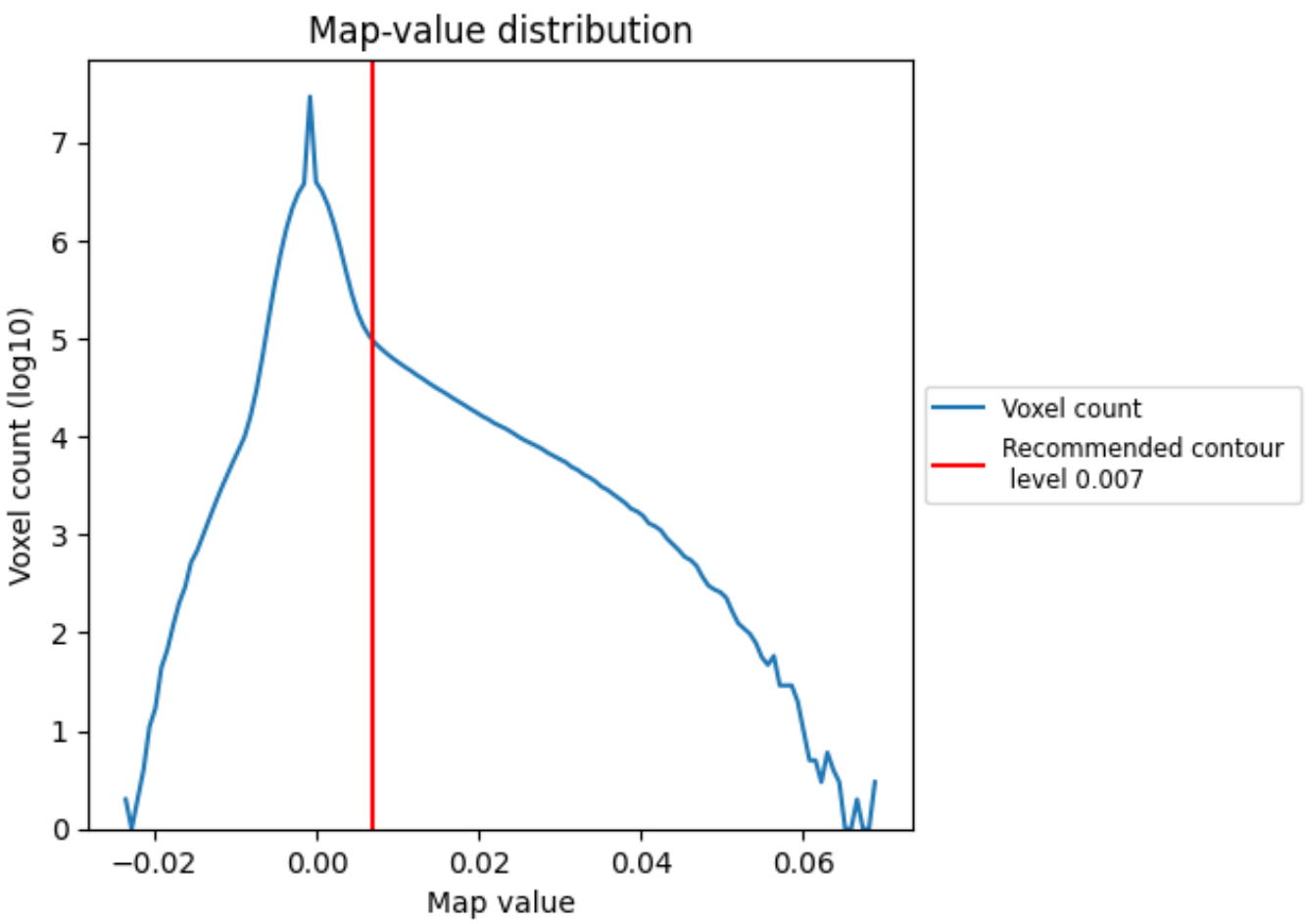
6.6 Mask visualisation (i)

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

7 Map analysis (i)

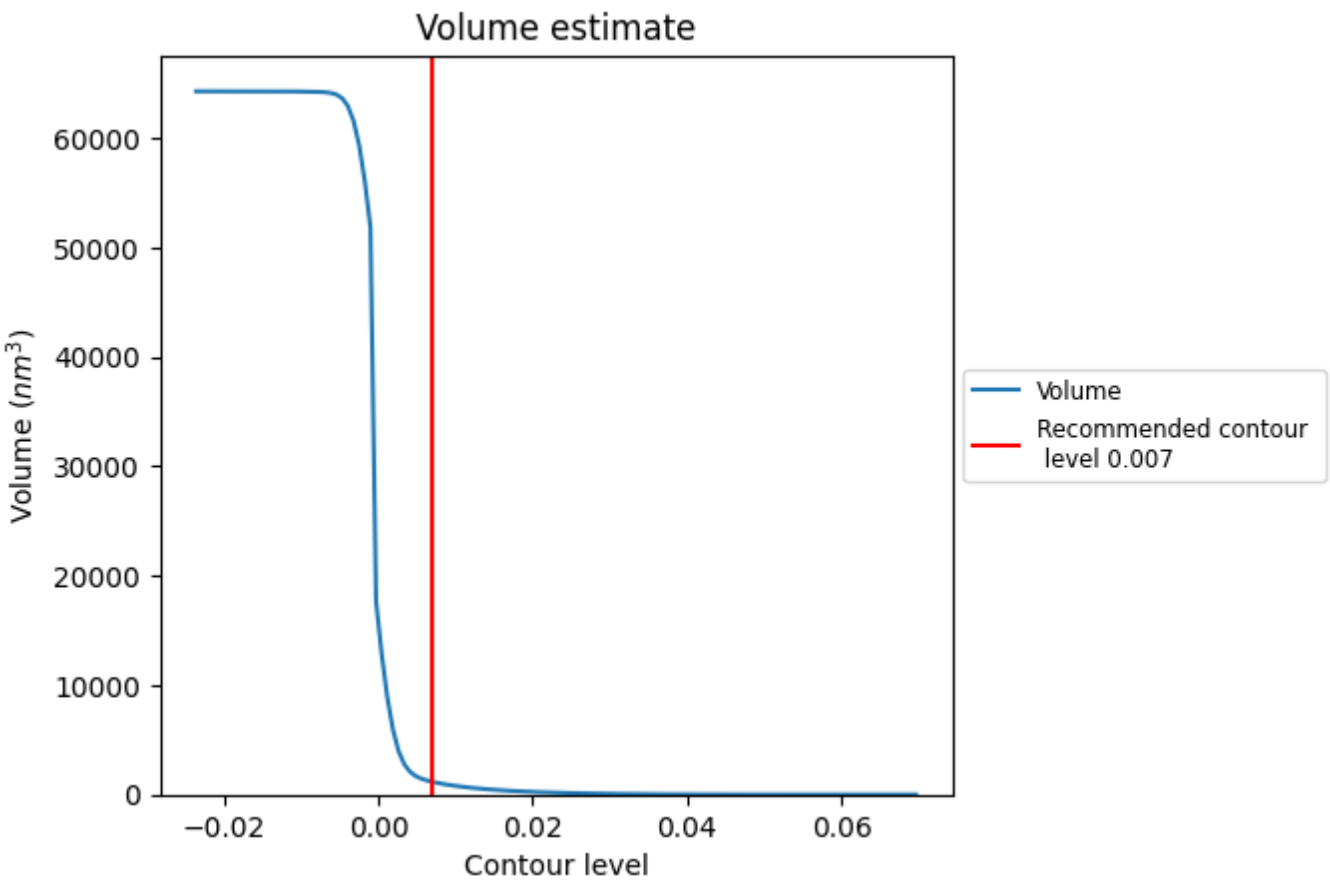
This section contains the results of statistical analysis of the map.

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.

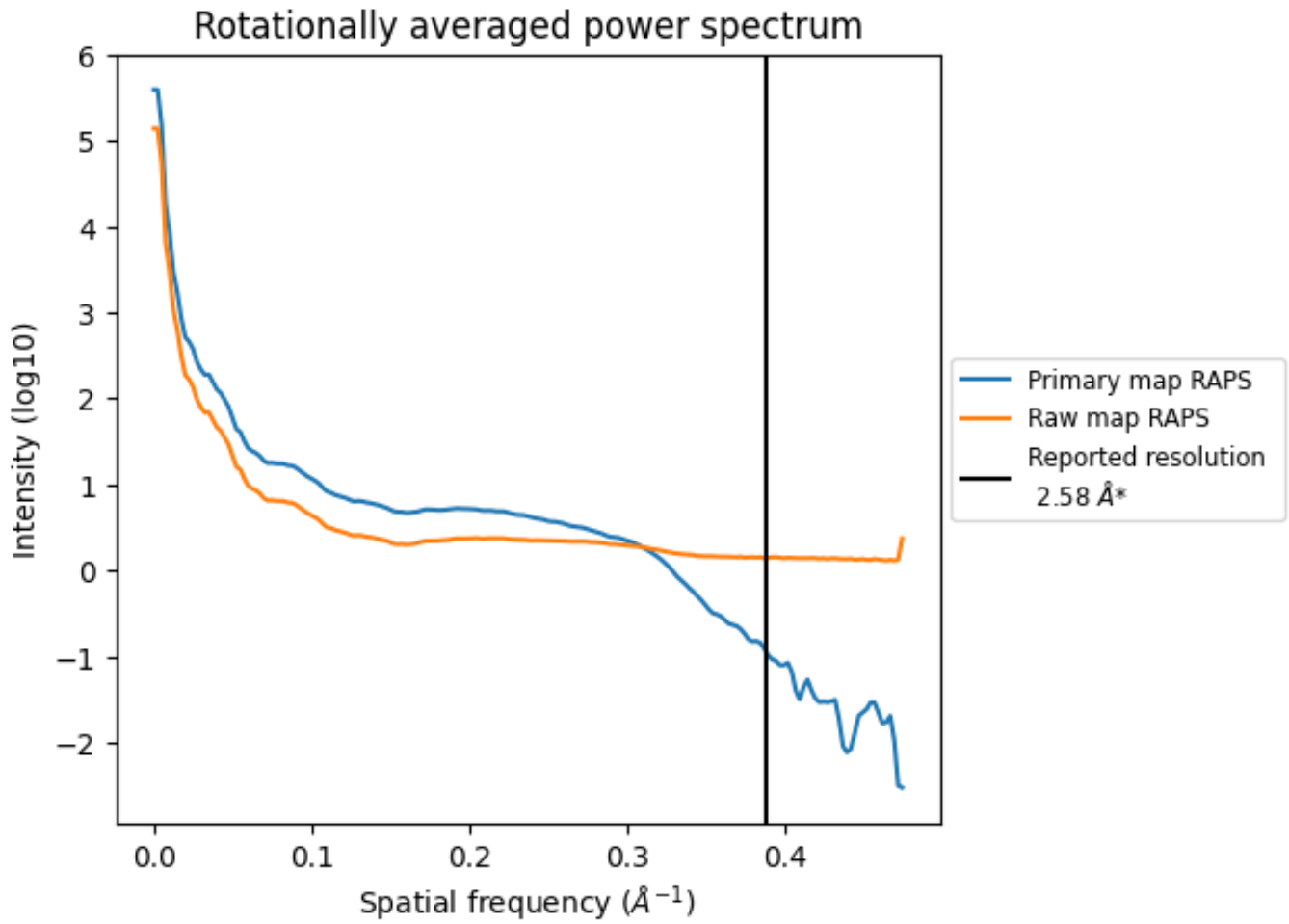
7.2 Volume estimate (i)



The volume at the recommended contour level is 1165 nm^3; this corresponds to an approximate mass of 1052 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)

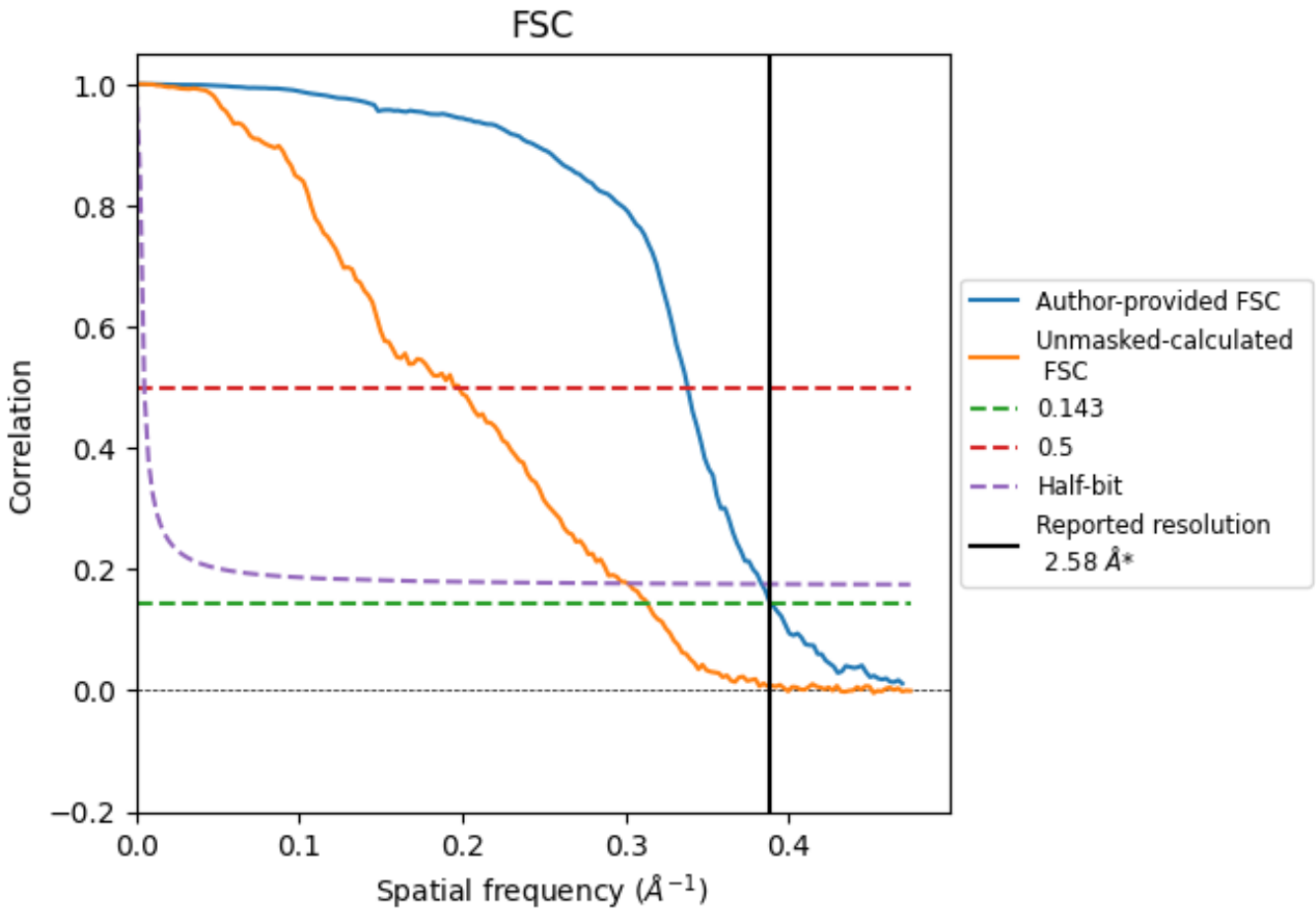


*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

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 0.388 Å^{-1}

8.2 Resolution estimates (i)

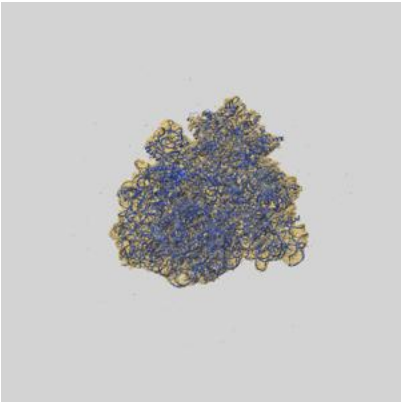
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.96	2.61
Unmasked-calculated*	3.19	5.06	3.32

*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 3.19 differs from the reported value 2.58 by more than 10 %

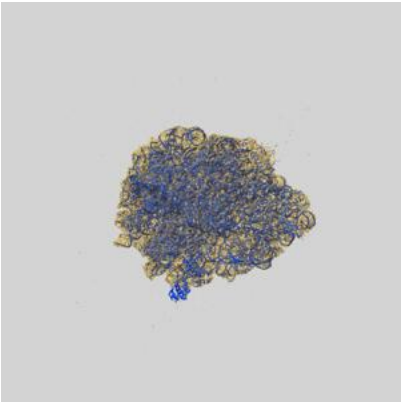
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26486 and PDB model 7UG7. Per-residue inclusion information can be found in section 3 on page 19.

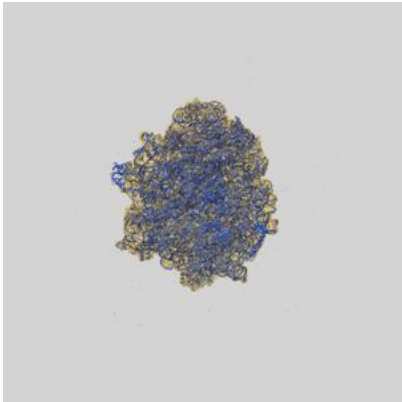
9.1 Map-model overlay (i)



X



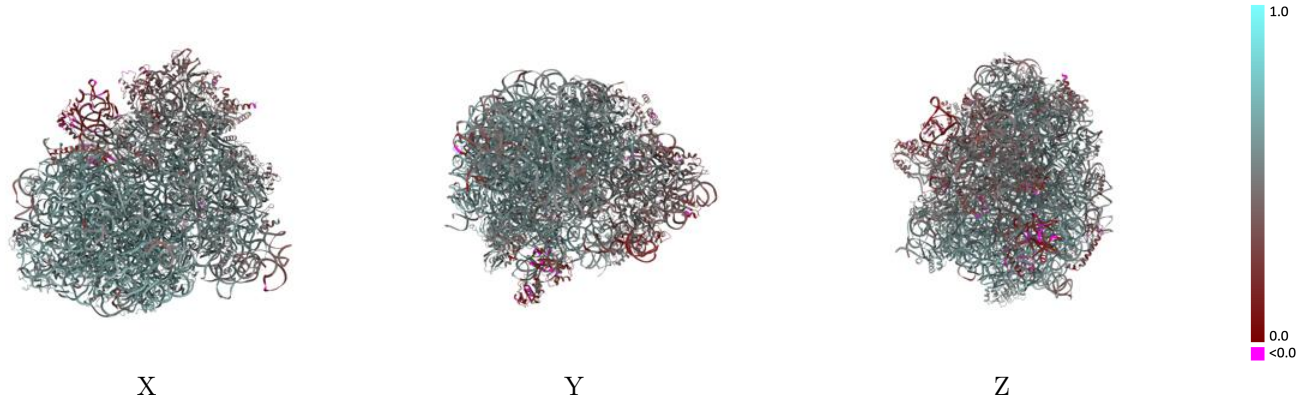
Y



Z

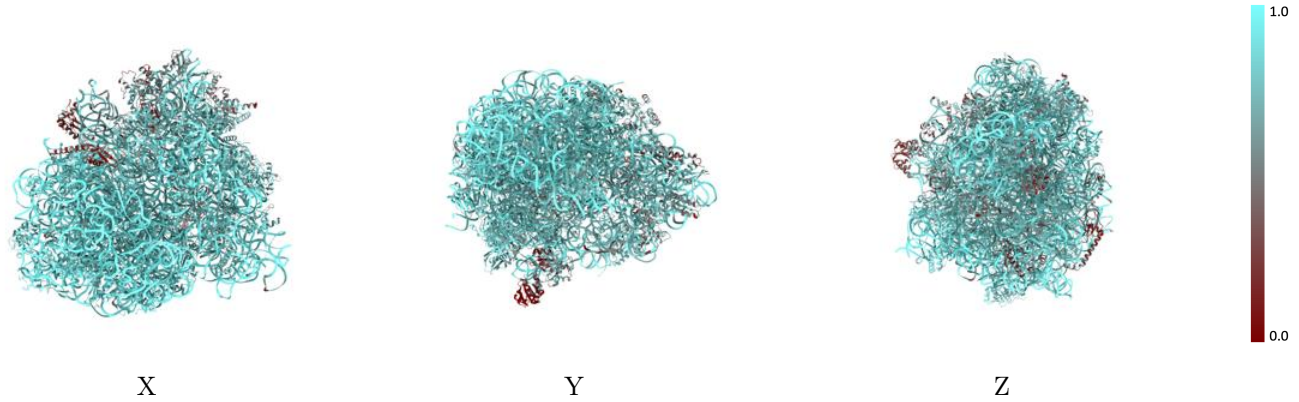
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



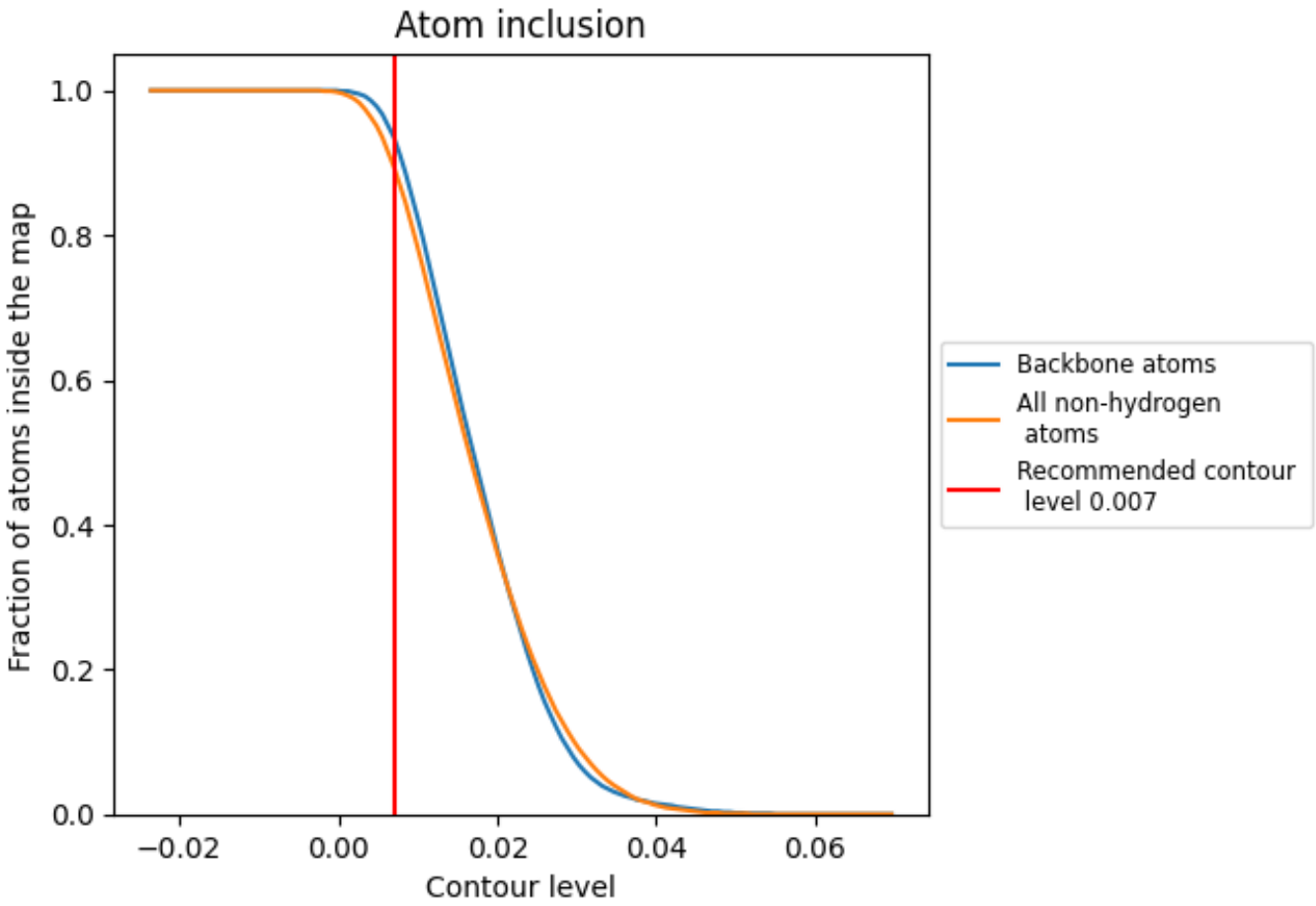
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.5360
16	0.9480	0.5160
23	0.9750	0.5870
5	0.9820	0.5590
B	0.8810	0.5290
Dt	0.8580	0.4840
EF	0.7300	0.4720
LA	0.2660	0.1840
LB	0.9300	0.6080
LC	0.9170	0.6030
LD	0.8930	0.5790
LE	0.7430	0.4420
LF	0.8430	0.5340
LI	0.3580	0.3090
LJ	0.2030	0.2680
LK	0.4100	0.2060
LM	0.9240	0.6070
LN	0.9050	0.6070
LO	0.8920	0.5760
LP	0.9200	0.6060
LQ	0.9590	0.6110
LR	0.8720	0.5370
LS	0.8730	0.5780
LT	0.9560	0.6110
LU	0.8810	0.5760
LV	0.9170	0.5980
LW	0.8660	0.5730
LX	0.8910	0.5620
LY	0.8640	0.5530
La	0.8930	0.6010
Lb	0.9200	0.5940
Lc	0.8590	0.5450
Ld	0.8880	0.5830
Le	0.5970	0.3510
Lf	0.8900	0.5880

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Chain	Atom inclusion	Q-score
Lg	0.8580	0.5680
Lh	0.9440	0.6170
Li	0.9490	0.6180
Lj	0.8940	0.5900
Pt	0.8270	0.4850
SB	0.6330	0.4010
SC	0.6780	0.4370
SD	0.7750	0.4740
SE	0.8280	0.5140
SF	0.7120	0.4390
SG	0.4260	0.3060
SH	0.8060	0.5050
SI	0.6530	0.3970
SJ	0.5990	0.3670
SK	0.7890	0.4950
SL	0.8250	0.5600
SM	0.5660	0.3200
SN	0.7400	0.4080
SO	0.8350	0.5110
SP	0.7960	0.5000
SQ	0.8050	0.5320
SR	0.7860	0.4870
SS	0.6920	0.4060
ST	0.8180	0.5100
SU	0.7160	0.4650
mR	0.7570	0.4550