



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2024 – 03:37 pm BST

PDB ID : 6ZTO
EMDB ID : EMD-11422
Title : E. coli 70S-RNAP expressome complex in uncoupled state 1
Authors : Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on : 2020-07-20
Resolution : 3.00 Å(reported)
Based on initial models : 6ALH, 4YBB

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

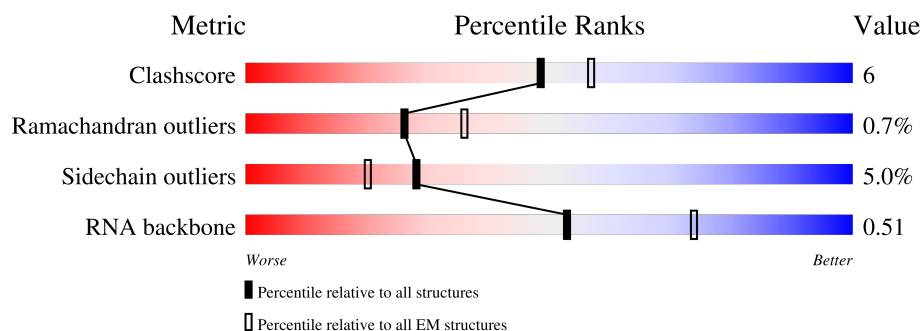
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	131	
7	AG	156	

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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	53	
23	AW	77	
24	AX	76	
25	BA	2904	
26	BB	120	
27	BC	273	
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	
32	BH	149	

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Mol	Chain	Length	Quality of chain
33	BK	142	
34	BL	123	
35	BM	144	
36	BN	136	
37	BO	127	
38	BP	117	
39	BQ	115	
40	BR	118	
41	BS	103	
42	BT	110	
43	BU	100	
44	BV	104	
45	BW	94	
46	BX	85	
47	BY	78	
48	BZ	63	
49	B1	59	
50	B2	57	
51	B3	55	
52	B4	46	
53	B5	65	
54	B6	50	
55	B7	70	
56	CN	39	
57	CT	39	

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Mol	Chain	Length	Quality of chain
58	CA	329	
58	CB	329	
59	CC	1342	
60	CD	1407	
61	CE	91	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 172846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0
			32909	14684	6037	10655	1533		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	209	Total	C	N	O	S	0	0
			1640	1038	308	291	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	156	Total	C	N	O	S	0	0
			1148	715	217	210	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP A0A090BZW5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	100	Total	C	N	O	S	0	0
			800	500	153	146	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	66	Total	C	N	O	S	0	0
			545	344	102	98	1		

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	27	Total	C	N	O	P	0	0
			572	256	102	187	27		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0
			1630	730	290	533	76	1		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2900	Total	C	N	O	P	0	0
			62270	27786	11456	20128	2900		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	77	VAL	ILE	conflict	UNP P02413

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BQ	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BU	96	Total	C	N	O	S	0	0
			764	484	142	136	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BV	103	Total	C	N	O	0	0
			789	498	148	143		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	B3	53	Total	C	N	O	0	0
			436	281	80	75		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	46	Total	C	N	O	S	0	0
			376	228	89	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B6	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B7	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 56 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CN	30	Total	C	N	O	P	0	0
			618	294	114	180	30		

- Molecule 57 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CT	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CA	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
58	CB	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CC	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CD	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

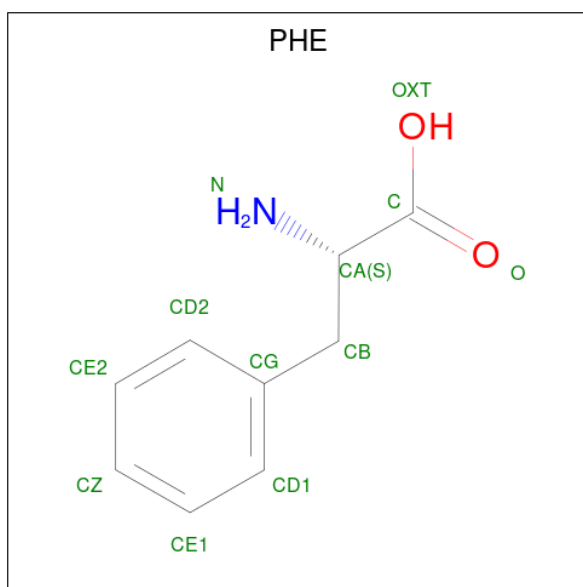
- Molecule 61 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CE	61	Total	C	N	O	S	0	0
			478	295	90	92	1		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	AA	143	Total	Mg	0
			143	143	
62	AI	1	Total	Mg	0
			1	1	
62	AL	1	Total	Mg	0
			1	1	
62	AM	1	Total	Mg	0
			1	1	
62	AW	5	Total	Mg	0
			5	5	
62	AX	1	Total	Mg	0
			1	1	
62	BA	317	Total	Mg	0
			317	317	
62	BB	9	Total	Mg	0
			9	9	
62	BC	3	Total	Mg	0
			3	3	
62	BN	1	Total	Mg	0
			1	1	
62	BO	1	Total	Mg	0
			1	1	
62	BQ	1	Total	Mg	0
			1	1	
62	BV	1	Total	Mg	0
			1	1	
62	BX	1	Total	Mg	0
			1	1	
62	CD	1	Total	Mg	0
			1	1	

- Molecule 63 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
63	AX	1	Total	C	N	O	0
			11	9	1	1	

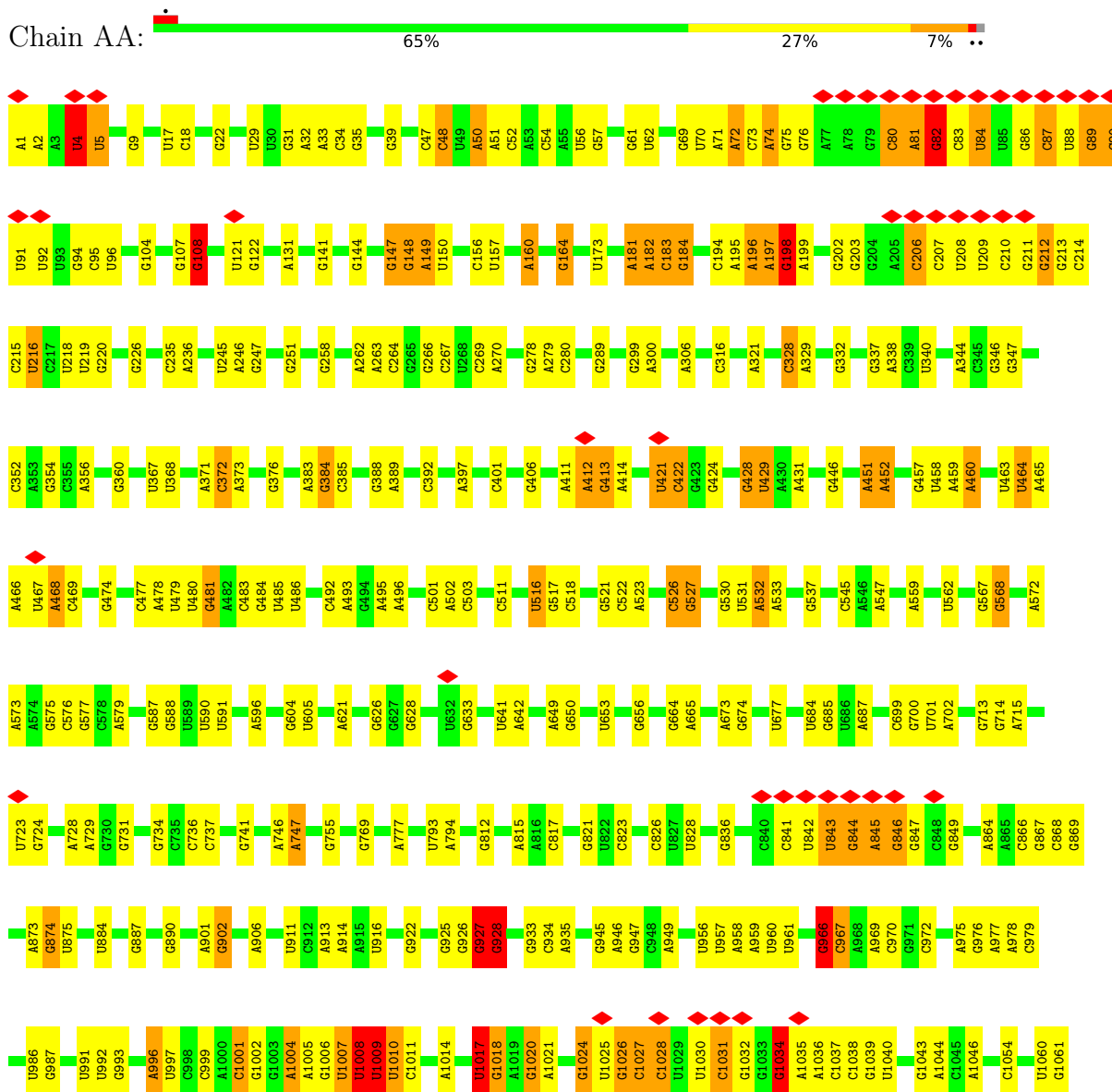
- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

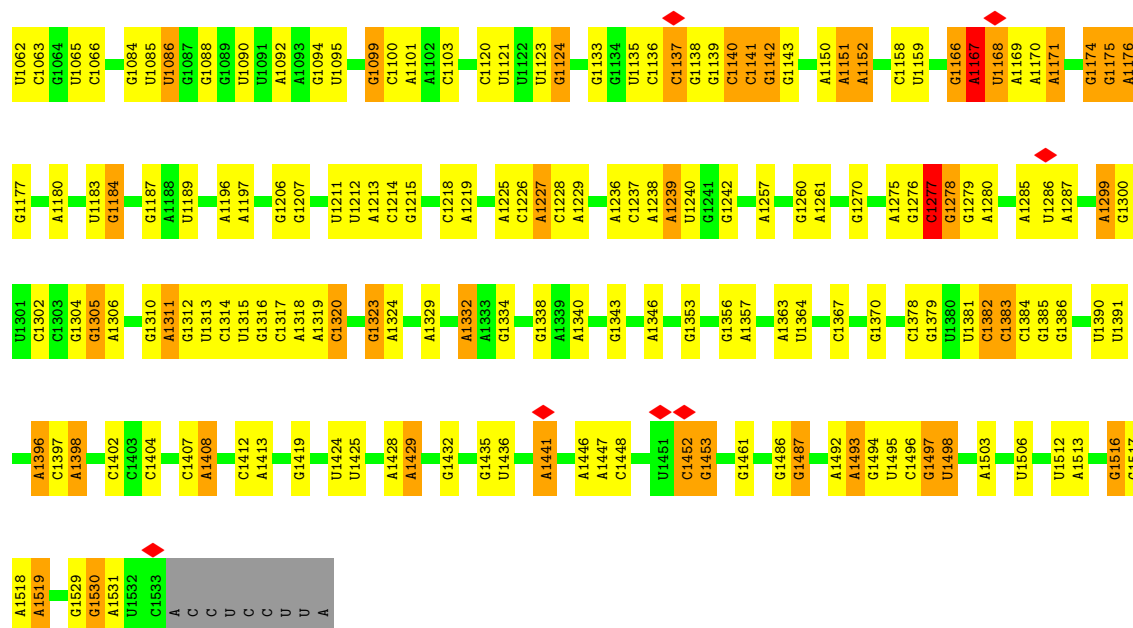
Mol	Chain	Residues	Atoms		AltConf
64	B6	1	Total	Zn	0
			1	1	
64	B7	1	Total	Zn	0
			1	1	
64	CD	2	Total	Zn	0
			2	2	

3 Residue-property plots

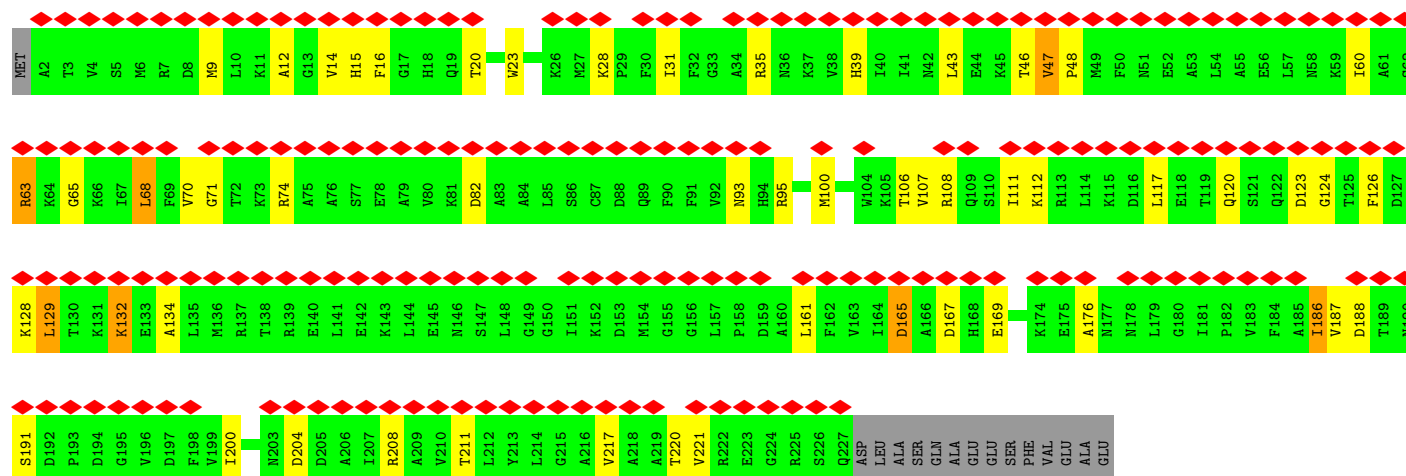
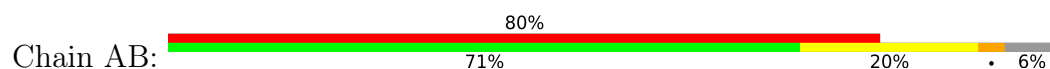
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

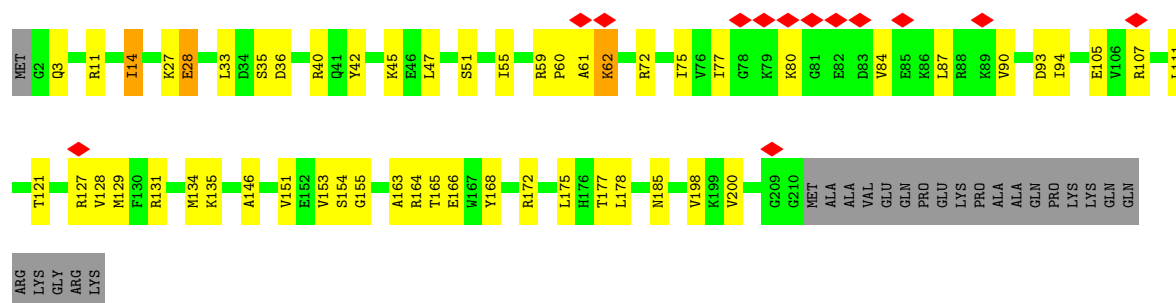




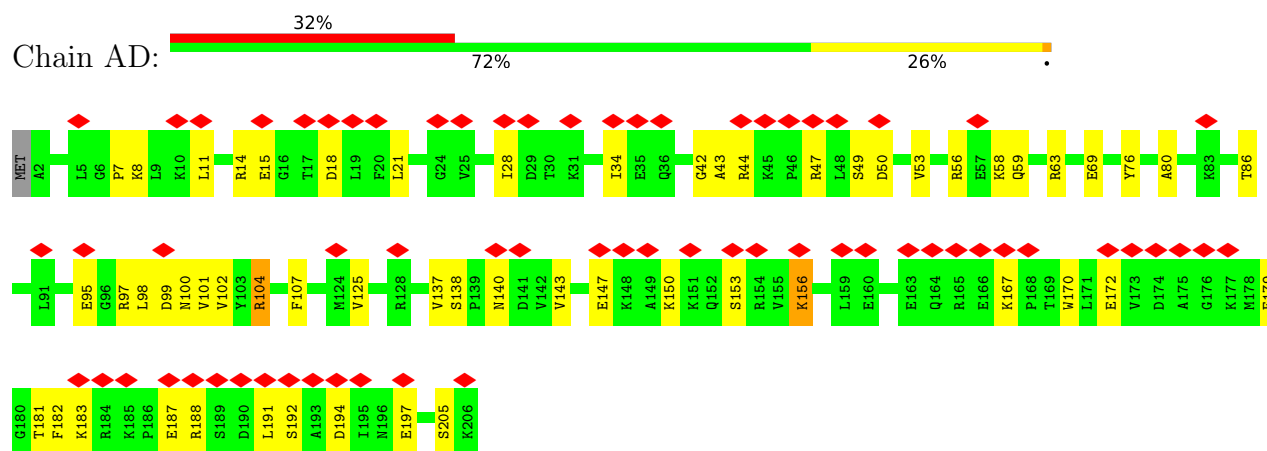
• Molecule 2: 30S ribosomal protein S2



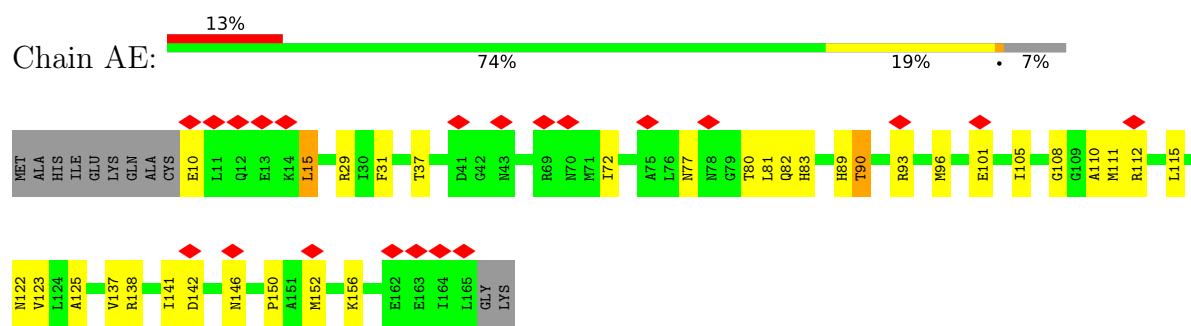
• Molecule 3: 30S ribosomal protein S3



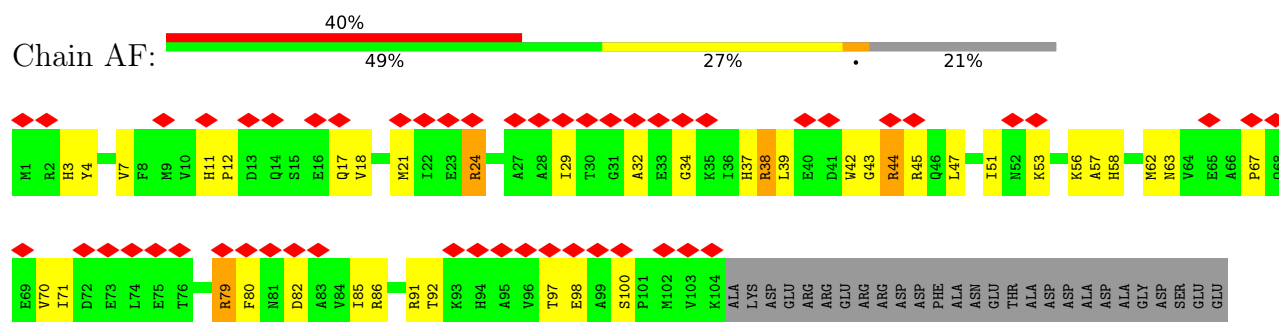
- Molecule 4: 30S ribosomal protein S4



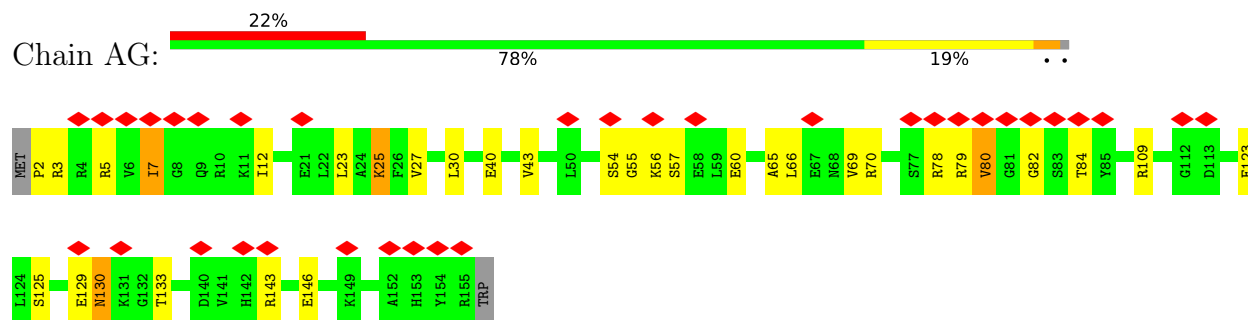
- Molecule 5: 30S ribosomal protein S5



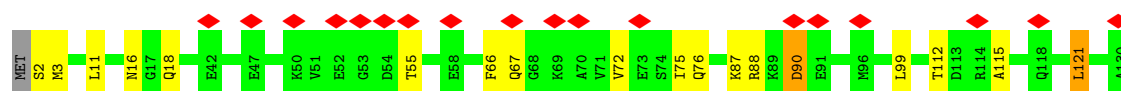
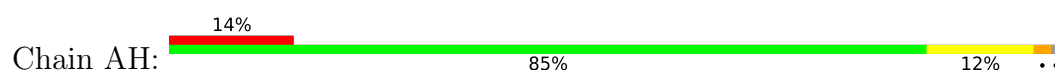
- Molecule 6: 30S ribosomal protein S6



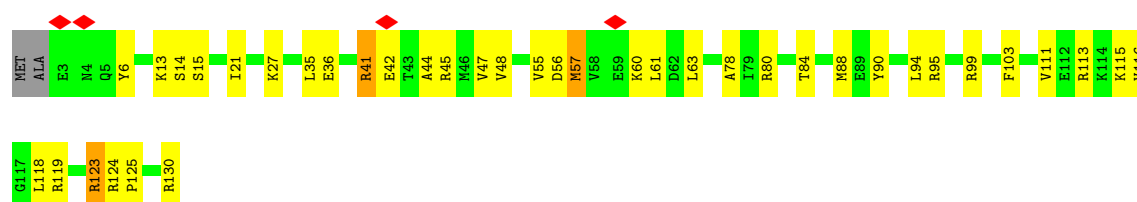
- Molecule 7: 30S ribosomal protein S7



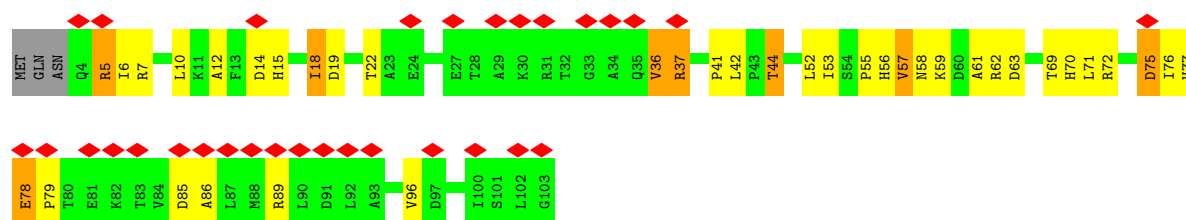
- Molecule 8: 30S ribosomal protein S8



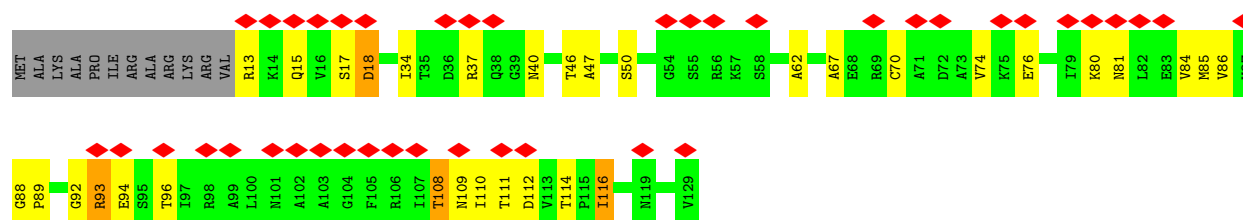
• Molecule 9: 30S ribosomal protein S9



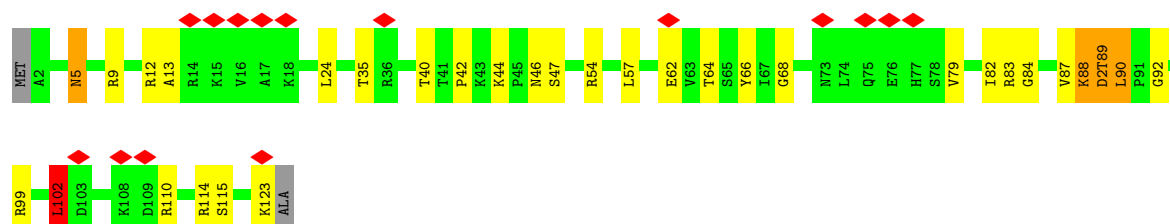
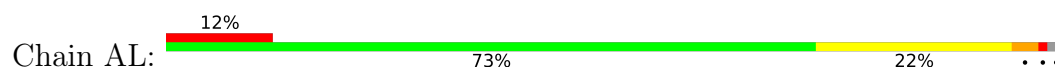
• Molecule 10: 30S ribosomal protein S10



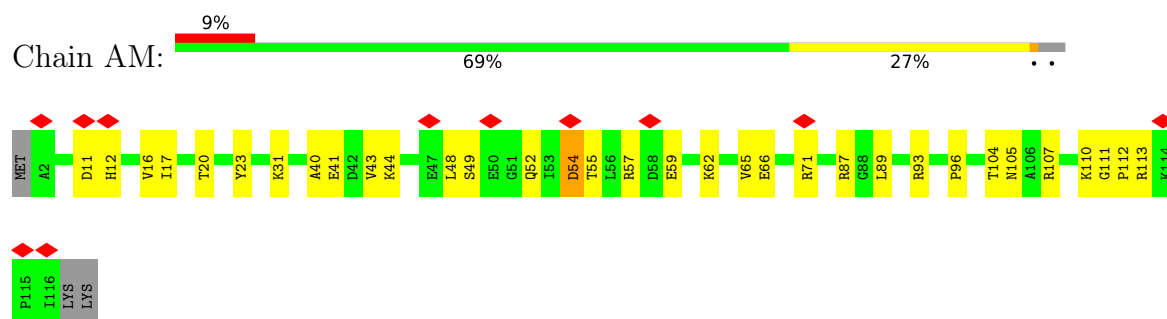
• Molecule 11: 30S ribosomal protein S11



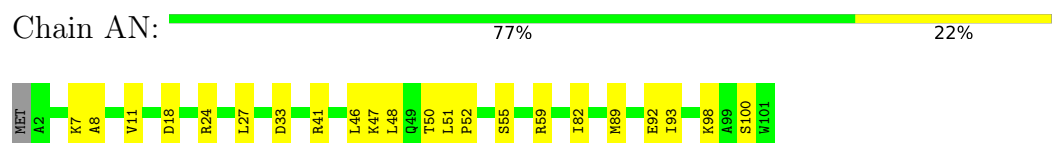
• Molecule 12: 30S ribosomal protein S12



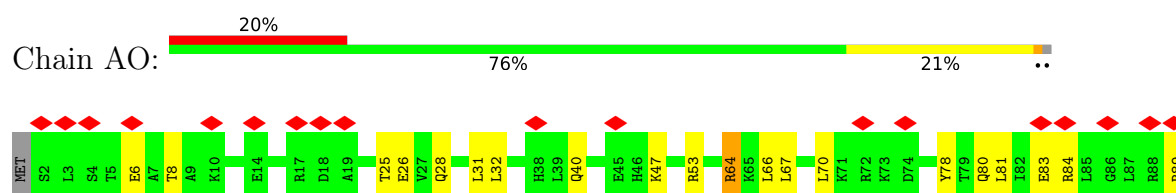
- Molecule 13: 30S ribosomal protein S13



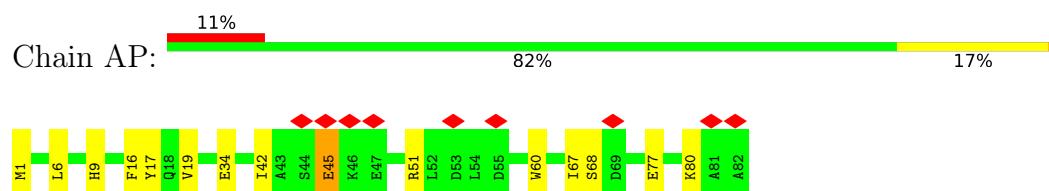
- Molecule 14: 30S ribosomal protein S14



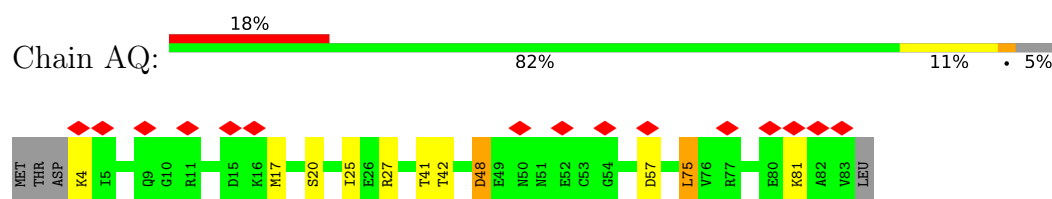
- Molecule 15: 30S ribosomal protein S15



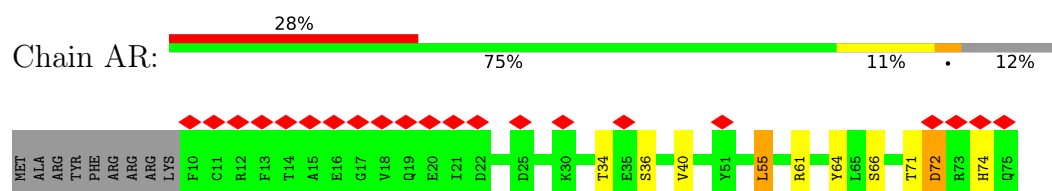
- Molecule 16: 30S ribosomal protein S16



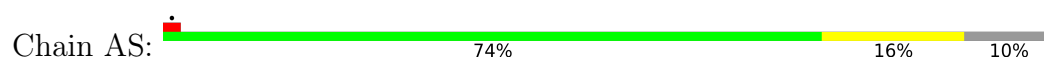
- Molecule 17: 30S ribosomal protein S17



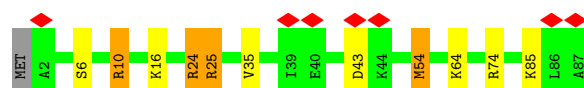
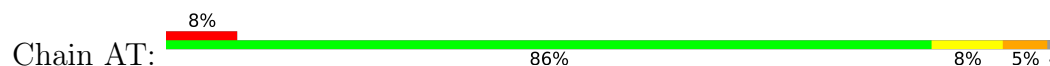
- Molecule 18: 30S ribosomal protein S18



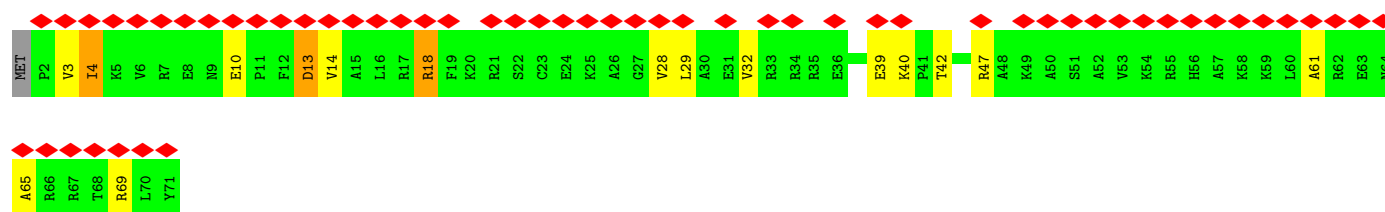
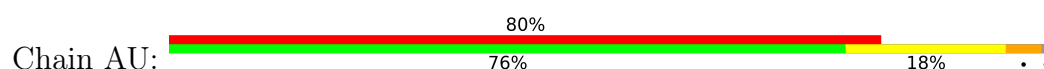
- Molecule 19: 30S ribosomal protein S19



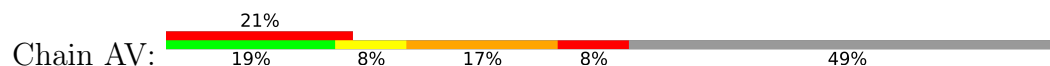
- Molecule 20: 30S ribosomal protein S20



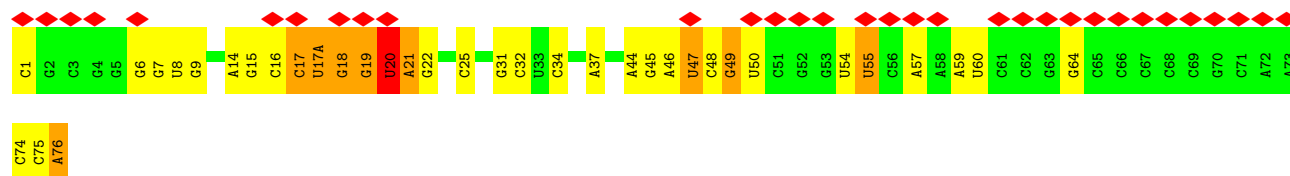
- Molecule 21: 30S ribosomal protein S21



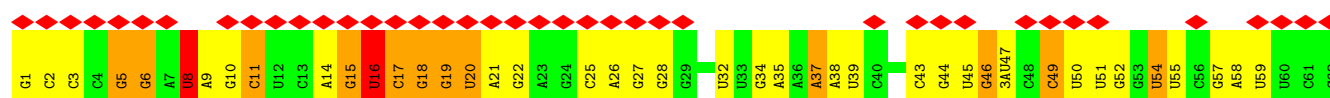
- Molecule 22: mRNA



- Molecule 23: tRNA(fmet) P-site

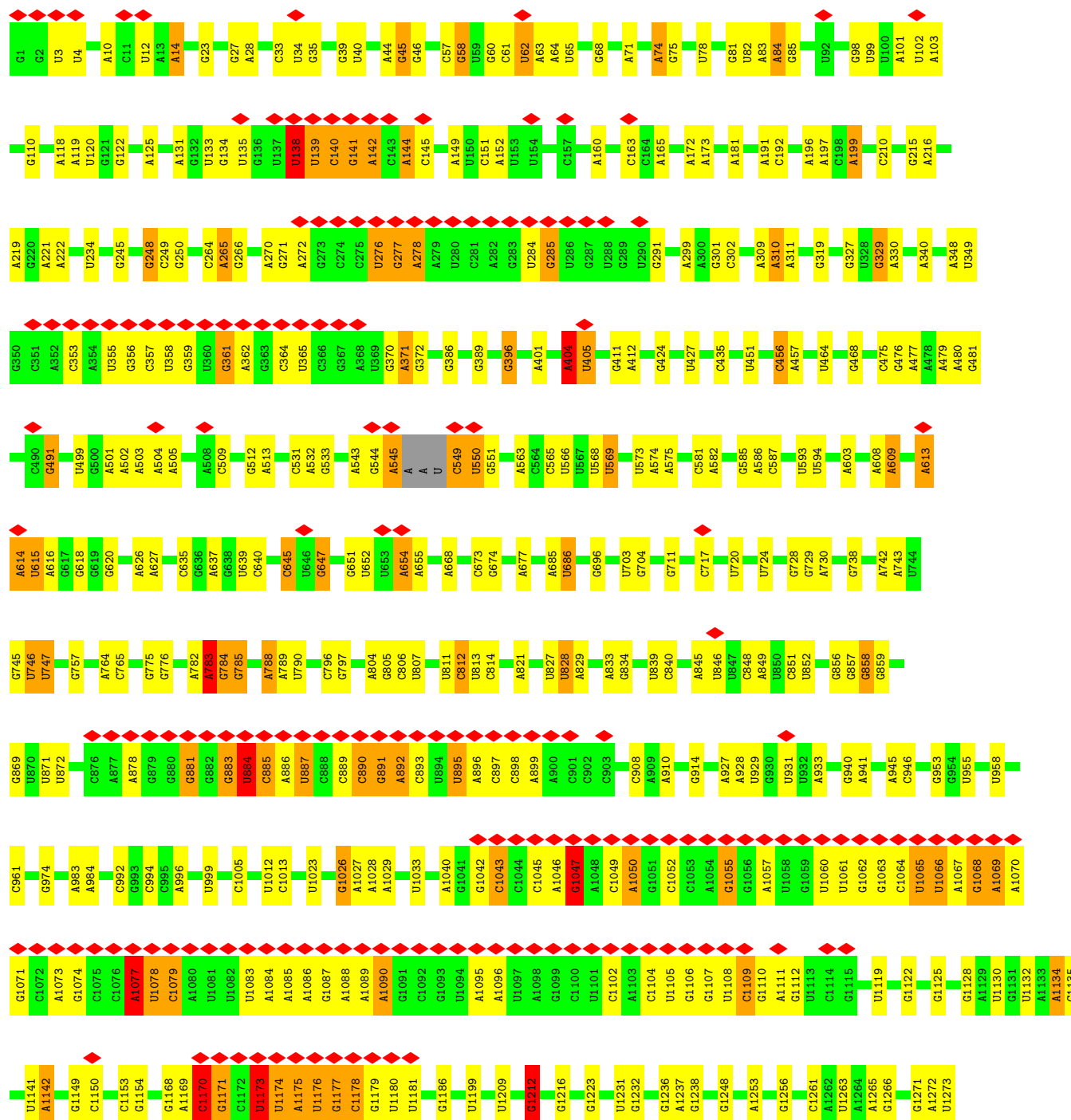


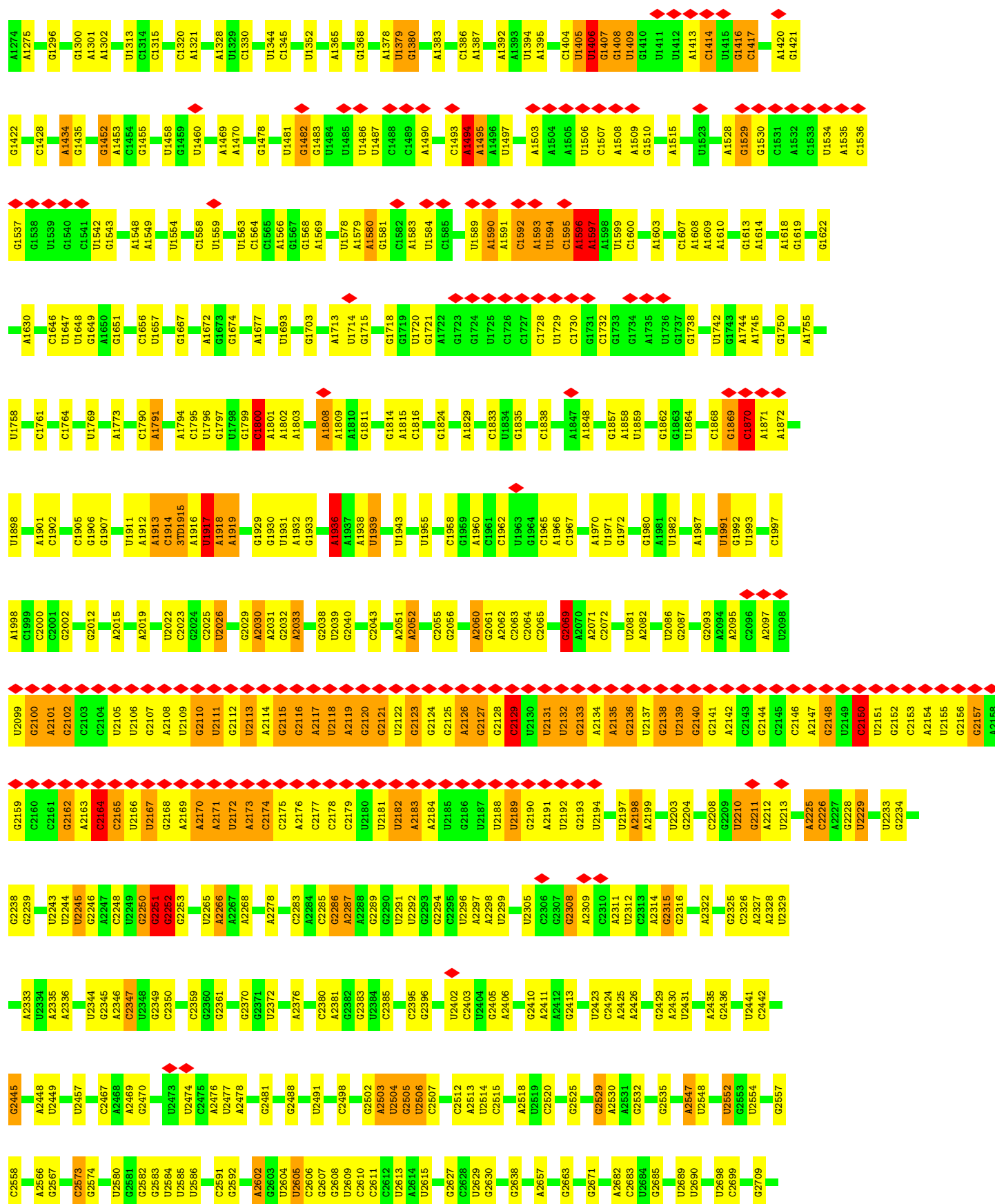
- Molecule 24: Phe-NH-tRNA(Phe) A-site

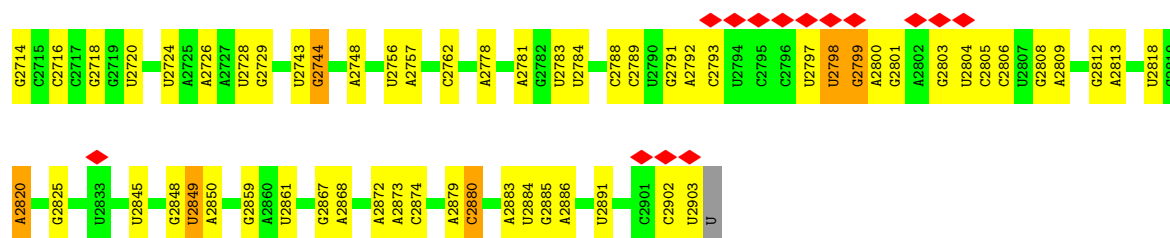




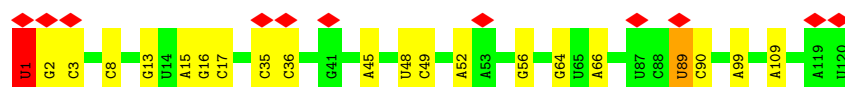
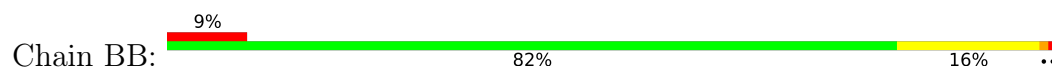
• Molecule 25: 23S ribosomal RNA



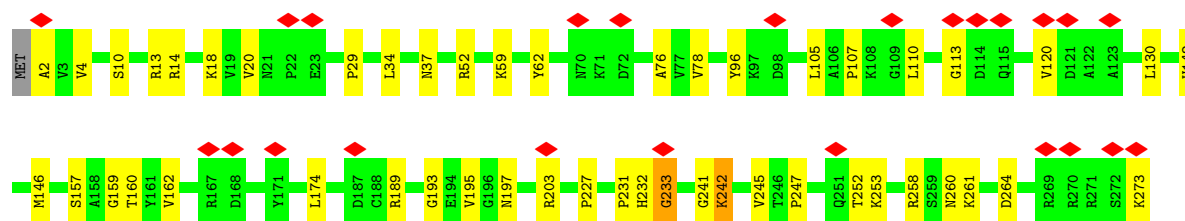
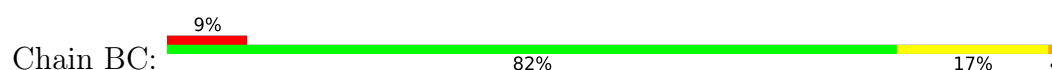




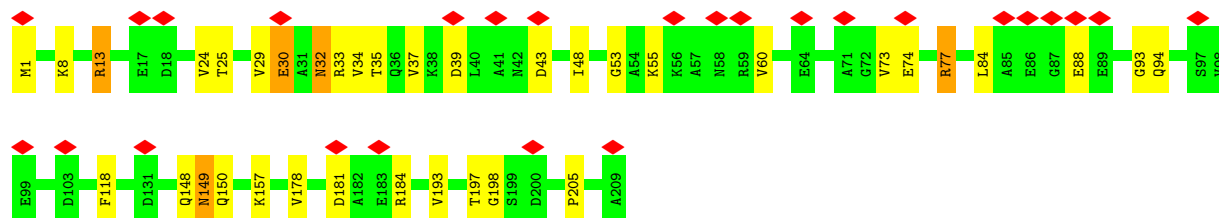
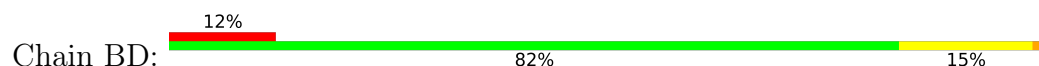
• Molecule 26: 5S ribosomal RNA



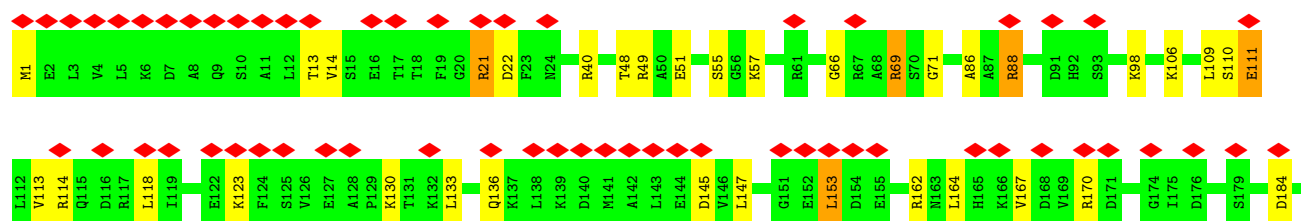
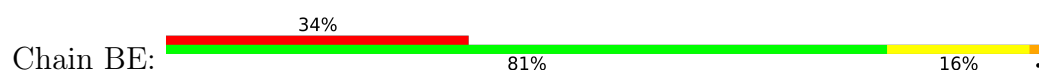
• Molecule 27: 50S ribosomal protein L2

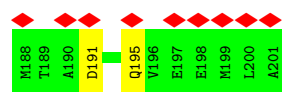


• Molecule 28: 50S ribosomal protein L3



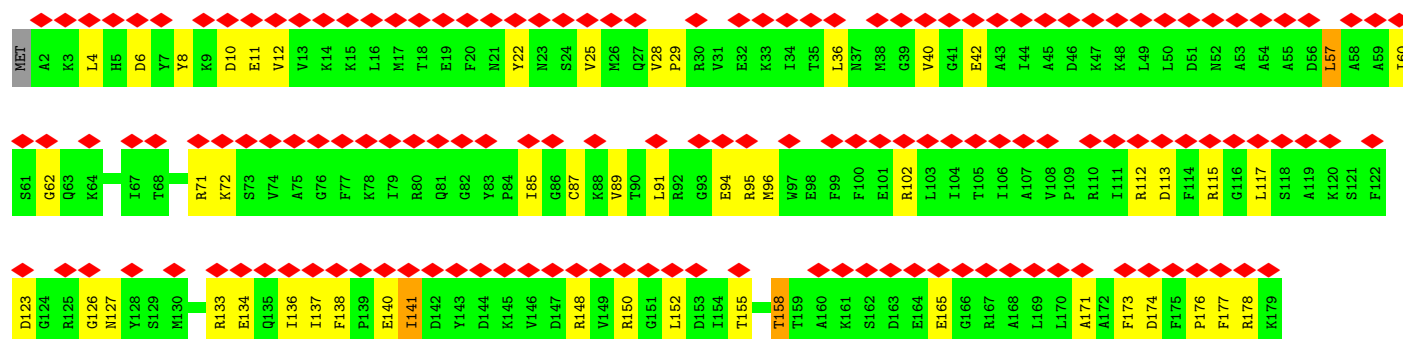
• Molecule 29: 50S ribosomal protein L4





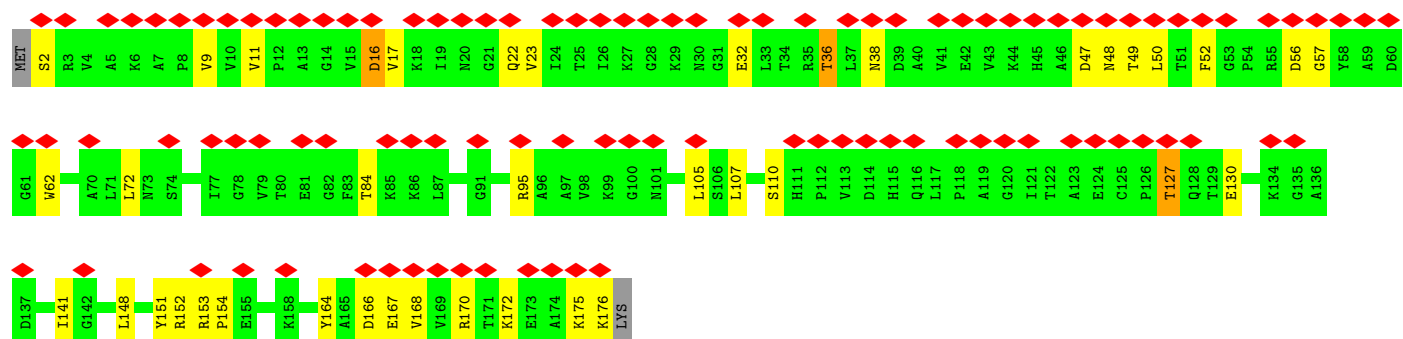
• Molecule 30: 50S ribosomal protein L5

Chain BF:



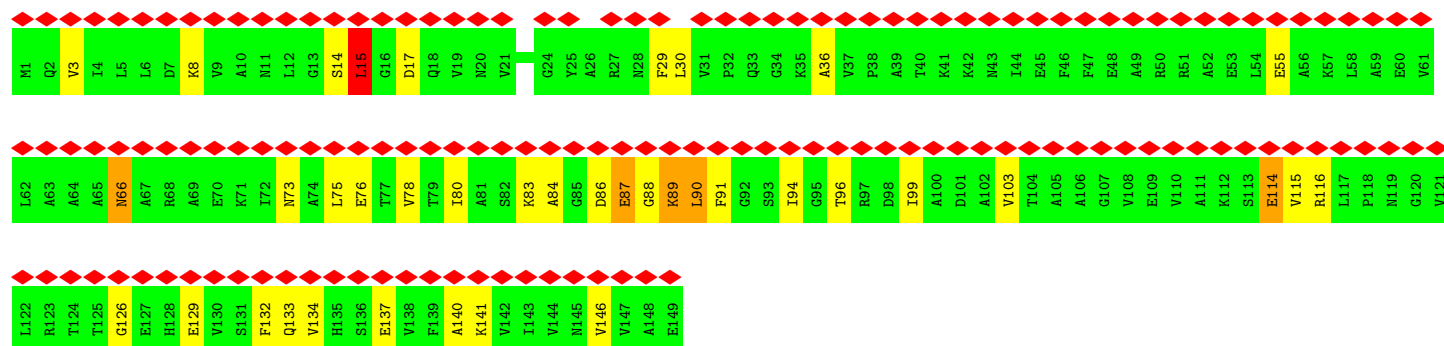
• Molecule 31: 50S ribosomal protein L6

Chain BG:

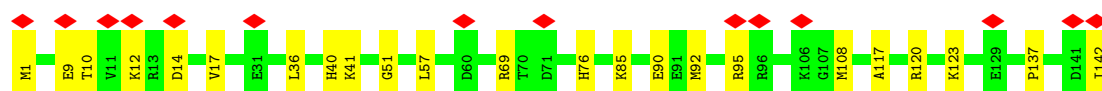
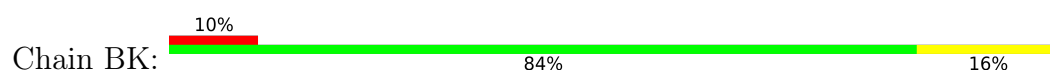


• Molecule 32: 50S ribosomal protein L9

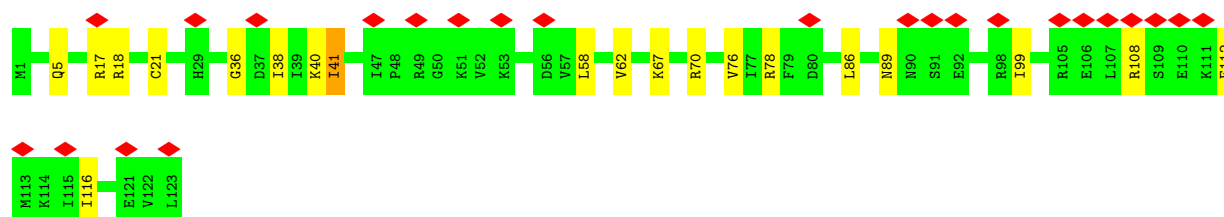
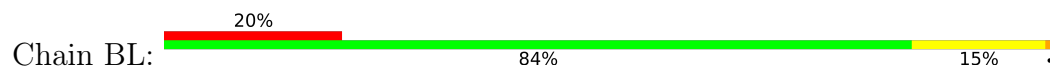
Chain BH:



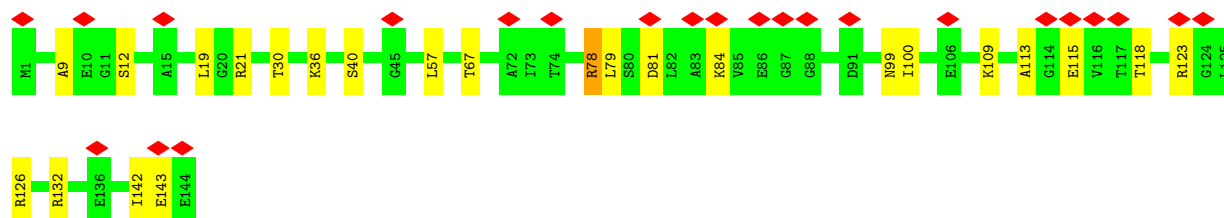
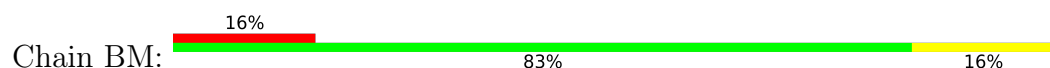
• Molecule 33: 50S ribosomal protein L13



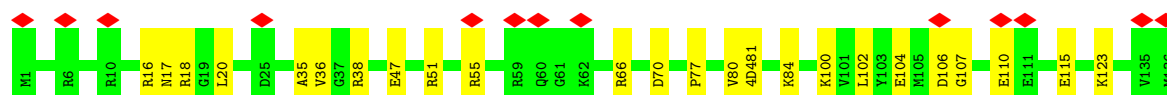
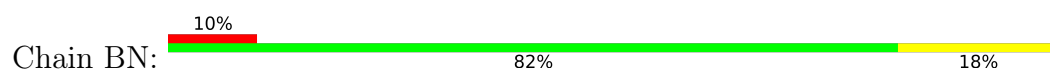
- Molecule 34: 50S ribosomal protein L14



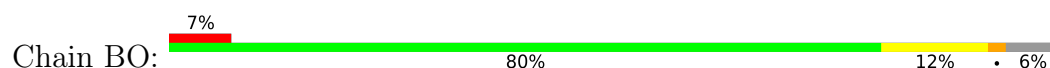
- Molecule 35: 50S ribosomal protein L15



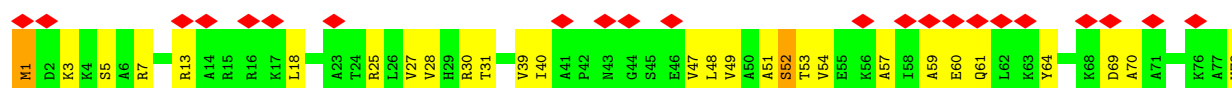
- Molecule 36: 50S ribosomal protein L16

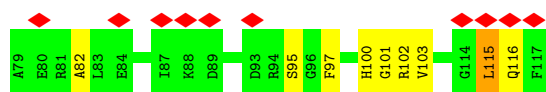


- Molecule 37: 50S ribosomal protein L17

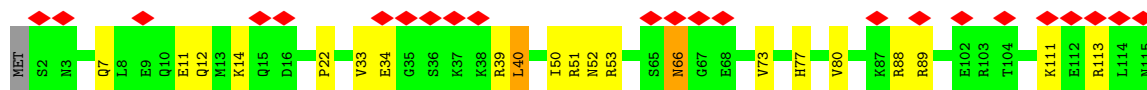
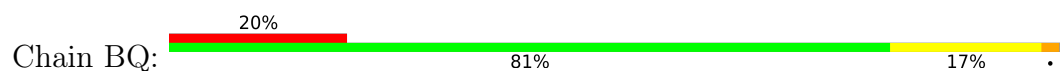


- Molecule 38: 50S ribosomal protein L18

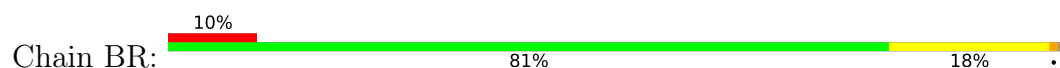




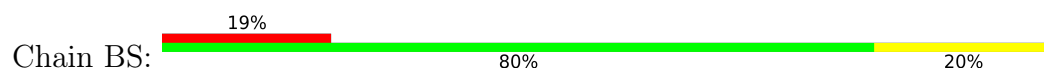
- Molecule 39: 50S ribosomal protein L19



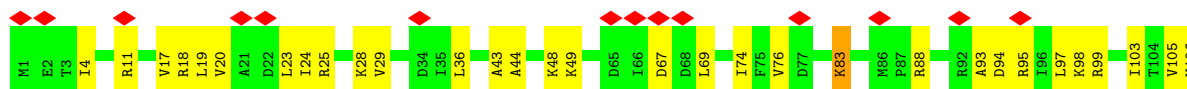
- Molecule 40: 50S ribosomal protein L20



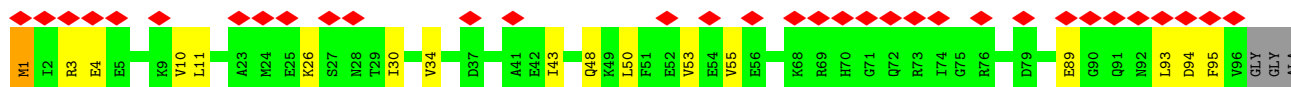
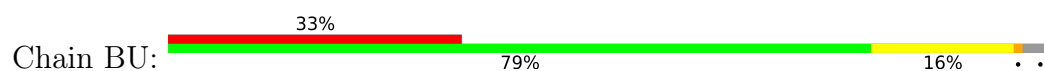
- Molecule 41: 50S ribosomal protein L21



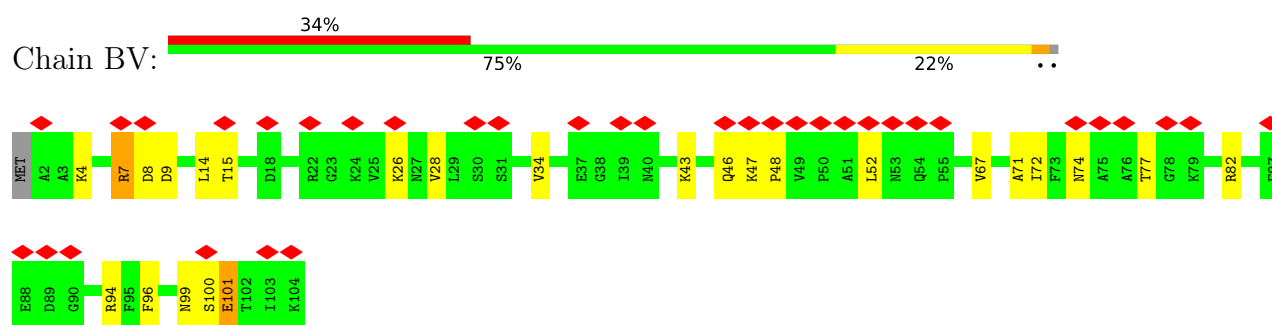
- Molecule 42: 50S ribosomal protein L22



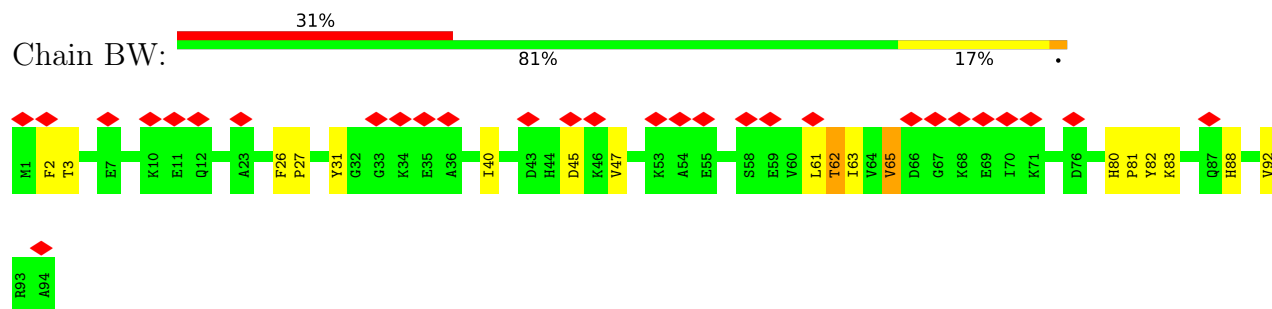
- Molecule 43: 50S ribosomal protein L23



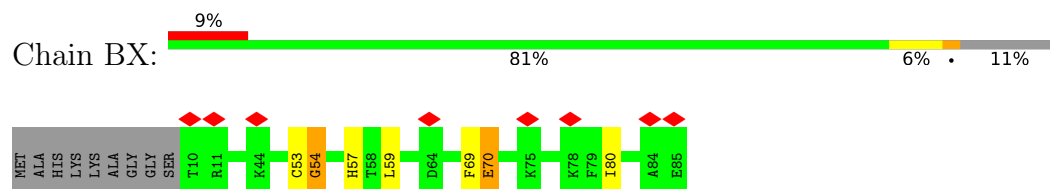
- Molecule 44: 50S ribosomal protein L24



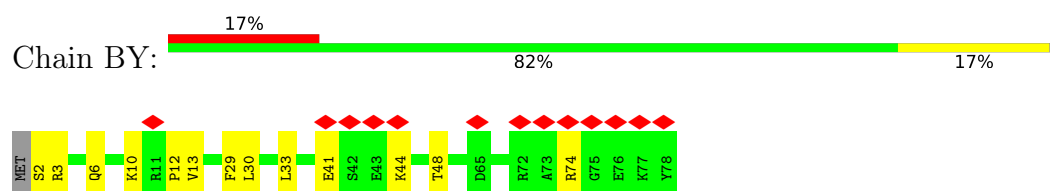
- Molecule 45: 50S ribosomal protein L25



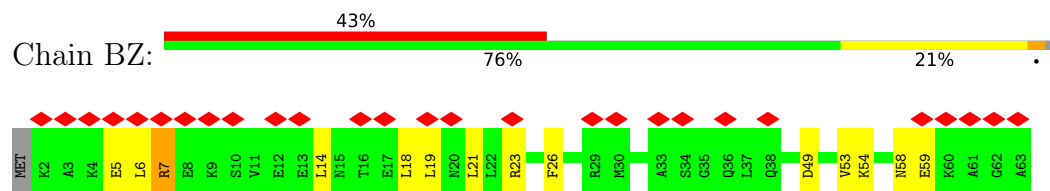
- Molecule 46: 50S ribosomal protein L27



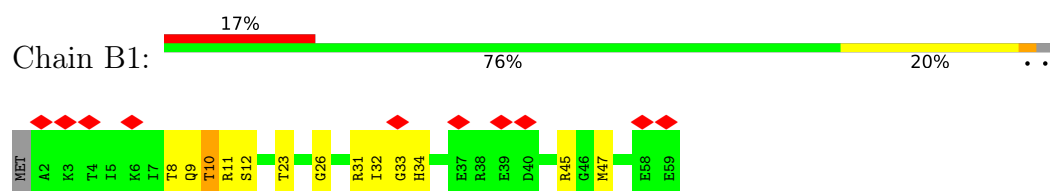
- Molecule 47: 50S ribosomal protein L28



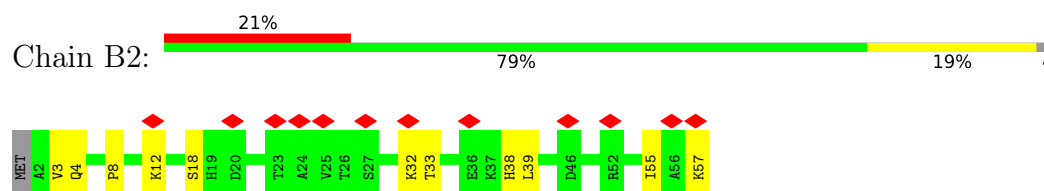
- Molecule 48: 50S ribosomal protein L29



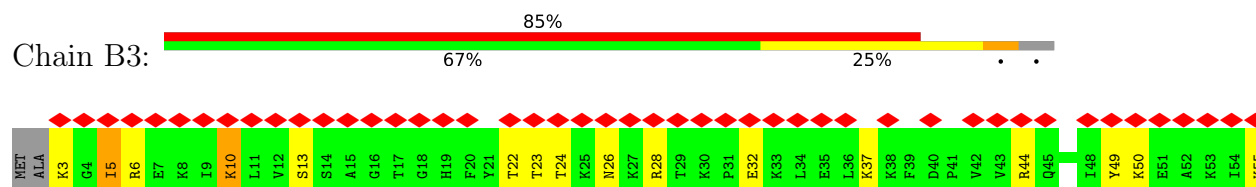
- Molecule 49: 50S ribosomal protein L30



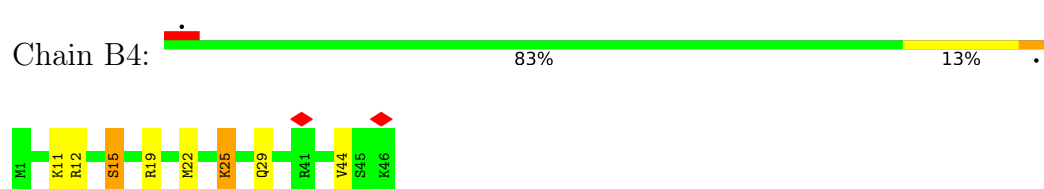
- Molecule 50: 50S ribosomal protein L32



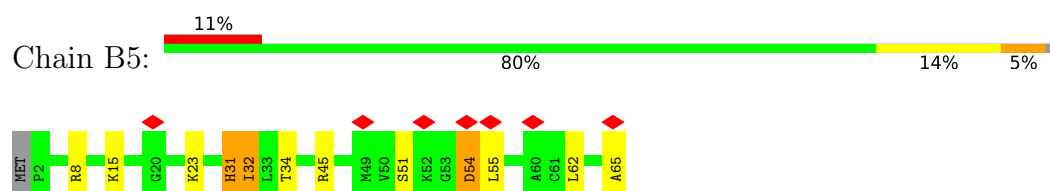
- Molecule 51: 50S ribosomal protein L33



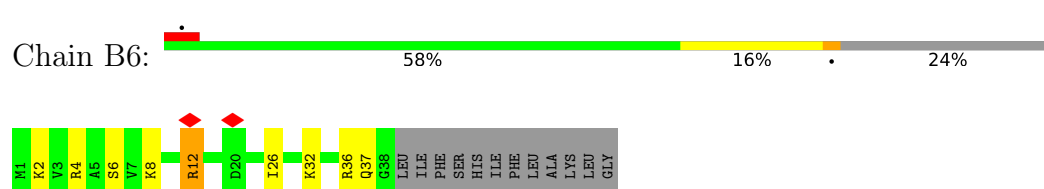
- Molecule 52: 50S ribosomal protein L34



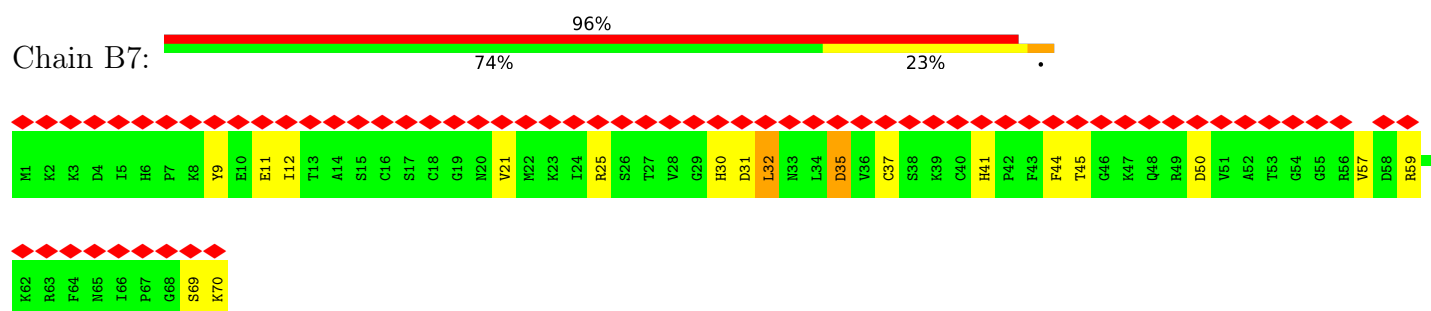
- Molecule 53: 50S ribosomal protein L35



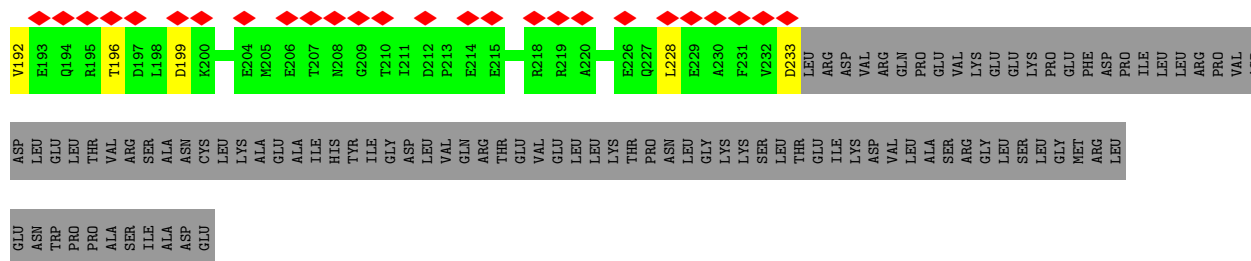
- Molecule 54: 50S ribosomal protein L36



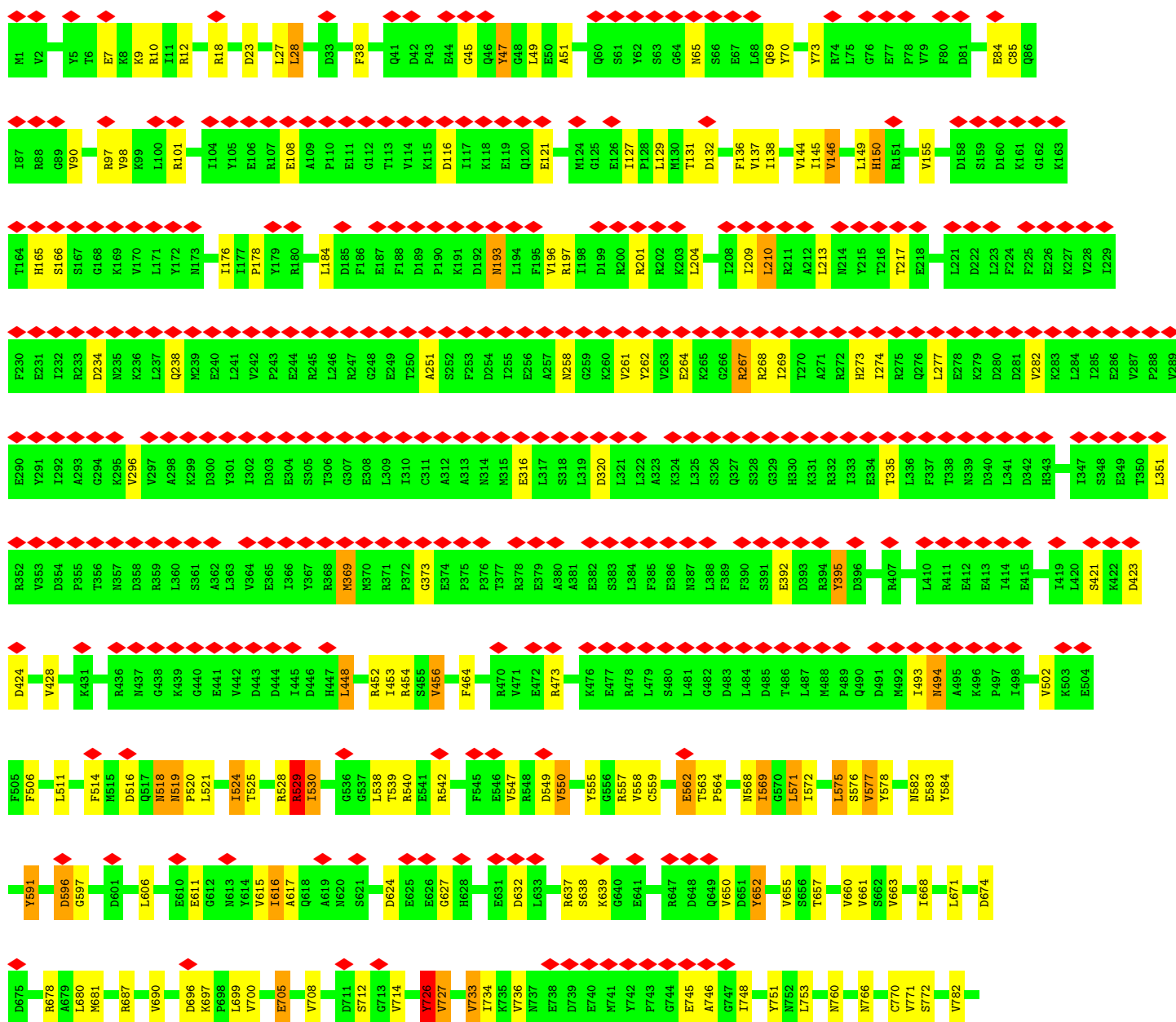
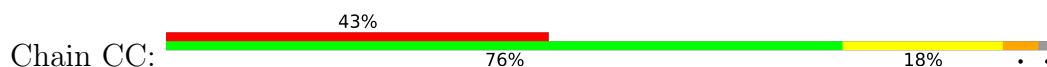
- Molecule 55: 50S ribosomal protein L31

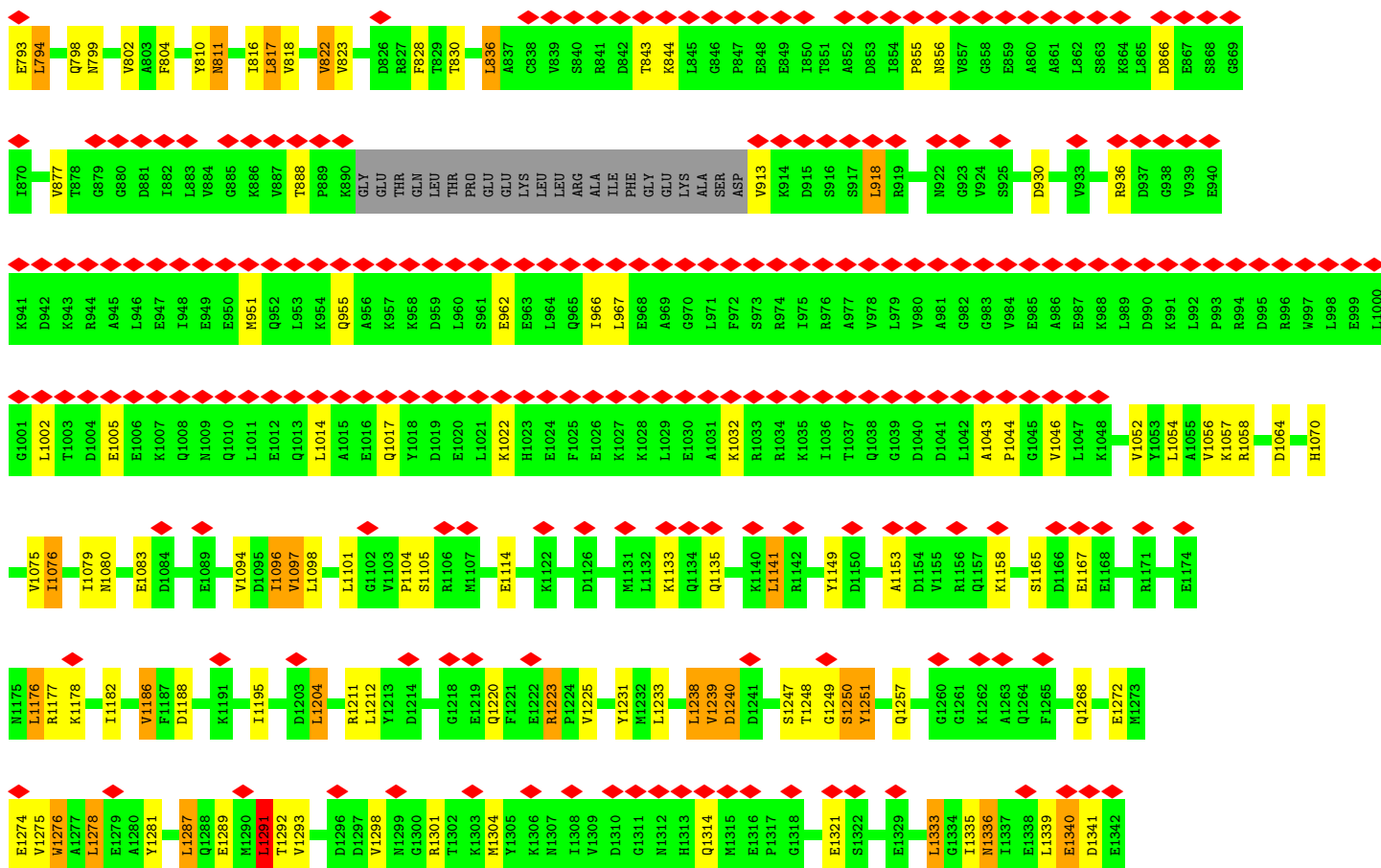


- Molecule 56: Non-template DNA strand

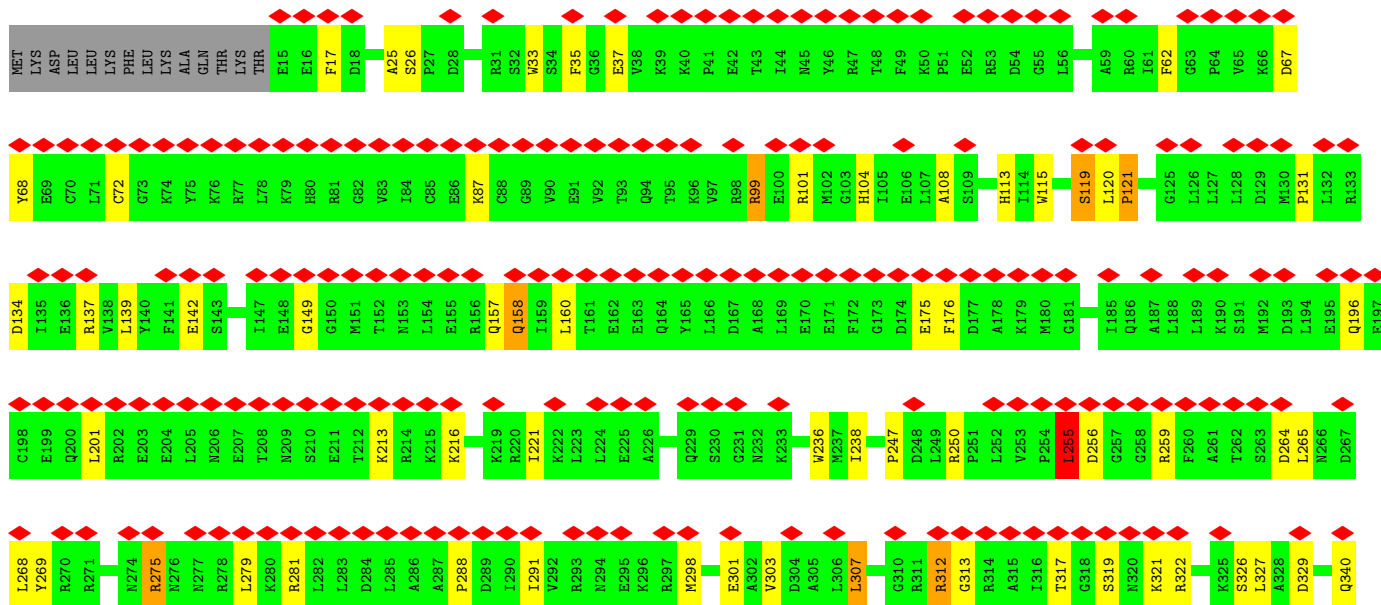
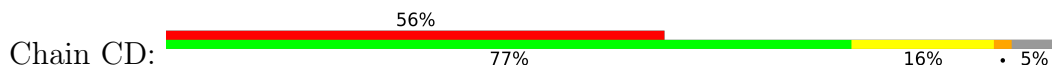


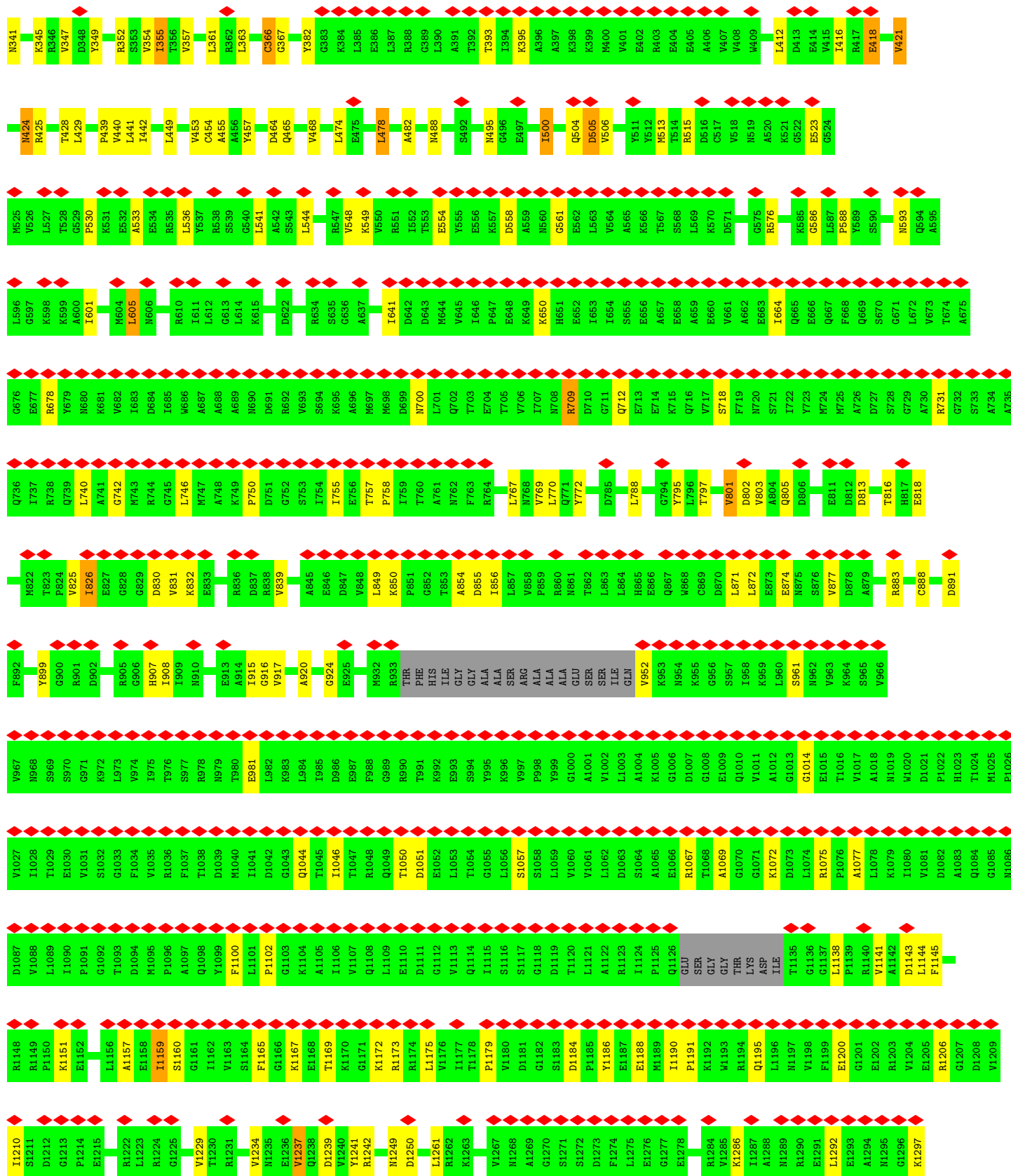
• Molecule 59: DNA-directed RNA polymerase subunit beta



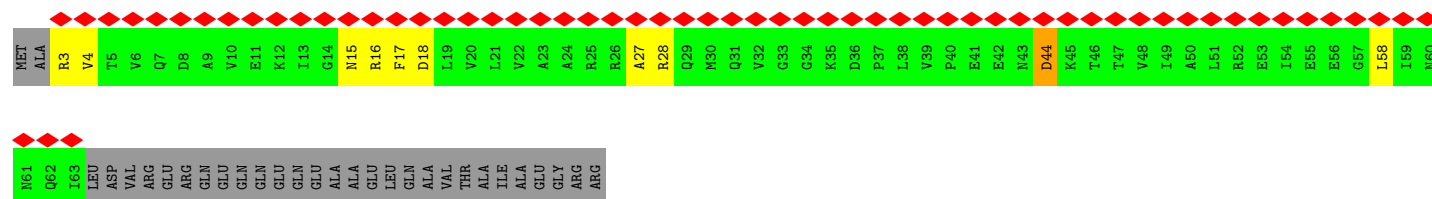


• Molecule 60: DNA-directed RNA polymerase subunit beta'





- Molecule 61: DNA-directed RNA polymerase subunit omega



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32195	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.947	Depositor
Minimum map value	-0.436	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	547.04004, 547.04004, 547.04004	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 1MG, G7M, H2U, MA6, OMG, 5MU, 3TD, 3AU, OMC, MIA, PSU, MEQ, 4OC, 7MG, 4SU, 4D4, UR3, D2T, 5MC, MG, ZN, 6MZ, 2MA, 2MG

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	AA	1.04	0/36569	0.95	44/57044 (0.1%)
2	AB	0.34	0/1796	0.53	0/2420
3	AC	0.52	0/1667	0.60	0/2246
4	AD	0.40	0/1665	0.54	0/2227
5	AE	0.45	0/1161	0.60	0/1563
6	AF	0.41	0/867	0.59	0/1171
7	AG	0.38	0/1230	0.59	2/1649 (0.1%)
8	AH	0.43	0/989	0.55	1/1326 (0.1%)
9	AI	0.56	0/1043	0.67	0/1387
10	AJ	0.50	0/810	0.69	0/1094
11	AK	0.39	0/893	0.56	0/1205
12	AL	0.48	0/954	0.68	0/1279
13	AM	0.43	0/900	0.62	1/1204 (0.1%)
14	AN	0.52	0/817	0.55	0/1088
15	AO	0.39	0/722	0.53	0/964
16	AP	0.48	0/659	0.54	0/884
17	AQ	0.45	0/657	0.59	0/881
18	AR	0.41	0/554	0.65	1/743 (0.1%)
19	AS	0.51	0/680	0.62	0/915
20	AT	0.41	0/676	0.53	0/895
21	AU	0.35	0/598	0.54	0/792
22	AV	1.98	28/637 (4.4%)	1.78	32/987 (3.2%)
23	AW	0.75	1/1725 (0.1%)	0.94	1/2687 (0.0%)
24	AX	0.58	1/1584 (0.1%)	0.84	1/2463 (0.0%)
25	BA	0.87	2/69165 (0.0%)	0.94	80/107893 (0.1%)
26	BB	0.74	0/2872	0.86	3/4478 (0.1%)
27	BC	0.46	0/2131	0.59	0/2863
28	BD	0.45	0/1576	0.57	0/2119
29	BE	0.40	0/1571	0.60	2/2113 (0.1%)
30	BF	0.35	0/1444	0.53	0/1937
31	BG	0.37	0/1333	0.57	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BH	0.29	0/1122	0.62	1/1515 (0.1%)
33	BK	0.43	0/1152	0.53	0/1551
34	BL	0.44	0/956	0.62	0/1279
35	BM	0.41	0/1061	0.62	0/1412
36	BN	0.41	0/1081	0.55	0/1443
37	BO	0.45	0/973	0.61	0/1301
38	BP	0.38	0/910	0.59	0/1219
39	BQ	0.43	0/929	0.56	0/1242
40	BR	0.51	0/960	0.56	0/1278
41	BS	0.44	0/829	0.62	0/1107
42	BT	0.41	0/864	0.60	0/1156
43	BU	0.38	0/771	0.53	0/1031
44	BV	0.38	0/797	0.53	0/1062
45	BW	0.40	0/766	0.56	0/1025
46	BX	0.43	0/589	0.52	0/779
47	BY	0.43	0/635	0.53	0/848
48	BZ	0.32	0/502	0.53	0/667
49	B1	0.37	0/453	0.56	0/605
50	B2	0.43	0/450	0.60	0/599
51	B3	0.34	0/443	0.61	0/587
52	B4	0.42	0/379	0.55	0/496
53	B5	0.40	0/513	0.62	0/676
54	B6	0.46	0/302	0.58	0/397
55	B7	0.31	0/559	0.67	0/745
56	CN	1.77	12/693 (1.7%)	1.24	3/1068 (0.3%)
57	CT	2.53	38/676 (5.6%)	1.33	9/1039 (0.9%)
58	CA	1.13	7/1797 (0.4%)	0.91	2/2436 (0.1%)
58	CB	0.80	1/1703 (0.1%)	0.86	3/2308 (0.1%)
59	CC	1.41	120/10581 (1.1%)	0.97	31/14275 (0.2%)
60	CD	1.12	58/10532 (0.6%)	0.91	15/14219 (0.1%)
61	CE	0.55	0/480	0.73	0/647
All	All	0.90	268/184403 (0.1%)	0.88	232/272334 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
5	AE	0	1
13	AM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	AV	0	1
25	BA	0	1
37	BO	0	1
46	BX	0	1
53	B5	0	1
All	All	0	8

The worst 5 of 268 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	1	C	OP3-P	-10.67	1.48	1.61
24	AX	1	G	OP3-P	-10.59	1.48	1.61
57	CT	18	DC	C3'-O3'	-10.26	1.30	1.44
60	CD	1357	ILE	C-N	-9.72	1.15	1.34
57	CT	14	DC	C3'-O3'	-9.51	1.31	1.44

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1027	C	C2-N1-C1'	12.29	132.32	118.80
57	CT	19	DG	O4'-C1'-N9	10.11	115.07	108.00
1	AA	1027	C	C6-N1-C1'	-9.76	109.09	120.80
22	AV	52	C	C6-N1-C2	-9.48	116.51	120.30
1	AA	812	G	O4'-C1'-N9	9.05	115.44	108.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1034	G	Sidechain
5	AE	89	HIS	Peptide
13	AM	65	VAL	Peptide
22	AV	45	C	Sidechain
25	BA	138	U	Sidechain

5.2 Too-close contacts

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	AA	32909	0	16580	275	0
2	AB	1765	0	1792	36	0
3	AC	1640	0	1713	27	0
4	AD	1643	0	1707	31	0
5	AE	1148	0	1195	19	0
6	AF	848	0	846	29	0
7	AG	1214	0	1267	18	0
8	AH	979	0	1031	10	0
9	AI	1031	0	1076	30	0
10	AJ	800	0	839	28	0
11	AK	877	0	887	25	0
12	AL	951	0	1012	25	0
13	AM	891	0	952	21	0
14	AN	805	0	844	13	0
15	AO	714	0	734	11	0
16	AP	649	0	666	8	0
17	AQ	648	0	691	6	0
18	AR	545	0	560	5	0
19	AS	663	0	688	11	0
20	AT	670	0	719	11	0
21	AU	590	0	629	12	0
22	AV	572	0	294	20	0
23	AW	1645	0	842	13	0
24	AX	1630	0	838	30	0
25	BA	62270	0	31335	443	0
26	BB	2569	0	1301	9	0
27	BC	2092	0	2167	32	0
28	BD	1566	0	1618	24	0
29	BE	1552	0	1618	23	0
30	BF	1420	0	1457	32	0
31	BG	1313	0	1358	20	0
32	BH	1111	0	1148	31	0
33	BK	1129	0	1162	10	0
34	BL	947	0	1023	11	0
35	BM	1052	0	1127	11	0
36	BN	1075	0	1155	13	0
37	BO	960	0	1000	12	0
38	BP	900	0	935	22	0
39	BQ	917	0	962	13	0
40	BR	947	0	1019	16	0
41	BS	816	0	839	10	0
42	BT	857	0	922	26	0
43	BU	764	0	829	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	789	0	843	14	0
45	BW	753	0	780	11	0
46	BX	582	0	598	4	0
47	BY	625	0	652	6	0
48	BZ	501	0	531	8	0
49	B1	449	0	488	6	0
50	B2	444	0	458	7	0
51	B3	436	0	477	13	0
52	B4	376	0	414	7	0
53	B5	504	0	572	9	0
54	B6	301	0	340	4	0
55	B7	549	0	551	14	0
56	CN	618	0	339	29	0
57	CT	606	0	338	37	0
58	CA	1775	0	1800	17	0
58	CB	1684	0	1713	19	0
59	CC	10415	0	10432	164	0
60	CD	10375	0	10597	147	0
61	CE	478	0	496	7	0
62	AA	143	0	0	0	0
62	AI	1	0	0	0	0
62	AL	1	0	0	0	0
62	AM	1	0	0	0	0
62	AW	5	0	0	0	0
62	AX	1	0	0	0	0
62	BA	317	0	0	0	0
62	BB	9	0	0	0	0
62	BC	3	0	0	0	0
62	BN	1	0	0	0	0
62	BO	1	0	0	0	0
62	BQ	1	0	0	0	0
62	BV	1	0	0	0	0
62	BX	1	0	0	0	0
62	CD	1	0	0	0	0
63	AX	11	0	8	1	0
64	B6	1	0	0	0	0
64	B7	1	0	0	0	0
64	CD	2	0	0	0	0
All	All	172846	0	123804	1795	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 6.

The worst 5 of 1795 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)
25:BA:2285:C:OP2	51:B3:6:ARG:NH1	1.99	0.94
1:AA:481:G:O2'	1:AA:483:C:N4	2.01	0.93
25:BA:1936:A:H2	25:BA:1943:U:H3	1.16	0.92
1:AA:411:A:H4'	1:AA:412:A:H5'	1.53	0.90
18:AR:36:SER:HA	18:AR:72:ASP:HB2	1.52	0.90

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	AB	224/241 (93%)	210 (94%)	13 (6%)	1 (0%)	34	72
3	AC	207/233 (89%)	197 (95%)	6 (3%)	4 (2%)	8	36
4	AD	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	29	68
5	AE	154/167 (92%)	145 (94%)	7 (4%)	2 (1%)	12	45
6	AF	102/131 (78%)	97 (95%)	5 (5%)	0	100	100
7	AG	152/156 (97%)	144 (95%)	6 (4%)	2 (1%)	12	45
8	AH	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	126/130 (97%)	111 (88%)	12 (10%)	3 (2%)	6	29
10	AJ	98/103 (95%)	90 (92%)	5 (5%)	3 (3%)	4	23
11	AK	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	17	55
12	AL	119/124 (96%)	109 (92%)	8 (7%)	2 (2%)	9	39
13	AM	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	AP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	AQ	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
18	AR	64/75 (85%)	61 (95%)	2 (3%)	1 (2%)	9	40
19	AS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	AU	68/71 (96%)	68 (100%)	0	0	100	100
27	BC	270/273 (99%)	249 (92%)	18 (7%)	3 (1%)	14	50
28	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	68
29	BE	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
30	BF	176/179 (98%)	163 (93%)	10 (6%)	3 (2%)	9	39
31	BG	173/177 (98%)	159 (92%)	13 (8%)	1 (1%)	25	64
32	BH	147/149 (99%)	134 (91%)	10 (7%)	3 (2%)	7	34
33	BK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	BL	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
35	BM	142/144 (99%)	132 (93%)	8 (6%)	2 (1%)	11	43
36	BN	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
37	BO	118/127 (93%)	108 (92%)	10 (8%)	0	100	100
38	BP	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	17	55
39	BQ	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
40	BR	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
41	BS	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15	53
42	BT	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	BU	94/100 (94%)	88 (94%)	5 (5%)	1 (1%)	14	50
44	BV	101/104 (97%)	97 (96%)	3 (3%)	1 (1%)	15	53
45	BW	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	BX	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
47	BY	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	BZ	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
49	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	B2	54/57 (95%)	54 (100%)	0	0	100	100
51	B3	51/55 (93%)	47 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	B4	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
53	B5	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	9	40
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
55	B7	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
58	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
58	CB	215/329 (65%)	204 (95%)	10 (5%)	1 (0%)	29	68
59	CC	1316/1342 (98%)	1196 (91%)	111 (8%)	9 (1%)	22	60
60	CD	1327/1407 (94%)	1222 (92%)	95 (7%)	10 (1%)	19	57
61	CE	59/91 (65%)	53 (90%)	4 (7%)	2 (3%)	3	20
All	All	8766/9396 (93%)	8198 (94%)	508 (6%)	60 (1%)	26	60

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AG	56	LYS
9	AI	56	ASP
10	AJ	57	VAL
11	AK	93	ARG
12	AL	88	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	187/199 (94%)	174 (93%)	13 (7%)	15	47
3	AC	171/190 (90%)	161 (94%)	10 (6%)	20	55
4	AD	172/173 (99%)	162 (94%)	10 (6%)	20	55
5	AE	118/126 (94%)	110 (93%)	8 (7%)	16	48
6	AF	91/112 (81%)	85 (93%)	6 (7%)	16	49
7	AG	127/129 (98%)	119 (94%)	8 (6%)	18	51
8	AH	104/105 (99%)	97 (93%)	7 (7%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AI	106/107 (99%)	101 (95%)	5 (5%)	26	63
10	AJ	87/90 (97%)	78 (90%)	9 (10%)	7	28
11	AK	90/99 (91%)	82 (91%)	8 (9%)	9	35
12	AL	102/103 (99%)	95 (93%)	7 (7%)	15	48
13	AM	93/96 (97%)	88 (95%)	5 (5%)	22	57
14	AN	83/84 (99%)	78 (94%)	5 (6%)	19	53
15	AO	76/77 (99%)	73 (96%)	3 (4%)	32	69
16	AP	65/65 (100%)	61 (94%)	4 (6%)	18	52
17	AQ	74/78 (95%)	70 (95%)	4 (5%)	22	57
18	AR	57/65 (88%)	54 (95%)	3 (5%)	22	58
19	AS	72/79 (91%)	71 (99%)	1 (1%)	67	88
20	AT	65/66 (98%)	59 (91%)	6 (9%)	9	34
21	AU	60/61 (98%)	54 (90%)	6 (10%)	7	29
27	BC	217/218 (100%)	212 (98%)	5 (2%)	50	80
28	BD	163/163 (100%)	155 (95%)	8 (5%)	25	61
29	BE	165/165 (100%)	155 (94%)	10 (6%)	18	53
30	BF	149/150 (99%)	139 (93%)	10 (7%)	16	49
31	BG	136/138 (99%)	124 (91%)	12 (9%)	10	36
32	BH	114/114 (100%)	106 (93%)	8 (7%)	15	47
33	BK	116/116 (100%)	111 (96%)	5 (4%)	29	66
34	BL	104/104 (100%)	98 (94%)	6 (6%)	20	55
35	BM	103/103 (100%)	95 (92%)	8 (8%)	12	42
36	BN	108/108 (100%)	102 (94%)	6 (6%)	21	56
37	BO	100/103 (97%)	95 (95%)	5 (5%)	24	60
38	BP	87/87 (100%)	81 (93%)	6 (7%)	15	48
39	BQ	99/100 (99%)	92 (93%)	7 (7%)	14	46
40	BR	89/90 (99%)	84 (94%)	5 (6%)	21	56
41	BS	84/84 (100%)	79 (94%)	5 (6%)	19	53
42	BT	93/93 (100%)	87 (94%)	6 (6%)	17	50
43	BU	83/84 (99%)	79 (95%)	4 (5%)	25	62
44	BV	84/85 (99%)	78 (93%)	6 (7%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BW	78/78 (100%)	74 (95%)	4 (5%)	24	60
46	BX	58/63 (92%)	57 (98%)	1 (2%)	60	85
47	BY	67/68 (98%)	64 (96%)	3 (4%)	27	64
48	BZ	54/55 (98%)	51 (94%)	3 (6%)	21	56
49	B1	48/49 (98%)	45 (94%)	3 (6%)	18	51
50	B2	47/48 (98%)	46 (98%)	1 (2%)	53	82
51	B3	48/49 (98%)	43 (90%)	5 (10%)	7	27
52	B4	37/38 (97%)	34 (92%)	3 (8%)	11	40
53	B5	51/52 (98%)	47 (92%)	4 (8%)	12	42
54	B6	34/44 (77%)	30 (88%)	4 (12%)	5	22
55	B7	62/62 (100%)	59 (95%)	3 (5%)	25	62
58	CA	197/286 (69%)	193 (98%)	4 (2%)	55	83
58	CB	187/286 (65%)	177 (95%)	10 (5%)	22	58
59	CC	1139/1157 (98%)	1097 (96%)	42 (4%)	34	70
60	CD	1118/1168 (96%)	1097 (98%)	21 (2%)	57	84
61	CE	52/75 (69%)	48 (92%)	4 (8%)	13	42
All	All	7371/7787 (95%)	7006 (95%)	365 (5%)	28	60

5 of 365 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BS	39	LEU
58	CA	101	THR
42	BT	109	ASP
48	BZ	59	GLU
59	CC	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
44	BV	54	GLN
44	BV	74	ASN
32	BH	73	ASN
41	BS	43	ASN
43	BU	48	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	292 (19%)	28 (1%)
22	AV	25/53 (47%)	9 (36%)	1 (4%)
23	AW	76/77 (98%)	22 (28%)	8 (10%)
24	AX	73/76 (96%)	16 (21%)	1 (1%)
25	BA	2895/2904 (99%)	557 (19%)	65 (2%)
26	BB	120/120 (100%)	12 (10%)	1 (0%)
All	All	4718/4772 (98%)	908 (19%)	104 (2%)

5 of 908 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	29	U

5 of 104 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	984	A
25	BA	1379	U
25	BA	2756	U
25	BA	1060	U
25	BA	1111	A

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

53 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
25	2MG	BA	2445	29,25	18,26,27	2.24	7 (38%)	16,38,41	1.75	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	H2U	AX	20	24	18,21,22	3.12	5 (27%)	21,30,33	1.95	5 (23%)
1	MA6	AA	1518	1	18,26,27	1.33	3 (16%)	19,38,41	4.05	2 (10%)
24	PSU	AX	32	24	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
1	2MG	AA	1207	1,62	18,26,27	2.32	7 (38%)	16,38,41	1.72	4 (25%)
25	H2U	BA	2449	25	18,21,22	2.85	5 (27%)	21,30,33	2.13	5 (23%)
1	2MG	AA	1516	1	18,26,27	2.27	7 (38%)	16,38,41	1.64	4 (25%)
24	PSU	AX	39	24	18,21,22	1.05	1 (5%)	22,30,33	1.85	5 (22%)
24	MIA	AX	37	24	22,29,32	2.86	4 (18%)	22,41,47	2.73	7 (31%)
25	OMC	BA	2498	62,25	19,22,23	2.81	7 (36%)	26,31,34	0.96	1 (3%)
25	2MA	BA	2503	62,25	17,25,26	2.59	7 (41%)	17,37,40	1.52	4 (23%)
23	5MU	AW	54	23	19,22,23	1.39	5 (26%)	28,32,35	2.11	6 (21%)
25	5MU	BA	1939	62,25	19,22,23	1.46	4 (21%)	28,32,35	2.32	6 (21%)
1	PSU	AA	516	1	18,21,22	1.14	2 (11%)	22,30,33	2.15	6 (27%)
24	3AU	AX	47	24	18,21,29	3.43	8 (44%)	26,30,43	1.72	5 (19%)
23	OMC	AW	32	23	19,22,23	2.81	8 (42%)	26,31,34	0.78	0
25	3TD	BA	1915	25	18,22,23	4.42	10 (55%)	22,32,35	2.19	4 (18%)
1	UR3	AA	1498	1	19,22,23	2.50	6 (31%)	26,32,35	1.25	2 (7%)
25	5MC	BA	1962	25	18,22,23	3.75	7 (38%)	26,32,35	1.08	4 (15%)
25	PSU	BA	2457	25	18,21,22	1.12	2 (11%)	22,30,33	2.00	5 (22%)
25	1MG	BA	745	25	18,26,27	2.60	5 (27%)	19,39,42	1.45	3 (15%)
1	5MC	AA	967	1	18,22,23	3.75	7 (38%)	26,32,35	1.04	2 (7%)
25	PSU	BA	955	25	18,21,22	1.11	2 (11%)	22,30,33	1.94	5 (22%)
1	5MC	AA	1407	1	18,22,23	3.77	7 (38%)	26,32,35	1.07	2 (7%)
25	PSU	BA	1911	25	18,21,22	1.09	1 (5%)	22,30,33	1.85	4 (18%)
23	H2U	AW	20	23	18,21,22	3.00	5 (27%)	21,30,33	2.25	6 (28%)
24	7MG	AX	46	24	22,26,27	3.86	10 (45%)	29,39,42	2.00	9 (31%)
25	OMU	BA	2552	25	19,22,23	2.83	7 (36%)	26,31,34	1.76	4 (15%)
25	PSU	BA	2605	25	18,21,22	1.08	2 (11%)	22,30,33	1.90	4 (18%)
25	5MU	BA	747	25	19,22,23	1.40	4 (21%)	28,32,35	2.28	6 (21%)
1	2MG	AA	966	1	18,26,27	2.30	7 (38%)	16,38,41	1.75	5 (31%)
1	G7M	AA	527	1	20,26,27	2.17	8 (40%)	17,39,42	1.32	2 (11%)
23	PSU	AW	55	23	18,21,22	1.07	1 (5%)	22,30,33	1.86	6 (27%)
25	6MZ	BA	2030	25	18,25,26	1.92	2 (11%)	16,36,39	2.50	3 (18%)
24	H2U	AX	16	24	18,21,22	3.02	5 (27%)	21,30,33	2.05	5 (23%)
24	PSU	AX	55	24	18,21,22	1.05	1 (5%)	22,30,33	1.87	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	BA	2580	25	18,21,22	1.09	3 (16%)	22,30,33	2.07	6 (27%)
28	MEQ	BD	150	28	8,9,10	0.89	0	5,10,12	0.55	0
25	G7M	BA	2069	25	20,26,27	2.28	8 (40%)	17,39,42	1.31	3 (17%)
23	4SU	AW	8	23	18,21,22	4.08	8 (44%)	26,30,33	2.30	5 (19%)
1	4OC	AA	1402	1,62	20,23,24	3.24	9 (45%)	26,32,35	0.97	1 (3%)
25	PSU	BA	1917	25	18,21,22	1.07	2 (11%)	22,30,33	1.87	5 (22%)
25	2MG	BA	1835	25	18,26,27	2.26	7 (38%)	16,38,41	1.79	4 (25%)
24	4SU	AX	8	24	18,21,22	4.08	8 (44%)	26,30,33	2.34	5 (19%)
36	4D4	BN	81	36	9,11,12	2.51	3 (33%)	8,13,15	0.83	0
25	OMG	BA	2251	25,23	18,26,27	2.56	8 (44%)	19,38,41	1.54	4 (21%)
12	D2T	AL	89	12	7,9,10	1.01	0	6,11,13	2.45	4 (66%)
24	5MU	AX	54	24	19,22,23	1.36	5 (26%)	28,32,35	2.06	7 (25%)
25	6MZ	BA	1618	25	18,25,26	1.86	3 (16%)	16,36,39	2.37	4 (25%)
25	PSU	BA	2604	25	18,21,22	1.05	1 (5%)	22,30,33	1.91	5 (22%)
25	PSU	BA	2504	25	18,21,22	1.04	1 (5%)	22,30,33	1.91	4 (18%)
1	MA6	AA	1519	1	18,26,27	1.33	3 (16%)	19,38,41	4.10	2 (10%)
25	PSU	BA	746	62,25	18,21,22	1.07	3 (16%)	22,30,33	1.97	7 (31%)

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
25	2MG	BA	2445	29,25	-	2/5/27/28	0/3/3/3
24	H2U	AX	20	24	-	3/7/38/39	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1,62	-	1/5/27/28	0/3/3/3
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	4/9/31/34	0/3/3/3
25	OMC	BA	2498	62,25	-	2/9/27/28	0/2/2/2
25	2MA	BA	2503	62,25	-	2/3/25/26	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
25	5MU	BA	1939	62,25	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	516	1	-	2/7/25/26	0/2/2/2
24	3AU	AX	47	24	-	2/7/25/35	0/2/2/2
23	OMC	AW	32	23	-	0/9/27/28	0/2/2/2
25	3TD	BA	1915	25	-	2/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
25	5MC	BA	1962	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
25	PSU	BA	955	25	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
23	H2U	AW	20	23	-	2/7/38/39	0/2/2/2
24	7MG	AX	46	24	-	3/7/37/38	0/3/3/3
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2
25	PSU	BA	2605	25	-	0/7/25/26	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
24	H2U	AX	16	24	-	3/7/38/39	0/2/2/2
24	PSU	AX	55	24	-	1/7/25/26	0/2/2/2
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
28	MEQ	BD	150	28	-	2/8/9/11	-
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1,62	-	0/9/29/30	0/2/2/2
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/5/27/28	0/3/3/3
24	4SU	AX	8	24	-	2/7/25/26	0/2/2/2
36	4D4	BN	81	36	-	7/11/12/14	-
25	OMG	BA	2251	25,23	-	1/5/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
25	6MZ	BA	1618	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	2504	25	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
25	PSU	BA	746	62,25	-	2/7/25/26	0/2/2/2

The worst 5 of 252 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.77	1.49	1.35
24	AX	37	MIA	C13-C14	9.69	1.60	1.32
25	BA	1915	3TD	C2-N1	9.63	1.49	1.37
1	AA	1407	5MC	C6-C5	9.59	1.50	1.34
24	AX	20	H2U	C2-N1	9.57	1.49	1.35

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-16.64	99.54	117.06
1	AA	1518	MA6	N1-C6-N6	-16.52	99.67	117.06
24	AX	8	4SU	C4-N3-C2	-8.27	119.31	127.34
24	AX	37	MIA	C12-C13-C14	-8.16	111.27	127.14
23	AW	8	4SU	C4-N3-C2	-8.08	119.49	127.34

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
24	AX	37	MIA	C12-C13-C14-C15
24	AX	37	MIA	C12-C13-C14-C16

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1516	2MG	1	0
24	AX	37	MIA	3	0
25	BA	2503	2MA	1	0
25	BA	1915	3TD	1	0
1	AA	1498	UR3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	967	5MC	1	0
23	AW	20	H2U	2	0
25	BA	2605	PSU	1	0
1	AA	966	2MG	2	0
1	AA	527	G7M	2	0
23	AW	55	PSU	1	0
25	BA	2030	6MZ	1	0
24	AX	16	H2U	3	0
28	BD	150	MEQ	2	0
25	BA	2069	G7M	2	0
25	BA	1917	PSU	3	0
24	AX	8	4SU	1	0
25	BA	2251	OMG	1	0
12	AL	89	D2T	2	0
24	AX	54	5MU	1	0
1	AA	1519	MA6	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 492 ligands modelled in this entry, 491 are monoatomic - leaving 1 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	$\# Z > 2$
63	PHE	AX	101	24	10,11,12	0.62	0	10,13,15	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PHE	AX	101	24	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	AX	101	PHE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
60	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.15

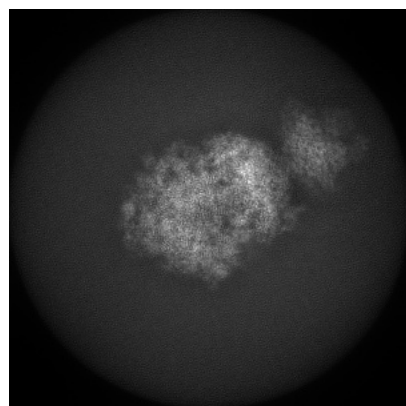
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11422. These allow visual inspection of the internal detail of the map and identification of artifacts.

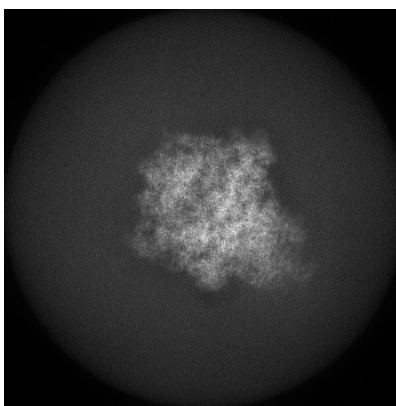
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

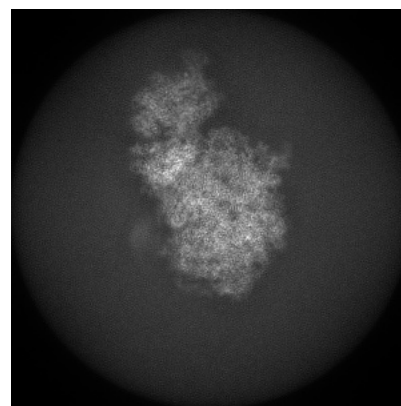
6.1.1 Primary map



X

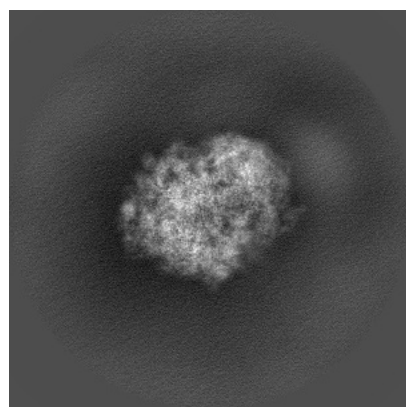


Y

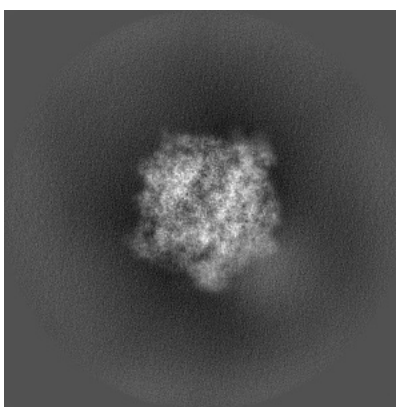


Z

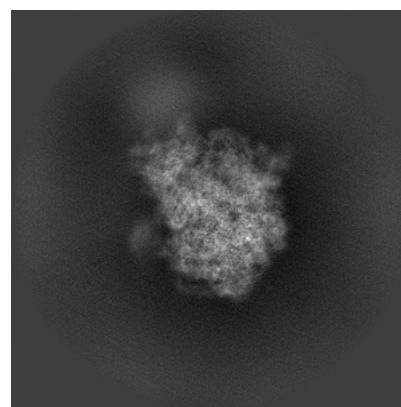
6.1.2 Raw map



X



Y

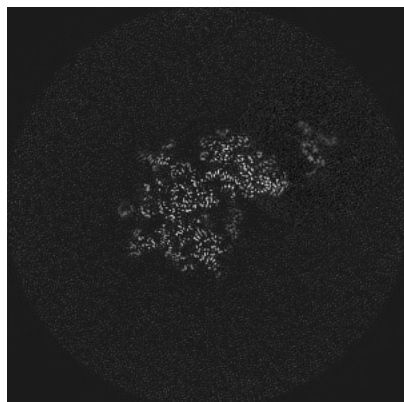


Z

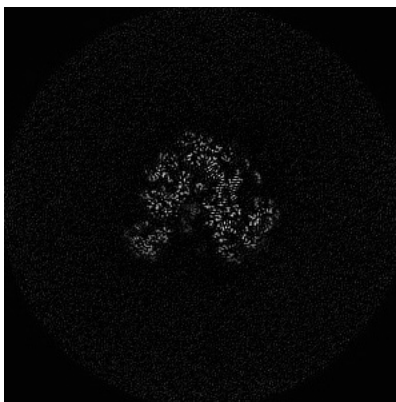
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

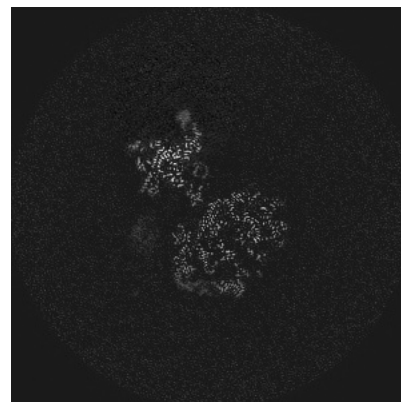
6.2.1 Primary map



X Index: 260

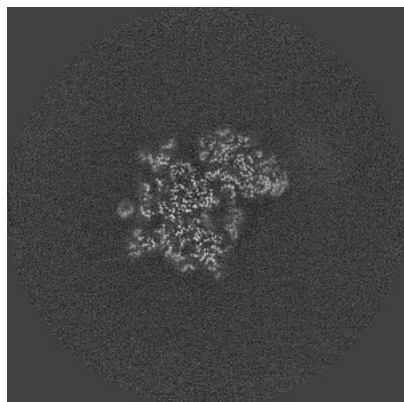


Y Index: 260

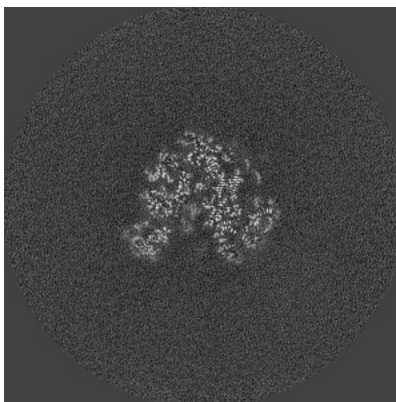


Z Index: 260

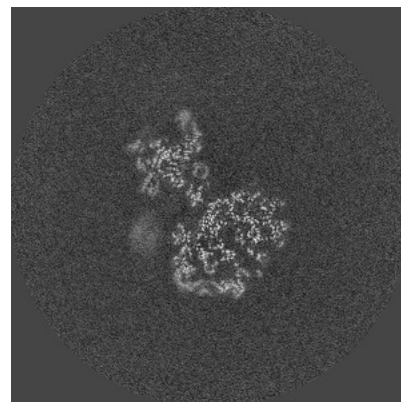
6.2.2 Raw map



X Index: 260



Y Index: 260

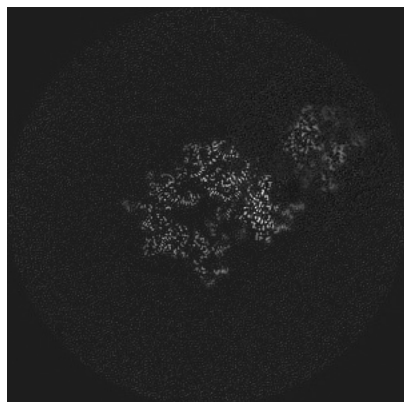


Z Index: 260

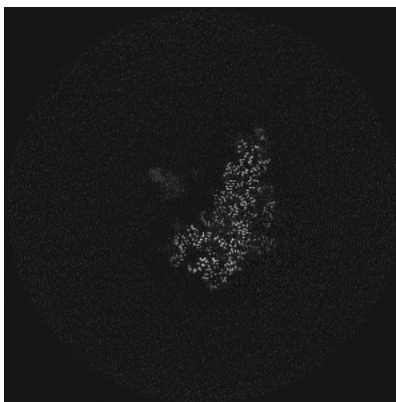
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

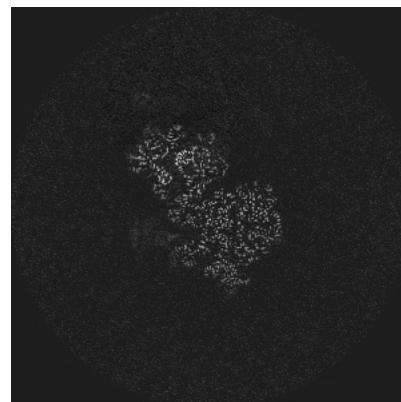
6.3.1 Primary map



X Index: 227

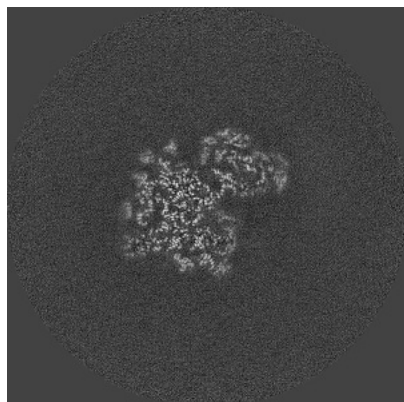


Y Index: 312

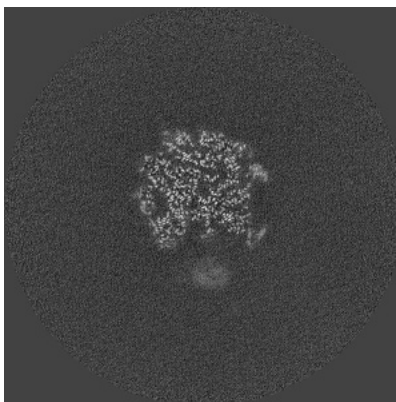


Z Index: 277

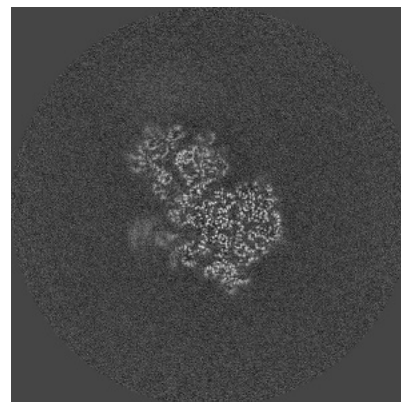
6.3.2 Raw map



X Index: 266



Y Index: 231

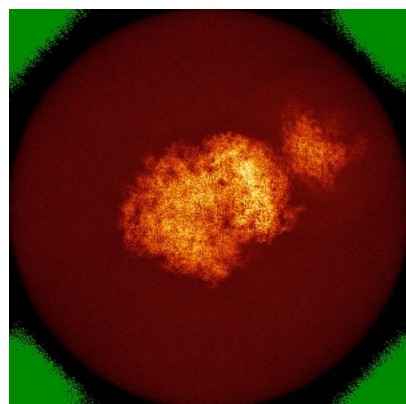


Z Index: 277

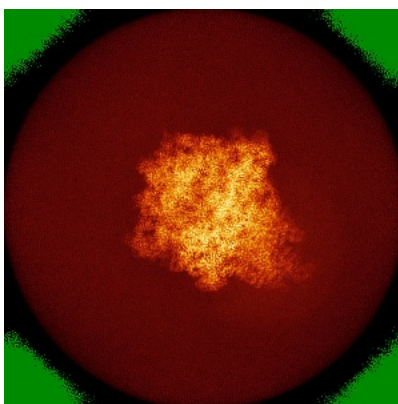
The images above show the largest variance slices of the map in three orthogonal directions.

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

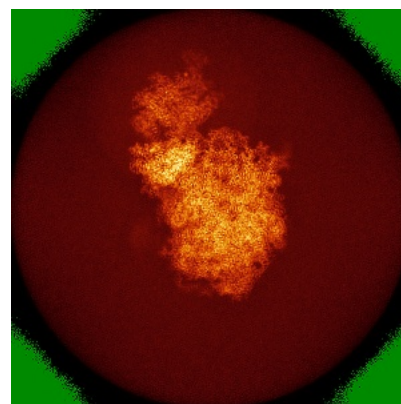
6.4.1 Primary map



X

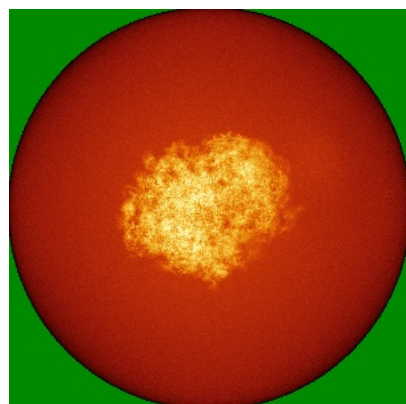


Y

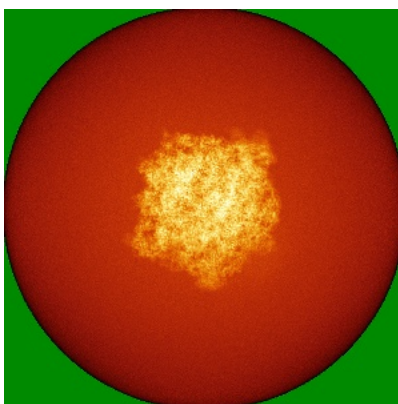


Z

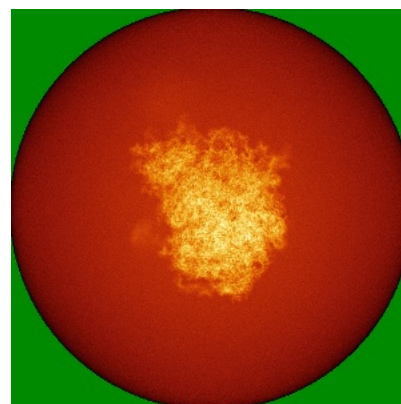
6.4.2 Raw map



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 0.5. 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.

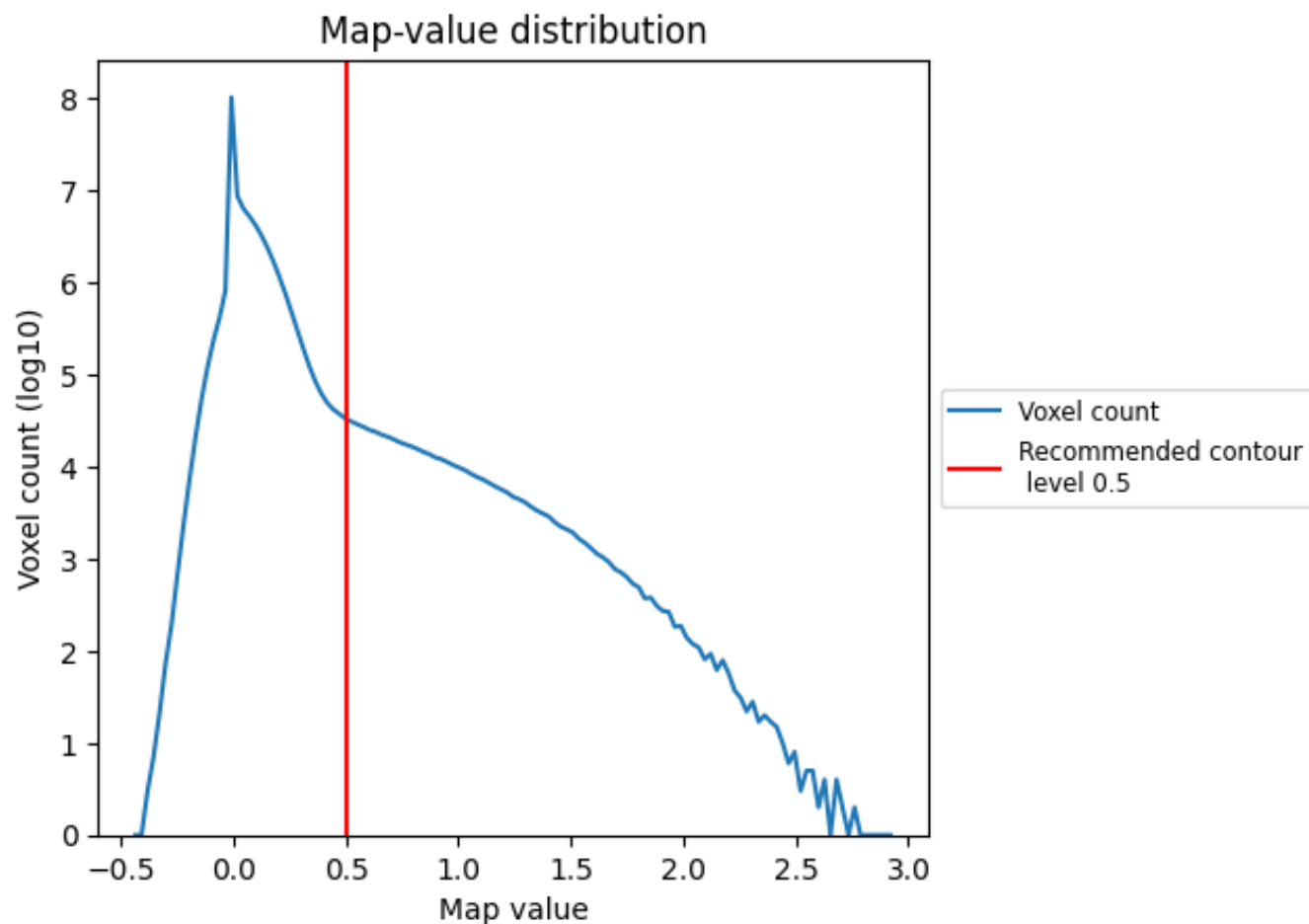
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

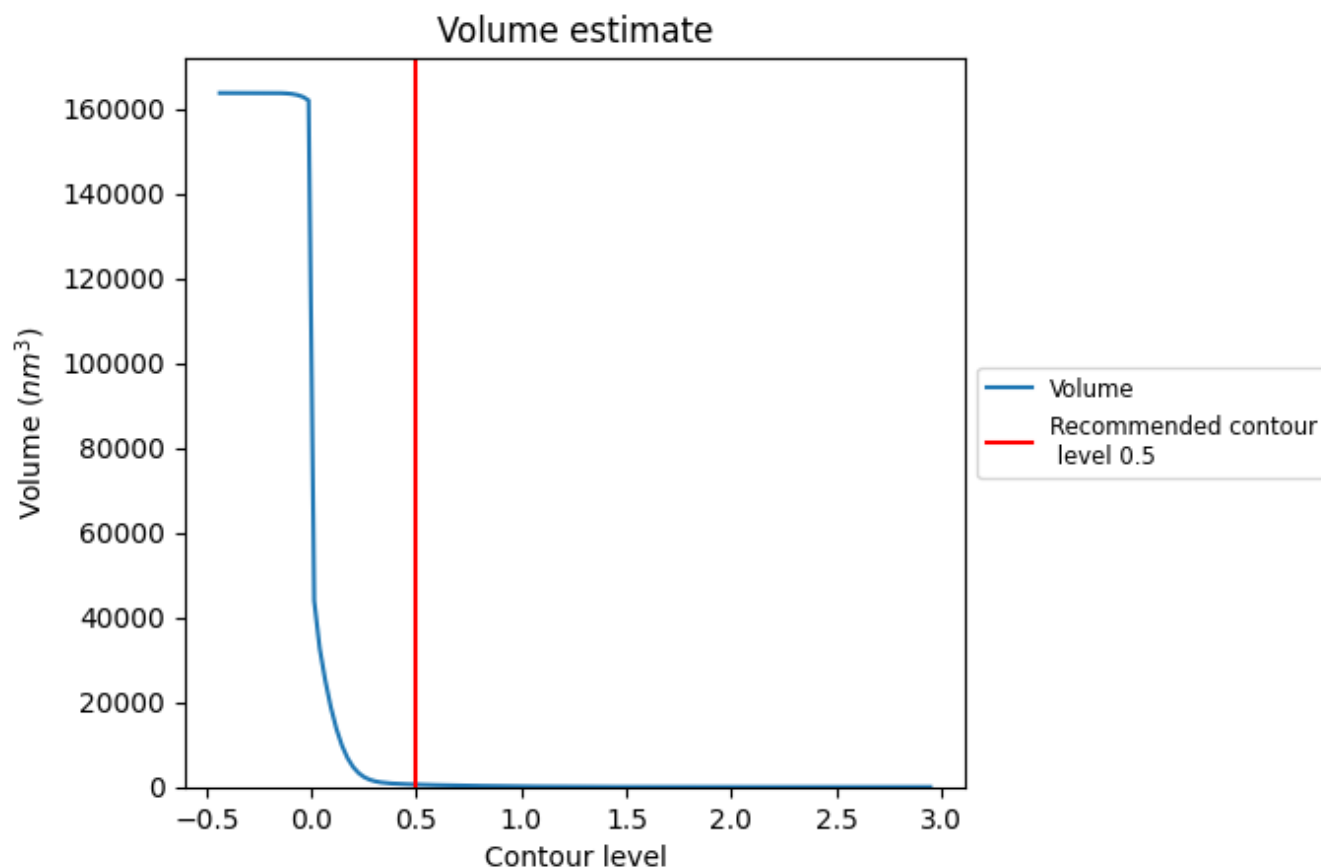
This section contains the results of statistical analysis of the map.

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.

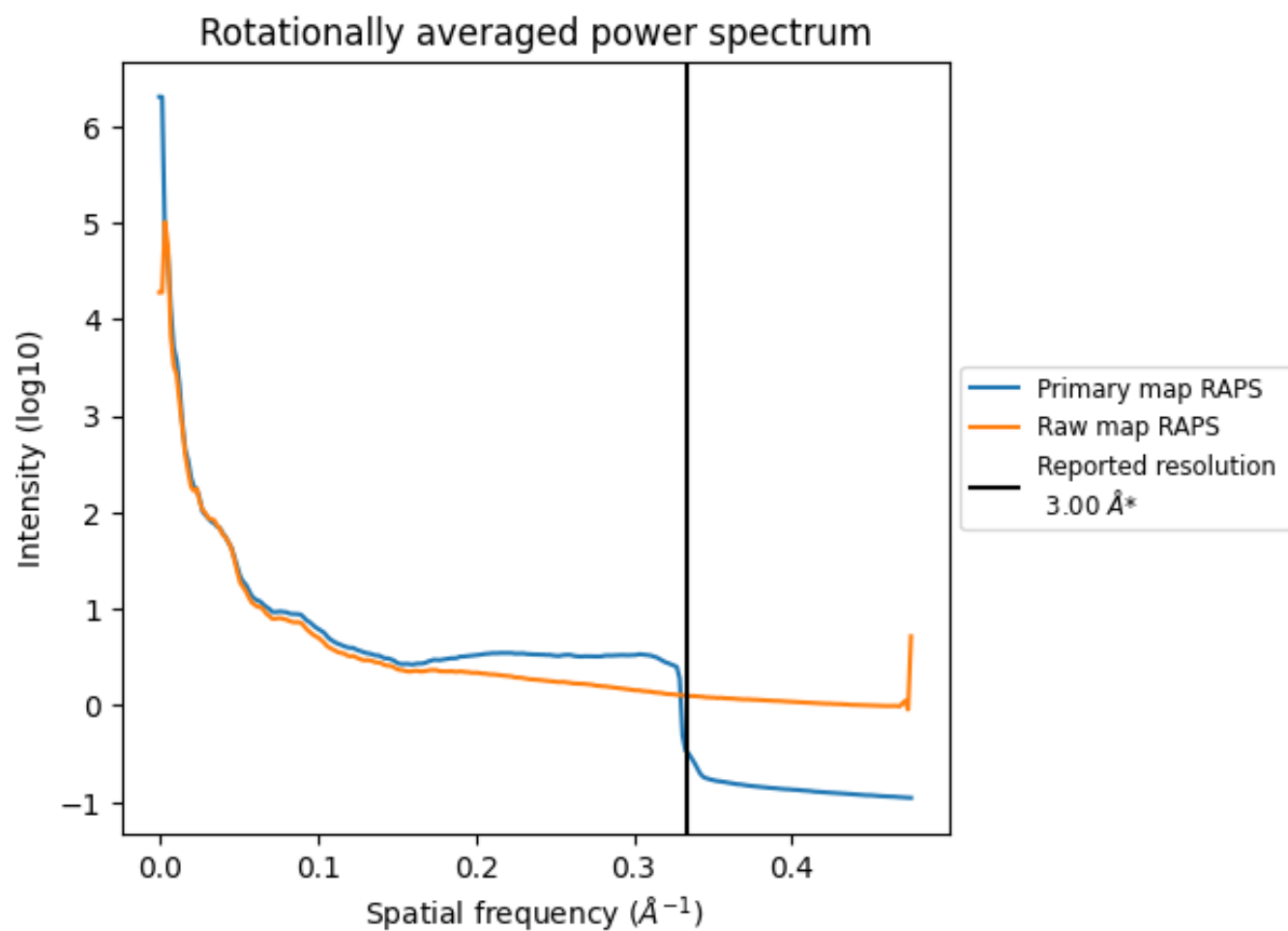
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 568 nm^3 ; this corresponds to an approximate mass of 513 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

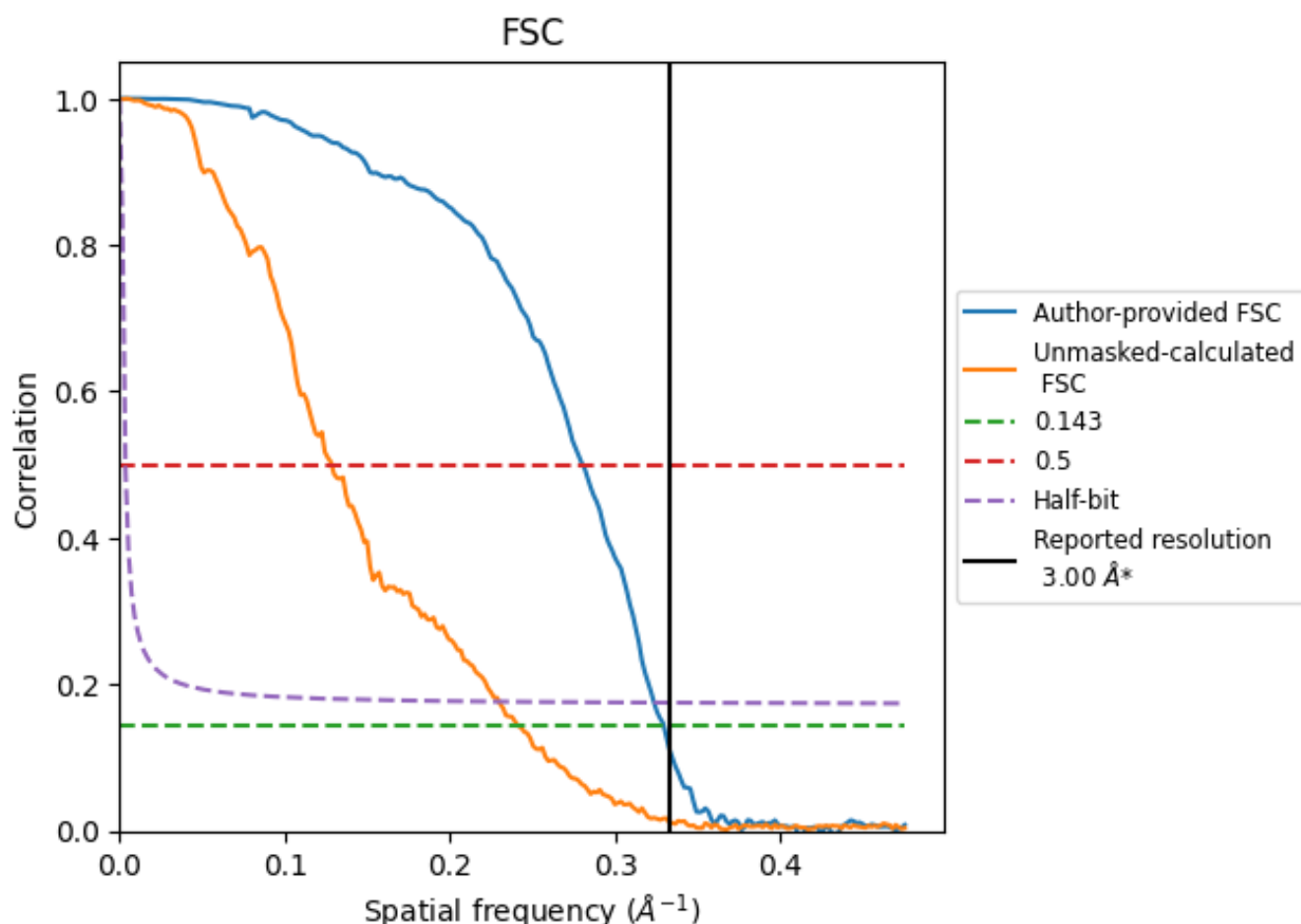


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

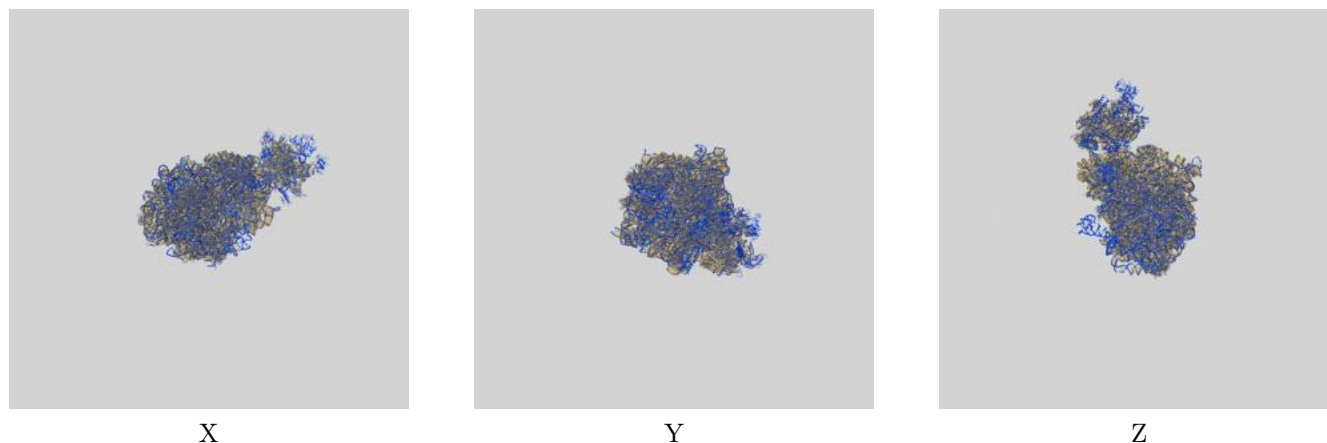
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.57	3.09
Unmasked-calculated*	4.14	7.79	4.35

*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 4.14 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

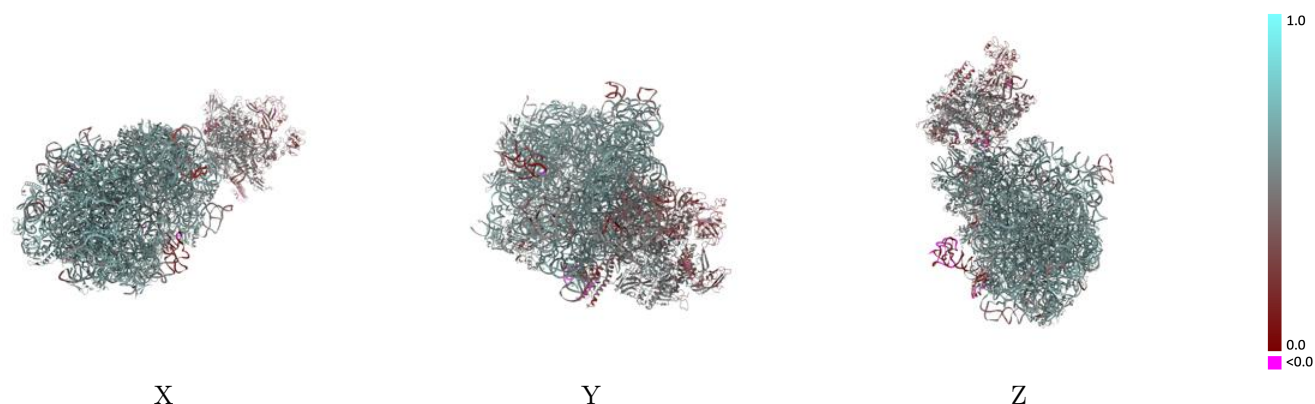
This section contains information regarding the fit between EMDB map EMD-11422 and PDB model 6ZTO. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



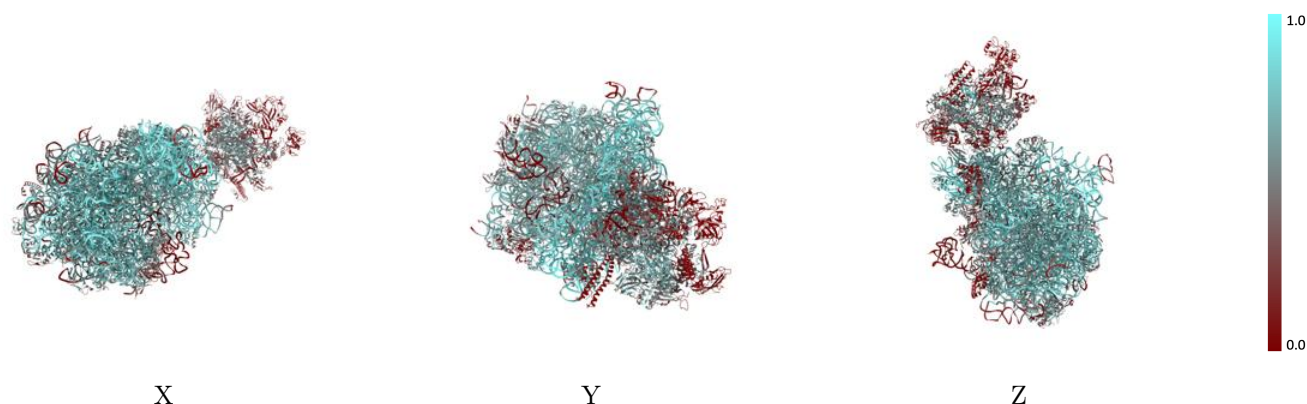
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



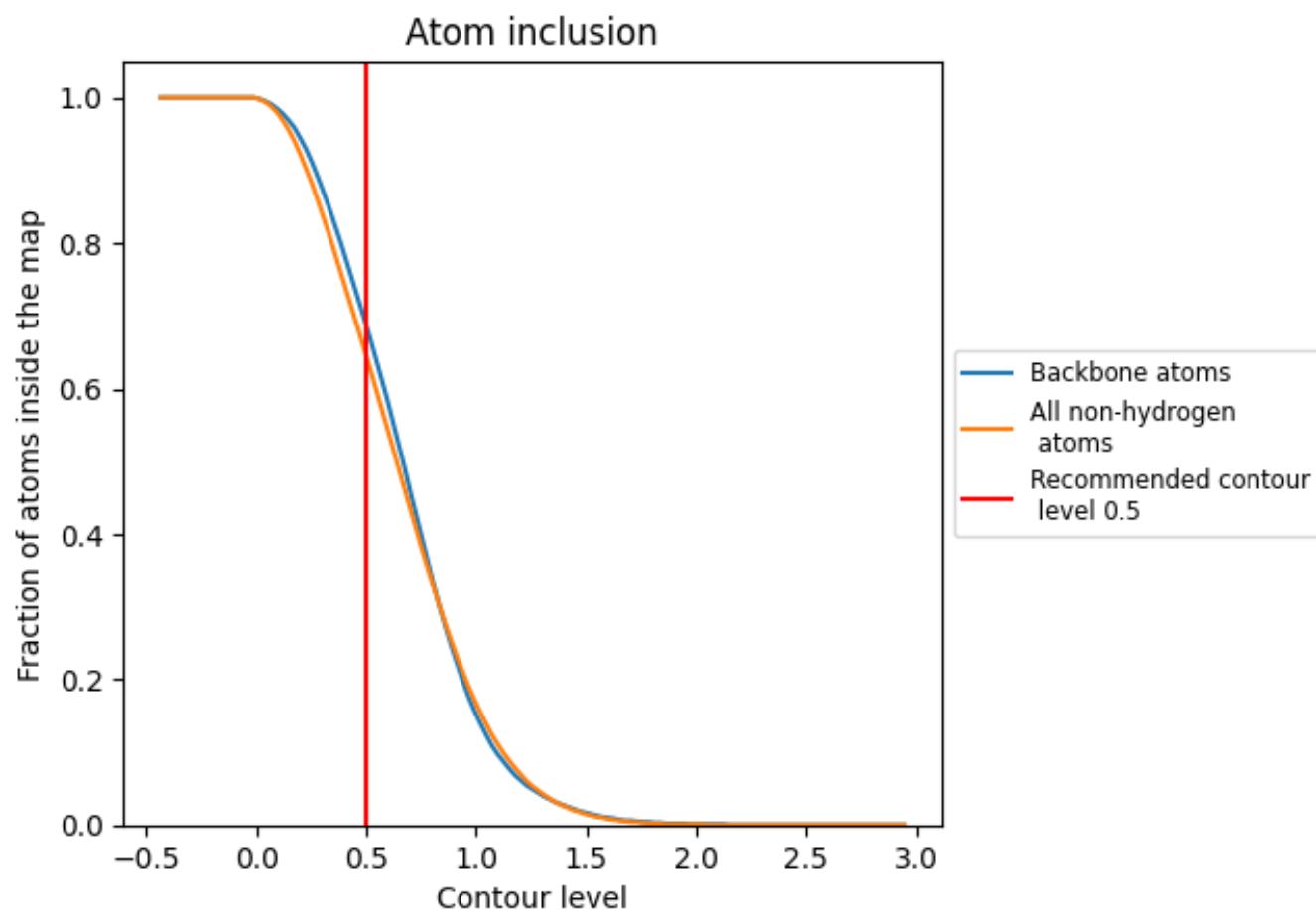
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

























































The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.5460
AA	 0.8620	 0.5860
AB	 0.2100	 0.4730
AC	 0.7040	 0.5730
AD	 0.5130	 0.5360
AE	 0.6160	 0.5630
AF	 0.4440	 0.5200
AG	 0.5630	 0.5210
AH	 0.6200	 0.5740
AI	 0.7820	 0.5750
AJ	 0.5570	 0.5130
AK	 0.5130	 0.5450
AL	 0.6510	 0.5840
AM	 0.6830	 0.5500
AN	 0.7830	 0.5840
AO	 0.5730	 0.5670
AP	 0.6920	 0.5750
AQ	 0.6120	 0.5610
AR	 0.4900	 0.4890
AS	 0.7710	 0.5720
AT	 0.6730	 0.5650
AU	 0.2410	 0.4870
AV	 0.4910	 0.4780
AW	 0.4880	 0.5310
AX	 0.2890	 0.5250
B1	 0.5790	 0.5800
B2	 0.6030	 0.5850
B3	 0.1590	 0.5180
B4	 0.7200	 0.6100
B5	 0.6820	 0.6140
B6	 0.6640	 0.5950
B7	 0.0670	 0.4020
BA	 0.7310	 0.5750
BB	 0.6990	 0.5900
BC	 0.6560	 0.6040



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Chain	Atom inclusion	Q-score
BD	 0.6460	 0.5980
BE	 0.5100	 0.5700
BF	 0.2480	 0.4980
BG	 0.3540	 0.5290
BH	 0.0320	 0.2420
BK	 0.6590	 0.5930
BL	 0.6120	 0.5920
BM	 0.5930	 0.5850
BN	 0.6300	 0.6000
BO	 0.7020	 0.6090
BP	 0.5320	 0.5620
BQ	 0.5880	 0.5860
BR	 0.6840	 0.6000
BS	 0.5970	 0.5870
BT	 0.6080	 0.5860
BU	 0.4880	 0.5470
BV	 0.4720	 0.5520
BW	 0.5430	 0.5580
BX	 0.6440	 0.6050
BY	 0.6010	 0.5930
BZ	 0.4440	 0.5440
CA	 0.4020	 0.4420
CB	 0.2010	 0.4110
CC	 0.4240	 0.4390
CD	 0.3200	 0.4040
CE	 0.0000	 0.1650
CN	 0.1570	 0.2800
CT	 0.3750	 0.3590