



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 05:50 am GMT

PDB ID : 8RCS
EMDB ID : EMD-19058
Title : Escherichia coli paused disome complex (Rotated disome interface class 1)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-12-07
Resolution : 4.46 Å (reported)
Based on initial model : 7N1P

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

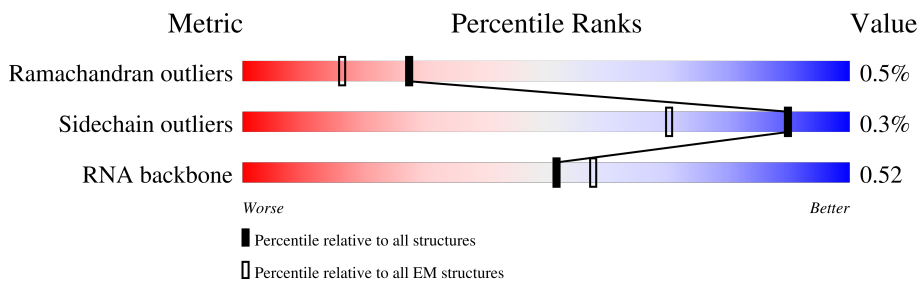
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.46 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	12	78	
2	32	59	
3	4	70	
3	41	70	
4	62	65	
5	71	2904	
5	72	2904	
6	82	120	

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Mol	Chain	Length	Quality of chain
7	A1	1542	70% 30%
7	A2	1542	73% 26%
8	B	241	59% 95%
8	B2	241	30% 94% 6%
9	C1	233	38% 90% 9%
9	C2	233	24% 91% 9%
10	D1	206	49% 98%
10	D2	206	51% 98%
11	E1	167	51% 95% 5%
11	E2	167	24% 95% 5%
12	F1	135	59% 79% 21%
12	F2	135	43% 78% 21%
13	G1	179	46% 87% 13%
13	G2	179	24% 81% 5% 14%
14	H1	130	37% 99%
14	H2	130	24% 99%
15	I1	130	25% 98%
15	I2	130	20% 99%
16	J1	103	39% 99%
16	J2	103	28% 92% 5%
17	K1	129	50% 88% 11%
17	K2	129	39% 90% 9%
18	L1	124	31% 98%
18	L2	124	18% 99%
19	M1	118	43% 97%

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Mol	Chain	Length	Quality of chain
19	M2	118	34% 99%
20	N1	101	26% 99%
20	N2	101	8% 99%
21	O1	89	35% 99%
21	O2	89	25% 98%
22	P1	82	37% 99%
23	Q1	84	38% 95% 5%
23	Q2	84	27% 94% 5%
24	R1	75	56% 97%
24	R2	75	63% 96%
25	S1	92	43% 90% 10%
25	S2	92	17% 90% 10%
26	T1	87	21% 94% 5%
27	U1	71	55% 97%
27	U2	71	45% 99%
28	V2	59	63% 31% 66%
29	W	76	5% 54% 37% 9%
30	W1	76	7% 26% 16% 57%
31	Y	76	93% 68% 29%
32	Y1	76	37% 38% 8% 53%
33	Z1	557	98%
34	a2	234	85% 93% 5%
35	b2	273	41% 99%
36	e2	179	54% 99%
37	g2	55	49% 95% 5%

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Mol	Chain	Length	Quality of chain
38	h2	136	
39	i2	149	
40	l2	46	
41	o2	144	
42	p	10	
43	r2	117	
44	z2	85	

2 Entry composition i

There are 48 unique types of molecules in this entry. The entry contains 187319 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 protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	12	77	625	388	129	106	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	32	58	449	281	87	79	2	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	68	533	330	101	96	6	0	0
3	41	14	118	74	26	18		0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	62	64	504	323	105	74	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	71	19	406	182	73	132	19	0	0
5	72	2904	62355	27824	11468	20159	2904	0	0

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	82	120	2569	1144	468	837	120	0	0

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A1	1542	33092	14767	6064	10719	1542	0	0
7	A2	1537	32990	14721	6049	10683	1537	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B	233	1815	1145	325	337	8	0	0
8	B2	227	1776	1123	318	327	8	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C1	213	1665	1054	312	295	4	0	0
9	C2	212	1658	1049	311	294	4	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D1	205	1643	1026	315	298	4	0	0
10	D2	205	1643	1026	315	298	4	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E1	158	1166	725	220	215	6	0	0
11	E2	158	1166	725	220	215	6	0	0

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		
12	F2	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G1	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		
13	G2	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
14	H2	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
15	I2	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J1	102	Total	C	N	O	S	0	0
			817	509	157	150	1		
16	J2	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K1	115	Total	C	N	O	S	0	0
			857	528	168	158	3		
17	K2	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L1	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
18	L2	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M1	115	Total	C	N	O	S	0	0
			891	552	179	157	3		
19	M2	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		
20	N2	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
21	O2	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q1	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
23	Q2	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R1	74	Total	C	N	O	S	0	0
			624	395	122	105	2		
24	R2	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S1	83	Total	C	N	O	S	0	0
			663	424	126	111	2		
25	S2	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U1	70	Total	C	N	O	S	0	0
			590	366	125	98	1		
27	U2	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	59	Total	C	N	O	P	0	0
			1272	569	242	402	59		

- Molecule 29 is a RNA chain called tRNA-Trp (P/E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
29	W	76	1630	730	286	536	76	2	0	0

- Molecule 30 is a RNA chain called tRNA-Phe (P/E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
30	W1	33	718	324	133	226	33	2	0	0

- Molecule 31 is a RNA chain called tRNA-Ala (A/P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	Y	76	1628	726	293	533	76	0	0

- Molecule 32 is a RNA chain called tRNA-Val (A/P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
32	Y1	36	778	348	142	252	36	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y1	34	CM0	U	variant	GB 1847302804

- Molecule 33 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Z1	9	75	49	10	16	0	0

- Molecule 34 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	a2	223	1661	1039	302	314	6	0	0

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	b2	271	2082	1288	423	364	7	0	0

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	e2	178	1420	905	251	258	6	0	0

- Molecule 37 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	g2	52	427	275	78	74	0	0

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h2	136	1085	692	209	178	6	1	0

- Molecule 39 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i2	149	1111	699	197	214	1	0	0

- Molecule 40 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l2	46	377	228	90	57	2	0	0

- Molecule 41 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	o2	51	377	231	83	62	1	0	0

- Molecule 42 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	p	10	76	47	18	11	0	0

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	r2	116	891	552	178	161	0	0

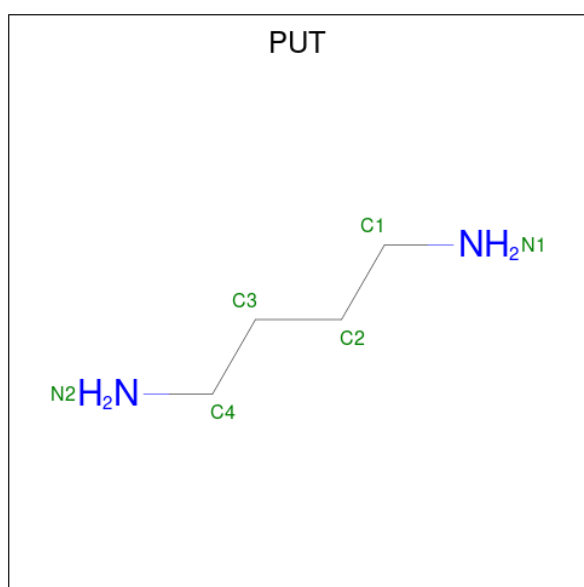
- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	z2	76	582	360	117	104	1	0	0

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

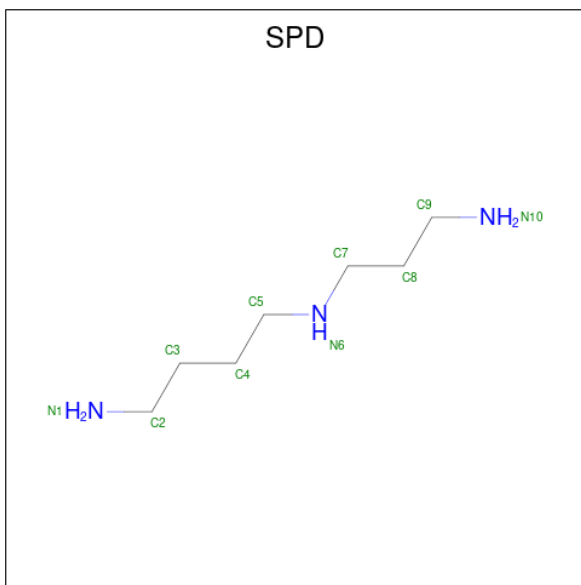
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
45	4	1	1	1	0
45	B	1	1	1	0

- Molecule 46 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
46	72	1	Total	C	N	0
			6	4	2	
46	72	1	Total	C	N	0
			6	4	2	

- Molecule 47 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
47	72	1	Total	C	N	0
			10	7	3	

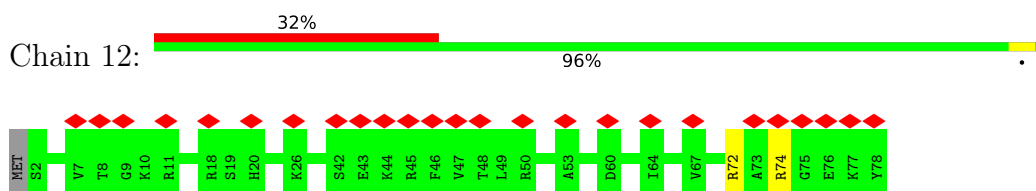
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	72	165	Total	Mg	0
			165	165	
48	A1	60	Total	Mg	0
			60	60	
48	A2	41	Total	Mg	0
			41	41	
48	N2	1	Total	Mg	0
			1	1	
48	Y	1	Total	Mg	0
			1	1	
48	o2	1	Total	Mg	0
			1	1	

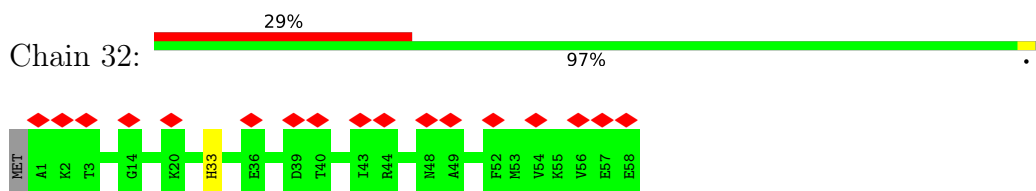
3 Residue-property plots [i](#)

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

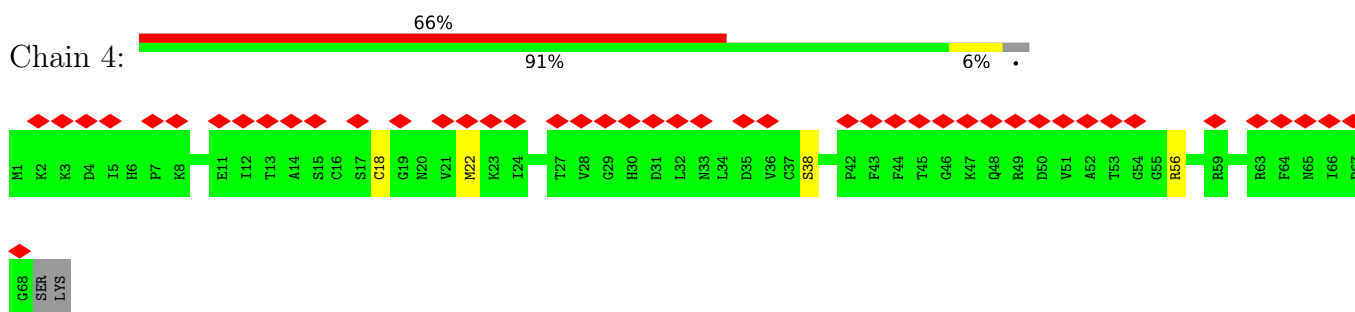
- Molecule 1: 50S ribosomal protein L28



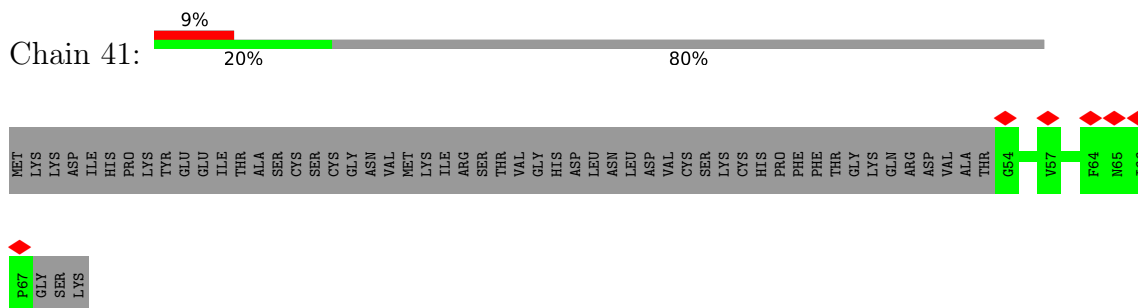
- Molecule 2: 50S ribosomal protein L30

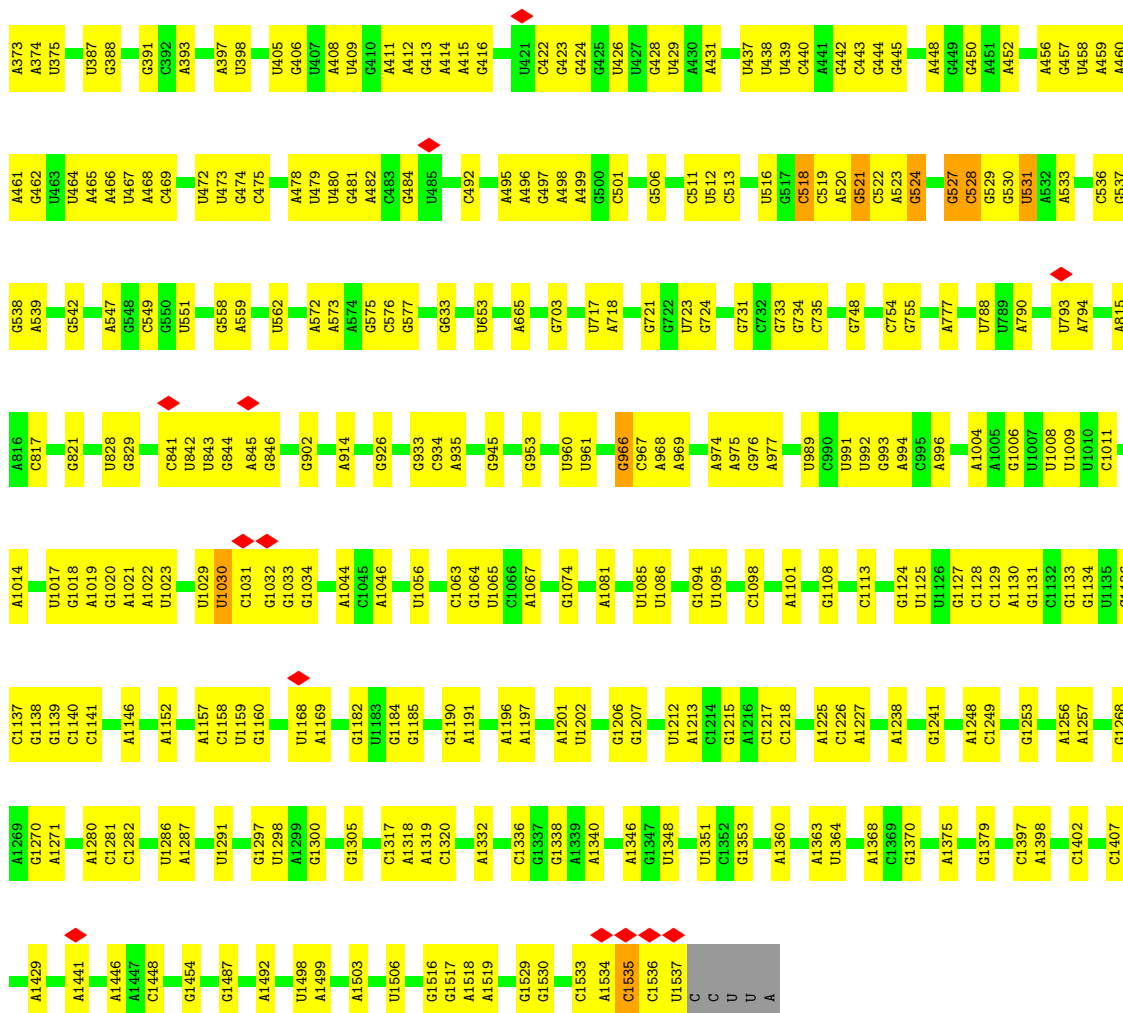


- Molecule 3: Large ribosomal subunit protein bL31A

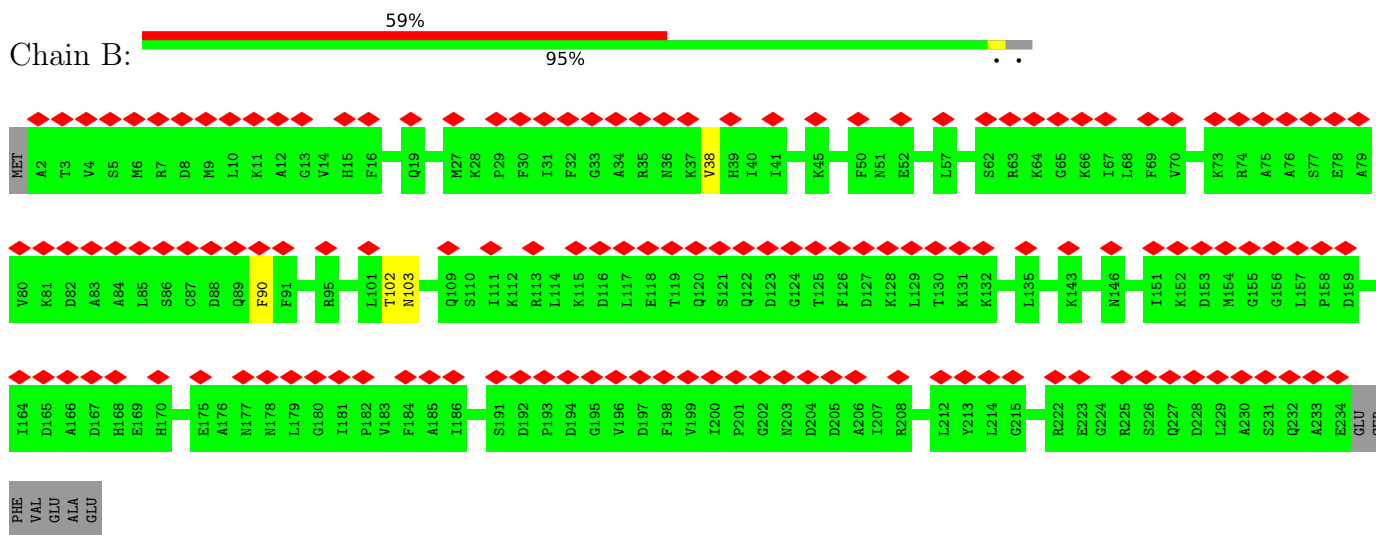


- Molecule 3: Large ribosomal subunit protein bL31A



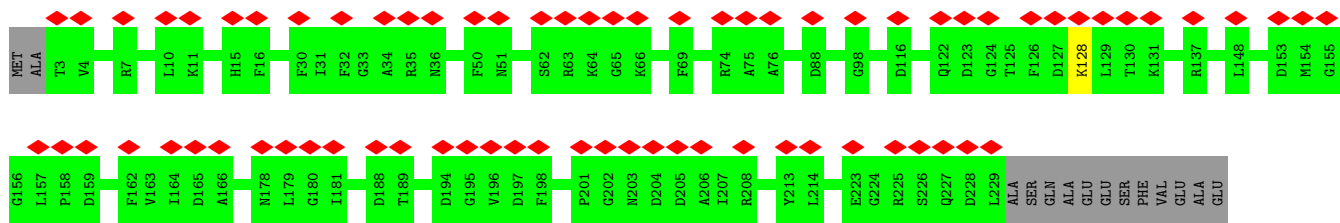


• Molecule 8: Small ribosomal subunit protein uS2

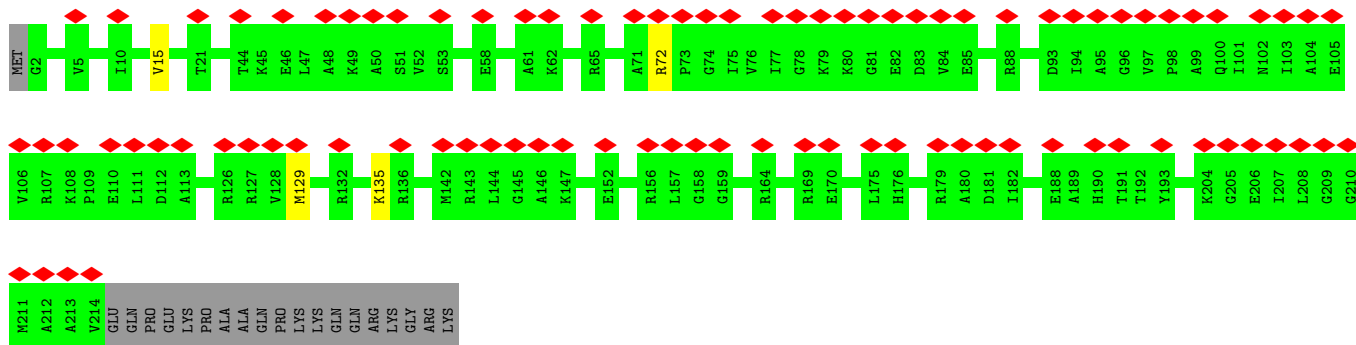
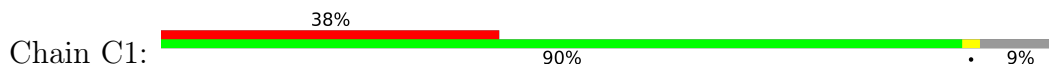


• Molecule 8: Small ribosomal subunit protein uS2

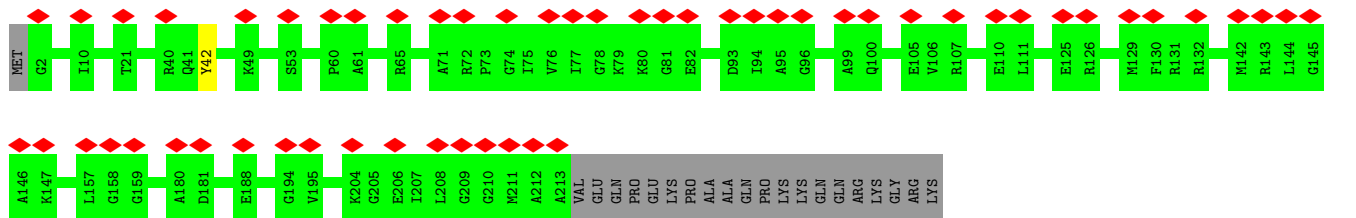
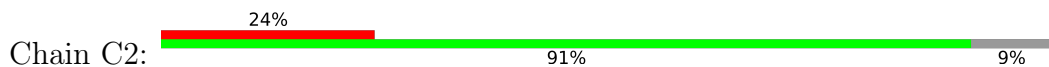




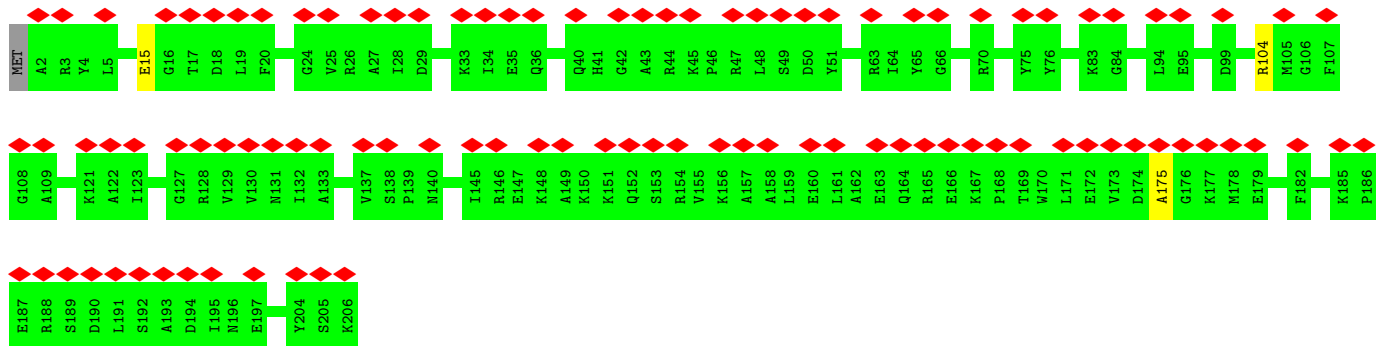
• Molecule 9: Small ribosomal subunit protein uS3



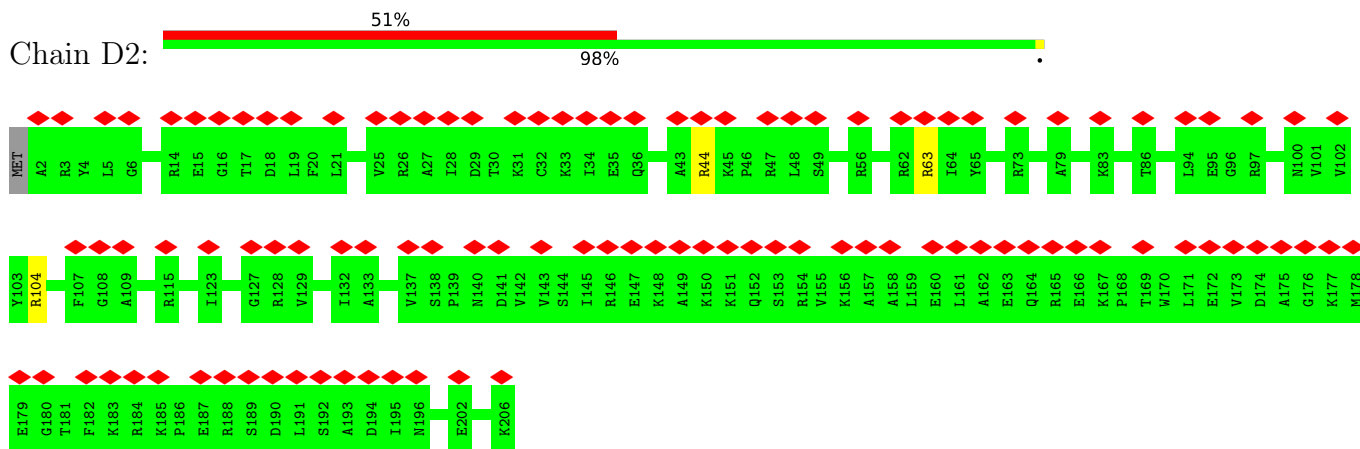
• Molecule 9: Small ribosomal subunit protein uS3



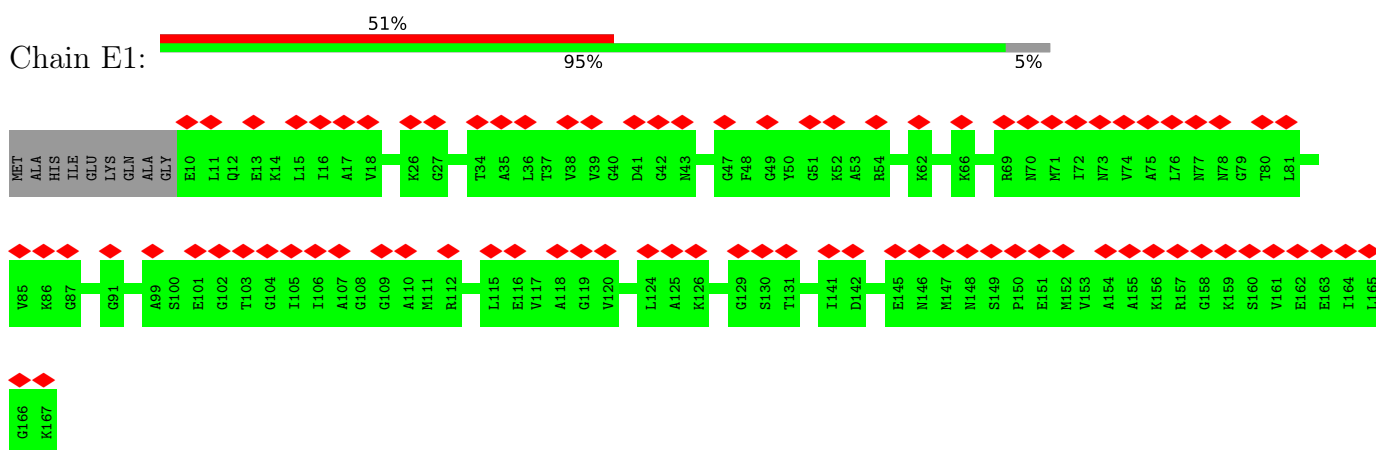
• Molecule 10: Small ribosomal subunit protein uS4



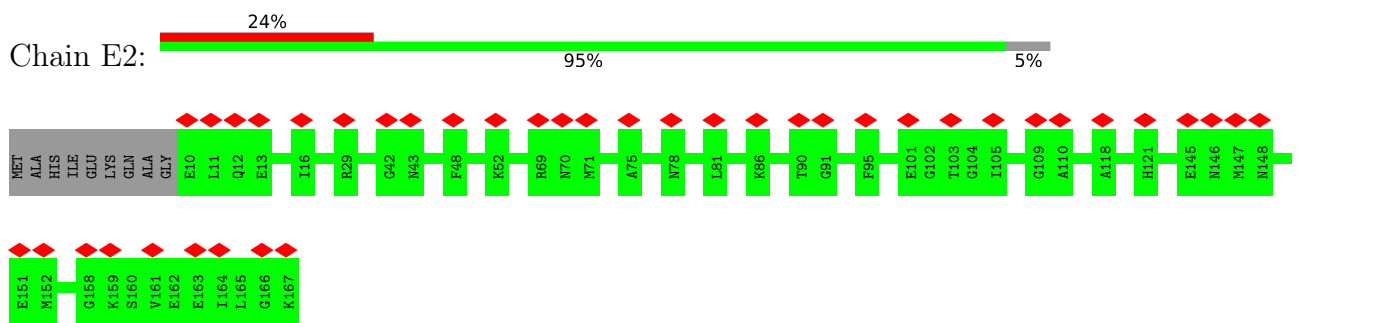
• Molecule 10: Small ribosomal subunit protein uS4



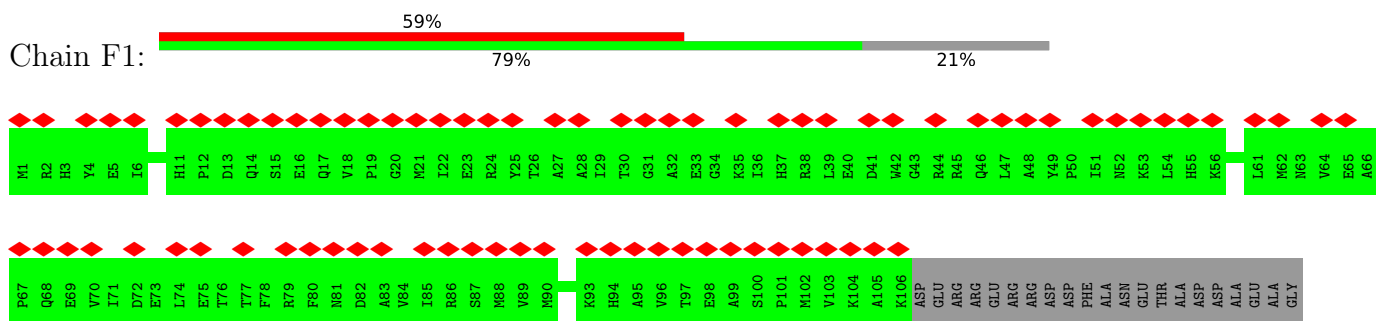
• Molecule 11: Small ribosomal subunit protein uS5



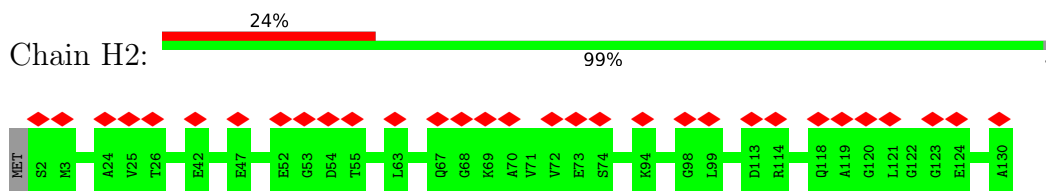
• Molecule 11: Small ribosomal subunit protein uS5



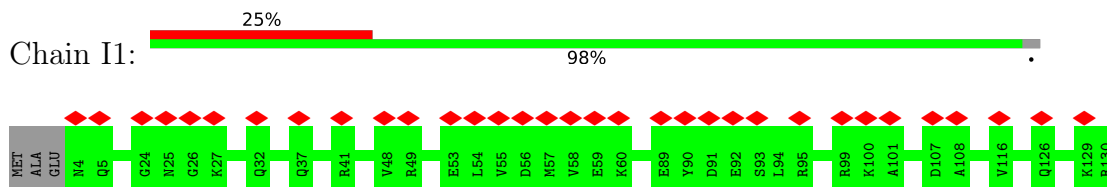
• Molecule 12: 30S ribosomal protein S6



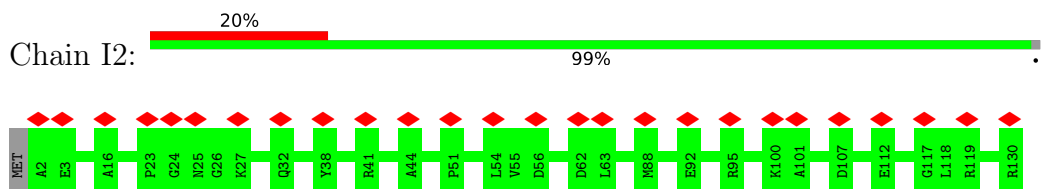
- Molecule 14: Small ribosomal subunit protein uS8



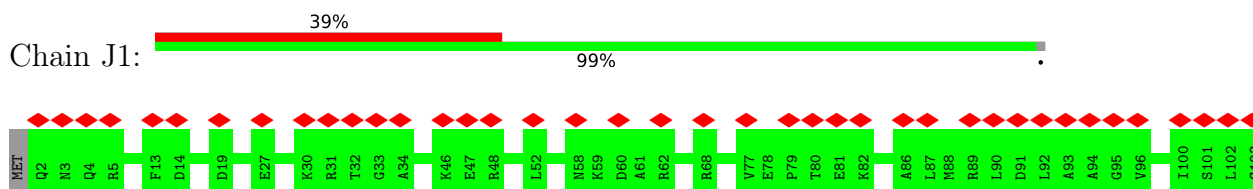
- Molecule 15: Small ribosomal subunit protein uS9



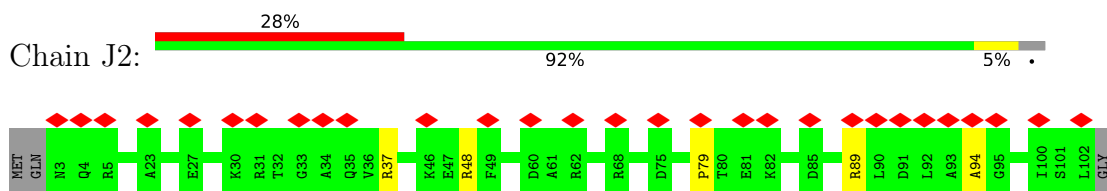
- Molecule 15: Small ribosomal subunit protein uS9



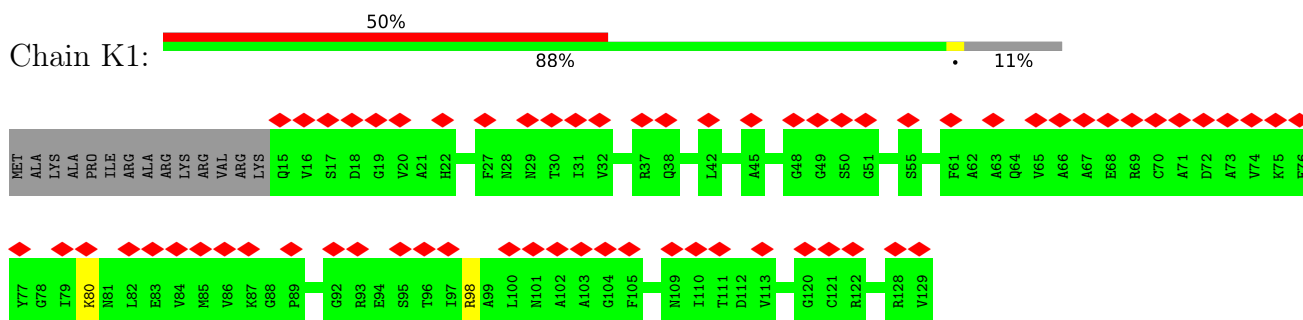
- Molecule 16: 30S ribosomal protein S10



- Molecule 16: 30S ribosomal protein S10

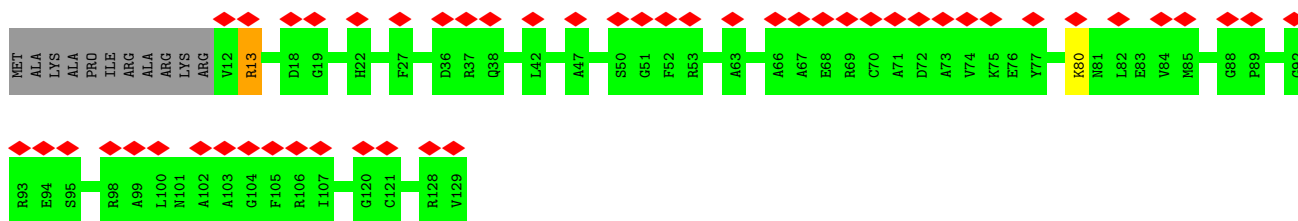


- Molecule 17: Small ribosomal subunit protein uS11



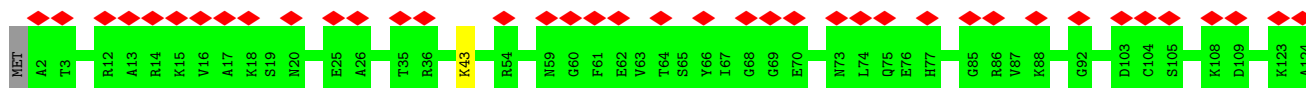
- Molecule 17: Small ribosomal subunit protein uS11

Chain K2: 39% 90% 9%



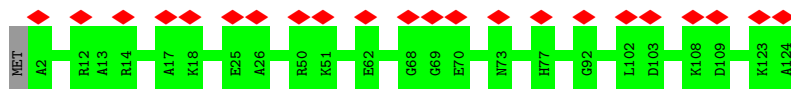
- Molecule 18: Small ribosomal subunit protein uS12

Chain L1: 31% 98%



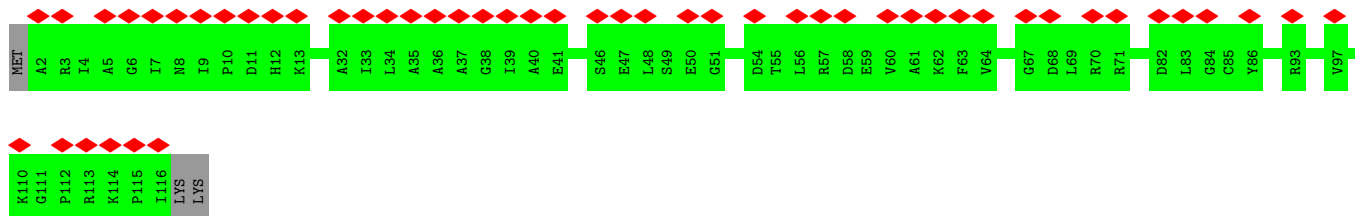
- Molecule 18: Small ribosomal subunit protein uS12

Chain L2: 18% 99%



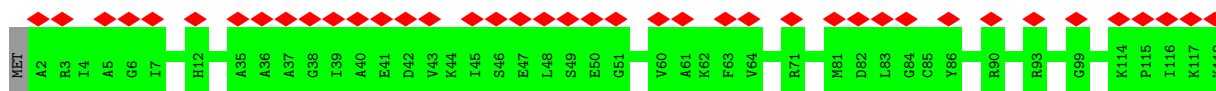
- Molecule 19: Small ribosomal subunit protein uS13

Chain M1: 43% 97%



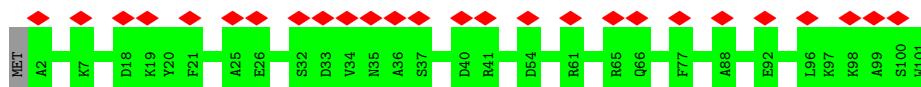
- Molecule 19: Small ribosomal subunit protein uS13

Chain M2: 34% 99%

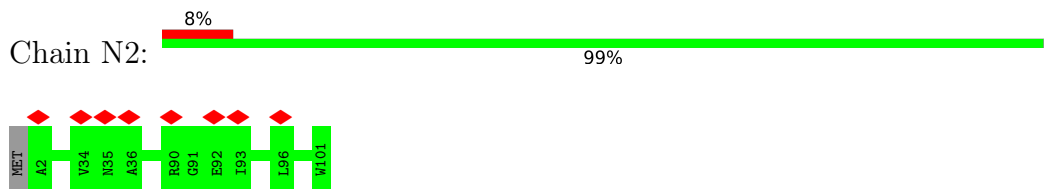


- Molecule 20: Small ribosomal subunit protein uS14

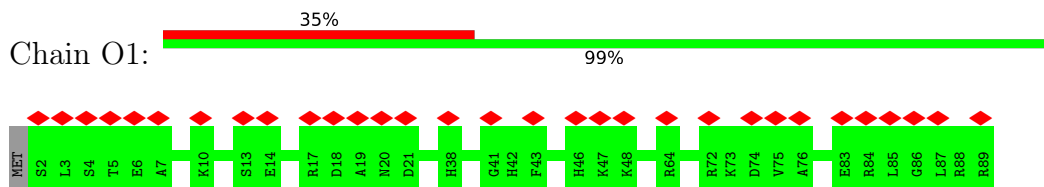
Chain N1: 26% 99%



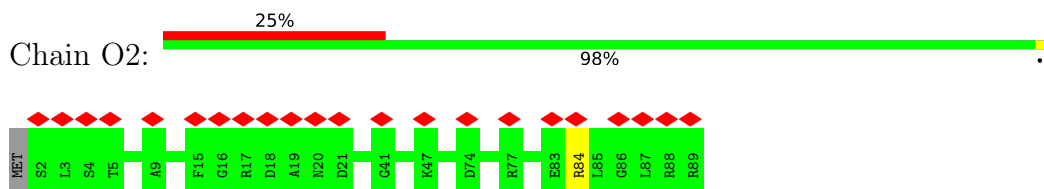
- Molecule 20: Small ribosomal subunit protein uS14



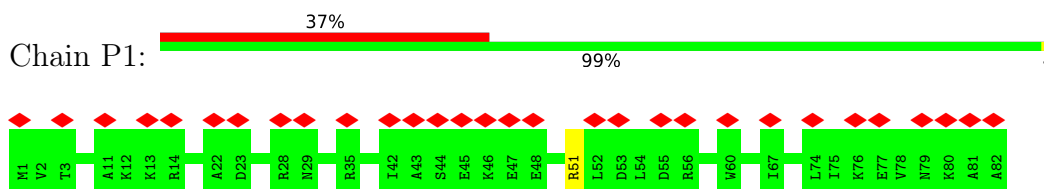
- Molecule 21: 30S ribosomal protein S15



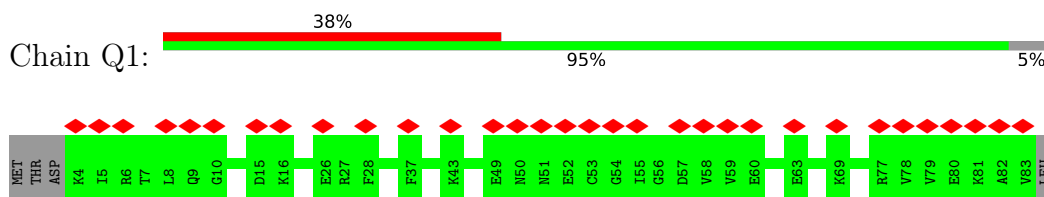
- Molecule 21: 30S ribosomal protein S15



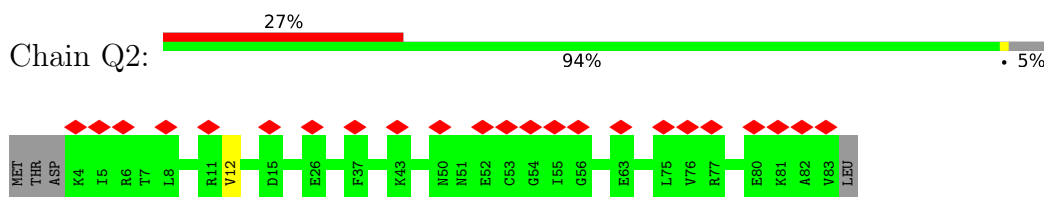
- Molecule 22: 30S ribosomal protein S16



- Molecule 23: Small ribosomal subunit protein uS17

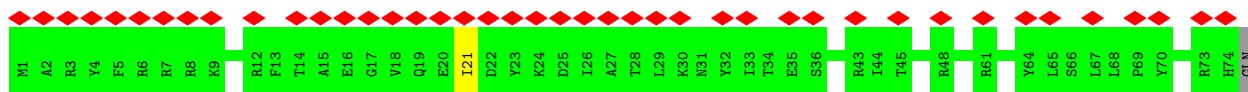


- Molecule 23: Small ribosomal subunit protein uS17

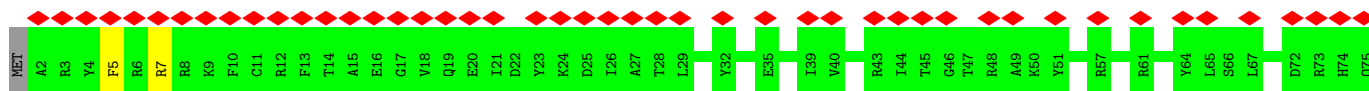


- Molecule 24: Small ribosomal subunit protein bS18

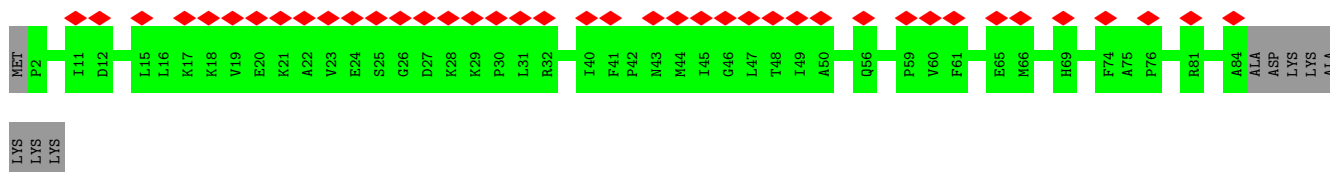
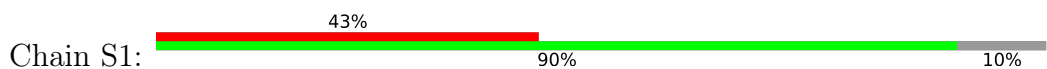




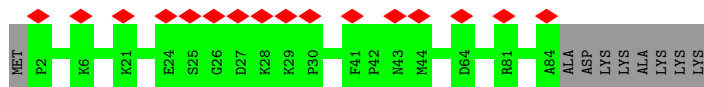
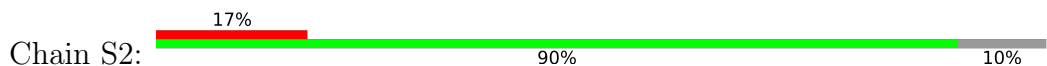
- Molecule 24: Small ribosomal subunit protein bS18



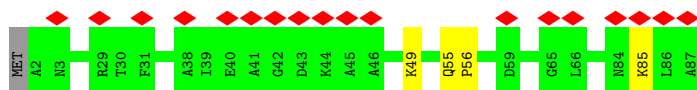
- Molecule 25: Small ribosomal subunit protein uS19



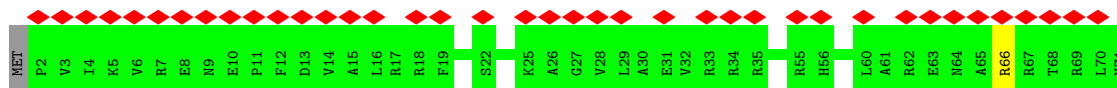
- Molecule 25: Small ribosomal subunit protein uS19



- Molecule 26: Small ribosomal subunit protein bS20



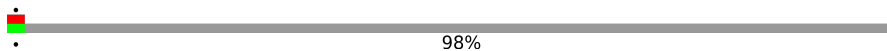
- Molecule 27: 30S ribosomal protein S21



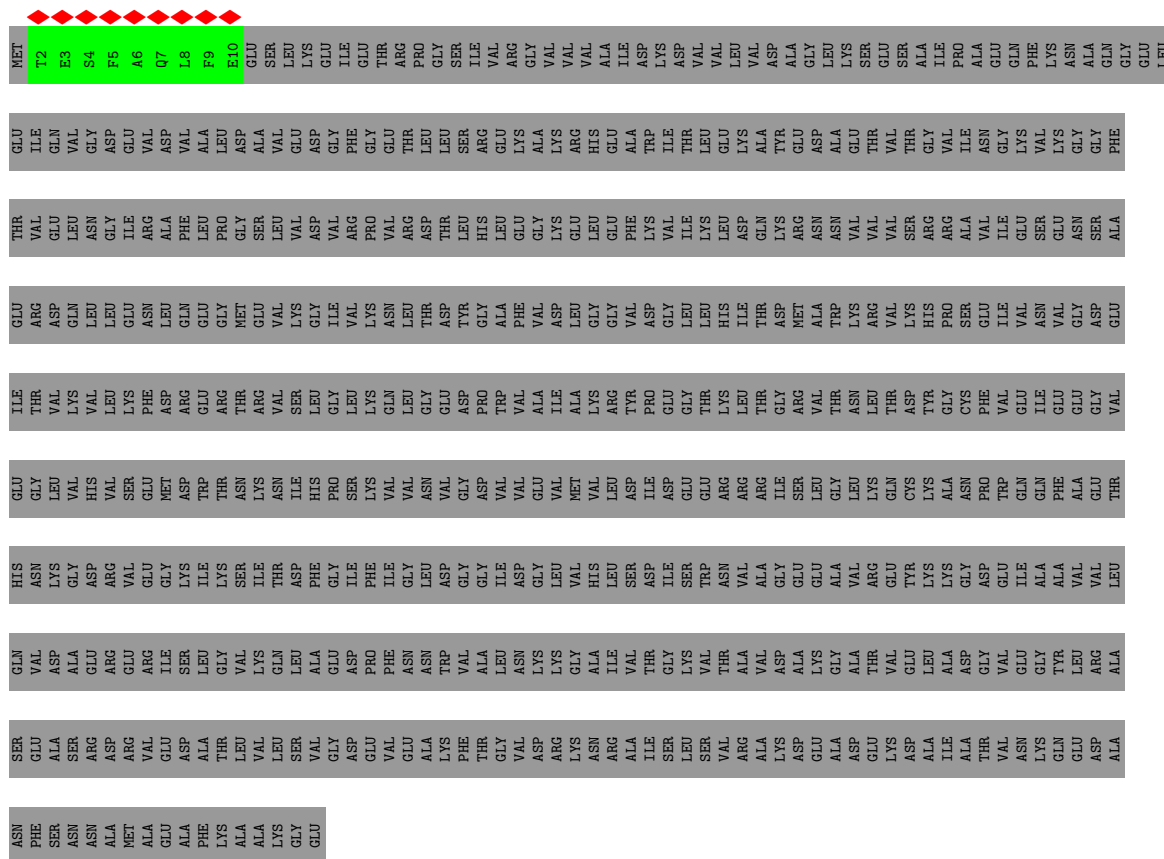
- Molecule 27: 30S ribosomal protein S21



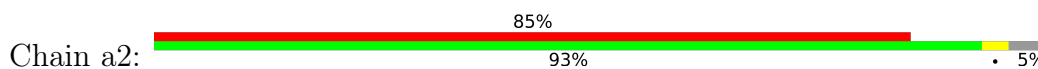
Chain Z1:



98%



• Molecule 34: Large ribosomal subunit protein uL1

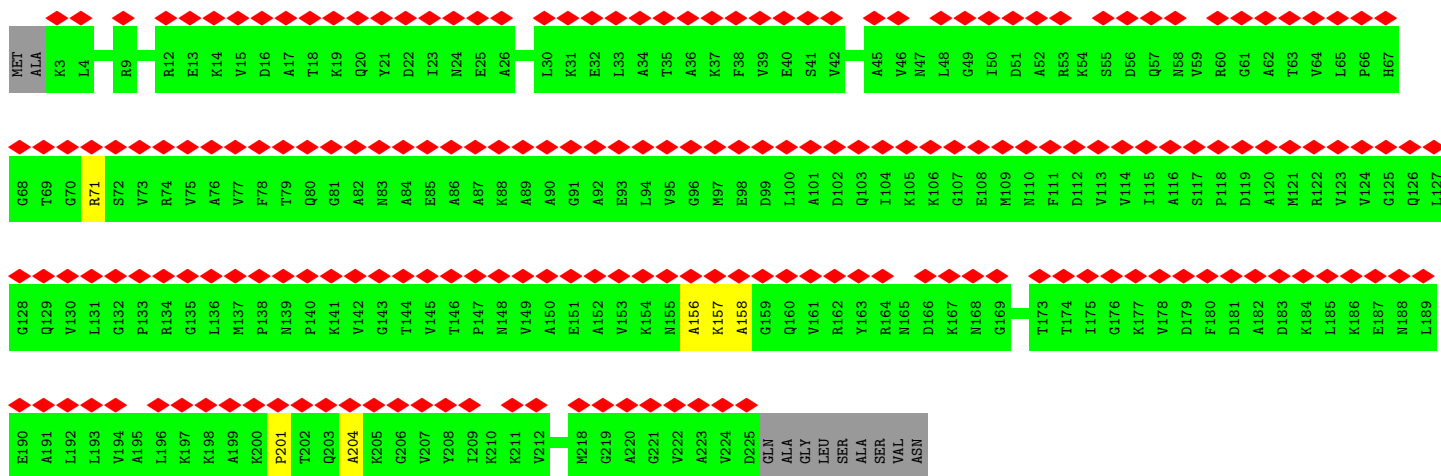


Chain a2:

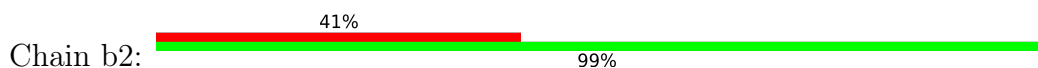
85%

93%

5%



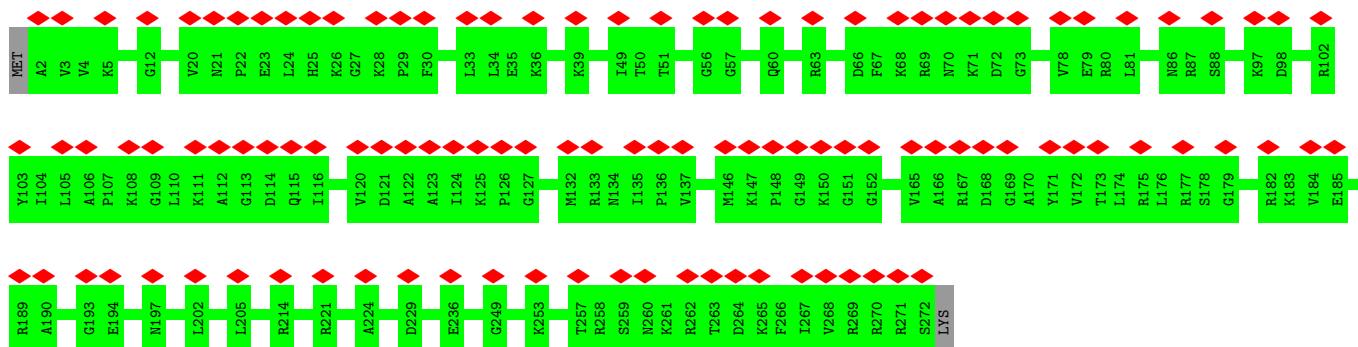
• Molecule 35: 50S ribosomal protein L2



Chain b2:

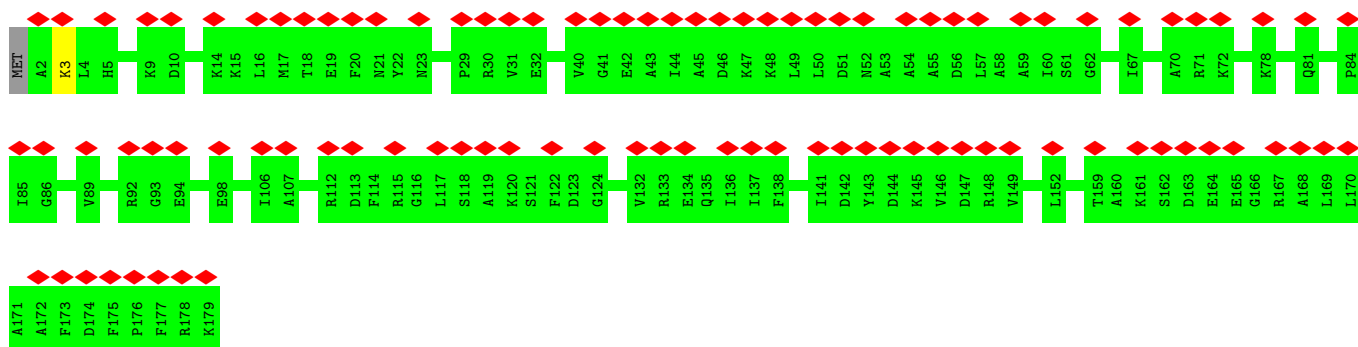
41%

99%



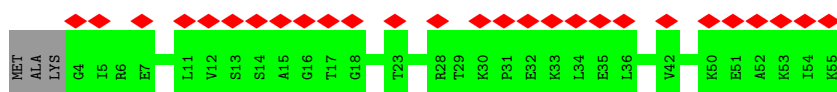
- Molecule 36: 50S ribosomal protein L5

Chain e2: 54% 99%



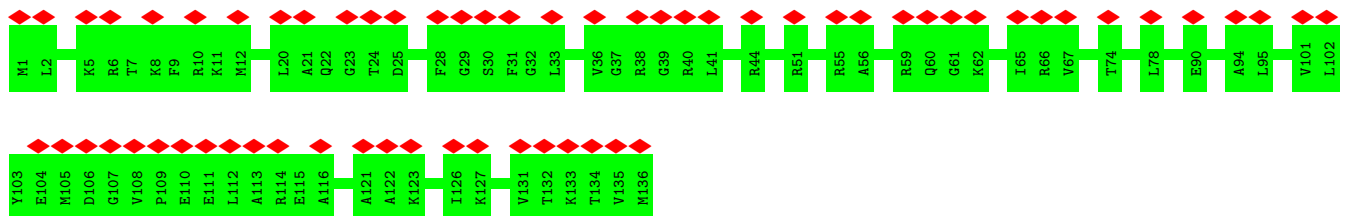
- Molecule 37: 50S ribosomal protein L33

Chain g2: 49% 95% 5%



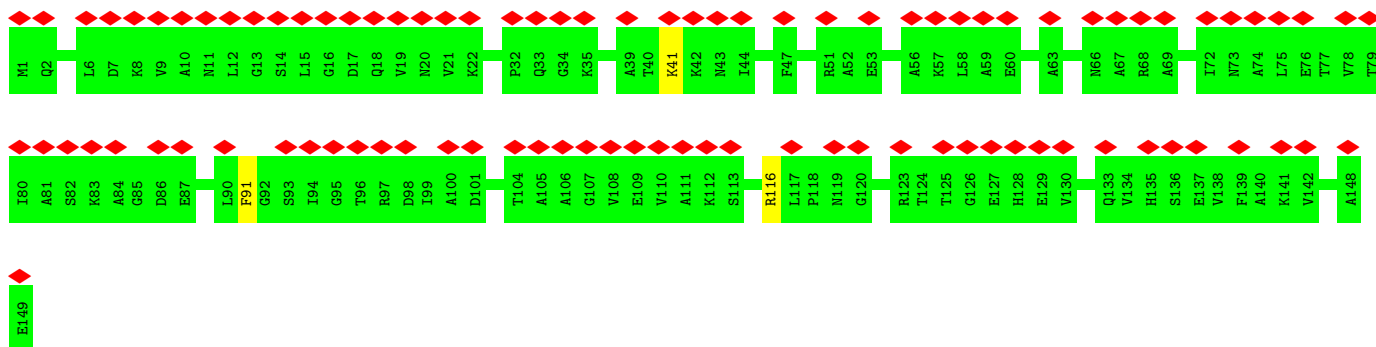
- Molecule 38: 50S ribosomal protein L16

Chain h2: 46% 100%

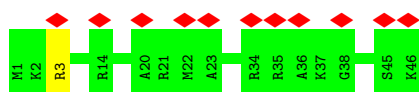


- Molecule 39: 50S ribosomal protein L9

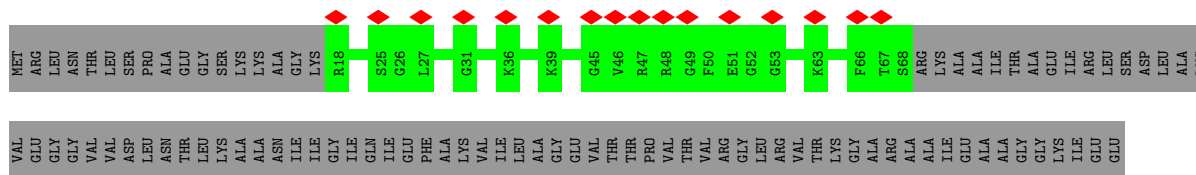
Chain i2: 62% 98%



• Molecule 40: 50S ribosomal protein L34



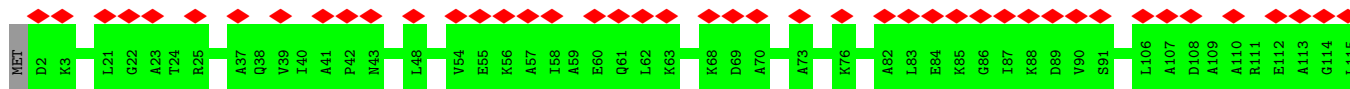
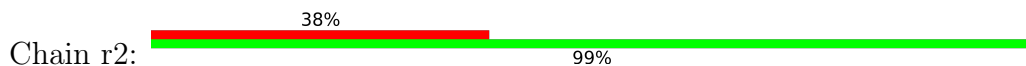
• Molecule 41: 50S ribosomal protein L15



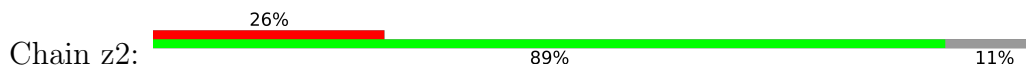
• Molecule 42: Nascent chain

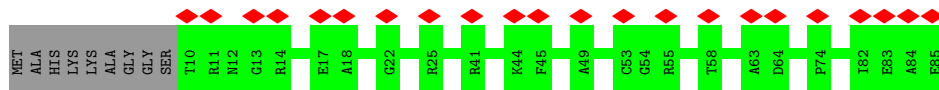


• Molecule 43: 50S ribosomal protein L18



• Molecule 44: 50S ribosomal protein L27





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10748	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	18.257	Depositor
Minimum map value	-5.431	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.924	Depositor
Recommended contour level	5.5	Depositor
Map size (\AA)	744.12, 744.12, 744.12	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.59, 1.59, 1.59	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: 7MG, 2MA, ZN, MIA, UR3, 1MG, OMC, SPD, 2MG, 5MU, 6MZ, MA6, 4OC, 4SU, G7M, H2U, OMU, MG, PUT, PSU, 3TD, CM0, 5MC, OMG

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	12	0.25	0/635	0.63	0/848
2	32	0.22	0/453	0.52	0/605
3	4	0.37	0/543	0.65	1/726 (0.1%)
3	41	0.25	0/120	0.60	0/158
4	62	0.24	0/513	0.56	0/676
5	71	0.16	0/429	0.69	0/664
5	72	0.18	1/69306 (0.0%)	0.70	12/108116 (0.0%)
6	82	0.18	0/2872	0.73	2/4478 (0.0%)
7	A1	0.24	0/36794	0.77	7/57392 (0.0%)
7	A2	0.24	0/36681	0.76	16/57217 (0.0%)
8	B	0.24	0/1846	0.53	0/2488
8	B2	0.25	0/1807	0.50	0/2435
9	C1	0.26	0/1692	0.55	0/2280
9	C2	0.29	0/1685	0.61	0/2270
10	D1	0.25	0/1665	0.53	0/2227
10	D2	0.25	0/1665	0.54	0/2227
11	E1	0.26	0/1179	0.52	0/1584
11	E2	0.26	0/1179	0.52	0/1584
12	F1	0.24	0/881	0.51	0/1189
12	F2	0.25	0/881	0.51	0/1189
13	G1	0.24	0/1246	0.53	0/1672
13	G2	0.28	0/1230	0.58	0/1649
14	H1	0.25	0/989	0.53	0/1326
14	H2	0.25	0/989	0.53	0/1326
15	I1	0.25	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.25	0/827	0.61	0/1117
16	J2	0.25	0/813	0.63	0/1100
17	K1	0.26	0/873	0.56	0/1180
17	K2	0.28	0/900	0.57	0/1215
18	L1	0.26	0/969	0.60	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	L2	0.26	0/969	0.61	0/1300
19	M1	0.25	0/900	0.57	0/1204
19	M2	0.24	0/919	0.58	0/1226
20	N1	0.26	0/817	0.60	0/1088
20	N2	0.25	0/817	0.57	0/1088
21	O1	0.23	0/722	0.55	0/964
21	O2	0.23	0/722	0.57	0/964
22	P1	0.25	0/659	0.60	0/884
23	Q1	0.27	0/657	0.58	0/881
23	Q2	0.25	0/657	0.58	0/881
24	R1	0.24	0/635	0.57	0/849
24	R2	0.25	0/637	0.62	0/851
25	S1	0.25	0/680	0.52	0/915
25	S2	0.26	0/680	0.53	0/915
26	T1	0.25	0/676	0.53	0/895
27	U1	0.26	0/598	0.61	0/792
27	U2	0.25	0/598	0.58	0/792
28	V2	0.32	0/1427	0.92	6/2224 (0.3%)
29	W	0.40	1/1604 (0.1%)	1.29	5/2496 (0.2%)
30	W1	0.28	0/677	0.89	0/1052
31	Y	0.35	1/1725 (0.1%)	0.79	2/2687 (0.1%)
32	Y1	0.20	0/786	0.79	0/1216
33	Z1	0.26	0/76	0.35	0/101
34	a2	0.24	0/1676	0.49	0/2259
35	b2	0.26	0/2121	0.59	0/2852
36	e2	0.25	0/1444	0.52	0/1937
37	g2	0.25	0/434	0.51	0/576
38	h2	0.25	0/1104	0.57	0/1474
39	i2	0.26	0/1122	0.55	0/1515
40	l2	0.24	0/380	0.63	0/498
41	o2	0.26	0/383	0.67	0/501
42	p	0.72	0/77	0.64	0/104
43	r2	0.25	0/901	0.59	0/1209
44	z2	0.26	0/589	0.54	0/779
All	All	0.23	3/202613 (0.0%)	0.71	51/304976 (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
1	12	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	1
9	C2	0	1
10	D1	0	2
10	D2	0	1
13	G2	0	3
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
34	a2	0	1
39	i2	0	1
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	1	G	OP3-P	-10.65	1.48	1.61
31	Y	1	G	OP3-P	-10.59	1.48	1.61
29	W	1	A	OP3-P	-10.58	1.48	1.61

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	43	G	O5'-P-OP2	-28.03	77.06	110.70
29	W	43	G	OP1-P-OP2	-27.59	78.22	119.60
29	W	43	G	O5'-P-OP1	15.97	129.86	110.70
29	W	42	G	OP1-P-O3'	-14.70	72.86	105.20
29	W	42	G	OP2-P-O3'	14.49	137.08	105.20

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	12	74	ARG	Sidechain
3	4	56	ARG	Sidechain
9	C2	42	TYR	Mainchain
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
1	12	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	34
3	4	66/70 (94%)	55 (83%)	11 (17%)	0	100	100
3	41	12/70 (17%)	10 (83%)	2 (17%)	0	100	100
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	B	231/241 (96%)	193 (84%)	34 (15%)	4 (2%)	7	36
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100	100
9	C1	211/233 (91%)	185 (88%)	24 (11%)	2 (1%)	14	51
9	C2	210/233 (90%)	185 (88%)	25 (12%)	0	100	100
10	D1	203/206 (98%)	183 (90%)	19 (9%)	1 (0%)	25	64
10	D2	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
11	E1	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
11	E2	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
12	F1	104/135 (77%)	104 (100%)	0	0	100	100
12	F2	104/135 (77%)	80 (77%)	23 (22%)	1 (1%)	13	49
13	G1	153/179 (86%)	151 (99%)	2 (1%)	0	100	100
13	G2	152/179 (85%)	122 (80%)	24 (16%)	6 (4%)	2	19
14	H1	127/130 (98%)	127 (100%)	0	0	100	100
14	H2	127/130 (98%)	127 (100%)	0	0	100	100
15	I1	125/130 (96%)	103 (82%)	22 (18%)	0	100	100
15	I2	127/130 (98%)	117 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J1	100/103 (97%)	92 (92%)	8 (8%)	0	100	100
16	J2	98/103 (95%)	86 (88%)	9 (9%)	3 (3%)	3	22
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	14	51
17	K2	116/129 (90%)	100 (86%)	15 (13%)	1 (1%)	14	51
18	L1	121/124 (98%)	115 (95%)	5 (4%)	1 (1%)	16	54
18	L2	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M1	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	M2	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
20	N1	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
20	N2	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
21	O1	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	O2	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P1	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
23	Q1	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
23	Q2	78/84 (93%)	75 (96%)	2 (3%)	1 (1%)	10	42
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9	40
24	R2	72/75 (96%)	53 (74%)	18 (25%)	1 (1%)	9	40
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
25	S2	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	5	28
27	U1	68/71 (96%)	58 (85%)	10 (15%)	0	100	100
27	U2	68/71 (96%)	60 (88%)	8 (12%)	0	100	100
33	Z1	7/557 (1%)	7 (100%)	0	0	100	100
34	a2	221/234 (94%)	201 (91%)	15 (7%)	5 (2%)	5	29
35	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
36	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
37	g2	50/55 (91%)	50 (100%)	0	0	100	100
38	h2	135/136 (99%)	135 (100%)	0	0	100	100
39	i2	147/149 (99%)	120 (82%)	25 (17%)	2 (1%)	9	40
40	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
41	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	p	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
43	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
44	z2	74/85 (87%)	74 (100%)	0	0	100	100
All	All	6206/7310 (85%)	5715 (92%)	458 (7%)	33 (0%)	27	64

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
13	G2	18	PHE
13	G2	35	LYS
13	G2	146	GLU
23	Q2	12	VAL

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	
1	12	67/68 (98%)	66 (98%)	1 (2%)	60	75
2	32	48/49 (98%)	48 (100%)	0	100	100
3	4	60/62 (97%)	58 (97%)	2 (3%)	33	54
3	41	12/62 (19%)	12 (100%)	0	100	100
4	62	51/52 (98%)	51 (100%)	0	100	100
8	B	192/199 (96%)	192 (100%)	0	100	100
8	B2	189/199 (95%)	188 (100%)	1 (0%)	86	89
9	C1	173/190 (91%)	171 (99%)	2 (1%)	67	79
9	C2	172/190 (90%)	172 (100%)	0	100	100
10	D1	172/173 (99%)	172 (100%)	0	100	100
10	D2	172/173 (99%)	170 (99%)	2 (1%)	67	79
11	E1	120/126 (95%)	120 (100%)	0	100	100
11	E2	120/126 (95%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	F1	92/116 (79%)	92 (100%)	0	100	100
12	F2	92/116 (79%)	92 (100%)	0	100	100
13	G1	128/147 (87%)	128 (100%)	0	100	100
13	G2	127/147 (86%)	127 (100%)	0	100	100
14	H1	104/105 (99%)	104 (100%)	0	100	100
14	H2	104/105 (99%)	104 (100%)	0	100	100
15	I1	105/107 (98%)	105 (100%)	0	100	100
15	I2	106/107 (99%)	106 (100%)	0	100	100
16	J1	89/90 (99%)	89 (100%)	0	100	100
16	J2	88/90 (98%)	88 (100%)	0	100	100
17	K1	88/99 (89%)	88 (100%)	0	100	100
17	K2	91/99 (92%)	90 (99%)	1 (1%)	70	80
18	L1	103/104 (99%)	103 (100%)	0	100	100
18	L2	103/104 (99%)	103 (100%)	0	100	100
19	M1	93/96 (97%)	93 (100%)	0	100	100
19	M2	95/96 (99%)	95 (100%)	0	100	100
20	N1	83/84 (99%)	83 (100%)	0	100	100
20	N2	83/84 (99%)	83 (100%)	0	100	100
21	O1	76/77 (99%)	76 (100%)	0	100	100
21	O2	76/77 (99%)	76 (100%)	0	100	100
22	P1	65/65 (100%)	65 (100%)	0	100	100
23	Q1	74/78 (95%)	74 (100%)	0	100	100
23	Q2	74/78 (95%)	74 (100%)	0	100	100
24	R1	64/65 (98%)	64 (100%)	0	100	100
24	R2	64/65 (98%)	63 (98%)	1 (2%)	58	74
25	S1	72/79 (91%)	72 (100%)	0	100	100
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	63 (97%)	2 (3%)	35	55
27	U1	60/61 (98%)	59 (98%)	1 (2%)	56	72
27	U2	60/61 (98%)	60 (100%)	0	100	100
33	Z1	8/461 (2%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	a2	174/181 (96%)	174 (100%)	0	100	100
35	b2	216/218 (99%)	216 (100%)	0	100	100
36	e2	149/150 (99%)	148 (99%)	1 (1%)	81	87
37	g2	47/49 (96%)	47 (100%)	0	100	100
38	h2	110/109 (101%)	110 (100%)	0	100	100
39	i2	114/114 (100%)	114 (100%)	0	100	100
40	l2	38/38 (100%)	37 (97%)	1 (3%)	41	61
41	o2	35/103 (34%)	35 (100%)	0	100	100
42	p	5/5 (100%)	2 (40%)	3 (60%)	0	0
43	r2	86/87 (99%)	86 (100%)	0	100	100
44	z2	58/63 (92%)	58 (100%)	0	100	100
All	All	5184/5994 (86%)	5166 (100%)	18 (0%)	90	91

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	l2	3	ARG
42	p	35	TRP
42	p	34	ARG
17	K2	13	ARG
36	e2	3	LYS

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

Mol	Chain	Res	Type
18	L2	29	GLN
35	b2	243	HIS
15	I1	75	GLN
15	I2	75	GLN
17	K1	40	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	58/59 (98%)	39 (67%)	8 (13%)
29	W	74/76 (97%)	28 (37%)	3 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	W1	31/76 (40%)	7 (22%)	2 (6%)
31	Y	75/76 (98%)	19 (25%)	2 (2%)
32	Y1	32/76 (42%)	5 (15%)	2 (6%)
5	71	17/2904 (0%)	1 (5%)	0
5	72	2899/2904 (99%)	458 (15%)	36 (1%)
6	82	119/120 (99%)	21 (17%)	3 (2%)
7	A1	1538/1542 (99%)	445 (28%)	36 (2%)
7	A2	1533/1542 (99%)	392 (25%)	30 (1%)
All	All	6376/9375 (68%)	1415 (22%)	122 (1%)

5 of 1415 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1907	G
5	72	10	A
5	72	15	G
5	72	34	U
5	72	44	A

5 of 122 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A1	686	U
28	V2	39	A
7	A1	1440	U
28	V2	37	A
31	Y	17	H2U

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

64 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
5	3TD	71	1915	5	19,22,23	4.07	7 (36%)	21,32,35	1.75	3 (14%)
7	UR3	A1	1498	7	19,22,23	2.77	8 (42%)	26,32,35	1.28	1 (3%)
30	MIA	W1	37	30	24,31,32	2.34	3 (12%)	26,44,47	2.74	7 (26%)
7	2MG	A1	1516	7	18,26,27	2.86	7 (38%)	16,38,41	1.35	3 (18%)
7	G7M	A2	527	7	20,26,27	6.09	12 (60%)	17,39,42	1.54	4 (23%)
5	1MG	72	745	5	18,26,27	2.74	6 (33%)	19,39,42	1.45	3 (15%)
31	5MU	Y	54	31	19,22,23	4.12	14 (73%)	28,32,35	3.97	12 (42%)
7	5MC	A2	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.00	2 (7%)
7	MA6	A1	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.39	3 (15%)
7	2MG	A2	966	7	18,26,27	2.84	7 (38%)	16,38,41	1.35	3 (18%)
5	PSU	72	746	5	18,21,22	0.91	1 (5%)	22,30,33	0.61	0
5	PSU	72	2580	5	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
31	PSU	Y	55	31	18,21,22	5.79	14 (77%)	22,30,33	1.98	5 (22%)
5	PSU	72	2604	5	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)
5	6MZ	72	1618	5	18,25,26	2.04	2 (11%)	16,36,39	2.27	4 (25%)
29	H2U	W	17	29	18,21,22	3.06	5 (27%)	21,30,33	2.02	5 (23%)
29	PSU	W	32	29	18,21,22	4.66	8 (44%)	22,30,33	1.88	5 (22%)
7	MA6	A2	1519	7	18,26,27	1.06	2 (11%)	19,38,41	3.38	3 (15%)
7	2MG	A1	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.32	3 (18%)
7	4OC	A2	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.91	1 (3%)
29	4SU	W	8	29	18,21,22	3.81	7 (38%)	26,30,33	2.28	4 (15%)
29	H2U	W	20	29	18,21,22	3.06	5 (27%)	21,30,33	2.03	5 (23%)
7	2MG	A1	966	7	18,26,27	2.84	7 (38%)	16,38,41	1.41	4 (25%)
29	G7M	W	46	29	20,26,27	2.81	7 (35%)	17,39,42	1.11	1 (5%)
5	6MZ	72	2030	5	18,25,26	2.07	4 (22%)	16,36,39	2.33	3 (18%)
29	PSU	W	55	29	18,21,22	5.78	13 (72%)	22,30,33	2.12	5 (22%)
30	G7M	W1	46	30	20,26,27	2.82	7 (35%)	17,39,42	1.13	1 (5%)
5	3TD	72	1915	5	19,22,23	0.83	1 (5%)	21,32,35	0.70	0
7	2MG	A2	1516	7	18,26,27	2.85	7 (38%)	16,38,41	1.36	3 (18%)
7	G7M	A1	527	7	20,26,27	2.80	8 (40%)	17,39,42	1.02	1 (5%)
7	MA6	A2	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.37	3 (15%)
29	H2U	W	16	29	18,21,22	3.04	5 (27%)	21,30,33	1.99	5 (23%)
5	PSU	72	2605	5	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	2MG	72	1835	5	18,26,27	2.84	7 (38%)	16,38,41	1.45	4 (25%)
5	H2U	72	2449	5,48	18,21,22	3.05	5 (27%)	21,30,33	2.05	5 (23%)
5	OMC	72	2498	5,48	19,22,23	3.29	8 (42%)	26,31,34	0.75	0
29	MIA	W	37	29	24,31,32	2.28	3 (12%)	26,44,47	3.01	8 (30%)
5	2MA	72	2503	5,48	17,25,26	2.65	5 (29%)	17,37,40	1.33	2 (11%)
7	5MC	A1	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.02	2 (7%)
7	5MC	A1	1407	7	18,22,23	4.04	7 (38%)	26,32,35	0.96	2 (7%)
5	PSU	72	2504	5,48	18,21,22	4.69	8 (44%)	22,30,33	1.85	5 (22%)
31	G7M	Y	46	31	20,26,27	2.82	8 (40%)	17,39,42	1.10	1 (5%)
29	5MU	W	54	29	19,22,23	4.11	14 (73%)	28,32,35	3.89	14 (50%)
7	MA6	A1	1519	7	18,26,27	1.07	2 (11%)	19,38,41	3.40	3 (15%)
7	2MG	A2	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.38	3 (18%)
7	UR3	A2	1498	7	19,22,23	2.78	8 (42%)	26,32,35	1.33	3 (11%)
32	6MZ	Y1	37	32	18,25,26	2.05	4 (22%)	16,36,39	2.44	4 (25%)
30	PSU	W1	32	30	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
32	CM0	Y1	34	32	23,26,27	3.74	6 (26%)	27,37,40	1.60	3 (11%)
5	OMG	72	2251	5,31	18,26,27	2.84	7 (38%)	19,38,41	1.53	4 (21%)
5	PSU	72	955	5	18,21,22	4.68	8 (44%)	22,30,33	1.87	5 (22%)
32	7MG	Y1	46	32	22,26,27	3.89	10 (45%)	29,39,42	2.03	9 (31%)
31	H2U	Y	17	31	18,21,22	3.09	5 (27%)	21,30,33	2.02	5 (23%)
5	2MG	72	2445	5	18,26,27	2.85	7 (38%)	16,38,41	1.37	3 (18%)
5	PSU	72	2457	5	18,21,22	4.65	8 (44%)	22,30,33	1.89	5 (22%)
5	G7M	72	2069	5	20,26,27	2.79	8 (40%)	17,39,42	1.03	1 (5%)
30	4SU	W1	8	30	18,21,22	3.80	7 (38%)	26,30,33	2.24	5 (19%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
5	5MU	72	1939	5	19,22,23	4.16	15 (78%)	28,32,35	4.12	12 (42%)
30	PSU	W1	39	30	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
7	4OC	A1	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.89	1 (3%)
5	5MC	72	1962	5	18,22,23	4.04	7 (38%)	26,32,35	1.05	2 (7%)
5	5MU	72	747	5	19,22,23	0.27	0	28,32,35	0.58	0
7	5MC	A2	1407	7	18,22,23	4.04	7 (38%)	26,32,35	0.96	2 (7%)

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
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
30	MIA	W1	37	30	-	6/11/33/34	0/3/3/3
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
7	G7M	A2	527	7	-	2/3/25/26	0/3/3/3
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
31	5MU	Y	54	31	-	0/7/25/26	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
7	MA6	A1	1518	7	-	3/7/29/30	0/3/3/3
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
5	PSU	72	746	5	-	4/7/25/26	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
31	PSU	Y	55	31	-	2/7/25/26	0/2/2/2
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
29	H2U	W	17	29	-	2/7/38/39	0/2/2/2
29	PSU	W	32	29	-	3/7/25/26	0/2/2/2
7	MA6	A2	1519	7	-	2/7/29/30	0/3/3/3
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
29	4SU	W	8	29	-	0/7/25/26	0/2/2/2
29	H2U	W	20	29	-	3/7/38/39	0/2/2/2
7	2MG	A1	966	7	-	0/5/27/28	0/3/3/3
29	G7M	W	46	29	-	1/3/25/26	0/3/3/3
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
29	PSU	W	55	29	-	1/7/25/26	0/2/2/2
30	G7M	W1	46	30	-	2/3/25/26	0/3/3/3
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3
7	MA6	A2	1518	7	-	0/7/29/30	0/3/3/3
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3
5	H2U	72	2449	5,48	-	0/7/38/39	0/2/2/2
5	OMC	72	2498	5,48	-	2/9/27/28	0/2/2/2
29	MIA	W	37	29	-	6/11/33/34	0/3/3/3
5	2MA	72	2503	5,48	-	0/3/25/26	0/3/3/3
7	5MC	A1	967	7	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
5	PSU	72	2504	5,48	-	0/7/25/26	0/2/2/2
31	G7M	Y	46	31	-	2/3/25/26	0/3/3/3
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2
7	MA6	A1	1519	7	-	4/7/29/30	0/3/3/3
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
32	CM0	Y1	34	32	-	4/12/30/31	0/2/2/2
5	OMG	72	2251	5,31	-	3/5/27/28	0/3/3/3
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
31	H2U	Y	17	31	-	7/7/38/39	0/2/2/2
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
5	PSU	72	2457	5	-	0/7/25/26	0/2/2/2
5	G7M	72	2069	5	-	2/3/25/26	0/3/3/3
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
5	5MU	72	1939	5	-	2/7/25/26	0/2/2/2
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
7	4OC	A1	1402	7	-	1/9/29/30	0/2/2/2
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
5	5MU	72	747	5	-	1/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2

The worst 5 of 437 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	527	G7M	C2'-C1'	-18.04	1.26	1.53
32	Y1	34	CM0	C6-C5	12.73	1.48	1.34
5	71	1915	3TD	C6-C5	12.65	1.50	1.35
5	72	955	PSU	C6-C5	12.25	1.49	1.35
5	72	2504	PSU	C6-C5	12.20	1.49	1.35

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A1	1519	MA6	N1-C6-N6	-12.36	104.05	117.06
7	A2	1519	MA6	N1-C6-N6	-12.35	104.06	117.06

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A1	1518	MA6	N1-C6-N6	-12.22	104.19	117.06
7	A2	1518	MA6	N1-C6-N6	-12.12	104.30	117.06
29	W	37	MIA	C11-S10-C2	11.00	110.48	102.27

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	1402	4OC	C1'-C2'-O2'-CM2
7	A1	1518	MA6	C5-C6-N6-C9
7	A1	1518	MA6	C5-C6-N6-C10
7	A1	1519	MA6	C3'-C4'-C5'-O5'
7	A2	527	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 271 are monoatomic - leaving 3 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	$\# Z > 2$
46	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.52	0
47	SPD	72	3003	-	9,9,9	0.33	0	8,8,8	0.88	0
46	PUT	72	3002	-	5,5,5	0.25	0	4,4,4	0.54	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
46	PUT	72	3001	-	-	1/3/3/3	-
47	SPD	72	3003	-	-	0/7/7/7	-
46	PUT	72	3002	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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.

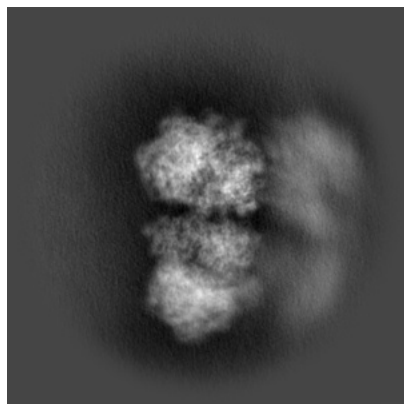
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19058. These allow visual inspection of the internal detail of the map and identification of artifacts.

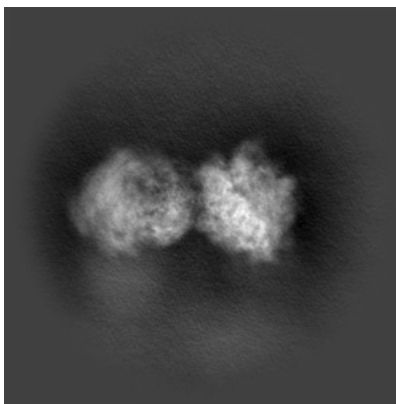
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

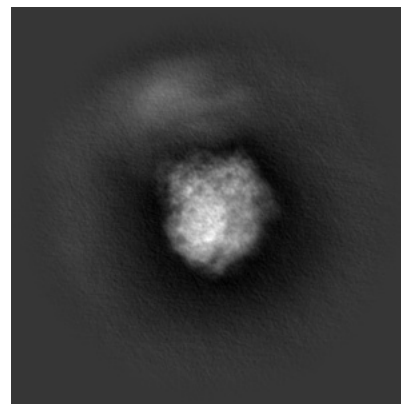
6.1.1 Primary map



X

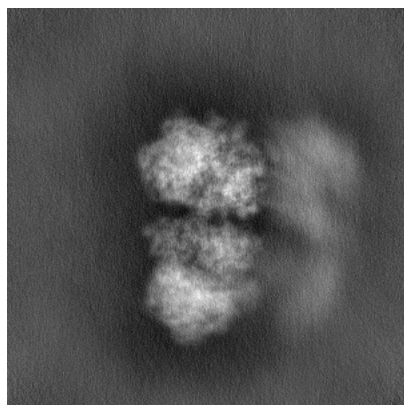


Y

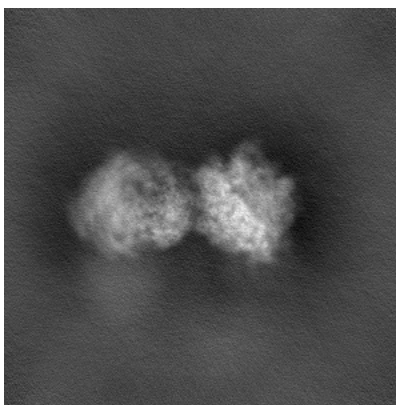


Z

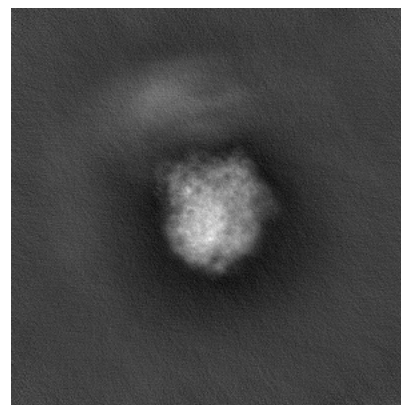
6.1.2 Raw map



X



Y

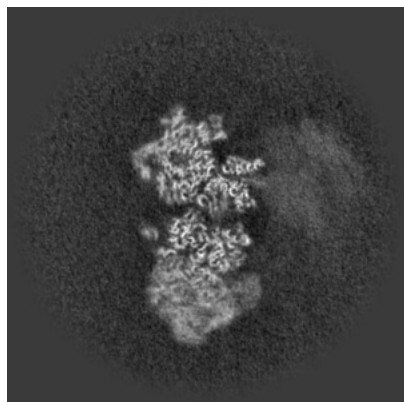


Z

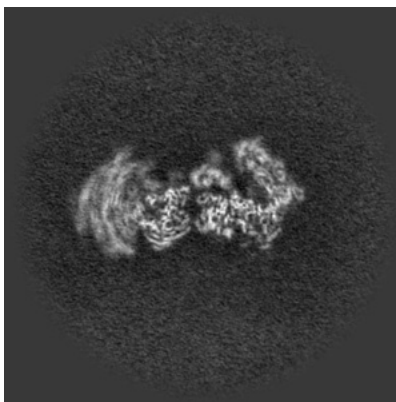
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

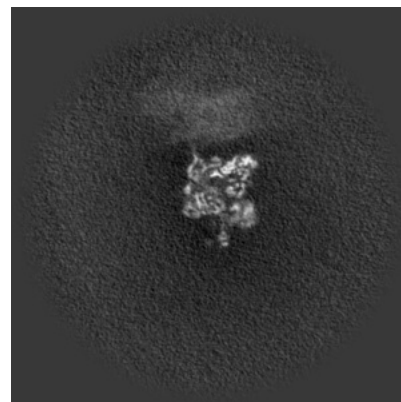
6.2.1 Primary map



X Index: 234

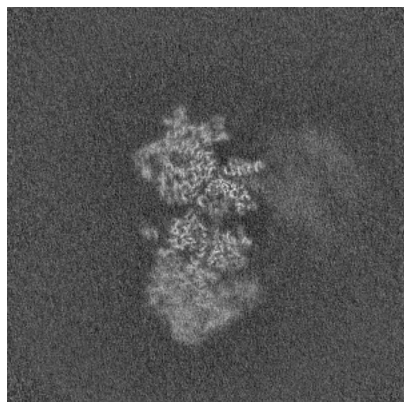


Y Index: 234

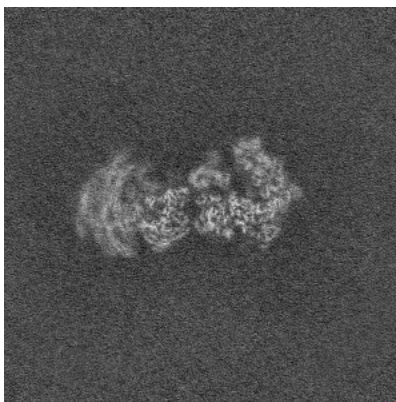


Z Index: 234

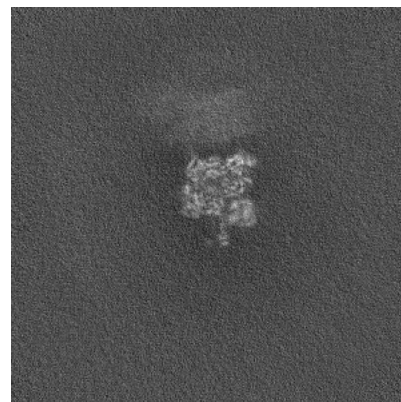
6.2.2 Raw map



X Index: 234



Y Index: 234

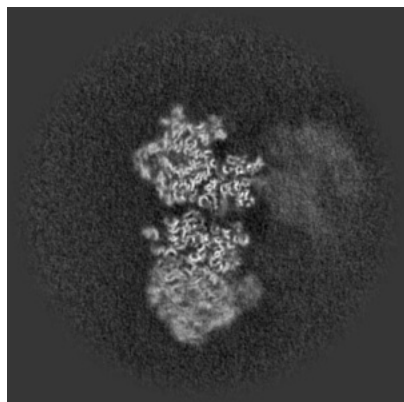


Z Index: 234

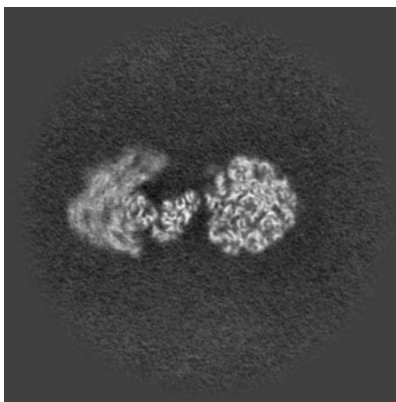
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

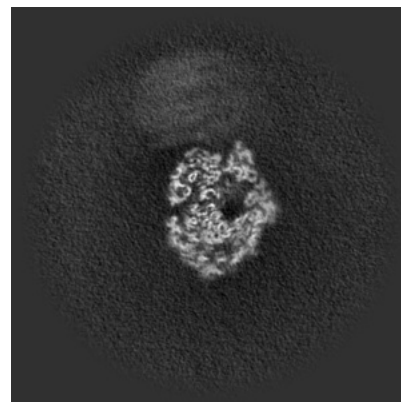
6.3.1 Primary map



X Index: 232

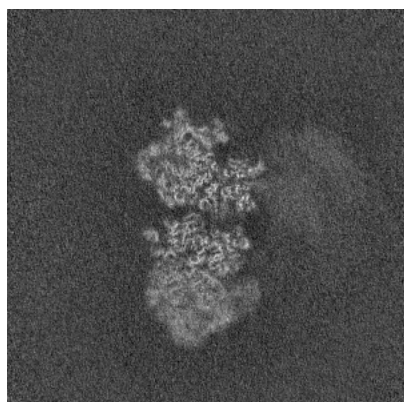


Y Index: 208

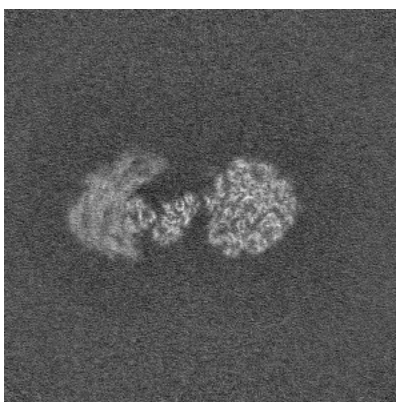


Z Index: 278

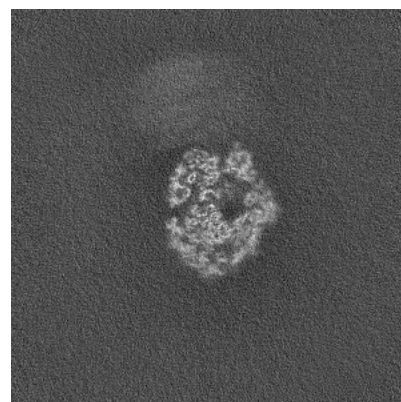
6.3.2 Raw map



X Index: 231



Y Index: 209

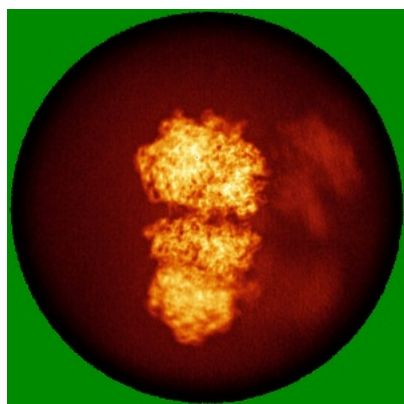


Z Index: 277

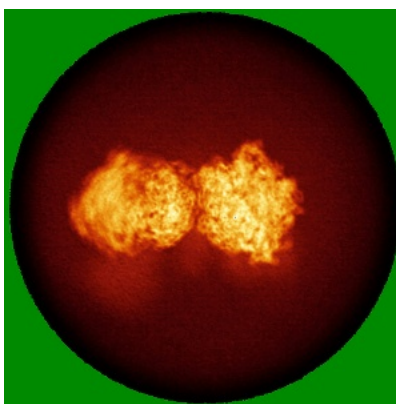
The images above show the largest variance slices of the map in three orthogonal directions.

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

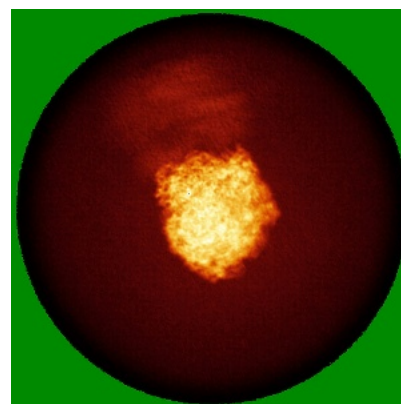
6.4.1 Primary map



X

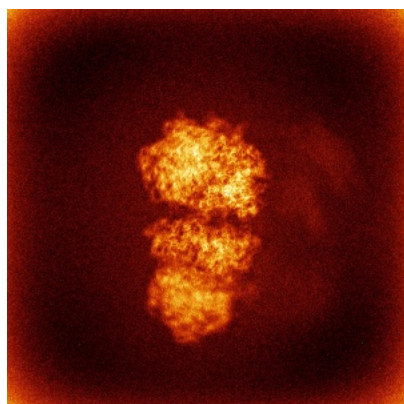


Y

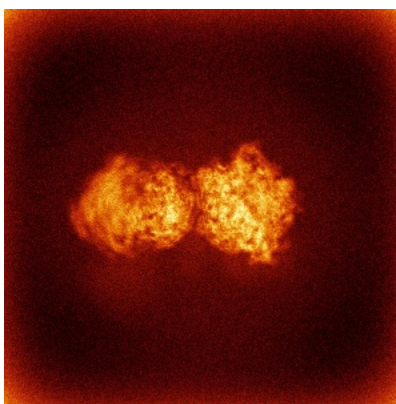


Z

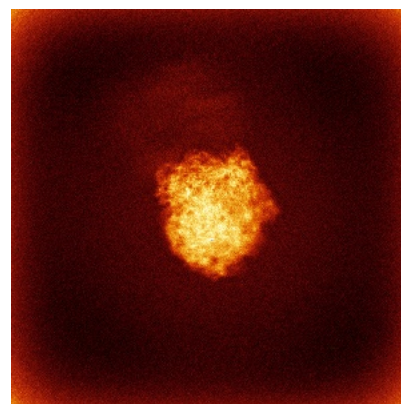
6.4.2 Raw map



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](#)

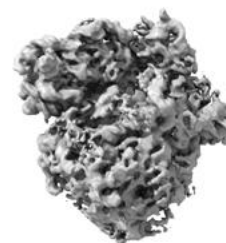
6.5.1 Primary map



X



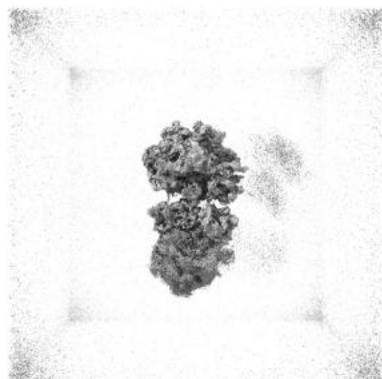
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

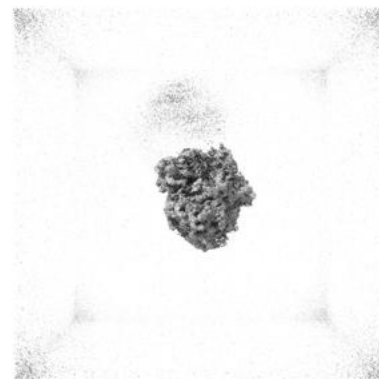
6.5.2 Raw map



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.

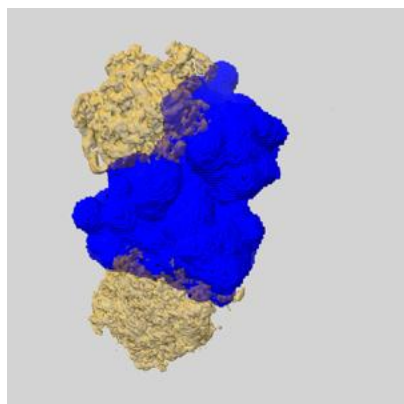
6.6 Mask visualisation [i](#)

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

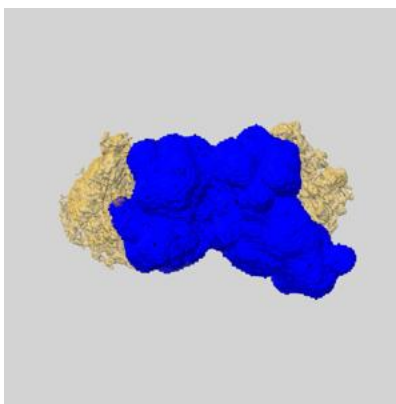
A mask typically either:

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

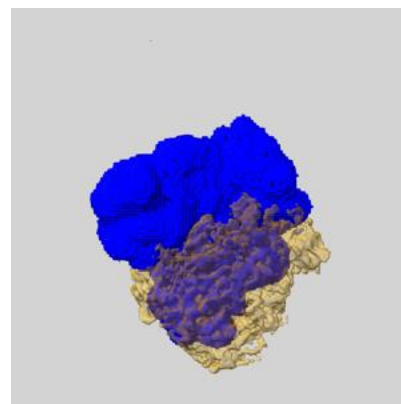
6.6.1 emd_19058_msk_1.map [i](#)



X



Y

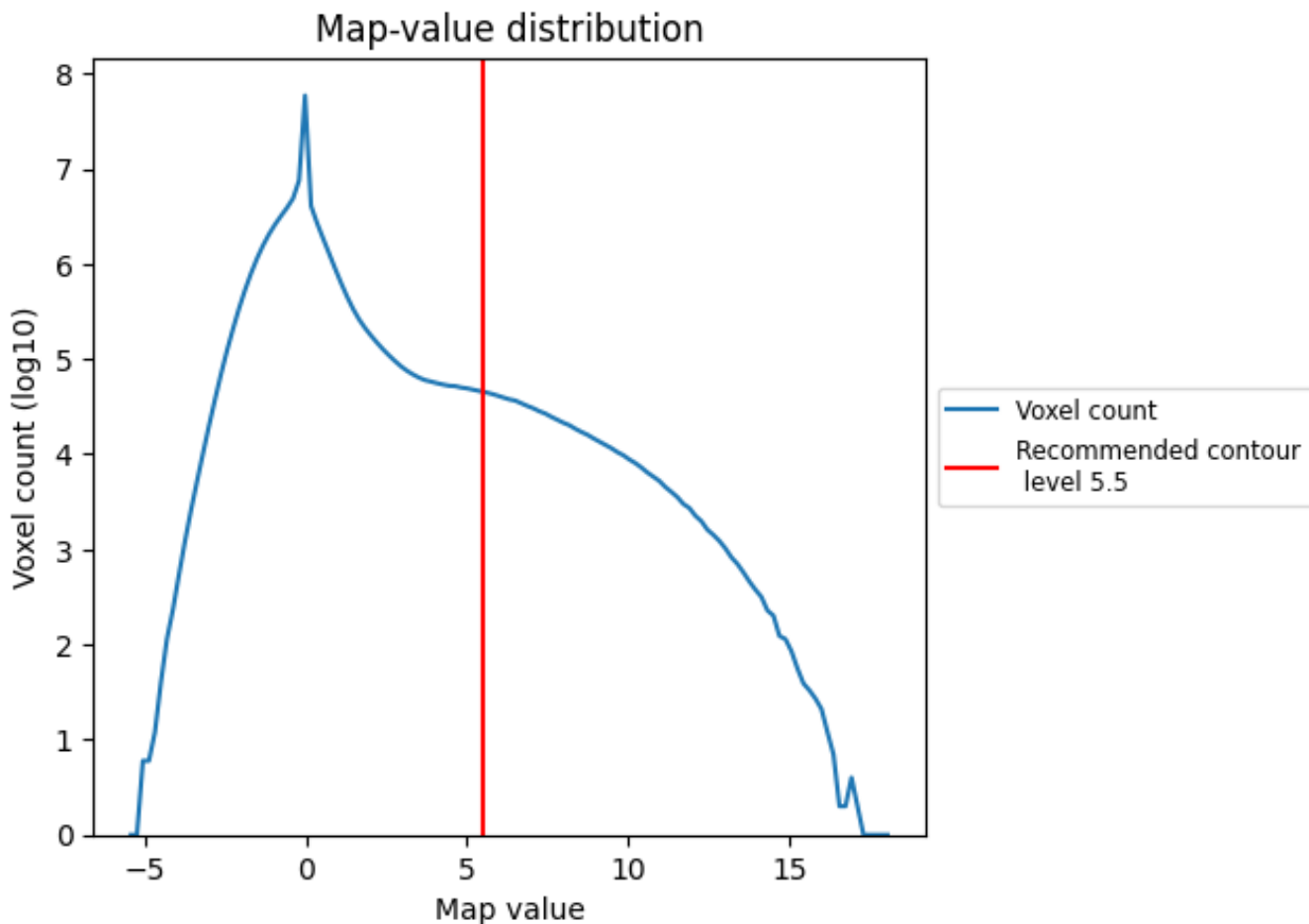


Z

7 Map analysis [i](#)

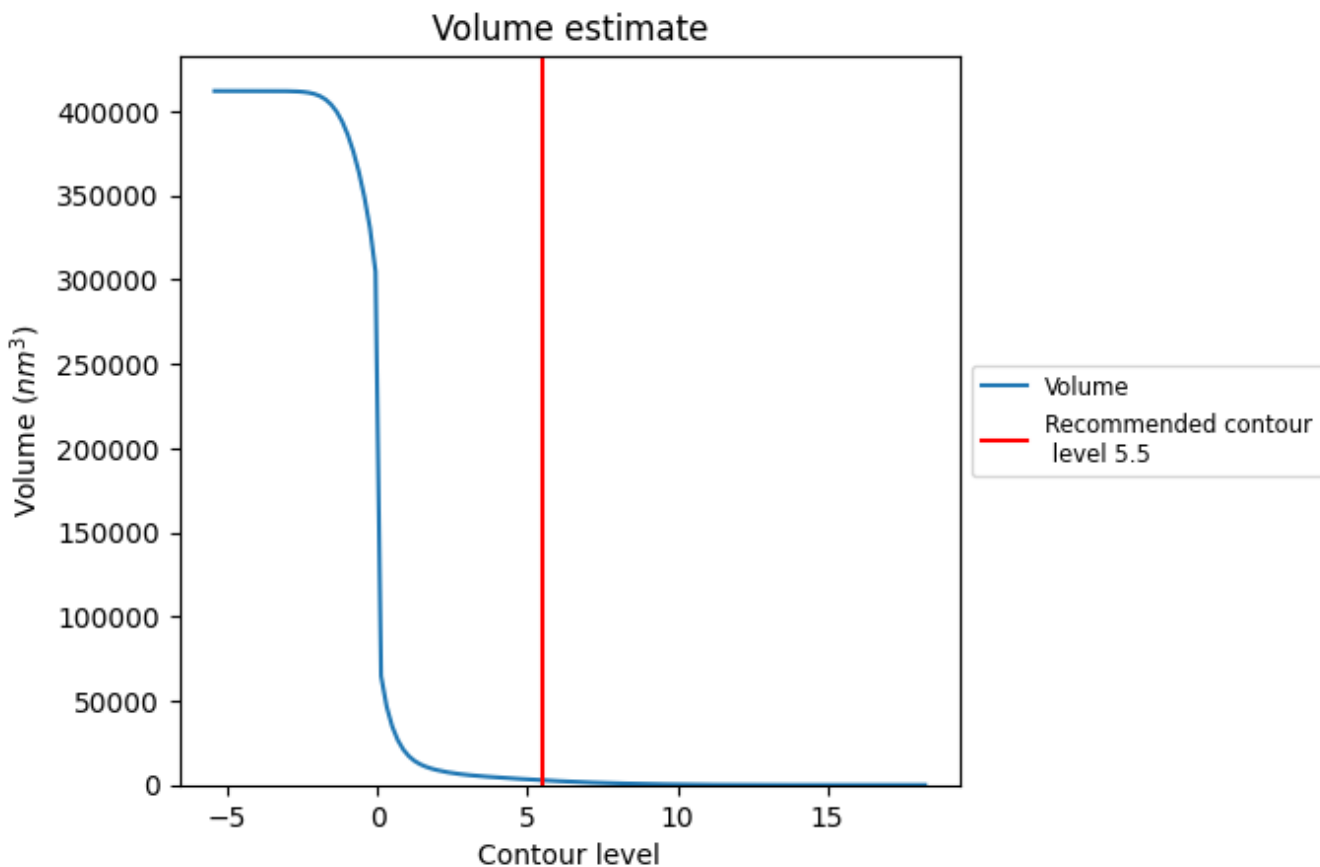
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

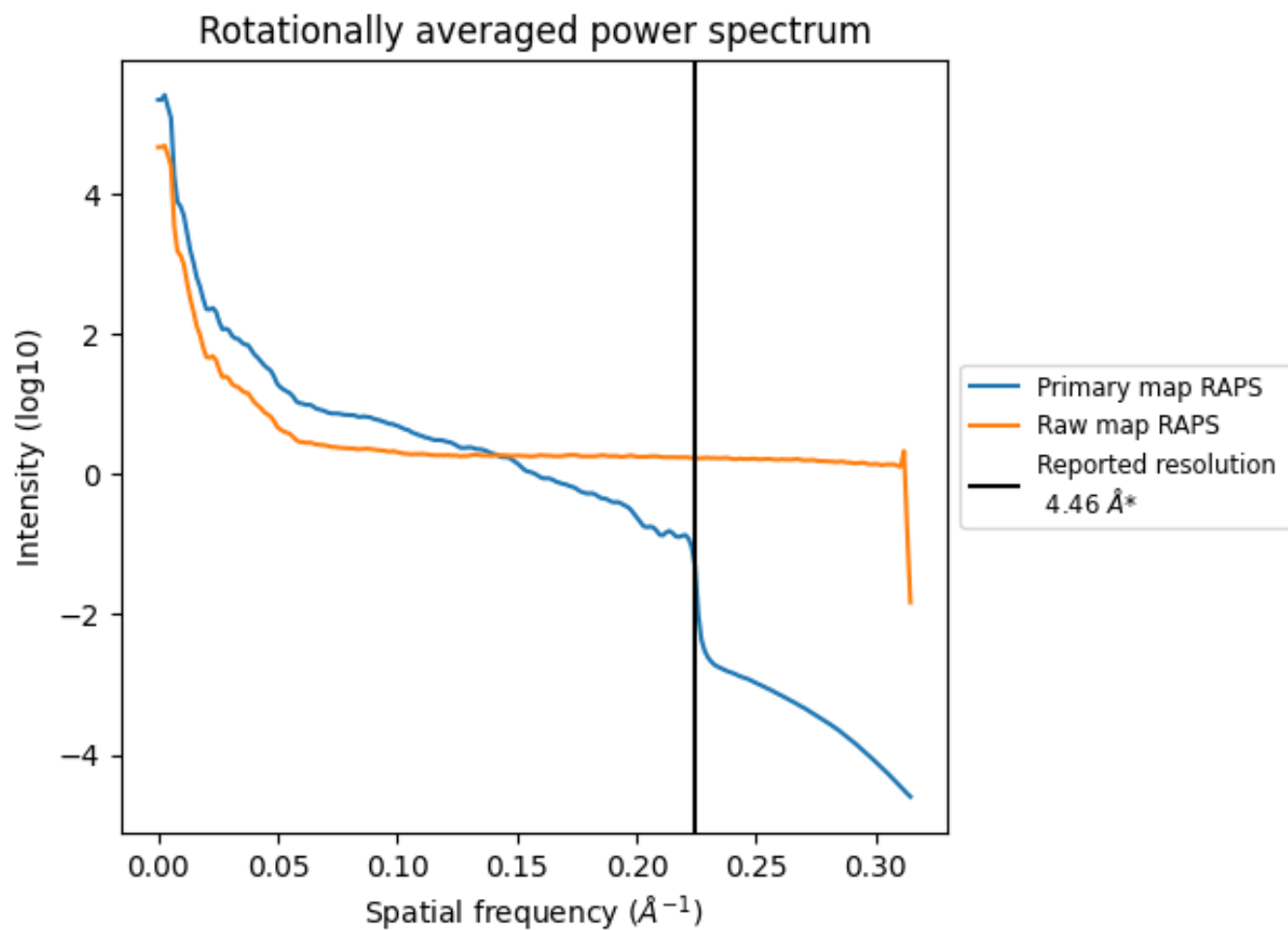
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2813 nm^3 ; this corresponds to an approximate mass of 2541 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

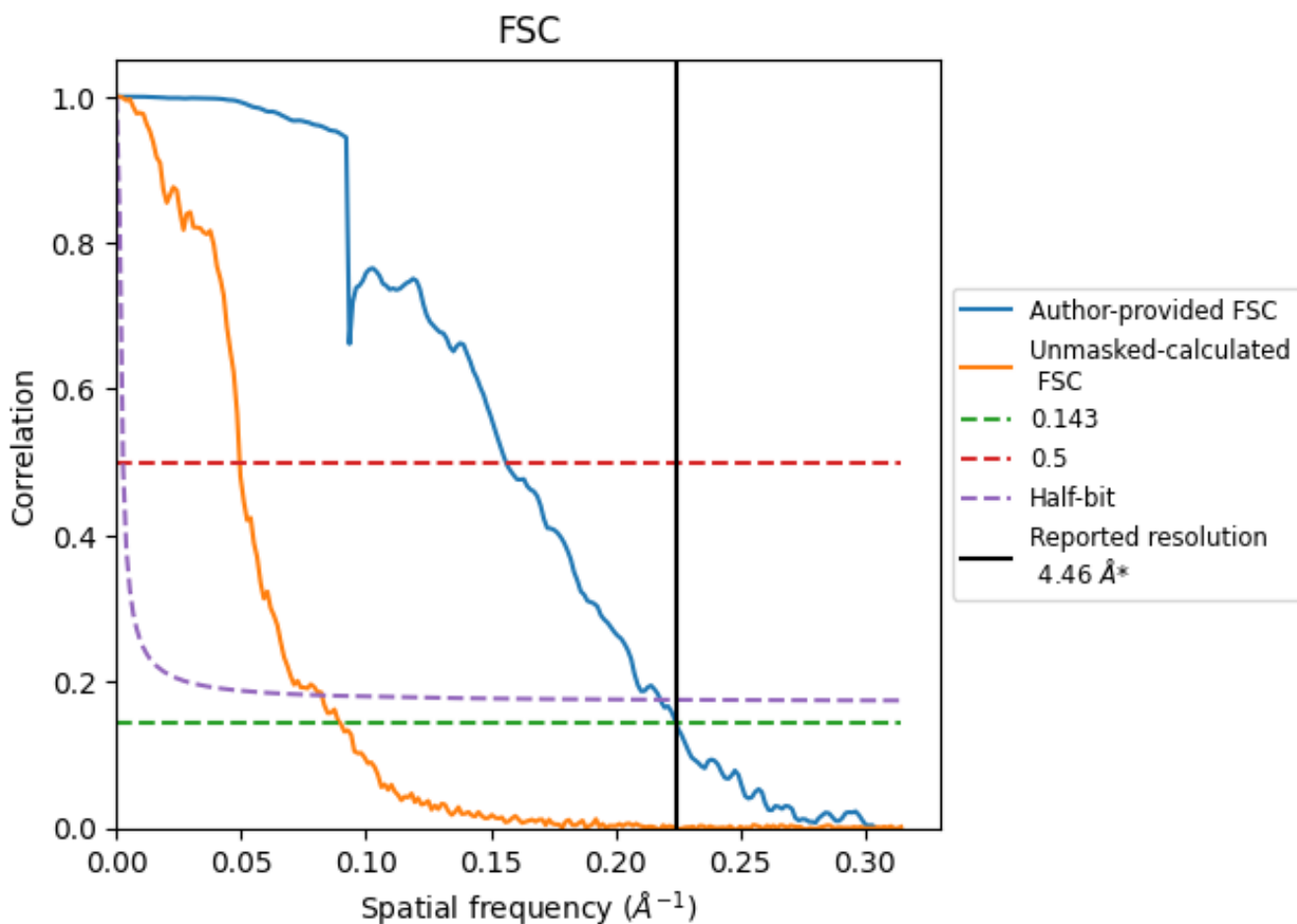


*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

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 0.224 Å⁻¹

8.2 Resolution estimates [i](#)

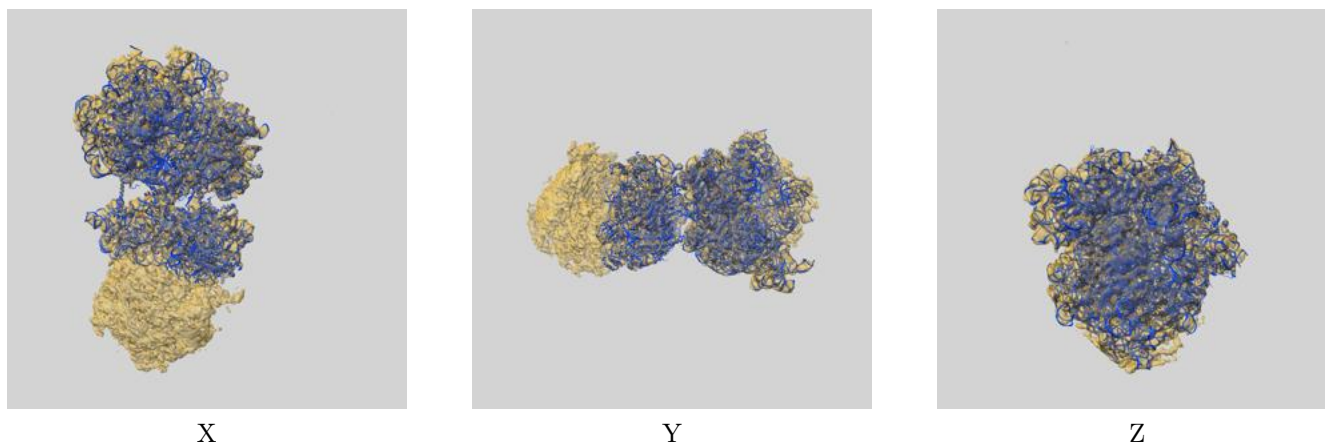
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.46	-	-
Author-provided FSC curve	4.46	6.41	4.59
Unmasked-calculated*	11.15	20.24	12.15

*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 11.15 differs from the reported value 4.46 by more than 10 %

9 Map-model fit [i](#)

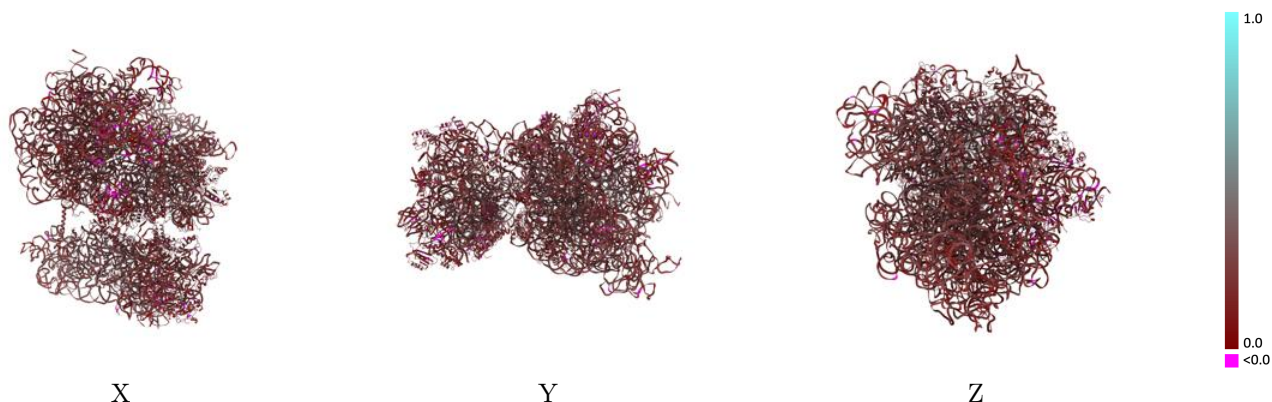
This section contains information regarding the fit between EMDB map EMD-19058 and PDB model 8RCS. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



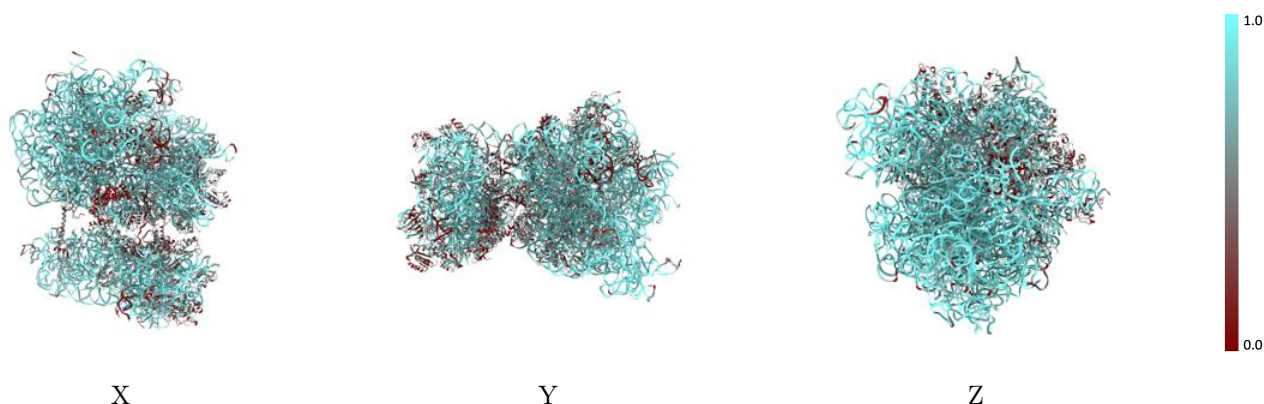
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



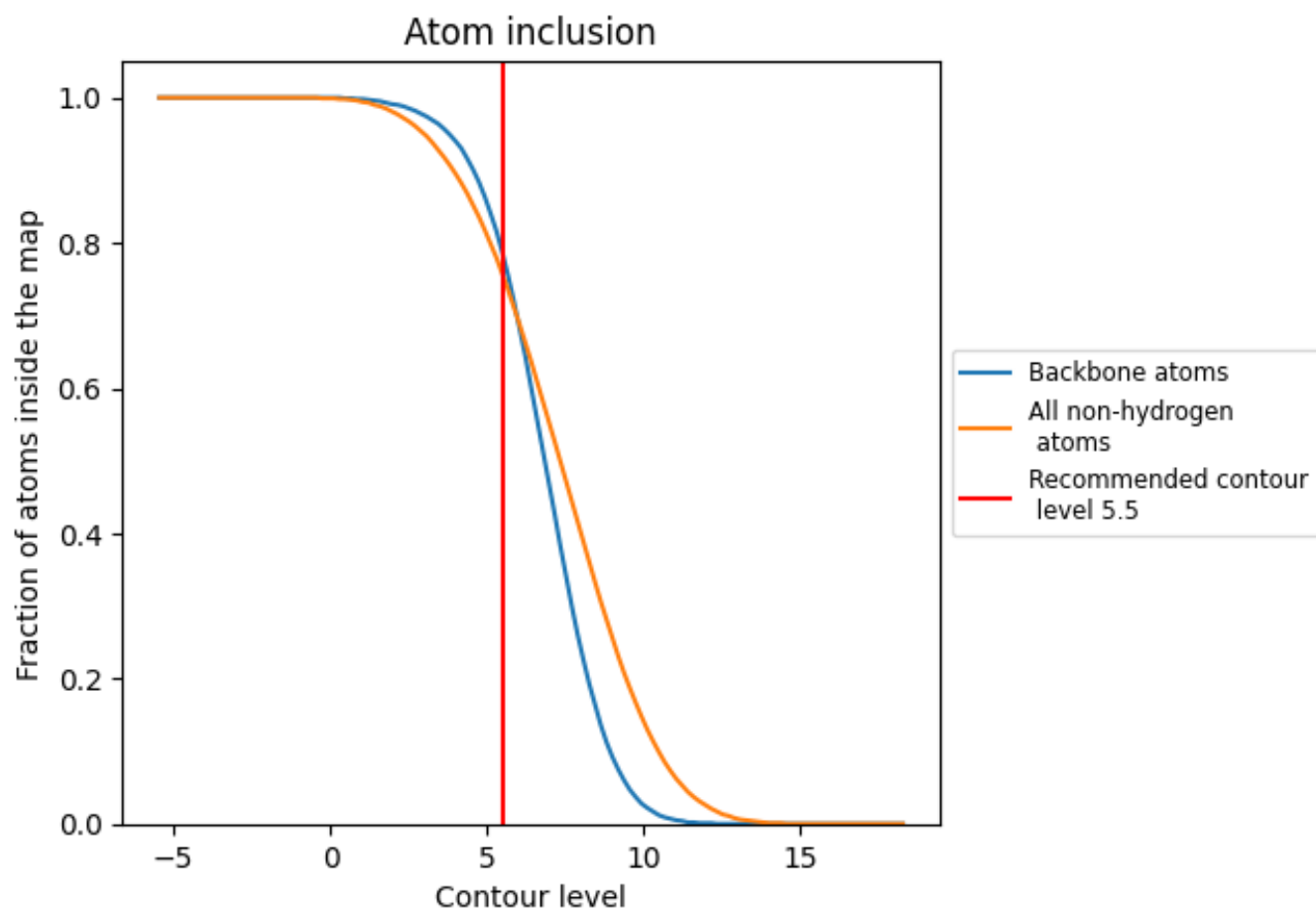
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 76% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.2180
12	 0.5070	 0.1680
32	 0.5290	 0.1480
4	 0.2980	 0.1790
41	 0.4200	 0.1170
62	 0.4970	 0.1430
71	 0.8450	 0.2240
72	 0.8780	 0.2160
82	 0.8650	 0.1880
A1	 0.8880	 0.2410
A2	 0.9090	 0.2580
B	 0.3240	 0.1820
B2	 0.4600	 0.2080
C1	 0.4260	 0.2170
C2	 0.5350	 0.2230
D1	 0.4100	 0.1840
D2	 0.3910	 0.1920
E1	 0.3630	 0.2090
E2	 0.5240	 0.2310
F1	 0.2410	 0.1600
F2	 0.3570	 0.2020
G1	 0.3980	 0.1620
G2	 0.4920	 0.2020
H1	 0.4480	 0.1740
H2	 0.5210	 0.2020
I1	 0.5380	 0.1880
I2	 0.5600	 0.2020
J1	 0.4310	 0.1840
J2	 0.4950	 0.2130
K1	 0.3570	 0.1750
K2	 0.4300	 0.2200
L1	 0.4980	 0.2220
L2	 0.5760	 0.2270
M1	 0.4620	 0.1640
M2	 0.4950	 0.1870



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Chain	Atom inclusion	Q-score
N1	 0.5450	 0.1770
N2	 0.6250	 0.1940
O1	 0.4880	 0.1710
O2	 0.5170	 0.1850
P1	 0.4700	 0.2050
Q1	 0.4620	 0.1770
Q2	 0.5000	 0.1960
R1	 0.3380	 0.1660
R2	 0.3290	 0.1830
S1	 0.4390	 0.1330
S2	 0.6110	 0.2030
T1	 0.5760	 0.1660
U1	 0.3550	 0.1650
U2	 0.3960	 0.1910
V2	 0.3700	 0.1890
W	 0.8040	 0.2290
W1	 0.7310	 0.1870
Y	 0.0650	 0.1340
Y1	 0.2280	 0.1870
Z1	 0.0000	 0.1070
a2	 0.1170	 0.1060
b2	 0.4670	 0.1930
e2	 0.3810	 0.1460
g2	 0.4220	 0.1360
h2	 0.4230	 0.1710
i2	 0.2950	 0.2000
l2	 0.5690	 0.1690
o2	 0.5730	 0.1260
p	 0.0280	 -0.0080
r2	 0.5000	 0.1180
z2	 0.5710	 0.1210