



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 12:58 pm BST

PDB ID : 7PJY / pdb_00007pjy
EMDB ID : EMD-13464
Title : Structure of the 70S-EF-G-GDP ribosome complex with tRNAs in chimeric state 1 (CHI1-EF-G-GDP)
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on : 2021-08-24
Resolution : 3.10 Å (reported)
Based on initial models : 5J9Z, 4AQY, 5LZD, 6YSS

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:

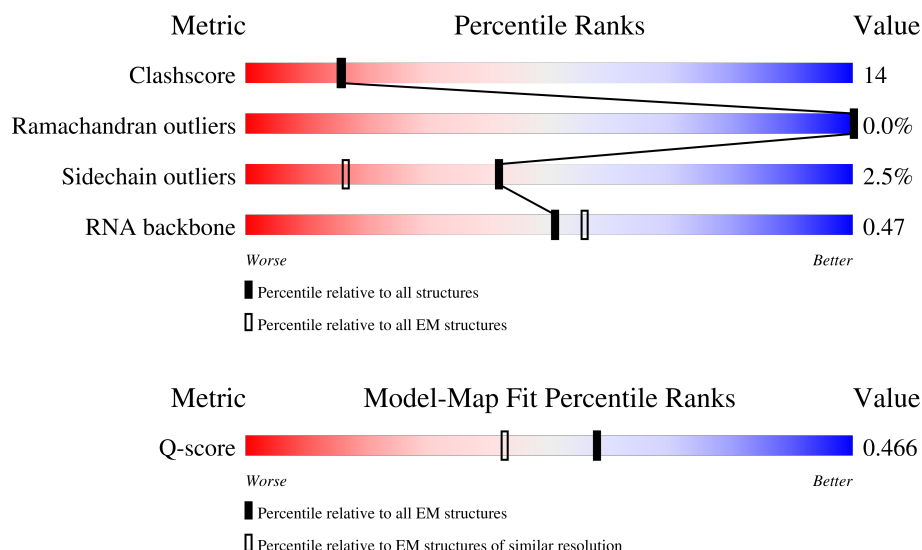
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	0	57	 65% 33%
2	1	55	 56% 35% 9%

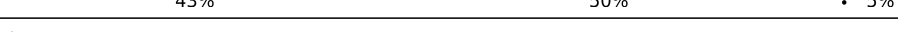
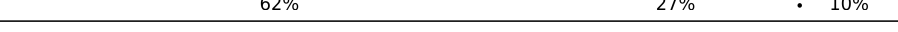
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Mol	Chain	Length	Quality of chain
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	
9	B	120	
10	C	273	
11	D	209	
12	E	201	
13	F	179	
14	G	177	
15	H	149	
16	I	142	
17	J	142	
18	K	123	
19	L	144	
20	M	136	
21	N	127	
22	O	117	
23	P	115	
24	Q	118	
25	R	103	
26	S	110	
27	T	100	

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Mol	Chain	Length	Quality of chain
28	U	104	
29	V	94	
30	W	85	
31	X	78	
32	Y	63	
33	Z	59	
34	a	1542	
35	b	240	
36	c	233	
37	d	206	
38	e	167	
39	f	135	
40	g	179	
41	h	130	
42	i	130	
43	j	103	
44	k	129	
45	l	124	
46	m	118	
47	n	102	
48	o	89	
49	p	82	
50	q	84	
51	r	75	
52	s	92	

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Mol	Chain	Length	Quality of chain
53	t	87	60% 38%
54	u	71	68% 20% 8%
55	v	77	43% 36% 19%
56	w	76	37% 49% 12%
57	x	704	7% 50% 44% 5%
58	y	2	50% 50%
59	z	33	21% 6% 70%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153095 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 L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62338	27816	11471	20148	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 15 is a protein called 50S ribosomal protein L9.

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

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

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	697	Total	C	N	O	S	1	0
			5416	3413	938	1040	25		

- Molecule 58 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	10	Total	C	N	O	P	0	0
			208	93	29	76	10		

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Mg	0
			1	1	
60	1	1	Total	Mg	0
			1	1	
60	6	1	Total	Mg	0
			1	1	
60	A	267	Total	Mg	0
			267	267	
60	B	6	Total	Mg	0
			6	6	
60	C	3	Total	Mg	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
60	D	1	Total 1	Mg 1	0
60	M	1	Total 1	Mg 1	0
60	O	1	Total 1	Mg 1	0
60	P	1	Total 1	Mg 1	0
60	a	34	Total 34	Mg 34	0
60	w	1	Total 1	Mg 1	0

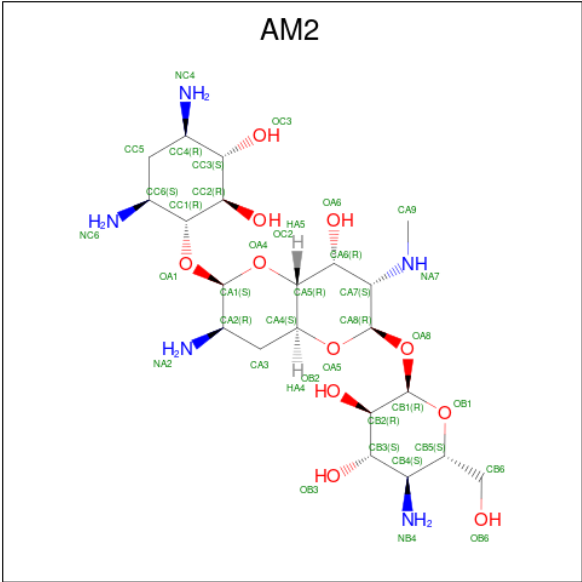
- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	4	1	Total 1	Zn 1	0
61	6	1	Total 1	Zn 1	0

- Molecule 62 is SODIUM ION (CCD ID: NA) (formula: Na).

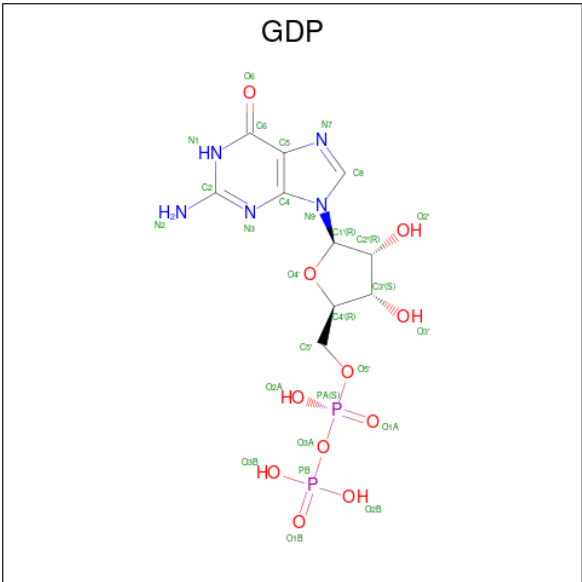
Mol	Chain	Residues	Atoms		AltConf
62	B	1	Total 1	Na 1	0

- Molecule 63 is APRAMYCIN (CCD ID: AM2) (formula: C₂₁H₄₁N₅O₁₁).



Mol	Chain	Residues	Atoms				AltConf
63	a	1	Total	C	N	O	0
			37	21	5	11	
63	a	1	Total	C	N	O	0
			37	21	5	11	
63	a	1	Total	C	N	O	0
			37	21	5	11	
63	a	1	Total	C	N	O	0
			37	21	5	11	

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

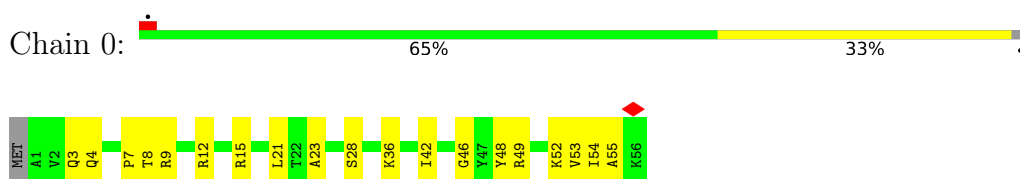


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	x	1	28	10	5	11	2	0

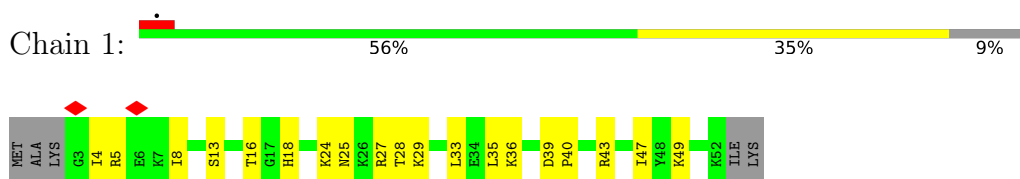
3 Residue-property plots [i](#)

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

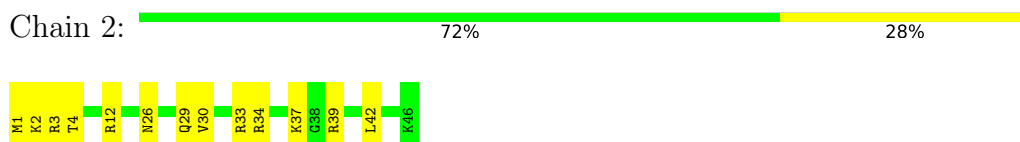
- Molecule 1: 50S ribosomal protein L32



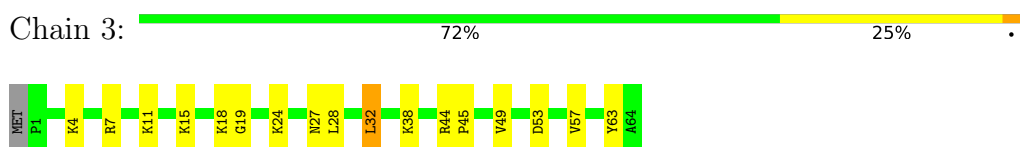
- Molecule 2: 50S ribosomal protein L33



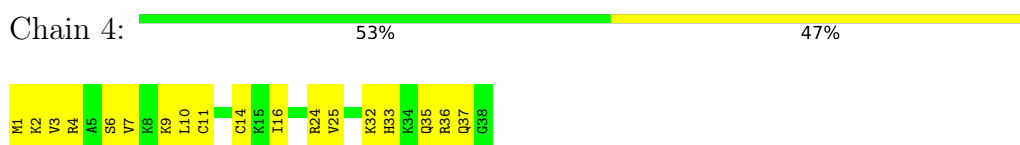
- Molecule 3: 50S ribosomal protein L34



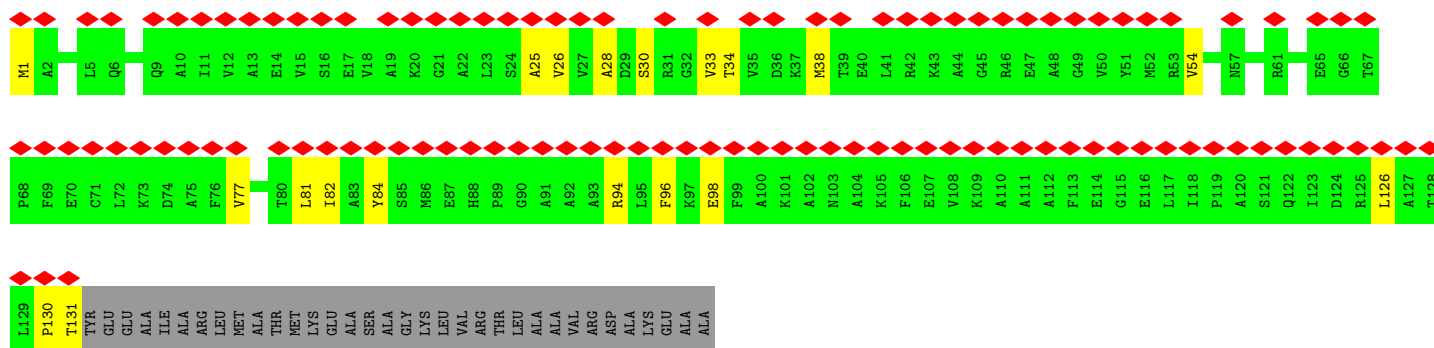
- Molecule 4: 50S ribosomal protein L35



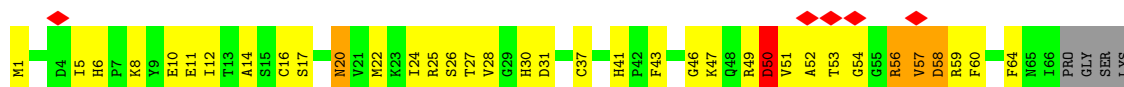
- Molecule 5: 50S ribosomal protein L36



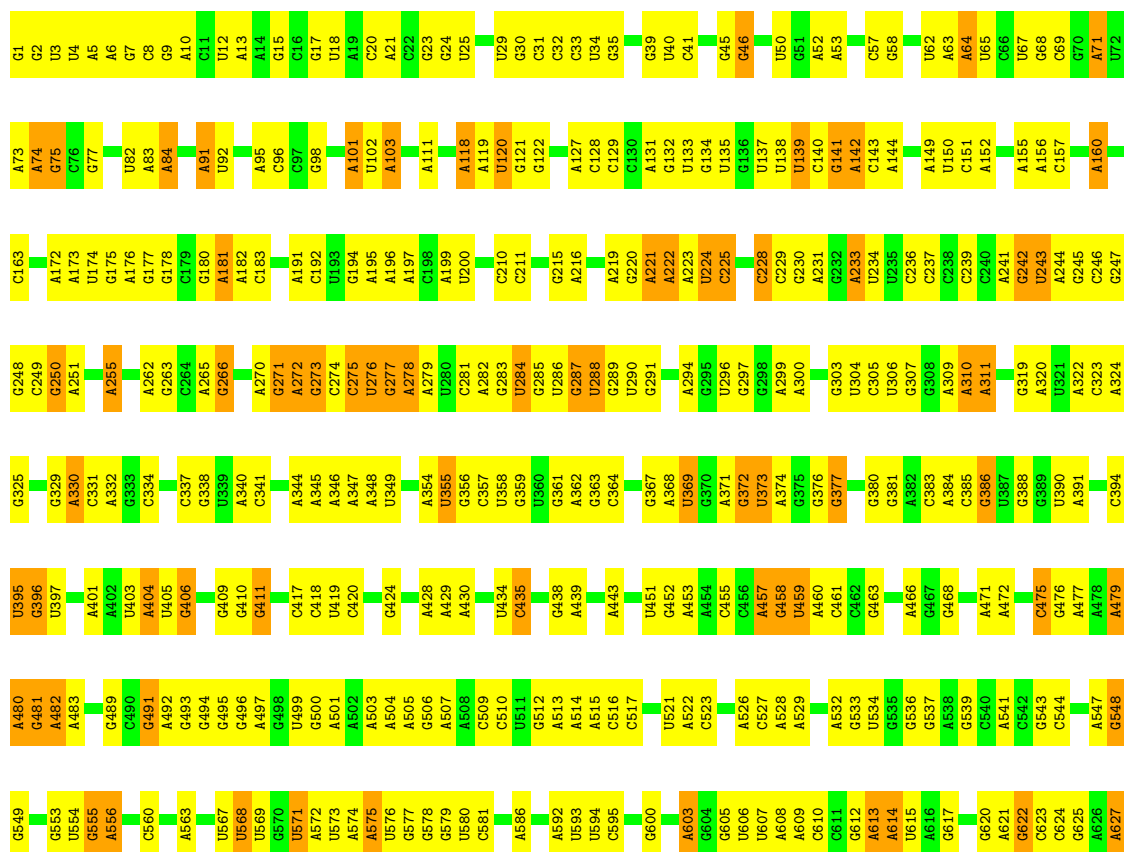
- Molecule 6: 50S ribosomal protein L10



• Molecule 7: 50S ribosomal protein L31

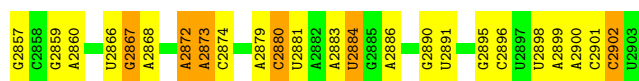


• Molecule 8: 23S ribosomal RNA

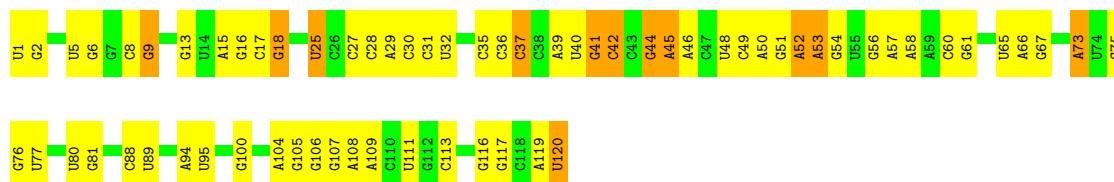


G1666	G1667	C1585	G1424	G1341	U1249	C1164	G1087	G1024	A947	U872	C791	A699	G628
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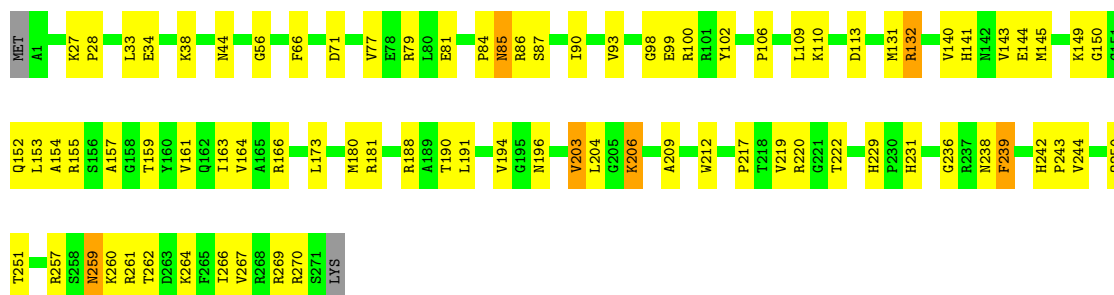




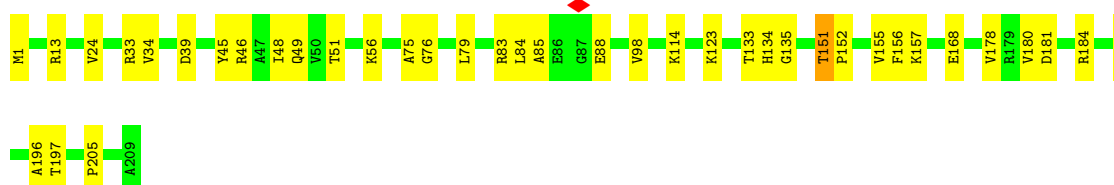
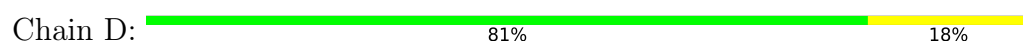
• Molecule 9: 5S ribosomal RNA



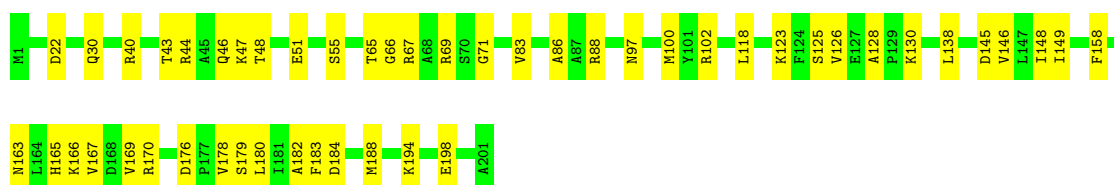
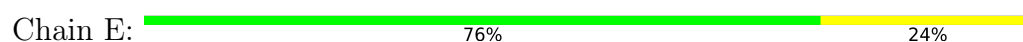
• Molecule 10: 50S ribosomal protein L2



• Molecule 11: 50S ribosomal protein L3

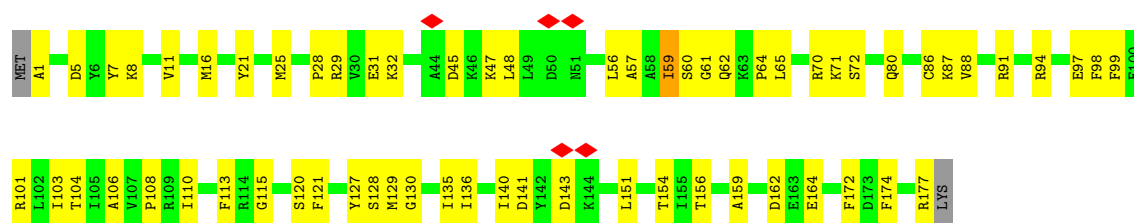


• Molecule 12: 50S ribosomal protein L4



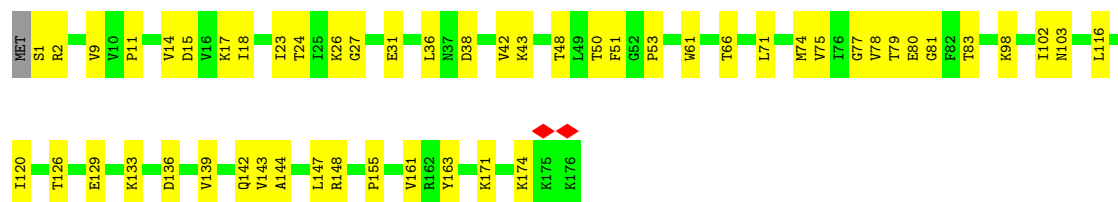
• Molecule 13: 50S ribosomal protein L5

Chain F:  64% 35%

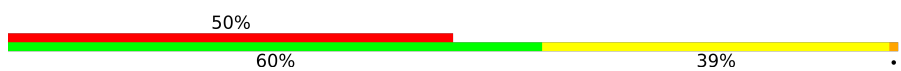


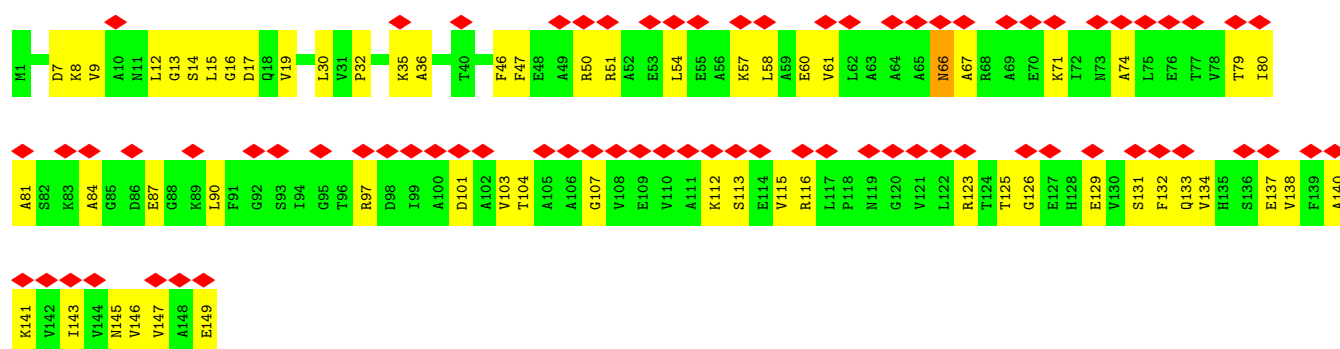
- Molecule 14: 50S ribosomal protein L6

Chain G:  70% 29%

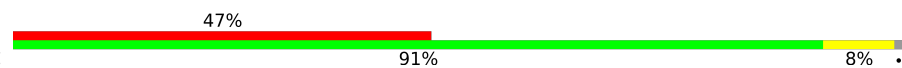


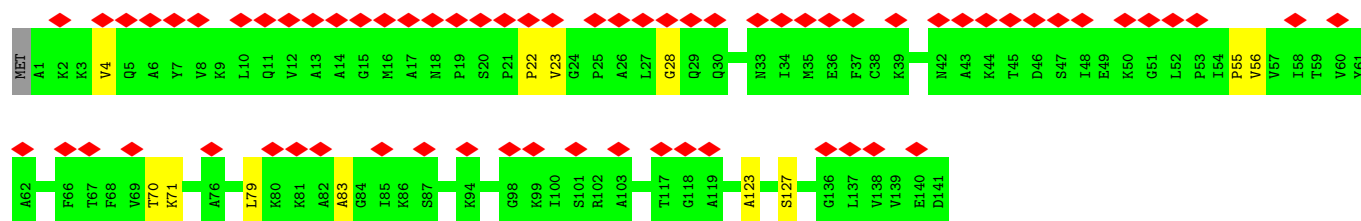
- Molecule 15: 50S ribosomal protein L9

Chain H:  50% 60% 39%



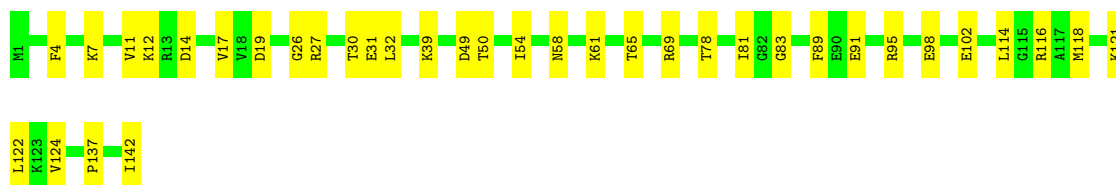
- Molecule 16: 50S ribosomal protein L11

Chain I:  47% 91% 8%



- Molecule 17: 50S ribosomal protein L13

Chain J:  75% 25%



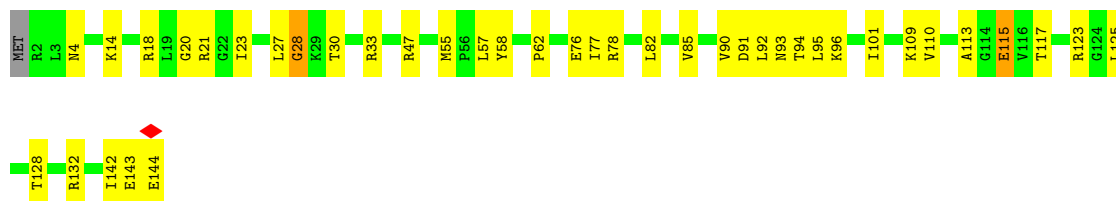
- Molecule 18: 50S ribosomal protein L14

Chain K: 67% 33% .



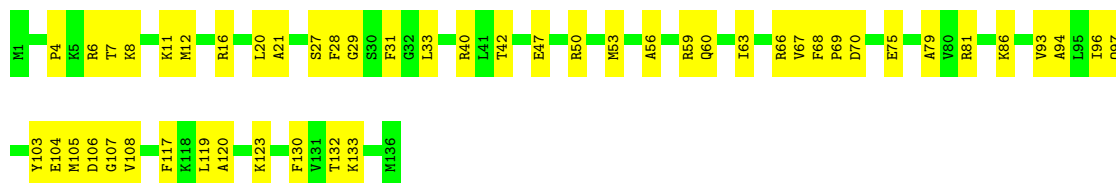
- Molecule 19: 50S ribosomal protein L15

Chain L: 72% 26% ..



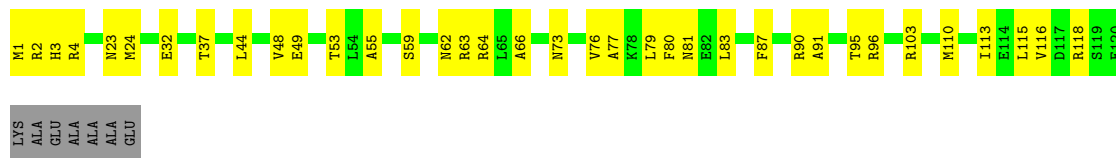
- Molecule 20: 50S ribosomal protein L16

Chain M: 64% 36%



- Molecule 21: 50S ribosomal protein L17

Chain N: 66% 28% 6%



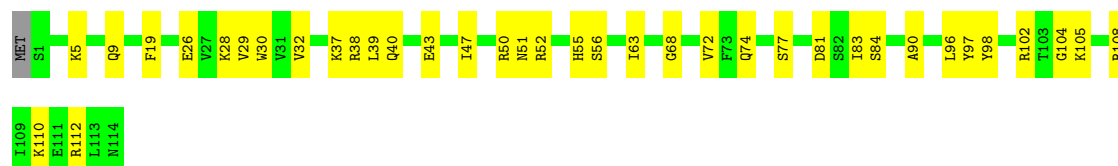
- Molecule 22: 50S ribosomal protein L18

Chain O: 66% 32% ..



- Molecule 23: 50S ribosomal protein L19

Chain P: 67% 32%



- Molecule 24: 50S ribosomal protein L20

Chain Q: 73% 26%



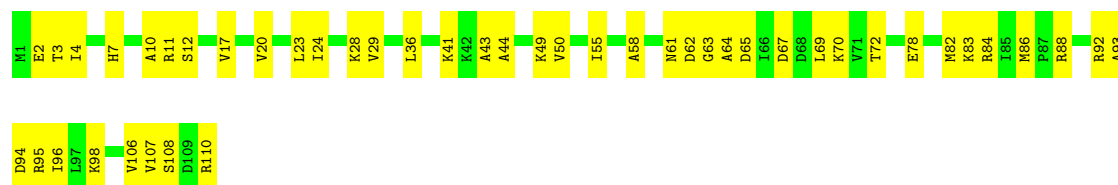
- Molecule 25: 50S ribosomal protein L21

Chain R: 71% 26%



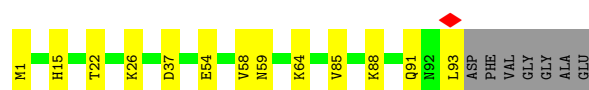
- Molecule 26: 50S ribosomal protein L22

Chain S: 58% 42%



- Molecule 27: 50S ribosomal protein L23

Chain T: 80% 13% 7%



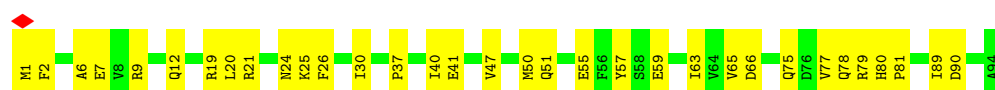
- Molecule 28: 50S ribosomal protein L24

Chain U:  69% 29%



- Molecule 29: 50S ribosomal protein L25

Chain V:  65% 35%



- Molecule 30: 50S ribosomal protein L27

Chain W:  65% 24% 12%



- Molecule 31: 50S ribosomal protein L28

Chain X:  72% 27%



- Molecule 32: 50S ribosomal protein L29

Chain Y:  70% 27%



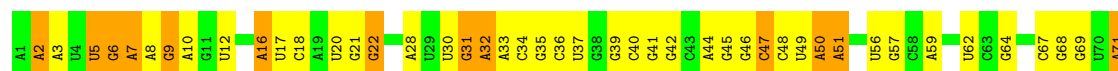
- Molecule 33: 50S ribosomal protein L30

Chain Z:  71% 27%

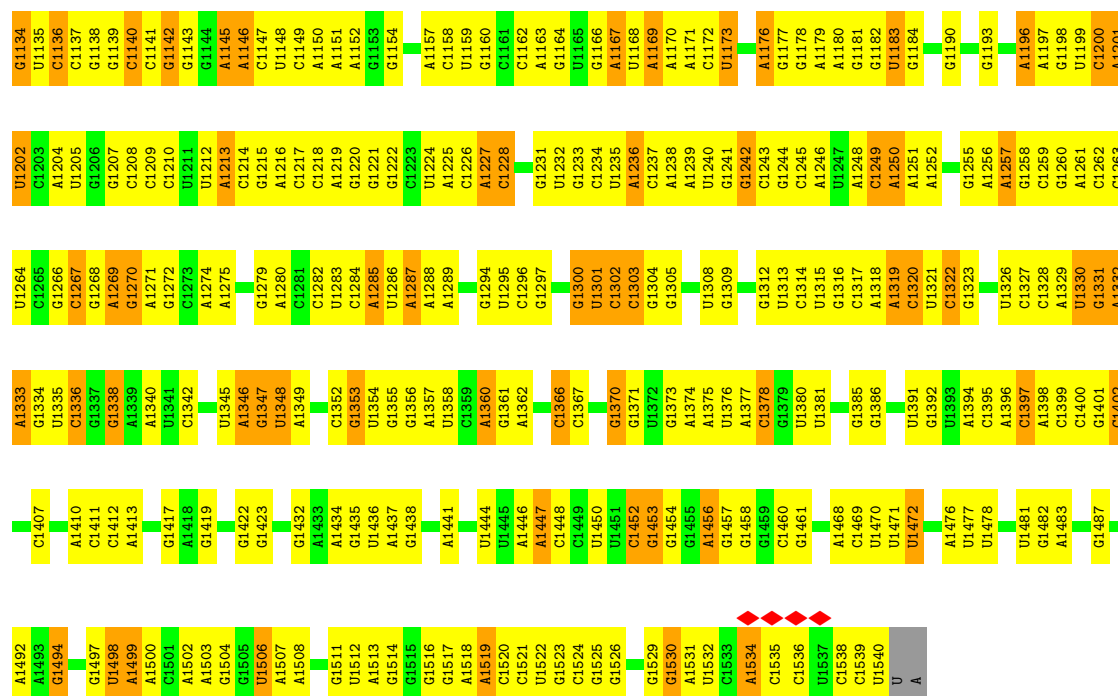


- Molecule 34: 16S ribosomal RNA

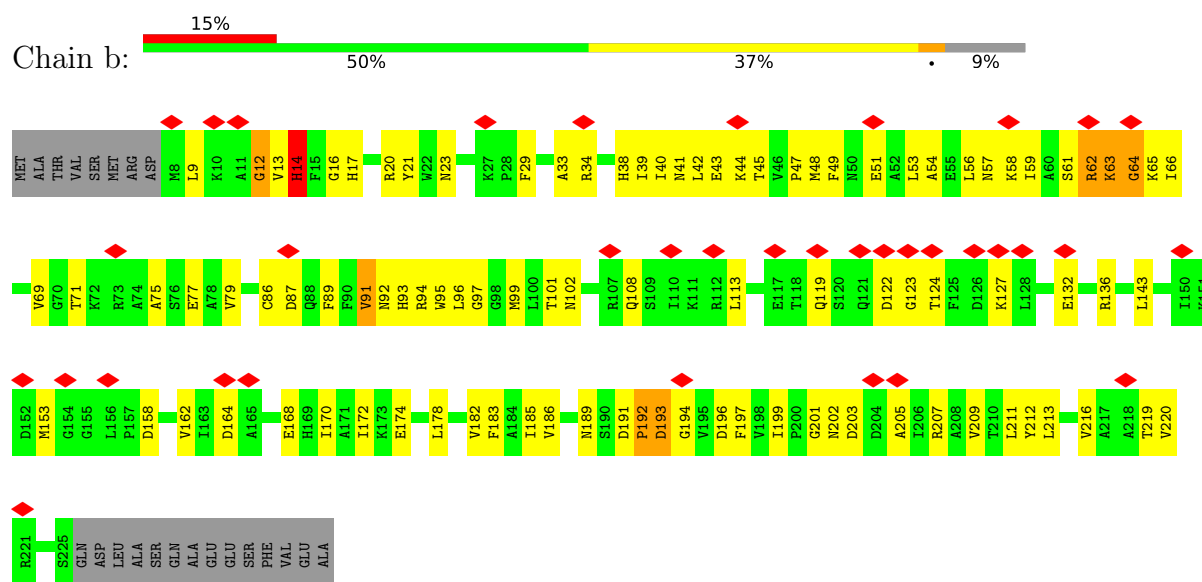
Chain a:  32% 51% 16%



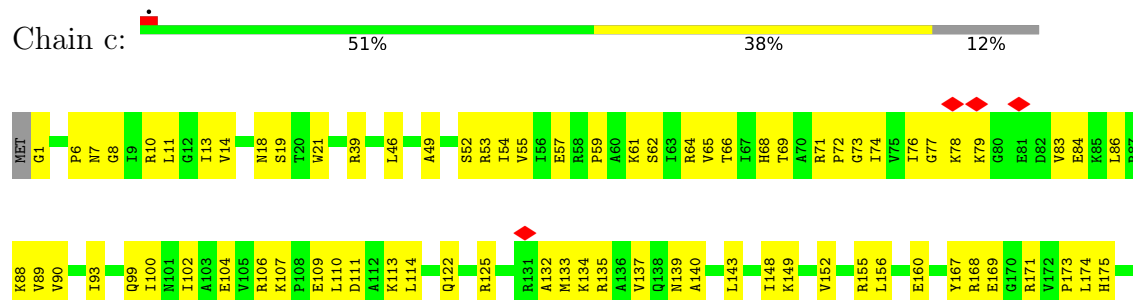
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G926	G927	C931	G932	G933	C934	A935	G939	G940	G941	G944	G945	A946	A947	A948	A949	U952	U953	A958	U959	U960	U961	G962	G963	A964	U965	G966	G967	G968	G969	G970	G971	G972	A973	A974	A975	G976	A977	C978	C979	C980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061																																																																																																																																																	
G844	A845	G846	G847	G848	G849	G850	U855	U856	U857	U858	U859	A864	A865	A866	A867	A868	A869	U870	U871	U872	A873	A874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061																																																									
U757	C758	A759	A766	A767	A768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996																																	
A622	C623	C624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756																																																																																																																																				
U428	U429	A430	A431	A432	A433	U434	A435	A436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554																																																																																																																																												
A356	G357	U358	G359	G360	G361	G362	A363	A364	A365	A366	U367	C372	A373	A374	U375	G376	G377	G378	C379	C380	C381	A382	A383	G384	G385	G386	A387	U388	A389	U389	U390	G391	C392	U393	U394	U395	U396	U397	U398	G399	C400	C401	C402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554																																																																							
C284	G289	G290	G291	G292	G293	G294	U295	U296	U297	U298	U299	U300	U301	U302	U303	U304	U305	U306	U307	U308	U309	U310	U311	U312	U313	U314	U315	U316	U317	U318	U319	U320	U321	U322	U323	U324	U325	U326	U327	U328	U329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554
G211	G212	G213	C214	C215	U216	U217	U218	U219	U220	U221	U222	U223	U224	U225	U226	U227	U228	U229	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239																																																																																																																																																																																																																																														

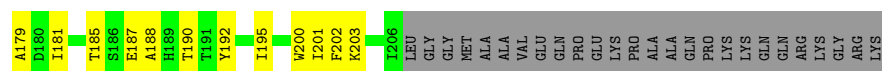


• Molecule 35: 30S ribosomal protein S2



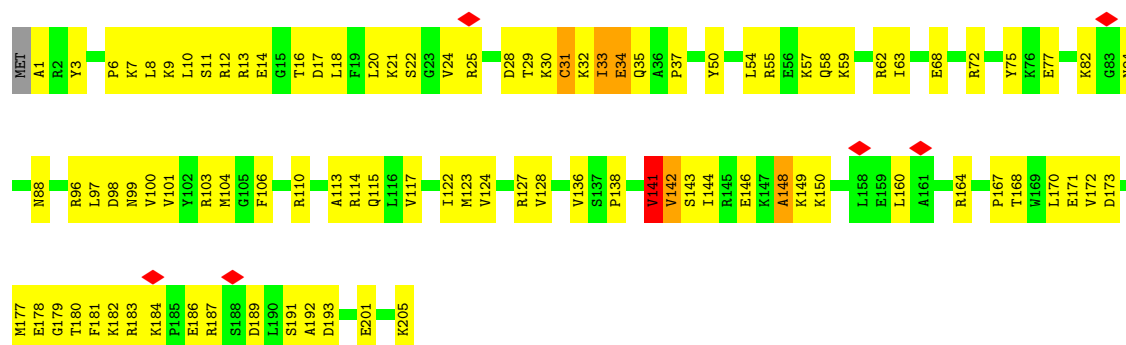
• Molecule 36: 30S ribosomal protein S3





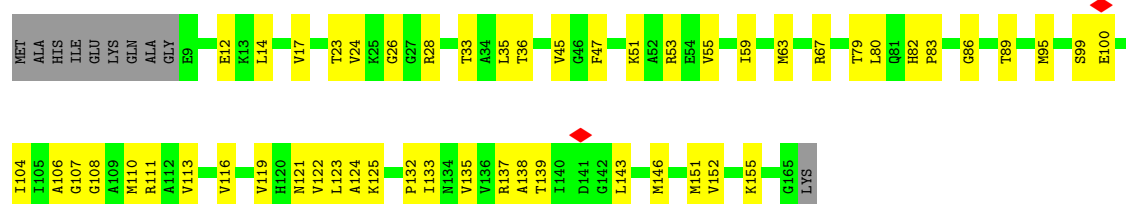
• Molecule 37: 30S ribosomal protein S4

Chain d: 53% 44%



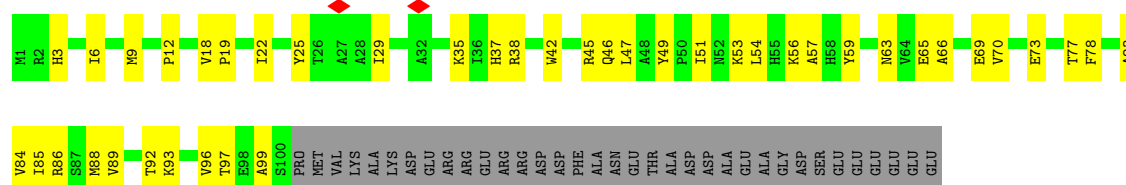
• Molecule 38: 30S ribosomal protein S5

Chain e: 63% 31% 6%



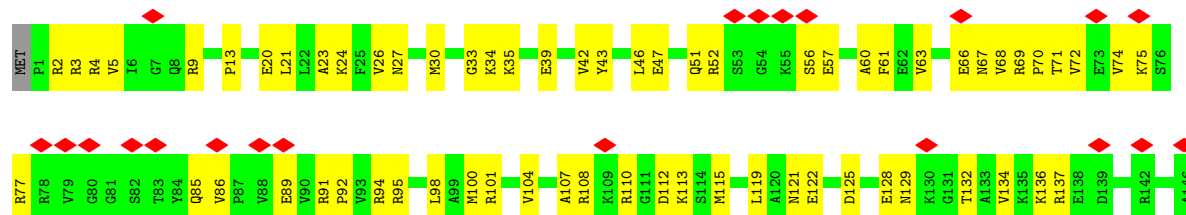
• Molecule 39: 30S ribosomal protein S6, fully modified isoform

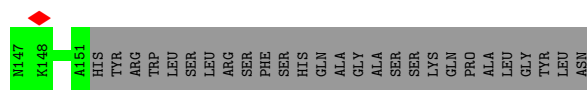
Chain f: 43% 31% 26%



• Molecule 40: 30S ribosomal protein S7

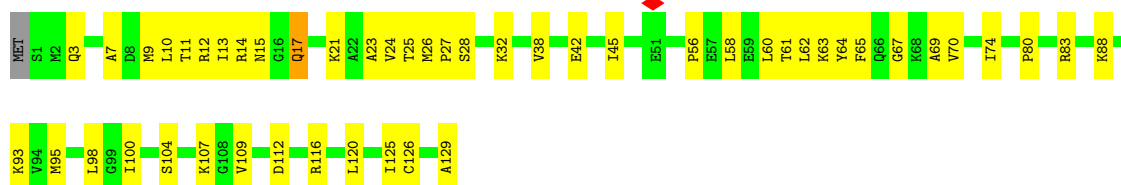
Chain g: 12% 48% 36% 16%





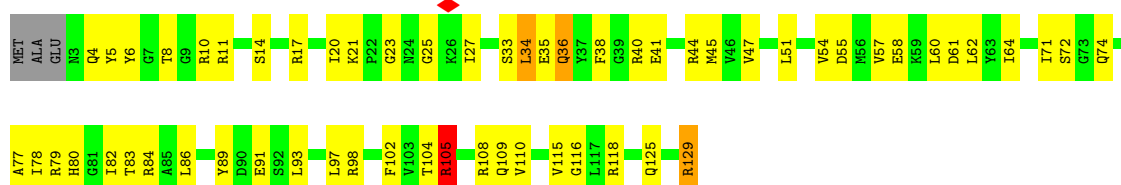
- Molecule 41: 30S ribosomal protein S8

Chain h: 62% 37%



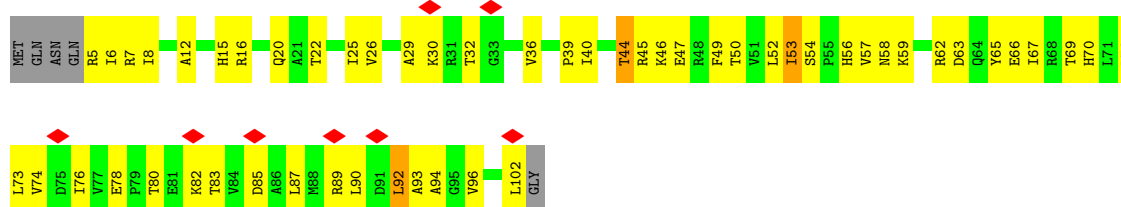
- Molecule 42: 30S ribosomal protein S9

Chain i: 52% 42%



- Molecule 43: 30S ribosomal protein S10

Chain j: 8% 43% 50% 5%



- Molecule 44: 30S ribosomal protein S11

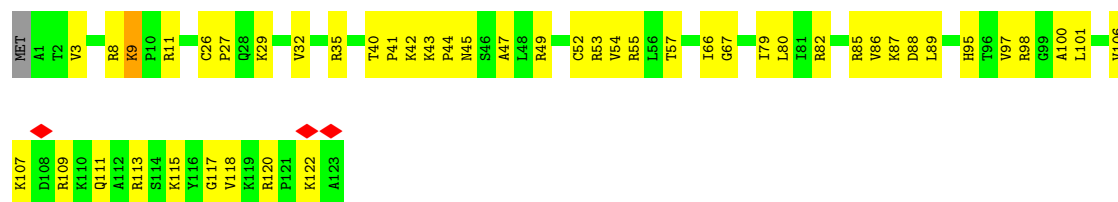
Chain k: 62% 27% 10%



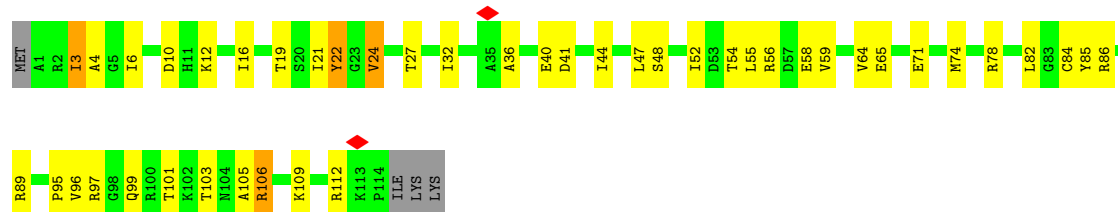
- Molecule 45: 30S ribosomal protein S12

Chain l: 61% 37%





• Molecule 46: 30S ribosomal protein S13



• Molecule 47: 30S ribosomal protein S14



• Molecule 48: 30S ribosomal protein S15



• Molecule 49: 30S ribosomal protein S16



• Molecule 50: 30S ribosomal protein S17





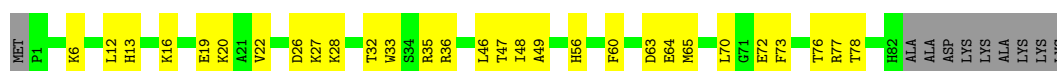
- Molecule 51: 30S ribosomal protein S18

Chain r:



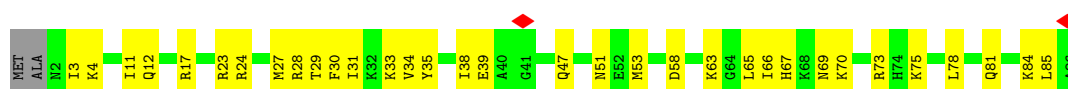
- Molecule 52: 30S ribosomal protein S19

Chain s:



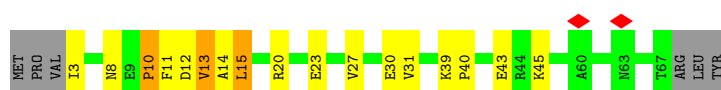
- Molecule 53: 30S ribosomal protein S20

Chain t:



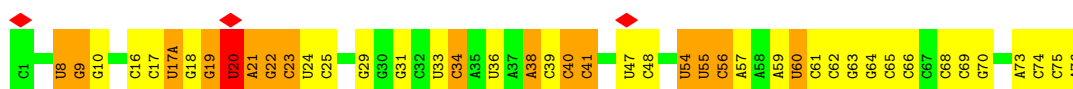
- Molecule 54: 30S ribosomal protein S21

Chain u:



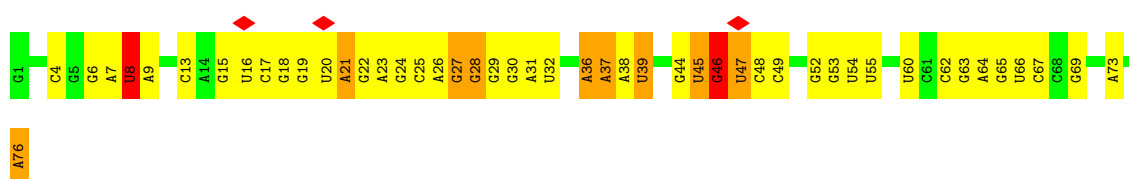
- Molecule 55: P-site tRNA(fMet)

Chain v:

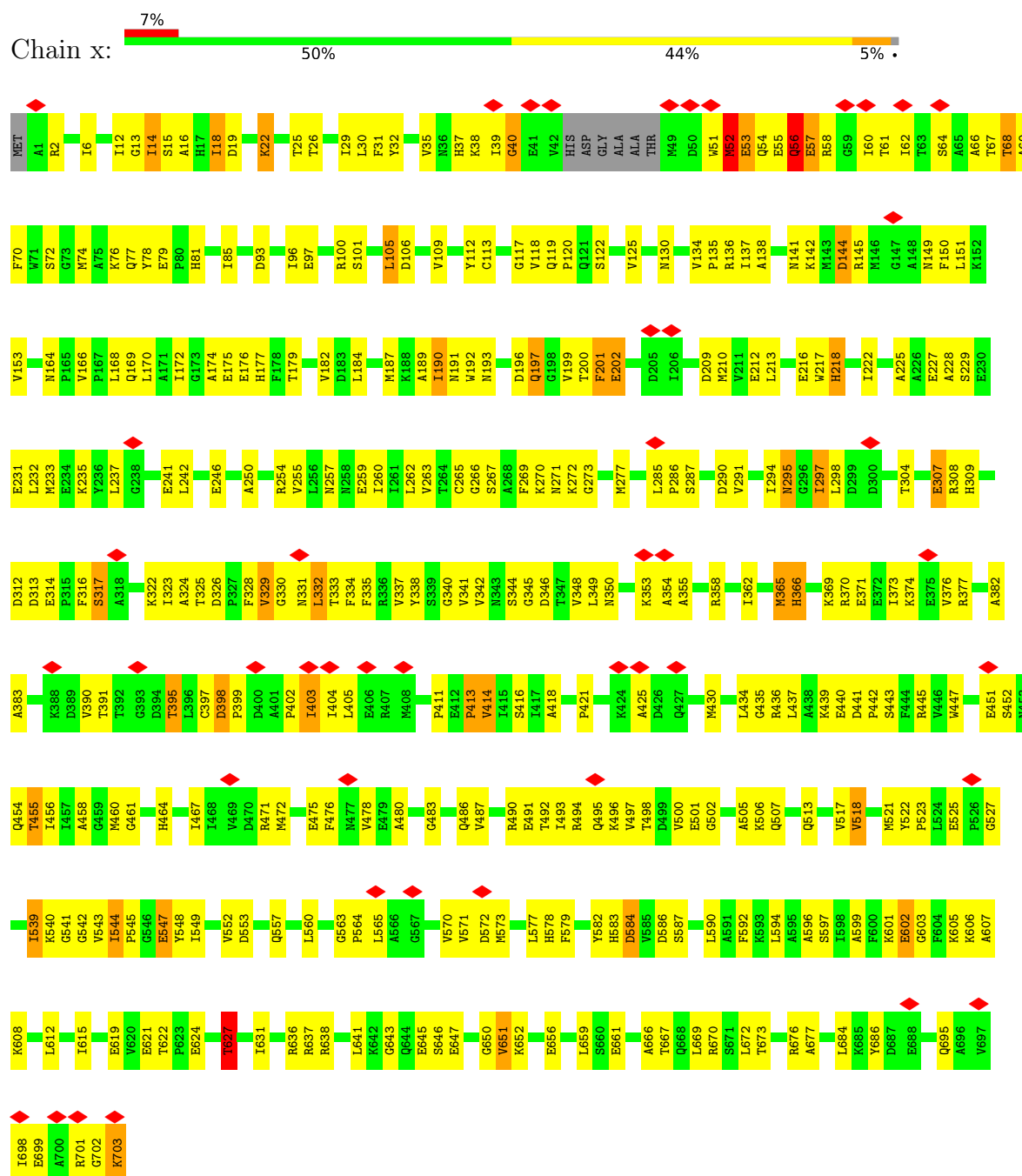


- Molecule 56: P-site fMet-Phe-tRNA(Phe)

Chain w:



- Molecule 57: Elongation factor G



- Molecule 58: Dipeptide (FME-PHE)



- Molecule 59: mRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23737	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	15.892	Depositor
Minimum map value	-8.596	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6525, 0.6525, 0.6525	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, AM2, MA6, 2MA, FME, 2MG, PSU, OMU, G7M, 5MC, UR3, 3TD, 4OC, OMC, 6MZ, 5MU, MIA, 4SU, OMG, MG, 1MG, GDP, NA

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	0	0.31	0/450	0.47	0/599
2	1	0.24	0/416	0.43	0/554
3	2	0.33	0/380	0.47	0/498
4	3	0.41	0/513	0.66	1/676 (0.1%)
5	4	0.30	0/303	0.54	0/397
6	5	0.33	0/646	0.78	3/898 (0.3%)
7	6	0.47	0/531	1.10	8/709 (1.1%)
8	A	0.33	1/69266 (0.0%)	0.38	8/108055 (0.0%)
9	B	0.25	0/2873	0.32	0/4478
10	C	0.46	0/2121	0.69	6/2852 (0.2%)
11	D	0.38	0/1586	0.54	2/2134 (0.1%)
12	E	0.39	0/1571	0.54	0/2113
13	F	0.30	0/1434	0.49	0/1926
14	G	0.28	0/1343	0.51	0/1816
15	H	0.35	0/1122	0.76	2/1515 (0.1%)
16	I	1.06	0/692	1.29	2/960 (0.2%)
17	J	0.30	0/1152	0.43	0/1551
18	K	0.42	0/947	0.52	1/1268 (0.1%)
19	L	0.49	0/1054	0.71	2/1403 (0.1%)
20	M	0.36	0/1093	0.53	0/1460
21	N	0.33	0/973	0.56	1/1301 (0.1%)
22	O	0.36	0/902	0.73	4/1209 (0.3%)
23	P	0.37	0/929	0.55	0/1242
24	Q	0.34	0/960	0.41	0/1278
25	R	0.67	3/829 (0.4%)	0.89	6/1107 (0.5%)
26	S	0.38	0/864	0.71	5/1156 (0.4%)
27	T	0.44	0/744	0.60	1/994 (0.1%)
28	U	0.34	0/787	0.52	0/1051
29	V	0.27	0/766	0.42	0/1025
30	W	0.31	0/582	0.45	0/769
31	X	0.37	0/635	0.53	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.40	0/510	0.54	1/677 (0.1%)
33	Z	0.28	0/453	0.42	0/605
34	a	0.29	6/36725 (0.0%)	0.41	24/57285 (0.0%)
35	b	0.44	0/1735	0.86	8/2338 (0.3%)
36	c	0.23	0/1651	0.46	0/2225
37	d	0.42	0/1665	0.75	7/2227 (0.3%)
38	e	0.35	0/1154	0.60	0/1554
39	f	0.21	0/835	0.49	0/1128
40	g	0.25	0/1195	0.49	0/1602
41	h	0.36	0/989	0.70	3/1326 (0.2%)
42	i	0.47	0/1034	0.77	2/1375 (0.1%)
43	j	0.40	0/796	0.75	2/1077 (0.2%)
44	k	0.23	0/885	0.47	0/1195
45	l	0.46	0/969	0.83	7/1300 (0.5%)
46	m	0.45	0/892	0.76	2/1193 (0.2%)
47	n	0.49	0/811	0.78	2/1081 (0.2%)
48	o	0.23	0/722	0.44	0/964
49	p	0.46	0/659	0.82	4/884 (0.5%)
50	q	0.45	0/657	0.80	3/881 (0.3%)
51	r	0.54	0/544	0.91	7/731 (1.0%)
52	s	0.48	0/675	0.88	4/908 (0.4%)
53	t	0.23	0/671	0.43	0/888
54	u	0.36	0/512	1.13	6/683 (0.9%)
55	v	0.41	3/1767 (0.2%)	0.42	0/2750
56	w	0.37	1/1650 (0.1%)	0.55	0/2569
57	x	0.79	2/5516 (0.0%)	1.20	31/7460 (0.4%)
58	y	0.12	0/11	0.73	0/13
59	z	0.47	0/230	0.65	0/355
All	All	0.37	16/164377 (0.0%)	0.52	165/245116 (0.1%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1081	A	O3'-P	8.21	1.73	1.61
55	v	20	U	C5-C6	7.56	1.49	1.34
25	R	49	ILE	CA-C	-7.54	1.44	1.52
34	a	921	U	C5'-C4'	6.68	1.61	1.51
25	R	57	GLY	CA-C	-6.12	1.43	1.52

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	903	C	P-O3'-C3'	26.12	159.38	120.20
54	u	13	VAL	N-CA-C	-16.13	96.84	112.17
10	C	238	ASN	N-CA-C	14.34	127.00	111.36
57	x	304	THR	N-CA-C	-13.74	92.33	109.65
57	x	56	GLN	N-CA-C	-12.14	98.10	113.16

There are no chirality outliers.

There are no planarity outliers.

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	0	444	0	461	18	0
2	1	409	0	440	12	0
3	2	377	0	418	14	0
4	3	504	0	574	17	0
5	4	302	0	340	14	0
6	5	647	0	336	11	0
7	6	522	0	521	33	0
8	A	62338	0	31367	1254	0
9	B	2570	0	1301	54	0
10	C	2082	0	2157	62	0
11	D	1565	0	1616	30	0
12	E	1552	0	1619	37	0
13	F	1410	0	1447	46	0
14	G	1323	0	1374	36	0
15	H	1111	0	1148	47	0
16	I	693	0	347	7	0
17	J	1129	0	1162	27	0
18	K	938	0	1012	36	0
19	L	1045	0	1117	31	0
20	M	1074	0	1157	40	0
21	N	960	0	1000	27	0
22	O	892	0	923	31	0
23	P	917	0	965	27	0
24	Q	947	0	1022	27	0
25	R	816	0	839	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	S	857	0	922	41	0
27	T	738	0	807	11	0
28	U	779	0	834	20	0
29	V	753	0	780	25	0
30	W	575	0	592	15	0
31	X	625	0	655	19	0
32	Y	509	0	543	11	0
33	Z	449	0	491	12	0
34	a	33050	0	16653	910	0
35	b	1704	0	1732	65	0
36	c	1624	0	1699	65	0
37	d	1643	0	1710	77	0
38	e	1141	0	1170	47	0
39	f	817	0	808	35	0
40	g	1181	0	1240	58	0
41	h	979	0	1034	41	0
42	i	1022	0	1070	45	0
43	j	786	0	828	51	0
44	k	869	0	878	36	0
45	l	955	0	1019	32	0
46	m	883	0	944	36	0
47	n	799	0	841	34	0
48	o	714	0	737	24	0
49	p	649	0	666	28	0
50	q	648	0	691	24	0
51	r	535	0	552	18	0
52	s	658	0	685	24	0
53	t	665	0	714	25	0
54	u	506	0	502	9	0
55	v	1642	0	837	27	0
56	w	1631	0	838	40	0
57	x	5416	0	5398	218	0
58	y	21	0	19	1	0
59	z	208	0	104	3	0
60	0	1	0	0	0	0
60	1	1	0	0	0	0
60	6	1	0	0	0	0
60	A	267	0	0	0	0
60	B	6	0	0	0	0
60	C	3	0	0	0	0
60	D	1	0	0	0	0
60	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	O	1	0	0	1	0
60	P	1	0	0	0	0
60	a	34	0	0	0	0
60	w	1	0	0	0	0
61	4	1	0	0	0	0
61	6	1	0	0	0	0
62	B	1	0	0	0	0
63	a	148	0	164	2	0
64	x	28	0	12	1	0
All	All	153095	0	103832	3620	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 14.

The worst 5 of 3620 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)
8:A:1915:3TD:C1'	8:A:1915:3TD:O4'	1.68	1.16
34:a:438:U:C2	34:a:496:A:N6	2.30	0.99
8:A:2100:G:H1	8:A:2189:U:H3	1.10	0.97
34:a:409:U:H3	34:a:433:G:H1	1.15	0.93
34:a:1498:UR3:O2'	34:a:1499:A:OP2	1.88	0.92

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	
1	0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
4	3	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
5	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
6	5	129/165 (78%)	112 (87%)	17 (13%)	0	100	100
7	6	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
10	C	269/273 (98%)	249 (93%)	20 (7%)	0	100	100
11	D	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
12	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
13	F	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
14	G	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
15	H	147/149 (99%)	125 (85%)	22 (15%)	0	100	100
16	I	139/142 (98%)	126 (91%)	12 (9%)	1 (1%)	18	49
17	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	K	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
19	L	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
20	M	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
21	N	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
22	O	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
23	P	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
24	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
25	R	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	12	41
26	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
27	T	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
28	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
29	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	W	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
31	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
32	Y	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
33	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
35	b	216/240 (90%)	193 (89%)	23 (11%)	0	100	100
36	c	204/233 (88%)	196 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	d	203/206 (98%)	188 (93%)	15 (7%)	0	100	100
38	e	155/167 (93%)	143 (92%)	12 (8%)	0	100	100
39	f	98/135 (73%)	91 (93%)	7 (7%)	0	100	100
40	g	149/179 (83%)	133 (89%)	16 (11%)	0	100	100
41	h	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
42	i	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
43	j	96/103 (93%)	80 (83%)	16 (17%)	0	100	100
44	k	114/129 (88%)	103 (90%)	11 (10%)	0	100	100
45	l	121/124 (98%)	105 (87%)	16 (13%)	0	100	100
46	m	112/118 (95%)	104 (93%)	8 (7%)	0	100	100
47	n	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
48	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
49	p	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
50	q	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
51	r	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
52	s	80/92 (87%)	75 (94%)	5 (6%)	0	100	100
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	55 (87%)	8 (13%)	0	100	100
57	x	694/704 (99%)	632 (91%)	61 (9%)	1 (0%)	48	78
All	All	6544/6924 (94%)	6062 (93%)	479 (7%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	R	51	VAL
57	x	403	ILE
16	I	22	PRO

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	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	49 (96%)	2 (4%)	28	60
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	56 (95%)	3 (5%)	21	52
10	C	216/218 (99%)	212 (98%)	4 (2%)	50	73
11	D	164/164 (100%)	164 (100%)	0	100	100
12	E	165/165 (100%)	163 (99%)	2 (1%)	63	78
13	F	148/150 (99%)	147 (99%)	1 (1%)	76	82
14	G	137/138 (99%)	137 (100%)	0	100	100
15	H	114/114 (100%)	113 (99%)	1 (1%)	70	80
17	J	116/116 (100%)	116 (100%)	0	100	100
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	99 (97%)	3 (3%)	37	66
20	M	109/109 (100%)	108 (99%)	1 (1%)	70	80
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	85 (99%)	1 (1%)	63	78
23	P	99/100 (99%)	99 (100%)	0	100	100
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	82 (98%)	2 (2%)	43	69
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	78 (98%)	2 (2%)	42	69
28	U	83/85 (98%)	83 (100%)	0	100	100
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	67 (100%)	0	100	100
32	Y	55/55 (100%)	53 (96%)	2 (4%)	31	62
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	170 (94%)	10 (6%)	19	49
36	c	170/190 (90%)	170 (100%)	0	100	100
37	d	172/173 (99%)	166 (96%)	6 (4%)	32	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	e	114/126 (90%)	114 (100%)	0	100	100
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	123 (99%)	1 (1%)	73	81
41	h	104/105 (99%)	103 (99%)	1 (1%)	68	79
42	i	105/107 (98%)	99 (94%)	6 (6%)	18	49
43	j	86/90 (96%)	83 (96%)	3 (4%)	32	62
44	k	89/99 (90%)	88 (99%)	1 (1%)	65	78
45	l	103/104 (99%)	102 (99%)	1 (1%)	68	79
46	m	92/96 (96%)	88 (96%)	4 (4%)	26	57
47	n	79/84 (94%)	79 (100%)	0	100	100
48	o	76/77 (99%)	75 (99%)	1 (1%)	61	77
49	p	65/65 (100%)	62 (95%)	3 (5%)	24	55
50	q	74/78 (95%)	71 (96%)	3 (4%)	27	59
51	r	56/65 (86%)	51 (91%)	5 (9%)	9	33
52	s	72/79 (91%)	72 (100%)	0	100	100
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	44 (96%)	2 (4%)	26	57
57	x	575/578 (100%)	514 (89%)	61 (11%)	6	26
58	y	1/1 (100%)	1 (100%)	0	100	100
All	All	5202/5408 (96%)	5070 (98%)	132 (2%)	42	69

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	x	452	SER
57	x	544	ILE
57	x	701	ARG
43	j	44	THR
42	i	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
36	c	2	GLN

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Mol	Chain	Res	Type
40	g	67	ASN
57	x	695	GLN
39	f	3	HIS
40	g	129	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1539/1542 (99%)	442 (28%)	0
55	v	76/77 (98%)	24 (31%)	0
56	w	75/76 (98%)	21 (28%)	0
59	z	9/33 (27%)	2 (22%)	0
8	A	2902/2903 (99%)	574 (19%)	34 (1%)
9	B	119/120 (99%)	21 (17%)	3 (2%)
All	All	4720/4751 (99%)	1084 (22%)	37 (0%)

5 of 1084 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	34	U
8	A	35	G
8	A	46	G
8	A	50	U

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	2324	U
9	B	52	A
8	A	2405	G
8	A	2779	U
8	A	1090	A

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

45 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
8	PSU	A	2604	8	18,21,22	1.06	1 (5%)	22,30,33	1.72	2 (9%)
8	PSU	A	2504	8	18,21,22	1.14	2 (11%)	22,30,33	1.84	4 (18%)
8	2MG	A	2445	8	23,26,27	1.32	3 (13%)	32,38,41	2.35	10 (31%)
56	G7M	w	46	56	23,26,27	2.62	8 (34%)	35,39,42	2.25	10 (28%)
34	MA6	a	1518	34	23,26,27	1.47	5 (21%)	34,38,41	2.75	12 (35%)
55	PSU	v	55	55	18,21,22	1.36	3 (16%)	22,30,33	1.96	4 (18%)
8	PSU	A	2457	8	18,21,22	0.98	2 (11%)	22,30,33	1.88	6 (27%)
8	5MC	A	1962	8	18,22,23	3.65	7 (38%)	26,32,35	0.97	1 (3%)
8	5MC	A	747	8	18,22,23	3.62	7 (38%)	26,32,35	1.14	1 (3%)
8	2MA	A	2503	8,60	22,25,26	3.72	8 (36%)	33,37,40	2.19	7 (21%)
8	PSU	A	2580	8,60	18,21,22	1.11	3 (16%)	22,30,33	1.89	6 (27%)
34	5MC	a	1407	34	18,22,23	1.03	2 (11%)	26,32,35	1.57	7 (26%)
8	2MG	A	1835	8	23,26,27	2.91	8 (34%)	32,38,41	2.26	10 (31%)
58	FME	y	101	58	8,9,10	0.96	0	7,9,11	1.17	1 (14%)
8	PSU	A	746	8,60	18,21,22	1.09	2 (11%)	22,30,33	1.81	5 (22%)
34	UR3	a	1498	34,60	19,22,23	2.69	6 (31%)	26,32,35	1.57	4 (15%)
8	5MU	A	1939	8	19,22,23	4.68	7 (36%)	28,32,35	3.76	9 (32%)
56	PSU	w	55	56	18,21,22	1.43	2 (11%)	22,30,33	1.98	3 (13%)
34	PSU	a	516	34	18,21,22	0.99	1 (5%)	22,30,33	1.79	5 (22%)
8	OMG	A	2251	56,8,60	23,26,27	2.35	9 (39%)	33,38,41	1.86	8 (24%)
34	2MG	a	1207	34	23,26,27	2.95	8 (34%)	32,38,41	2.23	11 (34%)
8	G7M	A	2069	8	23,26,27	2.56	8 (34%)	35,39,42	2.22	10 (28%)
8	PSU	A	955	8	18,21,22	1.07	2 (11%)	22,30,33	1.75	4 (18%)
55	4SU	v	8	55	18,21,22	3.61	7 (38%)	26,30,33	2.32	5 (19%)
56	MIA	w	37	56	28,31,32	2.53	7 (25%)	40,44,47	3.76	18 (45%)
8	PSU	A	1911	8	18,21,22	1.39	3 (16%)	22,30,33	2.01	4 (18%)
8	6MZ	A	1618	8	22,25,26	2.97	5 (22%)	30,36,39	4.28	14 (46%)
8	6MZ	A	2030	8	22,25,26	3.01	6 (27%)	30,36,39	4.47	14 (46%)
8	PSU	A	2605	8	18,21,22	1.02	1 (5%)	22,30,33	1.78	2 (9%)
34	2MG	a	966	34	23,26,27	1.39	4 (17%)	32,38,41	2.31	8 (25%)
34	MA6	a	1519	34	23,26,27	1.43	5 (21%)	34,38,41	2.84	12 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	2MG	a	1516	34	23,26,27	2.95	9 (39%)	32,38,41	2.28	12 (37%)
8	PSU	A	1917	8	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
56	5MU	w	54	56	19,22,23	1.40	4 (21%)	28,32,35	1.94	6 (21%)
55	5MU	v	54	55	19,22,23	4.85	7 (36%)	28,32,35	3.60	9 (32%)
34	G7M	a	527	34	23,26,27	2.61	8 (34%)	35,39,42	2.28	10 (28%)
8	1MG	A	745	8	22,26,27	2.66	6 (27%)	33,39,42	2.10	8 (24%)
34	5MC	a	967	34	18,22,23	3.73	7 (38%)	26,32,35	1.03	2 (7%)
8	OMC	A	2498	8,60	19,22,23	2.92	7 (36%)	26,31,34	0.83	0
56	PSU	w	32	56	18,21,22	1.03	1 (5%)	22,30,33	1.71	4 (18%)
56	4SU	w	8	56	18,21,22	3.62	7 (38%)	26,30,33	2.22	4 (15%)
8	3TD	A	1915	8	18,22,23	7.37	11 (61%)	22,32,35	1.72	3 (13%)
34	4OC	a	1402	34	20,23,24	3.00	8 (40%)	26,32,35	0.82	1 (3%)
8	OMU	A	2552	8,60	19,22,23	2.94	8 (42%)	26,31,34	1.78	5 (19%)
56	PSU	w	39	56	18,21,22	1.04	1 (5%)	22,30,33	1.72	4 (18%)

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
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/9/27/28	0/3/3/3
56	G7M	w	46	56	-	2/7/25/26	0/3/3/3
34	MA6	a	1518	34	-	1/11/29/30	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	2/7/25/26	0/2/2/2
8	5MC	A	747	8	-	1/7/25/26	0/2/2/2
8	2MA	A	2503	8,60	-	3/7/25/26	0/3/3/3
8	PSU	A	2580	8,60	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/9/27/28	0/3/3/3
58	FME	y	101	58	-	5/7/9/11	-
8	PSU	A	746	8,60	-	2/7/25/26	0/2/2/2
34	UR3	a	1498	34,60	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	5MU	A	1939	8	-	2/7/25/26	0/2/2/2
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
8	OMG	A	2251	56,8,60	-	1/9/27/28	0/3/3/3
34	2MG	a	1207	34	-	0/9/27/28	0/3/3/3
8	G7M	A	2069	8	-	1/7/25/26	0/3/3/3
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
56	MIA	w	37	56	-	3/15/33/34	0/3/3/3
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	0/9/27/28	0/3/3/3
8	6MZ	A	2030	8	-	2/9/27/28	0/3/3/3
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	2/9/27/28	0/3/3/3
34	MA6	a	1519	34	-	1/11/29/30	0/3/3/3
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
34	G7M	a	527	34	-	0/7/25/26	0/3/3/3
8	1MG	A	745	8	-	0/7/25/26	0/3/3/3
34	5MC	a	967	34	-	2/7/25/26	0/2/2/2
8	OMC	A	2498	8,60	-	0/9/27/28	0/2/2/2
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	3/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	0/9/29/30	0/2/2/2
8	OMU	A	2552	8,60	-	2/9/27/28	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2

The worst 5 of 227 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	O4'-C1'	18.04	1.68	1.43
8	A	1915	3TD	C2'-C1'	-15.17	1.34	1.53
8	A	1915	3TD	C6-C5	13.53	1.51	1.35
8	A	2030	6MZ	C6-N6	12.17	1.47	1.34
8	A	1618	6MZ	C6-N6	12.15	1.47	1.34

The worst 5 of 289 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2030	6MZ	C4-N9-C8	14.14	121.05	105.73
8	A	1618	6MZ	C4-N9-C8	13.04	119.86	105.73
56	w	37	MIA	C11-S10-C2	-12.51	92.92	102.27
8	A	1939	5MU	C5-C4-N3	12.43	125.92	115.31
55	v	54	5MU	C5-C4-N3	12.19	125.72	115.31

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	967	5MC	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
55	v	54	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

22 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	w	46	G7M	4	0
55	v	55	PSU	1	0
8	A	2457	PSU	1	0
8	A	2503	2MA	1	0
58	y	101	FME	1	0
8	A	746	PSU	1	0
34	a	1498	UR3	3	0
8	A	1939	5MU	1	0
34	a	516	PSU	2	0
8	A	2251	OMG	1	0
8	A	955	PSU	1	0
56	w	37	MIA	6	0
8	A	2030	6MZ	1	0
34	a	966	2MG	2	0
34	a	527	G7M	1	0
34	a	967	5MC	1	0
8	A	2498	OMC	1	0
56	w	8	4SU	1	0
8	A	1915	3TD	1	0
34	a	1402	4OC	2	0
8	A	2552	OMU	2	0
56	w	39	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 326 ligands modelled in this entry, 321 are monoatomic - leaving 5 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$
64	GDP	x	801	-	28,30,30	1.44	5 (17%)	44,47,47	2.20	16 (36%)
63	AM2	a	1628	-	40,40,40	0.18	0	53,60,60	0.57	0
63	AM2	a	1620	-	40,40,40	0.50	0	53,60,60	0.92	2 (3%)
63	AM2	a	1626	-	40,40,40	0.20	0	53,60,60	0.83	1 (1%)
63	AM2	a	1636	-	40,40,40	0.15	0	53,60,60	0.64	1 (1%)

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
64	GDP	x	801	-	-	2/16/32/32	0/3/3/3
63	AM2	a	1628	-	-	4/12/84/84	1/4/4/4
63	AM2	a	1620	-	-	5/12/84/84	0/4/4/4
63	AM2	a	1626	-	-	3/12/84/84	1/4/4/4
63	AM2	a	1636	-	-	7/12/84/84	1/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	x	801	GDP	C6-N1	-3.76	1.31	1.38
64	x	801	GDP	C4-N9	-3.16	1.29	1.38
64	x	801	GDP	C5-N7	-2.35	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	x	801	GDP	C5-C4	2.12	1.44	1.38
64	x	801	GDP	C2-N1	-2.07	1.32	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	x	801	GDP	C6-C5-N7	5.04	139.63	130.25
64	x	801	GDP	C5-C4-N3	-4.74	120.77	128.46
64	x	801	GDP	C2-N3-C4	4.66	120.60	112.30
64	x	801	GDP	PA-O3A-PB	-4.02	119.04	132.83
63	a	1626	AM2	CA5-CA6-CA7	-3.50	102.47	110.62

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	a	1620	AM2	CA8-CA7-NA7-CA9
63	a	1626	AM2	CA2-CA1-OA1-CC1
63	a	1628	AM2	CA2-CA1-OA1-CC1
63	a	1628	AM2	CA7-CA8-OA8-CB1
63	a	1636	AM2	CA7-CA8-OA8-CB1

All (3) ring outliers are listed below:

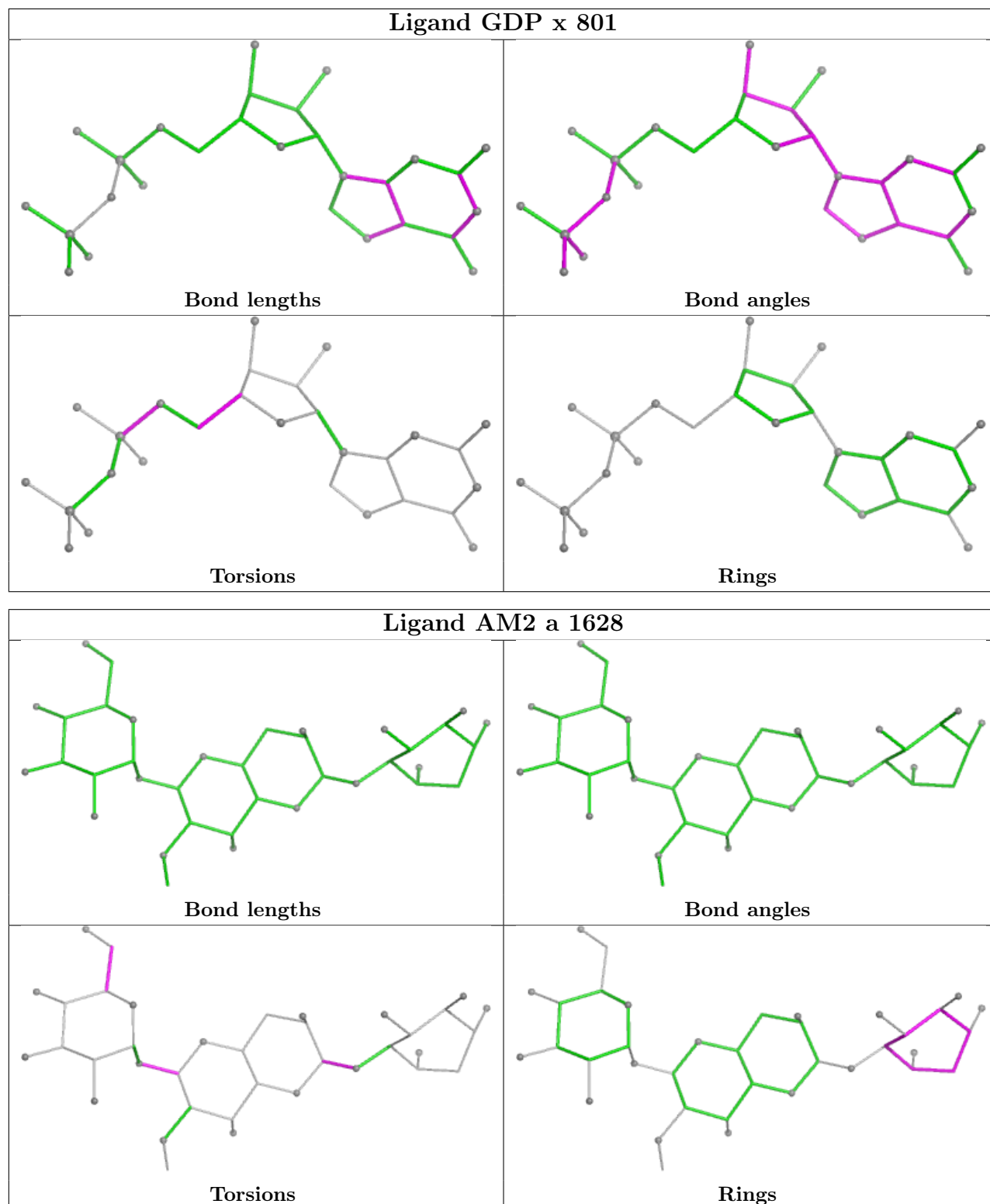
Mol	Chain	Res	Type	Atoms
63	a	1626	AM2	CC1-CC2-CC3-CC4-CC5-CC6
63	a	1628	AM2	CC1-CC2-CC3-CC4-CC5-CC6
63	a	1636	AM2	CA1-CA2-CA3-CA4-CA5-OA4

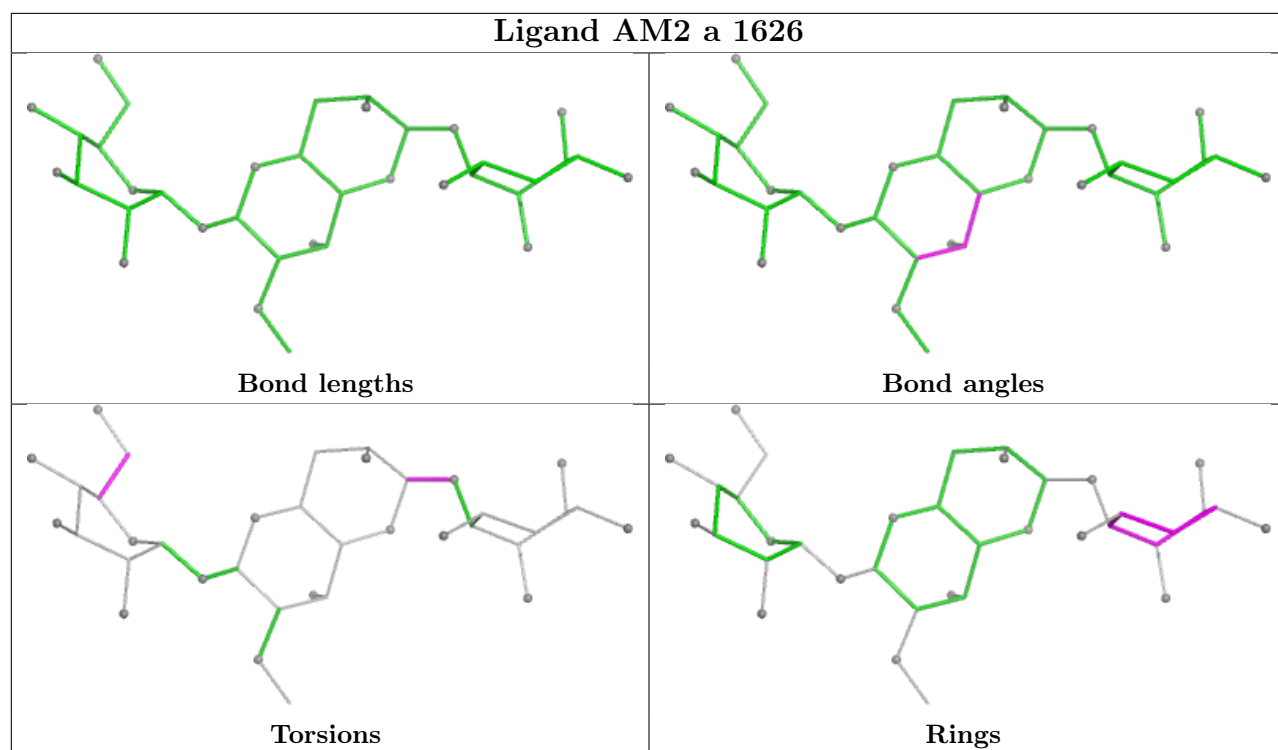
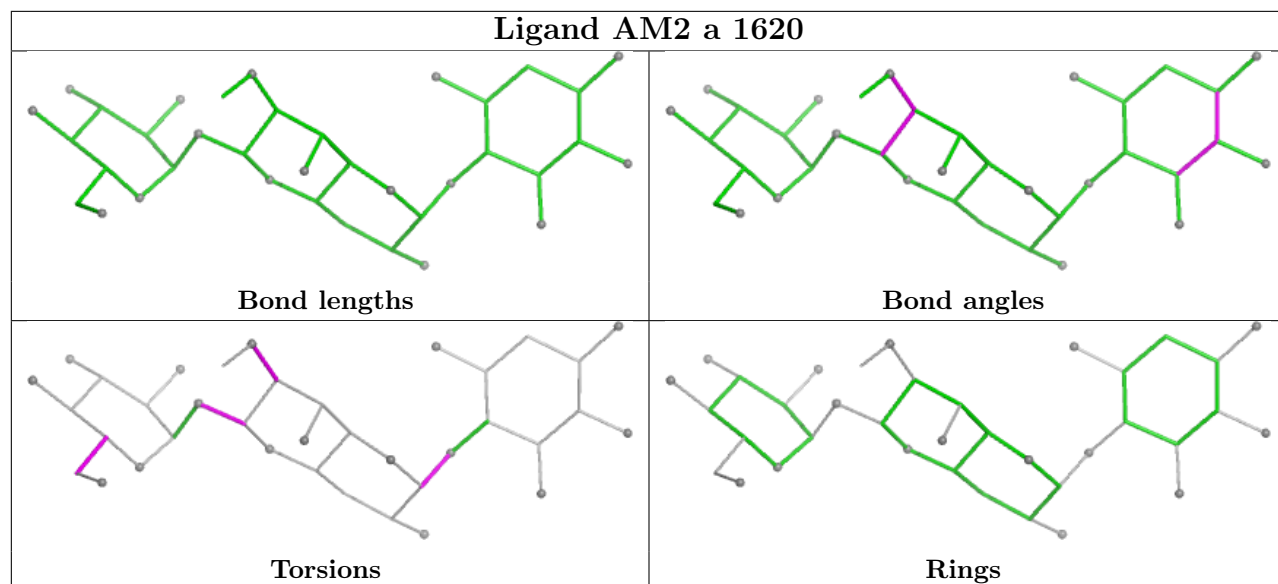
2 monomers are involved in 3 short contacts:

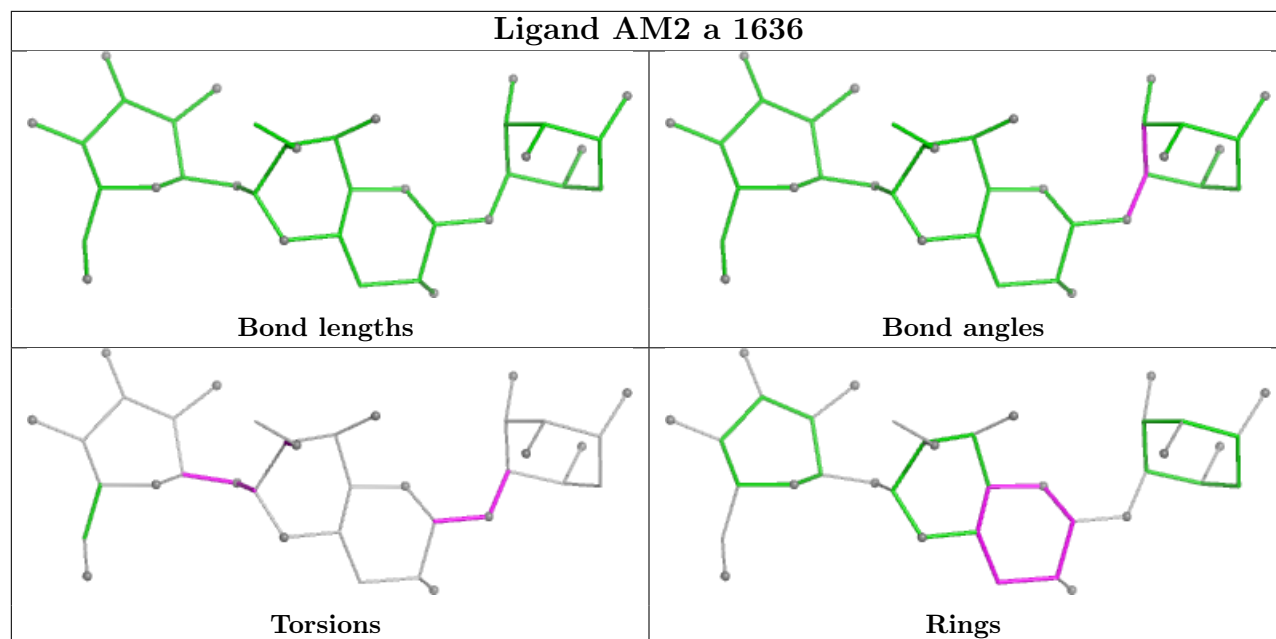
Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	x	801	GDP	1	0
63	a	1620	AM2	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

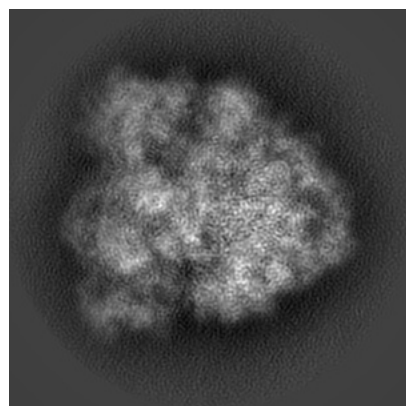
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13464. These allow visual inspection of the internal detail of the map and identification of artifacts.

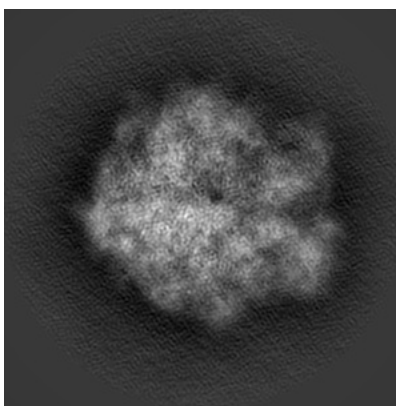
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

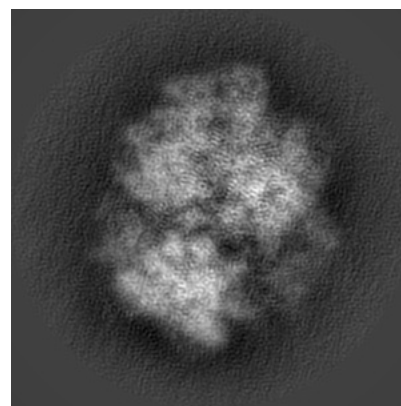
6.1.1 Primary map



X

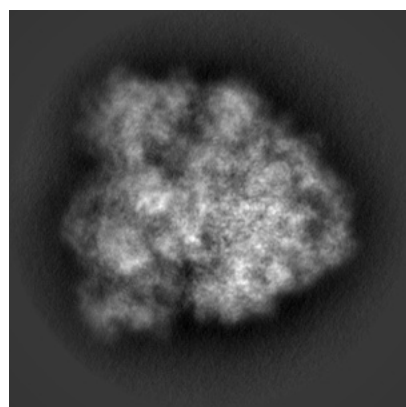


Y

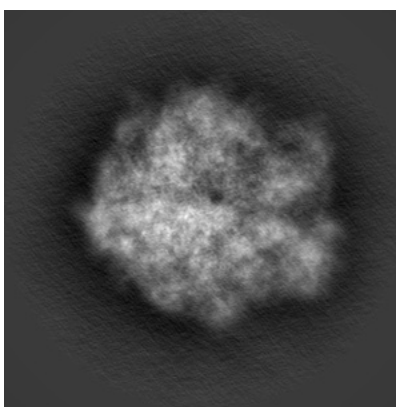


Z

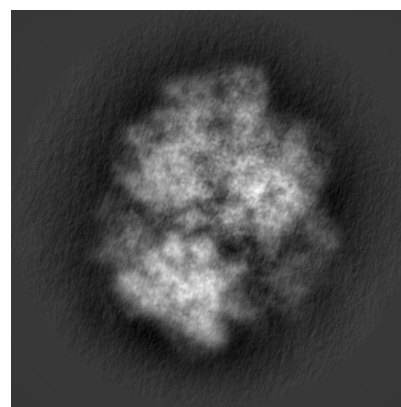
6.1.2 Raw map



X



Y

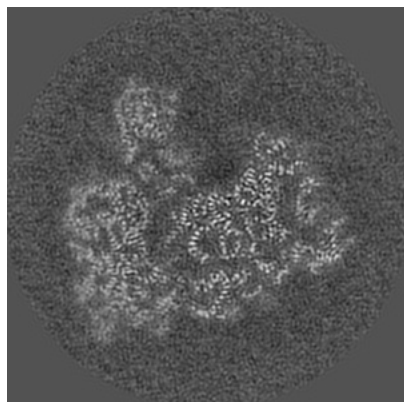


Z

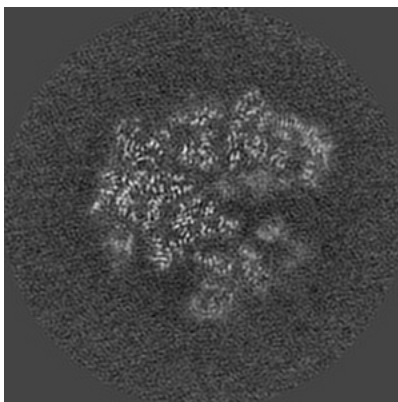
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

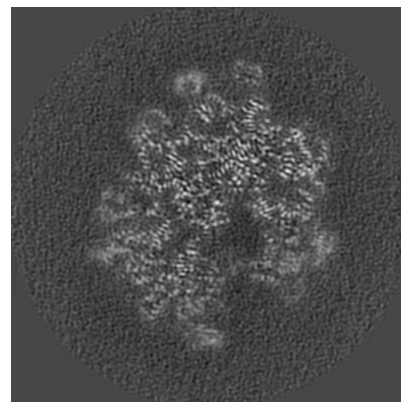
6.2.1 Primary map



X Index: 256

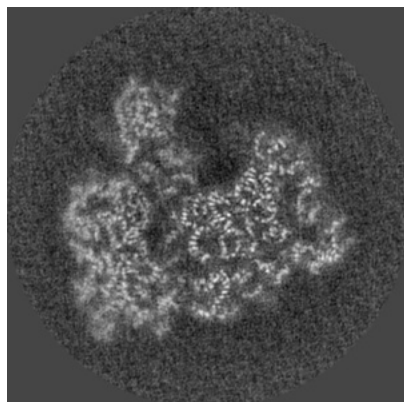


Y Index: 256

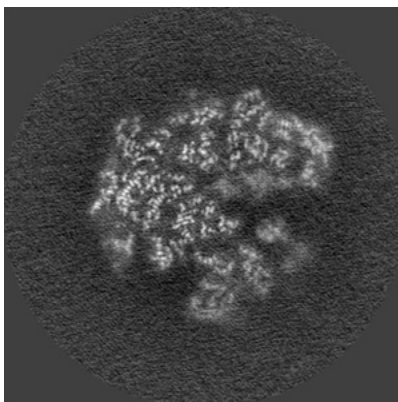


Z Index: 256

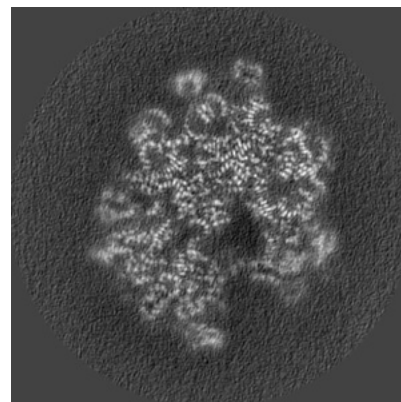
6.2.2 Raw map



X Index: 144



Y Index: 144

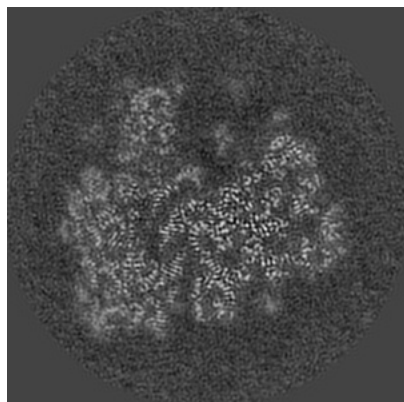


Z Index: 144

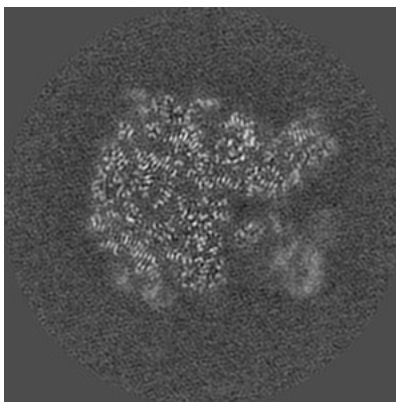
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

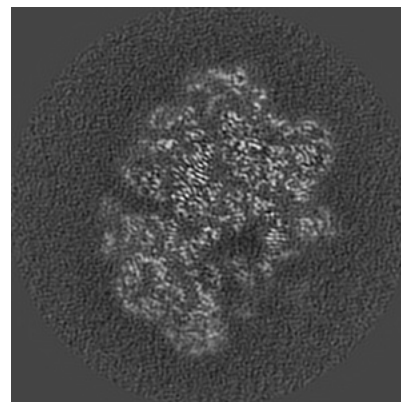
6.3.1 Primary map



X Index: 246

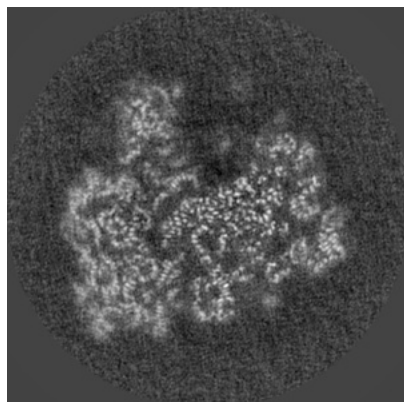


Y Index: 289

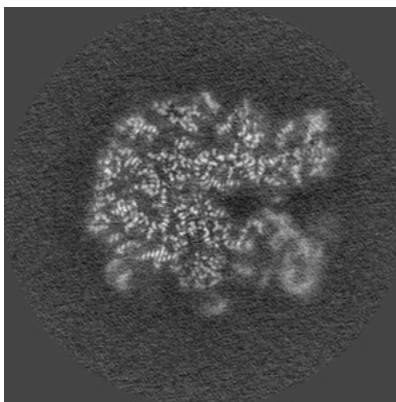


Z Index: 238

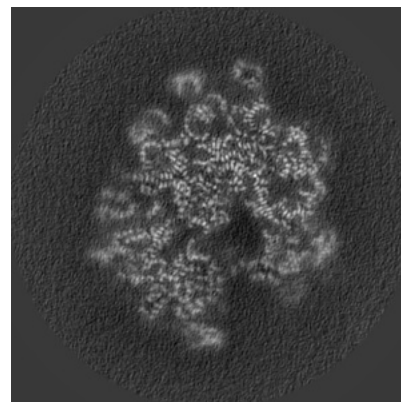
6.3.2 Raw map



X Index: 141



Y Index: 157

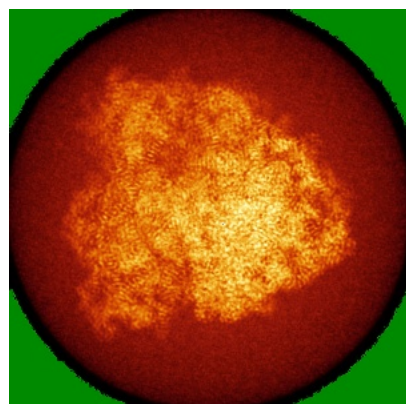


Z Index: 145

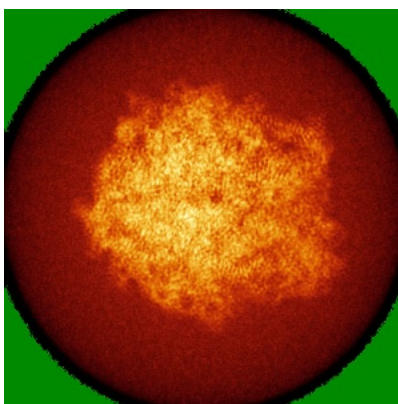
The images above show the largest variance slices of the map in three orthogonal directions.

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

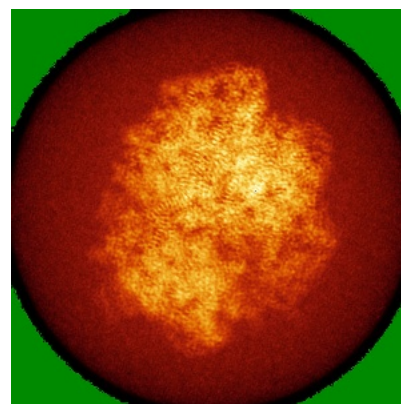
6.4.1 Primary map



X

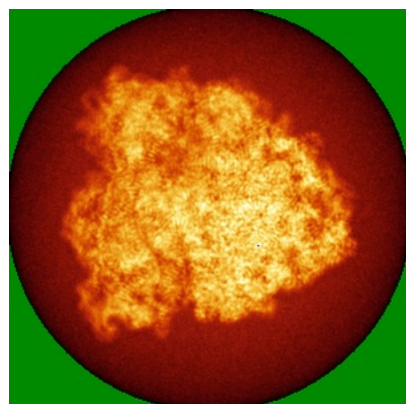


Y

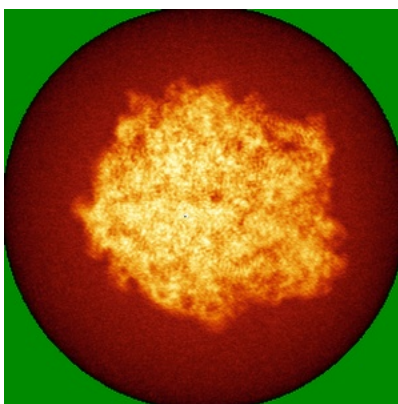


Z

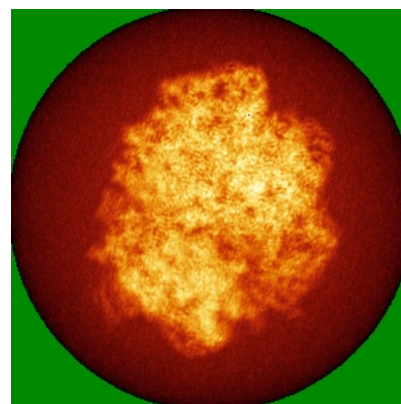
6.4.2 Raw map



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](#)

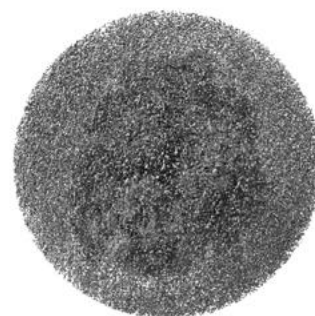
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. 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.

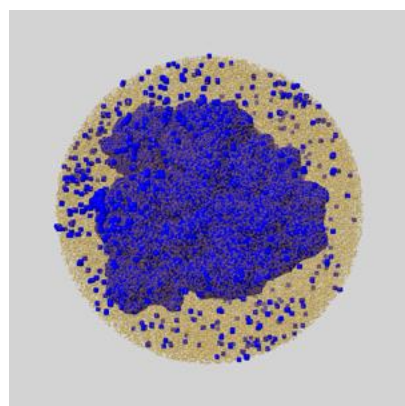
6.6 Mask visualisation [i](#)

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

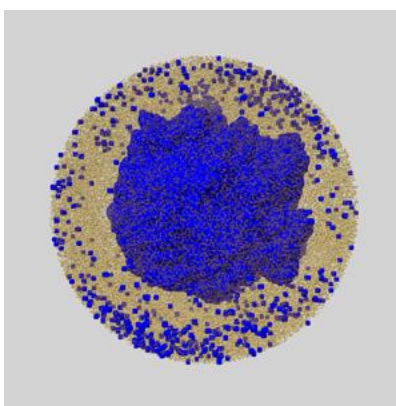
A mask typically either:

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

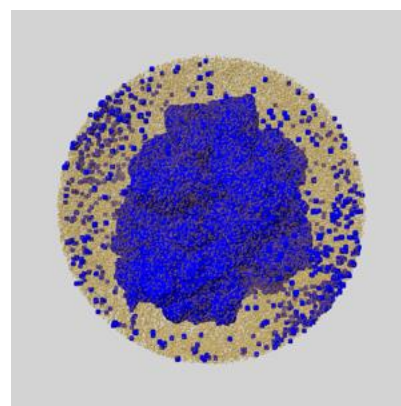
6.6.1 emd_13464_msk_1.map [i](#)



X



Y

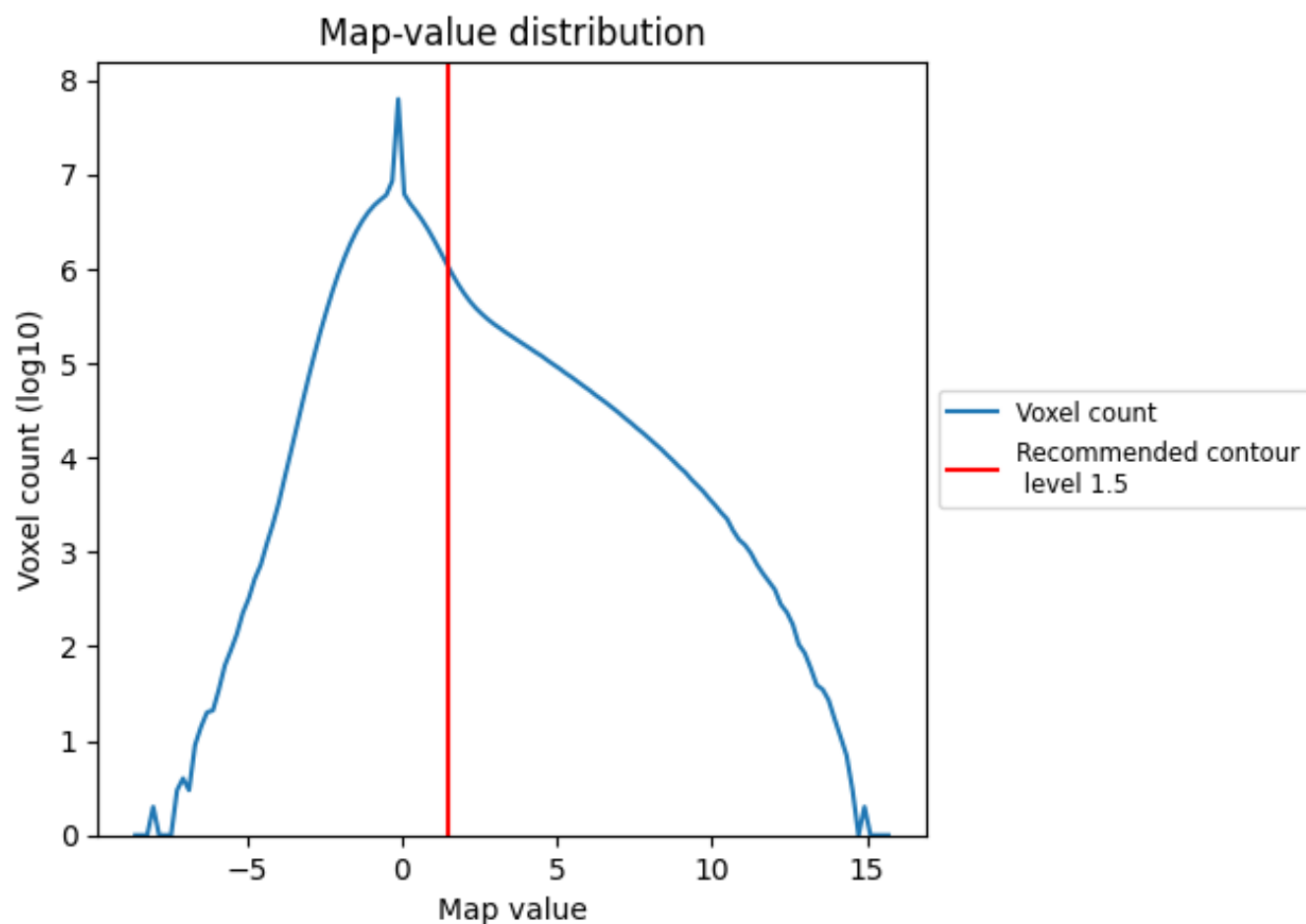


Z

7 Map analysis [i](#)

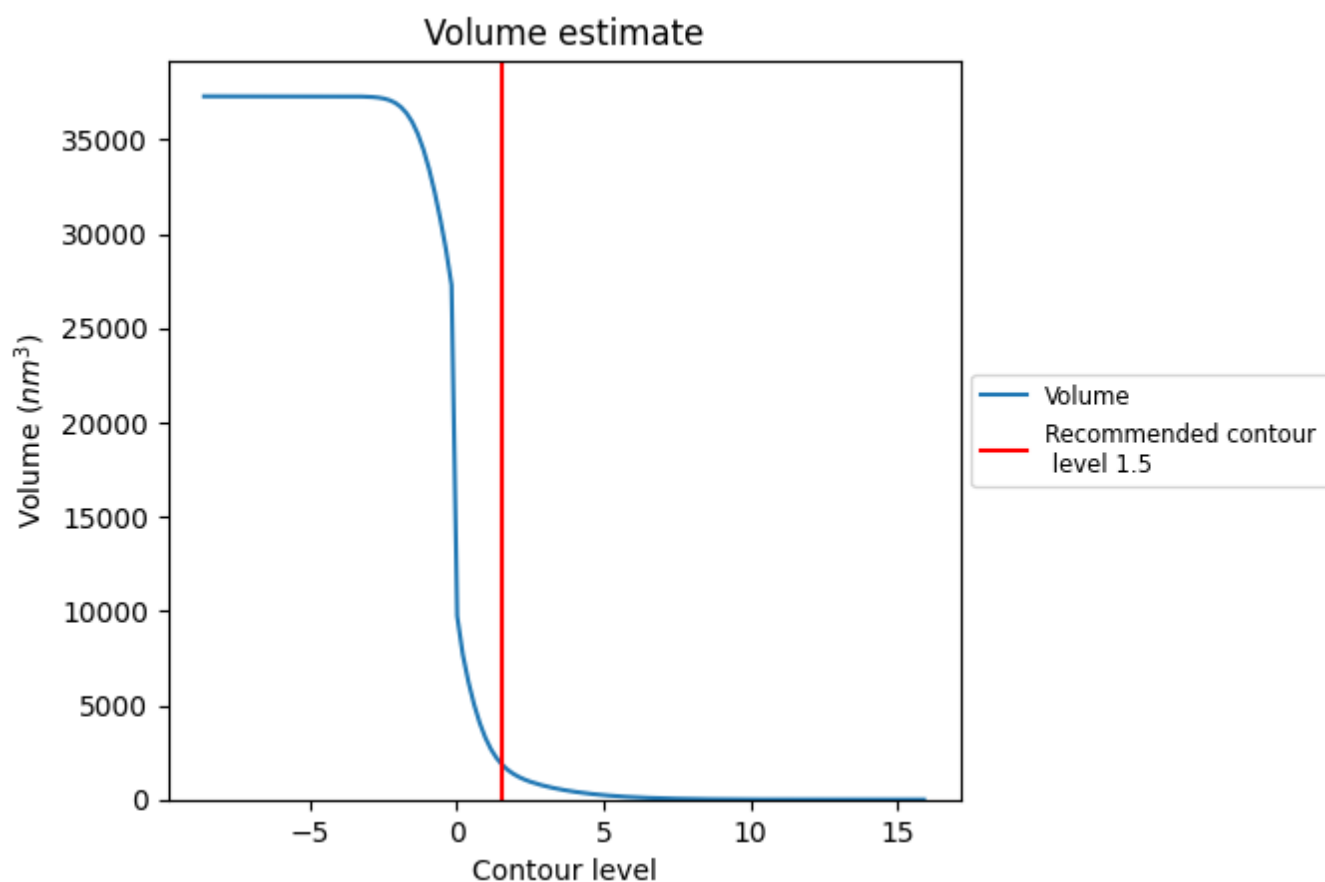
This section contains the results of statistical analysis of the map.

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.

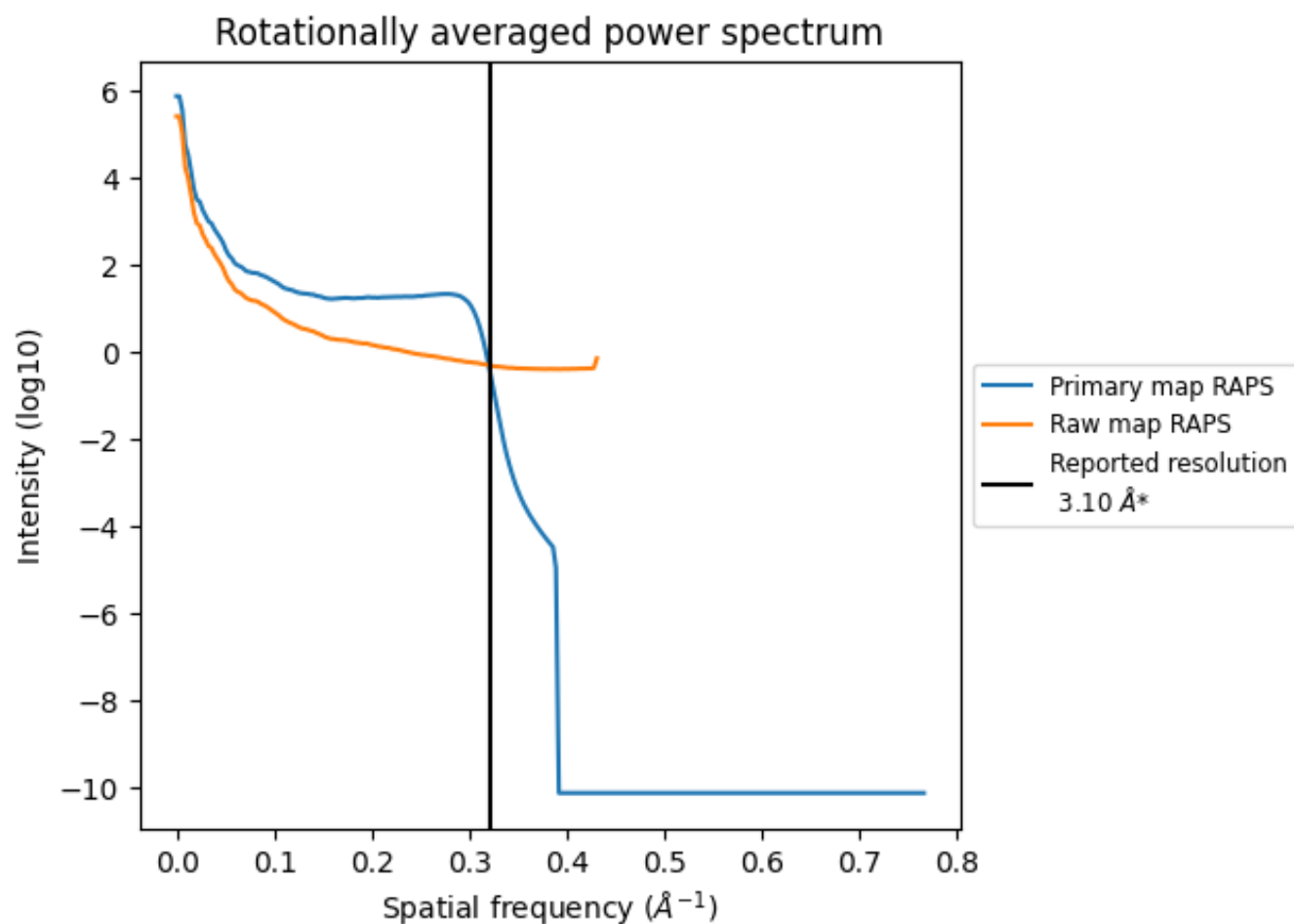
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1926 nm³; this corresponds to an approximate mass of 1740 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 ⓘ

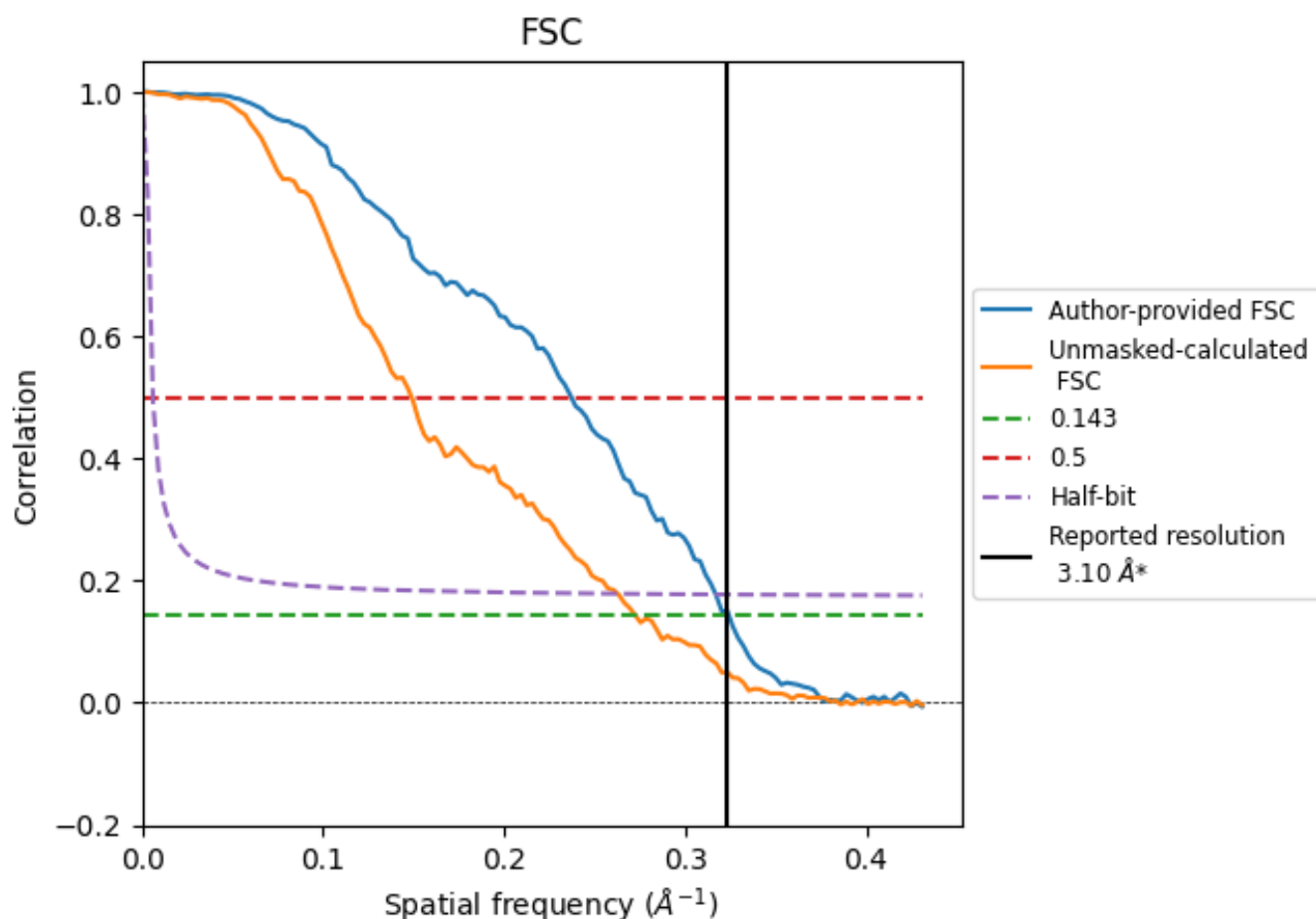


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

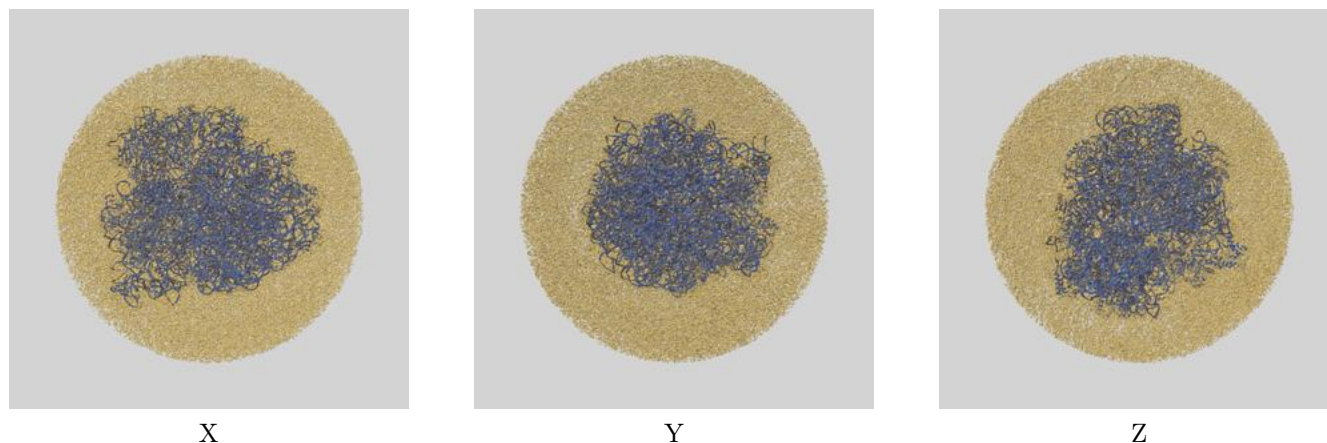
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	4.22	3.15
Unmasked-calculated*	3.67	6.72	3.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

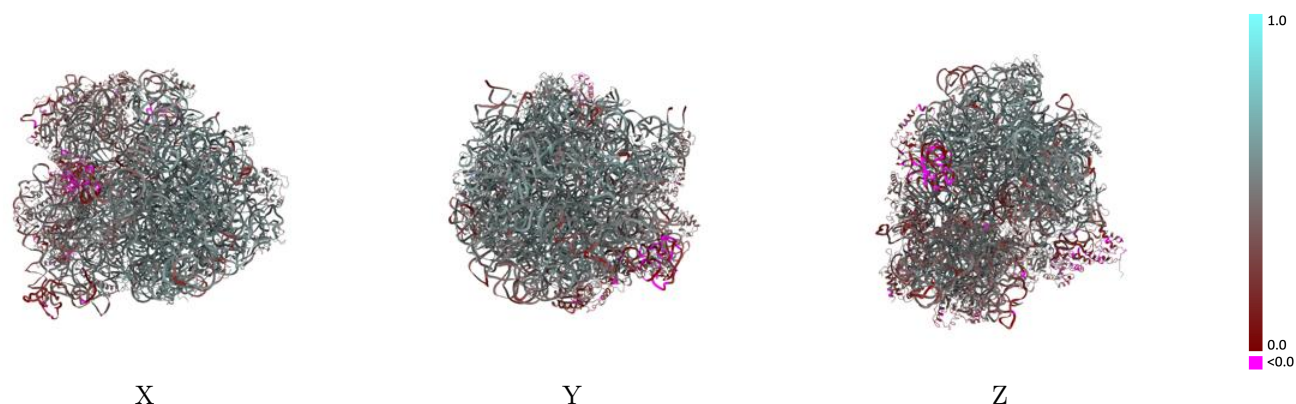
This section contains information regarding the fit between EMDB map EMD-13464 and PDB model 7PJY. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



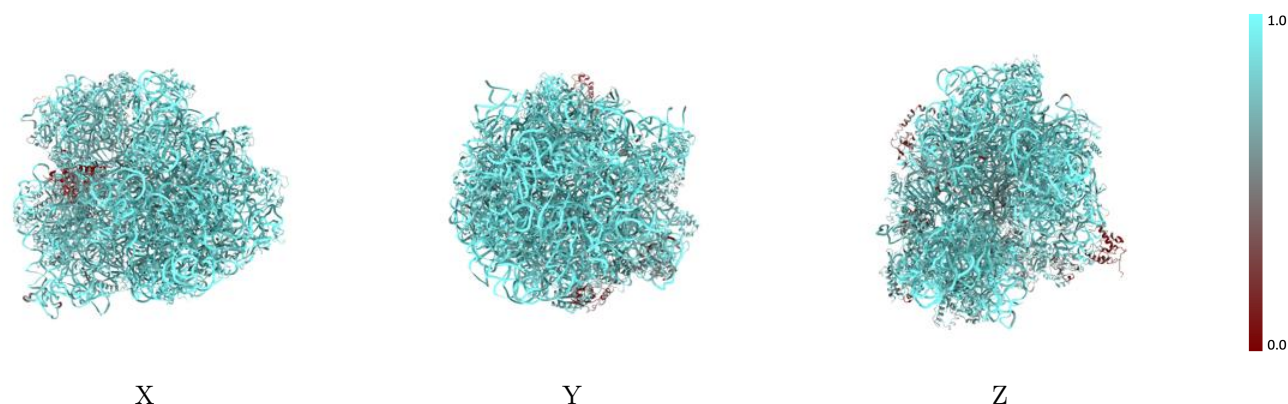
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



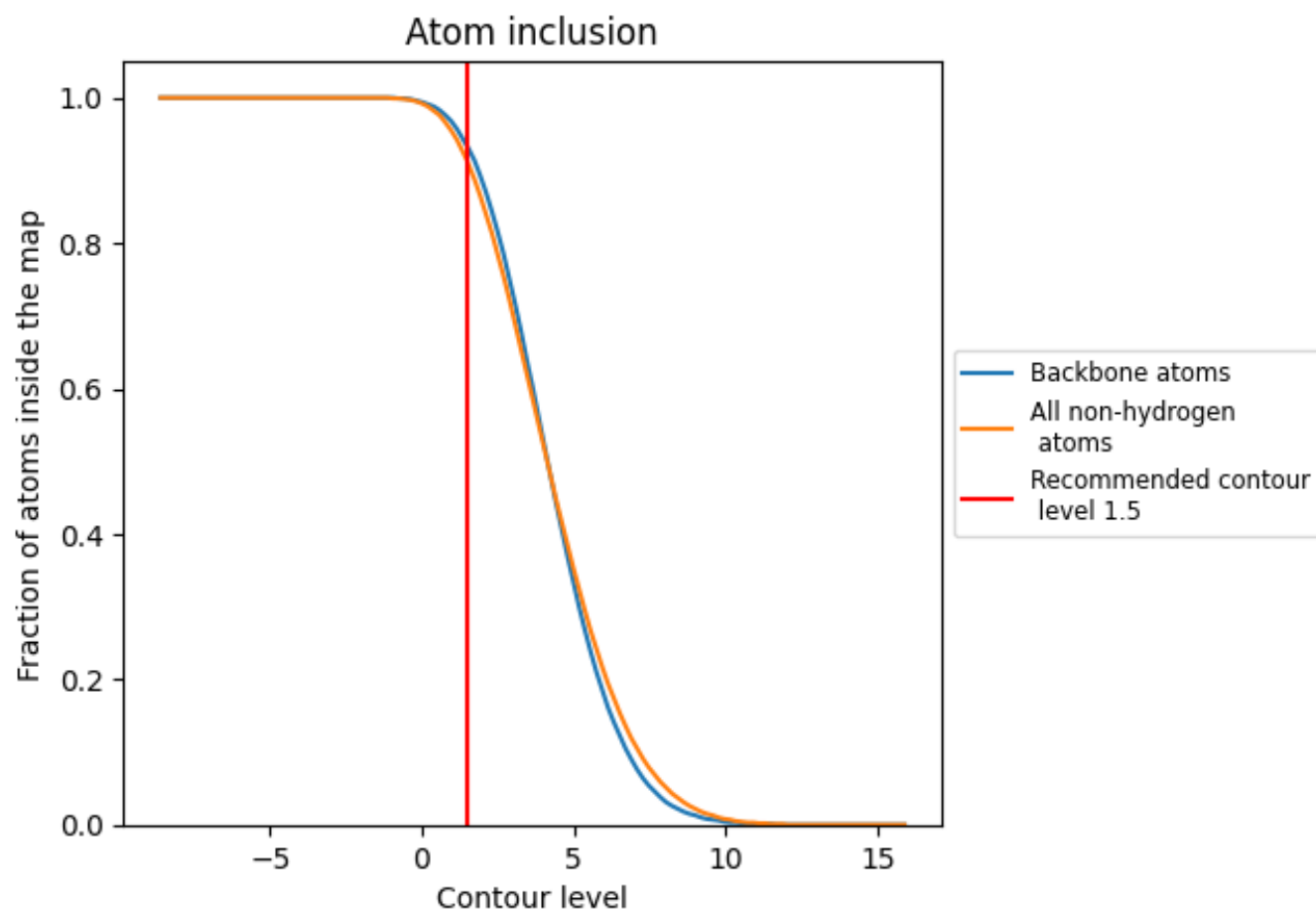
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.4660
0	 0.8930	 0.5200
1	 0.8460	 0.4870
2	 0.9210	 0.5610
3	 0.9370	 0.5640
4	 0.9350	 0.5350
5	 0.2230	 0.1450
6	 0.7800	 0.3320
A	 0.9630	 0.5030
B	 0.9700	 0.4890
C	 0.9130	 0.5380
D	 0.9140	 0.5310
E	 0.8900	 0.5000
F	 0.8310	 0.4070
G	 0.8590	 0.4270
H	 0.4430	 0.2690
I	 0.4990	 0.1370
J	 0.9270	 0.5300
K	 0.8640	 0.5270
L	 0.9060	 0.5210
M	 0.9060	 0.5220
N	 0.9480	 0.5380
O	 0.9050	 0.4780
P	 0.8950	 0.5300
Q	 0.9450	 0.5390
R	 0.9360	 0.5170
S	 0.8930	 0.5230
T	 0.9020	 0.4920
U	 0.9240	 0.4840
V	 0.8960	 0.5000
W	 0.9270	 0.5360
X	 0.8930	 0.5300
Y	 0.8910	 0.4570
Z	 0.9040	 0.5140
a	 0.9500	 0.4470



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Chain	Atom inclusion	Q-score
b	 0.6370	 0.3260
c	 0.8250	 0.4090
d	 0.8190	 0.3700
e	 0.8840	 0.4660
f	 0.8230	 0.3520
g	 0.6650	 0.2930
h	 0.8740	 0.4560
i	 0.8840	 0.3860
j	 0.7830	 0.3630
k	 0.8140	 0.4230
l	 0.8280	 0.4950
m	 0.8270	 0.3860
n	 0.8890	 0.4390
o	 0.8590	 0.4340
p	 0.8740	 0.4590
q	 0.8700	 0.4520
r	 0.8850	 0.4370
s	 0.8550	 0.4080
t	 0.8710	 0.4360
u	 0.7440	 0.3750
v	 0.8820	 0.4250
w	 0.7520	 0.3370
x	 0.7600	 0.3750
y	 0.6190	 0.3720
z	 0.9090	 0.5080