



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 10:49 PM JST

PDB ID : 8Y5R / pdb_00008y5r
EMDB ID : EMD-38947
Title : E.coli Transcription translation coupling complex in TTC-B state 5 (subclass 1) containing mRNA with 27-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and fusidic acid
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.
Deposited on : 2024-01-31
Resolution : 4.50 Å(reported)

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.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.45.1

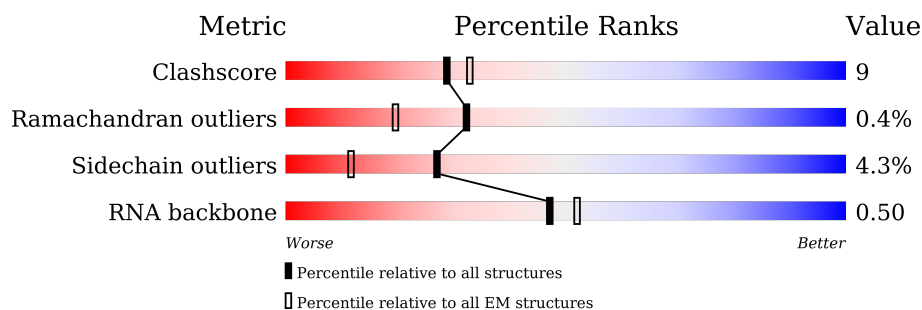
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





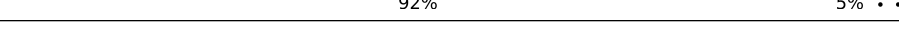


The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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	A	70	 80% 14% 6%
2	B	57	 77% 21% 2%
3	C	55	 84% 7% 9%
4	D	46	 76% 22% 2% 2%
5	E	65	 92% 5% 3% 2%
6	F	38	 74% 24% 2% 2%
7	G	241	 66% 23% 10%



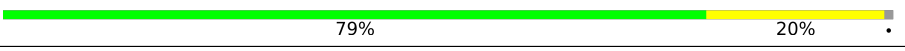
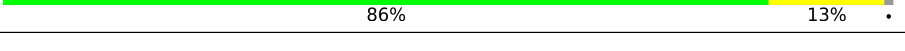
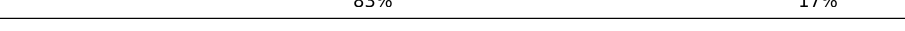
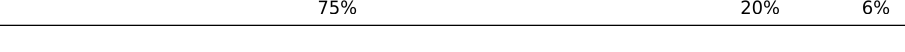
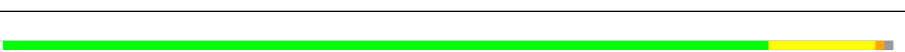




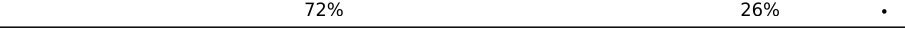




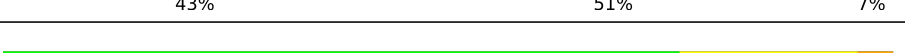


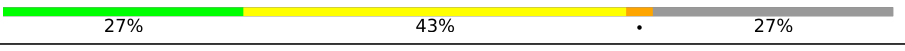
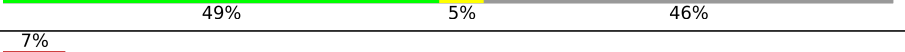
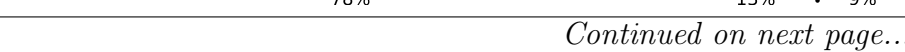



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	233	
9	I	206	
10	J	167	
11	K	135	
12	L	179	
13	M	130	
14	N	130	
15	O	103	
16	P	129	
17	Q	124	
18	R	118	
19	S	101	
20	T	89	
21	U	82	
22	V	84	
23	W	75	
24	X	92	
25	Y	87	
26	Z	71	
27	b	273	
28	c	209	
29	d	201	
30	e	179	
31	f	177	
32	g	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	i	142	
34	j	142	
35	k	123	
36	l	144	
37	m	136	
38	n	127	
39	o	117	
40	p	115	
41	q	118	
42	r	103	
43	s	110	
44	t	100	
45	u	104	
46	v	94	
47	w	85	
48	x	78	
49	y	63	
50	z	59	
51	1	2904	
52	2	120	
53	3	1542	
54	4	44	
55	8	37	
56	9	37	
57	A1	329	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NA	495	
62	NG	181	
63	5	76	
64	6	77	
65	0	716	

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 181797 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 L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	66	Total	C	N	O	S	0	0
			521	323	98	94	6		

- Molecule 2 is a protein called 50S ribosomal protein L32.

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

- Molecule 3 is a protein called 50S ribosomal protein L33.

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

- Molecule 4 is a protein called 50S ribosomal protein L34.

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

- Molecule 5 is a protein called 50S ribosomal protein L35.

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

- Molecule 6 is a protein called 50S ribosomal protein L36.

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

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called 30S ribosomal protein S3.

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

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

- Molecule 12 is a protein called 30S ribosomal protein S7.

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

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

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

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

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

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

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

- Molecule 22 is a protein called 30S ribosomal protein S17.

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

- Molecule 23 is a protein called 30S ribosomal protein S18.

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

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	52	Total	C	N	O	S	0	0
			400	256	73	70	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1929590828

- Molecule 52 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	U	conflict	GB NR_103249

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	39	Total	C	N	O	P	0	0
			809	362	113	295	39		

- Molecule 55 is a DNA chain called templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	27	Total	C	N	O	P	0	0
			539	257	88	167	27		

- Molecule 56 is a DNA chain called non-templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	9	20	Total	C	N	O	P	0	0
			417	195	84	118	20		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	A1	301	Total	C	N	O	S	0	0
			2088	1293	380	409	6		
57	A2	288	Total	C	N	O	S	0	0
			2029	1257	366	400	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B1	1335	Total	C	N	O	S	0	0
			10353	6509	1842	1955	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B2	1340	Total	C	N	O	S	0	0
			10546	6616	1839	2048	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	W0	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 61 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	NA	492	Total	C	N	O	0	0
			2432	1448	492	492		

- Molecule 62 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	NG	154	Total	C	N	O	0	0
			758	450	154	154		

- Molecule 63 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 64 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
64	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 65 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	0	673	Total	C	N	O	S	0	0
			5211	3289	900	999	23		

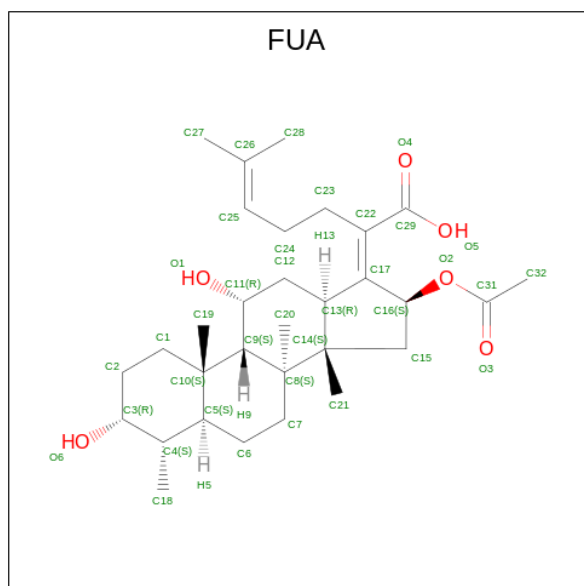
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	705	GLY	-	expression tag	UNP P0A6M8
0	706	SER	-	expression tag	UNP P0A6M8
0	707	SER	-	expression tag	UNP P0A6M8
0	708	GLY	-	expression tag	UNP P0A6M8
0	709	HIS	-	expression tag	UNP P0A6M8
0	710	HIS	-	expression tag	UNP P0A6M8
0	711	HIS	-	expression tag	UNP P0A6M8
0	712	HIS	-	expression tag	UNP P0A6M8
0	713	HIS	-	expression tag	UNP P0A6M8
0	714	HIS	-	expression tag	UNP P0A6M8
0	715	HIS	-	expression tag	UNP P0A6M8
0	716	HIS	-	expression tag	UNP P0A6M8

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

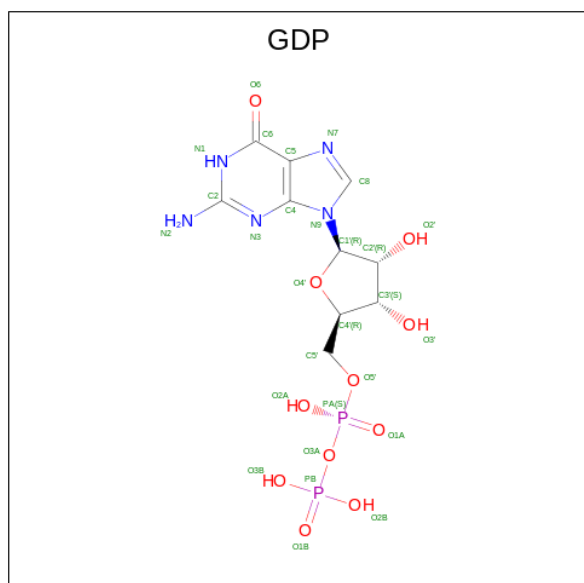
Mol	Chain	Residues	Atoms		AltConf
66	B1	1	Total	Mg	0
			1	1	

- Molecule 67 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
67	0	1	Total	C	O	0
			37	31	6	

- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).




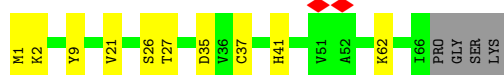
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
68	0	1	28	10	5	11	2	0

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 L31

Chain A: 




- Molecule 2: 50S ribosomal protein L32

Chain B: 



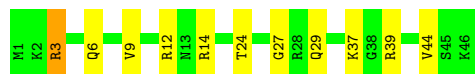
- Molecule 3: 50S ribosomal protein L33

Chain C: 



- Molecule 4: 50S ribosomal protein L34

Chain D: 



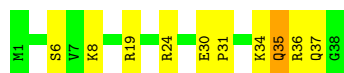
- Molecule 5: 50S ribosomal protein L35

Chain E: 



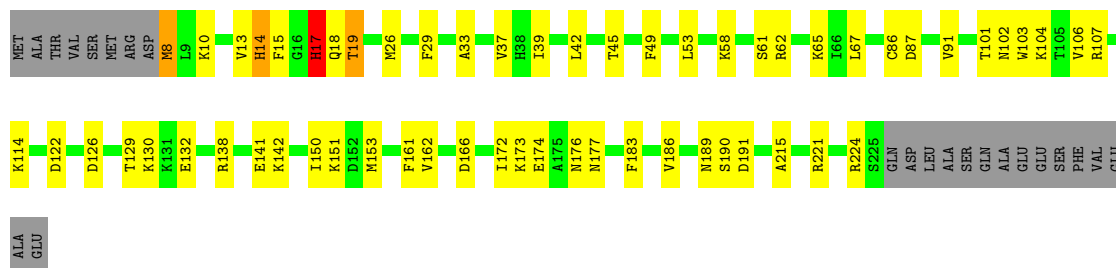
- Molecule 6: 50S ribosomal protein L36

Chain F:  74% 24% .



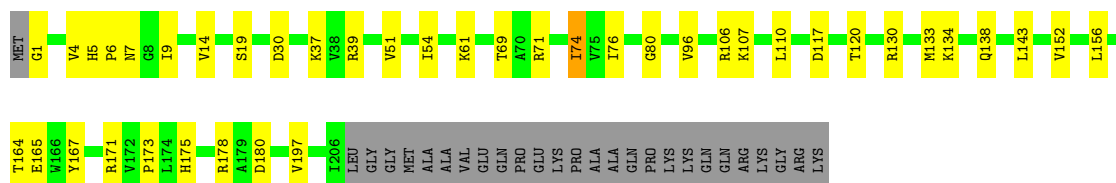
- Molecule 7: 30S ribosomal protein S2

Chain G:  66% 23% . 10%



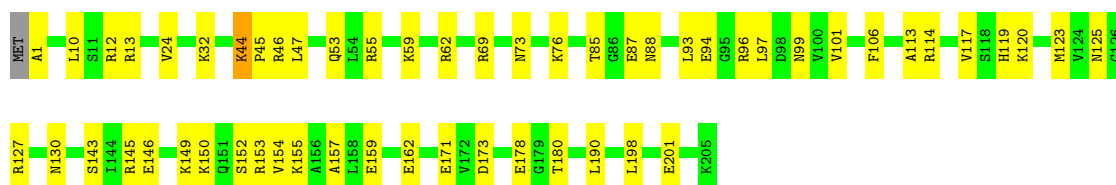
- Molecule 8: 30S ribosomal protein S3

Chain H:  71% 17% 12%




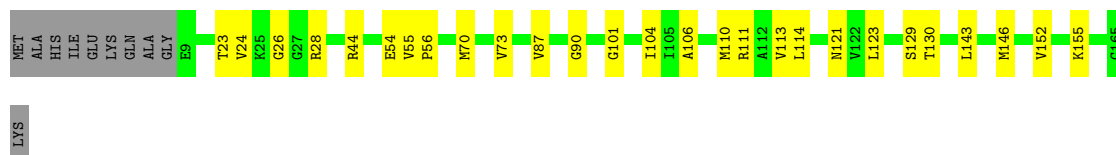
- Molecule 9: 30S ribosomal protein S4

Chain I:  73% 26%



- Molecule 10: 30S ribosomal protein S5

Chain J:  78% 16% 6%



- Molecule 11: 30S ribosomal protein S6, fully modified isoform



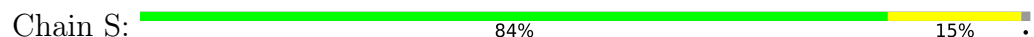
- Molecule 17: 30S ribosomal protein S12



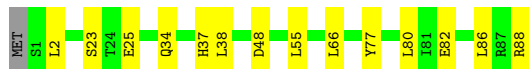
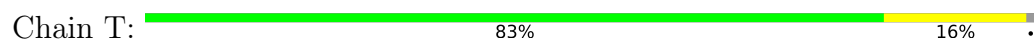
- Molecule 18: 30S ribosomal protein S13



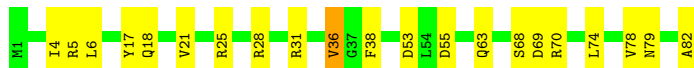
- Molecule 19: 30S ribosomal protein S14



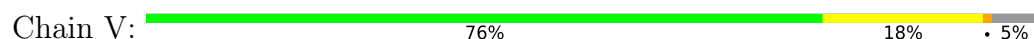
- Molecule 20: 30S ribosomal protein S15

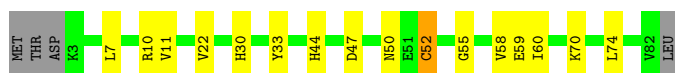


- Molecule 21: 30S ribosomal protein S16



- Molecule 22: 30S ribosomal protein S17





- Molecule 23: 30S ribosomal protein S18

Chain W: 67% 19% 13%



- Molecule 24: 30S ribosomal protein S19

Chain X: 73% 13% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y: 76% 22%



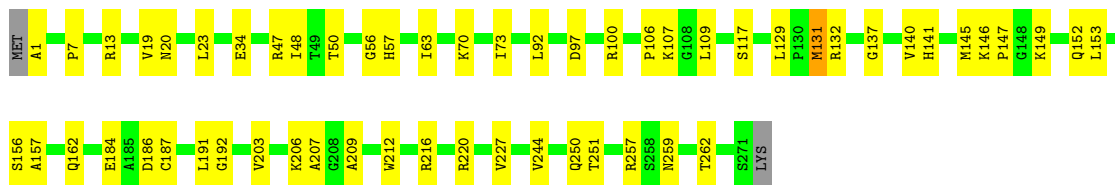
- Molecule 26: 30S ribosomal protein S21

Chain Z: 56% 34% 8%



- Molecule 27: 50S ribosomal protein L2

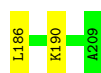
Chain b: 79% 20%



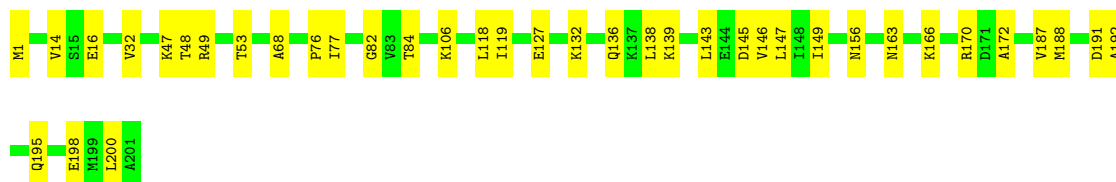
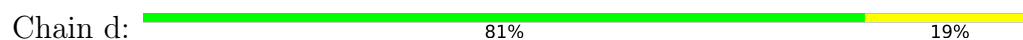
- Molecule 28: 50S ribosomal protein L3

Chain c: 83% 17%

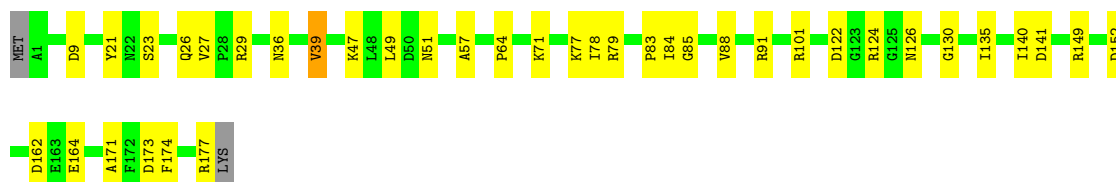
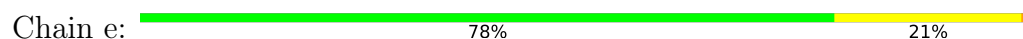




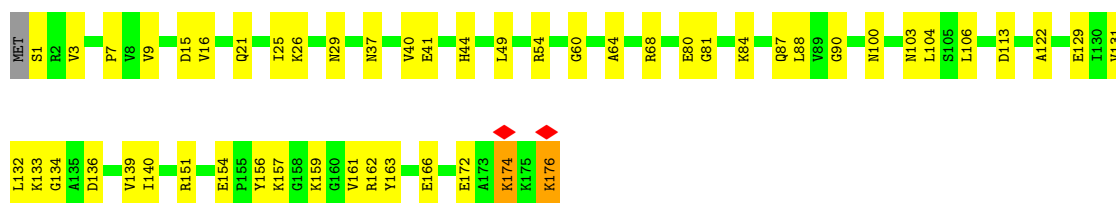
- Molecule 29: 50S ribosomal protein L4



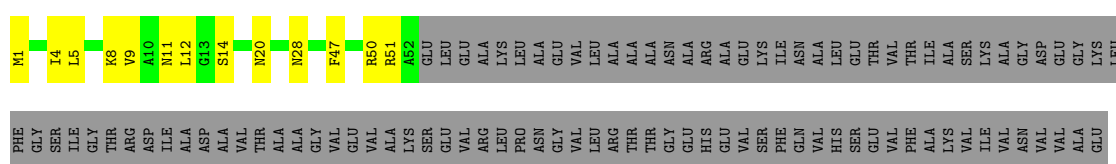
- Molecule 30: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L6

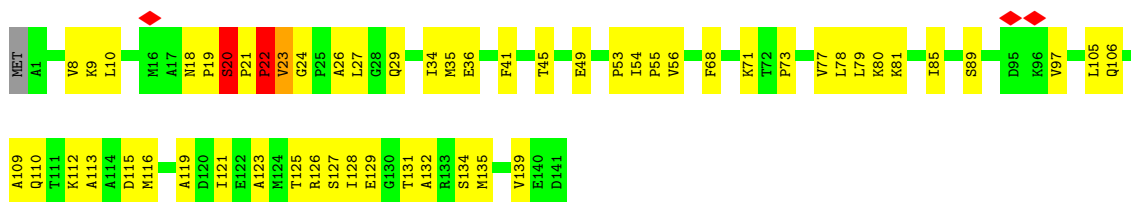


- Molecule 32: 50S ribosomal protein L9

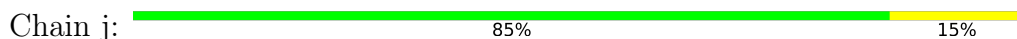


- Molecule 33: 50S ribosomal protein L11





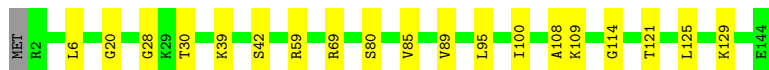
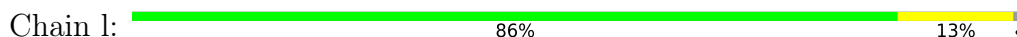
- Molecule 34: 50S ribosomal protein L13



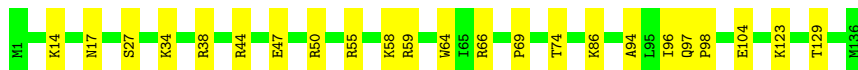
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



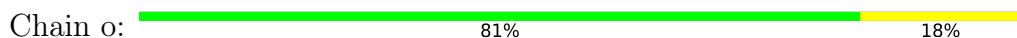
- Molecule 37: 50S ribosomal protein L16




- Molecule 38: 50S ribosomal protein L17

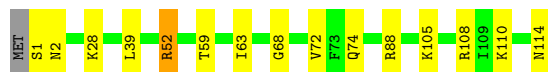


- Molecule 39: 50S ribosomal protein L18




- Molecule 40: 50S ribosomal protein L19

Chain p:  86% 12% ..



- Molecule 41: 50S ribosomal protein L20

Chain q:  83% 15% ..




- Molecule 42: 50S ribosomal protein L21

Chain r:  77% 23%



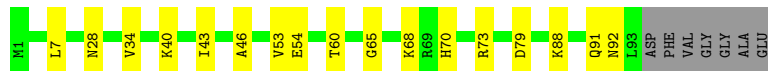
- Molecule 43: 50S ribosomal protein L22

Chain s:  85% 15%



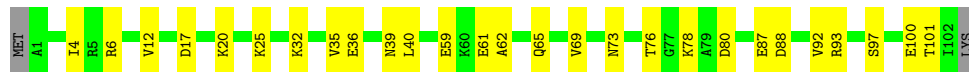
- Molecule 44: 50S ribosomal protein L23

Chain t:  76% 17% 7%




- Molecule 45: 50S ribosomal protein L24

Chain u:  72% 26% .



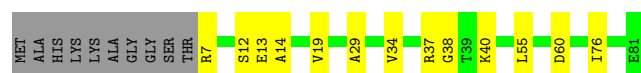
- Molecule 46: 50S ribosomal protein L25

Chain v:  85% 15%



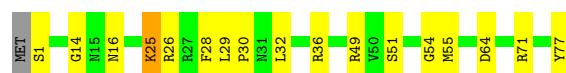
- Molecule 47: 50S ribosomal protein L27

Chain w:  73% 15% 12%




- Molecule 48: 50S ribosomal protein L28

Chain x:  77% 21% ..




- Molecule 49: 50S ribosomal protein L29

Chain y:  78% 22%



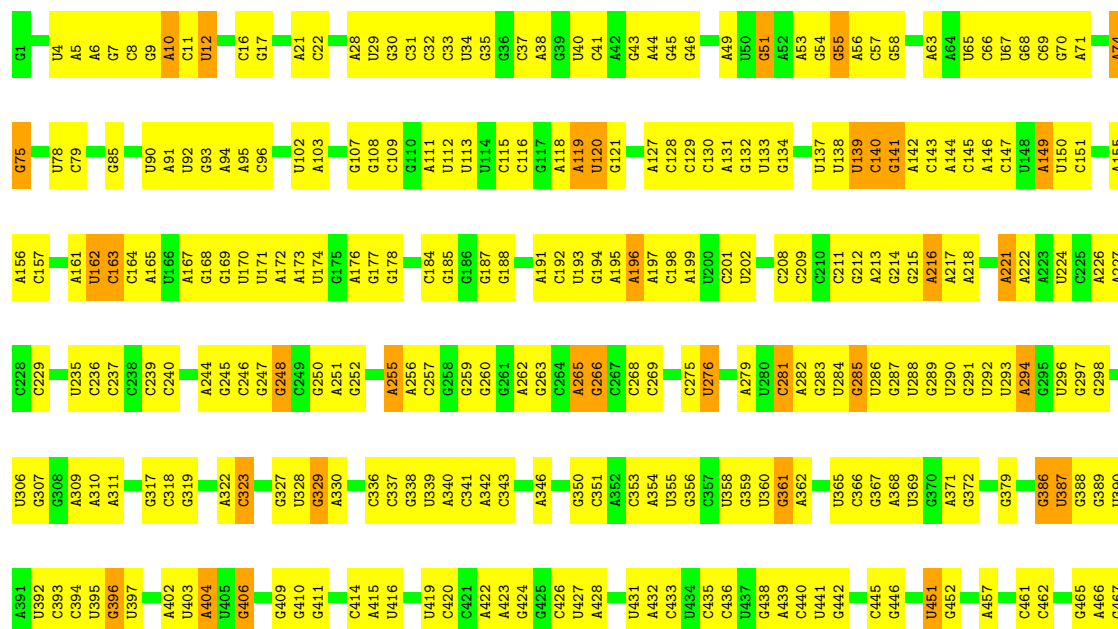
- Molecule 50: 50S ribosomal protein L30

Chain z:  76% 22% .



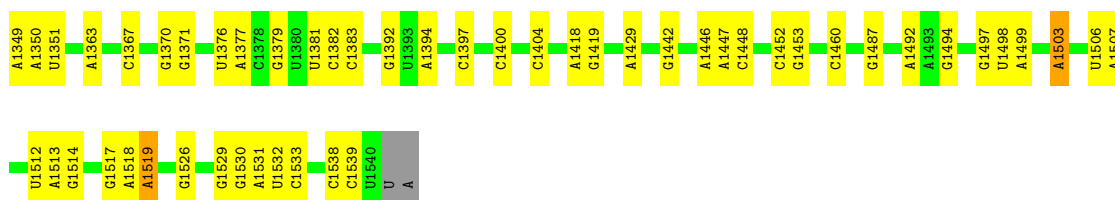
- Molecule 51: 23S rRNA

Chain 1:  43% 51% 7%

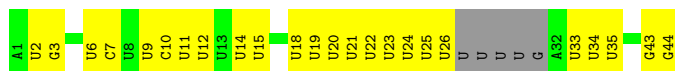


A1572	A1573	C1574	C1575	U1576	G1577	G1578	A1579	A1580	G1581	C1582	A1583	G1588	A1589	U1590	A1591	A1592	A1593	U1594	A1595	A1596	A1597	A1598	U1599	C1600	G1601	U1602	A1603	C1604	C1605	C1606	C1607	A1608	A1614	C1615	A1616	C1625	A1626	A1634	G1642	G1643	C1644	G1645	G1646	U1647	U1648	G1651	U1662	G1663	G1666	C1667	A1668	A1669								
C1428	G1429	G1430	G1438	A1439	G1443	A1434	C1435	G1436	C1437	U1438	C1439	U1440	G1441	U1442	U1443	A1365	A1366	A1367	G1368	G1448	G1449	G1450	C1451	G1452	G1453	C1454	C1461	C1462	C1463	G1464	G1465	U1466	U1467	U1468	U1469	A1470	C1480	U1481	G1482	G1483	U1484	U1485	U1486	U1487	A1488	C1489	U1490	G1491	C1492	G1493	U1494	A1495	A1496	U1497	G1500	U1501	A1502	G1503	A1504	A1505
U1336	G1337	G1338	G1339	G1343	A1344	C1345	G1346	A1347	C1348	C1349	U1352	G1352	A1353	A1354	A1355	A1356	A1357	G1358	G1377	A1378	U1379	G1380	G1381	G1382	A1383	A1384	C1385	G1386	A1387	G1388	U1389	U1390	U1394	U1400	G1401	U1402	A1403	C1404	U1405	U1406	U1409	U1410	U1411	U1412	G1413	G1414	U1415	A1416	C1417	G1418	U1419	A1420	G1425	G1426	A1427					
C1270	G1271	A1272	U1273	G1274	A1275	C1276	G1279	G1280	G1281	U1282	G1283	A1284	A1285	A1286	A1287	G1288	C1289	G1292	U1294	C1295	G1296	C1297	G1298	G1299	G1300	A1301	A1302	C1306	G1309	G1310	G1311	C1314	C1315	U1316	G1317	U1318	C1319	C1320	A1321	C1322	C1323	A1237	G1238	G1239	U1240	A1246	A1247	A1253	A1254	U1255	G1256	C1257	U1258	G1259	G1333	G1334	C1335			
U1176	G1177	G1178	G1179	U1180	U1181	U1182	U1183	U1184	G1185	G1186	G1187	U1188	G1189	A1194	G1194	G1195	G1196	G1197	U1198	U1199	C1200	A1204	A1205	U1209	G1210	G1211	G1212	A1213	U1219	G1220	G1225	A1230	U1231	G1232	C1233	A1237	G1154	A1155	A1156	G1157	G1160	C1161	G1162	G1163	C1164	A1165	G1166	G1167	C1168	U1169	G1170	G1171	C1172	U1173	U1174	A1175				
C1043	G1044	C1045	A1046	G1047	A1048	C1049	A1050	A1054	G1055	G1056	A1057	U1058	U1059	U1060	A1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	G1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	G1100	U1101	C1102	A1103	C1104		
C957	U958	A959	A960	C961	C968	A972	A973	G974	A975	A979	A980	A981	A982	A983	A984	C985	G989	C993	C994	C995	A996	C1005	A1009	G1010	G1011	U1012	C1013	A1014	U1015	U1019	A1020	A1021	G1022	U1023	G1024	G1025	A1026	A1027	G1031	A1032	U1033	U1034	U1035	A1036	G1037	U1038	A1039	A1040	G1041	C1042										
G879	C885	A886	U887	U888	C889	C890	C891	C892	C893	A894	U895	A896	C897	C898	A899	A900	C901	C902	A904	A905	U906	G907	C908	A909	A910	A911	C840	G841	U842	A845	U846	U847	C848	A849	U850	C851	U852	C853	C854	G855	U932	C935	A936	C937	G938	G939	G940	A941	G942	C946	A947	U955	G956							
G805	G809	U810	U811	C812	U813	C814	C815	A819	A820	A821	A825	U826	U827	U828	A829	G830	G831	U832	A833	C834	C835	G836	C908	A909	A910	A911	C840	G841	U842	A845	U846	U847	C848	A849	U850	C851	U852	C853	C854	G855	G858	G859	U860	G864	C865	U870	U871	U872	C873	C876	A877	A878								
U709	G712	G713	A718	C719	U720	A721	C722	C723	U724	G725	A727	A728	C729	A730	C736	G745	U746	C747	A752	G757	C758	G759	A760	U761	C761	C762	C763	C764	G774	G775	U779	G780	A781	G782	A783	G784	C785	A788	U789	C791	A792	A793	A794	C795	C796	A800	G801													
G548	G549	C550	G551	U552	G553	U554	G555	A556	C557	U558	U562	A563	U566	U567	U568	U569	G570	U571	A572	U573	A574	A575	U580	A586	A590	U591	U592	U593	U594	C595	U596	G597	A526	C527	A528	A529	G530	C531	A532	G533	U534	G535	G536	G537	A538	G539	C540	C541	C542	C543	C544	U545	U546	A547						

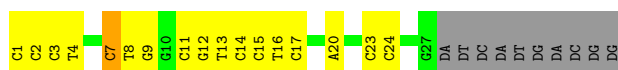
U2804	G2729	G2642	A2566	A2468	C2385	U2305	C2226	G2159	G2093	C1990	C1908	G1823	G1750	C1670
C2805	G2730	G2643	G2567	A2469	A2386	C2306	A2227	C2160	A2094	U1991	C1909	U1827	U1751	U1671
C2806	G2731	G2644	G2568	G2470	A2387	A2309	G2230	C2161	A2095	C2096	U1911	U1828	G1752	A1672
A2810	G2732	G2645	G2569	A2471	A2388	C2310	U2233	A2163	C2097	U1993	A1912	A1829	G1753	G1673
G2811	G2733	G2646	G2570	A2476	U2390	A2311	U2234	C2164	A2098	C1987	A1914	C1832	C1674	C1675
G2812	G2734	G2647	A2572	A2482	G2391	U2312	G2236	C2165	U2099	C1998	U1915	A1676	A1677	A1678
G2813	G2735	G2648	G2573	C2483	A2392	C2313	G2237	C2166	A2101	U1999	A1916	C1768	A1679	U1680
A2814	A2736	G2649	G2574	G2493	U2393	A2314	G2238	U2187	G2102	C1988	U1917	G1766	U1681	G1681
G2815	G2737	C2395	G2575	G2488	C2396	G2316	G2239	U2188	G2103	U1991	A1918	U1765	G1675	G1682
G2816	G2738	G2396	G2576	U2489	G2397	U2321	G2240	A2170	G2104	A2013	A1919	G1845	G1766	G1683
A2820	A2741	C2397	A2577	G2490	U2402	U2322	U2241	A2171	C2105	A2014	C1920	G1846	G1767	G1684
C2827	G2742	G2658	G2578	U2491	U2403	G2325	G2242	U2172	U2106	A2015	G1921	G1847	U1768	G1685
G2828	U2743	G2659	C2579	U2492	C2404	G2326	U2243	A2173	G2107	U2016	U1922	G1848	G1769	G1686
A2829	G2744	G2660	U2580	G2493	U2405	A2327	U2244	C2174	U2108	A2017	U1923	U1769	G1770	G1687
G2830	G2745	G2661	G2581	C2496	G2406	A2328	A2247	U2180	G2110	A2020	C1924	U1771	G1771	G1688
G2831	G2746	G2662	G2582	A2497	A2407	A2329	U2248	U2181	G2111	C2021	A1927	A1772	G1702	G1703
G2832	A2747	G2663	G2583	C2498	A2408	U2330	U2249	U2182	G2112	U2022	A1928	A1773	G1704	G1705
G2833	A2748	G2664	G2584	C2499	A2409	G2331	G2250	A2183	U2113	C2023	G1929	C1774	G1706	G1707
G2834	A2749	A2670	U2585	G2502	A2411	A2332	U2251	U2184	G2114	C2024	U1930	U1775	G1708	G1709
A2835	G2750	G2671	U2586	G2503	A2412	A2333	U2252	U2185	G2115	C2025	U1931	G1776	G1710	A1711
U2837	U2751	U2672	A2587	G2504	G2413	A2334	U2253	U2186	U2116	G2026	U1932	A1780	A1712	A1713
G2838	G2752	C2676	U2593	G2505	C2420	A2335	U2254	U2187	U2117	G2027	G1935	G1863	G1714	G1715
G2839	A2753	A2679	C2594	U2506	G2421	A2336	U2255	U2188	U2118	A2028	A1936	U1864	U1781	U1716
C2840	A2754	U2680	G2595	C2507	G2422	G2337	C2260	U2189	U2119	C2029	A1937	U1865	U1782	G1717
G2843	A2755	C2681	A2598	G2510	U2423	C2338	A2267	G2190	G2120	C2030	A1938	U1866	A1783	G1718
G2844	G2756	G2682	G2599	U2511	C2424	C2339	A2268	A2191	G2121	C2031	U1939	G1867	G1784	G1719
U2845	A2760	C2683	A2600	G2512	A2425	A2340	G2271	G2192	G2122	C2032	U1940	G1868	A1785	G1720
G2846	U2684	U2684	C2601	A2516	A2426	G2345	G2272	G2193	G2123	C2033	G1942	G1869	A1786	G1721
U2847	U2685	A2602	G2602	C2517	C2427	A2346	G2273	G2194	G2124	C2034	U1943	G1870	A1787	G1722
G2848	A2764	C2687	U2618	U2518	G2428	U2347	G2274	U2195	G2125	C2035	U1944	C1788	G1723	G1724
U2849	A2765	G2688	G2610	G2520	A2429	U2348	G2275	G2196	G2126	C2036	G1945	A1872	G1725	U1726
A2850	U2768	U2690	C2611	G2521	A2430	U2349	A2278	U2197	G2127	C2037	G1946	G1873	C1727	C1728
G2851	G2773	G2697	G2612	C2522	A2431	C2350	G2279	A2198	U2130	C2043	U1947	G1874	U1729	C1729
C2853	G2774	G2698	U2613	U2523	A2432	G2351	A2280	A2199	U2131	C2044	A1952	G1875	G1730	G1731
C2858	A2776	U2700	G2614	G2524	A2433	A2352	A2281	C2200	U2132	G2048	A1953	G1878	G1732	G1733
G2859	G2777	G2701	U2615	U2525	A2434	G2353	G2282	G2201	G2133	C2049	G1954	G1879	G1734	G1735
A2860	A2778	G2702	G2616	U2526	A2435	G2354	C2283	U2202	A2134	C2050	U1955	U1882	A1735	U1736
U2861	U2779	U2703	U2617	U2527	G2436	G2355	A2284	G2203	U2137	A2051	G1956	U1883	G1807	G1737
G2867	G2782	U2707	G2618	A2534	G2437	G2356	C2285	A2204	G2138	A2052	U1957	G1884	A1808	G1738
A2868	U2783	G2708	C2619	C2539	U2441	C2362	A2286	C2208	G2141	G2053	U1963	A1885	A1809	A1739
G2869	U2784	G2709	G2620	G2540	G2445	G2363	A2287	G2209	G2142	C2054	G1964	G1886	U1812	G1740
C2870	A2785	G2710	G2621	G2541	G2446	C2364	G2288	U2210	G2143	C2055	G1965	U1887	G1813	U1741
C2871	G2786	G2711	U2622	U2542	G2447	G2365	G2289	A2211	C2144	G2056	C1966	G1888	C1816	U1742
A2872	G2787	C2712	G2623	A2547	A2448	A2366	U2291	G2212	C2145	A2060	C1967	G1889	G1817	A1743
G2873	G2788	U2713	U2624	U2548	G2449	C2367	U2292	U2213	A2147	G2061	G1968	A1890	U1818	A1744
C2874	C2789	G2714	U2625	U2549	G2450	C2368	G2293	C2214	G2148	G2062	A1969	U1891	G1819	A1745
G2876	A2792	G2715	G2626	U2550	G2451	G2371	G2294	G2215	U2149	G2063	U1970	C1893	A1820	A1746
A2879	C2793	G2716	G2627	G2551	U2457	U2372	U2295	G2216	C2150	C2064	U1971	C1894	U1821	U1747
U2884	U2798	U2720	U2628	U2552	G2458	G2379	U2296	G2217	G2151	U2073	G1972	C1895	G1822	G1748
G2885	A2799	G2721	G2629	U2553	G2459	A2381	A2297	G2218	G2152	U2074	A1978	C1902	C1905	A1823
C2886	U2800	C2723	U2630	U2554	G2460	G2382	U2298	G2219	G2153	U2075	G1983	C1903	G1906	G1749
C2888	G2801	G2726	G2631	U2555	G2461	G2383	U2299	G2220	G2154	C2091	G1984	C1904	U1907	



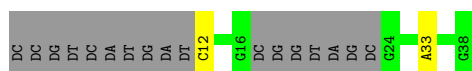
- Molecule 54: mRNA



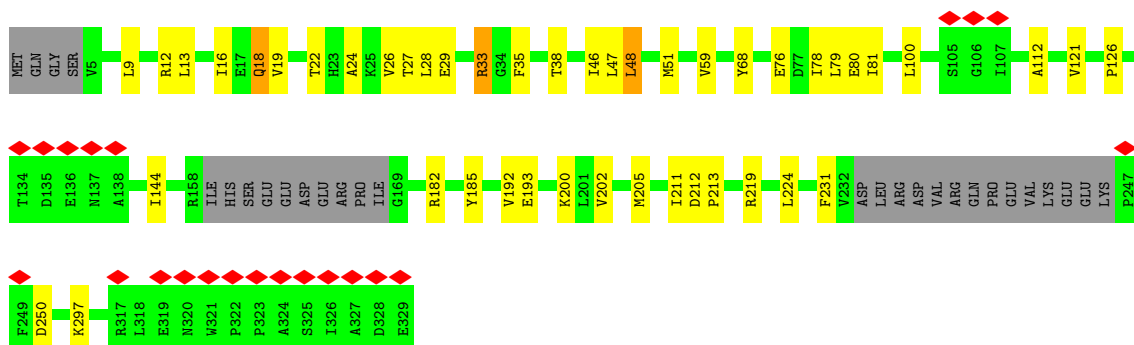
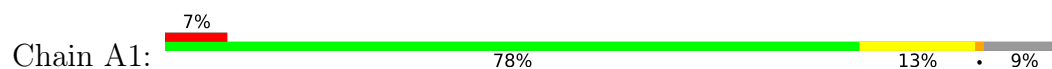
- Molecule 55: template DNA strand



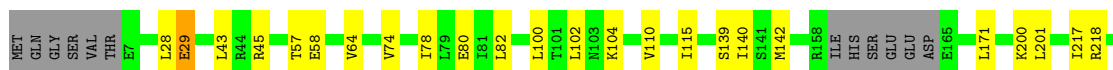
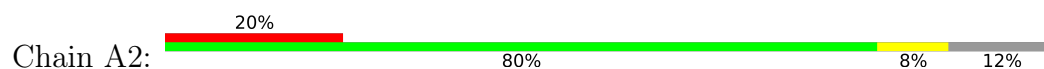
- Molecule 56: non-template DNA strand

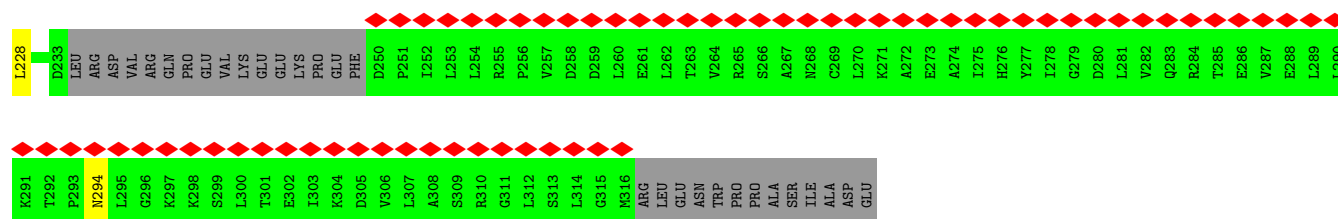


- Molecule 57: DNA-directed RNA polymerase subunit alpha

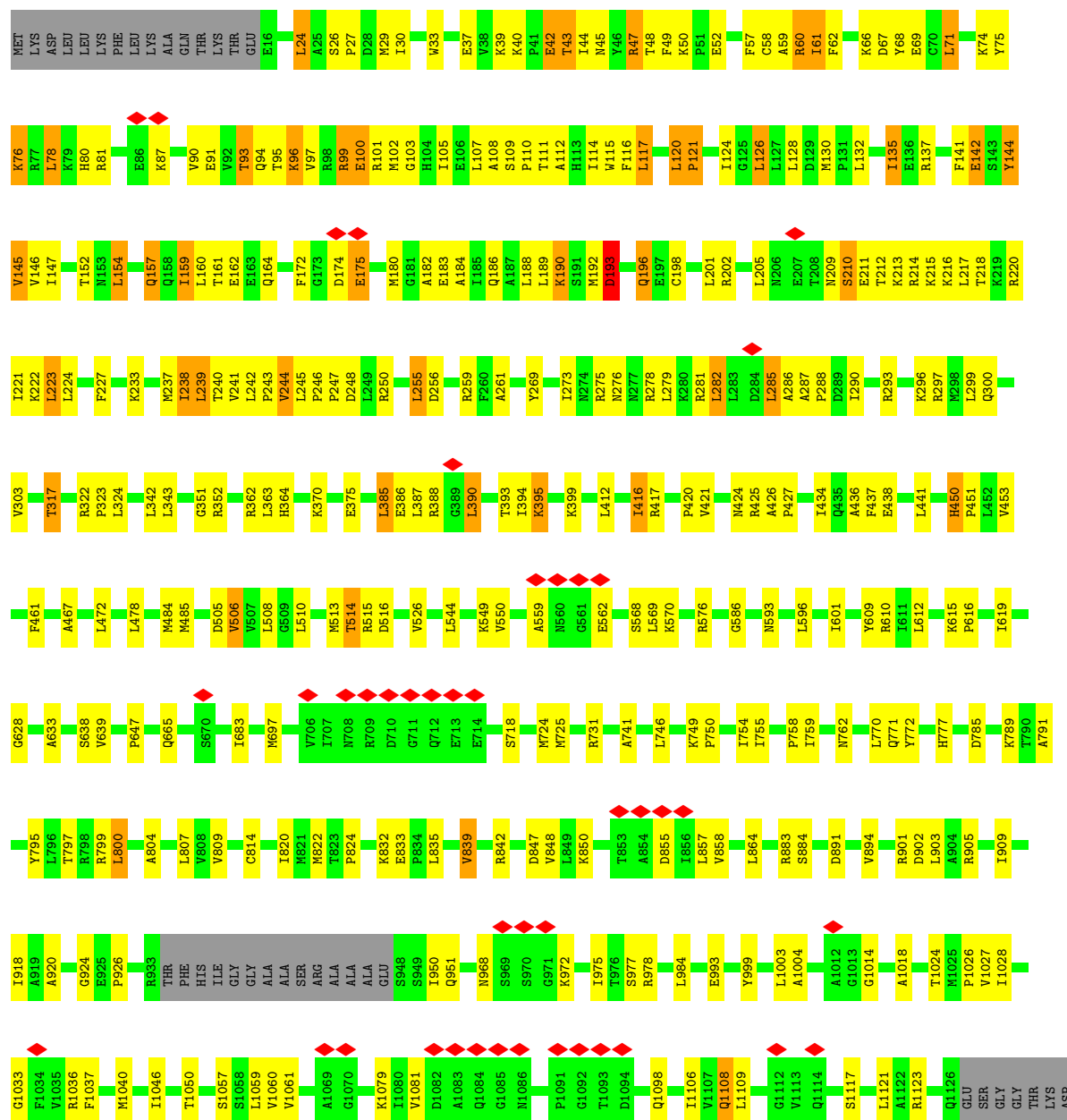


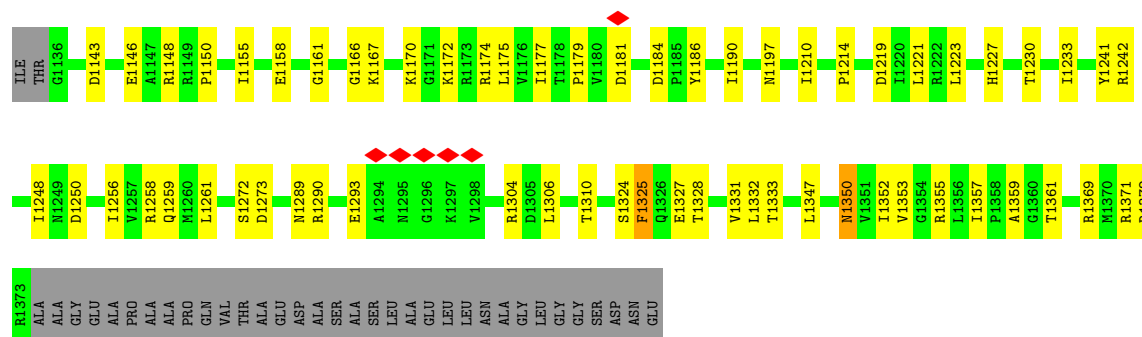
- Molecule 57: DNA-directed RNA polymerase subunit alpha



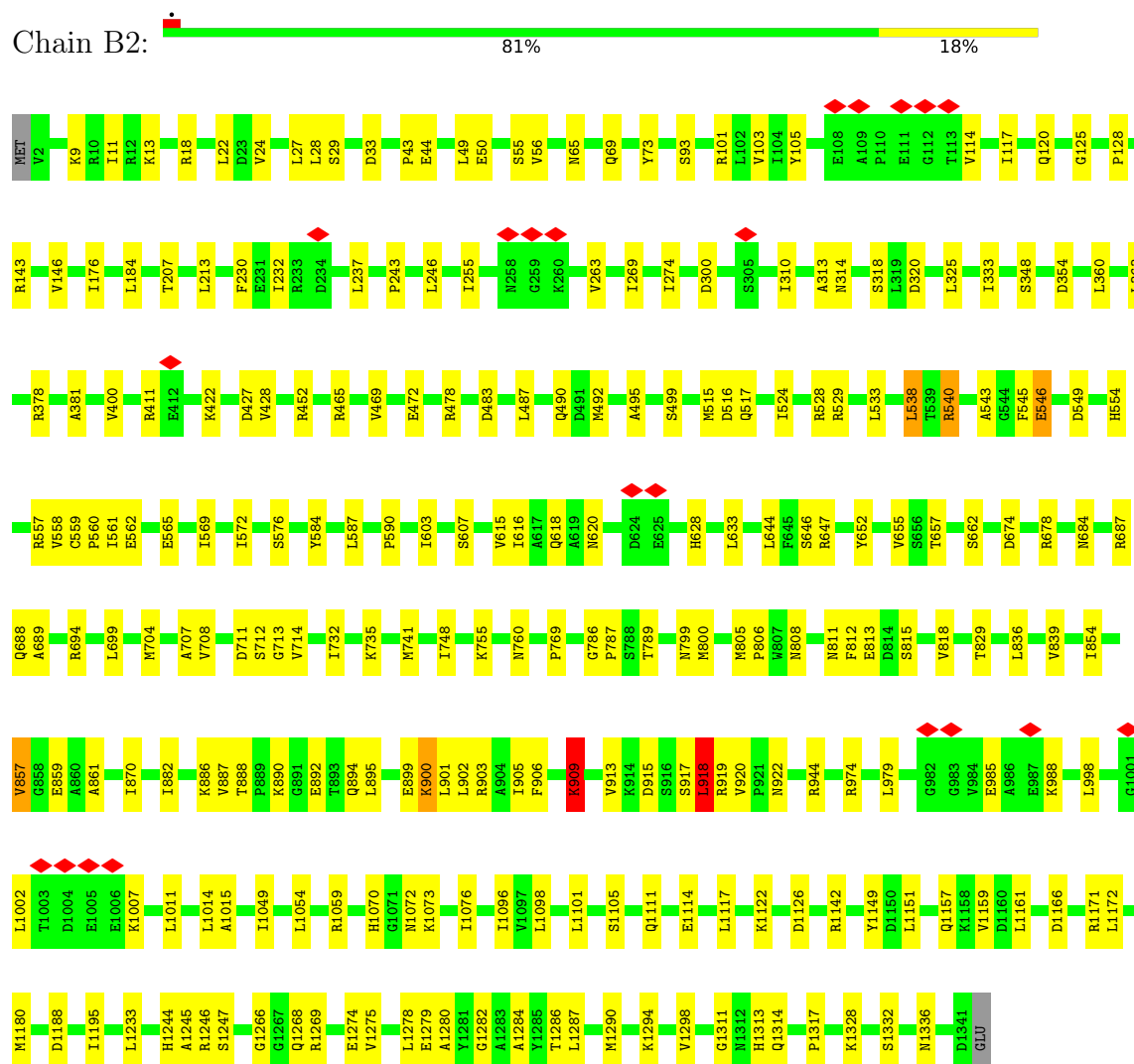


• Molecule 58: DNA-directed RNA polymerase subunit beta'

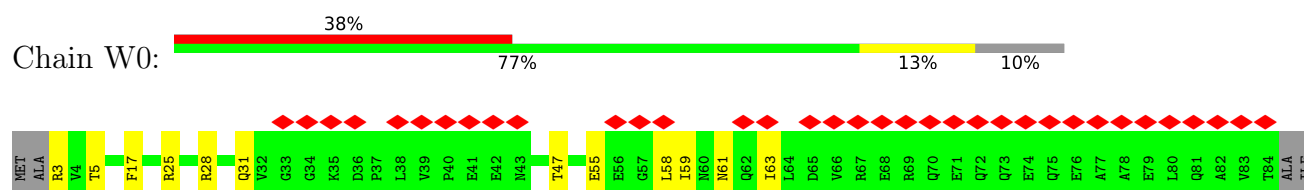


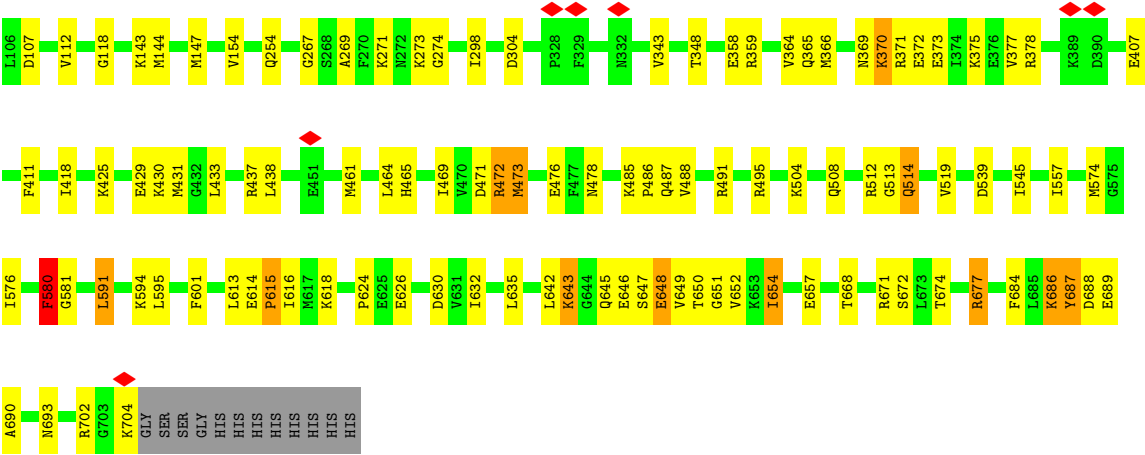


• Molecule 59: DNA-directed RNA polymerase subunit beta



• Molecule 60: DNA-directed RNA polymerase subunit omega





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	609587	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.007	Depositor
Map size (\AA)	753.60004, 753.60004, 753.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.57, 1.57, 1.57	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, FUA

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	A	0.26	0/530	0.54	0/707
2	B	0.40	0/450	0.60	0/599
3	C	0.27	0/416	0.52	0/554
4	D	0.47	0/380	0.76	2/498 (0.4%)
5	E	0.53	0/513	0.60	0/676
6	F	0.58	0/303	0.66	0/397
7	G	0.37	0/1735	0.64	0/2338
8	H	0.34	0/1651	0.55	0/2225
9	I	0.35	0/1665	0.71	0/2227
10	J	0.38	0/1169	0.68	2/1573 (0.1%)
11	K	0.46	0/835	0.77	0/1128
12	L	0.30	0/1195	0.66	3/1602 (0.2%)
13	M	0.35	0/989	0.52	0/1326
14	N	0.47	0/1034	0.77	0/1375
15	O	0.50	0/796	0.78	2/1077 (0.2%)
16	P	0.45	0/885	0.64	1/1195 (0.1%)
17	Q	0.50	0/969	0.86	2/1300 (0.2%)
18	R	0.33	0/892	0.73	2/1193 (0.2%)
19	S	0.33	0/817	0.61	0/1088
20	T	0.49	0/722	0.64	0/964
21	U	0.30	0/659	0.71	2/884 (0.2%)
22	V	0.44	0/657	0.71	0/881
23	W	0.54	0/544	0.74	1/731 (0.1%)
24	X	0.28	0/652	0.55	0/877
25	Y	0.28	0/671	0.52	0/888
26	Z	0.66	0/550	1.01	2/728 (0.3%)
27	b	0.49	0/2121	0.64	0/2852
28	c	0.42	0/1586	0.59	2/2134 (0.1%)
29	d	0.43	0/1571	0.62	0/2113
30	e	0.43	0/1434	0.65	2/1926 (0.1%)
31	f	0.35	0/1343	0.55	0/1816
32	g	0.32	0/405	0.75	0/544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.51	0/1046	0.87	3/1410 (0.2%)
34	j	0.41	0/1152	0.55	1/1551 (0.1%)
35	k	0.45	0/947	0.66	0/1268
36	l	0.40	0/1054	0.63	0/1403
37	m	0.56	0/1093	0.74	0/1460
38	n	0.46	0/973	0.72	1/1301 (0.1%)
39	o	0.32	0/902	0.51	0/1209
40	p	0.42	0/929	0.63	0/1242
41	q	0.52	0/960	0.62	1/1278 (0.1%)
42	r	0.45	0/829	0.69	0/1107
43	s	0.43	0/864	0.58	0/1156
44	t	0.33	0/744	0.52	0/994
45	u	0.46	0/787	0.75	0/1051
46	v	0.34	0/766	0.51	0/1025
47	w	0.40	0/582	0.52	0/769
48	x	0.43	0/635	0.63	1/848 (0.1%)
49	y	0.29	0/510	0.64	0/677
50	z	0.41	0/453	0.53	0/605
51	1	0.51	0/69796	0.62	21/108888 (0.0%)
52	2	0.43	0/2872	0.46	0/4479
53	3	0.42	0/36963	0.43	0/57662
54	4	0.52	0/896	0.68	0/1387
55	8	0.56	0/599	0.71	1/919 (0.1%)
56	9	0.49	0/468	0.53	0/719
57	A1	0.55	0/2106	0.81	0/2868
57	A2	0.49	0/2048	0.76	0/2786
58	B1	0.57	4/10510 (0.0%)	0.75	8/14196 (0.1%)
59	B2	0.46	0/10714	0.67	0/14459
60	W0	0.30	0/652	0.60	0/879
61	NA	0.78	0/2431	1.22	0/3385
62	NG	1.12	0/756	1.07	0/1048
63	5	0.57	0/1812	0.85	1/2823 (0.0%)
64	6	0.39	0/1832	0.57	1/2855 (0.0%)
65	0	0.84	0/5308	1.17	6/7181 (0.1%)
All	All	0.49	4/195128 (0.0%)	0.64	68/287304 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B1	1350	ASN	CG-ND2	-5.28	1.22	1.33
58	B1	1108	GLN	CD-OE1	5.18	1.33	1.23
58	B1	424	ASN	CG-ND2	-5.13	1.22	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B1	665	GLN	CD-OE1	5.04	1.33	1.23

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	0	580	PHE	CA-CB-CG	9.59	123.39	113.80
16	P	73	VAL	N-CA-C	-9.05	104.52	113.20
41	q	33	VAL	N-CA-C	-8.73	104.78	112.12
12	L	64	ALA	N-CA-C	-7.68	105.07	114.75
51	1	1130	U	C2'-C3'-O3'	7.63	120.94	109.50

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	A	521	0	520	8	0
2	B	444	0	461	10	0
3	C	409	0	440	3	0
4	D	377	0	418	9	0
5	E	504	0	574	2	0
6	F	302	0	343	5	0
7	G	1704	0	1732	39	0
8	H	1624	0	1699	27	0
9	I	1643	0	1710	34	0
10	J	1156	0	1199	17	0
11	K	817	0	808	16	0
12	L	1181	0	1240	19	0
13	M	979	0	1034	9	0
14	N	1022	0	1070	21	0
15	O	786	0	828	15	0
16	P	869	0	878	20	0
17	Q	955	0	1019	24	0
18	R	883	0	944	20	0
19	S	805	0	847	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	714	0	737	7	0
21	U	649	0	666	16	0
22	V	648	0	691	9	0
23	W	535	0	552	7	0
24	X	637	0	665	8	0
25	Y	665	0	714	12	0
26	Z	544	0	579	12	0
27	b	2082	0	2157	45	0
28	c	1565	0	1616	32	0
29	d	1552	0	1619	27	0
30	e	1410	0	1447	22	0
31	f	1323	0	1374	30	0
32	g	400	0	423	7	0
33	i	1032	0	1088	36	0
34	j	1129	0	1162	20	0
35	k	938	0	1012	19	0
36	l	1045	0	1117	15	0
37	m	1074	0	1157	13	0
38	n	960	0	1000	18	0
39	o	892	0	923	15	0
40	p	917	0	965	12	0
41	q	947	0	1022	10	0
42	r	816	0	839	14	0
43	s	857	0	922	11	0
44	t	738	0	807	9	0
45	u	779	0	834	14	0
46	v	753	0	780	9	0
47	w	575	0	592	9	0
48	x	625	0	655	11	0
49	y	509	0	543	11	0
50	z	449	0	491	9	0
51	1	62317	0	31346	1455	0
52	2	2568	0	1303	15	0
53	3	33012	0	16618	185	0
54	4	809	0	404	4	0
55	8	539	0	305	27	0
56	9	417	0	224	2	0
57	A1	2088	0	1895	24	0
57	A2	2029	0	1864	18	0
58	B1	10353	0	10548	322	0
59	B2	10546	0	10550	164	0
60	W0	650	0	658	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	NA	2432	0	1171	3	0
62	NG	758	0	334	10	0
63	5	1622	0	821	28	0
64	6	1640	0	837	20	0
65	0	5211	0	5200	46	0
66	B1	1	0	0	0	0
67	0	37	0	47	0	0
68	0	28	0	12	0	0
All	All	181797	0	131050	2821	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 9.

The worst 5 of 2821 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)
51:1:275:C:H2'	51:1:276:U:H4'	1.37	1.07
51:1:1672:A:C2	51:1:2582:G:H5'	1.95	1.02
51:1:1666:G:H2'	51:1:1667:G:H5'	1.41	1.01
58:B1:750:PRO:HB3	59:B2:549:ASP:OD2	1.60	1.01
51:1:1082:U:H3'	51:1:1083:U:H5''	1.41	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	64/70 (91%)	59 (92%)	5 (8%)	0	100	100
2	B	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	2	20
3	C	48/55 (87%)	41 (85%)	7 (15%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
5	E	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
6	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	G	216/241 (90%)	187 (87%)	27 (12%)	2 (1%)	14	51
8	H	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
9	I	203/206 (98%)	172 (85%)	30 (15%)	1 (0%)	25	64
10	J	155/167 (93%)	138 (89%)	17 (11%)	0	100	100
11	K	98/135 (73%)	84 (86%)	14 (14%)	0	100	100
12	L	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
13	M	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
14	N	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
15	O	96/103 (93%)	87 (91%)	8 (8%)	1 (1%)	13	49
16	P	114/129 (88%)	100 (88%)	13 (11%)	1 (1%)	14	51
17	Q	121/124 (98%)	94 (78%)	27 (22%)	0	100	100
18	R	112/118 (95%)	98 (88%)	13 (12%)	1 (1%)	14	51
19	S	98/101 (97%)	83 (85%)	15 (15%)	0	100	100
20	T	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
21	U	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
22	V	78/84 (93%)	69 (88%)	8 (10%)	1 (1%)	10	42
23	W	63/75 (84%)	56 (89%)	5 (8%)	2 (3%)	3	21
24	X	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
25	Y	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
26	Z	63/71 (89%)	44 (70%)	18 (29%)	1 (2%)	8	37
27	b	269/273 (98%)	244 (91%)	25 (9%)	0	100	100
28	c	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
31	f	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
32	g	50/149 (34%)	44 (88%)	5 (10%)	1 (2%)	6	32
33	i	139/142 (98%)	110 (79%)	26 (19%)	3 (2%)	5	29
34	j	140/142 (99%)	128 (91%)	12 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	k	120/123 (98%)	106 (88%)	14 (12%)	0	100	100
36	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
37	m	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
38	n	118/127 (93%)	103 (87%)	15 (13%)	0	100	100
39	o	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
40	p	112/115 (97%)	102 (91%)	10 (9%)	0	100	100
41	q	115/118 (98%)	110 (96%)	3 (3%)	2 (2%)	7	36
42	r	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
43	s	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
44	t	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
45	u	100/104 (96%)	84 (84%)	15 (15%)	1 (1%)	13	49
46	v	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
47	w	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
48	x	75/78 (96%)	72 (96%)	2 (3%)	1 (1%)	10	42
49	y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
50	z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
57	A1	295/329 (90%)	273 (92%)	21 (7%)	1 (0%)	37	72
57	A2	282/329 (86%)	272 (96%)	10 (4%)	0	100	100
58	B1	1329/1407 (94%)	1202 (90%)	123 (9%)	4 (0%)	37	72
59	B2	1338/1342 (100%)	1203 (90%)	130 (10%)	5 (0%)	30	68
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	474 (97%)	14 (3%)	2 (0%)	30	68
62	NG	150/181 (83%)	133 (89%)	10 (7%)	7 (5%)	2	17
65	0	669/716 (93%)	625 (93%)	43 (6%)	1 (0%)	48	83
All	All	10253/10945 (94%)	9283 (90%)	930 (9%)	40 (0%)	32	68

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
48	x	25	LYS
58	B1	121	PRO
61	NA	187	ARG
61	NA	188	PRO
62	NG	102	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	A	58/62 (94%)	57 (98%)	1 (2%)	56	72
2	B	47/48 (98%)	47 (100%)	0	100	100
3	C	45/49 (92%)	44 (98%)	1 (2%)	47	65
4	D	38/38 (100%)	37 (97%)	1 (3%)	41	61
5	E	51/52 (98%)	49 (96%)	2 (4%)	27	49
6	F	34/34 (100%)	30 (88%)	4 (12%)	4	17
7	G	180/199 (90%)	174 (97%)	6 (3%)	33	54
8	H	170/190 (90%)	167 (98%)	3 (2%)	54	71
9	I	172/173 (99%)	168 (98%)	4 (2%)	45	64
10	J	119/126 (94%)	117 (98%)	2 (2%)	56	72
11	K	87/116 (75%)	82 (94%)	5 (6%)	17	39
12	L	124/147 (84%)	124 (100%)	0	100	100
13	M	104/105 (99%)	103 (99%)	1 (1%)	73	81
14	N	105/107 (98%)	95 (90%)	10 (10%)	7	23
15	O	86/90 (96%)	78 (91%)	8 (9%)	7	24
16	P	89/99 (90%)	86 (97%)	3 (3%)	32	53
17	Q	103/104 (99%)	98 (95%)	5 (5%)	21	43
18	R	92/96 (96%)	91 (99%)	1 (1%)	70	80
19	S	83/84 (99%)	83 (100%)	0	100	100
20	T	76/77 (99%)	73 (96%)	3 (4%)	27	49
21	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
22	V	74/78 (95%)	72 (97%)	2 (3%)	40	60
23	W	56/65 (86%)	52 (93%)	4 (7%)	12	32
24	X	70/79 (89%)	70 (100%)	0	100	100
25	Y	65/66 (98%)	64 (98%)	1 (2%)	60	75
26	Z	55/61 (90%)	47 (86%)	8 (14%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	b	216/218 (99%)	212 (98%)	4 (2%)	52	69
28	c	164/164 (100%)	164 (100%)	0	100	100
29	d	165/165 (100%)	162 (98%)	3 (2%)	54	71
30	e	148/150 (99%)	142 (96%)	6 (4%)	26	48
31	f	137/138 (99%)	132 (96%)	5 (4%)	30	52
32	g	41/114 (36%)	38 (93%)	3 (7%)	11	31
33	i	109/110 (99%)	100 (92%)	9 (8%)	9	28
34	j	116/116 (100%)	116 (100%)	0	100	100
35	k	103/104 (99%)	103 (100%)	0	100	100
36	l	102/103 (99%)	101 (99%)	1 (1%)	73	81
37	m	109/109 (100%)	103 (94%)	6 (6%)	18	40
38	n	100/103 (97%)	99 (99%)	1 (1%)	73	81
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	98 (99%)	1 (1%)	73	81
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	53
42	r	84/84 (100%)	82 (98%)	2 (2%)	44	63
43	s	93/93 (100%)	92 (99%)	1 (1%)	70	80
44	t	80/84 (95%)	80 (100%)	0	100	100
45	u	83/85 (98%)	79 (95%)	4 (5%)	21	43
46	v	78/78 (100%)	77 (99%)	1 (1%)	65	77
47	w	57/63 (90%)	57 (100%)	0	100	100
48	x	67/68 (98%)	67 (100%)	0	100	100
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	46 (96%)	2 (4%)	25	47
57	A1	185/286 (65%)	174 (94%)	11 (6%)	16	38
57	A2	186/286 (65%)	184 (99%)	2 (1%)	70	80
58	B1	1110/1168 (95%)	1017 (92%)	93 (8%)	9	28
59	B2	1150/1157 (99%)	1118 (97%)	32 (3%)	38	59
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	75
65	0	553/588 (94%)	482 (87%)	71 (13%)	3	15
All	All	7931/8500 (93%)	7593 (96%)	338 (4%)	27	47

5 of 338 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
58	B1	1328	THR
65	0	369	ASN
59	B2	483	ASP
59	B2	915	ASP
65	0	471	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
59	B2	343	HIS
59	B2	808	ASN
65	0	367	HIS
27	b	69	ASN
27	b	24	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	398 (13%)	16 (0%)
52	2	119/120 (99%)	17 (14%)	1 (0%)
53	3	1538/1542 (99%)	253 (16%)	4 (0%)
54	4	37/44 (84%)	21 (56%)	2 (5%)
63	5	75/76 (98%)	39 (52%)	6 (8%)
64	6	76/77 (98%)	27 (35%)	2 (2%)
All	All	4747/4763 (99%)	755 (15%)	31 (0%)

5 of 755 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A
51	1	12	U
51	1	34	U
51	1	35	G
51	1	46	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	1	2326	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	5	57	G
53	3	4	U
64	6	33	U
63	5	32	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
68	GDP	0	801	-	24,30,30	0.90	1 (4%)	30,47,47	1.39	5 (16%)
67	FUA	0	800	-	39,40,40	1.67	3 (7%)	49,64,64	1.13	3 (6%)

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
68	GDP	0	801	-	-	2/12/32/32	0/3/3/3
67	FUA	0	800	-	-	9/15/92/92	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	0	800	FUA	C29-C22	-9.59	1.34	1.47
67	0	800	FUA	O5-C29	-2.46	1.23	1.30
68	0	801	GDP	C6-N1	-2.31	1.34	1.37
67	0	800	FUA	C9-C11	2.24	1.57	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	0	801	GDP	C3'-C2'-C1'	2.89	105.33	100.98
68	0	801	GDP	PA-O3A-PB	-2.62	123.84	132.83
68	0	801	GDP	C5-C6-N1	2.59	118.52	113.95
67	0	800	FUA	C14-C8-C9	-2.54	104.42	109.40
67	0	800	FUA	C8-C9-C10	2.51	118.92	116.34

There are no chirality outliers.

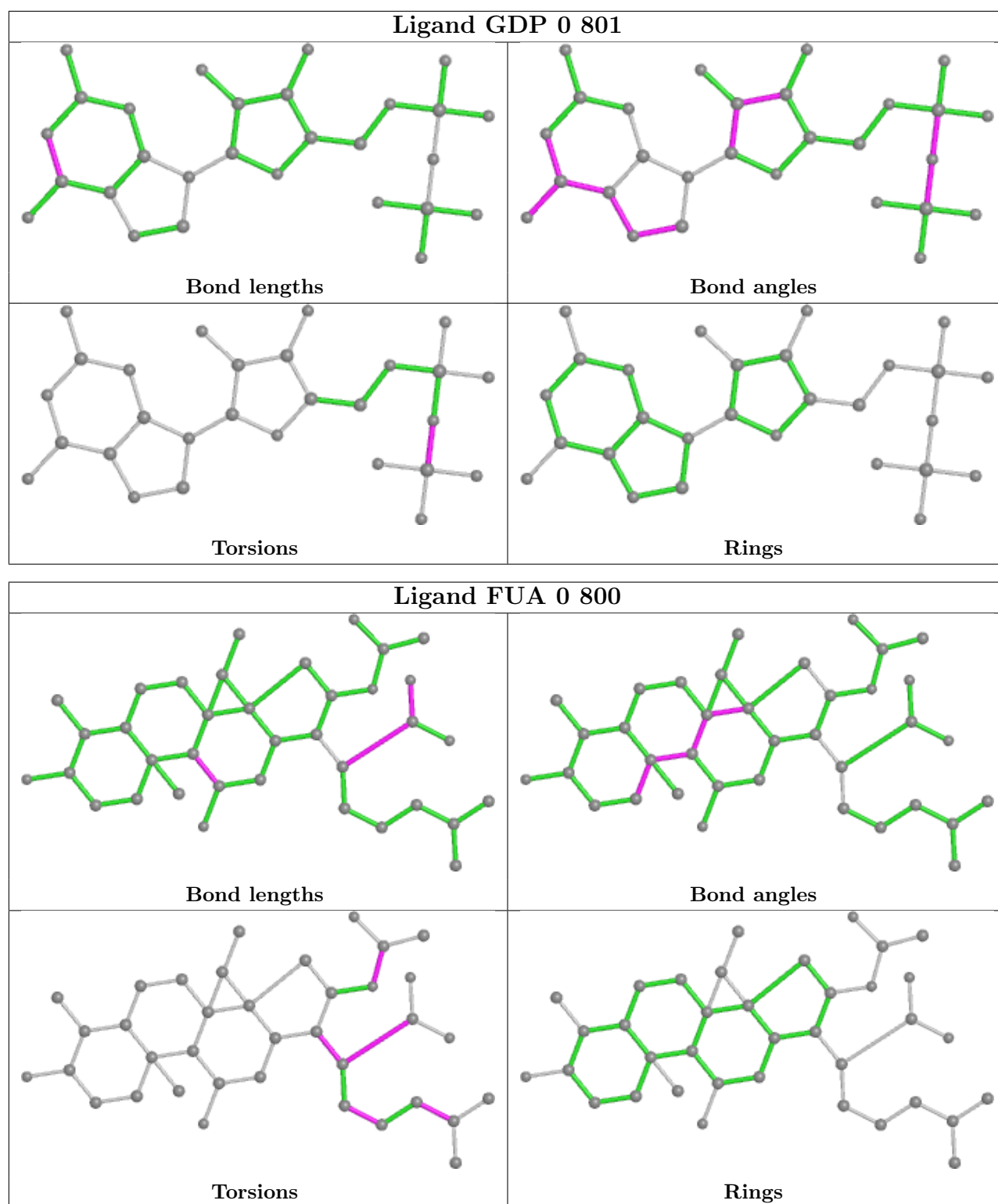
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
67	0	800	FUA	C13-C17-C22-C29
67	0	800	FUA	C23-C22-C29-O4
67	0	800	FUA	C23-C22-C29-O5
67	0	800	FUA	C22-C23-C24-C25
67	0	800	FUA	C24-C25-C26-C27

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

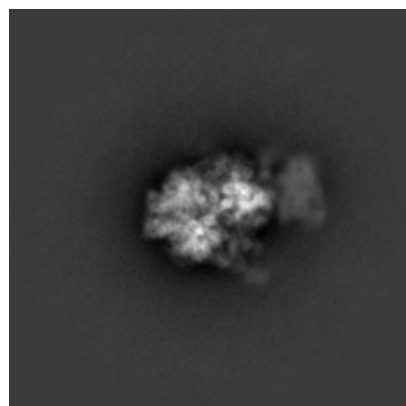
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38947. These allow visual inspection of the internal detail of the map and identification of artifacts.

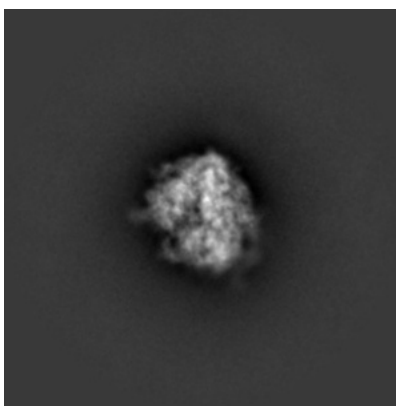
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

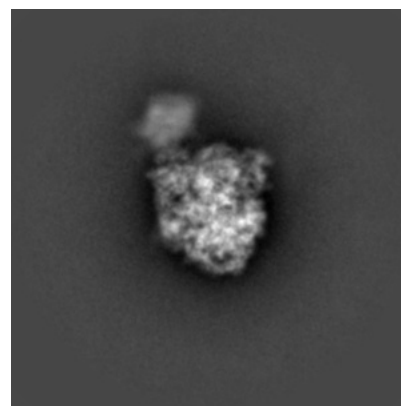
6.1.1 Primary map



X

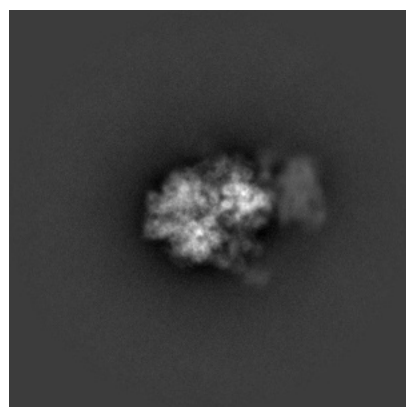


Y

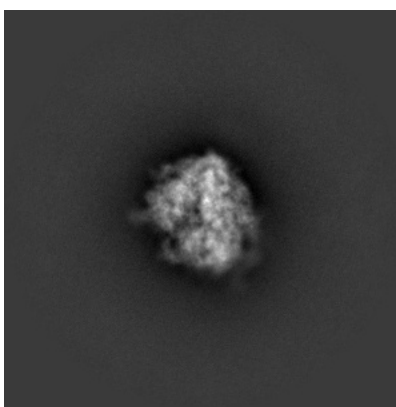


Z

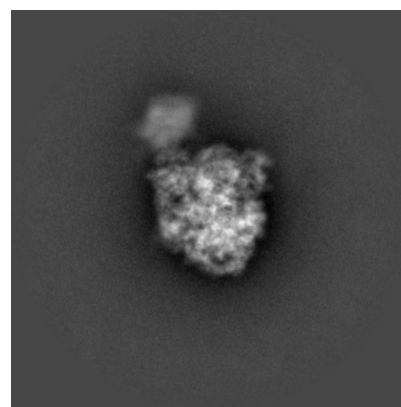
6.1.2 Raw map



X



Y

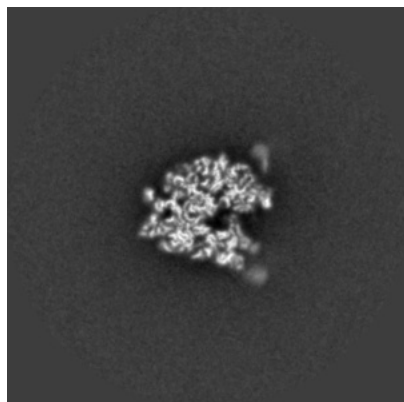


Z

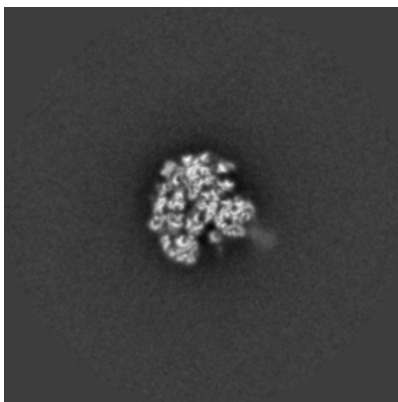
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

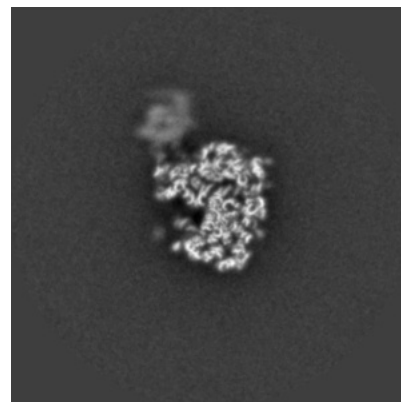
6.2.1 Primary map



X Index: 240

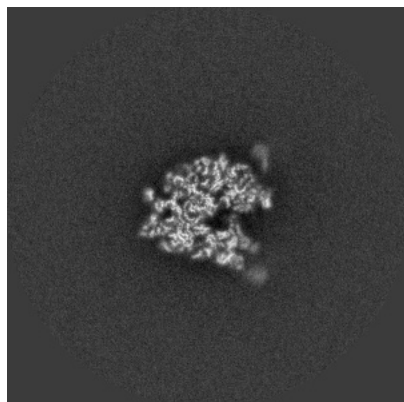


Y Index: 240

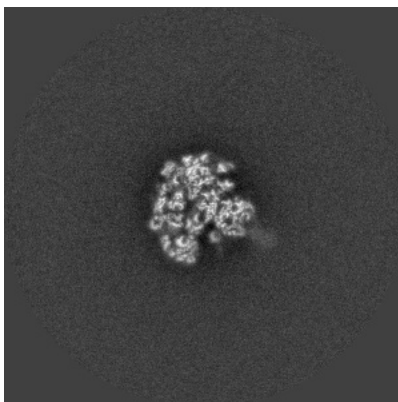


Z Index: 240

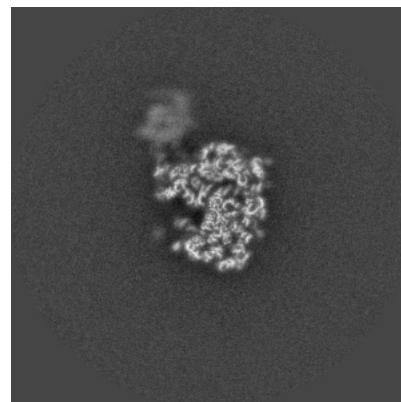
6.2.2 Raw map



X Index: 240



Y Index: 240

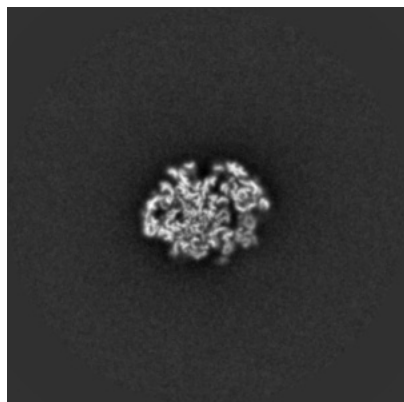


Z Index: 240

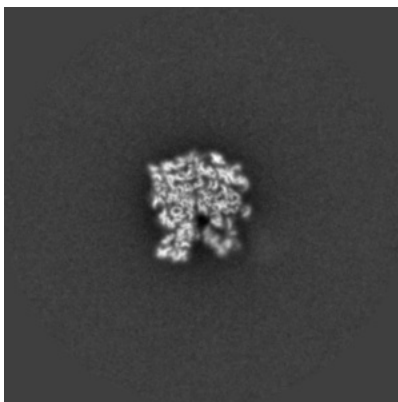
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

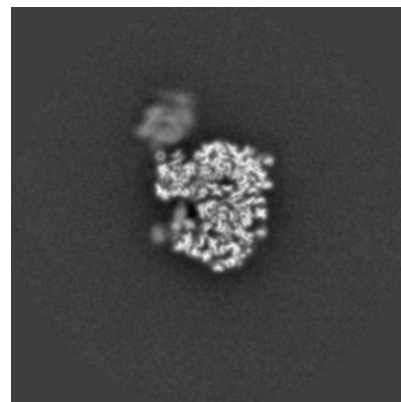
6.3.1 Primary map



X Index: 265

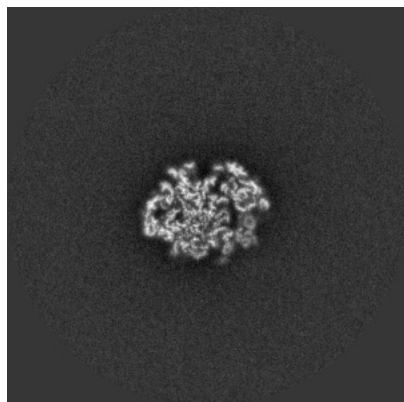


Y Index: 224

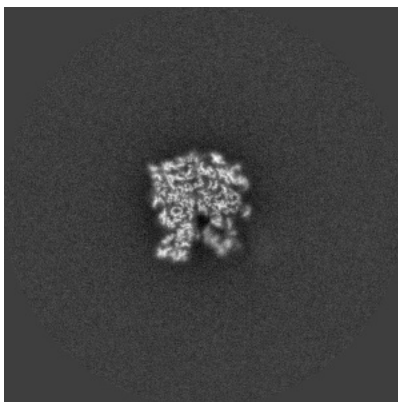


Z Index: 246

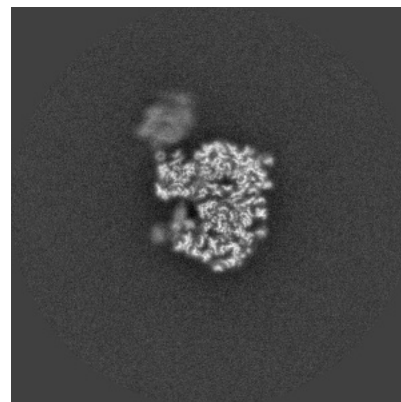
6.3.2 Raw map



X Index: 265



Y Index: 224

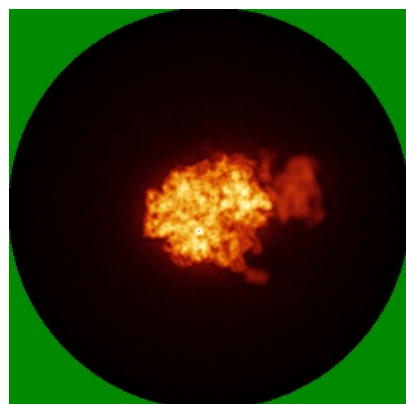


Z Index: 246

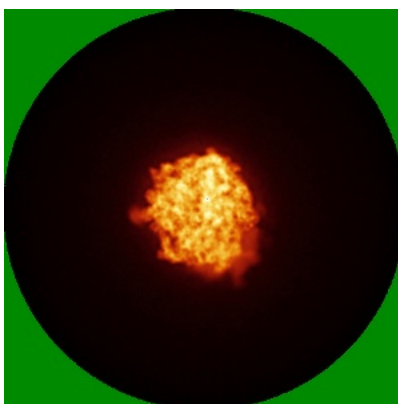
The images above show the largest variance slices of the map in three orthogonal directions.

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

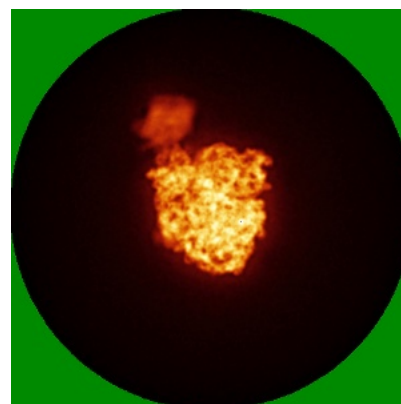
6.4.1 Primary map



X

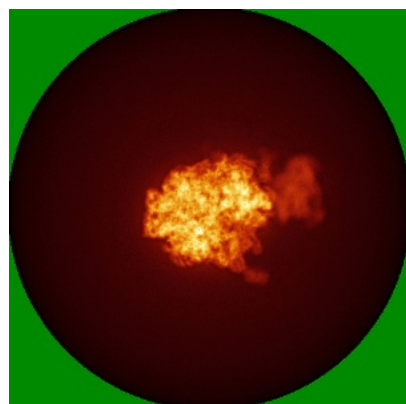


Y

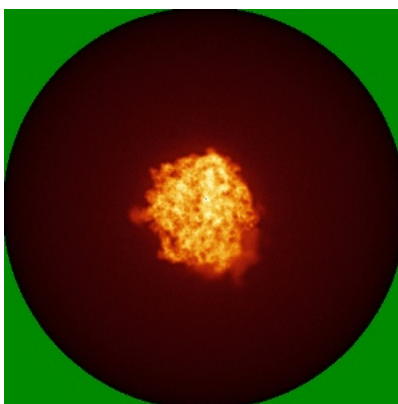


Z

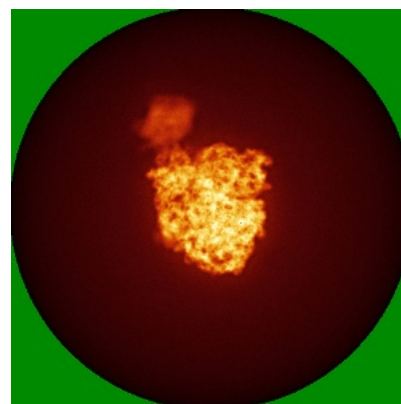
6.4.2 Raw map



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.

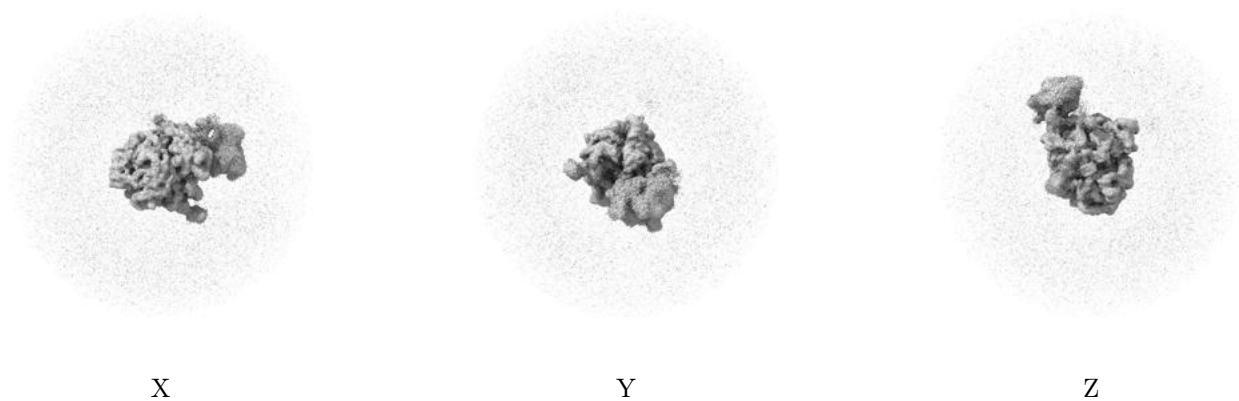
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

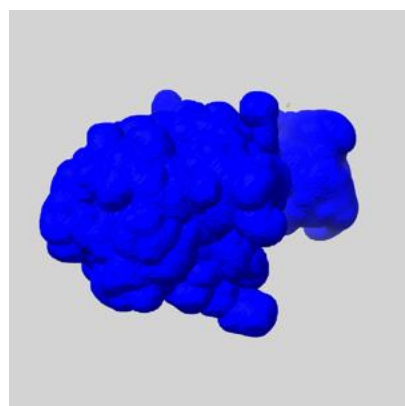
6.6 Mask visualisation [i](#)

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

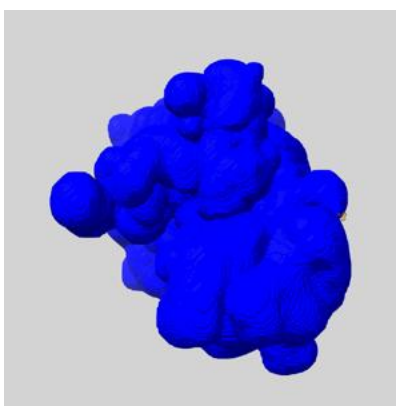
A mask typically either:

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

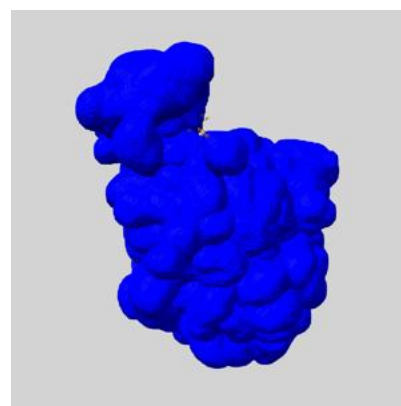
6.6.1 emd_38947_msk_1.map [i](#)



X



Y

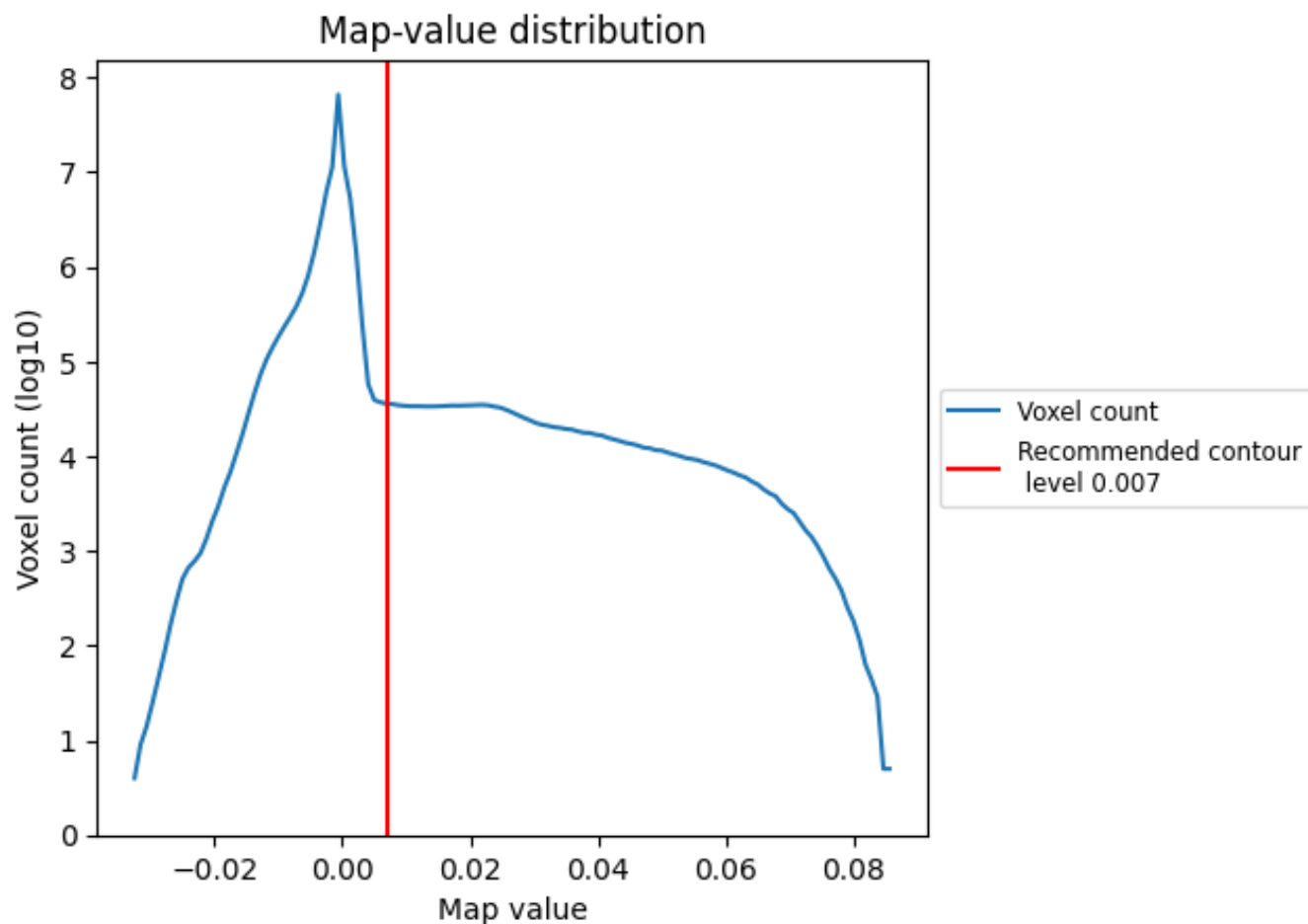


Z

7 Map analysis [i](#)

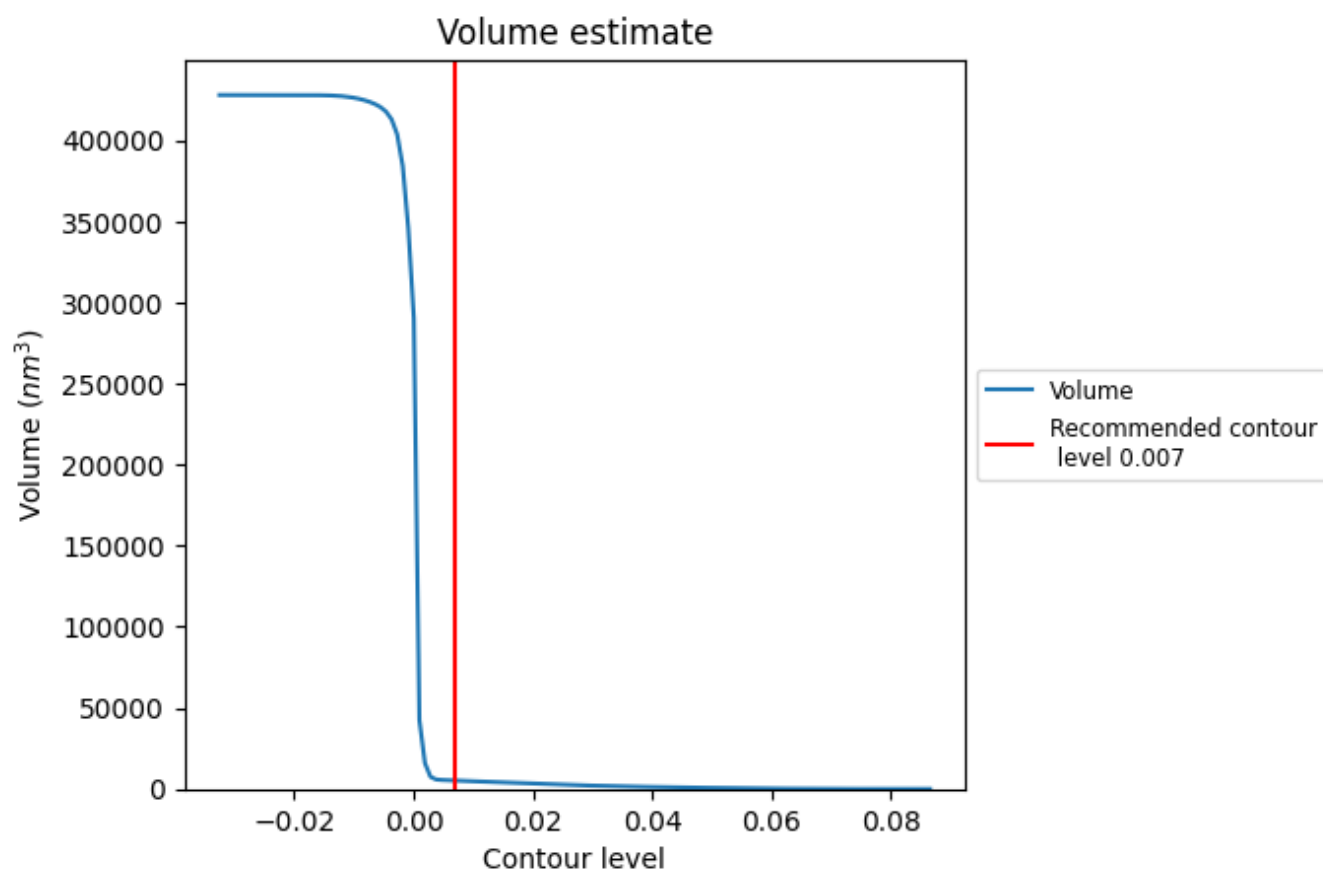
This section contains the results of statistical analysis of the map.

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.

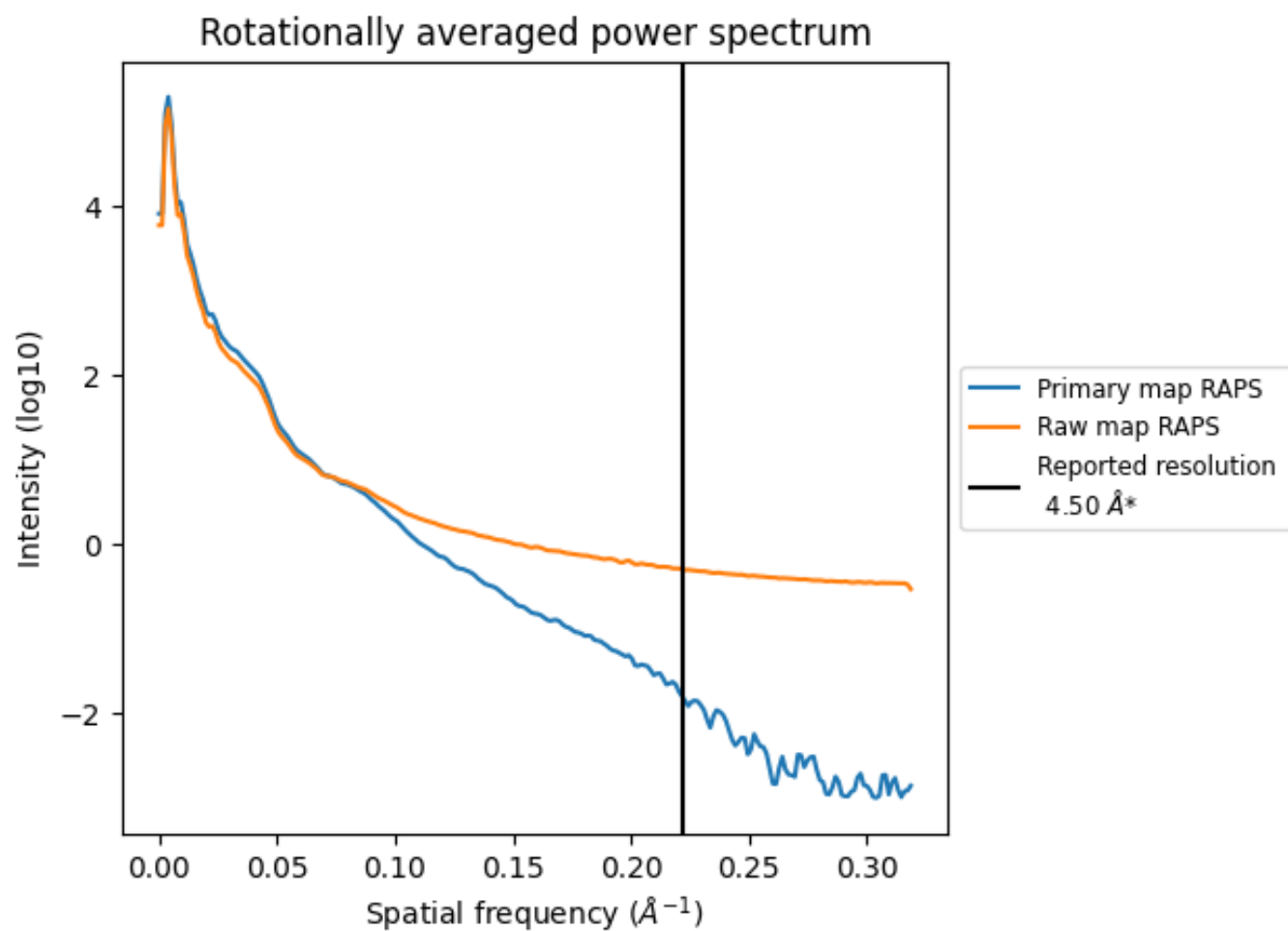
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5179 nm^3 ; this corresponds to an approximate mass of 4678 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](#)

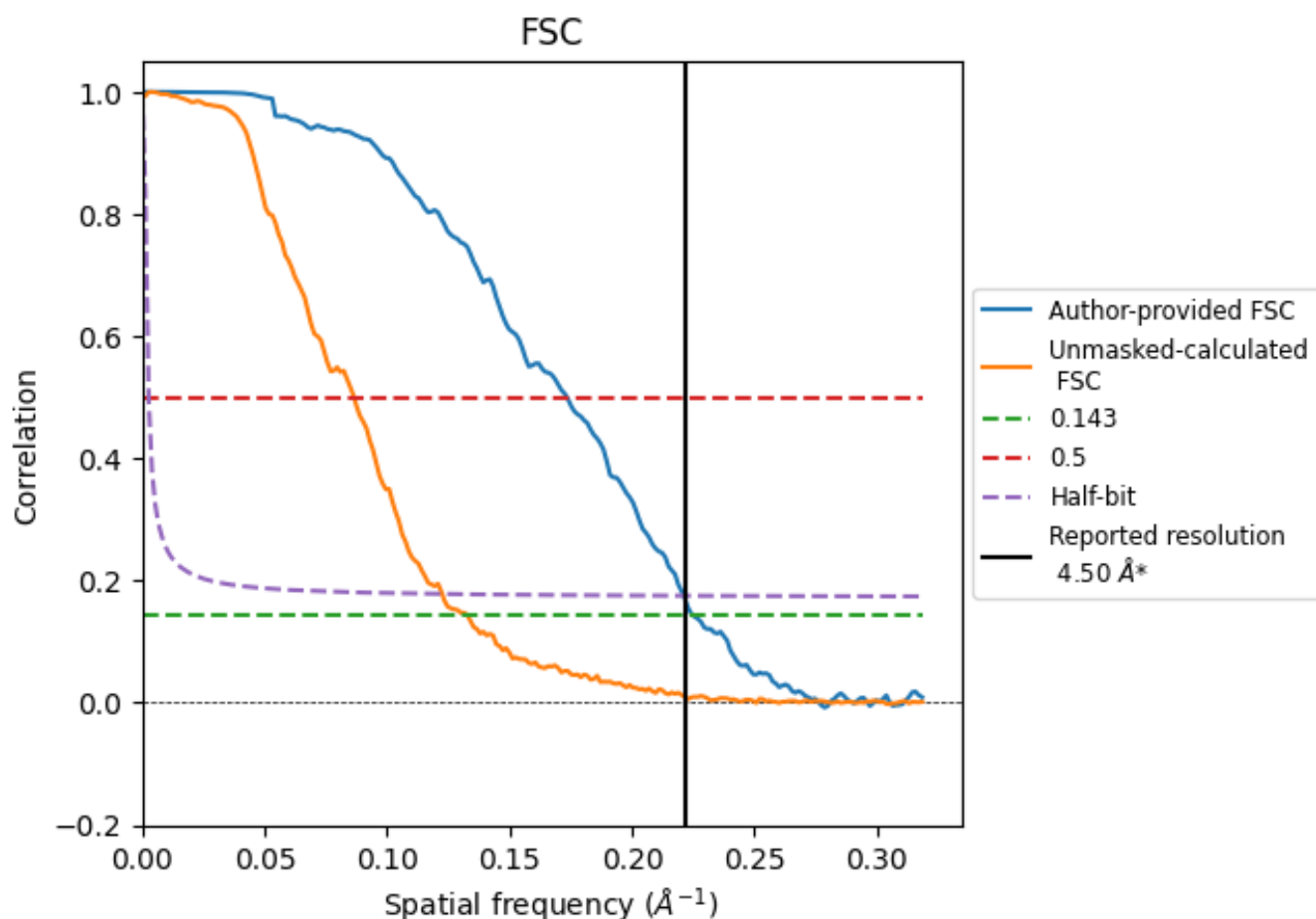


*Reported resolution corresponds to spatial frequency of 0.222 \AA^{-1}

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

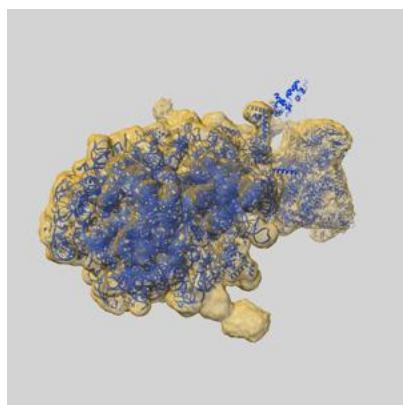
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.45	5.77	4.52
Unmasked-calculated*	7.53	11.57	8.16

*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 7.53 differs from the reported value 4.5 by more than 10 %

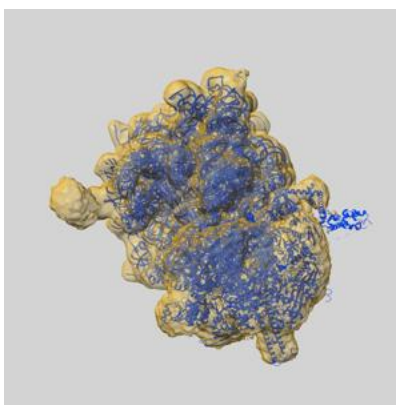
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38947 and PDB model 8Y5R. Per-residue inclusion information can be found in section [3](#) on page [18](#).

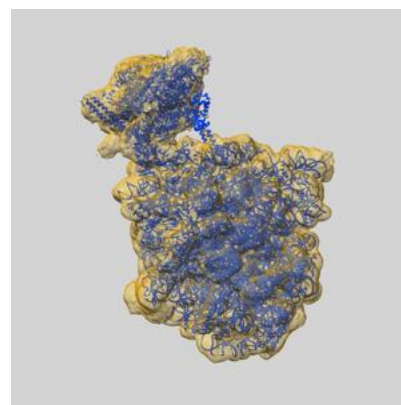
9.1 Map-model overlay [i](#)



X



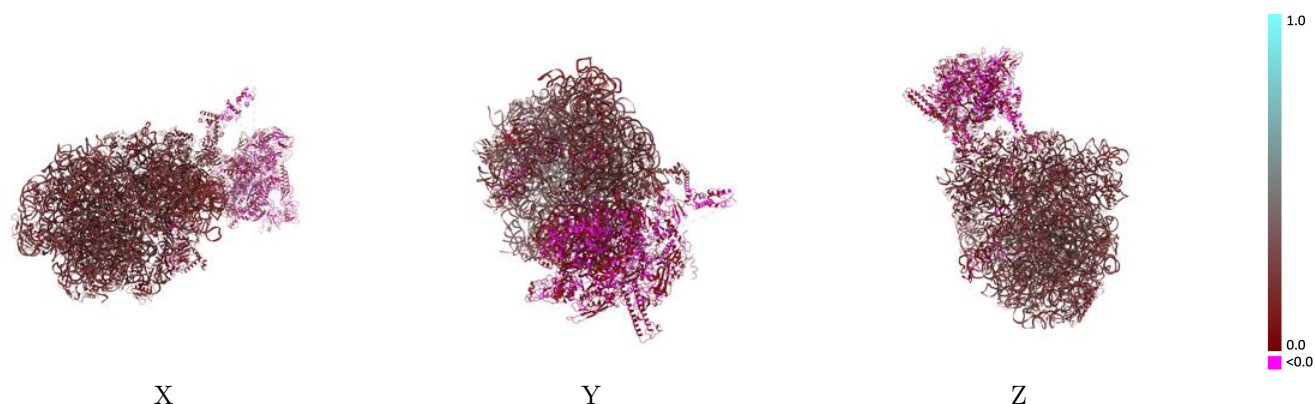
Y



Z

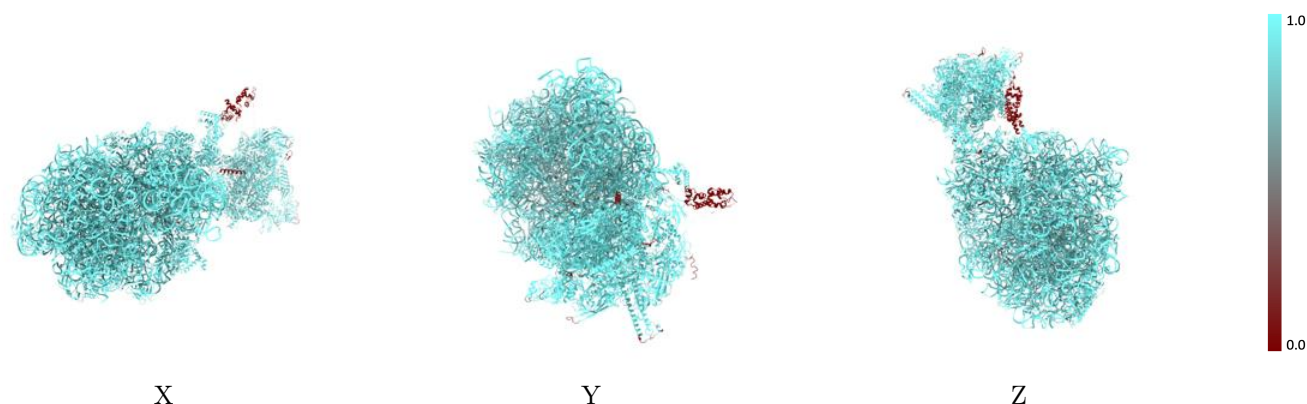
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



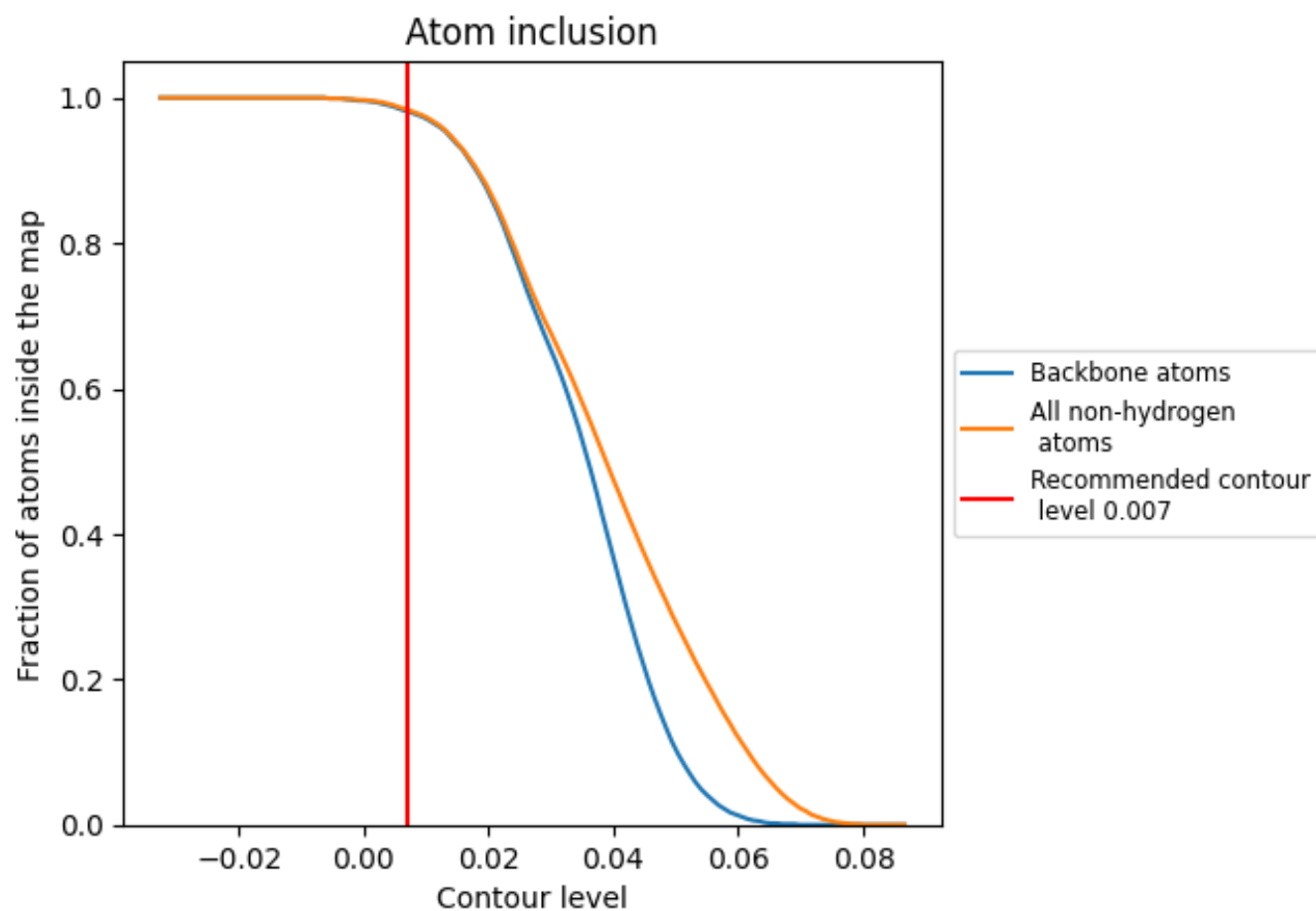
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

































































The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9840	 0.1860
0	 0.9620	 0.1590
1	 0.9990	 0.2370
2	 1.0000	 0.2190
3	 0.9990	 0.2220
4	 0.9600	 0.0710
5	 0.9770	 0.1390
6	 0.8350	 0.0860
8	 1.0000	 0.0480
9	 1.0000	 0.0880
A	 0.9780	 0.1340
A1	 0.9270	 0.0570
A2	 0.8330	 0.0560
B	 0.9950	 0.1950
B1	 0.9580	 0.0460
B2	 0.9760	 0.0550
C	 0.9850	 0.1850
D	 0.9860	 0.1780
E	 1.0000	 0.1740
F	 1.0000	 0.1580
G	 0.9900	 0.1840
H	 0.9780	 0.1770
I	 0.9980	 0.1480
J	 0.9930	 0.1970
K	 0.9940	 0.1890
L	 0.9940	 0.1930
M	 0.9850	 0.1870
N	 0.9990	 0.1660
NA	 0.8350	 0.1560
NG	 0.9140	 0.0750
O	 1.0000	 0.1410
P	 0.9980	 0.2010
Q	 0.9460	 0.1560
R	 0.9990	 0.1670
S	 0.9970	 0.1300



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	 0.9940	 0.1650
U	 0.9980	 0.1540
V	 0.9870	 0.1840
W	 0.9980	 0.1550
W0	 0.5610	 0.0450
X	 0.9870	 0.1100
Y	 0.9950	 0.1780
Z	 0.9770	 0.1500
b	 0.9950	 0.2210
c	 0.9950	 0.1920
d	 0.9960	 0.1930
e	 0.9910	 0.1700
f	 0.9780	 0.1860
g	 0.9980	 0.1820
i	 0.9560	 0.0900
j	 0.9960	 0.1930
k	 0.9880	 0.2310
l	 1.0000	 0.1900
m	 0.9880	 0.2080
n	 1.0000	 0.1840
o	 1.0000	 0.1720
p	 0.9870	 0.2130
q	 0.9990	 0.1670
r	 0.9960	 0.1940
s	 0.9920	 0.1970
t	 0.9890	 0.1840
u	 0.9950	 0.1700
v	 0.9970	 0.1800
w	 1.0000	 0.1690
x	 1.0000	 0.1940
y	 1.0000	 0.1660
z	 0.9950	 0.1960