



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 03:32 PM EDT

PDB ID : 5WE4 / pdb_00005we4
EMDB ID : EMD-8814
Title : 70S ribosome-EF-Tu wt complex with GppNHp
Authors : Fislage, M.; Brown, Z.; Frank, J.
Deposited on : 2017-07-07
Resolution : 3.10 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:

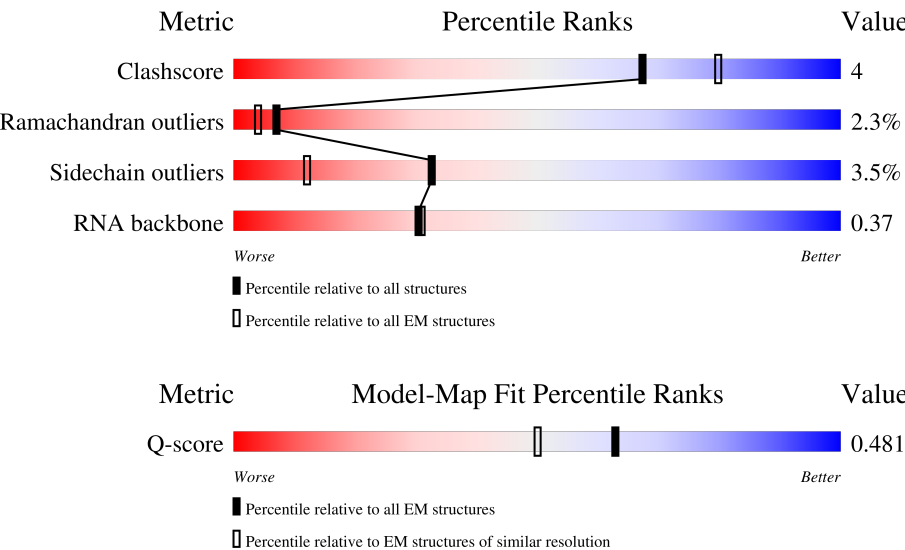
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 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.



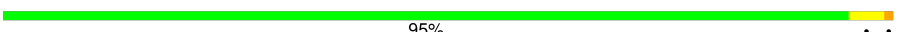
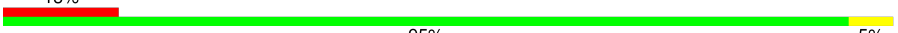
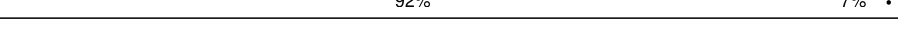
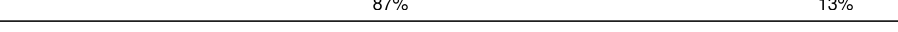
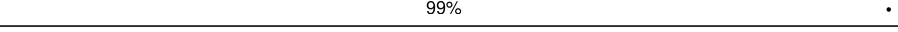
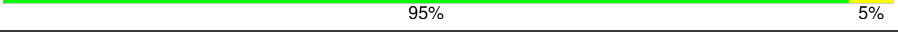
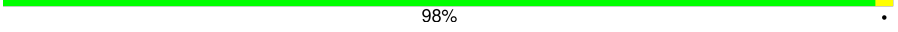
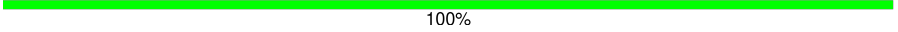
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A	2903	63% 30% 7%
2	B	120	67% 26% 8%
3	C	271	92% 8%

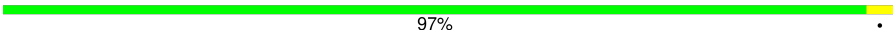
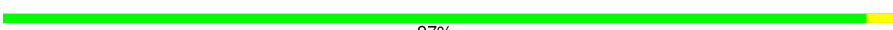
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Mol	Chain	Length	Quality of chain
4	D	208	 93% 6%
5	E	200	 93% 6%
6	F	177	 95% . .
7	G	174	 94% 6%
8	H	149	 13% 95% 5%
9	I	141	 24% 84% 12% . .
10	J	141	 94% 6% .
11	K	122	 86% 14%
12	L	143	 89% 10% .
13	M	136	 95% . .
14	N	119	 93% 6% .
15	O	116	 94% 5% .
16	P	114	 90% 10%
17	Q	115	 88% 11% .
18	R	102	 85% 15%
19	S	109	 92% 7% .
20	T	92	 87% 13%
21	U	102	 92% 8%
22	V	92	 99% .
23	W	75	 92% 8%
24	X	77	 95% 5%
25	Y	60	 98% .
26	Z	56	 100%
27	0	55	 84% 15% .
28	1	51	 94% 6%

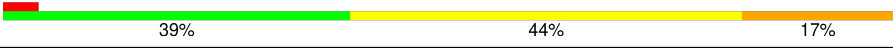
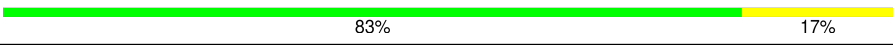
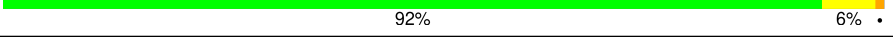
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Mol	Chain	Length	Quality of chain
29	2	45	 80% 18% .
30	3	64	 97% .
31	4	38	 92% 8%
32	5	131	 76% 72% 26% .
33	6	66	 97% .
34	a	1540	 62% 31% 7%
35	b	218	 97% .
36	c	206	 95% . .
37	d	205	 97% .
38	e	157	 93% 6% .
39	f	100	 84% 13% .
40	g	151	 93% 7%
41	h	129	 93% 7%
42	i	127	 91% 8% .
43	j	98	 87% 12% .
44	k	116	 94% 6%
45	l	121	 85% 12% .
46	m	115	 93% 7%
47	n	101	 88% 11% .
48	o	88	 92% 5% .
49	p	82	 91% 9%
50	q	80	 90% 10%
51	r	65	 83% 15% .
52	s	79	 87% 13%
53	t	85	 89% 9% .

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Mol	Chain	Length	Quality of chain
54	u	65	
55	v	77	
55	w	77	
56	x	12	
57	y	76	
58	z	393	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2900	Total	C	N	O	P	0	0
			62277	27788	11459	20130	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 731469900
A	1723	G	A	conflict	GB 731469900
A	1847	G	A	conflict	GB 731469900

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1174070234

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1557	974	287	293	3		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1544	969	282	289	4		

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O		0	0
			933	595	190	148			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total	C	N	O	S	0	0
			739	471	135	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total	C	N	O	S	0	0
			494	305	96	91	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	51	Total	C	N	O	S	0	0
			417	269	76	72			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

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	1	0
			1164	724	221	213	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

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	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	115	Total	C	N	O	S	0	0
			891	552	179	157	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
			810	502	165	140	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	79	Total	C	N	O	S	0	0
			637	408	120	107	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
			544	335	117	91	1		

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0
55	w	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	42	85	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3036	1918	524	581	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	47	ASN	ASP	conflict	UNP P0CE48

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	A	1181	Total 1181	Mg 1181	0
59	B	31	Total 31	Mg 31	0
59	C	1	Total 1	Mg 1	0
59	K	1	Total 1	Mg 1	0
59	L	2	Total 2	Mg 2	0
59	M	1	Total 1	Mg 1	0
59	Q	1	Total 1	Mg 1	0
59	R	1	Total 1	Mg 1	0
59	S	1	Total 1	Mg 1	0
59	T	2	Total 2	Mg 2	0
59	0	2	Total 2	Mg 2	0
59	1	1	Total 1	Mg 1	0
59	3	1	Total 1	Mg 1	0
59	4	1	Total 1	Mg 1	0
59	a	373	Total 373	Mg 373	0
59	d	1	Total 1	Mg 1	0
59	h	1	Total 1	Mg 1	0
59	i	1	Total 1	Mg 1	0
59	s	1	Total 1	Mg 1	0
59	u	1	Total 1	Mg 1	0
59	v	7	Total 7	Mg 7	0
59	w	1	Total 1	Mg 1	0

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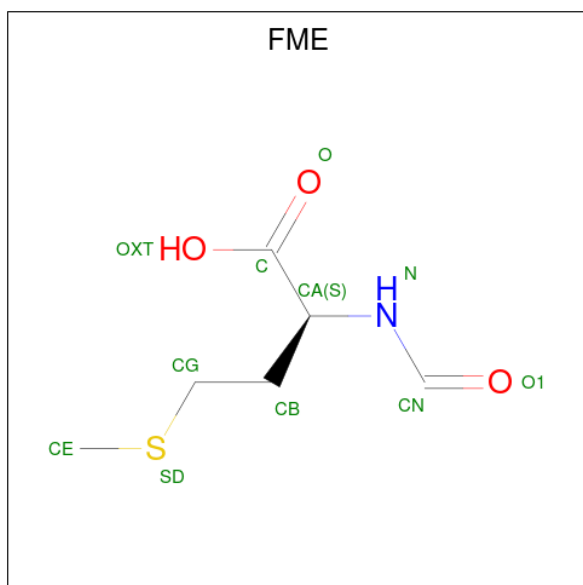
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Mol	Chain	Residues	Atoms		AltConf
59	y	4	Total	Mg	0
			4	4	
59	z	1	Total	Mg	0
			1	1	

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

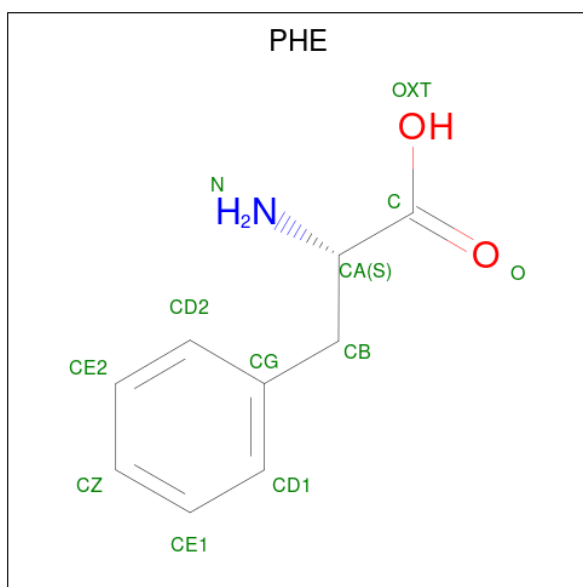
Mol	Chain	Residues	Atoms		AltConf
60	A	1	Total	K	0
			1	1	

- Molecule 61 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



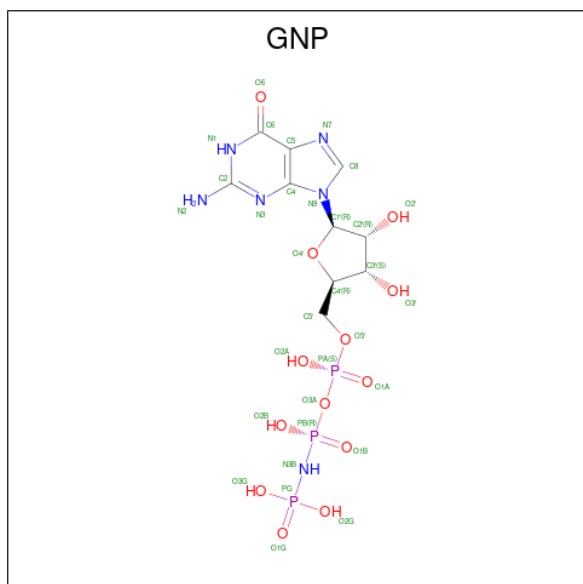
Mol	Chain	Residues	Atoms					AltConf
61	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	A	751	Total O 751 751	0
64	B	11	Total O 11 11	0
64	C	9	Total O 9 9	0
64	E	5	Total O 5 5	0
64	J	2	Total O 2 2	0
64	K	2	Total O 2 2	0
64	L	6	Total O 6 6	0
64	M	1	Total O 1 1	0
64	N	3	Total O 3 3	0
64	O	1	Total O 1 1	0
64	P	2	Total O 2 2	0
64	Q	3	Total O 3 3	0
64	R	1	Total O 1 1	0
64	S	2	Total O 2 2	0
64	T	3	Total O 3 3	0
64	U	2	Total O 2 2	0
64	W	1	Total O 1 1	0
64	X	1	Total O 1 1	0
64	Y	1	Total O 1 1	0
64	Z	3	Total O 3 3	0
64	2	5	Total O 5 5	0
64	3	4	Total O 4 4	0

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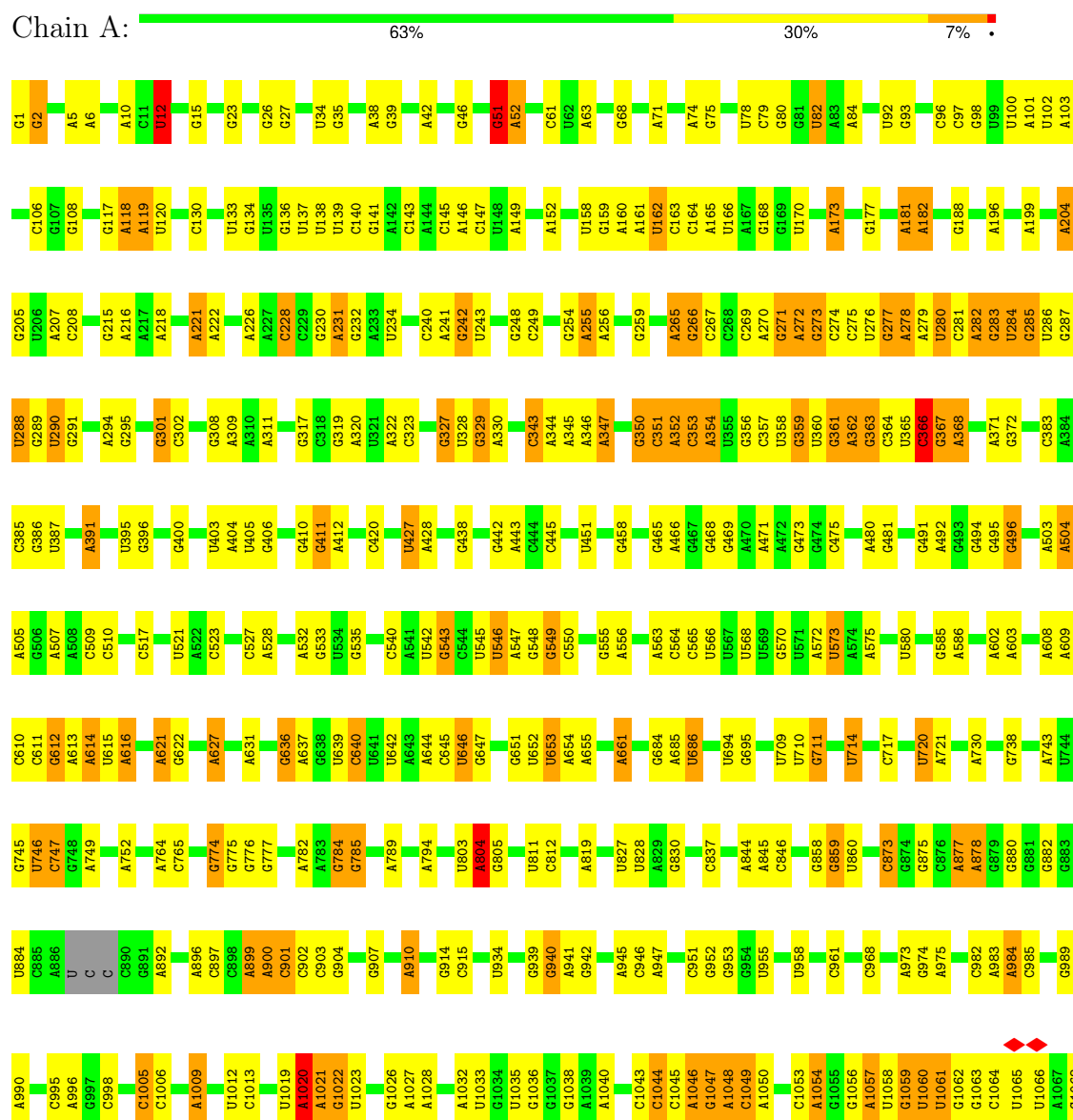
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
64	4	1	Total 1	O 1	0
64	a	160	Total 160	O 160	0
64	i	2	Total 2	O 2	0
64	j	1	Total 1	O 1	0
64	o	1	Total 1	O 1	0
64	p	1	Total 1	O 1	0
64	s	2	Total 2	O 2	0
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	v	3	Total 3	O 3	0
64	w	1	Total 1	O 1	0
64	y	3	Total 3	O 3	0

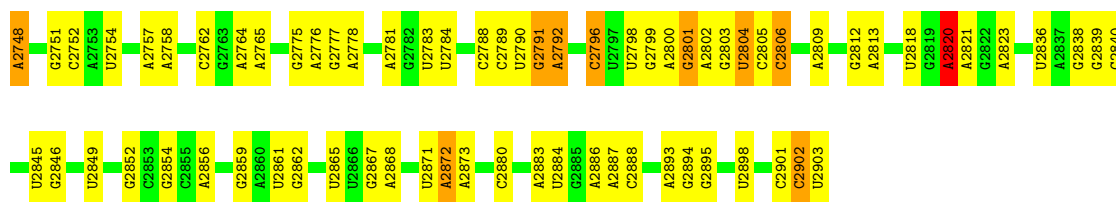
3 Residue-property plots

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

• Molecule 1: 23S rRNA

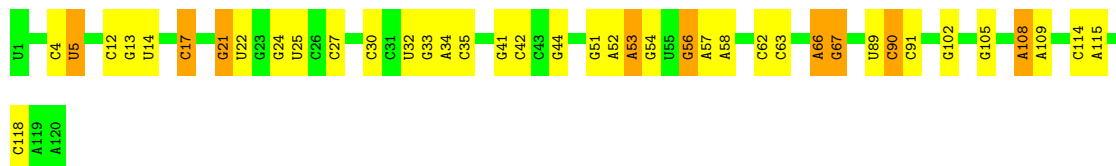


G2624	G2495	A2406	G2294	C2446	A2033	U1917	U1818	G1580	A1496	U1411	G1152	A1069
G2627	C2496	A2407	G2295	A2147	G2038	A1918	A1819	G1581	A1504	U1412	C1153	A1070
C2628	C2497	U2408	U2296	G2148	U2039	A1919	A1829	C1582	A1505	C1413	G1168	C1072
U2629	A2297	G2412	A2297	G2157	A1927	A1927	C1832	A1583	U1506	C1414	U1294	G1071
A2634	U2305	G2413	A2042	G2162	A1928	C1929	C1833	U1584	C1507	U1415	G1300	C1075
A2639	A2309	C2414	C2043	C2163	G1929	G1930	U1834	A1585	A1508	U1416	G1301	C1076
C2652	A2310	A2418	C2055	A2163	U1931	G1931	U1835	G1587	A1509	C1417	A1301	C1077
U2653	A2311	U2419	G2056	C2164	A1932	C1932	U1836	G1588	G1510	U1418	C1306	U1077
A2654	A2311	U2418	G2056	C2164	A1932	C1932	U1836	G1588	G1510	U1419	U1173	U1078
A2657	G2318	U2423	A2059	A2170	G1933	G1933	U1841	U1589	A1515	U1420	U1174	U1079
C2658	G2319	U2424	A2060	A2171	A1936	A1936	U1842	A1591	G1516	U1421	A1175	A1080
A2673	G2324	U2441	G2061	A2172	A1937	A1937	G1847	C1592	G1517	A427	U1176	U1081
G2674	U2324	U2442	A2062	A2173	A1938	A1938	G1847	A1593	C1518	C1428	C1177	U1082
A2675	G2325	U2443	A2063	A2174	U1939	G1735	A1853	U1594	G1522	C1429	C1178	U1083
C2676	G2326	U2444	G2069	A2175	U1940	C1736	A1854	C1595	U1523	U1430	G1179	A1084
C2677	A2327	U2445	A2070	C2176	C1941	U1736	U1855	A1596	G1524	A1431	U1180	A1085
A2678	A2328	U2446	A2071	C2177	C1942	G1738	G1857	A1597	C1525	U1432	U1183	G1087
A2679	U2329	U2447	C2072	U2182	C1942	A1739	A1858	A1603	C1526	A1433	U1184	A1088
G2686	G2332	U2448	A2077	G2183	U1955	A1739	U1859	U1608	G1527	A1434	G1190	A1089
U2687	U2332	U2449	U2194	G2184	C1962	G1743	G1860	A1609	G1528	U1435	G1337	A1090
C2688	U2333	U2450	U2195	U2194	U1963	G1743	G1861	A1610	A1529	G1441	G1338	U1097
U2689	U2334	U2451	U2196	U2195	U1964	G1750	G1862	A1613	G1530	G1447	U1343	U1101
C2691	A2335	U2452	A2080	A2198	G1965	U1751	G1863	G1613	A1532	C1452	U1344	C1102
G2694	A2336	U2453	U2092	G2204	C1966	C1752	U1864	U1616	U1534	A1453	C1345	A1103
U2707	A2337	U2454	G2093	A2205	U1967	A1755	U1865	A1617	U1535	A1454	U1352	U1104
C2712	A2338	U2455	C2096	A2206	A1970	U1758	G1867	C1618	C1536	C1455	C1363	U1105
U2713	A2339	U2456	C2097	C2207	U1971	U1759	G1868	G1619	G1537	U1456	U1226	G1106
C2715	A2340	U2457	U2098	C2208	G1972	G1764	C1870	G1622	G1538	U1457	G1227	G1107
C2716	G2345	U2458	G2102	A2211	U1977	A1773	A1871	U1647	U1539	U1458	U1227	U1108
G2719	C2350	U2459	C2103	U2212	A1977	G1773	C1874	G1642	U1542	U1459	G1236	C1109
U2720	U2356	U2460	U2105	U2220	U1980	G1776	A1875	G1643	A1544	U1460	U1240	A1111
A2724	G2361	U2461	U2106	U2221	A1981	U1779	A1876	U1647	A1545	U1466	G1248	G1115
C2725	U2362	U2462	U2107	G2221	U1982	U1780	C1881	U1648	G1546	U1467	U1249	G1116
A2726	G2363	U2463	U2108	A2225	U1983	U1781	U1882	G1649	C1547	U1468	C1257	C1117
U2727	G2364	U2464	G2110	C2226	U1991	U1782	U1883	A1548	A1549	A1469	U1258	G1131
C2728	G2365	U2465	U2111	U2227	G1992	U1783	G1884	A1654	A1549	U1470	A1263	U1119
A2733	G2366	U2466	G2112	G2228	U1993	A1784	G1888	A1659	G1555	U1475	G1266	C1135
C2735	G2367	U2467	U2113	G2229	C1997	A1791	A1889	G1659	C1556	U1476	G1266	C1135
U2736	G2371	U2468	U2118	G2230	U2012	C1795	A1890	G1674	C1557	U1477	G1266	C1135
A2737	A2378	U2469	A2119	G2231	G2013	C1796	A1891	C1675	C1558	A1478	U1271	G1139
U2738	G2379	U2470	G2120	G2232	A2013	U1796	C1895	U1676	U1559	U1479	U1272	C1140
A2739	G2383	U2471	G2121	G2233	A2020	G1800	A1900	A1677	G1560	U1482	U1273	U1141
C2742	U2384	U2472	G2127	A2273	C2021	A1801	G1906	U1693	C1565	G1483	C1404	A1142
U2743	G2385	U2473	U2131	A2274	U2022	A1802	G1907	C1694	A1566	U1484	U1403	A1143
C2744	G2386	U2474	U2132	A2275	C2023	A1803	G1908	G1695	G1567	U1485	U1273	C1144
U2745	G2387	U2475	U2133	A2276	G2027	A1804	U1911	G1696	G1568	A1490	U1406	A1145
A2746	G2388	U2476	G2134	A2277	U2028	A1805	U1912	U1714	A1569	U1491	G1407	C1278
C2747	A2392	U2477	A2134	A2278	G2029	G1811	A1913	G1715	A1572	G1492	U1408	G1279
U2748	U2402	U2478	G2141	G2286	A2030	C1816	3TD1915	U1716	U1578	A1493	G1409	C1283
A2749	C2403	U2479	G2142	A2287	A2031	C1817	A1916	A1717	A1579	U1494	U1409	C1150
U2750	U2404	U2480	C2145	A2288	G2032	A1916	A1916	G1718	A1579	A1495	G1410	A1151



- Molecule 2: 5S rRNA

Chain B: 67% 26% 8%



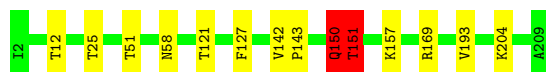
- Molecule 3: 50S ribosomal protein L2

Chain C: 92% 8%



- Molecule 4: 50S ribosomal protein L3

Chain D: 93% 6%



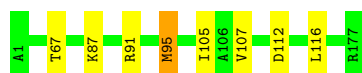
- Molecule 5: 50S ribosomal protein L4

Chain E: 93% 6%



- Molecule 6: 50S ribosomal protein L5

Chain F: 95%

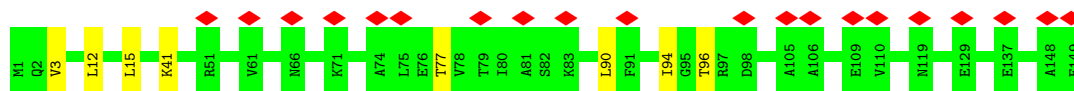


- Molecule 7: 50S ribosomal protein L6

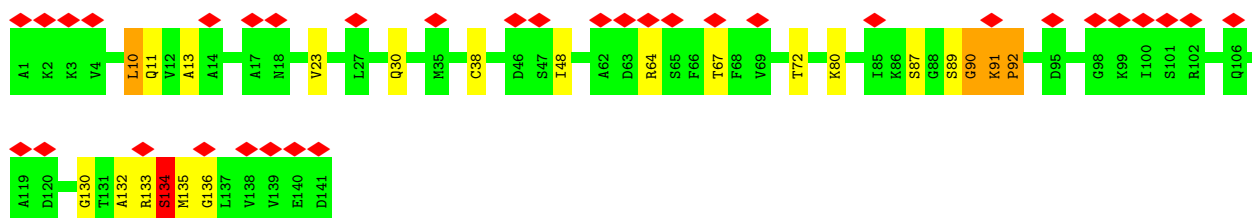
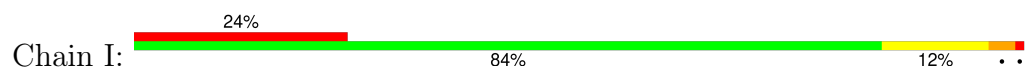
Chain G: 94% 6%



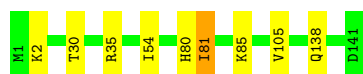
- Molecule 8: 50S ribosomal protein L9



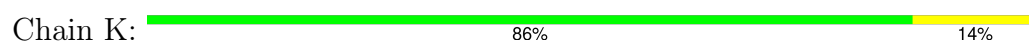
- Molecule 9: 50S ribosomal protein L11



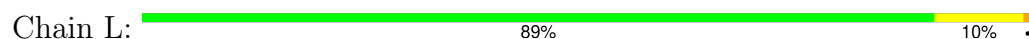
- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L14



- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



• Molecule 14: 50S ribosomal protein L17

Chain N:  93% 6%

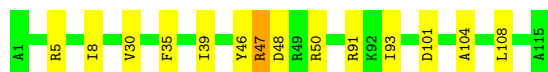
• Molecule 15: 50S ribosomal protein L18

Chain O:  94% 5%

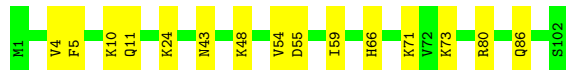
• Molecule 16: 50S ribosomal protein L19

Chain P:  90% 10%

• Molecule 17: 50S ribosomal protein L20

Chain Q:  88% 11%

• Molecule 18: 50S ribosomal protein L21

Chain R:  85% 15%

• Molecule 19: 50S ribosomal protein L22

Chain S:  92% 7%

• Molecule 20: 50S ribosomal protein L23

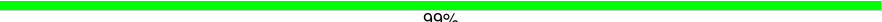
Chain T:  87% 13%

• Molecule 21: 50S ribosomal protein L24

Chain U:  92% 8%



- Molecule 22: 50S ribosomal protein L25

Chain V:  99% .

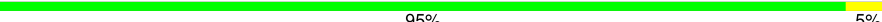


- Molecule 23: 50S ribosomal protein L27

Chain W:  92% 8%

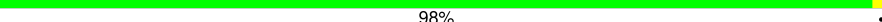


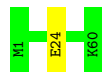
- Molecule 24: 50S ribosomal protein L28

Chain X:  95% 5%



- Molecule 25: 50S ribosomal protein L29

Chain Y:  98% .



- Molecule 26: 50S ribosomal protein L30

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L32

Chain 0:  84% 15% .



- Molecule 28: 50S ribosomal protein L33

Chain 1:  94% 6%



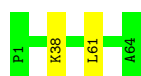
- Molecule 29: 50S ribosomal protein L34

Chain 2: 80% 18% .



- Molecule 30: 50S ribosomal protein L35

Chain 3: 97% .



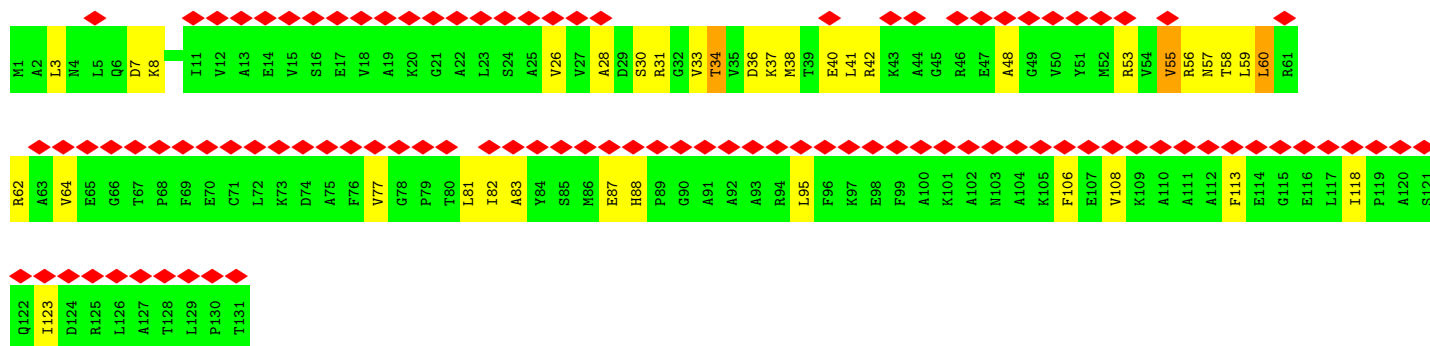
- Molecule 31: 50S ribosomal protein L36

Chain 4: 92% 8% .



- Molecule 32: 50S ribosomal protein L10

Chain 5: 76% 72% 26% .



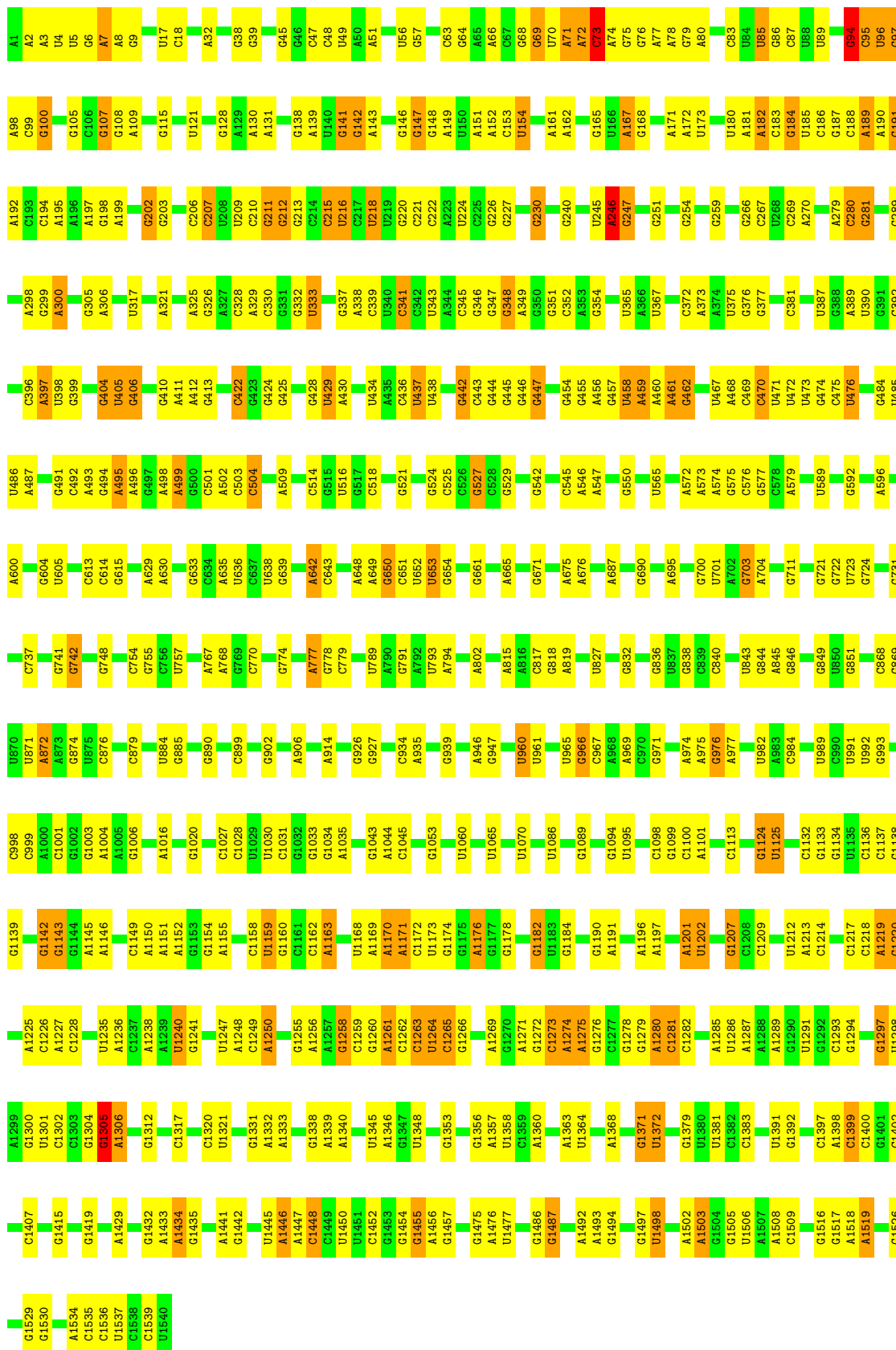
- Molecule 33: 50S ribosomal protein L31

Chain 6: 97% .

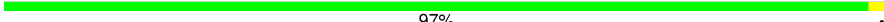


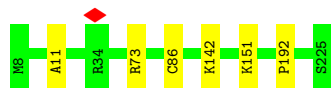
- Molecule 34: 16S rRNA

Chain a: 62% 31% 7% .

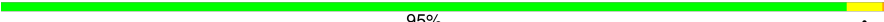


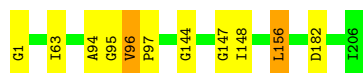
- Molecule 35: 30S ribosomal protein S2

Chain b:  97% .

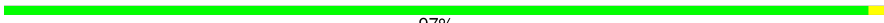


- Molecule 36: 30S ribosomal protein S3

Chain c:  95% . .



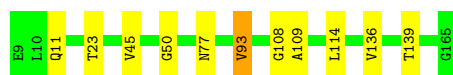
- Molecule 37: 30S ribosomal protein S4

Chain d:  97% .



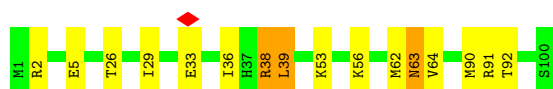
- Molecule 38: 30S ribosomal protein S5

Chain e:  93% 6% .



- Molecule 39: 30S ribosomal protein S6

Chain f:  84% 13% .



- Molecule 40: 30S ribosomal protein S7

Chain g:  93% 7%

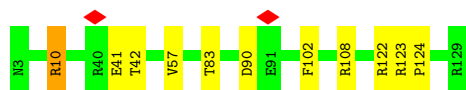


- Molecule 41: 30S ribosomal protein S8

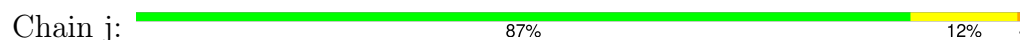
Chain h:  93% 7%



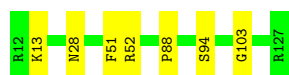
- Molecule 42: 30S ribosomal protein S9



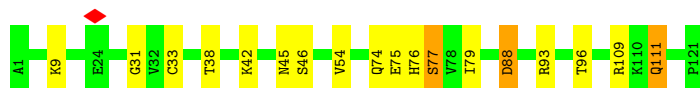
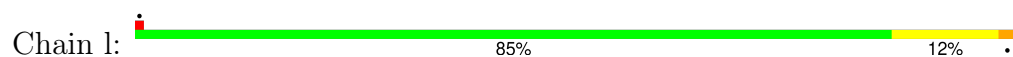
- Molecule 43: 30S ribosomal protein S10



- Molecule 44: 30S ribosomal protein S11



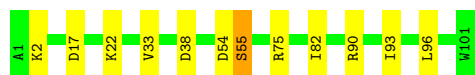
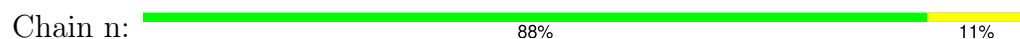
- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



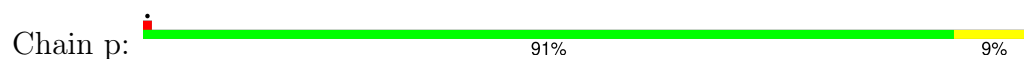
- Molecule 47: 30S ribosomal protein S14



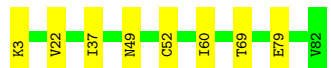
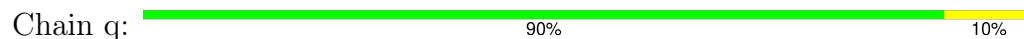
- Molecule 48: 30S ribosomal protein S15



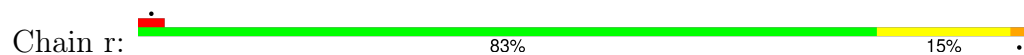
- Molecule 49: 30S ribosomal protein S16



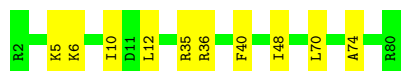
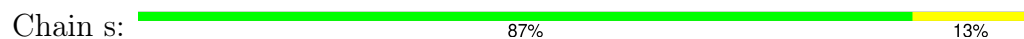
- Molecule 50: 30S ribosomal protein S17



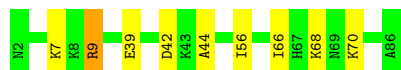
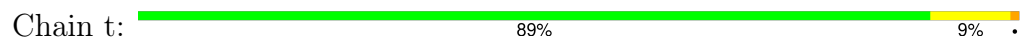
- Molecule 51: 30S ribosomal protein S18



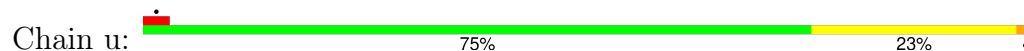
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S21

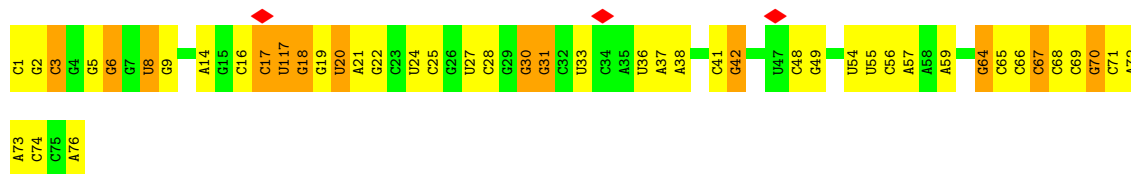


- Molecule 55: tRNA-fMet



- Molecule 55: tRNA-fMet

Chain w:  39% 44% 17%



- Molecule 56: mRNA

Chain x:  83% 17%



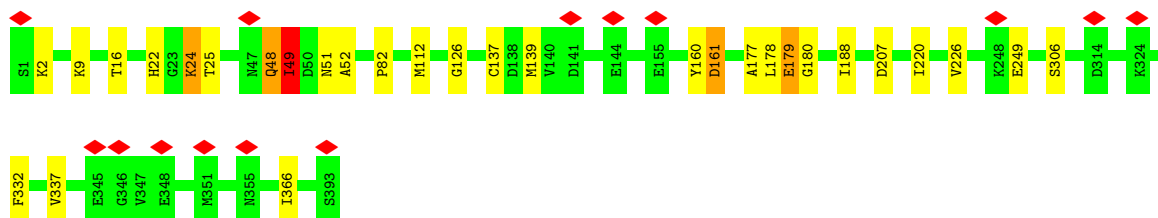
- Molecule 57: Phe-tRNA-Phe

Chain y:  53% 38% 8%



- Molecule 58: Elongation factor Tu 2

Chain z:  92% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.307	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.00677	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.38	0/69174	0.75	49/107907 (0.0%)
2	B	0.39	0/2876	0.72	0/4483
3	C	0.49	0/2121	0.77	0/2852
4	D	0.49	0/1578	0.79	2/2124 (0.1%)
5	E	0.50	0/1563	0.82	0/2103
6	F	0.53	0/1434	0.82	1/1926 (0.1%)
7	G	0.53	0/1324	0.73	0/1794
8	H	0.58	0/1122	0.77	0/1515
9	I	0.69	0/1046	0.94	2/1410 (0.1%)
10	J	0.49	0/1143	0.78	0/1540
11	K	0.51	0/947	0.78	0/1268
12	L	0.51	0/1052	0.85	0/1401
13	M	0.50	0/1093	0.79	0/1460
14	N	0.52	0/964	0.84	0/1289
15	O	0.51	0/902	0.86	0/1209
16	P	0.49	0/929	0.75	0/1242
17	Q	0.49	0/946	0.88	0/1260
18	R	0.47	0/823	0.71	0/1100
19	S	0.51	0/852	0.87	0/1142
20	T	0.50	0/736	0.80	0/984
21	U	0.49	0/787	0.74	0/1051
22	V	0.47	0/752	0.75	0/1008
23	W	0.48	0/579	0.71	0/767
24	X	0.48	0/635	0.72	0/848
25	Y	0.53	0/495	0.85	0/658
26	Z	0.52	0/438	0.78	0/586
27	0	0.47	0/440	0.86	0/588
28	1	0.50	0/424	0.67	0/565
29	2	0.51	0/370	1.00	0/487
30	3	0.47	0/513	0.84	0/676
31	4	0.46	0/303	0.73	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.71	0/1001	0.91	0/1350
33	6	0.57	0/531	0.79	0/709
34	a	0.38	0/36725	0.74	22/57285 (0.0%)
35	b	0.56	0/1735	0.79	0/2338
36	c	0.52	0/1651	0.80	0/2225
37	d	0.56	0/1665	0.81	0/2227
38	e	0.51	0/1180	0.83	0/1587
39	f	0.55	0/835	0.79	0/1128
40	g	0.53	0/1195	0.82	0/1602
41	h	0.50	0/989	0.79	0/1326
42	i	0.57	0/1034	0.78	0/1375
43	j	0.56	0/796	0.77	0/1077
44	k	0.51	0/885	0.79	0/1195
45	l	0.54	0/954	0.79	0/1282
46	m	0.55	0/900	0.84	0/1204
47	n	0.54	0/822	0.78	0/1095
48	o	0.52	0/722	0.87	0/964
49	p	0.54	0/659	0.77	0/884
50	q	0.55	0/657	0.75	0/881
51	r	0.56	0/544	0.81	0/731
52	s	0.55	0/652	0.76	0/877
53	t	0.54	0/671	0.88	0/888
54	u	0.63	0/550	0.91	0/728
55	v	0.41	1/1747 (0.1%)	0.72	0/2721
55	w	0.58	1/1747 (0.1%)	0.91	5/2721 (0.2%)
56	x	0.37	0/280	0.67	0/433
57	y	0.40	0/1607	0.71	1/2501 (0.0%)
58	z	0.57	0/3092	0.81	1/4183 (0.0%)
All	All	0.44	2/164187 (0.0%)	0.76	83/245157 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1
32	5	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-17.24	1.35	1.61
55	v	7	4SU	O3'-P	5.77	1.62	1.56

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	O3'-P-O5'	21.67	136.50	104.00
58	z	49	ILE	N-CA-C	-12.11	98.49	110.72
1	A	242	G	C2'-C3'-O3'	11.32	126.49	109.50
1	A	1378	A	C4'-C3'-O3'	10.04	124.46	109.40
1	A	1022	G	C2'-C3'-O3'	10.01	124.51	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	5	30	SER	Peptide
9	I	134	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	0	31340	456	0
2	B	2572	0	1302	19	0
3	C	2082	0	2157	6	0
4	D	1557	0	1604	5	0
5	E	1544	0	1607	5	0
6	F	1410	0	1447	1	0
7	G	1304	0	1348	5	0
8	H	1111	0	1148	1	0
9	I	1032	0	1088	15	0
10	J	1120	0	1151	2	0
11	K	938	0	1012	5	0
12	L	1043	0	1123	6	0
13	M	1074	0	1157	6	0
14	N	951	0	994	3	0
15	O	892	0	923	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	917	0	965	4	0
17	Q	933	0	1006	9	0
18	R	810	0	834	4	0
19	S	845	0	909	2	0
20	T	730	0	795	4	0
21	U	779	0	834	1	0
22	V	739	0	763	0	0
23	W	572	0	593	1	0
24	X	625	0	655	1	0
25	Y	494	0	530	0	0
26	Z	434	0	477	0	0
27	0	434	0	448	6	0
28	1	417	0	451	1	0
29	2	367	0	405	6	0
30	3	504	0	574	1	0
31	4	302	0	343	2	0
32	5	988	0	1025	34	0
33	6	522	0	524	0	0
34	a	33050	0	16656	247	0
35	b	1704	0	1732	1	0
36	c	1624	0	1699	3	0
37	d	1643	0	1710	3	0
38	e	1164	0	1212	1	0
39	f	817	0	808	11	0
40	g	1181	0	1240	2	0
41	h	979	0	1034	4	0
42	i	1022	0	1070	3	0
43	j	786	0	828	3	0
44	k	869	0	878	1	0
45	l	940	0	1001	5	0
46	m	891	0	955	3	0
47	n	810	0	852	4	0
48	o	714	0	737	3	0
49	p	649	0	666	1	0
50	q	648	0	691	1	0
51	r	535	0	552	2	0
52	s	637	0	665	5	0
53	t	665	0	714	3	0
54	u	544	0	579	4	0
55	v	1644	0	840	15	0
55	w	1644	0	840	23	0
56	x	252	0	129	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	y	1632	0	843	8	0
58	z	3036	0	3053	14	0
59	0	2	0	0	0	0
59	1	1	0	0	0	0
59	3	1	0	0	0	0
59	4	1	0	0	0	0
59	A	1181	0	0	0	0
59	B	31	0	0	0	0
59	C	1	0	0	0	0
59	K	1	0	0	0	0
59	L	2	0	0	0	0
59	M	1	0	0	0	0
59	Q	1	0	0	0	0
59	R	1	0	0	0	0
59	S	1	0	0	0	0
59	T	2	0	0	0	0
59	a	373	0	0	0	0
59	d	1	0	0	0	0
59	h	1	0	0	0	0
59	i	1	0	0	0	0
59	s	1	0	0	0	0
59	u	1	0	0	0	0
59	v	7	0	0	0	0
59	w	1	0	0	0	0
59	y	4	0	0	0	0
59	z	1	0	0	0	0
60	A	1	0	0	0	0
61	v	10	0	10	0	0
62	z	11	0	8	0	0
63	z	32	0	13	0	0
64	2	5	0	0	0	0
64	3	4	0	0	0	0
64	4	1	0	0	0	0
64	A	751	0	0	0	0
64	B	11	0	0	0	0
64	C	9	0	0	0	0
64	E	5	0	0	0	0
64	J	2	0	0	0	0
64	K	2	0	0	0	0
64	L	6	0	0	1	0
64	M	1	0	0	0	0
64	N	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	O	1	0	0	0	0
64	P	2	0	0	0	0
64	Q	3	0	0	0	0
64	R	1	0	0	0	0
64	S	2	0	0	0	0
64	T	3	0	0	0	0
64	U	2	0	0	0	0
64	W	1	0	0	0	0
64	X	1	0	0	0	0
64	Y	1	0	0	0	0
64	Z	3	0	0	0	0
64	a	160	0	0	0	0
64	i	2	0	0	0	0
64	j	1	0	0	0	0
64	o	1	0	0	0	0
64	p	1	0	0	0	0
64	s	2	0	0	0	0
64	t	1	0	0	0	0
64	u	1	0	0	0	0
64	v	3	0	0	0	0
64	w	1	0	0	0	0
64	y	3	0	0	0	0
All	All	155067	0	103547	892	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 892 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)
1:A:1021:A:N1	1:A:1141:U:O4	1.58	1.34
1:A:289:G:N1	1:A:351:C:N3	1.84	1.26
34:a:437:U:N3	34:a:495:A:N6	1.87	1.23
1:A:711:G:O6	1:A:720:U:N3	1.72	1.21
34:a:437:U:C4	34:a:495:A:C6	2.33	1.16

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	
3	C	269/271 (99%)	240 (89%)	27 (10%)	2 (1%)	18	49
4	D	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	24	57
5	E	198/200 (99%)	181 (91%)	15 (8%)	2 (1%)	12	41
6	F	175/177 (99%)	156 (89%)	19 (11%)	0	100	100
7	G	172/174 (99%)	159 (92%)	13 (8%)	0	100	100
8	H	147/149 (99%)	125 (85%)	19 (13%)	3 (2%)	6	25
9	I	139/141 (99%)	104 (75%)	29 (21%)	6 (4%)	2	12
10	J	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	9	34
11	K	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	3	17
12	L	141/143 (99%)	117 (83%)	19 (14%)	5 (4%)	3	16
13	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	8	32
14	N	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	4	21
15	O	114/116 (98%)	107 (94%)	6 (5%)	1 (1%)	14	44
16	P	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
17	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
18	R	100/102 (98%)	84 (84%)	13 (13%)	3 (3%)	3	19
19	S	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	14	44
20	T	90/92 (98%)	79 (88%)	9 (10%)	2 (2%)	5	24
21	U	100/102 (98%)	87 (87%)	11 (11%)	2 (2%)	6	25
22	V	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	11	39
23	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	9	34
24	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
25	Y	58/60 (97%)	54 (93%)	3 (5%)	1 (2%)	7	30
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	45 (85%)	7 (13%)	1 (2%)	6	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
29	2	43/45 (96%)	40 (93%)	3 (7%)	0	100	100
30	3	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	96 (74%)	24 (19%)	9 (7%)	1	5
33	6	64/66 (97%)	56 (88%)	7 (11%)	1 (2%)	7	30
35	b	216/218 (99%)	187 (87%)	24 (11%)	5 (2%)	5	23
36	c	204/206 (99%)	180 (88%)	18 (9%)	6 (3%)	3	19
37	d	203/205 (99%)	182 (90%)	19 (9%)	2 (1%)	12	41
38	e	156/157 (99%)	136 (87%)	16 (10%)	4 (3%)	4	21
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	13
40	g	149/151 (99%)	131 (88%)	13 (9%)	5 (3%)	3	16
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	94 (75%)	27 (22%)	4 (3%)	3	18
43	j	96/98 (98%)	70 (73%)	20 (21%)	6 (6%)	1	6
44	k	114/116 (98%)	101 (89%)	8 (7%)	5 (4%)	2	12
45	l	119/121 (98%)	94 (79%)	19 (16%)	6 (5%)	1	11
46	m	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	6	28
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	1	10
48	o	86/88 (98%)	77 (90%)	6 (7%)	3 (4%)	3	16
49	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4	21
50	q	78/80 (98%)	67 (86%)	8 (10%)	3 (4%)	2	15
51	r	63/65 (97%)	51 (81%)	10 (16%)	2 (3%)	3	18
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	4	22
54	u	63/65 (97%)	39 (62%)	14 (22%)	10 (16%)	0	0
58	z	391/393 (100%)	350 (90%)	29 (7%)	12 (3%)	3	18
All	All	6219/6322 (98%)	5469 (88%)	609 (10%)	141 (2%)	7	23

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	81	ILE

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Mol	Chain	Res	Type
11	K	89	ASN
32	5	55	VAL
32	5	123	ILE
33	6	4	ASP

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	
3	C	216/216 (100%)	208 (96%)	8 (4%)	30	61
4	D	163/163 (100%)	155 (95%)	8 (5%)	22	53
5	E	164/164 (100%)	159 (97%)	5 (3%)	36	65
6	F	148/148 (100%)	142 (96%)	6 (4%)	27	59
7	G	135/135 (100%)	133 (98%)	2 (2%)	57	75
8	H	114/114 (100%)	111 (97%)	3 (3%)	40	68
9	I	109/109 (100%)	103 (94%)	6 (6%)	19	50
10	J	115/115 (100%)	110 (96%)	5 (4%)	26	57
11	K	103/103 (100%)	99 (96%)	4 (4%)	28	60
12	L	102/102 (100%)	94 (92%)	8 (8%)	11	38
13	M	109/109 (100%)	107 (98%)	2 (2%)	51	73
14	N	99/99 (100%)	95 (96%)	4 (4%)	28	60
15	O	86/86 (100%)	84 (98%)	2 (2%)	44	70
16	P	99/99 (100%)	95 (96%)	4 (4%)	28	60
17	Q	88/88 (100%)	84 (96%)	4 (4%)	24	56
18	R	84/84 (100%)	77 (92%)	7 (8%)	10	35
19	S	92/92 (100%)	87 (95%)	5 (5%)	20	50
20	T	79/79 (100%)	75 (95%)	4 (5%)	21	52
21	U	83/83 (100%)	79 (95%)	4 (5%)	23	54
22	V	77/77 (100%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	57/57 (100%)	54 (95%)	3 (5%)	20	51
24	X	67/67 (100%)	65 (97%)	2 (3%)	36	65
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	47 (100%)	0	100	100
27	0	46/46 (100%)	44 (96%)	2 (4%)	26	57
28	1	46/46 (100%)	44 (96%)	2 (4%)	26	57
29	2	37/37 (100%)	33 (89%)	4 (11%)	6	25
30	3	51/51 (100%)	50 (98%)	1 (2%)	48	72
31	4	34/34 (100%)	33 (97%)	1 (3%)	37	66
32	5	100/100 (100%)	96 (96%)	4 (4%)	28	60
33	6	59/59 (100%)	58 (98%)	1 (2%)	53	74
35	b	180/180 (100%)	180 (100%)	0	100	100
36	c	170/170 (100%)	168 (99%)	2 (1%)	63	78
37	d	172/172 (100%)	170 (99%)	2 (1%)	63	78
38	e	120/119 (101%)	114 (95%)	6 (5%)	22	53
39	f	87/87 (100%)	83 (95%)	4 (5%)	24	55
40	g	124/124 (100%)	121 (98%)	3 (2%)	43	69
41	h	104/104 (100%)	101 (97%)	3 (3%)	37	66
42	i	105/105 (100%)	102 (97%)	3 (3%)	37	66
43	j	86/86 (100%)	83 (96%)	3 (4%)	32	62
44	k	89/89 (100%)	88 (99%)	1 (1%)	65	78
45	l	102/102 (100%)	96 (94%)	6 (6%)	18	48
46	m	93/93 (100%)	91 (98%)	2 (2%)	45	71
47	n	83/83 (100%)	81 (98%)	2 (2%)	43	69
48	o	76/76 (100%)	73 (96%)	3 (4%)	28	60
49	p	65/65 (100%)	62 (95%)	3 (5%)	24	55
50	q	74/74 (100%)	71 (96%)	3 (4%)	27	59
51	r	56/56 (100%)	50 (89%)	6 (11%)	6	25
52	s	70/70 (100%)	67 (96%)	3 (4%)	26	57
53	t	65/65 (100%)	60 (92%)	5 (8%)	12	38
54	u	55/55 (100%)	53 (96%)	2 (4%)	31	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	z	326/326 (100%)	317 (97%)	9 (3%)	38	66
All	All	5166/5165 (100%)	4984 (96%)	182 (4%)	32	62

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	e	11	GLN
45	l	111	GLN
38	e	136	VAL
41	h	120	LEU
48	o	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
51	r	73	HIS
53	t	47	GLN
58	z	329	GLN
21	U	53	GLN
21	U	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	757 (26%)	78 (2%)
2	B	119/120 (99%)	29 (24%)	3 (2%)
34	a	1539/1540 (99%)	429 (27%)	0
55	v	76/77 (98%)	21 (27%)	0
55	w	76/77 (98%)	36 (47%)	0
56	x	11/12 (91%)	1 (9%)	0
57	y	75/76 (98%)	29 (38%)	0
All	All	4793/4805 (99%)	1302 (27%)	81 (1%)

5 of 1302 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	5	A
1	A	6	A

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Mol	Chain	Res	Type
1	A	10	A
1	A	12	U

5 of 81 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1558	C
1	A	2391	G
1	A	1647	U
1	A	1918	A
1	A	2712	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	2604	1	18,21,22	1.36	3 (16%)	21,30,33	1.86	4 (19%)
34	MA6	a	1518	34	23,26,27	1.79	6 (26%)	33,38,41	2.25	11 (33%)
1	2MG	A	1835	1	23,26,27	1.34	4 (17%)	33,38,41	2.27	9 (27%)
34	7MG	a	527	34	23,26,27	1.44	3 (13%)	27,39,42	2.55	8 (29%)
1	OMG	A	2251	1,55,59	23,26,27	1.28	3 (13%)	32,38,41	1.85	5 (15%)
1	PSU	A	955	1	18,21,22	1.43	3 (16%)	21,30,33	2.08	4 (19%)
1	7MG	A	2069	1,59	23,26,27	1.47	4 (17%)	27,39,42	2.51	10 (37%)
57	PSU	y	39	57	18,21,22	1.47	2 (11%)	21,30,33	1.93	4 (19%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.41	4 (21%)
1	PSU	A	2504	1	18,21,22	1.43	2 (11%)	21,30,33	2.07	4 (19%)
1	PSU	A	2605	1	18,21,22	1.42	2 (11%)	21,30,33	2.02	4 (19%)
1	H2U	A	2449	1	18,21,22	1.12	2 (11%)	19,30,33	1.70	4 (21%)
34	UR3	a	1498	34	19,22,23	1.11	2 (10%)	26,32,35	1.94	5 (19%)
1	1MG	A	745	1	23,26,27	1.31	3 (13%)	33,39,42	1.98	8 (24%)

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	1.29	4 (17%)	33,38,41	2.29	9 (27%)
57	PSU	y	55	57	18,21,22	1.40	2 (11%)	21,30,33	2.08	5 (23%)
57	MIA	y	37	57	28,31,32	2.29	6 (21%)	38,44,47	2.87	19 (50%)
1	OMC	A	2498	1,59	19,22,23	0.84	1 (5%)	25,31,34	1.38	3 (12%)
1	OMU	A	2552	1,59	19,22,23	1.33	3 (15%)	25,31,34	2.18	9 (36%)
55	PSU	v	55	55	18,21,22	1.34	3 (16%)	21,30,33	2.00	5 (23%)
34	4OC	a	1402	34	20,23,24	0.80	0	25,32,35	1.35	4 (16%)
55	PSU	w	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.03	5 (23%)
1	2MG	A	2445	1,59	23,26,27	1.27	4 (17%)	33,38,41	2.19	8 (24%)
1	PSU	A	2580	1	18,21,22	1.48	3 (16%)	21,30,33	2.00	5 (23%)
1	3TD	A	1915	1	19,22,23	7.07	14 (73%)	23,32,35	2.03	5 (21%)
34	5MC	a	1407	34	19,22,23	1.77	2 (10%)	26,32,35	1.60	4 (15%)
57	4SU	y	8	57	18,21,22	1.85	5 (27%)	25,30,33	2.36	7 (28%)
34	2MG	a	1207	34	23,26,27	1.24	3 (13%)	33,38,41	2.92	10 (30%)
57	7MG	y	46	57	23,26,27	1.41	3 (13%)	27,39,42	2.49	7 (25%)
34	5MC	a	967	34	19,22,23	1.96	2 (10%)	26,32,35	1.45	4 (15%)
57	5MU	y	54	57	19,22,23	1.42	4 (21%)	27,32,35	2.07	8 (29%)
1	6MZ	A	1618	1	22,25,26	1.43	5 (22%)	29,36,39	2.50	13 (44%)
34	PSU	a	516	34	18,21,22	1.38	2 (11%)	21,30,33	2.11	5 (23%)
55	H2U	v	20	55	18,21,22	0.81	1 (5%)	19,30,33	1.64	3 (15%)
55	5MU	v	54	55	19,22,23	1.45	5 (26%)	27,32,35	1.98	9 (33%)
1	PSU	A	1917	1	18,21,22	1.45	2 (11%)	21,30,33	1.99	5 (23%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.47	4 (21%)
1	PSU	A	2457	1,59	18,21,22	1.54	3 (16%)	21,30,33	2.08	5 (23%)
1	PSU	A	746	1,59	18,21,22	1.37	2 (11%)	21,30,33	1.98	3 (14%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.62	2 (10%)
1	6MZ	A	2030	1,59	22,25,26	1.53	4 (18%)	29,36,39	2.30	10 (34%)
57	PSU	y	32	57	18,21,22	1.36	2 (11%)	21,30,33	2.19	5 (23%)
34	2MG	a	966	34	23,26,27	1.33	4 (17%)	33,38,41	2.66	11 (33%)
1	5MU	A	1939	1	19,22,23	1.35	3 (15%)	27,32,35	2.03	8 (29%)
55	4SU	w	8	55	18,21,22	1.83	5 (27%)	25,30,33	2.23	6 (24%)
34	MA6	a	1519	34,59	23,26,27	1.67	5 (21%)	33,38,41	2.46	12 (36%)
55	4SU	v	7	55	18,21,22	1.80	5 (27%)	25,30,33	2.47	7 (28%)
1	5MC	A	1962	1	19,22,23	1.77	2 (10%)	26,32,35	1.54	4 (15%)
55	5MU	w	54	55	19,22,23	1.50	4 (21%)	27,32,35	2.08	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	A	2503	1,59	22,25,26	1.50	4 (18%)	32,37,40	2.30	8 (25%)
1	5MC	A	747	1	19,22,23	1.75	3 (15%)	26,32,35	1.56	6 (23%)
1	PSU	A	1911	1	18,21,22	1.42	2 (11%)	21,30,33	2.12	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
1	OMG	A	2251	1,55,59	-	0/9/27/28	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	7MG	A	2069	1,59	-	3/7/37/38	0/3/3/3
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
57	MIA	y	37	57	-	3/15/33/34	0/3/3/3
1	OMC	A	2498	1,59	-	0/9/27/28	0/2/2/2
1	OMU	A	2552	1,59	-	2/9/27/28	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
55	PSU	w	55	55	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1,59	-	2/9/27/28	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	1/9/27/28	0/3/3/3
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	2/9/27/28	0/3/3/3
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
1	PSU	A	2457	1,59	-	2/7/25/26	0/2/2/2
1	PSU	A	746	1,59	-	1/7/25/26	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
1	6MZ	A	2030	1,59	-	3/9/27/28	0/3/3/3
57	PSU	y	32	57	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
34	MA6	a	1519	34,59	-	3/11/29/30	0/3/3/3
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
55	5MU	w	54	55	-	1/7/25/26	0/2/2/2
1	2MA	A	2503	1,59	-	2/7/25/26	0/3/3/3
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.55	1.66	1.43
1	A	1915	3TD	C6-C5	15.60	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.39	1.34	1.53
1	A	1915	3TD	C2-N1	8.57	1.47	1.37
34	a	967	5MC	C5-C4	7.37	1.49	1.44

The worst 5 of 341 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1207	2MG	C2-N3-C4	8.60	122.76	112.00
34	a	966	2MG	C2-N3-C4	8.51	122.64	112.00
57	y	46	7MG	N9-C4-N3	8.15	137.40	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	N9-C4-N3	8.14	137.39	125.46
34	a	1207	2MG	N1-C2-N2	8.12	124.84	116.56

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1618	6MZ	O4'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	1498	UR3	1	0
57	y	37	MIA	1	0
1	A	2498	OMC	3	0
1	A	1915	3TD	1	0
1	A	1618	6MZ	5	0
1	A	2030	6MZ	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1622 ligands modelled in this entry, 1619 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	PHE	z	401	-	10,11,12	0.45	0	8,13,15	0.18	0
63	GNP	z	402	59	34,34,34	2.46	9 (26%)	47,54,54	1.86	9 (19%)
61	FME	v	101	-	8,9,10	0.61	0	8,9,11	1.77	2 (25%)

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
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
63	GNP	z	402	59	-	6/18/38/38	0/3/3/3
61	FME	v	101	-	-	2/7/9/11	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GNP	PG-O1G	10.06	1.61	1.46
63	z	402	GNP	PG-N3B	4.48	1.75	1.63
63	z	402	GNP	PB-N3B	4.47	1.75	1.63
63	z	402	GNP	C5-C4	3.24	1.47	1.38
63	z	402	GNP	PG-O3G	-3.18	1.48	1.56

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GNP	C5-C4-N3	-6.06	118.75	128.39
63	z	402	GNP	C2-N3-C4	5.24	121.32	112.30
63	z	402	GNP	N9-C4-N3	4.66	135.26	125.95
61	v	101	FME	C-CA-N	3.64	116.53	109.50
63	z	402	GNP	C6-C5-N7	3.42	136.51	130.29

There are no chirality outliers.

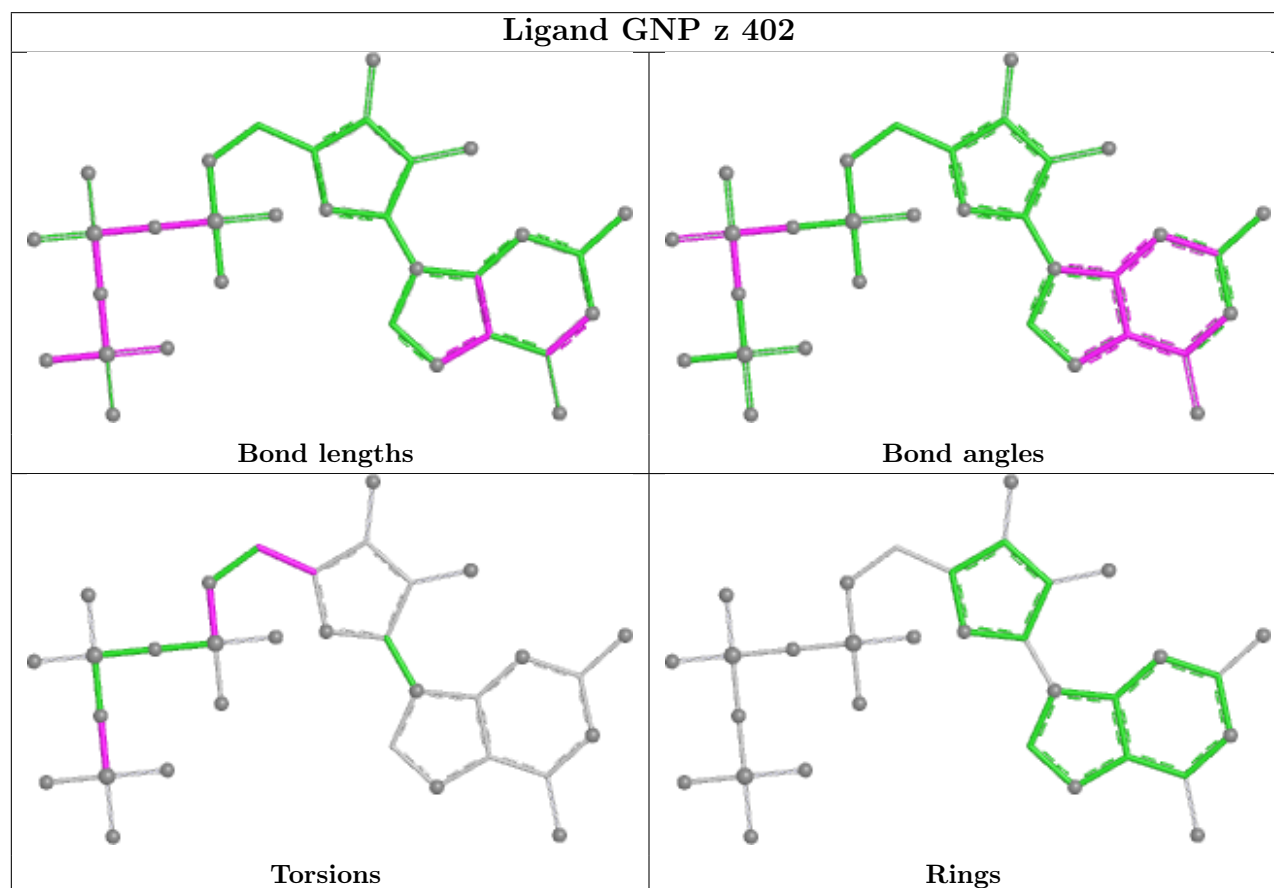
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	v	101	FME	O1-CN-N-CA
62	z	401	PHE	O-C-CA-CB
63	z	402	GNP	PB-N3B-PG-O1G
63	z	402	GNP	O4'-C4'-C5'-O5'
63	z	402	GNP	C3'-C4'-C5'-O5'

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
55	w	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1618:6MZ	O3'	1619:G	P	2.24
1	A	2030:6MZ	O3'	2031:A	P	1.77
1	w	117:U	O3'	18:G	P	1.35

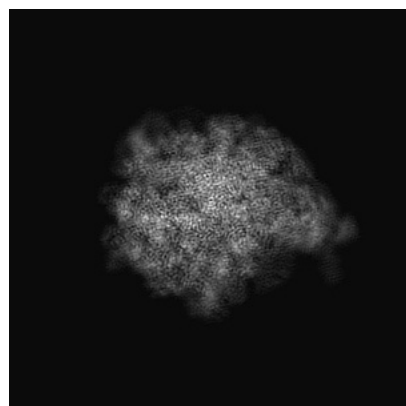
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8814. These allow visual inspection of the internal detail of the map and identification of artifacts.

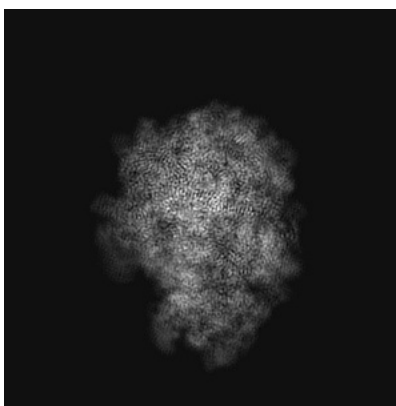
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

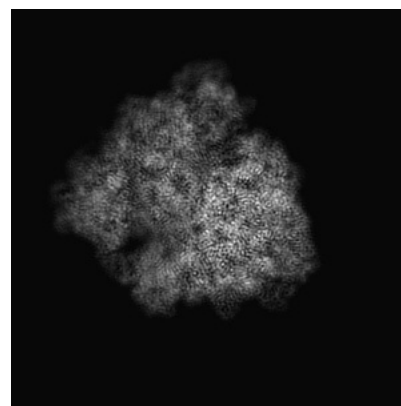
6.1.1 Primary map



X

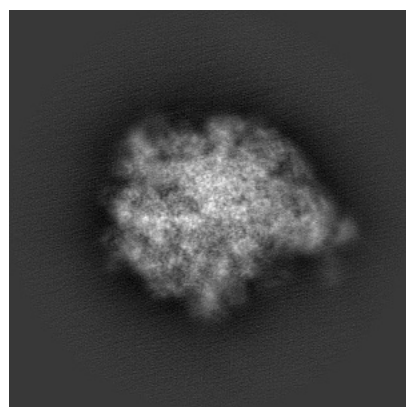


Y

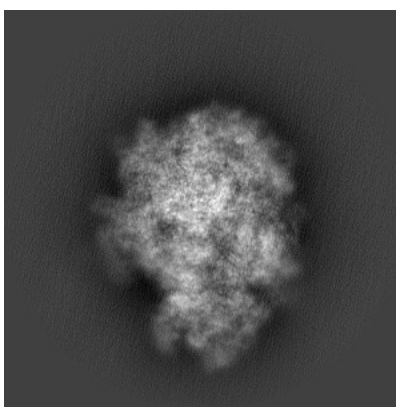


Z

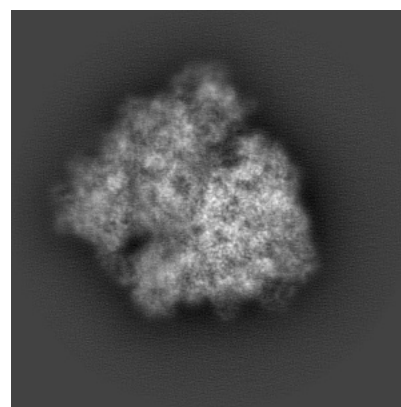
6.1.2 Raw map



X



Y

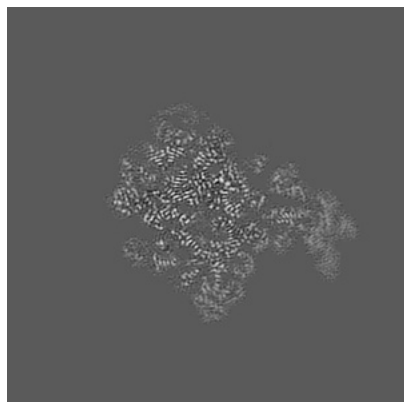


Z

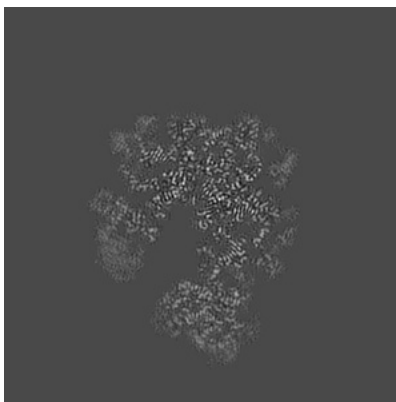
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

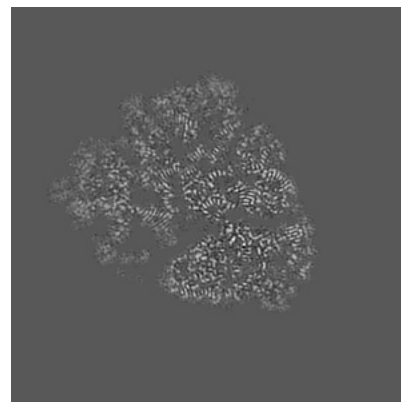
6.2.1 Primary map



X Index: 199

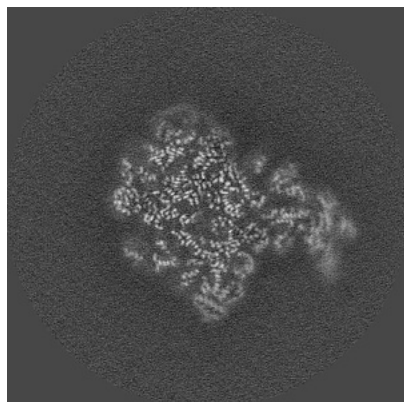


Y Index: 199

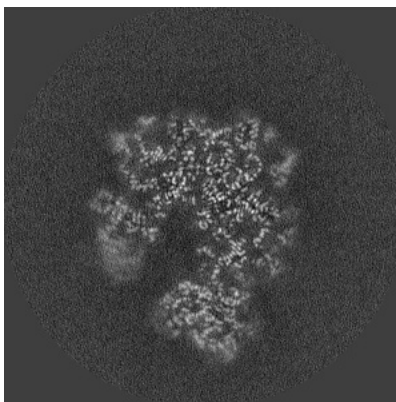


Z Index: 199

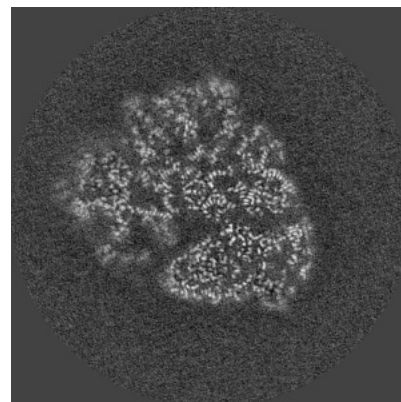
6.2.2 Raw map



X Index: 199



Y Index: 199

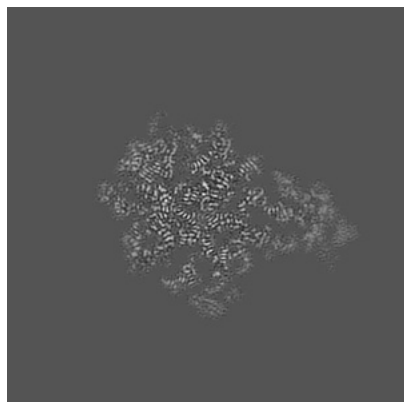


Z Index: 199

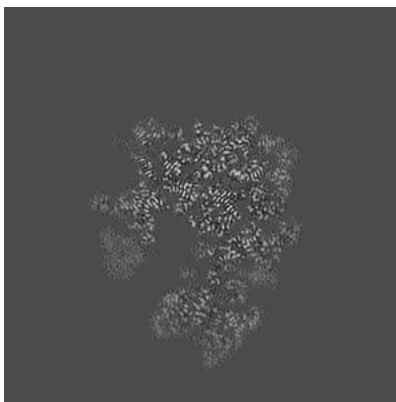
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

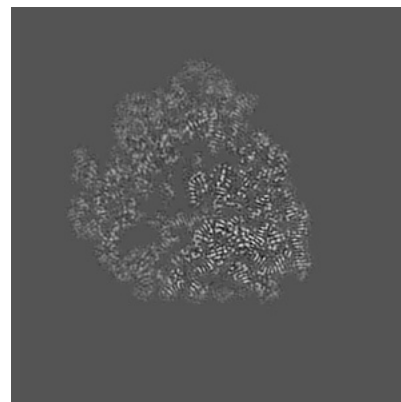
6.3.1 Primary map



X Index: 208

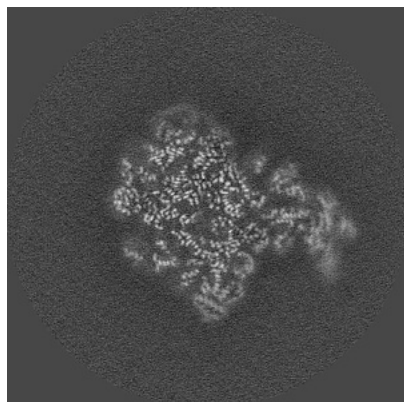


Y Index: 208

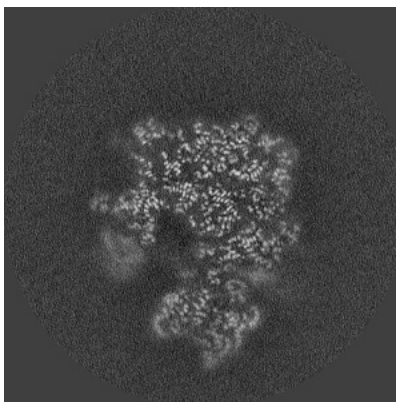


Z Index: 189

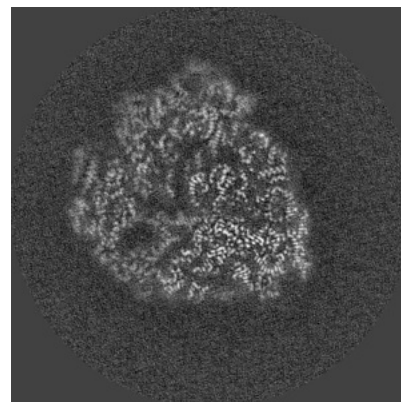
6.3.2 Raw map



X Index: 199



Y Index: 208

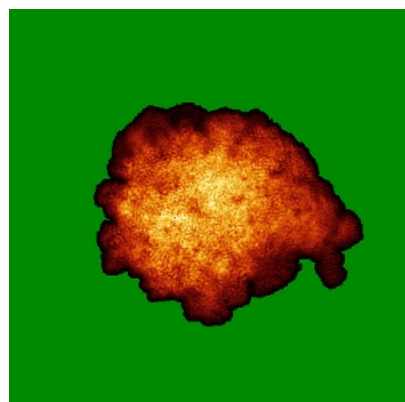


Z Index: 190

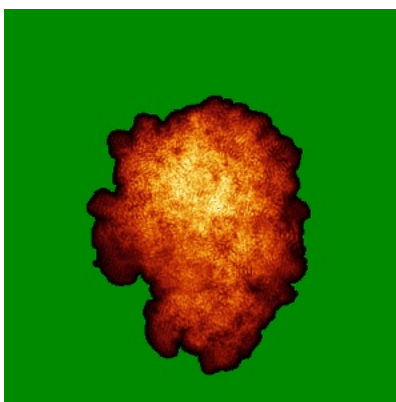
The images above show the largest variance slices of the map in three orthogonal directions.

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

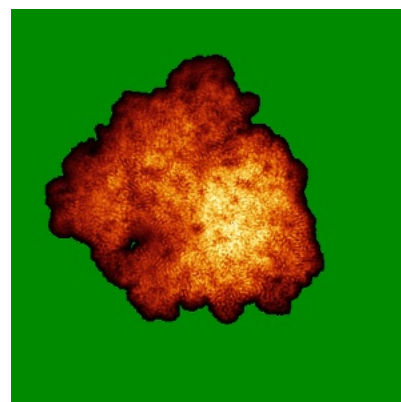
6.4.1 Primary map



X

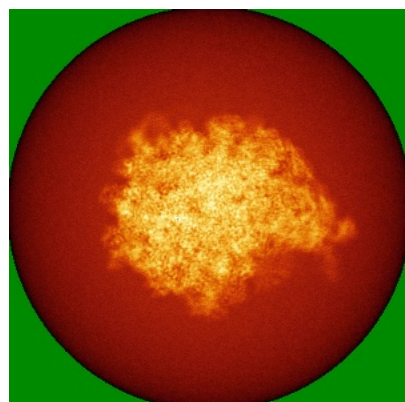


Y

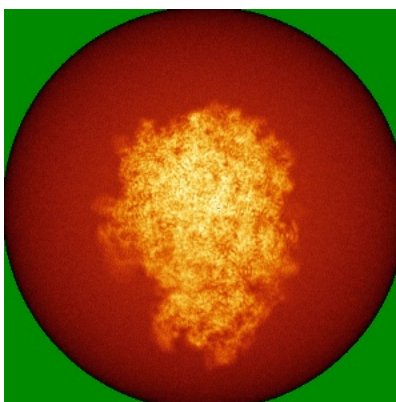


Z

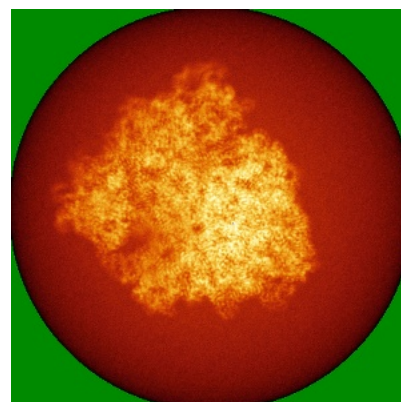
6.4.2 Raw map



X



Y

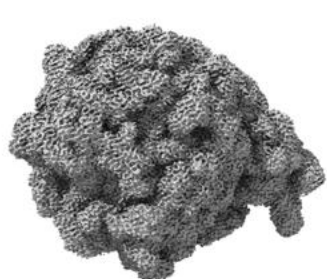


Z

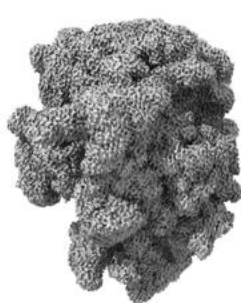
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

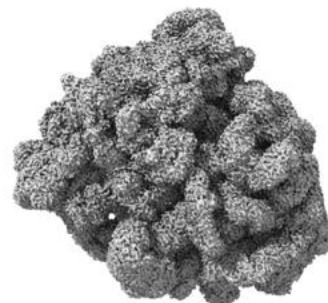
6.5.1 Primary map



X



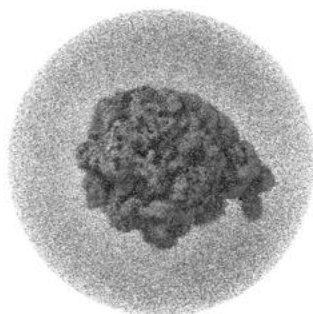
Y



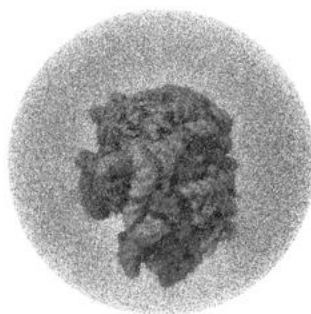
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00677. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

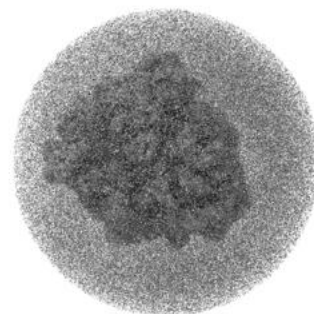
6.5.2 Raw map



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.

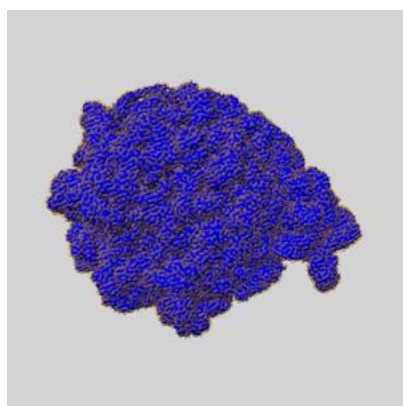
6.6 Mask visualisation [i](#)

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

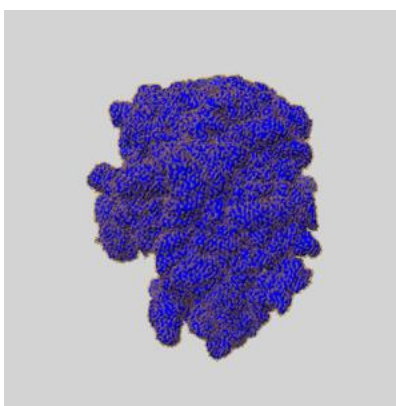
A mask typically either:

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

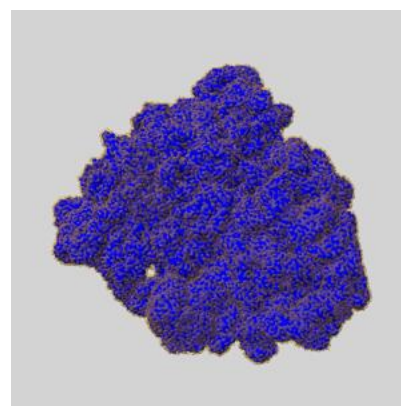
6.6.1 emd_8814_msk_1.map [i](#)



X



Y

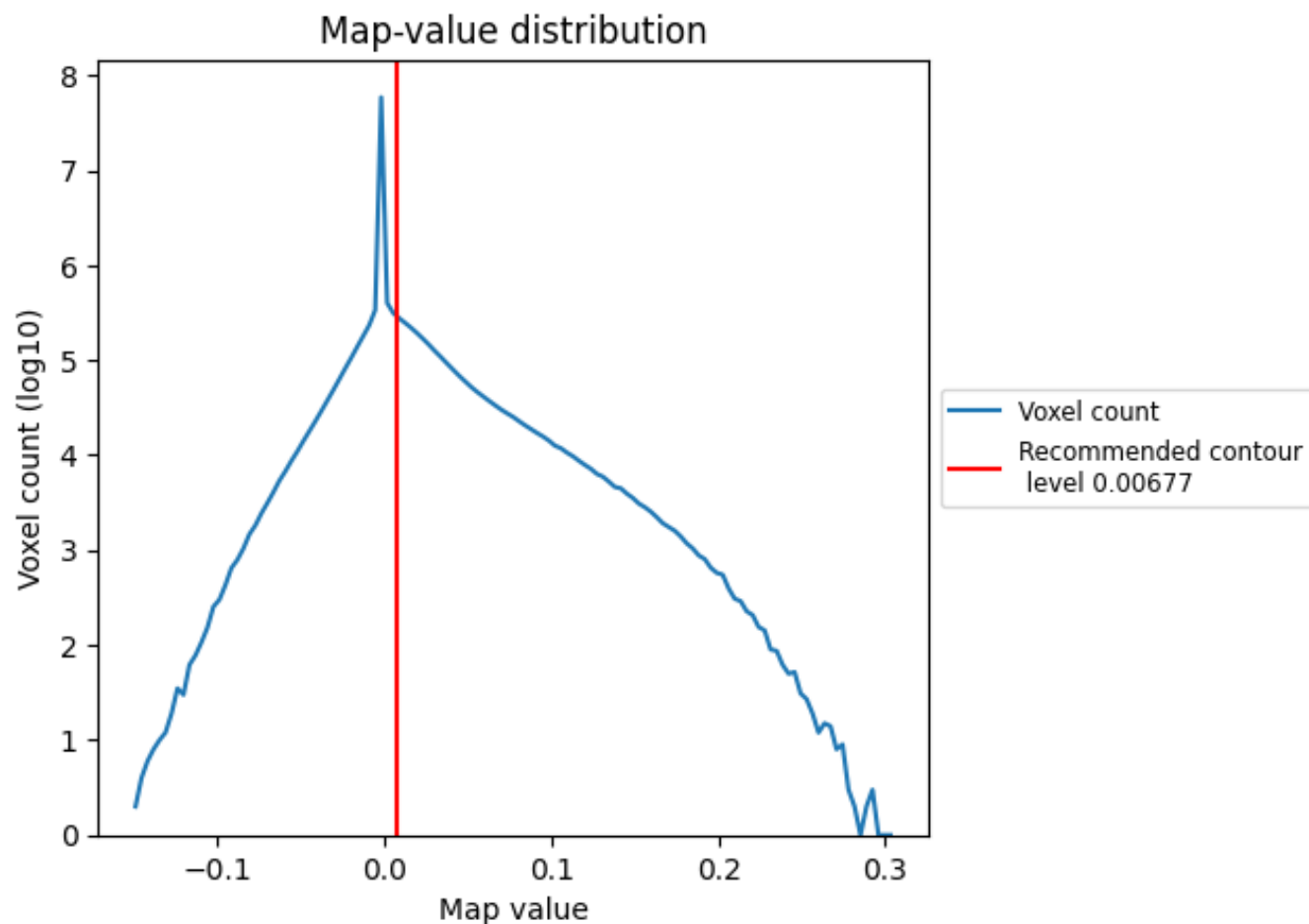


Z

7 Map analysis [i](#)

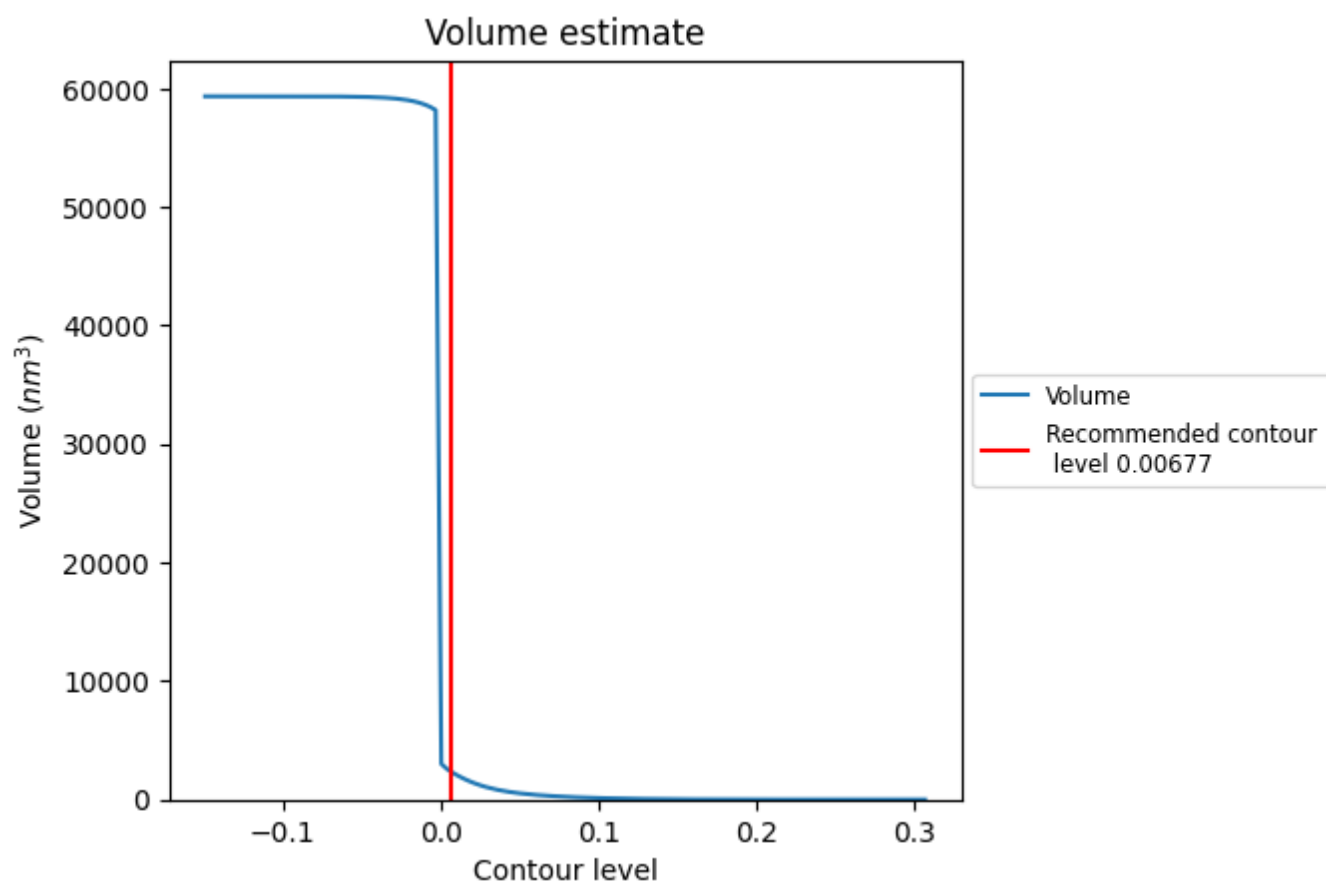
This section contains the results of statistical analysis of the map.

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.

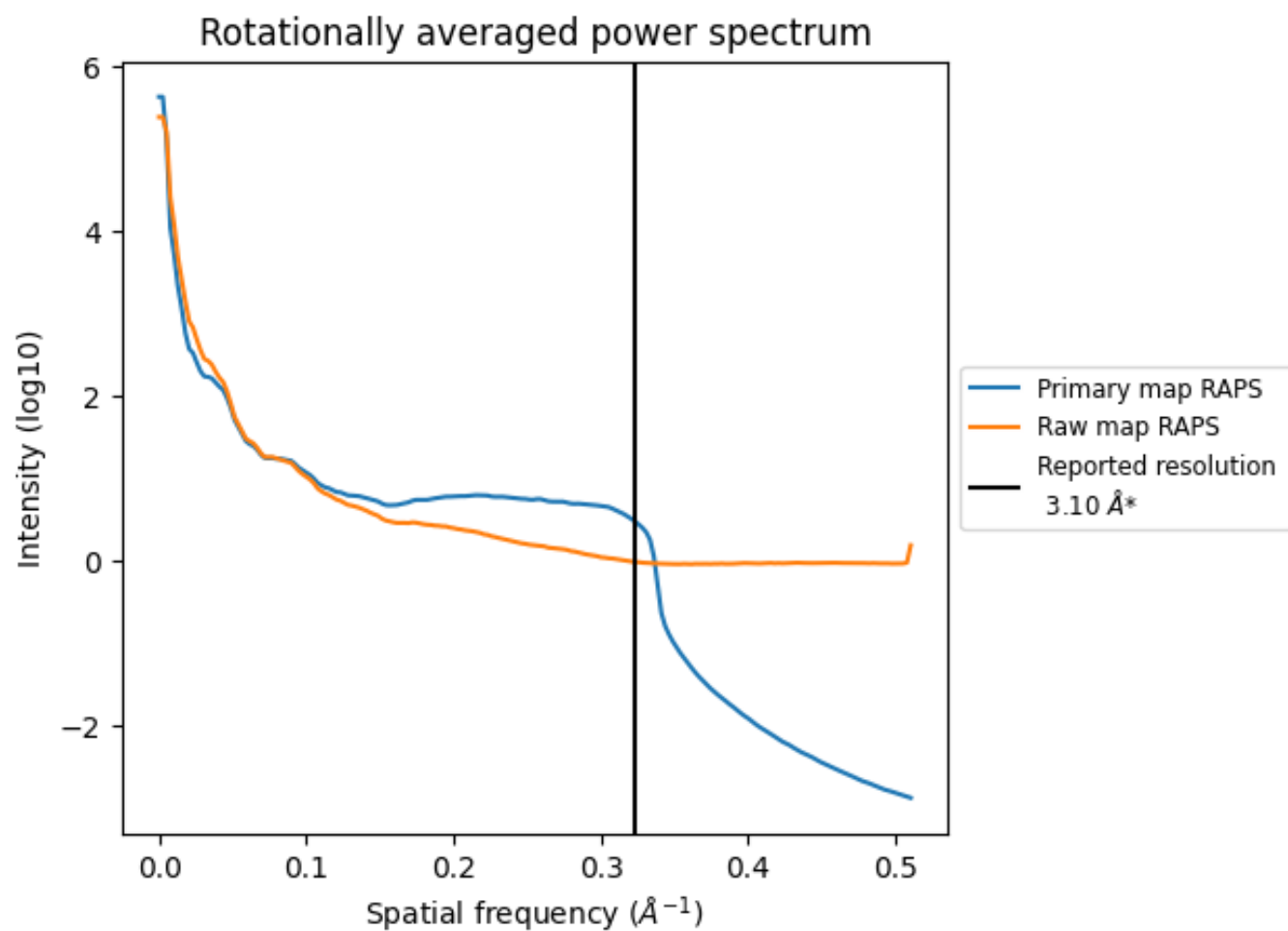
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2337 nm³; this corresponds to an approximate mass of 2111 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 ⓘ

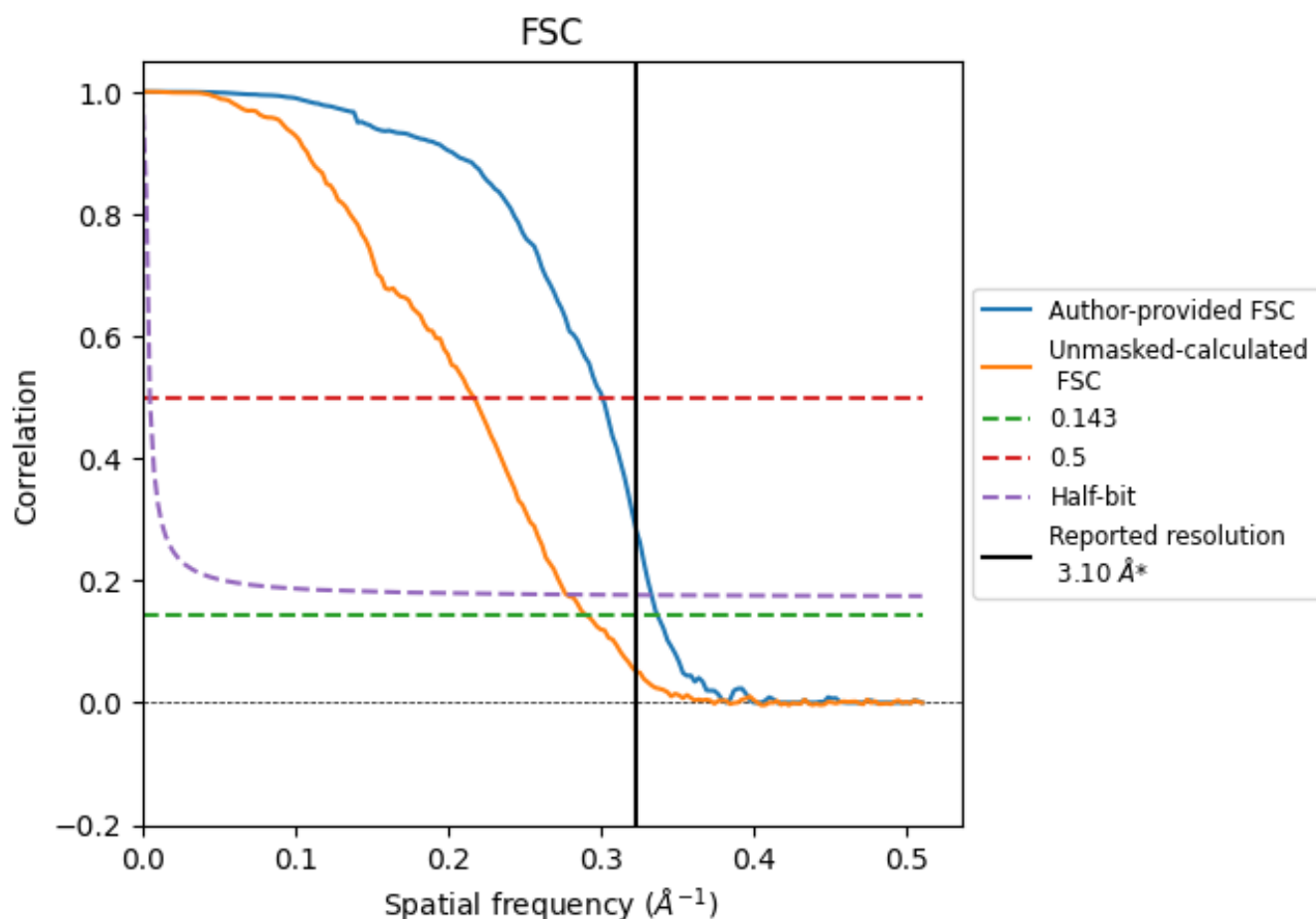


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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

8.2 Resolution estimates [i](#)

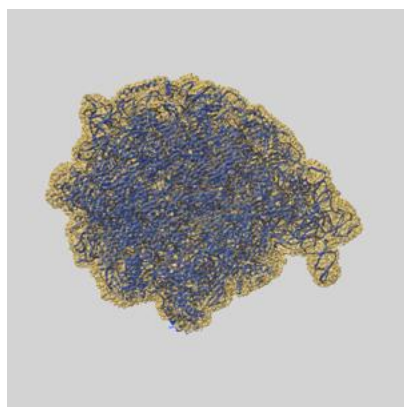
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	2.97	3.32	3.00
Unmasked-calculated*	3.44	4.61	3.60

*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 3.44 differs from the reported value 3.1 by more than 10 %

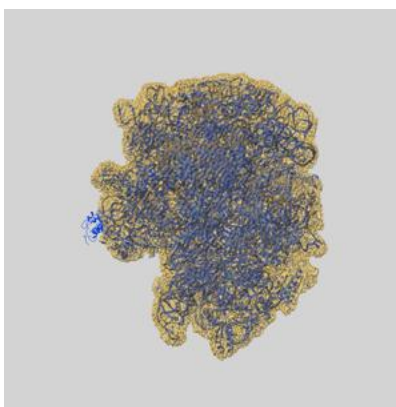
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8814 and PDB model 5WE4. Per-residue inclusion information can be found in section [3](#) on page [20](#).

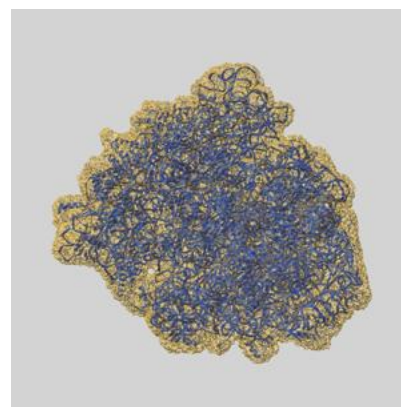
9.1 Map-model overlay [i](#)



X



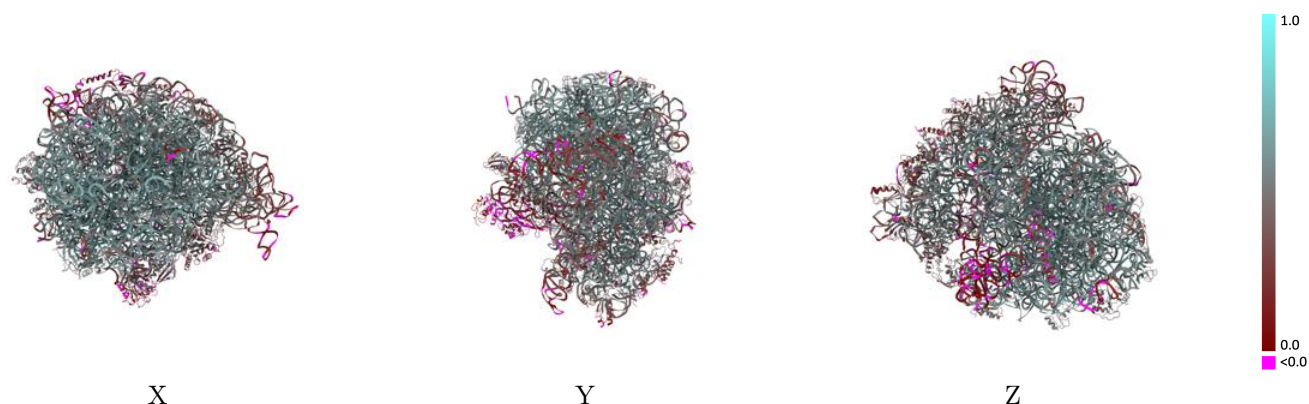
Y



Z

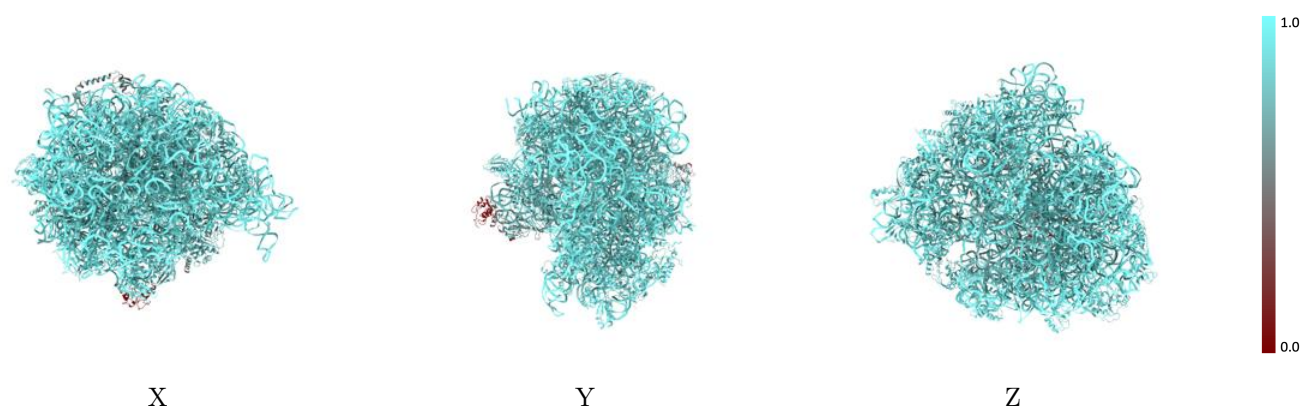
The images above show the 3D surface view of the map at the recommended contour level 0.00677 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



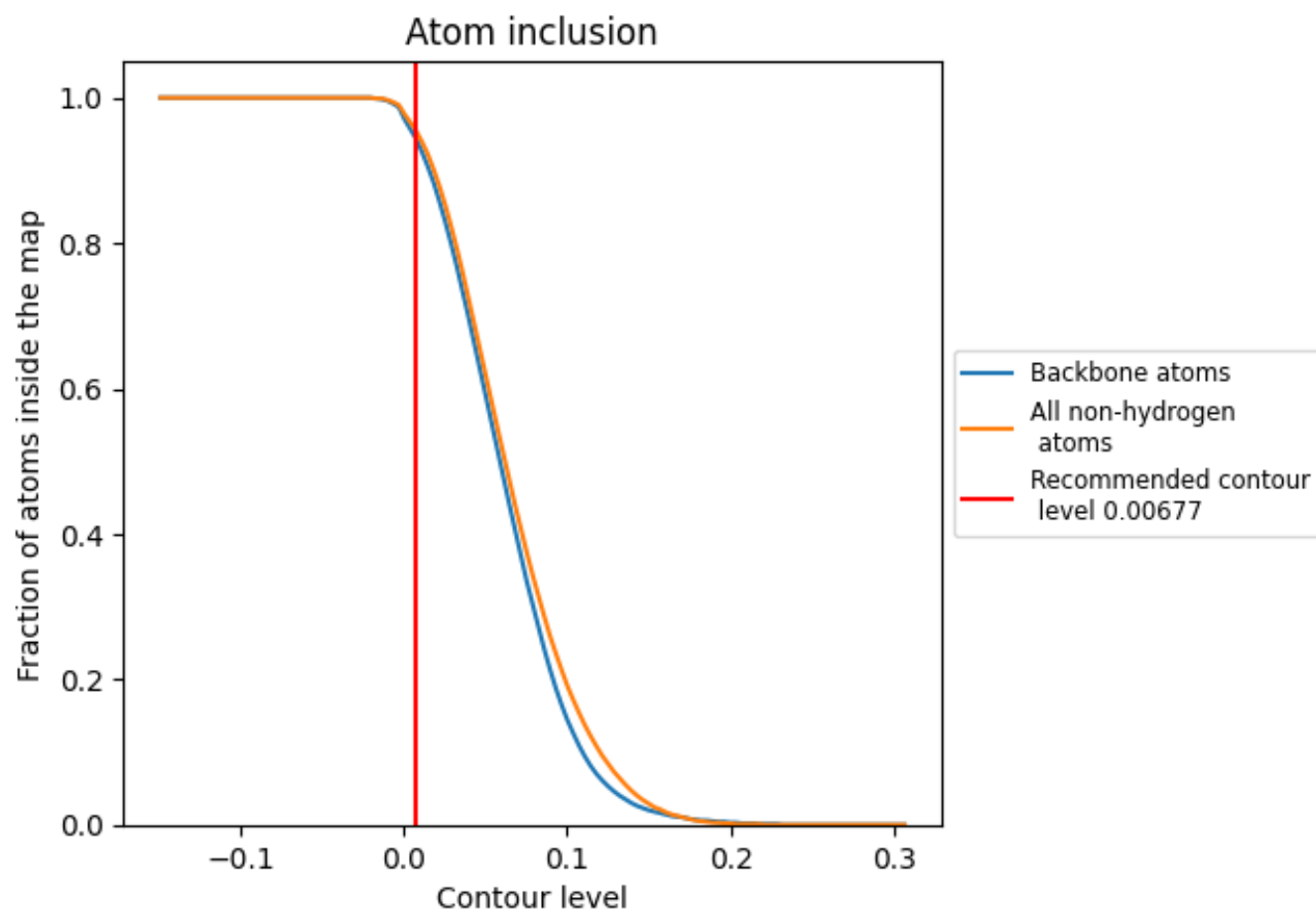
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00677).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.00677) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.4810
0	 0.9620	 0.5180
1	 0.9510	 0.4830
2	 0.9800	 0.5960
3	 0.9780	 0.5800
4	 0.9660	 0.5270
5	 0.1930	 -0.0150
6	 0.8590	 0.2790
A	 0.9860	 0.5370
B	 0.9930	 0.5010
C	 0.9690	 0.5610
D	 0.9670	 0.5420
E	 0.9580	 0.5050
F	 0.9480	 0.4040
G	 0.9240	 0.3720
H	 0.6810	 0.1800
I	 0.5860	 0.0360
J	 0.9620	 0.5340
K	 0.9510	 0.5220
L	 0.9690	 0.5240
M	 0.9580	 0.5320
N	 0.9830	 0.5580
O	 0.9640	 0.4620
P	 0.9570	 0.5190
Q	 0.9720	 0.5670
R	 0.9610	 0.5120
S	 0.9770	 0.5500
T	 0.9320	 0.4640
U	 0.9510	 0.4710
V	 0.9420	 0.4660
W	 0.9680	 0.5420
X	 0.9570	 0.5450
Y	 0.9230	 0.4250
Z	 0.9550	 0.5250
a	 0.9870	 0.4870



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Chain	Atom inclusion	Q-score
b	 0.9050	 0.3400
c	 0.9360	 0.4370
d	 0.9130	 0.3180
e	 0.9460	 0.4860
f	 0.9110	 0.4000
g	 0.9110	 0.3590
h	 0.9490	 0.4850
i	 0.9280	 0.3820
j	 0.9160	 0.3340
k	 0.9570	 0.4700
l	 0.9340	 0.4540
m	 0.9460	 0.4210
n	 0.9400	 0.4220
o	 0.9420	 0.4460
p	 0.9120	 0.3620
q	 0.9420	 0.4140
r	 0.9360	 0.4610
s	 0.9570	 0.4380
t	 0.9290	 0.3770
u	 0.8150	 0.2750
v	 0.9760	 0.4880
w	 0.7620	 0.0970
x	 0.9680	 0.4610
y	 0.8980	 0.2860
z	 0.8150	 0.2680