



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 04:46 PM EDT

PDB ID : 5WDT / pdb_00005wdt
EMDB ID : EMD-8813
Title : 70S ribosome-EF-Tu H84A complex with GppNHp
Authors : Fislage, M.; Brown, Z.; Frank, J.
Deposited on : 2017-07-06
Resolution : 3.00 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:

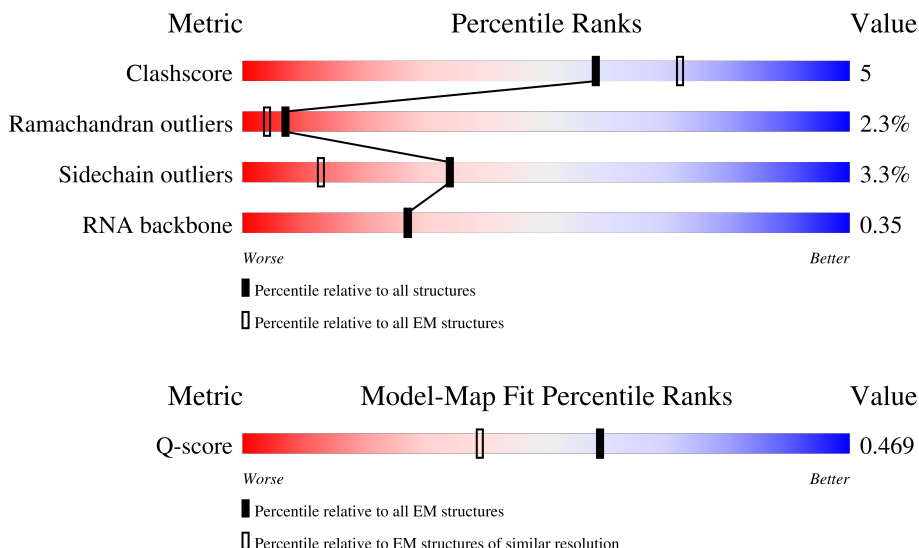
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



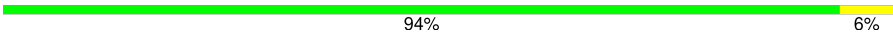
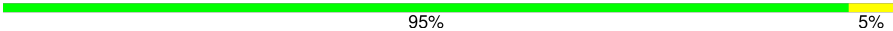
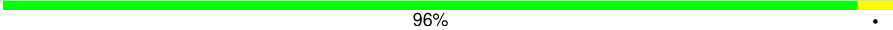
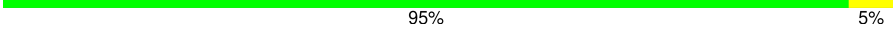
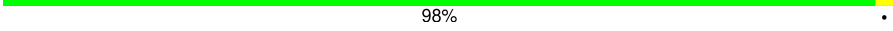
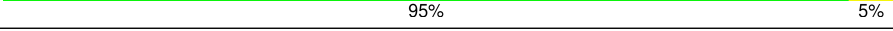
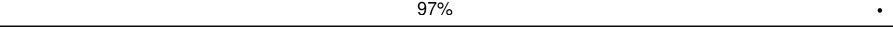
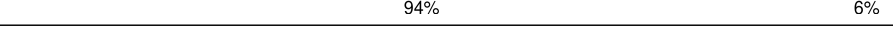
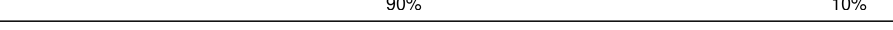
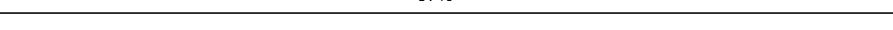
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	
2	B	120	
3	C	271	

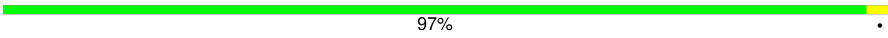
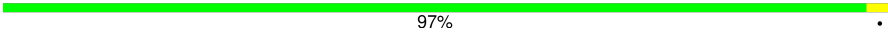
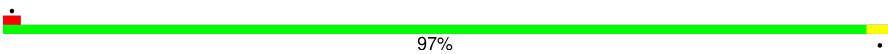
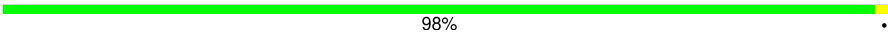
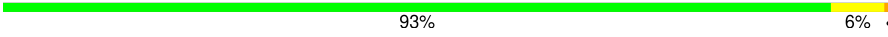
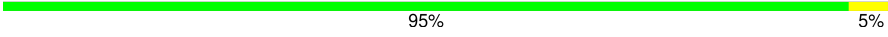
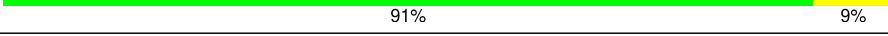
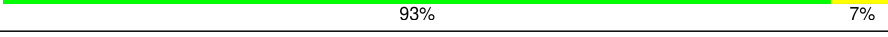
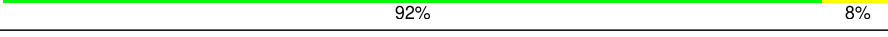
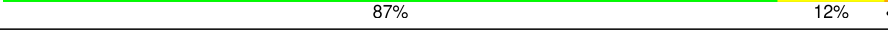
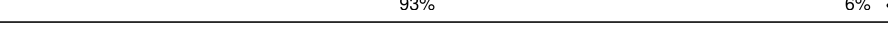
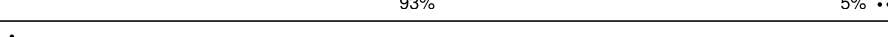
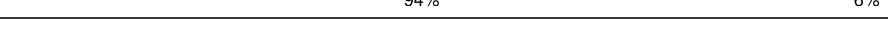
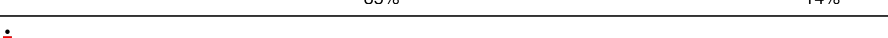
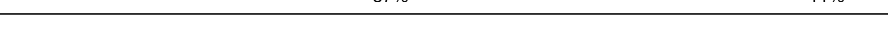
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Mol	Chain	Length	Quality of chain
4	D	208	 92% 7% .
5	E	200	 94% 6%
6	F	177	 95% 5%
7	G	174	 96% .
8	H	149	 6% 95% 5%
9	I	141	 26% 85% 12% .
10	J	141	 98% .
11	K	122	 85% 15%
12	L	143	 88% 10% .
13	M	136	 95% 5%
14	N	119	 97% .
15	O	116	 94% 6%
16	P	114	 91% 9%
17	Q	115	 90% 10% .
18	R	102	 90% 10%
19	S	109	 91% 9%
20	T	92	 92% 8%
21	U	102	 92% 8%
22	V	92	 97% ..
23	W	75	 96% .
24	X	77	 97% ..
25	Y	60	 98% .
26	Z	56	 98% .
27	0	55	 91% 9%
28	1	51	 100%

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Mol	Chain	Length	Quality of chain
29	2	45	
30	3	64	
31	4	38	
32	5	131	
33	6	66	
34	a	1540	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	115	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	

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Mol	Chain	Length	Quality of chain
54	u	65	 72%25%••
55	v	77	 66%26%8%•
55	w	77	 44%36%17%•
56	x	12	 83%17%
57	y	76	 51%39%8%•
58	z	393	 93%6%•

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155275 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 tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		

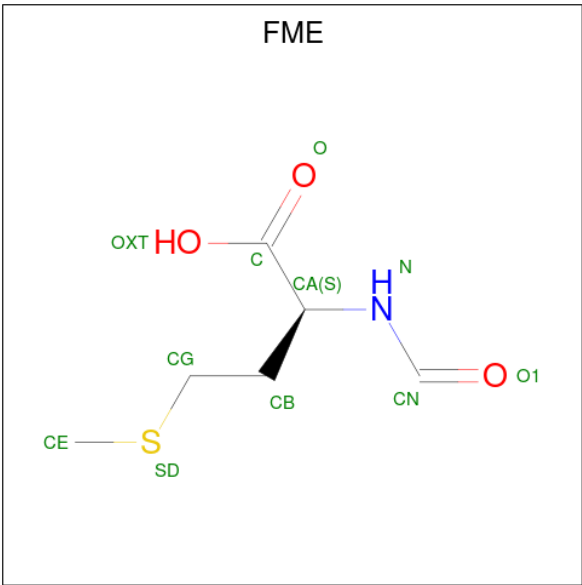
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	521	582	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP P0CE48

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	S	0
			10	6	1	2	1	

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

Mol	Chain	Residues	Atoms		AltConf
60	A	1325	Total	Mg	0
			1325	1325	
60	B	36	Total	Mg	0
			36	36	
60	C	3	Total	Mg	0
			3	3	
60	D	3	Total	Mg	0
			3	3	
60	E	3	Total	Mg	0
			3	3	
60	L	2	Total	Mg	0
			2	2	
60	M	1	Total	Mg	0
			1	1	
60	N	1	Total	Mg	0
			1	1	
60	Q	2	Total	Mg	0
			2	2	
60	R	1	Total	Mg	0
			1	1	
60	S	1	Total	Mg	0
			1	1	

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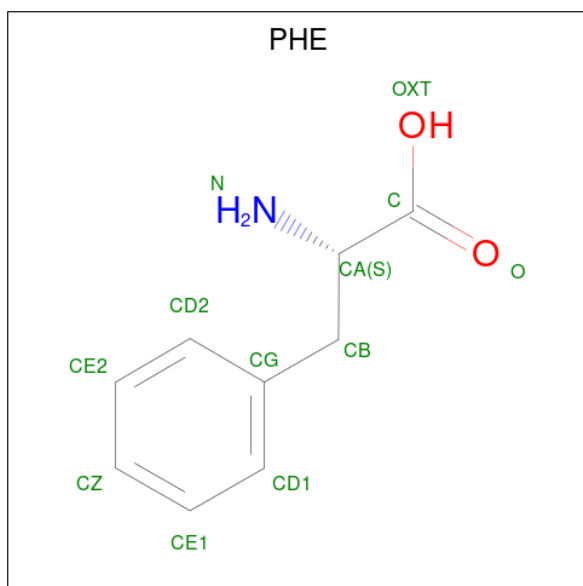
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Mol	Chain	Residues	Atoms		AltConf
60	T	1	Total 1	Mg 1	0
60	X	1	Total 1	Mg 1	0
60	Y	1	Total 1	Mg 1	0
60	Z	2	Total 2	Mg 2	0
60	0	2	Total 2	Mg 2	0
60	3	3	Total 3	Mg 3	0
60	4	1	Total 1	Mg 1	0
60	a	481	Total 481	Mg 481	0
60	d	1	Total 1	Mg 1	0
60	h	1	Total 1	Mg 1	0
60	i	3	Total 3	Mg 3	0
60	s	1	Total 1	Mg 1	0
60	t	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	12	Total 12	Mg 12	0
60	w	1	Total 1	Mg 1	0
60	x	1	Total 1	Mg 1	0
60	y	8	Total 8	Mg 8	0
60	z	4	Total 4	Mg 4	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

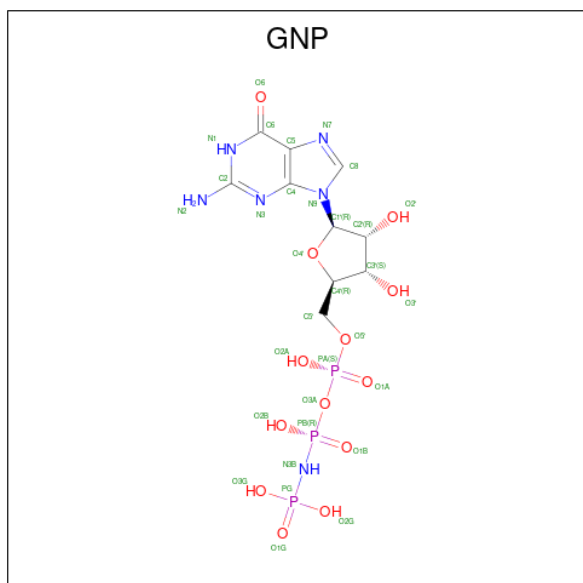
Mol	Chain	Residues	Atoms			AltConf
61	A	5	Total	K		0
			5	5		

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



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	653	Total	O	0
			653	653	
64	B	22	Total	O	0
			22	22	
64	C	7	Total	O	0
			7	7	
64	D	6	Total	O	0
			6	6	
64	E	6	Total	O	0
			6	6	
64	G	1	Total	O	0
			1	1	
64	J	1	Total	O	0
			1	1	
64	L	6	Total	O	0
			6	6	
64	M	1	Total	O	0
			1	1	
64	N	3	Total	O	0
			3	3	
64	P	1	Total	O	0
			1	1	
64	Q	4	Total	O	0
			4	4	
64	S	2	Total	O	0
			2	2	
64	U	3	Total	O	0
			3	3	
64	W	1	Total	O	0
			1	1	
64	X	3	Total	O	0
			3	3	
64	Y	1	Total	O	0
			1	1	
64	Z	2	Total	O	0
			2	2	
64	0	1	Total	O	0
			1	1	

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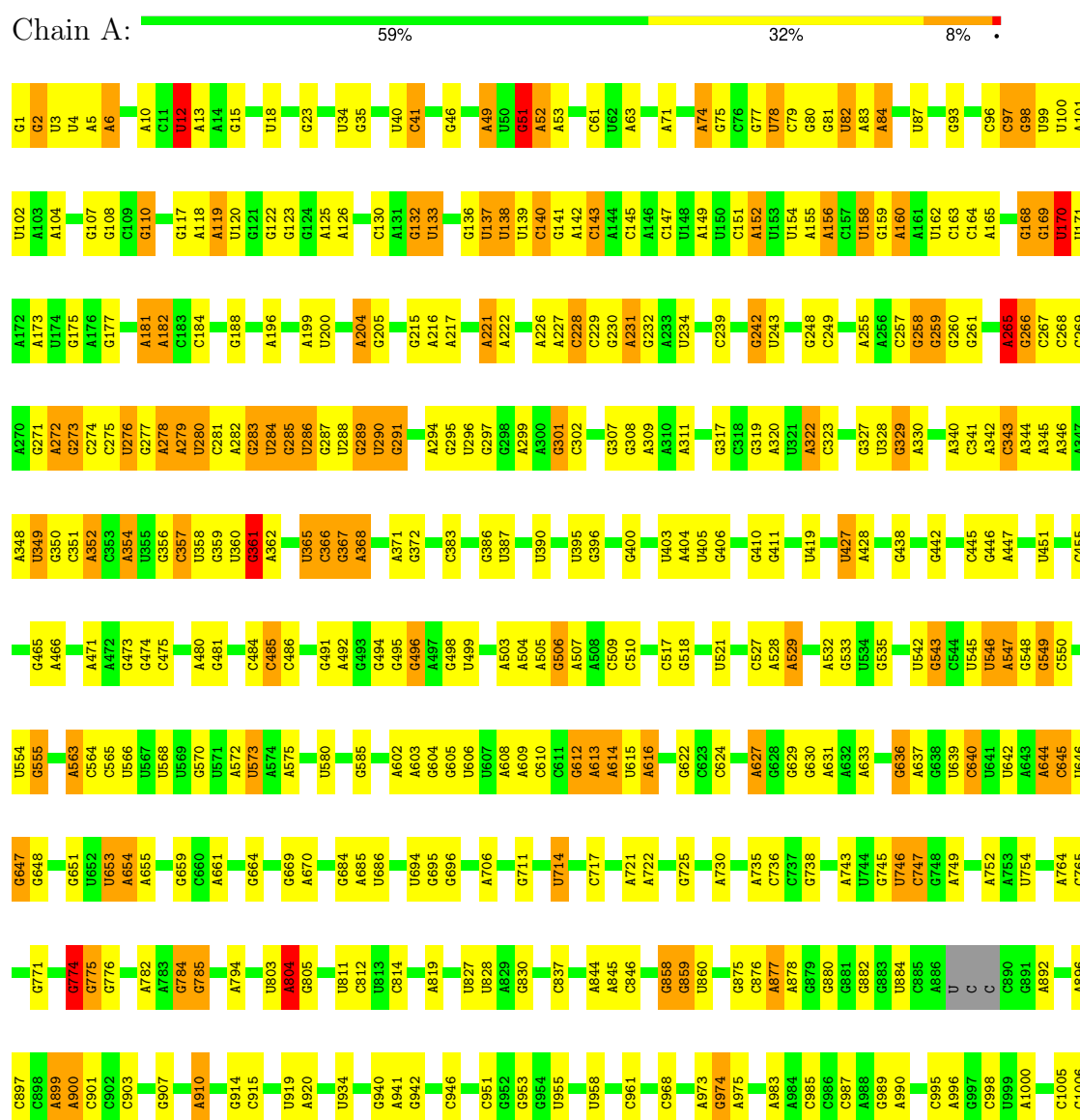
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Mol	Chain	Residues	Atoms		AltConf
64	2	4	Total 4	O 4	0
64	3	1	Total 1	O 1	0
64	4	1	Total 1	O 1	0
64	a	163	Total 163	O 163	0
64	d	1	Total 1	O 1	0
64	h	2	Total 2	O 2	0
64	k	1	Total 1	O 1	0
64	m	3	Total 3	O 3	0
64	o	1	Total 1	O 1	0
64	s	2	Total 2	O 2	0
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	v	9	Total 9	O 9	0
64	w	1	Total 1	O 1	0
64	x	1	Total 1	O 1	0
64	y	2	Total 2	O 2	0
64	z	2	Total 2	O 2	0

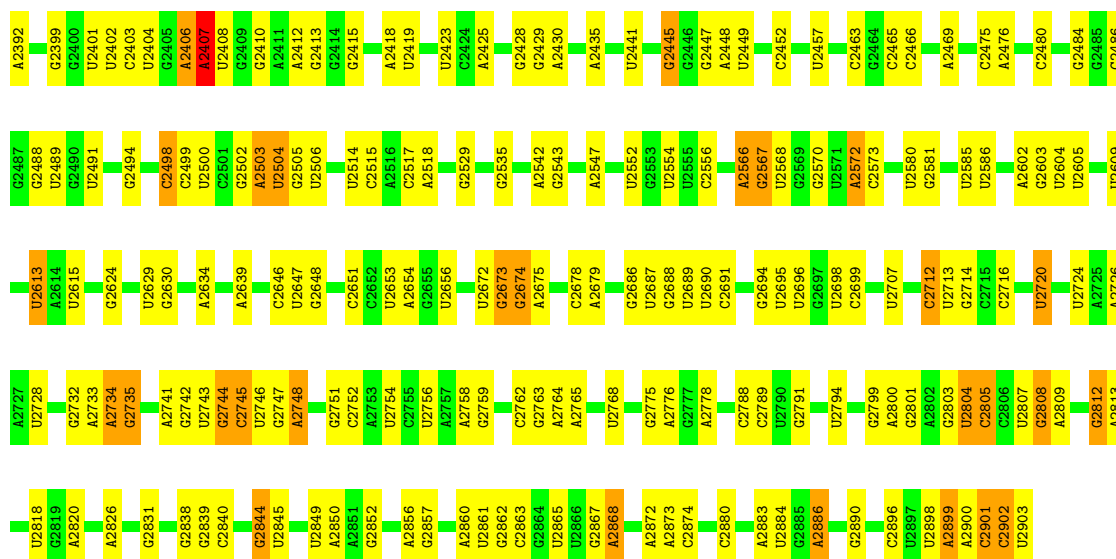
3 Residue-property plots

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

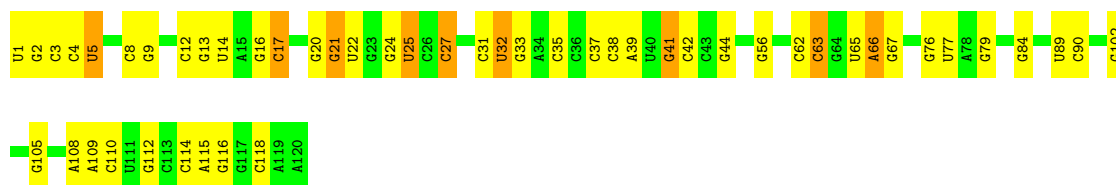


A2287	U2172	A2062	A1937	A1854	U1736	C1617	C1541	U1476	A1392	C1289	C1167	U1078	A1009
A2288	A2173	G2069	A1938	G1857	G1737	A1618	A1544	A1477	A1393	C1290	C1171	C1079	U1012
G2289	U2180	A2070	U1939	A1858	A1739	G1619	A1545	G1479	U1394	C1291	G1172	A1080	U1081
G2290	G2196	A2071	C1941	U1859	G1741	G1622	C1546	U1482	C1399	U1294	U1173	U1082	A1014
U2291	G2196	C2072	C1942	G1862	U1742	A1634	A1548	G1483	U1402	G1300	U1174	A1084	G1017
G2294	U2182	A2077	U1955	G1863	G1743	G1743	A1549	U1484	A1403	A1301	U1175	A1085	U1018
G2296	G2193	C2078	G1864	U1865	A1744	G1642	U1554	U1485	C1404	G1301	U1176	A1086	G1019
A2297	U2194	U2080	U1866	A1745	A1746	G1643	U1555	U1486	U1405	C1305	G1177	A1087	A1020
U2305	U2195	A2080	A1866	G1746	G1746	G1643	C1556	U1487	U1406	C1306	C1178	A1088	A1021
G2305	G2196	G1964	G1867	U1647	U1648	U1647	C1557	U1488	G1407	G1306	G1179	A1089	G1022
A2309	A2198	U2092	C1868	U1648	G1750	G1649	C1558	U1490	G1408	C1320	U1180	A1090	U1023
G2310	A2199	G2093	C1869	G1649	G1755	G1649	U1559	U1491	U1411	A1321	U1181	G1026	G1027
A2311	C2200	C2096	C1870	A1654	A1755	G1654	U1560	G1492	U1412	G1190	G1190	A1027	A1028
U2320	U2202	A2097	A1872	G1659	U1758	G1659	U1563	C1493	A1413	U1328	G1193	U1101	U1102
G2321	U2203	U2098	G1873	G1674	C1764	G1674	C1564	A1494	C1414	U1329	G1196	A1103	A1104
G2326	G2204	U2099	C1874	G1675	G1773	C1675	C1565	U1495	U1415	C1330	C1197	U1105	U1033
A2327	A2205	G2100	G1875	G1682	A1773	G1675	A1566	U1496	G1416	C1331	G1197	G1106	G1035
G2328	C2206	A2101	A1876	G1682	G1776	G1675	G1567	U1498	U1417	G1332	C1200	G1107	G1036
A2329	C2207	C2102	G1877	G1682	G1776	G1675	G1568	U1499	A1418	G1333	C1200	U1108	G1037
G2330	U2208	C2103	C1879	G1691	G1779	G1691	A1569	G1500	A1420	G1339	A1204	C1109	G1038
G2332	A2211	G2105	U1883	U1692	U1779	U1692	A1572	A1502	G1426	G1343	G1210	G1110	C1043
U2333	A2212	U2106	G1884	U1693	A1780	U1693	A1573	A1503	G1427	C1344	U1211	G1112	C1044
A2334	U2213	G2107	A1885	C1694	A1784	G1694	A1579	U1504	A1427	C1345	G1212	G1113	C1045
A2336	G2216	A2108	A1890	G1695	G1789	G1695	G1580	U1505	C1428	C1349	G1218	C1114	A1046
A2337	U2220	G2110	C1895	G1699	A1790	G1699	G1581	C1507	G1429	U1352	G1218	G1115	G1047
G2338	G2221	C2112	U1898	A1700	G1791	A1700	A1583	U1508	A1431	A1353	G1225	G1116	A1048
A2340	G2224	U2118	G1906	A1705	C1795	A1705	U1584	U1509	G1432	A1354	G1226	C1117	A1049
G2344	A2225	A2119	G1907	C1706	U1796	A1706	C1585	G1510	A1433	G1355	G1227	U1119	A1050
A2346	C2226	G2120	C1908	U1709	G1800	U1709	G1587	A1515	A1434	G1356	G1236	G1124	G1051
A2346	G2230	G2121	C1909	U1712	A1801	U1712	U1589	G1516	G1436	G1357	U1240	A1127	G1053
C2350	G2239	G2127	U1910	A1713	A1808	A1713	A1590	G1517	G1441	G1358	A1263	G1135	A1054
U2356	G2242	U2131	U1911	G1714	A1809	G1714	C1592	U1520	G1449	C1363	A1247	G1139	G1055
G2357	U2243	G2132	A1913	G1715	A1810	G1715	A1593	U1520	G1450	G1364	G1248	U1140	G1056
G2361	G2250	G2133	C1914	U1716	G1811	U1716	U1594	U1523	C1451	A1365	U1249	U1141	U1058
U2372	G2251	A2141	A1916	A1717	C1816	A1717	A1596	G1524	G1452	A1366	G1250	U1142	G1059
A2378	C2264	C2145	U1917	G1721	G1817	G1721	A1597	A1525	A1453	A1367	A1263	U1143	U1060
G2379	A2268	C2146	U1918	A1722	U1818	A1722	A1603	G1527	G1455	G1368	G1256	A1147	U1061
A2380	A2273	A2147	C1924	G1723	A1829	G1723	C1604	A1528	U1458	C1370	G1257	U1148	G1062
G2382	C2042	G2157	A1927	G1725	C1833	G1725	C1605	G1529	U1459	G1371	U1258	A1149	G1063
G2383	C2043	G2162	A1928	G1726	U1834	G1726	C1606	A1532	A1461	A1376	A1262	U1151	C1075
G2384	C2055	G2163	G1929	A1727	G1835	A1727	C1607	U1533	U1466	A1383	G1266	U1147	A1070
C2385	G2056	A2163	G1930	U1729	U1841	U1729	A1608	U1534	U1468	A1385	A1269	G1149	G1071
G2391	G2056	A2164	U1931	G1730	G1847	G1730	A1610	A1535	A1469	A1386	G1270	C1150	C1072
	A2059	A2170	A1932	G1731	U1852	C1732	G1613	G1537	A1470	C1386	A1272	A1151	C1076
	A2060	A2171	G1933	U1733	U1852	C1733	A1614	G1538	U1390	U1391	U1273	C1152	A1077
	G2286		A1936	G1735	A1853	G1735	A1616	G1540				C1153	



• Molecule 2: 5S rRNA

Chain B: 58% 34% 8%



• Molecule 3: 50S ribosomal protein L2

Chain C: 92% 8%



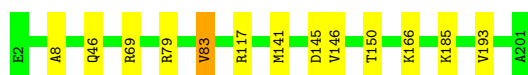
• Molecule 4: 50S ribosomal protein L3

Chain D: 92% 7%

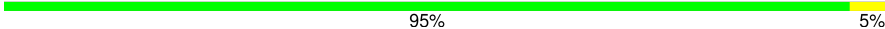


• Molecule 5: 50S ribosomal protein L4

Chain E: 94% 6%

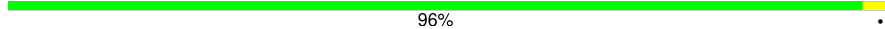


• Molecule 6: 50S ribosomal protein L5

Chain F:  95% 5%

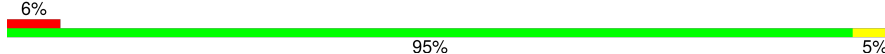


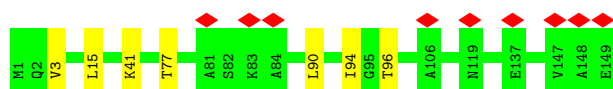
- Molecule 7: 50S ribosomal protein L6

Chain G:  96% .



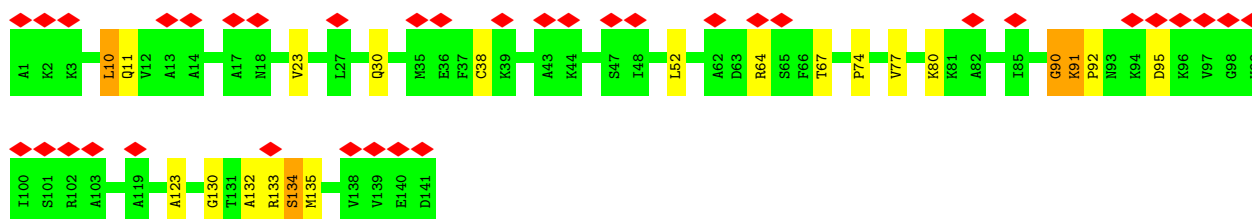
- Molecule 8: 50S ribosomal protein L9

Chain H:  6% 95% 5%

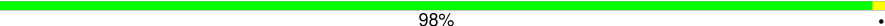


- Molecule 9: 50S ribosomal protein L11

Chain I:  26% 85% 12% .



- Molecule 10: 50S ribosomal protein L13

Chain J:  98% .



- Molecule 11: 50S ribosomal protein L14

Chain K:  85% 15%



- Molecule 12: 50S ribosomal protein L15

Chain L:  88% 10% .



- Molecule 13: 50S ribosomal protein L16

Chain M: 95% 5%



- Molecule 14: 50S ribosomal protein L17

Chain N: 97% .



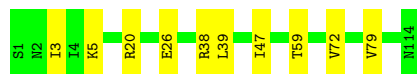
- Molecule 15: 50S ribosomal protein L18

Chain O: 94% 6%



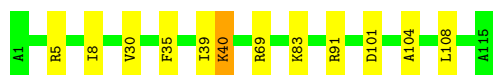
- Molecule 16: 50S ribosomal protein L19

Chain P: 91% 9%



- Molecule 17: 50S ribosomal protein L20

Chain Q: 90% 10% .



- Molecule 18: 50S ribosomal protein L21

Chain R: 90% 10%



- Molecule 19: 50S ribosomal protein L22

Chain S: 91% 9%



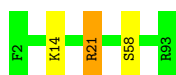
- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25



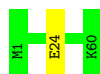
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28

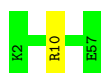


- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30





- Molecule 27: 50S ribosomal protein L32

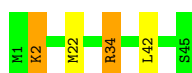


- Molecule 28: 50S ribosomal protein L33

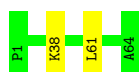


There are no outlier residues recorded for this chain.

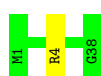
- Molecule 29: 50S ribosomal protein L34



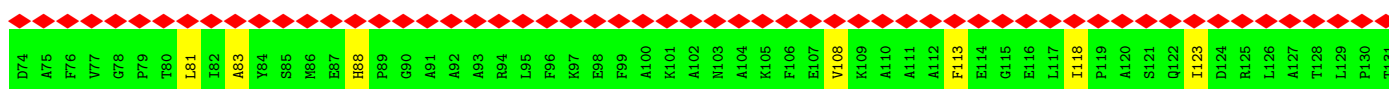
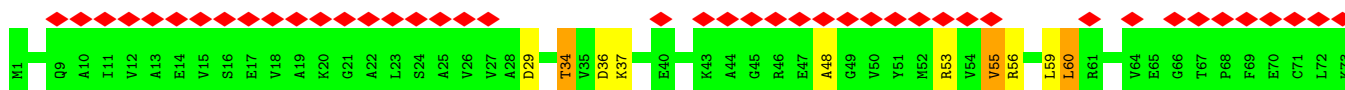
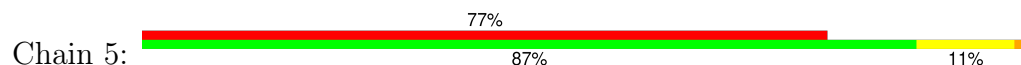
- Molecule 30: 50S ribosomal protein L35



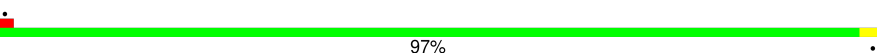
- Molecule 31: 50S ribosomal protein L36

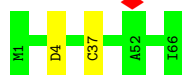


- Molecule 32: 50S ribosomal protein L10



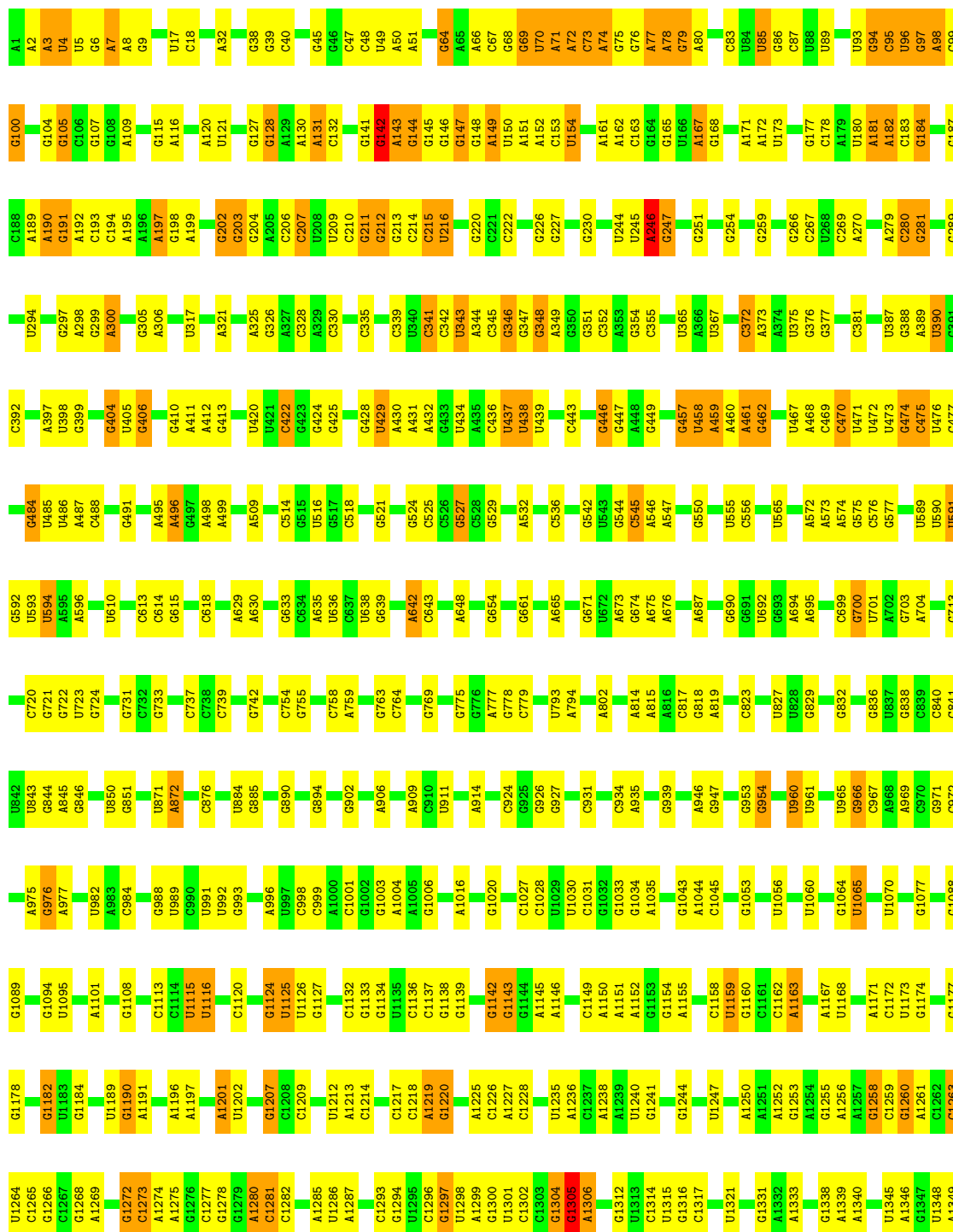
- Molecule 33: 50S ribosomal protein L31

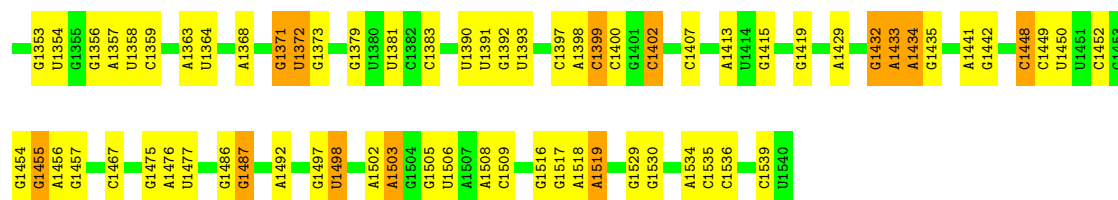
Chain 6:  97% .



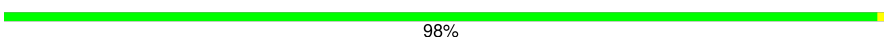
• Molecule 34: 16S rRNA

Chain a:  61% 31% 8%



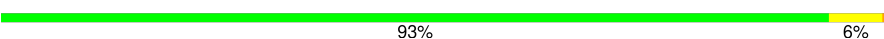


• Molecule 35: 30S ribosomal protein S2

Chain b:  98% .

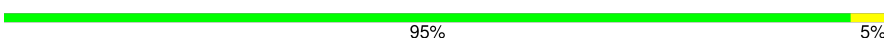


• Molecule 36: 30S ribosomal protein S3

Chain c:  93% 6% .



• Molecule 37: 30S ribosomal protein S4

Chain d:  95% 5% .



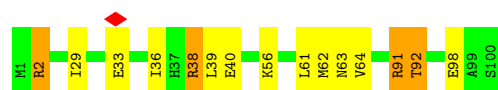
• Molecule 38: 30S ribosomal protein S5

Chain e:  89% 10% .



• Molecule 39: 30S ribosomal protein S6

Chain f:  85% 11% .

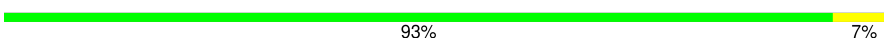


• Molecule 40: 30S ribosomal protein S7

Chain g:  91% 9% .

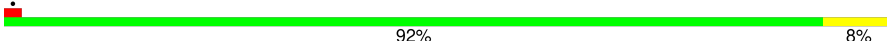


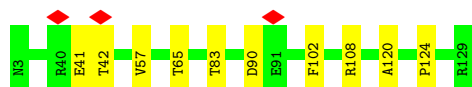
- Molecule 41: 30S ribosomal protein S8

Chain h:  93% 7%



- Molecule 42: 30S ribosomal protein S9

Chain i:  92% 8%



- Molecule 43: 30S ribosomal protein S10

Chain j:  87% 12%



- Molecule 44: 30S ribosomal protein S11

Chain k:  90% 10%



- Molecule 45: 30S ribosomal protein S12

Chain l:  85% 12%

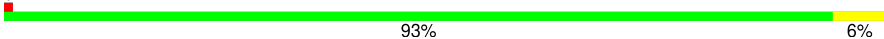


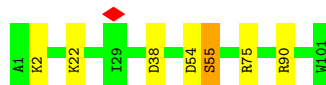
- Molecule 46: 30S ribosomal protein S13

Chain m:  90% 9%

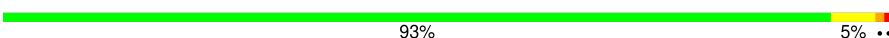


- Molecule 47: 30S ribosomal protein S14

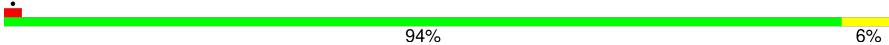
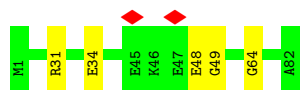
Chain n:  93% 6%



• Molecule 48: 30S ribosomal protein S15

Chain o:  93% 5% ..

• Molecule 49: 30S ribosomal protein S16

Chain p:  94% 6%

• Molecule 50: 30S ribosomal protein S17

Chain q:  89% 11%

• Molecule 51: 30S ribosomal protein S18

Chain r:  85% 14% .

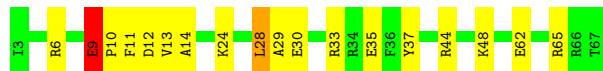
• Molecule 52: 30S ribosomal protein S19

Chain s:  87% 11% .

• Molecule 53: 30S ribosomal protein S20

Chain t:  89% 9% .

• Molecule 54: 30S ribosomal protein S21

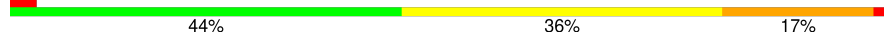
Chain u:  72% 25% ..

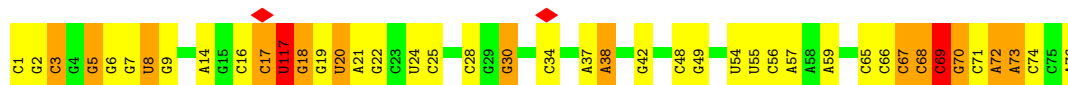
- Molecule 55: tRNA-fMet

Chain v:  66% 26% 8%



- Molecule 55: tRNA-fMet

Chain w:  44% 36% 17%



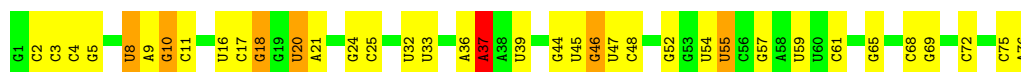
- Molecule 56: mRNA

Chain x:  83% 17%



- Molecule 57: tRNA-Phe

Chain y:  51% 39% 8%



- Molecule 58: Elongation factor Tu 2

Chain z:  93% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55276	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	0.247	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.00558	Depositor
Map size ($\text{\AA}$)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 1MG, UR3, H2U, 5MC, MA6, MG, 7MG, OMU, PSU, K, 2MG, 4SU, 6MZ, OMC, 3TD, 5MU, 2MA, OMG, 4OC, MIA, FME, GNP

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	0.73	39/107907 (0.0%)
2	B	0.39	0/2876	0.72	2/4483 (0.0%)
3	C	0.52	0/2121	0.76	0/2852
4	D	0.51	0/1578	0.77	0/2124
5	E	0.52	0/1563	0.82	0/2103
6	F	0.54	0/1434	0.81	0/1926
7	G	0.54	0/1324	0.74	0/1794
8	H	0.57	0/1122	0.77	0/1515
9	I	0.67	0/1046	0.92	2/1410 (0.1%)
10	J	0.52	0/1143	0.80	0/1540
11	K	0.53	0/947	0.75	0/1268
12	L	0.53	0/1052	0.85	0/1401
13	M	0.50	0/1093	0.78	0/1460
14	N	0.55	0/964	0.85	0/1289
15	O	0.54	0/902	0.85	0/1209
16	P	0.51	0/929	0.73	0/1242
17	Q	0.52	0/946	0.90	0/1260
18	R	0.49	0/823	0.66	0/1100
19	S	0.53	0/852	0.87	0/1142
20	T	0.52	0/736	0.76	0/984
21	U	0.51	0/787	0.74	0/1051
22	V	0.51	0/752	0.76	0/1008
23	W	0.47	0/579	0.70	0/767
24	X	0.49	0/635	0.74	0/848
25	Y	0.54	0/495	0.84	0/658
26	Z	0.55	0/438	0.79	0/586
27	0	0.49	0/440	0.81	0/588
28	1	0.50	0/424	0.68	0/565
29	2	0.53	0/370	1.00	0/487
30	3	0.52	0/513	0.86	0/676
31	4	0.47	0/303	0.71	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.64	0/1001	0.85	0/1350
33	6	0.56	0/531	0.78	0/709
34	a	0.38	0/36725	0.73	20/57285 (0.0%)
35	b	0.57	0/1735	0.78	0/2338
36	c	0.54	0/1651	0.80	0/2225
37	d	0.55	0/1665	0.80	0/2227
38	e	0.54	0/1180	0.82	0/1587
39	f	0.54	0/835	0.78	0/1128
40	g	0.54	0/1195	0.84	0/1602
41	h	0.53	0/989	0.81	0/1326
42	i	0.57	0/1034	0.78	0/1375
43	j	0.56	0/796	0.77	0/1077
44	k	0.54	0/885	0.79	0/1195
45	l	0.54	0/954	0.78	0/1282
46	m	0.57	0/900	0.84	0/1204
47	n	0.55	0/822	0.78	0/1095
48	o	0.54	0/722	0.91	1/964 (0.1%)
49	p	0.53	0/659	0.76	0/884
50	q	0.57	0/657	0.74	0/881
51	r	0.60	0/544	0.81	0/731
52	s	0.54	0/652	0.75	0/877
53	t	0.55	0/671	0.87	0/888
54	u	0.64	0/550	0.93	0/728
55	v	0.40	1/1747 (0.1%)	0.72	0/2721
55	w	0.47	2/1747 (0.1%)	1.01	6/2721 (0.2%)
56	x	0.36	0/280	0.67	0/433
57	y	0.39	0/1607	0.71	1/2501 (0.0%)
58	z	0.54	0/3086	0.79	0/4175
All	All	0.43	3/164181 (0.0%)	0.75	71/245149 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-7.86	1.49	1.61
55	w	17	C	O3'-P	6.49	1.70	1.61
55	v	7	4SU	O3'-P	5.27	1.61	1.56

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	O3'-P-O5'	29.36	148.04	104.00
1	A	2712	C	C2'-C3'-O3'	11.74	127.11	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	P-O3'-C3'	-11.12	103.52	120.20
1	A	242	G	C2'-C3'-O3'	10.12	124.68	109.50
1	A	51	G	C2'-C3'-O3'	9.53	123.80	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	62277	0	31340	646	0
2	B	2572	0	1302	27	0
3	C	2082	0	2157	5	0
4	D	1557	0	1604	7	0
5	E	1544	0	1607	4	0
6	F	1410	0	1447	1	0
7	G	1304	0	1348	3	0
8	H	1111	0	1148	1	0
9	I	1032	0	1088	13	0
10	J	1120	0	1151	1	0
11	K	938	0	1012	4	0
12	L	1043	0	1123	8	0
13	M	1074	0	1157	2	0
14	N	951	0	994	1	0
15	O	892	0	923	3	0
16	P	917	0	965	5	0
17	Q	933	0	1006	7	0
18	R	810	0	834	4	0
19	S	845	0	909	2	0
20	T	730	0	795	2	0
21	U	779	0	834	1	0
22	V	739	0	763	4	0
23	W	572	0	593	0	0
24	X	625	0	655	1	0
25	Y	494	0	530	0	0
26	Z	434	0	477	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	0	434	0	448	3	0
28	1	417	0	451	0	0
29	2	367	0	405	1	0
30	3	504	0	574	0	0
31	4	302	0	343	1	0
32	5	988	0	1025	8	0
33	6	522	0	524	0	0
34	a	33050	0	16656	274	0
35	b	1704	0	1732	0	0
36	c	1624	0	1699	4	0
37	d	1643	0	1710	5	0
38	e	1164	0	1212	2	0
39	f	817	0	808	17	0
40	g	1181	0	1240	2	0
41	h	979	0	1034	5	0
42	i	1022	0	1070	1	0
43	j	786	0	828	4	0
44	k	869	0	878	4	0
45	l	940	0	1001	5	0
46	m	891	0	955	4	0
47	n	810	0	852	1	0
48	o	714	0	737	3	0
49	p	649	0	666	0	0
50	q	648	0	691	2	0
51	r	535	0	552	2	0
52	s	637	0	665	6	0
53	t	665	0	714	4	0
54	u	544	0	579	6	0
55	v	1644	0	840	11	0
55	w	1644	0	840	67	0
56	x	252	0	129	1	0
57	y	1631	0	843	4	0
58	z	3031	0	3049	5	0
59	A	10	0	10	0	0
60	0	2	0	0	0	0
60	3	3	0	0	0	0
60	4	1	0	0	0	0
60	A	1325	0	0	0	0
60	B	36	0	0	0	0
60	C	3	0	0	0	0
60	D	3	0	0	0	0
60	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	L	2	0	0	0	0
60	M	1	0	0	0	0
60	N	1	0	0	0	0
60	Q	2	0	0	0	0
60	R	1	0	0	0	0
60	S	1	0	0	0	0
60	T	1	0	0	0	0
60	X	1	0	0	0	0
60	Y	1	0	0	0	0
60	Z	2	0	0	0	0
60	a	481	0	0	0	0
60	d	1	0	0	0	0
60	h	1	0	0	0	0
60	i	3	0	0	0	0
60	s	1	0	0	0	0
60	t	1	0	0	0	0
60	u	1	0	0	0	0
60	v	12	0	0	0	0
60	w	1	0	0	0	0
60	x	1	0	0	0	0
60	y	8	0	0	0	0
60	z	4	0	0	0	0
61	A	5	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	13	0	0
64	0	1	0	0	0	0
64	2	4	0	0	0	0
64	3	1	0	0	0	0
64	4	1	0	0	0	0
64	A	653	0	0	0	0
64	B	22	0	0	0	0
64	C	7	0	0	0	0
64	D	6	0	0	0	0
64	E	6	0	0	0	0
64	G	1	0	0	0	0
64	J	1	0	0	0	0
64	L	6	0	0	0	0
64	M	1	0	0	0	0
64	N	3	0	0	0	0
64	P	1	0	0	0	0
64	Q	4	0	0	0	0
64	S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	U	3	0	0	0	0
64	W	1	0	0	0	0
64	X	3	0	0	0	0
64	Y	1	0	0	0	0
64	Z	2	0	0	0	0
64	a	163	0	0	0	0
64	d	1	0	0	0	0
64	h	2	0	0	0	0
64	k	1	0	0	0	0
64	m	3	0	0	0	0
64	o	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	9	0	0	0	0
64	w	1	0	0	0	0
64	x	1	0	0	0	0
64	y	2	0	0	0	0
64	z	2	0	0	0	0
All	All	155275	0	103543	1133	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 5.

The worst 5 of 1133 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:1048:A:N1	1:A:1111:A:C6	1.73	1.54
1:A:1048:A:C2	1:A:1111:A:C6	1.97	1.49
1:A:283:G:N7	1:A:284:U:C2	1.87	1.40
1:A:1867:G:N1	1:A:1874:C:N3	1.68	1.38
1:A:1048:A:C2	1:A:1111:A:N1	1.90	1.38

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%)	242 (90%)	25 (9%)	2 (1%)	18	53
4	D	206/208 (99%)	191 (93%)	14 (7%)	1 (0%)	24	60
5	E	198/200 (99%)	179 (90%)	17 (9%)	2 (1%)	12	45
6	F	175/177 (99%)	155 (89%)	19 (11%)	1 (1%)	21	56
7	G	172/174 (99%)	159 (92%)	13 (8%)	0	100	100
8	H	147/149 (99%)	125 (85%)	19 (13%)	3 (2%)	6	28
9	I	139/141 (99%)	112 (81%)	24 (17%)	3 (2%)	5	26
10	J	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	53
11	K	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	3	17
12	L	141/143 (99%)	117 (83%)	20 (14%)	4 (3%)	4	21
13	M	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	8	35
14	N	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	7	32
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14	48
16	P	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
17	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
18	R	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	19
19	S	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	6	30
20	T	90/92 (98%)	78 (87%)	10 (11%)	2 (2%)	5	26
21	U	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	19
22	V	90/92 (98%)	84 (93%)	5 (6%)	1 (1%)	11	43
23	W	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
24	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
25	Y	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	32
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	48 (91%)	4 (8%)	1 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	5	25
30	3	62/64 (97%)	55 (89%)	7 (11%)	0	100	100
31	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
32	5	129/131 (98%)	99 (77%)	22 (17%)	8 (6%)	1	6
33	6	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	7	34
35	b	216/218 (99%)	187 (87%)	24 (11%)	5 (2%)	5	25
36	c	204/206 (99%)	184 (90%)	15 (7%)	5 (2%)	4	23
37	d	203/205 (99%)	182 (90%)	19 (9%)	2 (1%)	12	45
38	e	156/157 (99%)	131 (84%)	19 (12%)	6 (4%)	2	15
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	13
40	g	149/151 (99%)	130 (87%)	12 (8%)	7 (5%)	2	11
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	2	14
43	j	96/98 (98%)	73 (76%)	17 (18%)	6 (6%)	1	6
44	k	114/116 (98%)	99 (87%)	10 (9%)	5 (4%)	2	12
45	l	119/121 (98%)	98 (82%)	13 (11%)	8 (7%)	1	5
46	m	113/115 (98%)	103 (91%)	8 (7%)	2 (2%)	6	31
47	n	99/101 (98%)	82 (83%)	12 (12%)	5 (5%)	1	10
48	o	86/88 (98%)	78 (91%)	5 (6%)	3 (4%)	3	16
49	p	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	4	23
50	q	78/80 (98%)	70 (90%)	6 (8%)	2 (3%)	4	23
51	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	11
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	24
54	u	63/65 (97%)	40 (64%)	14 (22%)	9 (14%)	0	1
58	z	391/393 (100%)	352 (90%)	29 (7%)	10 (3%)	4	23
All	All	6219/6322 (98%)	5477 (88%)	602 (10%)	140 (2%)	7	25

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	83	VAL

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Mol	Chain	Res	Type
11	K	89	ASN
32	5	55	VAL
32	5	123	ILE
36	c	96	VAL

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%)	206 (95%)	10 (5%)	24	58
4	D	163/163 (100%)	154 (94%)	9 (6%)	19	53
5	E	164/164 (100%)	159 (97%)	5 (3%)	36	69
6	F	148/148 (100%)	143 (97%)	5 (3%)	32	66
7	G	135/135 (100%)	133 (98%)	2 (2%)	57	80
8	H	114/114 (100%)	112 (98%)	2 (2%)	51	77
9	I	109/109 (100%)	102 (94%)	7 (6%)	16	48
10	J	115/115 (100%)	114 (99%)	1 (1%)	70	85
11	K	103/103 (100%)	97 (94%)	6 (6%)	18	51
12	L	102/102 (100%)	94 (92%)	8 (8%)	11	39
13	M	109/109 (100%)	108 (99%)	1 (1%)	70	85
14	N	99/99 (100%)	98 (99%)	1 (1%)	68	84
15	O	86/86 (100%)	85 (99%)	1 (1%)	63	82
16	P	99/99 (100%)	95 (96%)	4 (4%)	28	62
17	Q	88/88 (100%)	83 (94%)	5 (6%)	18	52
18	R	84/84 (100%)	82 (98%)	2 (2%)	43	73
19	S	92/92 (100%)	88 (96%)	4 (4%)	26	60
20	T	79/79 (100%)	77 (98%)	2 (2%)	42	72
21	U	83/83 (100%)	80 (96%)	3 (4%)	31	65
22	V	77/77 (100%)	76 (99%)	1 (1%)	61	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	57/57 (100%)	54 (95%)	3 (5%)	20	54
24	X	67/67 (100%)	65 (97%)	2 (3%)	36	69
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	46 (98%)	1 (2%)	47	75
27	0	46/46 (100%)	45 (98%)	1 (2%)	45	74
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	37/37 (100%)	34 (92%)	3 (8%)	11	38
30	3	51/51 (100%)	49 (96%)	2 (4%)	28	62
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	97 (97%)	3 (3%)	36	69
33	6	59/59 (100%)	58 (98%)	1 (2%)	53	78
35	b	180/180 (100%)	180 (100%)	0	100	100
36	c	170/170 (100%)	165 (97%)	5 (3%)	37	70
37	d	172/172 (100%)	167 (97%)	5 (3%)	37	70
38	e	120/119 (101%)	111 (92%)	9 (8%)	12	41
39	f	87/87 (100%)	84 (97%)	3 (3%)	32	66
40	g	124/124 (100%)	119 (96%)	5 (4%)	28	62
41	h	104/104 (100%)	102 (98%)	2 (2%)	50	76
42	i	105/105 (100%)	102 (97%)	3 (3%)	37	70
43	j	86/86 (100%)	84 (98%)	2 (2%)	44	74
44	k	89/89 (100%)	87 (98%)	2 (2%)	45	74
45	l	102/102 (100%)	97 (95%)	5 (5%)	22	56
46	m	93/93 (100%)	91 (98%)	2 (2%)	45	74
47	n	83/83 (100%)	82 (99%)	1 (1%)	63	82
48	o	76/76 (100%)	73 (96%)	3 (4%)	28	62
49	p	65/65 (100%)	62 (95%)	3 (5%)	24	58
50	q	74/74 (100%)	71 (96%)	3 (4%)	27	61
51	r	56/56 (100%)	52 (93%)	4 (7%)	13	43
52	s	70/70 (100%)	67 (96%)	3 (4%)	26	60
53	t	65/65 (100%)	62 (95%)	3 (5%)	24	58
54	u	55/55 (100%)	51 (93%)	4 (7%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	z	325/325 (100%)	317 (98%)	8 (2%)	42	72
All	All	5165/5164 (100%)	4995 (97%)	170 (3%)	34	67

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	f	38	ARG
49	p	34	GLU
40	g	89	GLU
44	k	126	ARG
51	r	41	SER

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

Mol	Chain	Res	Type
49	p	9	HIS
51	r	51	GLN
58	z	301	HIS
19	S	9	HIS
18	R	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	806 (27%)	79 (2%)
2	B	119/120 (99%)	33 (27%)	4 (3%)
34	a	1539/1540 (99%)	442 (28%)	0
55	v	76/77 (98%)	17 (22%)	0
55	w	76/77 (98%)	35 (46%)	0
56	x	11/12 (91%)	1 (9%)	0
57	y	75/76 (98%)	29 (38%)	0
All	All	4793/4805 (99%)	1363 (28%)	83 (1%)

5 of 1363 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U

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

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1857	G
1	A	2566	A
1	A	1918	A
1	A	2333	A
1	A	2803	G

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	$\# Z > 2$
57	PSU	y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.10	5 (23%)
1	3TD	A	1915	1	19,22,23	7.08	14 (73%)	23,32,35	2.02	5 (21%)
55	PSU	w	55	55	18,21,22	1.32	2 (11%)	21,30,33	2.07	5 (23%)
55	5MU	w	54	55	19,22,23	1.50	4 (21%)	27,32,35	2.07	10 (37%)
57	H2U	y	16	57	18,21,22	0.81	1 (5%)	19,30,33	1.38	4 (21%)
1	PSU	A	746	1,60	18,21,22	1.42	2 (11%)	21,30,33	1.99	4 (19%)
1	7MG	A	2069	1,60	23,26,27	1.43	2 (8%)	27,39,42	2.53	11 (40%)
1	2MA	A	2503	1,60	22,25,26	1.62	4 (18%)	32,37,40	2.38	9 (28%)
1	OMG	A	2251	1,55,60	23,26,27	1.26	3 (13%)	32,38,41	1.95	6 (18%)
57	PSU	y	39	57	18,21,22	1.41	2 (11%)	21,30,33	1.99	4 (19%)
1	PSU	A	2504	1	18,21,22	1.43	2 (11%)	21,30,33	2.05	4 (19%)
34	2MG	a	1207	34	23,26,27	1.24	3 (13%)	33,38,41	2.84	10 (30%)
34	2MG	a	1516	34	23,26,27	1.27	3 (13%)	33,38,41	2.31	8 (24%)
1	PSU	A	2605	1	18,21,22	1.40	2 (11%)	21,30,33	2.05	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	4OC	a	1402	34	20,23,24	0.85	2 (10%)	25,32,35	1.32	4 (16%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.57	2 (10%)
57	4SU	y	8	57	18,21,22	1.85	5 (27%)	25,30,33	2.38	7 (28%)
1	OMU	A	2552	1,60	19,22,23	1.31	3 (15%)	25,31,34	2.04	9 (36%)
1	5MC	A	1962	1	19,22,23	2.00	2 (10%)	26,32,35	1.54	4 (15%)
1	5MC	A	747	1	19,22,23	1.91	2 (10%)	26,32,35	1.54	5 (19%)
1	2MG	A	1835	1	23,26,27	1.32	4 (17%)	33,38,41	2.27	7 (21%)
55	4SU	w	8	55	18,21,22	1.82	5 (27%)	25,30,33	2.22	5 (20%)
1	PSU	A	2457	1,60	18,21,22	1.44	2 (11%)	21,30,33	2.04	5 (23%)
1	PSU	A	2580	1	18,21,22	1.53	2 (11%)	21,30,33	2.13	5 (23%)
34	UR3	a	1498	34	19,22,23	1.14	1 (5%)	26,32,35	2.01	5 (19%)
57	5MU	y	54	57	19,22,23	1.43	4 (21%)	27,32,35	2.08	7 (25%)
1	2MG	A	2445	1,60	23,26,27	1.25	4 (17%)	33,38,41	2.32	8 (24%)
55	PSU	v	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.03	5 (23%)
34	2MG	a	966	34	23,26,27	1.32	4 (17%)	33,38,41	2.66	10 (30%)
34	7MG	a	527	34,60	23,26,27	1.41	2 (8%)	27,39,42	2.52	7 (25%)
1	PSU	A	2604	1	18,21,22	1.44	2 (11%)	21,30,33	1.94	4 (19%)
34	MA6	a	1518	34,60	23,26,27	1.76	6 (26%)	33,38,41	2.33	11 (33%)
1	PSU	A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.16	4 (19%)
1	OMC	A	2498	1,60	19,22,23	0.84	0	25,31,34	1.21	2 (8%)
1	6MZ	A	1618	1	22,25,26	1.53	4 (18%)	29,36,39	2.28	10 (34%)
1	1MG	A	745	1	23,26,27	1.41	4 (17%)	33,39,42	2.02	7 (21%)
34	5MC	a	1407	34	19,22,23	2.02	2 (10%)	26,32,35	1.62	5 (19%)
57	H2U	y	20	57	18,21,22	0.87	1 (5%)	19,30,33	1.48	4 (21%)
55	5MU	v	54	55	19,22,23	1.47	4 (21%)	27,32,35	1.94	8 (29%)
57	MIA	y	37	57	27,30,32	2.40	6 (22%)	38,42,47	2.81	16 (42%)
55	4SU	v	7	55	18,21,22	1.81	4 (22%)	25,30,33	2.36	6 (24%)
1	PSU	A	955	1	18,21,22	1.41	2 (11%)	21,30,33	2.06	4 (19%)
1	6MZ	A	2030	1,60	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
34	PSU	a	516	34	18,21,22	1.38	2 (11%)	21,30,33	2.16	5 (23%)
57	PSU	y	32	57,60	18,21,22	1.37	2 (11%)	21,30,33	2.05	5 (23%)
34	MA6	a	1519	34	23,26,27	1.71	6 (26%)	33,38,41	2.41	16 (48%)
55	H2U	v	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.68	3 (15%)
34	5MC	a	967	34	19,22,23	2.04	2 (10%)	26,32,35	1.55	5 (19%)
1	PSU	A	1917	1	18,21,22	1.45	2 (11%)	21,30,33	2.07	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	A	1939	1	19,22,23	1.48	4 (21%)	27,32,35	2.05	8 (29%)
57	7MG	y	46	57	23,26,27	1.41	3 (13%)	27,39,42	2.46	7 (25%)
1	H2U	A	2449	1	18,21,22	0.95	2 (11%)	19,30,33	1.74	4 (21%)

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
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	PSU	A	746	1,60	-	1/7/25/26	0/2/2/2
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3
1	2MA	A	2503	1,60	-	3/7/25/26	0/3/3/3
1	OMG	A	2251	1,55,60	-	0/9/27/28	0/3/3/3
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	1/9/27/28	0/3/3/3
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	OMU	A	2552	1,60	-	2/9/27/28	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	PSU	A	2457	1,60	-	2/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1,60	-	2/9/27/28	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	7MG	a	527	34,60	-	2/7/37/38	0/3/3/3
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34,60	-	4/11/29/30	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
1	6MZ	A	1618	1	-	2/9/27/28	0/3/3/3
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
57	MIA	y	37	57	-	4/14/32/34	0/3/3/3
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1,60	-	3/9/27/28	0/3/3/3
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
57	PSU	y	32	57,60	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	2/11/29/30	0/3/3/3
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.51	1.66	1.43
1	A	1915	3TD	C6-C5	15.64	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.44	1.34	1.53
1	A	1915	3TD	C2-N1	8.58	1.47	1.37
34	a	967	5MC	C5-C4	7.69	1.49	1.44

The worst 5 of 333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	966	2MG	C2-N3-C4	8.49	122.62	112.00
34	a	1207	2MG	C2-N3-C4	8.32	122.41	112.00
1	A	2503	2MA	C5-C4-N3	-8.12	118.62	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	N9-C4-N3	8.12	137.35	125.46
57	y	46	7MG	N9-C4-N3	8.09	137.32	125.46

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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'
1	A	1917	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	y	55	PSU	1	0
1	A	1915	3TD	1	0
1	A	2504	PSU	1	0
34	a	1498	UR3	1	0
1	A	2498	OMC	2	0
1	A	1618	6MZ	4	0
55	v	54	5MU	1	0
57	y	37	MIA	1	0
1	A	2030	6MZ	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1912 ligands modelled in this entry, 1909 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	$\# Z > 2$
63	GNP	z	402	60	34,34,34	2.41	7 (20%)	47,54,54	1.84	9 (19%)
62	PHE	z	401	-	10,11,12	0.45	0	8,13,15	0.17	0
59	FME	A	3001	-	8,9,10	0.63	0	8,9,11	1.92	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
63	GNP	z	402	60	-	2/18/38/38	0/3/3/3
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
59	FME	A	3001	-	-	2/7/9/11	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GNP	PG-O1G	10.09	1.61	1.46
63	z	402	GNP	PG-N3B	4.42	1.74	1.63
63	z	402	GNP	PB-N3B	4.23	1.74	1.63
63	z	402	GNP	PG-O2G	-3.25	1.48	1.56
63	z	402	GNP	C5-C4	3.12	1.47	1.38

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	-6.03	118.79	128.39
63	z	402	GNP	C2-N3-C4	5.18	121.22	112.30
63	z	402	GNP	N9-C4-N3	4.49	134.94	125.95
59	A	3001	FME	C-CA-N	4.03	117.28	109.50
63	z	402	GNP	C6-C5-N7	3.54	136.73	130.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	3001	FME	O1-CN-N-CA
62	z	401	PHE	O-C-CA-CB

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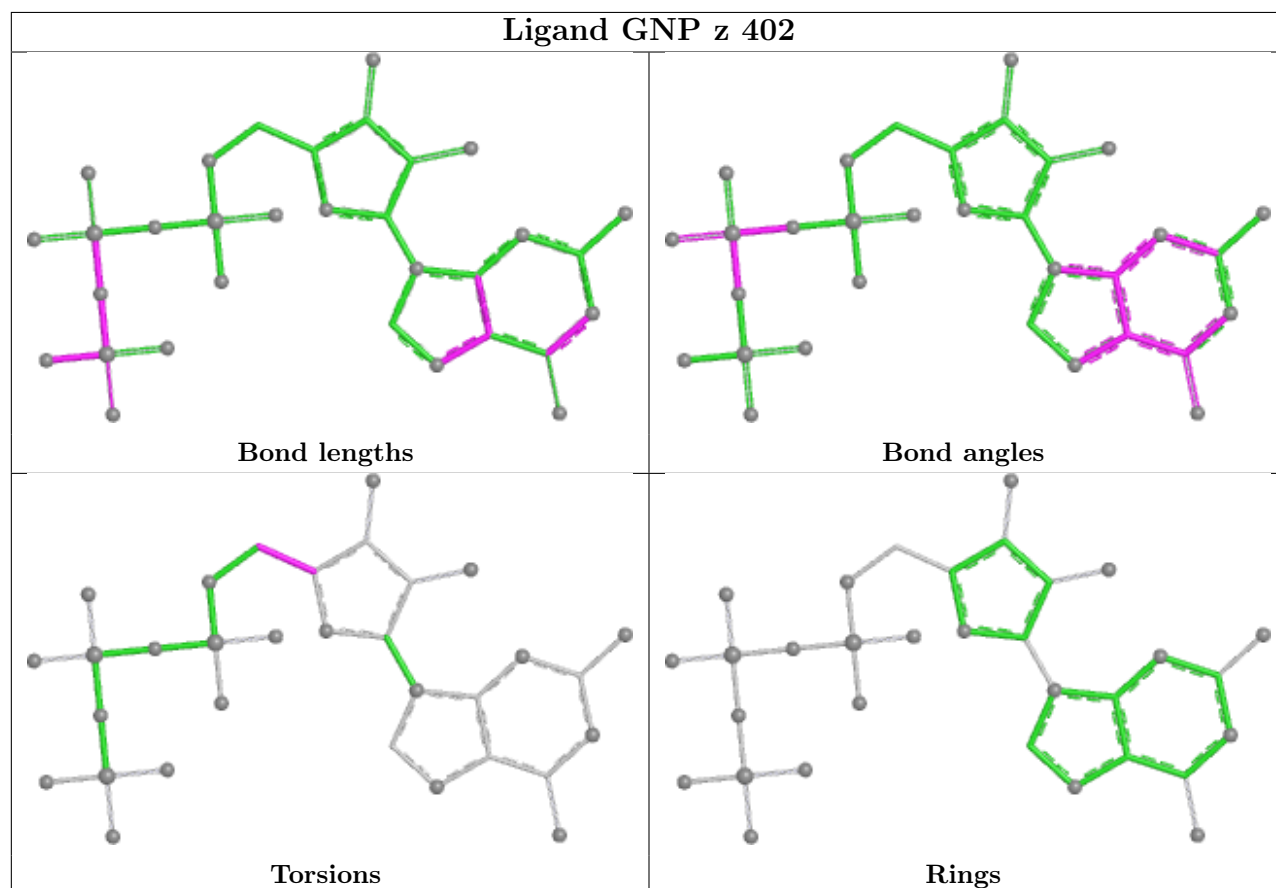
Continued from previous page...

Mol	Chain	Res	Type	Atoms
63	z	402	GNP	O4'-C4'-C5'-O5'
63	z	402	GNP	C3'-C4'-C5'-O5'
59	A	3001	FME	CA-CB-CG-SD

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2030:6MZ	O3'	2031:A	P	2.28
1	A	1618:6MZ	O3'	1619:G	P	1.81

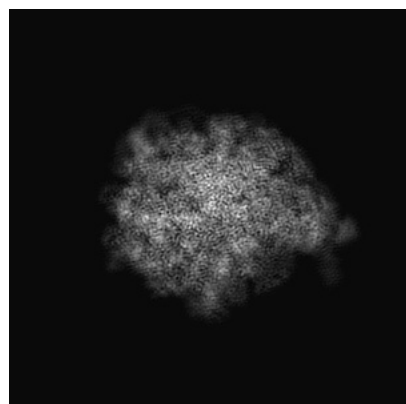
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8813. These allow visual inspection of the internal detail of the map and identification of artifacts.

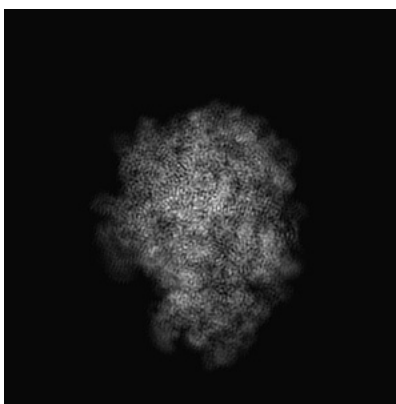
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

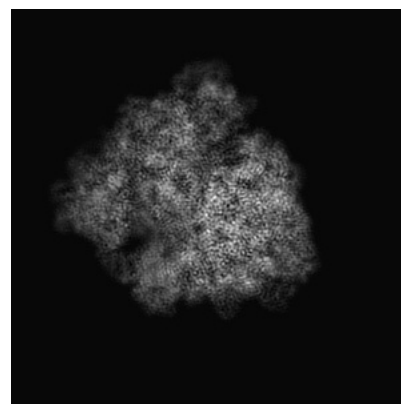
6.1.1 Primary map



X

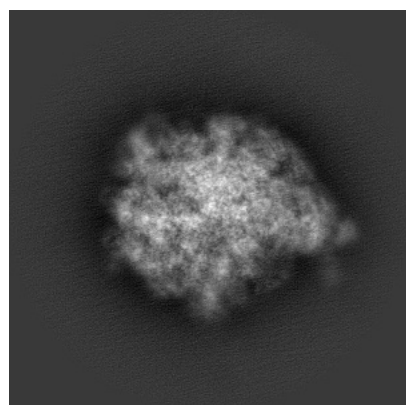


Y

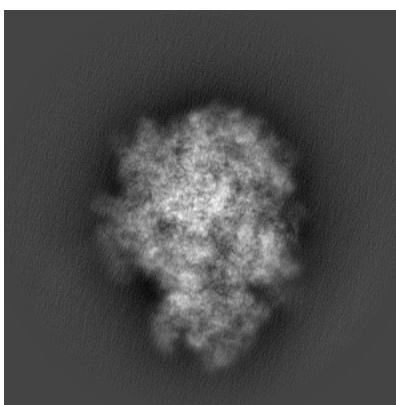


Z

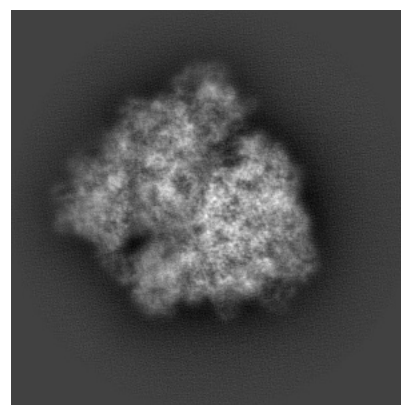
6.1.2 Raw map



X



Y

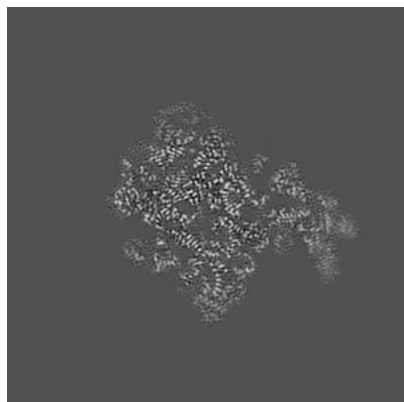


Z

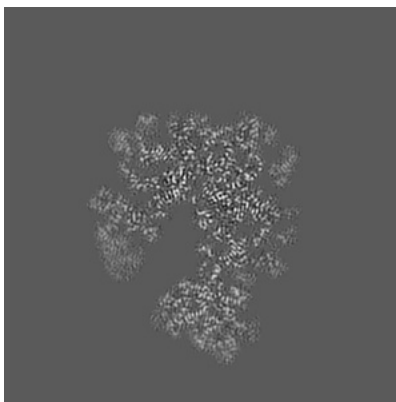
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

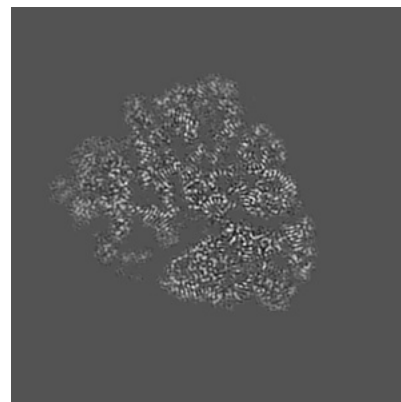
6.2.1 Primary map



X Index: 199

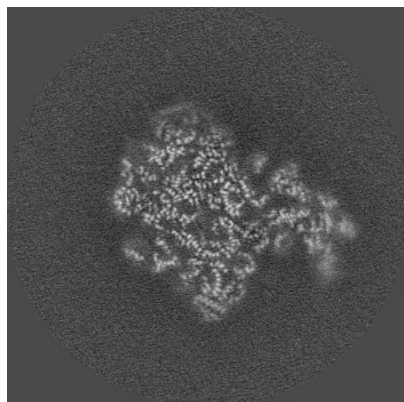


Y Index: 199

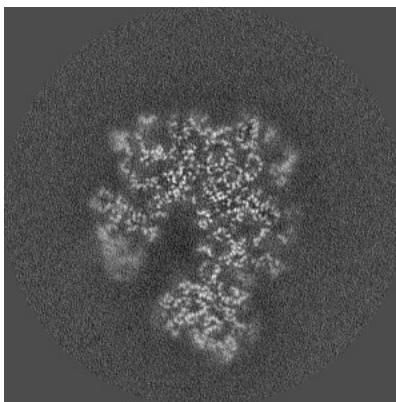


Z Index: 199

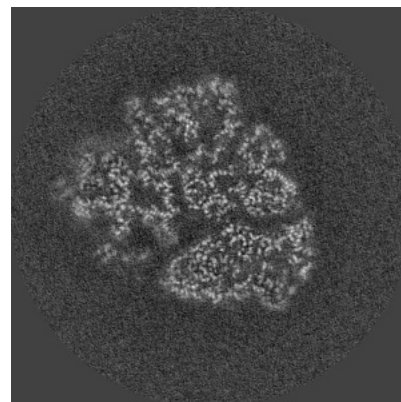
6.2.2 Raw map



X Index: 199



Y Index: 199

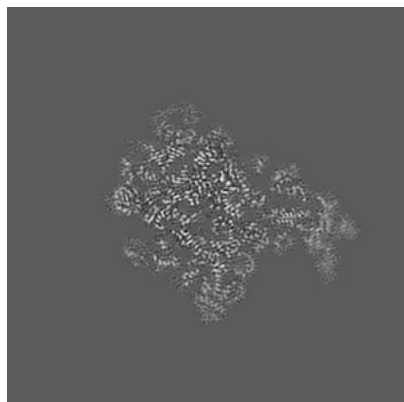


Z Index: 199

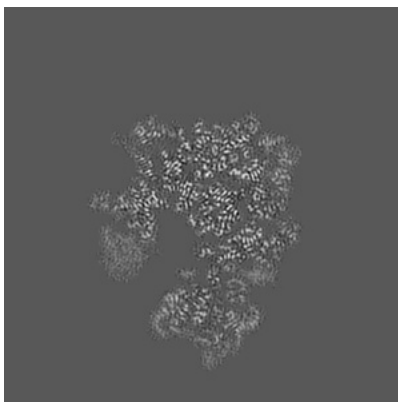
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

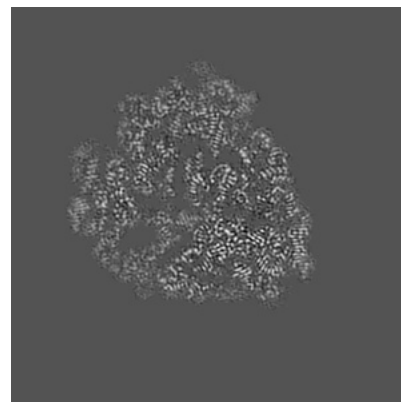
6.3.1 Primary map



X Index: 200

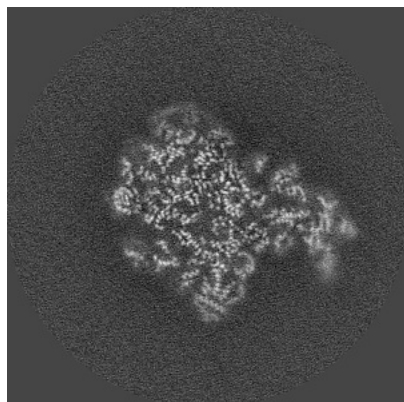


Y Index: 208

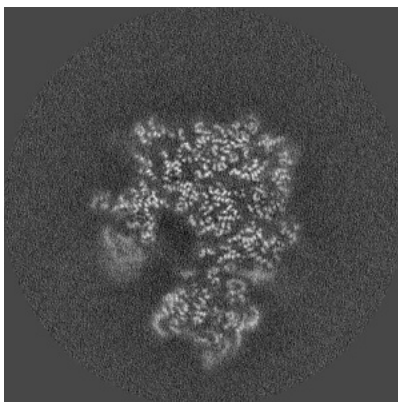


Z Index: 191

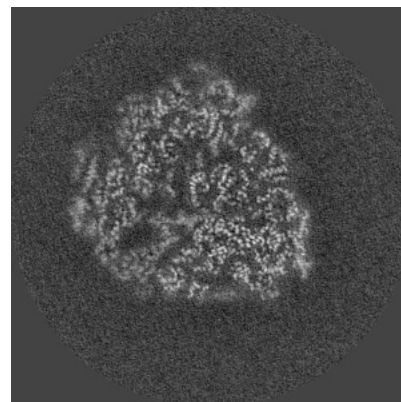
6.3.2 Raw map



X Index: 200



Y Index: 208

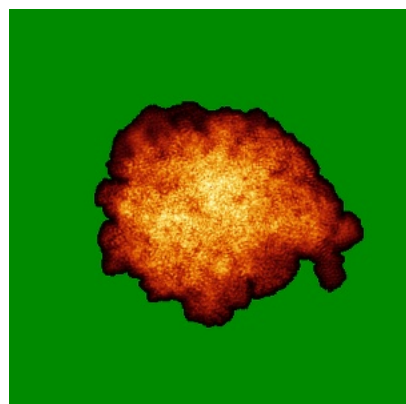


Z Index: 190

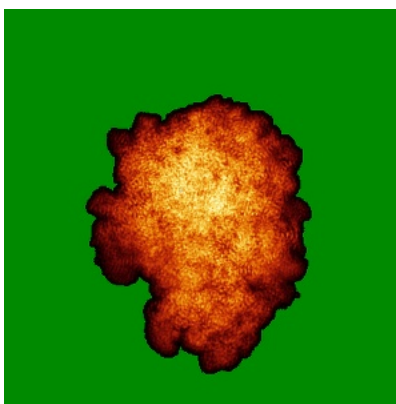
The images above show the largest variance slices of the map in three orthogonal directions.

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

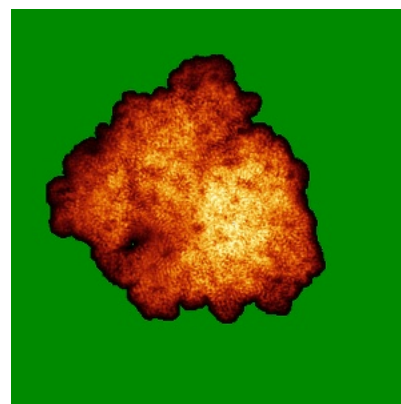
6.4.1 Primary map



X

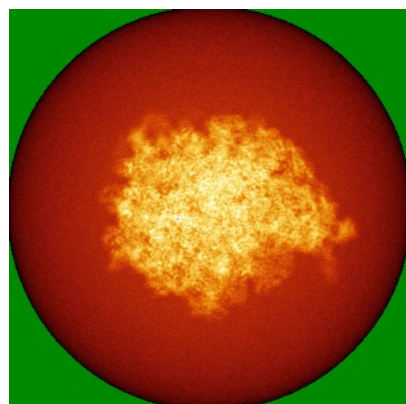


Y

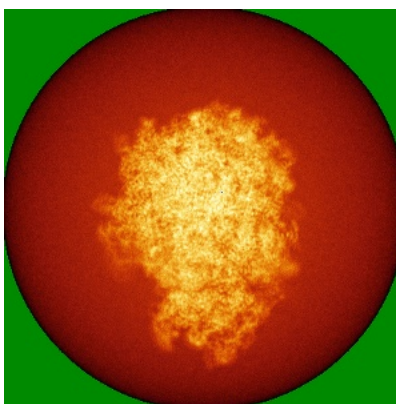


Z

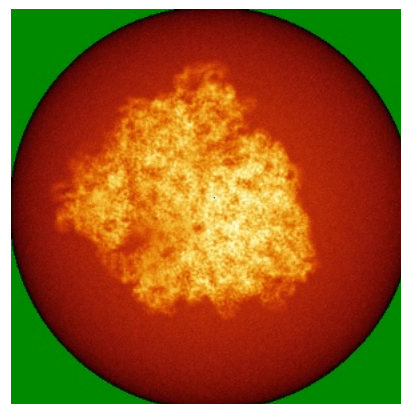
6.4.2 Raw map



X



Y



Z

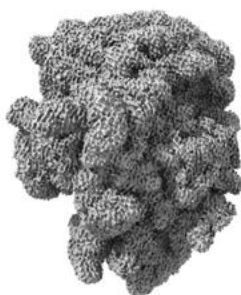
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

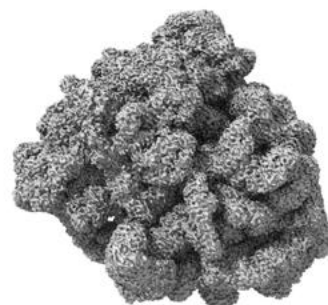
6.5.1 Primary map



X



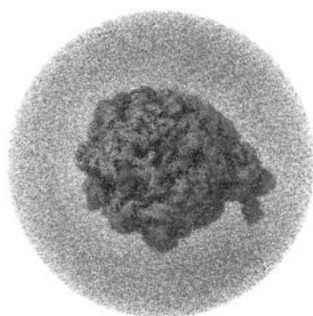
Y



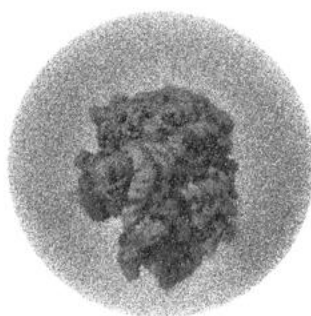
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00558. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

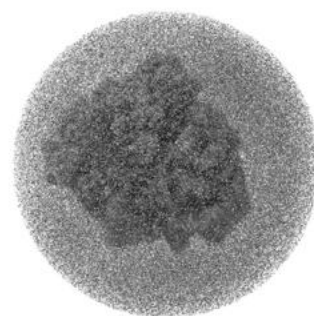
6.5.2 Raw map



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.

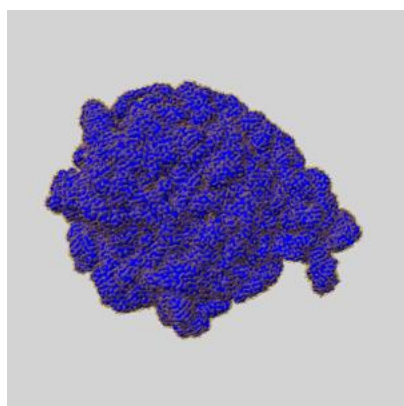
6.6 Mask visualisation [i](#)

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

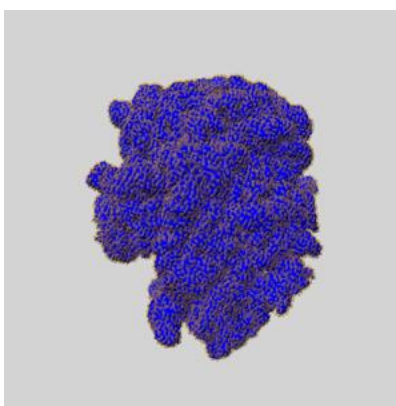
A mask typically either:

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

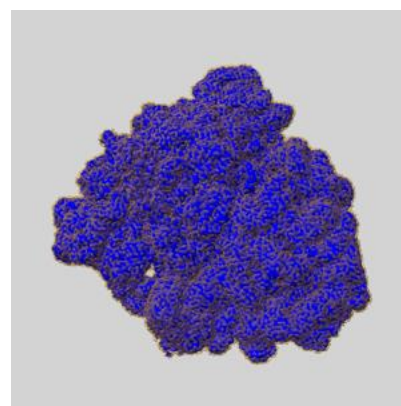
6.6.1 emd_8813_msk_1.map [i](#)



X



Y

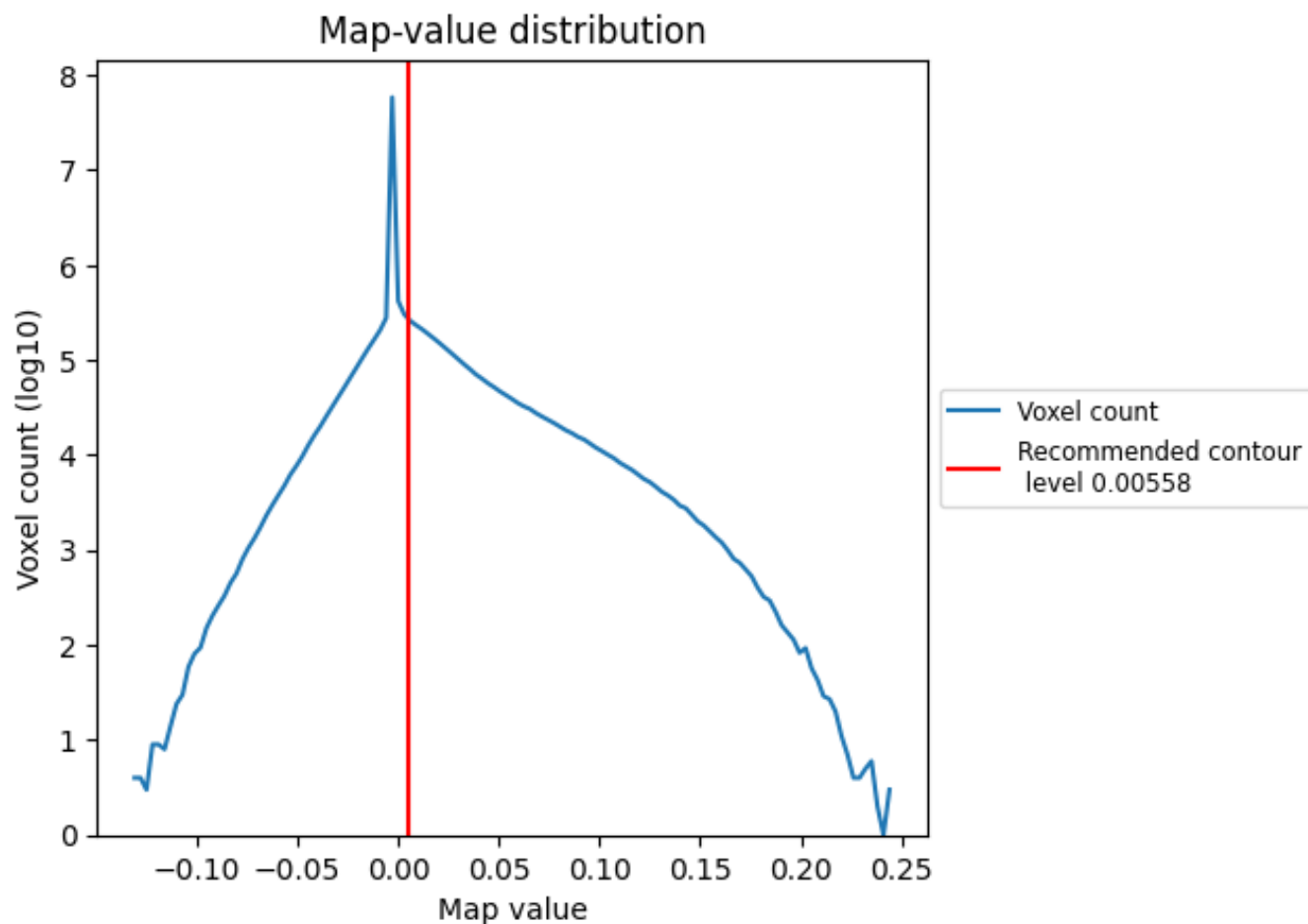


Z

7 Map analysis [i](#)

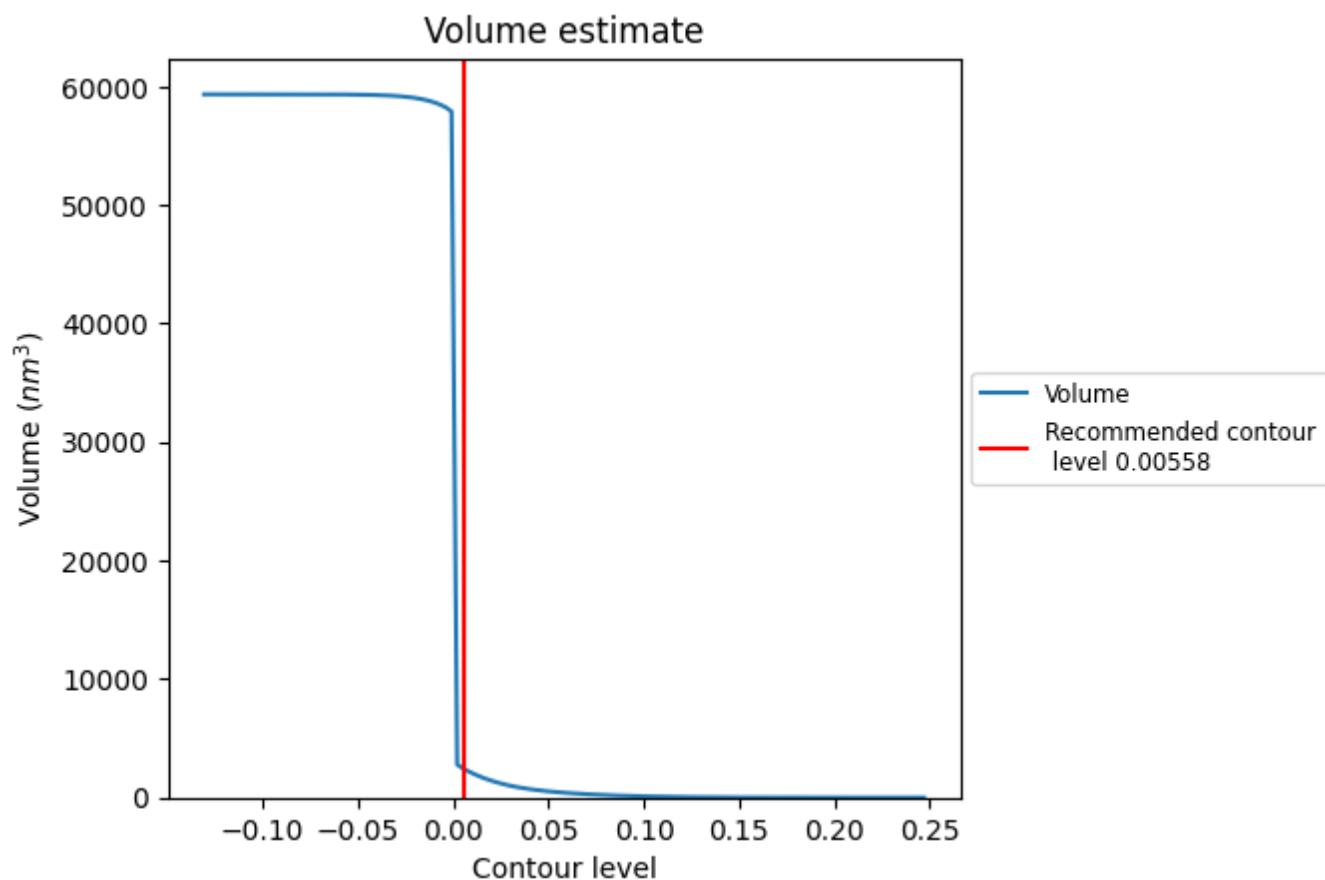
This section contains the results of statistical analysis of the map.

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.

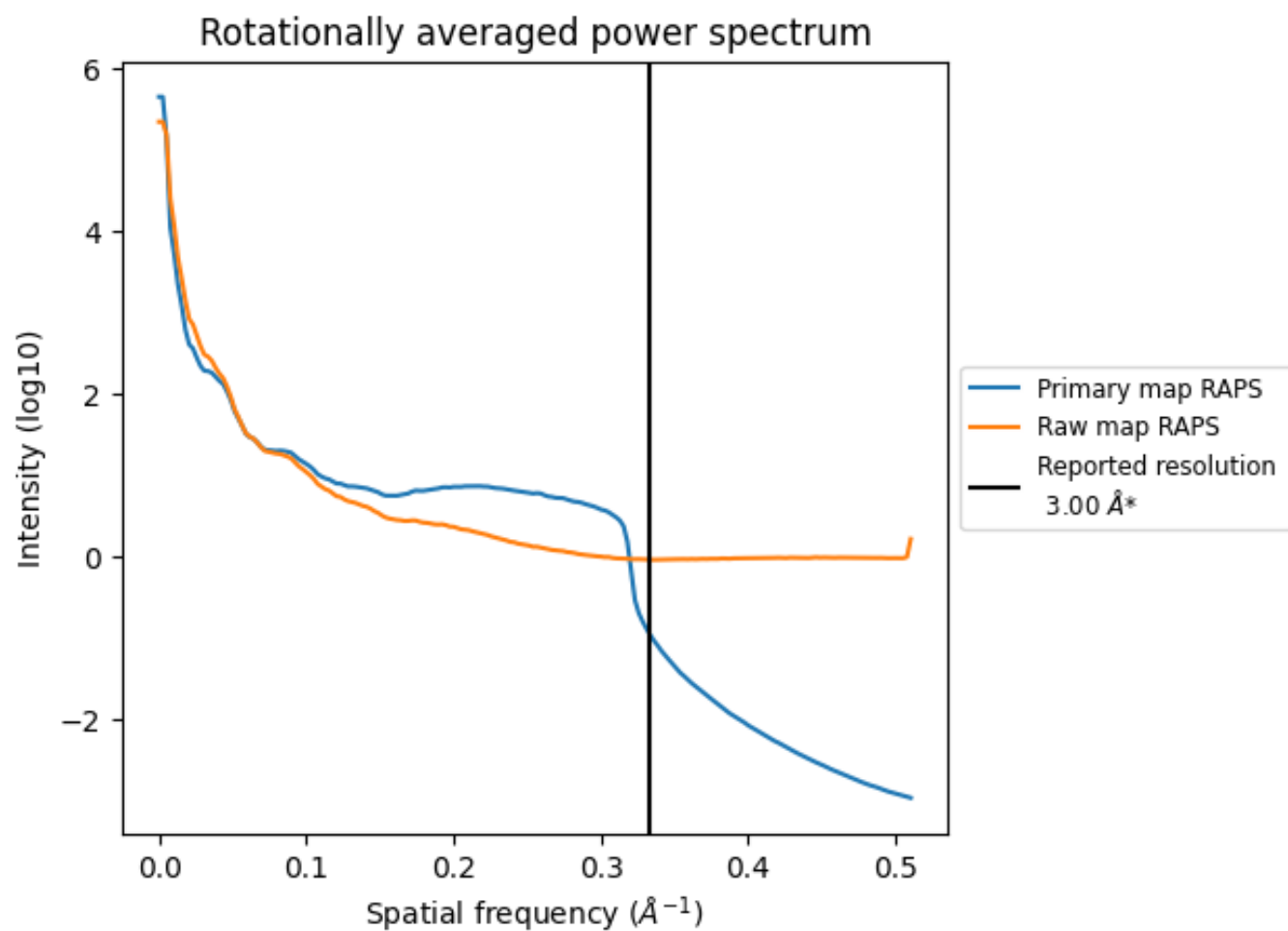
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2421 nm³; this corresponds to an approximate mass of 2187 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

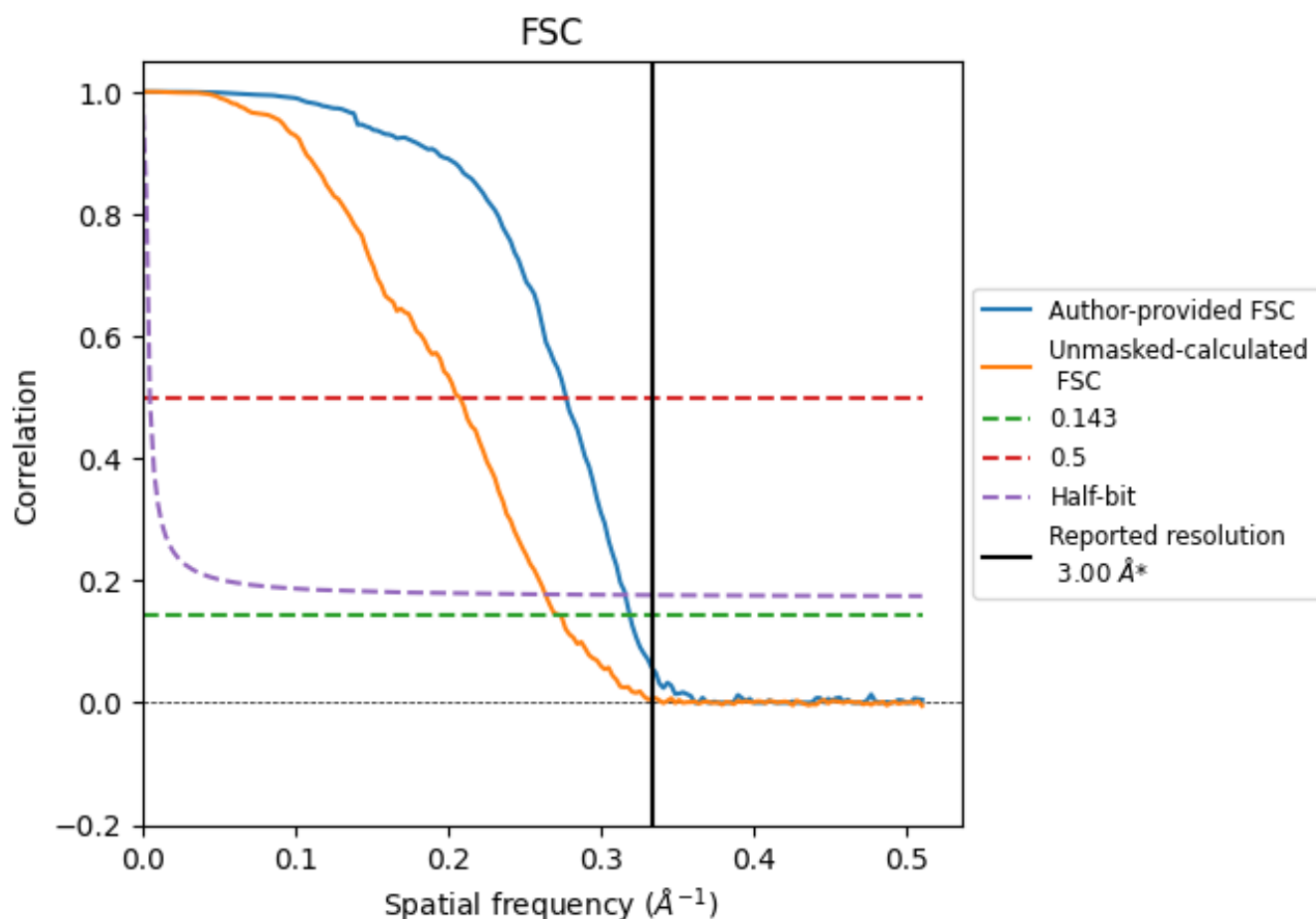


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

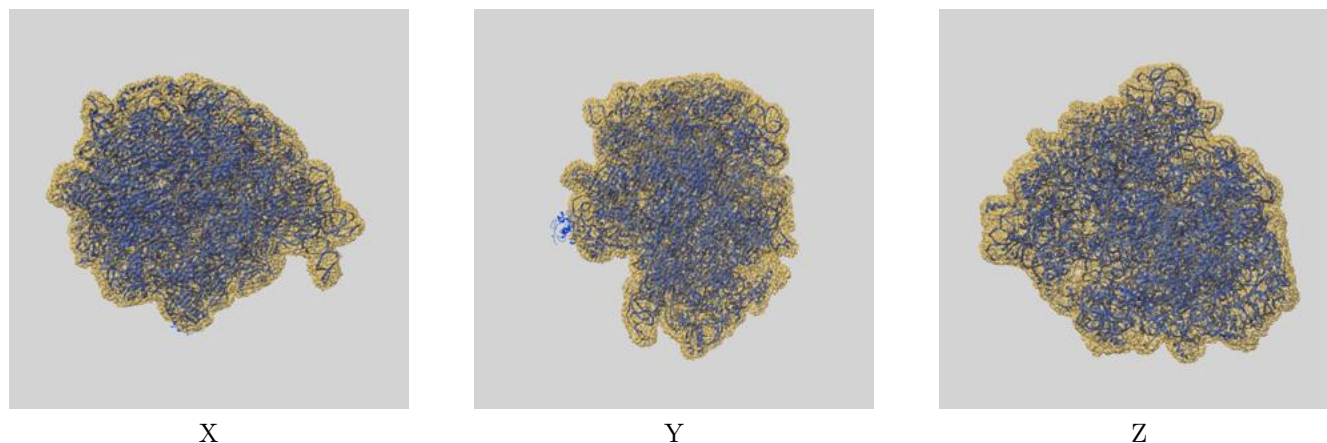
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.13	3.61	3.16
Unmasked-calculated*	3.66	4.82	3.79

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

9 Map-model fit [i](#)

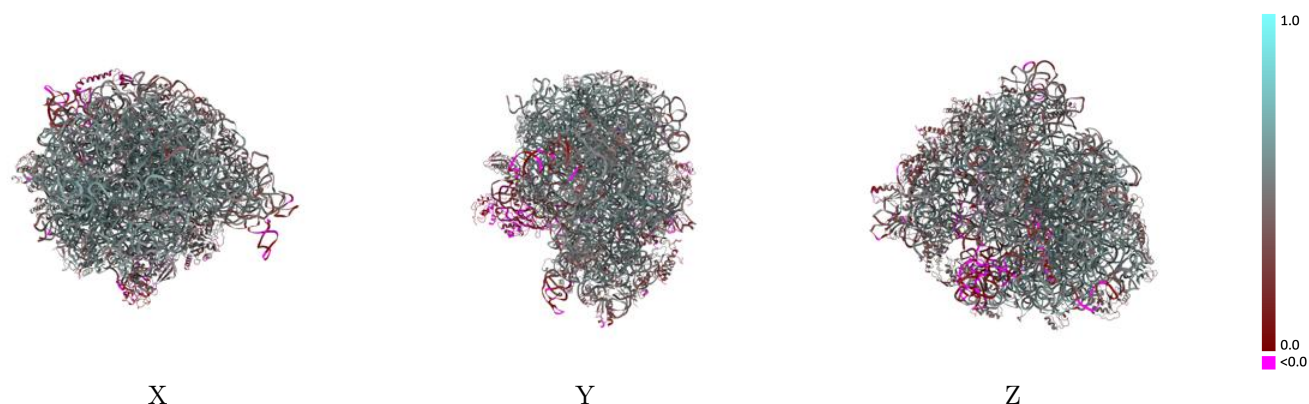
This section contains information regarding the fit between EMDB map EMD-8813 and PDB model 5WDT. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



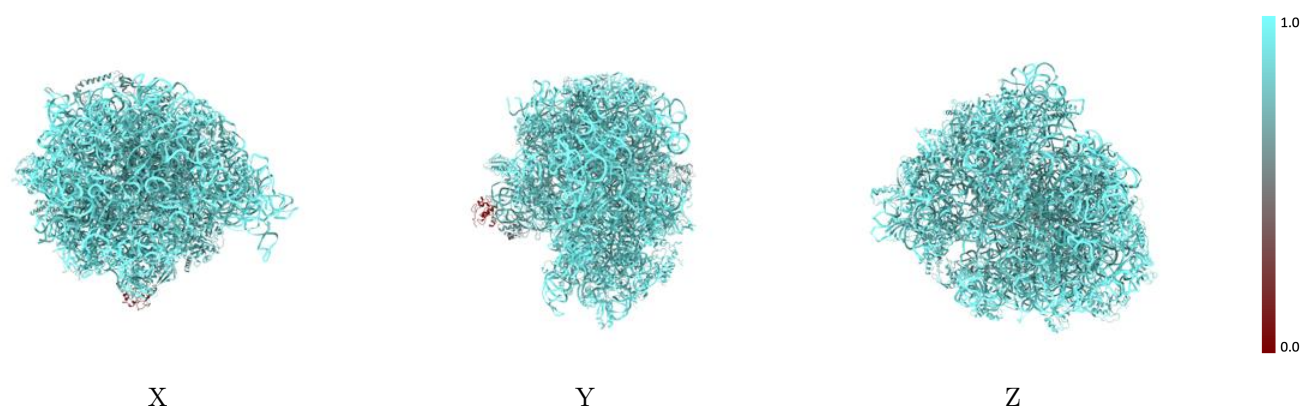
The images above show the 3D surface view of the map at the recommended contour level 0.00558 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



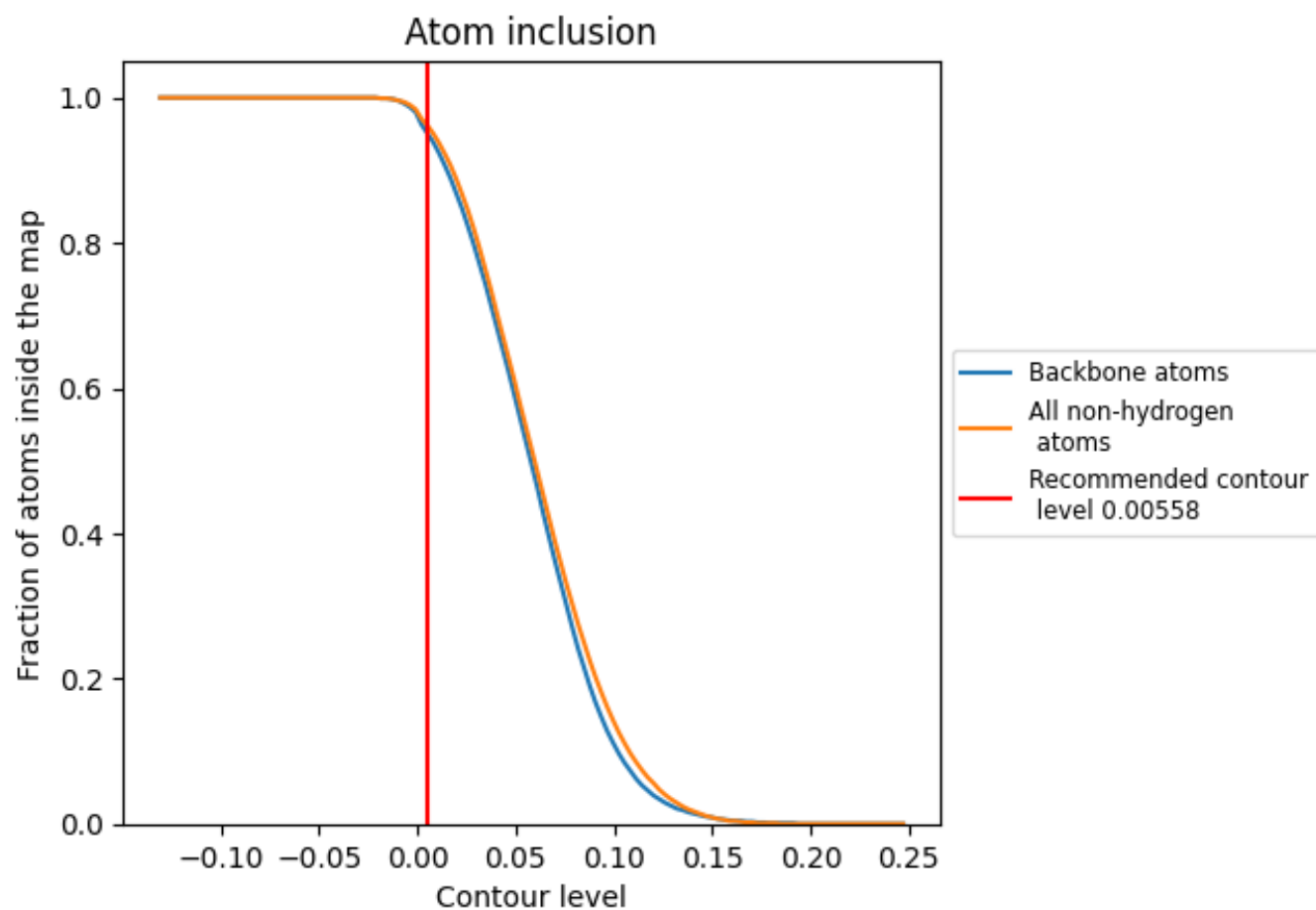
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00558).

9.4 Atom inclusion [i](#)



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 (0.00558) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.4690
0	 0.9430	 0.4710
1	 0.9540	 0.4730
2	 0.9680	 0.5660
3	 0.9680	 0.5520
4	 0.9760	 0.5170
5	 0.1950	 0.0080
6	 0.8810	 0.2830
A	 0.9860	 0.5100
B	 0.9950	 0.5060
C	 0.9660	 0.5260
D	 0.9680	 0.5190
E	 0.9510	 0.4730
F	 0.9270	 0.3960
G	 0.9410	 0.3910
H	 0.7410	 0.1690
I	 0.6250	 0.0170
J	 0.9720	 0.5140
K	 0.9380	 0.4980
L	 0.9460	 0.4800
M	 0.9550	 0.4980
N	 0.9690	 0.5250
O	 0.9570	 0.4340
P	 0.9400	 0.4850
Q	 0.9720	 0.5400
R	 0.9390	 0.4660
S	 0.9430	 0.5010
T	 0.9300	 0.4440
U	 0.9480	 0.4300
V	 0.9380	 0.4460
W	 0.9680	 0.5310
X	 0.9520	 0.5040
Y	 0.9300	 0.4080
Z	 0.9510	 0.4930
a	 0.9900	 0.4890



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.9040	 0.3380
c	 0.9450	 0.4310
d	 0.9350	 0.4110
e	 0.9440	 0.4610
f	 0.9150	 0.3890
g	 0.9150	 0.3550
h	 0.9510	 0.4730
i	 0.9220	 0.3720
j	 0.9260	 0.3410
k	 0.9470	 0.4480
l	 0.9450	 0.4870
m	 0.9400	 0.4100
n	 0.9550	 0.4370
o	 0.9540	 0.4570
p	 0.9310	 0.4280
q	 0.9290	 0.4380
r	 0.9180	 0.4040
s	 0.9530	 0.4390
t	 0.9430	 0.4210
u	 0.8110	 0.2700
v	 0.9680	 0.4680
w	 0.8190	 0.1030
x	 0.9840	 0.4830
y	 0.9490	 0.3620
z	 0.8850	 0.3280