



Full wwPDB EM Validation Report ⓘ

Nov 26, 2022 – 11:06 AM EST

PDB ID : 7SSD
EMDB ID : EMD-25407
Title : Mid translocation intermediate with EF-G bound with GDP (Structure IV)
Authors : Carbone, C.E.; Korostelev, A.A.
Deposited on : 2021-11-10
Resolution : 3.30 Å (reported)

This is a Full wwPDB EM Validation 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

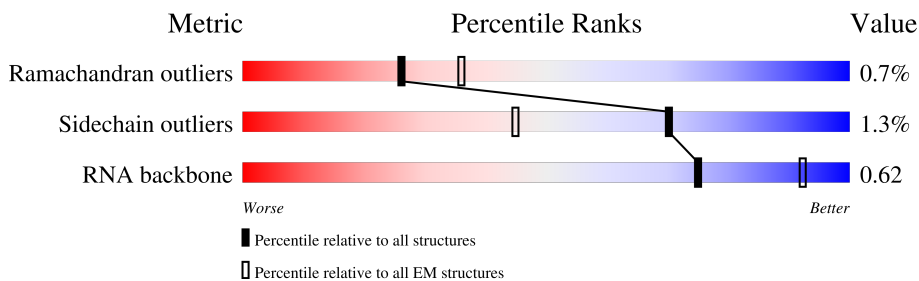
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	3	1539	87% (Green), 13% (Yellow)
2	1	2903	87% (Green), 13% (Yellow)
3	2	120	89% (Green), 11% (Yellow)
4	8	697	6% (Red), 93% (Green), 1% (Yellow), 1% (Grey)
5	6	77	78% (Green), 22% (Yellow)
6	b	271	97% (Green), 3% (Yellow)
7	c	209	99% (Green), 1% (Yellow)
8	d	201	98% (Green), 2% (Yellow)

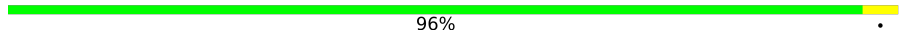
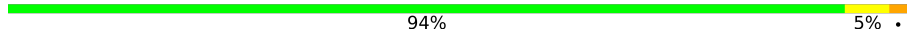
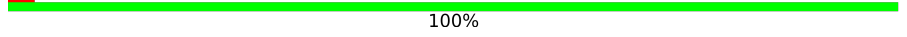



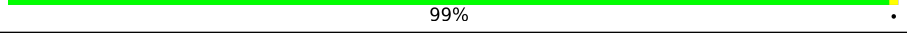
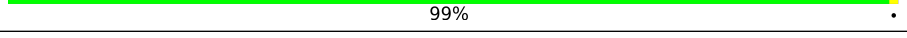
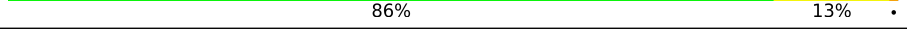
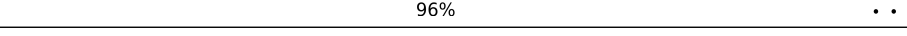
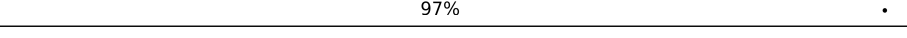
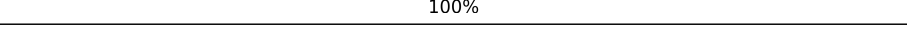
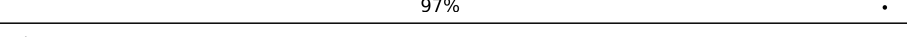
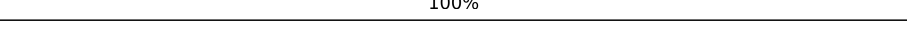
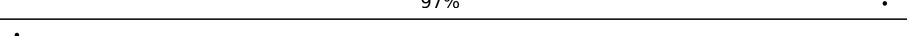
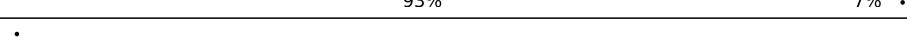
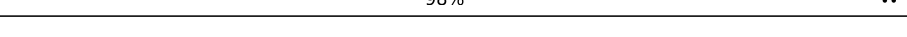
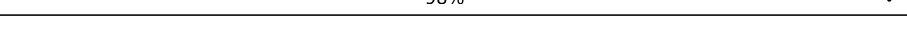
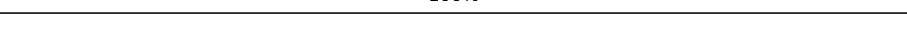






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Mol	Chain	Length	Quality of chain
9	e	177	96%
10	f	176	99%
11	g	149	98%
12	a	234	56% 43%
13	i	142	98%
14	j	142	100%
15	k	122	98%
16	l	143	98%
17	m	136	96%
18	n	120	99%
19	o	116	99%
20	p	114	100%
21	q	117	100%
22	r	103	97%
23	s	110	100%
24	t	93	99%
25	u	102	100%
26	v	94	100%
27	w	75	100%
28	x	77	100%
29	y	63	100%
30	z	58	98%
31	A	66	70% 30%
32	B	56	100%
33	C	50	100%

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Mol	Chain	Length	Quality of chain
34	D	46	 96%
35	E	64	 94% 5%
36	F	38	 100%
37	4	39	 36% 59%
38	5	77	 78% 22%
39	G	225	 89% 8%
40	H	206	 99%
41	I	205	 99%
42	J	157	 86% 13%
43	K	100	 96%
44	L	151	 97%
45	M	129	 100%
46	N	127	 97%
47	O	98	 100%
48	P	116	 97%
49	Q	123	 93% 7%
50	R	114	 98%
51	S	100	 98%
52	T	88	 100%
53	U	82	 98%
54	V	80	 95% 5%
55	W	65	 95% 5%
56	X	79	 96%
57	Y	85	 100%
58	Z	65	 94% 6%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 153049 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3	1539	33012	14725	6052	10697	1538	0	0

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	2903	62317	27801	11468	20146	2902	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 3 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 4 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	8	666	5157	3256	886	992	23	0	0

- Molecule 5 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

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

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

- Molecule 12 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 13 is a protein called 50S ribosomal protein L11.

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

- Molecule 14 is a protein called 50S ribosomal protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 16 is a protein called 50S ribosomal protein L15.

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

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 19 is a protein called 50S ribosomal protein L18.

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

- Molecule 20 is a protein called 50S ribosomal protein L19.

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

- Molecule 21 is a protein called 50S ribosomal protein L20.

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

- Molecule 22 is a protein called 50S ribosomal protein L21.

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

- Molecule 23 is a protein called 50S ribosomal protein L22.

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

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	t	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	u	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 26 is a protein called 50S ribosomal protein L25.

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

- Molecule 27 is a protein called 50S ribosomal protein L27.

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

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	46	Total	C	N	O	S	0	0
			355	221	62	66	6		

- Molecule 32 is a protein called 50S ribosomal protein L32.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 34 is a protein called 50S ribosomal protein L34.

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

- Molecule 35 is a protein called 50S ribosomal protein L35.

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

- Molecule 36 is a protein called 50S ribosomal protein L36.

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

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	16	Total	C	N	O	P	0	0
			350	156	70	108	16		

- Molecule 38 is a RNA chain called tRNA Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	77	Total	C	N	O	P	0	0
			1647	733	295	542	77		

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 57 is a protein called 30S ribosomal protein S20.

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

- Molecule 58 is a protein called 30S ribosomal protein S21.

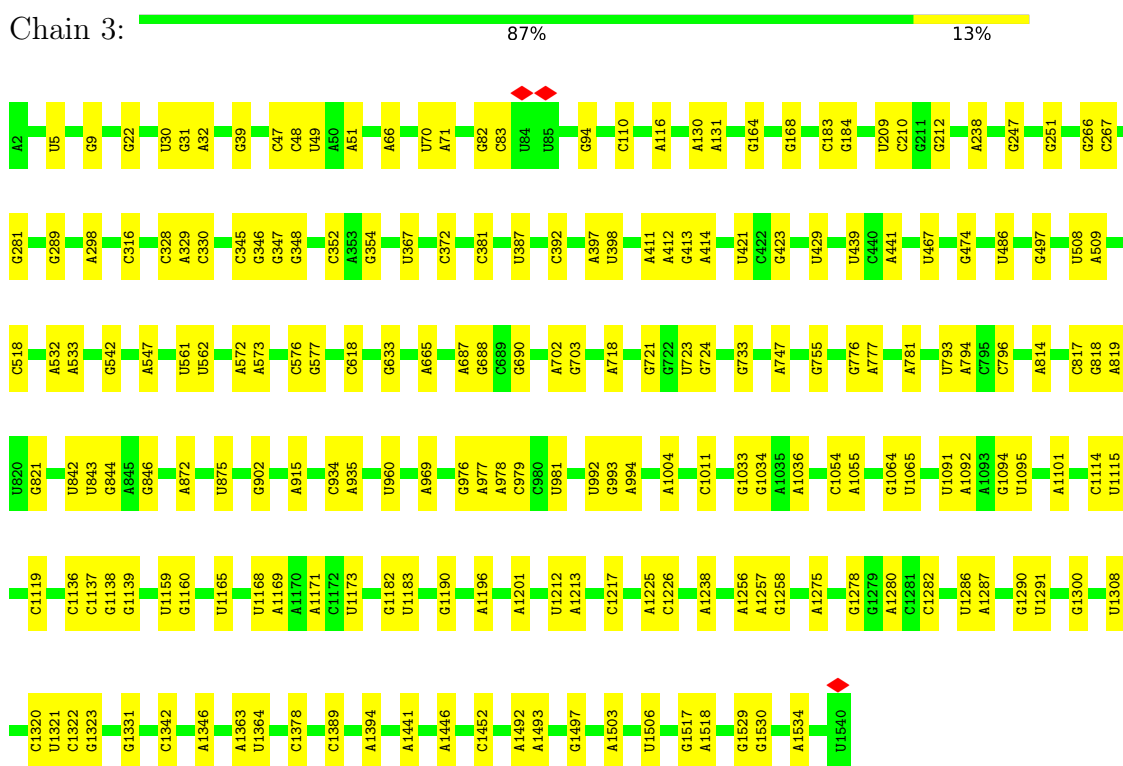
Mol	Chain	Residues	Atoms					AltConf	Trace
58	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).

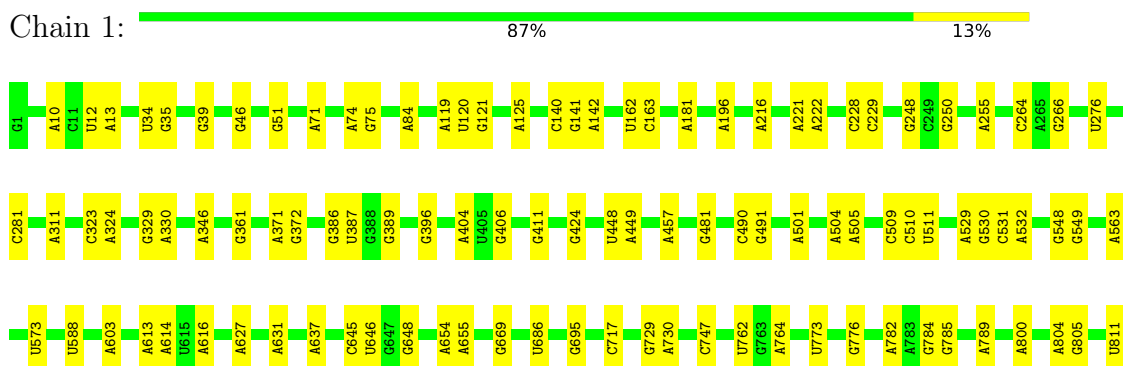
3 Residue-property plots [i](#)

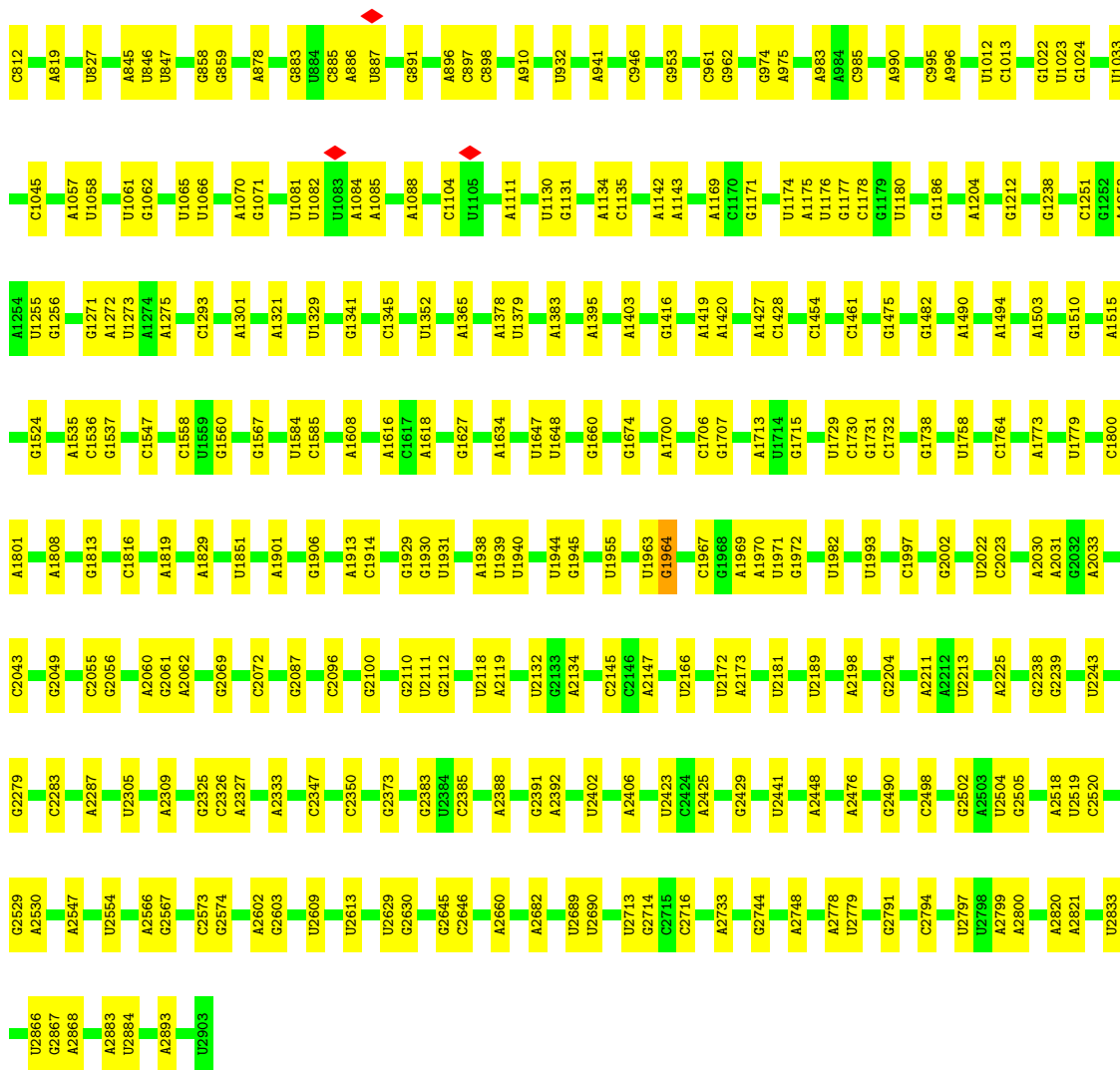
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 16S rRNA

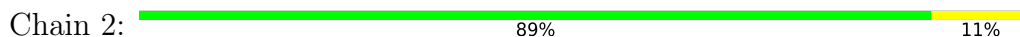


- Molecule 2: 23S rRNA

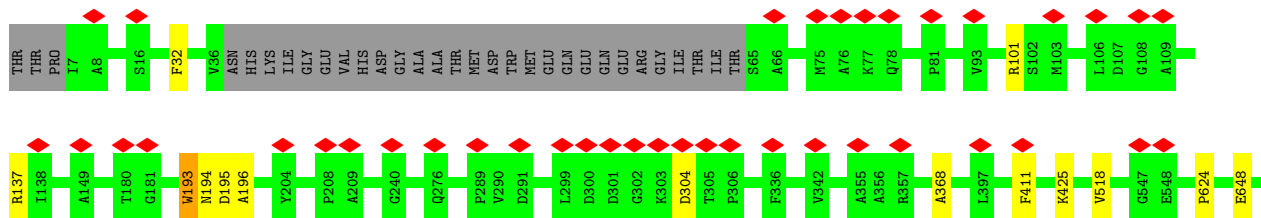




• Molecule 3: 5S RNA

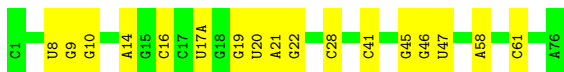
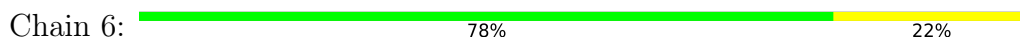


• Molecule 4: Elongation factor G

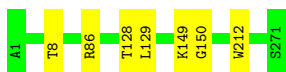




- Molecule 5: tRNA fMet



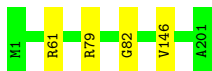
- Molecule 6: 50S ribosomal protein L2



- Molecule 7: 50S ribosomal protein L3



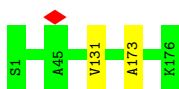
- Molecule 8: 50S ribosomal protein L4



- Molecule 9: 50S ribosomal protein L5



- Molecule 10: 50S ribosomal protein L6

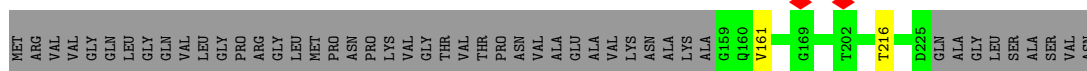
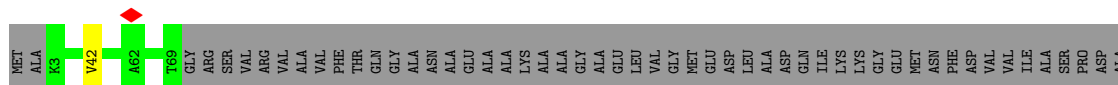


- Molecule 11: 50S ribosomal protein L9

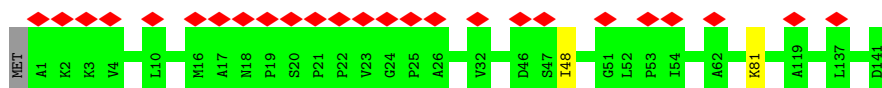




- Molecule 12: 50S ribosomal protein L1



- Molecule 13: 50S ribosomal protein L11



- Molecule 14: 50S ribosomal protein L13



There are no outlier residues recorded for this chain.

- Molecule 15: 50S ribosomal protein L14



- Molecule 16: 50S ribosomal protein L15

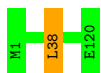


- Molecule 17: 50S ribosomal protein L16



- Molecule 18: 50S ribosomal protein L17

Chain n:  99%



- Molecule 19: 50S ribosomal protein L18

Chain o:  99%



- Molecule 20: 50S ribosomal protein L19

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 50S ribosomal protein L20

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: 50S ribosomal protein L21

Chain r:  97%



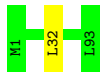
- Molecule 23: 50S ribosomal protein L22

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L23

Chain t:  99%



- Molecule 25: 50S ribosomal protein L24

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L25

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L27

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: 50S ribosomal protein L28

Chain x:  100%

There are no outlier residues recorded for this chain.

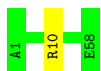
- Molecule 29: 50S ribosomal protein L29

Chain y:  100%

There are no outlier residues recorded for this chain.

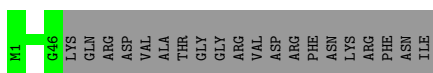
- Molecule 30: 50S ribosomal protein L30

Chain z:  98%



- Molecule 31: 50S ribosomal protein L31

Chain A:  70% 30%



- Molecule 32: 50S ribosomal protein L32

Chain B:  100%

There are no outlier residues recorded for this chain.

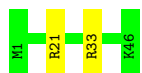
- Molecule 33: 50S ribosomal protein L33

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 50S ribosomal protein L34

Chain D:  96%



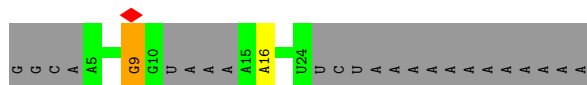
• Molecule 35: 50S ribosomal protein L35



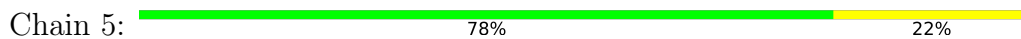
• Molecule 36: 50S ribosomal protein L36



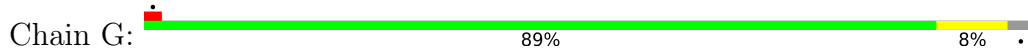
• Molecule 37: mRNA



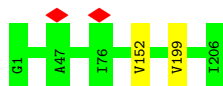
• Molecule 38: tRNA Pro



• Molecule 39: 30S ribosomal protein S2



• Molecule 40: 30S ribosomal protein S3



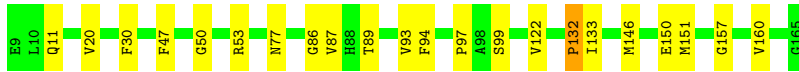
• Molecule 41: 30S ribosomal protein S4





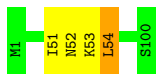
- Molecule 42: 30S ribosomal protein S5

Chain J: 86% 13%



- Molecule 43: 30S ribosomal protein S6

Chain K: 96%



- Molecule 44: 30S ribosomal protein S7

Chain L: 97%



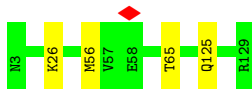
- Molecule 45: 30S ribosomal protein S8

Chain M: 100%

There are no outlier residues recorded for this chain.

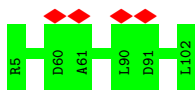
- Molecule 46: 30S ribosomal protein S9

Chain N: 97%



- Molecule 47: 30S ribosomal protein S10

Chain O: 100%

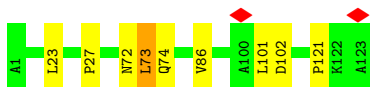
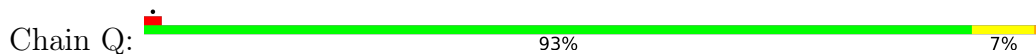


- Molecule 48: 30S ribosomal protein S11

Chain P: 97%



- Molecule 49: 30S ribosomal protein S12



- Molecule 50: 30S ribosomal protein S13



- Molecule 51: 30S ribosomal protein S14

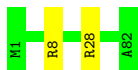


- Molecule 52: 30S ribosomal protein S15

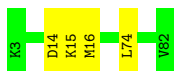


There are no outlier residues recorded for this chain.

- Molecule 53: 30S ribosomal protein S16



- Molecule 54: 30S ribosomal protein S17



- Molecule 55: 30S ribosomal protein S18





- Molecule 56: 30S ribosomal protein S19

Chain X:  96% ..



- Molecule 57: 30S ribosomal protein S20

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 30S ribosomal protein S21

Chain Z:  94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	27.032	Depositor
Minimum map value	-14.235	Depositor
Average map value	0.111	Depositor
Map value standard deviation	0.944	Depositor
Recommended contour level	0.7	Depositor
Map size (\AA)	370.5408, 370.5408, 370.5408	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8271, 0.8271, 0.8271	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	3	0.33	0/36963	0.66	0/57662
2	1	0.36	0/69796	0.66	0/108888
3	2	0.33	0/2872	0.66	0/4479
4	8	0.34	0/5253	0.65	3/7106 (0.0%)
5	6	0.35	0/1832	0.66	0/2855
6	b	0.52	0/2122	0.70	1/2852 (0.0%)
7	c	0.44	0/1586	0.66	0/2134
8	d	0.38	0/1571	0.63	0/2113
9	e	0.36	0/1435	0.67	2/1926 (0.1%)
10	f	0.33	0/1343	0.58	0/1816
11	g	0.33	0/1122	0.66	0/1515
12	a	0.30	0/1033	0.58	0/1387
13	i	0.31	0/1046	0.63	0/1410
14	j	0.43	0/1152	0.59	0/1551
15	k	0.45	0/948	0.75	1/1268 (0.1%)
16	l	0.40	0/1054	0.70	0/1403
17	m	0.46	0/1093	0.64	0/1460
18	n	0.44	0/974	0.71	1/1301 (0.1%)
19	o	0.34	0/902	0.56	0/1209
20	p	0.42	0/929	0.59	0/1242
21	q	0.46	0/960	0.53	0/1278
22	r	0.39	0/829	0.63	0/1107
23	s	0.40	0/864	0.60	0/1156
24	t	0.39	0/745	0.64	1/994 (0.1%)
25	u	0.38	0/788	0.58	0/1051
26	v	0.37	0/766	0.57	0/1025
27	w	0.41	0/582	0.61	0/769
28	x	0.45	0/635	0.62	0/848
29	y	0.32	0/510	0.58	0/677
30	z	0.34	0/453	0.67	0/605
31	A	0.31	0/362	0.61	0/485
32	B	0.42	0/450	0.64	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	C	0.39	0/417	0.59	0/554
34	D	0.46	0/380	0.78	1/498 (0.2%)
35	E	0.42	0/513	0.83	2/676 (0.3%)
36	F	0.45	0/303	0.73	0/397
37	4	0.66	0/392	0.73	0/608
38	5	0.38	0/1840	0.69	0/2868
39	G	0.35	0/1736	0.54	0/2338
40	H	0.33	0/1652	0.61	0/2225
41	I	0.32	0/1665	0.64	1/2227 (0.0%)
42	J	0.32	0/1170	0.55	0/1573
43	K	0.39	0/836	0.73	2/1128 (0.2%)
44	L	0.29	0/1196	0.58	0/1602
45	M	0.35	0/989	0.59	0/1326
46	N	0.34	0/1034	0.70	1/1375 (0.1%)
47	O	0.32	0/797	0.71	0/1077
48	P	0.35	0/886	0.64	1/1195 (0.1%)
49	Q	0.35	0/969	0.71	0/1300
50	R	0.31	0/893	0.62	0/1193
51	S	0.31	0/817	0.56	0/1088
52	T	0.35	0/722	0.61	0/964
53	U	0.32	0/659	0.68	0/884
54	V	0.38	0/658	0.68	1/881 (0.1%)
55	W	0.34	0/545	0.63	1/731 (0.1%)
56	X	0.34	0/653	0.68	1/877 (0.1%)
57	Y	0.30	0/671	0.57	0/888
58	Z	0.36	0/551	0.71	0/728
All	All	0.36	0/165914	0.66	20/247372 (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
2	1	0	3
4	8	0	5
7	c	0	1
8	d	0	2
9	e	0	1
10	f	0	1
11	g	0	1
16	l	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	m	0	2
22	r	0	1
30	z	0	1
35	E	0	1
37	4	0	1
41	I	0	1
43	K	0	1
44	L	0	1
46	N	0	1
49	Q	0	4
50	R	0	2
54	V	0	2
55	W	0	1
56	X	0	1
58	Z	0	3
All	All	0	38

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	8	195	ASP	CB-CG-OD1	9.24	126.62	118.30
41	I	4	LEU	CA-CB-CG	6.86	131.07	115.30
35	E	28	LEU	CA-CB-CG	6.63	130.56	115.30
35	E	32	LEU	CA-CB-CG	6.50	130.25	115.30
18	n	38	LEU	CA-CB-CG	6.27	129.72	115.30
15	k	8	LEU	CA-CB-CG	6.26	129.70	115.30
4	8	194	ASN	C-N-CA	5.86	136.35	121.70
6	b	129	LEU	CA-CB-CG	5.61	128.20	115.30
46	N	125	GLN	CA-CB-CG	5.47	125.43	113.40
9	e	173	ASP	CB-CG-OD1	5.42	123.18	118.30
43	K	52	ASN	C-N-CA	5.41	135.21	121.70
9	e	151	LEU	CA-CB-CG	5.31	127.51	115.30
24	t	32	LEU	CA-CB-CG	5.30	127.50	115.30
43	K	51	ILE	C-N-CA	5.29	134.93	121.70
54	V	74	LEU	CA-CB-CG	5.22	127.31	115.30
4	8	304	ASP	CB-CG-OD1	5.18	122.96	118.30
55	W	54	LEU	CA-CB-CG	5.16	127.17	115.30
48	P	81	LEU	CA-CB-CG	5.15	127.15	115.30
56	X	4	LEU	CB-CG-CD2	5.14	119.75	111.00
34	D	21	ARG	NE-CZ-NH2	5.05	122.83	120.30

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	1779	U	Sidechain
2	1	1964	G	Sidechain
2	1	511	U	Sidechain
37	4	9	G	Sidechain
4	8	193	TRP	Peptide
4	8	368	ALA	Peptide
4	8	411	PHE	Peptide
4	8	648	GLU	Peptide
4	8	698	VAL	Peptide
35	E	30	HIS	Peptide
41	I	18	LEU	Peptide
43	K	53	LYS	Peptide
44	L	148	LYS	Peptide
46	N	56	MET	Peptide
49	Q	101	LEU	Peptide
49	Q	121	PRO	Peptide
49	Q	72	ASN	Peptide
49	Q	73	LEU	Peptide
50	R	112	ARG	Peptide
50	R	95	PRO	Peptide
54	V	14	ASP	Peptide
54	V	15	LYS	Peptide
55	W	18	GLN	Peptide
56	X	78	THR	Peptide
58	Z	10	PRO	Peptide
58	Z	33	ARG	Peptide
58	Z	7	GLU	Peptide
7	c	133	THR	Peptide
8	d	79	ARG	Peptide
8	d	82	GLY	Peptide
9	e	20	ASN	Peptide
10	f	173	ALA	Peptide
11	g	2	GLN	Peptide
16	l	102	GLY	Peptide
17	m	57	VAL	Peptide
17	m	82	MET	Peptide
22	r	46	GLU	Peptide
30	z	10	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	8	662/697 (95%)	595 (90%)	65 (10%)	2 (0%)	41	71
6	b	269/271 (99%)	234 (87%)	33 (12%)	2 (1%)	22	54
7	c	207/209 (99%)	190 (92%)	16 (8%)	1 (0%)	29	61
8	d	199/201 (99%)	173 (87%)	25 (13%)	1 (0%)	29	61
9	e	175/177 (99%)	152 (87%)	23 (13%)	0	100	100
10	f	174/176 (99%)	152 (87%)	22 (13%)	0	100	100
11	g	147/149 (99%)	128 (87%)	19 (13%)	0	100	100
12	a	130/234 (56%)	118 (91%)	12 (9%)	0	100	100
13	i	139/142 (98%)	115 (83%)	24 (17%)	0	100	100
14	j	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
15	k	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19	51
16	l	141/143 (99%)	120 (85%)	20 (14%)	1 (1%)	22	54
17	m	134/136 (98%)	114 (85%)	18 (13%)	2 (2%)	10	38
18	n	118/120 (98%)	102 (86%)	16 (14%)	0	100	100
19	o	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
20	p	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
21	q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
22	r	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
23	s	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
24	t	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
25	u	100/102 (98%)	89 (89%)	11 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	v	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
27	w	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
28	x	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
29	y	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
30	z	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
31	A	44/66 (67%)	35 (80%)	9 (20%)	0	100	100
32	B	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
33	C	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
34	D	44/46 (96%)	38 (86%)	6 (14%)	0	100	100
35	E	62/64 (97%)	51 (82%)	9 (14%)	2 (3%)	4	22
36	F	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
39	G	216/225 (96%)	179 (83%)	28 (13%)	9 (4%)	3	17
40	H	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
41	I	203/205 (99%)	180 (89%)	22 (11%)	1 (0%)	29	61
42	J	155/157 (99%)	108 (70%)	32 (21%)	15 (10%)	0	3
43	K	98/100 (98%)	79 (81%)	18 (18%)	1 (1%)	15	46
44	L	149/151 (99%)	132 (89%)	17 (11%)	0	100	100
45	M	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
46	N	125/127 (98%)	107 (86%)	18 (14%)	0	100	100
47	O	96/98 (98%)	78 (81%)	18 (19%)	0	100	100
48	P	114/116 (98%)	99 (87%)	14 (12%)	1 (1%)	17	48
49	Q	121/123 (98%)	94 (78%)	23 (19%)	4 (3%)	4	22
50	R	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
51	S	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
52	T	86/88 (98%)	79 (92%)	7 (8%)	0	100	100
53	U	80/82 (98%)	64 (80%)	15 (19%)	1 (1%)	12	40
54	V	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
55	W	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
56	X	77/79 (98%)	64 (83%)	13 (17%)	0	100	100
57	Y	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
58	Z	63/65 (97%)	48 (76%)	14 (22%)	1 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6489/6756 (96%)	5692 (88%)	752 (12%)	45 (1%)	26	54

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	E	31	ILE
39	G	18	GLN
39	G	34	ARG
42	J	87	VAL
42	J	160	VAL
4	8	196	ALA
7	c	134	HIS
35	E	32	LEU
39	G	33	ALA
39	G	87	ASP
42	J	11	GLN
42	J	86	GLY
42	J	89	THR
42	J	93	VAL
42	J	99	SER
42	J	122	VAL
42	J	133	ILE
42	J	157	GLY
48	P	125	LYS
49	Q	73	LEU
49	Q	102	ASP
39	G	22	TRP
42	J	132	PRO
49	Q	74	GLN
53	U	28	ARG
15	k	25	LEU
17	m	82	MET
17	m	83	GLY
42	J	97	PRO
58	Z	8	ASN
6	b	149	LYS
8	d	61	ARG
16	l	103	ILE
42	J	77	ASN
6	b	150	GLY
39	G	47	PRO
42	J	50	GLY

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Mol	Chain	Res	Type
43	K	54	LEU
39	G	27	LYS
49	Q	27	PRO
39	G	157	PRO
4	8	624	PRO
39	G	123	GLY
41	I	131	ILE
42	J	20	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	8	548/574 (96%)	542 (99%)	6 (1%)	73	85
6	b	216/216 (100%)	212 (98%)	4 (2%)	57	77
7	c	164/164 (100%)	164 (100%)	0	100	100
8	d	165/165 (100%)	164 (99%)	1 (1%)	86	91
9	e	148/148 (100%)	143 (97%)	5 (3%)	37	65
10	f	137/137 (100%)	136 (99%)	1 (1%)	84	90
11	g	114/114 (100%)	112 (98%)	2 (2%)	59	78
12	a	110/181 (61%)	107 (97%)	3 (3%)	44	71
13	i	109/110 (99%)	107 (98%)	2 (2%)	59	78
14	j	116/116 (100%)	116 (100%)	0	100	100
15	k	103/103 (100%)	103 (100%)	0	100	100
16	l	102/102 (100%)	101 (99%)	1 (1%)	76	86
17	m	109/109 (100%)	107 (98%)	2 (2%)	59	78
18	n	100/100 (100%)	99 (99%)	1 (1%)	76	86
19	o	86/86 (100%)	85 (99%)	1 (1%)	71	83
20	p	99/99 (100%)	99 (100%)	0	100	100
21	q	89/89 (100%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	r	84/84 (100%)	82 (98%)	2 (2%)	49	73
23	s	93/93 (100%)	93 (100%)	0	100	100
24	t	80/80 (100%)	80 (100%)	0	100	100
25	u	83/83 (100%)	83 (100%)	0	100	100
26	v	78/78 (100%)	78 (100%)	0	100	100
27	w	57/57 (100%)	57 (100%)	0	100	100
28	x	67/67 (100%)	67 (100%)	0	100	100
29	y	55/55 (100%)	55 (100%)	0	100	100
30	z	48/48 (100%)	48 (100%)	0	100	100
31	A	42/59 (71%)	42 (100%)	0	100	100
32	B	47/47 (100%)	47 (100%)	0	100	100
33	C	45/45 (100%)	45 (100%)	0	100	100
34	D	38/38 (100%)	37 (97%)	1 (3%)	46	71
35	E	51/51 (100%)	51 (100%)	0	100	100
36	F	34/34 (100%)	34 (100%)	0	100	100
39	G	180/186 (97%)	171 (95%)	9 (5%)	24	55
40	H	170/170 (100%)	168 (99%)	2 (1%)	71	83
41	I	172/172 (100%)	171 (99%)	1 (1%)	86	91
42	J	119/119 (100%)	111 (93%)	8 (7%)	16	45
43	K	87/87 (100%)	86 (99%)	1 (1%)	73	85
44	L	124/124 (100%)	121 (98%)	3 (2%)	49	73
45	M	104/104 (100%)	104 (100%)	0	100	100
46	N	105/105 (100%)	103 (98%)	2 (2%)	57	77
47	O	86/86 (100%)	86 (100%)	0	100	100
48	P	89/89 (100%)	87 (98%)	2 (2%)	52	74
49	Q	103/103 (100%)	101 (98%)	2 (2%)	57	77
50	R	92/92 (100%)	91 (99%)	1 (1%)	73	85
51	S	83/83 (100%)	81 (98%)	2 (2%)	49	73
52	T	76/76 (100%)	76 (100%)	0	100	100
53	U	65/65 (100%)	64 (98%)	1 (2%)	65	81
54	V	74/74 (100%)	73 (99%)	1 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	W	56/56 (100%)	55 (98%)	1 (2%)	59	78
56	X	70/70 (100%)	68 (97%)	2 (3%)	42	69
57	Y	65/65 (100%)	65 (100%)	0	100	100
58	Z	55/55 (100%)	55 (100%)	0	100	100
All	All	5392/5513 (98%)	5322 (99%)	70 (1%)	70	82

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	8	32	PHE
4	8	101	ARG
4	8	137	ARG
4	8	193	TRP
4	8	425	LYS
4	8	518	VAL
6	b	8	THR
6	b	86	ARG
6	b	128	THR
6	b	212	TRP
8	d	146	VAL
9	e	29	ARG
9	e	49	LEU
9	e	114	ARG
9	e	144	LYS
9	e	151	LEU
10	f	131	VAL
11	g	50	ARG
11	g	112	LYS
12	a	42	VAL
12	a	161	VAL
12	a	216	THR
13	i	48	ILE
13	i	81	LYS
16	l	94	THR
17	m	10	ARG
17	m	13	HIS
18	n	38	LEU
19	o	53	THR
22	r	51	VAL
22	r	54	VAL
34	D	33	ARG

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Mol	Chain	Res	Type
39	G	21	TYR
39	G	65	LYS
39	G	94	ARG
39	G	126	ASP
39	G	136	ARG
39	G	158	ASP
39	G	188	THR
39	G	221	ARG
39	G	222	GLU
40	H	152	VAL
40	H	199	VAL
41	I	18	LEU
42	J	30	PHE
42	J	47	PHE
42	J	53	ARG
42	J	94	PHE
42	J	132	PRO
42	J	146	MET
42	J	150	GLU
42	J	151	MET
43	K	54	LEU
44	L	10	LYS
44	L	108	ARG
44	L	112	ASP
46	N	26	LYS
46	N	65	THR
48	P	107	THR
48	P	127	ARG
49	Q	23	LEU
49	Q	86	VAL
50	R	112	ARG
51	S	41	TRP
51	S	59	GLN
53	U	8	ARG
54	V	16	MET
55	W	11	ARG
56	X	4	LEU
56	X	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
4	8	92	HIS
4	8	129	GLN
4	8	192	ASN
4	8	221	ASN
4	8	351	ASN
4	8	455	GLN
4	8	496	GLN
4	8	627	ASN
6	b	89	ASN
6	b	114	GLN
6	b	127	ASN
6	b	196	ASN
6	b	250	GLN
7	c	94	GLN
7	c	148	GLN
8	d	9	GLN
8	d	94	GLN
8	d	97	ASN
10	f	29	ASN
11	g	2	GLN
12	a	188	ASN
13	i	104	GLN
13	i	110	GLN
14	j	40	HIS
14	j	58	ASN
14	j	132	HIS
14	j	136	GLN
15	k	3	GLN
17	m	3	GLN
18	n	11	ASN
19	o	61	GLN
20	p	2	ASN
20	p	9	GLN
20	p	114	ASN
21	q	43	GLN
21	q	51	GLN
22	r	11	GLN
22	r	18	GLN
22	r	82	HIS
23	s	7	HIS
23	s	15	GLN
24	t	15	HIS
24	t	48	GLN

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Mol	Chain	Res	Type
25	u	65	GLN
25	u	68	ASN
26	v	12	GLN
26	v	75	GLN
27	w	8	ASN
28	x	15	ASN
29	y	58	ASN
34	D	16	HIS
39	G	41	ASN
39	G	145	ASN
39	G	176	ASN
39	G	177	ASN
40	H	184	ASN
41	I	39	GLN
41	I	115	GLN
41	I	163	GLN
42	J	69	ASN
42	J	81	GLN
42	J	120	HIS
42	J	131	ASN
42	J	145	ASN
43	K	63	ASN
43	K	81	ASN
45	M	3	GLN
45	M	17	GLN
45	M	66	GLN
46	N	30	ASN
47	O	15	HIS
47	O	64	GLN
48	P	23	HIS
48	P	39	ASN
52	T	27	GLN
52	T	36	ASN
53	U	59	HIS
54	V	46	HIS
55	W	51	GLN
56	X	13	HIS
56	X	51	HIS
57	Y	67	HIS
57	Y	69	ASN
57	Y	77	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	1538/1539 (99%)	201 (13%)	2 (0%)
2	1	2902/2903 (99%)	383 (13%)	9 (0%)
3	2	119/120 (99%)	12 (10%)	1 (0%)
37	4	14/39 (35%)	2 (14%)	0
38	5	76/77 (98%)	17 (22%)	0
5	6	76/77 (98%)	17 (22%)	0
All	All	4725/4755 (99%)	632 (13%)	12 (0%)

All (632) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	5	U
1	3	9	G
1	3	22	G
1	3	30	U
1	3	31	G
1	3	32	A
1	3	39	G
1	3	47	C
1	3	48	C
1	3	49	U
1	3	51	A
1	3	66	A
1	3	71	A
1	3	82	G
1	3	83	C
1	3	94	G
1	3	110	C
1	3	116	A
1	3	130	A
1	3	131	A
1	3	164	G
1	3	168	G
1	3	183	C
1	3	184	G
1	3	209	U
1	3	210	C
1	3	212	G
1	3	238	A
1	3	247	G
1	3	251	G

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Mol	Chain	Res	Type
1	3	266	G
1	3	267	C
1	3	281	G
1	3	289	G
1	3	298	A
1	3	316	C
1	3	328	C
1	3	329	A
1	3	330	C
1	3	345	C
1	3	346	G
1	3	347	G
1	3	348	G
1	3	352	C
1	3	354	G
1	3	367	U
1	3	372	C
1	3	381	C
1	3	387	U
1	3	392	C
1	3	397	A
1	3	398	U
1	3	411	A
1	3	412	A
1	3	413	G
1	3	414	A
1	3	421	U
1	3	423	G
1	3	429	U
1	3	439	U
1	3	441	A
1	3	467	U
1	3	474	G
1	3	486	U
1	3	497	G
1	3	508	U
1	3	509	A
1	3	518	C
1	3	532	A
1	3	533	A
1	3	542	G
1	3	547	A

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Mol	Chain	Res	Type
1	3	561	U
1	3	562	U
1	3	572	A
1	3	573	A
1	3	576	C
1	3	577	G
1	3	618	C
1	3	633	G
1	3	665	A
1	3	687	A
1	3	688	G
1	3	690	G
1	3	702	A
1	3	703	G
1	3	718	A
1	3	721	G
1	3	723	U
1	3	724	G
1	3	733	G
1	3	747	A
1	3	755	G
1	3	776	G
1	3	777	A
1	3	781	A
1	3	793	U
1	3	794	A
1	3	796	C
1	3	814	A
1	3	817	C
1	3	818	G
1	3	819	A
1	3	821	G
1	3	842	U
1	3	843	U
1	3	844	G
1	3	846	G
1	3	872	A
1	3	875	U
1	3	902	G
1	3	915	A
1	3	934	C
1	3	935	A

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Mol	Chain	Res	Type
1	3	960	U
1	3	969	A
1	3	976	G
1	3	977	A
1	3	978	A
1	3	979	C
1	3	981	U
1	3	992	U
1	3	993	G
1	3	994	A
1	3	1004	A
1	3	1011	C
1	3	1033	G
1	3	1034	G
1	3	1036	A
1	3	1054	C
1	3	1055	A
1	3	1064	G
1	3	1065	U
1	3	1091	U
1	3	1092	A
1	3	1094	G
1	3	1095	U
1	3	1101	A
1	3	1114	C
1	3	1115	U
1	3	1119	C
1	3	1136	C
1	3	1137	C
1	3	1138	G
1	3	1139	G
1	3	1159	U
1	3	1160	G
1	3	1165	U
1	3	1168	U
1	3	1169	A
1	3	1171	A
1	3	1173	U
1	3	1182	G
1	3	1183	U
1	3	1190	G
1	3	1196	A

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Mol	Chain	Res	Type
1	3	1201	A
1	3	1212	U
1	3	1213	A
1	3	1217	C
1	3	1225	A
1	3	1226	C
1	3	1238	A
1	3	1256	A
1	3	1257	A
1	3	1258	G
1	3	1275	A
1	3	1278	G
1	3	1280	A
1	3	1282	C
1	3	1286	U
1	3	1287	A
1	3	1290	G
1	3	1291	U
1	3	1300	G
1	3	1308	U
1	3	1320	C
1	3	1321	U
1	3	1322	C
1	3	1323	G
1	3	1331	G
1	3	1342	C
1	3	1346	A
1	3	1363	A
1	3	1364	U
1	3	1378	C
1	3	1389	C
1	3	1394	A
1	3	1441	A
1	3	1446	A
1	3	1452	C
1	3	1492	A
1	3	1493	A
1	3	1497	G
1	3	1503	A
1	3	1506	U
1	3	1517	G
1	3	1518	A

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Mol	Chain	Res	Type
1	3	1529	G
1	3	1530	G
1	3	1534	A
2	1	10	A
2	1	12	U
2	1	13	A
2	1	34	U
2	1	35	G
2	1	39	G
2	1	46	G
2	1	51	G
2	1	71	A
2	1	74	A
2	1	75	G
2	1	84	A
2	1	119	A
2	1	120	U
2	1	121	G
2	1	125	A
2	1	140	C
2	1	141	G
2	1	142	A
2	1	162	U
2	1	163	C
2	1	181	A
2	1	196	A
2	1	216	A
2	1	221	A
2	1	222	A
2	1	228	C
2	1	229	C
2	1	248	G
2	1	250	G
2	1	255	A
2	1	264	C
2	1	266	G
2	1	276	U
2	1	281	C
2	1	311	A
2	1	323	C
2	1	324	A
2	1	329	G

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Mol	Chain	Res	Type
2	1	330	A
2	1	346	A
2	1	361	G
2	1	371	A
2	1	372	G
2	1	386	G
2	1	387	U
2	1	389	G
2	1	396	G
2	1	404	A
2	1	406	G
2	1	411	G
2	1	424	G
2	1	448	U
2	1	449	A
2	1	457	A
2	1	481	G
2	1	490	C
2	1	491	G
2	1	501	A
2	1	504	A
2	1	505	A
2	1	509	C
2	1	510	C
2	1	529	A
2	1	530	G
2	1	531	C
2	1	532	A
2	1	548	G
2	1	549	G
2	1	563	A
2	1	573	U
2	1	588	U
2	1	603	A
2	1	613	A
2	1	614	A
2	1	616	A
2	1	627	A
2	1	631	A
2	1	637	A
2	1	645	C
2	1	646	U

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Mol	Chain	Res	Type
2	1	648	G
2	1	654	A
2	1	655	A
2	1	669	G
2	1	686	U
2	1	695	G
2	1	717	C
2	1	729	G
2	1	730	A
2	1	747	C
2	1	762	U
2	1	764	A
2	1	773	U
2	1	776	G
2	1	782	A
2	1	784	G
2	1	785	G
2	1	789	A
2	1	800	A
2	1	804	A
2	1	805	G
2	1	811	U
2	1	812	C
2	1	819	A
2	1	827	U
2	1	845	A
2	1	846	U
2	1	847	U
2	1	858	G
2	1	859	G
2	1	878	A
2	1	883	G
2	1	885	C
2	1	886	A
2	1	887	U
2	1	891	G
2	1	896	A
2	1	897	C
2	1	898	C
2	1	910	A
2	1	932	U
2	1	941	A

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Mol	Chain	Res	Type
2	1	946	C
2	1	953	G
2	1	961	C
2	1	962	G
2	1	974	G
2	1	975	A
2	1	983	A
2	1	985	C
2	1	990	A
2	1	995	C
2	1	996	A
2	1	1012	U
2	1	1013	C
2	1	1022	G
2	1	1023	U
2	1	1024	G
2	1	1033	U
2	1	1045	C
2	1	1057	A
2	1	1058	U
2	1	1061	U
2	1	1062	G
2	1	1065	U
2	1	1066	U
2	1	1070	A
2	1	1071	G
2	1	1081	U
2	1	1082	U
2	1	1084	A
2	1	1085	A
2	1	1088	A
2	1	1104	C
2	1	1111	A
2	1	1131	G
2	1	1134	A
2	1	1135	C
2	1	1142	A
2	1	1143	A
2	1	1169	A
2	1	1171	G
2	1	1174	U
2	1	1175	A

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Mol	Chain	Res	Type
2	1	1176	U
2	1	1177	G
2	1	1178	C
2	1	1180	U
2	1	1186	G
2	1	1204	A
2	1	1212	G
2	1	1238	G
2	1	1251	C
2	1	1253	A
2	1	1255	U
2	1	1256	G
2	1	1271	G
2	1	1272	A
2	1	1273	U
2	1	1275	A
2	1	1293	C
2	1	1301	A
2	1	1321	A
2	1	1329	U
2	1	1341	G
2	1	1345	C
2	1	1352	U
2	1	1365	A
2	1	1378	A
2	1	1379	U
2	1	1383	A
2	1	1395	A
2	1	1403	A
2	1	1416	G
2	1	1419	A
2	1	1420	A
2	1	1427	A
2	1	1428	C
2	1	1454	C
2	1	1461	C
2	1	1475	G
2	1	1482	G
2	1	1490	A
2	1	1494	A
2	1	1503	A
2	1	1510	G

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Mol	Chain	Res	Type
2	1	1515	A
2	1	1524	G
2	1	1535	A
2	1	1536	C
2	1	1537	G
2	1	1547	C
2	1	1558	C
2	1	1560	G
2	1	1567	G
2	1	1584	U
2	1	1585	C
2	1	1608	A
2	1	1616	A
2	1	1618	A
2	1	1627	G
2	1	1634	A
2	1	1647	U
2	1	1648	U
2	1	1660	G
2	1	1674	G
2	1	1700	A
2	1	1706	C
2	1	1707	G
2	1	1713	A
2	1	1715	G
2	1	1729	U
2	1	1730	C
2	1	1731	G
2	1	1732	C
2	1	1738	G
2	1	1758	U
2	1	1764	C
2	1	1773	A
2	1	1800	C
2	1	1801	A
2	1	1808	A
2	1	1813	G
2	1	1816	C
2	1	1819	A
2	1	1829	A
2	1	1851	U
2	1	1901	A

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Mol	Chain	Res	Type
2	1	1906	G
2	1	1913	A
2	1	1914	C
2	1	1929	G
2	1	1931	U
2	1	1938	A
2	1	1939	U
2	1	1940	U
2	1	1944	U
2	1	1945	G
2	1	1955	U
2	1	1963	U
2	1	1964	G
2	1	1967	C
2	1	1969	A
2	1	1970	A
2	1	1971	U
2	1	1972	G
2	1	1982	U
2	1	1993	U
2	1	1997	C
2	1	2002	G
2	1	2022	U
2	1	2023	C
2	1	2030	A
2	1	2031	A
2	1	2033	A
2	1	2043	C
2	1	2049	G
2	1	2055	C
2	1	2056	G
2	1	2060	A
2	1	2061	G
2	1	2062	A
2	1	2069	G
2	1	2072	C
2	1	2087	G
2	1	2096	C
2	1	2100	G
2	1	2110	G
2	1	2111	U
2	1	2112	G

Continued on next page...

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Mol	Chain	Res	Type
2	1	2118	U
2	1	2119	A
2	1	2132	U
2	1	2134	A
2	1	2145	C
2	1	2147	A
2	1	2166	U
2	1	2172	U
2	1	2173	A
2	1	2181	U
2	1	2189	U
2	1	2198	A
2	1	2204	G
2	1	2211	A
2	1	2213	U
2	1	2225	A
2	1	2238	G
2	1	2239	G
2	1	2243	U
2	1	2279	G
2	1	2283	C
2	1	2287	A
2	1	2305	U
2	1	2309	A
2	1	2325	G
2	1	2327	A
2	1	2333	A
2	1	2347	C
2	1	2350	C
2	1	2373	G
2	1	2383	G
2	1	2385	C
2	1	2388	A
2	1	2391	G
2	1	2392	A
2	1	2402	U
2	1	2406	A
2	1	2423	U
2	1	2425	A
2	1	2429	G
2	1	2441	U
2	1	2448	A

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Mol	Chain	Res	Type
2	1	2476	A
2	1	2490	G
2	1	2498	C
2	1	2502	G
2	1	2504	U
2	1	2505	G
2	1	2518	A
2	1	2520	C
2	1	2529	G
2	1	2530	A
2	1	2547	A
2	1	2554	U
2	1	2566	A
2	1	2567	G
2	1	2573	C
2	1	2574	G
2	1	2602	A
2	1	2603	G
2	1	2609	U
2	1	2613	U
2	1	2629	U
2	1	2630	G
2	1	2645	G
2	1	2646	C
2	1	2660	A
2	1	2682	A
2	1	2689	U
2	1	2690	U
2	1	2713	U
2	1	2714	G
2	1	2716	C
2	1	2733	A
2	1	2744	G
2	1	2748	A
2	1	2778	A
2	1	2779	U
2	1	2791	G
2	1	2794	C
2	1	2797	U
2	1	2799	A
2	1	2800	A
2	1	2820	A

Continued on next page...

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Mol	Chain	Res	Type
2	1	2821	A
2	1	2833	U
2	1	2866	U
2	1	2867	G
2	1	2868	A
2	1	2883	A
2	1	2884	U
2	1	2893	A
3	2	2	G
3	2	4	C
3	2	15	A
3	2	24	G
3	2	35	C
3	2	41	G
3	2	44	G
3	2	53	A
3	2	84	G
3	2	89	U
3	2	90	C
3	2	109	A
5	6	8	U
5	6	9	G
5	6	10	G
5	6	14	A
5	6	16	C
5	6	17(A)	U
5	6	19	G
5	6	20	U
5	6	21	A
5	6	22	G
5	6	28	C
5	6	41	C
5	6	45	G
5	6	46	G
5	6	47	U
5	6	58	A
5	6	61	C
37	4	9	G
37	4	16	A
38	5	3	G
38	5	4	C
38	5	5	G

Continued on next page...

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Mol	Chain	Res	Type
38	5	6	A
38	5	8	U
38	5	16	C
38	5	17(A)	U
38	5	18	G
38	5	19	G
38	5	20	U
38	5	22	G
38	5	46	G
38	5	48	C
38	5	49	G
38	5	61	C
38	5	73	A
38	5	76	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	70	U
1	3	1257	A
2	1	490	C
2	1	784	G
2	1	896	A
2	1	1130	U
2	1	1730	C
2	1	1930	G
2	1	2326	C
2	1	2391	G
2	1	2519	U
3	2	88	C

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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
59	GDP	8	801	-	24,30,30	0.99	1 (4%)	30,47,47	1.35	4 (13%)

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
59	GDP	8	801	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	8	801	GDP	C6-N1	-2.84	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	8	801	GDP	PA-O3A-PB	-3.65	120.30	132.83
59	8	801	GDP	C3'-C2'-C1'	3.05	105.57	100.98
59	8	801	GDP	C5-C6-N1	2.32	118.05	113.95
59	8	801	GDP	C8-N7-C5	2.25	107.28	102.99

There are no chirality outliers.

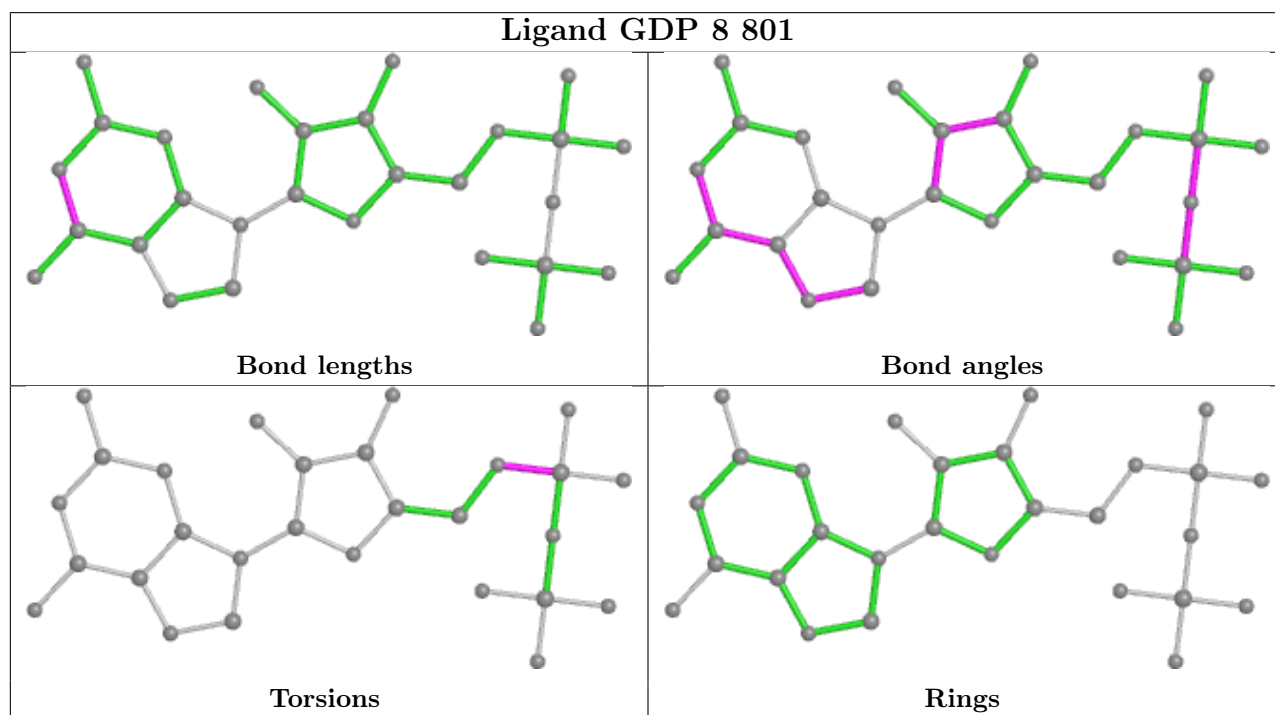
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	8	801	GDP	C5'-O5'-PA-O1A
59	8	801	GDP	C5'-O5'-PA-O3A
59	8	801	GDP	C5'-O5'-PA-O2A

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](#)

There are no chain breaks in this entry.

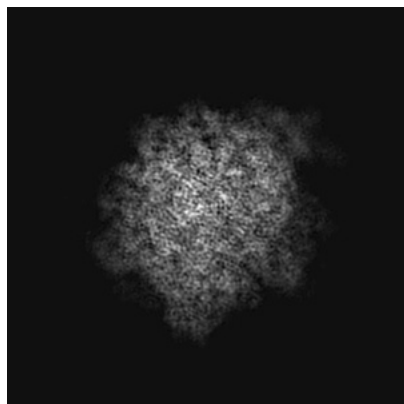
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25407. These allow visual inspection of the internal detail of the map and identification of artifacts.

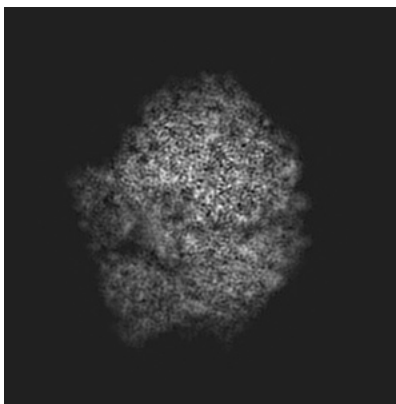
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

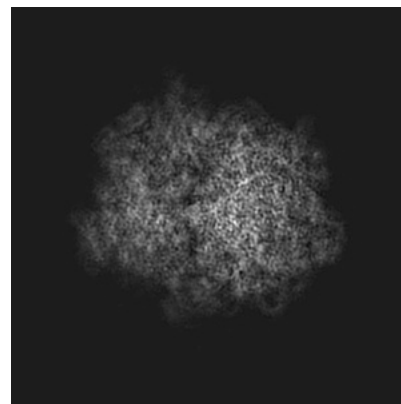
6.1.1 Primary map



X

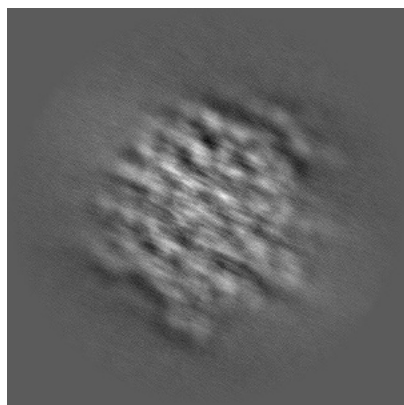


Y

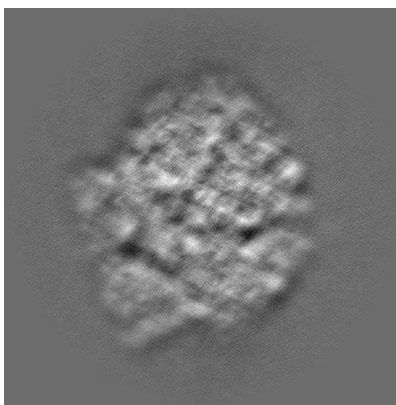


Z

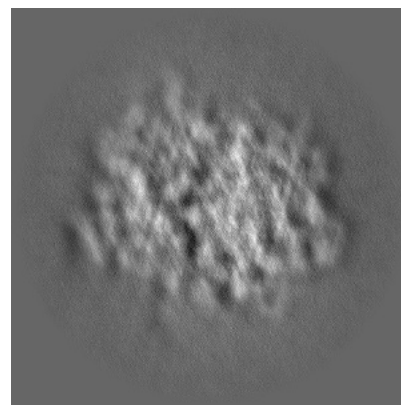
6.1.2 Raw map



X



Y

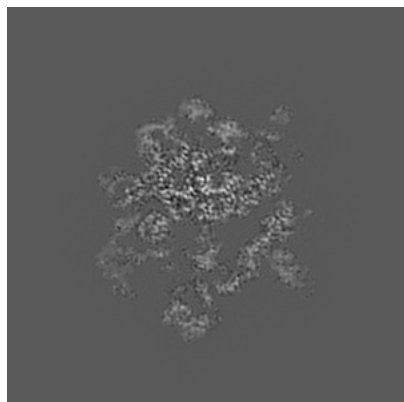


Z

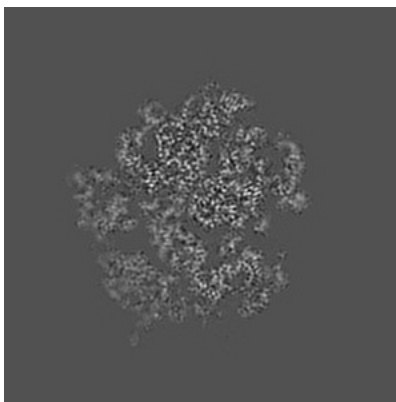
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

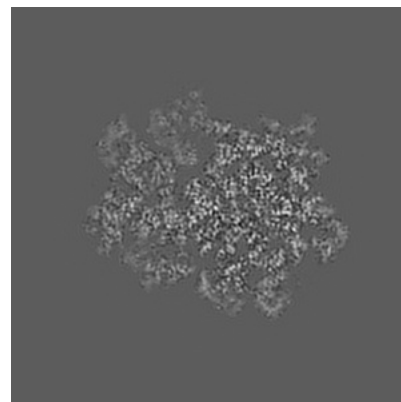
6.2.1 Primary map



X Index: 224

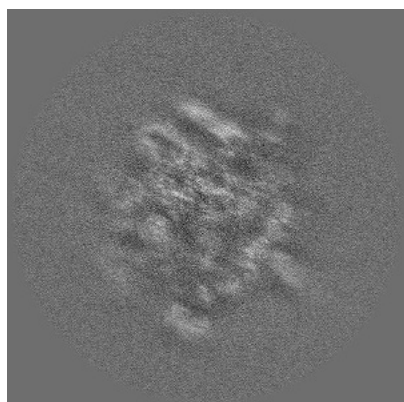


Y Index: 224

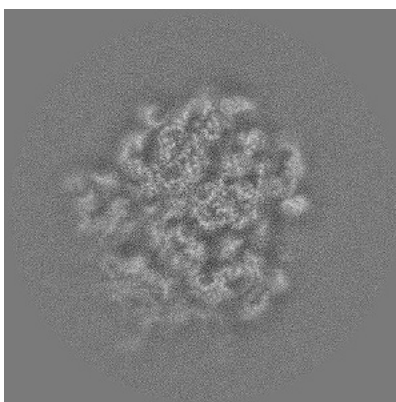


Z Index: 224

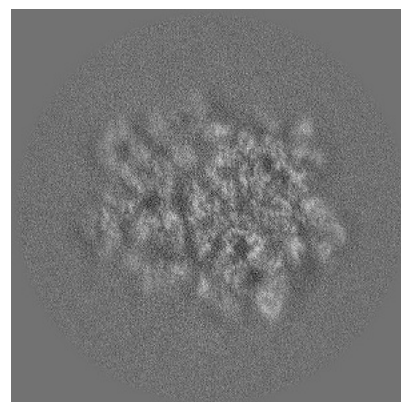
6.2.2 Raw map



X Index: 224



Y Index: 224

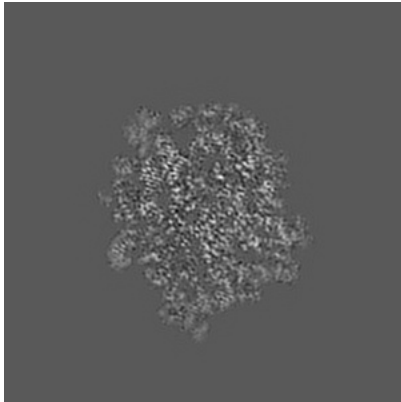


Z Index: 224

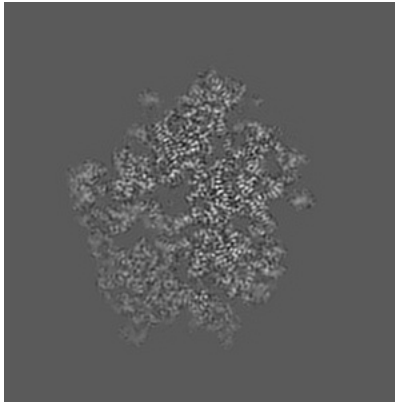
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

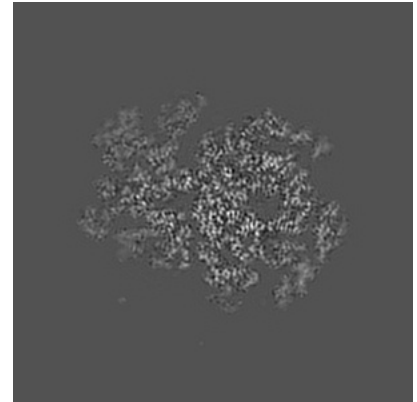
6.3.1 Primary map



X Index: 257

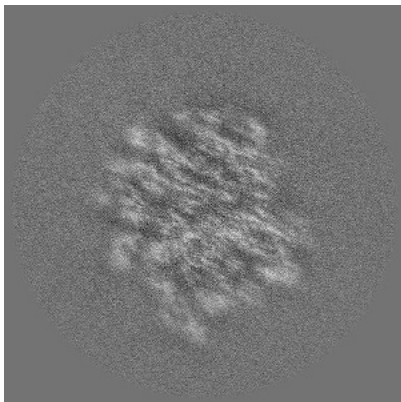


Y Index: 210

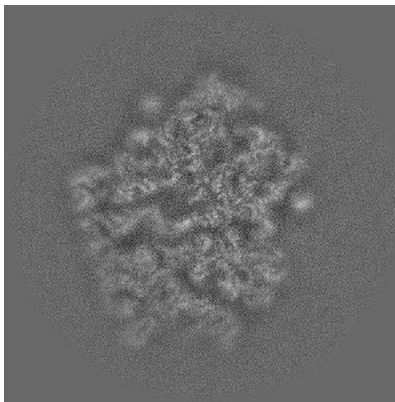


Z Index: 238

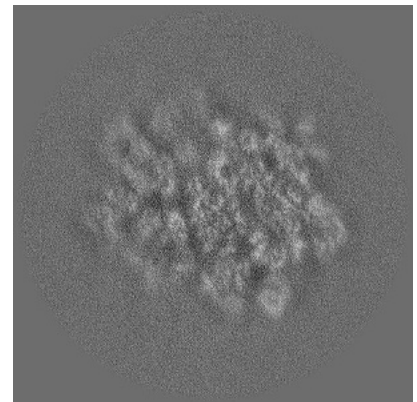
6.3.2 Raw map



X Index: 252



Y Index: 210

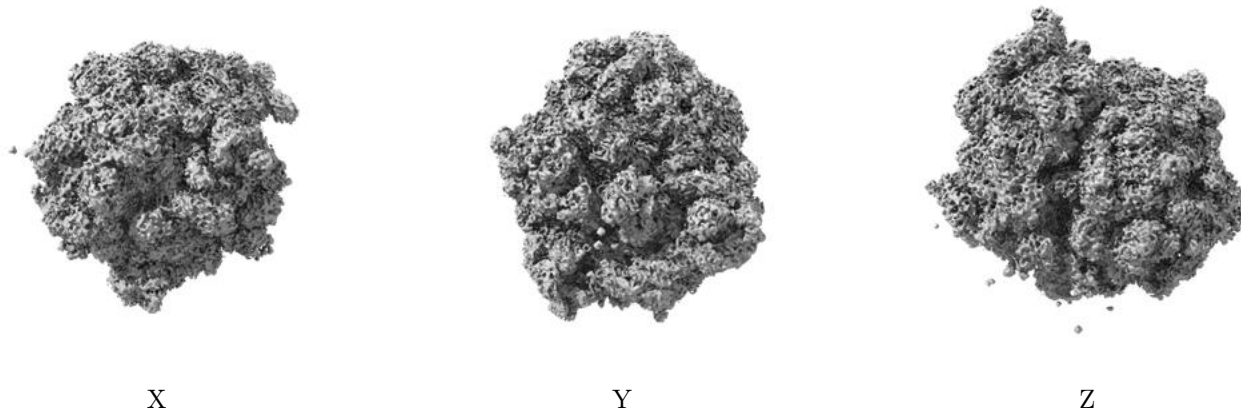


Z Index: 227

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

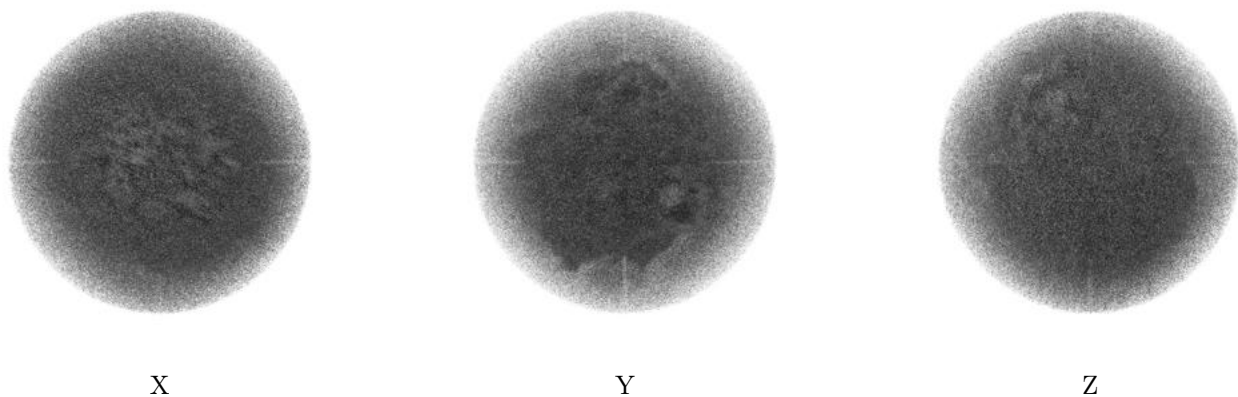
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

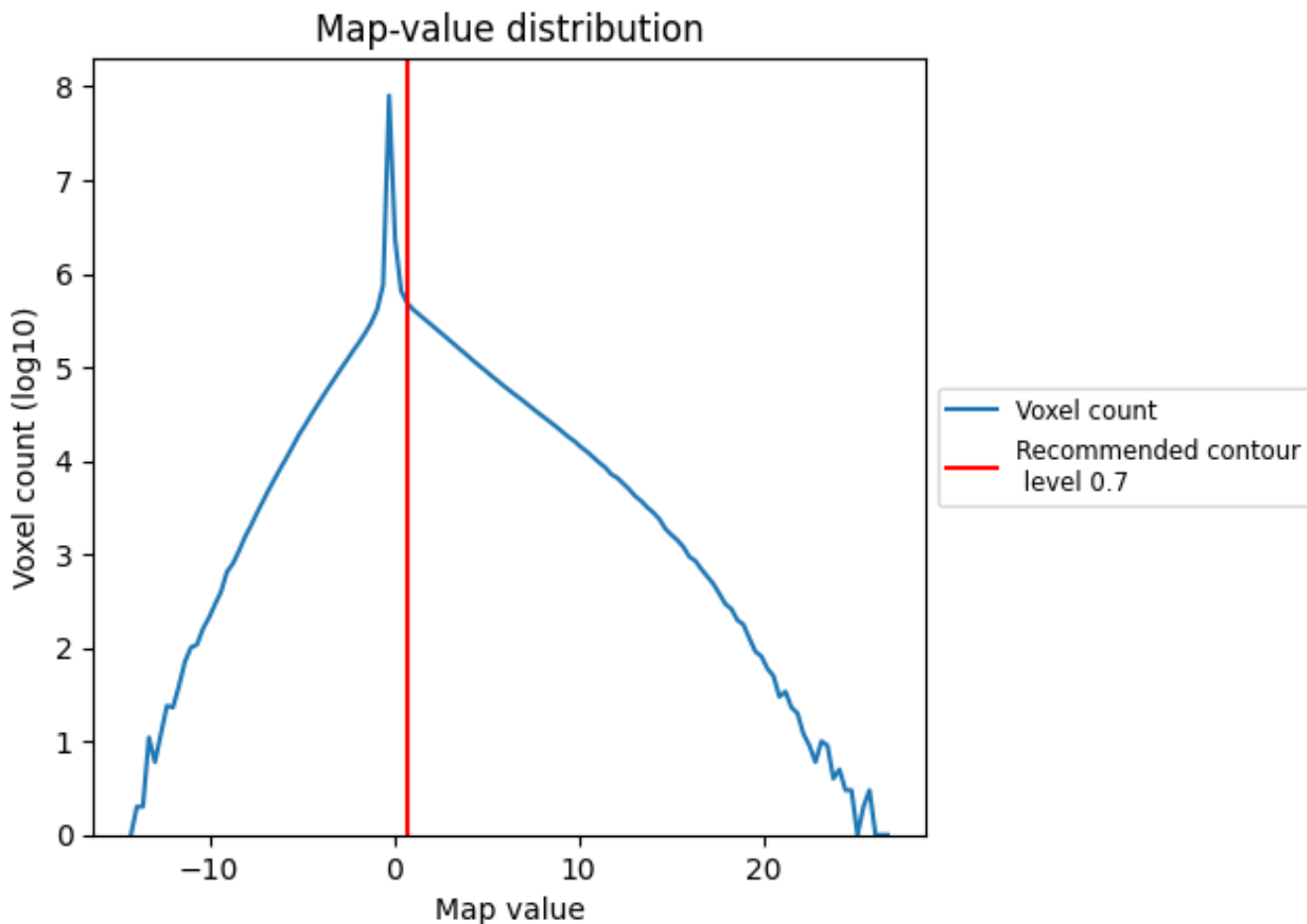
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

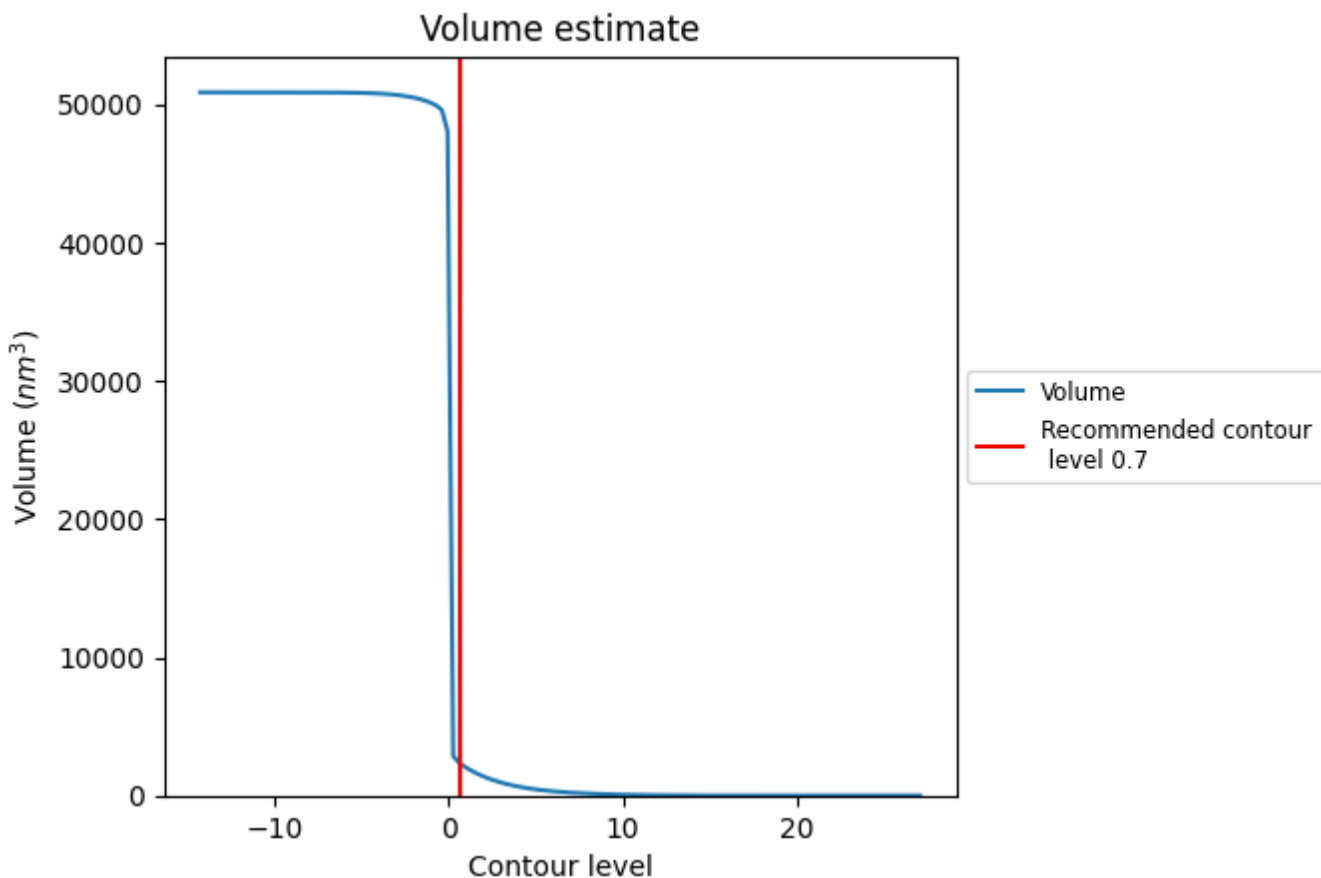
This section contains the results of statistical analysis of the map.

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.

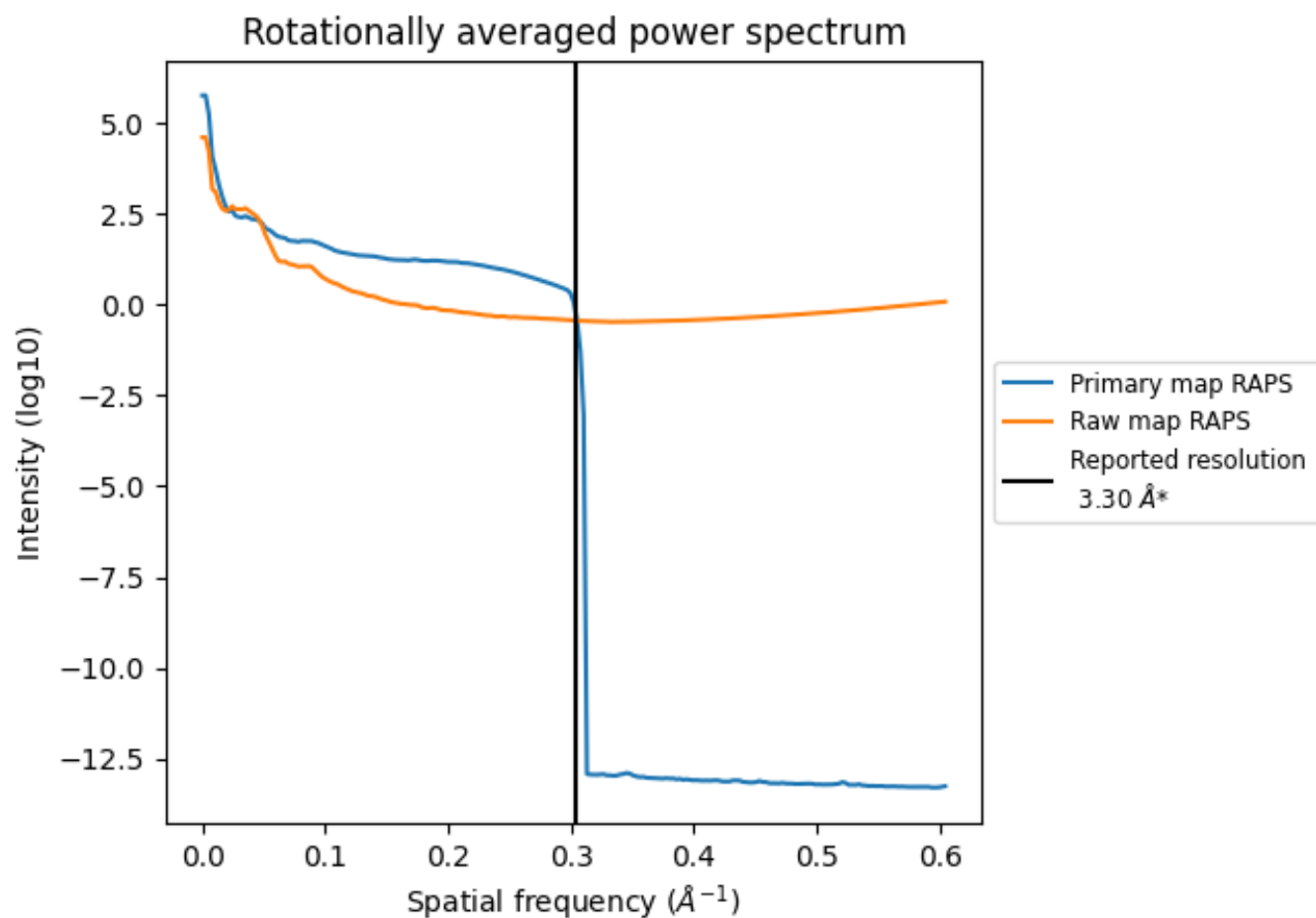
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2300 nm³; this corresponds to an approximate mass of 2078 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

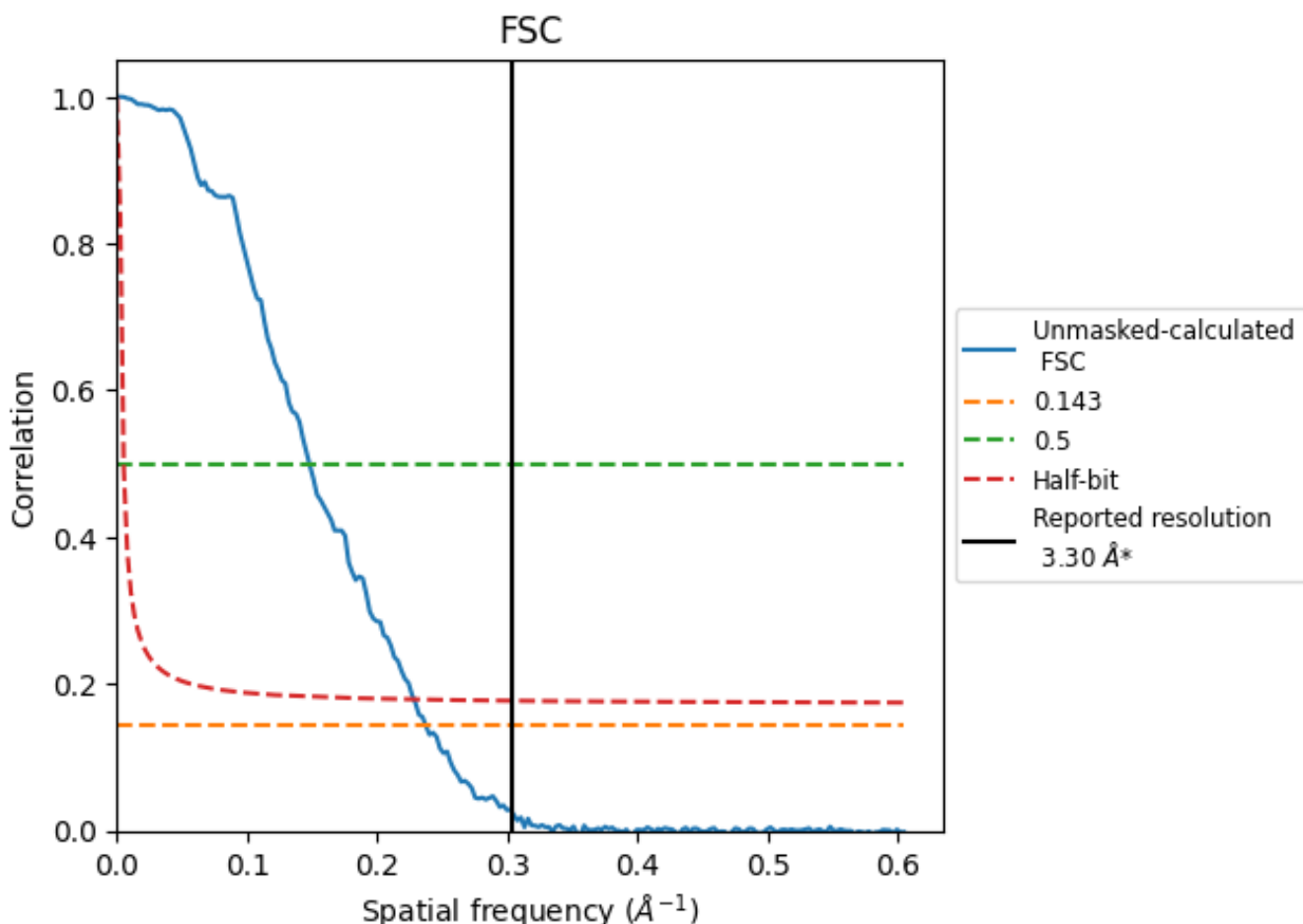


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303\AA^{-1}

8.2 Resolution estimates [i](#)

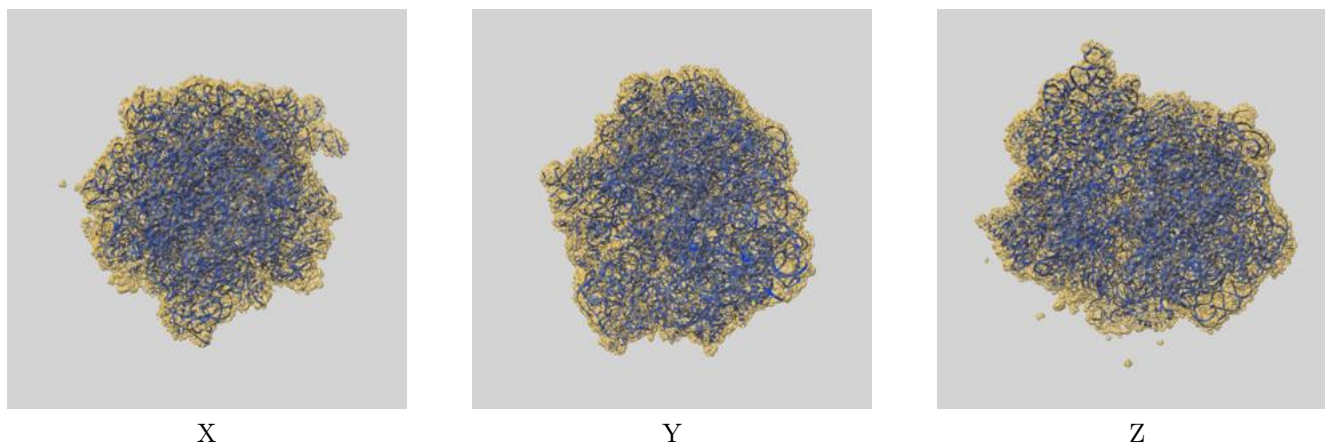
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.21	6.76	4.38

*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 4.21 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

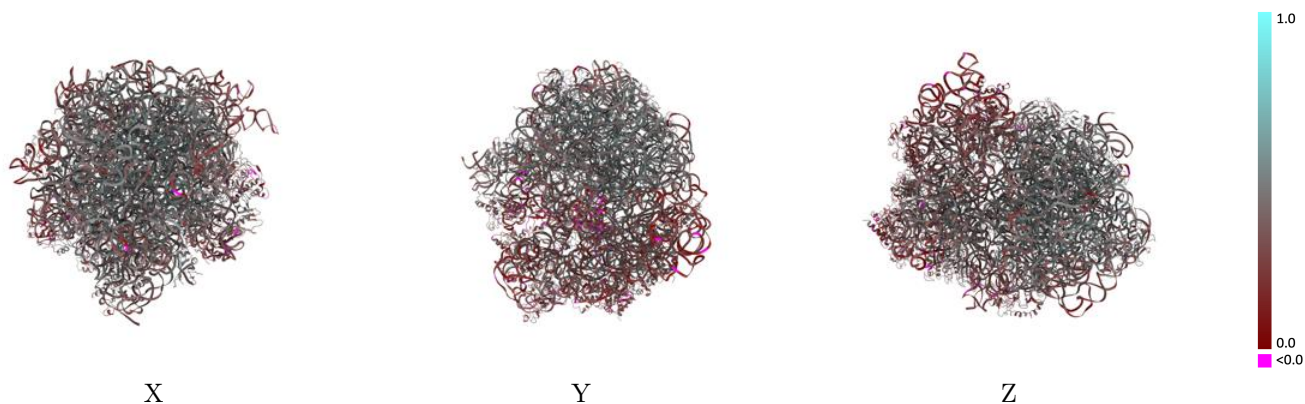
This section contains information regarding the fit between EMDB map EMD-25407 and PDB model 7SSD. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



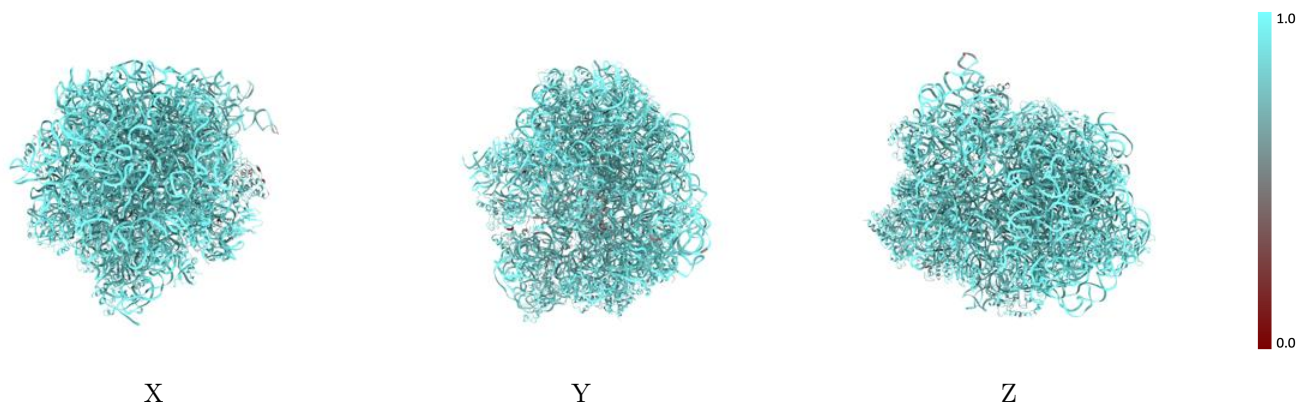
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



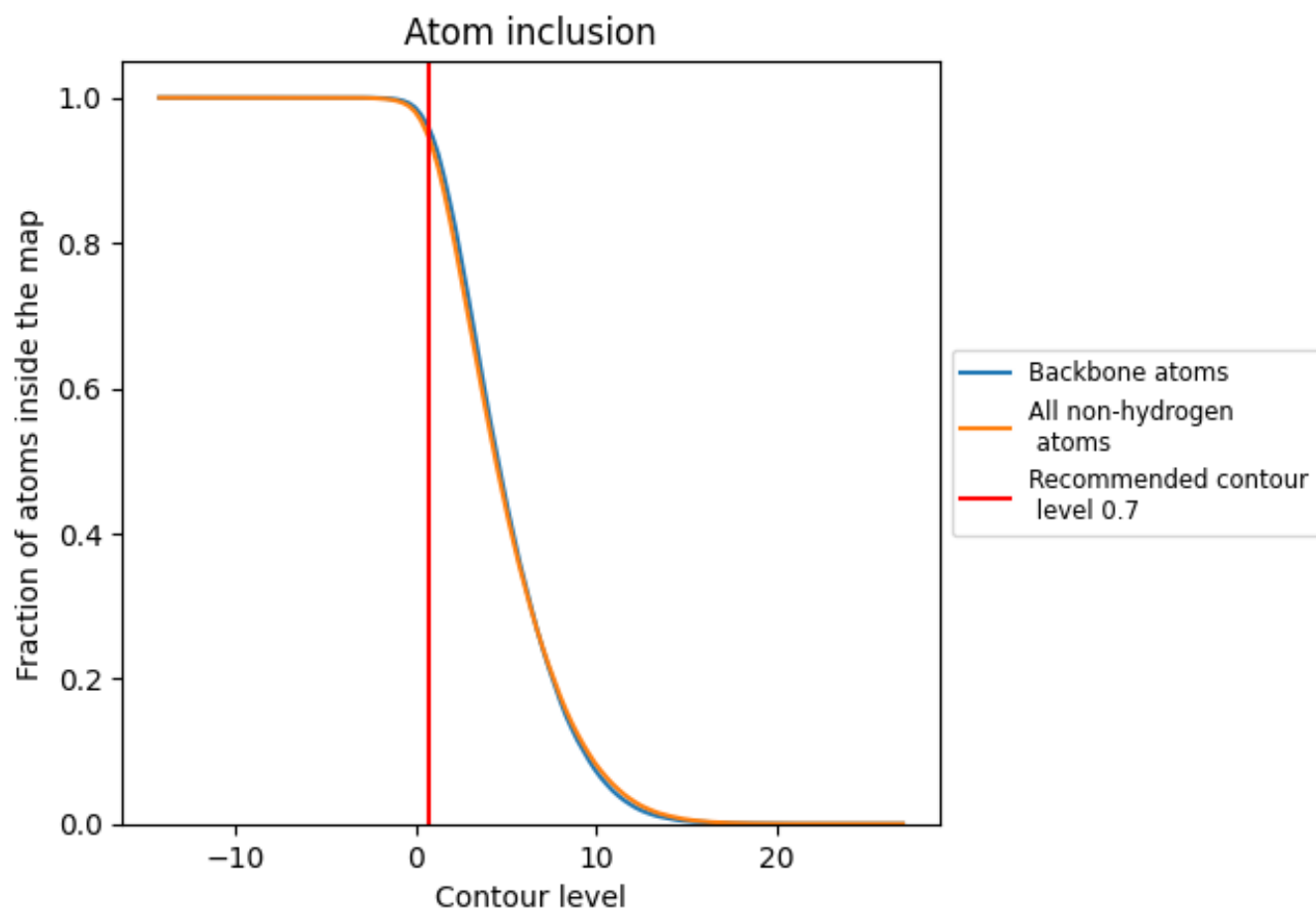
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9462	 0.3850
1	 0.9738	 0.4280
2	 0.9774	 0.3950
3	 0.9418	 0.3230
4	 0.8171	 0.1920
5	 0.9447	 0.3160
6	 0.9445	 0.3080
8	 0.8232	 0.2730
A	 0.9261	 0.3310
B	 0.9743	 0.4730
C	 0.8856	 0.3930
D	 0.9577	 0.5160
E	 0.9715	 0.5020
F	 0.9452	 0.4570
G	 0.8508	 0.2790
H	 0.8917	 0.3170
I	 0.9038	 0.2880
J	 0.9374	 0.3710
K	 0.9486	 0.3490
L	 0.8515	 0.2810
M	 0.9500	 0.4130
N	 0.8805	 0.3240
O	 0.8399	 0.2630
P	 0.9492	 0.3980
Q	 0.9034	 0.3800
R	 0.8615	 0.2820
S	 0.9096	 0.3160
T	 0.9536	 0.3960
U	 0.9250	 0.3660
V	 0.9384	 0.3650
W	 0.9612	 0.4030
X	 0.8666	 0.2880
Y	 0.9415	 0.3570
Z	 0.9131	 0.3540
a	 0.8543	 0.2550



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Chain	Atom inclusion	Q-score
b	 0.9668	 0.4920
c	 0.9623	 0.4710
d	 0.9592	 0.4490
e	 0.9192	 0.3470
f	 0.9537	 0.4090
g	 0.7911	 0.2970
i	 0.7427	 0.2190
j	 0.9645	 0.4840
k	 0.9639	 0.4720
l	 0.9705	 0.4640
m	 0.9587	 0.4640
n	 0.9577	 0.4670
o	 0.9571	 0.4220
p	 0.9606	 0.4690
q	 0.9692	 0.4820
r	 0.9611	 0.4440
s	 0.9809	 0.4840
t	 0.9654	 0.4670
u	 0.9583	 0.4140
v	 0.9621	 0.4350
w	 0.9589	 0.4860
x	 0.9667	 0.4770
y	 0.9376	 0.4040
z	 0.9680	 0.4630