Full wwPDB EM Validation Report

Apr 20, 2024 – 01:46 pm BST

PDB ID	:	8QOA
EMDB ID	:	EMD-18534
Title	:	Structure of SecM-stalled Escherichia coli 70S ribosome
Authors	:	Gersteuer, F.; Morici, M.; Wilson, D.N.
Deposited on	:	2023-09-28
Resolution	:	2.00 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:

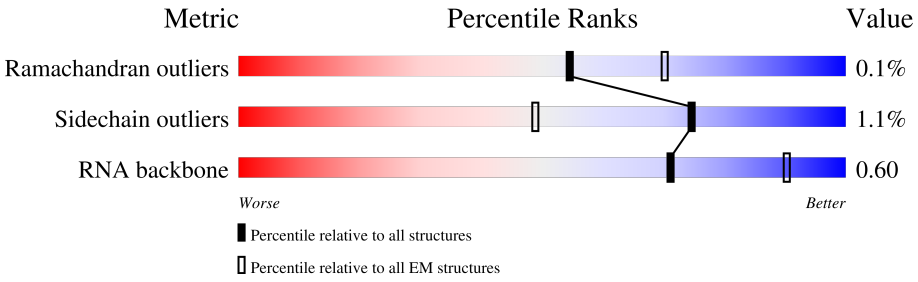
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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)
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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	89% 11%
2	1	46	96%
3	2	65	94% 5%
4	3	38	97%
5	5	2	50% 50%
6	B	241	91% 7%
7	C	233	88% 12%
8	D	206	97%

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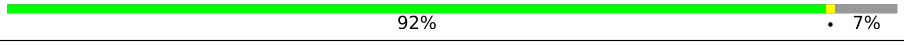
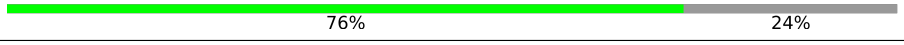
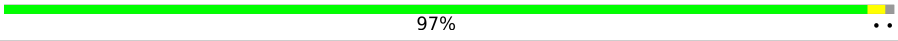
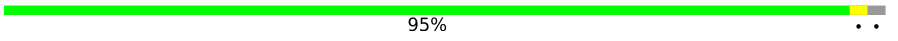
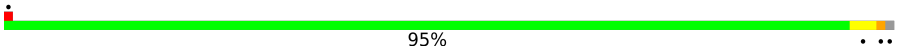
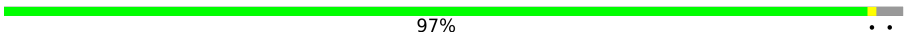
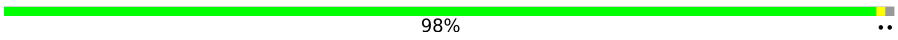
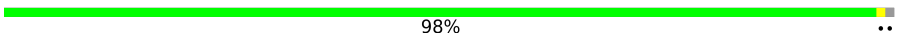
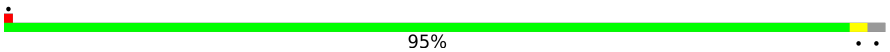
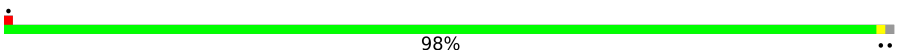
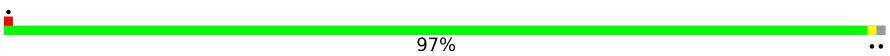
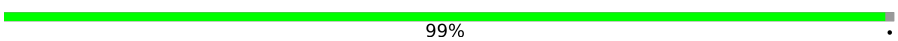
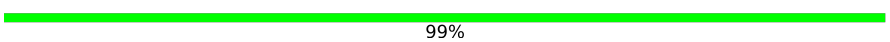
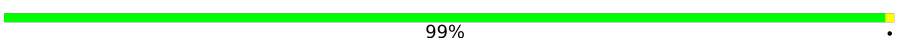
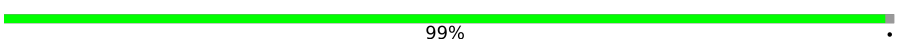
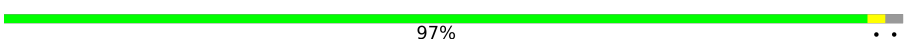
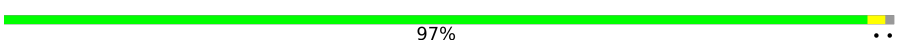
Mol	Chain	Length	Quality of chain
9	E	167	
10	F	135	
11	G	179	
12	H	130	
13	I	130	
14	L	124	
15	M	118	
16	N	101	
17	O	89	
18	P	82	
19	Q	84	
20	R	75	
21	S	92	
22	T	87	
23	U	71	
24	X	9	
25	Z	76	
26	b	120	
27	c	273	
28	d	209	
29	e	201	
30	f	179	
31	g	177	
32	h	149	
33	i	142	

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Mol	Chain	Length	Quality of chain
34	j	123	99%
35	k	144	100%
36	m	127	92% 7%
37	n	117	99%
38	o	115	97%
39	p	118	97%
40	q	103	99%
41	r	110	96%
42	s	100	93% 7%
43	t	104	96%
44	u	94	99%
45	v	85	98%
46	w	78	96%
47	x	63	94%
48	y	59	95% 5%
49	z	57	93% 7%
50	Y	77	81% 19%
51	4	70	86% 14%
52	a	2904	82% 12% 5%
53	A	1542	78% 18%
54	J	103	91% 5%
55	6	34	94% 6%
56	l	136	99%
57	K	129	88% 10%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 147750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	49	Total	C	N	O	0	0
			405	261	74	70		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

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

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 10 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	80	Total	C	N	O	0	0
			635	398	126	111		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	77	Total	C	N	O	S	0	0
			624	394	117	110	3		

- Molecule 20 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	9	Total	C	N	O	P	0	0
			189	84	31	65	9		

- Molecule 25 is a RNA chain called P-site tRNA-gly.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	76	Total	C	N	O	P	0	0
			1621	722	287	536	76		

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 27 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	208	Total	C	N	O	S	0	0
			1558	975	287	293	3		

- Molecule 29 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 32 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 33 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 36 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 39 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	84	Total	C	N	O	S	0	0
			628	388	126	113	1		

- Molecule 46 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	61	Total	C	N	O	S	0	0
			492	302	96	93	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	56	Total	C	N	O	S	0	0
			435	272	84	77	2		

- Molecule 49 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	53	Total	C	N	O	S	0	0
			421	254	90	76	1		

- Molecule 50 is a RNA chain called A-site tRNA-pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	77	Total	C	N	O	P	0	0
			1644	733	295	540	76		

- Molecule 51 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 52 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1513	Total	C	N	O	P	0	0
			32469	14484	5958	10514	1513		

- Molecule 54 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 55 is a protein called Secretion monitor.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	6	34	Total	C	N	O	0	0
			270	174	48	48		

- Molecule 56 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	variant	UNP P0ADY7

- Molecule 57 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	K	116	Total	C	N	O	S	0	0
			869	535	172	159	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	3	1	Total	Zn	0
			1	1	
58	4	1	Total	Zn	0
			1	1	

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	D	1	Total	K	0
			1	1	
59	F	1	Total	K	0
			1	1	
59	M	1	Total	K	0
			1	1	
59	Z	1	Total	K	0
			1	1	
59	c	3	Total	K	0
			3	3	
59	e	1	Total	K	0
			1	1	

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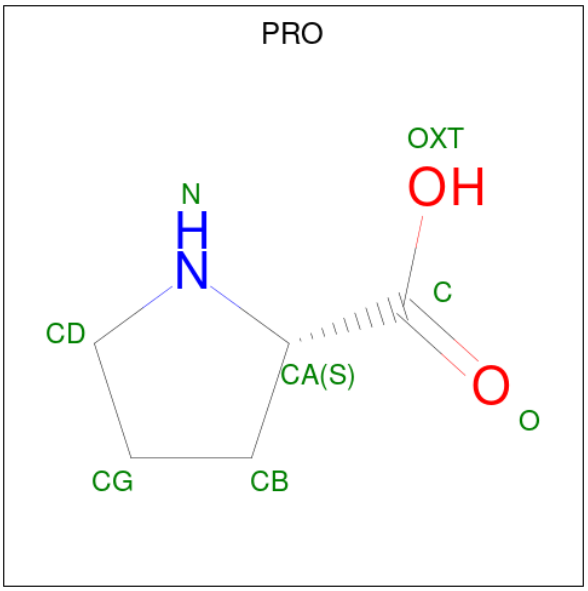
Mol	Chain	Residues	Atoms	AltConf
59	v	1	Total K 1 1	0
59	a	89	Total K 89 89	0
59	A	34	Total K 34 34	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
60	X	1	Total Mg 1 1	0
60	Z	1	Total Mg 1 1	0
60	b	5	Total Mg 5 5	0
60	c	2	Total Mg 2 2	0
60	d	1	Total Mg 1 1	0
60	p	1	Total Mg 1 1	0
60	z	1	Total Mg 1 1	0
60	a	217	Total Mg 217 217	0
60	A	59	Total Mg 59 59	0

- Molecule 61 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms	AltConf
61	Y	1	Total C N O 7 5 1 1	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	AltConf
62	0	9	Total O 9 9	0
62	1	19	Total O 19 19	0
62	2	23	Total O 23 23	0
62	3	5	Total O 5 5	0
62	5	2	Total O 2 2	0
62	C	1	Total O 1 1	0
62	D	2	Total O 2 2	0
62	E	4	Total O 4 4	0
62	G	1	Total O 1 1	0
62	H	4	Total O 4 4	0
62	L	11	Total O 11 11	0

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Mol	Chain	Residues	Atoms	AltConf
62	N	1	Total O 1 1	0
62	O	2	Total O 2 2	0
62	P	2	Total O 2 2	0
62	Q	1	Total O 1 1	0
62	R	3	Total O 3 3	0
62	T	1	Total O 1 1	0
62	U	2	Total O 2 2	0
62	X	5	Total O 5 5	0
62	Z	8	Total O 8 8	0
62	b	60	Total O 60 60	0
62	c	109	Total O 109 109	0
62	d	59	Total O 59 59	0
62	e	45	Total O 45 45	0
62	f	1	Total O 1 1	0
62	h	1	Total O 1 1	0
62	i	28	Total O 28 28	0
62	j	18	Total O 18 18	0
62	k	40	Total O 40 40	0
62	m	26	Total O 26 26	0
62	n	5	Total O 5 5	0
62	o	18	Total O 18 18	0

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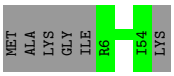
Mol	Chain	Residues	Atoms	AltConf
62	p	40	Total O 40 40	0
62	q	20	Total O 20 20	0
62	r	28	Total O 28 28	0
62	s	15	Total O 15 15	0
62	t	4	Total O 4 4	0
62	u	8	Total O 8 8	0
62	v	19	Total O 19 19	0
62	w	13	Total O 13 13	0
62	x	1	Total O 1 1	0
62	y	12	Total O 12 12	0
62	z	26	Total O 26 26	0
62	Y	4	Total O 4 4	0
62	a	4351	Total O 4351 4351	0
62	A	650	Total O 650 650	0
62	J	3	Total O 3 3	0
62	6	12	Total O 12 12	0
62	l	27	Total O 27 27	0
62	K	4	Total O 4 4	0

3 Residue-property plots (i)

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

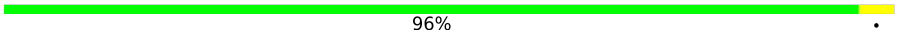
• Molecule 1: Large ribosomal subunit protein bL33

Chain 0:



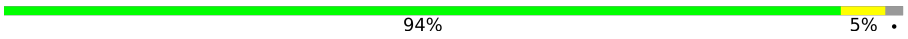
• Molecule 2: Large ribosomal subunit protein bL34

Chain 1:



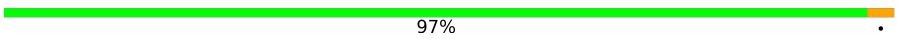
• Molecule 3: Large ribosomal subunit protein bL35

Chain 2:



• Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:

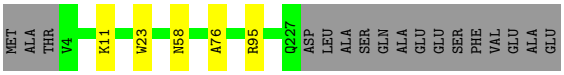


• Molecule 5: E-site tRNA

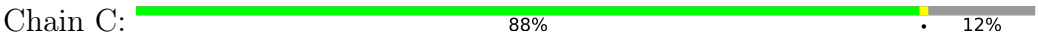
Chain 5:

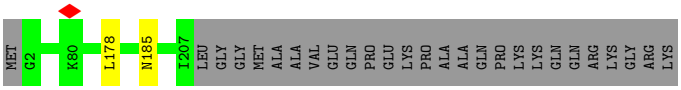
• Molecule 6: 30S ribosomal protein S2

Chain B:

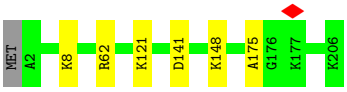


• Molecule 7: Small ribosomal subunit protein uS3

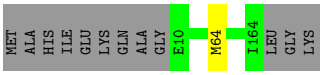




• Molecule 8: Small ribosomal subunit protein uS4

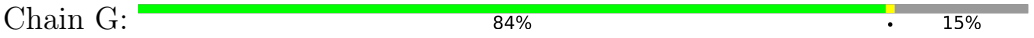


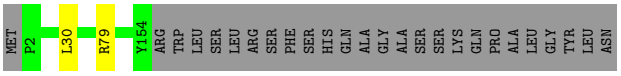
• Molecule 9: Small ribosomal subunit protein uS5



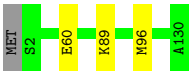
• Molecule 10: 30S ribosomal protein S6, fully modified isoform

• Molecule 11: 30S ribosomal protein S7

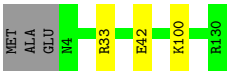




• Molecule 12: Small ribosomal subunit protein uS8

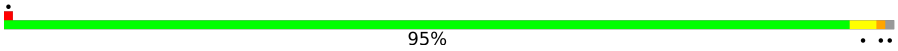


• Molecule 13: Small ribosomal subunit protein uS9



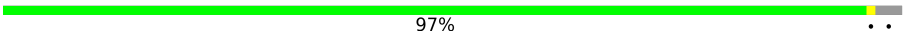
• Molecule 14: Small ribosomal subunit protein uS12

Chain L:



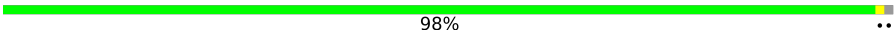
• Molecule 15: Small ribosomal subunit protein uS13

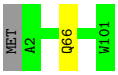
Chain M:



• Molecule 16: Small ribosomal subunit protein uS14

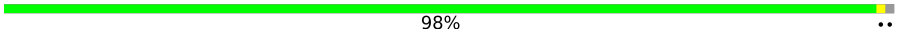
Chain N:





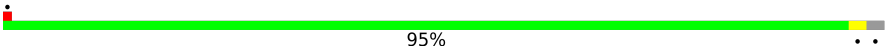
• Molecule 17: Small ribosomal subunit protein uS15

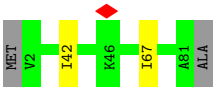
Chain O:



• Molecule 18: 30S ribosomal protein S16

Chain P:





• Molecule 19: Small ribosomal subunit protein uS17

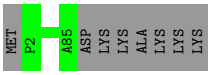
Chain Q:

• Molecule 20: Small ribosomal subunit protein bS18

Chain R:

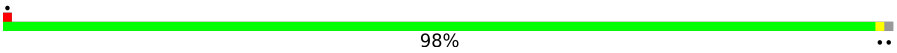
• Molecule 21: Small ribosomal subunit protein uS19

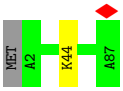
Chain S:



• Molecule 22: 30S ribosomal protein S20

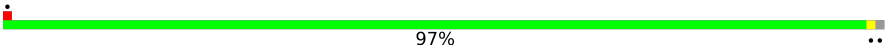
Chain T:

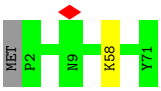




• Molecule 23: Small ribosomal subunit protein bS21

Chain U:





• Molecule 24: mRNA

Chain X:

• Molecule 25: P-site tRNA-gly

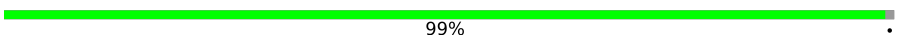
Chain Z:

• Molecule 26: 5S rRNA

Chain b:

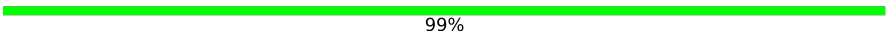
• Molecule 27: Large ribosomal subunit protein uL2

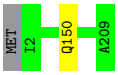
Chain c:



• Molecule 28: Large ribosomal subunit protein uL3

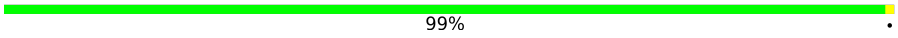
Chain d:





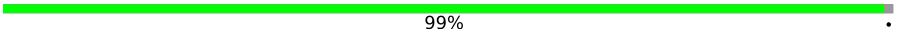
• Molecule 29: Large ribosomal subunit protein uL4

Chain e:



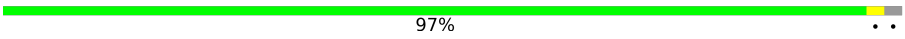
• Molecule 30: Large ribosomal subunit protein uL5

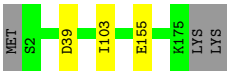
Chain f:



• Molecule 31: Large ribosomal subunit protein uL6

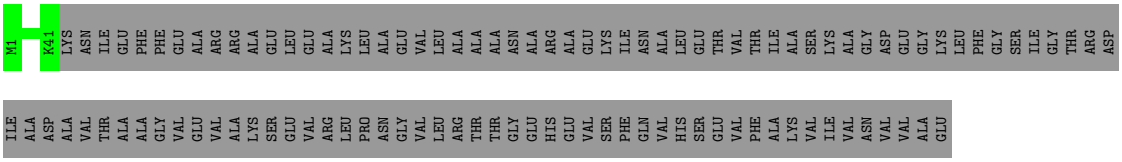
Chain g:





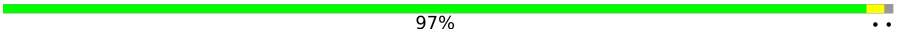
• Molecule 32: Large ribosomal subunit protein bL9

Chain h:



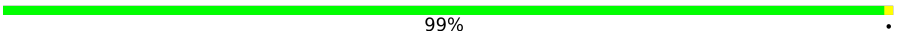
• Molecule 33: Large ribosomal subunit protein uL13

Chain i:



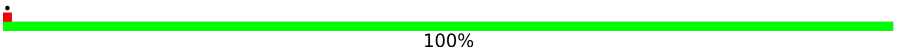
• Molecule 34: Large ribosomal subunit protein uL14

Chain j:



• Molecule 35: 50S ribosomal protein L15

Chain k:

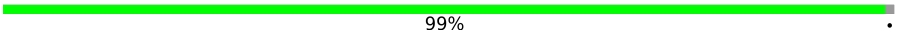


• Molecule 36: Large ribosomal subunit protein bL17

Chain m:

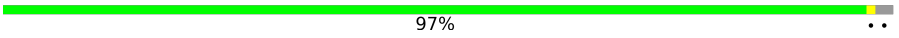
• Molecule 37: Large ribosomal subunit protein uL18

Chain n:



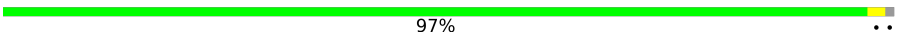
• Molecule 38: Large ribosomal subunit protein bL19

Chain o:



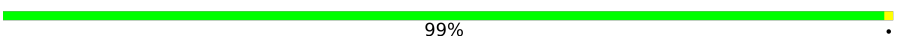
• Molecule 39: Large ribosomal subunit protein bL20

Chain p:



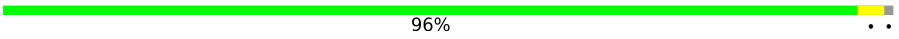
• Molecule 40: Large ribosomal subunit protein bL21

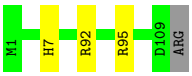
Chain q:



• Molecule 41: Large ribosomal subunit protein uL22

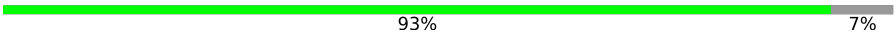
Chain r:





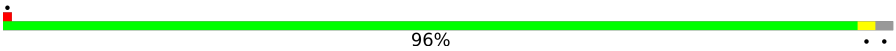
• Molecule 42: Large ribosomal subunit protein uL23

Chain s:



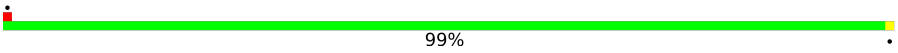
• Molecule 43: Large ribosomal subunit protein uL24

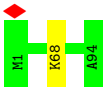
Chain t:



• Molecule 44: 50S ribosomal protein L25

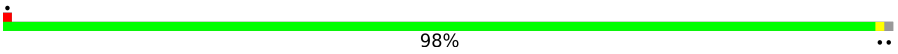
Chain u:

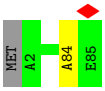




• Molecule 45: Large ribosomal subunit protein bL27

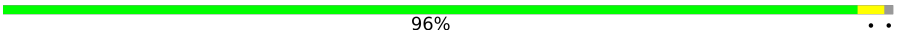
Chain v:

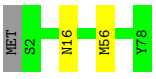




• Molecule 46: Large ribosomal subunit protein bL28

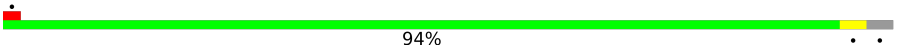
Chain w:

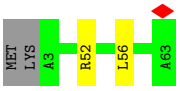




• Molecule 47: Large ribosomal subunit protein uL29

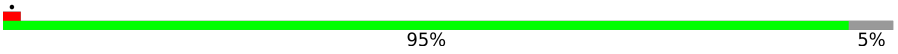
Chain x:

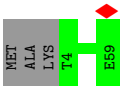




• Molecule 48: Large ribosomal subunit protein uL30

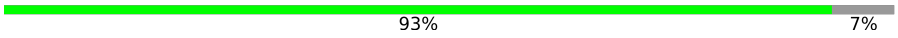
Chain y:

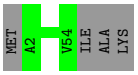




• Molecule 49: Large ribosomal subunit protein bL32

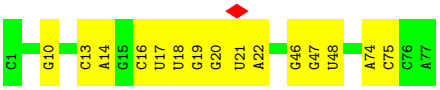
Chain z:





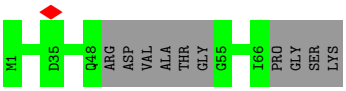
• Molecule 50: A-site tRNA-pro

Chain Y:



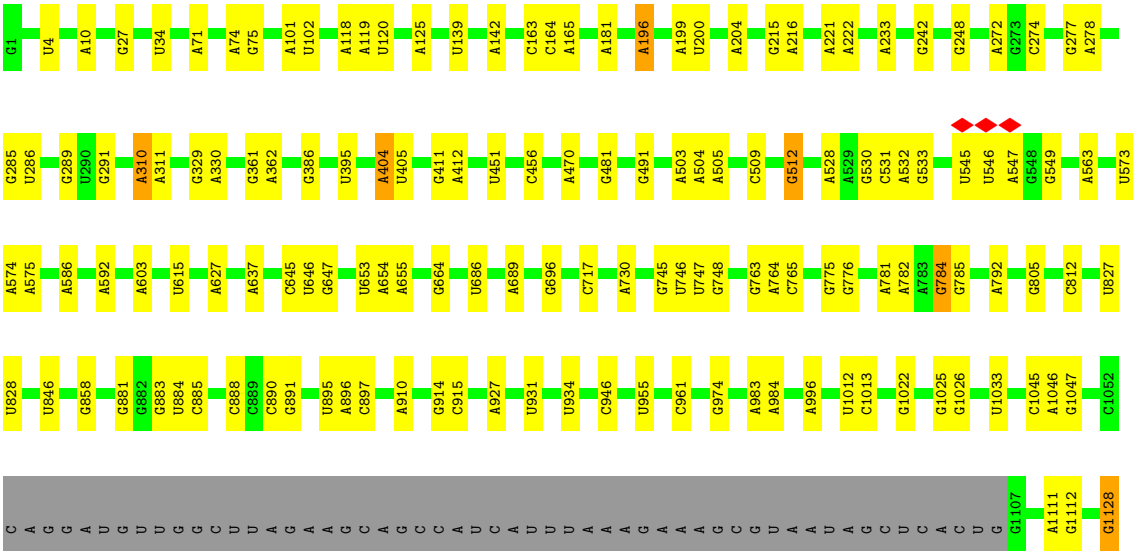
• Molecule 51: Large ribosomal subunit protein bL31A

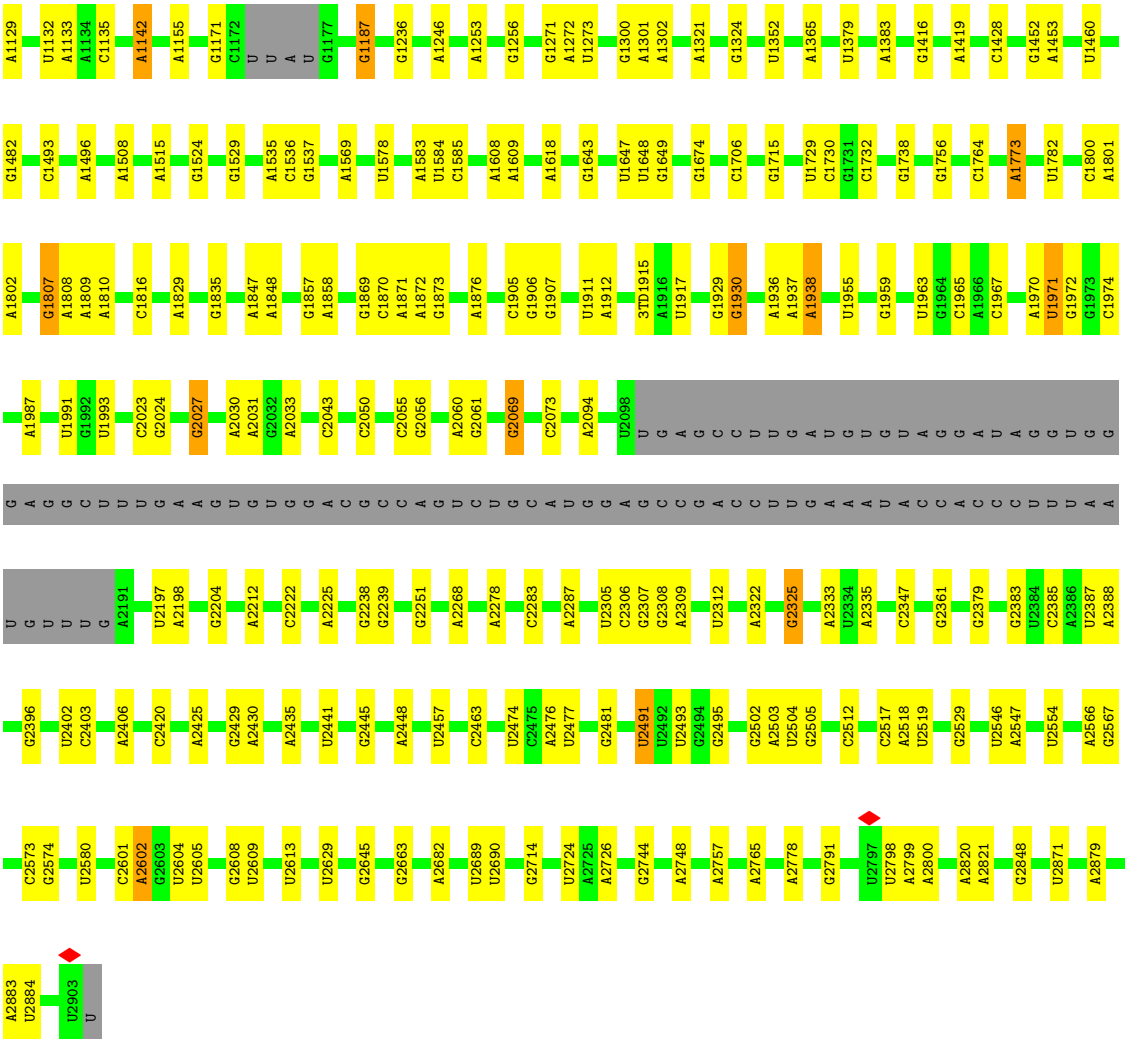
Chain 4:



• Molecule 52: 23S rRNA

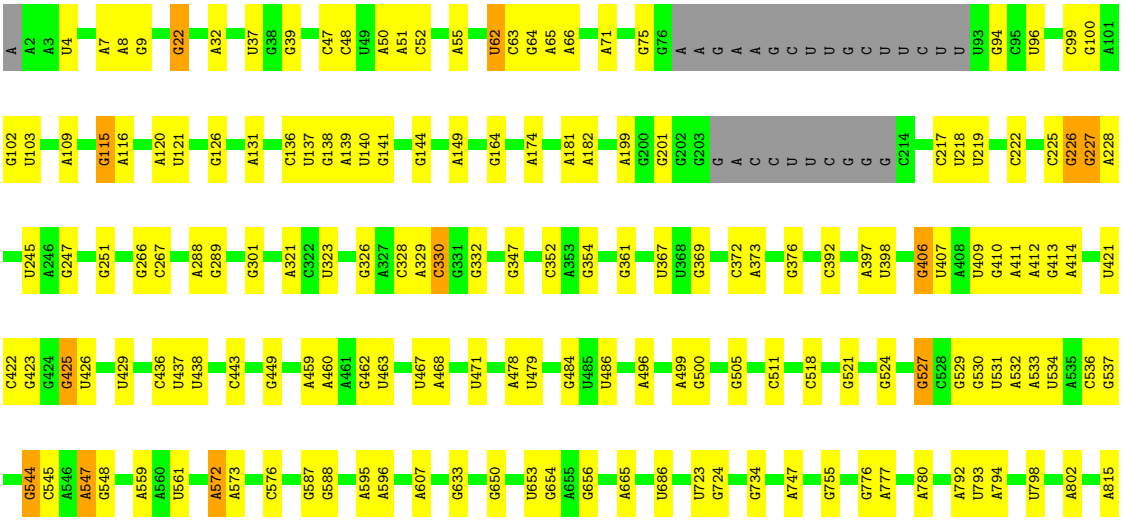
Chain a:

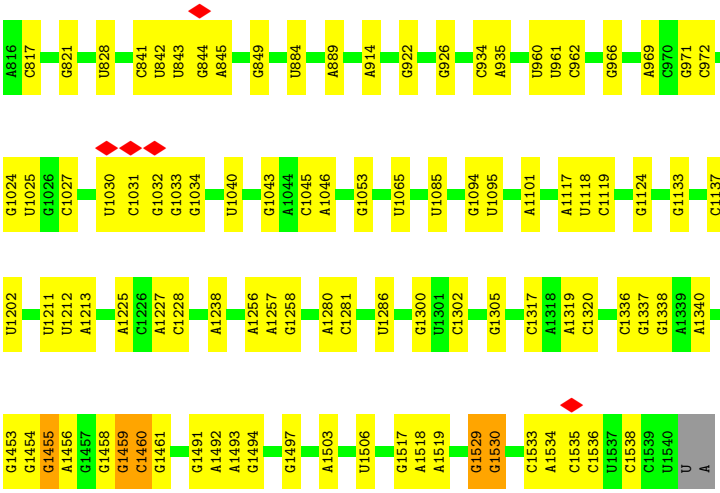




• Molecule 53: 16S rRNA

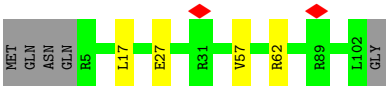
Chain A:





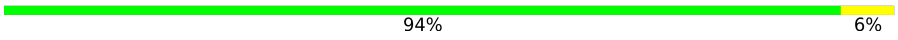
• Molecule 54: Small ribosomal subunit protein uS10

Chain J:



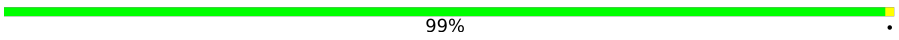
• Molecule 55: Secretion monitor

Chain 6:



• Molecule 56: Large ribosomal subunit protein uL16

Chain l:



• Molecule 57: Small ribosomal subunit protein uS11

Chain K:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300107	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00495	Depositor
Map size (Å)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: 2MG, K, OMG, OMU, ZN, MA6, 3TD, 5MC, PSU, IAS, MEQ, 2MA, 6MZ, D2T, MS6, OMC, H2U, 4D4, 5MU, MG, G7M, 1MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.31	0/412	0.63	0/549
2	1	0.32	0/380	0.76	0/498
3	2	0.31	0/513	0.69	0/676
4	3	0.30	0/303	0.73	0/397
5	5	0.78	0/46	1.05	0/69
6	B	0.29	0/1784	0.61	0/2403
7	C	0.28	0/1651	0.62	0/2225
8	D	0.30	0/1665	0.63	0/2227
9	E	0.30	0/1157	0.64	0/1557
10	F	0.29	0/858	0.62	0/1160
11	G	0.30	0/1219	0.65	0/1635
12	H	0.30	0/989	0.63	0/1326
13	I	0.31	0/1034	0.68	0/1375
14	L	0.32	0/960	0.75	0/1286
15	M	0.30	0/900	0.64	0/1204
16	N	0.30	0/817	0.60	0/1088
17	O	0.29	0/722	0.56	0/964
18	P	0.30	0/645	0.66	0/867
19	Q	0.28	0/633	0.66	0/849
20	R	0.29	0/553	0.64	0/742
21	S	0.31	0/685	0.61	0/922
22	T	0.28	0/676	0.56	0/895
23	U	0.28	0/597	0.68	0/792
24	X	0.66	0/209	1.19	0/323
25	Z	0.58	0/1810	1.13	0/2820
26	b	0.51	0/2850	1.16	2/4444 (0.0%)
27	c	0.31	0/2121	0.71	0/2852
28	d	0.30	0/1568	0.65	0/2109
29	e	0.29	0/1571	0.60	0/2113
30	f	0.29	0/1434	0.61	0/1926
31	g	0.30	0/1324	0.65	0/1794

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	h	0.31	0/306	0.69	0/413
33	i	0.30	0/1143	0.65	0/1540
34	j	0.30	0/955	0.69	0/1279
35	k	0.33	0/1062	0.62	0/1413
36	m	0.29	0/958	0.67	0/1281
37	n	0.29	0/902	0.62	0/1209
38	o	0.31	0/920	0.69	0/1231
39	p	0.30	0/960	0.66	0/1278
40	q	0.31	0/829	0.68	0/1107
41	r	0.28	0/852	0.63	0/1142
42	s	0.27	0/744	0.61	0/994
43	t	0.29	0/787	0.67	0/1051
44	u	0.30	0/766	0.63	0/1025
45	v	0.33	0/636	0.68	0/841
46	w	0.32	0/635	0.71	0/848
47	x	0.27	0/493	0.56	0/656
48	y	0.30	0/439	0.66	0/587
49	z	0.33	0/427	0.67	0/570
50	Y	0.60	0/1837	1.12	0/2864
51	4	0.31	0/488	0.64	0/649
52	a	0.49	0/65651	1.15	82/102413 (0.1%)
53	A	0.52	0/36272	1.14	38/56577 (0.1%)
54	J	0.28	0/796	0.66	0/1077
55	6	0.32	0/279	0.67	0/377
56	l	0.30	0/1073	0.69	0/1433
57	K	0.31	0/876	0.67	0/1181
All	All	0.46	0/153172	1.04	122/229123 (0.1%)

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
3	2	0	2
4	3	0	1
6	B	0	1
8	D	0	1
11	G	0	1
14	L	0	2
15	M	0	1
17	O	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	Q	0	1
29	e	0	1
33	i	0	2
36	m	0	1
38	o	0	1
39	p	0	2
41	r	0	1
46	w	0	1
47	x	0	1
52	a	0	1
54	J	0	1
All	All	0	23

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	a	574	A	O5'-P-OP1	-11.68	95.19	105.70
52	a	512	G	O4'-C1'-N9	11.43	117.34	108.20
53	A	115	G	P-O3'-C3'	9.42	131.00	119.70
26	b	7	G	O4'-C1'-N9	8.81	115.25	108.20
53	A	227	G	O4'-C1'-N9	8.76	115.21	108.20
52	a	2724	U	O5'-P-OP2	-8.68	97.89	105.70
53	A	288	A	O3'-P-O5'	-8.60	87.67	104.00
52	a	196	A	O5'-P-OP1	-8.48	98.07	105.70
52	a	503	A	O3'-P-O5'	-8.14	88.54	104.00
52	a	470	A	O5'-P-OP1	7.75	119.99	110.70
52	a	1025	G	O3'-P-O5'	7.69	118.61	104.00
52	a	2848	G	O4'-C1'-N9	7.67	114.33	108.20
52	a	2430	A	C1'-O4'-C4'	-7.50	103.90	109.90
52	a	2601	C	O3'-P-O5'	-7.49	89.77	104.00
52	a	1187	G	O5'-P-OP2	-7.47	98.97	105.70
52	a	574	A	O5'-P-OP2	7.46	119.65	110.70
53	A	406	G	C2'-C3'-O3'	7.44	125.86	109.50
52	a	1971	U	O3'-P-O5'	-7.38	89.98	104.00
52	a	1905	C	O3'-P-O5'	-7.38	89.98	104.00
53	A	1491	G	O3'-P-O5'	-7.35	90.03	104.00
52	a	204	A	O3'-P-O5'	-7.24	90.25	104.00
52	a	1936	A	O4'-C1'-N9	7.12	113.89	108.20
52	a	2027	G	O5'-P-OP2	-7.07	99.34	105.70
53	A	889	A	O3'-P-O5'	-6.89	90.92	104.00
52	a	395	U	O4'-C1'-N1	6.73	113.58	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	a	2073	C	O5'-P-OP2	-6.70	99.67	105.70
53	A	62	U	O4'-C1'-N1	6.66	113.53	108.20
53	A	1455	G	O4'-C1'-N9	6.63	113.50	108.20
52	a	2546	U	O3'-P-O5'	-6.59	91.49	104.00
52	a	2493	U	O3'-P-O5'	-6.55	91.56	104.00
53	A	406	G	P-O3'-C3'	6.55	127.56	119.70
52	a	984	A	O4'-C1'-N9	6.39	113.31	108.20
52	a	27	G	O4'-C1'-N9	6.33	113.26	108.20
53	A	425	G	C2'-C3'-O3'	6.33	123.82	113.70
53	A	547	A	P-O3'-C3'	6.20	127.14	119.70
53	A	301	G	O3'-P-O5'	-6.19	92.23	104.00
53	A	37	U	O4'-C1'-N1	6.18	113.14	108.20
53	A	1201	A	P-O3'-C3'	6.14	127.07	119.70
52	a	1847	A	O3'-P-O5'	-6.14	92.34	104.00
52	a	784	G	P-O3'-C3'	6.13	127.06	119.70
52	a	2094	A	O3'-P-O5'	-6.10	92.40	104.00
52	a	2517	C	O4'-C1'-N1	6.05	113.04	108.20
52	a	748	G	C1'-O4'-C4'	-6.05	105.06	109.90
53	A	1460	C	O4'-C1'-N1	5.99	112.99	108.20
52	a	1807	G	O5'-P-OP2	-5.99	100.31	105.70
52	a	2602	A	O5'-P-OP1	5.94	117.83	110.70
52	a	2050	C	O3'-P-O5'	-5.93	92.74	104.00
26	b	2	G	C2'-C3'-O3'	5.92	123.17	113.70
52	a	1142	A	O4'-C1'-N9	5.90	112.92	108.20
52	a	781	A	O3'-P-O5'	-5.85	92.88	104.00
52	a	1128	G	C1'-O4'-C4'	-5.85	105.22	109.90
52	a	2024	G	O5'-P-OP2	-5.84	100.44	105.70
52	a	528	A	O3'-P-O5'	-5.83	92.92	104.00
52	a	2278	A	O3'-P-O5'	-5.81	92.97	104.00
52	a	242	G	C3'-C2'-C1'	-5.79	96.86	101.50
53	A	561	U	O3'-P-O5'	-5.79	92.99	104.00
52	a	2871	U	O3'-P-O5'	-5.79	93.01	104.00
52	a	310	A	O3'-P-O5'	-5.78	93.02	104.00
53	A	323	U	O3'-P-O5'	-5.72	93.14	104.00
52	a	1857	G	O3'-P-O5'	-5.71	93.14	104.00
52	a	1236	G	O4'-C1'-N9	5.71	112.76	108.20
52	a	1324	G	O4'-C1'-N9	5.67	112.74	108.20
52	a	2574	G	O5'-P-OP2	-5.67	100.60	105.70
52	a	2879	A	O3'-P-O5'	-5.65	93.26	104.00
52	a	2495	G	OP2-P-O3'	5.65	117.63	105.20
52	a	2197	U	O3'-P-O5'	-5.65	93.27	104.00
53	A	1530	G	O4'-C1'-N9	5.64	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	977	A	O3'-P-O5'	-5.64	93.28	104.00
52	a	2645	G	O4'-C1'-N9	5.63	112.70	108.20
52	a	1643	G	O3'-P-O5'	-5.60	93.36	104.00
53	A	22	G	O5'-P-OP2	-5.60	100.66	105.70
52	a	1974	C	O3'-P-O5'	-5.57	93.42	104.00
52	a	2608	G	O5'-P-OP2	-5.55	100.70	105.70
52	a	2463	C	O3'-P-O5'	-5.54	93.47	104.00
52	a	1773	A	O5'-P-OP2	-5.52	100.73	105.70
52	a	2222	C	O3'-P-O5'	-5.51	93.53	104.00
53	A	527	G7M	O3'-P-O5'	-5.49	93.56	104.00
53	A	218	U	O4'-C1'-N1	5.45	112.56	108.20
52	a	512	G	C1'-O4'-C4'	-5.43	105.55	109.90
52	a	1246	A	O3'-P-O5'	-5.42	93.69	104.00
52	a	1936	A	C1'-O4'-C4'	-5.41	105.57	109.90
52	a	2420	C	O5'-P-OP2	-5.40	100.84	105.70
52	a	528	A	OP2-P-O3'	5.39	117.06	105.20
52	a	1810	A	O3'-P-O5'	-5.39	93.75	104.00
53	A	1199	U	O3'-P-O5'	-5.39	93.77	104.00
52	a	664	G	O5'-P-OP2	-5.38	100.86	105.70
53	A	1529	G	O3'-P-O5'	-5.37	93.81	104.00
52	a	404	A	P-O3'-C3'	5.36	126.13	119.70
53	A	1117	A	O3'-P-O5'	-5.36	93.82	104.00
53	A	780	A	O3'-P-O5'	-5.35	93.84	104.00
53	A	115	G	C2'-C3'-O3'	5.35	122.25	113.70
52	a	784	G	OP1-P-O3'	5.32	116.91	105.20
52	a	2512	C	O4'-C1'-N1	5.31	112.45	108.20
53	A	544	G	C2'-C3'-O3'	5.30	122.19	113.70
52	a	1706	C	O4'-C1'-N1	5.30	112.44	108.20
52	a	1496	A	O3'-P-O5'	-5.29	93.94	104.00
52	a	2361	G	O5'-P-OP2	-5.28	100.95	105.70
53	A	1459	G	O4'-C1'-N9	5.26	112.41	108.20
52	a	1930	G	C3'-C2'-C1'	-5.24	97.31	101.50
52	a	763	G	O3'-P-O5'	-5.24	94.05	104.00
52	a	277	G	P-O3'-C3'	5.23	125.98	119.70
52	a	2481	G	O4'-C1'-N9	5.21	112.36	108.20
52	a	1802	A	O5'-P-OP1	-5.19	101.03	105.70
53	A	686	U	C3'-C2'-C1'	-5.18	97.36	101.50
52	a	2519	U	O3'-P-O5'	-5.17	94.19	104.00
53	A	792	A	O4'-C1'-N9	5.16	112.33	108.20
53	A	1347	G	C3'-C2'-C1'	-5.16	97.37	101.50
52	a	1959	G	O3'-P-O5'	-5.16	94.20	104.00
52	a	2387	U	O5'-P-OP2	-5.16	101.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	a	2491	U	C1'-O4'-C4'	-5.16	105.77	109.90
52	a	2477	U	O3'-P-O5'	-5.16	94.21	104.00
53	A	572	A	O4'-C1'-N9	-5.15	104.08	108.20
52	a	689	A	OP2-P-O3'	5.13	116.49	105.20
53	A	1346	A	O4'-C1'-N9	5.13	112.31	108.20
53	A	547	A	C1'-O4'-C4'	-5.12	105.80	109.90
52	a	2325	G	O3'-P-O5'	-5.11	94.29	104.00
52	a	1938	A	O4'-C1'-N9	5.08	112.26	108.20
53	A	330	C	O4'-C1'-N1	5.08	112.26	108.20
53	A	798	U	O3'-P-O5'	-5.04	94.43	104.00
52	a	2388	A	OP2-P-O3'	5.03	116.25	105.20
53	A	226	G	O4'-C1'-N9	5.02	112.22	108.20
52	a	1756	G	O5'-P-OP2	-5.01	101.19	105.70

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	13	ARG	Sidechain
3	2	8	ARG	Sidechain
4	3	36	ARG	Sidechain
6	B	95	ARG	Sidechain
8	D	62	ARG	Sidechain
11	G	79	ARG	Sidechain
54	J	62	ARG	Sidechain
14	L	109	ASP	Peptide
14	L	110	ARG	Sidechain
15	M	90	ARG	Sidechain
17	O	72	ARG	Sidechain
19	Q	27	ARG	Sidechain
52	a	512	G	Sidechain
29	e	67	ARG	Sidechain
33	i	95	ARG	Sidechain
33	i	96	ARG	Sidechain
36	m	4	ARG	Sidechain
38	o	53	ARG	Sidechain
39	p	13	ARG	Sidechain
39	p	51	ARG	Sidechain
41	r	92	ARG	Sidechain
46	w	16	ASN	Peptide
47	x	52	ARG	Sidechain

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	
1	0	47/55 (86%)	47 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
6	B	222/241 (92%)	214 (96%)	7 (3%)	1 (0%)	29	23
7	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
8	D	203/206 (98%)	194 (96%)	7 (3%)	2 (1%)	15	9
9	E	153/167 (92%)	144 (94%)	9 (6%)	0	100	100
10	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
11	G	151/179 (84%)	145 (96%)	6 (4%)	0	100	100
12	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
13	I	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
14	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
15	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
16	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
17	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
18	P	78/82 (95%)	73 (94%)	5 (6%)	0	100	100
19	Q	75/84 (89%)	70 (93%)	5 (7%)	0	100	100
20	R	64/75 (85%)	64 (100%)	0	0	100	100
21	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
22	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
27	c	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
28	d	205/209 (98%)	198 (97%)	7 (3%)	0	100	100
29	e	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
30	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
31	g	172/177 (97%)	163 (95%)	8 (5%)	1 (1%)	25	19
32	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
33	i	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
34	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
35	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
36	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
37	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
38	o	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
39	p	115/118 (98%)	115 (100%)	0	0	100	100
40	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
41	r	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
42	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
43	t	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
44	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
45	v	82/85 (96%)	79 (96%)	2 (2%)	1 (1%)	13	7
46	w	75/78 (96%)	75 (100%)	0	0	100	100
47	x	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
48	y	54/59 (92%)	53 (98%)	1 (2%)	0	100	100
49	z	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
51	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
54	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	15	9
55	6	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
56	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
57	K	112/129 (87%)	103 (92%)	9 (8%)	0	100	100
All	All	5500/5947 (92%)	5306 (96%)	188 (3%)	6 (0%)	54	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	121	LYS
6	B	76	ALA
45	v	84	ALA
54	J	57	VAL
31	g	39	ASP
8	D	175	ALA

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	
1	0	45/49 (92%)	45 (100%)	0	100	100
2	1	38/38 (100%)	36 (95%)	2 (5%)	22	18
3	2	51/52 (98%)	50 (98%)	1 (2%)	55	58
4	3	34/34 (100%)	33 (97%)	1 (3%)	42	43
6	B	186/199 (94%)	183 (98%)	3 (2%)	62	67
7	C	170/190 (90%)	168 (99%)	2 (1%)	71	76
8	D	172/173 (99%)	169 (98%)	3 (2%)	60	65
9	E	118/126 (94%)	117 (99%)	1 (1%)	81	86
10	F	90/116 (78%)	90 (100%)	0	100	100
11	G	126/147 (86%)	125 (99%)	1 (1%)	81	86
12	H	104/105 (99%)	101 (97%)	3 (3%)	42	43
13	I	105/107 (98%)	102 (97%)	3 (3%)	42	43
14	L	102/103 (99%)	99 (97%)	3 (3%)	42	43
15	M	93/96 (97%)	93 (100%)	0	100	100
16	N	83/84 (99%)	82 (99%)	1 (1%)	71	76
17	O	76/77 (99%)	76 (100%)	0	100	100
18	P	64/65 (98%)	62 (97%)	2 (3%)	40	40
19	Q	71/78 (91%)	70 (99%)	1 (1%)	67	72
20	R	57/65 (88%)	57 (100%)	0	100	100
21	S	72/79 (91%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	T	65/66 (98%)	64 (98%)	1 (2%)	65 69
23	U	60/61 (98%)	59 (98%)	1 (2%)	60 65
27	c	216/218 (99%)	215 (100%)	1 (0%)	88 92
28	d	162/163 (99%)	162 (100%)	0	100 100
29	e	165/165 (100%)	164 (99%)	1 (1%)	86 90
30	f	148/150 (99%)	148 (100%)	0	100 100
31	g	135/138 (98%)	133 (98%)	2 (2%)	65 69
32	h	32/114 (28%)	32 (100%)	0	100 100
33	i	115/116 (99%)	114 (99%)	1 (1%)	78 83
34	j	104/104 (100%)	103 (99%)	1 (1%)	76 81
35	k	103/103 (100%)	103 (100%)	0	100 100
36	m	98/103 (95%)	98 (100%)	0	100 100
37	n	86/87 (99%)	86 (100%)	0	100 100
38	o	98/100 (98%)	98 (100%)	0	100 100
39	p	89/90 (99%)	89 (100%)	0	100 100
40	q	84/84 (100%)	83 (99%)	1 (1%)	71 76
41	r	92/93 (99%)	90 (98%)	2 (2%)	52 55
42	s	80/84 (95%)	80 (100%)	0	100 100
43	t	83/85 (98%)	81 (98%)	2 (2%)	49 51
44	u	78/78 (100%)	77 (99%)	1 (1%)	69 74
45	v	61/63 (97%)	61 (100%)	0	100 100
46	w	67/68 (98%)	66 (98%)	1 (2%)	65 69
47	x	53/55 (96%)	52 (98%)	1 (2%)	57 61
48	y	47/49 (96%)	47 (100%)	0	100 100
49	z	45/48 (94%)	45 (100%)	0	100 100
51	4	55/62 (89%)	55 (100%)	0	100 100
54	J	86/90 (96%)	84 (98%)	2 (2%)	50 53
55	6	27/27 (100%)	25 (93%)	2 (7%)	13 9
56	l	107/107 (100%)	107 (100%)	0	100 100
57	K	88/98 (90%)	85 (97%)	3 (3%)	37 36
All	All	4586/4852 (94%)	4536 (99%)	50 (1%)	74 78

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	25	LYS
2	1	46	LYS
3	2	31	HIS
4	3	36	ARG
6	B	11	LYS
6	B	23	TRP
6	B	58	ASN
7	C	178	LEU
7	C	185	ASN
8	D	8	LYS
8	D	141	ASP
8	D	148	LYS
9	E	64	MET
11	G	30	LEU
12	H	60	GLU
12	H	89	LYS
12	H	96	MET
13	I	33	ARG
13	I	42	GLU
13	I	100	LYS
14	L	15	LYS
14	L	86	ARG
14	L	110	ARG
16	N	66	GLN
18	P	42	ILE
18	P	67	ILE
19	Q	17	MET
22	T	44	LYS
23	U	58	LYS
27	c	240	PHE
29	e	140	ASP
31	g	103	ILE
31	g	155	GLU
33	i	80	HIS
34	j	49	ARG
40	q	71	LYS
41	r	7	HIS
41	r	95	ARG
43	t	24	LYS
43	t	74	ASN
44	u	68	LYS
46	w	56	MET

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Mol	Chain	Res	Type
47	x	56	LEU
54	J	17	LEU
54	J	27	GLU
55	6	134	GLU
55	6	138	ARG
57	K	72	ASP
57	K	89	PRO
57	K	94	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	31	HIS
6	B	103	ASN
7	C	140	ASN
9	E	82	GLN
14	L	112	GLN
16	N	43	ASN
18	P	18	GLN
27	c	197	ASN
27	c	243	HIS
28	d	32	ASN
34	j	5	GLN
37	n	61	GLN
38	o	12	GLN
39	p	37	GLN
39	p	52	GLN
40	q	6	GLN
40	q	43	ASN
43	t	74	ASN
46	w	6	GLN
56	l	13	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	X	8/9 (88%)	1 (12%)	0
25	Z	75/76 (98%)	15 (20%)	4 (5%)
26	b	118/120 (98%)	15 (12%)	0
5	5	1/2 (50%)	1 (100%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	Y	76/77 (98%)	14 (18%)	4 (5%)
52	a	2745/2904 (94%)	290 (10%)	0
53	A	1508/1542 (97%)	268 (17%)	42 (2%)
All	All	4531/4730 (95%)	604 (13%)	50 (1%)

All (604) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	5	76	A
24	X	15	U
25	Z	6	A
25	Z	14	A
25	Z	17	U
25	Z	18	G
25	Z	20	U
25	Z	21	A
25	Z	37	A
25	Z	46	G
25	Z	47	U
25	Z	48	C
25	Z	49	G
25	Z	51	G
25	Z	52	A
25	Z	58	A
25	Z	76	A
26	b	2	G
26	b	3	C
26	b	4	C
26	b	7	G
26	b	8	C
26	b	25	U
26	b	35	C
26	b	44	G
26	b	45	A
26	b	56	G
26	b	67	G
26	b	89	U
26	b	90	C
26	b	99	A
26	b	109	A
50	Y	10	G
50	Y	14	A

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Mol	Chain	Res	Type
50	Y	16	C
50	Y	17	U
50	Y	18	U
50	Y	19	G
50	Y	20	G
50	Y	21	U
50	Y	22	A
50	Y	46	G
50	Y	47	G
50	Y	48	U
50	Y	74	A
50	Y	75	C
52	a	4	U
52	a	10	A
52	a	34	U
52	a	71	A
52	a	74	A
52	a	75	G
52	a	101	A
52	a	102	U
52	a	118	A
52	a	119	A
52	a	120	U
52	a	125	A
52	a	139	U
52	a	142	A
52	a	163	C
52	a	164	C
52	a	165	A
52	a	181	A
52	a	196	A
52	a	199	A
52	a	200	U
52	a	215	G
52	a	216	A
52	a	221	A
52	a	222	A
52	a	233	A
52	a	248	G
52	a	272	A
52	a	274	C
52	a	278	A

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Mol	Chain	Res	Type
52	a	285	G
52	a	286	U
52	a	289	G
52	a	291	G
52	a	310	A
52	a	311	A
52	a	329	G
52	a	330	A
52	a	361	G
52	a	362	A
52	a	386	G
52	a	404	A
52	a	405	U
52	a	411	G
52	a	412	A
52	a	451	U
52	a	456	C
52	a	481	G
52	a	491	G
52	a	504	A
52	a	505	A
52	a	509	C
52	a	530	G
52	a	531	C
52	a	532	A
52	a	533	G
52	a	545	U
52	a	546	U
52	a	547	A
52	a	549	G
52	a	563	A
52	a	573	U
52	a	575	A
52	a	586	A
52	a	592	A
52	a	603	A
52	a	615	U
52	a	627	A
52	a	637	A
52	a	645	C
52	a	646	U
52	a	647	G

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Mol	Chain	Res	Type
52	a	653	U
52	a	654	A
52	a	655	A
52	a	686	U
52	a	696	G
52	a	717	C
52	a	730	A
52	a	747	5MU
52	a	764	A
52	a	765	C
52	a	775	G
52	a	776	G
52	a	782	A
52	a	784	G
52	a	785	G
52	a	792	A
52	a	805	G
52	a	812	C
52	a	827	U
52	a	828	U
52	a	846	U
52	a	858	G
52	a	881	G
52	a	883	G
52	a	884	U
52	a	885	C
52	a	888	C
52	a	890	C
52	a	891	G
52	a	895	U
52	a	896	A
52	a	897	C
52	a	910	A
52	a	914	G
52	a	915	C
52	a	927	A
52	a	931	U
52	a	934	U
52	a	946	C
52	a	961	C
52	a	974	G
52	a	983	A

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Mol	Chain	Res	Type
52	a	996	A
52	a	1012	U
52	a	1013	C
52	a	1022	G
52	a	1026	G
52	a	1033	U
52	a	1045	C
52	a	1046	A
52	a	1047	G
52	a	1111	A
52	a	1112	G
52	a	1128	G
52	a	1129	A
52	a	1132	U
52	a	1133	A
52	a	1135	C
52	a	1142	A
52	a	1155	A
52	a	1171	G
52	a	1187	G
52	a	1253	A
52	a	1256	G
52	a	1271	G
52	a	1272	A
52	a	1273	U
52	a	1300	G
52	a	1301	A
52	a	1302	A
52	a	1321	A
52	a	1352	U
52	a	1365	A
52	a	1379	U
52	a	1383	A
52	a	1416	G
52	a	1419	A
52	a	1428	C
52	a	1452	G
52	a	1453	A
52	a	1460	U
52	a	1482	G
52	a	1493	C
52	a	1508	A

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Mol	Chain	Res	Type
52	a	1515	A
52	a	1524	G
52	a	1529	G
52	a	1535	A
52	a	1536	C
52	a	1537	G
52	a	1569	A
52	a	1578	U
52	a	1583	A
52	a	1584	U
52	a	1585	C
52	a	1608	A
52	a	1609	A
52	a	1647	U
52	a	1648	U
52	a	1649	G
52	a	1674	G
52	a	1715	G
52	a	1729	U
52	a	1730	C
52	a	1732	C
52	a	1738	G
52	a	1764	C
52	a	1773	A
52	a	1782	U
52	a	1800	C
52	a	1801	A
52	a	1807	G
52	a	1808	A
52	a	1809	A
52	a	1816	C
52	a	1829	A
52	a	1848	A
52	a	1858	A
52	a	1869	G
52	a	1870	C
52	a	1871	A
52	a	1872	A
52	a	1873	G
52	a	1876	A
52	a	1906	G
52	a	1907	G

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Mol	Chain	Res	Type
52	a	1912	A
52	a	1929	G
52	a	1930	G
52	a	1937	A
52	a	1938	A
52	a	1955	U
52	a	1963	U
52	a	1965	C
52	a	1967	C
52	a	1970	A
52	a	1971	U
52	a	1972	G
52	a	1987	A
52	a	1991	U
52	a	1993	U
52	a	2023	C
52	a	2027	G
52	a	2031	A
52	a	2033	A
52	a	2043	C
52	a	2055	C
52	a	2056	G
52	a	2060	A
52	a	2061	G
52	a	2069	G7M
52	a	2198	A
52	a	2204	G
52	a	2212	A
52	a	2225	A
52	a	2238	G
52	a	2239	G
52	a	2268	A
52	a	2283	C
52	a	2287	A
52	a	2305	U
52	a	2306	C
52	a	2307	G
52	a	2308	G
52	a	2309	A
52	a	2312	U
52	a	2322	A
52	a	2325	G

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Mol	Chain	Res	Type
52	a	2333	A
52	a	2335	A
52	a	2347	C
52	a	2379	G
52	a	2383	G
52	a	2385	C
52	a	2396	G
52	a	2402	U
52	a	2403	C
52	a	2406	A
52	a	2425	A
52	a	2429	G
52	a	2435	A
52	a	2441	U
52	a	2448	A
52	a	2474	U
52	a	2476	A
52	a	2491	U
52	a	2502	G
52	a	2505	G
52	a	2518	A
52	a	2529	G
52	a	2547	A
52	a	2554	U
52	a	2566	A
52	a	2567	G
52	a	2573	C
52	a	2602	A
52	a	2609	U
52	a	2613	U
52	a	2629	U
52	a	2663	G
52	a	2682	A
52	a	2689	U
52	a	2690	U
52	a	2714	G
52	a	2726	A
52	a	2744	G
52	a	2748	A
52	a	2757	A
52	a	2765	A
52	a	2778	A

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Mol	Chain	Res	Type
52	a	2791	G
52	a	2798	U
52	a	2799	A
52	a	2800	A
52	a	2820	A
52	a	2821	A
52	a	2883	A
52	a	2884	U
53	A	4	U
53	A	8	A
53	A	9	G
53	A	22	G
53	A	32	A
53	A	39	G
53	A	47	C
53	A	48	C
53	A	50	A
53	A	51	A
53	A	52	C
53	A	55	A
53	A	62	U
53	A	63	C
53	A	64	G
53	A	65	A
53	A	66	A
53	A	71	A
53	A	75	G
53	A	94	G
53	A	96	U
53	A	99	C
53	A	100	G
53	A	102	G
53	A	103	U
53	A	109	A
53	A	116	A
53	A	120	A
53	A	121	U
53	A	126	G
53	A	131	A
53	A	136	C
53	A	137	U
53	A	139	A

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Mol	Chain	Res	Type
53	A	140	U
53	A	141	G
53	A	144	G
53	A	149	A
53	A	164	G
53	A	174	A
53	A	181	A
53	A	182	A
53	A	201	G
53	A	217	C
53	A	219	U
53	A	222	C
53	A	225	C
53	A	226	G
53	A	227	G
53	A	228	A
53	A	245	U
53	A	247	G
53	A	251	G
53	A	266	G
53	A	267	C
53	A	289	G
53	A	321	A
53	A	326	G
53	A	328	C
53	A	329	A
53	A	330	C
53	A	332	G
53	A	347	G
53	A	352	C
53	A	354	G
53	A	367	U
53	A	369	G
53	A	372	C
53	A	373	A
53	A	376	G
53	A	392	C
53	A	397	A
53	A	398	U
53	A	406	G
53	A	407	U
53	A	410	G

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Mol	Chain	Res	Type
53	A	411	A
53	A	412	A
53	A	413	G
53	A	414	A
53	A	421	U
53	A	423	G
53	A	425	G
53	A	426	U
53	A	429	U
53	A	436	C
53	A	437	U
53	A	438	U
53	A	443	C
53	A	449	G
53	A	459	A
53	A	460	A
53	A	462	G
53	A	463	U
53	A	467	U
53	A	468	A
53	A	471	U
53	A	478	A
53	A	479	U
53	A	484	G
53	A	486	U
53	A	496	A
53	A	499	A
53	A	500	G
53	A	505	G
53	A	511	C
53	A	518	C
53	A	521	G
53	A	524	G
53	A	527	G7M
53	A	529	G
53	A	530	G
53	A	531	U
53	A	532	A
53	A	533	A
53	A	534	U
53	A	536	C
53	A	537	G

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Mol	Chain	Res	Type
53	A	545	C
53	A	548	G
53	A	559	A
53	A	572	A
53	A	573	A
53	A	576	C
53	A	588	G
53	A	595	A
53	A	596	A
53	A	607	A
53	A	633	G
53	A	650	G
53	A	653	U
53	A	654	G
53	A	656	G
53	A	665	A
53	A	723	U
53	A	724	G
53	A	734	G
53	A	747	A
53	A	755	G
53	A	777	A
53	A	793	U
53	A	794	A
53	A	802	A
53	A	815	A
53	A	817	C
53	A	821	G
53	A	828	U
53	A	841	C
53	A	842	U
53	A	843	U
53	A	844	G
53	A	845	A
53	A	849	G
53	A	914	A
53	A	922	G
53	A	926	G
53	A	934	C
53	A	935	A
53	A	960	U
53	A	961	U

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Mol	Chain	Res	Type
53	A	962	C
53	A	966	G
53	A	969	A
53	A	971	G
53	A	972	C
53	A	975	A
53	A	976	G
53	A	977	A
53	A	984	C
53	A	993	G
53	A	1003	G
53	A	1004	A
53	A	1005	A
53	A	1006	G
53	A	1008	U
53	A	1009	U
53	A	1019	A
53	A	1022	A
53	A	1023	U
53	A	1024	G
53	A	1025	U
53	A	1027	C
53	A	1030	U
53	A	1031	C
53	A	1032	G
53	A	1033	G
53	A	1034	G
53	A	1040	U
53	A	1043	G
53	A	1045	C
53	A	1046	A
53	A	1053	G
53	A	1065	U
53	A	1085	U
53	A	1094	G
53	A	1095	U
53	A	1101	A
53	A	1118	U
53	A	1119	C
53	A	1124	G
53	A	1133	G
53	A	1137	C

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Mol	Chain	Res	Type
53	A	1139	G
53	A	1140	C
53	A	1141	C
53	A	1145	A
53	A	1159	U
53	A	1168	U
53	A	1169	A
53	A	1171	A
53	A	1184	G
53	A	1196	A
53	A	1197	A
53	A	1200	C
53	A	1202	U
53	A	1211	U
53	A	1212	U
53	A	1213	A
53	A	1227	A
53	A	1228	C
53	A	1238	A
53	A	1256	A
53	A	1257	A
53	A	1258	G
53	A	1280	A
53	A	1286	U
53	A	1300	G
53	A	1302	C
53	A	1305	G
53	A	1317	C
53	A	1319	A
53	A	1320	C
53	A	1336	C
53	A	1337	G
53	A	1338	G
53	A	1340	A
53	A	1346	A
53	A	1353	G
53	A	1363	A
53	A	1370	G
53	A	1379	G
53	A	1397	C
53	A	1419	G
53	A	1447	A

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Mol	Chain	Res	Type
53	A	1448	C
53	A	1450	U
53	A	1451	U
53	A	1452	C
53	A	1453	G
53	A	1454	G
53	A	1455	G
53	A	1456	A
53	A	1458	G
53	A	1459	G
53	A	1460	C
53	A	1461	G
53	A	1492	A
53	A	1494	G
53	A	1497	G
53	A	1503	A
53	A	1506	U
53	A	1517	G
53	A	1529	G
53	A	1530	G
53	A	1533	C
53	A	1534	A
53	A	1535	C
53	A	1538	C

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	Z	18	G
25	Z	47	U
25	Z	48	C
25	Z	51	G
50	Y	13	C
50	Y	16	C
50	Y	18	U
50	Y	20	G
53	A	7	A
53	A	65	A
53	A	115	G
53	A	121	U
53	A	136	C
53	A	138	G

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Mol	Chain	Res	Type
53	A	139	A
53	A	181	A
53	A	199	A
53	A	328	C
53	A	361	G
53	A	367	U
53	A	397	A
53	A	406	G
53	A	409	U
53	A	422	C
53	A	425	G
53	A	499	A
53	A	531	U
53	A	532	A
53	A	533	A
53	A	544	G
53	A	547	A
53	A	587	G
53	A	653	U
53	A	776	G
53	A	793	U
53	A	843	U
53	A	884	U
53	A	971	G
53	A	992	U
53	A	1024	G
53	A	1045	C
53	A	1124	G
53	A	1201	A
53	A	1211	U
53	A	1225	A
53	A	1256	A
53	A	1281	C
53	A	1319	A
53	A	1493	A
53	A	1536	C

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

31 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	$\#\|Z\| > 2$
52	OMU	a	2552	52,60	19,22,23	0.27	0	26,31,34	0.48	0
52	PSU	a	2604	52	18,21,22	0.96	1 (5%)	22,30,33	0.83	1 (4%)
52	6MZ	a	2030	52	18,25,26	0.75	0	16,36,39	0.89	1 (6%)
52	PSU	a	2605	52	18,21,22	0.98	1 (5%)	22,30,33	0.90	0
52	PSU	a	955	52	18,21,22	0.91	1 (5%)	22,30,33	0.75	0
52	2MG	a	2445	52	18,26,27	1.01	1 (5%)	16,38,41	0.86	0
53	MA6	A	1519	53	18,26,27	0.80	1 (5%)	19,38,41	0.76	0
52	PSU	a	1917	52	18,21,22	0.96	1 (5%)	22,30,33	0.61	0
52	5MC	a	1962	52	18,22,23	0.33	0	26,32,35	0.65	0
52	6MZ	a	1618	52	18,25,26	0.69	0	16,36,39	0.89	1 (6%)
52	2MA	a	2503	52,60,59	17,25,26	1.02	2 (11%)	17,37,40	1.09	1 (5%)
52	PSU	a	2580	52,59	18,21,22	1.01	1 (5%)	22,30,33	0.69	1 (4%)
28	MEQ	d	150	28	8,9,10	0.44	0	5,10,12	1.35	1 (20%)
53	MA6	A	1518	53	18,26,27	0.83	2 (11%)	19,38,41	0.64	0
14	D2T	L	89	14	7,9,10	0.93	0	6,11,13	1.91	3 (50%)
52	PSU	a	1911	52	18,21,22	0.93	1 (5%)	22,30,33	0.62	0
52	3TD	a	1915	52	19,22,23	1.01	1 (5%)	21,32,35	0.70	0
52	PSU	a	2457	52	18,21,22	0.98	1 (5%)	22,30,33	0.64	0
53	G7M	A	527	53	20,26,27	1.10	2 (10%)	17,39,42	0.76	0
52	OMG	a	2251	52,25,59	18,26,27	0.99	2 (11%)	19,38,41	0.82	1 (5%)
52	1MG	a	745	52	18,26,27	1.03	2 (11%)	19,39,42	0.49	0
56	4D4	l	81	56	9,11,12	0.81	0	8,13,15	1.22	1 (12%)
52	PSU	a	746	52,60	18,21,22	1.00	1 (5%)	22,30,33	1.26	2 (9%)
52	5MU	a	747	52	19,22,23	0.30	0	28,32,35	0.49	0
52	2MG	a	1835	52	18,26,27	1.06	2 (11%)	16,38,41	0.72	0
52	5MU	a	1939	52,59	19,22,23	0.32	0	28,32,35	0.56	0
52	G7M	a	2069	52	20,26,27	1.10	3 (15%)	17,39,42	0.58	0
52	PSU	a	2504	52,59	18,21,22	0.93	1 (5%)	22,30,33	0.86	1 (4%)
57	IAS	K	119	57	6,7,8	0.96	0	6,8,10	0.92	0
52	H2U	a	2449	52	18,21,22	0.59	0	21,30,33	0.62	0
52	OMC	a	2498	52,60	19,22,23	0.27	0	26,31,34	0.65	0

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
52	OMU	a	2552	52,60	-	0/9/27/28	0/2/2/2
52	PSU	a	2604	52	-	0/7/25/26	0/2/2/2
52	6MZ	a	2030	52	-	2/5/27/28	0/3/3/3
52	PSU	a	2605	52	-	0/7/25/26	0/2/2/2
52	PSU	a	955	52	-	0/7/25/26	0/2/2/2
52	2MG	a	2445	52	-	0/5/27/28	0/3/3/3
53	MA6	A	1519	53	-	2/7/29/30	0/3/3/3
52	PSU	a	1917	52	-	0/7/25/26	0/2/2/2
52	5MC	a	1962	52	-	0/7/25/26	0/2/2/2
52	6MZ	a	1618	52	-	0/5/27/28	0/3/3/3
52	2MA	a	2503	52,60,59	-	1/3/25/26	0/3/3/3
52	PSU	a	2580	52,59	-	0/7/25/26	0/2/2/2
28	MEQ	d	150	28	-	2/8/9/11	-
53	MA6	A	1518	53	-	0/7/29/30	0/3/3/3
14	D2T	L	89	14	-	4/7/12/14	-
52	PSU	a	1911	52	-	0/7/25/26	0/2/2/2
52	3TD	a	1915	52	-	0/7/25/26	0/2/2/2
52	PSU	a	2457	52	-	0/7/25/26	0/2/2/2
53	G7M	A	527	53	-	2/3/25/26	0/3/3/3
52	OMG	a	2251	52,25,59	-	0/5/27/28	0/3/3/3
52	1MG	a	745	52	-	0/3/25/26	0/3/3/3
56	4D4	l	81	56	-	1/11/12/14	-
52	PSU	a	746	52,60	-	1/7/25/26	0/2/2/2
52	5MU	a	747	52	-	0/7/25/26	0/2/2/2
52	2MG	a	1835	52	-	0/5/27/28	0/3/3/3
52	5MU	a	1939	52,59	-	0/7/25/26	0/2/2/2
52	G7M	a	2069	52	-	2/3/25/26	0/3/3/3
52	PSU	a	2504	52,59	-	0/7/25/26	0/2/2/2
57	IAS	K	119	57	-	0/7/7/8	-
52	H2U	a	2449	52	-	0/7/38/39	0/2/2/2
52	OMC	a	2498	52,60	-	0/9/27/28	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	2580	PSU	C6-C5	4.01	1.40	1.35
52	a	1915	3TD	C6-C5	3.86	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	1917	PSU	C6-C5	3.86	1.39	1.35
52	a	2457	PSU	C6-C5	3.84	1.39	1.35
52	a	746	PSU	C6-C5	3.83	1.39	1.35
52	a	1911	PSU	C6-C5	3.75	1.39	1.35
52	a	2605	PSU	C6-C5	3.73	1.39	1.35
52	a	2604	PSU	C6-C5	3.68	1.39	1.35
52	a	2504	PSU	C6-C5	3.60	1.39	1.35
52	a	955	PSU	C6-C5	3.55	1.39	1.35
53	A	527	G7M	C8-N9	3.49	1.39	1.33
52	a	2069	G7M	C8-N9	3.26	1.39	1.33
52	a	2503	2MA	C2-N3	2.81	1.37	1.31
52	a	2251	OMG	C5-C6	-2.70	1.41	1.47
52	a	1835	2MG	C5-C6	-2.59	1.42	1.47
52	a	2069	G7M	C8-N7	2.46	1.37	1.33
53	A	527	G7M	C8-N7	2.44	1.37	1.33
52	a	745	1MG	C6-N1	2.40	1.43	1.39
52	a	2445	2MG	C5-C6	-2.34	1.42	1.47
52	a	2503	2MA	C5-C4	-2.30	1.37	1.43
53	A	1518	MA6	C6-N1	2.19	1.36	1.33
52	a	745	1MG	C5-C4	-2.14	1.37	1.43
53	A	1519	MA6	C6-N1	2.14	1.36	1.33
53	A	1518	MA6	C8-N7	-2.06	1.31	1.34
52	a	2251	OMG	C8-N7	-2.04	1.31	1.35
52	a	1835	2MG	C8-N7	-2.02	1.31	1.35
52	a	2069	G7M	C5-C6	-2.02	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	a	746	PSU	C3'-C2'-C1'	3.41	105.61	101.64
52	a	2503	2MA	CM2-C2-N1	3.19	123.32	116.23
52	a	746	PSU	O3'-C3'-C4'	2.91	119.45	111.05
14	L	89	D2T	O-C-CA	-2.53	118.15	124.78
14	L	89	D2T	OD1-CG-CB	-2.50	117.21	122.44
52	a	2030	6MZ	C2-N1-C6	2.44	118.68	116.59
14	L	89	D2T	OD2-CG-CB	2.38	118.29	113.15
52	a	1618	6MZ	C2-N1-C6	2.34	118.60	116.59
52	a	2604	PSU	C2'-C3'-C4'	-2.29	98.19	102.64
52	a	2580	PSU	C3'-C2'-C1'	2.08	104.06	101.64
52	a	2251	OMG	O6-C6-C5	2.01	128.30	124.37
28	d	150	MEQ	OE1-CD-CG	-2.01	118.34	122.02
56	l	81	4D4	OB-CB-CG	-2.01	104.78	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	a	2504	PSU	C2'-C3'-C4'	-2.00	98.75	102.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	L	89	D2T	CA-CB-CG-OD1
14	L	89	D2T	CA-CB-CG-OD2
53	A	527	G7M	O4'-C4'-C5'-O5'
53	A	527	G7M	C3'-C4'-C5'-O5'
53	A	1519	MA6	O4'-C4'-C5'-O5'
28	d	150	MEQ	NE2-CD-CG-CB
28	d	150	MEQ	OE1-CD-CG-CB
53	A	1519	MA6	C3'-C4'-C5'-O5'
52	a	2030	6MZ	O4'-C4'-C5'-O5'
52	a	2069	G7M	C4'-C5'-O5'-P
52	a	2030	6MZ	C3'-C4'-C5'-O5'
14	L	89	D2T	SB-CB-CG-OD2
14	L	89	D2T	CG-CB-SB-CB1
52	a	746	PSU	O4'-C1'-C5-C6
52	a	2069	G7M	O4'-C4'-C5'-O5'
52	a	2503	2MA	O4'-C4'-C5'-O5'
56	l	81	4D4	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 423 ligands modelled in this entry, 422 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
61	PRO	Y	101	50	5,7,8	0.60	0	7,8,10	0.80	0

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
61	PRO	Y	101	50	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

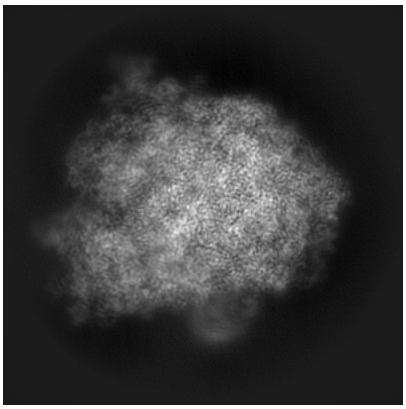
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18534. These allow visual inspection of the internal detail of the map and identification of artifacts.

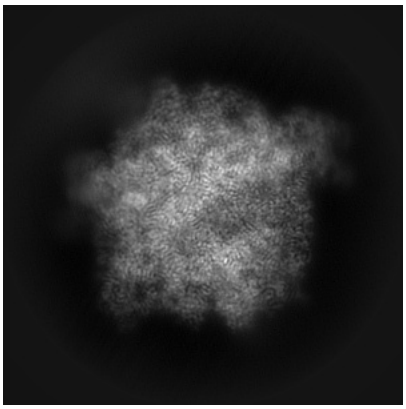
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

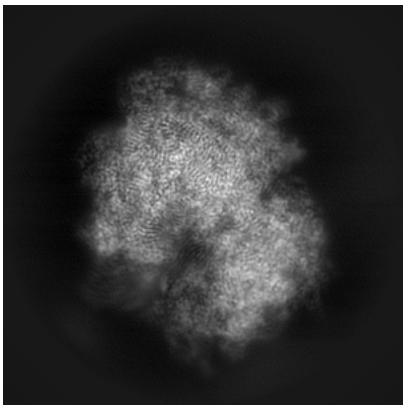
6.1.1 Primary map



X

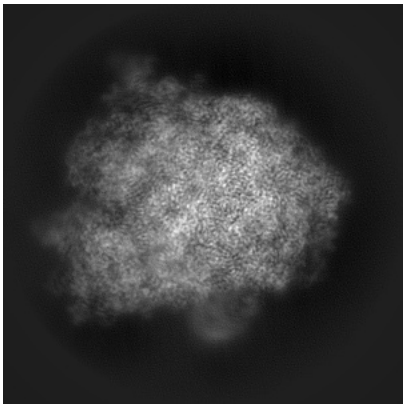


Y

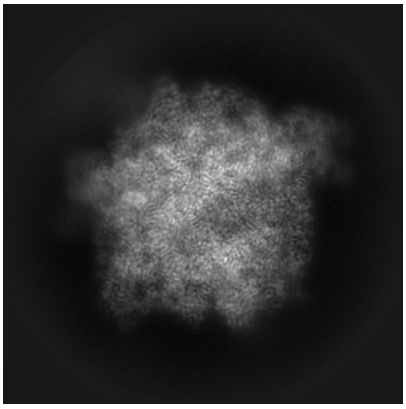


Z

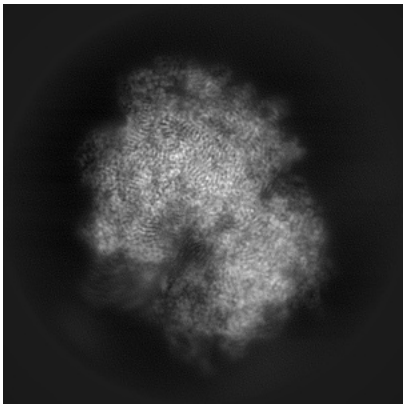
6.1.2 Raw map



X



Y

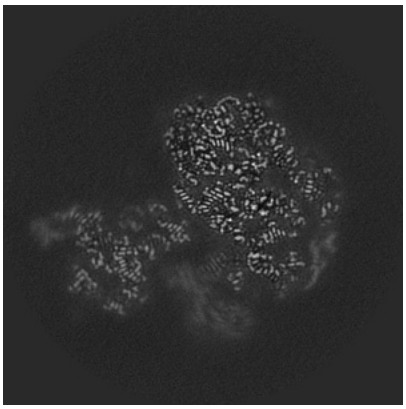


Z

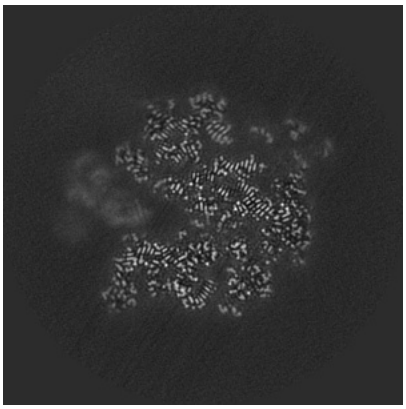
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

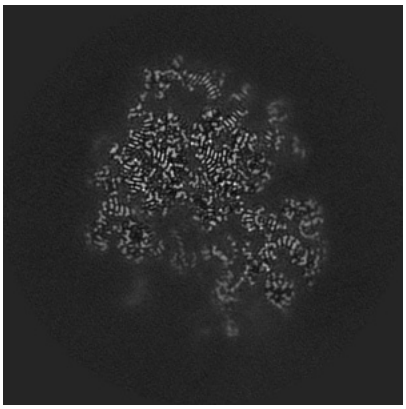
6.2.1 Primary map



X Index: 200

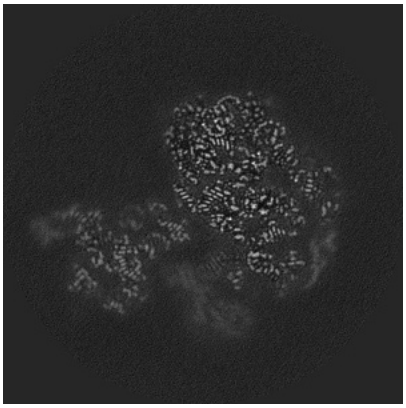


Y Index: 200

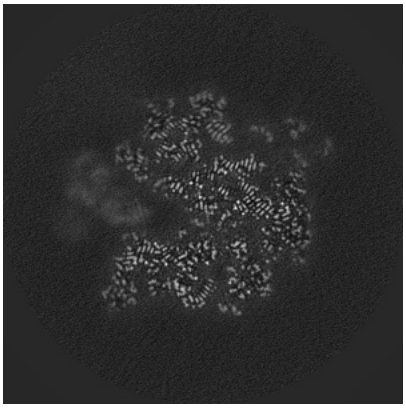


Z Index: 200

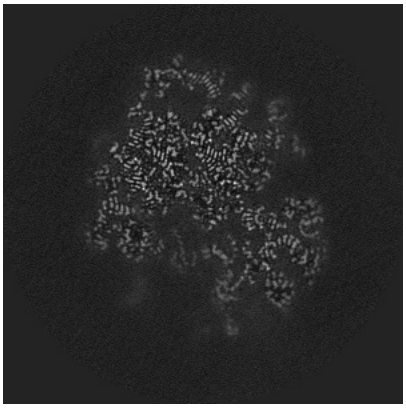
6.2.2 Raw map



X Index: 200



Y Index: 200

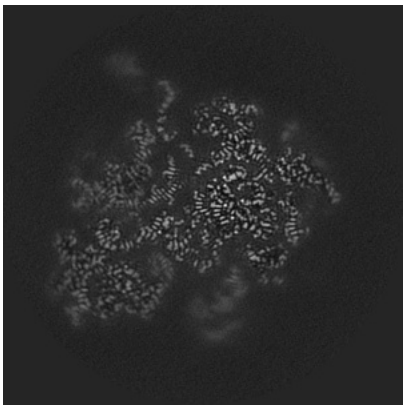


Z Index: 200

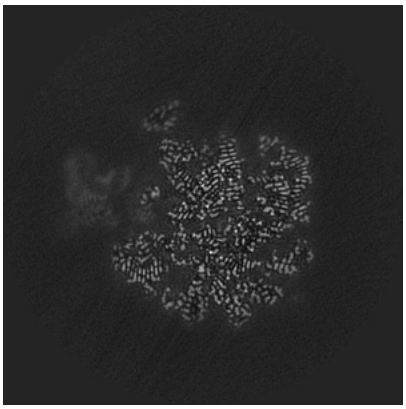
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

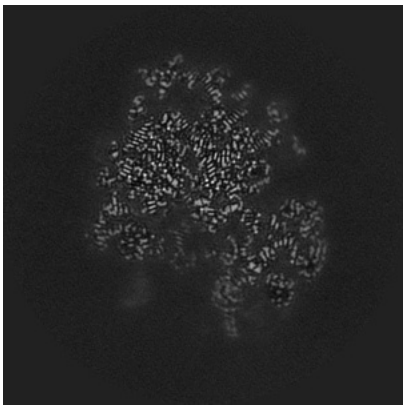
6.3.1 Primary map



X Index: 225

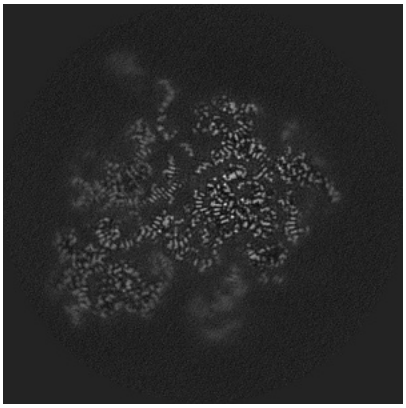


Y Index: 221

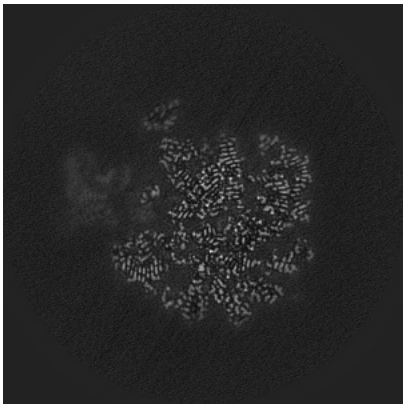


Z Index: 202

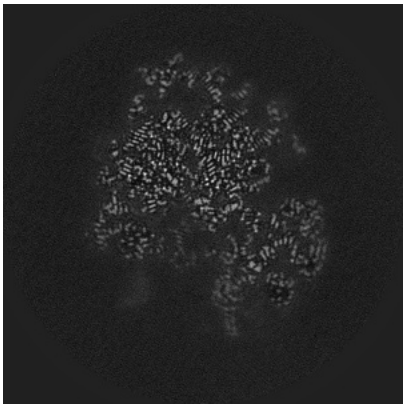
6.3.2 Raw map



X Index: 225



Y Index: 221

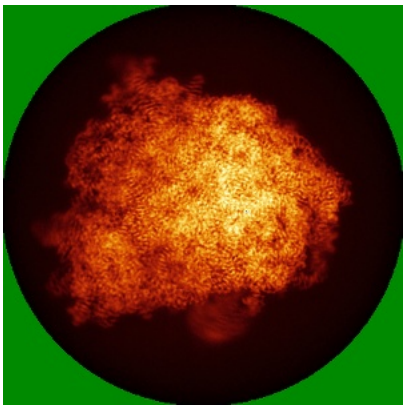


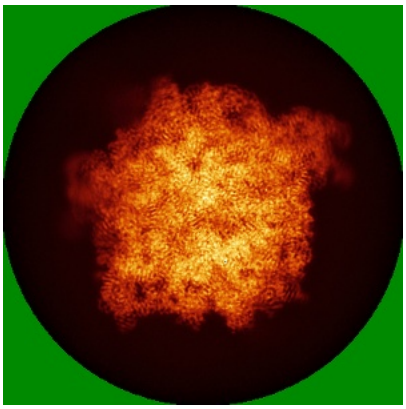
Z Index: 202

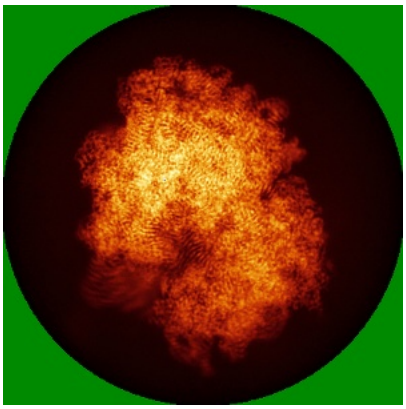
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

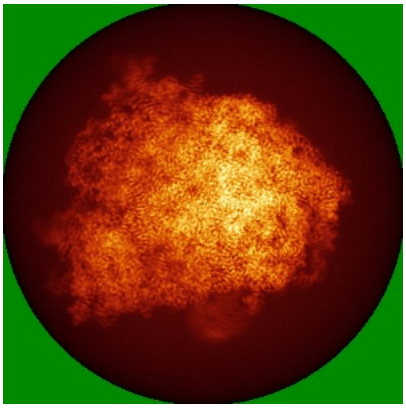
6.4.1 Primary map

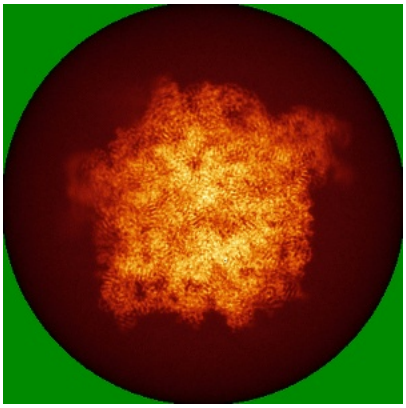

X

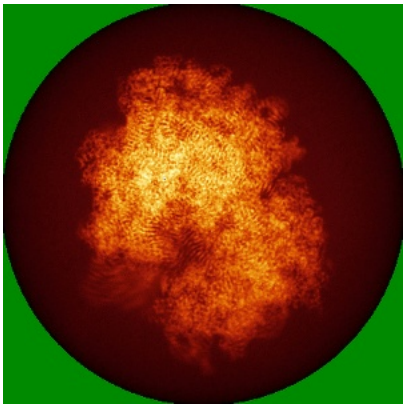

Y


Z

6.4.2 Raw map


X

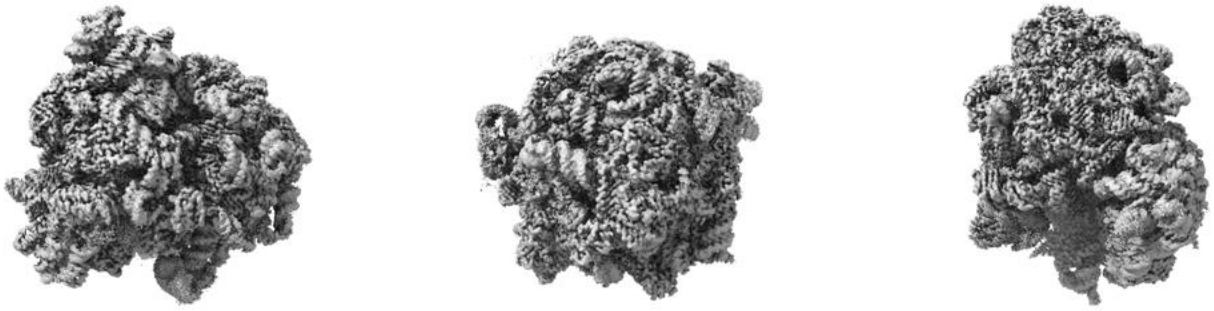

Y


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)

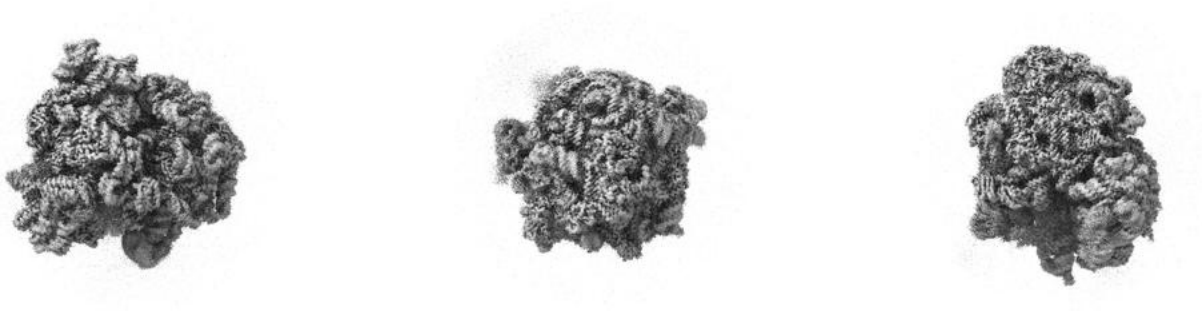
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00495. 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.

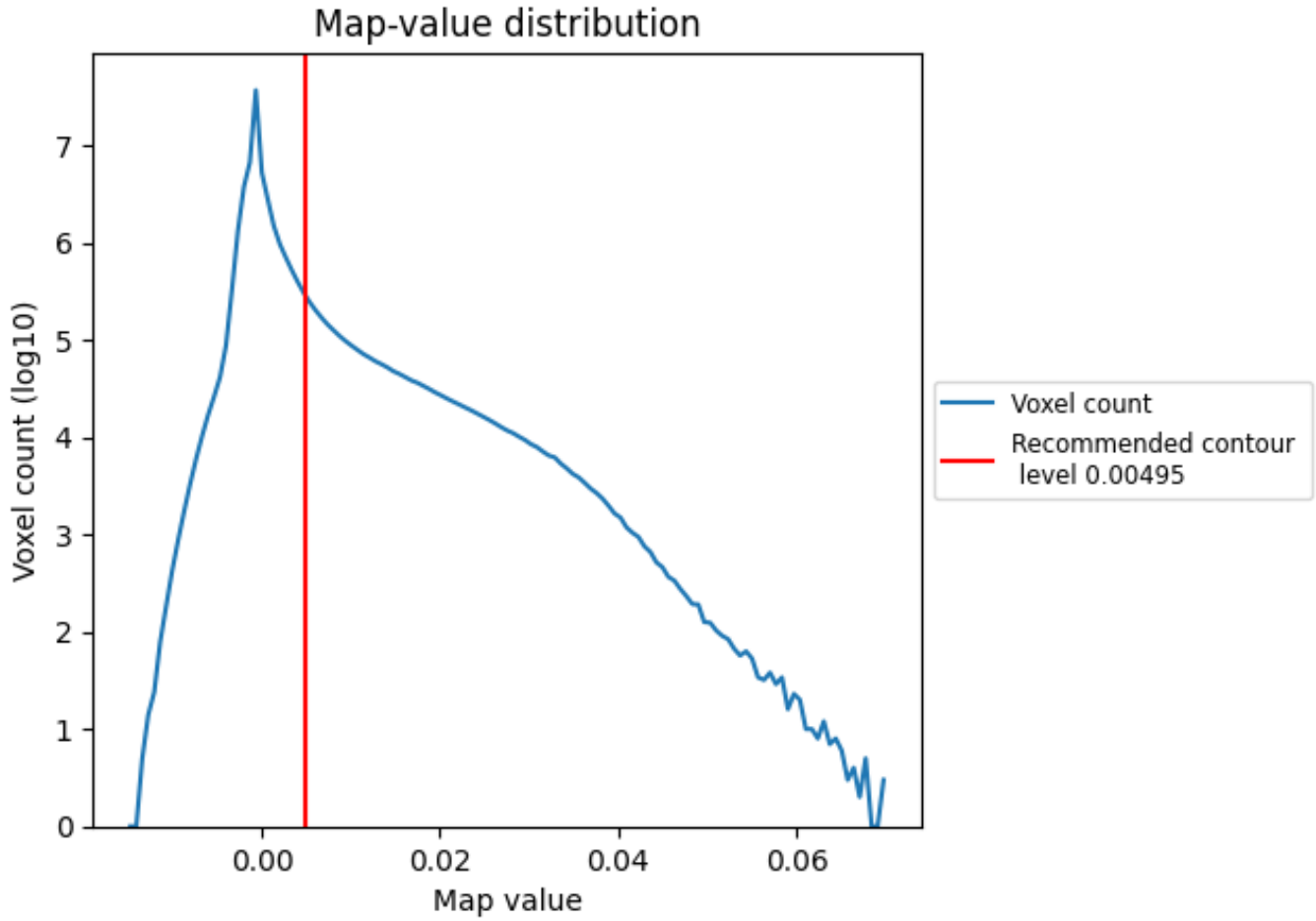
6.6 Mask visualisation (i)

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

7 Map analysis

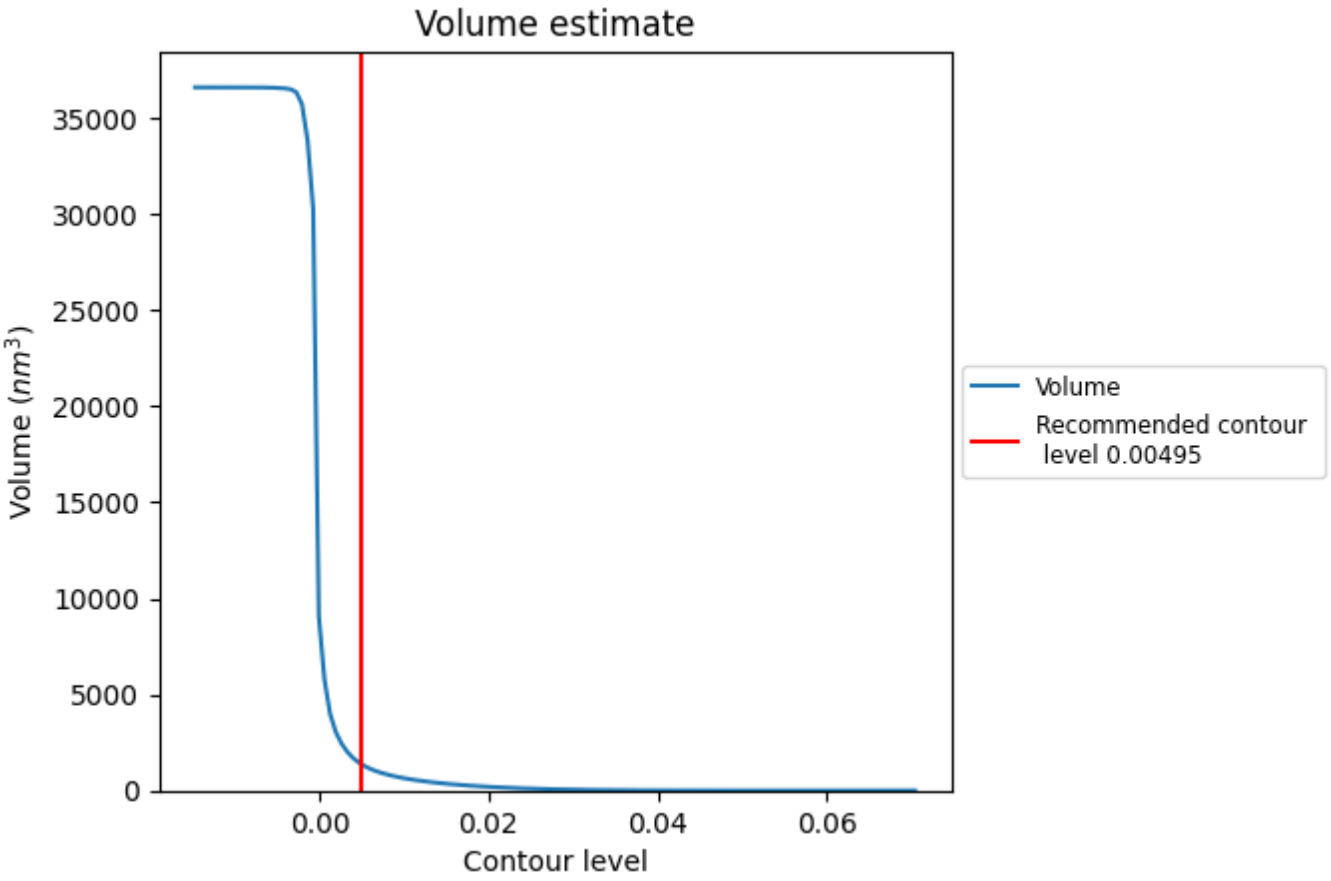
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

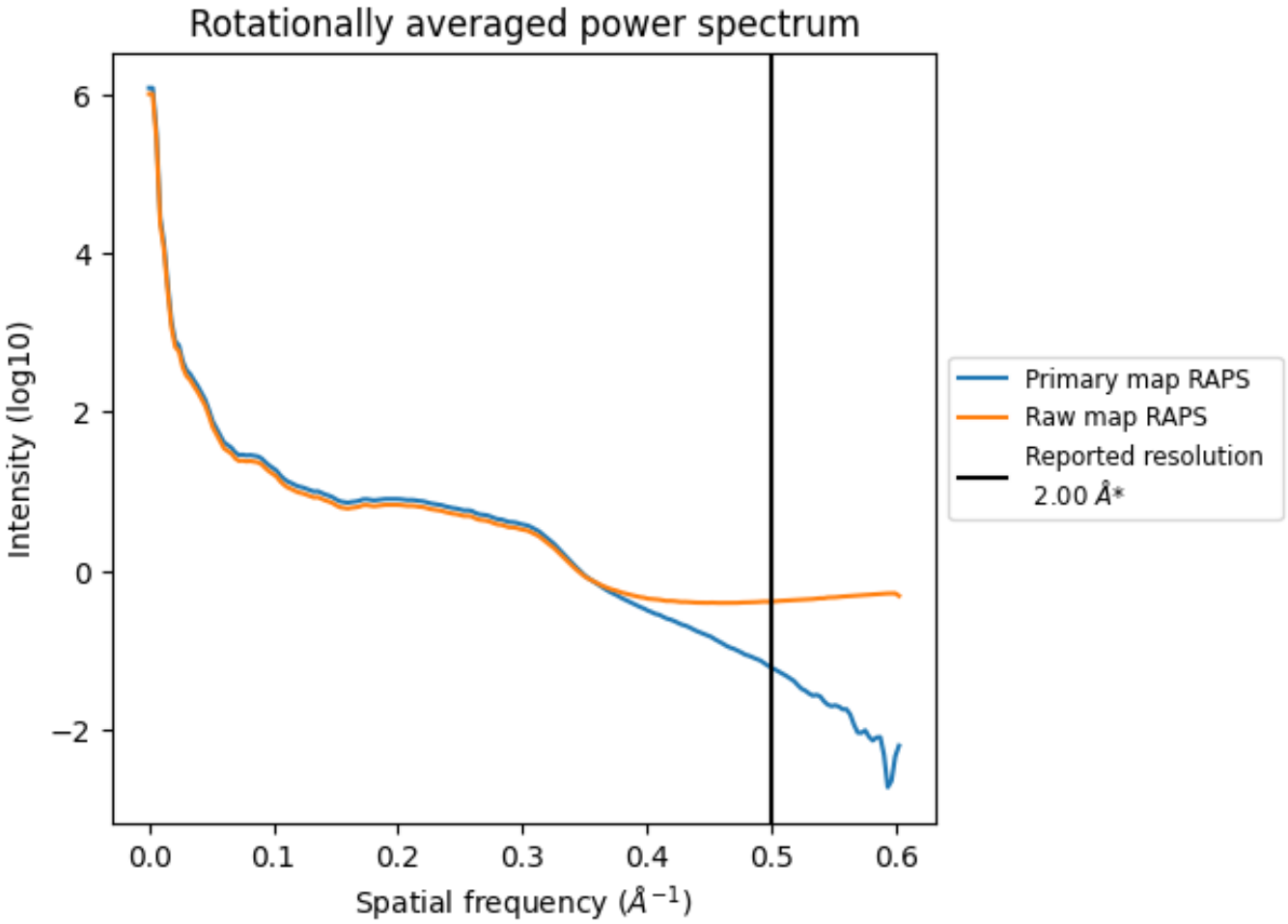
7.2 Volume estimate



The volume at the recommended contour level is 1377 nm^3; this corresponds to an approximate mass of 1244 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)

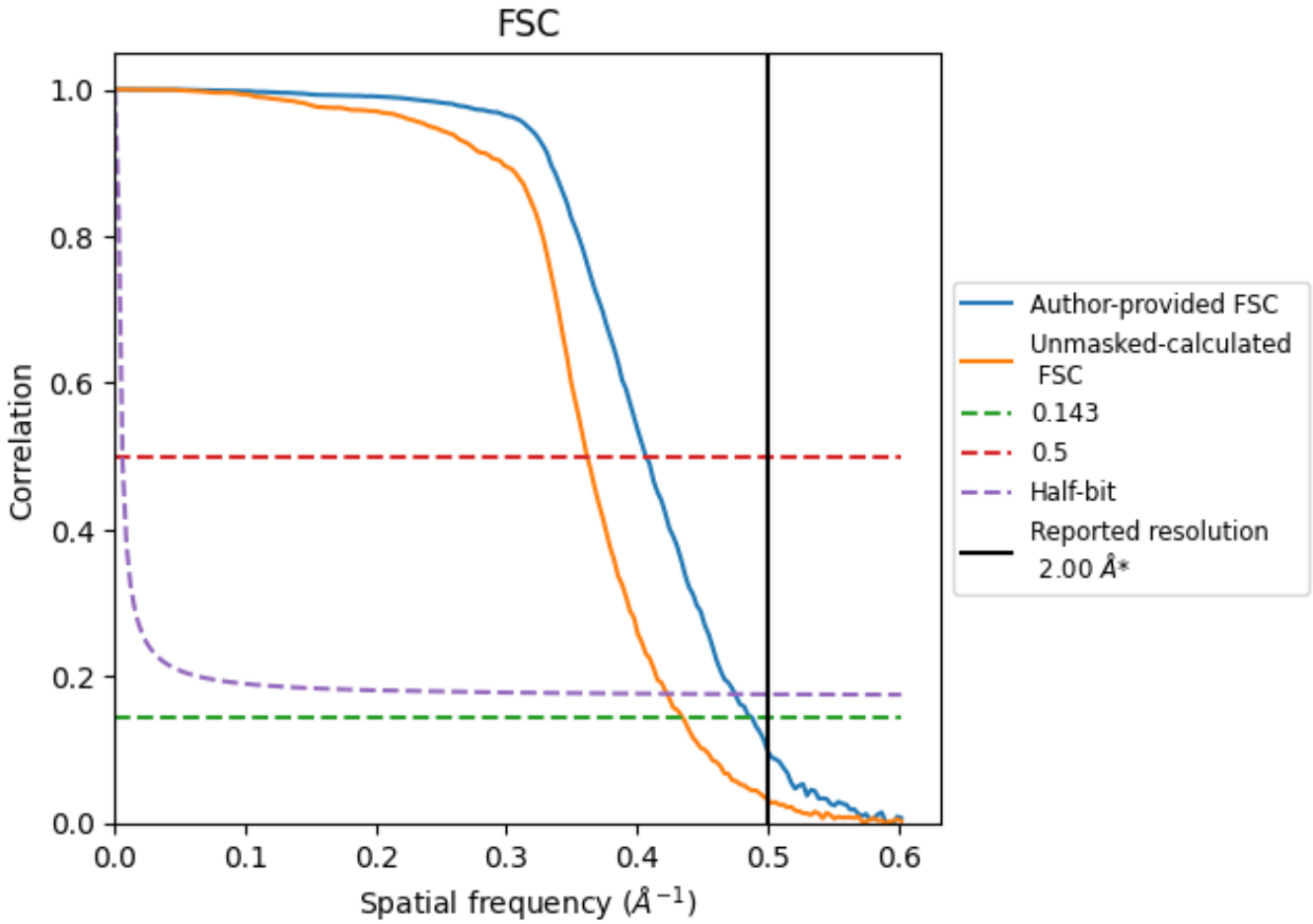


*Reported resolution corresponds to spatial frequency of 0.500 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.500 Å^{-1}

8.2 Resolution estimates (i)

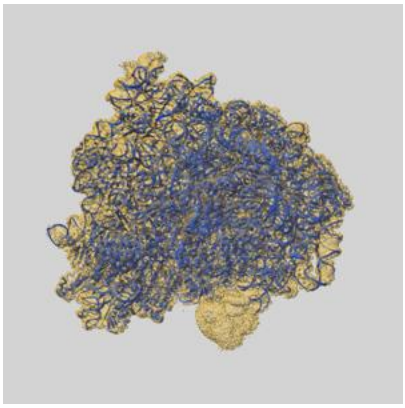
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	2.05	2.46	2.11
Unmasked-calculated*	2.30	2.76	2.37

*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 2.30 differs from the reported value 2.0 by more than 10 %

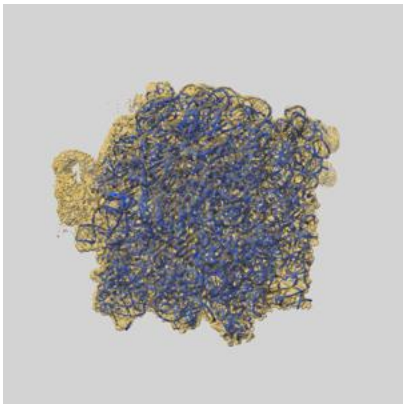
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18534 and PDB model 8QOA. Per-residue inclusion information can be found in section 3 on page 18.

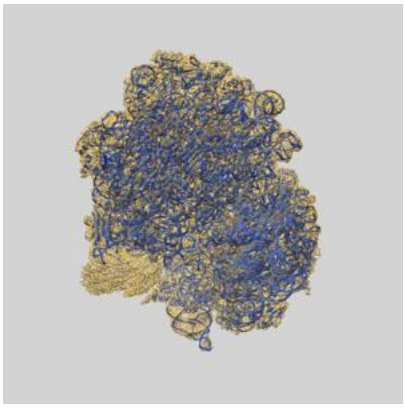
9.1 Map-model overlay



X



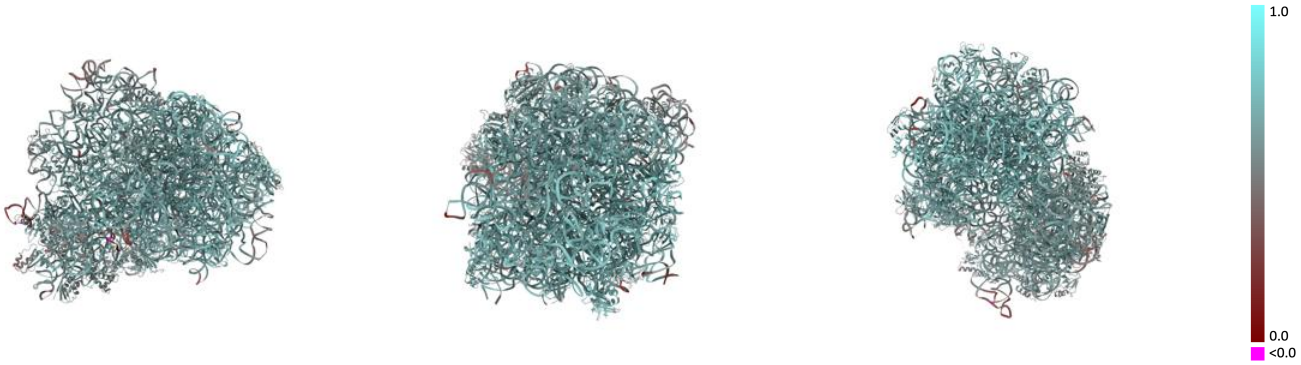
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00495 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.

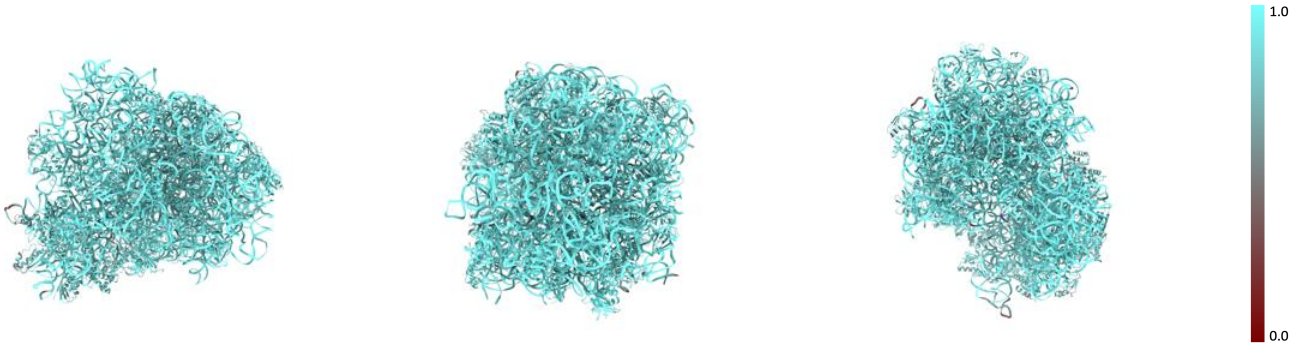
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

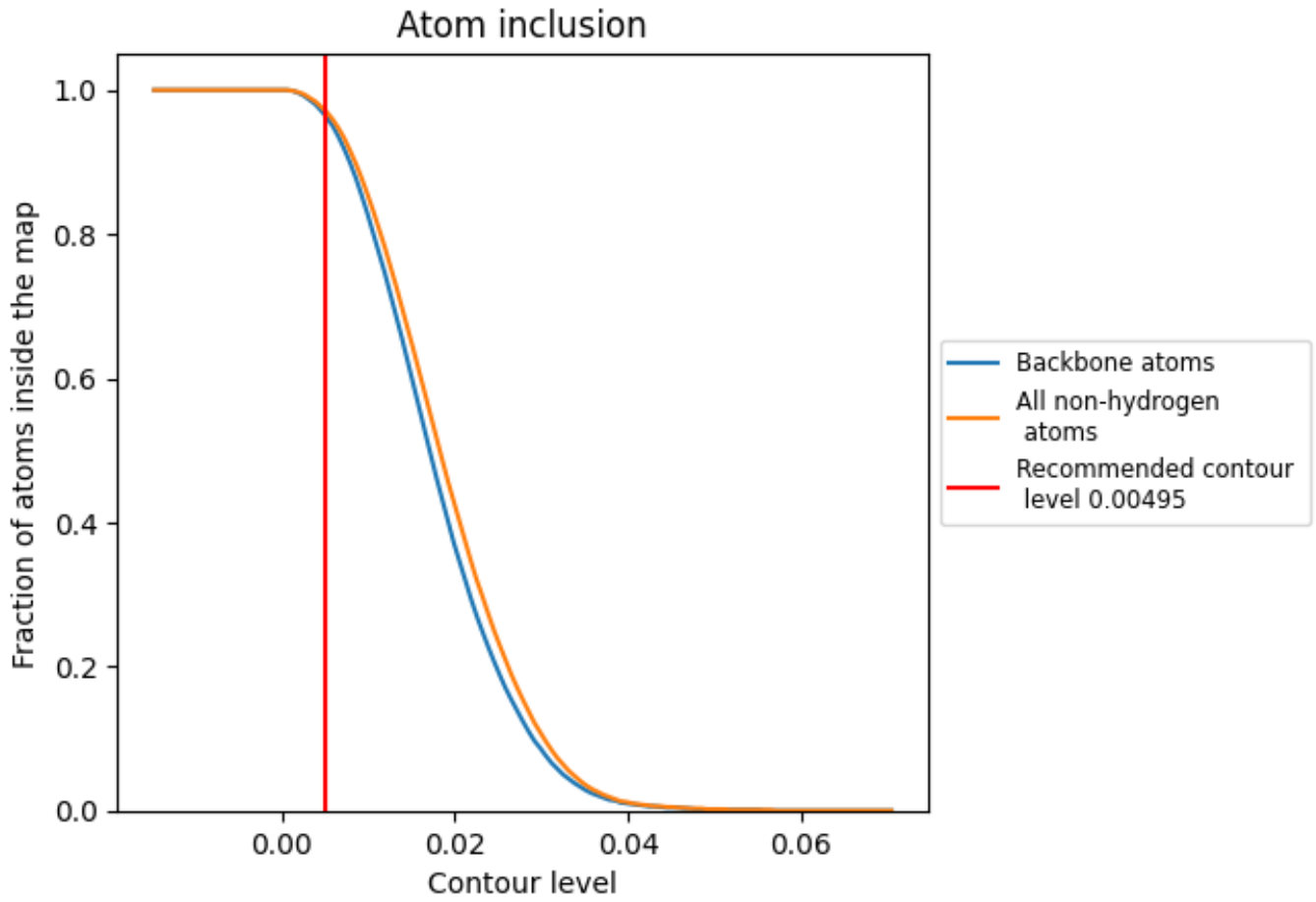
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.00495).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.00495) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9720	0.6520
0	0.9570	0.6700
1	0.9920	0.7250
2	0.9860	0.7170
3	0.9690	0.6830
4	0.8770	0.5370
5	1.0000	0.6750
6	0.9240	0.6320
A	0.9850	0.6200
B	0.8820	0.5680
C	0.9150	0.6000
D	0.8680	0.5700
E	0.9510	0.6510
F	0.9060	0.5890
G	0.9030	0.5630
H	0.9420	0.6380
I	0.9160	0.5850
J	0.8380	0.5430
K	0.9480	0.6300
L	0.9420	0.6040
M	0.9330	0.5940
N	0.9440	0.6050
O	0.9450	0.6310
P	0.9050	0.5820
Q	0.9240	0.5680
R	0.9410	0.6210
S	0.9170	0.5780
T	0.9210	0.5800
U	0.8610	0.5450
X	0.9840	0.6240
Y	0.9160	0.5970
Z	0.9670	0.5890
a	0.9950	0.6840
b	0.9950	0.6520
c	0.9800	0.7110

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.9660	0.6980
e	0.9350	0.6620
f	0.9160	0.5930
g	0.9190	0.5890
h	0.9230	0.6080
i	0.9760	0.7010
j	0.9700	0.6880
k	0.9690	0.6910
l	0.9750	0.6930
m	0.9910	0.7130
n	0.9370	0.6410
o	0.9610	0.6890
p	0.9880	0.7180
q	0.9400	0.6750
r	0.9650	0.6970
s	0.9360	0.6520
t	0.9350	0.6340
u	0.9110	0.6370
v	0.9640	0.6980
w	0.9750	0.6890
x	0.9080	0.6200
y	0.9460	0.6790
z	0.9800	0.7010