



Full wwPDB EM Validation Report ⓘ

Jul 11, 2024 – 02:00 PM EDT

PDB ID : 8FZE
EMDB ID : EMD-29621
Title : Cryo-EM structure of an E. coli non-rotated ribosome termination complex bound with RF1, P- and E-site tRNAPhe (State I-A)
Authors : Rybak, M.Y.; Li, L.; Lin, J.; Gagnon, M.G.
Deposited on : 2023-01-28
Resolution : 3.00 Å(reported)
Based on initial model : 7K00

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:

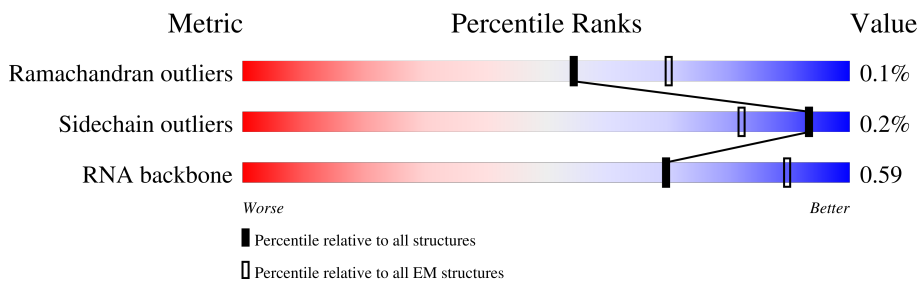
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.00 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.



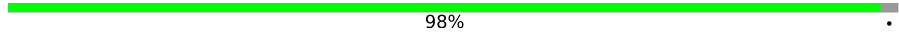
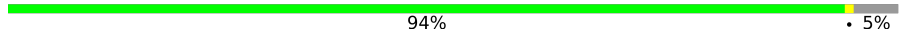

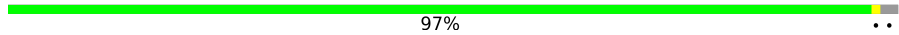
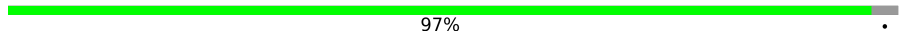
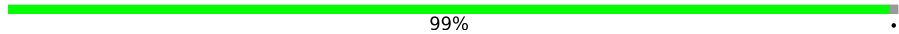
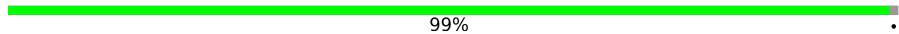
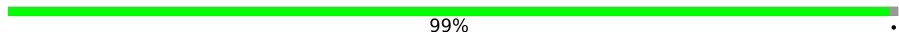
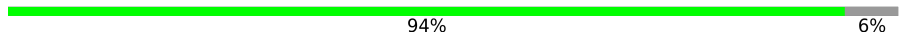


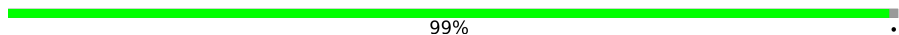




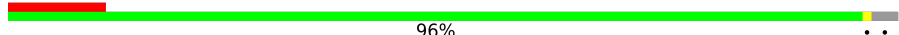


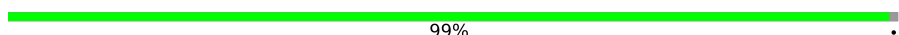
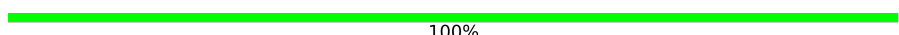
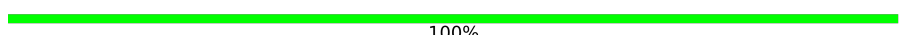
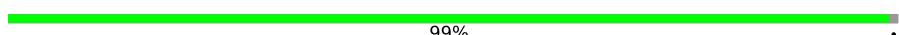
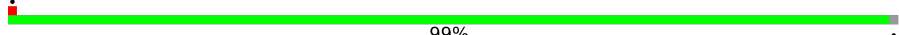

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	a	1542	
2	b	241	
3	c	233	
4	d	206	
5	e	167	
6	f	131	
7	g	156	
8	h	130	

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Mol	Chain	Length	Quality of chain
9	i	130	 98%
10	j	103	 94% 5%
11	k	129	 90% 9%
12	l	124	 97%
13	m	118	 97%
14	n	101	 99%
15	o	89	 99%
16	p	82	 99%
17	q	84	 94% 6%
18	r	75	 72% 28%
19	s	92	 90% 10%
20	t	87	 99%
21	u	71	 76% 23%
22	x	76	 71% 28%
22	y	76	 67% 28%
23	z	21	 38% 10% 52%
24	w	360	 11% 96%
25	A	2904	 86% 13%
26	B	120	 88% 12%
27	C	273	 99%
28	D	209	 100%
29	E	201	 100%
30	F	179	 99%
31	G	177	 99%
32	H	149	 7% 26% 74%

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Mol	Chain	Length	Quality of chain
33	I	165	24% 79% 21%
34	J	142	5% 99%
35	L	142	100%
36	M	123	99%
37	N	144	100%
38	O	136	99%
39	P	127	93% 7%
40	Q	117	99%
41	R	115	99%
42	S	118	99%
43	T	103	100%
44	U	110	100%
45	V	100	93% 7%
46	W	104	98%
47	X	94	100%
48	Y	85	88% 11%
49	Z	78	99%
50	1	63	97%
51	2	59	98%
52	3	70	86% 14%
53	4	57	96%
54	5	55	93% 7%
55	6	46	98%
56	7	65	95%
57	8	38	100%

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 150009 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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1528	32803	14637	6019	10619	1528	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	224	1754	1110	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	156	1152	717	217	212	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	152	1191	741	230	216	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	117	877	540	173	161	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	121	942	582	193	162	5	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			446	283	85	78		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 22 is a RNA chain called P-site phenylalanyl-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	x	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		
22	y	74	Total	C	N	O	P	S	0	0
			1584	707	285	517	74	1		

- Molecule 23 is a RNA chain called F-UAA mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	z	10	Total	C	N	O	P	0	0
			210	95	36	69	10		

- Molecule 24 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	349	Total	C	N	O	S	0	0
			2750	1679	513	545	13		

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

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

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 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

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

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 50S ribosomal protein L5.

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 50S ribosomal protein L6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	131	Total	C	N	O	S	0	0
			982	622	172	183	5		

- Molecule 34 is a protein called 50S ribosomal protein L11.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	N	144	1052	653	207	190	2	0	0

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	82	MS6	MET	conflict	UNP E6BI61

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called Ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	60	Total	C	N	O	S	0	0
			468	290	87	85	6		

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	5	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	a	121	Total	Mg	0
			121	121	
58	n	1	Total	Mg	0
			1	1	
58	x	2	Total	Mg	0
			2	2	
58	A	423	Total	Mg	0
			423	423	
58	B	10	Total	Mg	0
			10	10	
58	C	4	Total	Mg	0
			4	4	
58	N	1	Total	Mg	0
			1	1	
58	P	1	Total	Mg	0
			1	1	
58	S	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
58	V	1	Total 1	Mg 1	0
58	Y	1	Total 1	Mg 1	0
58	4	2	Total 2	Mg 2	0
58	6	1	Total 1	Mg 1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	3	1	Total 1	Zn 1	0
59	8	1	Total 1	Zn 1	0

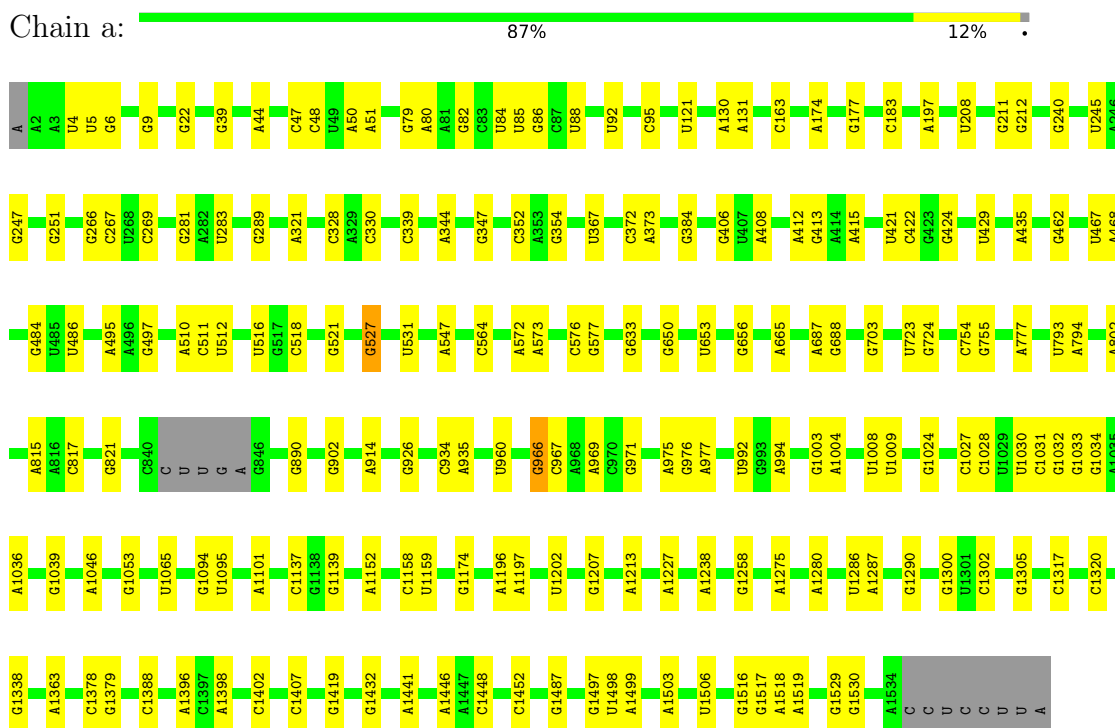
- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	a	17	Total 17	O 17	0
60	k	1	Total 1	O 1	0
60	y	1	Total 1	O 1	0
60	A	133	Total 133	O 133	0
60	B	4	Total 4	O 4	0
60	D	1	Total 1	O 1	0
60	6	1	Total 1	O 1	0
60	8	1	Total 1	O 1	0

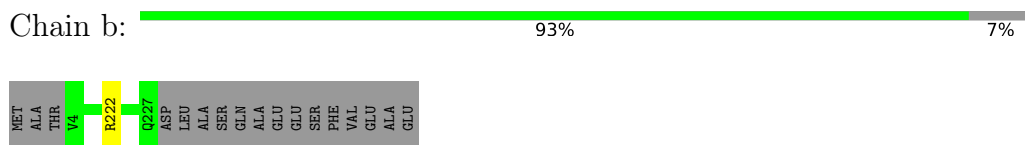
3 Residue-property plots i

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.

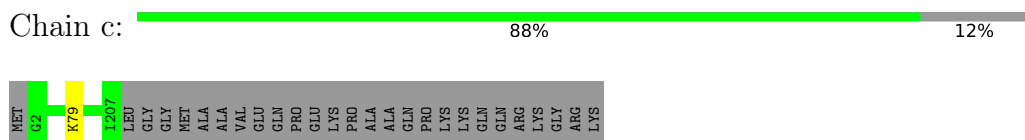
• Molecule 1: 16S Ribosomal RNA



• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



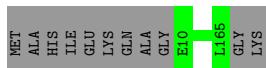
- Molecule 4: 30S ribosomal protein S4

Chain d:  99%




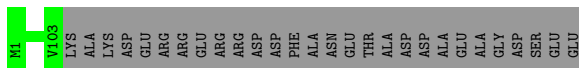
- Molecule 5: 30S ribosomal protein S5

Chain e:  93% 7%



- Molecule 6: 30S ribosomal protein S6

Chain f:  79% 21%



- Molecule 7: 30S ribosomal protein S7

Chain g:  97%



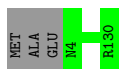
- Molecule 8: 30S ribosomal protein S8

Chain h:  99%



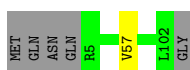
- Molecule 9: 30S ribosomal protein S9

Chain i:  98%



- Molecule 10: 30S ribosomal protein S10

Chain j:  94% 5%



- Molecule 11: 30S ribosomal protein S11

Chain k:  90% 9%



- Molecule 12: 30S ribosomal protein S12

Chain l:  97%



- Molecule 13: 30S ribosomal protein S13

Chain m:  97%



- Molecule 14: 30S ribosomal protein S14

Chain n:  99%



- Molecule 15: 30S ribosomal protein S15

Chain o:  99%



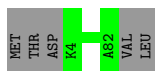
- Molecule 16: 30S ribosomal protein S16

Chain p:  99%

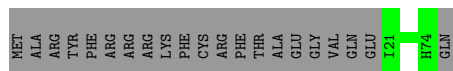


- Molecule 17: 30S ribosomal protein S17

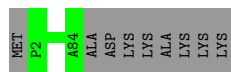
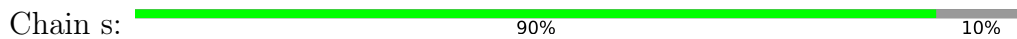
Chain q:  94% 6%



- Molecule 18: 30S ribosomal protein S18



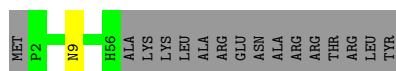
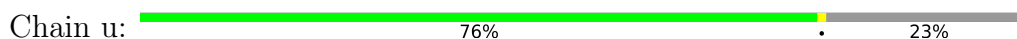
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



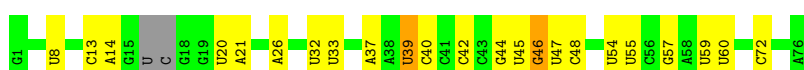
• Molecule 21: 30S ribosomal protein S21



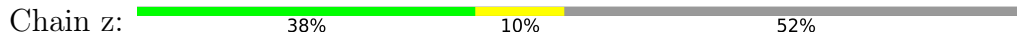
• Molecule 22: P-site phenylalanyl-tRNA



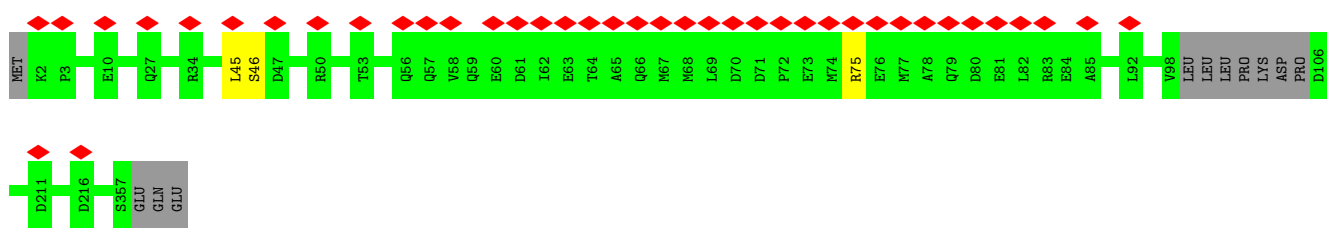
• Molecule 22: P-site phenylalanyl-tRNA



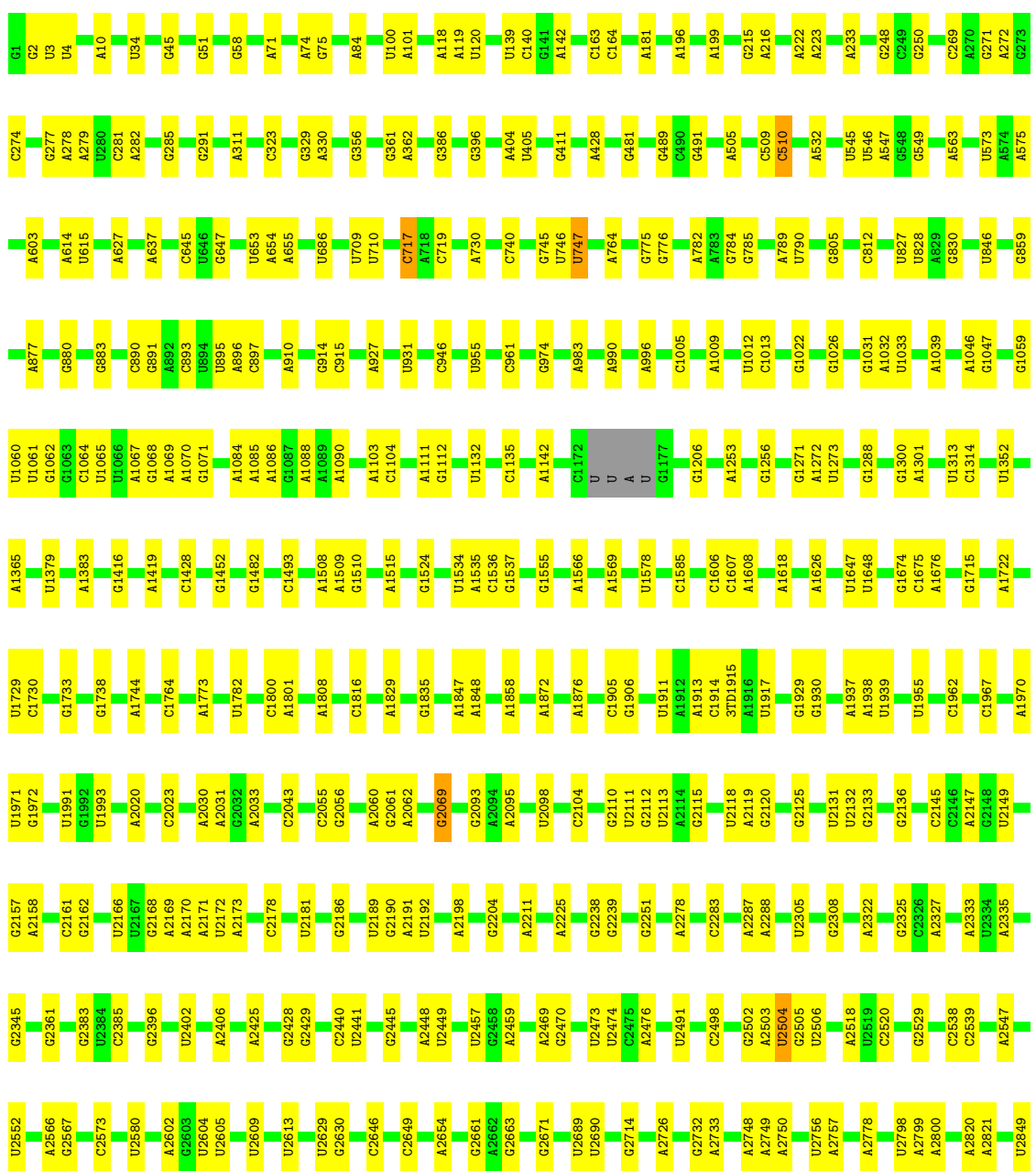
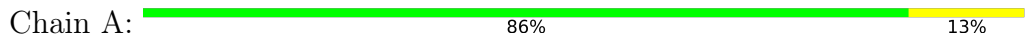
• Molecule 23: F-UAA mRNA

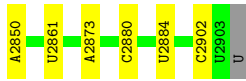


• Molecule 24: Peptide chain release factor 1



• Molecule 25: 23S Ribosomal RNA





- Molecule 26: 5S Ribosomal RNA

Chain B: 88% 12%



- Molecule 27: 50S ribosomal protein L2

Chain C: 99%



- Molecule 28: 50S ribosomal protein L3

Chain D: 100%



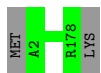
- Molecule 29: 50S ribosomal protein L4

Chain E: 100%



- Molecule 30: 50S ribosomal protein L5

Chain F: 99%



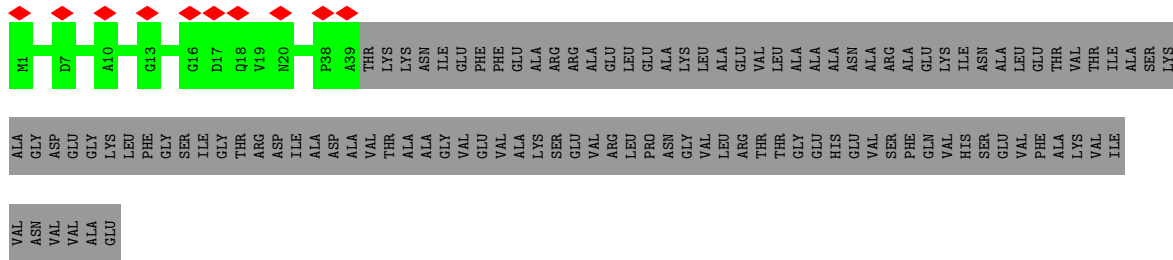
- Molecule 31: 50S ribosomal protein L6

Chain G: 99%

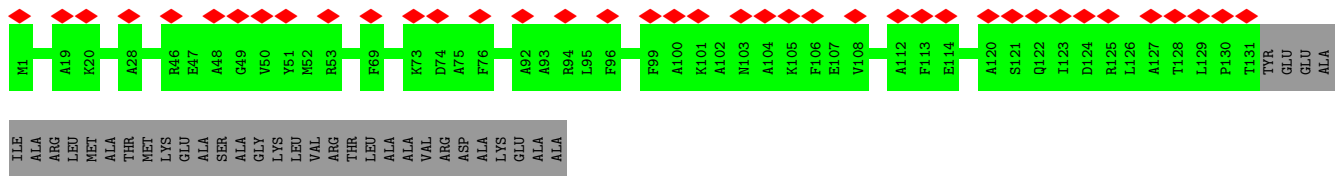
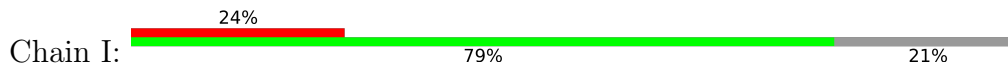


- Molecule 32: 50S ribosomal protein L9

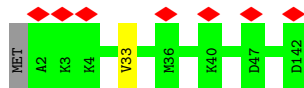
Chain H: 7% 26% 74%



- Molecule 33: 50S ribosomal protein L10



- Molecule 34: 50S ribosomal protein L11

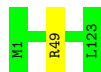


- Molecule 35: 50S ribosomal protein L13



There are no outlier residues recorded for this chain.

- Molecule 36: 50S ribosomal protein L14



- Molecule 37: 50S ribosomal protein L15



There are no outlier residues recorded for this chain.

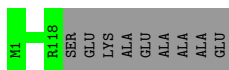
- Molecule 38: 50S ribosomal protein L16





- Molecule 39: 50S ribosomal protein L17

Chain P: 93% 7%



- Molecule 40: 50S ribosomal protein L18

Chain Q: 99%



- Molecule 41: 50S ribosomal protein L19

Chain R: 99%



- Molecule 42: 50S ribosomal protein L20

Chain S: 99%



- Molecule 43: Ribosomal protein L21

Chain T: 100%

There are no outlier residues recorded for this chain.

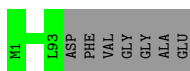
- Molecule 44: 50S ribosomal protein L22

Chain U: 100%

There are no outlier residues recorded for this chain.

- Molecule 45: 50S ribosomal protein L23

Chain V: 93% 7%



- Molecule 46: 50S ribosomal protein L24

Chain W:  98%




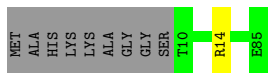
- Molecule 47: 50S ribosomal protein L25

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 50S ribosomal protein L27

Chain Y:  88% 11%



- Molecule 49: 50S ribosomal protein L28

Chain Z:  99%



- Molecule 50: 50S ribosomal protein L29

Chain 1:  97%




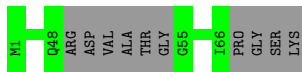
- Molecule 51: 50S ribosomal protein L30

Chain 2:  98%



- Molecule 52: 50S ribosomal protein L31

Chain 3:  86% 14%



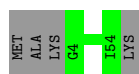
- Molecule 53: 50S ribosomal protein L32

Chain 4:  96% .



- Molecule 54: 50S ribosomal protein L33

Chain 5:  93% 7%



- Molecule 55: 50S ribosomal protein L34

Chain 6:  98% .



- Molecule 56: 50S ribosomal protein L35

Chain 7:  95% . .



- Molecule 57: 50S ribosomal protein L36

Chain 8:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.600	Depositor
Minimum map value	-0.505	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, OMU, 4OC, MS6, H2U, 3TD, OMG, IAS, 1MG, 4SU, ZN, G7M, MIA, MG, UR3, D2T, 2MG, MA6, OMC, 7MG, PSU, MEQ, 2MA, 6MZ, 5MU, 4D4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.24	0/36450	0.78	4/56856 (0.0%)
2	b	0.28	0/1785	0.53	0/2404
3	c	0.26	0/1651	0.55	0/2225
4	d	0.25	0/1665	0.53	0/2227
5	e	0.25	0/1165	0.53	0/1568
6	f	0.31	0/858	0.63	0/1160
7	g	0.24	0/1206	0.54	0/1617
8	h	0.26	0/989	0.54	0/1326
9	i	0.26	0/1034	0.57	0/1375
10	j	0.24	0/796	0.59	0/1077
11	k	0.26	0/884	0.56	0/1191
12	l	0.25	0/945	0.59	0/1268
13	m	0.25	0/900	0.59	0/1204
14	n	0.26	0/817	0.58	0/1088
15	o	0.25	0/722	0.55	0/964
16	p	0.25	0/653	0.56	0/877
17	q	0.25	0/650	0.57	0/871
18	r	0.25	0/453	0.55	0/609
19	s	0.26	0/680	0.52	0/915
20	t	0.25	0/676	0.51	0/895
21	u	0.26	0/467	0.65	1/620 (0.2%)
22	x	0.35	1/1651 (0.1%)	0.82	0/2569
22	y	0.22	0/1605	0.84	0/2497
23	z	0.24	0/234	0.79	0/361
24	w	0.25	0/2788	0.57	1/3753 (0.0%)
25	A	0.27	0/69147	0.80	8/107869 (0.0%)
26	B	0.31	1/2876 (0.0%)	0.81	0/4483
27	C	0.27	0/2121	0.59	0/2852
28	D	0.25	0/1576	0.54	0/2119
29	E	0.24	0/1571	0.51	0/2113
30	F	0.26	0/1434	0.55	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	G	0.25	0/1343	0.52	0/1816
32	H	0.23	0/290	0.49	0/392
33	I	0.26	0/995	0.56	0/1343
34	J	0.25	0/1046	0.51	0/1410
35	L	0.25	0/1152	0.50	0/1551
36	M	0.25	0/955	0.57	0/1279
37	N	0.25	0/1061	0.57	0/1412
38	O	0.25	0/1073	0.53	0/1433
39	P	0.24	0/958	0.57	0/1281
40	Q	0.25	0/902	0.55	0/1209
41	R	0.25	0/929	0.54	0/1242
42	S	0.25	0/960	0.51	0/1278
43	T	0.26	0/829	0.56	0/1107
44	U	0.24	0/864	0.53	0/1156
45	V	0.24	0/744	0.51	0/994
46	W	0.27	0/787	0.54	0/1051
47	X	0.25	0/766	0.52	0/1025
48	Y	0.25	0/589	0.56	0/779
49	Z	0.23	0/635	0.57	0/848
50	1	0.22	0/496	0.50	0/660
51	2	0.23	0/453	0.54	0/605
52	3	0.24	0/475	0.48	0/633
53	4	0.24	0/440	0.57	0/588
54	5	0.25	0/424	0.52	0/565
55	6	0.23	0/380	0.64	0/498
56	7	0.24	0/513	0.54	0/676
57	8	0.24	0/303	0.57	0/397
All	All	0.26	2/160811 (0.0%)	0.73	14/240107 (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
38	O	0	1
56	7	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	x	1	G	OP3-P	-10.65	1.48	1.61
26	B	1	U	OP3-P	-10.62	1.48	1.61

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	w	45	LEU	CA-CB-CG	7.18	131.82	115.30
25	A	1313	U	C2-N1-C1'	7.06	126.17	117.70
1	a	754	C	C2-N1-C1'	6.99	126.49	118.80
25	A	790	U	C2-N1-C1'	6.62	125.65	117.70
21	u	9	ASN	C-N-CA	-6.53	105.38	121.70
25	A	510	C	N1-C2-O2	6.21	122.62	118.90
1	a	1158	C	C2-N1-C1'	5.91	125.30	118.80
25	A	1314	C	C2-N1-C1'	5.22	124.54	118.80
1	a	330	C	C2-N1-C1'	5.19	124.51	118.80
25	A	1313	U	N1-C2-O2	5.16	126.41	122.80
1	a	754	C	C6-N1-C1'	-5.10	114.68	120.80
25	A	510	C	N3-C2-O2	-5.08	118.34	121.90
25	A	717	C	C2-N1-C1'	5.04	124.34	118.80
25	A	323	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	7	30	ARG	Peptide
38	O	81	4D4	Mainchain

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	
2	b	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
3	c	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
4	d	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
5	e	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
6	f	101/131 (77%)	97 (96%)	4 (4%)	0	100	100
7	g	150/156 (96%)	142 (95%)	8 (5%)	0	100	100
8	h	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	i	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
10	j	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	15	53
11	k	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
12	l	118/124 (95%)	112 (95%)	6 (5%)	0	100	100
13	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
14	n	98/101 (97%)	98 (100%)	0	0	100	100
15	o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	p	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
17	q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
18	r	52/75 (69%)	50 (96%)	2 (4%)	0	100	100
19	s	81/92 (88%)	77 (95%)	4 (5%)	0	100	100
20	t	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	u	53/71 (75%)	51 (96%)	2 (4%)	0	100	100
24	w	345/360 (96%)	322 (93%)	22 (6%)	1 (0%)	41	76
27	C	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
28	D	206/209 (99%)	203 (98%)	2 (1%)	1 (0%)	29	68
29	E	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
30	F	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
31	G	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
32	H	37/149 (25%)	35 (95%)	2 (5%)	0	100	100
33	I	129/165 (78%)	111 (86%)	18 (14%)	0	100	100
34	J	139/142 (98%)	122 (88%)	16 (12%)	1 (1%)	22	60
35	L	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
36	M	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
37	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	O	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
39	P	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
40	Q	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
41	R	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
42	S	115/118 (98%)	115 (100%)	0	0	100	100
43	T	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
44	U	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
45	V	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
46	W	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
47	X	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
48	Y	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
49	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
50	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
51	2	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
52	3	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
53	4	53/57 (93%)	52 (98%)	1 (2%)	0	100	100
54	5	49/55 (89%)	49 (100%)	0	0	100	100
55	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
56	7	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9	40
57	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	6057/6553 (92%)	5815 (96%)	237 (4%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	j	57	VAL
24	w	46	SER
28	D	149	ASN
34	J	33	VAL
56	7	32	ILE

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	
2	b	186/199 (94%)	185 (100%)	1 (0%)	88	96
3	c	170/190 (90%)	169 (99%)	1 (1%)	86	95
4	d	172/173 (99%)	171 (99%)	1 (1%)	86	95
5	e	119/126 (94%)	119 (100%)	0	100	100
6	f	90/112 (80%)	90 (100%)	0	100	100
7	g	125/129 (97%)	125 (100%)	0	100	100
8	h	104/105 (99%)	104 (100%)	0	100	100
9	i	105/107 (98%)	105 (100%)	0	100	100
10	j	86/90 (96%)	86 (100%)	0	100	100
11	k	89/98 (91%)	89 (100%)	0	100	100
12	l	101/103 (98%)	101 (100%)	0	100	100
13	m	93/96 (97%)	93 (100%)	0	100	100
14	n	83/84 (99%)	83 (100%)	0	100	100
15	o	76/77 (99%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	73/78 (94%)	73 (100%)	0	100	100
18	r	47/65 (72%)	47 (100%)	0	100	100
19	s	72/79 (91%)	72 (100%)	0	100	100
20	t	65/66 (98%)	65 (100%)	0	100	100
21	u	48/61 (79%)	48 (100%)	0	100	100
24	w	289/300 (96%)	288 (100%)	1 (0%)	92	97
27	C	216/218 (99%)	215 (100%)	1 (0%)	88	96
28	D	163/163 (100%)	163 (100%)	0	100	100
29	E	165/165 (100%)	164 (99%)	1 (1%)	86	95
30	F	148/150 (99%)	148 (100%)	0	100	100
31	G	137/138 (99%)	137 (100%)	0	100	100
32	H	30/114 (26%)	30 (100%)	0	100	100
33	I	99/123 (80%)	99 (100%)	0	100	100
34	J	109/110 (99%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	L	116/116 (100%)	116 (100%)	0	100	100
36	M	104/104 (100%)	103 (99%)	1 (1%)	76	91
37	N	103/103 (100%)	103 (100%)	0	100	100
38	O	107/107 (100%)	107 (100%)	0	100	100
39	P	98/103 (95%)	98 (100%)	0	100	100
40	Q	86/87 (99%)	86 (100%)	0	100	100
41	R	99/100 (99%)	99 (100%)	0	100	100
42	S	89/90 (99%)	89 (100%)	0	100	100
43	T	84/84 (100%)	84 (100%)	0	100	100
44	U	93/93 (100%)	93 (100%)	0	100	100
45	V	80/84 (95%)	80 (100%)	0	100	100
46	W	83/85 (98%)	83 (100%)	0	100	100
47	X	78/78 (100%)	78 (100%)	0	100	100
48	Y	58/63 (92%)	57 (98%)	1 (2%)	60	85
49	Z	67/68 (98%)	67 (100%)	0	100	100
50	1	54/55 (98%)	54 (100%)	0	100	100
51	2	48/49 (98%)	48 (100%)	0	100	100
52	3	53/62 (86%)	53 (100%)	0	100	100
53	4	46/48 (96%)	46 (100%)	0	100	100
54	5	46/49 (94%)	46 (100%)	0	100	100
55	6	38/38 (100%)	37 (97%)	1 (3%)	46	78
56	7	51/52 (98%)	51 (100%)	0	100	100
57	8	34/34 (100%)	34 (100%)	0	100	100
All	All	5040/5336 (94%)	5031 (100%)	9 (0%)	93	98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	222	ARG
3	c	79	LYS
4	d	184	ARG
24	w	75	ARG
27	C	111	LYS
29	E	6	LYS

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Mol	Chain	Res	Type
36	M	49	ARG
48	Y	14	ARG
55	6	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	15	HIS
2	b	39	HIS
2	b	177	ASN
2	b	178	ASN
3	c	140	ASN
4	d	36	GLN
4	d	40	GLN
4	d	74	ASN
4	d	131	ASN
5	e	12	GLN
5	e	19	ASN
5	e	70	ASN
5	e	73	ASN
5	e	77	ASN
5	e	83	HIS
6	f	37	HIS
7	g	122	ASN
8	h	38	ASN
9	i	81	HIS
9	i	126	GLN
10	j	58	ASN
11	k	28	ASN
11	k	38	GLN
11	k	81	ASN
12	l	46	ASN
12	l	77	HIS
12	l	96	HIS
13	m	105	ASN
14	n	4	GLN
14	n	60	GLN
15	o	40	GLN
15	o	51	HIS
16	p	9	HIS
18	r	52	GLN
19	s	83	HIS

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Mol	Chain	Res	Type
20	t	21	ASN
21	u	9	ASN
24	w	20	GLN
24	w	156	HIS
24	w	197	HIS
24	w	238	ASN
24	w	266	ASN
24	w	279	HIS
24	w	288	GLN
24	w	320	HIS
27	C	53	HIS
27	C	90	ASN
27	C	128	ASN
27	C	260	ASN
28	D	134	HIS
28	D	185	ASN
29	E	41	GLN
29	E	97	ASN
29	E	165	HIS
30	F	21	ASN
31	G	115	HIS
31	G	128	GLN
34	J	43	ASN
35	L	40	HIS
35	L	58	ASN
35	L	76	HIS
36	M	3	GLN
38	O	60	GLN
39	P	23	ASN
39	P	62	ASN
42	S	72	ASN
43	T	6	GLN
44	U	57	ASN
45	V	91	GLN
48	Y	46	HIS
48	Y	50	ASN
52	3	41	HIS
53	4	6	ASN
57	8	37	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1523/1542 (98%)	178 (11%)	0
22	x	74/76 (97%)	15 (20%)	0
22	y	71/76 (93%)	18 (25%)	0
23	z	9/21 (42%)	2 (22%)	0
25	A	2893/2904 (99%)	359 (12%)	13 (0%)
26	B	119/120 (99%)	11 (9%)	3 (2%)
All	All	4689/4739 (98%)	583 (12%)	16 (0%)

All (583) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	22	G
1	a	39	G
1	a	44	A
1	a	47	C
1	a	48	C
1	a	50	A
1	a	51	A
1	a	79	G
1	a	80	A
1	a	82	G
1	a	84	U
1	a	85	U
1	a	86	G
1	a	88	U
1	a	92	U
1	a	95	C
1	a	121	U
1	a	130	A
1	a	131	A
1	a	163	C
1	a	174	A
1	a	177	G
1	a	183	C
1	a	197	A
1	a	208	U
1	a	211	G
1	a	212	G
1	a	240	G

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Mol	Chain	Res	Type
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	269	C
1	a	281	G
1	a	283	U
1	a	289	G
1	a	321	A
1	a	328	C
1	a	339	C
1	a	344	A
1	a	347	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	372	C
1	a	373	A
1	a	384	G
1	a	406	G
1	a	408	A
1	a	412	A
1	a	413	G
1	a	415	A
1	a	421	U
1	a	422	C
1	a	424	G
1	a	429	U
1	a	435	A
1	a	462	G
1	a	467	U
1	a	468	A
1	a	484	G
1	a	486	U
1	a	495	A
1	a	497	G
1	a	510	A
1	a	511	C
1	a	512	U
1	a	518	C
1	a	521	G

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Mol	Chain	Res	Type
1	a	527	G7M
1	a	531	U
1	a	547	A
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	633	G
1	a	650	G
1	a	653	U
1	a	656	G
1	a	665	A
1	a	687	A
1	a	688	G
1	a	703	G
1	a	723	U
1	a	724	G
1	a	755	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	802	A
1	a	815	A
1	a	817	C
1	a	821	G
1	a	890	G
1	a	902	G
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	966	2MG
1	a	969	A
1	a	971	G
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	994	A
1	a	1003	G

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Mol	Chain	Res	Type
1	a	1004	A
1	a	1008	U
1	a	1009	U
1	a	1024	G
1	a	1027	C
1	a	1028	C
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1036	A
1	a	1039	G
1	a	1046	A
1	a	1053	G
1	a	1065	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1137	C
1	a	1139	G
1	a	1152	A
1	a	1159	U
1	a	1174	G
1	a	1196	A
1	a	1197	A
1	a	1202	U
1	a	1213	A
1	a	1227	A
1	a	1238	A
1	a	1258	G
1	a	1275	A
1	a	1280	A
1	a	1286	U
1	a	1287	A
1	a	1290	G
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1338	G

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Mol	Chain	Res	Type
1	a	1363	A
1	a	1378	C
1	a	1379	G
1	a	1388	C
1	a	1396	A
1	a	1398	A
1	a	1419	G
1	a	1432	G
1	a	1441	A
1	a	1446	A
1	a	1448	C
1	a	1452	C
1	a	1487	G
1	a	1497	G
1	a	1499	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1529	G
1	a	1530	G
22	x	12	U
22	x	13	C
22	x	16	U
22	x	17	C
22	x	19	G
22	x	20	U
22	x	22	G
22	x	38	A
22	x	44	G
22	x	45	U
22	x	47	U
22	x	48	C
22	x	49	C
22	x	55	PSU
22	x	76	A
22	y	13	C
22	y	14	A
22	y	20	U
22	y	21	A
22	y	26	A
22	y	33	U
22	y	39	PSU

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Mol	Chain	Res	Type
22	y	40	C
22	y	42	C
22	y	44	G
22	y	45	U
22	y	46	7MG
22	y	47	U
22	y	48	C
22	y	57	G
22	y	59	U
22	y	60	U
22	y	72	C
23	z	12	A
23	z	20	U
25	A	2	G
25	A	4	U
25	A	10	A
25	A	34	U
25	A	45	G
25	A	51	G
25	A	58	G
25	A	71	A
25	A	74	A
25	A	75	G
25	A	84	A
25	A	100	U
25	A	101	A
25	A	118	A
25	A	119	A
25	A	120	U
25	A	139	U
25	A	140	C
25	A	142	A
25	A	163	C
25	A	164	C
25	A	181	A
25	A	196	A
25	A	199	A
25	A	215	G
25	A	216	A
25	A	222	A
25	A	223	A
25	A	233	A

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Mol	Chain	Res	Type
25	A	248	G
25	A	250	G
25	A	269	C
25	A	271	G
25	A	272	A
25	A	274	C
25	A	277	G
25	A	278	A
25	A	279	A
25	A	281	C
25	A	282	A
25	A	285	G
25	A	291	G
25	A	311	A
25	A	329	G
25	A	330	A
25	A	356	G
25	A	361	G
25	A	362	A
25	A	386	G
25	A	396	G
25	A	404	A
25	A	405	U
25	A	411	G
25	A	428	A
25	A	481	G
25	A	489	G
25	A	491	G
25	A	505	A
25	A	509	C
25	A	510	C
25	A	532	A
25	A	546	U
25	A	547	A
25	A	549	G
25	A	563	A
25	A	573	U
25	A	575	A
25	A	603	A
25	A	614	A
25	A	615	U
25	A	627	A

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Mol	Chain	Res	Type
25	A	637	A
25	A	645	C
25	A	647	G
25	A	653	U
25	A	654	A
25	A	655	A
25	A	686	U
25	A	709	U
25	A	710	U
25	A	717	C
25	A	719	C
25	A	730	A
25	A	740	C
25	A	747	5MU
25	A	764	A
25	A	775	G
25	A	776	G
25	A	782	A
25	A	784	G
25	A	785	G
25	A	789	A
25	A	805	G
25	A	812	C
25	A	827	U
25	A	828	U
25	A	830	G
25	A	846	U
25	A	859	G
25	A	877	A
25	A	880	G
25	A	883	G
25	A	890	C
25	A	891	G
25	A	893	C
25	A	895	U
25	A	896	A
25	A	897	C
25	A	910	A
25	A	914	G
25	A	915	C
25	A	927	A
25	A	931	U

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Mol	Chain	Res	Type
25	A	946	C
25	A	961	C
25	A	974	G
25	A	983	A
25	A	990	A
25	A	996	A
25	A	1005	C
25	A	1009	A
25	A	1012	U
25	A	1013	C
25	A	1022	G
25	A	1026	G
25	A	1032	A
25	A	1033	U
25	A	1039	A
25	A	1046	A
25	A	1047	G
25	A	1059	G
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1064	C
25	A	1065	U
25	A	1067	A
25	A	1068	G
25	A	1069	A
25	A	1070	A
25	A	1071	G
25	A	1084	A
25	A	1085	A
25	A	1086	A
25	A	1088	A
25	A	1090	A
25	A	1103	A
25	A	1104	C
25	A	1111	A
25	A	1112	G
25	A	1132	U
25	A	1135	C
25	A	1142	A
25	A	1206	G
25	A	1253	A

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Mol	Chain	Res	Type
25	A	1256	G
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1288	G
25	A	1300	G
25	A	1301	A
25	A	1352	U
25	A	1365	A
25	A	1379	U
25	A	1383	A
25	A	1416	G
25	A	1419	A
25	A	1428	C
25	A	1452	G
25	A	1482	G
25	A	1493	C
25	A	1508	A
25	A	1509	A
25	A	1510	G
25	A	1515	A
25	A	1524	G
25	A	1534	U
25	A	1535	A
25	A	1536	C
25	A	1537	G
25	A	1555	G
25	A	1566	A
25	A	1569	A
25	A	1578	U
25	A	1585	C
25	A	1606	C
25	A	1607	C
25	A	1608	A
25	A	1626	A
25	A	1647	U
25	A	1648	U
25	A	1674	G
25	A	1675	C
25	A	1676	A
25	A	1715	G
25	A	1722	A

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Mol	Chain	Res	Type
25	A	1729	U
25	A	1730	C
25	A	1733	G
25	A	1738	G
25	A	1744	A
25	A	1764	C
25	A	1773	A
25	A	1782	U
25	A	1800	C
25	A	1801	A
25	A	1808	A
25	A	1816	C
25	A	1829	A
25	A	1847	A
25	A	1848	A
25	A	1858	A
25	A	1872	A
25	A	1876	A
25	A	1905	C
25	A	1906	G
25	A	1913	A
25	A	1914	C
25	A	1929	G
25	A	1930	G
25	A	1937	A
25	A	1938	A
25	A	1955	U
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1991	U
25	A	1993	U
25	A	2020	A
25	A	2023	C
25	A	2031	A
25	A	2033	A
25	A	2043	C
25	A	2055	C
25	A	2056	G
25	A	2060	A
25	A	2061	G

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Mol	Chain	Res	Type
25	A	2062	A
25	A	2069	G7M
25	A	2093	G
25	A	2095	A
25	A	2098	U
25	A	2104	C
25	A	2110	G
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2115	G
25	A	2118	U
25	A	2119	A
25	A	2120	G
25	A	2125	G
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2136	G
25	A	2145	C
25	A	2147	A
25	A	2149	U
25	A	2157	G
25	A	2158	A
25	A	2161	C
25	A	2162	G
25	A	2166	U
25	A	2168	G
25	A	2169	A
25	A	2170	A
25	A	2171	A
25	A	2172	U
25	A	2173	A
25	A	2178	C
25	A	2181	U
25	A	2186	G
25	A	2189	U
25	A	2190	G
25	A	2192	U
25	A	2198	A
25	A	2204	G
25	A	2211	A

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Mol	Chain	Res	Type
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2278	A
25	A	2283	C
25	A	2287	A
25	A	2288	A
25	A	2305	U
25	A	2308	G
25	A	2322	A
25	A	2325	G
25	A	2327	A
25	A	2333	A
25	A	2335	A
25	A	2345	G
25	A	2361	G
25	A	2383	G
25	A	2385	C
25	A	2396	G
25	A	2402	U
25	A	2406	A
25	A	2425	A
25	A	2428	G
25	A	2429	G
25	A	2440	C
25	A	2441	U
25	A	2448	A
25	A	2459	A
25	A	2469	A
25	A	2470	G
25	A	2474	U
25	A	2476	A
25	A	2491	U
25	A	2502	G
25	A	2504	PSU
25	A	2505	G
25	A	2506	U
25	A	2518	A
25	A	2520	C
25	A	2529	G
25	A	2539	C
25	A	2547	A

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Mol	Chain	Res	Type
25	A	2566	A
25	A	2567	G
25	A	2573	C
25	A	2602	A
25	A	2609	U
25	A	2613	U
25	A	2629	U
25	A	2630	G
25	A	2646	C
25	A	2649	C
25	A	2654	A
25	A	2661	G
25	A	2663	G
25	A	2671	G
25	A	2689	U
25	A	2690	U
25	A	2714	G
25	A	2726	A
25	A	2732	G
25	A	2733	A
25	A	2748	A
25	A	2749	A
25	A	2750	A
25	A	2757	A
25	A	2778	A
25	A	2798	U
25	A	2800	A
25	A	2820	A
25	A	2821	A
25	A	2849	U
25	A	2850	A
25	A	2861	U
25	A	2873	A
25	A	2880	C
25	A	2884	U
25	A	2902	C
26	B	4	C
26	B	35	C
26	B	44	G
26	B	45	A
26	B	53	A
26	B	56	G

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Mol	Chain	Res	Type
26	B	65	U
26	B	67	G
26	B	89	U
26	B	91	C
26	B	109	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	3	U
25	A	271	G
25	A	277	G
25	A	545	U
25	A	784	G
25	A	1031	G
25	A	1111	A
25	A	2189	U
25	A	2191	A
25	A	2473	U
25	A	2538	C
25	A	2756	U
25	A	2799	A
26	B	3	C
26	B	52	A
26	B	66	A

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

53 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
25	PSU	A	2580	25	18,21,22	1.39	3 (16%)	22,30,33	1.94	4 (18%)
25	OMC	A	2498	25,58	19,22,23	0.84	0	26,31,34	0.90	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	MIA	y	37	22	18,24,32	1.11	2 (11%)	18,35,47	1.34	2 (11%)
25	5MU	A	747	25	19,22,23	1.42	6 (31%)	28,32,35	2.08	6 (21%)
25	H2U	A	2449	25	18,21,22	1.09	3 (16%)	21,30,33	1.72	1 (4%)
22	5MU	y	54	22	19,22,23	1.43	5 (26%)	28,32,35	2.03	7 (25%)
25	PSU	A	2605	25	18,21,22	1.30	3 (16%)	22,30,33	1.83	3 (13%)
1	5MC	a	967	1	18,22,23	0.94	2 (11%)	26,32,35	1.16	2 (7%)
25	PSU	A	2457	25	18,21,22	1.33	2 (11%)	22,30,33	1.90	5 (22%)
25	5MU	A	1939	25	19,22,23	1.40	5 (26%)	28,32,35	2.15	6 (21%)
1	PSU	a	516	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
25	6MZ	A	2030	25	18,25,26	0.87	1 (5%)	16,36,39	2.17	4 (25%)
25	2MG	A	2445	25,58	18,26,27	0.94	1 (5%)	16,38,41	1.16	3 (18%)
25	PSU	A	1911	25	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
25	OMG	A	2251	25,22	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
25	PSU	A	1917	25	18,21,22	1.40	2 (11%)	22,30,33	1.82	3 (13%)
22	7MG	x	46	22	22,26,27	1.30	3 (13%)	29,39,42	2.56	7 (24%)
25	PSU	A	2604	25	18,21,22	1.38	3 (16%)	22,30,33	1.86	4 (18%)
25	3TD	A	1915	25,58	19,22,23	4.06	7 (36%)	21,32,35	1.71	3 (14%)
22	PSU	y	32	22	18,21,22	1.35	2 (11%)	22,30,33	1.90	5 (22%)
22	4SU	y	8	22	18,21,22	1.78	5 (27%)	26,30,33	2.26	5 (19%)
25	2MA	A	2503	25,58	17,25,26	1.00	1 (5%)	17,37,40	0.98	2 (11%)
25	5MC	A	1962	25,58	18,22,23	0.95	2 (11%)	26,32,35	1.17	2 (7%)
1	5MC	a	1407	1	18,22,23	0.95	2 (11%)	26,32,35	1.18	3 (11%)
25	PSU	A	746	25,58	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
1	MA6	a	1519	1	18,26,27	0.95	1 (5%)	19,38,41	1.94	6 (31%)
22	PSU	y	39	22	18,21,22	1.32	2 (11%)	22,30,33	1.92	3 (13%)
22	7MG	y	46	22	22,26,27	1.29	3 (13%)	29,39,42	2.57	8 (27%)
1	UR3	a	1498	1	19,22,23	0.97	0	26,32,35	1.46	2 (7%)
22	5MU	x	54	22	19,22,23	1.39	5 (26%)	28,32,35	2.16	6 (21%)
22	PSU	x	55	22	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
25	G7M	A	2069	25	20,26,27	1.22	2 (10%)	17,39,42	0.66	0
25	2MG	A	1835	25	18,26,27	0.91	1 (5%)	16,38,41	1.15	2 (12%)
38	4D4	O	81	38	9,11,12	2.59	3 (33%)	8,13,15	0.84	0
1	2MG	a	966	1	18,26,27	0.91	1 (5%)	16,38,41	1.19	3 (18%)
1	MA6	a	1518	1	18,26,27	0.95	1 (5%)	19,38,41	1.83	6 (31%)
25	6MZ	A	1618	25	18,25,26	0.88	1 (5%)	16,36,39	2.04	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	y	55	22	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
12	D2T	l	89	12	7,9,10	1.06	0	6,11,13	2.33	2 (33%)
22	PSU	x	32	22	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
22	4SU	x	8	22	18,21,22	1.83	5 (27%)	26,30,33	2.00	5 (19%)
25	PSU	A	955	25	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
28	MEQ	D	150	28	8,9,10	0.50	0	5,10,12	0.16	0
25	PSU	A	2504	25,58	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
11	IAS	k	119	11	6,7,8	0.97	0	6,8,10	1.26	1 (16%)
25	OMU	A	2552	25	19,22,23	1.22	3 (15%)	26,31,34	1.73	5 (19%)
22	PSU	x	39	22	18,21,22	1.29	2 (11%)	22,30,33	2.09	4 (18%)
1	G7M	a	527	1	20,26,27	1.22	2 (10%)	17,39,42	0.62	0
1	2MG	a	1207	1	18,26,27	0.90	1 (5%)	16,38,41	1.13	2 (12%)
25	1MG	A	745	25	18,26,27	0.73	0	19,39,42	1.13	2 (10%)
1	2MG	a	1516	1	18,26,27	0.90	1 (5%)	16,38,41	1.15	2 (12%)
22	MIA	x	37	22	24,31,32	2.23	4 (16%)	26,44,47	2.55	9 (34%)
1	4OC	a	1402	1	20,23,24	0.75	0	26,32,35	0.95	1 (3%)

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
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
25	OMC	A	2498	25,58	-	1/9/27/28	0/2/2/2
22	MIA	y	37	22	-	2/3/25/34	0/3/3/3
25	5MU	A	747	25	-	1/7/25/26	0/2/2/2
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
22	5MU	y	54	22	-	3/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
25	6MZ	A	2030	25	-	2/5/27/28	0/3/3/3
25	2MG	A	2445	25,58	-	0/5/27/28	0/3/3/3
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	OMG	A	2251	25,22	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	A	1917	25	-	2/7/25/26	0/2/2/2
22	7MG	x	46	22	-	2/7/37/38	0/3/3/3
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
25	3TD	A	1915	25,58	-	1/7/25/26	0/2/2/2
22	PSU	y	32	22	-	0/7/25/26	0/2/2/2
22	4SU	y	8	22	-	0/7/25/26	0/2/2/2
25	2MA	A	2503	25,58	-	1/3/25/26	0/3/3/3
25	5MC	A	1962	25,58	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
25	PSU	A	746	25,58	-	4/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	4/7/29/30	0/3/3/3
22	PSU	y	39	22	-	2/7/25/26	0/2/2/2
22	7MG	y	46	22	-	3/7/37/38	0/3/3/3
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
22	5MU	x	54	22	-	0/7/25/26	0/2/2/2
22	PSU	x	55	22	-	3/7/25/26	0/2/2/2
25	G7M	A	2069	25	-	1/3/25/26	0/3/3/3
25	2MG	A	1835	25	-	0/5/27/28	0/3/3/3
38	4D4	O	81	38	-	1/11/12/14	-
1	2MG	a	966	1	-	2/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	2/7/29/30	0/3/3/3
25	6MZ	A	1618	25	-	0/5/27/28	0/3/3/3
22	PSU	y	55	22	-	0/7/25/26	0/2/2/2
12	D2T	l	89	12	-	3/7/12/14	-
22	PSU	x	32	22	-	0/7/25/26	0/2/2/2
22	4SU	x	8	22	-	0/7/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
28	MEQ	D	150	28	-	2/8/9/11	-
25	PSU	A	2504	25,58	-	0/7/25/26	0/2/2/2
11	IAS	k	119	11	-	0/7/7/8	-
25	OMU	A	2552	25	-	0/9/27/28	0/2/2/2
22	PSU	x	39	22	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	-	2/3/25/26	0/3/3/3
1	2MG	a	1207	1	-	1/5/27/28	0/3/3/3
25	1MG	A	745	25	-	0/3/25/26	0/3/3/3
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
22	MIA	x	37	22	-	5/11/33/34	0/3/3/3
1	4OC	a	1402	1	-	3/9/29/30	0/2/2/2

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	12.01	1.49	1.35
25	A	1915	3TD	C2-N1	9.42	1.49	1.37
22	x	37	MIA	C13-C14	7.18	1.53	1.32
22	x	37	MIA	C2-S10	-6.88	1.69	1.75
38	O	81	4D4	CZ-NE	6.20	1.45	1.33
25	A	1915	3TD	C6-N1	5.92	1.46	1.36
25	A	1915	3TD	C2-N3	4.80	1.49	1.38
22	y	8	4SU	C4-S4	-4.68	1.59	1.68
22	x	8	4SU	C4-S4	-4.56	1.59	1.68
1	a	527	G7M	C5-C4	3.61	1.46	1.39
22	x	8	4SU	C4-N3	-3.60	1.33	1.37
25	A	2069	G7M	C5-C4	3.51	1.46	1.39
38	O	81	4D4	CZ-NH2	3.39	1.45	1.32
22	y	32	PSU	C6-C5	3.29	1.39	1.35
22	y	39	PSU	C6-C5	3.17	1.39	1.35
25	A	1917	PSU	C6-C5	3.17	1.39	1.35
25	A	1911	PSU	C6-C5	3.16	1.39	1.35
22	y	8	4SU	C4-N3	-3.16	1.34	1.37
22	y	55	PSU	C6-C5	3.14	1.39	1.35
25	A	2504	PSU	C6-C5	3.12	1.39	1.35
22	x	46	7MG	C4-N9	-3.07	1.34	1.37
25	A	955	PSU	C6-C5	3.04	1.38	1.35
25	A	746	PSU	C6-C5	3.03	1.38	1.35
22	x	55	PSU	C6-C5	3.02	1.38	1.35
22	y	46	7MG	C5-C4	2.99	1.47	1.38
25	A	2604	PSU	C6-C5	2.99	1.38	1.35
1	a	516	PSU	C6-C5	2.98	1.38	1.35
22	x	39	PSU	C6-C5	2.95	1.38	1.35
25	A	2580	PSU	C6-C5	2.93	1.38	1.35
22	x	32	PSU	C6-C5	2.92	1.38	1.35
22	x	46	7MG	C5-C4	2.90	1.47	1.38
25	A	747	5MU	C4-N3	-2.83	1.33	1.38
25	A	2604	PSU	C4-N3	-2.82	1.33	1.38
22	y	46	7MG	C4-N9	-2.80	1.34	1.37
22	x	8	4SU	C5-C4	-2.80	1.39	1.42
25	A	2449	H2U	C2-N3	-2.80	1.33	1.38
25	A	746	PSU	C4-N3	-2.78	1.33	1.38
25	A	955	PSU	C4-N3	-2.78	1.33	1.38
25	A	2457	PSU	C6-C5	2.78	1.38	1.35
25	A	747	5MU	C6-C5	2.74	1.39	1.34
22	y	8	4SU	C5-C4	-2.73	1.39	1.42
25	A	1939	5MU	C4-N3	-2.72	1.33	1.38
25	A	2457	PSU	C4-N3	-2.71	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C4-N3	2.71	1.46	1.40
25	A	2504	PSU	C4-N3	-2.70	1.33	1.38
25	A	2445	2MG	C6-N1	-2.70	1.33	1.37
22	x	32	PSU	C4-N3	-2.70	1.33	1.38
25	A	1911	PSU	C4-N3	-2.69	1.33	1.38
22	y	37	MIA	C5-C4	2.68	1.48	1.40
25	A	2552	OMU	C4-N3	-2.67	1.33	1.38
22	x	54	5MU	C4-N3	-2.67	1.33	1.38
22	y	54	5MU	C6-C5	2.67	1.39	1.34
22	y	54	5MU	C4-N3	-2.67	1.33	1.38
1	a	516	PSU	C4-N3	-2.66	1.33	1.38
25	A	2580	PSU	C4-N3	-2.66	1.33	1.38
1	a	1407	5MC	C6-C5	2.66	1.39	1.34
25	A	1917	PSU	C4-N3	-2.65	1.33	1.38
25	A	2605	PSU	C4-N3	-2.64	1.33	1.38
25	A	1962	5MC	C6-C5	2.64	1.38	1.34
22	y	32	PSU	C4-N3	-2.63	1.34	1.38
1	a	967	5MC	C6-C5	2.63	1.38	1.34
25	A	1835	2MG	C6-N1	-2.63	1.34	1.37
25	A	1939	5MU	C6-C5	2.62	1.38	1.34
25	A	2251	OMG	C6-N1	-2.62	1.34	1.37
22	y	55	PSU	C4-N3	-2.61	1.34	1.38
1	a	966	2MG	C6-N1	-2.60	1.34	1.37
22	x	54	5MU	C6-C5	2.57	1.38	1.34
22	x	55	PSU	C4-N3	-2.56	1.34	1.38
25	A	2069	G7M	C6-N1	-2.54	1.34	1.37
25	A	2449	H2U	C4-N3	-2.54	1.33	1.37
22	y	37	MIA	C2-N3	2.53	1.36	1.32
1	a	527	G7M	C6-N1	-2.53	1.34	1.37
22	y	54	5MU	C2-N1	2.52	1.42	1.38
1	a	1207	2MG	C6-N1	-2.52	1.34	1.37
25	A	2605	PSU	C6-C5	2.52	1.38	1.35
22	y	39	PSU	C4-N3	-2.48	1.34	1.38
25	A	1939	5MU	C6-N1	-2.45	1.33	1.38
1	a	1516	2MG	C6-N1	-2.43	1.34	1.37
1	a	1518	MA6	C5-C4	2.42	1.47	1.40
25	A	1962	5MC	C6-N1	-2.42	1.33	1.38
22	x	39	PSU	C4-N3	-2.40	1.34	1.38
25	A	1915	3TD	O2-C2	-2.40	1.18	1.23
25	A	1618	6MZ	C5-C4	2.37	1.47	1.40
1	a	1519	MA6	C5-C4	2.36	1.47	1.40
22	x	54	5MU	C6-N1	-2.36	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2030	6MZ	C5-C4	2.36	1.47	1.40
22	x	46	7MG	C6-N1	-2.35	1.34	1.38
22	x	8	4SU	C2-N3	-2.31	1.33	1.38
22	y	54	5MU	C4-C5	2.30	1.48	1.44
22	y	46	7MG	C6-N1	-2.30	1.34	1.38
25	A	747	5MU	C6-N1	-2.27	1.34	1.38
25	A	747	5MU	C4-C5	2.27	1.48	1.44
1	a	1407	5MC	C6-N1	-2.26	1.34	1.38
25	A	1939	5MU	C4-C5	2.25	1.48	1.44
22	x	54	5MU	C4-C5	2.24	1.48	1.44
22	x	54	5MU	C2-N1	2.24	1.42	1.38
22	x	37	MIA	C5-C4	2.24	1.46	1.40
1	a	967	5MC	C6-N1	-2.24	1.34	1.38
25	A	2552	OMU	C2-N3	-2.23	1.34	1.38
22	y	54	5MU	C6-N1	-2.23	1.34	1.38
38	O	81	4D4	CZ-NH1	-2.22	1.25	1.34
25	A	2580	PSU	O4'-C1'	-2.20	1.40	1.43
25	A	747	5MU	C2-N1	2.18	1.41	1.38
25	A	2503	2MA	C2-N3	2.16	1.35	1.31
22	y	8	4SU	C2-N1	2.14	1.41	1.38
25	A	2604	PSU	C2-N3	-2.14	1.33	1.37
25	A	1939	5MU	C2-N3	-2.11	1.34	1.38
22	y	8	4SU	C2-N3	-2.10	1.34	1.38
25	A	2605	PSU	C2-N3	-2.08	1.34	1.37
22	x	37	MIA	C6-N1	2.06	1.35	1.32
25	A	747	5MU	C2-N3	-2.05	1.34	1.38
25	A	2449	H2U	C2-N1	-2.04	1.32	1.35
22	x	8	4SU	C2-N1	2.03	1.41	1.38
25	A	2552	OMU	C5-C4	-2.02	1.39	1.43
25	A	1915	3TD	O4-C4	-2.01	1.18	1.23

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	46	7MG	N9-C4-N3	8.91	138.79	125.47
22	x	46	7MG	N9-C4-N3	8.87	138.74	125.47
22	x	37	MIA	C12-C13-C14	-8.15	111.29	127.14
25	A	2449	H2U	C4-N3-C2	-7.11	119.89	125.79
22	y	8	4SU	C4-N3-C2	-6.81	120.72	127.34
22	x	39	PSU	N1-C2-N3	6.39	122.37	115.13
22	y	8	4SU	C5-C4-N3	6.21	120.45	114.69
25	A	1911	PSU	N1-C2-N3	6.13	122.08	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	955	PSU	N1-C2-N3	6.11	122.05	115.13
1	a	1498	UR3	C4-N3-C2	-6.09	118.83	124.56
1	a	516	PSU	N1-C2-N3	6.02	121.95	115.13
25	A	746	PSU	N1-C2-N3	6.02	121.95	115.13
25	A	2030	6MZ	C2-N1-C6	5.96	121.70	116.59
22	x	55	PSU	N1-C2-N3	5.96	121.88	115.13
22	y	32	PSU	N1-C2-N3	5.95	121.87	115.13
25	A	2580	PSU	N1-C2-N3	5.95	121.87	115.13
25	A	2457	PSU	N1-C2-N3	5.92	121.84	115.13
25	A	1917	PSU	N1-C2-N3	5.92	121.83	115.13
22	y	55	PSU	N1-C2-N3	5.89	121.80	115.13
25	A	2504	PSU	N1-C2-N3	5.88	121.79	115.13
25	A	2604	PSU	N1-C2-N3	5.86	121.77	115.13
22	x	8	4SU	C4-N3-C2	-5.84	121.67	127.34
22	y	39	PSU	N1-C2-N3	5.84	121.75	115.13
22	x	32	PSU	N1-C2-N3	5.77	121.67	115.13
25	A	1618	6MZ	C2-N1-C6	5.76	121.53	116.59
22	x	8	4SU	C5-C4-N3	5.68	119.95	114.69
22	y	46	7MG	C5-C4-N3	-5.59	117.48	128.13
25	A	1939	5MU	C4-N3-C2	-5.50	120.23	127.35
25	A	2605	PSU	N1-C2-N3	5.48	121.34	115.13
22	x	54	5MU	C4-N3-C2	-5.46	120.28	127.35
22	x	46	7MG	C5-C4-N3	-5.42	117.79	128.13
22	x	46	7MG	N9-C8-N7	-5.35	95.73	103.38
25	A	747	5MU	C4-N3-C2	-5.25	120.55	127.35
25	A	1939	5MU	N3-C2-N1	5.22	121.82	114.89
25	A	747	5MU	N3-C2-N1	5.19	121.77	114.89
22	y	46	7MG	N9-C8-N7	-5.08	96.11	103.38
22	x	54	5MU	N3-C2-N1	5.08	121.63	114.89
25	A	1915	3TD	N1-C2-N3	5.07	120.14	116.14
22	y	54	5MU	C4-N3-C2	-4.76	121.18	127.35
22	y	54	5MU	N3-C2-N1	4.76	121.20	114.89
22	x	37	MIA	C2-N3-C4	4.68	121.77	115.32
22	x	39	PSU	C4-N3-C2	-4.67	119.61	126.34
25	A	2552	OMU	C4-N3-C2	-4.66	120.43	126.58
22	x	54	5MU	C5-C4-N3	4.57	119.22	115.31
22	y	46	7MG	C2-N3-C4	4.39	120.13	112.30
22	x	46	7MG	C2-N3-C4	4.36	120.08	112.30
25	A	1939	5MU	C5-C4-N3	4.32	119.00	115.31
25	A	2552	OMU	N3-C2-N1	4.32	120.62	114.89
25	A	747	5MU	C5-C4-N3	4.31	118.99	115.31
25	A	1939	5MU	C5-C6-N1	-4.30	118.91	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1518	MA6	N1-C6-N6	4.20	121.47	117.06
25	A	1915	3TD	C4-N3-C2	-4.18	120.08	124.61
22	y	8	4SU	C5-C4-S4	-4.15	119.12	124.47
25	A	955	PSU	C4-N3-C2	-4.14	120.38	126.34
25	A	746	PSU	C4-N3-C2	-4.12	120.40	126.34
22	y	54	5MU	C5-C4-N3	4.09	118.80	115.31
22	y	39	PSU	C4-N3-C2	-4.06	120.48	126.34
22	x	54	5MU	O4-C4-C5	-4.05	120.20	124.90
25	A	2457	PSU	C4-N3-C2	-4.04	120.51	126.34
25	A	2605	PSU	C4-N3-C2	-4.01	120.56	126.34
25	A	1911	PSU	C4-N3-C2	-4.00	120.58	126.34
22	x	39	PSU	O2-C2-N1	-3.99	118.40	122.79
1	a	516	PSU	C4-N3-C2	-3.98	120.61	126.34
25	A	2604	PSU	C4-N3-C2	-3.94	120.67	126.34
22	y	32	PSU	C4-N3-C2	-3.93	120.68	126.34
25	A	2504	PSU	C4-N3-C2	-3.92	120.69	126.34
25	A	2580	PSU	C4-N3-C2	-3.91	120.71	126.34
22	x	37	MIA	C15-C14-C13	-3.91	111.36	122.65
22	y	55	PSU	C4-N3-C2	-3.90	120.72	126.34
25	A	747	5MU	C5-C6-N1	-3.88	119.35	123.34
12	l	89	D2T	CB1-SB-CB	3.85	109.42	102.44
22	x	32	PSU	C4-N3-C2	-3.85	120.79	126.34
22	x	37	MIA	C16-C14-C13	-3.85	111.52	122.65
22	y	54	5MU	O4-C4-C5	-3.84	120.46	124.90
22	x	54	5MU	C5-C6-N1	-3.83	119.39	123.34
22	x	55	PSU	C4-N3-C2	-3.80	120.87	126.34
22	y	8	4SU	N3-C2-N1	3.78	119.91	114.89
25	A	2030	6MZ	C9-N6-C6	-3.78	119.62	122.87
25	A	1939	5MU	O4-C4-C5	-3.74	120.56	124.90
22	x	55	PSU	O2-C2-N1	-3.74	118.67	122.79
22	y	39	PSU	O2-C2-N1	-3.72	118.70	122.79
25	A	1962	5MC	C5-C6-N1	-3.64	119.59	123.34
25	A	747	5MU	O4-C4-C5	-3.64	120.68	124.90
25	A	2552	OMU	C5-C4-N3	3.61	120.23	114.84
25	A	1917	PSU	C4-N3-C2	-3.59	121.17	126.34
1	a	1407	5MC	C5-C6-N1	-3.49	119.75	123.34
1	a	1519	MA6	C10-N6-C6	-3.49	108.96	119.51
22	x	8	4SU	N3-C2-N1	3.49	119.52	114.89
25	A	1618	6MZ	C9-N6-C6	-3.46	119.89	122.87
1	a	967	5MC	C5-C6-N1	-3.46	119.78	123.34
25	A	2580	PSU	O2-C2-N1	-3.44	119.00	122.79
1	a	1519	MA6	C9-N6-C6	-3.43	109.14	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	516	PSU	O2-C2-N1	-3.36	119.09	122.79
25	A	746	PSU	O2-C2-N1	-3.35	119.10	122.79
22	y	32	PSU	O2-C2-N1	-3.33	119.12	122.79
25	A	1917	PSU	O2-C2-N1	-3.33	119.12	122.79
1	a	1518	MA6	C10-N6-C6	-3.33	109.43	119.51
22	y	37	MIA	N3-C2-N1	-3.31	123.50	128.68
25	A	2030	6MZ	C4-C5-N7	-3.30	105.96	109.40
22	y	55	PSU	O2-C2-N1	-3.30	119.16	122.79
1	a	1519	MA6	C4-C5-N7	-3.30	105.96	109.40
1	a	1519	MA6	N3-C2-N1	-3.29	123.54	128.68
25	A	1911	PSU	O2-C2-N1	-3.28	119.18	122.79
25	A	955	PSU	O2-C2-N1	-3.27	119.19	122.79
22	x	8	4SU	C5-C4-S4	-3.26	120.27	124.47
22	x	37	MIA	C4-C5-N7	-3.22	106.04	109.40
25	A	2457	PSU	O2-C2-N1	-3.20	119.27	122.79
25	A	2504	PSU	O2-C2-N1	-3.18	119.29	122.79
1	a	1518	MA6	C9-N6-C6	-3.16	109.95	119.51
22	y	54	5MU	C5-C6-N1	-3.09	120.16	123.34
1	a	1518	MA6	N3-C2-N1	-3.07	123.88	128.68
22	x	32	PSU	O2-C2-N1	-3.07	119.41	122.79
22	x	37	MIA	C5-C6-N1	-3.07	118.26	120.81
1	a	1519	MA6	N1-C6-N6	3.07	120.28	117.06
25	A	1618	6MZ	N3-C2-N1	-3.05	123.91	128.68
12	l	89	D2T	OD2-CG-CB	3.03	119.70	113.15
25	A	2605	PSU	O2-C2-N1	-3.02	119.46	122.79
25	A	2030	6MZ	N3-C2-N1	-2.95	124.06	128.68
25	A	2552	OMU	O4-C4-C5	-2.92	120.03	125.16
25	A	1618	6MZ	C4-C5-N7	-2.91	106.36	109.40
22	x	46	7MG	C5-C6-N1	2.89	116.07	110.99
22	y	54	5MU	C1'-N1-C2	2.86	122.74	117.57
25	A	2604	PSU	O2-C2-N1	-2.85	119.65	122.79
22	y	46	7MG	C5-C6-N1	2.85	116.01	110.99
1	a	1519	MA6	C10-N6-C9	-2.84	106.97	116.12
25	A	1939	5MU	O2-C2-N1	-2.77	119.11	122.79
1	a	1518	MA6	C4-C5-N7	-2.72	106.57	109.40
25	A	1962	5MC	C5-C4-N3	-2.62	118.85	121.67
1	a	967	5MC	C5-C4-N3	-2.60	118.87	121.67
1	a	1407	5MC	C5-C4-N3	-2.60	118.87	121.67
25	A	2580	PSU	O4'-C1'-C2'	2.50	108.67	105.14
22	x	37	MIA	C2-N1-C6	2.49	121.65	117.19
22	y	8	4SU	C1'-N1-C2	2.48	122.05	117.57
22	x	37	MIA	N3-C2-N1	-2.47	122.43	126.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	745	1MG	C5-C6-N1	2.47	117.62	113.90
25	A	2445	2MG	C8-N7-C5	2.47	107.70	102.99
11	k	119	IAS	OD1-CG-CB	-2.44	118.31	125.43
22	y	37	MIA	C4-C5-N7	-2.43	106.87	109.40
25	A	745	1MG	C8-N7-C5	2.43	107.61	102.99
22	y	54	5MU	C1'-N1-C6	-2.41	117.11	121.12
1	a	1516	2MG	C8-N7-C5	2.40	107.55	102.99
1	a	1402	4OC	C6-C5-C4	2.38	119.87	116.96
25	A	2251	OMG	C8-N7-C5	2.38	107.52	102.99
1	a	1207	2MG	C8-N7-C5	2.38	107.52	102.99
25	A	2503	2MA	C8-N7-C5	2.37	107.50	102.99
25	A	1835	2MG	C8-N7-C5	2.37	107.50	102.99
25	A	1835	2MG	C5-C6-N1	2.36	118.12	113.95
22	x	54	5MU	O2-C2-N1	-2.36	119.65	122.79
25	A	2445	2MG	C5-C6-N1	2.35	118.10	113.95
25	A	2503	2MA	C5-C6-N1	2.35	118.07	114.02
25	A	2552	OMU	O2-C2-N1	-2.33	119.69	122.79
1	a	1207	2MG	C5-C6-N1	2.33	118.06	113.95
1	a	1516	2MG	C5-C6-N1	2.31	118.03	113.95
1	a	966	2MG	C8-N7-C5	2.30	107.38	102.99
25	A	2251	OMG	C5-C6-N1	2.29	118.00	113.95
1	a	516	PSU	O4'-C1'-C2'	2.29	108.38	105.14
25	A	747	5MU	O2-C2-N1	-2.29	119.74	122.79
22	x	37	MIA	C11-S10-C2	-2.24	100.60	102.27
1	a	1518	MA6	C10-N6-C9	-2.23	108.93	116.12
22	y	46	7MG	O6-C6-C5	-2.23	122.07	127.54
1	a	1407	5MC	O2-C2-N3	-2.23	118.71	122.33
22	x	46	7MG	C5-C4-N9	-2.22	103.46	106.35
1	a	966	2MG	C5-C6-N1	2.21	117.85	113.95
25	A	2498	OMC	O2-C2-N3	-2.21	118.74	122.33
25	A	2457	PSU	O4'-C1'-C2'	2.19	108.23	105.14
25	A	955	PSU	C5-C6-N1	-2.18	118.84	122.11
22	x	39	PSU	C5-C6-N1	-2.17	118.85	122.11
22	x	46	7MG	O6-C6-C5	-2.14	122.29	127.54
25	A	2604	PSU	C5-C6-N1	-2.14	118.90	122.11
25	A	1915	3TD	C6-C5-C4	2.12	119.69	118.22
22	x	8	4SU	C1'-N1-C2	2.12	121.40	117.57
22	y	32	PSU	O4'-C1'-C2'	2.12	108.13	105.14
25	A	746	PSU	C5-C6-N1	-2.11	118.94	122.11
1	a	966	2MG	CM2-N2-C2	-2.08	119.26	123.86
22	y	46	7MG	CM7-N7-C5	2.06	131.71	126.40
25	A	2457	PSU	C5-C6-N1	-2.05	119.04	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	46	7MG	C5-C4-N9	-2.04	103.70	106.35
1	a	1498	UR3	C3U-N3-C4	2.02	120.78	117.89
22	y	32	PSU	C5-C6-N1	-2.02	119.08	122.11
25	A	1911	PSU	C5-C6-N1	-2.02	119.08	122.11
25	A	2445	2MG	CM2-N2-C2	-2.01	119.42	123.86

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1207	2MG	N3-C2-N2-CM2
1	a	1519	MA6	C5-C6-N6-C9
12	l	89	D2T	O-C-CA-CB
12	l	89	D2T	SB-CB-CG-OD2
22	x	37	MIA	N6-C12-C13-C14
22	x	37	MIA	C12-C13-C14-C15
22	x	37	MIA	C12-C13-C14-C16
22	y	37	MIA	O4'-C4'-C5'-O5'
22	y	39	PSU	C2'-C1'-C5-C6
22	y	46	7MG	C4'-C5'-O5'-P
25	A	746	PSU	C2'-C1'-C5-C4
25	A	746	PSU	C2'-C1'-C5-C6
25	A	746	PSU	O4'-C1'-C5-C6
1	a	1402	4OC	O4'-C4'-C5'-O5'
22	y	54	5MU	C3'-C4'-C5'-O5'
25	A	2030	6MZ	O4'-C4'-C5'-O5'
1	a	1402	4OC	C3'-C4'-C5'-O5'
1	a	1519	MA6	O4'-C4'-C5'-O5'
22	x	37	MIA	O4'-C4'-C5'-O5'
22	x	55	PSU	O4'-C4'-C5'-O5'
22	y	37	MIA	C3'-C4'-C5'-O5'
22	y	54	5MU	O4'-C4'-C5'-O5'
25	A	1917	PSU	C3'-C4'-C5'-O5'
25	A	1917	PSU	O4'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C9
22	y	46	7MG	C2'-C1'-N9-C8
28	D	150	MEQ	NE2-CD-CG-CB
22	x	55	PSU	C3'-C4'-C5'-O5'
28	D	150	MEQ	OE1-CD-CG-CB
1	a	527	G7M	C3'-C4'-C5'-O5'
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	1519	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	x	37	MIA	C3'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	966	2MG	C3'-C4'-C5'-O5'
22	y	46	7MG	C3'-C4'-C5'-O5'
12	l	89	D2T	CG-CB-SB-CB1
22	x	46	7MG	C2'-C1'-N9-C8
1	a	1402	4OC	C3'-C2'-O2'-CM2
22	x	55	PSU	C4'-C5'-O5'-P
1	a	966	2MG	O4'-C4'-C5'-O5'
25	A	2030	6MZ	C3'-C4'-C5'-O5'
38	O	81	4D4	CG-CD-NE-CZ
25	A	746	PSU	O4'-C1'-C5-C4
25	A	2498	OMC	C3'-C2'-O2'-CM2
25	A	1915	3TD	O4'-C4'-C5'-O5'
25	A	747	5MU	C3'-C4'-C5'-O5'
22	y	39	PSU	O4'-C1'-C5-C6
22	y	54	5MU	C2'-C1'-N1-C2
22	x	46	7MG	O4'-C1'-N9-C8
25	A	2069	G7M	O4'-C4'-C5'-O5'
25	A	2503	2MA	O4'-C4'-C5'-O5'
1	a	1518	MA6	N1-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 572 ligands modelled in this entry, 572 are monoatomic - leaving 0 for Mogul analysis.

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.

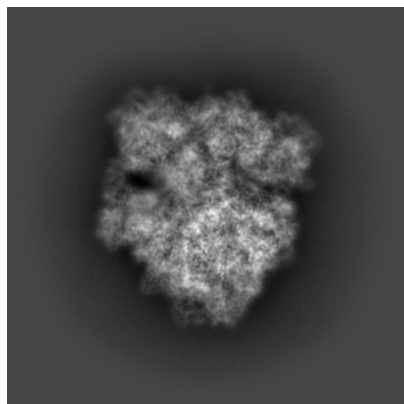
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29621. These allow visual inspection of the internal detail of the map and identification of artifacts.

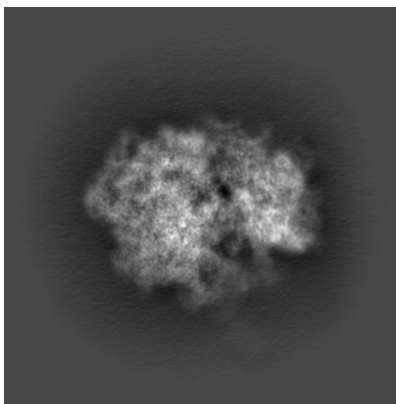
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

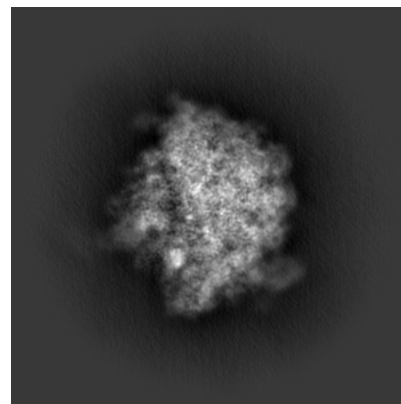
6.1.1 Primary map



X

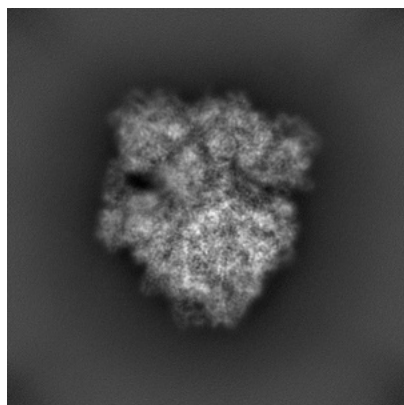


Y

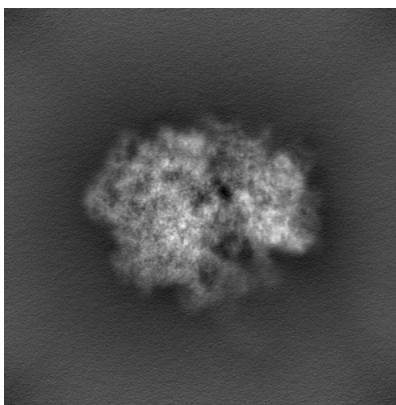


Z

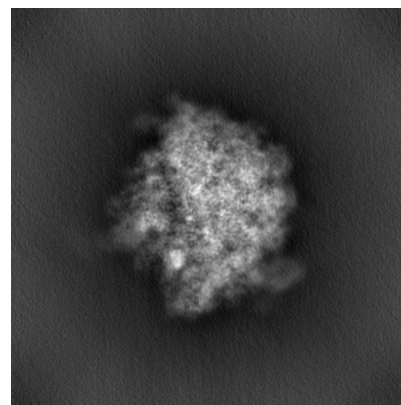
6.1.2 Raw map



X



Y

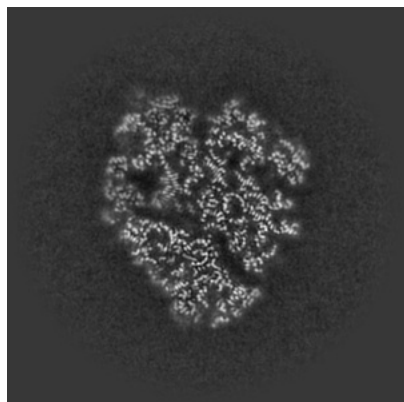


Z

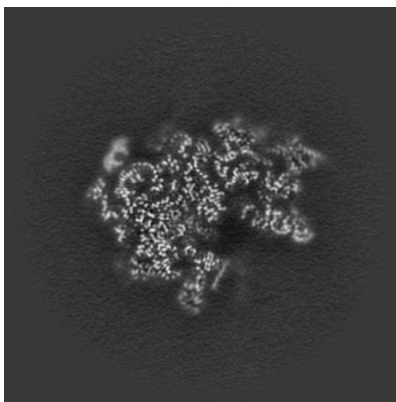
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

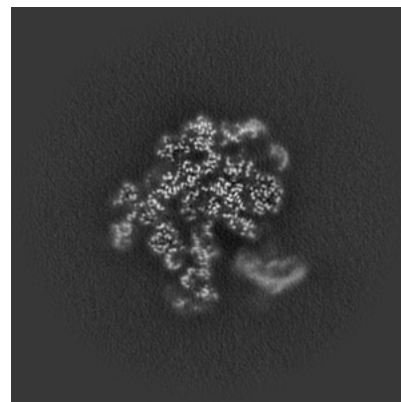
6.2.1 Primary map



X Index: 256

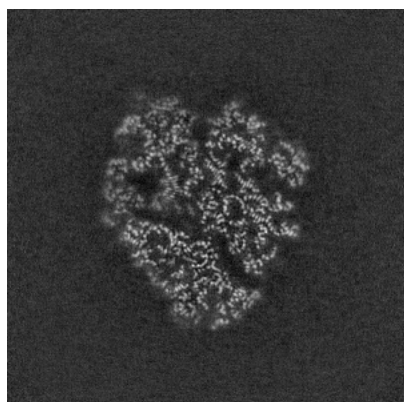


Y Index: 256

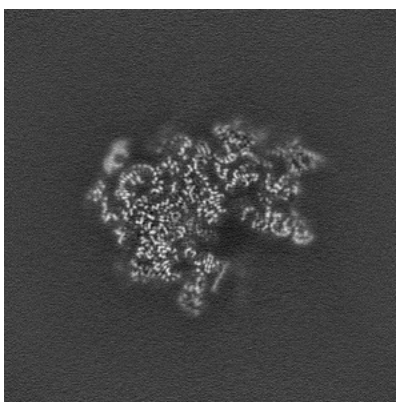


Z Index: 256

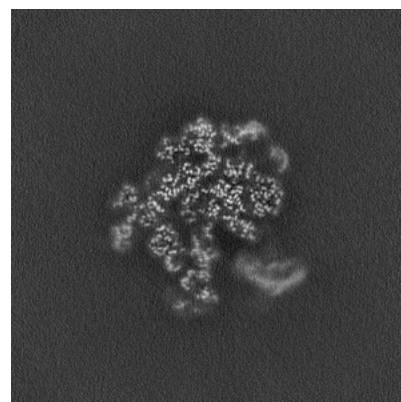
6.2.2 Raw map



X Index: 256



Y Index: 256

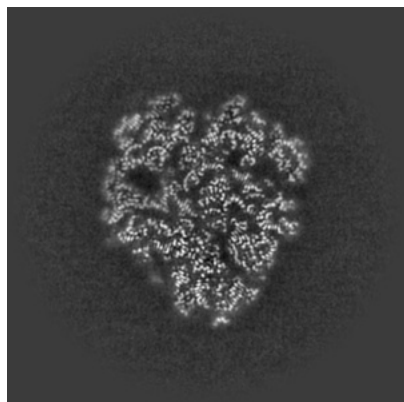


Z Index: 256

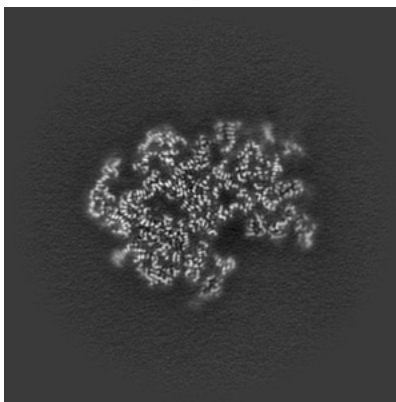
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

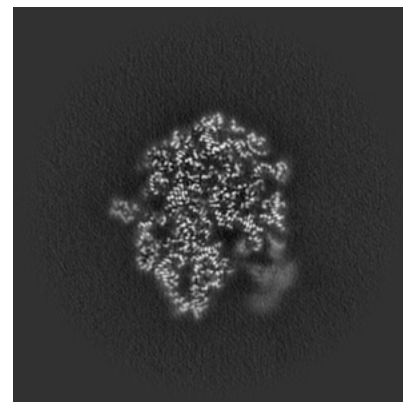
6.3.1 Primary map



X Index: 251

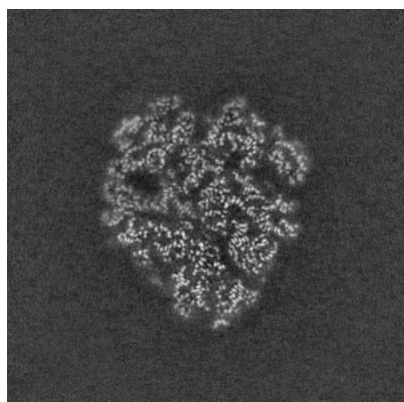


Y Index: 272

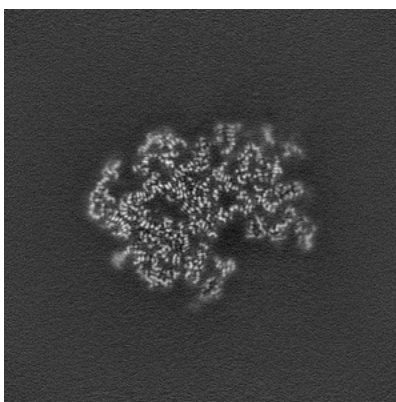


Z Index: 231

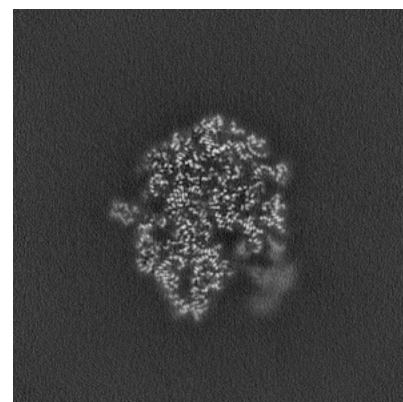
6.3.2 Raw map



X Index: 252



Y Index: 272

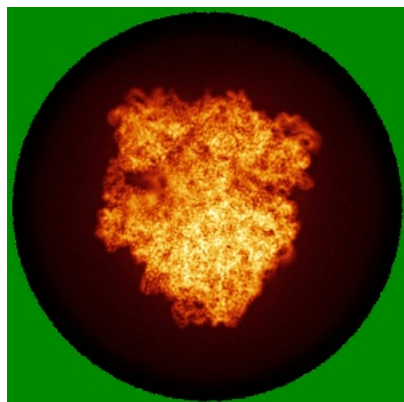


Z Index: 231

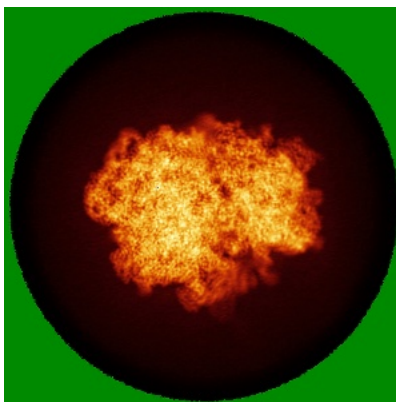
The images above show the largest variance slices of the map in three orthogonal directions.

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

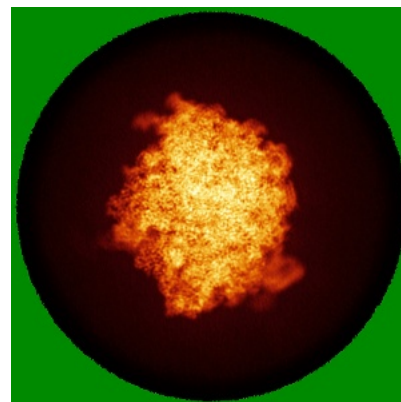
6.4.1 Primary map



X

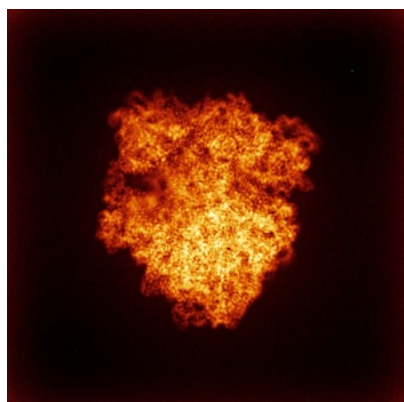


Y

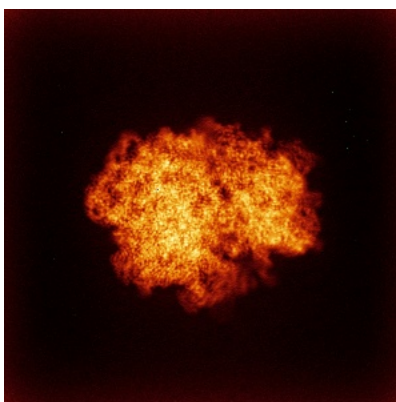


Z

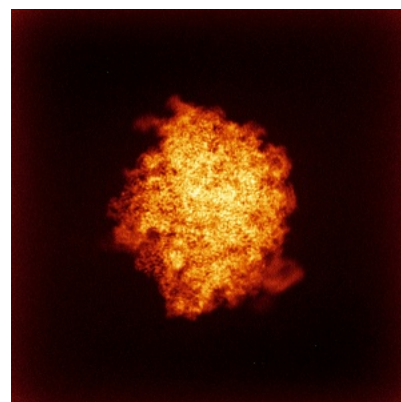
6.4.2 Raw map



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



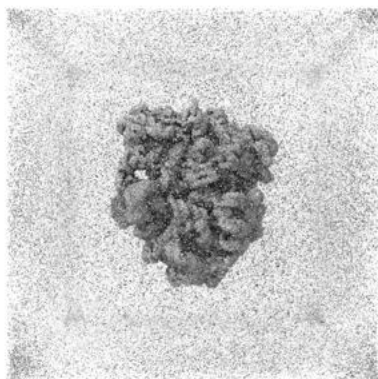
Y



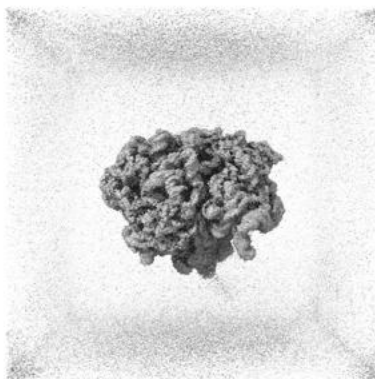
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

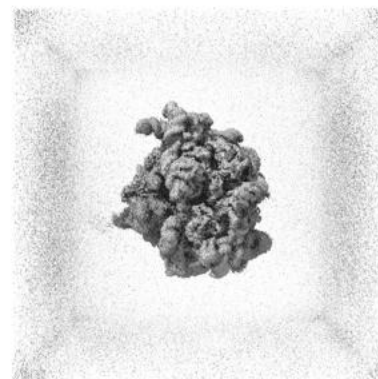
6.5.2 Raw map



X



Y



Z

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

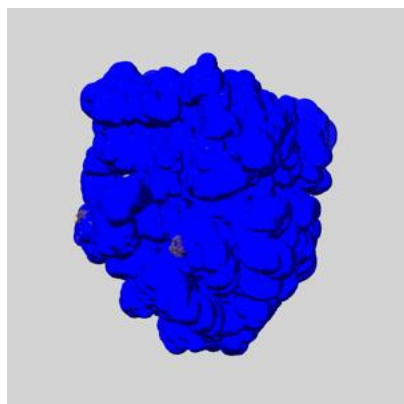
6.6 Mask visualisation [i](#)

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

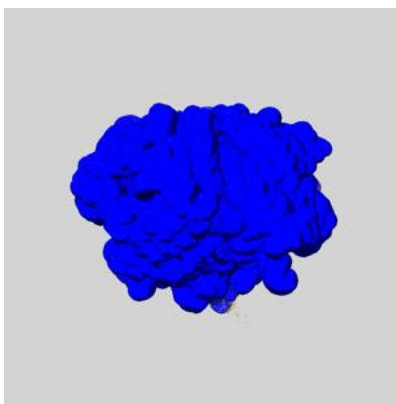
A mask typically either:

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

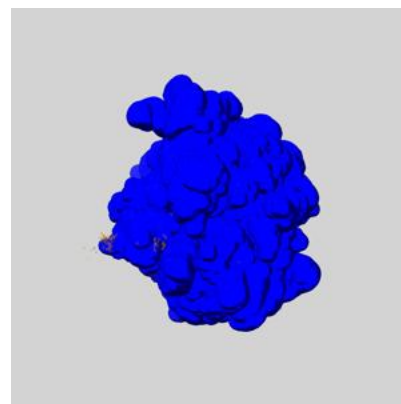
6.6.1 emd_29621_msk_1.map [i](#)



X



Y

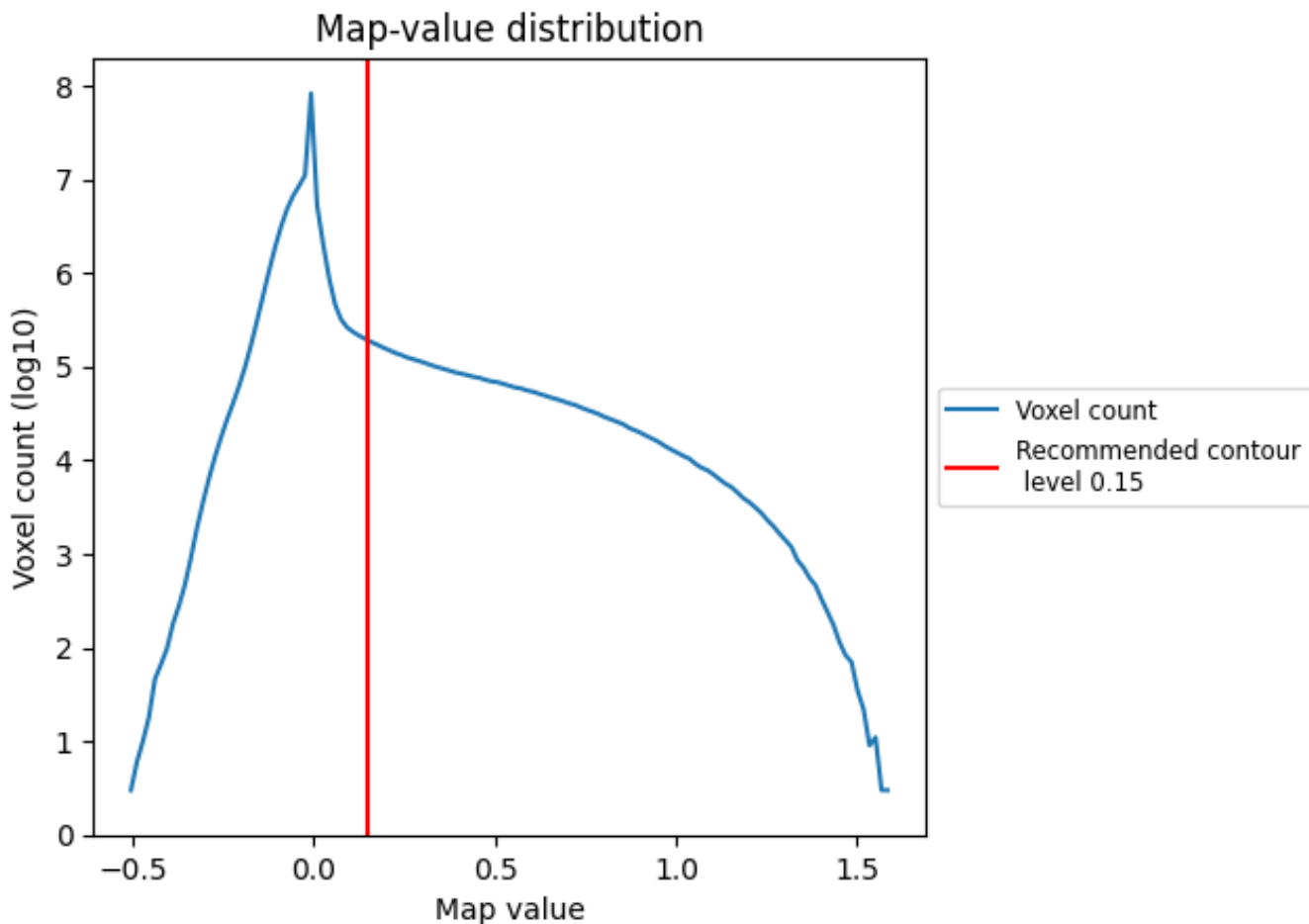


Z

7 Map analysis [i](#)

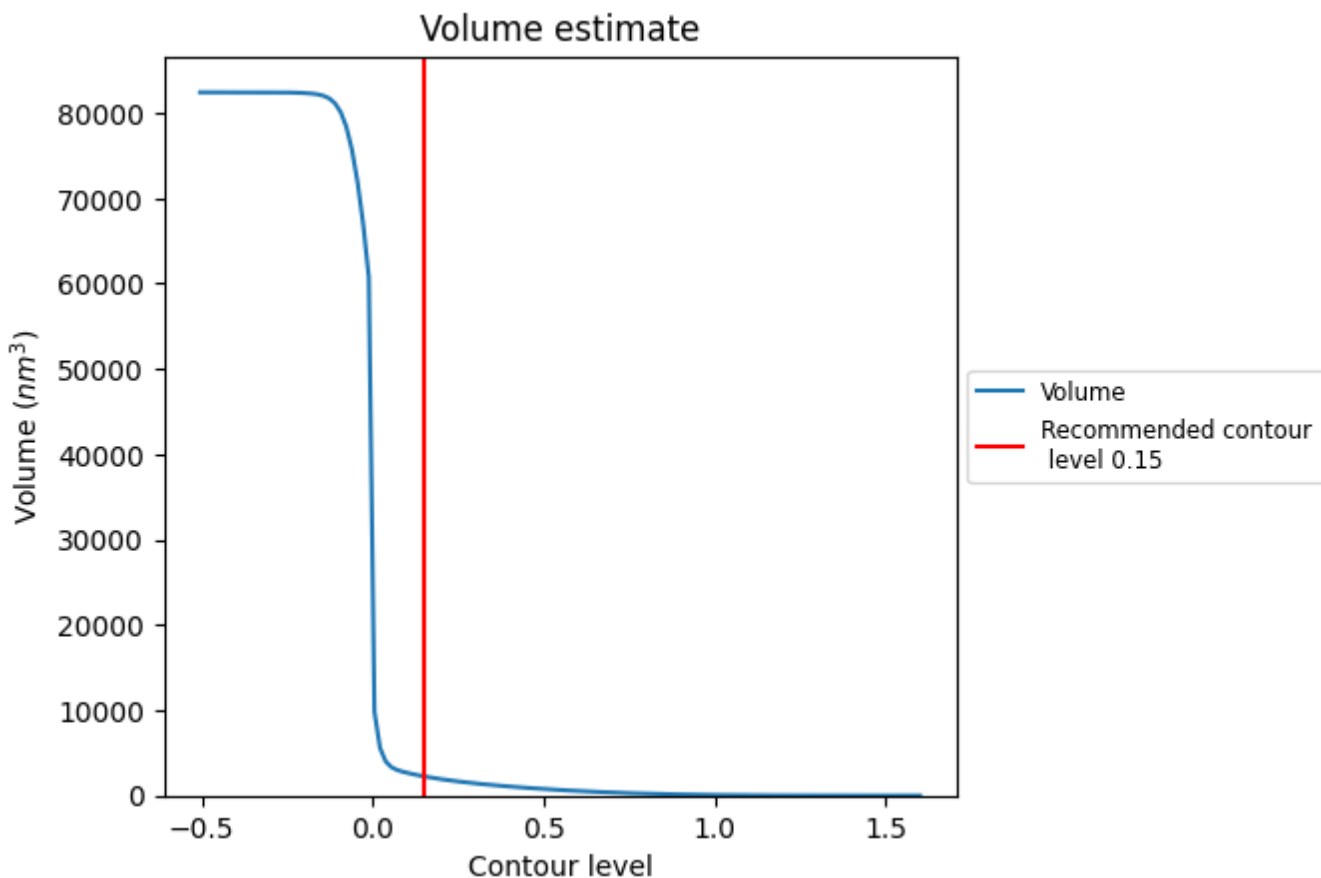
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

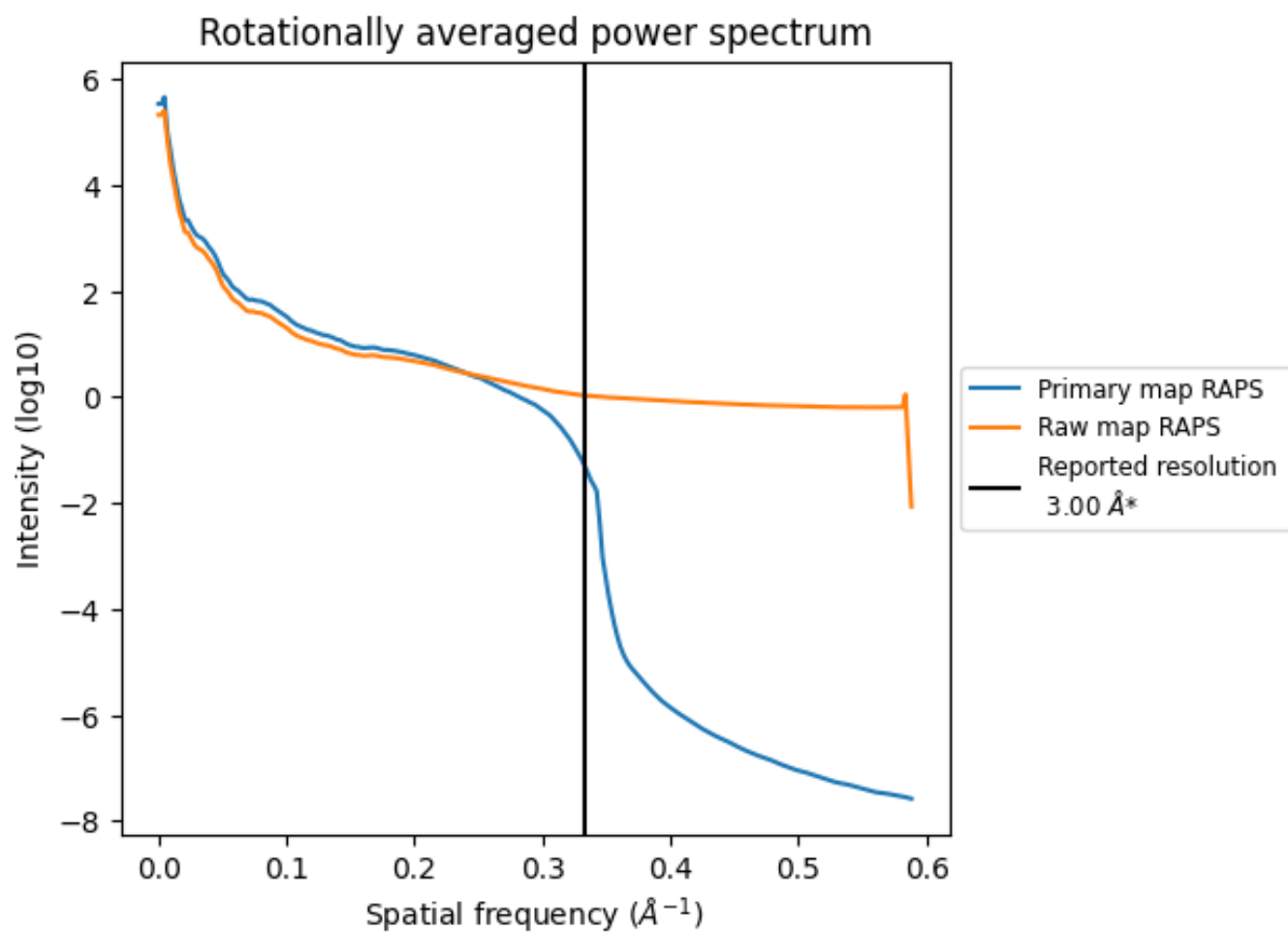
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2250 nm³; this corresponds to an approximate mass of 2033 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

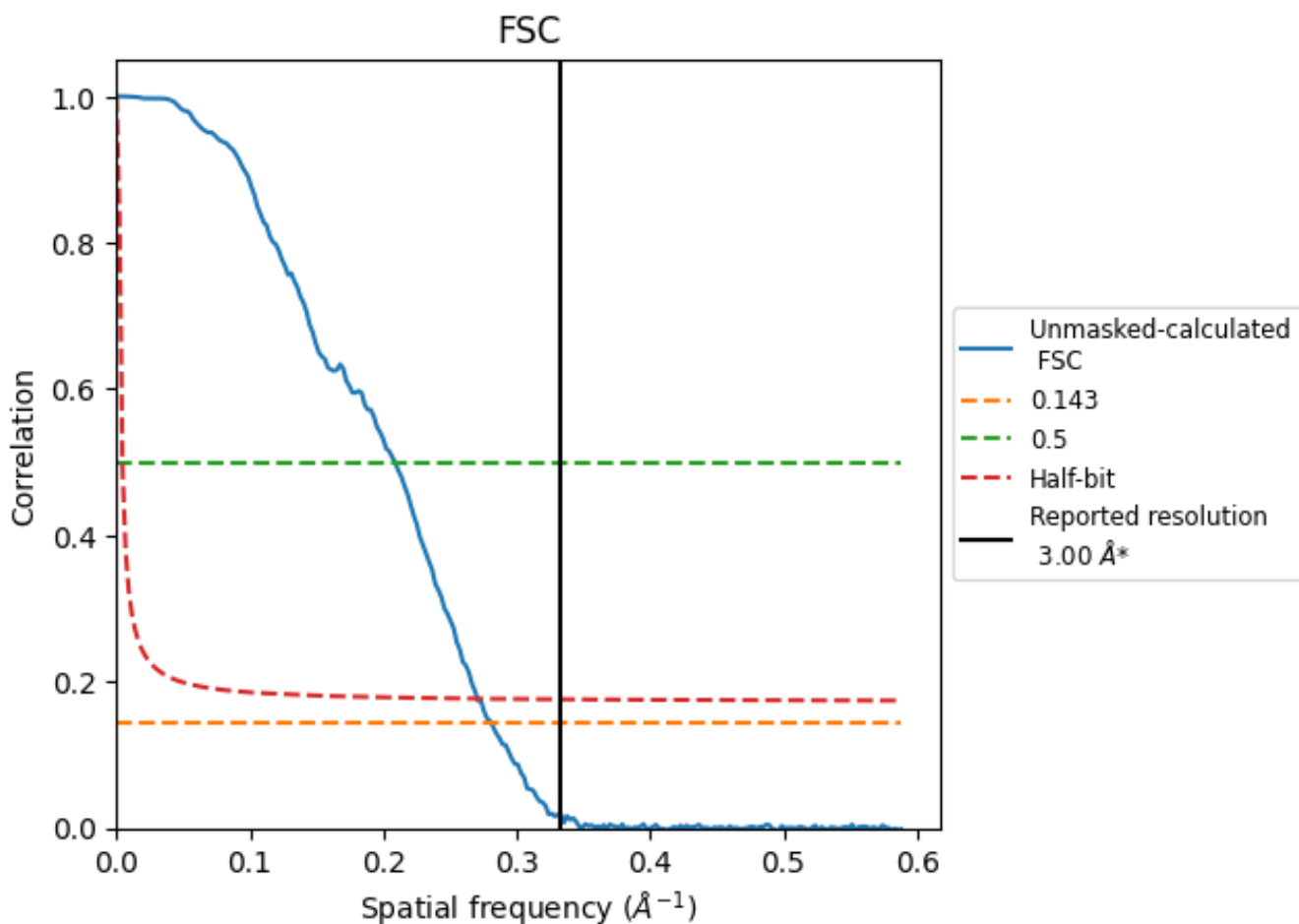


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

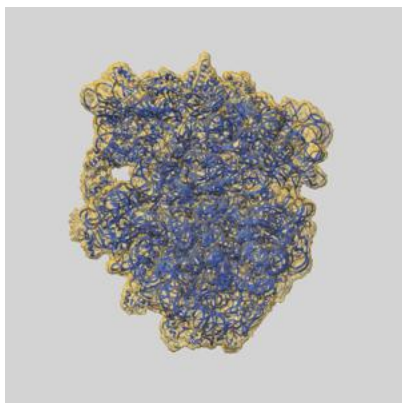
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.56	4.79	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.56 differs from the reported value 3.0 by more than 10 %

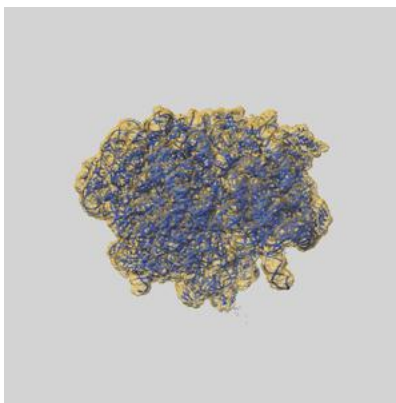
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29621 and PDB model 8FZE. Per-residue inclusion information can be found in section 3 on page 15.

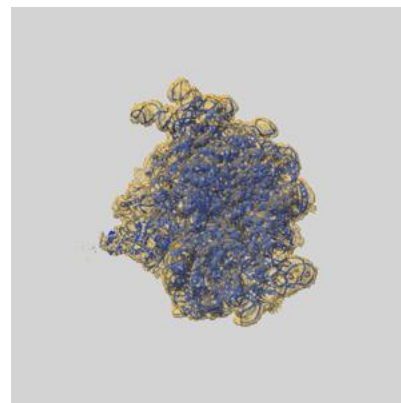
9.1 Map-model overlay [i](#)



X



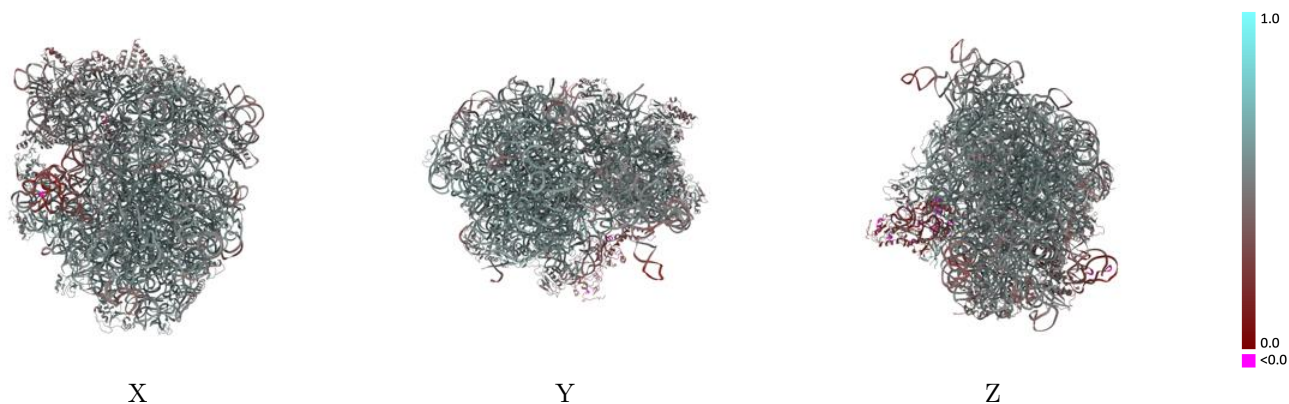
Y



Z

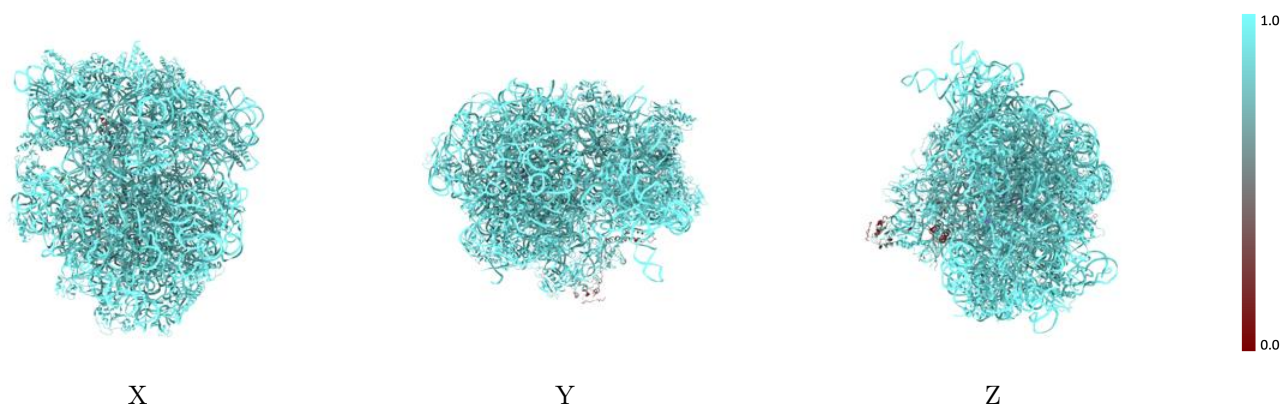
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



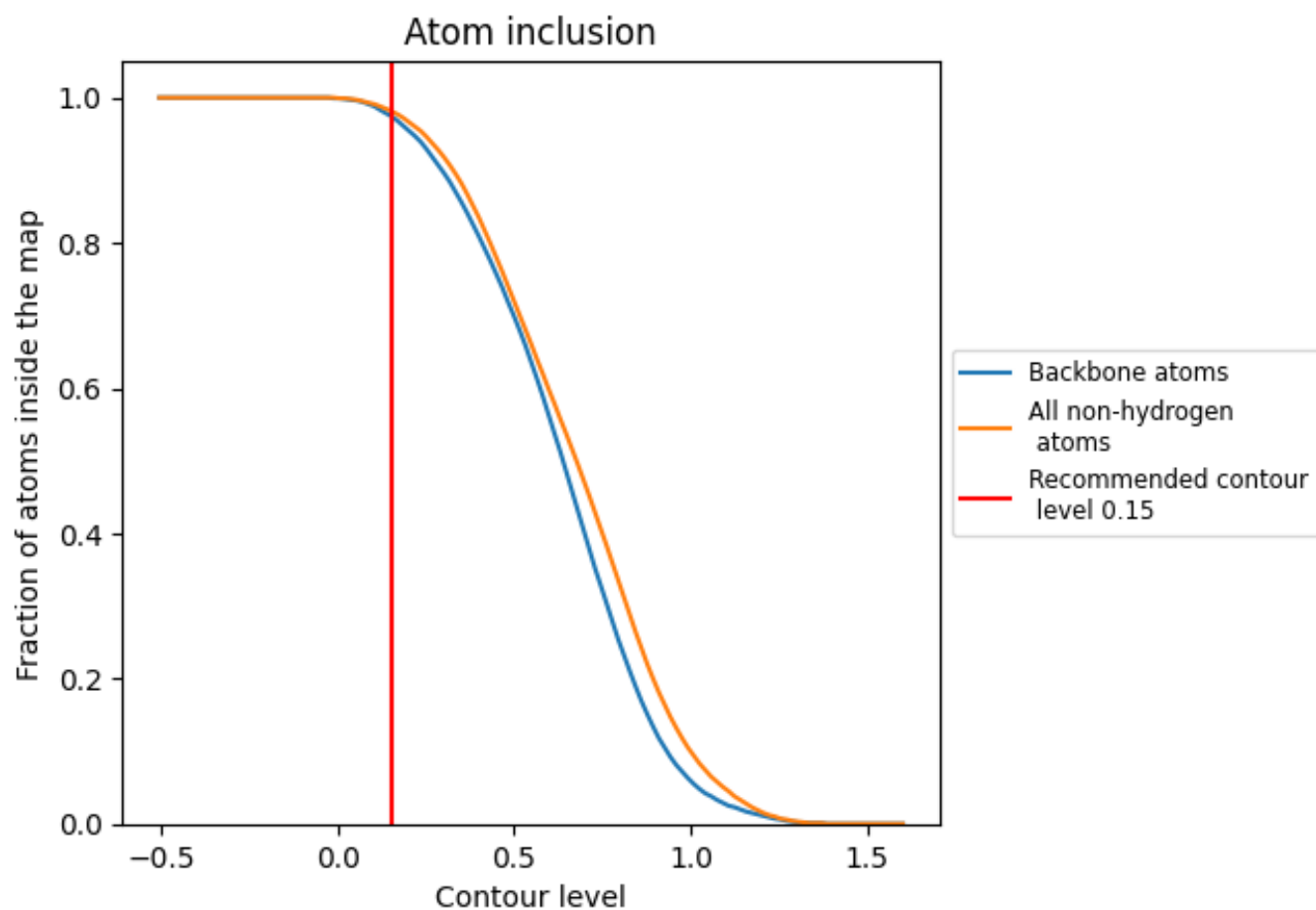
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

















































The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9820	 0.5110
1	 0.9830	 0.4930
2	 0.9840	 0.5540
3	 0.9700	 0.4660
4	 0.9910	 0.5660
5	 0.9580	 0.5280
6	 0.9750	 0.5710
7	 0.9720	 0.5760
8	 0.9690	 0.5490
A	 0.9980	 0.5280
B	 0.9990	 0.5150
C	 0.9680	 0.5630
D	 0.9770	 0.5570
E	 0.9860	 0.5350
F	 0.9610	 0.4870
G	 0.9720	 0.4770
H	 0.6300	 0.4470
I	 0.5830	 0.2150
J	 0.9070	 0.2090
L	 0.9820	 0.5510
M	 0.9670	 0.5520
N	 0.9800	 0.5530
O	 0.9710	 0.5560
P	 0.9890	 0.5670
Q	 0.9900	 0.5060
R	 0.9620	 0.5520
S	 0.9930	 0.5580
T	 0.9820	 0.5450
U	 0.9730	 0.5500
V	 0.9570	 0.5260
W	 0.9900	 0.5170
X	 0.9720	 0.5240
Y	 0.9610	 0.5590
Z	 0.9830	 0.5500
a	 0.9990	 0.5100



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.9620	 0.4410
c	 0.9450	 0.4850
d	 0.9800	 0.4790
e	 0.9730	 0.5170
f	 0.9730	 0.4750
g	 0.9580	 0.4470
h	 0.9760	 0.5220
i	 0.9760	 0.4690
j	 0.9620	 0.4440
k	 0.9670	 0.5110
l	 0.9540	 0.5440
m	 0.9790	 0.4850
n	 0.9830	 0.4910
o	 0.9640	 0.4910
p	 0.9840	 0.5190
q	 0.9790	 0.5180
r	 0.9700	 0.5070
s	 0.9800	 0.4740
t	 0.9620	 0.4870
u	 0.9390	 0.4760
w	 0.8060	 0.4010
x	 0.9880	 0.5190
y	 0.9650	 0.3260
z	 0.9810	 0.4960