



## Full wwPDB EM Validation Report ⓘ

Aug 10, 2023 – 09:26 pm BST

PDB ID : 8BHN  
EMDB ID : EMD-16062  
Title : Elongating E. coli 70S ribosome containing deacylated tRNA(iMet) in the P-site and m6AAA mRNA codon with cognate dipeptidyl-tRNA(Lys) in the A-site  
Authors : Koziej, L.; Glatt, S.  
Deposited on : 2022-10-31  
Resolution : 2.85 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

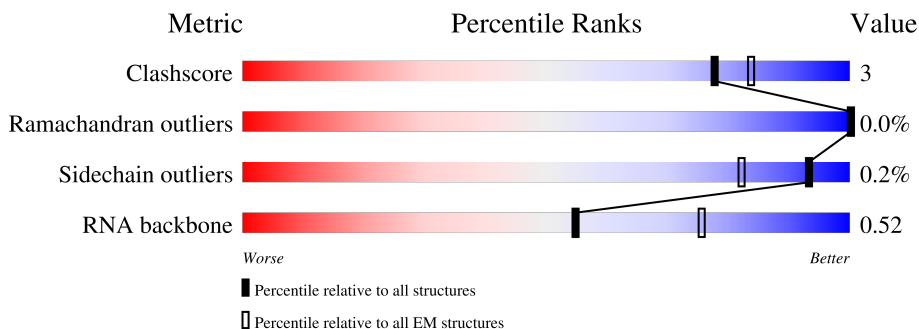
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

# 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 2.85 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)
Clashscore	158937	4297
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  $\geq 3$ , 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	273	96%
2	B	209	97%
3	C	201	92%
4	D	179	82%
5	E	177	90%
6	F	149	56%
7	G	142	92%

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Mol	Chain	Length	Quality of chain
8	H	123	90% 10%
9	I	144	97% .
10	J	136	91% 9%
11	K	127	89% . 7%
12	L	117	97% ..
13	M	115	99% .
14	N	118	98% ..
15	O	103	95% 5%
16	P	110	100%
17	Q	100	90% . 7%
18	R	104	6% 97% ..
19	S	94	91% 9%
20	T	85	88% 12%
21	U	78	95% . .
22	V	63	89% 6% 5%
23	W	59	92% 5% .
24	X	70	16% 69% 17% 14%
25	a	57	96% .
26	b	55	5% 91% . 7%
27	c	46	100%
28	d	65	97% ..
29	e	38	100%
30	f	241	5% 93% 7%
31	g	233	88% 12%
32	h	206	13% 100%

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Mol	Chain	Length	Quality of chain
33	i	167	93% 7%
34	j	131	81% 19% 6%
35	k	179	84% 16% 6%
36	l	130	99%
37	m	130	97% 6%
38	n	103	96%
39	o	129	91% 9%
40	p	124	99%
41	q	118	97%
42	r	101	99%
43	s	89	99%
44	t	82	100% 9%
45	u	84	95% 5%
46	v	75	88% 12% 15%
47	w	92	85% 14% 6%
48	x	87	98%
49	y	71	99%
50	0	2904	79% 14% 5% 6%
51	1	120	86% 13% 6%
52	2	1542	72% 20% 8% 6%
53	3	30	23% 7% 67% 6%
54	4	77	57% 30% 13% 12%
55	5	76	79% 12% 8% 6%
56	6	2	50% 50%

## 2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 238688 atoms, of which 96012 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	271	4236	1288	2154	423	364	7	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	208	3170	976	1611	287	292	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	201	3171	974	1619	283	290	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	177	2854	899	1444	249	256	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	173	2627	814	1332	237	242	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	149	2259	699	1148	197	214	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	142	2291	714	1162	212	199	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	123	1970	593	1023	181	167	6	0	0

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	144	2182	654	1129	207	190	2	0	0

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	136	2231	686	1157	205	177	6	0	0

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	118	1934	585	989	194	161	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
12	L	116	1815	552	923	178	162	0	0

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	M	114	1879	574	962	179	163	1	0	0

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
14	N	117	1966	604	1019	192	151	0	0

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	O	103	1655	516	839	153	145	2	0	0

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	P	110	1779	532	922	166	156	3	0	0

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	Q	93	1545	466	807	139	131	2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	H	N			O
18	R	102	1610	492	831	146	141	0	0

- Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	S	94	1533	479	780	137	134	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	T	75	1165	355	593	116	100	1	0	0

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	U	77	1277	388	652	129	106	2	0	0

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	V	60	1014	303	523	96	91	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	W	57	921	276	482	86	75	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	X	60	962	299	482	90	85	6	0	0

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	a	55	879	263	445	92	78	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			
26	b	51	868	269	451	76	72		0	0

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	c	46	795	228	418	90	57	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L35.



Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	d	64	1077	323	573	105	74	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	e	38	645	185	343	65	48	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	f	224	3533	1109	1780	315	321	8	0	0

- Molecule 31 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	g	206	3320	1028	1696	305	288	3	0	0

- Molecule 32 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	h	205	3350	1026	1707	315	298	4	0	0

- Molecule 33 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
33	i	155	2329	711	1185	216	211	6	0	0

- Molecule 34 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
34	j	106	1726	545	864	156	154	7	0	0

- Molecule 35 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
35	k	151	2419	735	1238	227	215	4	0	0

- Molecule 36 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
36	l	129	2010	616	1031	173	184	6	0	0

- Molecule 37 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
37	m	127	2092	634	1070	206	179	3	0	0

- Molecule 38 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
38	n	99	1631	498	836	152	144	1	0	0

- Molecule 39 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
39	o	117	1764	540	887	174	160	3	0	0

- Molecule 40 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
40	p	123	1971	590	1016	196	165	4	0	0

- Molecule 41 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
41	q	114	1824	546	941	178	156	3	0	0

- Molecule 42 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
42	r	100	1649	499	844	164	139	3	0	0

- Molecule 43 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
43	s	88	1448	439	734	144	130	1	0	0

- Molecule 44 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
44	t	82	1315	406	666	128	114	1	0	0

- Molecule 45 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
45	u	80	1339	411	691	121	113	3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
46	v	66	1109	345	565	102	96	1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
47	w	79	1302	408	665	120	107	2	0	0

- Molecule 48 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
48	x	86	1389	414	719	138	115	3	0	0

- Molecule 49 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
49	y	70	Total	C	H	N	O	S	0	0
			1219	366	629	125	98	1		

- Molecule 50 is a RNA chain called 23S rRNA RRLG-RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
50	0	2758	Total	C	H	N	O	P	0	0
			89005	26417	29786	10911	19134	2757		

- Molecule 51 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
51	1	120	Total	C	H	N	O	P	0	0
			3868	1144	1302	468	835	119		

- Molecule 52 is a RNA chain called 16S rRNA RRSB-RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
52	2	1534	Total	C	H	N	O	P	0	0
			49480	14681	16563	6041	10661	1534		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
53	3	10	Total	C	H	N	O	P	0	0
			325	98	109	41	67	10		

- Molecule 54 is a RNA chain called Deacylated P-site tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace		
54	4	77	Total	C	H	N	O	P	S	0	0
			2468	734	826	297	534	76	1		

- Molecule 55 is a RNA chain called Dipeptidyl A-site tRNA(Lys).

Mol	Chain	Residues	Atoms					AltConf	Trace		
55	5	76	Total	C	H	N	O	P	S	0	0
			2456	729	831	283	537	75	1		

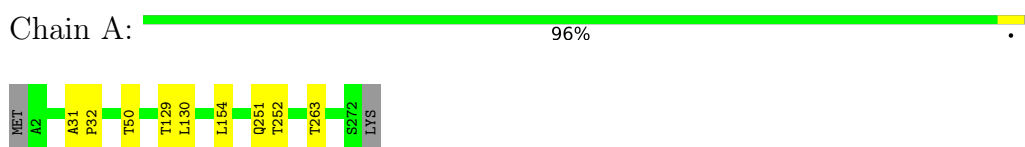
- Molecule 56 is a protein called fMet-Lys dipeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
56	6	2	37	12	18	3	3	1	0	0

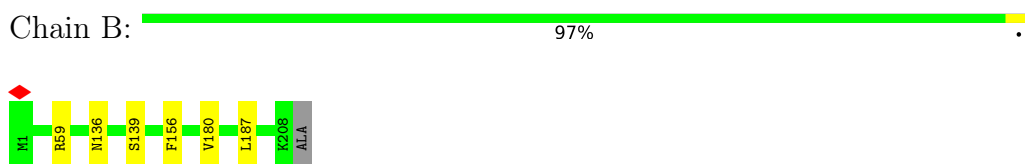
### 3 Residue-property plots

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

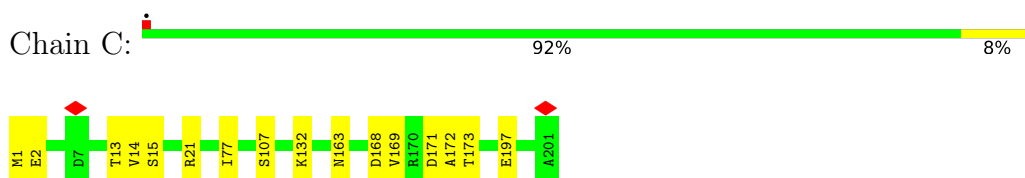
- Molecule 1: 50S ribosomal protein L2



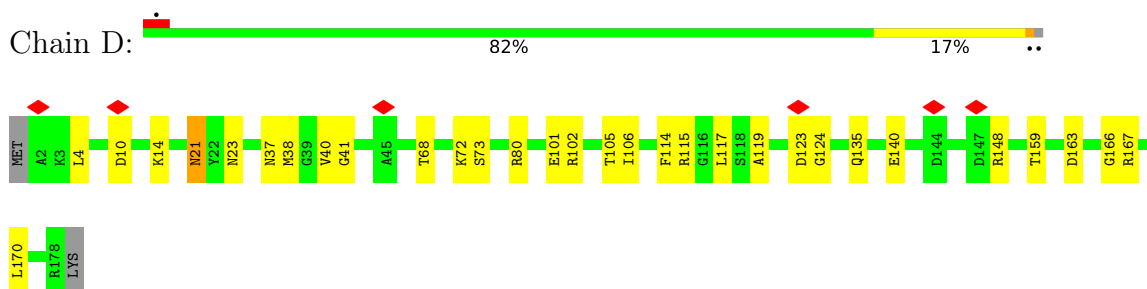
- Molecule 2: 50S ribosomal protein L3



- Molecule 3: 50S ribosomal protein L4



- Molecule 4: 50S ribosomal protein L5

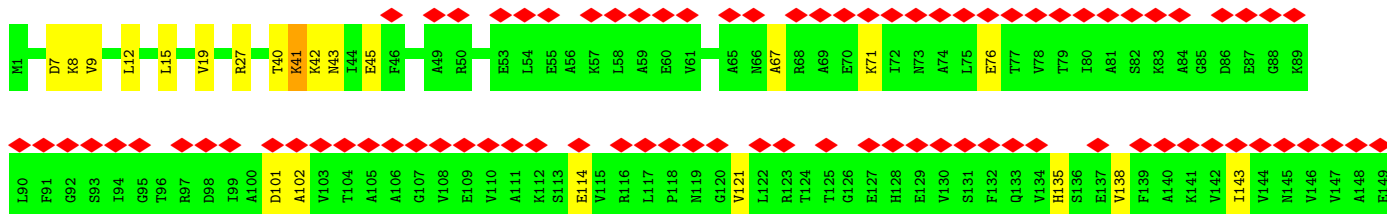
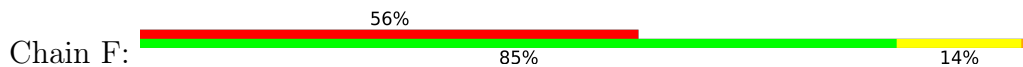


- Molecule 5: 50S ribosomal protein L6

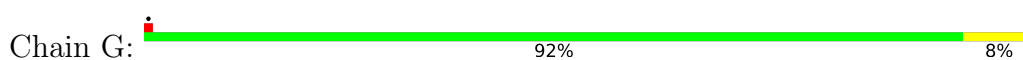




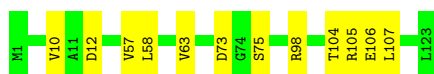
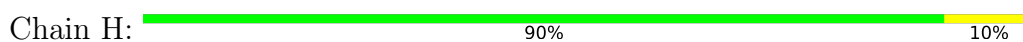
- Molecule 6: 50S ribosomal protein L9



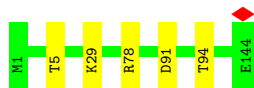
- Molecule 7: 50S ribosomal protein L13



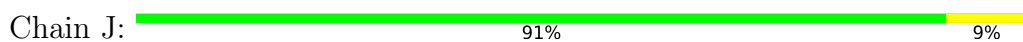
- Molecule 8: 50S ribosomal protein L14



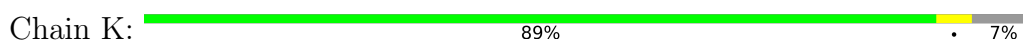
- Molecule 9: 50S ribosomal protein L15



- Molecule 10: 50S ribosomal protein L16

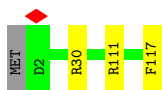


- Molecule 11: 50S ribosomal protein L17



- Molecule 12: 50S ribosomal protein L18

Chain L:  97%



- Molecule 13: 50S ribosomal protein L19

Chain M:  99%



- Molecule 14: 50S ribosomal protein L20

Chain N:  98%



- Molecule 15: 50S ribosomal protein L21

Chain O:  95%




- Molecule 16: 50S ribosomal protein L22

Chain P:  100%



- Molecule 17: 50S ribosomal protein L23

Chain Q:  90%



- Molecule 18: 50S ribosomal protein L24

Chain R:  6%

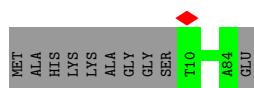
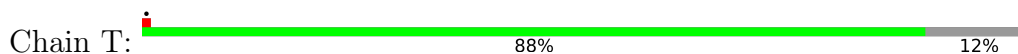




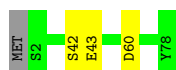
- Molecule 19: 50S ribosomal protein L25



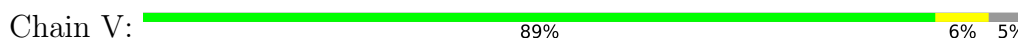
- Molecule 20: 50S ribosomal protein L27



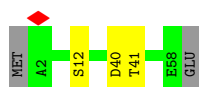
- Molecule 21: 50S ribosomal protein L28



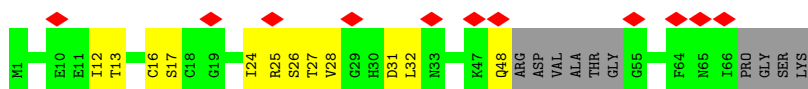
- Molecule 22: 50S ribosomal protein L29



- Molecule 23: 50S ribosomal protein L30



- Molecule 24: 50S ribosomal protein L31

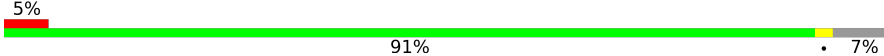


- Molecule 25: 50S ribosomal protein L32

Chain a:  96%



- Molecule 26: 50S ribosomal protein L33

Chain b:  5% 91% 7%



- Molecule 27: 50S ribosomal protein L34

Chain c:  100%



- Molecule 28: 50S ribosomal protein L35

Chain d:  97%

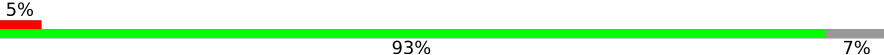


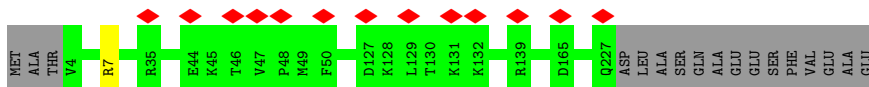
- Molecule 29: 50S ribosomal protein L36

Chain e:  100%


There are no outlier residues recorded for this chain.

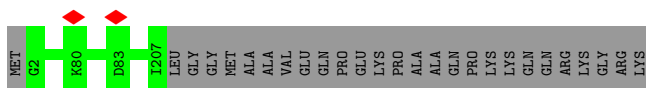
- Molecule 30: 30S ribosomal protein S2

Chain f:  5% 93% 7%

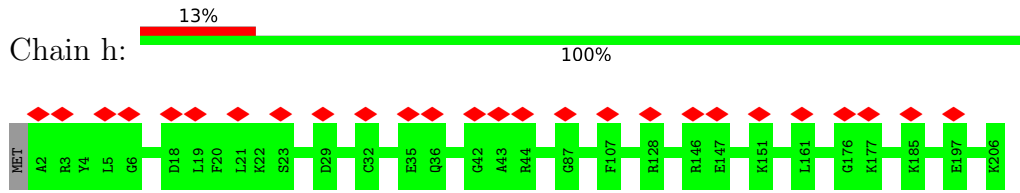


- Molecule 31: 30S ribosomal protein S3

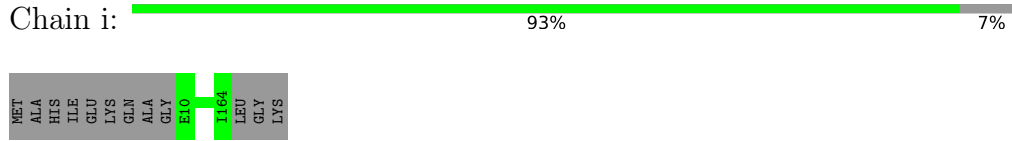
Chain g:  1% 88% 12%



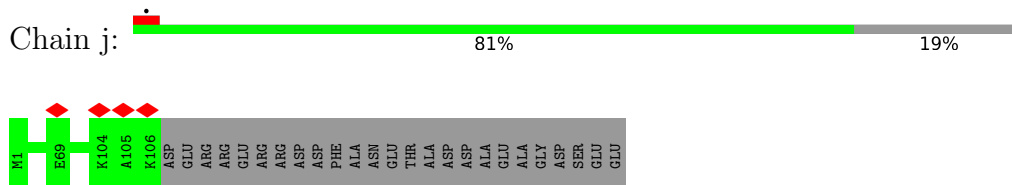
- Molecule 32: 30S ribosomal protein S4



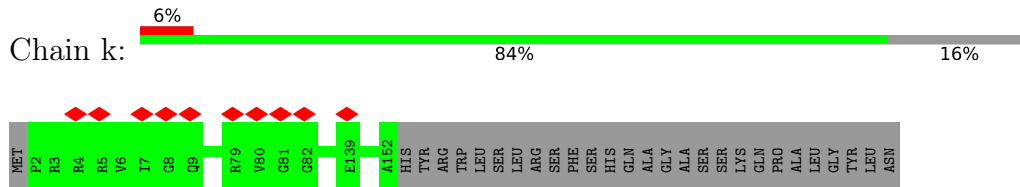
• Molecule 33: 30S ribosomal protein S5



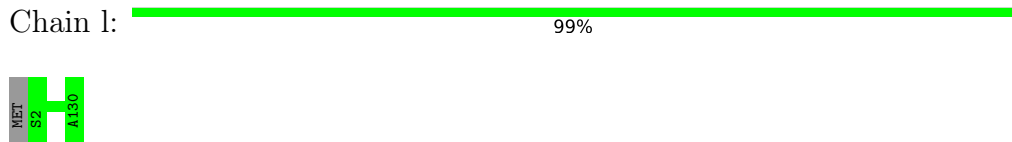
• Molecule 34: 30S ribosomal protein S6



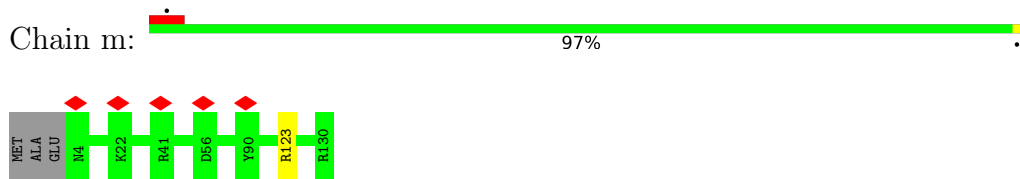
• Molecule 35: 30S ribosomal protein S7



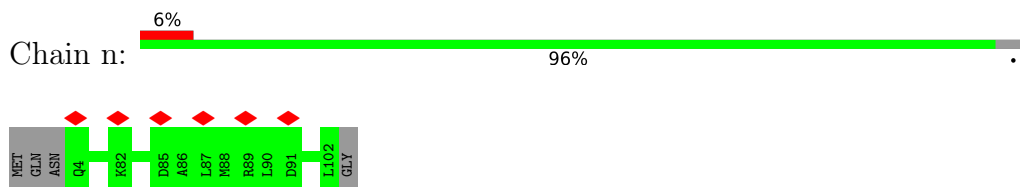
• Molecule 36: 30S ribosomal protein S8



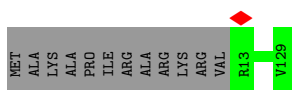
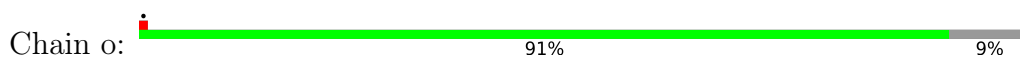
• Molecule 37: 30S ribosomal protein S9



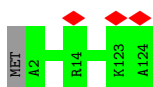
• Molecule 38: 30S ribosomal protein S10



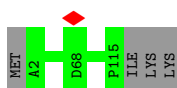
- Molecule 39: 30S ribosomal protein S11



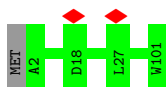
- Molecule 40: 30S ribosomal protein S12



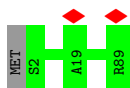
- Molecule 41: 30S ribosomal protein S13



- Molecule 42: 30S ribosomal protein S14



- Molecule 43: 30S ribosomal protein S15

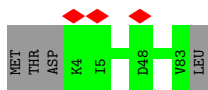


- Molecule 44: 30S ribosomal protein S16

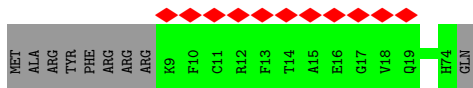
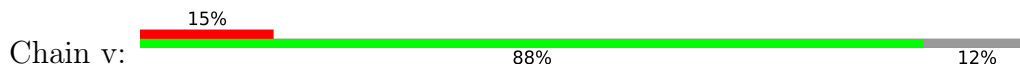


- Molecule 45: 30S ribosomal protein S17

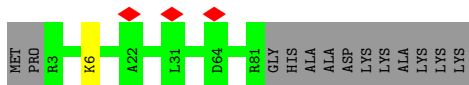
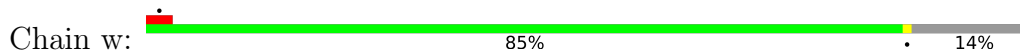




• Molecule 46: 30S ribosomal protein S18



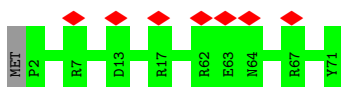
• Molecule 47: 30S ribosomal protein S19



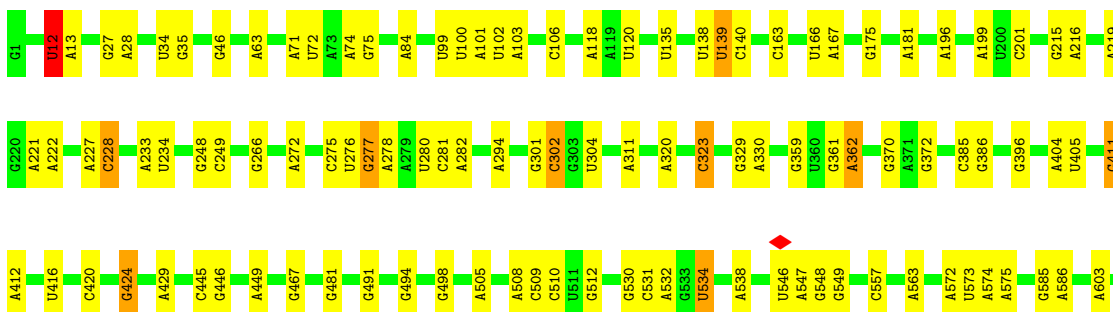
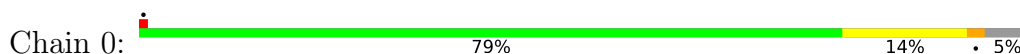
• Molecule 48: 30S ribosomal protein S20

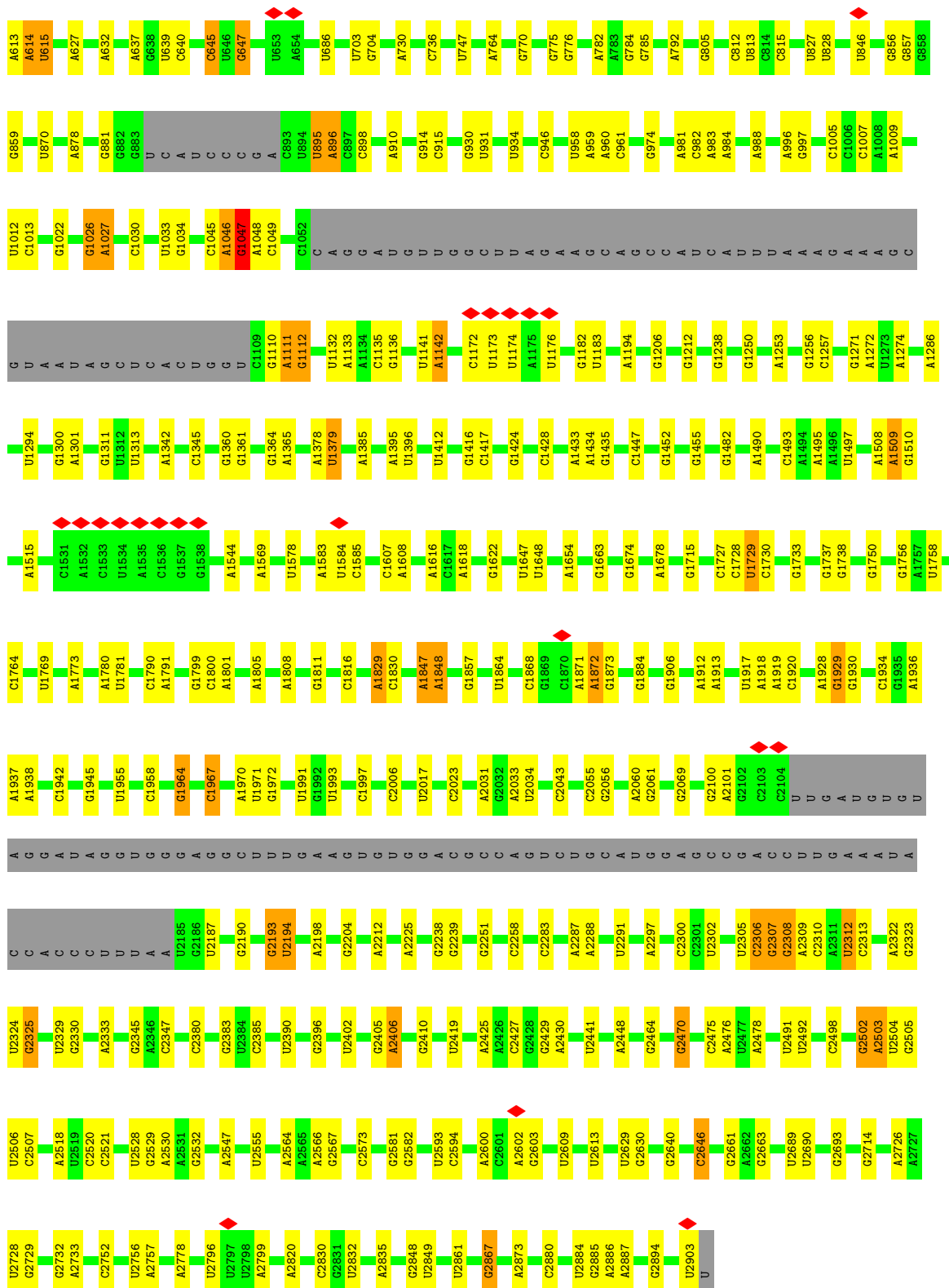


• Molecule 49: 30S ribosomal protein S21

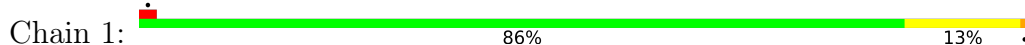


• Molecule 50: 23S rRNA RRLG-RRNA





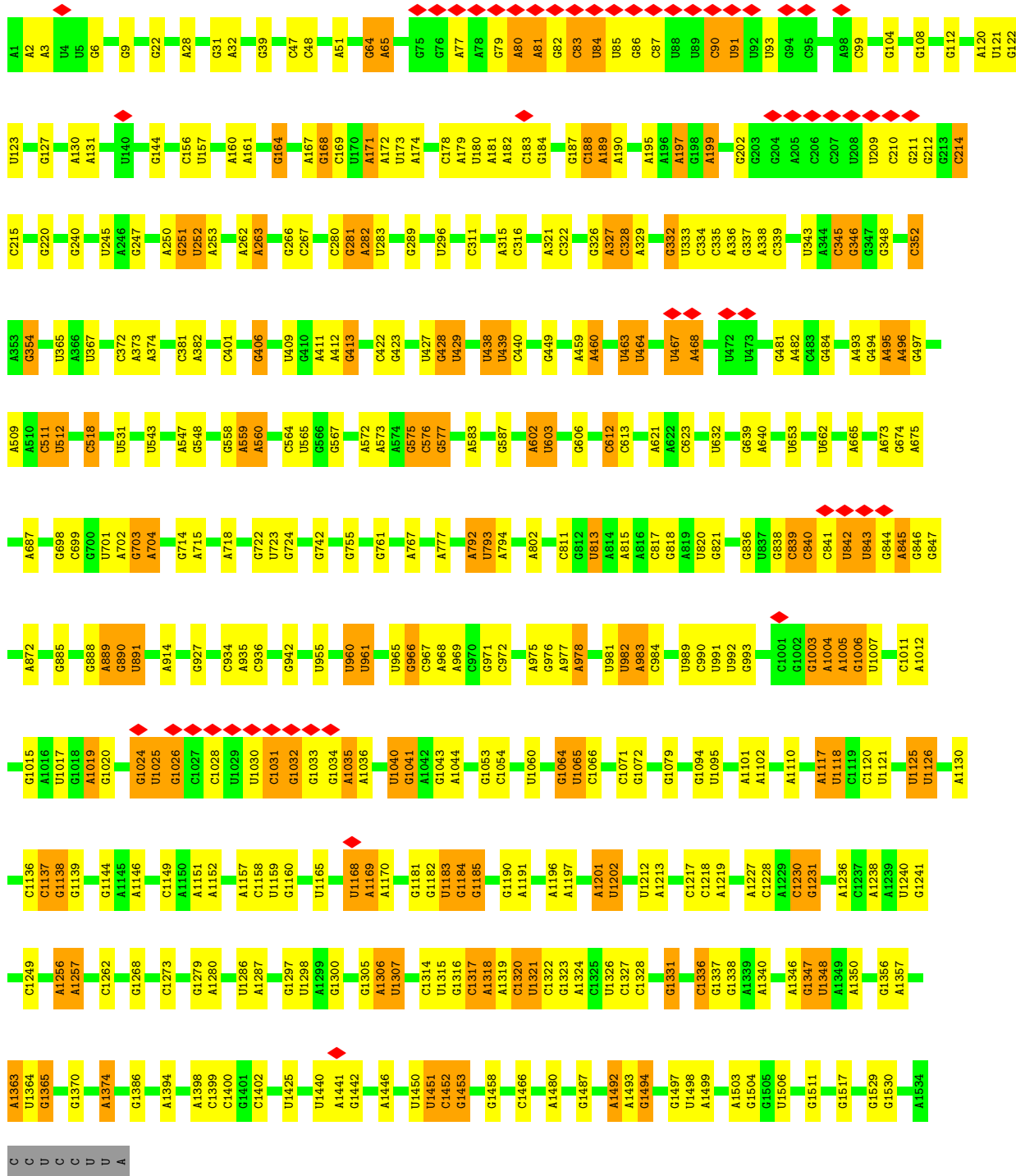
• Molecule 51: 5S rRNA





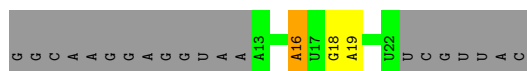
• Molecule 52: 16S rRNA RRSB-RRNA

Chain 2: 72% 20% 8%



• Molecule 53: mRNA

Chain 3:  23% 7% 67%




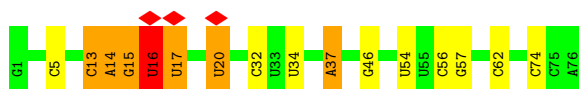
- Molecule 54: Deacylated P-site tRNA(fMet)

Chain 4:  12% 57% 30% 13%



- Molecule 55: Dipeptidyl A-site tRNA(Lys)

Chain 5:  79% 12% 8%



- Molecule 56: fMet-Lys dipeptide

Chain 6:  50% 50%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41219	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)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.434	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.103	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, FME, H2U, U8U, 6MZ, OMC, T6A, 5MU

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	0.27	0/2121	0.59	0/2852
2	B	0.26	0/1580	0.53	0/2127
3	C	0.26	0/1571	0.52	0/2113
4	D	0.26	0/1434	0.54	0/1926
5	E	0.25	0/1315	0.51	0/1783
6	F	0.25	0/1122	0.51	0/1515
7	G	0.27	0/1152	0.52	0/1551
8	H	0.26	0/956	0.59	0/1279
9	I	0.26	0/1062	0.59	0/1413
10	J	0.26	0/1093	0.58	0/1460
11	K	0.26	0/958	0.60	0/1281
12	L	0.26	0/902	0.56	0/1209
13	M	0.25	0/929	0.55	0/1242
14	N	0.29	0/960	0.56	0/1278
15	O	0.26	0/829	0.54	0/1107
16	P	0.25	0/864	0.54	0/1156
17	Q	0.25	0/744	0.52	0/994
18	R	0.25	0/787	0.51	0/1051
19	S	0.27	0/766	0.50	0/1025
20	T	0.25	0/579	0.55	0/767
21	U	0.25	0/635	0.60	0/848
22	V	0.25	0/492	0.53	0/655
23	W	0.24	0/443	0.54	0/593
24	X	0.27	0/488	0.51	0/649
25	a	0.24	0/440	0.58	0/588
26	b	0.25	0/424	0.50	0/565
27	c	0.26	0/380	0.66	0/498
28	d	0.25	0/513	0.57	0/676
29	e	0.26	0/303	0.59	0/397
30	f	0.26	0/1784	0.50	0/2403
31	g	0.25	0/1651	0.55	0/2225
32	h	0.29	0/1665	0.55	0/2227

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	i	0.26	0/1157	0.53	0/1557
34	j	0.25	0/881	0.52	0/1189
35	k	0.25	0/1195	0.56	0/1602
36	l	0.26	0/989	0.53	0/1326
37	m	0.26	0/1034	0.61	0/1375
38	n	0.24	0/805	0.57	0/1089
39	o	0.26	0/893	0.56	0/1205
40	p	0.25	0/969	0.59	0/1300
41	q	0.25	0/892	0.58	0/1193
42	r	0.25	0/817	0.57	0/1088
43	s	0.26	0/722	0.56	0/964
44	t	0.25	0/659	0.59	0/884
45	u	0.24	0/657	0.54	0/881
46	v	0.26	0/553	0.53	0/742
47	w	0.26	0/652	0.53	0/877
48	x	0.29	0/676	0.54	0/895
49	y	0.27	0/598	0.60	0/792
50	0	0.34	0/66326	0.77	4/103471 (0.0%)
51	1	0.29	0/2869	0.74	0/4474
52	2	0.33	0/36859	0.78	1/57501 (0.0%)
53	3	1.04	0/215	0.79	0/330
54	4	0.66	0/1766	0.72	0/2753
55	5	0.77	0/1663	0.72	0/2588
56	6	0.28	0/8	0.35	0/8
All	All	0.33	0/154797	0.72	5/231537 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	0	323	C	C2-N1-C1'	6.19	125.61	118.80
50	0	1313	U	C2-N1-C1'	5.80	124.67	117.70
50	0	12	U	C2-N1-C1'	5.60	124.42	117.70
50	0	1047	G	O4'-C1'-N9	5.44	112.55	108.20
52	2	1466	C	N3-C2-O2	-5.07	118.35	121.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2082	2154	2154	7	0
2	B	1559	1611	1611	6	0
3	C	1552	1619	1619	11	0
4	D	1410	1444	1444	39	0
5	E	1295	1332	1332	10	0
6	F	1111	1148	1148	15	0
7	G	1129	1162	1162	10	0
8	H	947	1023	1023	9	0
9	I	1053	1129	1129	5	0
10	J	1074	1157	1157	10	0
11	K	945	989	989	3	0
12	L	892	923	923	2	0
13	M	917	962	962	0	0
14	N	947	1019	1019	1	0
15	O	816	839	839	4	0
16	P	857	922	922	0	0
17	Q	738	807	807	2	0
18	R	779	831	831	1	0
19	S	753	780	780	4	0
20	T	572	593	593	0	0
21	U	625	652	652	3	0
22	V	491	523	523	3	0
23	W	439	482	482	2	0
24	X	480	482	482	8	0
25	a	434	445	445	0	0
26	b	417	451	451	0	0
27	c	377	418	418	0	0
28	d	504	573	572	0	0
29	e	302	343	343	0	0
30	f	1753	1780	1780	0	0
31	g	1624	1696	1696	0	0
32	h	1643	1707	1707	0	0
33	i	1144	1185	1185	0	0
34	j	862	864	864	0	0
35	k	1181	1238	1238	0	0
36	l	979	1031	1031	0	0
37	m	1022	1070	1070	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	n	795	836	836	0	0
39	o	877	887	887	0	0
40	p	955	1016	1016	0	0
41	q	883	941	941	0	0
42	r	805	844	844	0	0
43	s	714	734	734	0	0
44	t	649	666	666	0	0
45	u	648	691	691	0	0
46	v	544	565	565	0	0
47	w	637	665	665	0	0
48	x	670	719	719	0	0
49	y	590	629	629	0	0
50	0	59219	29786	29790	113	0
51	1	2566	1302	1302	4	0
52	2	32917	16563	16564	184	0
53	3	216	109	110	1	0
54	4	1642	826	841	28	0
55	5	1625	831	835	8	0
56	6	19	18	23	0	0
All	All	142676	96012	96041	445	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (445) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:ARG:HH12	54:4:56:C:N4	1.46	1.12
52:2:1183:U:O2'	52:2:1184:G:OP1	1.76	1.04
10:J:59:ARG:NH2	55:5:56:C:OP2	1.96	0.97
52:2:281:G:O2'	52:2:282:A:OP2	1.86	0.94
7:G:96:ARG:NH2	50:0:2640:G:OP1	2.03	0.91
52:2:1025:U:O2'	52:2:1026:G:O4'	1.88	0.91
4:D:10:ASP:O	4:D:14:LYS:NZ	2.03	0.91
4:D:80:ARG:NH1	54:4:56:C:N4	2.19	0.89
11:K:86:ARG:NH2	11:K:117:ASP:O	2.06	0.89
52:2:171:A:O2'	52:2:172:A:O4'	1.91	0.89
55:5:15:G:O2'	55:5:16:H2U:OP1	1.91	0.88
24:X:13:THR:OG1	24:X:31:ASP:OD1	1.90	0.88
21:U:42:SER:OG	21:U:43:GLU:OE1	1.92	0.86
4:D:80:ARG:NH1	54:4:56:C:H42	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:SER:OG	54:4:56:C:O4'	1.92	0.86
50:0:2306:C:OP2	50:0:2307:G:O2'	1.93	0.86
4:D:80:ARG:NH1	54:4:56:C:N3	2.24	0.85
4:D:80:ARG:HH12	54:4:56:C:H42	0.88	0.84
50:0:1026:G:O2'	50:0:1027:A:OP1	1.95	0.83
4:D:80:ARG:NH1	54:4:56:C:C4	2.47	0.82
52:2:1306:A:N6	52:2:1331:G:O2'	2.12	0.82
52:2:1125:U:O2'	52:2:1126:U:O2	1.99	0.81
50:0:1311:G:OP2	50:0:1311:G:N2	2.11	0.80
52:2:90:C:O2'	52:2:91:U:O5'	1.99	0.80
51:1:66:A:OP2	51:1:108:A:N6	2.15	0.80
50:0:1111:A:O2'	50:0:1112:G:OP2	1.99	0.78
54:4:51:C:N4	54:4:63:G:O6	2.15	0.78
4:D:73:SER:HG	54:4:56:C:C1'	1.96	0.78
52:2:1183:U:HO2'	52:2:1184:G:P	2.06	0.78
52:2:576:C:O2'	52:2:577:G:OP1	2.02	0.78
50:0:276:U:O2'	50:0:278:A:N7	2.17	0.78
52:2:467:U:O2'	52:2:468:A:OP1	2.03	0.77
10:J:59:ARG:NH2	55:5:56:C:H5''	2.00	0.76
12:L:111:ARG:NH1	12:L:117:PHE:O	2.19	0.76
52:2:427:U:OP2	52:2:428:G:O2'	2.04	0.76
3:C:21:ARG:NH1	3:C:107:SER:OG	2.18	0.76
52:2:251:G:O2'	52:2:252:U:OP2	2.03	0.76
54:4:6:G:O2'	54:4:49:G:OP2	2.04	0.75
50:0:895:U:O2'	50:0:896:A:OP1	2.04	0.75
50:0:1508:A:O2'	50:0:1509:A:O4'	2.04	0.75
5:E:47:ASP:OD1	5:E:48:ASN:N	2.20	0.74
52:2:1451:U:O2'	52:2:1452:C:OP1	2.03	0.73
6:F:7:ASP:OD1	6:F:8:LYS:N	2.24	0.71
52:2:1256:A:O2'	52:2:1257:A:OP2	2.09	0.71
52:2:167:A:N6	52:2:168:G:O6	2.24	0.70
55:5:13:C:O2'	55:5:14:A:OP1	2.08	0.70
52:2:845:A:O2'	52:2:846:G:O5'	2.10	0.70
10:J:106:ASP:OD1	10:J:107:GLY:N	2.25	0.69
52:2:1451:U:HO2'	52:2:1452:C:P	2.14	0.69
52:2:509:A:N3	52:2:543:U:O2'	2.26	0.69
50:0:1447:C:O2'	50:0:1544:A:N3	2.25	0.69
50:0:1871:A:O2'	50:0:1872:A:O5'	2.12	0.69
52:2:842:U:O2'	52:2:843:U:OP1	2.11	0.68
50:0:219:A:N3	50:0:234:U:O2'	2.25	0.68
52:2:401:C:O2'	52:2:621:A:N3	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:58:ASN:ND2	50:0:72:U:O4	2.26	0.68
52:2:558:G:OP2	52:2:559:A:O2'	2.10	0.68
50:0:1857:G:N2	50:0:1884:G:O2'	2.27	0.67
52:2:188:C:O2'	52:2:189:A:OP1	2.12	0.67
52:2:1003:G:O2'	52:2:1004:A:O5'	2.07	0.67
52:2:1320:C:O2'	52:2:1321:U:OP1	2.12	0.67
12:L:30:ARG:NH2	51:1:48:U:OP1	2.27	0.67
50:0:2581:G:N2	50:0:2581:G:OP2	2.27	0.67
2:B:59:ARG:NH1	50:0:2830:C:OP2	2.28	0.67
52:2:463:U:O2'	52:2:464:U:OP1	2.12	0.67
4:D:21:ASN:O	4:D:21:ASN:ND2	2.26	0.66
1:A:251:GLN:NE2	1:A:252:THR:O	2.28	0.66
50:0:2405:G:O2'	50:0:2406:A:OP1	2.12	0.66
50:0:1864:U:OP1	50:0:2410:G:O2'	2.15	0.65
50:0:2193:G:O2'	50:0:2194:U:OP1	2.13	0.65
52:2:65:A:O2'	52:2:199:A:O2'	2.15	0.65
50:0:2324:U:H3'	50:0:2325:G:C5'	2.27	0.64
52:2:1025:U:O2'	52:2:1026:G:N3	2.24	0.64
52:2:1363:A:O2'	52:2:1365:G:N7	2.31	0.64
50:0:1857:G:O2'	50:0:1884:G:N2	2.29	0.64
52:2:967:C:OP2	52:2:968:A:O2'	2.10	0.64
50:0:1964:G:O2'	50:0:1967:C:OP2	2.17	0.63
10:J:55:ARG:NH2	50:0:2470:G:OP1	2.31	0.63
55:5:13:C:HO2'	55:5:14:A:P	2.20	0.63
4:D:115:ARG:NH1	24:X:48:GLN:OE1	2.32	0.63
6:F:67:ALA:HB1	6:F:71:LYS:NZ	2.14	0.62
52:2:495:A:O2'	52:2:496:A:OP2	2.15	0.62
4:D:37:ASN:ND2	50:0:2313:C:O4'	2.29	0.62
50:0:2728:U:HO2'	50:0:2729:G:H8	1.48	0.62
52:2:281:G:HO2'	52:2:282:A:P	2.19	0.62
52:2:845:A:O2'	52:2:846:G:O4'	2.16	0.62
52:2:157:U:O2	52:2:164:G:O6	2.19	0.61
52:2:3:A:O2'	52:2:612:C:O2'	2.16	0.60
52:2:602:A:O2'	52:2:603:U:OP1	2.18	0.60
8:H:98:ARG:NH1	52:2:339:C:OP2	2.34	0.60
52:2:187:G:N2	52:2:190:A:OP2	2.35	0.60
50:0:895:U:HO2'	50:0:896:A:P	2.25	0.60
55:5:37:T6A:H152	55:5:37:T6A:O10	2.02	0.60
54:4:15:C:O2'	54:4:16:C:OP1	2.16	0.59
52:2:188:C:HO2'	52:2:189:A:P	2.26	0.59
52:2:1317:C:O2'	52:2:1318:A:OP1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:2:576:C:HO2'	52:2:577:G:P	2.24	0.59
52:2:888:G:H3'	52:2:889:A:H5''	1.84	0.59
10:J:59:ARG:HH22	55:5:56:C:H5''	1.68	0.58
52:2:189:A:O2'	52:2:190:A:O4'	2.16	0.58
24:X:16:CYS:SG	24:X:17:SER:N	2.76	0.58
52:2:168:G:O2'	52:2:169:C:O5'	2.21	0.58
50:0:370:G:O2'	50:0:424:G:OP1	2.20	0.58
52:2:79:G:N1	52:2:91:U:O2	2.34	0.58
19:S:45:ASP:OD1	19:S:46:LYS:N	2.37	0.58
52:2:511:C:O2'	52:2:512:U:OP2	2.15	0.58
52:2:1019:A:N6	52:2:1020:G:O6	2.37	0.58
4:D:80:ARG:HH22	54:4:56:C:N4	2.02	0.57
50:0:1495:A:N3	50:0:1578:U:O2'	2.37	0.57
4:D:73:SER:OG	54:4:56:C:C1'	2.50	0.57
50:0:1026:G:HO2'	50:0:1027:A:P	2.27	0.57
52:2:90:C:C2'	52:2:91:U:O5'	2.51	0.57
54:4:14:G:O2'	54:4:15:C:OP1	2.17	0.57
50:0:2193:G:HO2'	50:0:2194:U:P	2.28	0.56
51:1:14:U:OP2	51:1:70:C:O2'	2.22	0.56
50:0:27:G:O2'	50:0:28:A:OP2	2.20	0.56
52:2:1125:U:O2'	52:2:1126:U:P	2.63	0.56
52:2:1117:A:O2'	52:2:1118:U:OP1	2.24	0.56
3:C:14:VAL:HG13	3:C:197:GLU:OE2	2.06	0.56
9:I:5:THR:HG22	9:I:5:THR:O	2.05	0.56
52:2:844:G:P	52:2:844:G:H21	2.28	0.56
52:2:1031:C:O2'	52:2:1032:G:O5'	2.24	0.56
52:2:64:G:H4'	52:2:65:A:O5'	2.07	0.55
52:2:1320:C:O2'	52:2:1321:U:P	2.64	0.55
50:0:1385:A:O2'	50:0:1396:U:O2	2.24	0.55
50:0:2324:U:H3'	50:0:2325:G:H5''	1.88	0.55
52:2:197:A:O2'	52:2:220:G:N2	2.39	0.55
54:4:15:C:HO2'	54:4:16:C:P	2.29	0.54
52:2:2:A:N3	52:2:613:C:O2'	2.32	0.54
52:2:602:A:HO2'	52:2:603:U:P	2.30	0.54
52:2:839:C:O2'	52:2:840:C:OP1	2.23	0.54
4:D:123:ASP:OD1	4:D:124:GLY:N	2.41	0.54
50:0:1047:G:O2'	50:0:1048:A:OP2	2.21	0.54
50:0:2193:G:O2'	50:0:2194:U:P	2.65	0.54
52:2:1125:U:O2'	52:2:1126:U:OP1	2.25	0.54
50:0:614:A:O2'	50:0:615:U:OP2	2.24	0.54
52:2:28:A:O2'	52:2:296:U:OP1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:2:262:A:O2'	52:2:263:A:O5'	2.13	0.54
52:2:1137:C:O2'	52:2:1138:G:P	2.66	0.54
50:0:2100:G:O6	50:0:2101:A:N6	2.41	0.54
52:2:463:U:O2'	52:2:464:U:P	2.66	0.54
4:D:80:ARG:CZ	54:4:56:C:C4	2.91	0.54
52:2:602:A:O2'	52:2:603:U:P	2.66	0.54
52:2:1024:G:HO2'	52:2:1025:U:P	2.30	0.53
3:C:171:ASP:OD1	3:C:172:ALA:N	2.41	0.53
52:2:438:U:O2'	52:2:439:U:O5'	2.26	0.53
52:2:1040:U:O2'	52:2:1041:G:OP1	2.24	0.53
4:D:163:ASP:O	4:D:167:ARG:HG3	2.09	0.53
5:E:60:ASP:OD1	5:E:60:ASP:N	2.41	0.53
4:D:102:ARG:NH2	24:X:25:ARG:O	2.37	0.53
50:0:2258:C:O2'	50:0:2427:C:OP2	2.24	0.53
52:2:327:A:O2'	52:2:328:C:O4'	2.25	0.53
3:C:173:THR:HG22	3:C:173:THR:O	2.09	0.53
50:0:2796:U:H3	50:0:2799:A:H61	1.56	0.53
6:F:67:ALA:HB1	6:F:71:LYS:HZ3	1.73	0.52
52:2:673:A:H2'	52:2:674:G:C8	2.44	0.52
5:E:169:VAL:HG13	5:E:169:VAL:O	2.09	0.52
52:2:428:G:O2'	52:2:429:U:OP2	2.17	0.52
52:2:1305:G:H22	52:2:1331:G:H2'	1.74	0.52
6:F:101:ASP:OD1	6:F:102:ALA:N	2.43	0.52
50:0:2528:U:O2'	50:0:2530:A:OP1	2.17	0.52
50:0:1141:U:H4'	50:0:1142:A:O4'	2.10	0.52
52:2:890:G:O2'	52:2:891:U:P	2.68	0.52
52:2:1040:U:HO2'	52:2:1041:G:P	2.32	0.52
1:A:263:THR:O	1:A:263:THR:HG22	2.09	0.51
52:2:1028:C:O2'	52:2:1031:C:OP1	2.21	0.51
52:2:767:A:H8	52:2:1511:G:H21	1.59	0.51
50:0:895:U:O2'	50:0:896:A:P	2.69	0.51
4:D:68:THR:HG21	50:0:2312:U:O3'	2.11	0.51
7:G:88:THR:HG22	7:G:89:PHE:N	2.25	0.51
6:F:41:LYS:O	6:F:45:GLU:HG2	2.10	0.51
50:0:1047:G:HO2'	50:0:1048:A:P	2.34	0.51
6:F:121:VAL:HG12	6:F:121:VAL:O	2.11	0.51
50:0:282:A:N6	50:0:359:G:O6	2.43	0.51
52:2:1024:G:O2'	52:2:1025:U:O5'	2.27	0.50
4:D:80:ARG:NH2	54:4:56:C:N4	2.60	0.50
50:0:227:A:O2'	50:0:228:C:OP2	2.25	0.50
4:D:80:ARG:CZ	54:4:56:C:N4	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:0:12:U:H2'	50:0:12:U:O2	2.11	0.50
52:2:1320:C:HO2'	52:2:1321:U:P	2.34	0.50
4:D:114:PHE:CE1	4:D:117:LEU:HD12	2.46	0.50
52:2:818:G:O2'	52:2:820:U:O2	2.28	0.50
52:2:1117:A:O2'	52:2:1118:U:P	2.70	0.50
4:D:105:THR:OG1	4:D:106:ILE:HD12	2.12	0.50
52:2:83:C:O2'	52:2:84:U:P	2.69	0.50
52:2:966:G:N2	54:4:34:C:H5'	2.27	0.50
52:2:1201:A:H1'	52:2:1202:U:OP2	2.11	0.50
52:2:1137:C:O2'	52:2:1138:G:OP2	2.30	0.50
52:2:1347:G:C2'	52:2:1348:U:OP2	2.59	0.50
50:0:2193:G:H2'	50:0:2194:U:C6	2.47	0.49
52:2:1230:C:O2'	52:2:1231:G:P	2.70	0.49
3:C:1:MET:N	3:C:14:VAL:O	2.46	0.49
52:2:792:A:H1'	52:2:793:U:OP2	2.12	0.49
9:I:91:ASP:OD1	9:I:94:THR:HG23	2.13	0.49
52:2:438:U:HO2'	52:2:439:U:P	2.35	0.49
52:2:1498:U:OP2	53:3:16:A:O2'	2.30	0.49
50:0:278:A:N6	50:0:362:A:N7	2.61	0.49
52:2:123:U:OP1	52:2:311:C:O2'	2.29	0.49
52:2:463:U:HO2'	52:2:464:U:P	2.34	0.49
52:2:64:G:H5'	52:2:65:A:OP1	2.12	0.48
52:2:1326:U:C2	52:2:1327:C:C5	3.01	0.48
4:D:4:LEU:HD12	4:D:101:GLU:HB2	1.95	0.48
54:4:19:G:OP1	54:4:60:U:N3	2.44	0.48
5:E:104:ASN:ND2	5:E:114:ASP:OD1	2.44	0.48
50:0:1378:A:O2'	50:0:1379:U:OP2	2.26	0.48
50:0:411:G:OP2	50:0:2406:A:O2'	2.32	0.48
52:2:1011:C:N4	52:2:1017:U:O4	2.47	0.48
52:2:1314:C:H2'	52:2:1315:U:C6	2.49	0.48
4:D:159:THR:HG22	4:D:159:THR:O	2.12	0.48
7:G:100:VAL:HG23	7:G:101:ILE:N	2.28	0.48
52:2:188:C:O2'	52:2:189:A:P	2.72	0.48
52:2:373:A:C2	52:2:374:A:C8	3.01	0.48
54:4:58:A:O2'	54:4:60:U:OP2	2.20	0.48
3:C:168:ASP:OD1	3:C:169:VAL:N	2.47	0.48
50:0:1026:G:O2'	50:0:1027:A:P	2.71	0.48
50:0:1847:A:O2'	50:0:1848:A:O5'	2.32	0.48
9:I:78:ARG:NH1	50:0:627:A:OP1	2.42	0.48
50:0:138:U:O2'	50:0:139:U:OP2	2.26	0.48
50:0:1769:U:O2'	50:0:1958:C:OP1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:2:322:C:H42	52:2:329:A:H62	1.59	0.48
52:2:990:C:O2'	52:2:991:U:O4'	2.28	0.48
52:2:1005:A:O5'	52:2:1006:G:N2	2.47	0.48
3:C:2:GLU:OE2	3:C:13:THR:HG22	2.14	0.47
6:F:15:LEU:HD23	6:F:15:LEU:O	2.14	0.47
52:2:202:G:O2'	52:2:468:A:N3	2.47	0.47
52:2:841:C:N4	52:2:843:U:O4	2.47	0.47
10:J:14:LYS:NZ	50:0:958:U:OP2	2.46	0.47
6:F:27:ARG:NH1	21:U:60:ASP:OD2	2.47	0.47
7:G:37:ARG:NH1	50:0:1007:C:OP1	2.47	0.47
52:2:714:G:H2'	52:2:715:A:C8	2.49	0.47
10:J:6:ARG:NH2	50:0:870:U:OP1	2.47	0.47
50:0:1936:A:C2	50:0:1945:G:C6	3.02	0.47
52:2:459:A:H2'	52:2:460:A:H8	1.80	0.47
54:4:4:G:H1	54:4:68:C:H42	1.62	0.47
4:D:119:ALA:O	4:D:167:ARG:NH2	2.48	0.47
50:0:2532:G:N2	50:0:2663:G:O2'	2.48	0.47
52:2:982:U:O2'	52:2:983:A:OP2	2.23	0.47
2:B:180:VAL:HG22	2:B:187:LEU:CD1	2.45	0.47
52:2:792:A:H4'	52:2:793:U:O5'	2.15	0.47
8:H:57:VAL:C	8:H:58:LEU:HD12	2.35	0.47
5:E:12:PRO:O	5:E:15:VAL:HG22	2.15	0.46
54:4:22:G:O2'	54:4:23:C:OP2	2.29	0.46
2:B:156:PHE:CE1	7:G:81:ILE:HD13	2.49	0.46
51:1:45:A:C4	51:1:46:A:C8	3.03	0.46
52:2:1168:U:H3'	52:2:1169:A:H5'	1.96	0.46
50:0:1847:A:O2'	50:0:1848:A:H8	1.97	0.46
22:V:10:SER:OG	22:V:11:VAL:N	2.47	0.46
1:A:129:THR:C	1:A:130:LEU:HD12	2.36	0.46
7:G:97:PRO:O	7:G:100:VAL:HG22	2.16	0.46
50:0:1048:A:C2	50:0:1049:C:C5	3.04	0.46
52:2:64:G:N7	52:2:99:C:N4	2.64	0.46
54:4:10:A:O2'	54:4:11:G:OP1	2.32	0.46
19:S:63:ILE:HG22	19:S:65:VAL:HG13	1.98	0.46
52:2:493:A:H2'	52:2:494:G:O4'	2.16	0.46
4:D:37:ASN:OD1	4:D:38:MET:N	2.49	0.46
4:D:135:GLN:NE2	4:D:148:ARG:O	2.42	0.46
50:0:1433:A:O2'	50:0:1434:A:H5'	2.16	0.46
52:2:699:C:O2	52:2:699:C:O4'	2.33	0.46
52:2:703:G:C2'	52:2:704:A:OP2	2.64	0.46
4:D:40:VAL:HG23	4:D:41:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:114:PHE:HE1	4:D:117:LEU:HD12	1.80	0.46
18:R:49:VAL:HG13	18:R:49:VAL:O	2.16	0.46
50:0:703:U:H2'	50:0:704:G:O4'	2.16	0.46
7:G:65:THR:HG22	7:G:66:GLY:N	2.30	0.46
23:W:12:SER:OG	50:0:988:A:OP2	2.34	0.46
6:F:9:VAL:HG11	6:F:12:LEU:HD21	1.99	0.45
52:2:181:A:O2'	52:2:182:A:O4'	2.34	0.45
52:2:328:C:O2	52:2:328:C:C2'	2.63	0.45
4:D:123:ASP:O	50:0:2302:U:O2'	2.34	0.45
6:F:135:HIS:HB3	6:F:138:VAL:HG22	1.97	0.45
15:O:85:LYS:NZ	50:0:815:C:OP2	2.48	0.45
52:2:978:A:C4	52:2:1319:A:C2	3.04	0.45
52:2:1015:G:HO2'	52:2:1217:C:HO2'	1.64	0.45
50:0:1046:A:H3'	50:0:1047:G:H5'	1.99	0.45
52:2:1356:G:H2'	52:2:1357:A:C8	2.52	0.45
19:S:55:GLU:HB3	19:S:59:GLU:OE2	2.17	0.45
50:0:2646:C:OP2	50:0:2732:G:O2'	2.33	0.45
52:2:160:A:H2'	52:2:161:A:O4'	2.16	0.45
52:2:890:G:O2'	52:2:891:U:OP2	2.34	0.45
1:A:154:LEU:HD23	50:0:1799:G:N2	2.32	0.45
5:E:17:VAL:HG12	5:E:18:LYS:N	4.53	0.45
52:2:1256:A:HO2'	52:2:1257:A:P	2.38	0.45
14:N:49:ASP:CG	50:0:534:U:HO2'	2.20	0.45
50:0:1048:A:N7	50:0:1111:A:N6	2.65	0.45
15:O:37:GLU:HG3	15:O:37:GLU:O	2.16	0.45
24:X:12:ILE:HD12	24:X:32:LEU:HD13	1.98	0.45
52:2:332:G:C2	52:2:333:U:C6	3.05	0.45
52:2:1315:U:H2'	52:2:1316:G:O4'	2.17	0.45
50:0:2848:G:O2'	50:0:2867:G:N2	2.42	0.44
52:2:1120:C:O2	52:2:1120:C:O4'	2.35	0.44
55:5:32:C:O2	55:5:32:C:O5'	2.35	0.44
10:J:132:THR:HG22	10:J:133:LYS:N	2.32	0.44
50:0:301:G:O2'	50:0:302:C:OP2	2.35	0.44
50:0:984:A:N3	50:0:984:A:H2'	2.32	0.44
50:0:1607:C:N4	50:0:1622:G:OP2	2.50	0.44
52:2:65:A:N6	52:2:381:C:N3	2.65	0.44
52:2:559:A:H1'	52:2:560:A:OP2	2.16	0.44
52:2:1025:U:H2'	52:2:1026:G:H21	1.82	0.44
52:2:1184:G:H2'	52:2:1185:G:H5'	1.99	0.44
2:B:136:ASN:ND2	2:B:139:SER:O	2.49	0.44
4:D:140:GLU:OE1	4:D:140:GLU:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:0:2291:U:OP1	50:0:2380:C:O2'	2.36	0.44
50:0:2323:G:O2'	50:0:2324:U:H5'	2.18	0.44
52:2:1125:U:H2'	52:2:1126:U:H2'	1.98	0.44
4:D:21:ASN:HD22	4:D:21:ASN:C	2.16	0.44
52:2:575:G:H4'	52:2:576:C:O5'	2.17	0.44
52:2:90:C:H2'	52:2:91:U:O4'	2.17	0.44
52:2:890:G:C2'	52:2:891:U:OP2	2.66	0.44
54:4:7:4SU:S4	54:4:13:A:N7	2.91	0.44
50:0:2555:U:O2	50:0:2555:U:O4'	2.35	0.44
52:2:373:A:C2	52:2:482:A:N6	2.86	0.44
52:2:701:U:OP1	52:2:702:A:O2'	2.24	0.44
52:2:703:G:O2'	52:2:704:A:P	2.76	0.44
52:2:989:U:O2	52:2:989:U:O4'	2.36	0.44
5:E:166:ASP:OD1	5:E:166:ASP:N	2.50	0.43
6:F:40:THR:OG1	6:F:43:ASN:ND2	2.51	0.43
17:Q:11:LEU:O	22:V:29:ARG:NH1	2.51	0.43
50:0:106:C:HO2'	50:0:294:A:HO2'	1.65	0.43
52:2:80:A:O2'	52:2:81:A:O4'	2.36	0.43
52:2:337:G:H2'	52:2:338:A:C8	2.53	0.43
52:2:981:U:O2	52:2:981:U:O5'	2.36	0.43
52:2:1262:C:O4'	52:2:1262:C:O2	2.34	0.43
3:C:132:LYS:NZ	50:0:320:A:OP2	2.44	0.43
15:O:55:ASP:O	15:O:55:ASP:OD1	2.36	0.43
50:0:1182:G:H2'	50:0:1183:U:O4'	2.18	0.43
50:0:2521:C:O2'	50:0:2564:A:H8	2.01	0.43
4:D:166:GLY:O	4:D:170:LEU:HD13	2.19	0.43
52:2:1035:A:N3	52:2:1035:A:H2'	2.33	0.43
8:H:63:VAL:HG12	8:H:107:LEU:HD11	2.01	0.43
8:H:104:THR:HG22	8:H:106:GLU:OE1	2.18	0.43
52:2:606:G:N2	52:2:632:U:OP1	2.43	0.43
52:2:1230:C:H2'	52:2:1231:G:H8	1.82	0.43
52:2:1298:U:O2	52:2:1298:U:O4'	2.35	0.43
50:0:1912:A:O2'	52:2:1494:G:O2'	2.28	0.43
2:B:59:ARG:HG3	2:B:59:ARG:O	2.18	0.43
2:B:180:VAL:HG22	2:B:187:LEU:HD12	2.00	0.43
7:G:96:ARG:HG3	7:G:96:ARG:O	2.19	0.43
52:2:335:C:C2	52:2:336:A:C8	3.07	0.43
4:D:106:ILE:O	4:D:106:ILE:HG22	2.17	0.43
11:K:32:GLU:HG2	11:K:115:LEU:HD12	2.01	0.43
50:0:981:A:OP2	50:0:982:C:N4	2.41	0.43
50:0:2756:U:H4'	50:0:2757:A:OP1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:2:575:G:H1'	52:2:576:C:OP2	2.18	0.43
52:2:978:A:C5	52:2:1319:A:C2	3.06	0.43
52:2:1347:G:O2'	52:2:1348:U:P	2.76	0.43
50:0:445:C:H2'	50:0:446:G:O4'	2.19	0.43
52:2:345:C:H1'	52:2:346:G:OP2	2.19	0.43
7:G:65:THR:HG21	50:0:1141:U:H2'	2.01	0.43
50:0:100:U:O2	50:0:100:U:O4'	2.36	0.43
52:2:81:A:H2'	52:2:82:G:C8	2.54	0.43
52:2:214:C:C2	52:2:215:C:C5	3.07	0.43
52:2:467:U:H4'	52:2:468:A:OP2	2.19	0.43
52:2:1347:G:N2	52:2:1374:A:OP2	2.51	0.43
5:E:92:VAL:O	5:E:92:VAL:HG13	2.19	0.42
24:X:24:ILE:HG22	24:X:25:ARG:N	2.34	0.42
52:2:64:G:C5	52:2:99:C:N4	2.87	0.42
9:I:29:LYS:O	9:I:29:LYS:HG2	2.19	0.42
50:0:639:U:H2'	50:0:640:C:H6	1.84	0.42
50:0:645:C:H2'	50:0:647:G:N7	2.34	0.42
52:2:1040:U:O2'	52:2:1041:G:P	2.77	0.42
23:W:40:ASP:O	23:W:41:THR:HG23	2.19	0.42
50:0:1727:C:H2'	50:0:1728:C:O4'	2.19	0.42
52:2:1117:A:HO2'	52:2:1118:U:P	2.42	0.42
52:2:1120:C:C5	52:2:1121:U:C5	3.07	0.42
52:2:81:A:H2'	52:2:82:G:H8	1.84	0.42
6:F:41:LYS:HD2	6:F:42:LYS:N	2.34	0.42
52:2:411:A:C4	52:2:413:G:H1'	2.54	0.42
52:2:1064:G:H4'	52:2:1065:U:OP1	2.18	0.42
8:H:73:ASP:OD1	8:H:75:SER:OG	2.17	0.42
17:Q:65:GLY:N	17:Q:79:ASP:OD1	2.52	0.42
50:0:277:G:O2'	50:0:278:A:C4	2.73	0.42
50:0:1728:C:HO2'	50:0:1729:U:H6	1.65	0.42
52:2:1031:C:O2'	52:2:1032:G:O4'	2.29	0.42
52:2:1336:C:O2	52:2:1336:C:O4'	2.37	0.42
3:C:77:ILE:O	3:C:77:ILE:HG22	2.20	0.42
50:0:1928:A:H2'	50:0:1929:G:O4'	2.20	0.42
52:2:1249:C:O5'	52:2:1249:C:O2	2.37	0.42
4:D:21:ASN:ND2	4:D:21:ASN:C	2.73	0.42
50:0:1918:A:O2'	50:0:1920:C:N4	2.52	0.42
50:0:2593:U:C2	50:0:2594:C:C5	3.07	0.42
52:2:662:U:O2'	52:2:836:G:OP1	2.37	0.42
52:2:1452:C:O2'	52:2:1453:G:OP2	2.22	0.42
6:F:114:GLU:OE1	6:F:114:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:57:VAL:O	8:H:58:LEU:HD12	2.19	0.42
52:2:179:A:H2'	52:2:180:U:O4'	2.19	0.42
8:H:73:ASP:OD1	8:H:73:ASP:C	2.58	0.41
7:G:30:THR:HG21	50:0:1005:C:O2'	2.18	0.41
9:I:5:THR:O	9:I:5:THR:CG2	2.68	0.41
10:J:129:THR:HG22	10:J:130:PHE:N	2.35	0.41
19:S:2:PHE:HB2	19:S:61:LEU:HD22	2.03	0.41
52:2:352:C:O2'	52:2:354:G:OP1	2.30	0.41
1:A:50:THR:HG23	50:0:1805:A:N3	2.35	0.41
8:H:104:THR:HG22	8:H:105:ARG:N	2.35	0.41
52:2:674:G:H2'	52:2:675:A:H8	1.85	0.41
52:2:1071:C:H2'	52:2:1072:G:H8	1.85	0.41
52:2:1347:G:O2'	52:2:1348:U:OP2	2.39	0.41
4:D:72:LYS:HG3	4:D:73:SER:N	2.35	0.41
50:0:1111:A:C2'	50:0:1112:G:OP2	2.67	0.41
50:0:2308:G:N3	50:0:2308:G:H2'	2.36	0.41
50:0:2502:G:H5'	50:0:2503:A:H5''	2.01	0.41
21:U:43:GLU:OE1	21:U:43:GLU:N	2.53	0.41
24:X:26:SER:OG	24:X:27:THR:N	2.54	0.41
50:0:1791:A:C2	50:0:1829:A:H4'	2.55	0.41
52:2:518:C:O2	52:2:518:C:O4'	2.36	0.41
4:D:23:ASN:O	4:D:23:ASN:OD1	2.39	0.41
4:D:140:GLU:HA	24:X:28:VAL:HG22	2.02	0.41
50:0:1781:U:O2	50:0:1781:U:O4'	2.37	0.41
50:0:1790:C:H2'	50:0:1791:A:C8	2.55	0.41
52:2:83:C:O2'	52:2:84:U:OP1	2.36	0.41
52:2:413:G:H2'	52:2:428:G:N2	2.35	0.41
52:2:1327:C:C2	52:2:1328:C:C5	3.08	0.41
50:0:27:G:H22	50:0:512:G:H1'	1.84	0.41
50:0:1046:A:H3'	50:0:1047:G:C5'	2.50	0.41
52:2:960:U:C4'	52:2:961:U:OP2	2.69	0.41
11:K:30:ARG:HG3	11:K:30:ARG:NH1	2.36	0.41
3:C:14:VAL:HG12	3:C:15:SER:N	2.36	0.41
5:E:75:MET:O	5:E:79:VAL:HG23	2.21	0.41
10:J:24:THR:HG22	10:J:99:GLY:O	2.21	0.41
50:0:301:G:O2'	50:0:302:C:P	2.79	0.41
52:2:813:U:O2	52:2:813:U:O4'	2.38	0.41
52:2:1218:C:H2'	52:2:1219:A:C8	2.55	0.41
52:2:1323:G:H2'	52:2:1324:A:C8	2.56	0.41
54:4:14:G:N2	54:4:48:C:H42	2.19	0.41
6:F:12:LEU:HD12	6:F:19:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:0:2100:G:C6	50:0:2101:A:N6	2.89	0.40
52:2:79:G:C2	52:2:80:A:N6	2.89	0.40
52:2:406:G:C8	52:2:495:A:C2	3.09	0.40
52:2:1492:A:O2'	52:2:1493:A:O4'	2.27	0.40
1:A:31:ALA:HB3	1:A:32:PRO:HD3	2.04	0.40
6:F:76:GLU:O	6:F:143:ILE:HG22	2.20	0.40
8:H:10:VAL:HG12	8:H:12:ASP:OD1	2.22	0.40
15:O:27:ILE:HD13	15:O:33:VAL:HG22	2.02	0.40
50:0:856:G:H2'	50:0:857:G:C8	2.57	0.40
52:2:333:U:C2	52:2:334:C:C5	3.09	0.40
3:C:163:ASN:ND2	50:0:320:A:N3	2.69	0.40
5:E:79:VAL:O	5:E:79:VAL:HG12	2.21	0.40
50:0:1360:G:N7	50:0:1361:G:C8	2.90	0.40
52:2:1144:G:N2	52:2:1146:A:H62	2.20	0.40
52:2:1307:U:O5'	52:2:1307:U:O2	2.39	0.40
1:A:263:THR:O	1:A:263:THR:CG2	2.69	0.40
52:2:602:A:H2'	52:2:603:U:C6	2.57	0.40
54:4:22:G:O2'	54:4:23:C:P	2.79	0.40
50:0:2329:U:H2'	50:0:2330:G:C8	2.57	0.40
52:2:639:G:C2	52:2:640:A:N7	2.89	0.40
52:2:1340:A:O2'	54:4:31:G:O3'	2.38	0.40

There are no symmetry-related clashes.

## 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	A	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
2	B	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
3	C	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
4	D	175/179 (98%)	163 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	171/177 (97%)	162 (95%)	9 (5%)	0	100	100
6	F	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
7	G	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
8	H	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
9	I	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
10	J	134/136 (98%)	118 (88%)	16 (12%)	0	100	100
11	K	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
12	L	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
13	M	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
14	N	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
15	O	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
16	P	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
17	Q	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
18	R	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
19	S	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
20	T	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
21	U	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
22	V	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
23	W	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
24	X	56/70 (80%)	50 (89%)	6 (11%)	0	100	100
25	a	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
26	b	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
27	c	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
28	d	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9	28
29	e	36/38 (95%)	36 (100%)	0	0	100	100
30	f	222/241 (92%)	200 (90%)	22 (10%)	0	100	100
31	g	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
32	h	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
33	i	153/167 (92%)	147 (96%)	6 (4%)	0	100	100
34	j	104/131 (79%)	100 (96%)	4 (4%)	0	100	100
35	k	149/179 (83%)	144 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	l	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
37	m	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
38	n	97/103 (94%)	91 (94%)	6 (6%)	0	100	100
39	o	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
40	p	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
41	q	112/118 (95%)	97 (87%)	15 (13%)	0	100	100
42	r	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
43	s	86/89 (97%)	86 (100%)	0	0	100	100
44	t	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
45	u	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
46	v	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
47	w	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
48	x	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
49	y	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
All	All	5581/5909 (94%)	5310 (95%)	270 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	d	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	
1	A	216/218 (99%)	216 (100%)	0	100	100
2	B	164/164 (100%)	164 (100%)	0	100	100
3	C	165/165 (100%)	165 (100%)	0	100	100
4	D	148/150 (99%)	147 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	134/138 (97%)	134 (100%)	0	100	100
6	F	114/114 (100%)	113 (99%)	1 (1%)	78	92
7	G	116/116 (100%)	116 (100%)	0	100	100
8	H	104/104 (100%)	104 (100%)	0	100	100
9	I	103/103 (100%)	103 (100%)	0	100	100
10	J	109/109 (100%)	109 (100%)	0	100	100
11	K	98/103 (95%)	98 (100%)	0	100	100
12	L	86/87 (99%)	86 (100%)	0	100	100
13	M	99/100 (99%)	99 (100%)	0	100	100
14	N	89/90 (99%)	89 (100%)	0	100	100
15	O	84/84 (100%)	84 (100%)	0	100	100
16	P	93/93 (100%)	93 (100%)	0	100	100
17	Q	80/84 (95%)	80 (100%)	0	100	100
18	R	83/85 (98%)	83 (100%)	0	100	100
19	S	78/78 (100%)	78 (100%)	0	100	100
20	T	57/63 (90%)	57 (100%)	0	100	100
21	U	67/68 (98%)	67 (100%)	0	100	100
22	V	54/55 (98%)	54 (100%)	0	100	100
23	W	47/49 (96%)	47 (100%)	0	100	100
24	X	55/62 (89%)	55 (100%)	0	100	100
25	a	46/48 (96%)	46 (100%)	0	100	100
26	b	46/49 (94%)	45 (98%)	1 (2%)	52	79
27	c	38/38 (100%)	38 (100%)	0	100	100
28	d	51/52 (98%)	51 (100%)	0	100	100
29	e	34/34 (100%)	34 (100%)	0	100	100
30	f	186/199 (94%)	185 (100%)	1 (0%)	88	96
31	g	170/190 (90%)	170 (100%)	0	100	100
32	h	172/173 (99%)	172 (100%)	0	100	100
33	i	118/126 (94%)	118 (100%)	0	100	100
34	j	92/112 (82%)	92 (100%)	0	100	100
35	k	124/147 (84%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	l	104/105 (99%)	104 (100%)	0	100	100
37	m	105/107 (98%)	104 (99%)	1 (1%)	76	91
38	n	87/90 (97%)	87 (100%)	0	100	100
39	o	90/99 (91%)	90 (100%)	0	100	100
40	p	103/104 (99%)	103 (100%)	0	100	100
41	q	92/96 (96%)	92 (100%)	0	100	100
42	r	83/84 (99%)	83 (100%)	0	100	100
43	s	76/77 (99%)	76 (100%)	0	100	100
44	t	65/65 (100%)	65 (100%)	0	100	100
45	u	74/78 (95%)	74 (100%)	0	100	100
46	v	57/65 (88%)	57 (100%)	0	100	100
47	w	70/79 (89%)	69 (99%)	1 (1%)	67	86
48	x	65/66 (98%)	64 (98%)	1 (2%)	65	86
49	y	60/61 (98%)	60 (100%)	0	100	100
56	6	1/1 (100%)	1 (100%)	0	100	100
All	All	4652/4827 (96%)	4645 (100%)	7 (0%)	93	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	21	ASN
6	F	41	LYS
26	b	28	ARG
30	f	7	ARG
37	m	123	ARG
47	w	6	LYS
48	x	21	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
38	n	35	GLN
45	u	50	ASN
47	w	52	HIS
48	x	20	HIS
48	x	82	GLN

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	0	2754/2904 (94%)	351 (12%)	8 (0%)
51	1	119/120 (99%)	11 (9%)	0
52	2	1533/1542 (99%)	287 (18%)	53 (3%)
53	3	8/30 (26%)	2 (25%)	0
54	4	76/77 (98%)	16 (21%)	2 (2%)
55	5	74/76 (97%)	10 (13%)	2 (2%)
All	All	4564/4749 (96%)	677 (14%)	65 (1%)

All (677) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	0	12	U
50	0	13	A
50	0	34	U
50	0	35	G
50	0	46	G
50	0	63	A
50	0	71	A
50	0	74	A
50	0	75	G
50	0	84	A
50	0	99	U
50	0	101	A
50	0	102	U
50	0	103	A
50	0	118	A
50	0	120	U
50	0	135	U
50	0	139	U
50	0	140	C
50	0	163	C
50	0	166	U
50	0	167	A
50	0	175	G
50	0	181	A
50	0	196	A
50	0	199	A
50	0	201	C
50	0	215	G
50	0	216	A
50	0	221	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	222	A
50	0	228	C
50	0	233	A
50	0	248	G
50	0	249	C
50	0	266	G
50	0	272	A
50	0	275	C
50	0	277	G
50	0	280	U
50	0	281	C
50	0	302	C
50	0	304	U
50	0	311	A
50	0	323	C
50	0	329	G
50	0	330	A
50	0	361	G
50	0	362	A
50	0	372	G
50	0	385	C
50	0	386	G
50	0	396	G
50	0	404	A
50	0	405	U
50	0	411	G
50	0	412	A
50	0	416	U
50	0	420	C
50	0	424	G
50	0	429	A
50	0	449	A
50	0	467	G
50	0	481	G
50	0	491	G
50	0	494	G
50	0	498	G
50	0	505	A
50	0	508	A
50	0	509	C
50	0	510	C
50	0	530	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	531	C
50	0	532	A
50	0	534	U
50	0	538	A
50	0	547	A
50	0	548	G
50	0	549	G
50	0	557	C
50	0	563	A
50	0	572	A
50	0	573	U
50	0	574	A
50	0	575	A
50	0	585	G
50	0	586	A
50	0	603	A
50	0	613	A
50	0	614	A
50	0	615	U
50	0	632	A
50	0	637	A
50	0	645	C
50	0	647	G
50	0	686	U
50	0	730	A
50	0	736	C
50	0	747	U
50	0	764	A
50	0	770	G
50	0	775	G
50	0	776	G
50	0	782	A
50	0	784	G
50	0	785	G
50	0	792	A
50	0	805	G
50	0	812	C
50	0	813	U
50	0	827	U
50	0	828	U
50	0	846	U
50	0	859	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	878	A
50	0	881	G
50	0	895	U
50	0	896	A
50	0	898	C
50	0	910	A
50	0	914	G
50	0	915	C
50	0	930	G
50	0	931	U
50	0	934	U
50	0	946	C
50	0	959	A
50	0	961	C
50	0	974	G
50	0	983	A
50	0	996	A
50	0	997	G
50	0	1009	A
50	0	1012	U
50	0	1013	C
50	0	1022	G
50	0	1026	G
50	0	1027	A
50	0	1030	C
50	0	1033	U
50	0	1034	G
50	0	1045	C
50	0	1046	A
50	0	1047	G
50	0	1110	G
50	0	1111	A
50	0	1112	G
50	0	1132	U
50	0	1133	A
50	0	1135	C
50	0	1136	G
50	0	1142	A
50	0	1172	C
50	0	1173	U
50	0	1174	U
50	0	1176	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	1194	A
50	0	1206	G
50	0	1212	G
50	0	1238	G
50	0	1250	G
50	0	1253	A
50	0	1256	G
50	0	1257	C
50	0	1271	G
50	0	1272	A
50	0	1274	A
50	0	1286	A
50	0	1294	U
50	0	1300	G
50	0	1301	A
50	0	1342	A
50	0	1345	C
50	0	1364	G
50	0	1365	A
50	0	1379	U
50	0	1395	A
50	0	1412	U
50	0	1416	G
50	0	1417	C
50	0	1424	G
50	0	1428	C
50	0	1435	G
50	0	1452	G
50	0	1455	G
50	0	1482	G
50	0	1490	A
50	0	1493	C
50	0	1497	U
50	0	1509	A
50	0	1510	G
50	0	1515	A
50	0	1569	A
50	0	1583	A
50	0	1584	U
50	0	1585	C
50	0	1608	A
50	0	1616	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	1618	A
50	0	1647	U
50	0	1648	U
50	0	1654	A
50	0	1663	G
50	0	1674	G
50	0	1678	A
50	0	1715	G
50	0	1729	U
50	0	1730	C
50	0	1733	G
50	0	1737	G
50	0	1738	G
50	0	1750	G
50	0	1756	G
50	0	1758	U
50	0	1764	C
50	0	1773	A
50	0	1780	A
50	0	1800	C
50	0	1801	A
50	0	1808	A
50	0	1811	G
50	0	1816	C
50	0	1829	A
50	0	1830	C
50	0	1848	A
50	0	1868	C
50	0	1872	A
50	0	1873	G
50	0	1906	G
50	0	1913	A
50	0	1917	U
50	0	1919	A
50	0	1929	G
50	0	1930	G
50	0	1934	C
50	0	1937	A
50	0	1938	A
50	0	1942	C
50	0	1955	U
50	0	1964	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	1967	C
50	0	1970	A
50	0	1971	U
50	0	1972	G
50	0	1991	U
50	0	1993	U
50	0	1997	C
50	0	2006	C
50	0	2017	U
50	0	2023	C
50	0	2031	A
50	0	2033	A
50	0	2034	U
50	0	2043	C
50	0	2055	C
50	0	2056	G
50	0	2060	A
50	0	2061	G
50	0	2069	G
50	0	2187	U
50	0	2190	G
50	0	2194	U
50	0	2198	A
50	0	2204	G
50	0	2212	A
50	0	2225	A
50	0	2238	G
50	0	2239	G
50	0	2251	G
50	0	2283	C
50	0	2287	A
50	0	2288	A
50	0	2297	A
50	0	2300	C
50	0	2305	U
50	0	2306	C
50	0	2307	G
50	0	2308	G
50	0	2309	A
50	0	2310	C
50	0	2312	U
50	0	2322	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	2325	G
50	0	2333	A
50	0	2345	G
50	0	2347	C
50	0	2383	G
50	0	2385	C
50	0	2390	U
50	0	2396	G
50	0	2402	U
50	0	2406	A
50	0	2419	U
50	0	2425	A
50	0	2429	G
50	0	2430	A
50	0	2441	U
50	0	2448	A
50	0	2464	G
50	0	2470	G
50	0	2475	C
50	0	2476	A
50	0	2478	A
50	0	2491	U
50	0	2492	U
50	0	2498	C
50	0	2502	G
50	0	2503	A
50	0	2504	U
50	0	2505	G
50	0	2506	U
50	0	2507	C
50	0	2518	A
50	0	2520	C
50	0	2529	G
50	0	2547	A
50	0	2566	A
50	0	2567	G
50	0	2573	C
50	0	2582	G
50	0	2600	A
50	0	2602	A
50	0	2603	G
50	0	2609	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	2613	U
50	0	2629	U
50	0	2630	G
50	0	2646	C
50	0	2661	G
50	0	2689	U
50	0	2690	U
50	0	2693	G
50	0	2714	G
50	0	2726	A
50	0	2733	A
50	0	2752	C
50	0	2778	A
50	0	2820	A
50	0	2832	U
50	0	2835	A
50	0	2849	U
50	0	2861	U
50	0	2867	G
50	0	2873	A
50	0	2880	C
50	0	2884	U
50	0	2885	G
50	0	2886	A
50	0	2887	A
50	0	2894	G
50	0	2903	U
51	1	24	G
51	1	30	C
51	1	35	C
51	1	41	G
51	1	42	C
51	1	44	G
51	1	89	U
51	1	90	C
51	1	105	G
51	1	108	A
51	1	109	A
52	2	6	G
52	2	9	G
52	2	22	G
52	2	31	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	32	A
52	2	39	G
52	2	47	C
52	2	48	C
52	2	51	A
52	2	65	A
52	2	77	A
52	2	81	A
52	2	84	U
52	2	85	U
52	2	86	G
52	2	87	C
52	2	90	C
52	2	91	U
52	2	93	U
52	2	104	G
52	2	108	G
52	2	112	G
52	2	120	A
52	2	121	U
52	2	122	G
52	2	127	G
52	2	131	A
52	2	144	G
52	2	156	C
52	2	164	G
52	2	168	G
52	2	171	A
52	2	173	U
52	2	174	A
52	2	178	C
52	2	183	C
52	2	184	G
52	2	188	C
52	2	189	A
52	2	195	A
52	2	197	A
52	2	199	A
52	2	209	U
52	2	210	C
52	2	211	G
52	2	212	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	214	C
52	2	240	G
52	2	245	U
52	2	247	G
52	2	251	G
52	2	252	U
52	2	253	A
52	2	263	A
52	2	266	G
52	2	267	C
52	2	280	C
52	2	282	A
52	2	283	U
52	2	289	G
52	2	316	C
52	2	321	A
52	2	326	G
52	2	327	A
52	2	328	C
52	2	332	G
52	2	343	U
52	2	346	G
52	2	348	G
52	2	352	C
52	2	354	G
52	2	365	U
52	2	367	U
52	2	372	C
52	2	382	A
52	2	406	G
52	2	409	U
52	2	412	A
52	2	413	G
52	2	422	C
52	2	423	G
52	2	429	U
52	2	439	U
52	2	440	C
52	2	449	G
52	2	460	A
52	2	463	U
52	2	464	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	468	A
52	2	481	G
52	2	484	G
52	2	495	A
52	2	496	A
52	2	497	G
52	2	511	C
52	2	512	U
52	2	518	C
52	2	531	U
52	2	547	A
52	2	548	G
52	2	559	A
52	2	560	A
52	2	564	C
52	2	565	U
52	2	567	G
52	2	572	A
52	2	573	A
52	2	576	C
52	2	577	G
52	2	583	A
52	2	587	G
52	2	603	U
52	2	612	C
52	2	623	C
52	2	653	U
52	2	665	A
52	2	687	A
52	2	698	G
52	2	703	G
52	2	704	A
52	2	718	A
52	2	722	G
52	2	723	U
52	2	724	G
52	2	742	G
52	2	755	G
52	2	761	G
52	2	777	A
52	2	793	U
52	2	794	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	802	A
52	2	811	C
52	2	813	U
52	2	815	A
52	2	817	C
52	2	821	G
52	2	838	G
52	2	840	C
52	2	842	U
52	2	843	U
52	2	845	A
52	2	847	G
52	2	872	A
52	2	885	G
52	2	889	A
52	2	890	G
52	2	891	U
52	2	914	A
52	2	927	G
52	2	934	C
52	2	935	A
52	2	936	C
52	2	942	G
52	2	955	U
52	2	960	U
52	2	961	U
52	2	965	U
52	2	966	G
52	2	969	A
52	2	971	G
52	2	972	C
52	2	975	A
52	2	976	G
52	2	977	A
52	2	978	A
52	2	983	A
52	2	984	C
52	2	992	U
52	2	993	G
52	2	1004	A
52	2	1005	A
52	2	1006	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1007	U
52	2	1012	A
52	2	1019	A
52	2	1024	G
52	2	1025	U
52	2	1026	G
52	2	1030	U
52	2	1032	G
52	2	1033	G
52	2	1034	G
52	2	1035	A
52	2	1036	A
52	2	1041	G
52	2	1043	G
52	2	1044	A
52	2	1053	G
52	2	1054	C
52	2	1060	U
52	2	1064	G
52	2	1065	U
52	2	1066	C
52	2	1079	G
52	2	1094	G
52	2	1095	U
52	2	1101	A
52	2	1102	A
52	2	1110	A
52	2	1118	U
52	2	1126	U
52	2	1130	A
52	2	1136	C
52	2	1137	C
52	2	1138	G
52	2	1139	G
52	2	1149	C
52	2	1152	A
52	2	1158	C
52	2	1159	U
52	2	1160	G
52	2	1165	U
52	2	1168	U
52	2	1169	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1170	A
52	2	1181	G
52	2	1183	U
52	2	1184	G
52	2	1185	G
52	2	1191	A
52	2	1196	A
52	2	1197	A
52	2	1202	U
52	2	1212	U
52	2	1213	A
52	2	1227	A
52	2	1228	C
52	2	1231	G
52	2	1236	A
52	2	1238	A
52	2	1240	U
52	2	1241	G
52	2	1256	A
52	2	1257	A
52	2	1268	G
52	2	1273	C
52	2	1279	G
52	2	1280	A
52	2	1286	U
52	2	1287	A
52	2	1297	G
52	2	1300	G
52	2	1306	A
52	2	1307	U
52	2	1317	C
52	2	1318	A
52	2	1320	C
52	2	1321	U
52	2	1322	C
52	2	1331	G
52	2	1336	C
52	2	1337	G
52	2	1338	G
52	2	1346	A
52	2	1347	G
52	2	1348	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1350	A
52	2	1363	A
52	2	1365	G
52	2	1370	G
52	2	1374	A
52	2	1386	G
52	2	1394	A
52	2	1398	A
52	2	1400	C
52	2	1402	C
52	2	1425	U
52	2	1441	A
52	2	1442	G
52	2	1446	A
52	2	1450	U
52	2	1451	U
52	2	1452	C
52	2	1453	G
52	2	1458	G
52	2	1480	A
52	2	1487	G
52	2	1492	A
52	2	1494	G
52	2	1497	G
52	2	1499	A
52	2	1503	A
52	2	1504	G
52	2	1506	U
52	2	1517	G
52	2	1529	G
52	2	1530	G
53	3	16	A
53	3	18	G
54	4	8	G
54	4	11	G
54	4	15	C
54	4	16	C
54	4	18	G
54	4	19	G
54	4	21	A
54	4	22	G
54	4	23	C

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Mol	Chain	Res	Type
54	4	26	G
54	4	30	G
54	4	39	C
54	4	44	A
54	4	55	U
54	4	68	C
54	4	76	A
55	5	5	C
55	5	13	C
55	5	14	A
55	5	16	H2U
55	5	17	H2U
55	5	20	H2U
55	5	46	G
55	5	57	G
55	5	62	C
55	5	74	C

All (65) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	0	546	U
50	0	895	U
50	0	960	A
50	0	1026	G
50	0	1111	A
50	0	1847	A
50	0	2193	G
50	0	2307	G
52	2	64	G
52	2	80	A
52	2	83	C
52	2	130	A
52	2	188	C
52	2	210	C
52	2	250	A
52	2	251	G
52	2	281	G
52	2	315	A
52	2	345	C
52	2	422	C
52	2	428	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	438	U
52	2	463	U
52	2	467	U
52	2	495	A
52	2	559	A
52	2	575	G
52	2	602	A
52	2	703	G
52	2	792	A
52	2	839	C
52	2	842	U
52	2	890	G
52	2	960	U
52	2	982	U
52	2	992	U
52	2	1003	G
52	2	1024	G
52	2	1031	C
52	2	1040	U
52	2	1053	G
52	2	1117	A
52	2	1125	U
52	2	1136	C
52	2	1137	C
52	2	1151	A
52	2	1157	A
52	2	1182	G
52	2	1183	U
52	2	1190	G
52	2	1201	A
52	2	1230	C
52	2	1317	C
52	2	1320	C
52	2	1337	G
52	2	1347	G
52	2	1364	U
52	2	1399	C
52	2	1440	U
52	2	1451	U
52	2	1452	C
54	4	10	A
54	4	14	G

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Mol	Chain	Res	Type
55	5	13	C
55	5	15	G

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

11 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
54	5MU	4	54	54	19,22,23	1.41	6 (31%)	28,32,35	2.05	6 (21%)
53	6MZ	3	19	53,55	18,25,26	1.83	6 (33%)	16,36,39	1.90	4 (25%)
54	OMC	4	32	54	19,22,23	0.87	2 (10%)	26,31,34	0.75	0
55	5MU	5	54	55	19,22,23	1.42	4 (21%)	28,32,35	2.16	7 (25%)
55	H2U	5	17	55	18,21,22	0.97	2 (11%)	21,30,33	1.40	3 (14%)
55	T6A	5	37	55	27,34,35	0.98	1 (3%)	29,49,52	2.73	8 (27%)
55	H2U	5	20	55	18,21,22	0.97	2 (11%)	21,30,33	1.37	3 (14%)
55	H2U	5	16	55	18,21,22	0.96	2 (11%)	21,30,33	1.34	3 (14%)
54	4SU	4	7	54	18,21,22	1.79	4 (22%)	26,30,33	2.22	5 (19%)
55	U8U	5	34	53,55	19,24,25	1.69	3 (15%)	23,34,37	1.13	2 (8%)
56	FME	6	1	56	8,9,10	1.01	1 (12%)	7,9,11	1.23	1 (14%)

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
54	5MU	4	54	54	-	0/7/25/26	0/2/2/2
53	6MZ	3	19	53,55	-	2/5/27/28	0/3/3/3
54	OMC	4	32	54	-	0/9/27/28	0/2/2/2
55	5MU	5	54	55	-	0/7/25/26	0/2/2/2
55	H2U	5	17	55	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	T6A	5	37	55	-	6/19/41/42	0/3/3/3
55	H2U	5	20	55	-	3/7/38/39	0/2/2/2
55	H2U	5	16	55	-	1/7/38/39	0/2/2/2
54	4SU	4	7	54	-	1/7/25/26	0/2/2/2
55	U8U	5	34	53,55	-	2/9/28/29	0/2/2/2
56	FME	6	1	56	-	3/7/9/11	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	5	34	U8U	C2-S2	-5.44	1.59	1.67
53	3	19	6MZ	C6-N6	5.06	1.43	1.35
54	4	7	4SU	C4-S4	-4.55	1.59	1.68
54	4	7	4SU	C4-N3	-3.48	1.33	1.37
55	5	54	5MU	C4-N3	-3.15	1.33	1.38
55	5	34	U8U	C4-N3	-3.02	1.33	1.38
54	4	7	4SU	C5-C4	-2.81	1.38	1.42
54	4	54	5MU	C4-N3	-2.73	1.33	1.38
54	4	54	5MU	C6-C5	2.72	1.39	1.34
53	3	19	6MZ	C5-C4	-2.70	1.33	1.40
55	5	54	5MU	C6-N1	-2.61	1.33	1.38
54	4	7	4SU	C2-N3	-2.58	1.33	1.38
55	5	54	5MU	C2-N3	-2.57	1.33	1.38
53	3	19	6MZ	C6-N1	-2.53	1.30	1.34
55	5	20	H2U	C2-N3	-2.47	1.33	1.38
55	5	17	H2U	C2-N3	-2.46	1.33	1.38
55	5	16	H2U	C2-N3	-2.44	1.33	1.38
53	3	19	6MZ	C9-N6	-2.40	1.41	1.45
53	3	19	6MZ	C4-N3	-2.34	1.32	1.35
54	4	54	5MU	C4-C5	2.24	1.48	1.44
55	5	34	U8U	C6-N1	-2.24	1.34	1.38
55	5	54	5MU	C6-C5	2.13	1.38	1.34
55	5	37	T6A	C12-C13	-2.13	1.49	1.52
54	4	32	OMC	C5-C4	-2.12	1.38	1.42
54	4	54	5MU	C2-N3	-2.12	1.34	1.38
56	6	1	FME	CA-N	-2.09	1.43	1.46
54	4	54	5MU	C2-N1	2.08	1.41	1.38
55	5	17	H2U	C4-N3	-2.08	1.34	1.37
54	4	54	5MU	C6-N1	-2.07	1.34	1.38
55	5	16	H2U	C4-N3	-2.07	1.34	1.37
54	4	32	OMC	C6-N1	-2.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	5	20	H2U	C4-N3	-2.06	1.34	1.37
53	3	19	6MZ	C5-N7	-2.05	1.32	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	5	37	T6A	N6-C10-N11	8.92	126.22	113.76
54	4	7	4SU	C4-N3-C2	-6.84	120.69	127.34
55	5	37	T6A	C2-N1-C6	5.93	121.68	116.59
55	5	37	T6A	N6-C6-N1	5.80	126.49	118.72
54	4	7	4SU	C5-C4-N3	5.64	119.92	114.69
55	5	54	5MU	C4-N3-C2	-5.45	120.30	127.35
53	3	19	6MZ	N3-C2-N1	-5.30	120.39	128.68
55	5	54	5MU	N3-C2-N1	5.25	121.85	114.89
54	4	54	5MU	C4-N3-C2	-5.16	120.67	127.35
54	4	54	5MU	N3-C2-N1	5.13	121.70	114.89
55	5	37	T6A	O10-C10-N6	-4.86	115.41	123.62
55	5	54	5MU	C5-C4-N3	4.76	119.37	115.31
54	4	54	5MU	C5-C4-N3	4.39	119.06	115.31
54	4	7	4SU	N3-C2-N1	4.33	120.63	114.89
55	5	17	H2U	C4-N3-C2	-4.19	122.32	125.79
54	4	7	4SU	C5-C4-S4	-4.15	119.12	124.47
55	5	20	H2U	C4-N3-C2	-4.13	122.36	125.79
55	5	16	H2U	C4-N3-C2	-3.99	122.48	125.79
55	5	54	5MU	O4-C4-C5	-3.83	120.46	124.90
54	4	54	5MU	O4-C4-C5	-3.74	120.57	124.90
54	4	54	5MU	C5-C6-N1	-3.71	119.52	123.34
53	3	19	6MZ	C2-N1-C6	3.67	119.73	116.59
55	5	54	5MU	C5-C6-N1	-3.63	119.60	123.34
55	5	34	U8U	O4-C4-C5	-3.56	119.67	124.96
55	5	37	T6A	N3-C2-N1	-3.53	123.17	128.68
55	5	37	T6A	C14-C12-C13	-3.18	104.77	110.19
55	5	34	U8U	C5-C4-N3	2.87	119.00	114.97
55	5	17	H2U	C5-C4-N3	2.83	119.83	116.65
55	5	16	H2U	C5-C4-N3	2.79	119.79	116.65
55	5	37	T6A	C4-C5-N7	-2.74	106.54	109.40
54	4	54	5MU	O2-C2-N1	-2.72	119.17	122.79
55	5	20	H2U	C5-C4-N3	2.71	119.69	116.65
53	3	19	6MZ	C1'-N9-C4	-2.68	121.94	126.64
56	6	1	FME	C-CA-N	2.66	114.52	109.73
55	5	54	5MU	O2-C2-N1	-2.39	119.60	122.79
55	5	37	T6A	O10-C10-N11	-2.34	118.35	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	5	54	5MU	C5M-C5-C4	2.31	121.31	118.77
54	4	7	4SU	O2-C2-N1	-2.29	119.74	122.79
55	5	20	H2U	C5-C6-N1	-2.25	104.22	111.61
55	5	17	H2U	C5-C6-N1	-2.16	104.51	111.61
53	3	19	6MZ	C9-N6-C6	-2.13	121.04	122.87
55	5	16	H2U	C5-C6-N1	-2.02	104.94	111.61

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	5	17	H2U	O4'-C1'-N1-C2
55	5	17	H2U	O4'-C1'-N1-C6
55	5	20	H2U	O4'-C1'-N1-C2
55	5	20	H2U	O4'-C1'-N1-C6
55	5	34	U8U	N-C-C5-C4
55	5	37	T6A	N11-C12-C14-O14
55	5	37	T6A	N11-C12-C14-C15
55	5	37	T6A	C13-C12-C14-O14
55	5	37	T6A	C13-C12-C14-C15
53	3	19	6MZ	N1-C6-N6-C9
56	6	1	FME	O1-CN-N-CA
56	6	1	FME	N-CA-CB-CG
55	5	37	T6A	C13-C12-N11-C10
56	6	1	FME	C-CA-CB-CG
55	5	20	H2U	C4'-C5'-O5'-P
55	5	37	T6A	C14-C12-N11-C10
55	5	16	H2U	C4'-C5'-O5'-P
54	4	7	4SU	O4'-C4'-C5'-O5'
53	3	19	6MZ	C5-C6-N6-C9
55	5	17	H2U	O4'-C4'-C5'-O5'
55	5	34	U8U	N-C-C5-C6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	5	37	T6A	1	0
55	5	16	H2U	1	0
54	4	7	4SU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

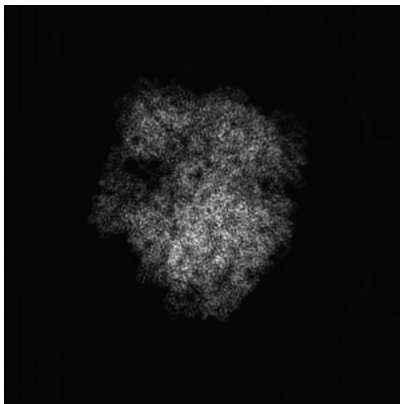
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16062. These allow visual inspection of the internal detail of the map and identification of artifacts.

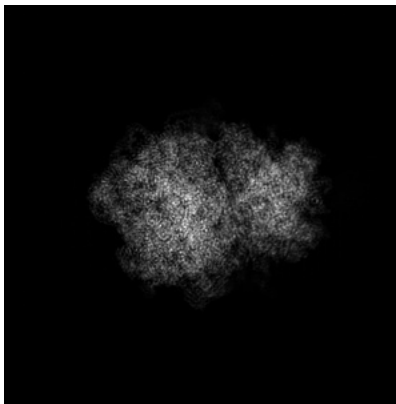
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

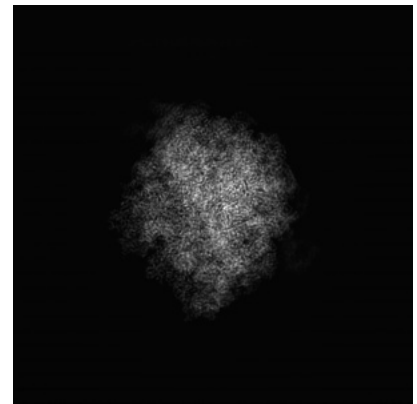
#### 6.1.1 Primary map



X

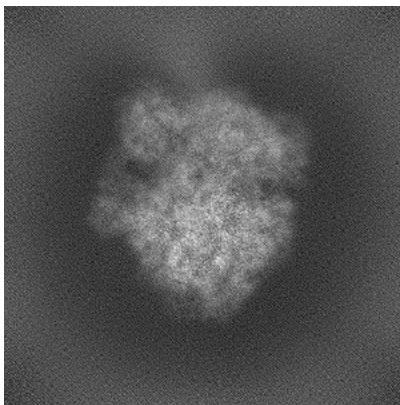


Y

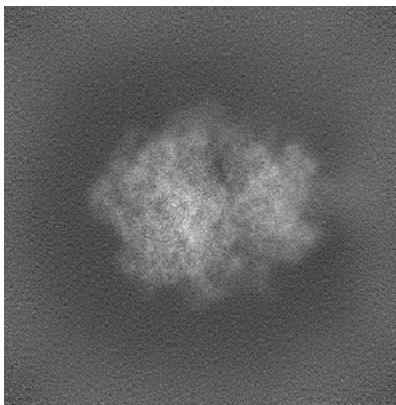


Z

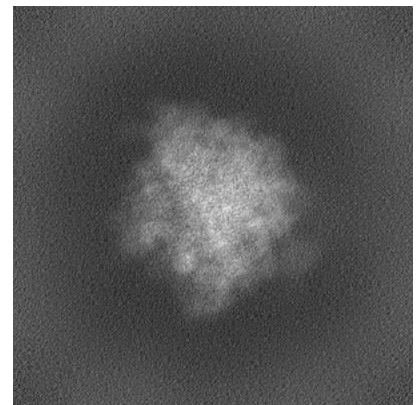
#### 6.1.2 Raw map



X



Y



Z

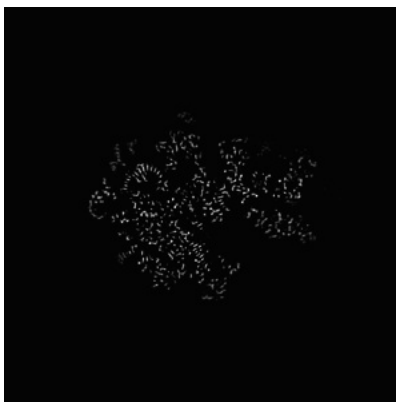
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 256

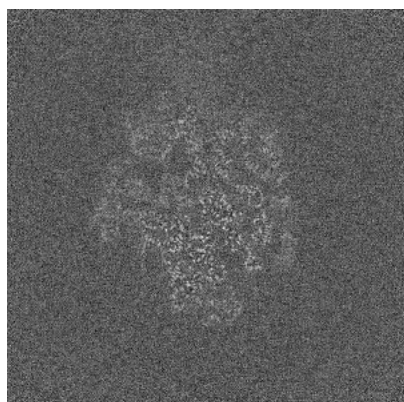


Y Index: 256

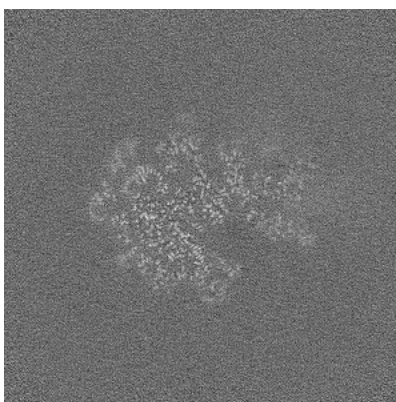


Z Index: 256

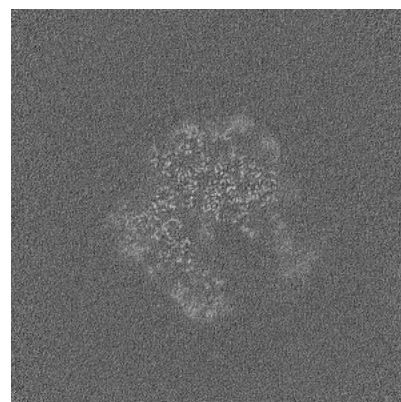
### 6.2.2 Raw map



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: 269

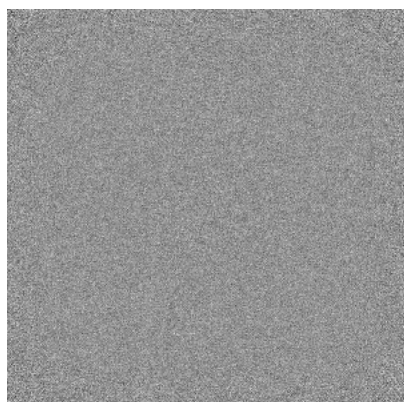


Y Index: 279

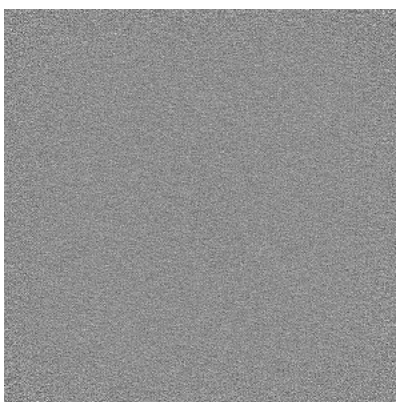


Z Index: 235

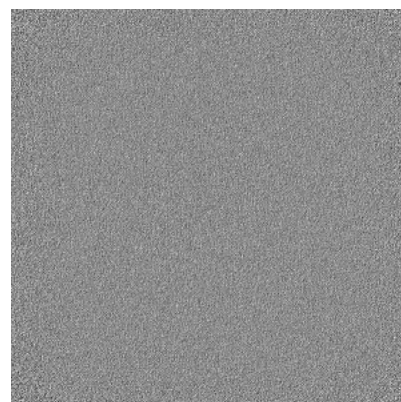
### 6.3.2 Raw map



X Index: 0



Y Index: 0

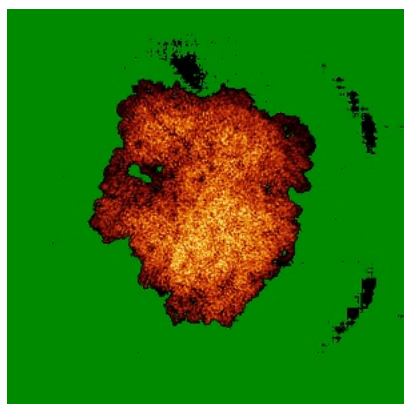


Z Index: 0

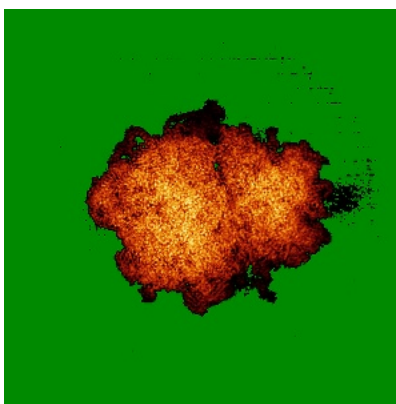
The images above show the largest variance slices of the map in three orthogonal directions.

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

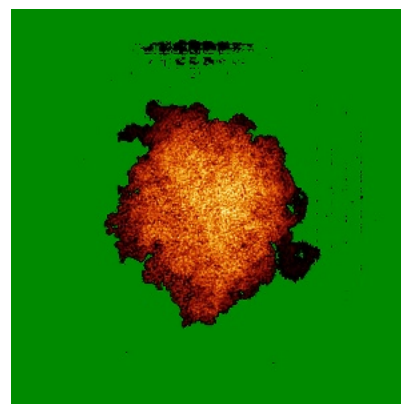
### 6.4.1 Primary map



X

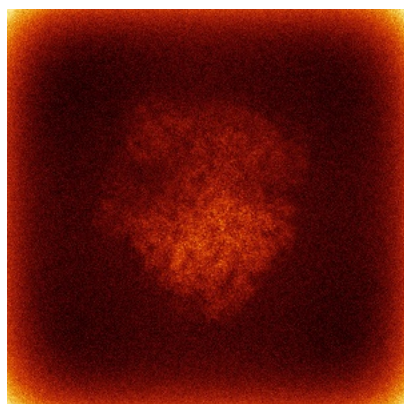


Y

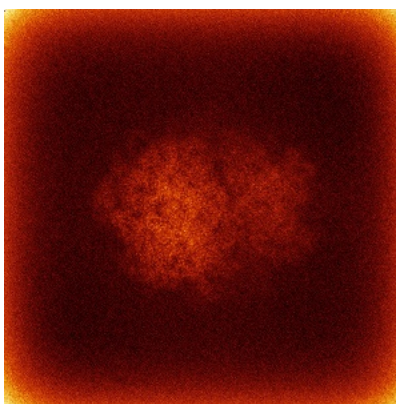


Z

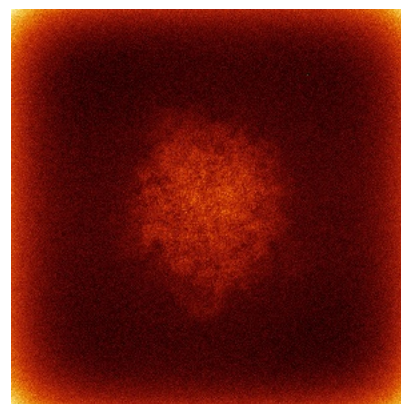
### 6.4.2 Raw map



X



Y

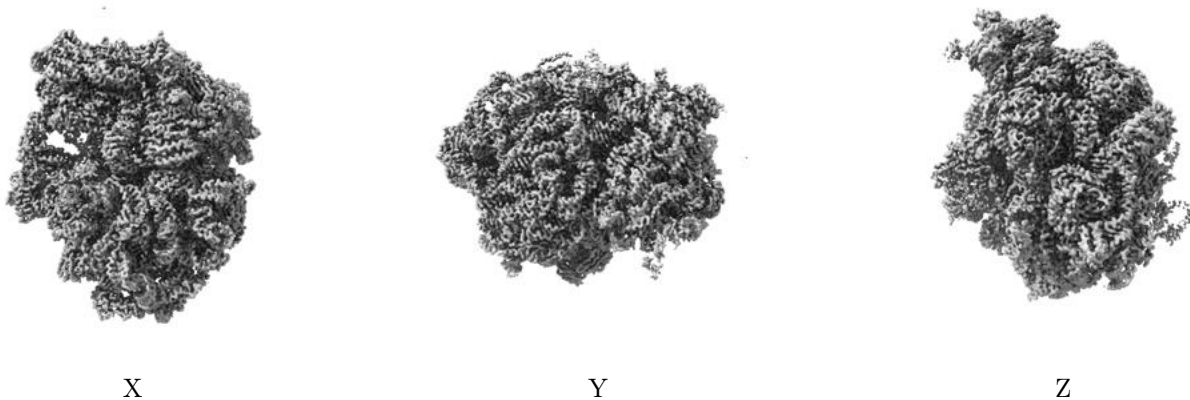


Z

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.

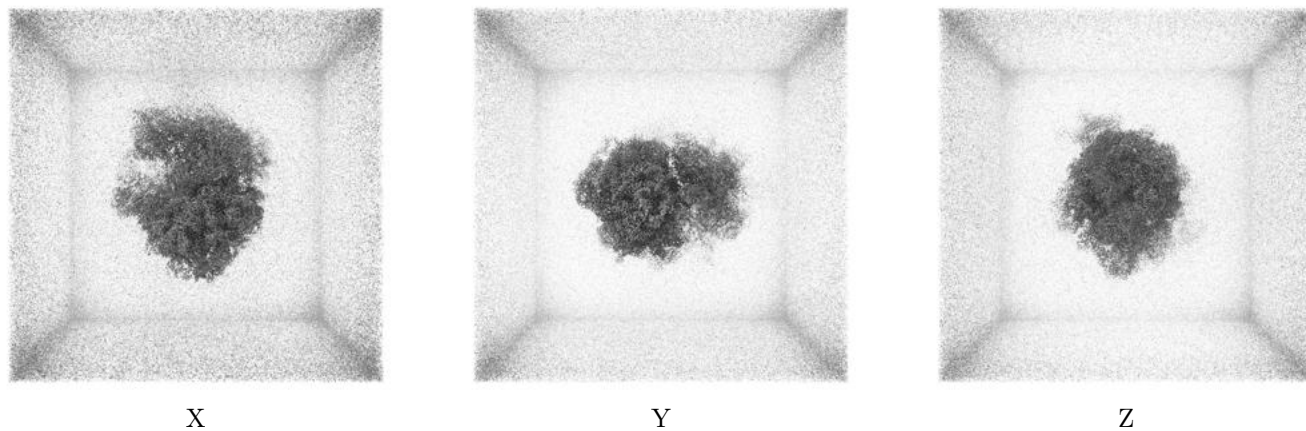
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.103. 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



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.



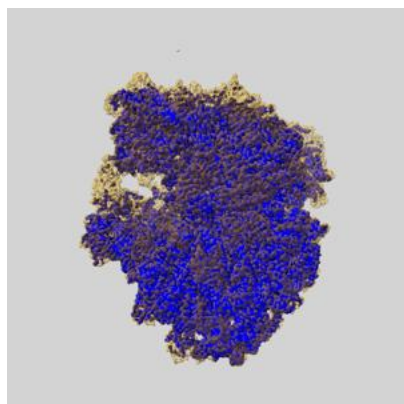
## 6.6 Mask visualisation [i](#)

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

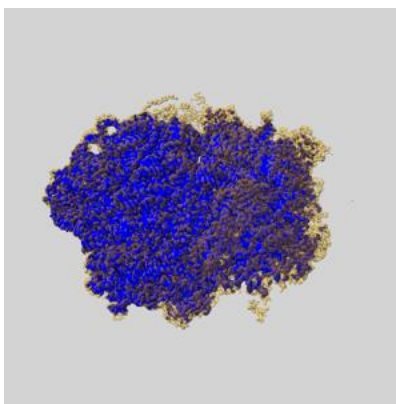
A mask typically either:

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

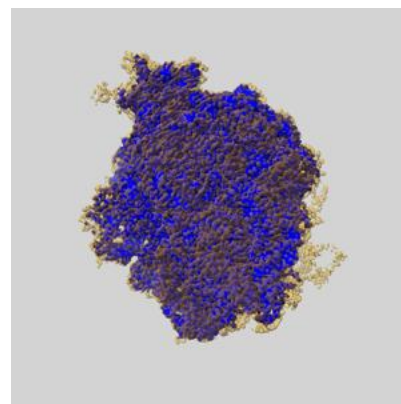
### 6.6.1 emd\_16062\_msk\_1.map [i](#)



X



Y

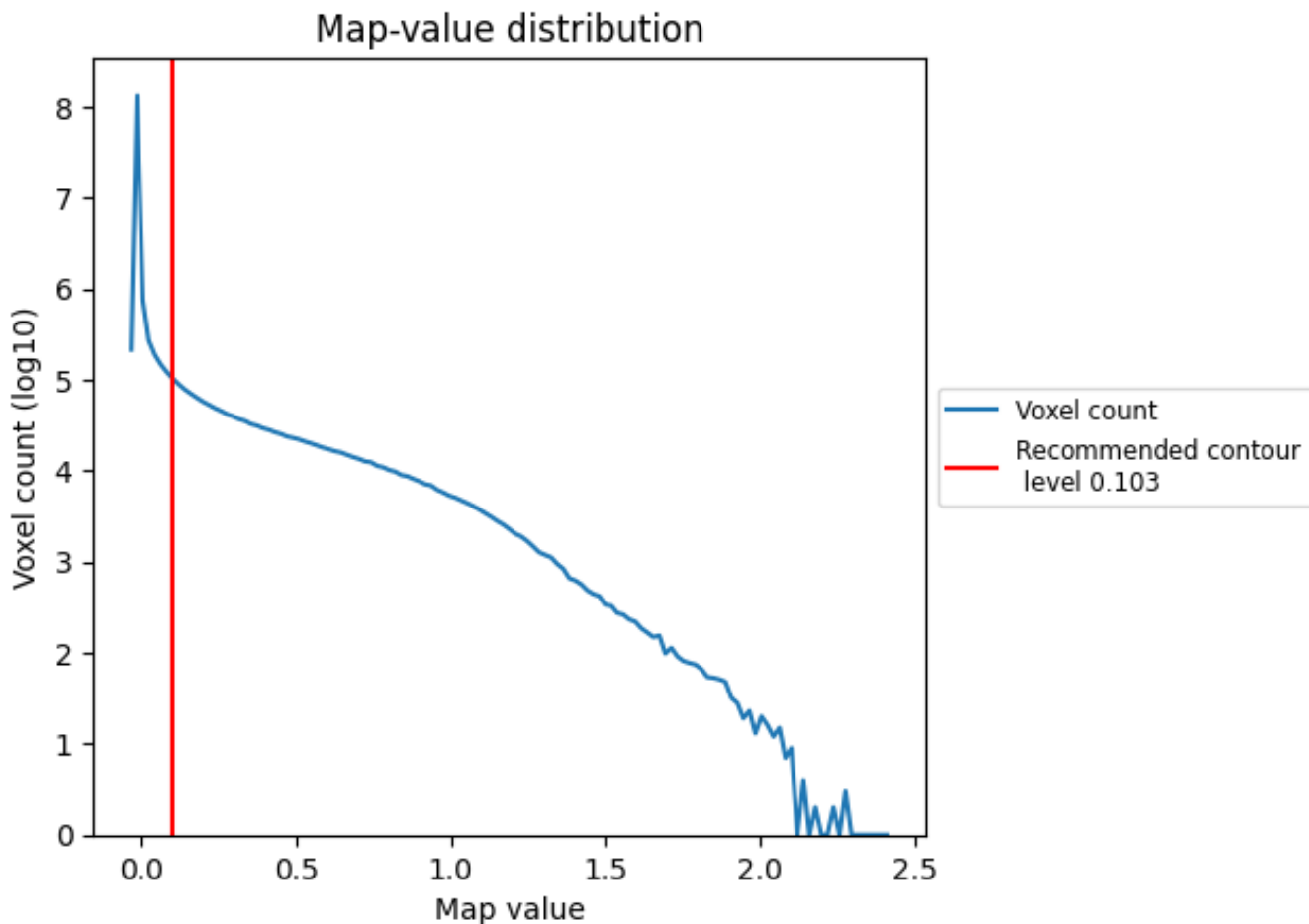


Z

## 7 Map analysis [i](#)

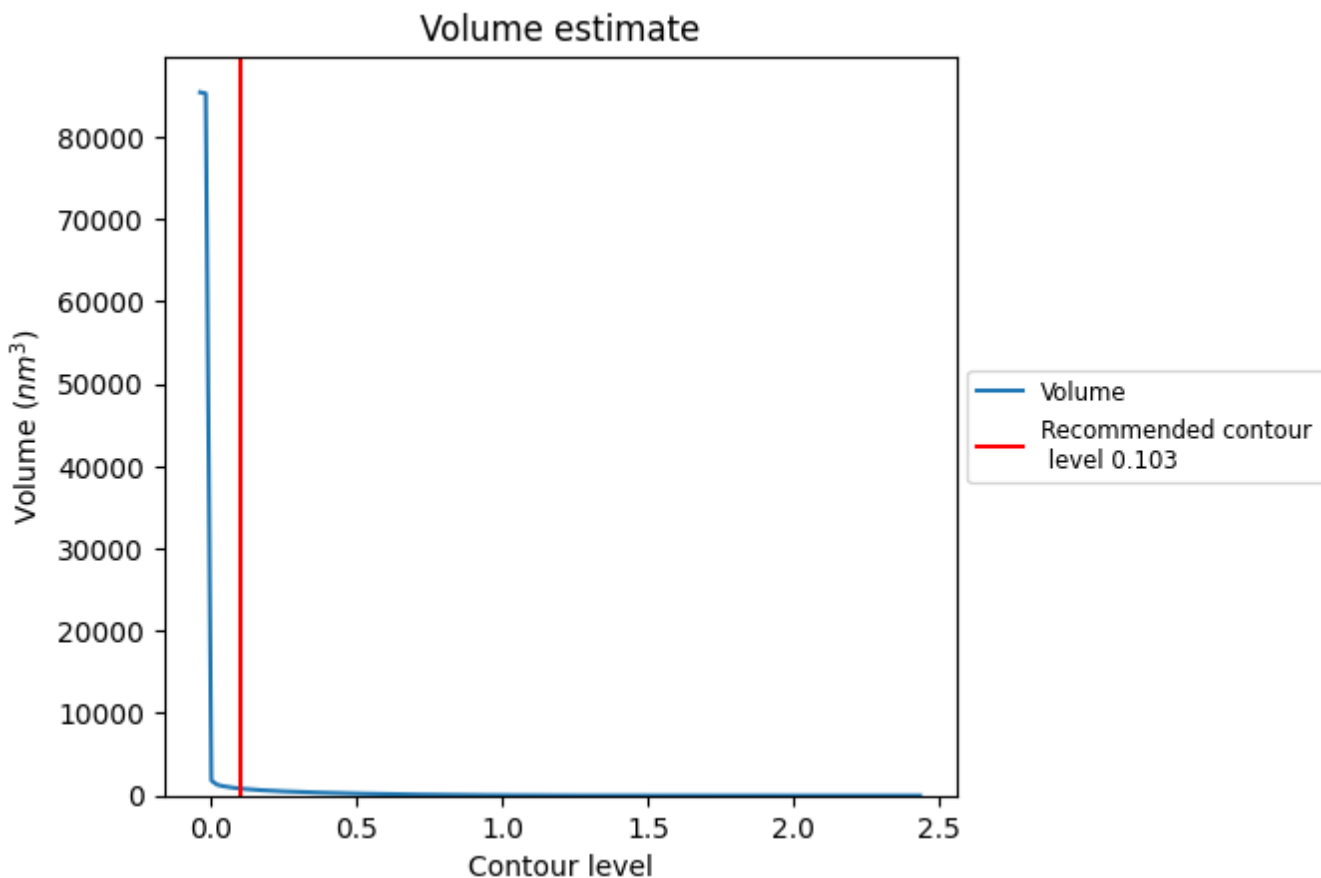
This section contains the results of statistical analysis of the map.

### 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.

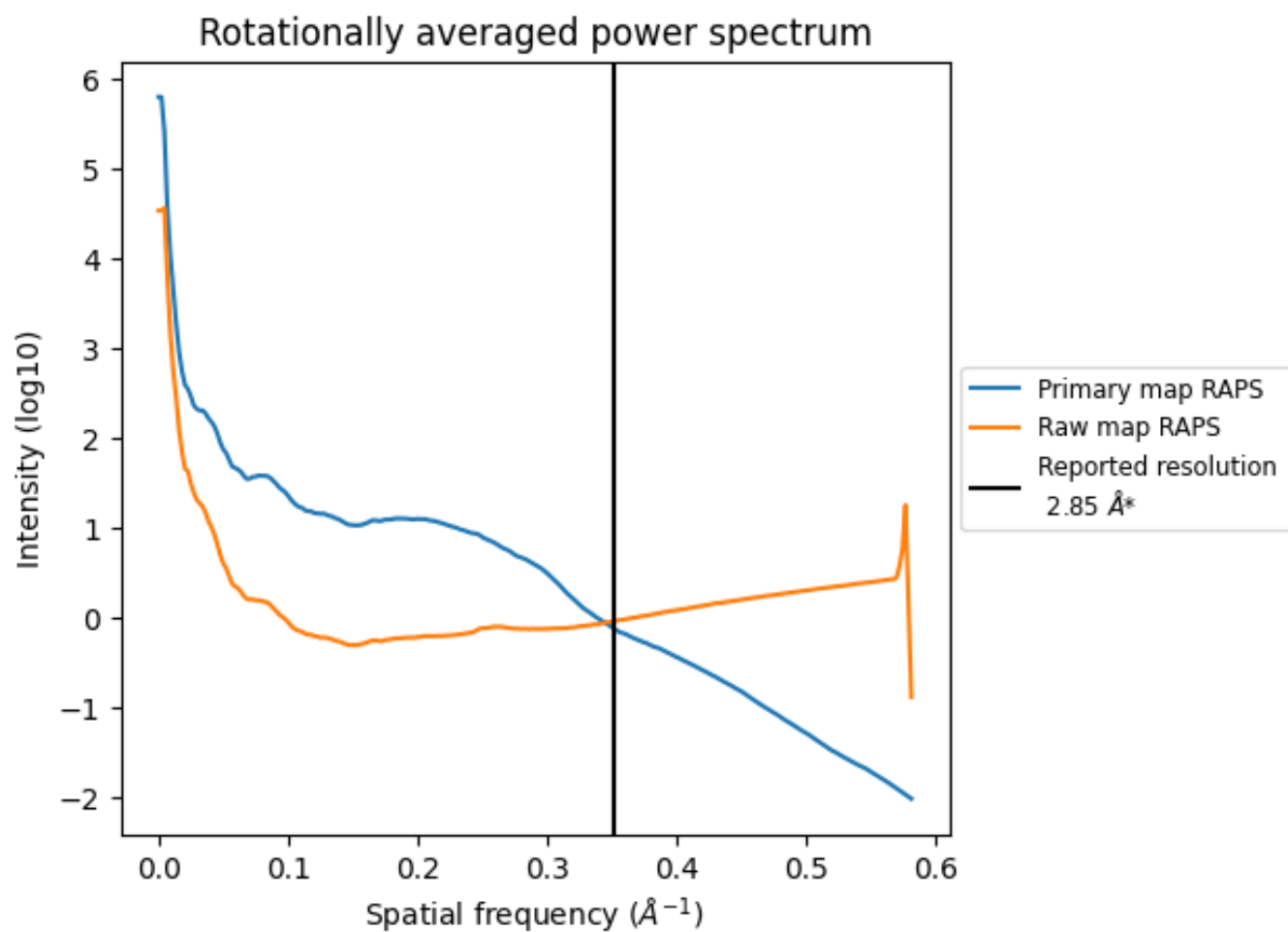
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 856  $\text{nm}^3$ ; this corresponds to an approximate mass of 773 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

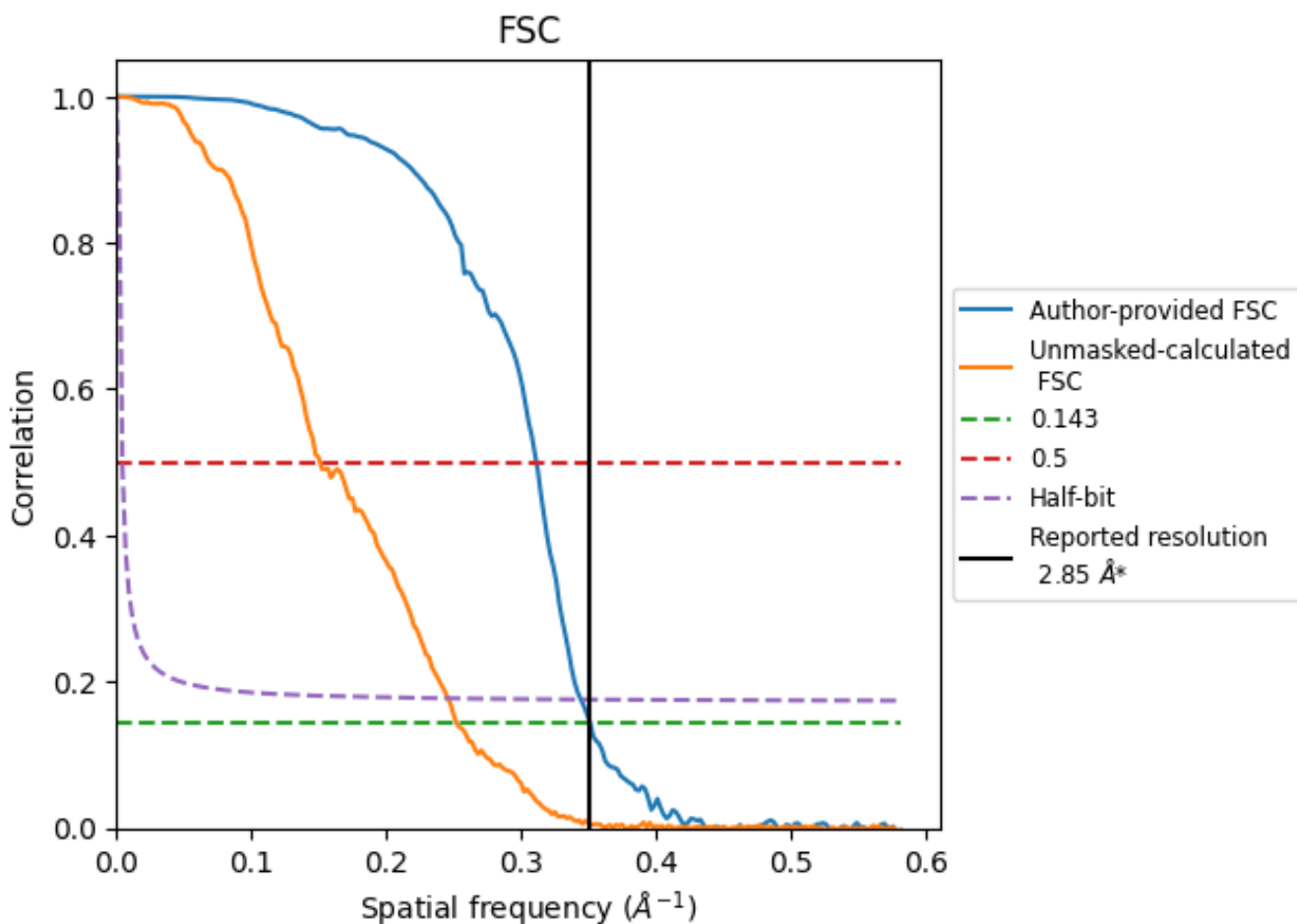


\*Reported resolution corresponds to spatial frequency of 0.351 Å<sup>-1</sup>

## 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 0.351 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

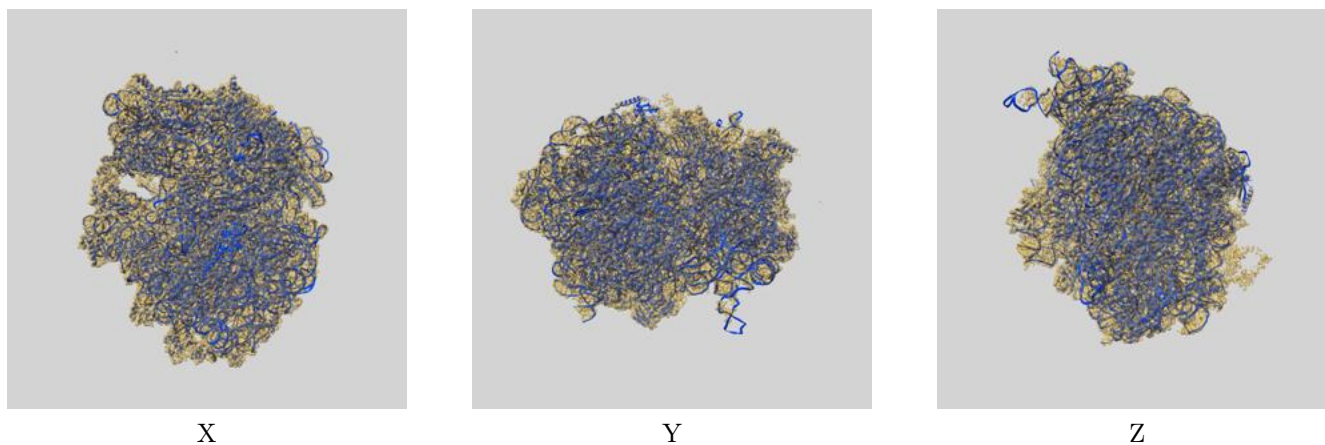
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.21	2.91
Unmasked-calculated*	3.97	6.63	4.07

\*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 3.97 differs from the reported value 2.85 by more than 10 %

## 9 Map-model fit [i](#)

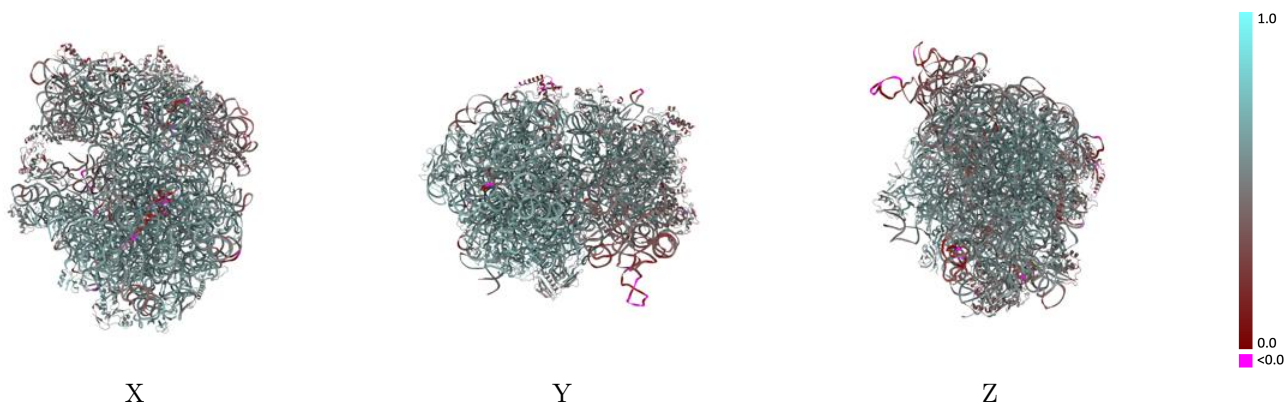
This section contains information regarding the fit between EMDB map EMD-16062 and PDB model 8BHN. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



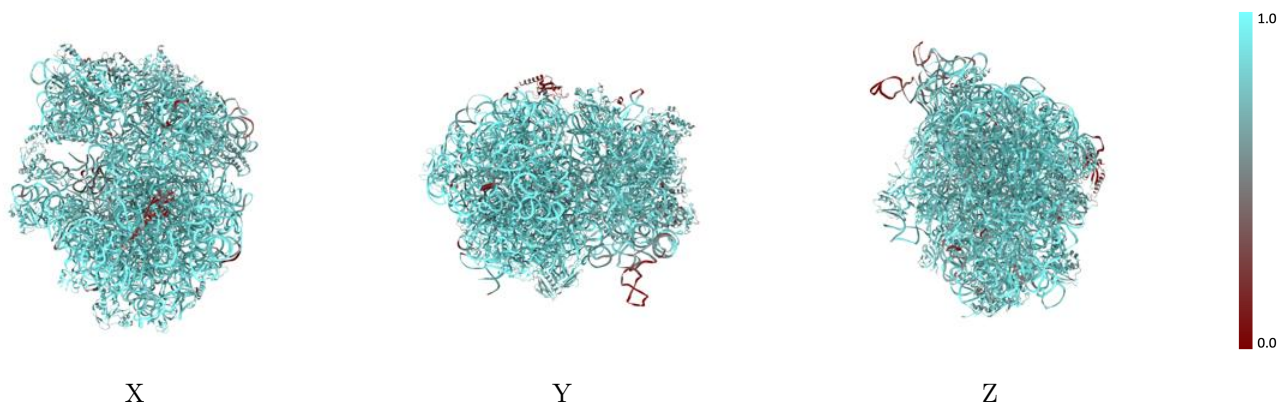
The images above show the 3D surface view of the map at the recommended contour level 0.103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

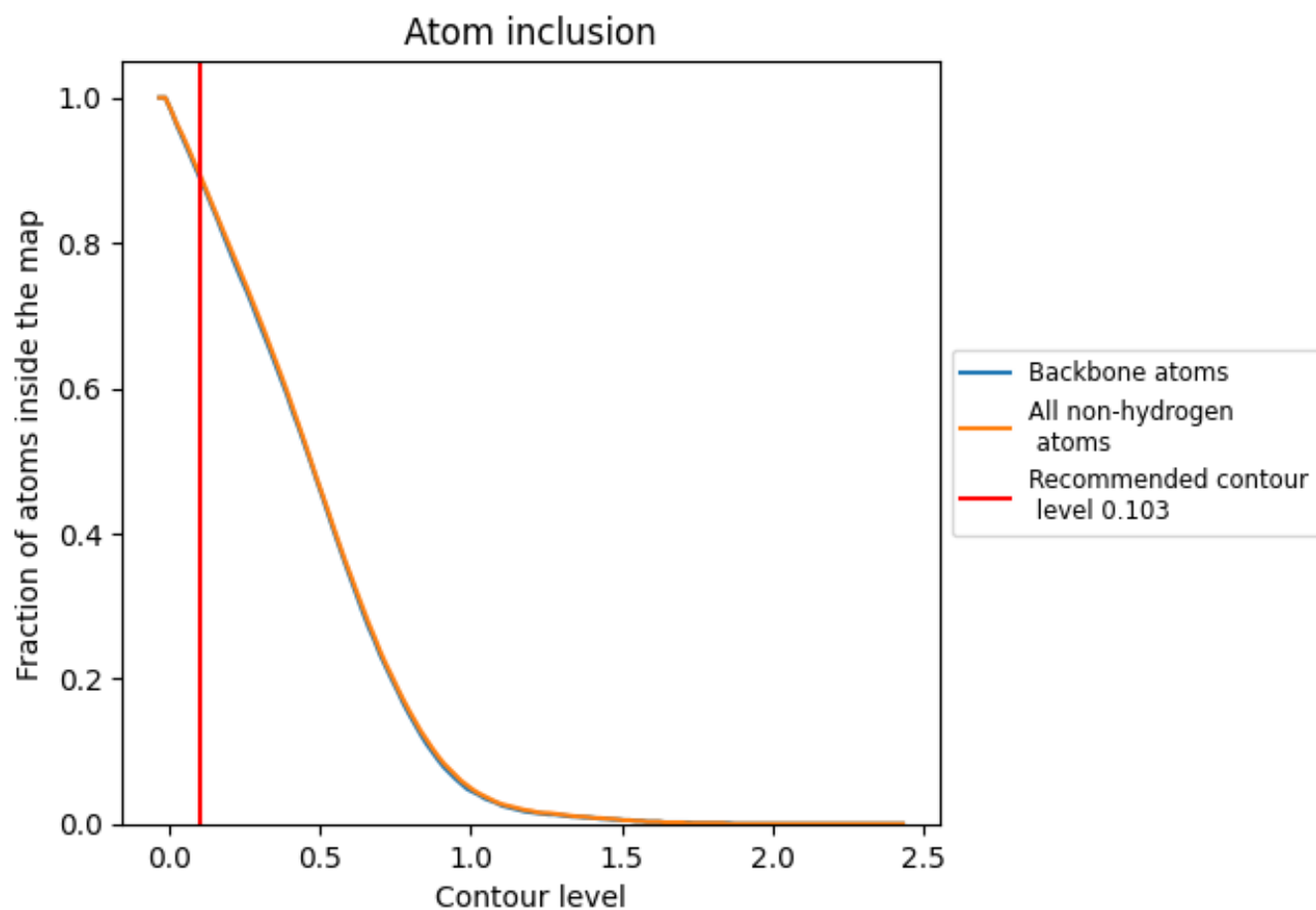
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.103).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.5480
0	 0.9480	 0.5890
1	 0.9230	 0.5430
2	 0.8800	 0.5050
3	 0.9490	 0.5990
4	 0.7330	 0.4540
5	 0.8840	 0.5350
6	 0.6840	 0.5600
A	 0.9400	 0.6270
B	 0.9190	 0.6130
C	 0.8910	 0.5790
D	 0.7610	 0.4320
E	 0.7970	 0.5070
F	 0.3890	 0.2870
G	 0.9260	 0.6090
H	 0.9210	 0.6060
I	 0.9150	 0.6110
J	 0.9090	 0.5960
K	 0.9390	 0.6250
L	 0.8360	 0.5230
M	 0.9170	 0.6000
N	 0.9210	 0.6180
O	 0.9030	 0.5950
P	 0.9040	 0.6050
Q	 0.8780	 0.5720
R	 0.8540	 0.5690
S	 0.8440	 0.5540
T	 0.9080	 0.6150
U	 0.9220	 0.6050
V	 0.8460	 0.5430
W	 0.9110	 0.5960
X	 0.6160	 0.3430
a	 0.9260	 0.6170
b	 0.8340	 0.5590
c	 0.9380	 0.6390



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Chain	Atom inclusion	Q-score
d	 0.9250	 0.6250
e	 0.9110	 0.6200
f	 0.7380	 0.4270
g	 0.8510	 0.5170
h	 0.6770	 0.4130
i	 0.8950	 0.5560
j	 0.8050	 0.4910
k	 0.7530	 0.4440
l	 0.8660	 0.5400
m	 0.7760	 0.4610
n	 0.7650	 0.4530
o	 0.8480	 0.5300
p	 0.8520	 0.5440
q	 0.8000	 0.4610
r	 0.8330	 0.5080
s	 0.8250	 0.4940
t	 0.7320	 0.4410
u	 0.8080	 0.4840
v	 0.7500	 0.4670
w	 0.7780	 0.4600
x	 0.7310	 0.4120
y	 0.7090	 0.4360