



Full wwPDB EM Validation Report ⓘ

Jun 15, 2026 – 10:55 am BST

PDB ID : 9RFW / pdb_00009rfw
EMDB ID : EMD-53943
Title : Manikomycin bound to the Escherichia coli 50S ribosomal subunit
Authors : Kaur, M.; Travin, D.; Berger, M.J.; Jangra, M.; Morici, M.; Safdari, H.A.; Guitor, A.K.; Koteva, K.; Xu, M.; Chen, X.; Vazquez-Laslop, N.; Mankin, A.S.; Wilson, D.N.; Wright, G.
Deposited on : 2025-06-05
Resolution : 2.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

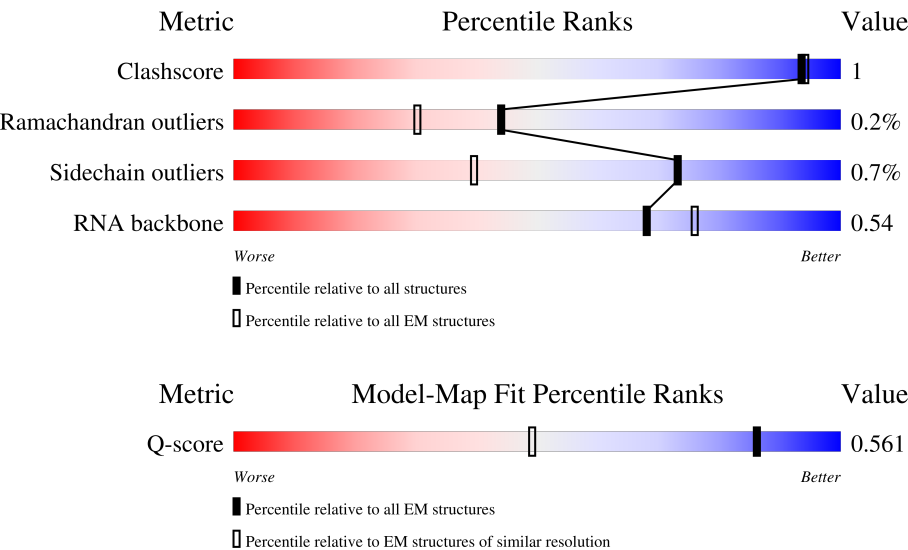
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 Å.

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



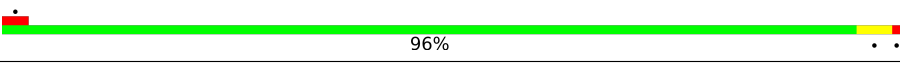
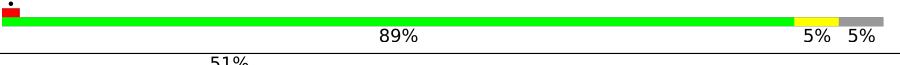
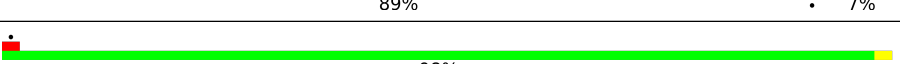
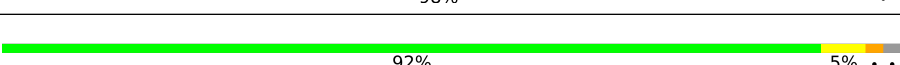
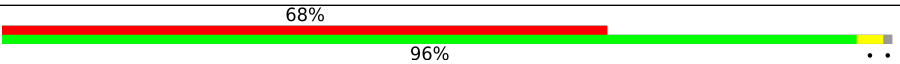
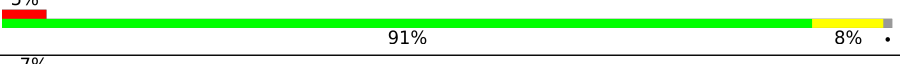
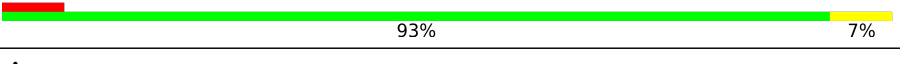
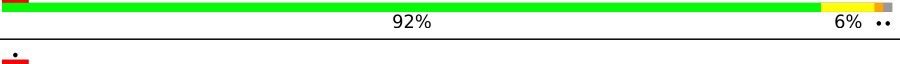
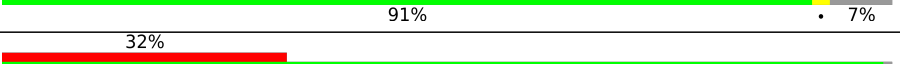
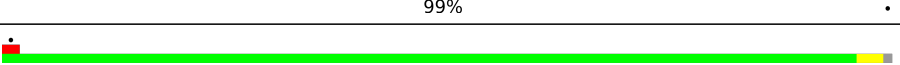
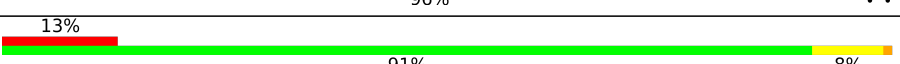
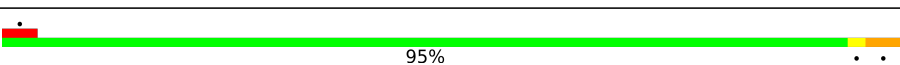
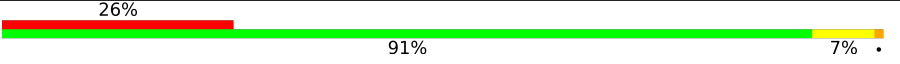
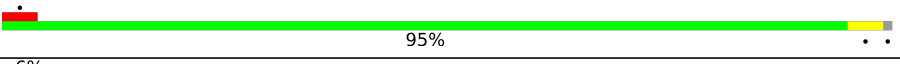
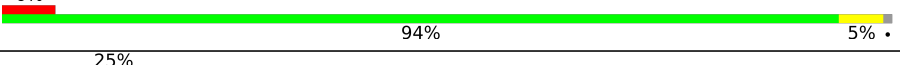
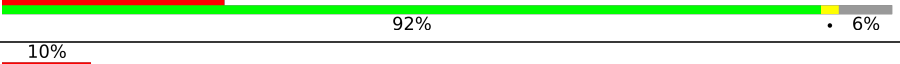
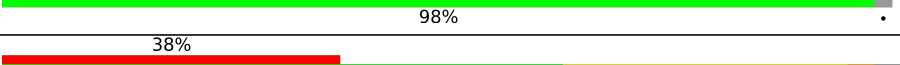
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	38	5% 89% 11%
2	c	273	95% 5%
3	d	209	8% 95%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	l	136	
5	z	57	
6	4	70	
7	a	2904	
8	b	120	
9	0	55	
10	1	46	
11	2	65	
12	f	179	
13	h	149	
14	i	142	
15	j	123	
16	k	144	
17	m	127	
18	n	117	
19	p	118	
20	q	103	
21	r	110	
22	u	94	
23	v	85	
24	w	78	
25	x	63	
26	y	59	
27	Y	76	
28	Z	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	e	201	
30	g	177	
31	o	115	
32	s	100	
33	t	104	
34	C	9	
34	D	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	3TD	a	1915	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 89357 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 2 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 3 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

- Molecule 5 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 6 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	54	Total	C	N	O	S	0	0
			439	274	82	77	6		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	2747	Total	C	N	O	P	0	0
			59004	26328	10878	19051	2747		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	114	Total	C	N	O	P	0	0
			2449	1090	454	791	114		

- Molecule 9 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 10 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 11 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 12 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 13 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	h	40	Total	C	N	O	S	0	0
			294	188	52	53	1		

- Molecule 14 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL14.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	k	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 17 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 24 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	59	Total	C	N	O	S	0	0
			486	300	95	90	1		

- Molecule 26 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 27 is a RNA chain called A-site tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	74	Total	C	N	O	P	0	0
			1576	704	283	516	73		

- Molecule 28 is a RNA chain called P-site tRNA-Val.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	74	Total	C	N	O	P	0	0
			1582	705	287	516	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	199	Total	C	N	O	S	0	0
			1538	966	280	287	5		

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	141	Total	C	N	O	S	0	0
			1058	666	194	196	2		

- Molecule 31 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	o	111	Total	C	N	O	S	0	0
			898	565	175	157	1		

- Molecule 32 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	s	86	Total	C	N	O	S	0	0
			687	437	129	119	2		

- Molecule 33 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	t	94	Total	C	N	O		0	0
			721	454	136	131			

- Molecule 34 is a protein called Manikomycin.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	C	9	Total	C	N	O		0	0
			84	50	22	12			
34	D	9	Total	C	N	O		0	0
			84	50	22	12			

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
35	3	1	Total 1	Zn 1	0
35	4	1	Total 1	Zn 1	0

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	c	1	Total 1	Mg 1	0
36	d	1	Total 1	Mg 1	0
36	z	1	Total 1	Mg 1	0
36	a	205	Total 205	Mg 205	0
36	b	5	Total 5	Mg 5	0

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
37	a	2	Total 2	K 2	0

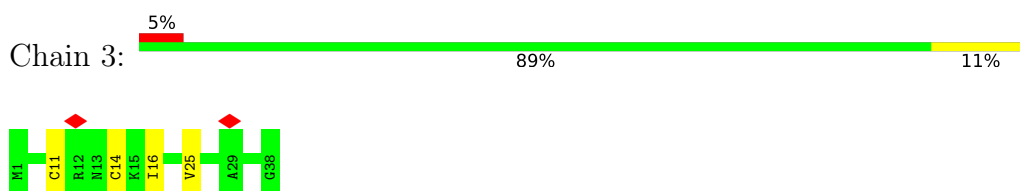
- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	a	59	Total 59	O 59	0
38	2	1	Total 1	O 1	0
38	w	1	Total 1	O 1	0
38	C	4	Total 4	O 4	0

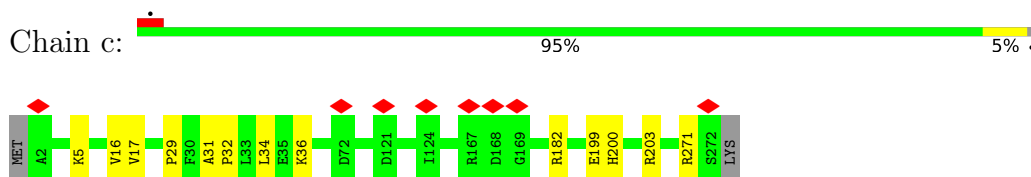
3 Residue-property plots [i](#)

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

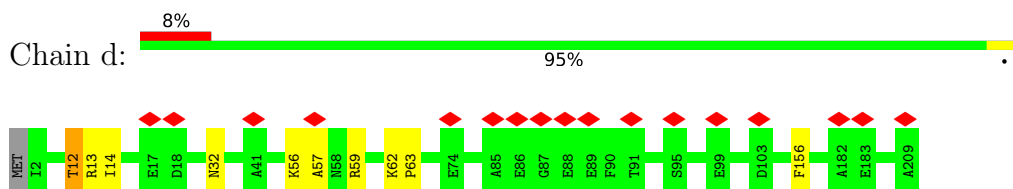
- Molecule 1: Large ribosomal subunit protein bL36A



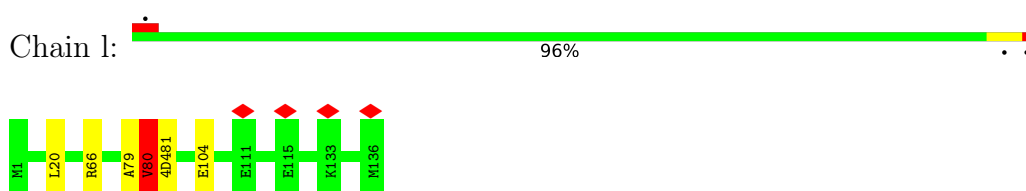
- Molecule 2: Large ribosomal subunit protein uL2



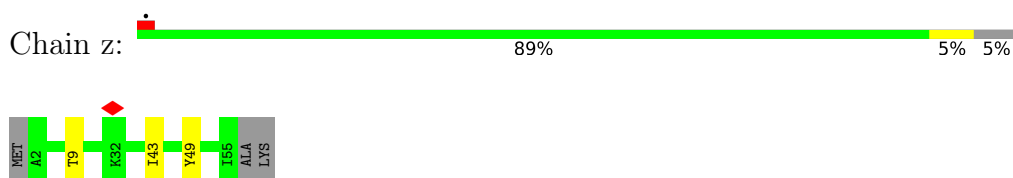
- Molecule 3: Large ribosomal subunit protein uL3



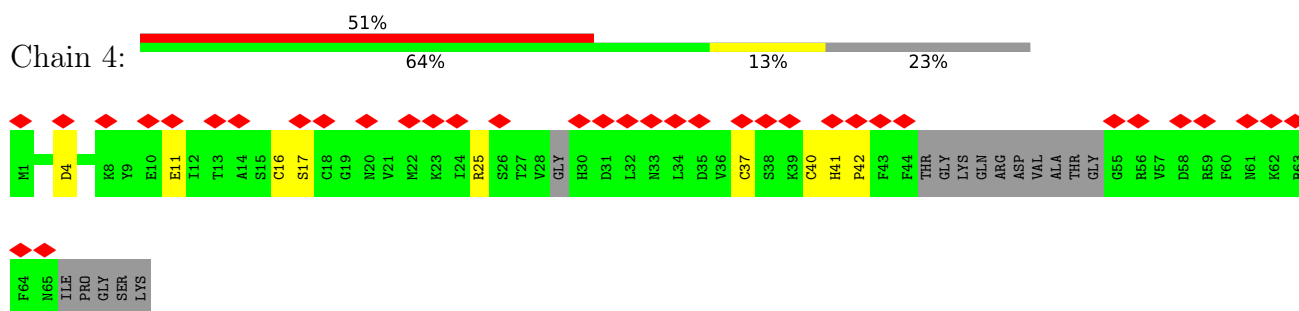
- Molecule 4: Large ribosomal subunit protein uL16



- Molecule 5: Large ribosomal subunit protein bL32

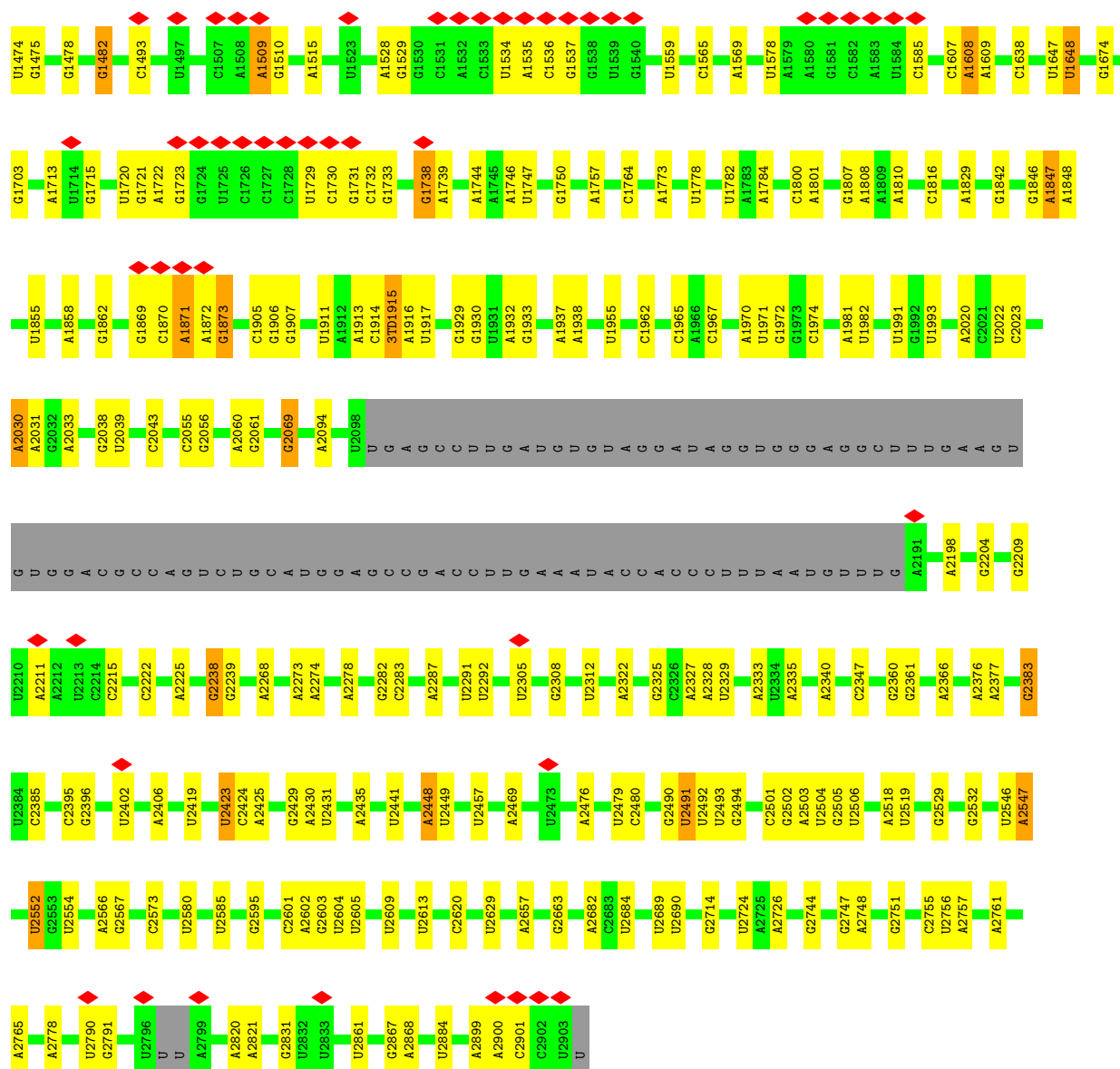


• Molecule 6: Large ribosomal subunit protein bL31A

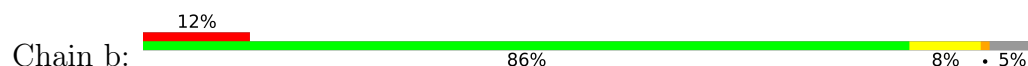


• Molecule 7: 23S rRNA

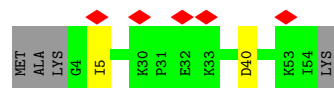
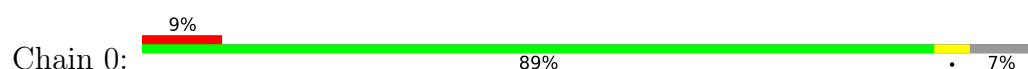




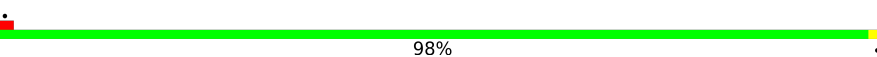
• Molecule 8: 5S rRNA

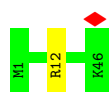


• Molecule 9: Large ribosomal subunit protein bL33



• Molecule 10: Large ribosomal subunit protein bL34

Chain 1:  98%

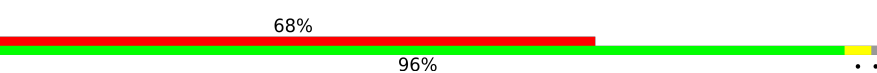


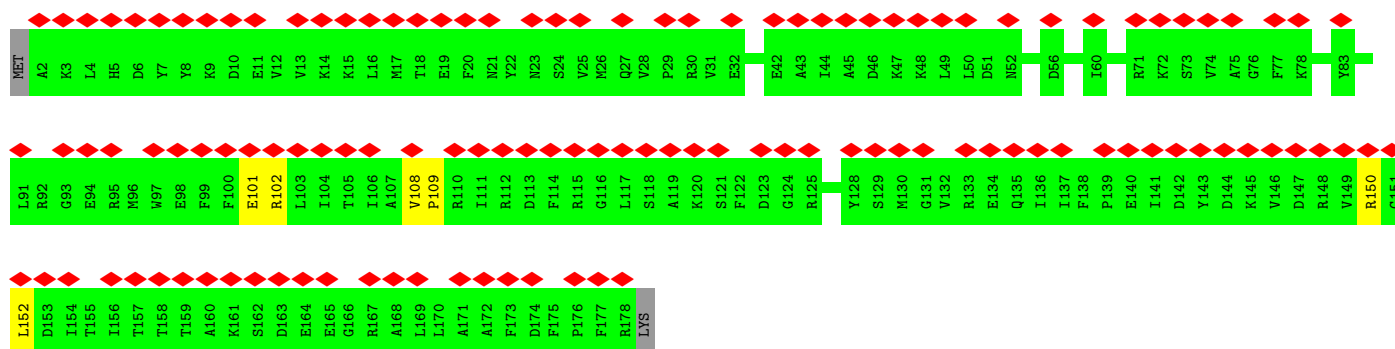
- Molecule 11: Large ribosomal subunit protein bL35

Chain 2:  92% 5% ..



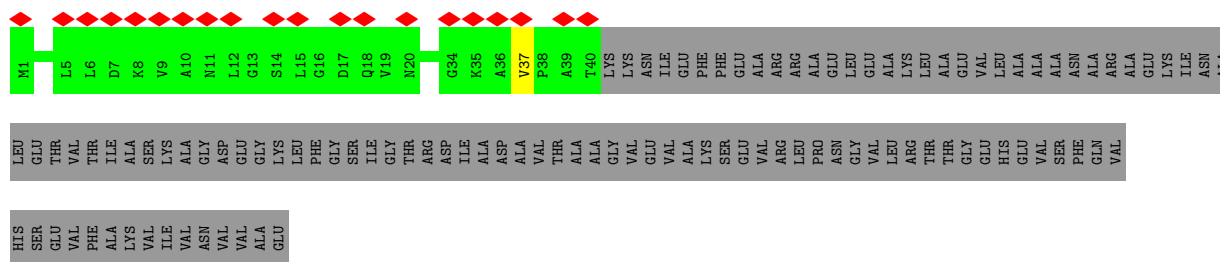
- Molecule 12: Large ribosomal subunit protein uL5

Chain f:  68% 96% ..



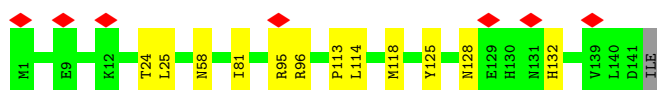
- Molecule 13: Large ribosomal subunit protein bL9

Chain h:  13% 26% 73%

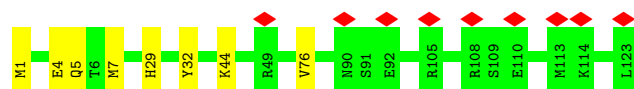
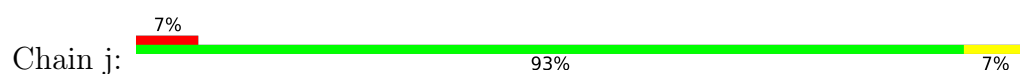


- Molecule 14: Large ribosomal subunit protein uL13

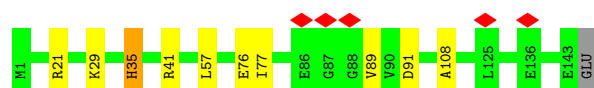
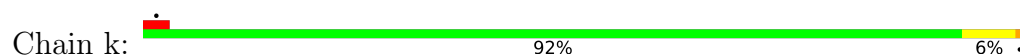
Chain i:  5% 91% 8% ..



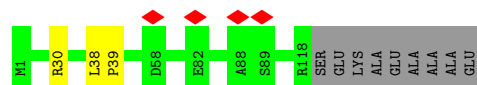
- Molecule 15: Large ribosomal subunit protein uL14



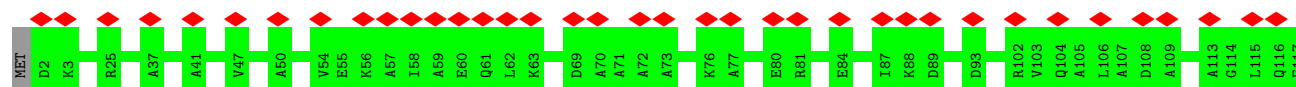
- Molecule 16: 50S ribosomal protein L15



- Molecule 17: Large ribosomal subunit protein bL17



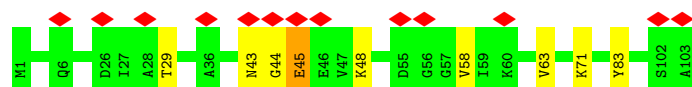
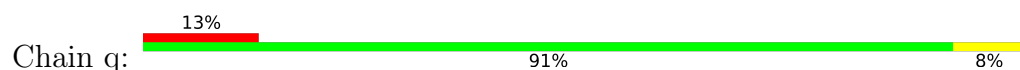
- Molecule 18: Large ribosomal subunit protein uL18



- Molecule 19: Large ribosomal subunit protein bL20

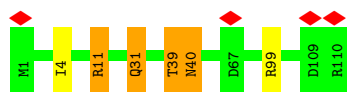


- Molecule 20: Large ribosomal subunit protein bL21

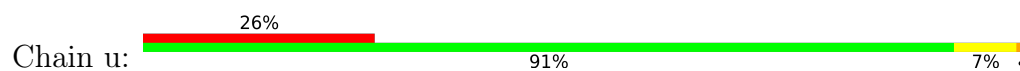


- Molecule 21: Large ribosomal subunit protein uL22





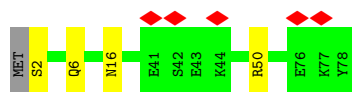
- Molecule 22: 50S ribosomal protein L25



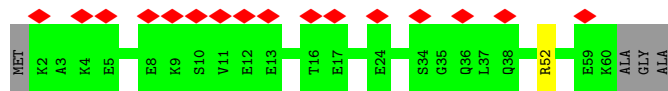
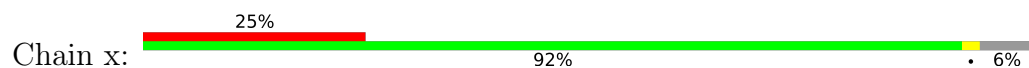
- Molecule 23: Large ribosomal subunit protein bL27



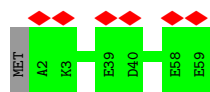
- Molecule 24: Large ribosomal subunit protein bL28



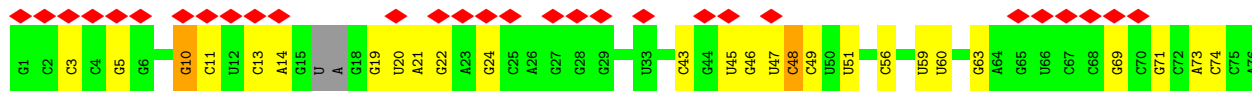
- Molecule 25: Large ribosomal subunit protein uL29



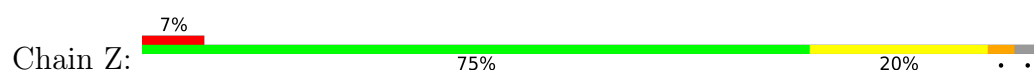
- Molecule 26: Large ribosomal subunit protein uL30



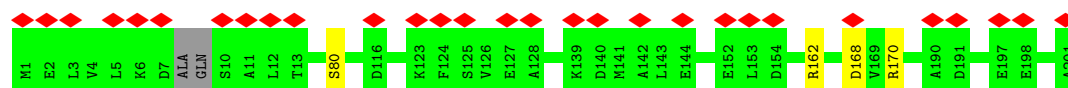
- Molecule 27: A-site tRNA-Phe



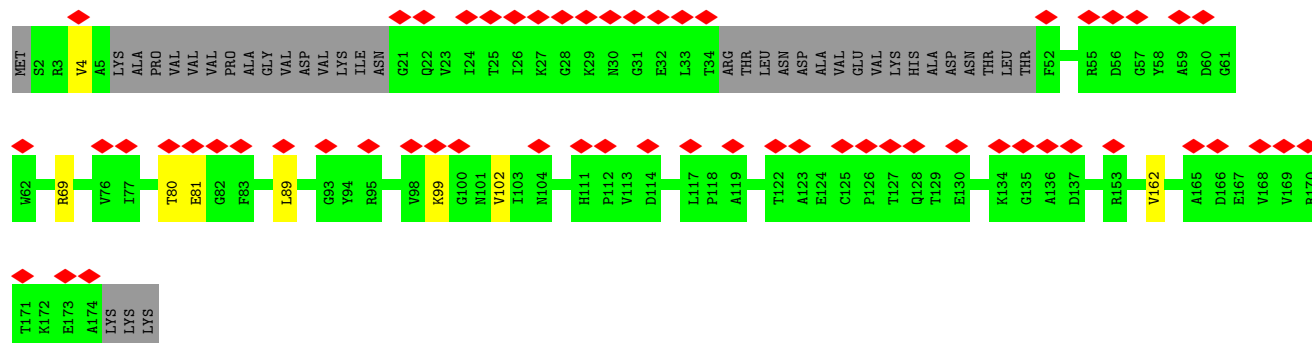
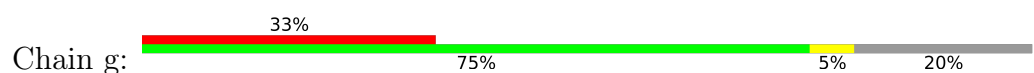
- Molecule 28: P-site tRNA-Val



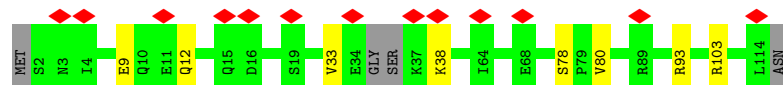
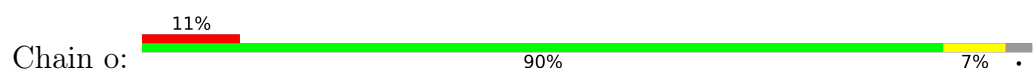
- Molecule 29: Large ribosomal subunit protein uL4



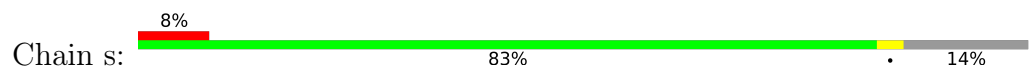
- Molecule 30: Large ribosomal subunit protein uL6



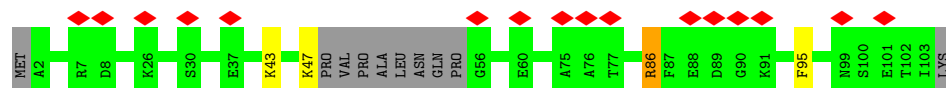
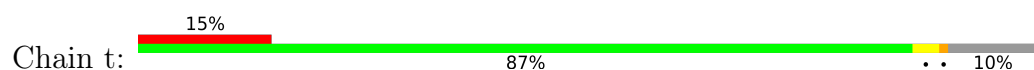
- Molecule 31: Large ribosomal subunit protein bL19



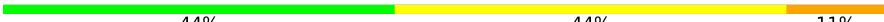
- Molecule 32: Large ribosomal subunit protein uL23



- Molecule 33: Large ribosomal subunit protein uL24



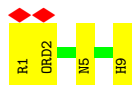
● Molecule 34: Manikomycin

Chain C:  44% 44% 11%



● Molecule 34: Manikomycin

Chain D:  22% 56% 44%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251301	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)	300	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.228	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0166	Depositor
Map size (Å)	359.424, 359.424, 359.424	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, OMC, K, 4D4, G7M, ORD, 1MG, 2MG, H2U, 2MA, OMG, DSG, DPN, MEQ, PSU, MG, MS6, DAR, ZN, 3TD, 5MC, 6MZ, 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	3	0.68	0/303	0.89	0/397
2	c	0.67	0/2121	0.85	0/2852
3	d	0.65	0/1568	0.84	0/2109
4	l	0.61	1/1073 (0.1%)	0.81	0/1433
5	z	0.68	0/435	0.89	0/581
6	4	0.51	0/446	0.80	0/592
7	a	0.53	2/65510 (0.0%)	0.90	71/102191 (0.1%)
8	b	0.53	0/2737	0.86	2/4262 (0.0%)
9	0	0.54	0/424	0.83	0/565
10	1	0.66	0/380	0.88	0/498
11	2	0.71	0/513	0.89	1/676 (0.1%)
12	f	0.48	0/1434	0.84	0/1926
13	h	0.50	0/297	0.79	0/402
14	i	0.61	0/1143	0.81	0/1540
15	j	0.57	0/955	0.84	0/1279
16	k	0.67	0/1052	0.87	1/1401 (0.1%)
17	m	0.63	0/958	0.87	0/1281
18	n	0.55	0/902	0.85	0/1209
19	p	0.65	0/960	0.84	0/1278
20	q	0.55	0/829	0.79	0/1107
21	r	0.64	0/864	0.83	1/1156 (0.1%)
22	u	0.52	0/766	0.82	0/1025
23	v	0.63	0/636	0.77	0/841
24	w	0.61	0/635	0.83	0/848
25	x	0.48	0/487	0.83	0/648
26	y	0.59	0/453	0.80	0/605
27	Y	0.54	0/1760	0.81	0/2740
28	Z	0.53	0/1767	0.85	1/2751 (0.0%)
29	e	0.59	0/1556	0.83	0/2091
30	g	0.51	0/1073	0.80	0/1447
31	o	0.61	0/909	0.82	1/1215 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	s	0.55	0/692	0.82	0/923
33	t	0.54	0/725	0.79	0/961
34	C	1.90	0/23	2.18	1/29 (3.4%)
34	D	2.08	1/23 (4.3%)	1.52	0/29
All	All	0.55	4/96409 (0.0%)	0.88	79/144888 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	c	0	1
4	l	0	1
7	a	0	7
12	f	0	1
16	k	0	1
17	m	0	1
21	r	0	2
23	v	0	1
24	w	0	1
25	x	0	1
29	e	0	1
31	o	0	1
33	t	0	1
34	D	0	1
All	All	0	21

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	9	HIS	ND1-CE1	6.68	1.39	1.32
4	l	80	VAL	C-O	-6.17	1.11	1.23
7	a	2069	G7M	O3'-P	5.34	1.61	1.56
7	a	2552	OMU	O3'-P	5.12	1.61	1.56

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	2490	G	O3'-P-O5'	-10.66	88.01	104.00
7	a	2546	U	O3'-P-O5'	-8.23	91.65	104.00
7	a	1025	G	O3'-P-O5'	8.22	116.34	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	9	HIS	CA-CB-CG	-8.03	105.77	113.80
7	a	204	A	O3'-P-O5'	-7.66	92.51	104.00
16	k	35	HIS	CB-CA-C	7.60	125.55	110.42
7	a	1025	G	C2'-C3'-O3'	7.40	120.59	109.50
7	a	528	A	O3'-P-O5'	-7.39	92.92	104.00
7	a	2601	C	O3'-P-O5'	-7.24	93.14	104.00
7	a	1905	C	O3'-P-O5'	-7.20	93.21	104.00
7	a	2492	U	O3'-P-O5'	-7.15	93.28	104.00
7	a	2479	U	O3'-P-O5'	-7.03	93.46	104.00
7	a	1565	C	O3'-P-O5'	-6.93	93.60	104.00
7	a	2501	C	O3'-P-O5'	-6.85	93.73	104.00
7	a	781	A	O3'-P-O5'	-6.74	93.90	104.00
7	a	1437	C	O3'-P-O5'	-6.52	94.23	104.00
7	a	1974	C	O3'-P-O5'	-6.47	94.30	104.00
7	a	1131	G	O3'-P-O5'	-6.40	94.40	104.00
7	a	579	G	O3'-P-O5'	-6.39	94.41	104.00
7	a	1359	A	O3'-P-O5'	-6.38	94.43	104.00
7	a	1373	A	O3'-P-O5'	-6.37	94.44	104.00
28	Z	8	U	O3'-P-O5'	-6.37	94.44	104.00
7	a	1246	A	O3'-P-O5'	-6.36	94.47	104.00
7	a	329	G	O3'-P-O5'	-6.35	94.47	104.00
7	a	2423	U	O3'-P-O5'	-6.29	94.57	104.00
7	a	1293	C	O3'-P-O5'	-6.28	94.58	104.00
7	a	2383	G	O3'-P-O5'	-6.27	94.59	104.00
7	a	2022	U	C1'-C2'-O2'	-6.25	102.43	111.80
7	a	2620	C	O3'-P-O5'	-6.16	94.77	104.00
7	a	2222	C	O3'-P-O5'	-6.14	94.79	104.00
7	a	1757	A	C4'-C3'-O3'	-6.12	103.82	113.00
7	a	1648	U	O3'-P-O5'	-6.11	94.84	104.00
31	o	93	ARG	CA-CB-CG	-6.03	102.05	114.10
7	a	385	C	O3'-P-O5'	-5.97	95.04	104.00
7	a	731	C	O3'-P-O5'	-5.96	95.06	104.00
7	a	2360	G	O3'-P-O5'	5.93	112.89	104.00
7	a	2094	A	O3'-P-O5'	-5.87	95.19	104.00
7	a	1270	C	C2'-C3'-O3'	-5.87	104.90	113.70
7	a	310	A	O3'-P-O5'	-5.80	95.31	104.00
7	a	248	G	C4'-C3'-O3'	-5.73	104.41	113.00
7	a	1289	C	O3'-P-O5'	-5.72	95.42	104.00
7	a	60	G	O3'-P-O5'	-5.71	95.44	104.00
8	b	90	C	O3'-P-O5'	-5.70	95.45	104.00
7	a	1356	G	O3'-P-O5'	-5.69	95.46	104.00
7	a	1358	G	O3'-P-O5'	-5.69	95.47	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	1638	C	O3'-P-O5'	-5.66	95.51	104.00
7	a	747	5MU	O3'-P-O5'	-5.65	95.53	104.00
7	a	2493	U	O3'-P-O5'	-5.62	95.58	104.00
7	a	2376	A	O3'-P-O5'	-5.58	95.63	104.00
7	a	621	A	O3'-P-O5'	-5.55	95.68	104.00
7	a	1385	A	O3'-P-O5'	-5.54	95.69	104.00
7	a	2519	U	O3'-P-O5'	-5.54	95.69	104.00
7	a	193	U	O3'-P-O5'	-5.52	95.72	104.00
7	a	1981	A	C2'-C3'-O3'	-5.52	105.42	113.70
7	a	1394	U	O3'-P-O5'	-5.51	95.73	104.00
21	r	39	THR	CA-CB-OG1	-5.49	101.36	109.60
7	a	495	G	O3'-P-O5'	-5.49	95.77	104.00
7	a	409	G	O3'-P-O5'	-5.45	95.82	104.00
7	a	816	C	O3'-P-O5'	-5.42	95.87	104.00
7	a	2278	A	O3'-P-O5'	-5.36	95.97	104.00
7	a	22	C	O3'-P-O5'	-5.34	96.00	104.00
7	a	1168	G	O3'-P-O5'	-5.33	96.00	104.00
7	a	404	A	C2'-C3'-O3'	5.33	117.50	109.50
7	a	673	C	O3'-P-O5'	-5.30	96.05	104.00
7	a	982	C	C2'-C3'-O3'	-5.27	105.80	113.70
7	a	2501	C	C4'-C3'-O3'	-5.24	105.15	113.00
7	a	1025	G	C4'-C3'-O3'	-5.22	101.57	109.40
7	a	784	G	C2'-C3'-O3'	-5.20	105.90	113.70
8	b	32	U	O3'-P-O5'	-5.14	96.28	104.00
7	a	2755	C	O3'-P-O5'	-5.14	96.29	104.00
7	a	2747	G	O3'-P-O5'	-5.12	96.31	104.00
7	a	1810	A	O3'-P-O5'	-5.10	96.36	104.00
7	a	748	G	C1'-O4'-C4'	-5.08	104.82	109.90
11	2	45	ARG	CB-CA-C	-5.08	104.76	113.04
7	a	808	G	O3'-P-O5'	-5.06	96.42	104.00
7	a	2761	A	O3'-P-O5'	-5.06	96.42	104.00
7	a	295	G	O3'-P-O5'	-5.04	96.45	104.00
7	a	1410	G	O3'-P-O5'	-5.02	96.47	104.00
7	a	1436	G	O3'-P-O5'	-5.01	96.48	104.00

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	D	1	DAR	Peptide
7	a	249	C	Sidechain
7	a	2595	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
7	a	395	U	Sidechain
7	a	463	G	Sidechain
7	a	512	G	Sidechain
7	a	575	A	Sidechain
7	a	980	A	Sidechain
2	c	271	ARG	Sidechain
29	e	162	ARG	Sidechain
12	f	150	ARG	Sidechain
16	k	41	ARG	Sidechain
4	l	80	VAL	Mainchain
17	m	30	ARG	Sidechain
31	o	103	ARG	Sidechain
21	r	11	ARG	Sidechain
21	r	4	ILE	Peptide
33	t	86	ARG	Sidechain
23	v	25	ARG	Sidechain
24	w	16	ASN	Peptide
25	x	52	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	3	302	0	340	3	0
2	c	2082	0	2154	6	0
3	d	1558	0	1606	7	0
4	l	1075	0	1145	3	0
5	z	429	0	440	3	0
6	4	439	0	432	4	0
7	a	59004	0	29705	108	0
8	b	2449	0	1242	3	0
9	0	417	0	451	1	0
10	1	377	0	418	1	0
11	2	504	0	572	2	0
12	f	1410	0	1444	2	0
13	h	294	0	314	0	0
14	i	1120	0	1151	7	0
15	j	946	0	1023	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	k	1043	0	1123	7	0
17	m	945	0	989	1	0
18	n	892	0	923	0	0
19	p	947	0	1019	3	0
20	q	816	0	839	5	0
21	r	857	0	922	4	0
22	u	753	0	780	4	0
23	v	628	0	642	1	0
24	w	625	0	652	1	0
25	x	486	0	518	0	0
26	y	449	0	488	0	0
27	Y	1576	0	802	7	0
28	Z	1582	0	803	1	0
29	e	1538	0	1605	1	0
30	g	1058	0	1081	3	0
31	o	898	0	947	4	0
32	s	687	0	761	2	0
33	t	721	0	770	3	0
34	C	84	0	83	3	0
34	D	84	0	83	1	0
35	3	1	0	0	0	0
35	4	1	0	0	0	0
36	a	205	0	0	0	0
36	b	5	0	0	0	0
36	c	1	0	0	0	0
36	d	1	0	0	0	0
36	z	1	0	0	0	0
37	a	2	0	0	0	0
38	2	1	0	0	0	0
38	C	4	0	0	0	0
38	a	59	0	0	1	0
38	w	1	0	0	0	0
All	All	89357	0	58267	184	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 1.

All (184) 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)
7:a:1915:3TD:O3'	7:a:1916:A:P	2.25	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:1915:3TD:HO3'	7:a:1916:A:P	1.98	0.87
7:a:1914:C:O3'	7:a:1915:3TD:P	2.34	0.85
7:a:12:U:H2'	7:a:12:U:O2	1.83	0.77
7:a:1914:C:HO3'	7:a:1915:3TD:P	2.09	0.75
7:a:1434:A:H2'	7:a:1435:G:C8	2.23	0.74
7:a:2419:U:O4	38:a:6301:HOH:O	2.06	0.72
7:a:483:A:H5''	33:t:47:LYS:HD2	1.72	0.70
7:a:896:A:H2'	27:Y:56:C:O2	1.92	0.69
6:4:37:CYS:N	6:4:40:CYS:SG	2.66	0.69
7:a:1914:C:O3'	7:a:1915:3TD:OP1	2.12	0.67
7:a:1434:A:H2'	7:a:1435:G:H8	1.60	0.66
7:a:549:G:H2'	7:a:550:C:H6	1.61	0.66
7:a:1915:3TD:O3'	7:a:1916:A:OP2	2.16	0.64
7:a:1915:3TD:O3'	7:a:1916:A:OP1	2.16	0.64
7:a:534:U:O2'	19:p:49:ASP:OD2	2.10	0.63
7:a:894:U:H2'	7:a:895:U:O4'	1.99	0.62
7:a:504:A:O2'	7:a:505:A:OP1	2.17	0.62
21:r:39:THR:O	21:r:40:ASN:HB2	2.00	0.61
24:w:6:GLN:HE21	24:w:50:ARG:H	1.50	0.60
22:u:9:ARG:HG2	22:u:41:GLU:HG2	1.83	0.59
27:Y:51:U:H3	27:Y:63:G:H1	1.51	0.58
7:a:568:U:H1'	7:a:2030:6MZ:H9C1	1.86	0.58
3:d:12:THR:HG22	3:d:13:ARG:H	1.68	0.58
5:z:9:THR:CG2	7:a:2020:A:H5'	2.34	0.58
7:a:504:A:O2'	7:a:505:A:P	2.63	0.57
20:q:29:THR:O	20:q:63:VAL:HB	2.04	0.57
7:a:558:U:OP1	14:i:113:PRO:HD2	2.05	0.57
7:a:1872:A:H3'	7:a:1873:G:O4'	2.07	0.55
3:d:156:PHE:CE1	14:i:81:ILE:HD13	2.42	0.54
14:i:95:ARG:HD3	14:i:96:ARG:NH2	2.22	0.54
20:q:29:THR:O	20:q:63:VAL:O	2.26	0.54
28:Z:9:A:O2'	28:Z:10:G:N7	2.41	0.53
7:a:1182:G:H2'	7:a:1183:U:O4'	2.08	0.53
7:a:549:G:H2'	7:a:550:C:C6	2.40	0.53
4:l:66:ARG:NH1	4:l:104:GLU:OE2	2.41	0.53
7:a:2900:A:H2'	7:a:2901:C:O4'	2.08	0.53
7:a:12:U:O2	7:a:12:U:C2'	2.57	0.52
21:r:31:GLN:HE21	21:r:31:GLN:HA	1.74	0.52
2:c:5:LYS:HD2	2:c:17:VAL:HG22	1.89	0.52
22:u:4:ILE:HG12	22:u:50:MET:HE1	1.92	0.52
31:o:78:SER:OG	31:o:80:VAL:HG12	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:2209:G:H1	7:a:2215:C:H42	1.58	0.52
7:a:784:G:H5'	7:a:785:G:OP1	2.10	0.51
7:a:1778:U:H2'	7:a:1784:A:N6	2.25	0.51
1:3:11:CYS:SG	1:3:14:CYS:N	2.83	0.51
7:a:1722:A:H2'	7:a:1723:G:O4'	2.10	0.51
4:l:79:ALA:HA	7:a:2494:G:O2'	2.11	0.51
7:a:1187:G:H5''	20:q:83:TYR:CE1	2.45	0.51
1:3:16:ILE:HD13	1:3:25:VAL:HG22	1.93	0.50
3:d:14:ILE:HA	31:o:12:GLN:HE22	1.75	0.50
3:d:59:ARG:NH2	7:a:2831:G:OP2	2.40	0.50
2:c:31:ALA:N	2:c:32:PRO:CD	2.75	0.49
7:a:2328:A:H2'	7:a:2329:U:C6	2.48	0.49
7:a:141:G:H2'	7:a:142:A:O4'	2.11	0.49
7:a:2395:C:O2'	34:C:9:HIS:ND1	2.31	0.49
7:a:2532:G:O2'	7:a:2657:A:N1	2.45	0.49
7:a:2756:U:H1'	7:a:2757:A:H5''	1.95	0.49
7:a:811:U:H2'	16:k:21:ARG:HA	1.95	0.49
6:4:11:GLU:HA	6:4:25:ARG:HA	1.95	0.48
16:k:77:ILE:HD13	16:k:108:ALA:HB1	1.95	0.48
7:a:1869:G:C6	7:a:1871:A:OP2	2.67	0.48
7:a:1433:A:H2'	7:a:1434:A:O4'	2.14	0.48
7:a:2209:G:H1	7:a:2215:C:N4	2.11	0.48
8:b:117:G:C6	8:b:118:C:C4	3.01	0.48
7:a:2:G:H2'	7:a:3:U:C6	2.49	0.47
3:d:12:THR:HG23	31:o:9:GLU:OE2	2.14	0.47
7:a:543:G:H5''	7:a:543:G:H8	1.79	0.47
14:i:58:ASN:HD21	14:i:128:ASN:HD22	1.63	0.47
7:a:1474:U:C4	7:a:1475:G:C6	3.03	0.47
15:j:1:MET:HE3	15:j:32:TYR:CZ	2.50	0.47
7:a:247:G:H4'	7:a:386:G:C5	2.49	0.47
27:Y:10:G:H2'	27:Y:11:C:C6	2.50	0.47
7:a:548:G:H2'	7:a:549:G:C1'	2.45	0.47
7:a:1045:C:O2	7:a:1045:C:O4'	2.31	0.47
7:a:1020:A:C2	7:a:1141:U:C2	3.04	0.46
34:C:5:DSG:O	34:C:6:DAR:C	2.63	0.46
7:a:570:G:H2'	7:a:2030:6MZ:N7	2.30	0.46
7:a:1607:C:H4'	7:a:1608:A:O5'	2.16	0.46
16:k:77:ILE:CD1	16:k:108:ALA:HB1	2.45	0.46
19:p:91:ASP:OD1	19:p:91:ASP:C	2.59	0.46
7:a:1185:G:H5''	7:a:1186:G:OP1	2.15	0.46
16:k:76:GLU:C	16:k:77:ILE:HD12	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:465:G:OP1	10:1:12:ARG:NH1	2.48	0.46
22:u:75:GLN:HB2	22:u:92:VAL:HG23	1.98	0.46
7:a:548:G:H2'	7:a:549:G:H1'	1.97	0.46
7:a:1129:A:N6	7:a:2491:U:OP1	2.47	0.46
7:a:1378:A:O2'	7:a:1380:G:N7	2.49	0.46
5:z:9:THR:HG21	7:a:2020:A:H5'	1.97	0.45
27:Y:59:U:H3'	27:Y:60:U:O2	2.17	0.45
11:2:27:ALA:O	11:2:28:ASN:HB2	2.16	0.45
7:a:493:G:H2'	7:a:494:G:O4'	2.17	0.45
7:a:1409:U:H2'	7:a:1410:G:O4'	2.17	0.45
7:a:2273:A:H2'	7:a:2274:A:C8	2.52	0.45
27:Y:48:C:H5''	27:Y:48:C:H6	1.82	0.45
7:a:2:G:C2	7:a:3:U:C2	3.05	0.45
7:a:644:A:H2'	7:a:645:C:O4'	2.17	0.45
7:a:788:A:OP1	7:a:790:U:H5	2.00	0.45
8:b:24:G:N7	8:b:56:G:H2'	2.31	0.45
7:a:895:U:H3'	7:a:896:A:H5'	1.99	0.45
7:a:1141:U:H4'	7:a:1142:A:O4'	2.18	0.44
7:a:1746:A:H2'	7:a:1747:U:C6	2.53	0.44
7:a:2552:OMU:H6	7:a:2552:OMU:O5'	2.18	0.44
32:s:48:GLN:HE21	32:s:55:VAL:H	1.66	0.44
2:c:29:PRO:HG2	2:c:34:LEU:HD11	1.98	0.44
30:g:89:LEU:HD22	30:g:162:VAL:HG22	1.99	0.44
7:a:896:A:H2'	27:Y:56:C:C2	2.53	0.44
7:a:2431:U:OP2	34:C:1:DAR:NH1	2.46	0.43
14:i:125:TYR:OH	14:i:132:HIS:NE2	2.47	0.43
20:q:43:ASN:O	20:q:44:GLY:C	2.61	0.43
7:a:851:C:H2'	7:a:852:U:C6	2.52	0.43
7:a:1050:A:H2'	7:a:1051:G:O4'	2.19	0.43
7:a:3:U:H2'	7:a:4:U:C6	2.53	0.43
7:a:1720:U:H2'	7:a:1721:G:O4'	2.18	0.43
4:l:20:LEU:HD13	22:u:81:PRO:HG2	2.00	0.43
8:b:117:G:H2'	8:b:118:C:O4'	2.18	0.43
27:Y:60:U:O2	27:Y:60:U:O5'	2.37	0.43
31:o:33:VAL:HG22	31:o:38:LYS:HG3	2.01	0.43
7:a:1021:A:N3	7:a:1021:A:H3'	2.34	0.43
30:g:80:THR:OG1	30:g:81:GLU:N	2.50	0.43
30:g:4:VAL:O	30:g:69:ARG:HG2	2.18	0.43
6:4:16:CYS:SG	6:4:17:SER:N	2.92	0.43
7:a:945:A:C4	7:a:2448:A:C2	3.07	0.43
7:a:2327:A:H2'	7:a:2328:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:1050:A:C2	7:a:2751:G:C4	3.06	0.43
7:a:1914:C:O3'	7:a:1915:3TD:OP2	2.33	0.43
15:j:4:GLU:O	15:j:5:GLN:HB2	2.18	0.43
2:c:5:LYS:NZ	2:c:16:VAL:O	2.49	0.42
3:d:62:LYS:N	3:d:63:PRO:CD	2.82	0.42
19:p:76:TYR:CZ	19:p:80:ILE:HG13	2.54	0.42
32:s:61:LEU:HD12	32:s:61:LEU:C	2.44	0.42
7:a:2038:G:H2'	7:a:2039:U:O4'	2.18	0.42
7:a:1046:A:H3'	7:a:1047:G:C5'	2.49	0.42
11:2:54:ASP:HB3	16:k:57:LEU:HD22	2.01	0.42
20:q:44:GLY:O	20:q:45:GLU:HB2	2.19	0.42
34:D:5:DSG:OD1	34:D:5:DSG:C	2.67	0.42
5:z:43:ILE:HG22	5:z:49:TYR:HB2	2.01	0.42
7:a:857:G:H2'	7:a:858:G:O4'	2.20	0.42
7:a:861:A:C2	7:a:917:A:C4	3.07	0.42
7:a:1872:A:C5	7:a:1873:G:H1'	2.54	0.42
7:a:1932:A:H2'	7:a:1933:G:O4'	2.20	0.42
7:a:2506:U:C2	7:a:2585:U:O4	2.72	0.42
29:e:168:ASP:OD2	29:e:170:ARG:NE	2.52	0.42
7:a:499:U:H5''	33:t:43:LYS:HE2	2.02	0.42
14:i:24:THR:O	14:i:25:LEU:C	2.63	0.42
7:a:273:G:C6	7:a:274:C:C4	3.08	0.42
1:3:11:CYS:N	1:3:14:CYS:SG	2.92	0.42
7:a:2684:U:H4'	15:j:76:VAL:CG2	2.50	0.42
7:a:191:A:H2'	7:a:192:C:C6	2.55	0.42
7:a:1914:C:H3'	7:a:1915:3TD:OP2	2.19	0.42
12:f:101:GLU:O	12:f:102:ARG:C	2.62	0.42
7:a:366:C:H2'	7:a:367:G:O4'	2.20	0.41
7:a:340:A:H2'	7:a:341:C:O4'	2.20	0.41
7:a:1738:G:HO2'	7:a:1739:A:H8	1.66	0.41
17:m:38:LEU:HB3	17:m:39:PRO:HD3	2.02	0.41
2:c:203:ARG:HH21	2:c:203:ARG:HG3	1.85	0.41
7:a:1528:A:H2'	7:a:1529:G:O4'	2.20	0.41
16:k:77:ILE:HD12	16:k:77:ILE:N	2.35	0.41
33:t:86:ARG:HG3	33:t:95:PHE:CE1	2.55	0.41
7:a:120:U:H5''	7:a:122:G:OP2	2.20	0.41
14:i:114:LEU:HG	14:i:118:MET:HE3	2.02	0.41
7:a:387:U:C4	7:a:388:G:O6	2.74	0.41
12:f:108:VAL:N	12:f:109:PRO:CD	2.83	0.41
2:c:199:GLU:O	2:c:200:HIS:C	2.63	0.41
7:a:1869:G:O2'	7:a:1872:A:N6	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:84:A:N1	7:a:98:G:O2'	2.48	0.41
9:0:40:ASP:OD1	9:0:40:ASP:C	2.64	0.41
21:r:39:THR:O	21:r:40:ASN:CB	2.63	0.41
7:a:2547:A:H4'	15:j:29:HIS:NE2	2.36	0.41
16:k:89:VAL:HG12	16:k:91:ASP:OD1	2.20	0.41
7:a:21:A:H2'	7:a:22:C:O4'	2.21	0.41
7:a:1482:G:H1'	7:a:1509:A:H61	1.86	0.41
7:a:2395:C:H2'	7:a:2396:G:O4'	2.21	0.41
15:j:7:MET:HE1	15:j:44:LYS:HG3	2.03	0.41
23:v:38:VAL:HG12	23:v:59:LEU:HB2	2.03	0.41
7:a:614:A:H3'	7:a:615:U:C5'	2.51	0.40
7:a:819:A:C4	7:a:1189:A:C2	3.09	0.40
7:a:2209:G:N2	7:a:2215:C:N3	2.67	0.40
7:a:2238:G:N3	7:a:2238:G:H2'	2.36	0.40
3:d:56:LYS:O	3:d:57:ALA:C	2.65	0.40
7:a:1846:G:C6	7:a:1847:A:C6	3.09	0.40
7:a:2291:U:H2'	7:a:2292:U:C6	2.56	0.40
6:4:41:HIS:HA	6:4:42:PRO:HD3	1.93	0.40
21:r:11:ARG:NH1	21:r:99:ARG:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	36/38 (95%)	36 (100%)	0	0	100	100
2	c	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
3	d	205/209 (98%)	199 (97%)	6 (3%)	0	100	100
4	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
5	z	52/57 (91%)	51 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	4	48/70 (69%)	45 (94%)	2 (4%)	1 (2%)	5	7
9	0	49/55 (89%)	49 (100%)	0	0	100	100
10	1	44/46 (96%)	44 (100%)	0	0	100	100
11	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	11
12	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
13	h	38/149 (26%)	34 (90%)	4 (10%)	0	100	100
14	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
15	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
16	k	141/144 (98%)	134 (95%)	5 (4%)	2 (1%)	9	13
17	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
18	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
19	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
20	q	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	12	20
21	r	108/110 (98%)	105 (97%)	2 (2%)	1 (1%)	14	22
22	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
23	v	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
24	w	75/78 (96%)	75 (100%)	0	0	100	100
25	x	57/63 (90%)	57 (100%)	0	0	100	100
26	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
29	e	195/201 (97%)	191 (98%)	4 (2%)	0	100	100
30	g	135/177 (76%)	129 (96%)	6 (4%)	0	100	100
31	o	107/115 (93%)	105 (98%)	2 (2%)	0	100	100
32	s	82/100 (82%)	80 (98%)	2 (2%)	0	100	100
33	t	90/104 (86%)	87 (97%)	3 (3%)	0	100	100
34	C	2/9 (22%)	2 (100%)	0	0	100	100
34	D	2/9 (22%)	2 (100%)	0	0	100	100
All	All	3040/3355 (91%)	2948 (97%)	86 (3%)	6 (0%)	44	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	r	40	ASN
6	4	4	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	2	28	ASN
16	k	35	HIS
16	k	29	LYS
20	q	45	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	34/34 (100%)	34 (100%)	0	100	100
2	c	216/218 (99%)	214 (99%)	2 (1%)	70	85
3	d	162/163 (99%)	160 (99%)	2 (1%)	63	81
4	l	107/107 (100%)	106 (99%)	1 (1%)	70	85
5	z	46/48 (96%)	46 (100%)	0	100	100
6	4	51/62 (82%)	51 (100%)	0	100	100
9	0	46/49 (94%)	45 (98%)	1 (2%)	45	67
10	1	38/38 (100%)	38 (100%)	0	100	100
11	2	51/52 (98%)	51 (100%)	0	100	100
12	f	148/150 (99%)	147 (99%)	1 (1%)	76	88
13	h	31/114 (27%)	30 (97%)	1 (3%)	34	56
14	i	115/116 (99%)	115 (100%)	0	100	100
15	j	104/104 (100%)	104 (100%)	0	100	100
16	k	102/103 (99%)	102 (100%)	0	100	100
17	m	98/103 (95%)	98 (100%)	0	100	100
18	n	86/87 (99%)	86 (100%)	0	100	100
19	p	89/90 (99%)	89 (100%)	0	100	100
20	q	84/84 (100%)	81 (96%)	3 (4%)	31	52
21	r	93/93 (100%)	92 (99%)	1 (1%)	65	82
22	u	78/78 (100%)	76 (97%)	2 (3%)	40	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	v	61/63 (97%)	61 (100%)	0	100	100
24	w	67/68 (98%)	66 (98%)	1 (2%)	57	77
25	x	54/55 (98%)	54 (100%)	0	100	100
26	y	48/49 (98%)	48 (100%)	0	100	100
29	e	164/165 (99%)	163 (99%)	1 (1%)	78	89
30	g	107/138 (78%)	105 (98%)	2 (2%)	50	71
31	o	97/100 (97%)	97 (100%)	0	100	100
32	s	75/84 (89%)	75 (100%)	0	100	100
33	t	76/85 (89%)	76 (100%)	0	100	100
34	C	3/3 (100%)	3 (100%)	0	100	100
34	D	3/3 (100%)	3 (100%)	0	100	100
All	All	2534/2706 (94%)	2516 (99%)	18 (1%)	73	88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	c	36	LYS
2	c	182	ARG
3	d	12	THR
3	d	32	ASN
4	l	80	VAL
9	o	5	ILE
12	f	152	LEU
13	h	37	VAL
20	q	48	LYS
20	q	58	VAL
20	q	71	LYS
21	r	31	GLN
22	u	41	GLU
22	u	65	VAL
24	w	2	SER
29	e	80	SER
30	g	99	LYS
30	g	102	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	13	ASN
2	c	53	HIS
2	c	90	ASN
2	c	197	ASN
3	d	58	ASN
4	l	60	GLN
4	l	97	GLN
5	z	6	ASN
6	4	33	ASN
6	4	65	ASN
9	0	45	GLN
14	i	47	HIS
14	i	128	ASN
14	i	138	GLN
18	n	29	HIS
19	p	52	GLN
19	p	72	ASN
21	r	9	HIS
21	r	31	GLN
21	r	40	ASN
22	u	5	ASN
22	u	24	ASN
22	u	49	ASN
24	w	6	GLN
24	w	36	HIS
25	x	27	ASN
25	x	58	ASN
26	y	9	GLN
29	e	136	GLN
30	g	104	ASN
31	o	7	GLN
31	o	12	GLN
32	s	48	GLN
33	t	74	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	Y	72/76 (94%)	19 (26%)	3 (4%)
28	Z	72/76 (94%)	16 (22%)	3 (4%)
7	a	2742/2904 (94%)	318 (11%)	0
8	b	110/120 (91%)	6 (5%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2996/3176 (94%)	359 (11%)	6 (0%)

All (359) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	a	2	G
7	a	10	A
7	a	34	U
7	a	42	A
7	a	58	G
7	a	63	A
7	a	71	A
7	a	74	A
7	a	75	G
7	a	86	G
7	a	101	A
7	a	102	U
7	a	118	A
7	a	119	A
7	a	120	U
7	a	125	A
7	a	126	A
7	a	139	U
7	a	140	C
7	a	141	G
7	a	142	A
7	a	163	C
7	a	165	A
7	a	181	A
7	a	196	A
7	a	199	A
7	a	200	U
7	a	215	G
7	a	216	A
7	a	221	A
7	a	222	A
7	a	233	A
7	a	248	G
7	a	249	C
7	a	250	G
7	a	265	A
7	a	272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	278	A
7	a	282	A
7	a	285	G
7	a	289	G
7	a	311	A
7	a	329	G
7	a	330	A
7	a	361	G
7	a	362	A
7	a	386	G
7	a	404	A
7	a	405	U
7	a	411	G
7	a	420	C
7	a	425	G
7	a	451	U
7	a	456	C
7	a	481	G
7	a	491	G
7	a	503	A
7	a	504	A
7	a	505	A
7	a	509	C
7	a	530	G
7	a	531	C
7	a	532	A
7	a	533	G
7	a	543	G
7	a	545	U
7	a	546	U
7	a	547	A
7	a	549	G
7	a	563	A
7	a	573	U
7	a	575	A
7	a	586	A
7	a	592	A
7	a	603	A
7	a	614	A
7	a	615	U
7	a	627	A
7	a	637	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	645	C
7	a	647	G
7	a	653	U
7	a	654	A
7	a	655	A
7	a	686	U
7	a	717	C
7	a	730	A
7	a	732	C
7	a	738	G
7	a	747	5MU
7	a	764	A
7	a	765	C
7	a	775	G
7	a	776	G
7	a	782	A
7	a	784	G
7	a	785	G
7	a	805	G
7	a	812	C
7	a	827	U
7	a	828	U
7	a	846	U
7	a	847	U
7	a	858	G
7	a	859	G
7	a	877	A
7	a	879	G
7	a	881	G
7	a	883	G
7	a	884	U
7	a	885	C
7	a	890	C
7	a	891	G
7	a	895	U
7	a	896	A
7	a	897	C
7	a	898	C
7	a	905	A
7	a	910	A
7	a	927	A
7	a	931	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	934	U
7	a	946	C
7	a	961	C
7	a	974	G
7	a	983	A
7	a	984	A
7	a	985	C
7	a	996	A
7	a	1009	A
7	a	1012	U
7	a	1013	C
7	a	1022	G
7	a	1025	G
7	a	1026	G
7	a	1033	U
7	a	1045	C
7	a	1047	G
7	a	1112	G
7	a	1115	G
7	a	1116	G
7	a	1122	G
7	a	1128	G
7	a	1129	A
7	a	1132	U
7	a	1133	A
7	a	1134	A
7	a	1135	C
7	a	1136	G
7	a	1142	A
7	a	1171	G
7	a	1253	A
7	a	1254	A
7	a	1256	G
7	a	1271	G
7	a	1272	A
7	a	1294	U
7	a	1300	G
7	a	1301	A
7	a	1338	G
7	a	1352	U
7	a	1357	C
7	a	1365	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	1379	U
7	a	1383	A
7	a	1409	U
7	a	1411	U
7	a	1416	G
7	a	1419	A
7	a	1421	G
7	a	1428	C
7	a	1452	G
7	a	1453	A
7	a	1478	G
7	a	1482	G
7	a	1493	C
7	a	1509	A
7	a	1510	G
7	a	1515	A
7	a	1534	U
7	a	1535	A
7	a	1536	C
7	a	1537	G
7	a	1559	U
7	a	1569	A
7	a	1578	U
7	a	1585	C
7	a	1608	A
7	a	1609	A
7	a	1647	U
7	a	1648	U
7	a	1674	G
7	a	1703	G
7	a	1713	A
7	a	1715	G
7	a	1729	U
7	a	1730	C
7	a	1731	G
7	a	1732	C
7	a	1733	G
7	a	1738	G
7	a	1744	A
7	a	1750	G
7	a	1764	C
7	a	1773	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	1782	U
7	a	1800	C
7	a	1801	A
7	a	1807	G
7	a	1808	A
7	a	1816	C
7	a	1829	A
7	a	1842	G
7	a	1847	A
7	a	1848	A
7	a	1855	U
7	a	1858	A
7	a	1862	G
7	a	1870	C
7	a	1871	A
7	a	1873	G
7	a	1906	G
7	a	1907	G
7	a	1913	A
7	a	1929	G
7	a	1930	G
7	a	1937	A
7	a	1938	A
7	a	1955	U
7	a	1965	C
7	a	1967	C
7	a	1970	A
7	a	1971	U
7	a	1972	G
7	a	1982	U
7	a	1991	U
7	a	1993	U
7	a	2023	C
7	a	2031	A
7	a	2033	A
7	a	2043	C
7	a	2055	C
7	a	2056	G
7	a	2060	A
7	a	2061	G
7	a	2069	G7M
7	a	2198	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	2204	G
7	a	2211	A
7	a	2225	A
7	a	2238	G
7	a	2239	G
7	a	2268	A
7	a	2282	G
7	a	2283	C
7	a	2287	A
7	a	2305	U
7	a	2308	G
7	a	2312	U
7	a	2322	A
7	a	2325	G
7	a	2333	A
7	a	2335	A
7	a	2340	A
7	a	2347	C
7	a	2361	G
7	a	2366	A
7	a	2377	A
7	a	2383	G
7	a	2385	C
7	a	2402	U
7	a	2406	A
7	a	2423	U
7	a	2424	C
7	a	2425	A
7	a	2429	G
7	a	2430	A
7	a	2435	A
7	a	2441	U
7	a	2448	A
7	a	2469	A
7	a	2476	A
7	a	2480	C
7	a	2491	U
7	a	2502	G
7	a	2505	G
7	a	2518	A
7	a	2529	G
7	a	2547	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	2554	U
7	a	2566	A
7	a	2567	G
7	a	2573	C
7	a	2602	A
7	a	2603	G
7	a	2609	U
7	a	2613	U
7	a	2629	U
7	a	2663	G
7	a	2682	A
7	a	2689	U
7	a	2690	U
7	a	2714	G
7	a	2724	U
7	a	2726	A
7	a	2744	G
7	a	2748	A
7	a	2765	A
7	a	2778	A
7	a	2790	U
7	a	2791	G
7	a	2820	A
7	a	2821	A
7	a	2861	U
7	a	2867	G
7	a	2868	A
7	a	2884	U
7	a	2899	A
8	b	44	G
8	b	45	A
8	b	56	G
8	b	64	G
8	b	99	A
8	b	109	A
27	Y	3	C
27	Y	5	G
27	Y	10	G
27	Y	14	A
27	Y	19	G
27	Y	20	U
27	Y	21	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	Y	22	G
27	Y	24	G
27	Y	43	C
27	Y	45	U
27	Y	46	G
27	Y	47	U
27	Y	48	C
27	Y	49	C
27	Y	69	G
27	Y	71	G
27	Y	73	A
27	Y	74	C
28	Z	6	A
28	Z	7	U
28	Z	9	A
28	Z	10	G
28	Z	19	G
28	Z	21	A
28	Z	22	G
28	Z	42	G
28	Z	46	G
28	Z	47	U
28	Z	48	C
28	Z	49	G
28	Z	51	C
28	Z	58	A
28	Z	68	C
28	Z	76	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	Y	13	C
27	Y	20	U
27	Y	47	U
28	Z	6	A
28	Z	9	A
28	Z	48	C

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

Of 39 non-standard protein/DNA/RNA residues modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 37 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PSU	a	1917	7	18,21,22	0.82	1 (5%)	22,30,33	0.68	0
7	PSU	a	2504	7	18,21,22	0.93	1 (5%)	22,30,33	0.87	0
7	2MG	a	1835	7	23,26,27	0.37	0	32,38,41	0.47	0
7	PSU	a	955	7	18,21,22	0.90	1 (5%)	22,30,33	0.75	0
7	H2U	a	2449	7	18,21,22	0.78	1 (5%)	21,30,33	1.00	2 (9%)
7	G7M	a	2069	7	23,26,27	0.74	1 (4%)	35,39,42	0.63	0
7	2MG	a	2445	7	23,26,27	0.49	0	32,38,41	0.39	0
7	PSU	a	2457	7	18,21,22	0.89	1 (5%)	22,30,33	0.68	0
7	5MC	a	1962	7	18,22,23	0.48	0	26,32,35	0.69	1 (3%)
7	PSU	a	2580	36,7	18,21,22	0.80	1 (5%)	22,30,33	0.96	1 (4%)
7	OMC	a	2498	36,7	19,22,23	0.41	0	26,31,34	0.46	0
7	PSU	a	2605	7	18,21,22	0.87	2 (11%)	22,30,33	0.91	0
7	PSU	a	2604	7	18,21,22	0.91	1 (5%)	22,30,33	0.83	1 (4%)
7	2MA	a	2503	36,7	22,25,26	0.43	0	33,37,40	0.69	1 (3%)
7	3TD	a	1915	-	18,22,23	0.81	1 (5%)	22,32,35	0.77	0
7	5MU	a	747	7	19,22,23	0.44	0	28,32,35	0.60	1 (3%)
7	OMU	a	2552	7	19,22,23	0.43	0	26,31,34	0.51	0
4	MS6	l	82	4	5,7,8	0.25	0	2,7,9	0.06	0
4	4D4	l	81	4	9,11,12	0.48	0	8,13,15	1.08	1 (12%)
7	5MU	a	1939	7	19,22,23	0.49	0	28,32,35	0.41	0
7	OMG	a	2251	28,7	23,26,27	0.36	0	33,38,41	0.47	0
34	ORD	C	2	34	6,7,8	1.12	1 (16%)	2,7,9	0.49	0
7	1MG	a	745	7	22,26,27	0.61	0	33,39,42	0.53	0
7	PSU	a	746	36,7	18,21,22	0.96	1 (5%)	22,30,33	0.67	0
34	ORD	D	2	34	6,7,8	1.18	1 (16%)	2,7,9	0.95	0
7	PSU	a	1911	7	18,21,22	0.93	1 (5%)	22,30,33	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MEQ	d	150	3	8,9,10	0.55	0	5,10,12	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PSU	a	1917	7	-	0/7/25/26	0/2/2/2
7	PSU	a	2504	7	-	0/7/25/26	0/2/2/2
7	2MG	a	1835	7	-	0/9/27/28	0/3/3/3
7	PSU	a	955	7	-	0/7/25/26	0/2/2/2
7	H2U	a	2449	7	-	0/7/38/39	0/2/2/2
7	G7M	a	2069	7	-	2/7/25/26	0/3/3/3
7	2MG	a	2445	7	-	0/9/27/28	0/3/3/3
7	PSU	a	2457	7	-	0/7/25/26	0/2/2/2
7	5MC	a	1962	7	-	0/7/25/26	0/2/2/2
7	PSU	a	2580	36,7	-	0/7/25/26	0/2/2/2
7	OMC	a	2498	36,7	-	0/9/27/28	0/2/2/2
7	PSU	a	2605	7	-	0/7/25/26	0/2/2/2
7	PSU	a	2604	7	-	0/7/25/26	0/2/2/2
7	2MA	a	2503	36,7	-	2/7/25/26	0/3/3/3
7	3TD	a	1915	-	-	0/7/25/26	0/2/2/2
7	5MU	a	747	7	-	0/7/25/26	0/2/2/2
7	OMU	a	2552	7	-	0/9/27/28	0/2/2/2
4	MS6	l	82	4	-	1/4/6/8	-
4	4D4	l	81	4	-	4/11/12/14	-
7	5MU	a	1939	7	-	0/7/25/26	0/2/2/2
7	OMG	a	2251	28,7	-	0/9/27/28	0/3/3/3
34	ORD	C	2	34	-	0/5/6/8	-
7	1MG	a	745	7	-	0/7/25/26	0/3/3/3
7	PSU	a	746	36,7	-	1/7/25/26	0/2/2/2
34	ORD	D	2	34	-	2/5/6/8	-
7	PSU	a	1911	7	-	0/7/25/26	0/2/2/2
3	MEQ	d	150	3	-	2/8/9/11	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	1911	PSU	C6-C5	3.43	1.39	1.35
7	a	1917	PSU	C6-C5	3.09	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	1915	3TD	C6-C5	3.09	1.38	1.35
7	a	746	PSU	C6-C5	3.07	1.38	1.35
7	a	2604	PSU	C6-C5	3.04	1.38	1.35
7	a	2580	PSU	C6-C5	2.92	1.38	1.35
7	a	955	PSU	C6-C5	2.85	1.38	1.35
7	a	2457	PSU	C6-C5	2.84	1.38	1.35
7	a	2504	PSU	C6-C5	2.65	1.38	1.35
7	a	2605	PSU	C6-C5	2.56	1.38	1.35
34	D	2	ORD	O-C	2.55	1.30	1.19
7	a	2069	G7M	C8-N7	2.39	1.37	1.33
34	C	2	ORD	O-C	2.27	1.29	1.19
7	a	2449	H2U	C2-N3	-2.17	1.34	1.38
7	a	2605	PSU	C4-C5	-2.13	1.38	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	2580	PSU	C3'-C2'-C1'	3.02	105.15	101.64
7	a	2449	H2U	N3-C2-N1	2.77	119.58	116.65
4	l	81	4D4	CB-CA-C	-2.44	107.88	111.77
7	a	747	5MU	O3'-C3'-C4'	-2.36	104.23	111.05
7	a	2449	H2U	O2-C2-N1	-2.35	120.15	123.11
7	a	1962	5MC	C5-C6-N1	-2.31	120.97	123.34
7	a	2503	2MA	C5-C4-N3	-2.20	124.72	127.19
7	a	2604	PSU	C2'-C3'-C4'	-2.11	98.54	102.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	D	2	ORD	O-C-CA-CB
3	d	150	MEQ	OE1-CD-CG-CB
3	d	150	MEQ	NE2-CD-CG-CB
4	l	81	4D4	OB-CB-CG-CD
34	D	2	ORD	N-CA-CB-CG
4	l	81	4D4	CA-CB-CG-CD
4	l	81	4D4	CG-CD-NE-CZ
7	a	2069	G7M	O4'-C4'-C5'-O5'
7	a	746	PSU	O4'-C1'-C5-C6
7	a	2503	2MA	O4'-C4'-C5'-O5'
7	a	2503	2MA	O4'-C1'-N9-C8
4	l	82	MS6	CB-CG-SD-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	l	81	4D4	O-C-CA-CB
7	a	2069	G7M	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	a	1915	3TD	9	0
7	a	2552	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 217 ligands modelled in this entry, 217 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	a	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1914:C	O3'	1915:3TD	P	2.34
1	a	1915:3TD	O3'	1916:A	P	2.25

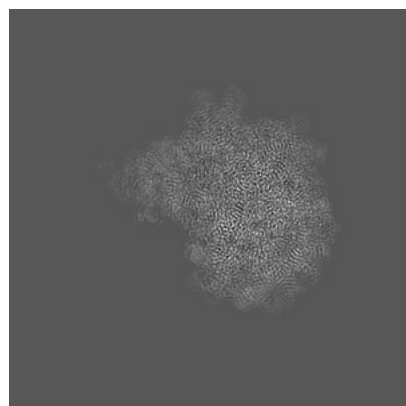
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53943. These allow visual inspection of the internal detail of the map and identification of artifacts.

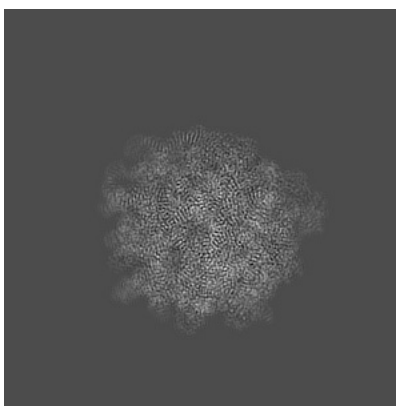
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

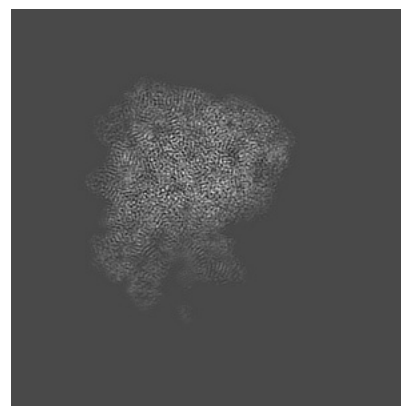
6.1.1 Primary map



X

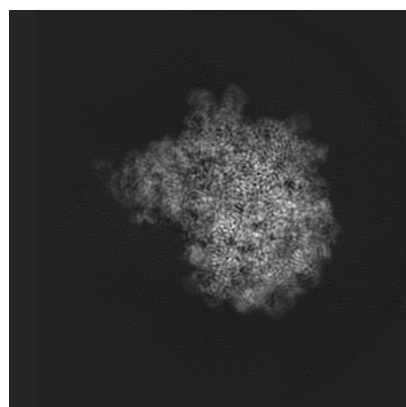


Y

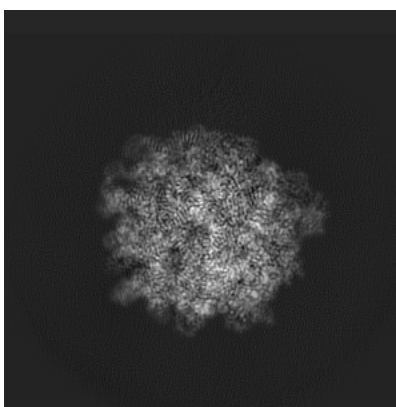


Z

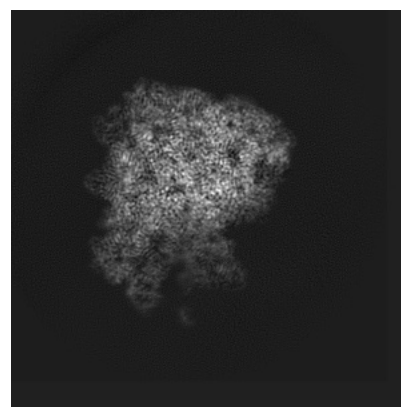
6.1.2 Raw map



X



Y

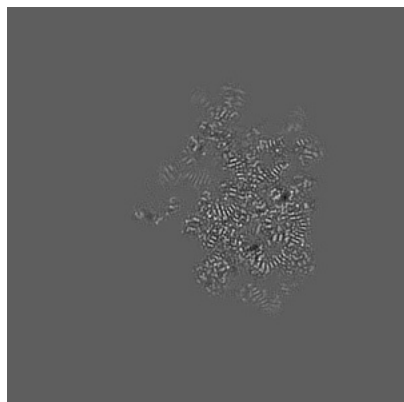


Z

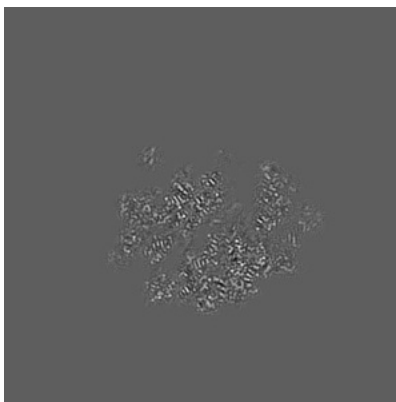
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

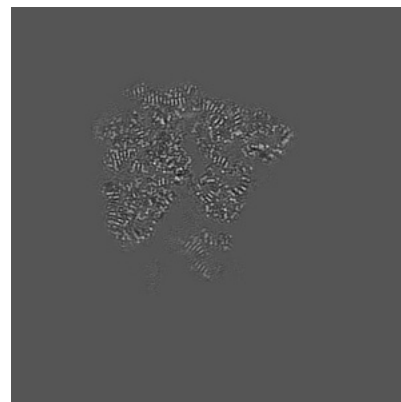
6.2.1 Primary map



X Index: 216

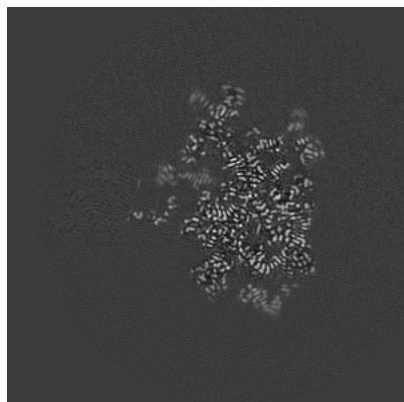


Y Index: 216

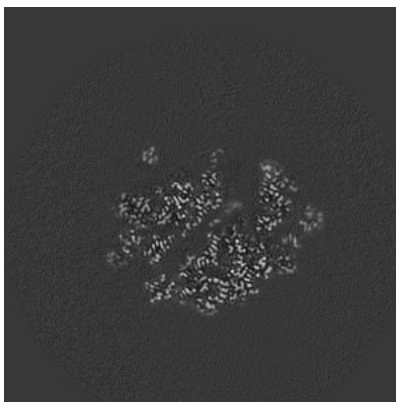


Z Index: 216

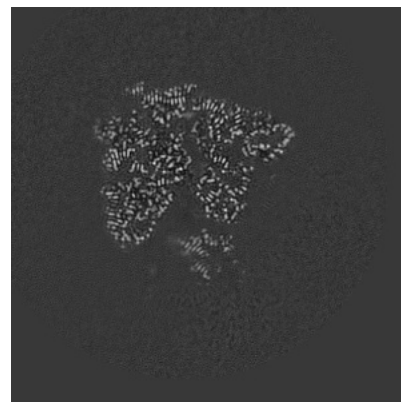
6.2.2 Raw map



X Index: 216



Y Index: 216

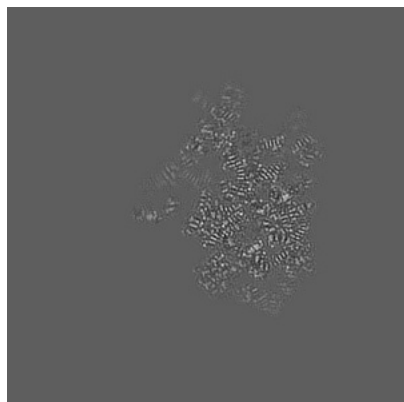


Z Index: 216

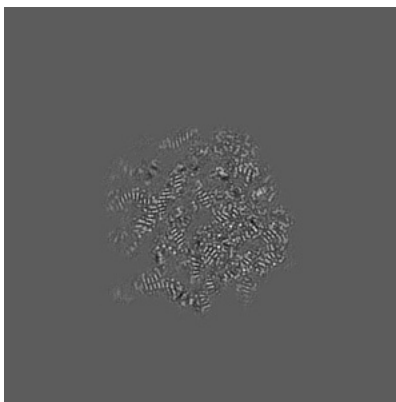
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

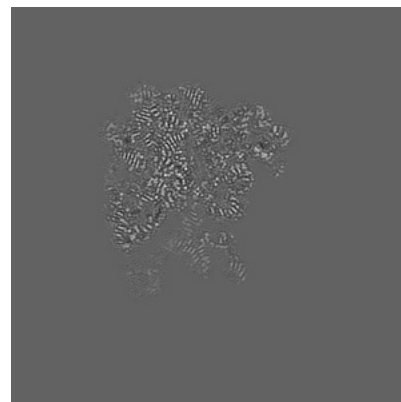
6.3.1 Primary map



X Index: 218

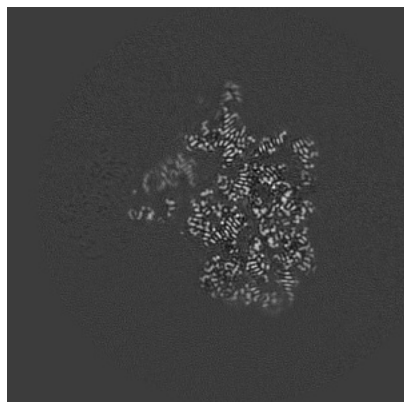


Y Index: 266

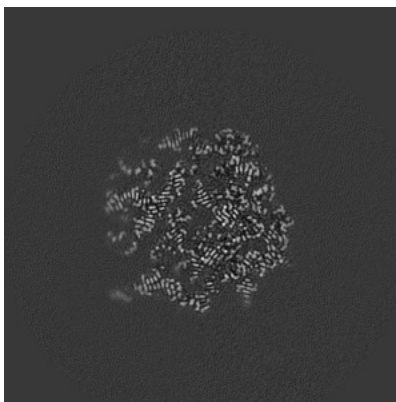


Z Index: 223

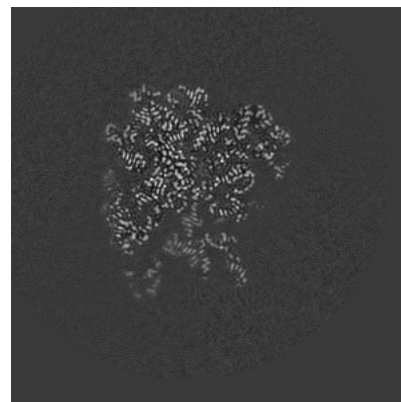
6.3.2 Raw map



X Index: 223



Y Index: 267

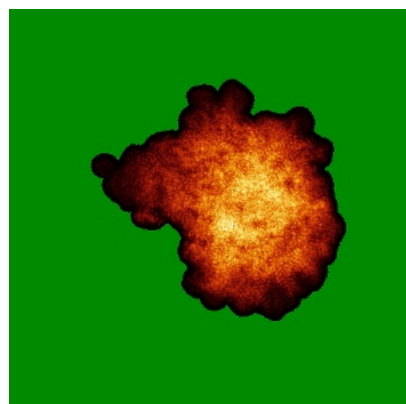


Z Index: 224

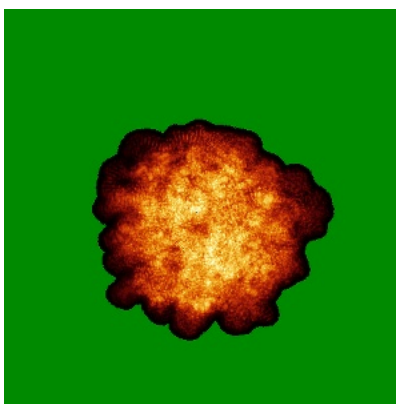
The images above show the largest variance slices of the map in three orthogonal directions.

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

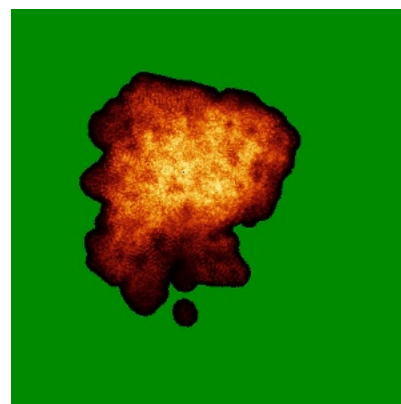
6.4.1 Primary map



X

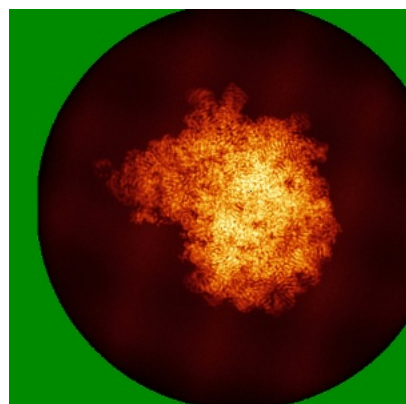


Y

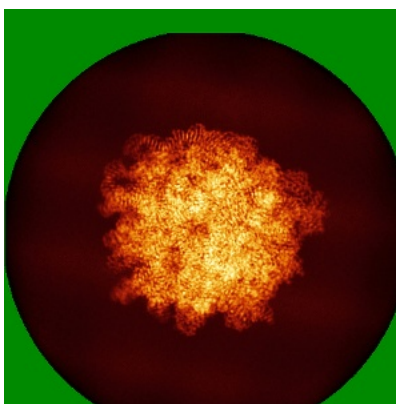


Z

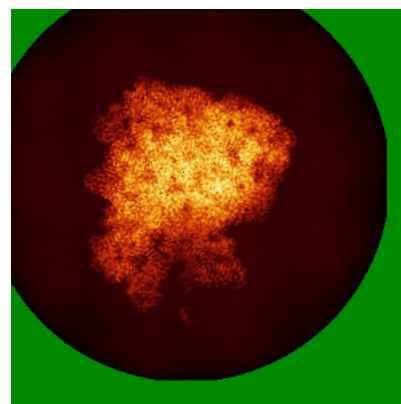
6.4.2 Raw map



X



Y

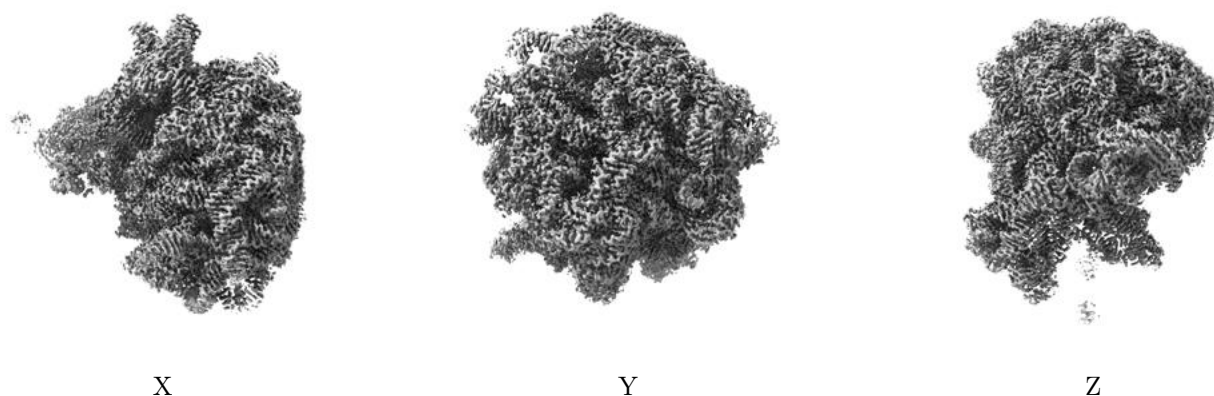


Z

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.

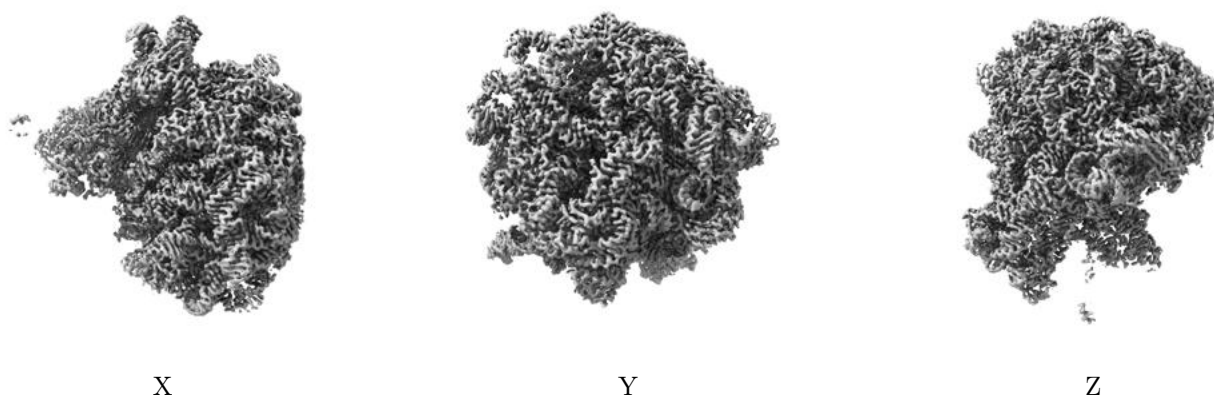
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0166. 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.

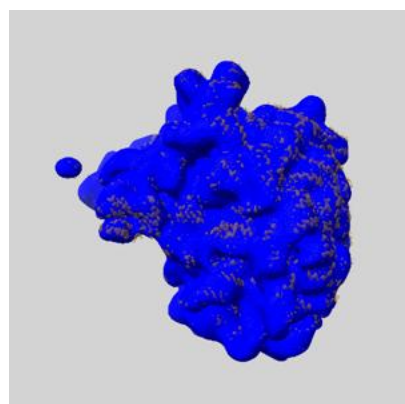
6.6 Mask visualisation [i](#)

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

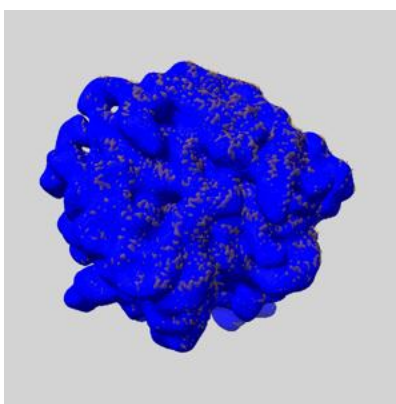
A mask typically either:

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

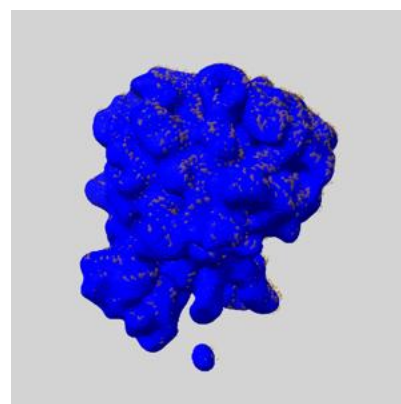
6.6.1 emd_53943_msk_1.map [i](#)



X



Y

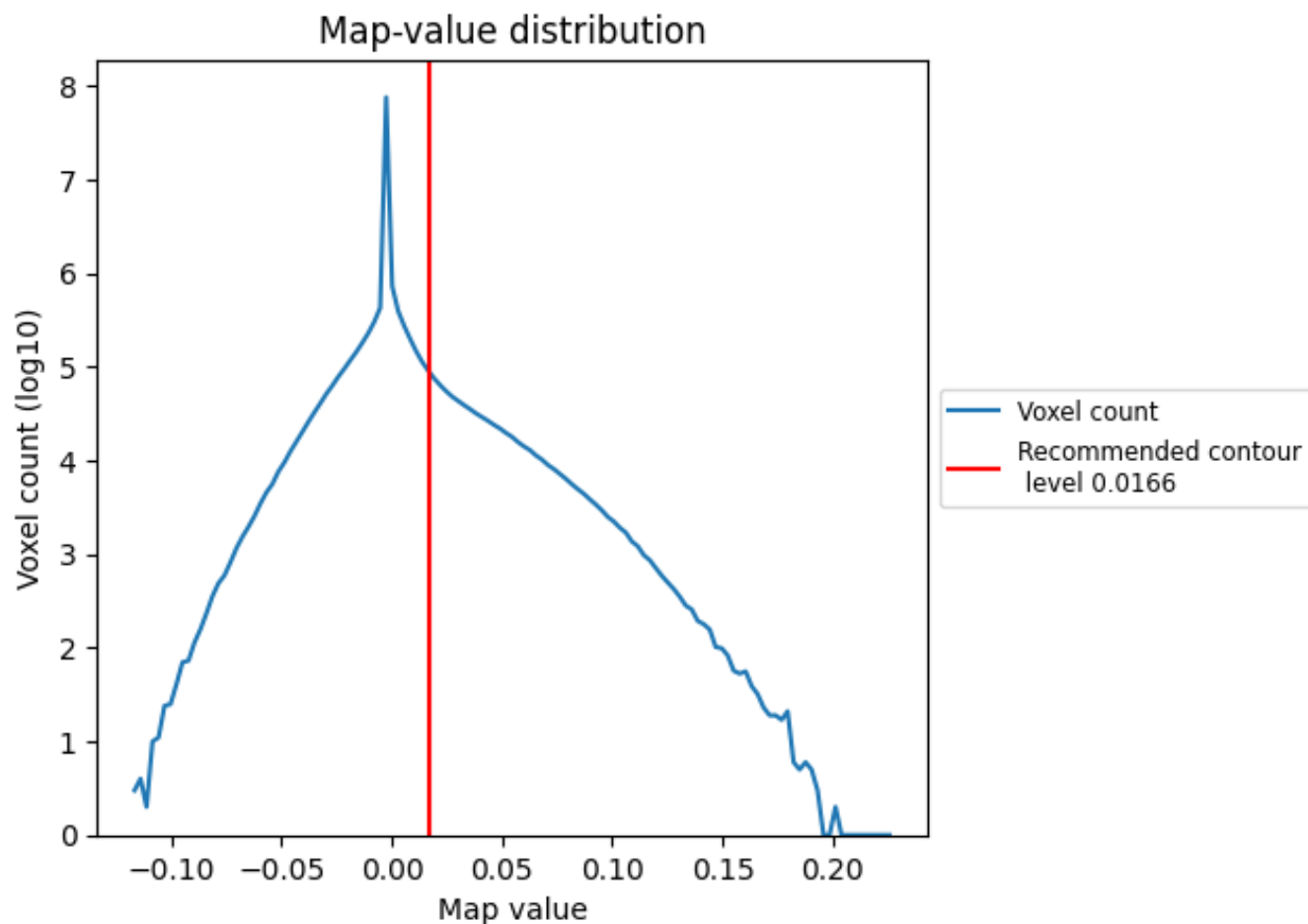


Z

7 Map analysis [i](#)

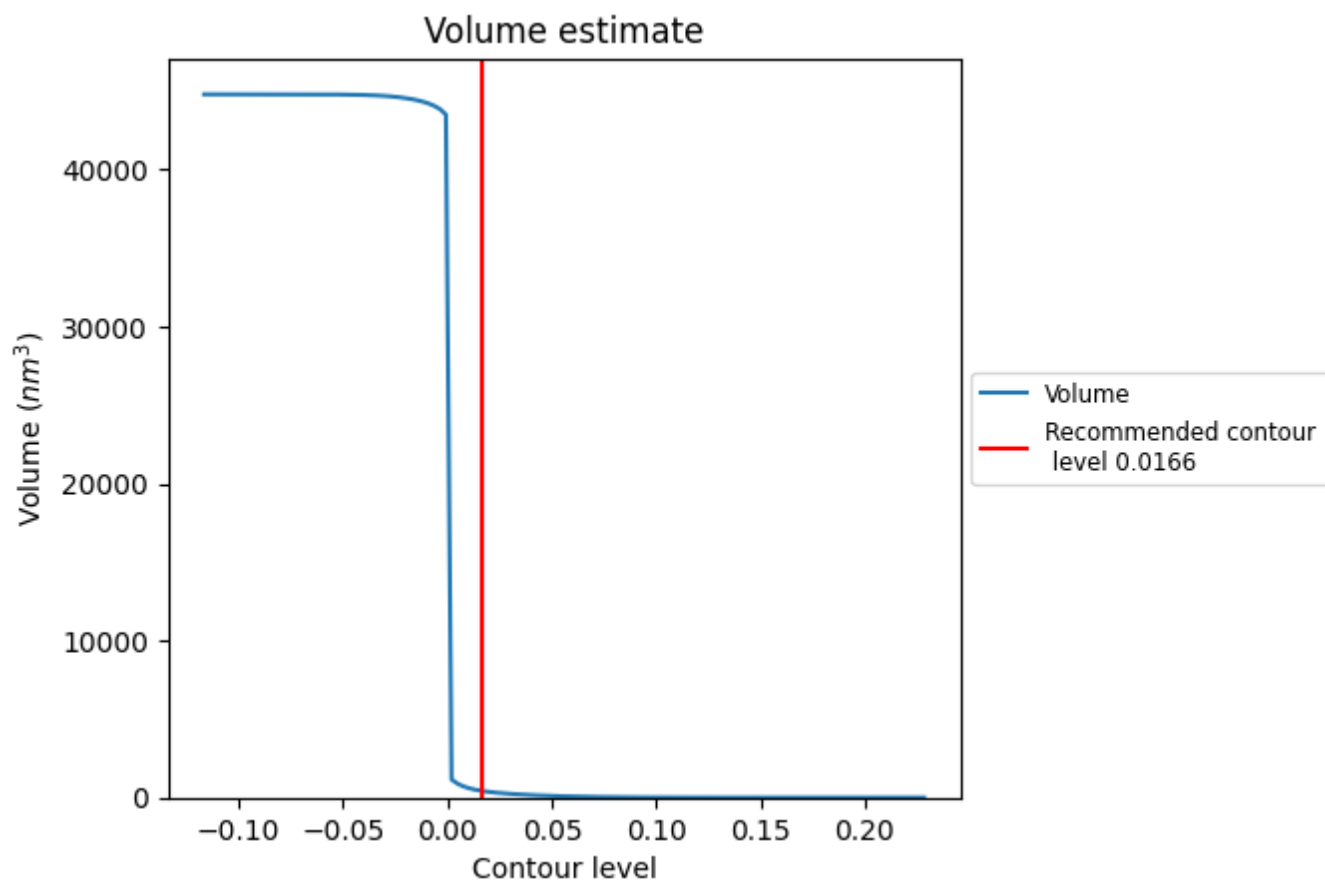
This section contains the results of statistical analysis of the map.

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.

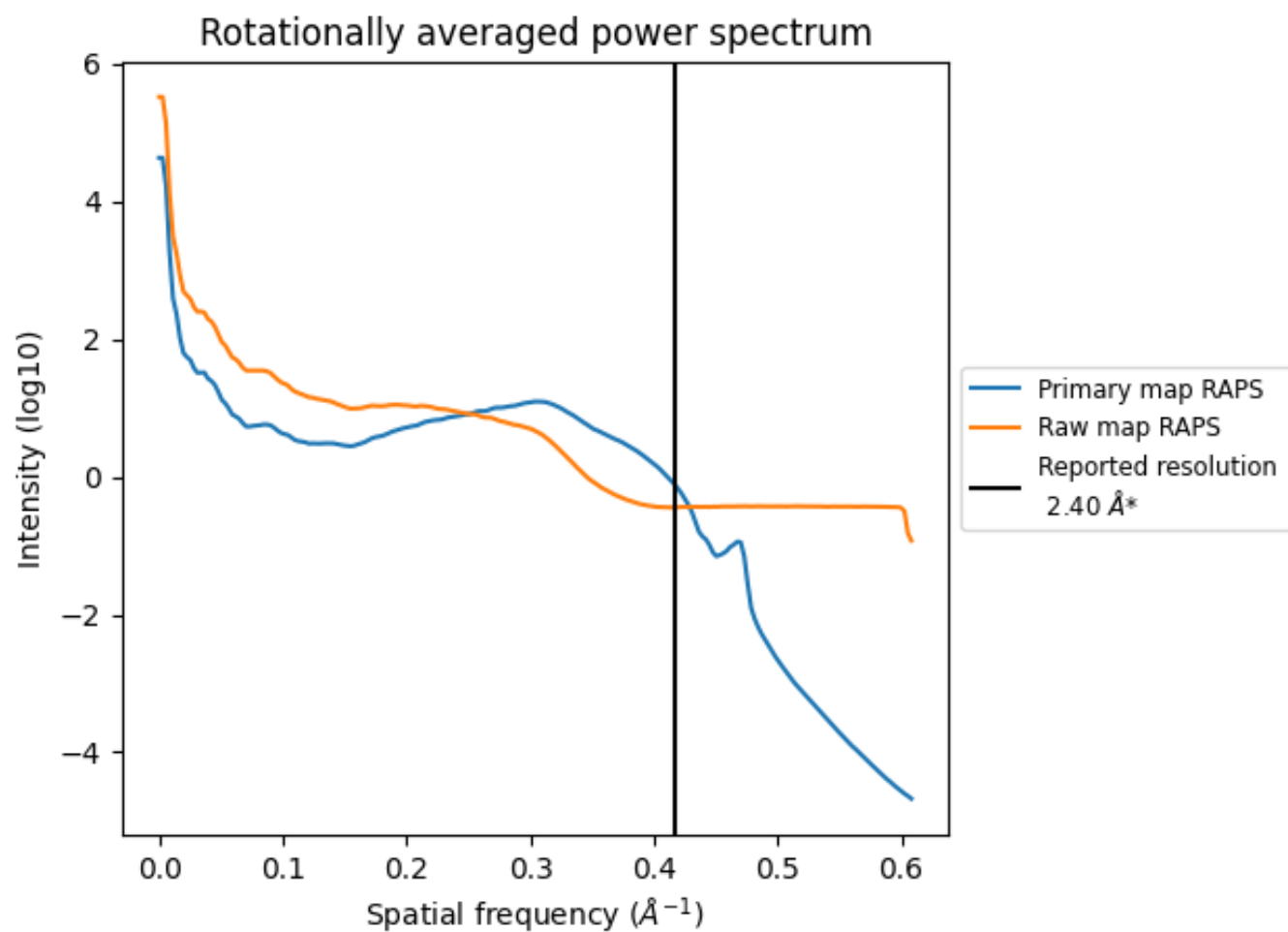
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm^3 ; this corresponds to an approximate mass of 382 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

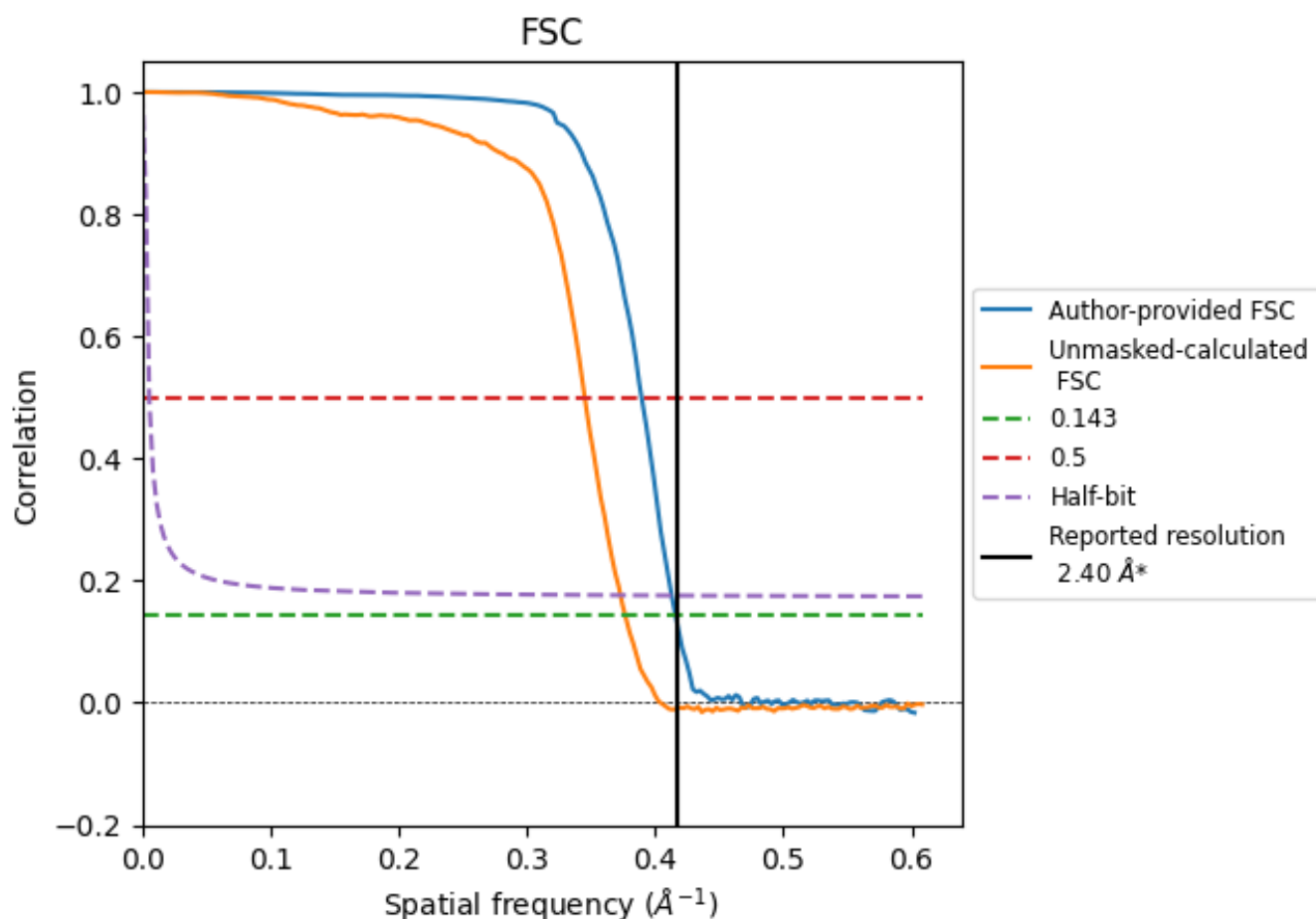


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.417 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

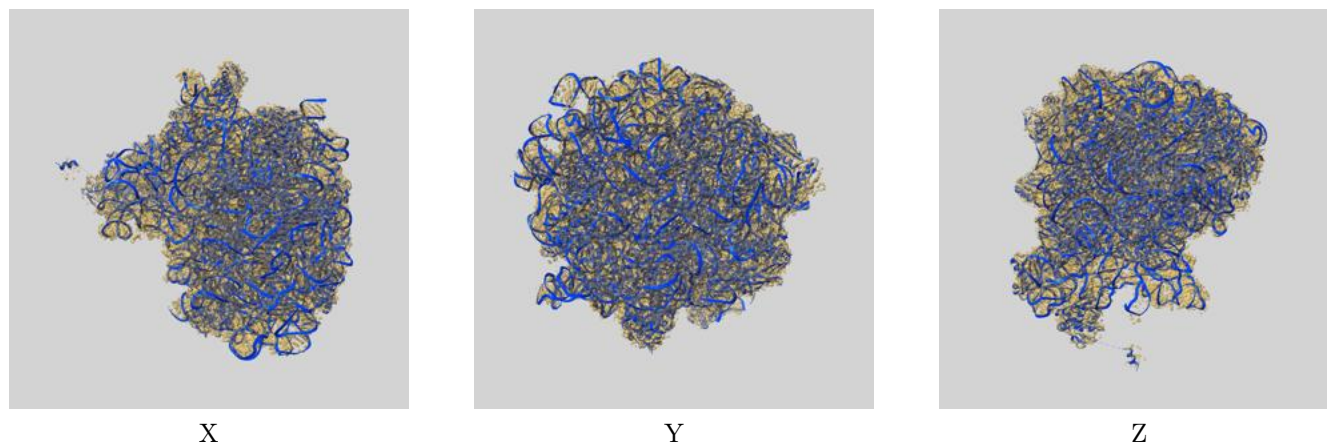
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.57	2.42
Unmasked-calculated*	2.65	2.90	2.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.65 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

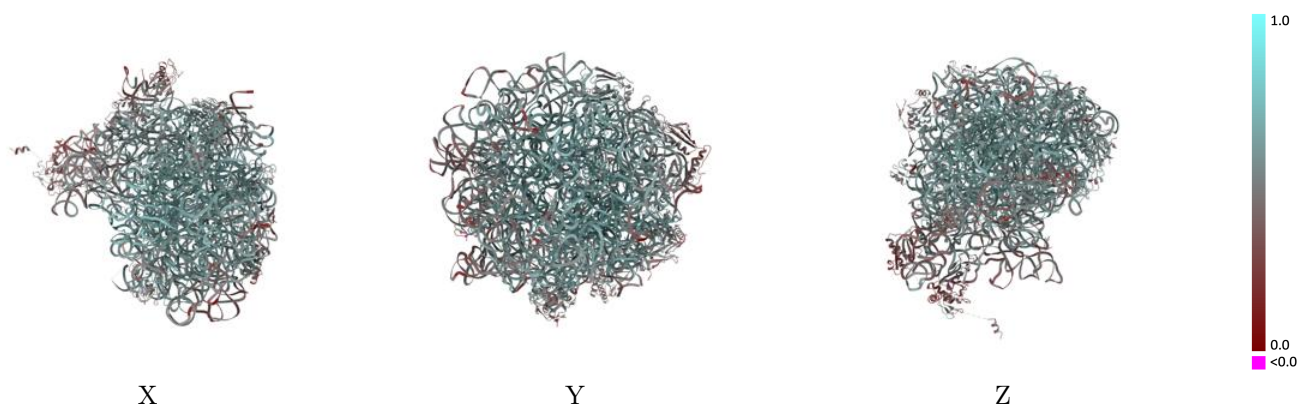
This section contains information regarding the fit between EMDB map EMD-53943 and PDB model 9RFW. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



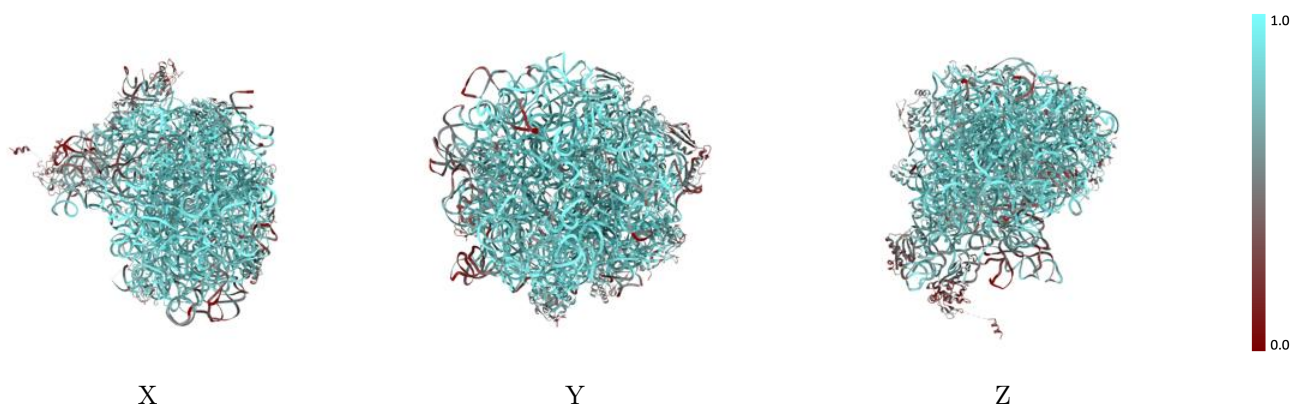
The images above show the 3D surface view of the map at the recommended contour level 0.0166 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



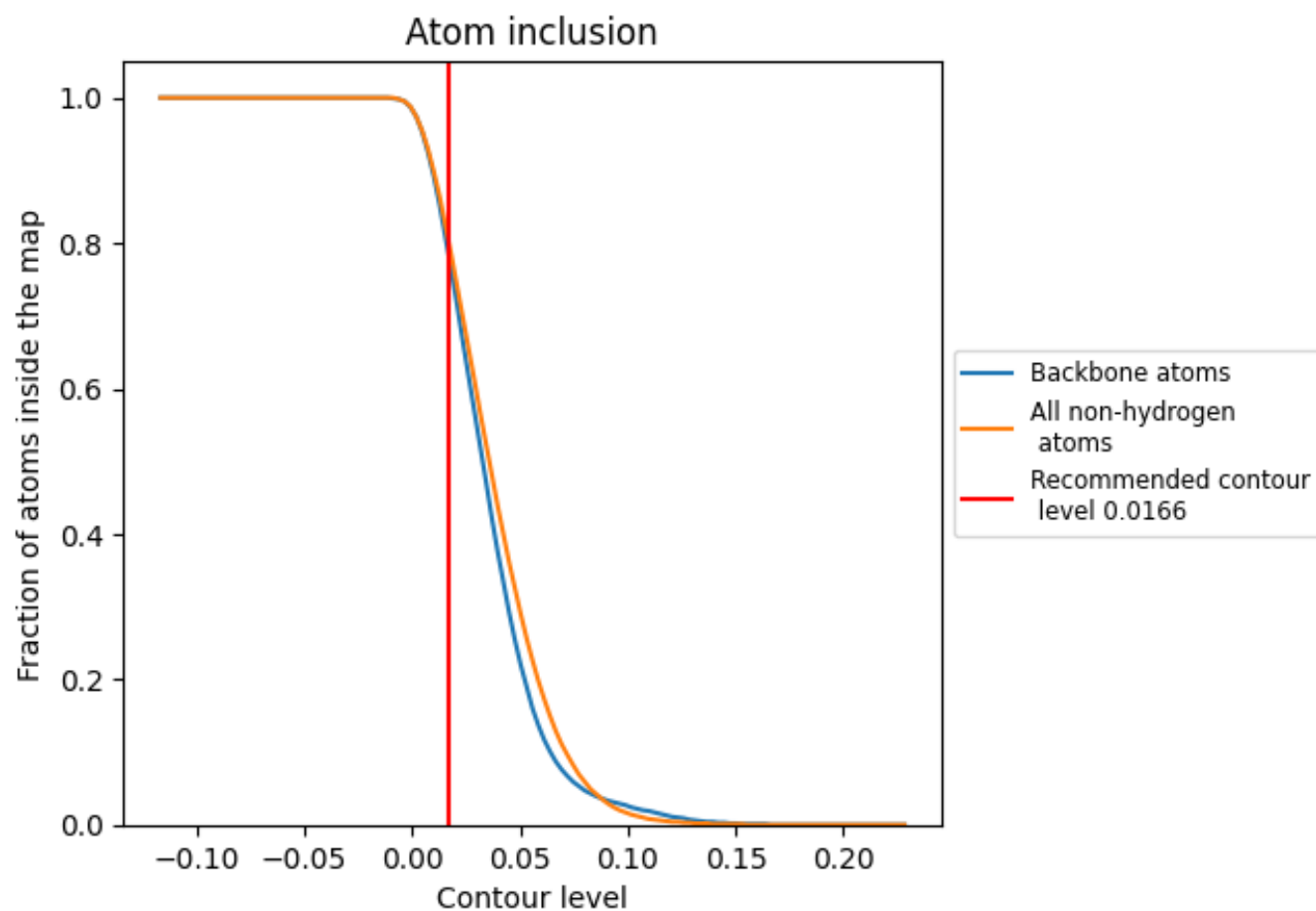
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0166).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 81% 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 (0.0166) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.5610
0	 0.7310	 0.5420
1	 0.9440	 0.6580
2	 0.9530	 0.6470
3	 0.8230	 0.5400
4	 0.3430	 0.4310
C	 0.9490	 0.6450
D	 0.6920	 0.5860
Y	 0.5090	 0.4700
Z	 0.6290	 0.4730
a	 0.8600	 0.5860
b	 0.6820	 0.4260
c	 0.8620	 0.5910
d	 0.8120	 0.5650
e	 0.7420	 0.5360
f	 0.3200	 0.3020
g	 0.4410	 0.3760
h	 0.4470	 0.3890
i	 0.8530	 0.5780
j	 0.8010	 0.5650
k	 0.8260	 0.5850
l	 0.8310	 0.5820
m	 0.8700	 0.5890
n	 0.4980	 0.3720
o	 0.7050	 0.5020
p	 0.8630	 0.6010
q	 0.7430	 0.5220
r	 0.8540	 0.6200
s	 0.7170	 0.5060
t	 0.6420	 0.4340
u	 0.6150	 0.4540
v	 0.8140	 0.5700
w	 0.8070	 0.5840
x	 0.5530	 0.4060
y	 0.8030	 0.5780
z	 0.8500	 0.6160

