



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 07:01 am BST

PDB ID : 8CEU / pdb_00008ceu
EMDB ID : EMD-16613
Title : Retapamulin and Capreomycin bound to the 50S subunit
Authors : Paternoga, H.; Beckert, B.; Wilson, D.N.
Deposited on : 2023-02-02
Resolution : 1.83 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:

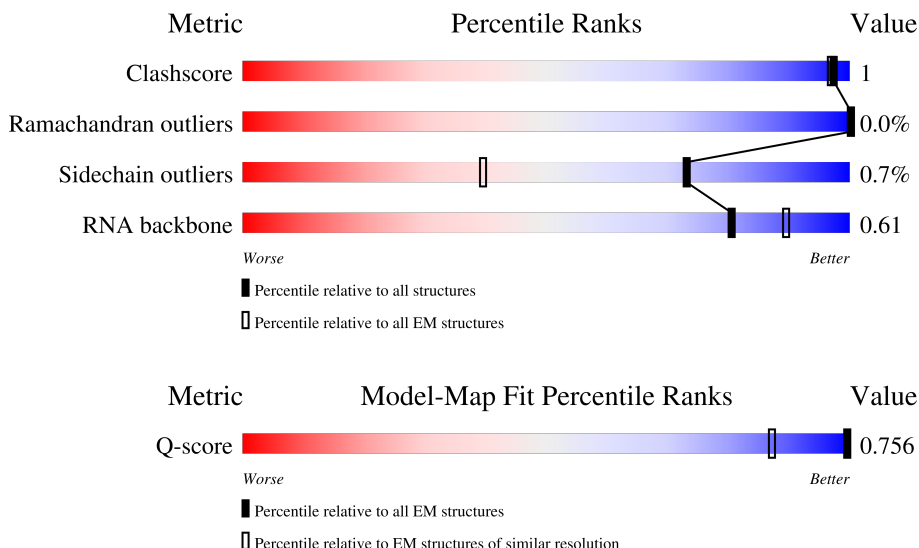
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 1.83 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	903 (1.33 - 2.33)

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	0	55	15% 91% 7%
2	1	46	98%
3	2	65	97%

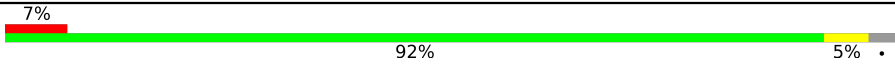
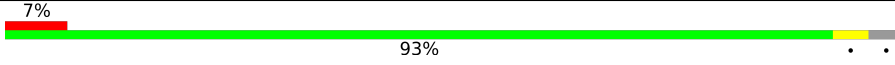
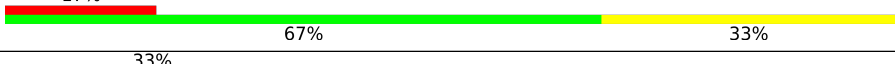
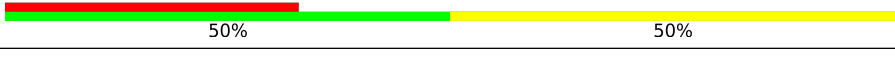
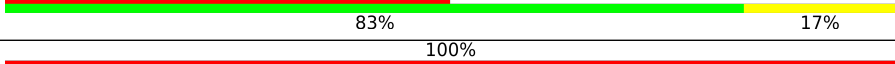
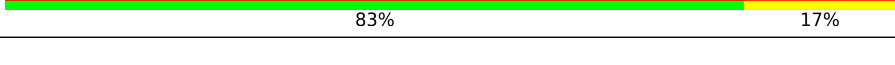
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Mol	Chain	Length	Quality of chain
4	3	38	
5	a	2904	
6	b	120	
7	c	273	
8	d	209	
9	e	201	
10	f	179	
11	g	177	
12	h	149	
13	i	142	
14	j	123	
15	k	144	
16	l	136	
17	m	127	
18	n	117	
19	o	115	
20	p	118	
21	q	103	
22	r	110	
23	s	100	
24	t	104	
25	u	94	
26	v	85	
27	w	78	
28	x	63	

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Mol	Chain	Length	Quality of chain
29	y	59	
30	z	57	
31	C	6	
31	D	6	
31	E	6	
31	F	6	
31	G	6	
31	H	6	
31	I	6	
31	V	6	

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
33	G34	a	3001	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 92830 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

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

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

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

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

- Molecule 5 is a RNA chain called 23S rRNA.

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

- Molecule 6 is a RNA chain called 5S rRNA.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	189	Total	C	N	O	S	0	0
			1463	918	269	271	5		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	121	Total	C	N	O	S	0	0
			974	625	169	174	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	172	Total	C	N	O	S	0	0
			1291	813	237	239	2		

- Molecule 12 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

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

There is a discrepancy between the modelled and reference sequences:

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

- 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 bL19.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	100	Total	C	N	O	S	0	0
			794	504	150	138	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	t	95	Total	C	N	O	0	0
			728	459	137	132		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 26 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	v	77	Total	C	N	O	S	0	0
			576	357	115	103	1		

- Molecule 27 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	y	57	Total	C	N	O	S	0	0
			444	278	86	78	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL32.

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

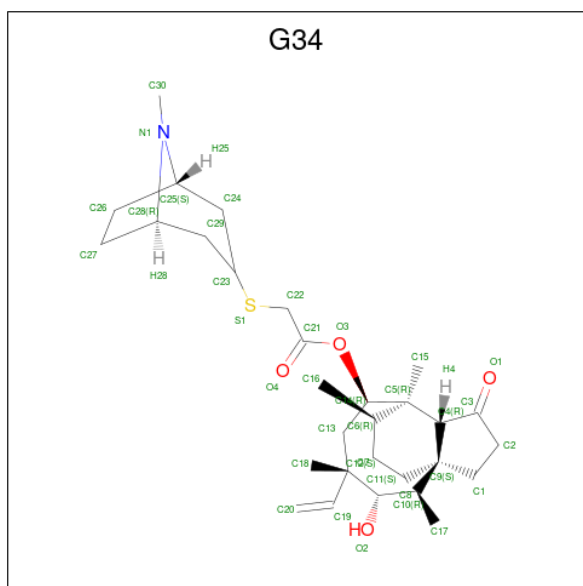
- Molecule 31 is a protein called Capreomycin IA.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	V	6	Total	C	N	O	0	0
			47	25	14	8		
31	C	6	Total	C	N	O	0	0
			47	25	14	8		
31	D	6	Total	C	N	O	0	0
			47	25	14	8		
31	E	6	Total	C	N	O	0	0
			47	25	14	8		
31	F	6	Total	C	N	O	0	0
			47	25	14	8		
31	G	6	Total	C	N	O	0	0
			47	25	14	8		
31	H	6	Total	C	N	O	0	0
			47	25	14	8		
31	I	6	Total	C	N	O	0	0
			47	25	14	8		

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	3	1	Total	Zn	0
			1	1	

- Molecule 33 is Retapamulin (CCD ID: G34) (formula: $C_{30}H_{47}NO_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	N	O	S	0
			36	30	1	4	1	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	a	209	Total	Mg	0
			209	209	
34	b	5	Total	Mg	0
			5	5	
34	c	2	Total	Mg	0
			2	2	
34	d	1	Total	Mg	0
			1	1	
34	p	1	Total	Mg	0
			1	1	
34	v	1	Total	Mg	0
			1	1	
34	z	1	Total	Mg	0
			1	1	

- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
35	a	75	Total K 75 75	0
35	c	3	Total K 3 3	0
35	e	1	Total K 1 1	0
35	t	1	Total K 1 1	0
35	v	1	Total K 1 1	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	0	11	Total O 11 11	0
36	1	31	Total O 31 31	0
36	2	29	Total O 29 29	0
36	3	10	Total O 10 10	0
36	a	5806	Total O 5806 5806	0
36	b	92	Total O 92 92	0
36	c	121	Total O 121 121	0
36	d	87	Total O 87 87	0
36	e	58	Total O 58 58	0
36	i	43	Total O 43 43	0
36	j	35	Total O 35 35	0
36	k	67	Total O 67 67	0
36	l	57	Total O 57 57	0
36	m	48	Total O 48 48	0

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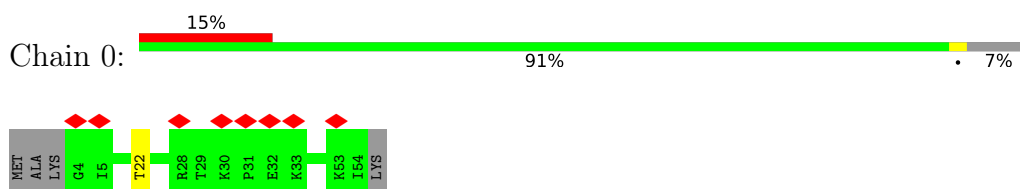
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Mol	Chain	Residues	Atoms		AltConf
36	n	6	Total 6	O 6	0
36	o	36	Total 36	O 36	0
36	p	63	Total 63	O 63	0
36	q	27	Total 27	O 27	0
36	r	42	Total 42	O 42	0
36	s	25	Total 25	O 25	0
36	t	13	Total 13	O 13	0
36	u	16	Total 16	O 16	0
36	v	27	Total 27	O 27	0
36	w	23	Total 23	O 23	0
36	x	5	Total 5	O 5	0
36	y	10	Total 10	O 10	0
36	z	35	Total 35	O 35	0
36	F	1	Total 1	O 1	0
36	G	3	Total 3	O 3	0
36	H	2	Total 2	O 2	0
36	I	1	Total 1	O 1	0

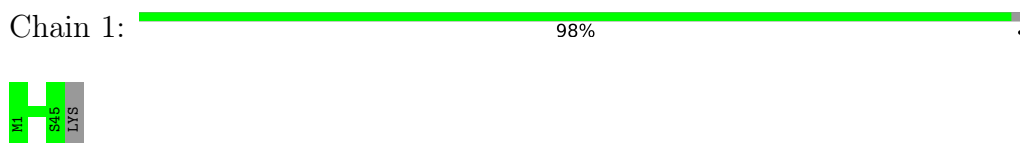
3 Residue-property plots [i](#)

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

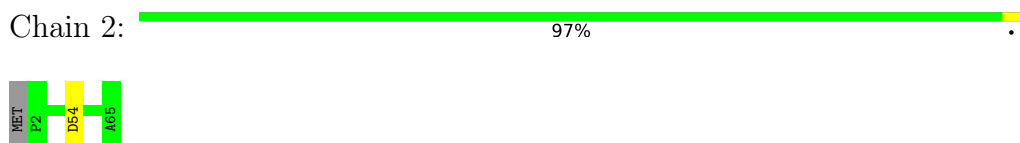
- Molecule 1: Large ribosomal subunit protein bL33



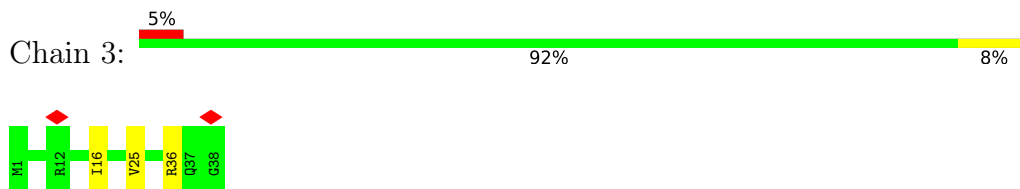
- Molecule 2: Large ribosomal subunit protein bL34



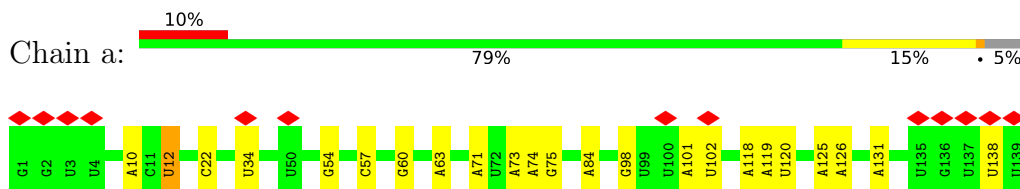
- Molecule 3: Large ribosomal subunit protein bL35

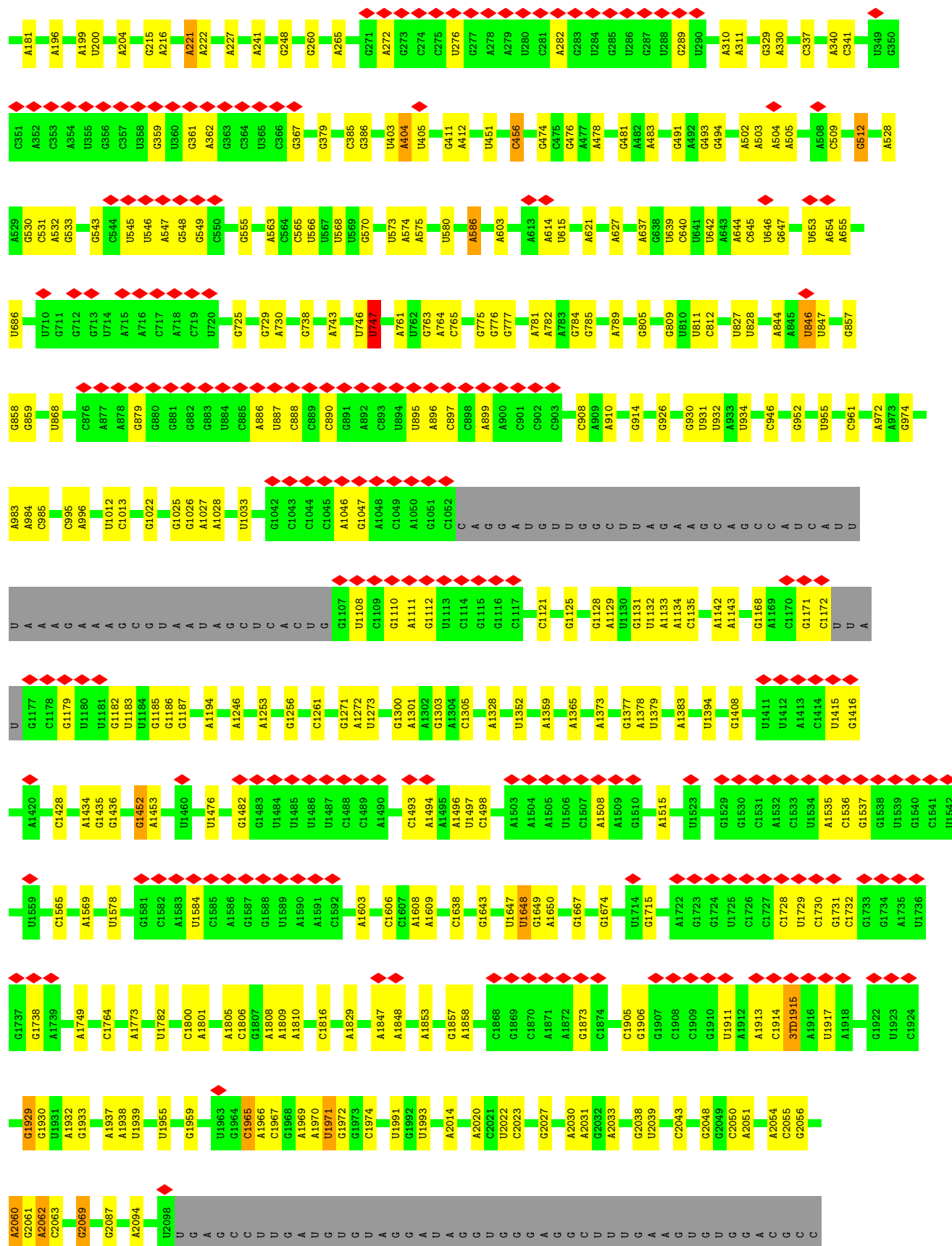


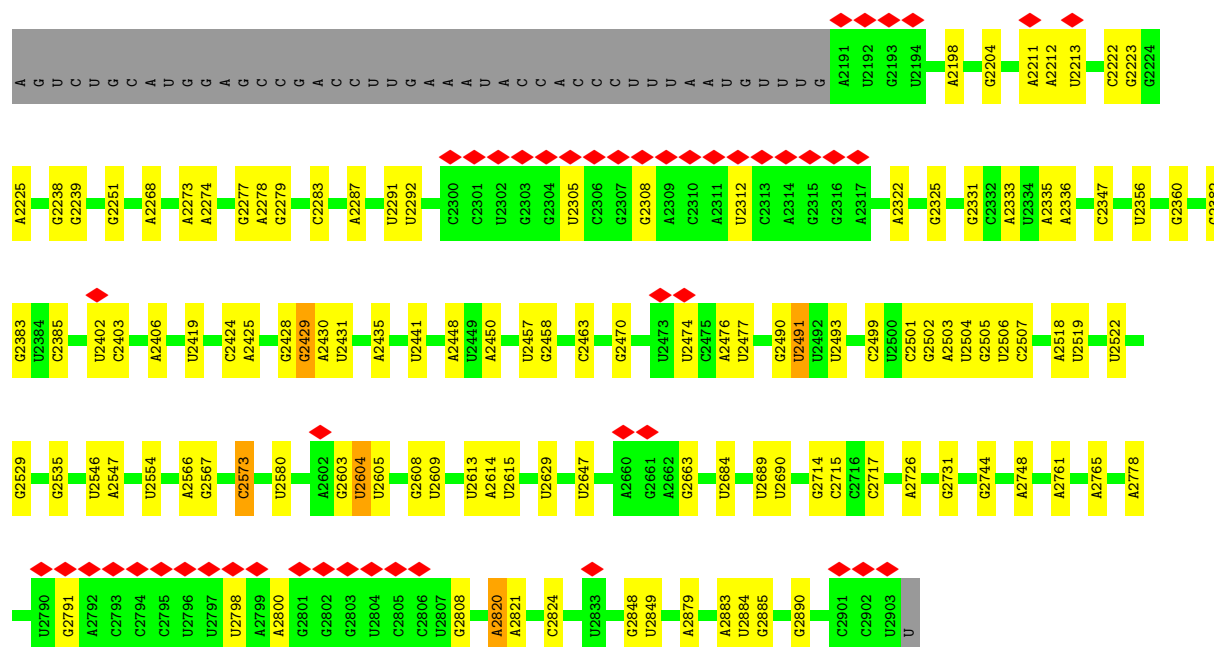
- Molecule 4: Large ribosomal subunit protein bL36A



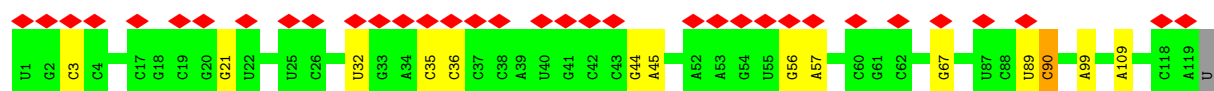
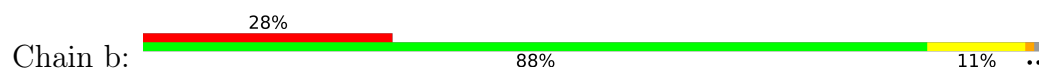
- Molecule 5: 23S rRNA



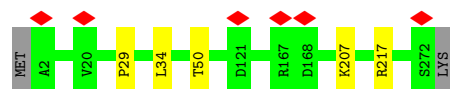




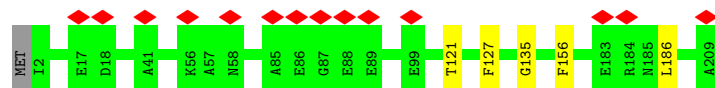
- Molecule 6: 5S rRNA



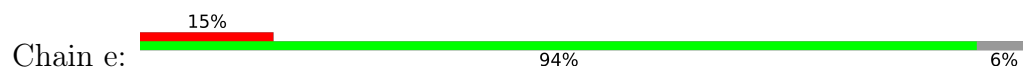
- Molecule 7: Large ribosomal subunit protein uL2



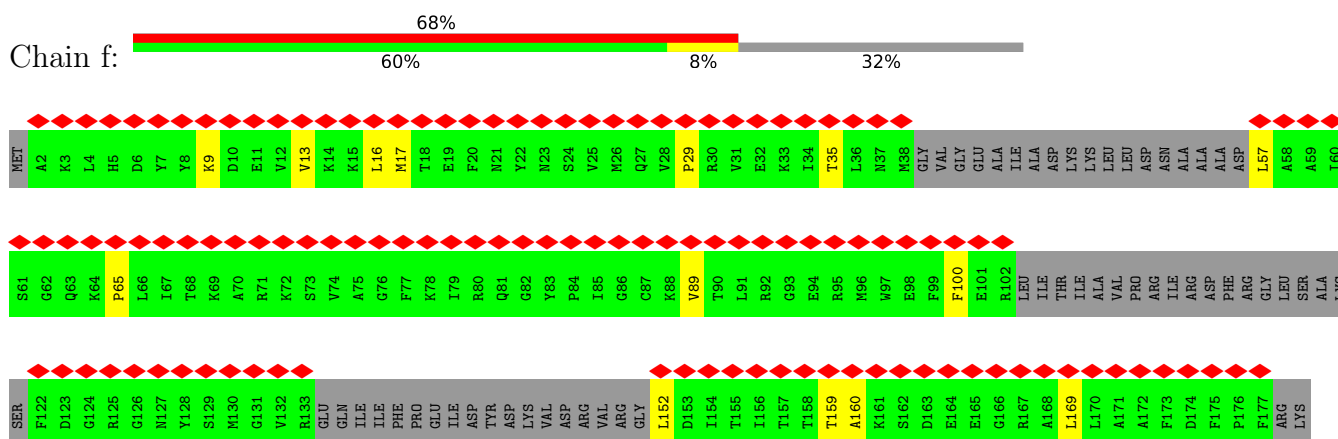
- Molecule 8: Large ribosomal subunit protein uL3



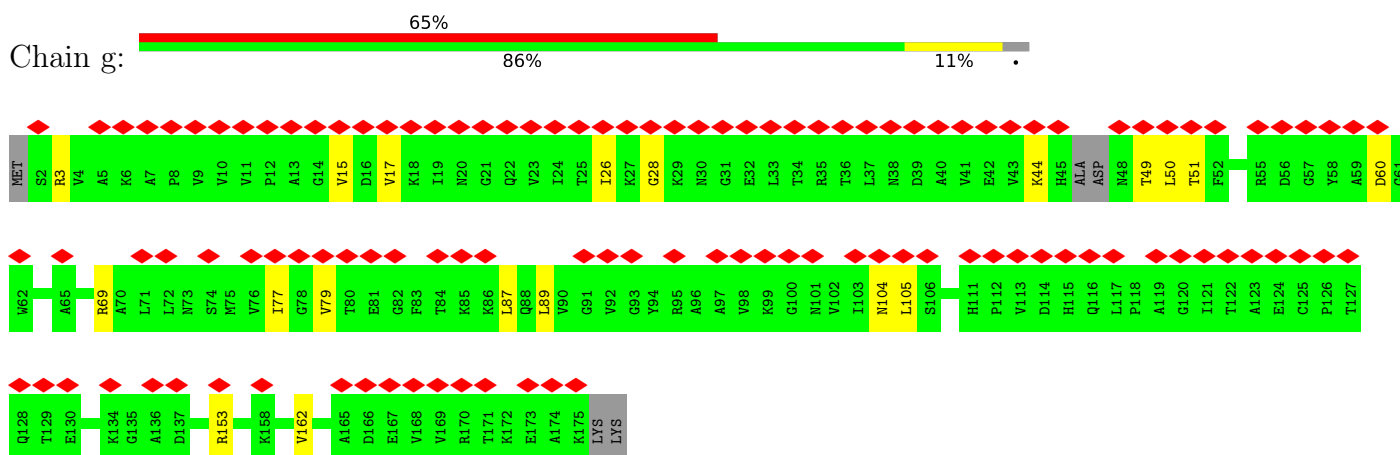
- Molecule 9: Large ribosomal subunit protein uL4



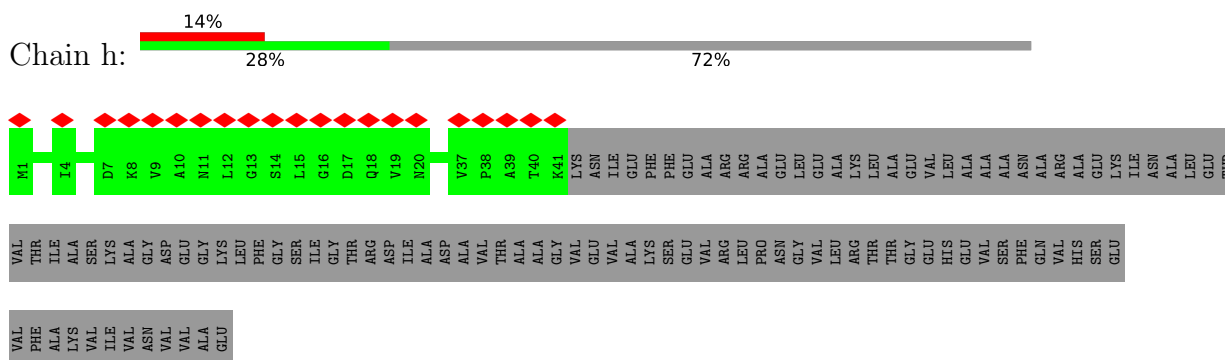
- Molecule 10: Large ribosomal subunit protein uL5



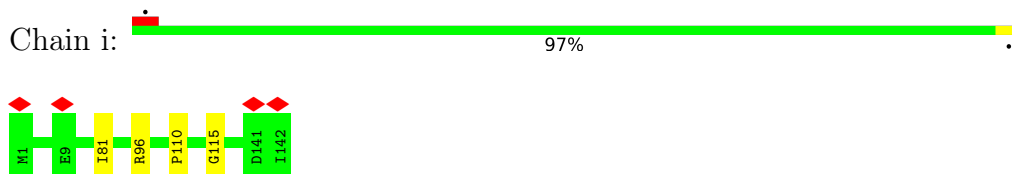
- Molecule 11: Large ribosomal subunit protein uL6



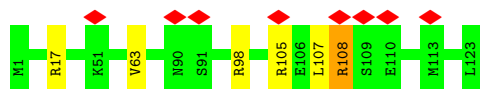
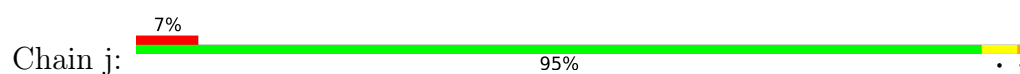
- Molecule 12: Large ribosomal subunit protein bL9



- Molecule 13: Large ribosomal subunit protein uL13



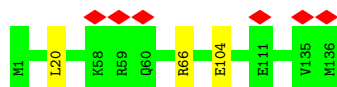
- Molecule 14: Large ribosomal subunit protein uL14



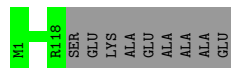
- Molecule 15: 50S ribosomal protein L15



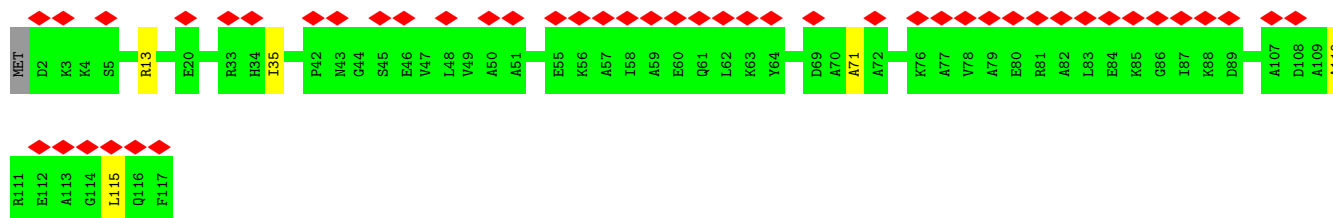
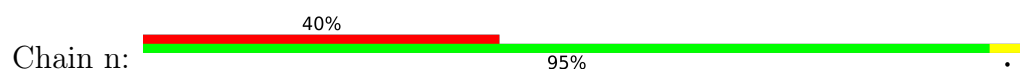
- Molecule 16: Large ribosomal subunit protein uL16



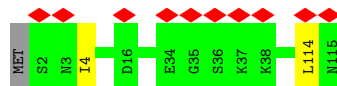
- Molecule 17: Large ribosomal subunit protein bL17



- Molecule 18: Large ribosomal subunit protein uL18



- Molecule 19: Large ribosomal subunit protein bL19

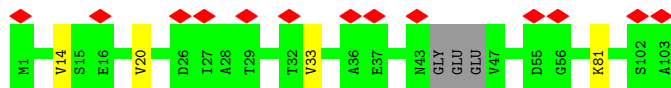
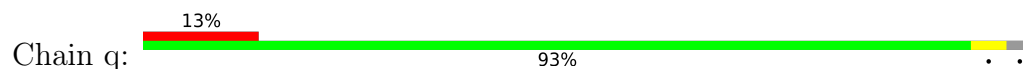


- Molecule 20: Large ribosomal subunit protein bL20

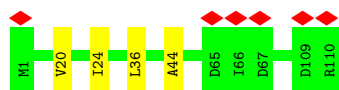




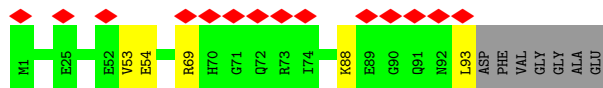
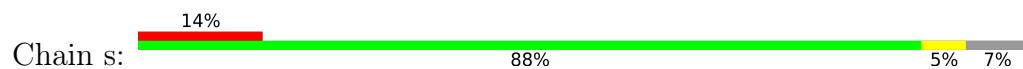
- Molecule 21: Large ribosomal subunit protein bL21



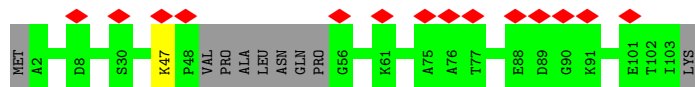
- Molecule 22: Large ribosomal subunit protein uL22



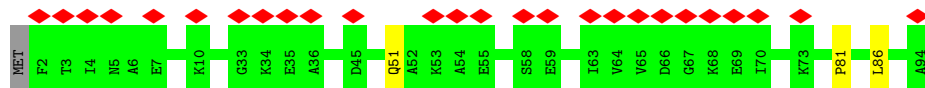
- Molecule 23: Large ribosomal subunit protein uL23



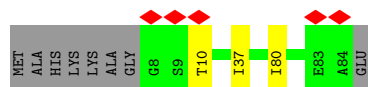
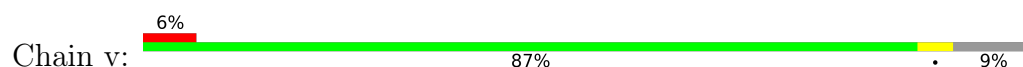
- Molecule 24: Large ribosomal subunit protein uL24



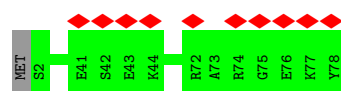
- Molecule 25: 50S ribosomal protein L25



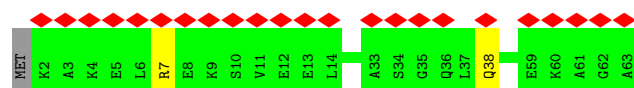
- Molecule 26: Large ribosomal subunit protein bL27



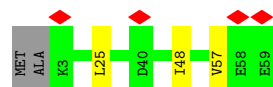
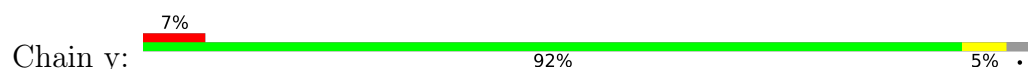
- Molecule 27: Large ribosomal subunit protein bL28



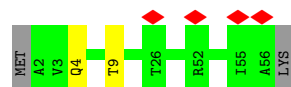
- Molecule 28: Large ribosomal subunit protein uL29



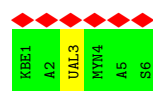
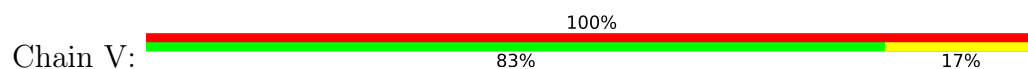
- Molecule 29: Large ribosomal subunit protein uL30



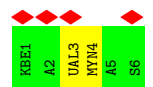
- Molecule 30: Large ribosomal subunit protein bL32



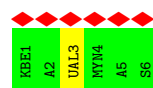
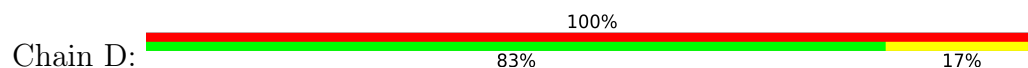
- Molecule 31: Capreomycin IA



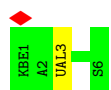
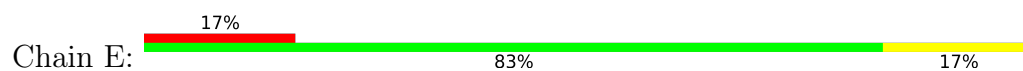
- Molecule 31: Capreomycin IA



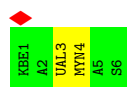
- Molecule 31: Capreomycin IA



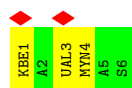
● Molecule 31: Capreomycin IA



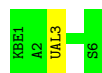
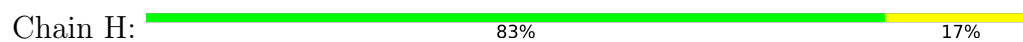
● Molecule 31: Capreomycin IA



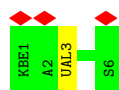
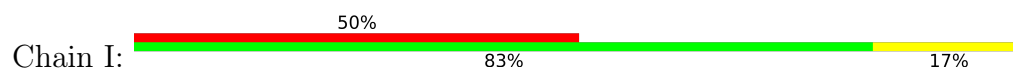
● Molecule 31: Capreomycin IA



● Molecule 31: Capreomycin IA



● Molecule 31: Capreomycin IA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179724	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72, 0.72, 0.72	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, G34, 2MA, UAL, KBE, 3TD, ZN, OMG, H2U, OMC, G7M, MG, 6MZ, 2MG, MS6, PSU, OMU, 5MC, 4D4, MEQ, K, MYN, DPP, 1MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.46	0/424	0.87	0/565
2	1	0.48	0/370	0.88	0/487
3	2	0.50	0/513	0.97	0/676
4	3	0.51	0/303	0.83	0/397
5	a	0.50	0/65651	0.98	121/102413 (0.1%)
6	b	0.55	0/2850	0.92	1/4444 (0.0%)
7	c	0.51	0/2121	0.88	0/2852
8	d	0.48	0/1568	0.88	0/2109
9	e	0.49	0/1481	0.96	0/1989
10	f	0.53	0/990	0.97	1/1323 (0.1%)
11	g	0.53	0/1310	1.03	1/1773 (0.1%)
12	h	0.53	0/306	0.95	0/413
13	i	0.50	0/1152	0.90	0/1551
14	j	0.48	0/955	0.92	0/1279
15	k	0.51	0/1062	0.88	0/1413
16	l	0.47	0/1073	0.89	0/1433
17	m	0.49	0/958	0.94	0/1281
18	n	0.52	0/902	0.99	0/1209
19	o	0.49	0/929	0.81	0/1242
20	p	0.48	0/960	0.99	0/1278
21	q	0.50	0/806	0.82	0/1075
22	r	0.50	0/864	0.91	0/1156
23	s	0.47	0/744	0.88	0/994
24	t	0.49	0/733	0.91	0/973
25	u	0.50	0/758	0.96	0/1015
26	v	0.49	0/583	0.84	0/773
27	w	0.49	0/635	0.91	0/848
28	x	0.47	0/502	1.04	0/667
29	y	0.50	0/448	0.95	0/598
30	z	0.50	0/440	0.87	0/588
31	C	0.18	0/5	0.34	0/5

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	D	0.19	0/5	0.44	0/5
31	E	0.23	0/5	0.45	0/5
31	F	0.19	0/5	0.69	0/5
31	G	0.20	0/5	0.69	0/5
31	H	0.25	0/5	0.51	0/5
31	I	0.16	0/5	0.39	0/5
31	V	0.21	0/5	0.44	0/5
All	All	0.50	0/92431	0.96	124/138854 (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
4	3	0	1
5	a	0	1
7	c	0	1
11	g	0	3
13	i	0	1
14	j	0	3
18	n	0	1
20	p	0	1
23	s	0	1
28	x	0	1
All	All	0	14

There are no bond length outliers.

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	2429	G	O3'-P-O5'	-9.02	90.47	104.00
5	a	1905	C	O3'-P-O5'	-8.87	90.70	104.00
5	a	1373	A	O3'-P-O5'	-8.81	90.78	104.00
5	a	1971	U	O3'-P-O5'	-8.29	91.57	104.00
5	a	2050	C	O3'-P-O5'	-8.19	91.71	104.00
5	a	2820	A	C4'-C3'-O3'	-8.01	100.98	113.00
5	a	781	A	O3'-P-O5'	-7.66	92.51	104.00
5	a	204	A	O3'-P-O5'	-7.33	93.01	104.00
5	a	2546	U	O3'-P-O5'	-7.18	93.22	104.00
5	a	1847	A	O3'-P-O5'	-7.14	93.28	104.00
5	a	1246	A	O3'-P-O5'	-7.05	93.42	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	1810	A	O3'-P-O5'	-6.99	93.51	104.00
5	a	1186	G	O3'-P-O5'	-6.96	93.56	104.00
5	a	1408	G	O3'-P-O5'	-6.92	93.62	104.00
5	a	2062	A	O3'-P-O5'	-6.86	93.71	104.00
5	a	310	A	O3'-P-O5'	-6.78	93.83	104.00
5	a	1025	G	O3'-P-O5'	6.76	114.14	104.00
5	a	1974	C	O3'-P-O5'	-6.72	93.92	104.00
5	a	2094	A	O3'-P-O5'	-6.72	93.92	104.00
5	a	1452	G	O3'-P-O5'	-6.70	93.95	104.00
5	a	2356	U	O3'-P-O5'	-6.67	93.99	104.00
5	a	2463	C	O3'-P-O5'	-6.67	93.99	104.00
5	a	1650	A	O3'-P-O5'	-6.65	94.03	104.00
5	a	2717	C	O3'-P-O5'	-6.60	94.10	104.00
5	a	2519	U	O3'-P-O5'	-6.59	94.12	104.00
5	a	2761	A	O3'-P-O5'	-6.54	94.18	104.00
5	a	1131	G	O3'-P-O5'	-6.53	94.20	104.00
5	a	763	G	O3'-P-O5'	-6.40	94.41	104.00
5	a	1187	G	O3'-P-O5'	-6.40	94.41	104.00
5	a	2808	G	O3'-P-O5'	-6.39	94.41	104.00
5	a	2501	C	O3'-P-O5'	-6.38	94.42	104.00
5	a	2278	A	O3'-P-O5'	-6.35	94.48	104.00
5	a	1496	A	O3'-P-O5'	-6.24	94.64	104.00
5	a	1969	A	O3'-P-O5'	-6.23	94.65	104.00
5	a	2477	U	O3'-P-O5'	-6.18	94.72	104.00
5	a	1185	G	O3'-P-O5'	-6.13	94.80	104.00
5	a	1806	C	O3'-P-O5'	-6.13	94.81	104.00
5	a	995	C	O3'-P-O5'	-6.12	94.81	104.00
5	a	1606	C	O3'-P-O5'	-6.12	94.81	104.00
5	a	1134	A	O3'-P-O5'	-6.06	94.91	104.00
5	a	1638	C	O3'-P-O5'	-6.03	94.96	104.00
5	a	1377	G	O3'-P-O5'	-5.99	95.02	104.00
5	a	2382	G	O3'-P-O5'	-5.97	95.04	104.00
5	a	761	A	O3'-P-O5'	-5.95	95.08	104.00
5	a	952	G	O3'-P-O5'	-5.89	95.16	104.00
5	a	379	G	O3'-P-O5'	-5.89	95.16	104.00
5	a	260	G	O3'-P-O5'	-5.88	95.19	104.00
5	a	528	A	O3'-P-O5'	-5.87	95.19	104.00
5	a	1959	G	O3'-P-O5'	-5.85	95.23	104.00
5	a	1643	G	O3'-P-O5'	-5.84	95.24	104.00
5	a	474	G	O3'-P-O5'	-5.83	95.26	104.00
5	a	2048	G	O3'-P-O5'	-5.82	95.28	104.00
5	a	926	G	O3'-P-O5'	-5.80	95.30	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	404	A	C2'-C3'-O3'	5.78	118.18	109.50
5	a	2715	C	O3'-P-O5'	-5.76	95.36	104.00
5	a	2493	U	O3'-P-O5'	-5.75	95.38	104.00
5	a	2491	U	C2'-C3'-O3'	5.75	118.12	109.50
5	a	512	G	O4'-C1'-N9	5.69	116.74	108.20
5	a	60	G	O3'-P-O5'	-5.69	95.46	104.00
5	a	2731	G	O3'-P-O5'	-5.66	95.51	104.00
5	a	972	A	O3'-P-O5'	-5.65	95.52	104.00
5	a	2573	C	O3'-P-O5'	-5.63	95.56	104.00
5	a	1261	C	O3'-P-O5'	-5.62	95.56	104.00
5	a	1121	C	O3'-P-O5'	-5.62	95.56	104.00
5	a	2684	U	O3'-P-O5'	-5.59	95.62	104.00
5	a	385	C	O3'-P-O5'	-5.58	95.63	104.00
5	a	2614	A	O3'-P-O5'	-5.54	95.69	104.00
5	a	1359	A	O3'-P-O5'	-5.54	95.69	104.00
5	a	227	A	O3'-P-O5'	-5.53	95.71	104.00
5	a	2060	A	O3'-P-O5'	-5.52	95.72	104.00
5	a	22	C	O3'-P-O5'	-5.52	95.72	104.00
5	a	57	C	O3'-P-O5'	-5.52	95.73	104.00
5	a	2222	C	O3'-P-O5'	-5.48	95.78	104.00
5	a	2022	U	O3'-P-O5'	-5.48	95.78	104.00
5	a	1168	G	O3'-P-O5'	-5.45	95.83	104.00
5	a	2360	G	O3'-P-O5'	-5.45	95.83	104.00
5	a	2490	G	O3'-P-O5'	-5.45	95.83	104.00
5	a	844	A	O3'-P-O5'	-5.43	95.86	104.00
5	a	1328	A	O3'-P-O5'	-5.43	95.86	104.00
5	a	2608	G	O3'-P-O5'	-5.43	95.86	104.00
5	a	241	A	O3'-P-O5'	-5.41	95.88	104.00
5	a	868	U	O3'-P-O5'	-5.39	95.92	104.00
5	a	2051	A	O3'-P-O5'	-5.39	95.92	104.00
5	a	1305	C	O3'-P-O5'	-5.38	95.94	104.00
5	a	1929	G	O3'-P-O5'	-5.35	95.97	104.00
5	a	555	G	O3'-P-O5'	-5.35	95.97	104.00
5	a	2848	G	O3'-P-O5'	-5.32	96.02	104.00
5	a	1966	A	O3'-P-O5'	-5.30	96.05	104.00
5	a	12	U	N1-C1'-C2'	5.28	119.92	112.00
5	a	2890	G	O3'-P-O5'	-5.28	96.08	104.00
5	a	2879	A	O3'-P-O5'	-5.25	96.13	104.00
5	a	221	A	O3'-P-O5'	-5.22	96.17	104.00
5	a	1857	G	O3'-P-O5'	-5.21	96.18	104.00
5	a	2428	G	O3'-P-O5'	-5.21	96.19	104.00
5	a	621	A	O3'-P-O5'	-5.20	96.20	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	2279	G	O3'-P-O5'	-5.20	96.20	104.00
5	a	337	C	O3'-P-O5'	-5.19	96.22	104.00
5	a	2849	U	O3'-P-O5'	-5.17	96.24	104.00
6	b	90	C	O3'-P-O5'	-5.17	96.24	104.00
5	a	73	A	O3'-P-O5'	-5.17	96.25	104.00
5	a	1749	A	O3'-P-O5'	-5.15	96.28	104.00
5	a	1565	C	O3'-P-O5'	-5.14	96.29	104.00
5	a	846	U	O3'-P-O5'	-5.12	96.32	104.00
5	a	2277	G	O3'-P-O5'	-5.12	96.33	104.00
5	a	1378	A	O3'-P-O5'	-5.11	96.33	104.00
5	a	2824	C	O3'-P-O5'	-5.11	96.33	104.00
5	a	781	A	C4'-C3'-O3'	-5.08	105.38	113.00
5	a	1648	U	O3'-P-O5'	-5.08	96.38	104.00
5	a	478	A	O3'-P-O5'	-5.08	96.38	104.00
5	a	54	G	O3'-P-O5'	-5.07	96.39	104.00
5	a	1187	G	C4'-C3'-O3'	-5.07	105.40	113.00
5	a	1194	A	O3'-P-O5'	-5.07	96.40	104.00
5	a	2458	G	O3'-P-O5'	-5.06	96.41	104.00
5	a	1965	C	O5'-P-OP2	-5.05	92.84	108.00
5	a	725	G	C4'-C3'-O3'	-5.05	105.42	113.00
5	a	1667	G	O3'-P-O5'	-5.05	96.43	104.00
5	a	2054	A	O3'-P-O5'	-5.05	96.43	104.00
5	a	747	5MU	O3'-P-O5'	-5.05	96.43	104.00
5	a	1436	G	O3'-P-O5'	-5.04	96.44	104.00
5	a	2885	G	O3'-P-O5'	-5.02	96.46	104.00
5	a	908	C	O3'-P-O5'	-5.02	96.47	104.00
10	f	100	PHE	CA-CB-CG	5.02	118.82	113.80
5	a	456	C	O3'-P-O5'	-5.01	96.48	104.00
11	g	60	ASP	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	36	ARG	Sidechain
5	a	512	G	Sidechain
7	c	217	ARG	Sidechain
11	g	153	ARG	Sidechain
11	g	3	ARG	Sidechain
11	g	69	ARG	Sidechain
13	i	96	ARG	Sidechain
14	j	108	ARG	Sidechain

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Mol	Chain	Res	Type	Group
14	j	17	ARG	Sidechain
14	j	98	ARG	Sidechain
18	n	13	ARG	Sidechain
20	p	51	ARG	Sidechain
23	s	69	ARG	Sidechain
28	x	7	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	0	417	0	451	1	0
2	1	367	0	405	0	0
3	2	504	0	572	1	0
4	3	302	0	340	1	0
5	a	59130	0	29739	40	0
6	b	2549	0	1291	0	0
7	c	2082	0	2153	3	0
8	d	1558	0	1606	4	0
9	e	1463	0	1523	1	0
10	f	974	0	989	4	0
11	g	1291	0	1335	5	0
12	h	303	0	327	0	0
13	i	1129	0	1162	2	0
14	j	946	0	1023	2	0
15	k	1053	0	1129	4	0
16	l	1075	0	1145	2	0
17	m	945	0	989	0	0
18	n	892	0	923	2	0
19	o	917	0	962	1	0
20	p	947	0	1019	2	0
21	q	794	0	823	3	0
22	r	857	0	922	2	0
23	s	738	0	807	2	0
24	t	728	0	776	1	0
25	u	745	0	768	2	0
26	v	576	0	590	1	0
27	w	625	0	652	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	x	501	0	531	0	0
29	y	444	0	483	2	0
30	z	434	0	445	2	0
31	C	47	0	40	0	0
31	D	47	0	40	0	0
31	E	47	0	39	0	0
31	F	47	0	39	0	0
31	G	47	0	39	0	0
31	H	47	0	39	0	0
31	I	47	0	39	0	0
31	V	47	0	40	0	0
32	3	1	0	0	0	0
33	a	36	0	47	3	0
34	a	209	0	0	0	0
34	b	5	0	0	0	0
34	c	2	0	0	0	0
34	d	1	0	0	0	0
34	p	1	0	0	0	0
34	v	1	0	0	0	0
34	z	1	0	0	0	0
35	a	75	0	0	0	0
35	c	3	0	0	0	0
35	e	1	0	0	0	0
35	t	1	0	0	0	0
35	v	1	0	0	0	0
36	0	11	0	0	0	0
36	1	31	0	0	0	0
36	2	29	0	0	0	0
36	3	10	0	0	0	0
36	F	1	0	0	0	0
36	G	3	0	0	0	0
36	H	2	0	0	0	0
36	I	1	0	0	0	0
36	a	5806	0	0	0	0
36	b	92	0	0	0	0
36	c	121	0	0	0	0
36	d	87	0	0	0	0
36	e	58	0	0	1	0
36	i	43	0	0	0	0
36	j	35	0	0	0	0
36	k	67	0	0	0	0
36	l	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	m	48	0	0	0	0
36	n	6	0	0	0	0
36	o	36	0	0	0	0
36	p	63	0	0	0	0
36	q	27	0	0	1	0
36	r	42	0	0	0	0
36	s	25	0	0	0	0
36	t	13	0	0	0	0
36	u	16	0	0	0	0
36	v	27	0	0	0	0
36	w	23	0	0	0	0
36	x	5	0	0	0	0
36	y	10	0	0	0	0
36	z	35	0	0	0	0
All	All	92830	0	56242	78	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 (78) 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)
10:f:29:PRO:HB3	10:f:160:ALA:HB2	1.70	0.72
5:a:568:U:H1'	5:a:2030:6MZ:H9C1	1.74	0.70
7:c:29:PRO:HG2	7:c:34:LEU:HD11	1.77	0.65
10:f:29:PRO:HB2	10:f:169:LEU:HD22	1.82	0.60
15:k:77:ILE:HD13	15:k:108:ALA:HB1	1.85	0.57
16:l:20:LEU:HD13	25:u:81:PRO:HG2	1.86	0.57
5:a:1939:5MU:OP1	5:a:2604:PSU:O2'	2.23	0.56
11:g:15:VAL:HG12	11:g:28:GLY:HA3	1.88	0.55
5:a:483:A:H5''	24:t:47:LYS:HD2	1.88	0.55
5:a:811:U:H2'	15:k:21:ARG:HA	1.89	0.53
5:a:12:U:H2'	5:a:12:U:O2	2.09	0.53
26:v:37:ILE:HG21	26:v:80:ILE:HG21	1.92	0.51
14:j:105:ARG:HG3	14:j:108:ARG:HG3	1.93	0.51
5:a:2020:A:H5'	30:z:9:THR:CG2	2.41	0.50
11:g:17:VAL:HG11	11:g:50:LEU:HD21	1.92	0.50
5:a:857:G:H2'	5:a:858:G:O4'	2.12	0.50
5:a:476:G:H4'	5:a:502:A:N1	2.28	0.49
5:a:2063:C:O2	5:a:2450:A:N1	2.46	0.49
22:r:20:VAL:HG11	22:r:44:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:3001:G34:H10	33:a:3001:G34:H14	1.94	0.48
20:p:76:TYR:CZ	20:p:80:ILE:HG13	2.48	0.48
5:a:493:G:H2'	5:a:494:G:O4'	2.13	0.48
11:g:26:ILE:HG22	11:g:79:VAL:HG21	1.96	0.48
3:2:54:ASP:HB3	15:k:57:LEU:HD22	1.95	0.47
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.96	0.47
5:a:586:A:N1	5:a:809:G:O2'	2.45	0.47
21:q:81:LYS:NZ	36:q:201:HOH:O	2.47	0.47
5:a:580:U:O3'	20:p:31:VAL:HG13	2.15	0.47
5:a:1853:A:N1	5:a:2087:G:H1'	2.30	0.47
5:a:1434:A:H2'	5:a:1435:G:C8	2.50	0.46
10:f:16:LEU:HD13	10:f:29:PRO:HG2	1.97	0.46
5:a:2273:A:H2'	5:a:2274:A:C8	2.49	0.46
5:a:1028:A:N6	5:a:1125:G:H2'	2.30	0.46
8:d:156:PHE:CE1	13:i:81:ILE:HD13	2.51	0.46
33:a:3001:G34:C21	33:a:3001:G34:H163	2.46	0.46
5:a:2291:U:H2'	5:a:2292:U:C6	2.52	0.45
5:a:2038:G:H2'	5:a:2039:U:O4'	2.16	0.45
5:a:1182:G:H2'	5:a:1183:U:O4'	2.17	0.45
5:a:729:G:C6	7:c:207:LYS:HB2	2.51	0.45
5:a:340:A:H2'	5:a:341:C:O4'	2.17	0.44
5:a:930:G:H1'	29:y:25:LEU:HD11	1.99	0.44
14:j:63:VAL:HG12	14:j:107:LEU:HD11	2.00	0.44
5:a:1026:G:H2'	5:a:1027:A:C8	2.53	0.44
1:0:22:THR:HG21	5:a:2419:U:H4'	2.00	0.44
9:e:65:THR:OG1	36:e:401:HOH:O	2.21	0.44
23:s:53:VAL:HG11	23:s:93:LEU:HG	1.99	0.44
5:a:743:A:OP1	8:d:135:GLY:HA2	2.18	0.43
5:a:157:C:H2'	5:a:158:U:O4'	2.18	0.43
5:a:1932:A:H2'	5:a:1933:G:O4'	2.18	0.43
5:a:642:U:O2'	5:a:644:A:N7	2.46	0.43
16:l:66:ARG:NH1	16:l:104:GLU:OE2	2.52	0.43
21:q:14:VAL:HG11	21:q:20:VAL:HG21	1.99	0.43
33:a:3001:G34:H131	33:a:3001:G34:H4	1.93	0.42
11:g:44:LYS:HB2	11:g:51:THR:HB	2.01	0.42
23:s:54:GLU:HB3	23:s:88:LYS:HD2	2.01	0.42
5:a:2030:6MZ:C2	5:a:2499:C:H5''	2.50	0.42
29:y:48:ILE:HG21	29:y:57:VAL:HG21	2.01	0.42
15:k:77:ILE:HD11	15:k:101:ILE:HG21	2.01	0.42
13:i:110:PRO:O	13:i:115:GLY:HA3	2.20	0.41
5:a:639:U:H2'	5:a:640:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:f:57:LEU:HD23	10:f:65:PRO:HB3	2.02	0.41
18:n:35:ILE:HG21	18:n:71:ALA:HA	2.02	0.41
5:a:1394:U:H4'	5:a:1603:A:H4'	2.02	0.41
5:a:1805:A:N3	7:c:50:THR:HB	2.35	0.41
11:g:89:LEU:HD22	11:g:162:VAL:HG22	2.03	0.41
5:a:747:5MU:O2	5:a:2014:A:H1'	2.19	0.41
25:u:51:GLN:HG2	25:u:86:LEU:HD11	2.02	0.41
5:a:565:C:H2'	5:a:566:U:O4'	2.21	0.41
5:a:568:U:O4	21:q:81:LYS:NZ	2.53	0.41
5:a:2615:U:C2	30:z:4:GLN:HA	2.56	0.41
8:d:121:THR:HB	8:d:127:PHE:CD2	2.56	0.41
18:n:110:ALA:HB1	18:n:115:LEU:HD12	2.02	0.41
22:r:24:ILE:HD13	22:r:36:LEU:HD11	2.03	0.41
8:d:186:LEU:HD11	19:o:4:ILE:HG23	2.02	0.40
5:a:570:G:H2'	5:a:2030:6MZ:N7	2.35	0.40
5:a:2522:U:O2'	5:a:2647:U:OP1	2.36	0.40
5:a:84:A:N1	5:a:98:G:O2'	2.45	0.40
5:a:2331:G:O2'	5:a:2336:A:N1	2.47	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	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
7	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
8	d	205/209 (98%)	198 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	e	186/201 (92%)	182 (98%)	4 (2%)	0	100	100
10	f	113/179 (63%)	106 (94%)	7 (6%)	0	100	100
11	g	168/177 (95%)	157 (94%)	10 (6%)	1 (1%)	21	9
12	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
13	i	140/142 (99%)	140 (100%)	0	0	100	100
14	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
15	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
16	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
17	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
18	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
19	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
20	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	q	96/103 (93%)	95 (99%)	1 (1%)	0	100	100
22	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
23	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
24	t	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
25	u	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
26	v	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
27	w	75/78 (96%)	75 (100%)	0	0	100	100
28	x	60/63 (95%)	60 (100%)	0	0	100	100
29	y	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
30	z	53/57 (93%)	52 (98%)	1 (2%)	0	100	100
All	All	2957/3267 (90%)	2874 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	g	49	THR

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	0	46/49 (94%)	46 (100%)	0	100	100
2	1	37/38 (97%)	37 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
7	c	216/218 (99%)	216 (100%)	0	100	100
8	d	162/163 (99%)	162 (100%)	0	100	100
9	e	155/165 (94%)	155 (100%)	0	100	100
10	f	103/150 (69%)	96 (93%)	7 (7%)	14	3
11	g	134/138 (97%)	130 (97%)	4 (3%)	36	19
12	h	32/114 (28%)	32 (100%)	0	100	100
13	i	116/116 (100%)	116 (100%)	0	100	100
14	j	104/104 (100%)	104 (100%)	0	100	100
15	k	103/103 (100%)	102 (99%)	1 (1%)	68	58
16	l	107/107 (100%)	107 (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	o	99/100 (99%)	98 (99%)	1 (1%)	68	58
20	p	89/90 (99%)	89 (100%)	0	100	100
21	q	82/84 (98%)	81 (99%)	1 (1%)	63	51
22	r	93/93 (100%)	93 (100%)	0	100	100
23	s	80/84 (95%)	80 (100%)	0	100	100
24	t	77/85 (91%)	77 (100%)	0	100	100
25	u	77/78 (99%)	77 (100%)	0	100	100
26	v	57/63 (90%)	56 (98%)	1 (2%)	51	35
27	w	67/68 (98%)	67 (100%)	0	100	100
28	x	54/55 (98%)	53 (98%)	1 (2%)	50	34
29	y	48/49 (98%)	48 (100%)	0	100	100
30	z	46/48 (96%)	46 (100%)	0	100	100
31	C	1/1 (100%)	1 (100%)	0	100	100
31	D	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	E	1/1 (100%)	1 (100%)	0	100	100
31	F	1/1 (100%)	1 (100%)	0	100	100
31	G	1/1 (100%)	1 (100%)	0	100	100
31	H	1/1 (100%)	1 (100%)	0	100	100
31	I	1/1 (100%)	1 (100%)	0	100	100
31	V	1/1 (100%)	1 (100%)	0	100	100
All	All	2461/2646 (93%)	2445 (99%)	16 (1%)	73	68

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	f	9	LYS
10	f	13	VAL
10	f	17	MET
10	f	35	THR
10	f	89	VAL
10	f	152	LEU
10	f	159	THR
11	g	77	ILE
11	g	87	LEU
11	g	104	ASN
11	g	105	LEU
15	k	91	ASP
19	o	114	LEU
21	q	33	VAL
26	v	10	THR
28	x	38	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
7	c	153	GLN
8	d	36	GLN
9	e	94	GLN
11	g	30	ASN
11	g	104	ASN
11	g	115	HIS
13	i	58	ASN
13	i	128	ASN

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Mol	Chain	Res	Type
14	j	3	GLN
15	k	104	GLN
16	l	60	GLN
17	m	18	GLN
18	n	29	HIS
19	o	10	GLN
19	o	41	GLN
19	o	52	ASN
21	q	86	GLN
22	r	9	HIS
25	u	49	ASN
27	w	17	ASN
28	x	15	ASN
28	x	20	ASN
28	x	27	ASN
28	x	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	a	2749/2904 (94%)	291 (10%)	0
6	b	118/120 (98%)	14 (11%)	0
All	All	2867/3024 (94%)	305 (10%)	0

All (305) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	a	10	A
5	a	34	U
5	a	63	A
5	a	71	A
5	a	74	A
5	a	75	G
5	a	101	A
5	a	102	U
5	a	118	A
5	a	119	A
5	a	120	U
5	a	125	A
5	a	126	A
5	a	131	A

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Mol	Chain	Res	Type
5	a	138	U
5	a	140	C
5	a	163	C
5	a	181	A
5	a	196	A
5	a	199	A
5	a	200	U
5	a	215	G
5	a	216	A
5	a	221	A
5	a	222	A
5	a	248	G
5	a	265	A
5	a	272	A
5	a	276	U
5	a	282	A
5	a	289	G
5	a	311	A
5	a	329	G
5	a	330	A
5	a	359	G
5	a	361	G
5	a	362	A
5	a	367	G
5	a	386	G
5	a	403	U
5	a	404	A
5	a	405	U
5	a	411	G
5	a	412	A
5	a	451	U
5	a	456	C
5	a	481	G
5	a	491	G
5	a	503	A
5	a	504	A
5	a	505	A
5	a	509	C
5	a	530	G
5	a	531	C
5	a	532	A
5	a	533	G

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Mol	Chain	Res	Type
5	a	543	G
5	a	545	U
5	a	546	U
5	a	547	A
5	a	548	G
5	a	549	G
5	a	563	A
5	a	573	U
5	a	574	A
5	a	575	A
5	a	586	A
5	a	603	A
5	a	614	A
5	a	615	U
5	a	627	A
5	a	637	A
5	a	645	C
5	a	646	U
5	a	647	G
5	a	653	U
5	a	654	A
5	a	655	A
5	a	686	U
5	a	730	A
5	a	738	G
5	a	747	5MU
5	a	764	A
5	a	765	C
5	a	775	G
5	a	776	G
5	a	777	G
5	a	782	A
5	a	784	G
5	a	785	G
5	a	789	A
5	a	805	G
5	a	812	C
5	a	827	U
5	a	828	U
5	a	846	U
5	a	847	U
5	a	859	G

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Mol	Chain	Res	Type
5	a	879	G
5	a	886	A
5	a	887	U
5	a	888	C
5	a	890	C
5	a	895	U
5	a	896	A
5	a	897	C
5	a	899	A
5	a	910	A
5	a	914	G
5	a	931	U
5	a	932	U
5	a	934	U
5	a	946	C
5	a	961	C
5	a	974	G
5	a	983	A
5	a	984	A
5	a	985	C
5	a	996	A
5	a	1012	U
5	a	1013	C
5	a	1022	G
5	a	1033	U
5	a	1046	A
5	a	1047	G
5	a	1108	U
5	a	1110	G
5	a	1111	A
5	a	1112	G
5	a	1128	G
5	a	1129	A
5	a	1132	U
5	a	1133	A
5	a	1135	C
5	a	1142	A
5	a	1143	A
5	a	1171	G
5	a	1172	C
5	a	1179	G
5	a	1253	A

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Mol	Chain	Res	Type
5	a	1256	G
5	a	1271	G
5	a	1272	A
5	a	1273	U
5	a	1300	G
5	a	1301	A
5	a	1303	G
5	a	1352	U
5	a	1365	A
5	a	1379	U
5	a	1383	A
5	a	1415	U
5	a	1416	G
5	a	1428	C
5	a	1452	G
5	a	1453	A
5	a	1476	U
5	a	1482	G
5	a	1493	C
5	a	1494	A
5	a	1497	U
5	a	1498	C
5	a	1508	A
5	a	1515	A
5	a	1535	A
5	a	1536	C
5	a	1537	G
5	a	1569	A
5	a	1578	U
5	a	1584	U
5	a	1608	A
5	a	1609	A
5	a	1647	U
5	a	1648	U
5	a	1649	G
5	a	1674	G
5	a	1715	G
5	a	1728	C
5	a	1729	U
5	a	1730	C
5	a	1731	G
5	a	1732	C

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Mol	Chain	Res	Type
5	a	1738	G
5	a	1764	C
5	a	1773	A
5	a	1782	U
5	a	1800	C
5	a	1801	A
5	a	1808	A
5	a	1809	A
5	a	1816	C
5	a	1829	A
5	a	1848	A
5	a	1858	A
5	a	1873	G
5	a	1906	G
5	a	1913	A
5	a	1914	C
5	a	1915	3TD
5	a	1929	G
5	a	1930	G
5	a	1937	A
5	a	1938	A
5	a	1955	U
5	a	1965	C
5	a	1967	C
5	a	1970	A
5	a	1971	U
5	a	1972	G
5	a	1991	U
5	a	1993	U
5	a	2023	C
5	a	2027	G
5	a	2031	A
5	a	2033	A
5	a	2043	C
5	a	2055	C
5	a	2056	G
5	a	2060	A
5	a	2061	G
5	a	2062	A
5	a	2069	G7M
5	a	2198	A
5	a	2204	G

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Mol	Chain	Res	Type
5	a	2211	A
5	a	2212	A
5	a	2213	U
5	a	2223	G
5	a	2225	A
5	a	2238	G
5	a	2239	G
5	a	2268	A
5	a	2283	C
5	a	2287	A
5	a	2305	U
5	a	2308	G
5	a	2312	U
5	a	2322	A
5	a	2325	G
5	a	2333	A
5	a	2335	A
5	a	2347	C
5	a	2383	G
5	a	2385	C
5	a	2402	U
5	a	2403	C
5	a	2406	A
5	a	2424	C
5	a	2425	A
5	a	2429	G
5	a	2430	A
5	a	2431	U
5	a	2435	A
5	a	2441	U
5	a	2448	A
5	a	2470	G
5	a	2474	U
5	a	2476	A
5	a	2491	U
5	a	2502	G
5	a	2505	G
5	a	2506	U
5	a	2507	C
5	a	2518	A
5	a	2529	G
5	a	2535	G

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Mol	Chain	Res	Type
5	a	2547	A
5	a	2554	U
5	a	2566	A
5	a	2567	G
5	a	2573	C
5	a	2603	G
5	a	2609	U
5	a	2613	U
5	a	2629	U
5	a	2663	G
5	a	2689	U
5	a	2690	U
5	a	2714	G
5	a	2726	A
5	a	2744	G
5	a	2748	A
5	a	2765	A
5	a	2778	A
5	a	2791	G
5	a	2798	U
5	a	2800	A
5	a	2820	A
5	a	2821	A
5	a	2883	A
5	a	2884	U
6	b	3	C
6	b	21	G
6	b	32	U
6	b	35	C
6	b	36	C
6	b	44	G
6	b	45	A
6	b	56	G
6	b	57	A
6	b	67	G
6	b	89	U
6	b	90	C
6	b	99	A
6	b	109	A

There are no RNA pucker outliers to report.

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

67 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
31	MYN	E	4	31	7,11,12	0.51	0	6,14,16	1.18	0
31	KBE	D	1	31	8,8,9	0.65	0	7,8,10	0.79	0
5	H2U	a	2449	5	18,21,22	0.56	0	21,30,33	0.74	0
31	DPP	D	2	31	3,5,6	0.74	0	1,5,7	0.01	0
5	G7M	a	2069	5	23,26,27	0.73	1 (4%)	35,39,42	0.68	0
5	OMG	a	2251	5,35	23,26,27	0.34	0	33,38,41	0.60	1 (3%)
5	6MZ	a	2030	5	22,25,26	0.49	0	30,36,39	0.74	0
31	KBE	V	1	31	8,8,9	0.75	0	7,8,10	0.79	0
31	DPP	C	2	31	3,5,6	0.77	0	1,5,7	0.18	0
31	DPP	I	2	31	3,5,6	0.74	0	1,5,7	0.03	0
31	MYN	F	4	31	7,11,12	0.46	0	6,14,16	1.33	2 (33%)
16	4D4	l	81	16	9,11,12	0.48	0	8,13,15	0.76	0
5	PSU	a	2605	5	18,21,22	1.01	1 (5%)	22,30,33	0.84	1 (4%)
31	KBE	H	1	31	8,8,9	0.57	0	7,8,10	0.65	0
31	DPP	H	5	31	3,5,6	0.65	0	1,5,7	0.17	0
31	DPP	E	5	31	3,5,6	0.68	0	1,5,7	0.21	0
31	MYN	D	4	31	7,11,12	0.52	0	6,14,16	0.83	0
5	PSU	a	2604	5	18,21,22	0.89	1 (5%)	22,30,33	0.77	1 (4%)
31	MYN	G	4	31	7,11,12	0.52	0	6,14,16	1.37	2 (33%)
31	KBE	F	1	31	8,8,9	0.64	0	7,8,10	0.71	0
5	2MA	a	2503	5,34,35	22,25,26	0.98	2 (9%)	33,37,40	1.24	4 (12%)
31	MYN	C	4	31	7,11,12	0.52	0	6,14,16	1.79	2 (33%)
31	DPP	F	2	31	3,5,6	0.73	0	1,5,7	0.16	0
31	UAL	C	3	31	7,8,9	1.42	1 (14%)	5,9,11	2.02	1 (20%)
31	DPP	D	5	31	3,5,6	0.66	0	1,5,7	0.26	0
5	OMU	a	2552	5	19,22,23	0.23	0	26,31,34	0.43	0
31	UAL	I	3	31	7,8,9	1.34	1 (14%)	5,9,11	2.18	1 (20%)
16	MS6	l	82	16	5,7,8	0.24	0	2,7,9	0.23	0
5	PSU	a	955	5	18,21,22	0.93	1 (5%)	22,30,33	0.67	0
31	DPP	C	5	31	3,5,6	0.64	0	1,5,7	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	a	1917	5	18,21,22	0.95	1 (5%)	22,30,33	0.62	0
5	5MU	a	1939	5,35	19,22,23	0.32	0	28,32,35	0.45	0
5	PSU	a	2504	5,35	18,21,22	0.89	1 (5%)	22,30,33	0.70	0
31	DPP	E	2	31	3,5,6	0.71	0	1,5,7	0.06	0
31	UAL	E	3	31	7,8,9	1.36	1 (14%)	5,9,11	2.32	1 (20%)
31	DPP	G	2	31	3,5,6	0.75	0	1,5,7	0.04	0
5	3TD	a	1915	5	18,22,23	1.02	1 (5%)	22,32,35	0.79	0
5	PSU	a	746	5,34	18,21,22	0.95	1 (5%)	22,30,33	0.59	0
5	2MG	a	1835	5	23,26,27	0.40	0	32,38,41	0.47	0
31	DPP	H	2	31	3,5,6	0.75	0	1,5,7	0.03	0
31	UAL	F	3	31	7,8,9	1.48	1 (14%)	5,9,11	2.26	1 (20%)
5	2MG	a	2445	5	23,26,27	0.42	0	32,38,41	0.52	0
8	MEQ	d	150	8	8,9,10	0.42	0	5,10,12	1.20	0
5	1MG	a	745	5	22,26,27	0.56	0	33,39,42	0.55	0
31	DPP	V	2	31	3,5,6	0.72	0	1,5,7	0.18	0
31	KBE	G	1	31	8,8,9	0.70	0	7,8,10	1.22	1 (14%)
31	MYN	V	4	31	7,11,12	0.64	0	6,14,16	1.12	0
31	KBE	C	1	31	8,8,9	0.69	0	7,8,10	0.62	0
31	DPP	I	5	31	3,5,6	0.66	0	1,5,7	0.23	0
31	KBE	I	1	31	8,8,9	0.51	0	7,8,10	0.62	0
5	5MC	a	1962	5	18,22,23	0.36	0	26,32,35	0.72	0
5	PSU	a	1911	5	18,21,22	0.96	1 (5%)	22,30,33	0.61	0
31	UAL	V	3	31	7,8,9	1.42	1 (14%)	5,9,11	1.95	1 (20%)
31	KBE	E	1	31	8,8,9	0.60	0	7,8,10	0.87	0
31	UAL	D	3	31	7,8,9	1.45	1 (14%)	5,9,11	2.16	1 (20%)
5	PSU	a	2457	5	18,21,22	1.00	1 (5%)	22,30,33	0.62	0
31	UAL	G	3	31	7,8,9	1.39	1 (14%)	5,9,11	2.06	1 (20%)
31	UAL	H	3	31	7,8,9	1.32	1 (14%)	5,9,11	2.30	1 (20%)
31	MYN	H	4	31	7,11,12	0.56	0	6,14,16	1.16	0
5	PSU	a	2580	5,35	18,21,22	1.01	1 (5%)	22,30,33	0.74	0
31	MYN	I	4	31	7,11,12	0.54	0	6,14,16	1.04	0
31	DPP	V	5	31	3,5,6	0.64	0	1,5,7	0.30	0
31	DPP	G	5	31	3,5,6	0.65	0	1,5,7	0.23	0
5	5MU	a	747	5	19,22,23	0.32	0	28,32,35	0.50	0
5	6MZ	a	1618	5	22,25,26	0.48	0	30,36,39	0.58	0
31	DPP	F	5	31	3,5,6	0.65	0	1,5,7	0.25	0
5	OMC	a	2498	5,34	19,22,23	0.28	0	26,31,34	0.61	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
31	MYN	E	4	31	-	0/1/16/18	0/1/1/1
31	KBE	D	1	31	-	3/7/7/8	-
5	H2U	a	2449	5	-	0/7/38/39	0/2/2/2
31	DPP	D	2	31	-	0/2/4/6	-
5	G7M	a	2069	5	-	2/7/25/26	0/3/3/3
5	OMG	a	2251	5,35	-	0/9/27/28	0/3/3/3
5	6MZ	a	2030	5	-	2/9/27/28	0/3/3/3
31	KBE	V	1	31	-	2/7/7/8	-
31	DPP	C	2	31	-	2/2/4/6	-
31	DPP	I	2	31	-	1/2/4/6	-
31	MYN	F	4	31	-	0/1/16/18	0/1/1/1
16	4D4	l	81	16	-	1/11/12/14	-
5	PSU	a	2605	5	-	0/7/25/26	0/2/2/2
31	KBE	H	1	31	-	0/7/7/8	-
31	DPP	H	5	31	-	0/2/4/6	-
31	DPP	E	5	31	-	0/2/4/6	-
31	MYN	D	4	31	-	0/1/16/18	0/1/1/1
5	PSU	a	2604	5	-	0/7/25/26	0/2/2/2
31	MYN	G	4	31	-	0/1/16/18	0/1/1/1
31	KBE	F	1	31	-	0/7/7/8	-
5	2MA	a	2503	5,34,35	-	2/7/25/26	0/3/3/3
31	MYN	C	4	31	-	0/1/16/18	0/1/1/1
31	DPP	F	2	31	-	2/2/4/6	-
31	UAL	C	3	31	-	0/3/7/9	-
31	DPP	D	5	31	-	0/2/4/6	-
5	OMU	a	2552	5	-	0/9/27/28	0/2/2/2
31	UAL	I	3	31	-	1/3/7/9	-
16	MS6	l	82	16	-	1/4/6/8	-
5	PSU	a	955	5	-	0/7/25/26	0/2/2/2
31	DPP	C	5	31	-	0/2/4/6	-
5	PSU	a	1917	5	-	0/7/25/26	0/2/2/2
5	5MU	a	1939	5,35	-	0/7/25/26	0/2/2/2
5	PSU	a	2504	5,35	-	0/7/25/26	0/2/2/2
31	DPP	E	2	31	-	2/2/4/6	-
31	UAL	E	3	31	-	0/3/7/9	-
31	DPP	G	2	31	-	0/2/4/6	-
5	3TD	a	1915	5	-	2/7/25/26	0/2/2/2
5	PSU	a	746	5,34	-	2/7/25/26	0/2/2/2
5	2MG	a	1835	5	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DPP	H	2	31	-	0/2/4/6	-
31	UAL	F	3	31	-	1/3/7/9	-
5	2MG	a	2445	5	-	0/9/27/28	0/3/3/3
8	MEQ	d	150	8	-	2/8/9/11	-
5	1MG	a	745	5	-	0/7/25/26	0/3/3/3
31	DPP	V	2	31	-	0/2/4/6	-
31	KBE	G	1	31	-	2/7/7/8	-
31	MYN	V	4	31	-	1/1/16/18	0/1/1/1
31	KBE	C	1	31	-	2/7/7/8	-
31	DPP	I	5	31	-	0/2/4/6	-
31	KBE	I	1	31	-	1/7/7/8	-
5	5MC	a	1962	5	-	1/7/25/26	0/2/2/2
5	PSU	a	1911	5	-	0/7/25/26	0/2/2/2
31	UAL	V	3	31	-	0/3/7/9	-
31	KBE	E	1	31	-	2/7/7/8	-
31	UAL	D	3	31	-	2/3/7/9	-
5	PSU	a	2457	5	-	0/7/25/26	0/2/2/2
31	UAL	G	3	31	-	0/3/7/9	-
31	UAL	H	3	31	-	1/3/7/9	-
31	MYN	H	4	31	-	0/1/16/18	0/1/1/1
5	PSU	a	2580	5,35	-	0/7/25/26	0/2/2/2
31	MYN	I	4	31	-	0/1/16/18	0/1/1/1
31	DPP	V	5	31	-	0/2/4/6	-
31	DPP	G	5	31	-	0/2/4/6	-
5	5MU	a	747	5	-	0/7/25/26	0/2/2/2
5	6MZ	a	1618	5	-	0/9/27/28	0/3/3/3
31	DPP	F	5	31	-	0/2/4/6	-
5	OMC	a	2498	5,34	-	0/9/27/28	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	2580	PSU	C6-C5	4.04	1.40	1.35
5	a	2457	PSU	C6-C5	4.00	1.40	1.35
5	a	2605	PSU	C6-C5	3.91	1.39	1.35
5	a	1915	3TD	C6-C5	3.88	1.39	1.35
5	a	746	PSU	C6-C5	3.84	1.39	1.35
5	a	1911	PSU	C6-C5	3.83	1.39	1.35
5	a	1917	PSU	C6-C5	3.76	1.39	1.35
5	a	955	PSU	C6-C5	3.63	1.39	1.35
5	a	2504	PSU	C6-C5	3.51	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	2604	PSU	C6-C5	3.50	1.39	1.35
31	D	3	UAL	CA-N	3.10	1.43	1.35
31	F	3	UAL	CA-N	3.05	1.42	1.35
31	H	3	UAL	CA-N	3.03	1.42	1.35
31	I	3	UAL	CA-N	3.02	1.42	1.35
31	C	3	UAL	CA-N	2.98	1.42	1.35
31	E	3	UAL	CA-N	2.96	1.42	1.35
31	G	3	UAL	CA-N	2.93	1.42	1.35
31	V	3	UAL	CA-N	2.91	1.42	1.35
5	a	2069	G7M	C8-N7	2.73	1.38	1.33
5	a	2503	2MA	C2-N1	2.56	1.38	1.34
5	a	2503	2MA	C6-N6	-2.06	1.29	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	H	3	UAL	O-C-CA	-5.09	118.92	125.39
31	E	3	UAL	O-C-CA	-5.05	118.97	125.39
31	F	3	UAL	O-C-CA	-4.97	119.07	125.39
31	I	3	UAL	O-C-CA	-4.82	119.27	125.39
31	D	3	UAL	O-C-CA	-4.61	119.53	125.39
31	G	3	UAL	O-C-CA	-4.55	119.61	125.39
31	C	3	UAL	O-C-CA	-4.40	119.80	125.39
31	V	3	UAL	O-C-CA	-4.29	119.93	125.39
5	a	2503	2MA	CM2-C2-N1	4.25	123.79	117.15
31	G	1	KBE	CB-CA-C	2.77	116.34	112.25
5	a	2503	2MA	C2-N1-C6	2.71	122.31	118.08
31	C	4	MYN	CD-CG-CB	2.59	113.90	109.83
5	a	2503	2MA	N3-C2-N1	-2.54	121.05	125.72
5	a	2604	PSU	C2'-C3'-C4'	-2.43	97.92	102.64
5	a	2503	2MA	C5-C4-N3	-2.40	124.49	127.19
31	F	4	MYN	CA-CB-N1	-2.29	107.71	111.41
31	C	4	MYN	O-C-CA	-2.27	118.84	124.78
5	a	2251	OMG	O2'-C2'-C1'	2.20	113.37	109.08
31	G	4	MYN	CD-CG-CB	2.17	113.25	109.83
5	a	2605	PSU	C2'-C3'-C4'	-2.06	98.63	102.64
31	G	4	MYN	O-C-CA	-2.04	119.44	124.78
31	F	4	MYN	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	746	PSU	C2'-C1'-C5-C4
31	V	1	KBE	N-CB-CG-CD
31	C	1	KBE	C-CA-CB-N
31	C	1	KBE	C-CA-CB-CG
31	D	1	KBE	C-CA-CB-N
31	D	1	KBE	C-CA-CB-CG
31	E	1	KBE	C-CA-CB-N
31	G	1	KBE	CA-CB-CG-CD
31	C	2	DPP	N-CA-CB-NG
31	E	2	DPP	N-CA-CB-NG
31	F	2	DPP	N-CA-CB-NG
31	F	2	DPP	C-CA-CB-NG
31	F	3	UAL	CA-CB-N1-C1
5	a	2030	6MZ	O4'-C4'-C5'-O5'
5	a	1915	3TD	C3'-C4'-C5'-O5'
5	a	1915	3TD	O4'-C4'-C5'-O5'
8	d	150	MEQ	NE2-CD-CG-CB
8	d	150	MEQ	OE1-CD-CG-CB
31	I	1	KBE	O-C-CA-CB
5	a	2030	6MZ	C3'-C4'-C5'-O5'
31	G	1	KBE	CE-CD-CG-CB
31	D	3	UAL	O2-C1-N1-CB
31	D	3	UAL	N2-C1-N1-CB
31	H	3	UAL	CA-CB-N1-C1
31	I	3	UAL	CA-CB-N1-C1
31	V	1	KBE	CA-CB-CG-CD
31	C	2	DPP	C-CA-CB-NG
31	E	2	DPP	C-CA-CB-NG
16	l	82	MS6	CB-CG-SD-CE
5	a	2069	G7M	C4'-C5'-O5'-P
31	D	1	KBE	O-C-CA-CB
31	E	1	KBE	O-C-CA-CB
31	V	4	MYN	O-C-CA-CB
5	a	746	PSU	O4'-C1'-C5-C6
5	a	2503	2MA	C4'-C5'-O5'-P
5	a	2069	G7M	O4'-C4'-C5'-O5'
5	a	2503	2MA	O4'-C4'-C5'-O5'
16	l	81	4D4	O-C-CA-CB
31	I	2	DPP	N-CA-CB-NG
5	a	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	a	2030	6MZ	3	0
5	a	2604	PSU	1	0
5	a	1939	5MU	1	0
5	a	747	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 303 ligands modelled in this entry, 302 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	G34	a	3001	-	40,40,40	0.65	1 (2%)	58,64,64	1.01	4 (6%)

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
33	G34	a	3001	-	1/1/14/15	0/12/94/94	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	3001	G34	C12-C11	2.10	1.57	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	3001	G34	C12-C11-C10	2.96	117.48	114.58

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	3001	G34	C13-C12-C11	2.48	115.13	112.70
33	a	3001	G34	O3-C14-C13	2.40	108.83	106.24
33	a	3001	G34	C18-C12-C13	-2.12	104.02	105.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	a	3001	G34	C23

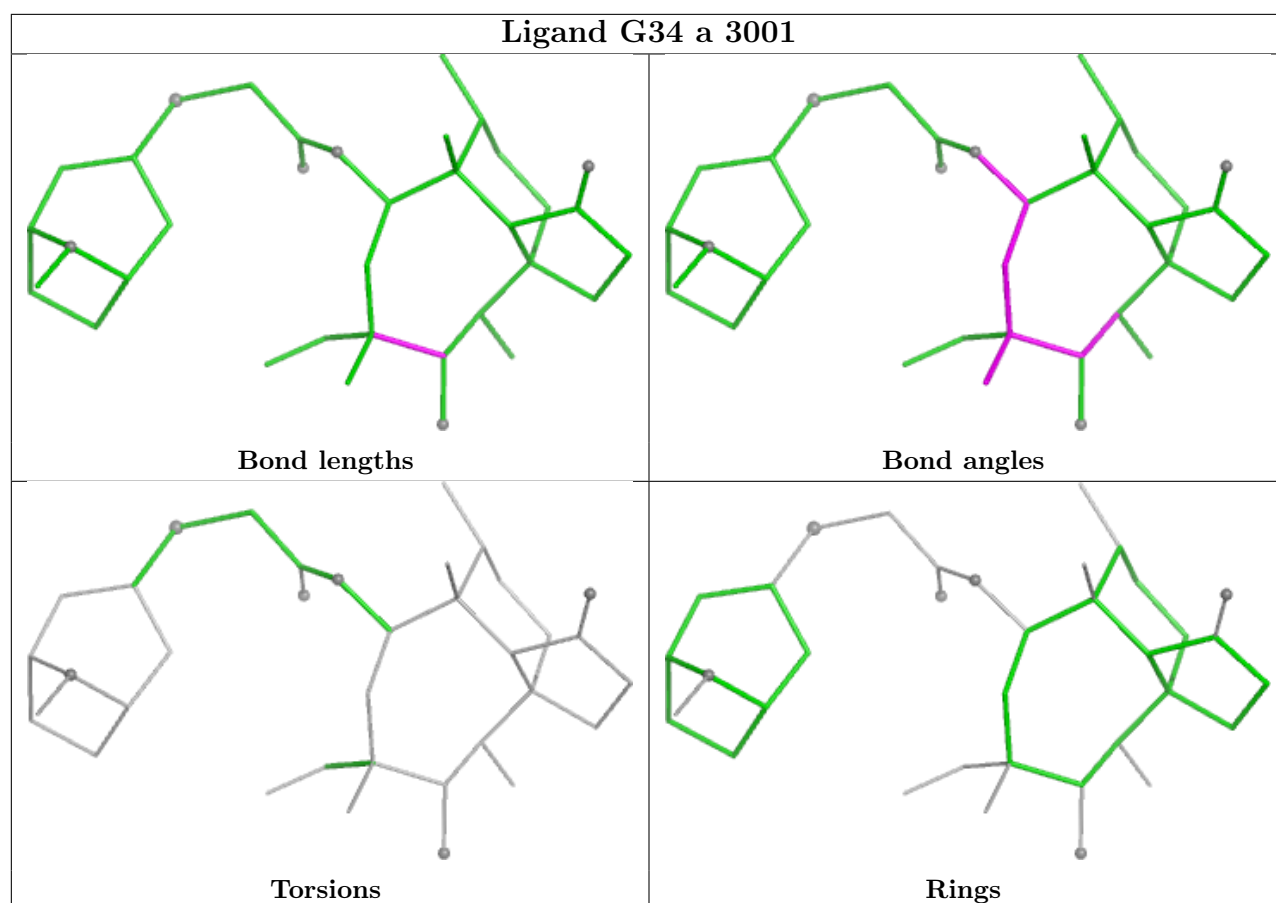
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	3001	G34	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

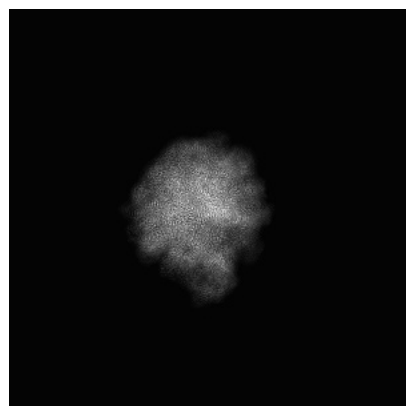
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16613. These allow visual inspection of the internal detail of the map and identification of artifacts.

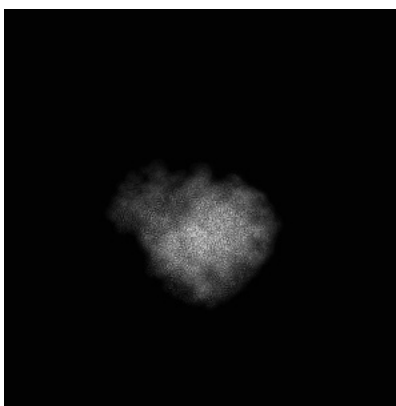
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

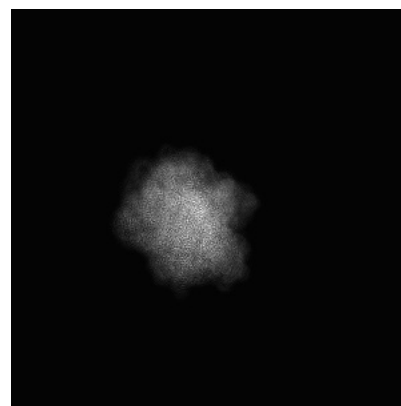
6.1.1 Primary map



X

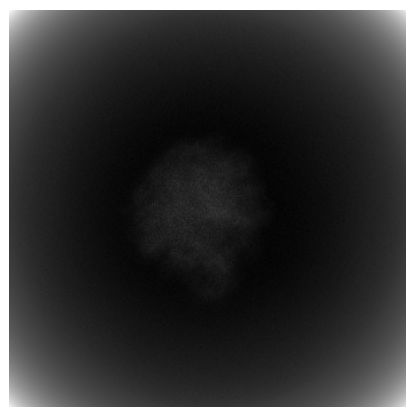


Y

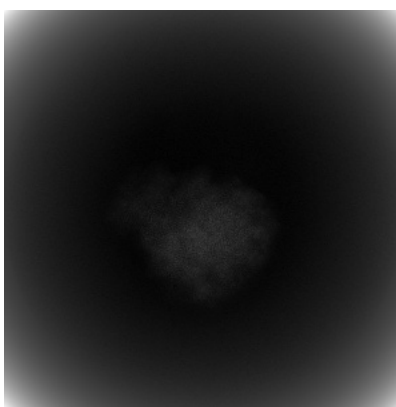


Z

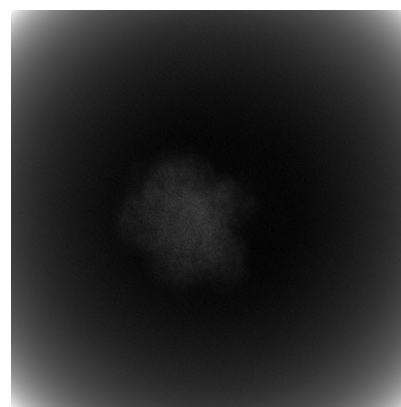
6.1.2 Raw map



X



Y

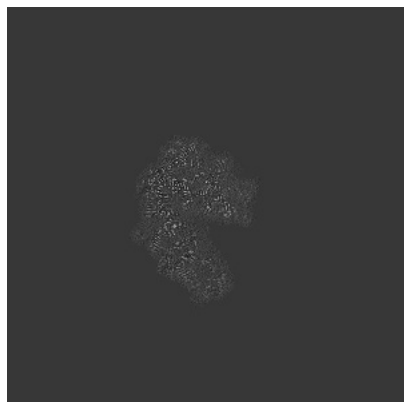


Z

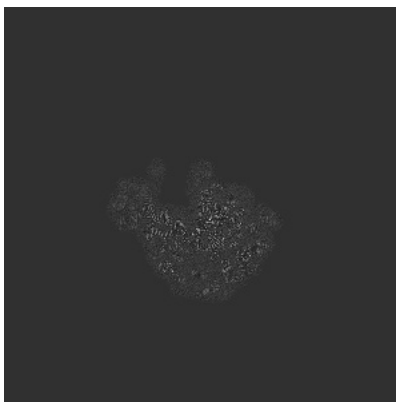
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

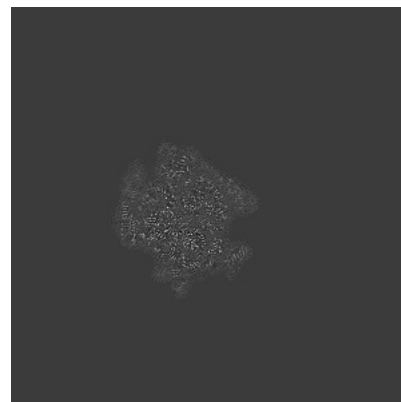
6.2.1 Primary map



X Index: 360

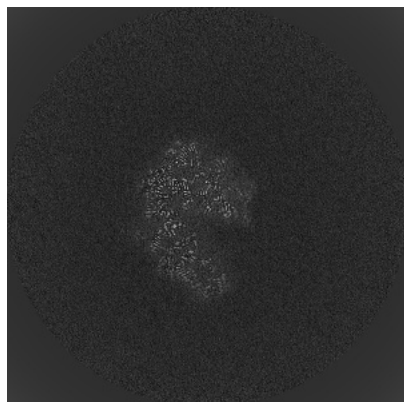


Y Index: 360

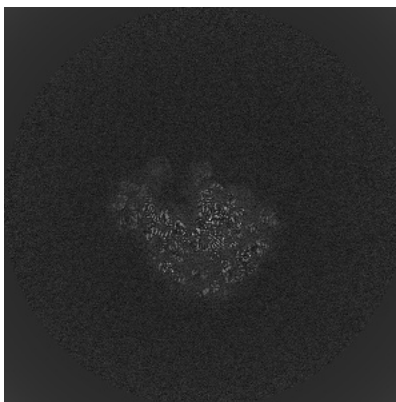


Z Index: 360

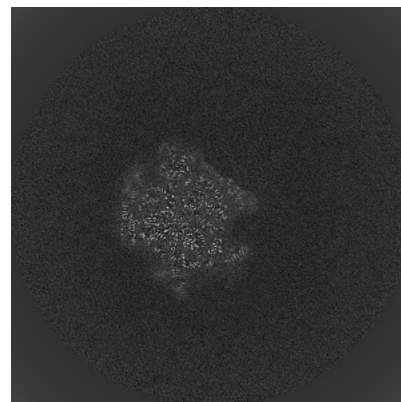
6.2.2 Raw map



X Index: 360



Y Index: 360

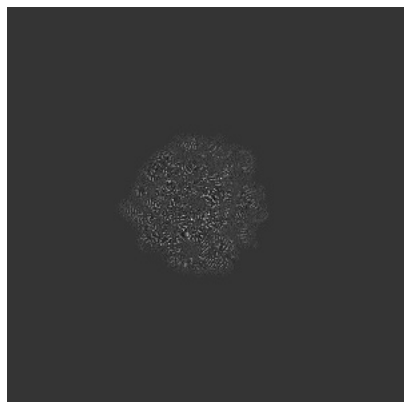


Z Index: 360

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

6.3 Largest variance slices [i](#)

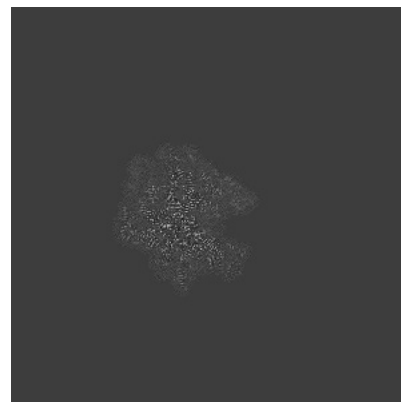
6.3.1 Primary map



X Index: 310

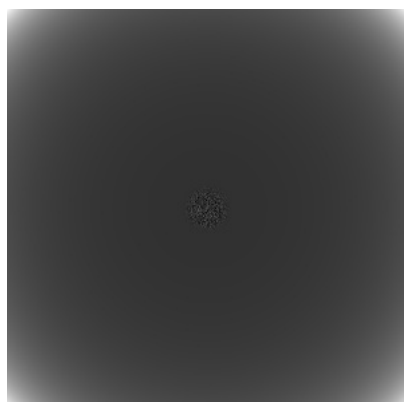


Y Index: 306

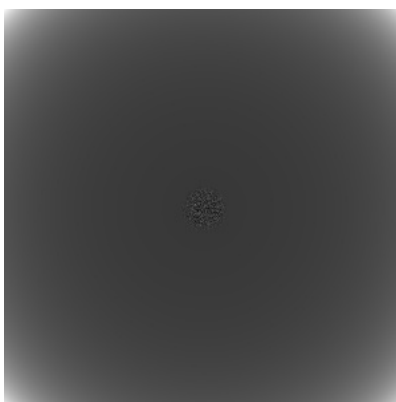


Z Index: 349

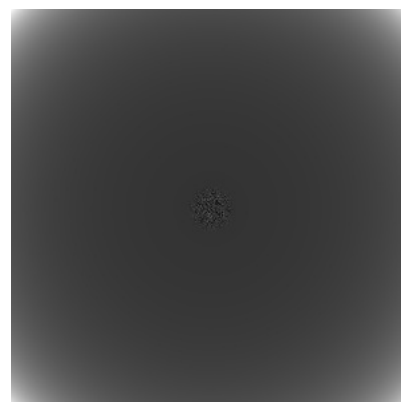
6.3.2 Raw map



X Index: 0



Y Index: 0

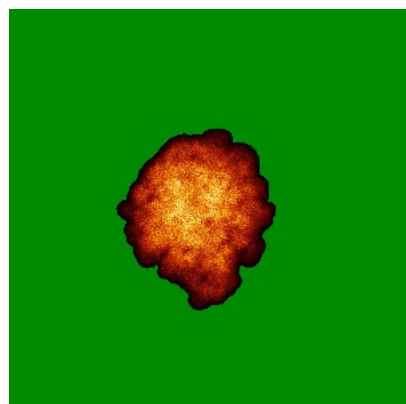


Z Index: 0

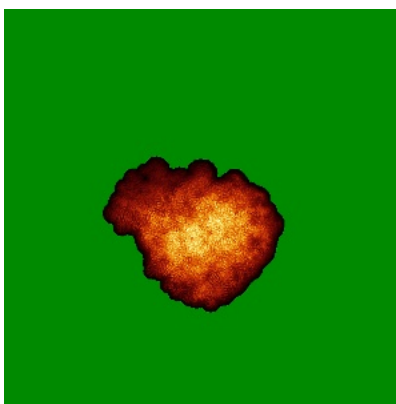
The images above show the largest variance slices of the map in three orthogonal directions.

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

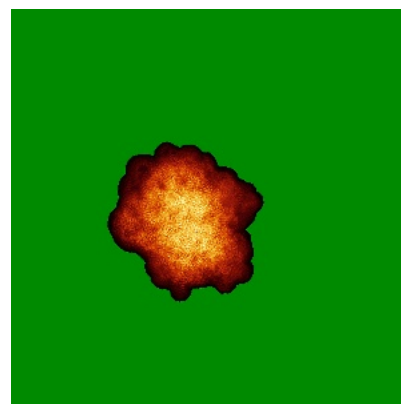
6.4.1 Primary map



X

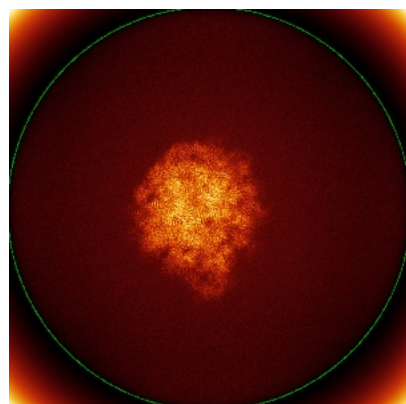


Y

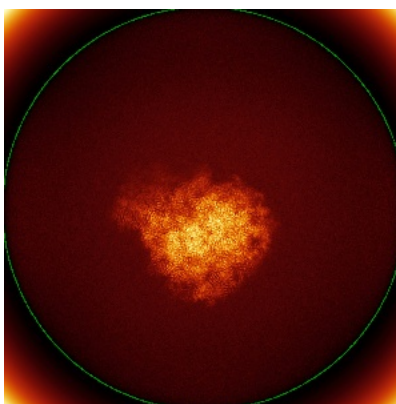


Z

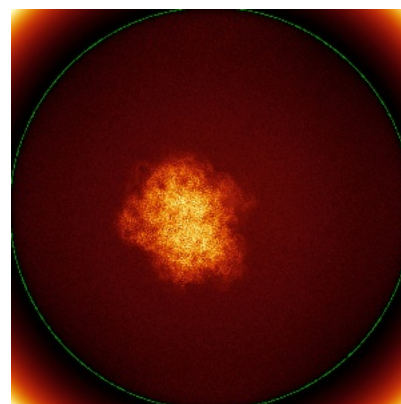
6.4.2 Raw map



X



Y

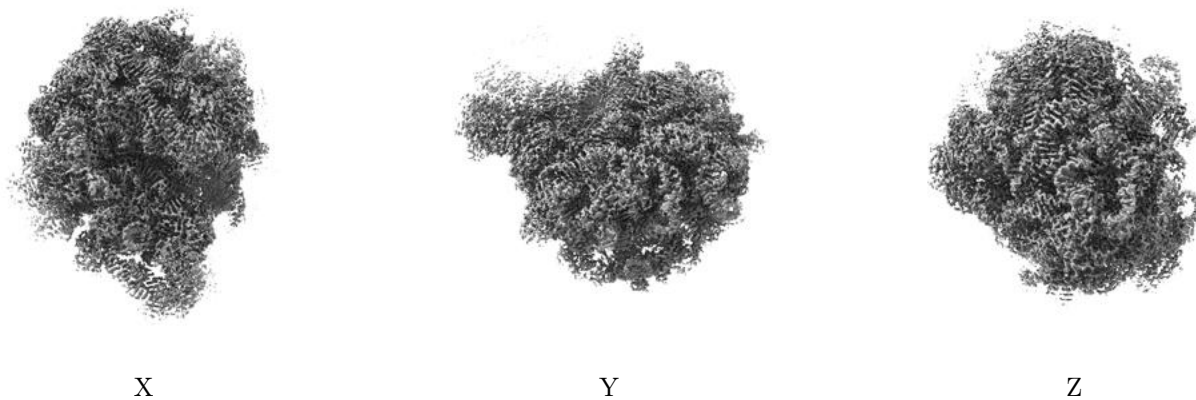


Z

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.

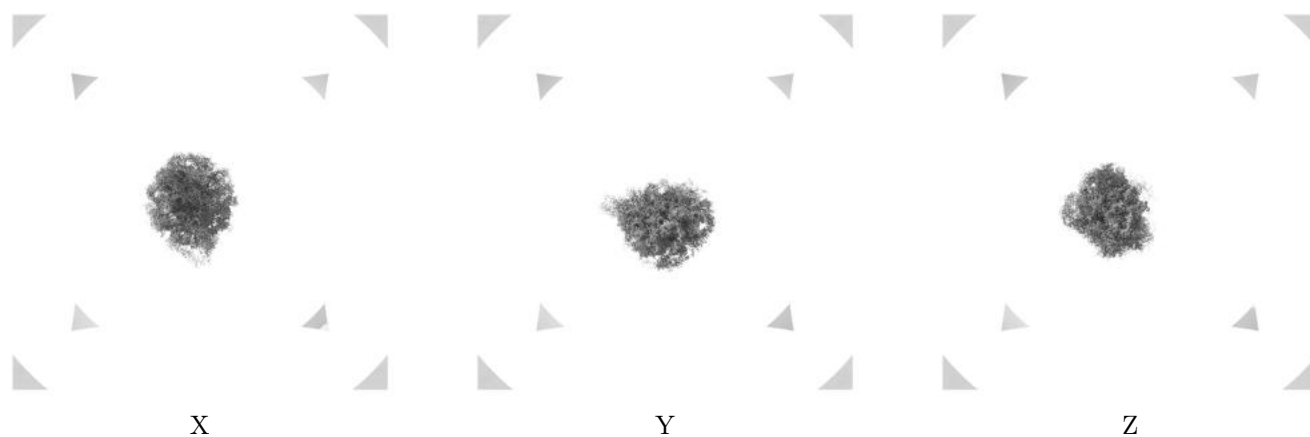
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

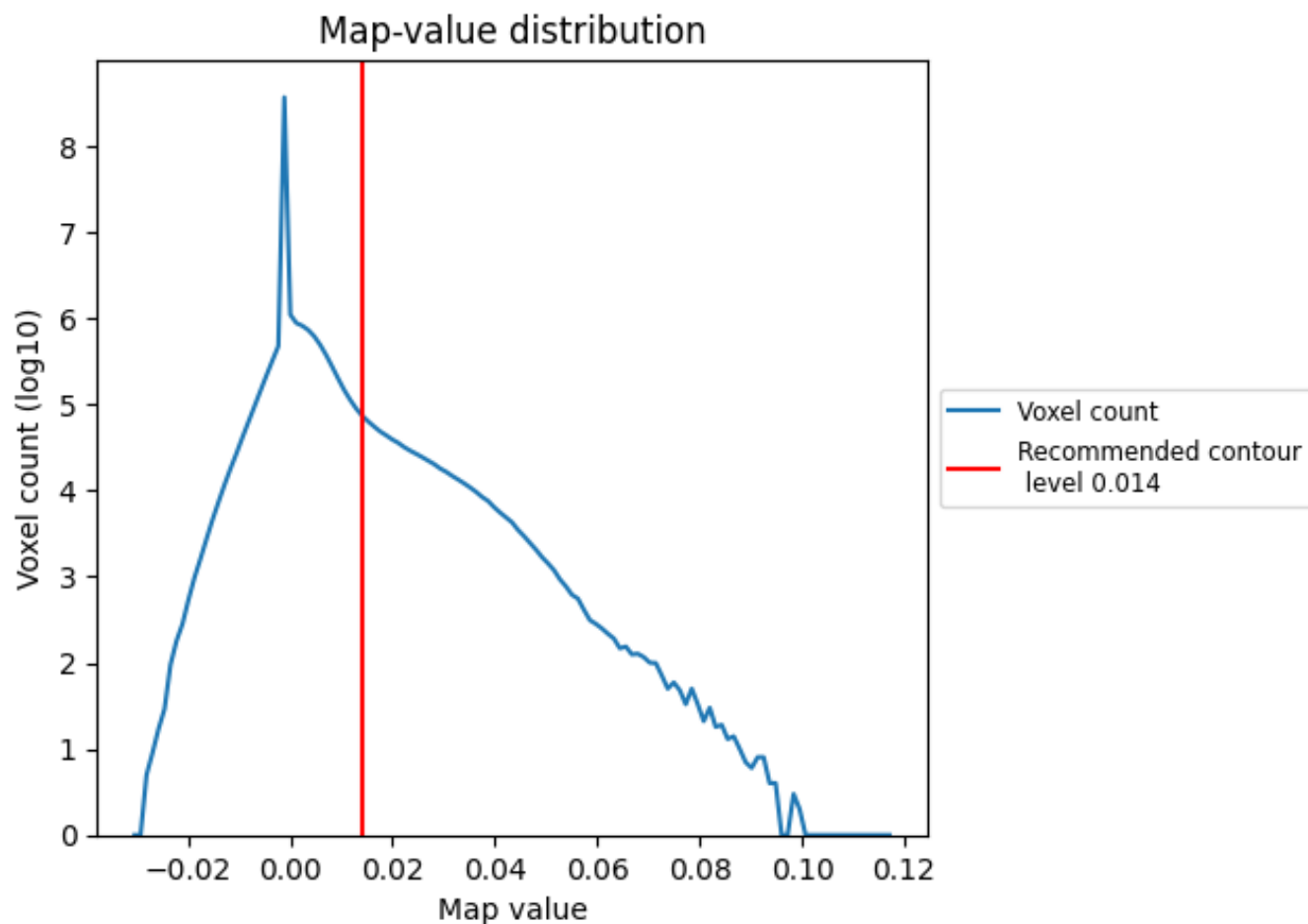
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

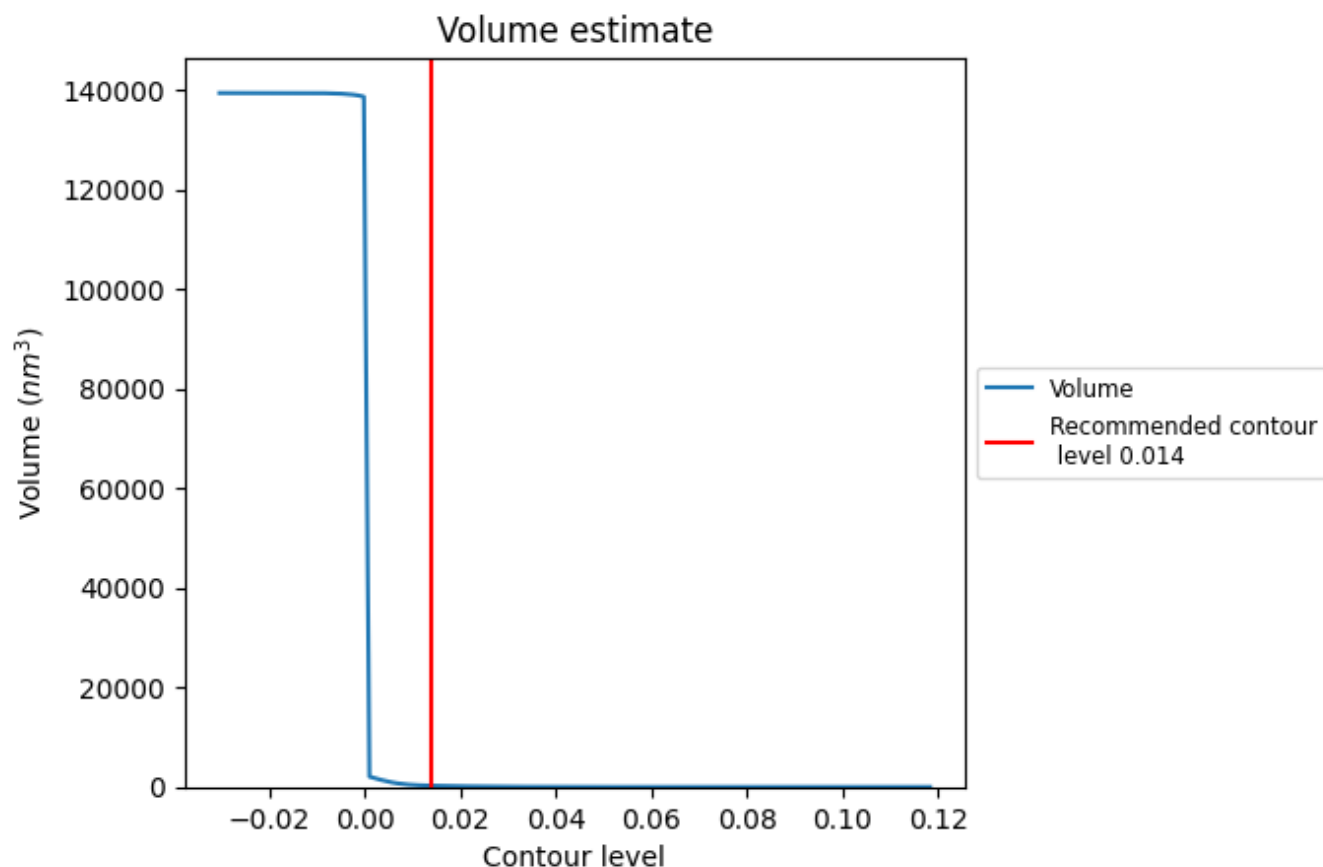
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

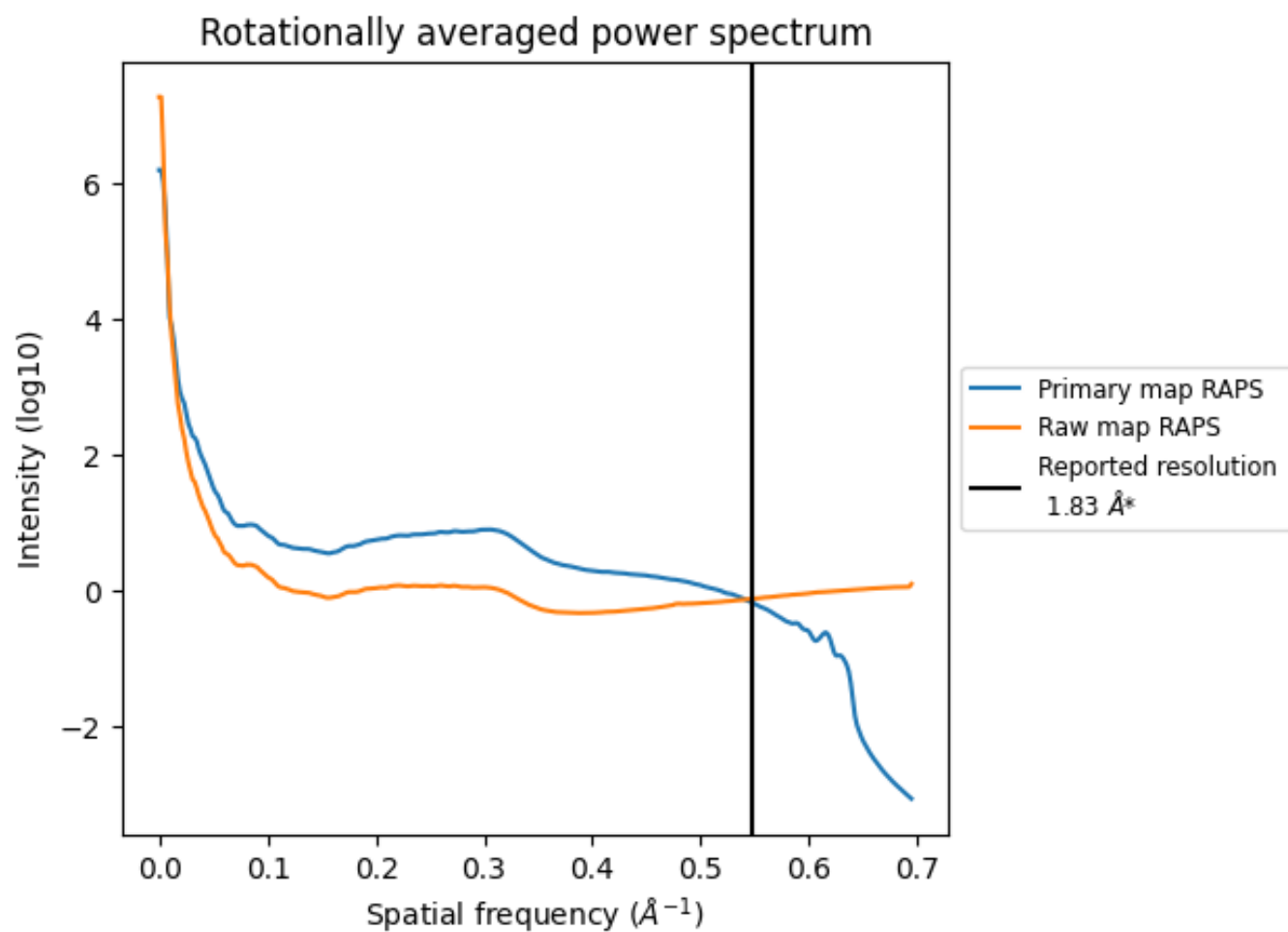
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 nm^3 ; this corresponds to an approximate mass of 227 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 ⓘ

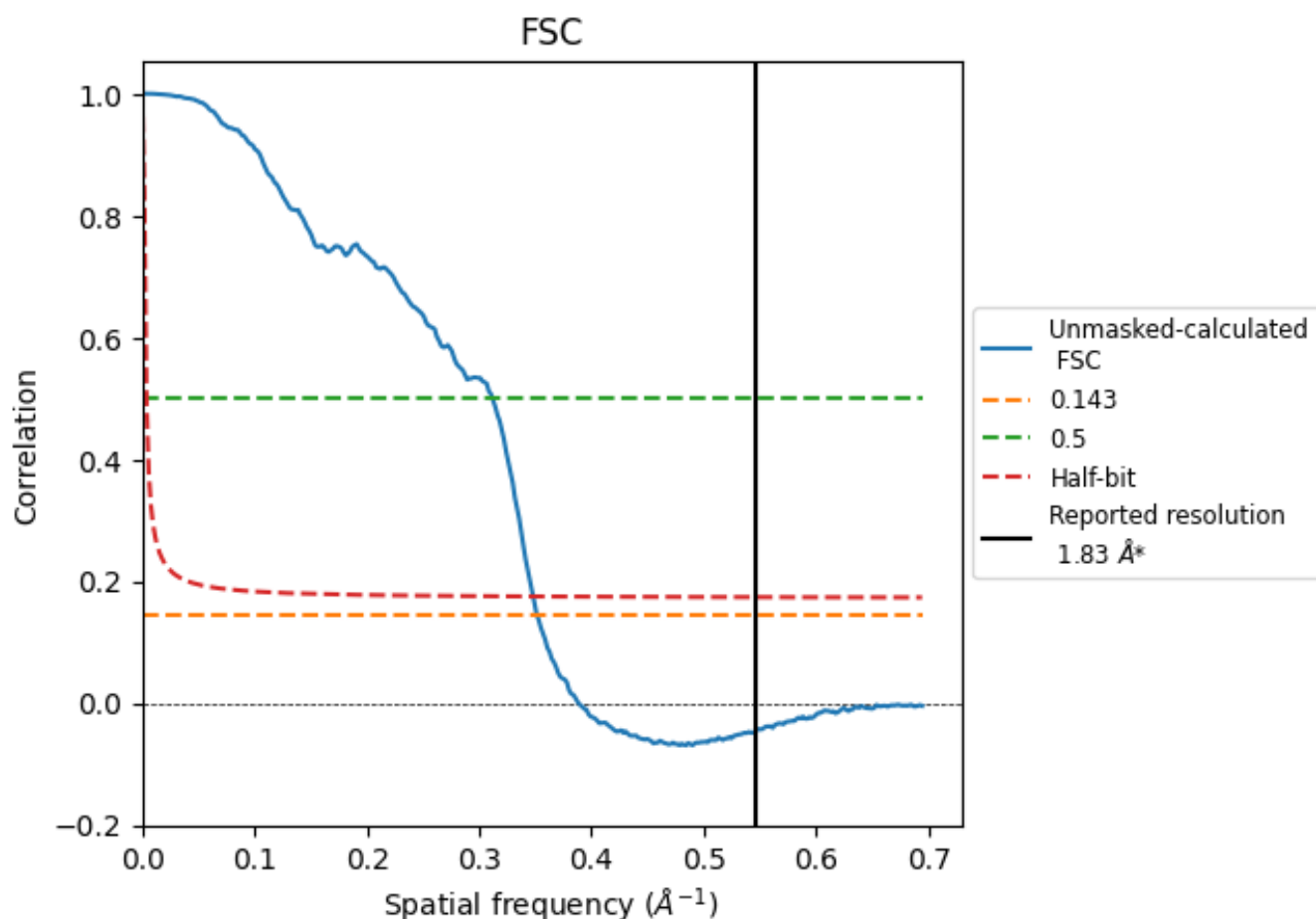


*Reported resolution corresponds to spatial frequency of 0.546 Å⁻¹

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 0.546 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

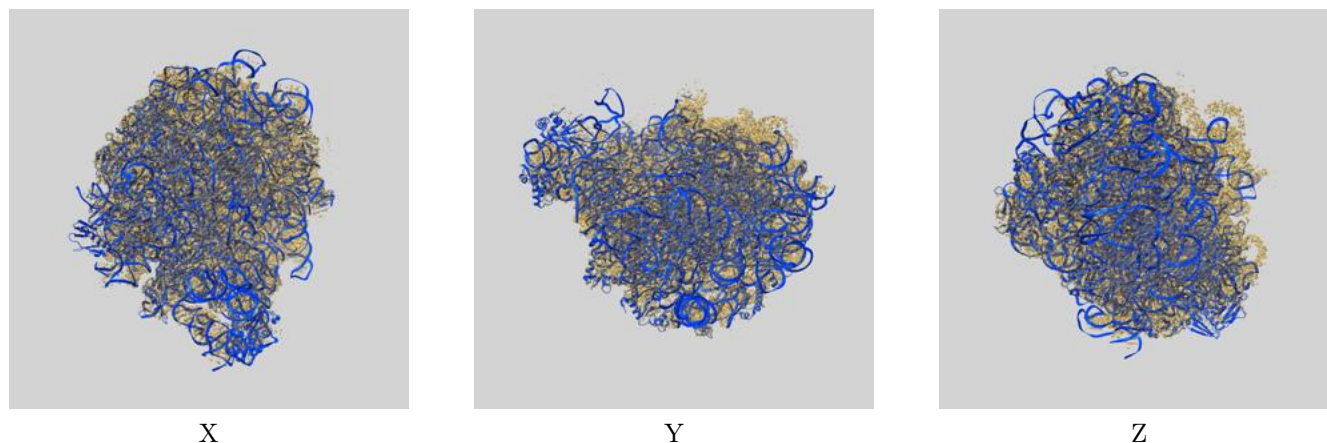
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	3.21	2.87

*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 2.84 differs from the reported value 1.83 by more than 10 %

9 Map-model fit [i](#)

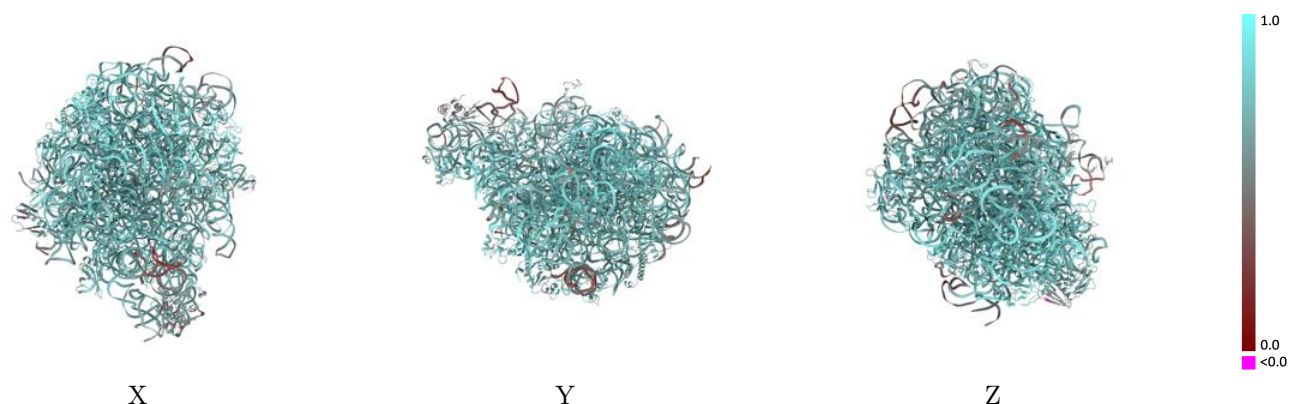
This section contains information regarding the fit between EMDB map EMD-16613 and PDB model 8CEU. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



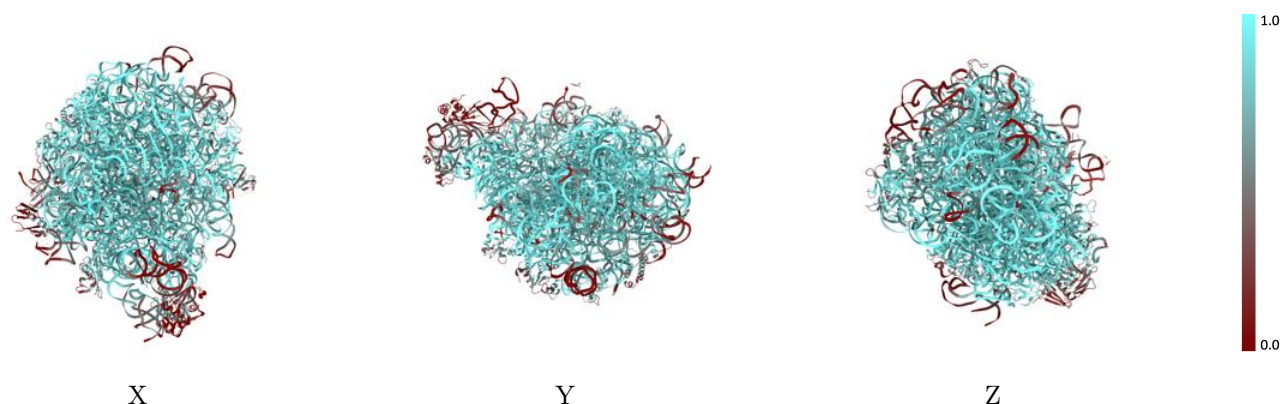
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



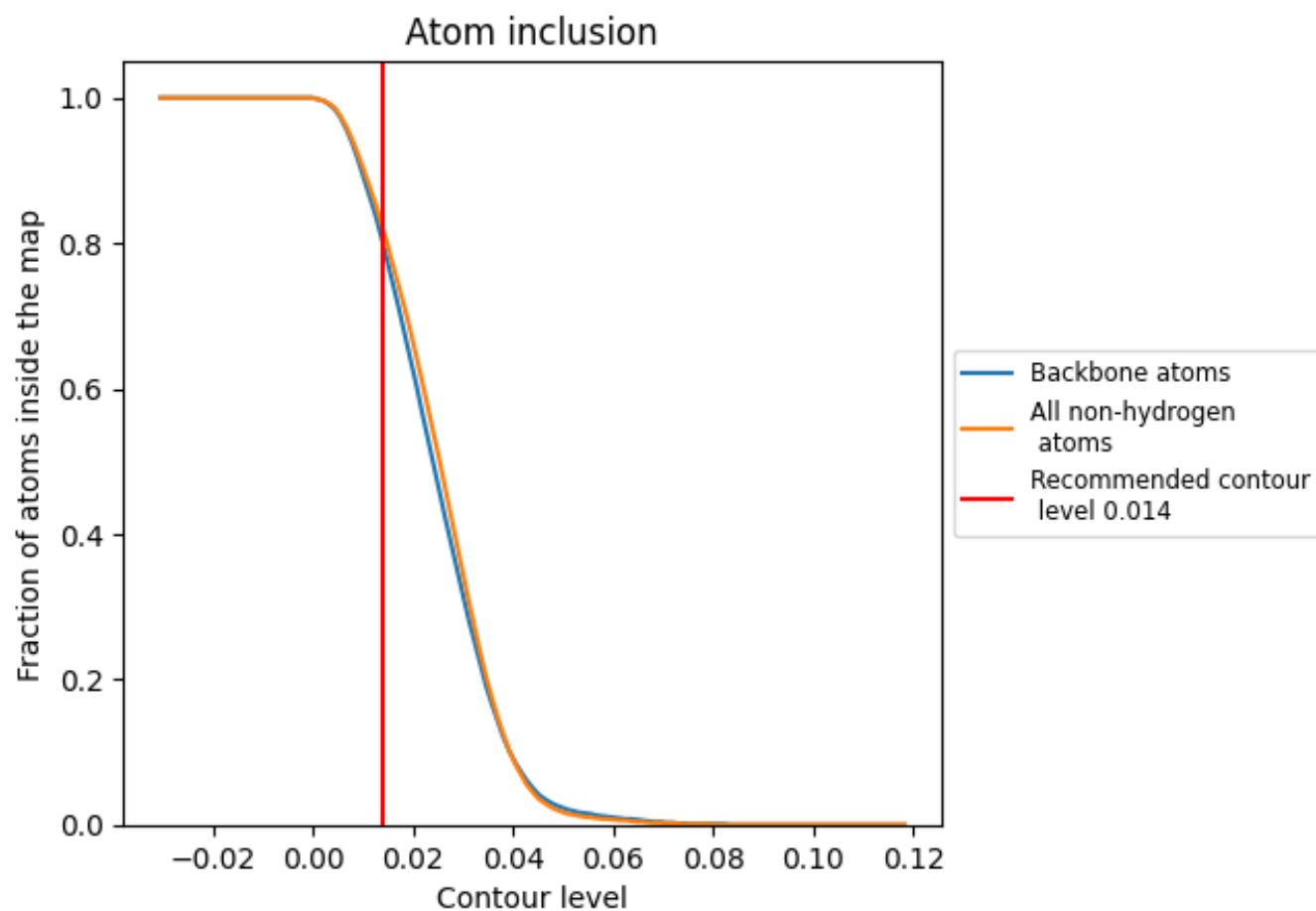
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 82% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.7560
0	 0.7340	 0.7410
1	 0.9800	 0.8370
2	 0.9530	 0.8220
3	 0.8360	 0.7760
C	 0.2340	 0.6000
D	 0.1280	 0.5330
E	 0.6600	 0.7230
F	 0.5110	 0.6620
G	 0.6380	 0.7010
H	 0.7450	 0.7330
I	 0.5320	 0.7070
V	 0.1060	 0.4950
a	 0.8610	 0.7610
b	 0.6030	 0.6730
c	 0.9040	 0.8080
d	 0.8610	 0.7920
e	 0.7400	 0.7540
f	 0.0820	 0.5030
g	 0.3190	 0.6170
h	 0.4700	 0.6470
i	 0.8700	 0.7860
j	 0.8240	 0.7840
k	 0.8120	 0.7710
l	 0.8410	 0.7810
m	 0.9540	 0.8240
n	 0.5160	 0.6950
o	 0.8060	 0.7820
p	 0.9140	 0.8070
q	 0.7430	 0.7540
r	 0.8640	 0.7920
s	 0.7330	 0.7460
t	 0.7000	 0.7260
u	 0.6220	 0.7140
v	 0.8780	 0.7950



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Chain	Atom inclusion	Q-score
w	 0.8040	 0.7780
x	 0.5750	 0.6970
y	 0.8100	 0.7660
z	 0.8470	 0.7820