



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2026 – 06:15 pm BST

PDB ID : 9TEY / pdb_00009tey
EMDB ID : EMD-55847
Title : DalDro bound to the terminating Escherichia coli 70S ribosome
Authors : Berger, M.J.; Safdari, H.A.; Wilson, D.N.
Deposited on : 2025-11-26
Resolution : 3.11 Å(reported)

This is a wwPDB EM Validation Summary 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:

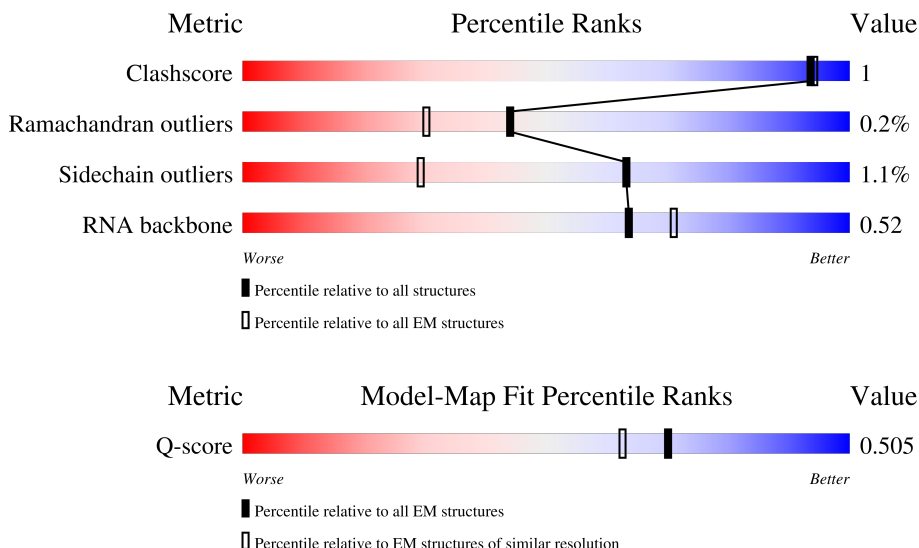
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.11 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	14465 (2.61 - 3.61)

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	5% 93% 7%
2	1	46	89% 11%
3	2	65	92% 6%

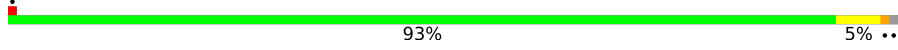
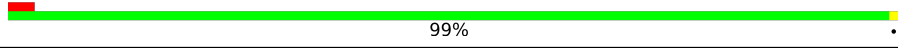
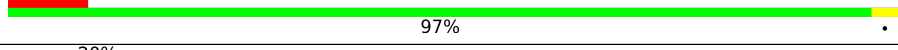
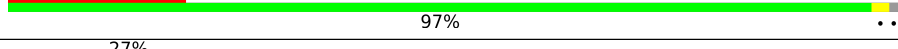
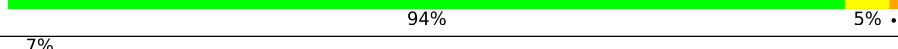
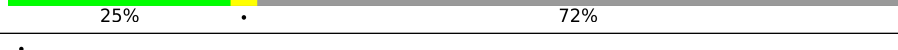
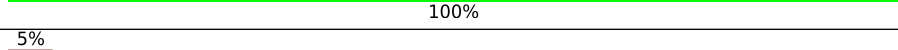
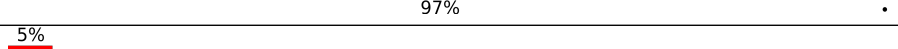
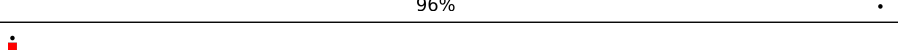
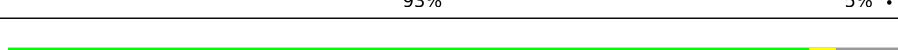
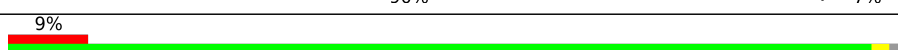
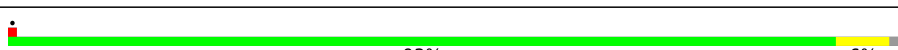
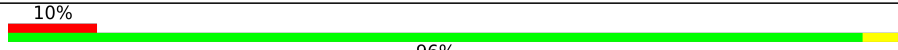
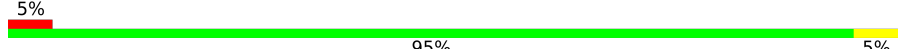
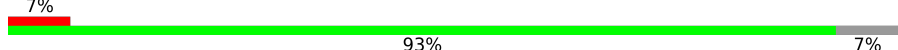
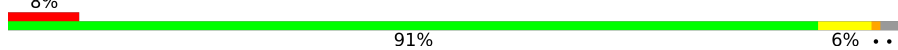
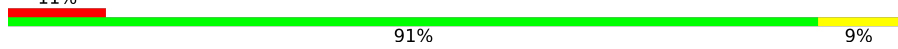
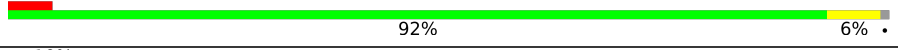
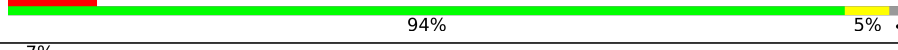
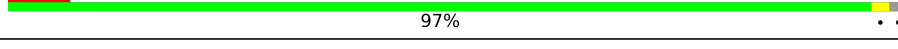
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Mol	Chain	Length	Quality of chain
4	3	38	
5	8	20	
6	B	241	
7	C	233	
8	D	206	
9	E	167	
10	F	135	
11	G	179	
12	H	130	
13	I	130	
14	J	103	
15	K	129	
16	L	124	
17	M	118	
18	N	101	
19	O	89	
20	P	82	
21	Q	84	
22	R	75	
23	S	92	
24	T	87	
25	U	71	
26	W	360	
27	Z	76	
28	Y	120	

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Mol	Chain	Length	Quality of chain
28	b	120	
29	c	273	
30	d	209	
31	e	201	
32	f	179	
33	g	177	
34	h	149	
35	i	142	
36	j	123	
37	k	144	
38	l	136	
39	m	127	
40	n	117	
41	o	115	
42	p	118	
43	q	103	
44	r	110	
45	s	100	
46	t	104	
47	u	94	
48	v	85	
49	w	78	
50	x	63	
51	y	59	
52	z	57	

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Mol	Chain	Length	Quality of chain
53	4	70	
54	V	2904	
55	A	1542	

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
15	IAS	K	119	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 141915 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	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

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

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

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

- Molecule 5 is a protein called Drosocin.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	8	9	Total	C	N	O	0	0
			74	46	17	11		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	1	HIS	-	insertion	UNP P36193
8	2	ASP	LYS	conflict	UNP P36193
8	3	LYS	PRO	conflict	UNP P36193

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Chain	Residue	Modelled	Actual	Comment	Reference
8	4	PRO	ARG	conflict	UNP P36193
8	7	LEU	SER	conflict	UNP P36193

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 20 is a protein called 30S ribosomal protein S16.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 22 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 24 is a protein called 30S ribosomal protein S20.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 26 is a protein called Peptide chain release factor RF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	254	Total	C	N	O	S	0	0
			1977	1207	376	386	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		
28	Y	9	Total	C	N	O	P	0	0
			188	85	31	63	9		

- Molecule 29 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	270	Total	C	N	O	S	0	0
			2076	1285	422	362	7		

- Molecule 30 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 34 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL14.

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

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

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 39 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL24.

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

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

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	v	77	Total	C	N	O	S	
			582	360	115	106	1	0

- Molecule 49 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 53 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	59	Total	C	N	O	S	0	0
			472	294	89	84	5		

- Molecule 54 is a RNA chain called 23S rRNA.

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

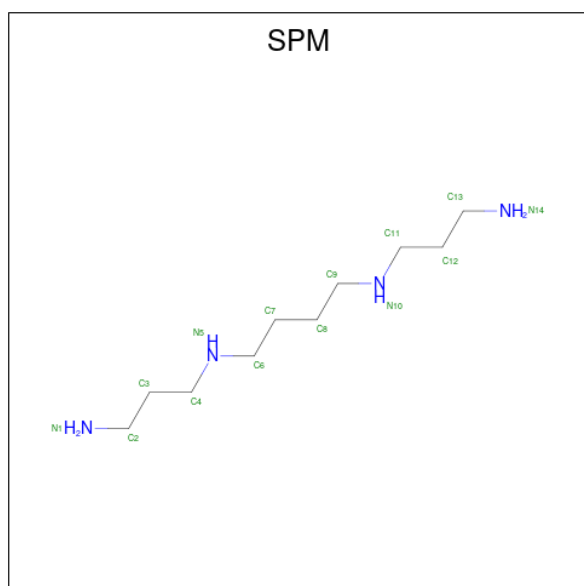
- Molecule 55 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
57	V	1	Total	C	N	0
			14	10	4	

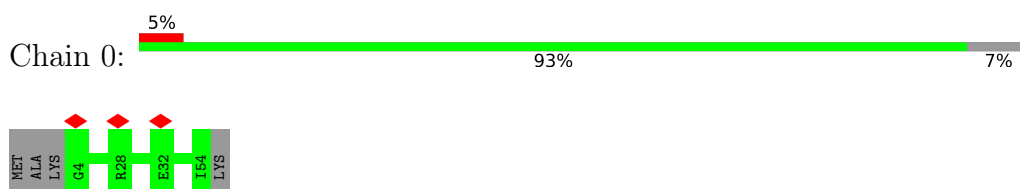
- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	A	1	Total	O	0
			1	1	
58	Y	5	Total	O	0
			5	5	

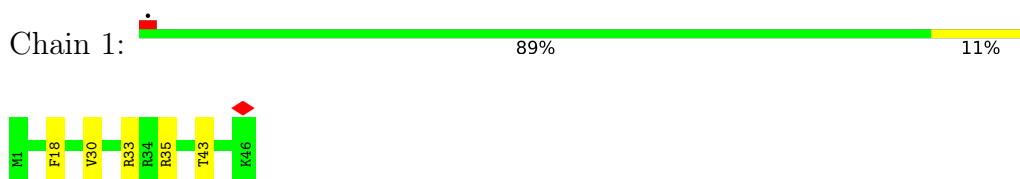
3 Residue-property plots [i](#)

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.

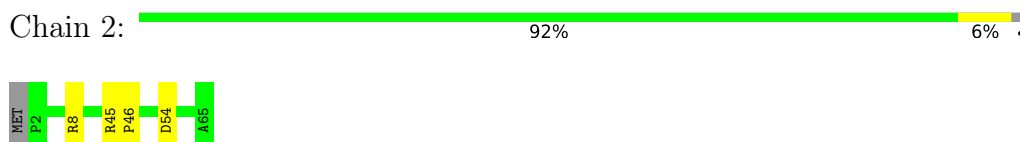
- Molecule 1: Large ribosomal subunit protein bL33



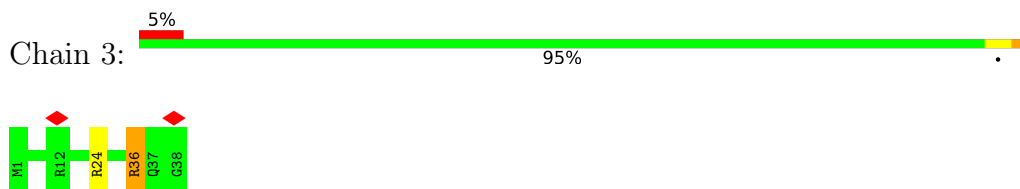
- Molecule 2: Large ribosomal subunit protein bL34



- Molecule 3: Large ribosomal subunit protein bL35



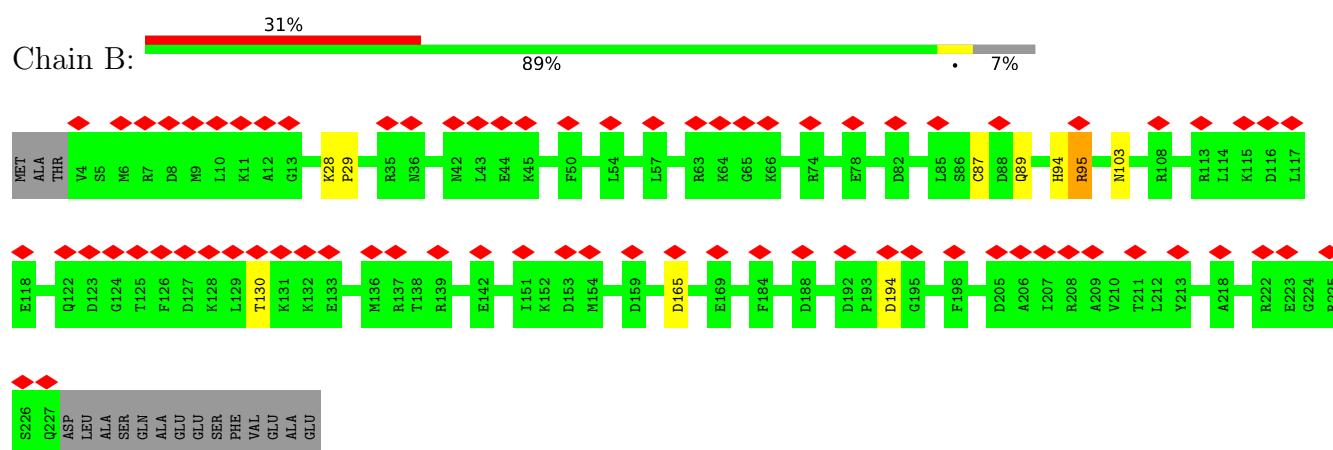
- Molecule 4: Large ribosomal subunit protein bL36A



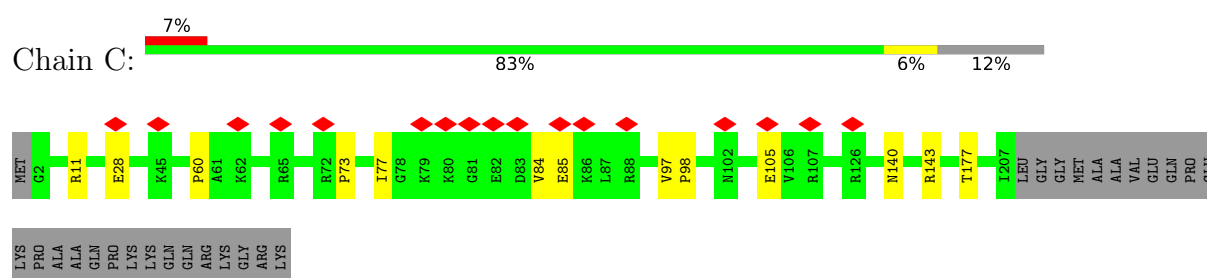
- Molecule 5: Drosocin



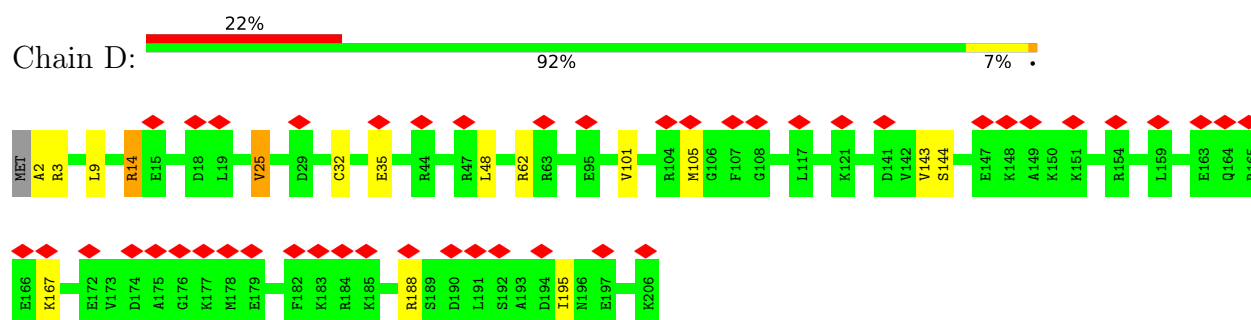
- Molecule 6: 30S ribosomal protein S2



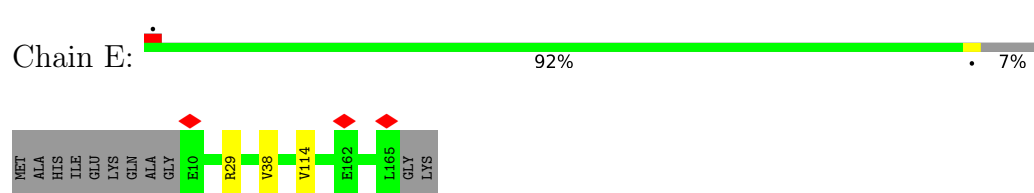
- Molecule 7: Small ribosomal subunit protein uS3



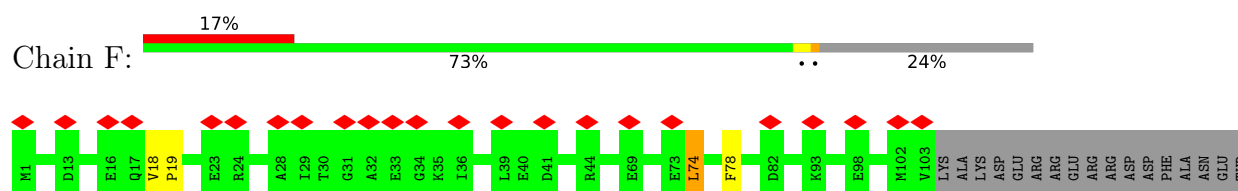
- Molecule 8: Small ribosomal subunit protein uS4



- Molecule 9: Small ribosomal subunit protein uS5

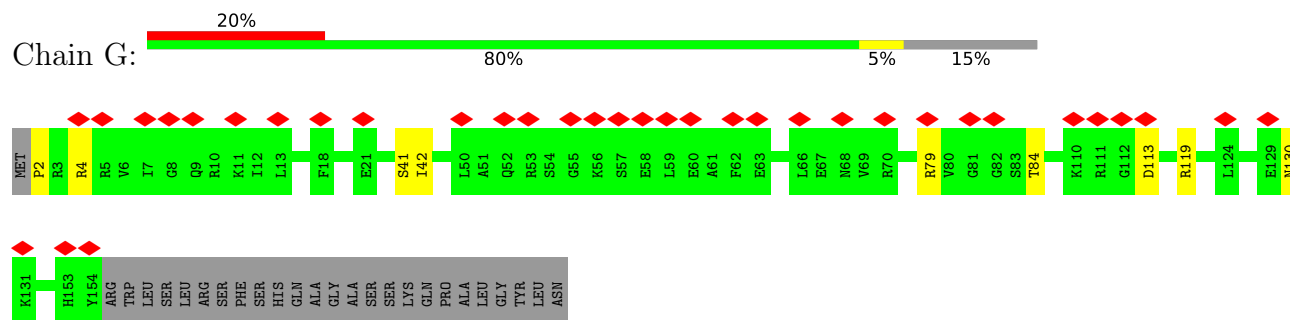


- Molecule 10: 30S ribosomal protein S6, fully modified isoform

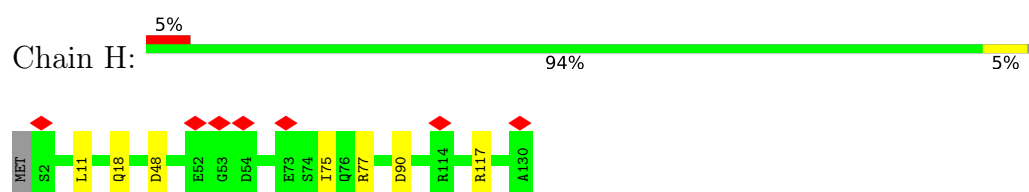


ALA
ASP
ASP
ALA
GLU
ALA
GLY
ASP
SER
GLU
GLU
GLU
GLU

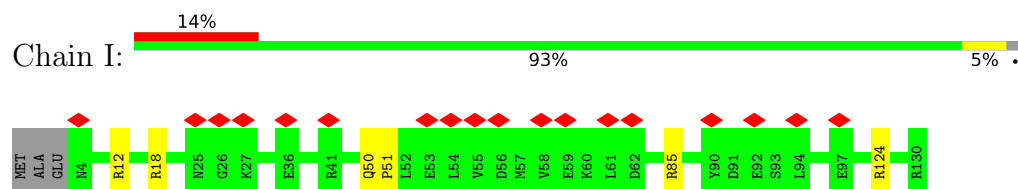
- Molecule 11: 30S ribosomal protein S7



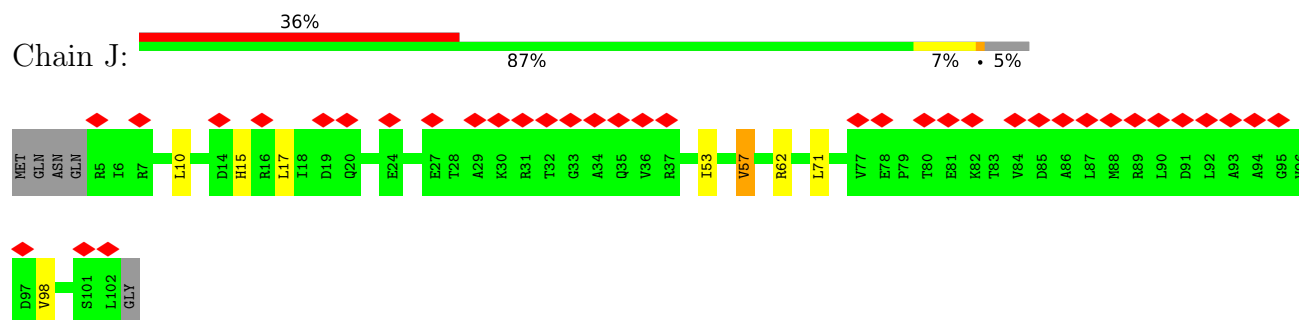
- Molecule 12: Small ribosomal subunit protein uS8



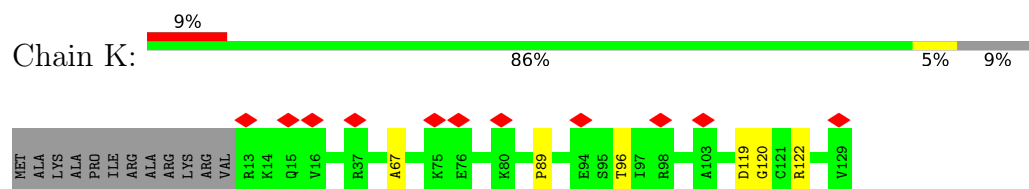
- Molecule 13: Small ribosomal subunit protein uS9



- Molecule 14: Small ribosomal subunit protein uS10



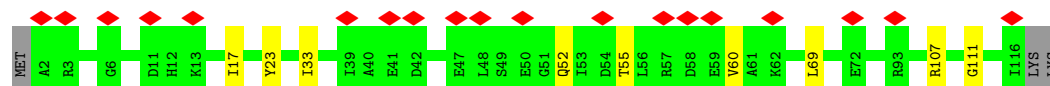
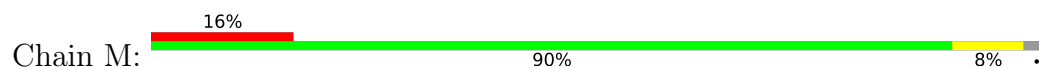
- Molecule 15: Small ribosomal subunit protein uS11



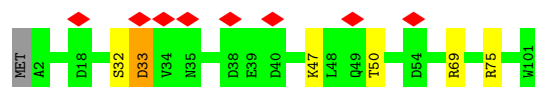
- Molecule 16: Small ribosomal subunit protein uS12



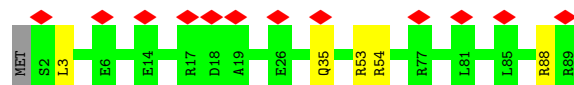
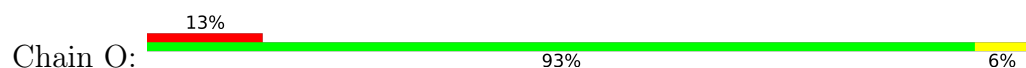
- Molecule 17: Small ribosomal subunit protein uS13



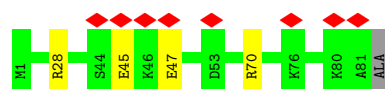
- Molecule 18: Small ribosomal subunit protein uS14



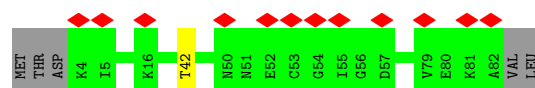
- Molecule 19: Small ribosomal subunit protein uS15



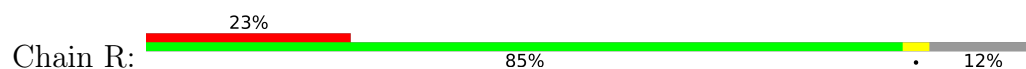
- Molecule 20: 30S ribosomal protein S16



- Molecule 21: Small ribosomal subunit protein uS17

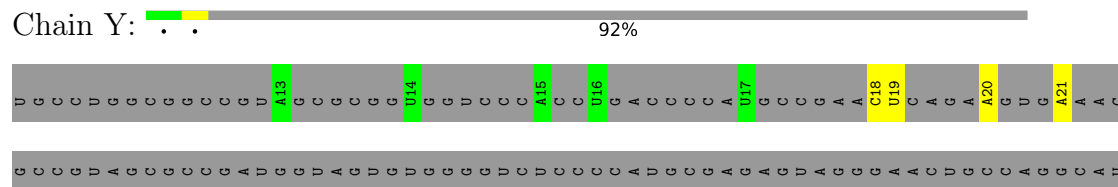


- Molecule 22: Small ribosomal subunit protein bS18

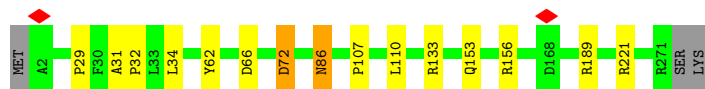
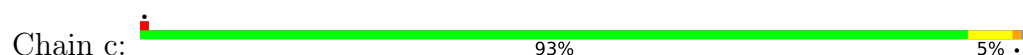




- Molecule 28: 5S rRNA



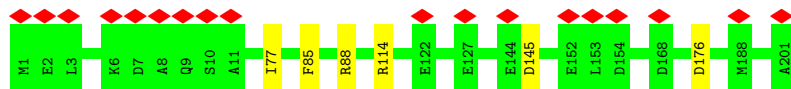
- Molecule 29: Large ribosomal subunit protein uL2



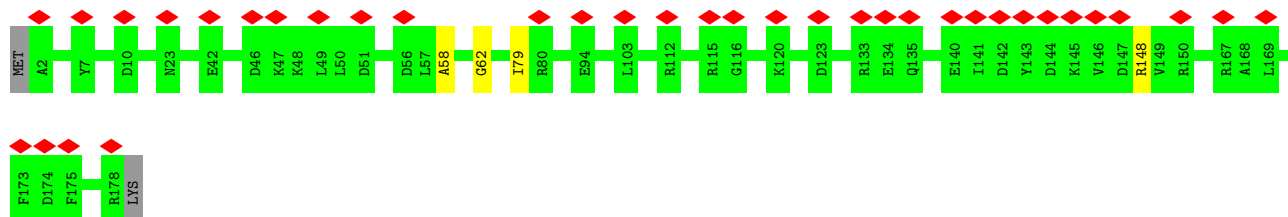
- Molecule 30: Large ribosomal subunit protein uL3



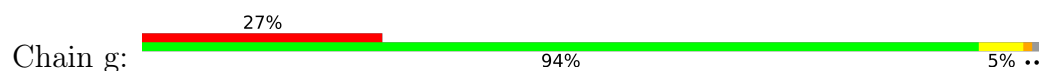
- Molecule 31: Large ribosomal subunit protein uL4

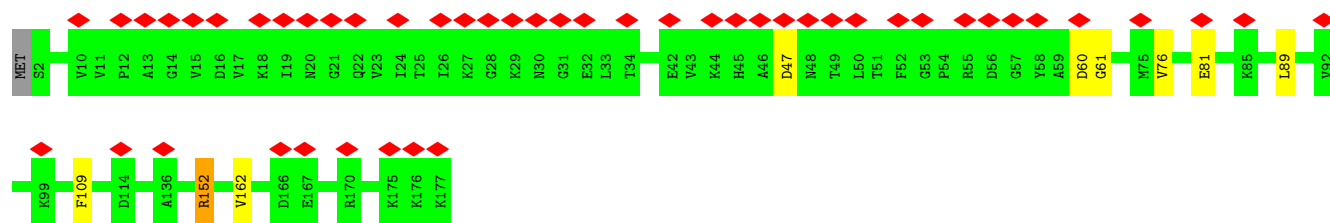


- Molecule 32: Large ribosomal subunit protein uL5

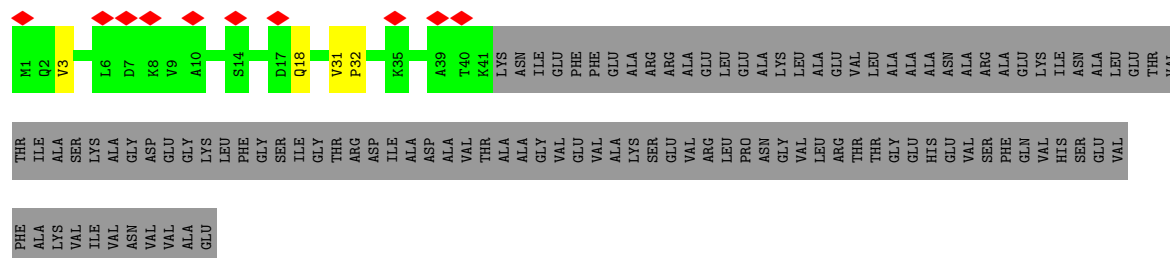


- Molecule 33: Large ribosomal subunit protein uL6

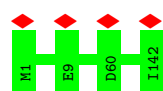




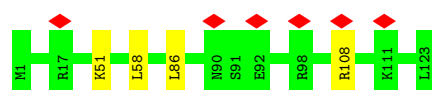
- Molecule 34: Large ribosomal subunit protein bL9



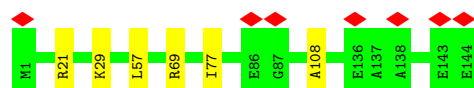
- Molecule 35: Large ribosomal subunit protein uL13



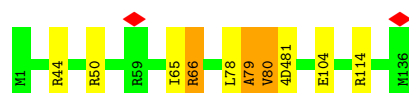
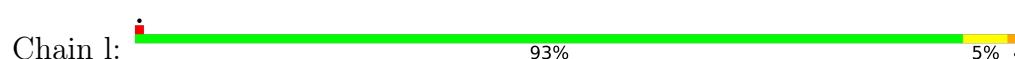
- Molecule 36: Large ribosomal subunit protein uL14



- Molecule 37: 50S ribosomal protein L15

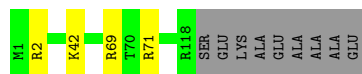


- Molecule 38: Large ribosomal subunit protein uL16

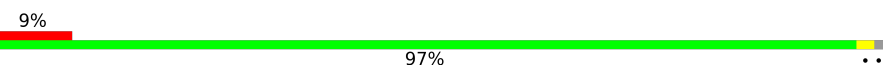


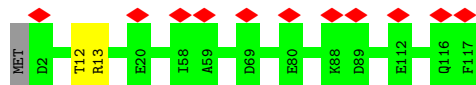
- Molecule 39: Large ribosomal subunit protein bL17

Chain m:  90% 7%

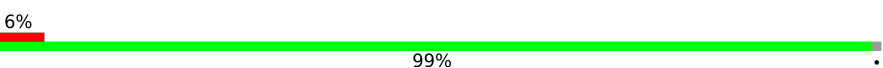


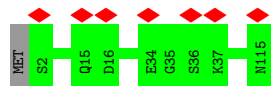
- Molecule 40: Large ribosomal subunit protein uL18

Chain n:  9% 97%

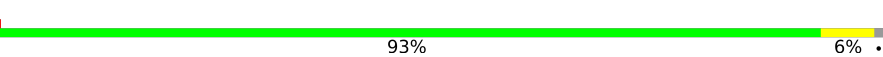


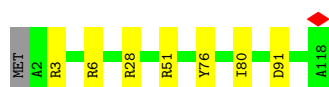
- Molecule 41: Large ribosomal subunit protein bL19

Chain o:  6% 99%

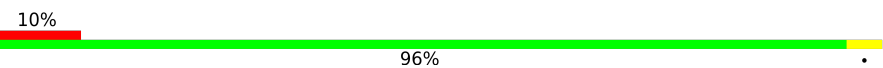


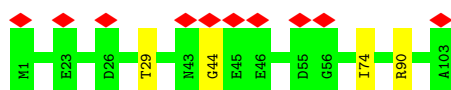
- Molecule 42: Large ribosomal subunit protein bL20

Chain p:  93% 6%

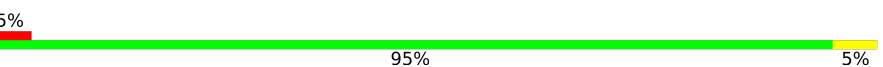


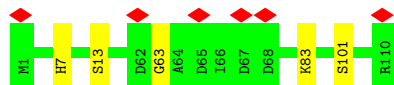
- Molecule 43: Large ribosomal subunit protein bL21

Chain q:  10% 96%



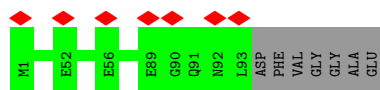
- Molecule 44: Large ribosomal subunit protein uL22

Chain r:  5% 95% 5%

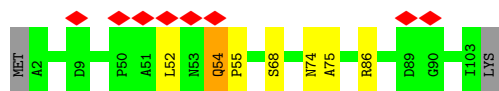
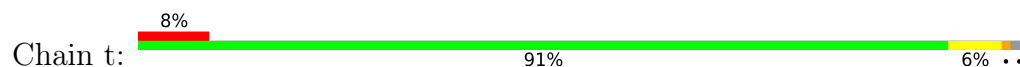


- Molecule 45: Large ribosomal subunit protein uL23

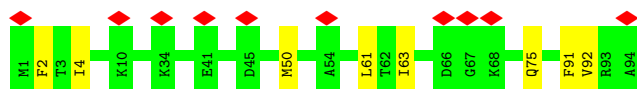
Chain s:  7% 93% 7%



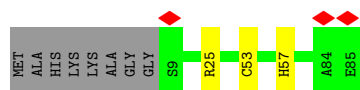
- Molecule 46: Large ribosomal subunit protein uL24



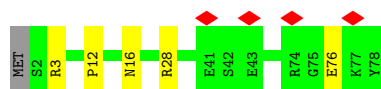
- Molecule 47: 50S ribosomal protein L25



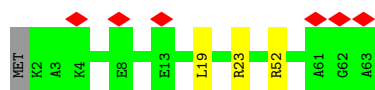
- Molecule 48: Large ribosomal subunit protein bL27



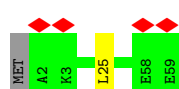
- Molecule 49: Large ribosomal subunit protein bL28



- Molecule 50: Large ribosomal subunit protein uL29

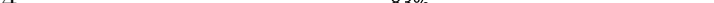


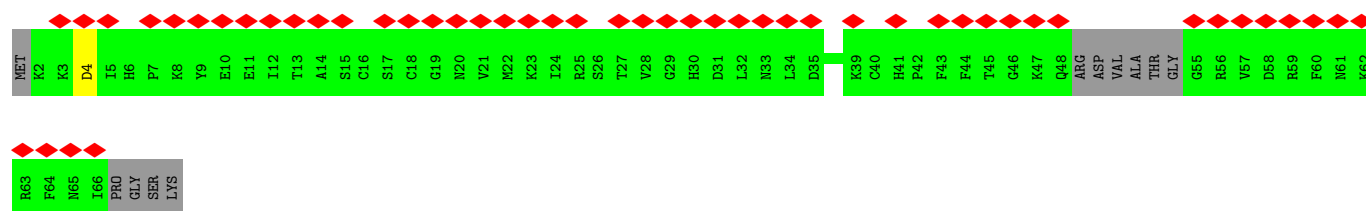
- Molecule 51: Large ribosomal subunit protein uL30



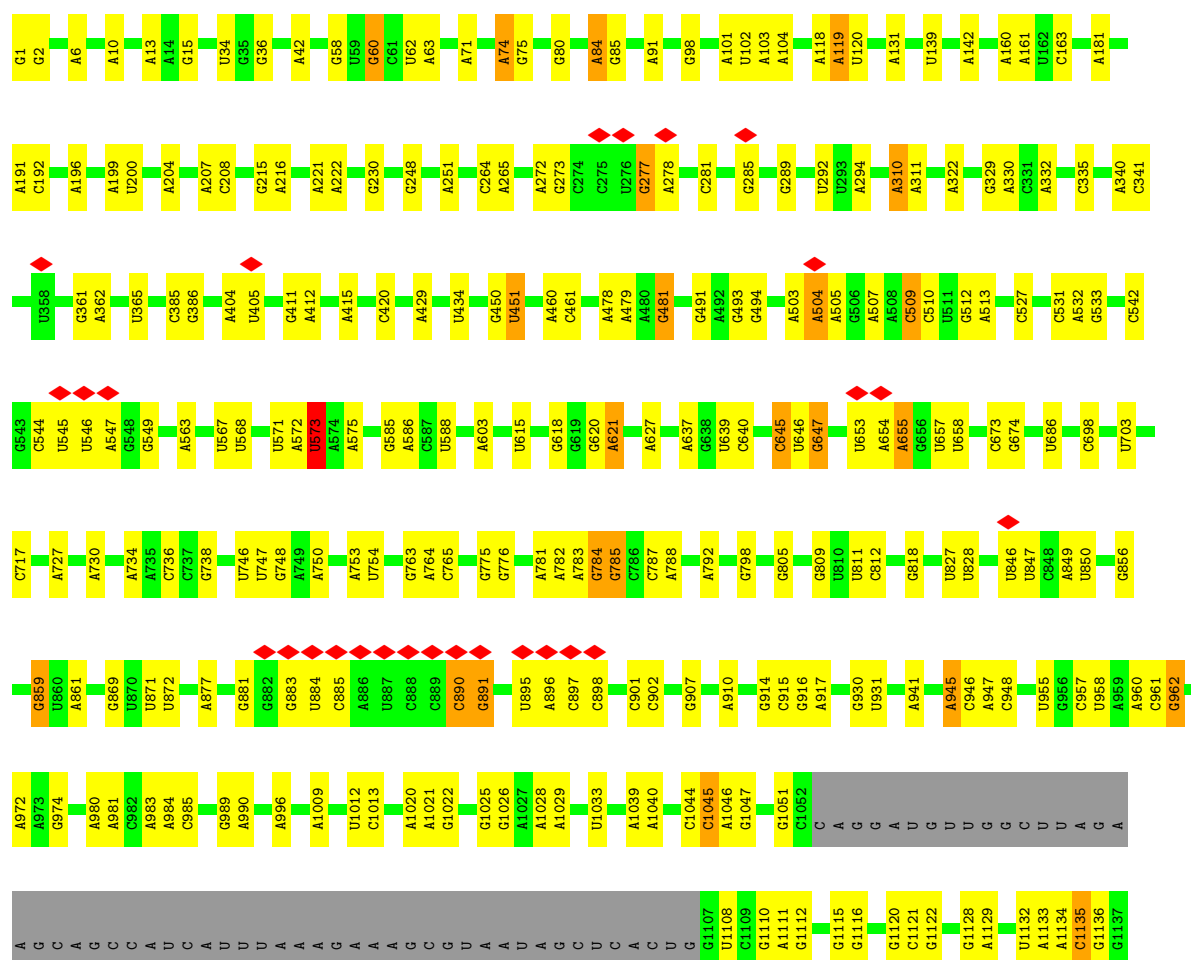
- Molecule 52: Large ribosomal subunit protein bL32

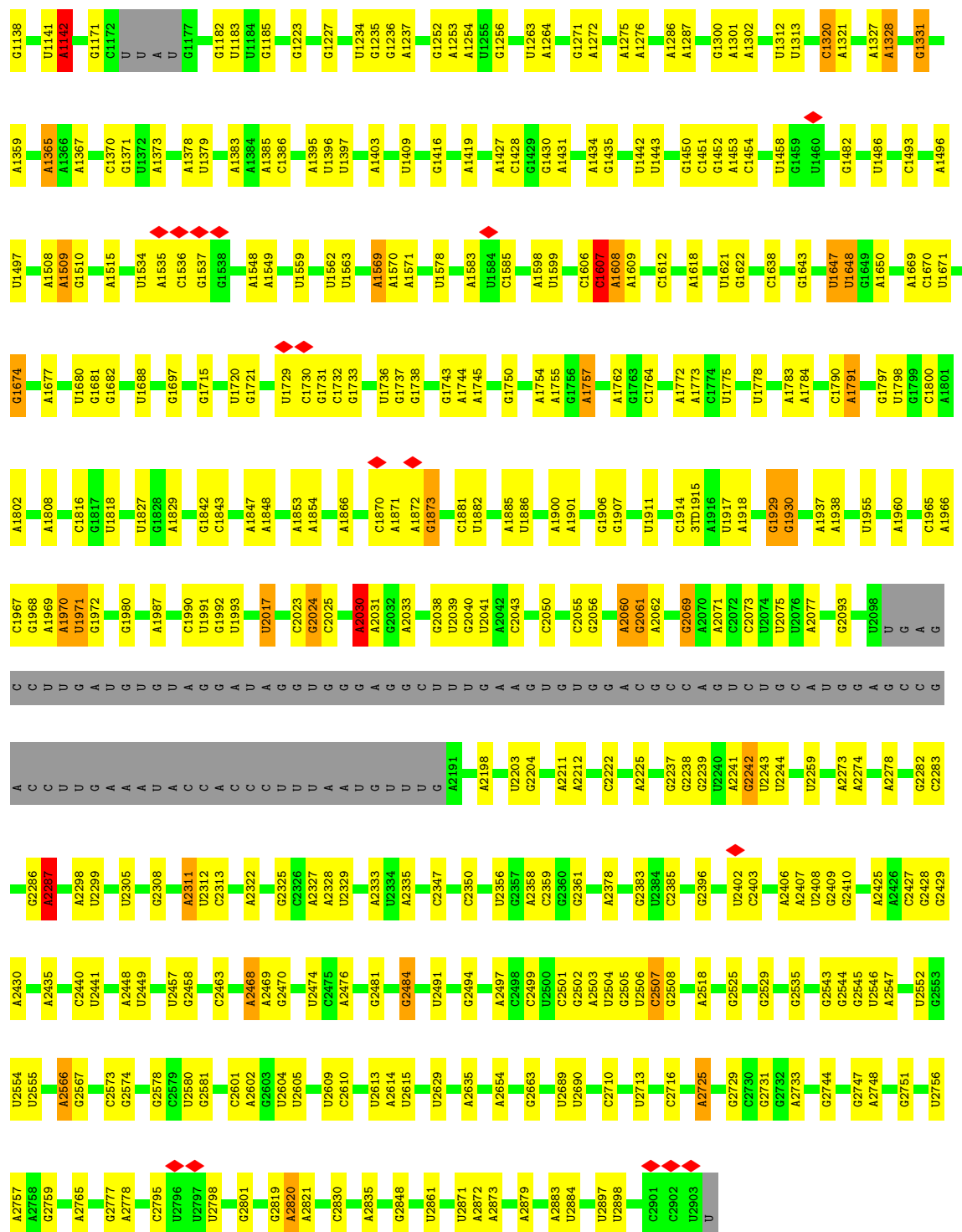
Diagram illustrating the protein structure of the A2V3Q4R10I43Y49A56Lys mutant. The structure shows the N-terminus (MET) and C-terminus (LYS). The mutant residues are highlighted in red: A2, V3, Q4, R10, I43, Y49, and A56. The wild-type residues are shown in grey: MET, LYS, and the residues between the mutant sites.

- Chain 4:  71% 83% 16%



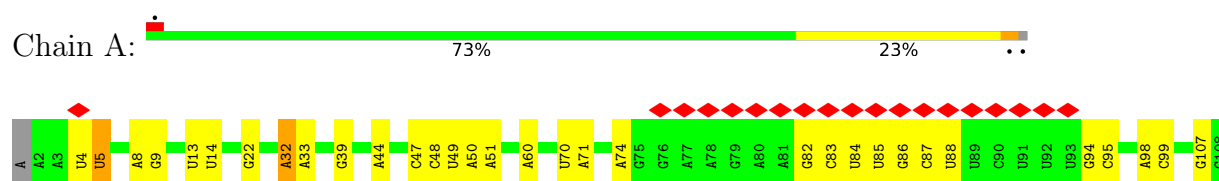
- Chain V: 73% 20% 5%

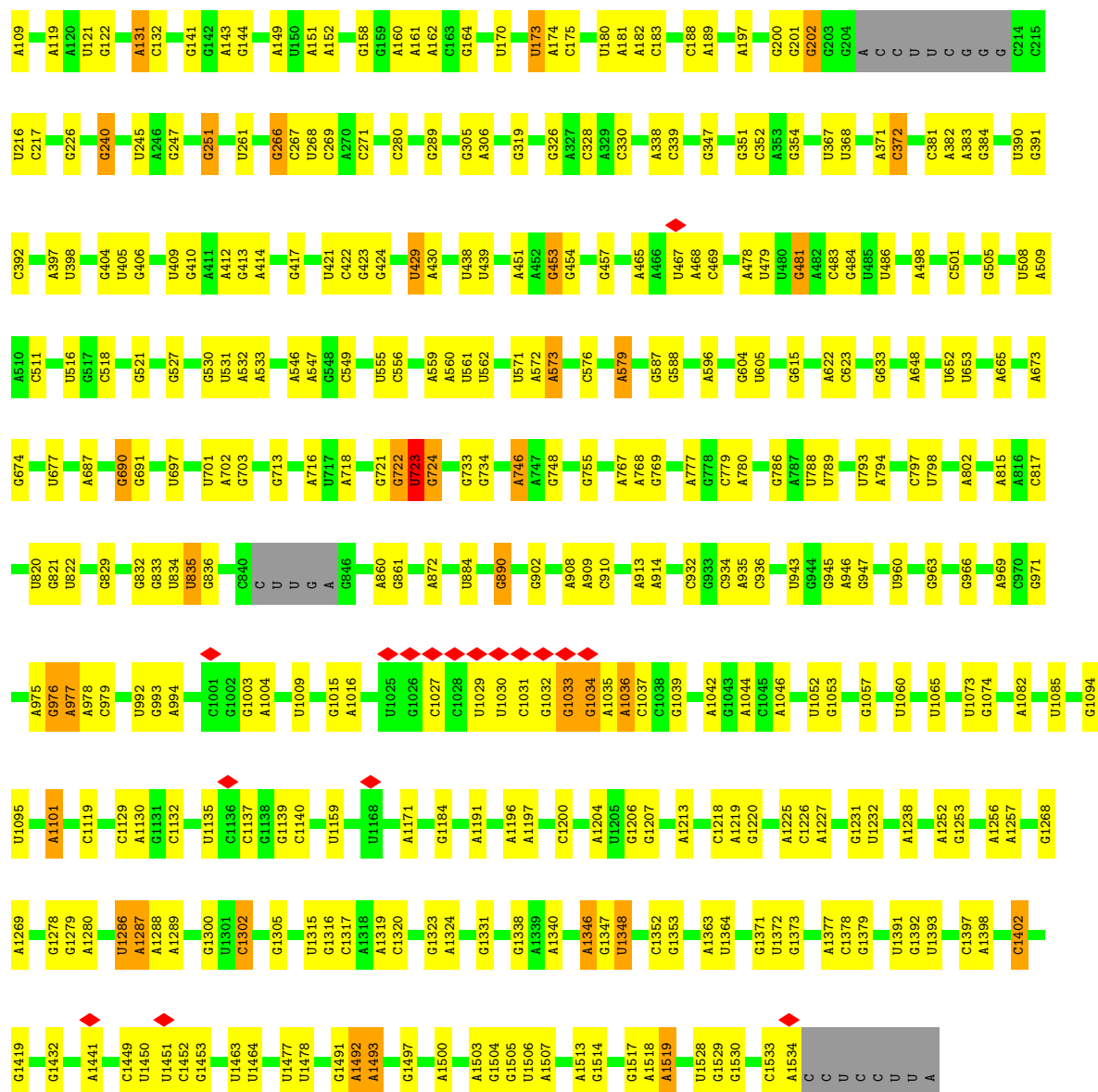




• Molecule 55: 16S rRNA

Chain A:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70345	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 ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.60	0/424	0.85	0/565
2	1	0.66	0/380	1.01	0/498
3	2	0.67	0/513	0.95	0/676
4	3	0.59	0/303	0.86	0/397
5	8	0.68	0/76	0.96	0/103
6	B	0.56	0/1784	0.98	0/2403
7	C	0.57	0/1651	0.90	0/2225
8	D	0.54	0/1665	0.94	0/2227
9	E	0.58	0/1165	0.92	0/1568
10	F	0.55	0/858	0.87	0/1160
11	G	0.57	0/1219	0.96	0/1635
12	H	0.58	0/989	0.92	0/1326
13	I	0.56	0/1034	0.92	0/1375
14	J	0.56	0/796	0.89	0/1077
15	K	0.60	0/884	0.88	0/1191
16	L	0.59	0/960	0.89	0/1286
17	M	0.57	0/900	1.01	0/1204
18	N	0.57	0/817	0.95	0/1088
19	O	0.56	0/722	0.95	0/964
20	P	0.57	0/653	0.90	0/877
21	Q	0.56	0/650	0.84	0/871
22	R	0.58	0/553	1.00	0/742
23	S	0.60	0/685	0.87	0/922
24	T	0.58	0/676	1.01	0/895
25	U	0.58	0/597	1.00	0/792
26	W	0.60	0/2007	0.89	0/2702
27	Z	0.62	0/1813	0.89	2/2823 (0.1%)
28	Y	0.63	0/209	1.05	1/322 (0.3%)
28	b	0.59	0/2850	0.88	4/4444 (0.1%)
29	c	0.64	0/2115	0.93	1/2844 (0.0%)
30	d	0.60	0/1576	0.87	0/2119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	e	0.59	0/1571	0.96	1/2113 (0.0%)
32	f	0.54	0/1434	0.92	0/1926
33	g	0.57	0/1343	0.90	0/1816
34	h	0.55	0/306	0.96	0/413
35	i	0.60	0/1152	0.90	0/1551
36	j	0.60	0/955	0.92	0/1279
37	k	0.61	0/1062	0.88	0/1413
38	l	0.58	0/1073	0.92	0/1433
39	m	0.61	0/958	0.96	1/1281 (0.1%)
40	n	0.58	0/902	0.92	0/1209
41	o	0.60	0/929	0.82	0/1242
42	p	0.61	0/960	0.94	0/1278
43	q	0.59	0/829	0.80	0/1107
44	r	0.61	0/864	0.95	0/1156
45	s	0.59	0/744	0.86	0/994
46	t	0.55	0/787	0.88	0/1051
47	u	0.56	0/766	0.84	0/1025
48	v	0.59	0/589	0.88	0/780
49	w	0.61	0/635	0.87	0/848
50	x	0.52	0/502	1.00	0/667
51	y	0.60	0/453	1.00	0/605
52	z	0.62	0/440	0.94	0/588
53	4	0.60	0/480	0.87	0/639
54	V	0.60	1/65651 (0.0%)	0.95	131/102413 (0.1%)
55	A	0.59	0/36236	0.90	38/56520 (0.1%)
All	All	0.59	1/153145 (0.0%)	0.93	179/228668 (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	1	0	1
3	2	0	1
4	3	0	2
6	B	0	1
8	D	0	3
9	E	0	1
11	G	0	1
12	H	0	2
13	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	J	0	1
15	K	0	1
18	N	0	2
19	O	0	2
20	P	0	1
24	T	0	1
26	W	0	2
29	c	0	4
31	e	0	2
33	g	0	1
36	j	0	1
37	k	0	1
38	l	0	3
39	m	0	1
42	p	0	2
43	q	0	1
44	r	0	1
46	t	0	1
48	v	0	1
49	w	0	1
50	x	0	2
52	z	0	1
54	V	0	1
All	All	0	49

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	V	2552	OMU	O3'-P	5.14	1.61	1.56

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	V	1969	A	O3'-P-O5'	-10.19	88.72	104.00
54	V	1606	C	O3'-P-O5'	-9.54	89.69	104.00
54	V	818	G	O3'-P-O5'	-9.03	90.46	104.00
54	V	1607	C	C2'-C3'-O3'	8.37	122.06	109.50
54	V	2614	A	O3'-P-O5'	-8.23	91.65	104.00

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	35	ARG	Sidechain
3	2	8	ARG	Sidechain
4	3	24	ARG	Sidechain
4	3	36	ARG	Sidechain
6	B	130	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	0	0
2	1	377	0	418	2	0
3	2	504	0	572	2	0
4	3	302	0	340	0	0
5	8	74	0	78	0	0
6	B	1753	0	1780	4	0
7	C	1624	0	1696	5	0
8	D	1643	0	1707	6	0
9	E	1152	0	1196	1	0
10	F	839	0	833	2	0
11	G	1203	0	1254	4	0
12	H	979	0	1031	1	0
13	I	1022	0	1070	2	0
14	J	786	0	828	3	0
15	K	877	0	884	6	0
16	L	957	0	1017	1	0
17	M	891	0	952	5	0
18	N	805	0	844	2	0
19	O	714	0	734	2	0
20	P	643	0	661	2	0
21	Q	641	0	682	0	0
22	R	544	0	565	1	0
23	S	668	0	693	0	0
24	T	670	0	719	0	0
25	U	589	0	629	0	0
26	W	1977	0	1932	8	0
27	Z	1623	0	821	1	0
28	Y	188	0	96	4	0
28	b	2549	0	1291	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c	2076	0	2149	7	0
30	d	1566	0	1618	2	0
31	e	1552	0	1619	2	0
32	f	1410	0	1444	2	0
33	g	1323	0	1371	2	0
34	h	303	0	327	2	0
35	i	1129	0	1162	0	0
36	j	946	0	1023	1	0
37	k	1053	0	1129	3	0
38	l	1075	0	1145	3	0
39	m	945	0	989	1	0
40	n	892	0	923	1	0
41	o	917	0	962	0	0
42	p	947	0	1019	4	0
43	q	816	0	839	1	0
44	r	857	0	922	0	0
45	s	738	0	807	0	0
46	t	779	0	831	2	0
47	u	753	0	780	4	0
48	v	582	0	593	1	0
49	w	625	0	652	2	0
50	x	501	0	531	1	0
51	y	449	0	488	1	0
52	z	434	0	445	2	0
53	4	472	0	467	0	0
54	V	59130	0	29769	113	0
55	A	32612	0	16432	103	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	V	14	0	26	0	0
58	A	1	0	0	0	0
58	Y	5	0	0	0	0
All	All	141915	0	96236	298	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.

The worst 5 of 298 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)
32:f:79:ILE:HD11	54:V:2311:A:N3	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:119:IAS:CG	15:K:120:GLY:N	2.46	0.79
54:V:568:U:H1'	54:V:2030:6MZ:H9C1	1.75	0.68
29:c:62:TYR:HA	29:c:86:ASN:HD21	1.61	0.65
15:K:119:IAS:CG	15:K:120:GLY:CA	2.77	0.62

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%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	8	7/20 (35%)	4 (57%)	3 (43%)	0	100	100
6	B	222/241 (92%)	204 (92%)	15 (7%)	3 (1%)	9	31
7	C	204/233 (88%)	189 (93%)	14 (7%)	1 (0%)	24	55
8	D	203/206 (98%)	195 (96%)	7 (3%)	1 (0%)	24	55
9	E	154/167 (92%)	145 (94%)	9 (6%)	0	100	100
10	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
11	G	151/179 (84%)	145 (96%)	6 (4%)	0	100	100
12	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
13	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
14	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	39
15	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
16	L	120/124 (97%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
18	N	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	12	39
19	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
20	P	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
21	Q	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
22	R	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
23	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
24	T	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
25	U	68/71 (96%)	68 (100%)	0	0	100	100
26	W	252/360 (70%)	242 (96%)	10 (4%)	0	100	100
29	c	268/273 (98%)	253 (94%)	15 (6%)	0	100	100
30	d	206/209 (99%)	192 (93%)	14 (7%)	0	100	100
31	e	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
32	f	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
33	g	174/177 (98%)	163 (94%)	10 (6%)	1 (1%)	21	50
34	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
35	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
36	j	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
37	k	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	18	47
38	l	132/136 (97%)	126 (96%)	4 (3%)	2 (2%)	8	30
39	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
40	n	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
41	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
42	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
43	q	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	12	39
44	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
45	s	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
46	t	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
47	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
48	v	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
49	w	75/78 (96%)	72 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	x	60/63 (95%)	60 (100%)	0	0	100	100
51	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
52	z	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
53	4	55/70 (79%)	52 (94%)	2 (4%)	1 (2%)	6	26
All	All	5736/6293 (91%)	5455 (95%)	268 (5%)	13 (0%)	44	71

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	l	80	VAL
8	D	25	VAL
14	J	57	VAL
18	N	33	ASP
6	B	87	CYS

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	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	63
5	8	9/19 (47%)	9 (100%)	0	100	100
6	B	186/199 (94%)	185 (100%)	1 (0%)	81	83
7	C	170/190 (90%)	168 (99%)	2 (1%)	63	76
8	D	172/173 (99%)	166 (96%)	6 (4%)	32	60
9	E	119/126 (94%)	119 (100%)	0	100	100
10	F	90/116 (78%)	89 (99%)	1 (1%)	65	76
11	G	126/147 (86%)	123 (98%)	3 (2%)	43	67
12	H	104/105 (99%)	101 (97%)	3 (3%)	37	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	I	105/107 (98%)	105 (100%)	0	100	100
14	J	86/90 (96%)	83 (96%)	3 (4%)	32	60
15	K	89/98 (91%)	88 (99%)	1 (1%)	65	76
16	L	102/103 (99%)	102 (100%)	0	100	100
17	M	93/96 (97%)	93 (100%)	0	100	100
18	N	83/84 (99%)	83 (100%)	0	100	100
19	O	76/77 (99%)	76 (100%)	0	100	100
20	P	65/65 (100%)	64 (98%)	1 (2%)	57	73
21	Q	73/78 (94%)	72 (99%)	1 (1%)	59	74
22	R	57/65 (88%)	57 (100%)	0	100	100
23	S	72/79 (91%)	70 (97%)	2 (3%)	38	64
24	T	65/66 (98%)	65 (100%)	0	100	100
25	U	60/61 (98%)	59 (98%)	1 (2%)	53	72
26	W	205/300 (68%)	201 (98%)	4 (2%)	48	70
29	c	215/218 (99%)	212 (99%)	3 (1%)	59	74
30	d	163/163 (100%)	163 (100%)	0	100	100
31	e	165/165 (100%)	164 (99%)	1 (1%)	78	81
32	f	148/150 (99%)	147 (99%)	1 (1%)	76	80
33	g	137/138 (99%)	133 (97%)	4 (3%)	37	63
34	h	32/114 (28%)	32 (100%)	0	100	100
35	i	116/116 (100%)	116 (100%)	0	100	100
36	j	104/104 (100%)	103 (99%)	1 (1%)	68	77
37	k	103/103 (100%)	103 (100%)	0	100	100
38	l	107/107 (100%)	105 (98%)	2 (2%)	50	71
39	m	98/103 (95%)	98 (100%)	0	100	100
40	n	86/87 (99%)	86 (100%)	0	100	100
41	o	99/100 (99%)	99 (100%)	0	100	100
42	p	89/90 (99%)	89 (100%)	0	100	100
43	q	84/84 (100%)	83 (99%)	1 (1%)	63	76
44	r	93/93 (100%)	89 (96%)	4 (4%)	26	55
45	s	80/84 (95%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	t	83/85 (98%)	80 (96%)	3 (4%)	31	59
47	u	78/78 (100%)	77 (99%)	1 (1%)	61	75
48	v	58/63 (92%)	58 (100%)	0	100	100
49	w	67/68 (98%)	66 (98%)	1 (2%)	57	73
50	x	54/55 (98%)	54 (100%)	0	100	100
51	y	48/49 (98%)	48 (100%)	0	100	100
52	z	46/48 (96%)	46 (100%)	0	100	100
53	4	54/62 (87%)	54 (100%)	0	100	100
All	All	4783/5144 (93%)	4731 (99%)	52 (1%)	63	76

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	W	259	ASP
33	g	47	ASP
46	t	68	SER
26	W	313	PRO
29	c	86	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
37	k	104	GLN
47	u	49	ASN
38	l	17	ASN
44	r	40	ASN
53	4	20	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	Z	75/76 (98%)	16 (21%)	4 (5%)
28	Y	8/120 (6%)	2 (25%)	1 (12%)
28	b	118/120 (98%)	13 (11%)	0
54	V	2750/2904 (94%)	354 (12%)	51 (1%)
55	A	1516/1542 (98%)	224 (14%)	27 (1%)
All	All	4467/4762 (93%)	609 (13%)	83 (1%)

5 of 609 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	Z	8	U
27	Z	17	C
27	Z	18	G
27	Z	19	G
27	Z	21	A

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	A	70	U
55	A	884	U
55	A	94	G
55	A	532	A
55	A	1035	A

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

40 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	$\# Z > 2$
55	MA6	A	1519	55	23,26,27	0.32	0	34,38,41	0.75	1 (2%)
54	2MG	V	1835	54	23,26,27	0.38	0	32,38,41	0.67	0
54	PSU	V	1917	54	18,21,22	1.04	2 (11%)	22,30,33	0.66	0
30	MEQ	d	150	30	8,9,10	0.52	0	5,10,12	1.02	0
54	PSU	V	2605	54	18,21,22	0.92	1 (5%)	22,30,33	0.82	0
16	D2T	L	89	16	7,9,10	0.94	0	6,11,13	1.53	2 (33%)
54	OMU	V	2552	54	19,22,23	0.31	0	26,31,34	0.46	0
54	PSU	V	2504	54	18,21,22	0.97	1 (5%)	22,30,33	0.85	0
54	1MG	V	745	54	22,26,27	0.64	0	33,39,42	0.56	0
55	2MG	A	1207	55	23,26,27	0.39	0	32,38,41	0.41	0
55	UR3	A	1498	55	19,22,23	0.43	0	26,32,35	0.69	0
55	2MG	A	1516	55	23,26,27	0.36	0	32,38,41	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	2MA	V	2503	54	22,25,26	0.40	0	33,37,40	0.74	1 (3%)
15	IAS	K	119	15	6,7,8	0.88	0	6,8,10	1.00	0
54	PSU	V	2604	54	18,21,22	0.91	1 (5%)	22,30,33	1.01	2 (9%)
54	H2U	V	2449	54	18,21,22	0.49	0	21,30,33	0.97	3 (14%)
54	2MG	V	2445	54	23,26,27	0.48	0	32,38,41	0.51	0
55	5MC	A	967	55	18,22,23	0.34	0	26,32,35	0.56	0
54	PSU	V	2580	54	18,21,22	1.06	1 (5%)	22,30,33	0.80	0
54	5MU	V	747	54	19,22,23	0.34	0	28,32,35	0.54	0
54	PSU	V	746	54	18,21,22	1.10	1 (5%)	22,30,33	0.91	1 (4%)
38	4D4	l	81	38	9,11,12	0.78	0	8,13,15	1.50	1 (12%)
54	OMC	V	2498	54	19,22,23	0.44	0	26,31,34	0.48	0
54	3TD	V	1915	54	18,22,23	0.86	1 (5%)	22,32,35	0.79	0
54	5MU	V	1939	54	19,22,23	0.49	0	28,32,35	0.57	0
55	MA6	A	1518	55	23,26,27	0.34	0	34,38,41	0.67	1 (2%)
55	4OC	A	1402	55	20,23,24	0.47	0	26,32,35	0.72	0
54	5MC	V	1962	54	18,22,23	0.37	0	26,32,35	0.56	0
38	MS6	l	82	38	5,7,8	0.36	0	2,7,9	0.52	0
55	5MC	A	1407	55	18,22,23	0.35	0	26,32,35	0.75	0
54	6MZ	V	2030	54	22,25,26	0.95	1 (4%)	30,36,39	0.62	0
55	2MG	A	966	55	23,26,27	0.48	0	32,38,41	0.42	0
54	PSU	V	955	54	18,21,22	0.81	1 (5%)	22,30,33	0.66	0
55	PSU	A	516	55	18,21,22	0.82	1 (5%)	22,30,33	0.69	0
54	6MZ	V	1618	54	22,25,26	0.64	1 (4%)	30,36,39	0.57	0
54	PSU	V	1911	54	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
54	G7M	V	2069	54	23,26,27	0.67	1 (4%)	35,39,42	0.69	1 (2%)
55	G7M	A	527	55	23,26,27	0.67	1 (4%)	35,39,42	0.71	0
54	OMG	V	2251	27,54	23,26,27	0.47	0	33,38,41	0.54	0
54	PSU	V	2457	54	18,21,22	0.96	1 (5%)	22,30,33	0.73	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
55	MA6	A	1519	55	-	4/11/29/30	0/3/3/3
54	2MG	V	1835	54	-	0/9/27/28	0/3/3/3
54	PSU	V	1917	54	-	0/7/25/26	0/2/2/2
30	MEQ	d	150	30	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	V	2605	54	-	0/7/25/26	0/2/2/2
16	D2T	L	89	16	-	1/7/12/14	-
54	OMU	V	2552	54	-	0/9/27/28	0/2/2/2
54	PSU	V	2504	54	-	0/7/25/26	0/2/2/2
54	1MG	V	745	54	-	0/7/25/26	0/3/3/3
55	2MG	A	1207	55	-	0/9/27/28	0/3/3/3
55	UR3	A	1498	55	-	0/7/25/26	0/2/2/2
55	2MG	A	1516	55	-	0/9/27/28	0/3/3/3
54	2MA	V	2503	54	-	2/7/25/26	0/3/3/3
15	IAS	K	119	15	-	0/7/7/8	-
54	PSU	V	2604	54	-	0/7/25/26	0/2/2/2
54	H2U	V	2449	54	-	0/7/38/39	0/2/2/2
54	2MG	V	2445	54	-	0/9/27/28	0/3/3/3
55	5MC	A	967	55	-	0/7/25/26	0/2/2/2
54	PSU	V	2580	54	-	0/7/25/26	0/2/2/2
54	5MU	V	747	54	-	1/7/25/26	0/2/2/2
54	PSU	V	746	54	-	1/7/25/26	0/2/2/2
38	4D4	I	81	38	-	1/11/12/14	-
54	OMC	V	2498	54	-	0/9/27/28	0/2/2/2
54	3TD	V	1915	54	-	0/7/25/26	0/2/2/2
54	5MU	V	1939	54	-	0/7/25/26	0/2/2/2
55	MA6	A	1518	55	-	0/11/29/30	0/3/3/3
55	4OC	A	1402	55	-	2/9/29/30	0/2/2/2
54	5MC	V	1962	54	-	0/7/25/26	0/2/2/2
38	MS6	I	82	38	-	1/4/6/8	-
55	5MC	A	1407	55	-	0/7/25/26	0/2/2/2
54	6MZ	V	2030	54	-	1/9/27/28	0/3/3/3
55	2MG	A	966	55	-	0/9/27/28	0/3/3/3
54	PSU	V	955	54	-	0/7/25/26	0/2/2/2
55	PSU	A	516	55	-	0/7/25/26	0/2/2/2
54	6MZ	V	1618	54	-	0/9/27/28	0/3/3/3
54	PSU	V	1911	54	-	0/7/25/26	0/2/2/2
54	G7M	V	2069	54	-	2/7/25/26	0/3/3/3
55	G7M	A	527	55	-	1/7/25/26	0/3/3/3
54	OMG	V	2251	27,54	-	3/9/27/28	0/3/3/3
54	PSU	V	2457	54	-	0/7/25/26	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	V	746	PSU	C6-C5	3.71	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	V	2580	PSU	C6-C5	3.50	1.39	1.35
54	V	2030	6MZ	C6-N6	-3.45	1.30	1.34
54	V	1915	3TD	C6-C5	3.40	1.39	1.35
54	V	1917	PSU	C6-C5	3.35	1.39	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	l	81	4D4	CB-CA-C	3.89	117.99	111.77
55	A	1518	MA6	C2-N1-C6	2.90	118.61	111.75
55	A	1519	MA6	C2-N1-C6	2.81	118.38	111.75
54	V	2604	PSU	C2'-C3'-C4'	-2.54	97.70	102.64
54	V	2503	2MA	C5-C4-N3	-2.44	124.45	127.19

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	1519	MA6	O4'-C4'-C5'-O5'
55	A	1402	4OC	O4'-C4'-C5'-O5'
55	A	1519	MA6	C3'-C4'-C5'-O5'
55	A	1402	4OC	C3'-C4'-C5'-O5'
30	d	150	MEQ	OE1-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A	1207	2MG	1	0
15	K	119	IAS	4	0
55	A	1402	4OC	1	0
54	V	2030	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	$\# Z > 2$
57	SPM	V	3001	-	13,13,13	0.23	0	12,12,12	0.18	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
57	SPM	V	3001	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	V	3001	SPM	C7-C8-C9-N10
57	V	3001	SPM	C8-C9-N10-C11

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
15	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	119:IAS	CG	120:GLY	N	2.46

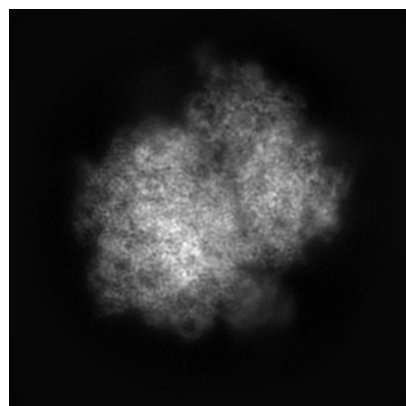
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55847. These allow visual inspection of the internal detail of the map and identification of artifacts.

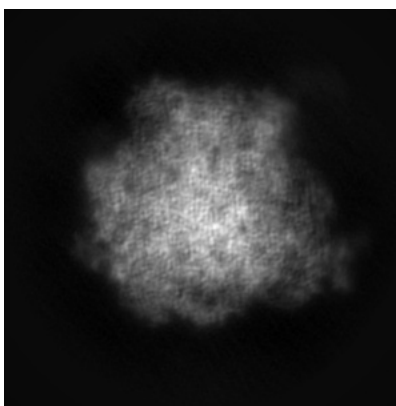
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

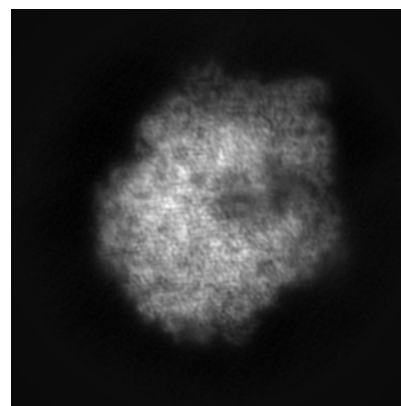
6.1.1 Primary map



X

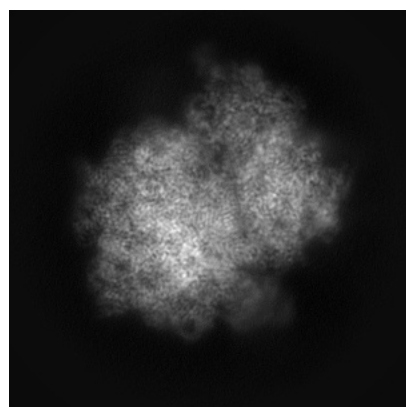


Y

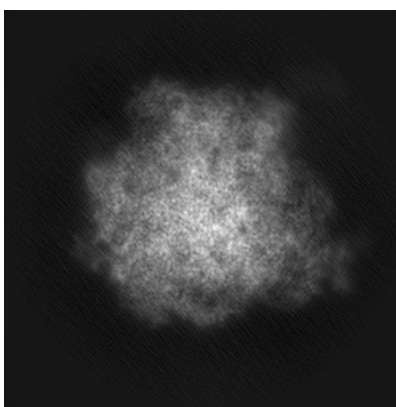


Z

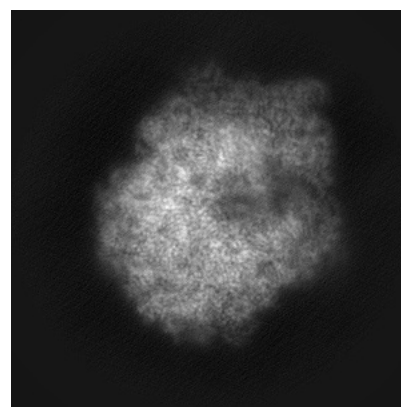
6.1.2 Raw map



X



Y

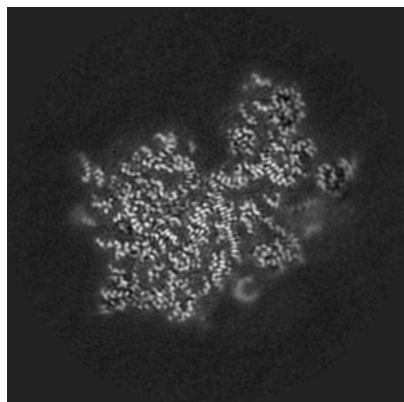


Z

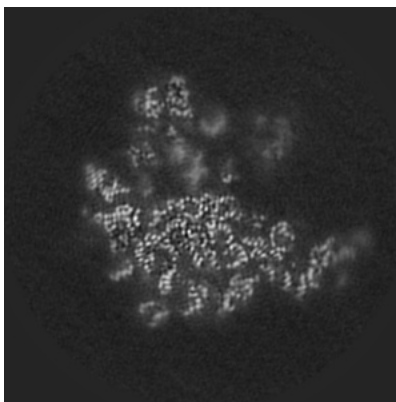
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

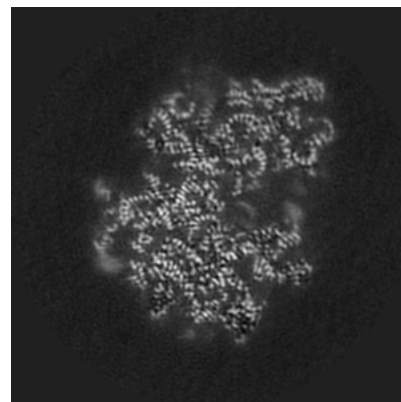
6.2.1 Primary map



X Index: 208

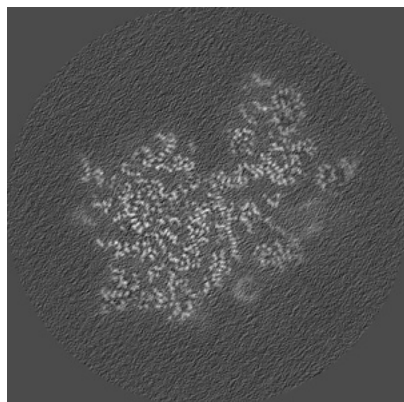


Y Index: 208

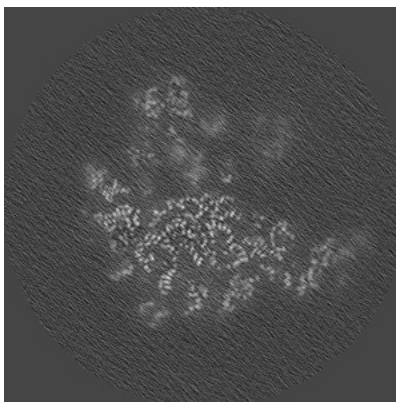


Z Index: 208

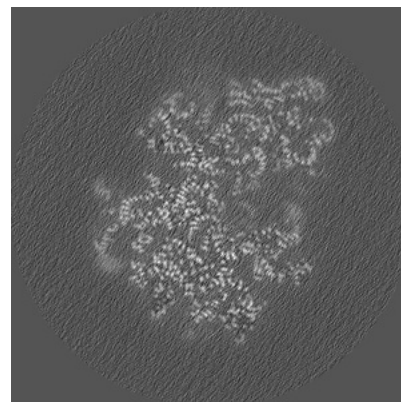
6.2.2 Raw map



X Index: 208



Y Index: 208

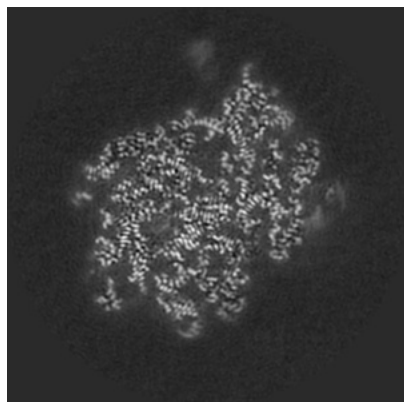


Z Index: 208

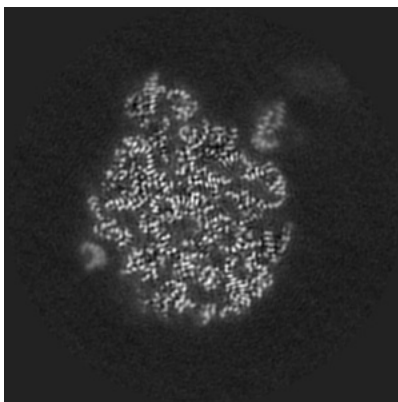
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

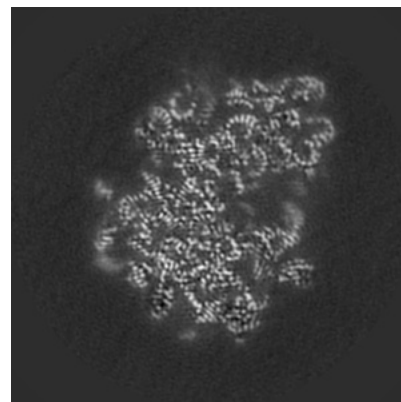
6.3.1 Primary map



X Index: 179

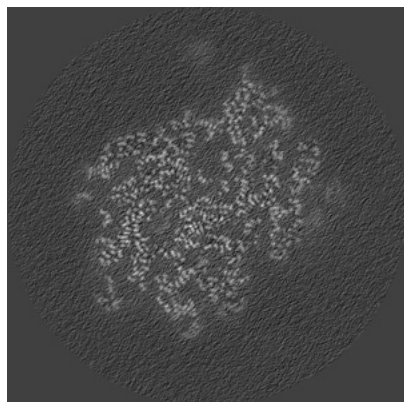


Y Index: 170

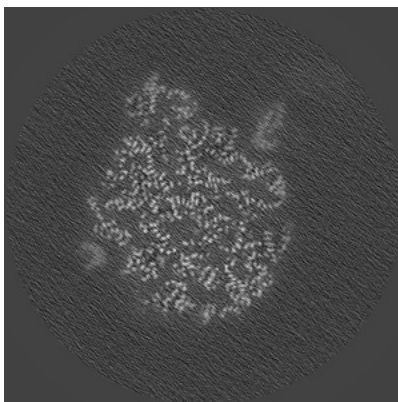


Z Index: 210

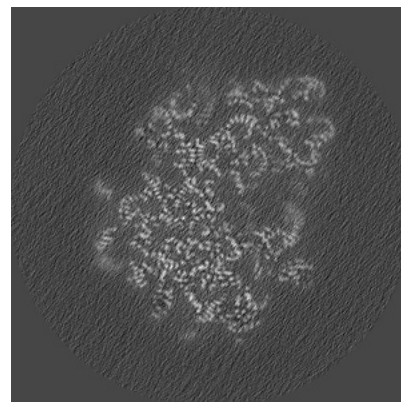
6.3.2 Raw map



X Index: 180



Y Index: 170

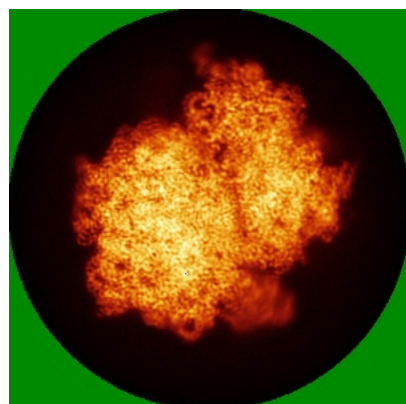


Z Index: 210

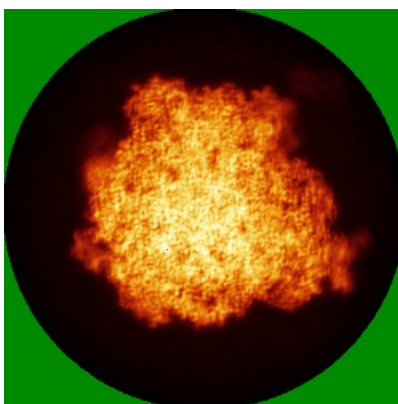
The images above show the largest variance slices of the map in three orthogonal directions.

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

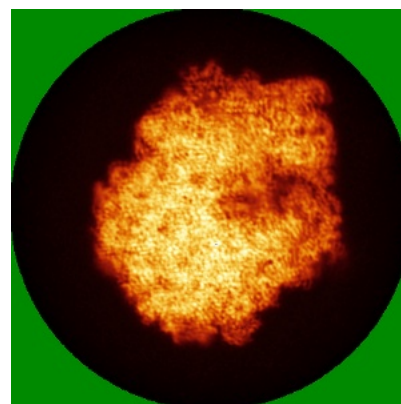
6.4.1 Primary map



X

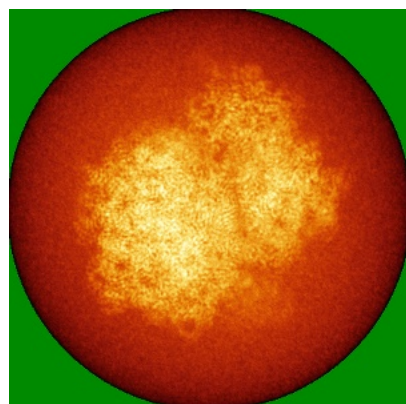


Y

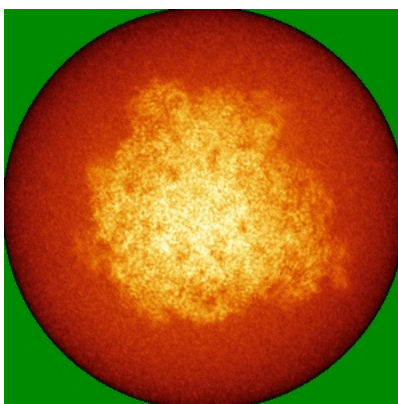


Z

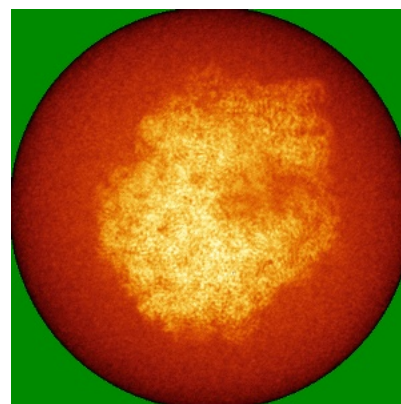
6.4.2 Raw map



X



Y

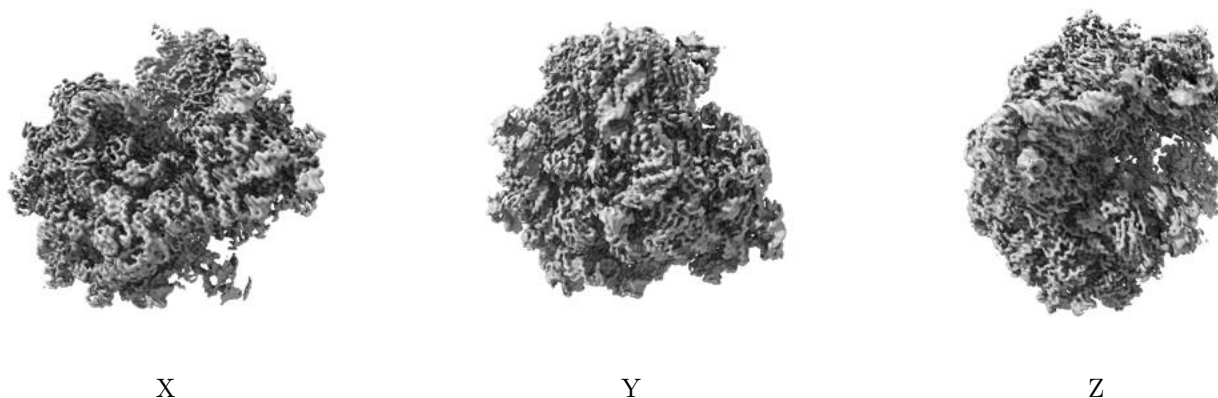


Z

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 0.015. 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.

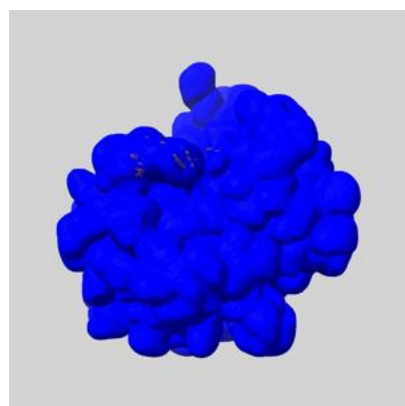
6.6 Mask visualisation [i](#)

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

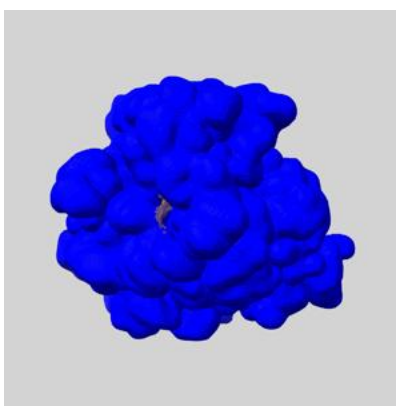
A mask typically either:

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

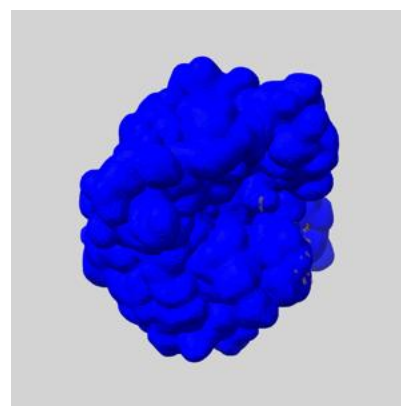
6.6.1 emd_55847_msk_1.map [i](#)



X



Y

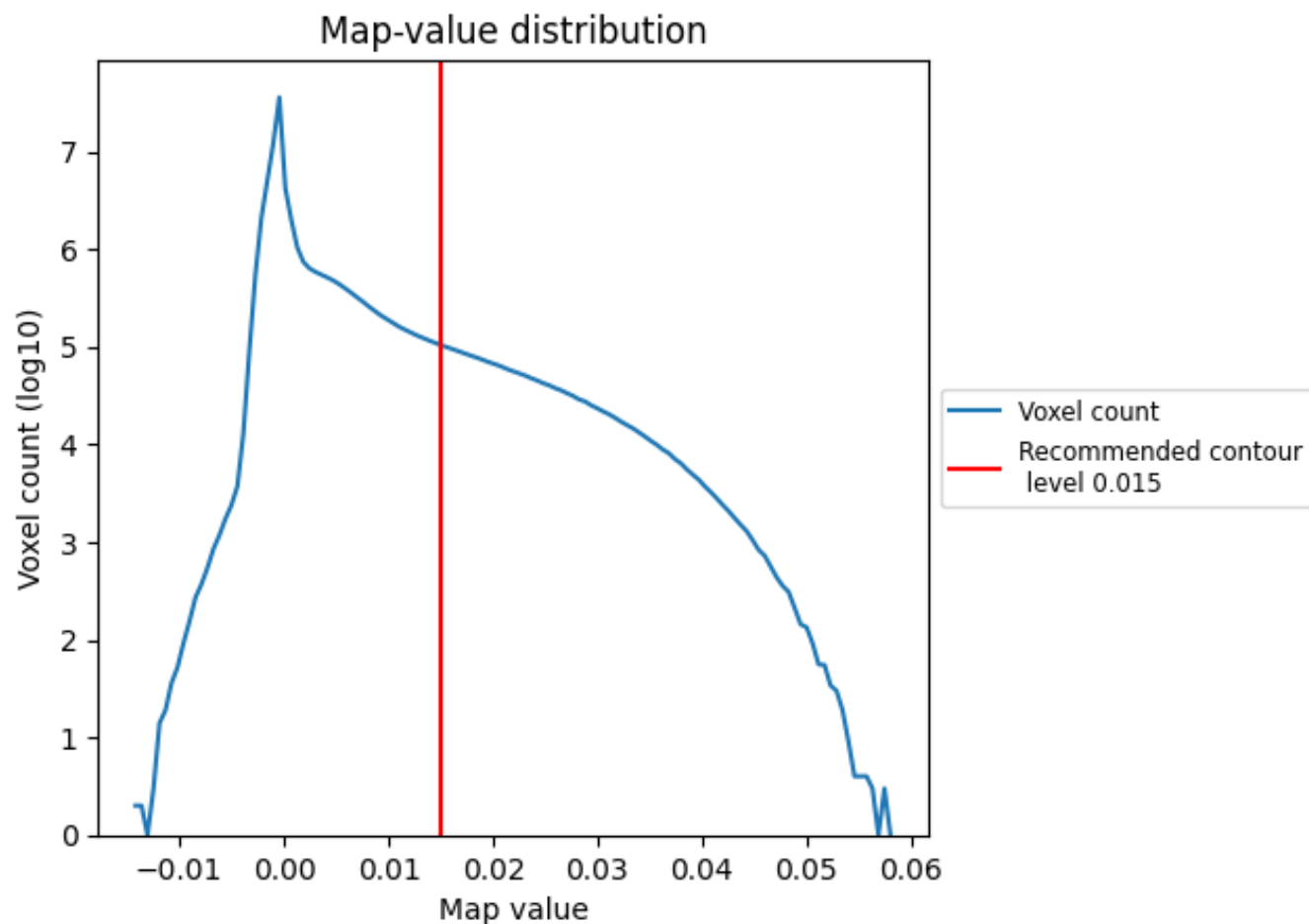


Z

7 Map analysis [i](#)

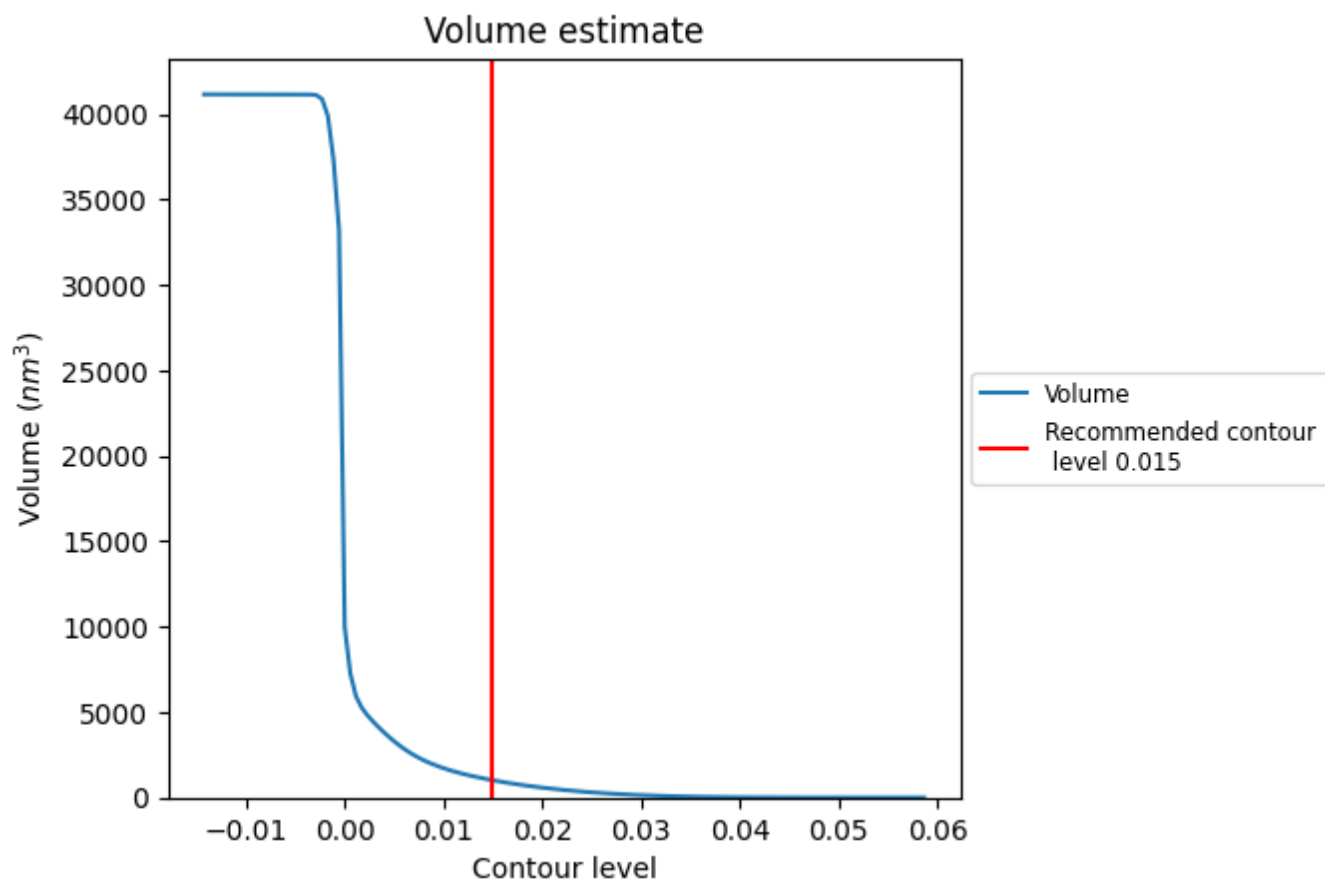
This section contains the results of statistical analysis of the map.

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.

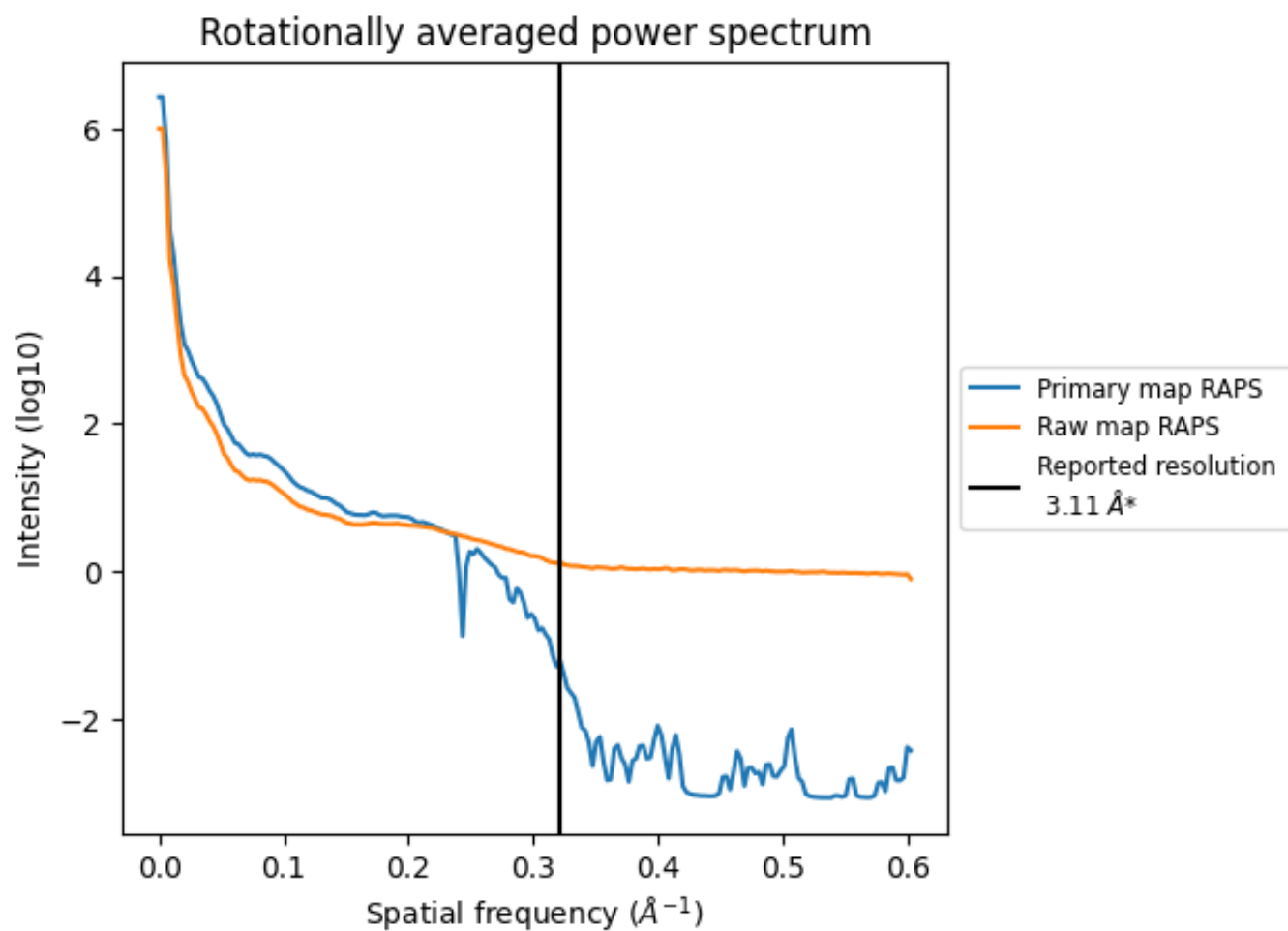
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1012 nm^3 ; this corresponds to an approximate mass of 915 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 ⓘ

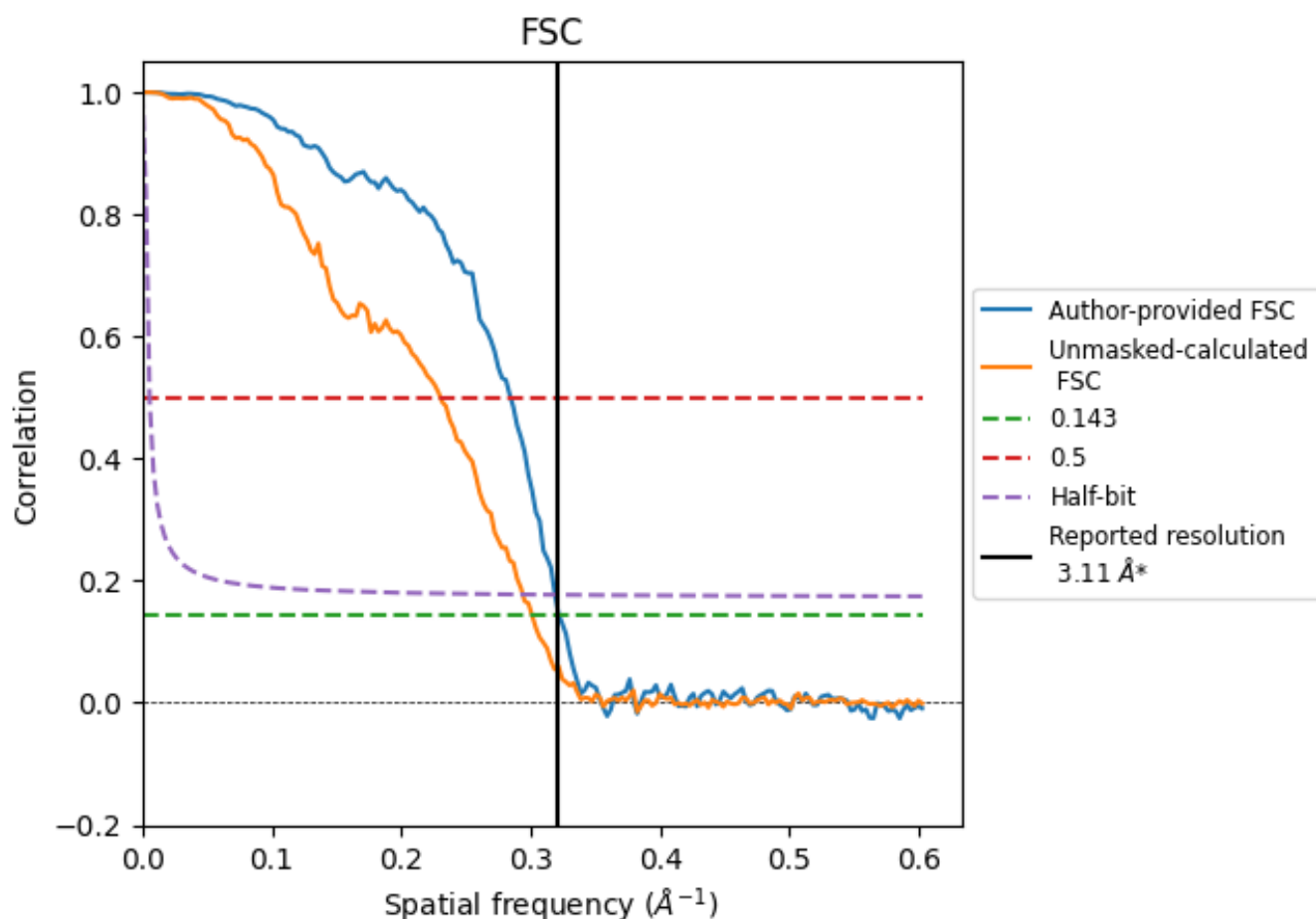


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

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 0.322 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

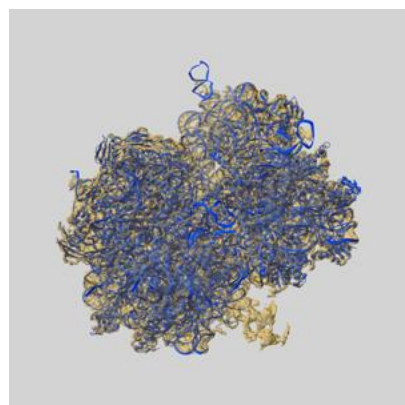
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.51	3.14
Unmasked-calculated*	3.32	4.34	3.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

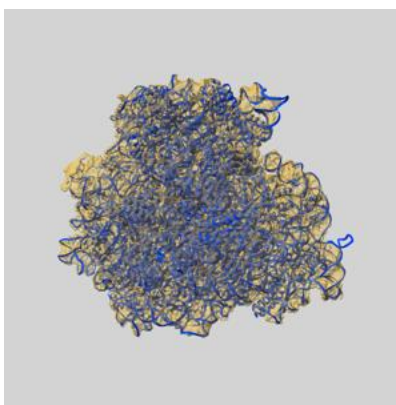
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55847 and PDB model 9TEY. Per-residue inclusion information can be found in section 3 on page 16.

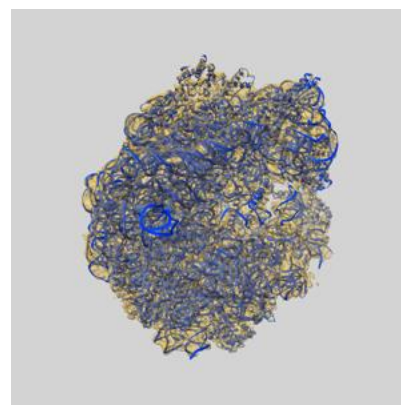
9.1 Map-model overlay [i](#)



X



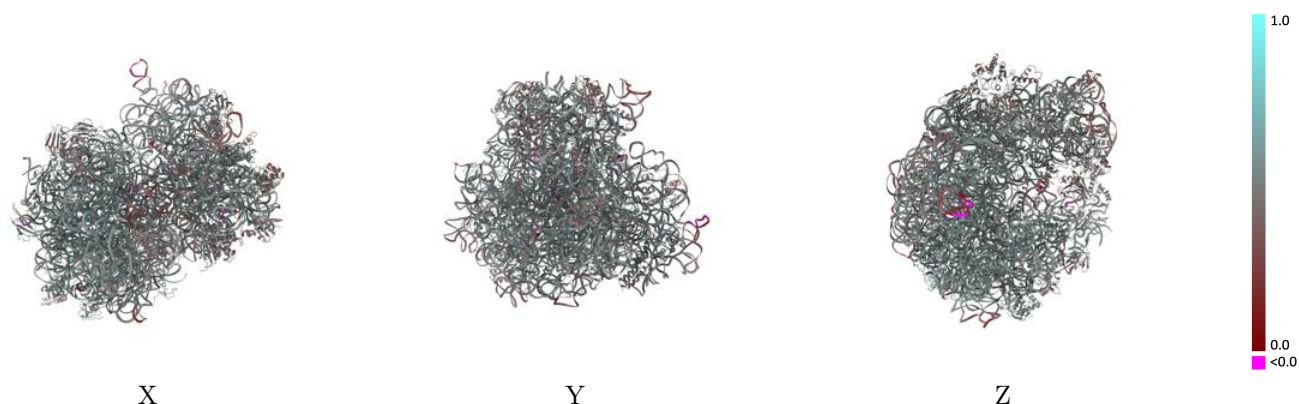
Y



Z

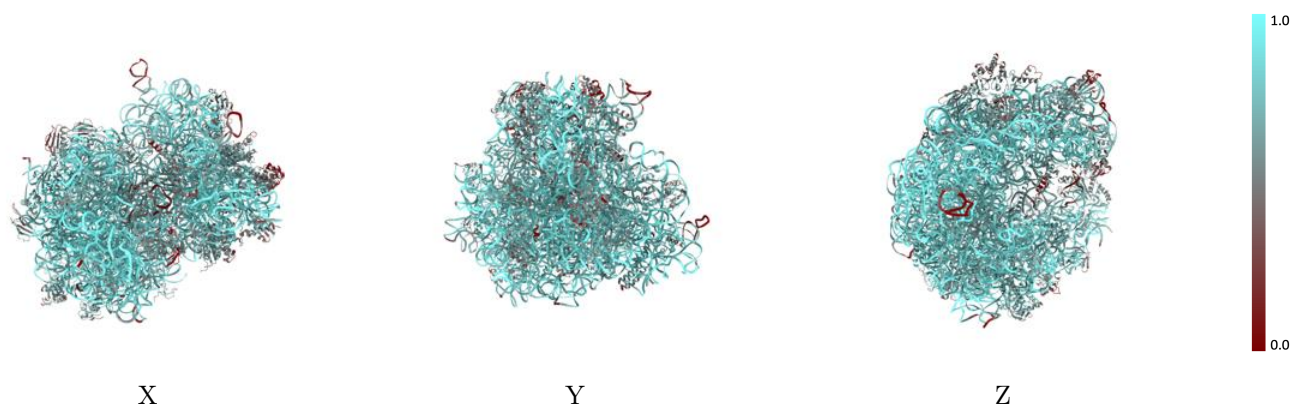
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



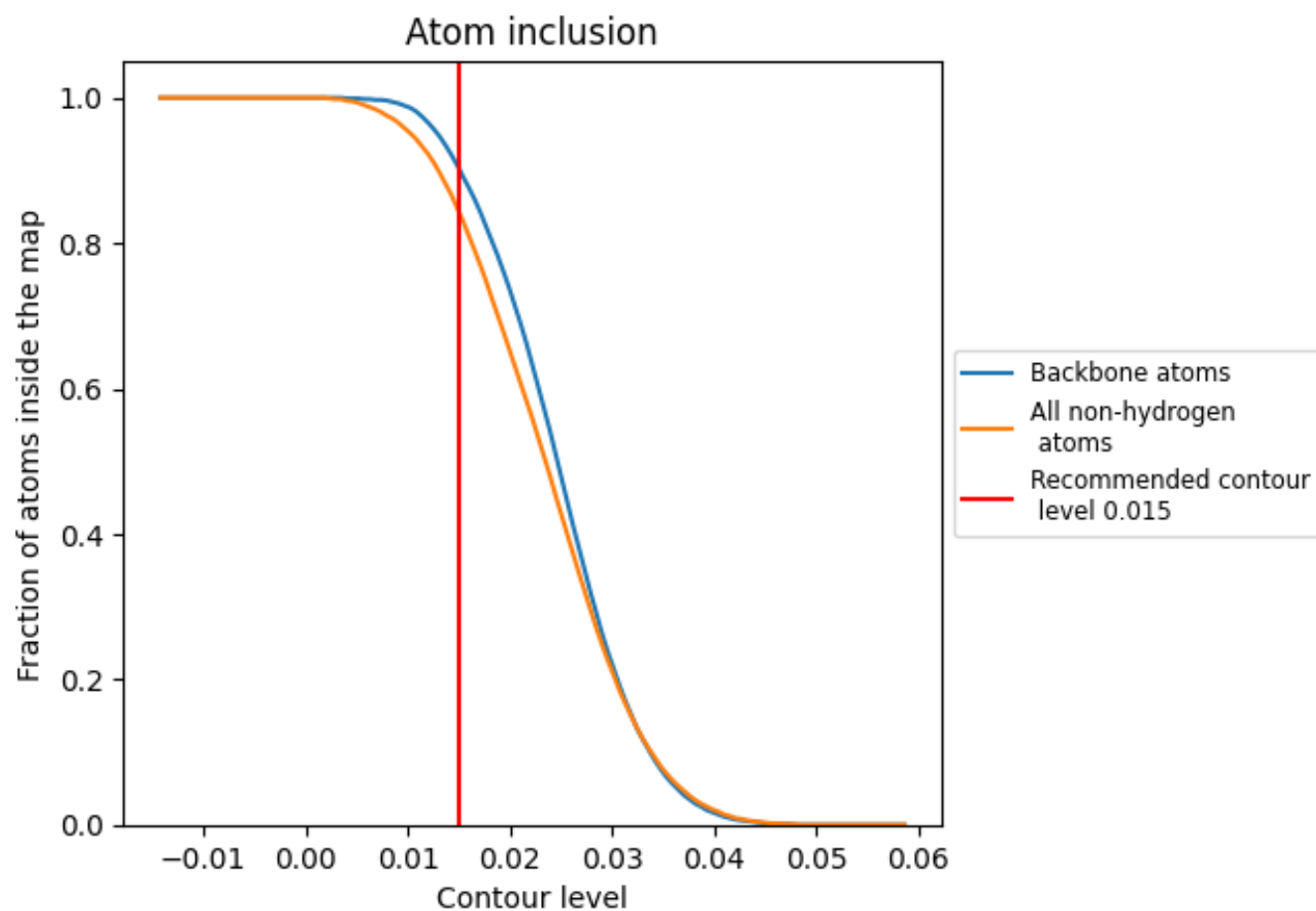
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.5050
0	 0.7090	 0.4960
1	 0.8840	 0.5300
2	 0.8660	 0.5490
3	 0.7410	 0.5110
4	 0.2150	 0.4340
8	 0.8430	 0.5340
A	 0.9080	 0.4980
B	 0.4850	 0.4430
C	 0.6350	 0.4930
D	 0.5810	 0.4690
E	 0.7280	 0.5030
F	 0.5890	 0.4710
G	 0.5540	 0.4450
H	 0.6690	 0.5040
I	 0.6360	 0.4700
J	 0.5070	 0.4540
K	 0.6790	 0.4950
L	 0.7040	 0.5070
M	 0.6310	 0.4790
N	 0.6910	 0.4910
O	 0.6680	 0.4810
P	 0.7070	 0.5060
Q	 0.6420	 0.4710
R	 0.5540	 0.4230
S	 0.6040	 0.4650
T	 0.6850	 0.4730
U	 0.5010	 0.4360
V	 0.9400	 0.5190
W	 0.6400	 0.4790
Y	 0.9200	 0.5190
Z	 0.7050	 0.4120
b	 0.9060	 0.5140
c	 0.8170	 0.5350
d	 0.7520	 0.5320



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Chain	Atom inclusion	Q-score
e	 0.6980	 0.5100
f	 0.5550	 0.4500
g	 0.5300	 0.4550
h	 0.6070	 0.4720
i	 0.7580	 0.5240
j	 0.6900	 0.5220
k	 0.7360	 0.5270
l	 0.7710	 0.5250
m	 0.8230	 0.5340
n	 0.6800	 0.4890
o	 0.7070	 0.5230
p	 0.8070	 0.5310
q	 0.6850	 0.5210
r	 0.7390	 0.5210
s	 0.6910	 0.5010
t	 0.6390	 0.4900
u	 0.6530	 0.5060
v	 0.8060	 0.5290
w	 0.7890	 0.5250
x	 0.6670	 0.4610
y	 0.7140	 0.5160
z	 0.8040	 0.5340