Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 05:56 pm BST

PDB ID	:	9GS9
EMDB ID	:	EMD-51543
Title	:	Tn7016 PseCAST QCascade
Authors	:	Lampe, G.D.; Liang, A.R.; Zhang, D.J.; Fernandez, I.S.; Sternberg, S.H.
Deposited on	:	2024-09-13
Resolution	:	2.60 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:

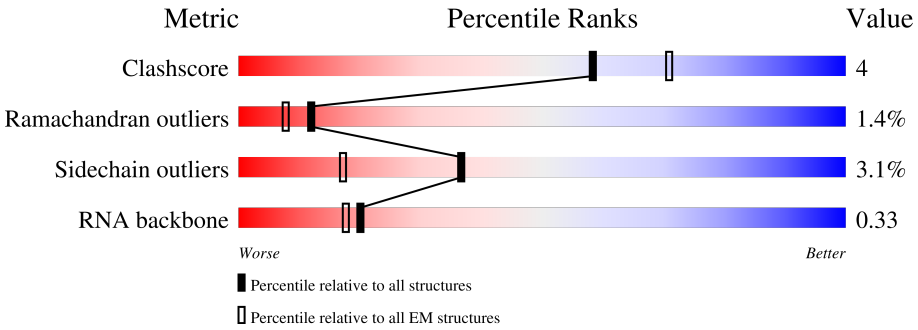
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	1	60	48% 38% 12% ·
2	2	74	5% 35% 18% 47%
3	3	11	82% 18%
4	A	695	15% 90% 8% ·
5	B	350	94% · ·
5	C	350	96% · ·
5	D	350	97% · ·

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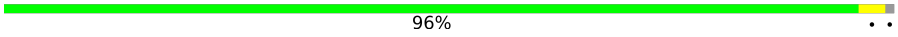
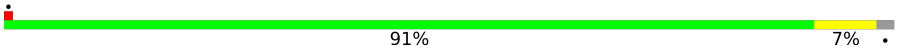
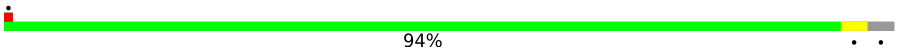
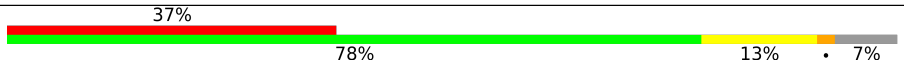
Mol	Chain	Length	Quality of chain
5	E	350	
5	F	350	
5	G	350	
6	H	203	
7	I	432	
7	J	432	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31710 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	60	Total	C	N	O	P	0	0
			1291	577	243	412	59		

- Molecule 2 is a DNA chain called T-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	39	Total	C	N	O	P	0	0
			793	376	140	238	39		

- Molecule 3 is a DNA chain called NT-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	11	Total	C	N	O	P	0	0
			222	105	45	61	11		

- Molecule 4 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	694	Total	C	N	O	S	0	0
			5013	3180	885	927	21		

- Molecule 5 is a protein called Cas7.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	341	Total	C	N	O	S	0	0
			2723	1740	454	519	10		
5	C	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
5	D	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
5	E	345	Total	C	N	O	S	0	0
			2768	1769	461	526	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	344	Total	C	N	O	S	0	0
			2763	1766	460	525	12		
5	G	307	Total	C	N	O	S	0	0
			2477	1585	411	470	11		

- Molecule 6 is a protein called Cas6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	197	Total	C	N	O	S	0	0
			1592	1014	277	292	9		

- Molecule 7 is a protein called TniQ.1.

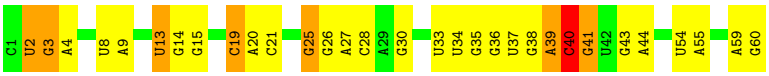
Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	402	Total	C	N	O	S	0	0
			3261	2085	554	606	16		
7	J	401	Total	C	N	O	S	0	0
			3253	2079	553	605	16		

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.

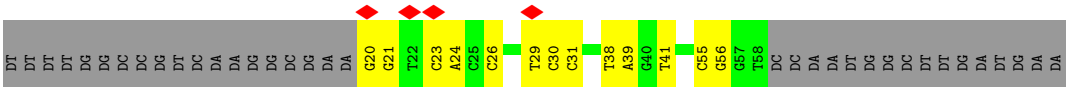
- Molecule 1: crRNA

Chain 1:



- Molecule 2: T-DNA

Chain 2:

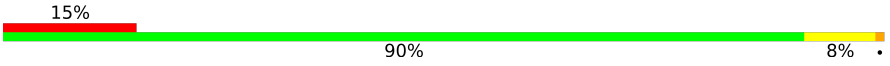


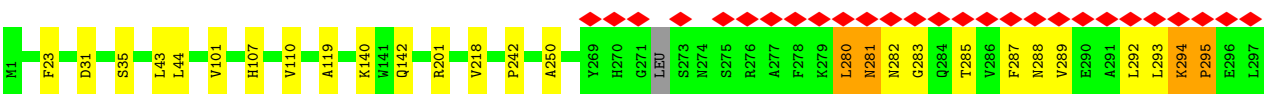
- Molecule 3: NT-DNA

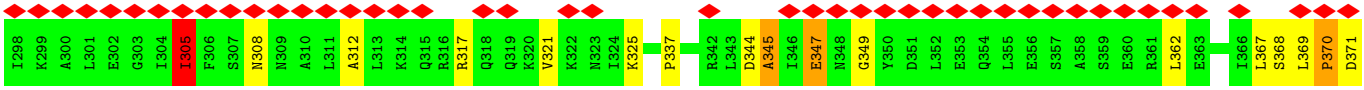
Chain 3:

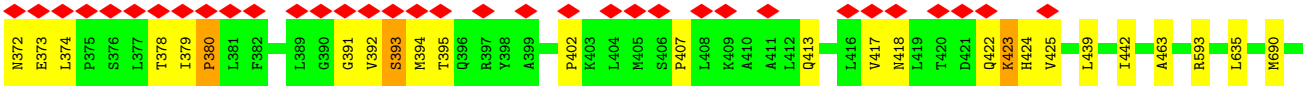
- Molecule 4: Cas8

Chain A:



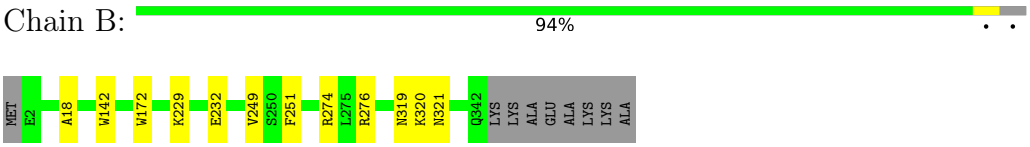






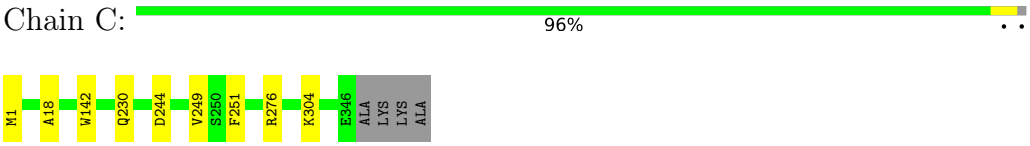
- Molecule 5: Cas7.1

Chain B:



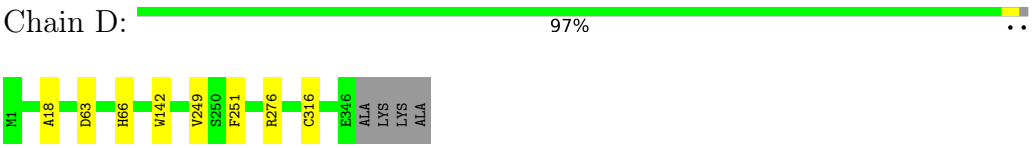
- Molecule 5: Cas7.1

Chain C:



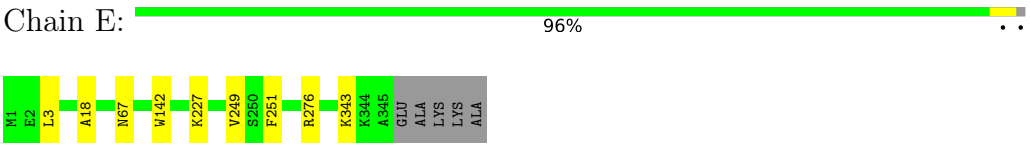
- Molecule 5: Cas7.1

Chain D:



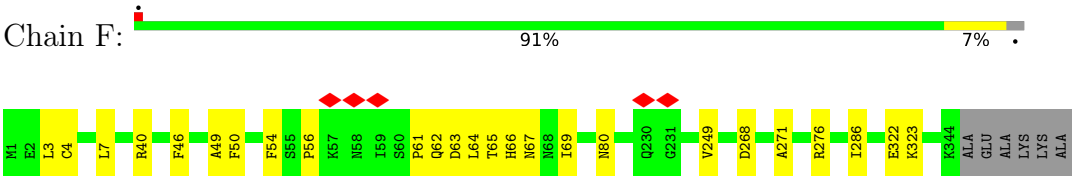
- Molecule 5: Cas7.1

Chain E:



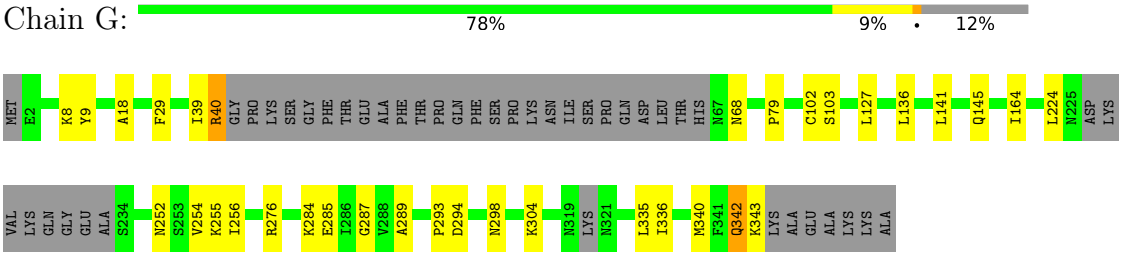
- Molecule 5: Cas7.1

Chain F:



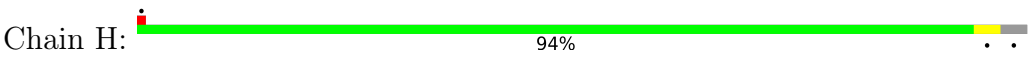
- Molecule 5: Cas7.1

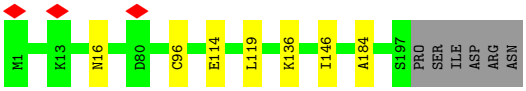
Chain G:



- Molecule 6: Cas6

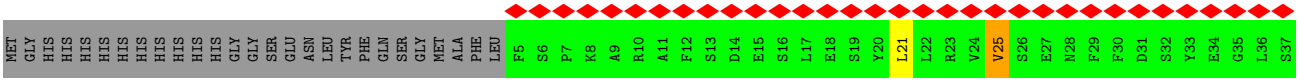
Chain H:

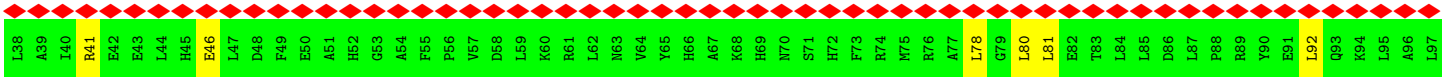


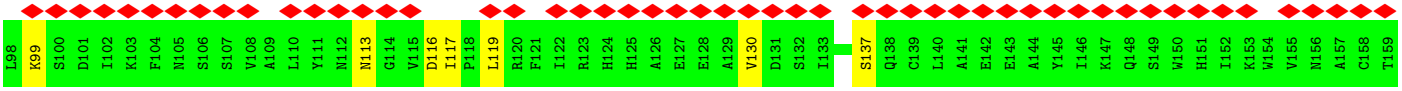


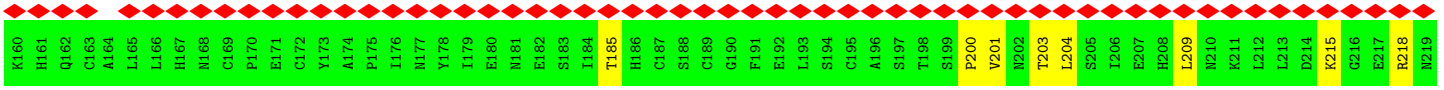
• Molecule 7: TniQ.1

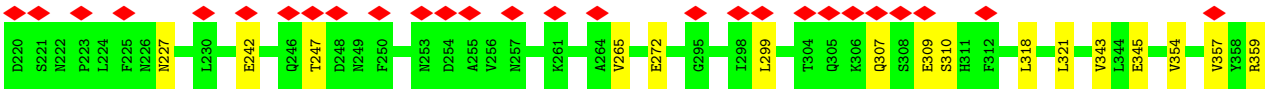
Chain I:

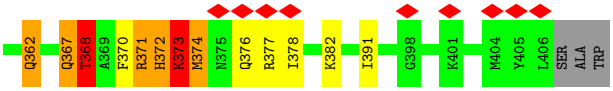






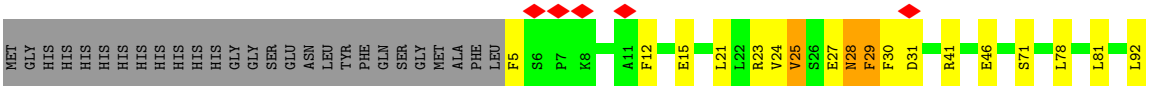


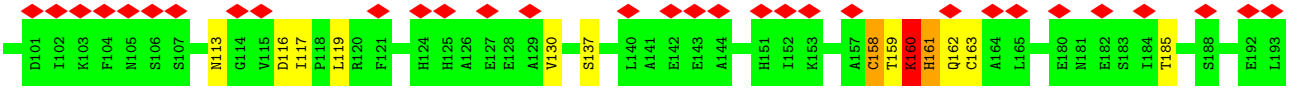


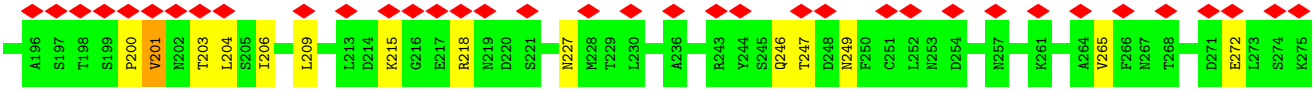


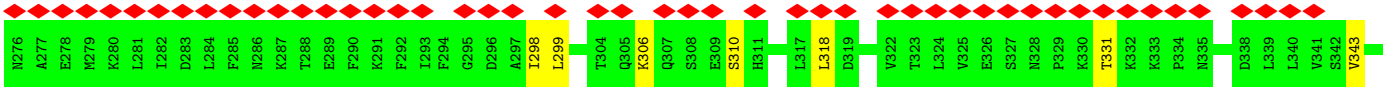
• Molecule 7: TniQ.1

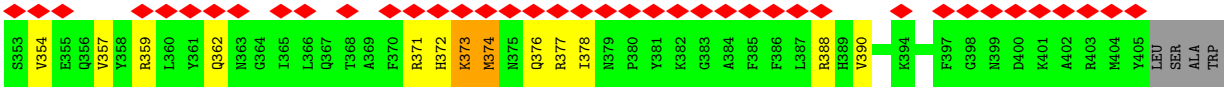
Chain J:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150000	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	373.53, 373.53, 373.53	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2451, 1.2451, 1.2451	Depositor

5 Model quality

5.1 Standard geometry

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	1	2.33	1/1447 (0.1%)	1.15	7/2258 (0.3%)
2	2	0.28	0/886	0.90	0/1364
3	3	0.30	0/249	0.84	0/380
4	A	0.73	0/5107	0.81	6/6948 (0.1%)
5	B	0.69	0/2788	0.74	0/3777
5	C	0.67	0/2842	0.74	0/3846
5	D	0.67	0/2842	0.74	0/3846
5	E	0.67	0/2833	0.73	0/3834
5	F	0.68	0/2828	0.75	0/3827
5	G	0.69	0/2531	0.75	1/3423 (0.0%)
6	H	0.70	1/1626 (0.1%)	0.77	0/2189
7	I	0.70	0/3338	0.80	2/4520 (0.0%)
7	J	0.84	1/3330 (0.0%)	1.07	4/4509 (0.1%)
All	All	0.84	3/32647 (0.0%)	0.83	20/44721 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	15
5	B	0	1
5	D	0	1
5	F	0	1
7	I	0	1
7	J	0	1
All	All	0	20

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	40	C	O3'-P	-87.97	0.55	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	28	ASN	C-N	27.38	1.97	1.34
6	H	114	GLU	CD-OE2	5.36	1.31	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	28	ASN	O-C-N	-39.10	60.14	122.70
1	1	40	C	OP1-P-O3'	-27.74	44.18	105.20
7	J	28	ASN	CA-C-N	26.48	175.46	117.20
1	1	40	C	P-O3'-C3'	25.04	149.75	119.70
1	1	40	C	O3'-P-O5'	14.29	131.16	104.00
7	J	28	ASN	C-N-CA	-11.94	91.84	121.70
1	1	25	G	C2'-C3'-O3'	8.81	128.88	109.50
4	A	295	PRO	N-CA-CB	6.85	111.53	103.30
7	I	373	LYS	CB-CA-C	6.64	123.69	110.40
1	1	40	C	OP2-P-O3'	6.61	119.74	105.20
4	A	402	PRO	N-CA-CB	6.04	110.55	103.30
1	1	13	U	C2'-C3'-O3'	6.01	123.32	113.70
1	1	19	C	C2'-C3'-O3'	6.00	123.30	113.70
4	A	407	PRO	N-CA-CB	5.83	110.29	103.30
4	A	337	PRO	N-CA-CB	5.80	110.26	103.30
4	A	370	PRO	N-CA-CB	5.54	109.95	103.30
4	A	380	PRO	N-CA-CB	5.22	109.57	103.30
5	G	39	ILE	C-N-CA	5.17	134.63	121.70
7	I	373	LYS	C-N-CA	5.06	134.35	121.70
7	J	160	LYS	C-N-CA	-5.01	109.16	121.70

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	280	LEU	Peptide
4	A	281	ASN	Peptide
4	A	282	ASN	Peptide
4	A	283	GLY	Peptide
4	A	289	VAL	Peptide
4	A	294	LYS	Peptide
4	A	305	ILE	Peptide
4	A	345	ALA	Peptide
4	A	347	GLU	Peptide
4	A	349	GLY	Peptide
4	A	367	LEU	Peptide

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Mol	Chain	Res	Type	Group
4	A	391	GLY	Peptide
4	A	393	SER	Peptide
4	A	418	ASN	Peptide
4	A	423	LYS	Peptide
5	B	319	ASN	Peptide
5	D	316	CYS	Peptide
5	F	322	GLU	Peptide
7	I	367	GLN	Mainchain
7	J	158	CYS	Peptide

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	1	1291	0	648	43	0
2	2	793	0	439	67	0
3	3	222	0	122	1	0
4	A	5013	0	4539	26	0
5	B	2723	0	2652	3	0
5	C	2777	0	2730	3	0
5	D	2777	0	2728	2	0
5	E	2768	0	2724	2	0
5	F	2763	0	2716	50	0
5	G	2477	0	2426	73	0
6	H	1592	0	1581	5	0
7	I	3261	0	3187	87	0
7	J	3253	0	3177	49	0
All	All	31710	0	29669	271	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 4.

All (271) 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)
1:1:39:A:C8	5:G:224:LEU:HD23	1.20	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:39:A:C5	5:G:224:LEU:HD22	1.42	1.49
2:2:20:DG:C4'	7:I:371:ARG:H	1.25	1.45
1:1:39:A:C8	5:G:224:LEU:CD2	1.97	1.45
2:2:20:DG:C4'	7:I:371:ARG:N	1.80	1.45
1:1:39:A:C5	5:G:224:LEU:CD2	2.13	1.30
5:F:62:GLN:OE1	7:I:371:ARG:NH1	1.68	1.25
2:2:20:DG:H5"	7:I:370:PHE:CB	1.69	1.22
1:1:39:A:N7	5:G:224:LEU:CD2	2.03	1.20
1:1:39:A:C4	5:G:224:LEU:CD2	2.23	1.20
7:J:28:ASN:O	7:J:29:PHE:N	1.73	1.20
7:J:28:ASN:C	7:J:29:PHE:N	1.97	1.18
2:2:20:DG:H5'	7:I:370:PHE:CA	1.74	1.16
7:J:159:THR:O	7:J:161:HIS:N	1.77	1.15
5:F:61:PRO:CG	7:I:362:GLN:OE1	1.91	1.15
5:G:40:ARG:NH2	5:G:68:ASN:O	1.78	1.14
2:2:20:DG:C5'	7:I:370:PHE:HB2	1.75	1.14
2:2:20:DG:H4'	7:I:371:ARG:N	1.58	1.13
1:1:39:A:N7	5:G:224:LEU:HD22	1.63	1.12
2:2:26:DC:H5"	5:G:343:LYS:HB2	1.26	1.11
1:1:39:A:N9	5:G:224:LEU:CD2	2.13	1.11
7:J:5:PHE:CD1	7:J:29:PHE:CE2	2.22	1.11
2:2:23:DC:O2	5:F:69:ILE:HB	1.51	1.08
7:J:160:LYS:NZ	7:J:161:HIS:ND1	2.01	1.07
7:J:160:LYS:NZ	7:J:161:HIS:CG	2.23	1.06
2:2:20:DG:C5'	7:I:371:ARG:N	2.17	1.06
7:J:5:PHE:CG	7:J:29:PHE:CE2	2.29	1.06
2:2:20:DG:H5'	7:I:370:PHE:HA	1.33	1.04
2:2:20:DG:C5'	7:I:371:ARG:H	1.70	1.04
5:F:66:HIS:CE1	7:I:373:LYS:CE	2.18	1.04
7:J:160:LYS:NZ	7:J:161:HIS:HB2	1.72	1.04
5:F:286:ILE:HA	5:G:102:CYS:O	1.60	1.02
1:1:39:A:C4	5:G:224:LEU:HD21	1.93	0.99
2:2:20:DG:C5'	7:I:370:PHE:CB	2.35	0.99
7:I:372:HIS:HB2	7:I:376:GLN:HB3	1.44	0.98
5:F:65:THR:HG21	5:G:287:GLY:CA	1.92	0.98
2:2:20:DG:C5'	7:I:370:PHE:CA	2.40	0.98
2:2:20:DG:O4'	7:I:371:ARG:N	1.88	0.96
5:F:65:THR:HG21	5:G:287:GLY:C	1.84	0.96
7:J:160:LYS:NZ	7:J:161:HIS:CB	2.29	0.96
7:J:28:ASN:C	7:J:29:PHE:CB	2.34	0.96
5:F:66:HIS:CE1	7:I:373:LYS:HE2	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:61:PRO:CB	7:I:362:GLN:OE1	2.15	0.95
1:1:39:A:N9	5:G:224:LEU:HD23	1.78	0.94
1:1:39:A:N7	5:G:224:LEU:HD23	1.71	0.93
5:F:65:THR:HG21	5:G:287:GLY:HA2	1.51	0.93
7:J:5:PHE:CG	7:J:29:PHE:HE2	1.84	0.93
5:F:62:GLN:OE1	7:I:371:ARG:CZ	2.17	0.92
5:F:64:LEU:HD22	5:G:289:ALA:HB2	1.48	0.92
2:2:21:DG:O4'	7:I:373:LYS:CD	2.00	0.91
5:F:66:HIS:CE1	7:I:373:LYS:HG3	2.05	0.91
5:F:66:HIS:NE2	7:I:373:LYS:CD	2.25	0.90
7:J:160:LYS:HZ2	7:J:161:HIS:CG	1.84	0.90
7:J:160:LYS:HZ1	7:J:161:HIS:CB	1.82	0.90
2:2:20:DG:H4'	7:I:371:ARG:CA	2.03	0.89
7:J:5:PHE:CE1	7:J:29:PHE:CD2	2.47	0.88
1:1:35:G:H1'	5:G:8:LYS:HE3	1.55	0.87
5:F:61:PRO:HG2	7:I:362:GLN:OE1	1.73	0.87
1:1:35:G:C2	5:G:340:MET:SD	2.68	0.86
2:2:21:DG:O4'	7:I:373:LYS:HD3	1.74	0.86
7:J:28:ASN:C	7:J:29:PHE:HB3	1.95	0.85
2:2:20:DG:H5"	7:I:370:PHE:HB2	0.87	0.85
7:J:160:LYS:NZ	7:J:160:LYS:O	2.07	0.85
7:J:160:LYS:CE	7:J:161:HIS:HB2	2.07	0.84
1:1:40:C:N3	2:2:21:DG:O6	2.11	0.84
2:2:20:DG:O4'	7:I:371:ARG:HB2	1.77	0.83
7:I:370:PHE:CZ	7:I:382:LYS:NZ	2.46	0.83
5:F:49:ALA:HB1	5:G:293:PRO:CG	2.06	0.83
7:I:370:PHE:HZ	7:I:382:LYS:NZ	1.75	0.83
2:2:20:DG:C4'	7:I:371:ARG:CA	2.56	0.83
1:1:39:A:N9	5:G:224:LEU:HD21	1.91	0.82
2:2:20:DG:H4'	7:I:371:ARG:O	1.79	0.82
7:I:372:HIS:CD2	7:I:376:GLN:O	2.33	0.81
2:2:26:DC:H5"	5:G:343:LYS:CB	2.08	0.81
2:2:20:DG:H4'	7:I:371:ARG:C	2.01	0.80
7:J:5:PHE:CD1	7:J:29:PHE:CD2	2.69	0.80
2:2:20:DG:C1'	7:I:371:ARG:HB2	2.12	0.80
4:A:317:ARG:O	4:A:321:VAL:N	2.12	0.80
7:J:160:LYS:HZ1	7:J:161:HIS:CG	1.92	0.80
2:2:20:DG:H5'	7:I:371:ARG:N	1.95	0.79
2:2:20:DG:C5'	7:I:370:PHE:C	2.51	0.79
7:J:28:ASN:C	7:J:29:PHE:CA	2.50	0.79
2:2:20:DG:O4'	7:I:371:ARG:CB	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:66:HIS:CE1	7:I:373:LYS:CD	2.68	0.76
5:F:61:PRO:HB3	7:I:362:GLN:OE1	1.84	0.76
5:F:61:PRO:HG3	7:I:362:GLN:OE1	1.85	0.76
5:F:66:HIS:CE1	7:I:373:LYS:CG	2.68	0.76
4:A:292:LEU:HA	4:A:293:LEU:C	2.06	0.76
2:2:26:DC:C5'	5:G:343:LYS:HB2	2.13	0.74
2:2:20:DG:H5'	7:I:370:PHE:C	2.08	0.73
7:J:159:THR:C	7:J:161:HIS:N	2.34	0.72
7:J:159:THR:C	7:J:161:HIS:H	1.87	0.72
2:2:20:DG:C1'	7:I:371:ARG:CB	2.68	0.72
7:I:373:LYS:HE2	7:I:373:LYS:HA	1.71	0.72
1:1:39:A:OP1	5:G:252:ASN:ND2	2.21	0.71
7:J:12:PHE:HE1	7:J:23:ARG:NH1	1.89	0.71
2:2:21:DG:C1'	7:I:373:LYS:HD3	2.20	0.70
5:F:49:ALA:HB1	5:G:293:PRO:HG3	1.72	0.70
5:F:66:HIS:NE2	7:I:373:LYS:HG3	2.04	0.70
1:1:36:G:C4	2:2:24:DA:N1	2.60	0.70
7:J:27:GLU:O	7:J:29:PHE:HD1	1.75	0.70
5:F:67:ASN:OD1	5:G:284:LYS:NZ	2.24	0.70
5:F:66:HIS:NE2	7:I:373:LYS:HD3	2.06	0.69
7:I:372:HIS:CB	7:I:376:GLN:HB3	2.20	0.68
7:I:373:LYS:CE	7:I:373:LYS:HA	2.22	0.68
2:2:20:DG:O4'	7:I:371:ARG:CA	2.40	0.68
5:G:136:LEU:HD22	5:G:164:ILE:HD11	1.75	0.68
4:A:305:ILE:HA	4:A:312:ALA:HB2	1.75	0.68
7:I:371:ARG:HH11	7:I:372:HIS:H	1.41	0.68
5:F:66:HIS:NE2	7:I:373:LYS:CG	2.57	0.67
1:1:40:C:O2'	1:1:41:G:O5'	2.12	0.67
7:J:160:LYS:HZ1	7:J:161:HIS:HB2	1.47	0.67
5:G:40:ARG:HG2	6:H:146:ILE:HG23	1.78	0.65
1:1:39:A:C6	5:G:224:LEU:HD22	2.25	0.65
7:J:27:GLU:O	7:J:29:PHE:CD1	2.48	0.65
7:J:5:PHE:CE1	7:J:29:PHE:CG	2.73	0.65
7:J:159:THR:O	7:J:162:GLN:N	2.31	0.63
2:2:20:DG:O3'	7:I:371:ARG:O	2.16	0.63
1:1:36:G:C5	2:2:24:DA:C6	2.87	0.63
2:2:20:DG:H1'	7:I:371:ARG:CB	2.29	0.62
2:2:26:DC:H5"	5:G:343:LYS:HD3	1.80	0.62
1:1:37:U:H3'	5:G:254:VAL:CG1	2.30	0.62
1:1:35:G:C1'	5:G:8:LYS:HE3	2.27	0.62
2:2:23:DC:O2	5:F:69:ILE:CB	2.38	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:35:G:N3	5:G:340:MET:SD	2.73	0.61
2:2:26:DC:O2	5:G:340:MET:SD	2.58	0.61
7:I:372:HIS:CD2	7:I:376:GLN:HB3	2.36	0.61
7:J:12:PHE:CE1	7:J:23:ARG:NH1	2.69	0.61
7:J:12:PHE:HE1	7:J:23:ARG:CZ	2.14	0.60
7:J:160:LYS:HE3	7:J:161:HIS:HB2	1.84	0.59
2:2:41:DT:H73	5:C:230:GLN:HB3	1.84	0.59
1:1:40:C:OP1	5:G:255:LYS:NZ	2.36	0.58
2:2:26:DC:C4'	5:G:343:LYS:C	2.72	0.58
2:2:20:DG:C4'	7:I:371:ARG:O	2.50	0.58
4:A:378:THR:O	4:A:380:PRO:N	2.37	0.57
2:2:30:DC:H1'	2:2:31:DC:C5	2.39	0.57
5:G:141:LEU:O	5:G:145:GLN:HB2	2.03	0.57
7:I:372:HIS:HD2	7:I:376:GLN:CA	2.16	0.57
1:1:36:G:C6	2:2:24:DA:C6	2.92	0.57
7:I:370:PHE:CZ	7:I:382:LYS:CE	2.88	0.57
1:1:36:G:N3	2:2:24:DA:C2	2.73	0.56
1:1:37:U:O2'	5:F:40:ARG:O	2.23	0.56
4:A:439:LEU:HB3	4:A:442:ILE:HD11	1.88	0.56
5:F:50:PHE:HZ	5:G:298:ASN:ND2	2.03	0.56
1:1:38:G:N1	5:G:285:GLU:OE2	2.35	0.55
2:2:26:DC:H4'	5:G:343:LYS:C	2.27	0.55
5:F:65:THR:CG2	5:G:287:GLY:C	2.69	0.55
7:I:367:GLN:O	7:I:368:THR:O	2.25	0.55
4:A:293:LEU:HA	4:A:294:LYS:HA	1.89	0.55
7:I:373:LYS:HE2	7:I:374:MET:H	1.72	0.55
2:2:21:DG:H5'	7:I:371:ARG:O	2.07	0.55
4:A:305:ILE:HA	4:A:312:ALA:CB	2.37	0.54
5:F:63:ASP:HB3	7:I:374:MET:CE	2.16	0.54
2:2:20:DG:H5'	7:I:371:ARG:H	1.56	0.54
5:G:127:LEU:HD13	5:G:336:ILE:HD12	1.89	0.54
1:1:30:G:H1	2:2:31:DC:N4	2.05	0.54
7:J:373:LYS:HE2	7:J:373:LYS:HA	1.88	0.54
2:2:26:DC:C5'	5:G:343:LYS:HD3	2.38	0.54
5:F:286:ILE:CA	5:G:102:CYS:O	2.47	0.54
5:F:54:PHE:CE1	5:G:304:LYS:NZ	2.71	0.53
7:J:160:LYS:HZ2	7:J:161:HIS:CB	2.11	0.53
5:F:50:PHE:HZ	5:G:298:ASN:HD21	1.56	0.53
4:A:369:LEU:O	4:A:370:PRO:C	2.46	0.53
4:A:321:VAL:O	4:A:325:LYS:N	2.41	0.53
7:J:160:LYS:HE3	7:J:163:CYS:SG	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:36:G:C4	2:2:24:DA:C2	2.98	0.52
1:1:36:G:C5	2:2:24:DA:N1	2.78	0.52
5:F:64:LEU:HD22	5:G:289:ALA:CB	2.30	0.52
7:I:367:GLN:C	7:I:368:THR:O	2.46	0.52
2:2:20:DG:H1'	7:I:371:ARG:HB2	1.86	0.52
4:A:292:LEU:CA	4:A:293:LEU:C	2.78	0.52
5:F:65:THR:CG2	5:G:287:GLY:HA2	2.33	0.51
7:J:159:THR:HA	7:J:206:ILE:HD11	1.91	0.51
7:J:162:GLN:HE21	7:J:201:VAL:HG21	1.74	0.51
5:F:56:PRO:HG2	5:G:294:ASP:HA	1.93	0.51
7:I:372:HIS:CD2	7:I:376:GLN:CB	2.94	0.51
2:2:20:DG:H1'	7:I:371:ARG:HB3	1.90	0.51
7:J:24:VAL:O	7:J:29:PHE:HE1	1.94	0.51
5:E:3:LEU:HB2	5:E:343:LYS:HB2	1.92	0.50
7:I:372:HIS:HD2	7:I:376:GLN:CB	2.24	0.50
7:I:372:HIS:CG	7:I:376:GLN:HB3	2.46	0.50
5:C:18:ALA:HB3	5:C:251:PHE:HB2	1.93	0.50
5:F:49:ALA:HB1	5:G:293:PRO:HG2	1.91	0.50
7:I:372:HIS:HD2	7:I:376:GLN:N	2.10	0.50
7:J:12:PHE:HD1	7:J:15:GLU:OE1	1.95	0.49
7:I:371:ARG:HD3	7:I:372:HIS:N	2.27	0.49
5:G:340:MET:O	5:G:340:MET:HG2	2.12	0.49
4:A:370:PRO:O	4:A:373:GLU:N	2.45	0.49
7:I:372:HIS:HB2	7:I:376:GLN:CB	2.30	0.49
7:I:372:HIS:HD2	7:I:376:GLN:O	1.91	0.49
5:D:63:ASP:HA	5:D:66:HIS:CD2	2.48	0.49
1:1:36:G:C2	2:2:24:DA:C2	3.01	0.48
5:F:4:CYS:HB2	5:F:7:LEU:HB2	1.95	0.48
2:2:31:DC:O2	2:2:31:DC:C2'	2.62	0.48
5:G:40:ARG:HG2	6:H:146:ILE:CG2	2.44	0.48
5:G:9:TYR:CZ	5:G:335:LEU:HD22	2.48	0.48
1:1:2:U:H1'	4:A:463:ALA:HA	1.97	0.47
4:A:368:SER:CA	4:A:369:LEU:HA	2.43	0.47
5:F:69:ILE:HD12	5:G:224:LEU:HD13	1.95	0.47
1:1:34:U:O2'	5:G:8:LYS:NZ	2.46	0.47
2:2:21:DG:H1'	5:F:66:HIS:NE2	2.29	0.47
5:G:40:ARG:NH2	5:G:68:ASN:CB	2.78	0.47
5:F:66:HIS:HE1	7:I:373:LYS:HG3	1.73	0.47
5:F:80:ASN:ND2	5:G:29:PHE:CD2	2.83	0.47
7:J:372:HIS:HB2	7:J:376:GLN:HB3	1.96	0.47
7:I:370:PHE:CZ	7:I:382:LYS:HE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:28:ASN:C	7:J:29:PHE:HB2	2.33	0.46
5:F:64:LEU:CA	7:I:374:MET:CE	2.59	0.46
4:A:101:VAL:HG21	4:A:635:LEU:HB3	1.97	0.46
7:J:160:LYS:HG2	7:J:161:HIS:ND1	2.31	0.46
4:A:293:LEU:CA	4:A:294:LYS:HA	2.45	0.46
4:A:369:LEU:O	4:A:374:LEU:N	2.48	0.46
1:1:35:G:C1'	5:G:8:LYS:CE	2.94	0.46
5:G:40:ARG:CG	6:H:146:ILE:HG23	2.44	0.46
7:I:370:PHE:O	7:I:370:PHE:CD1	2.69	0.46
1:1:30:G:N1	2:2:31:DC:N4	2.64	0.45
5:F:63:ASP:HB3	7:I:374:MET:HE2	1.97	0.45
5:G:40:ARG:NH2	5:G:68:ASN:HB2	2.31	0.45
5:G:79:PRO:HG3	6:H:119:LEU:HD13	1.99	0.45
7:I:372:HIS:CG	7:I:372:HIS:O	2.69	0.45
2:2:38:DT:H2"	2:2:39:DA:H5'	1.99	0.45
7:I:21:LEU:O	7:I:25:VAL:HG23	2.16	0.45
4:A:370:PRO:C	4:A:371:ASP:HA	2.37	0.45
1:1:37:U:H2'	5:G:254:VAL:HG11	1.99	0.45
7:J:246:GLN:HE21	7:J:249:ASN:HD22	1.64	0.45
4:A:107:HIS:HB3	4:A:110:VAL:HG22	1.99	0.44
4:A:317:ARG:O	4:A:321:VAL:CB	2.66	0.44
5:C:1:MET:N	5:C:304:LYS:O	2.50	0.44
4:A:31:ASP:HA	4:A:140:LYS:HB3	1.99	0.44
5:F:49:ALA:CB	5:G:293:PRO:HG3	2.46	0.44
7:J:27:GLU:O	7:J:29:PHE:HB3	2.16	0.44
7:J:158:CYS:O	7:J:206:ILE:HD11	2.17	0.44
2:2:21:DG:H1'	7:I:373:LYS:HD3	1.98	0.43
2:2:55:DC:H2"	2:2:56:DG:C8	2.53	0.43
1:1:39:A:C8	5:G:224:LEU:HA	2.54	0.43
1:1:54:U:C5	6:H:119:LEU:HD11	2.54	0.43
5:B:229:LYS:HB2	5:B:232:GLU:HG2	2.01	0.43
5:F:46:PHE:CG	5:G:342:GLN:HG2	2.54	0.43
7:I:373:LYS:HE2	7:I:374:MET:N	2.34	0.43
5:E:18:ALA:HB3	5:E:251:PHE:HB2	2.00	0.42
1:1:35:G:O4'	5:G:8:LYS:NZ	2.50	0.42
2:2:20:DG:C3'	7:I:371:ARG:O	2.67	0.42
5:F:66:HIS:HD1	7:I:374:MET:HB2	1.84	0.42
4:A:368:SER:CB	4:A:369:LEU:HA	2.50	0.42
5:F:50:PHE:CZ	5:G:298:ASN:ND2	2.85	0.42
7:J:373:LYS:HA	7:J:373:LYS:CE	2.49	0.42
7:I:307:GLN:HB3	7:I:309:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:321:LEU:HB3	7:I:391:ILE:HD11	2.01	0.42
2:2:26:DC:H5"	5:G:343:LYS:CD	2.47	0.41
5:F:268:ASP:HB3	5:F:271:ALA:HB2	2.01	0.41
5:G:18:ALA:CB	5:G:256:ILE:HD11	2.50	0.41
1:1:37:U:H5"	5:G:254:VAL:HG13	2.02	0.41
7:J:29:PHE:CE2	7:J:30:PHE:HD2	2.38	0.41
2:2:26:DC:H5"	5:G:343:LYS:CG	2.50	0.41
2:2:29:DT:H4'	2:2:30:DC:C5'	2.51	0.41
7:J:21:LEU:O	7:J:25:VAL:HG23	2.21	0.41
4:A:242:PRO:HB2	4:A:250:ALA:HA	2.02	0.41
7:I:372:HIS:O	7:I:372:HIS:ND1	2.54	0.41
3:3:2:DC:H2"	3:3:3:DC:C5	2.56	0.41
5:F:286:ILE:O	5:G:103:SER:HA	2.21	0.41
4:A:413:GLN:O	4:A:417:VAL:N	2.47	0.41
5:B:172:TRP:CE2	5:B:274:ARG:HD3	2.55	0.41
5:D:18:ALA:HB3	5:D:251:PHE:HB2	2.02	0.41
7:J:246:GLN:NE2	7:J:249:ASN:HD22	2.19	0.41
4:A:368:SER:HA	4:A:369:LEU:HA	2.02	0.40
4:A:119:ALA:HB3	4:A:218:VAL:HG22	2.02	0.40
7:J:160:LYS:HD3	7:J:160:LYS:N	2.35	0.40
1:1:2:U:H3'	1:1:3:G:H5"	2.04	0.40
1:1:37:U:N3	2:2:24:DA:C6	2.90	0.40
4:A:23:PHE:CE1	4:A:43:LEU:HD11	2.57	0.40
5:B:18:ALA:HB3	5:B:251:PHE:HB2	2.03	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
4	A	678/695 (98%)	609 (90%)	46 (7%)	23 (3%)	3 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	339/350 (97%)	326 (96%)	11 (3%)	2 (1%)	22	43
5	C	344/350 (98%)	330 (96%)	12 (4%)	2 (1%)	22	43
5	D	344/350 (98%)	335 (97%)	8 (2%)	1 (0%)	37	59
5	E	343/350 (98%)	335 (98%)	7 (2%)	1 (0%)	37	59
5	F	342/350 (98%)	326 (95%)	15 (4%)	1 (0%)	37	59
5	G	299/350 (85%)	286 (96%)	12 (4%)	1 (0%)	37	59
6	H	195/203 (96%)	182 (93%)	11 (6%)	2 (1%)	13	29
7	I	398/432 (92%)	366 (92%)	24 (6%)	8 (2%)	6	12
7	J	397/432 (92%)	362 (91%)	24 (6%)	11 (3%)	4	7
All	All	3679/3862 (95%)	3457 (94%)	170 (5%)	52 (1%)	12	19

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	142	GLN
4	A	281	ASN
4	A	287	PHE
4	A	295	PRO
4	A	345	ALA
4	A	362	LEU
4	A	372	ASN
4	A	379	ILE
4	A	422	GLN
4	A	424	HIS
5	F	3	LEU
5	G	342	GLN
7	I	218	ARG
7	I	227	ASN
7	I	368	THR
7	I	374	MET
7	J	29	PHE
7	J	160	LYS
7	J	218	ARG
4	A	288	ASN
4	A	305	ILE
4	A	347	GLU
4	A	393	SER
4	A	394	MET
6	H	96	CYS

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Mol	Chain	Res	Type
6	H	184	ALA
7	I	113	ASN
7	I	200	PRO
7	I	203	THR
7	J	161	HIS
7	J	200	PRO
7	J	203	THR
7	J	227	ASN
4	A	280	LEU
4	A	308	ASN
5	B	142	TRP
5	C	244	ASP
7	I	215	LYS
7	J	113	ASN
7	J	215	LYS
7	J	374	MET
4	A	285	THR
4	A	344	ASP
4	A	395	THR
5	C	142	TRP
5	D	142	TRP
7	J	388	ARG
4	A	392	VAL
4	A	423	LYS
4	A	425	VAL
5	B	320	LYS
5	E	142	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	456/614 (74%)	451 (99%)	5 (1%)	70 86
5	B	296/307 (96%)	293 (99%)	3 (1%)	73 88
5	C	305/307 (99%)	303 (99%)	2 (1%)	81 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	D	305/307 (99%)	303 (99%)	2 (1%)	81 93
5	E	304/307 (99%)	300 (99%)	4 (1%)	65 84
5	F	304/307 (99%)	301 (99%)	3 (1%)	73 88
5	G	272/307 (89%)	270 (99%)	2 (1%)	81 93
6	H	173/179 (97%)	171 (99%)	2 (1%)	67 85
7	I	359/383 (94%)	323 (90%)	36 (10%)	6 13
7	J	358/383 (94%)	320 (89%)	38 (11%)	5 11
All	All	3132/3401 (92%)	3035 (97%)	97 (3%)	37 62

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	35	SER
4	A	44	LEU
4	A	201	ARG
4	A	593	ARG
4	A	690	MET
5	B	249	VAL
5	B	276	ARG
5	B	321	ASN
5	C	249	VAL
5	C	276	ARG
5	D	249	VAL
5	D	276	ARG
5	E	67	ASN
5	E	227	LYS
5	E	249	VAL
5	E	276	ARG
5	F	249	VAL
5	F	276	ARG
5	F	323	LYS
5	G	40	ARG
5	G	276	ARG
6	H	16	ASN
6	H	136	LYS
7	I	25	VAL
7	I	41	ARG
7	I	46	GLU
7	I	78	LEU
7	I	80	LEU

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Mol	Chain	Res	Type
7	I	81	LEU
7	I	92	LEU
7	I	99	LYS
7	I	116	ASP
7	I	117	ILE
7	I	119	LEU
7	I	130	VAL
7	I	137	SER
7	I	185	THR
7	I	201	VAL
7	I	204	LEU
7	I	209	LEU
7	I	242	GLU
7	I	247	THR
7	I	265	VAL
7	I	272	GLU
7	I	299	LEU
7	I	310	SER
7	I	318	LEU
7	I	343	VAL
7	I	345	GLU
7	I	354	VAL
7	I	357	VAL
7	I	359	ARG
7	I	362	GLN
7	I	368	THR
7	I	371	ARG
7	I	372	HIS
7	I	373	LYS
7	I	377	ARG
7	I	378	ILE
7	J	25	VAL
7	J	31	ASP
7	J	41	ARG
7	J	46	GLU
7	J	71	SER
7	J	78	LEU
7	J	81	LEU
7	J	92	LEU
7	J	116	ASP
7	J	117	ILE
7	J	119	LEU

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Mol	Chain	Res	Type
7	J	130	VAL
7	J	137	SER
7	J	160	LYS
7	J	185	THR
7	J	201	VAL
7	J	204	LEU
7	J	209	LEU
7	J	247	THR
7	J	265	VAL
7	J	272	GLU
7	J	298	ILE
7	J	299	LEU
7	J	306	LYS
7	J	310	SER
7	J	318	LEU
7	J	331	THR
7	J	343	VAL
7	J	354	VAL
7	J	357	VAL
7	J	359	ARG
7	J	362	GLN
7	J	371	ARG
7	J	373	LYS
7	J	374	MET
7	J	377	ARG
7	J	378	ILE
7	J	390	VAL

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

Mol	Chain	Res	Type
4	A	115	ASN
5	B	62	GLN
5	B	93	GLN
5	C	67	ASN
5	C	93	GLN
5	C	298	ASN
5	D	66	HIS
5	D	93	GLN
5	D	230	GLN
5	D	298	ASN
5	E	93	GLN

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Mol	Chain	Res	Type
5	E	298	ASN
5	F	93	GLN
5	F	298	ASN
5	G	321	ASN
6	H	16	ASN
6	H	166	GLN
7	I	52	HIS
7	I	168	ASN
7	I	210	ASN
7	I	246	GLN
7	J	52	HIS
7	J	162	GLN
7	J	246	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	59/60 (98%)	23 (38%)	7 (11%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	3	G
1	1	4	A
1	1	8	U
1	1	9	A
1	1	13	U
1	1	14	G
1	1	15	G
1	1	19	C
1	1	20	A
1	1	21	C
1	1	25	G
1	1	26	G
1	1	27	A
1	1	28	C
1	1	33	U
1	1	39	A
1	1	40	C
1	1	41	G
1	1	43	G

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Mol	Chain	Res	Type
1	1	44	A
1	1	55	A
1	1	59	A
1	1	60	G

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	3	G
1	1	13	U
1	1	19	C
1	1	25	G
1	1	40	C
1	1	43	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	A	7

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Mol	Chain	Number of breaks
7	J	2
7	I	1
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	431:ASP	C	432:GLU	N	7.62
1	A	401:HIS	C	402:PRO	N	5.03
1	A	369:LEU	C	370:PRO	N	4.46
1	A	368:SER	C	369:LEU	N	4.43
1	A	293:LEU	C	294:LYS	N	4.29
1	A	370:PRO	C	371:ASP	N	3.80
1	I	190:GLY	C	191:PHE	N	3.60
1	J	190:GLY	C	191:PHE	N	3.60
1	A	274:ASN	C	275:SER	N	3.12
1	J	28:ASN	C	29:PHE	N	1.97
1	1	40:C	O3'	41:G	P	0.55

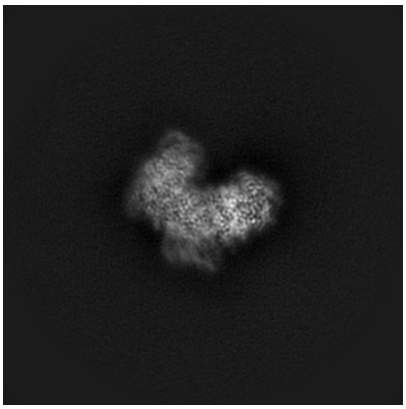
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51543. These allow visual inspection of the internal detail of the map and identification of artifacts.

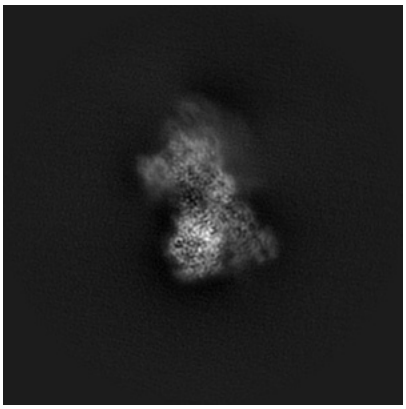
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

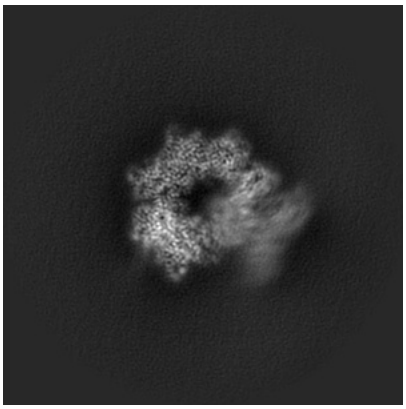
6.1.1 Primary map



X

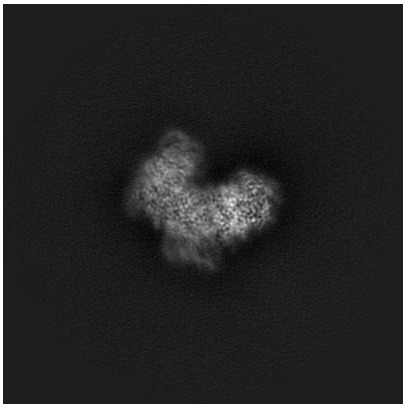


Y

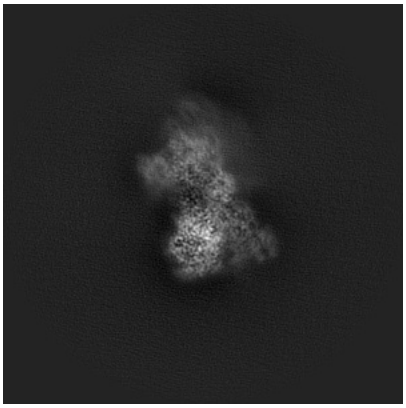


Z

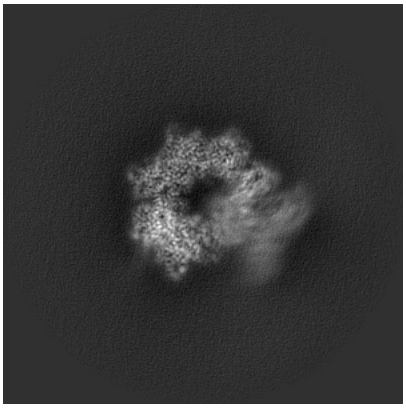
6.1.2 Raw map



X



Y

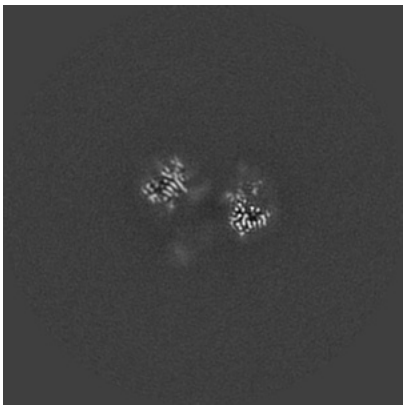


Z

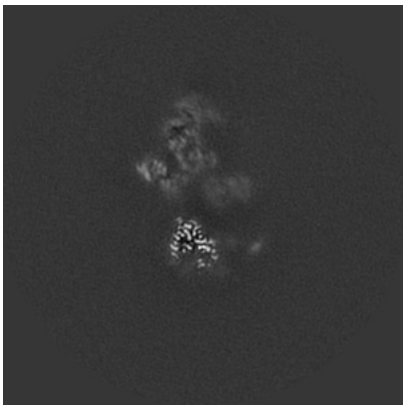
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

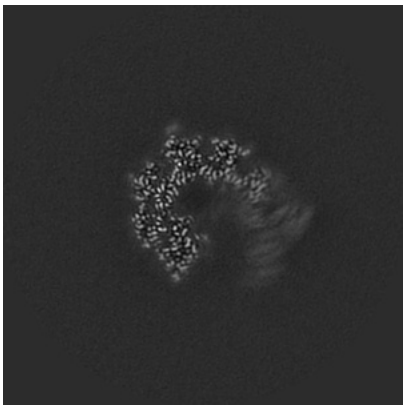
6.2.1 Primary map



X Index: 150

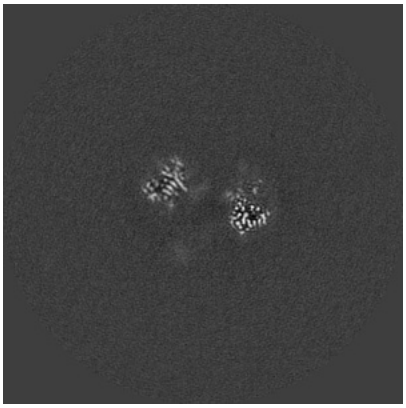


Y Index: 150



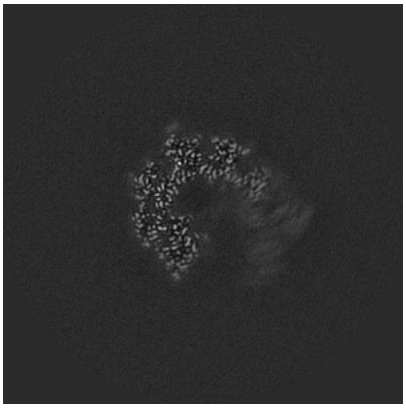
Z Index: 150

6.2.2 Raw map



X Index: 150

Y Index: 150



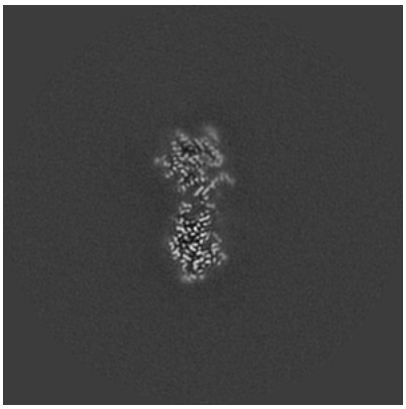
Z Index: 150

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

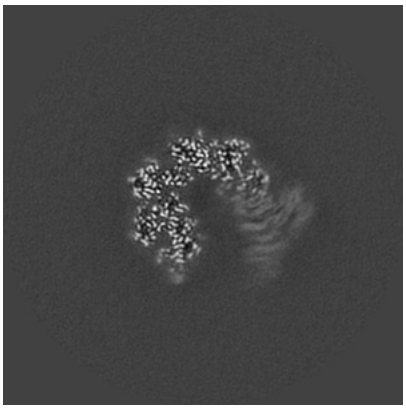
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 124



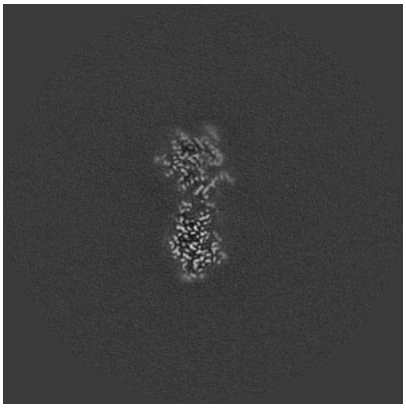
Y Index: 171



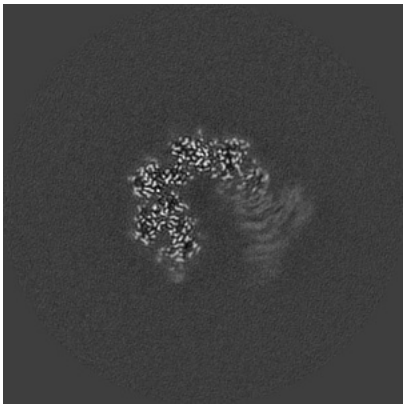
Z Index: 145

6.3.2 Raw map

X Index: 124



Y Index: 171

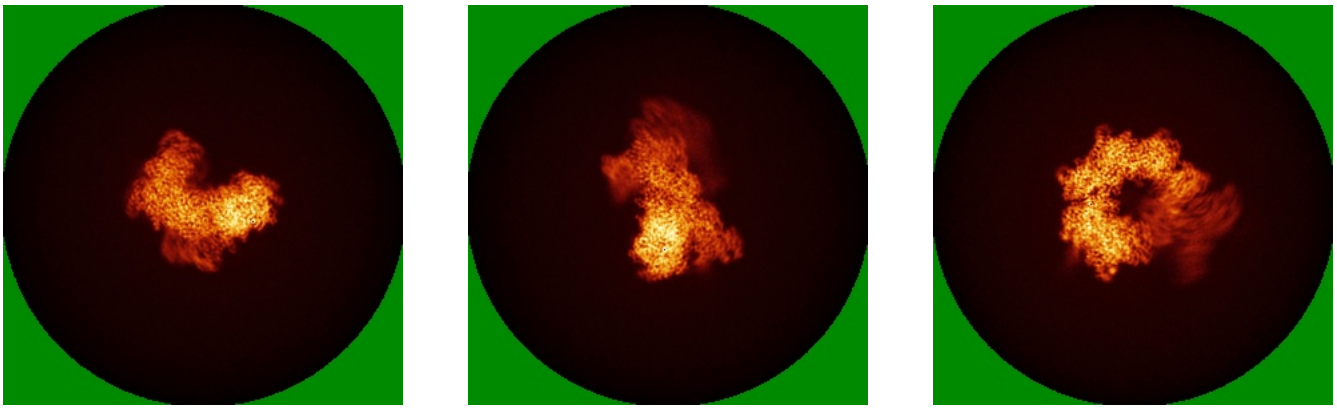


Z Index: 145

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

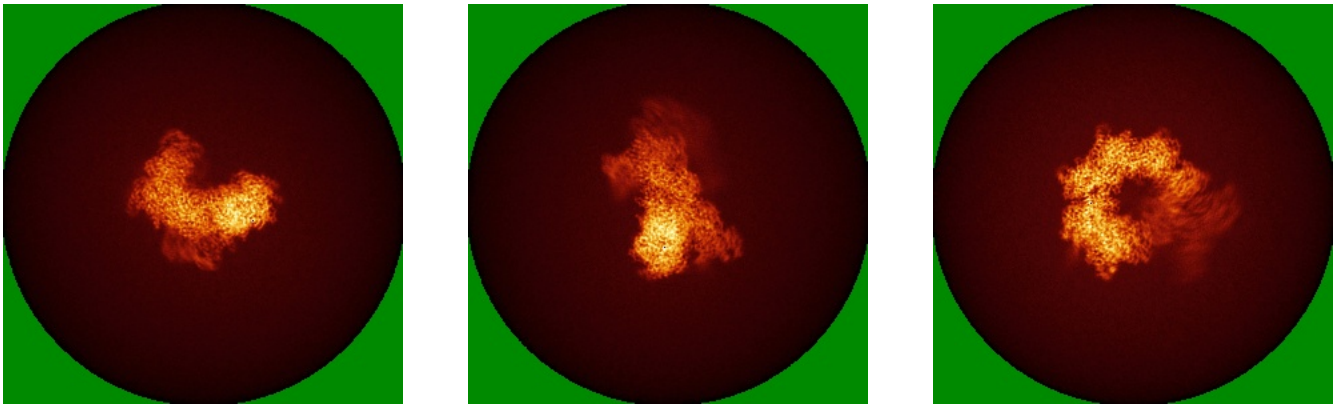
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

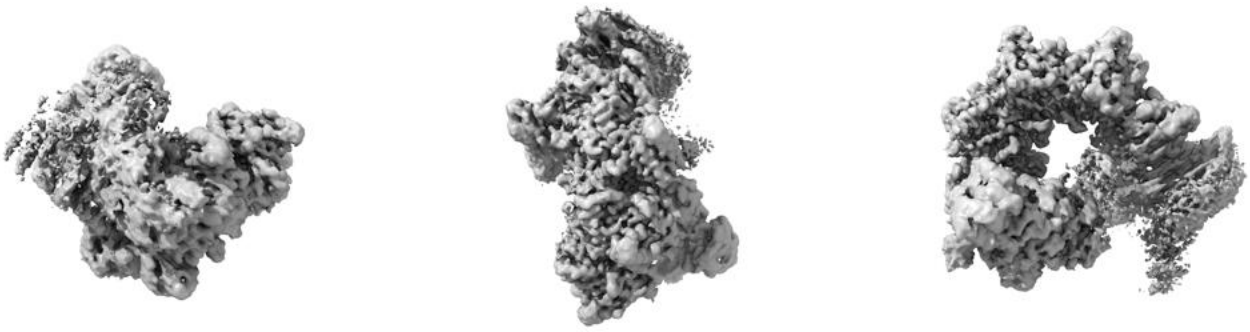


X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

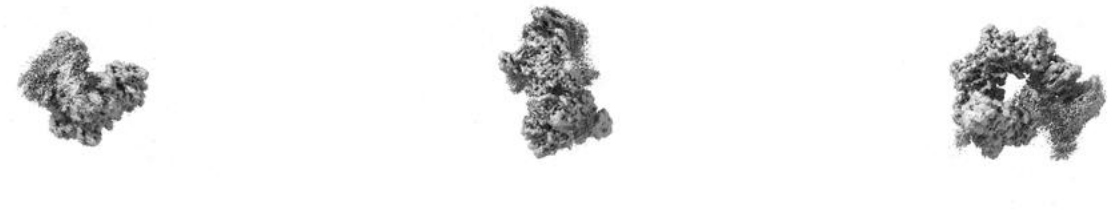
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

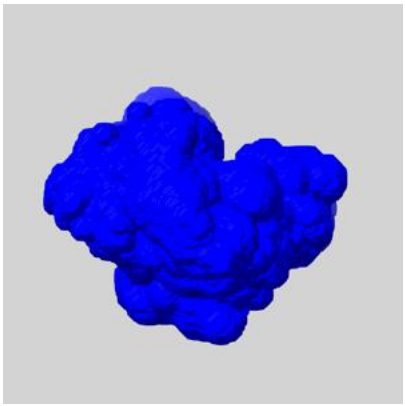
6.6 Mask visualisation (i)

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

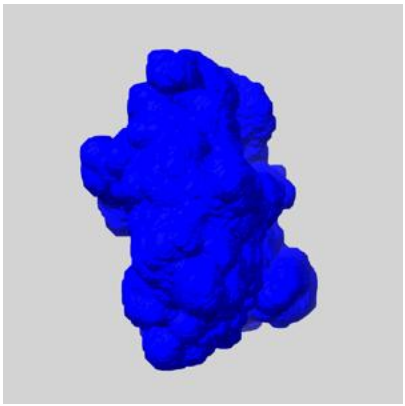
A mask typically either:

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

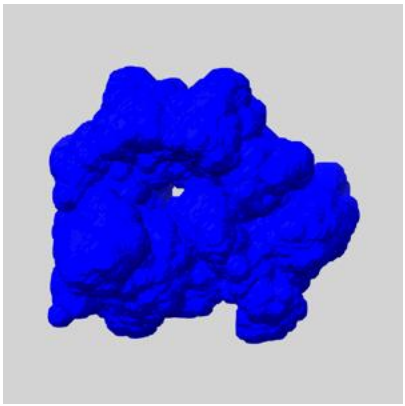
6.6.1 emd_51543_msk_1.map (i)



X



Y

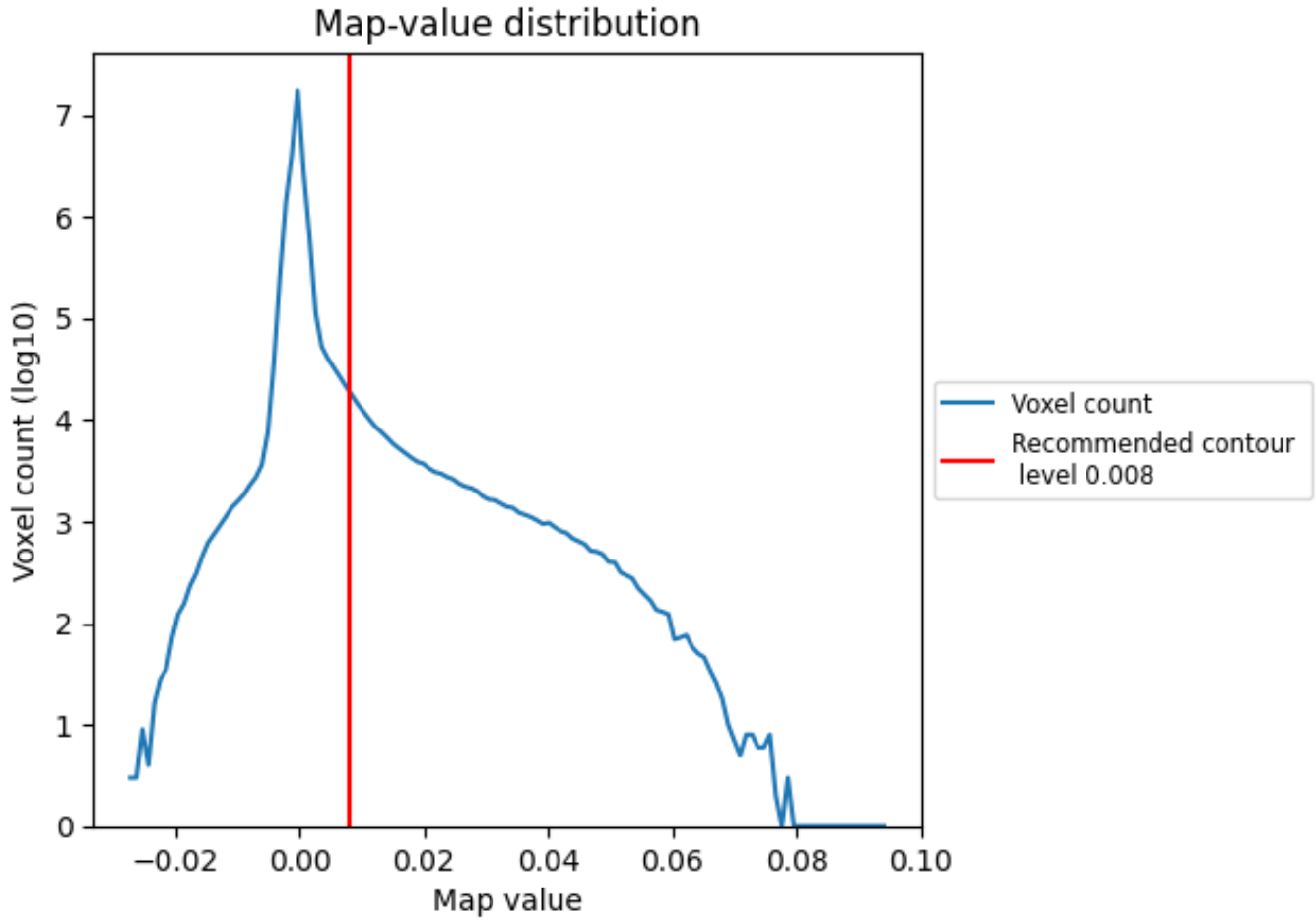


Z

7 Map analysis

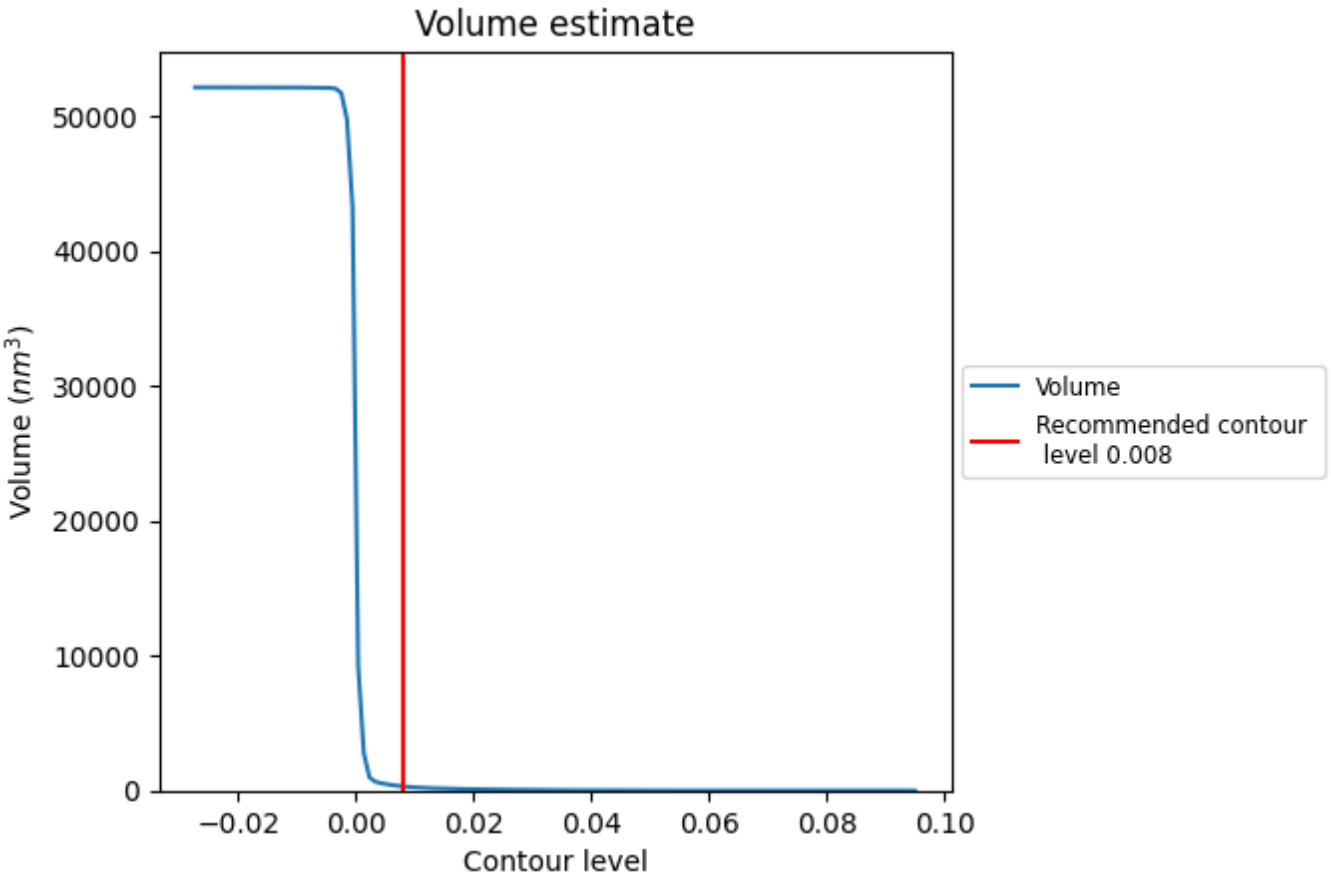
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

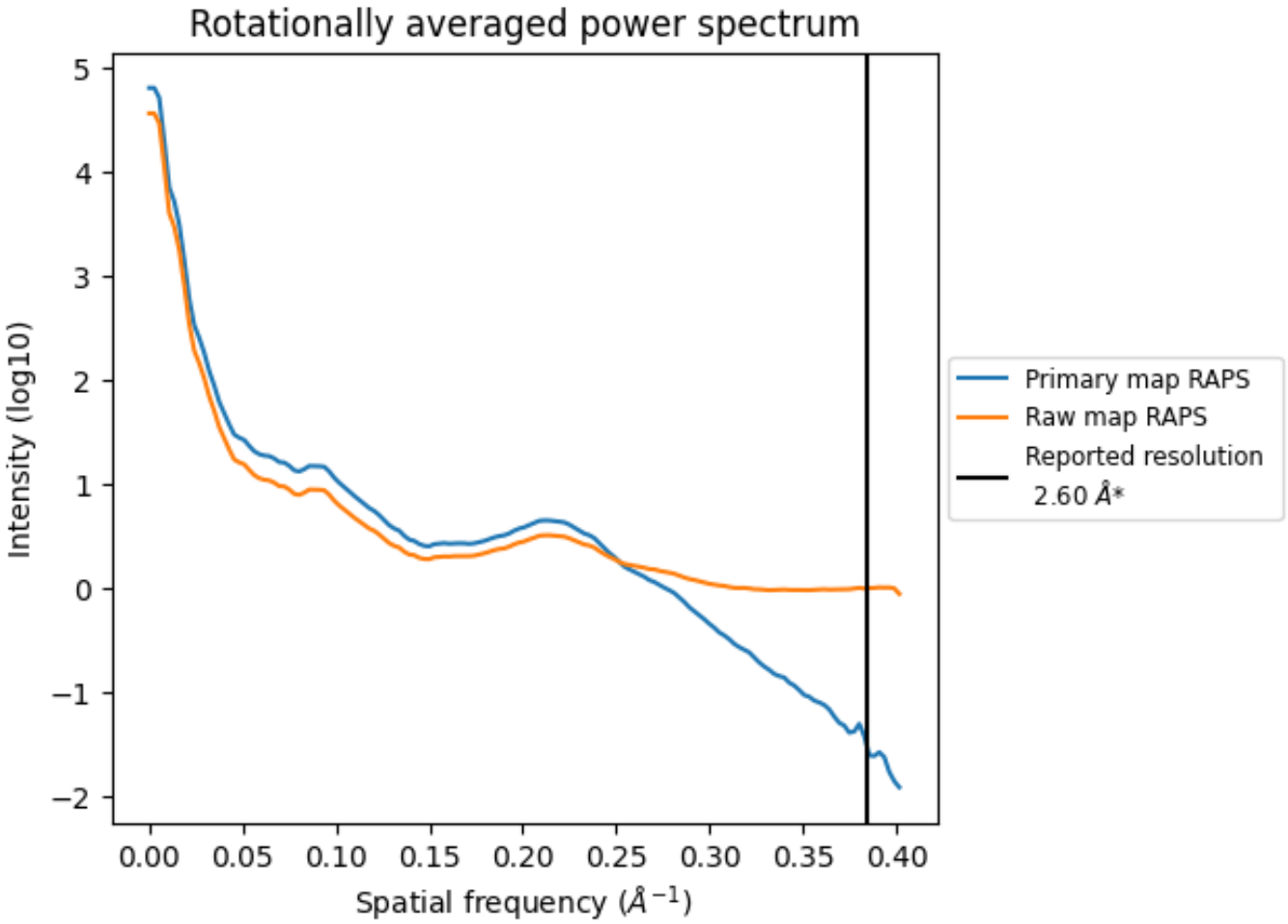
7.2 Volume estimate



The volume at the recommended contour level is 307 nm^3; this corresponds to an approximate mass of 277 kDa.

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

7.3 Rotationally averaged power spectrum (i)

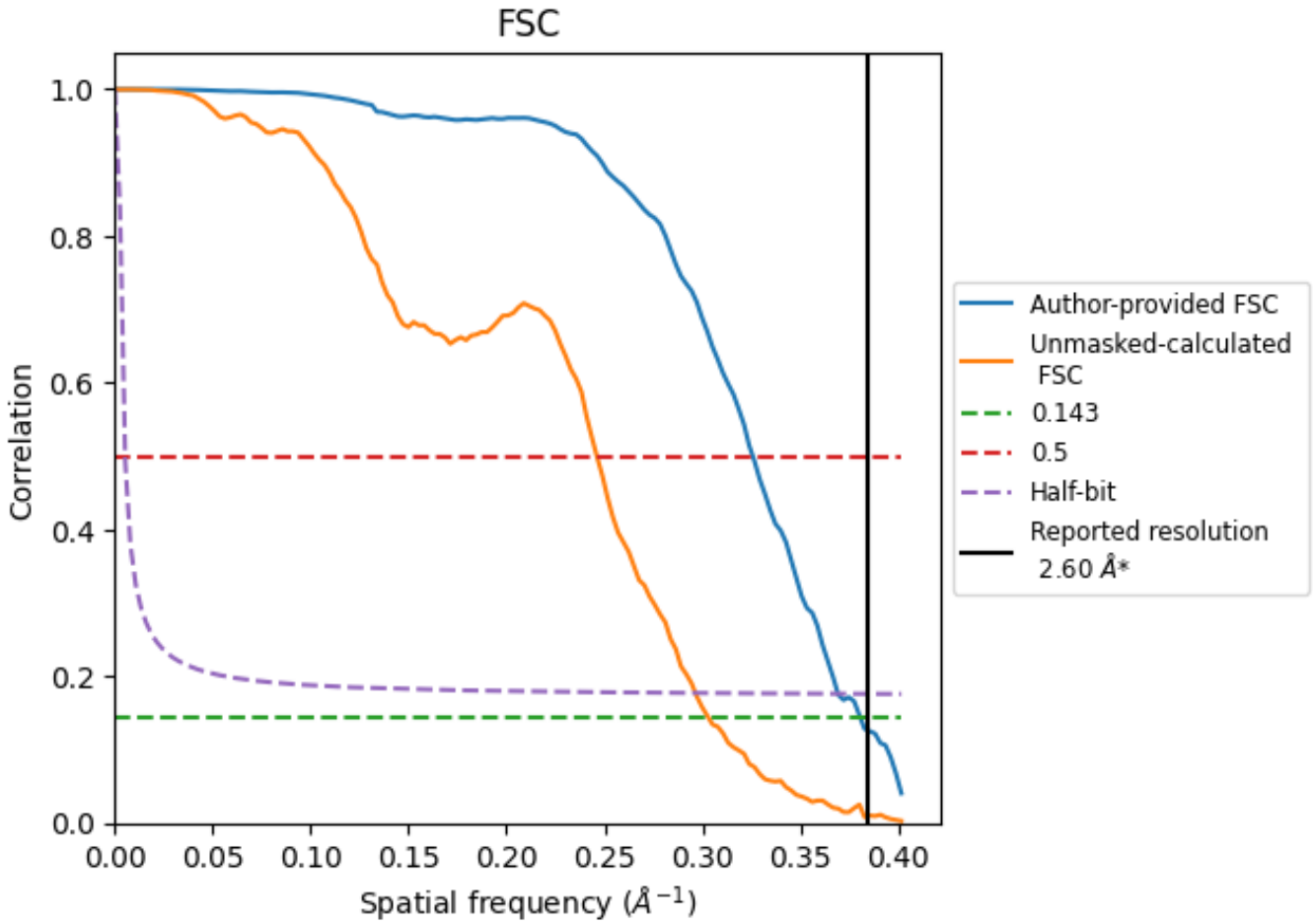


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

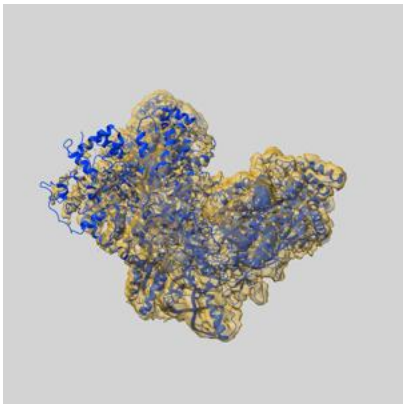
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.63	3.07	2.71
Unmasked-calculated*	3.30	4.06	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.6 by more than 10 %

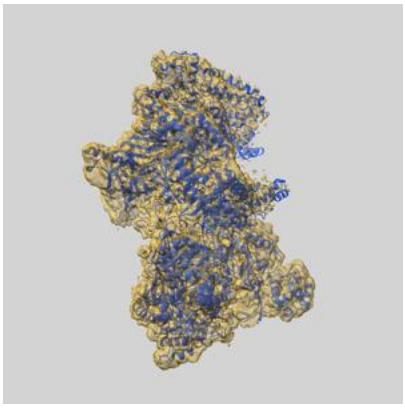
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51543 and PDB model 9GS9. Per-residue inclusion information can be found in section 3 on page 6.

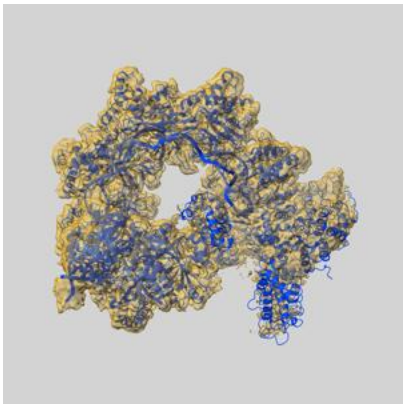
9.1 Map-model overlay



X



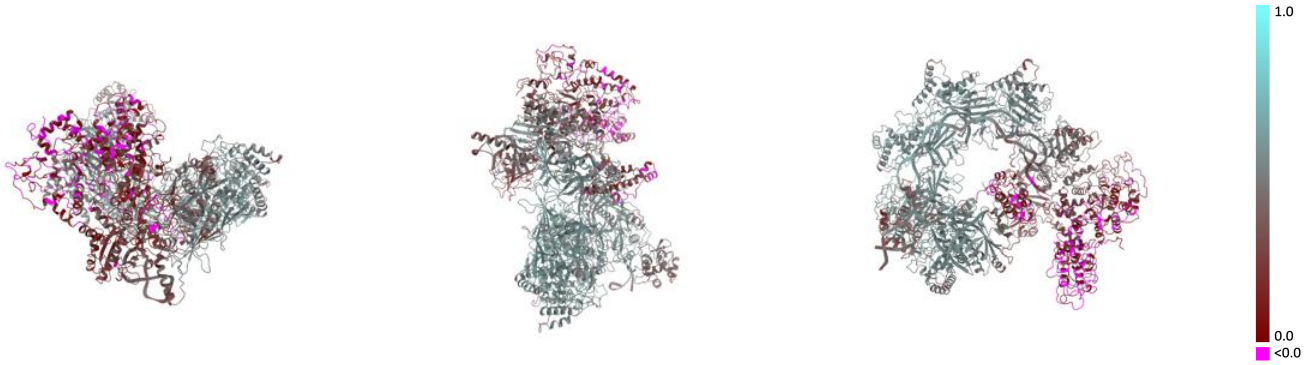
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

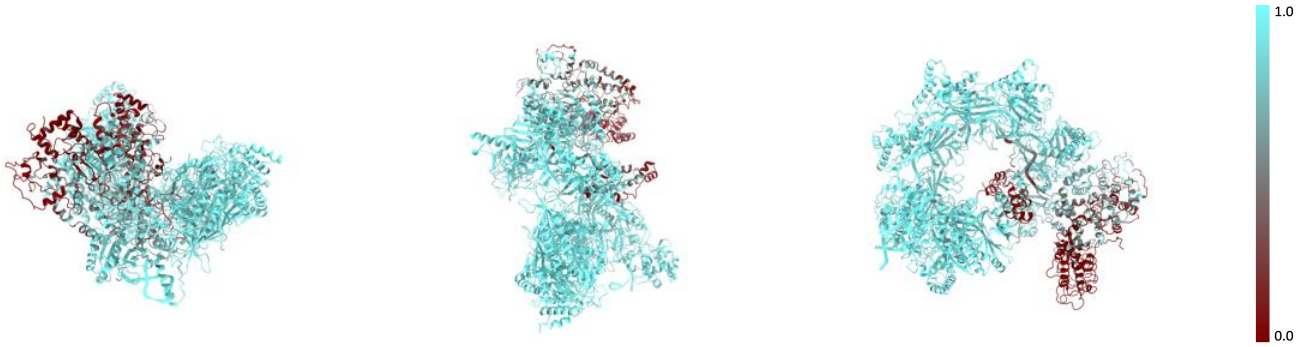
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

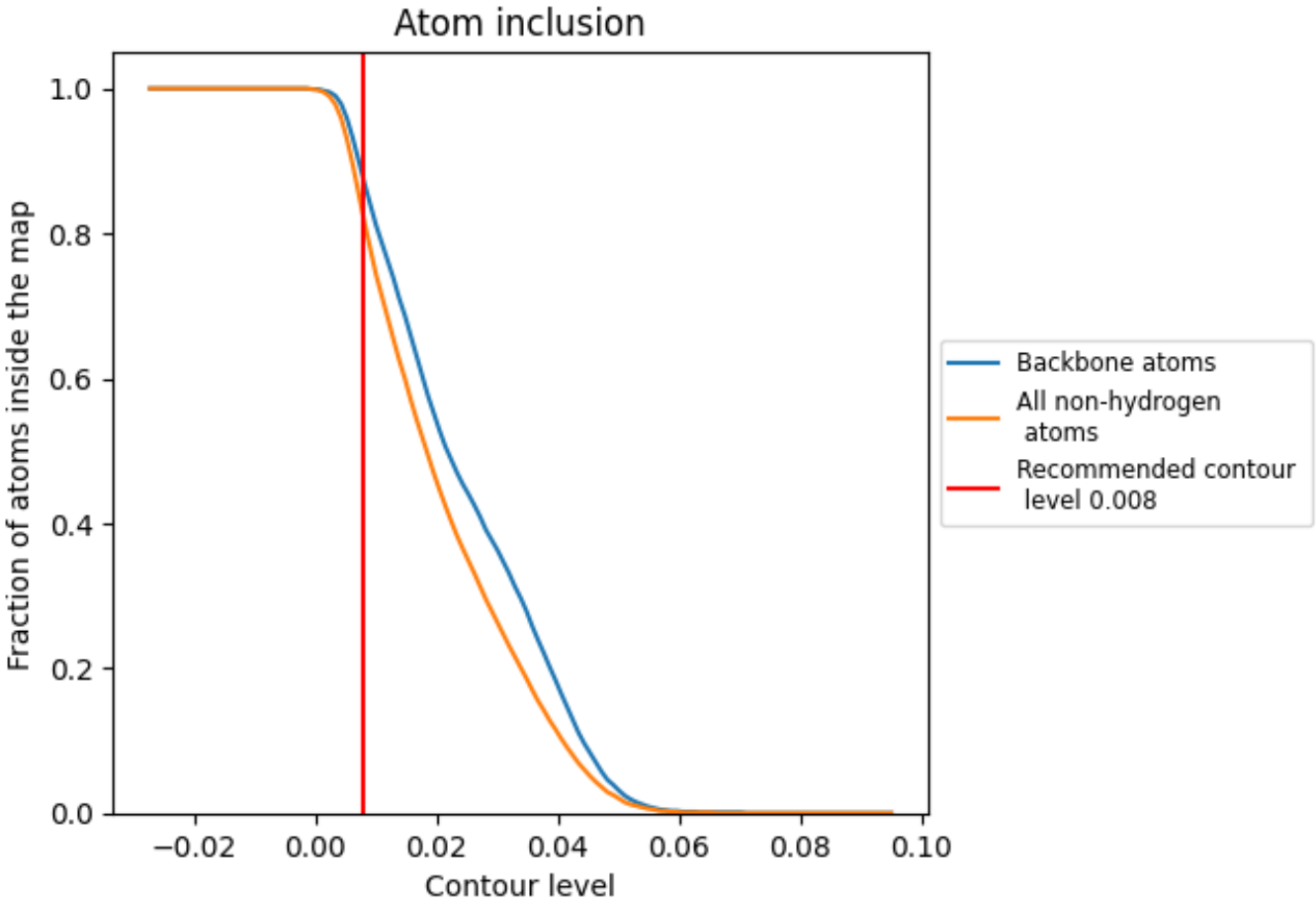
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 87% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.4220
1	0.9910	0.5070
2	0.7990	0.4650
3	0.9960	0.4670
A	0.8530	0.4440
B	0.9540	0.5440
C	0.9590	0.5600
D	0.9580	0.5630
E	0.9560	0.5570
F	0.9290	0.5130
G	0.9090	0.4500
H	0.8830	0.2830
I	0.3350	0.1070
J	0.5020	0.1690