



Full wwPDB EM Validation Report ⓘ

Jan 27, 2025 – 07:05 PM EST

PDB ID : 9C2D
EMDB ID : EMD-45155
Title : Bacteriophage Sf14 Capsid Icosahedral reconstruction
Authors : Subramanian, S.; Kerns, H.R.; Braverman, S.G.; Doore, S.M.
Deposited on : 2024-05-30
Resolution : 3.20 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) : 2.40

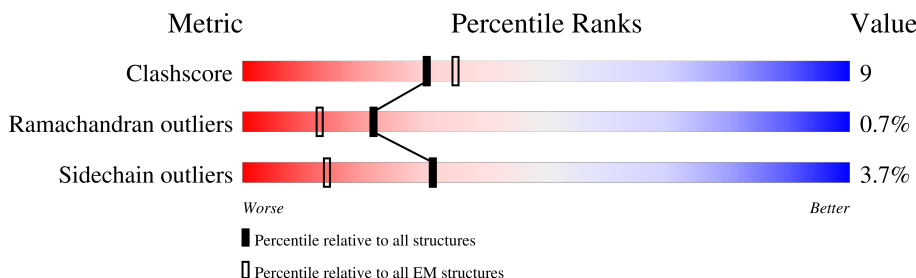
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





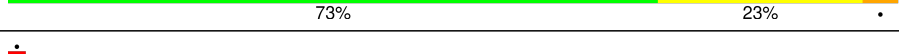
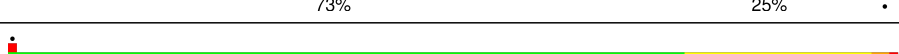
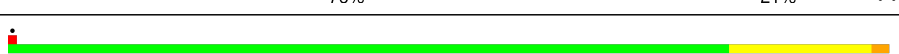

The reported resolution of this entry is 3.20 Å.

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.




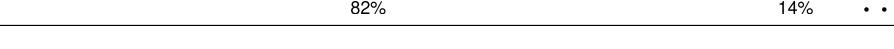
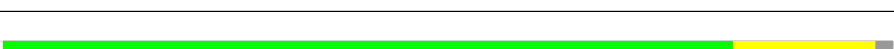


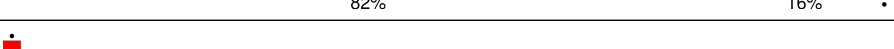



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	367	
1	B	367	
1	C	367	
1	D	367	
1	E	367	
1	F	367	
1	G	367	
1	H	367	

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Mol	Chain	Length	Quality of chain
1	I	367	
2	J	125	
2	K	125	
2	L	125	
2	M	125	
2	N	125	
2	O	125	
2	P	125	
2	Q	125	
2	R	125	
3	S	372	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35316 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	366	Total	C	N	O	S	0	0
			2906	1845	493	556	12		
1	B	366	Total	C	N	O	S	0	0
			2890	1838	484	555	13		
1	C	366	Total	C	N	O	S	0	0
			2895	1839	493	550	13		
1	D	366	Total	C	N	O	S	0	0
			2845	1807	481	545	12		
1	E	366	Total	C	N	O	S	0	0
			2877	1830	485	549	13		
1	F	366	Total	C	N	O	S	0	0
			2898	1842	488	555	13		
1	G	366	Total	C	N	O	S	0	0
			2903	1843	491	556	13		
1	H	366	Total	C	N	O	S	0	0
			2910	1847	492	559	12		
1	I	356	Total	C	N	O	S	0	0
			2817	1791	474	539	13		

- Molecule 2 is a protein called Structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	122	Total	C	N	O	S	0	0
			917	583	154	179	1		
2	K	123	Total	C	N	O	S	0	0
			939	597	157	184	1		
2	L	123	Total	C	N	O	S	0	0
			935	595	156	183	1		
2	M	123	Total	C	N	O	S	0	0
			939	597	157	184	1		
2	N	123	Total	C	N	O	S	0	0
			937	596	157	183	1		
2	O	124	Total	C	N	O	S	0	0
			943	601	158	183	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	123	Total	C	N	O	S	0	0
			926	588	156	181	1		
2	Q	123	Total	C	N	O	S	0	0
			935	595	157	182	1		
2	R	123	Total	C	N	O	S	0	0
			939	597	157	184	1		

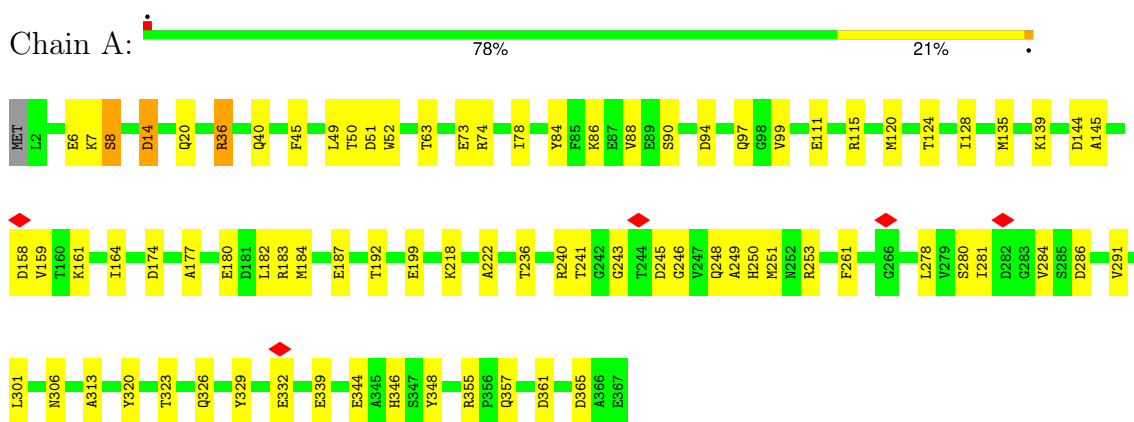
- Molecule 3 is a protein called Tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	120	Total	C	N	O	S	0	0
			965	633	150	179	3		

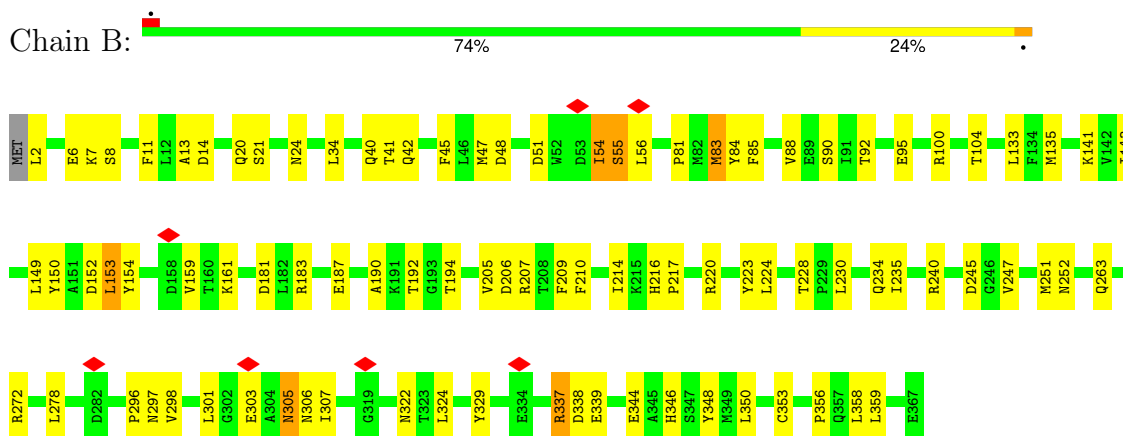
3 Residue-property plots

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

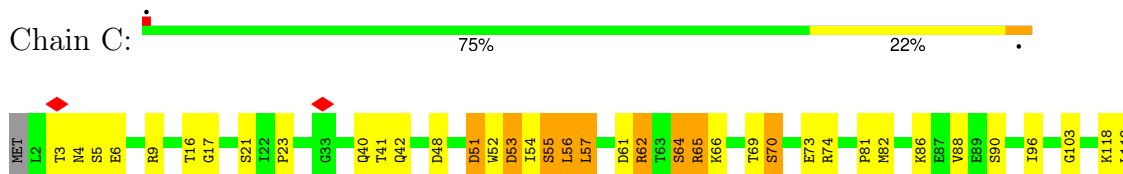
• Molecule 1: Major capsid protein

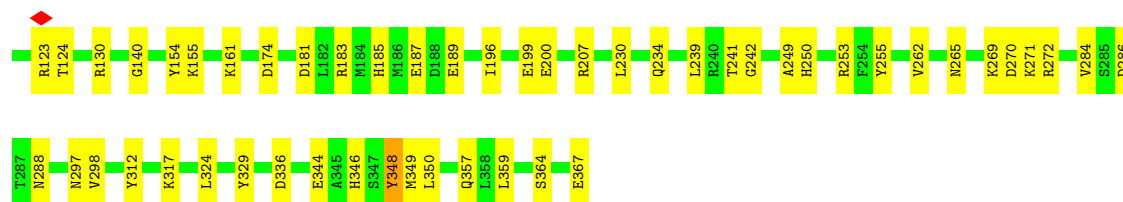


• Molecule 1: Major capsid protein

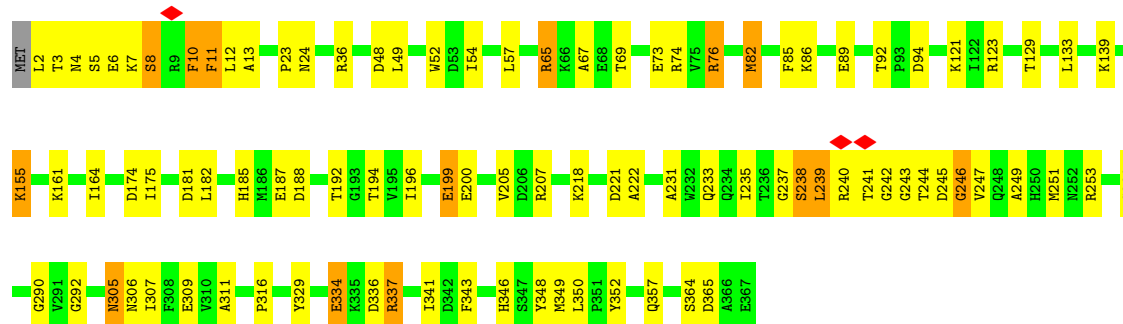


• Molecule 1: Major capsid protein

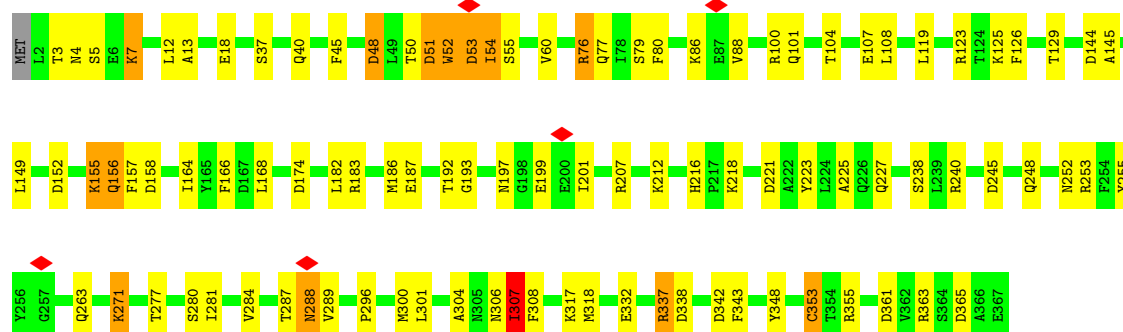




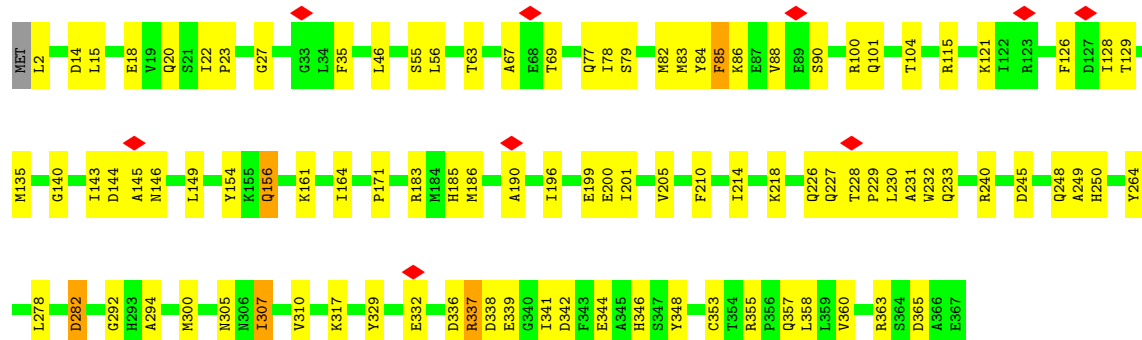
• Molecule 1: Major capsid protein



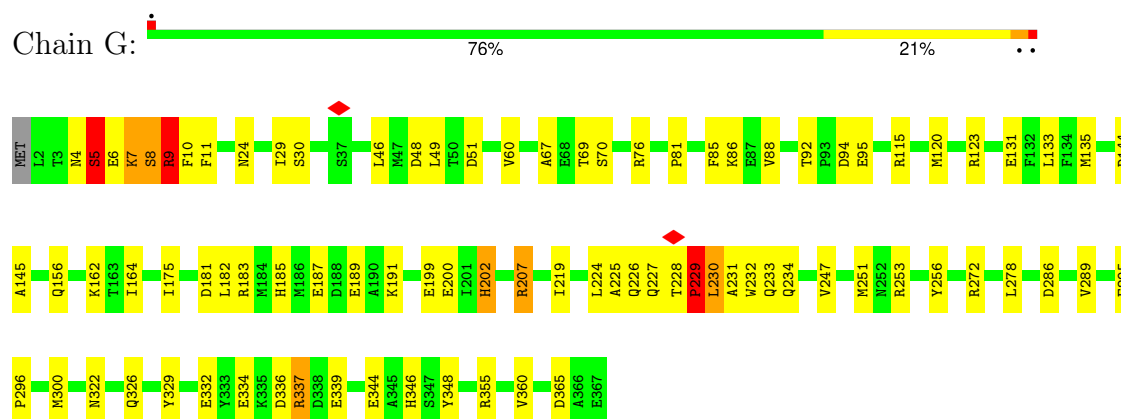
• Molecule 1: Major capsid protein



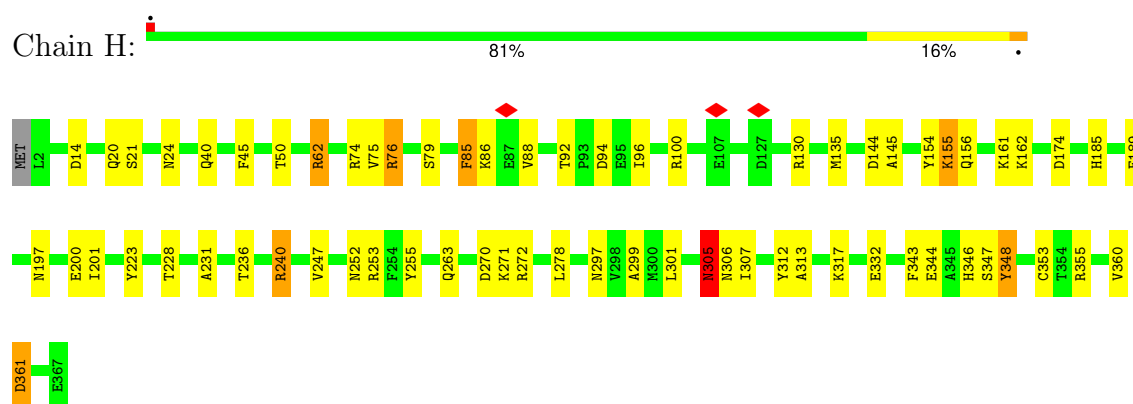
• Molecule 1: Major capsid protein



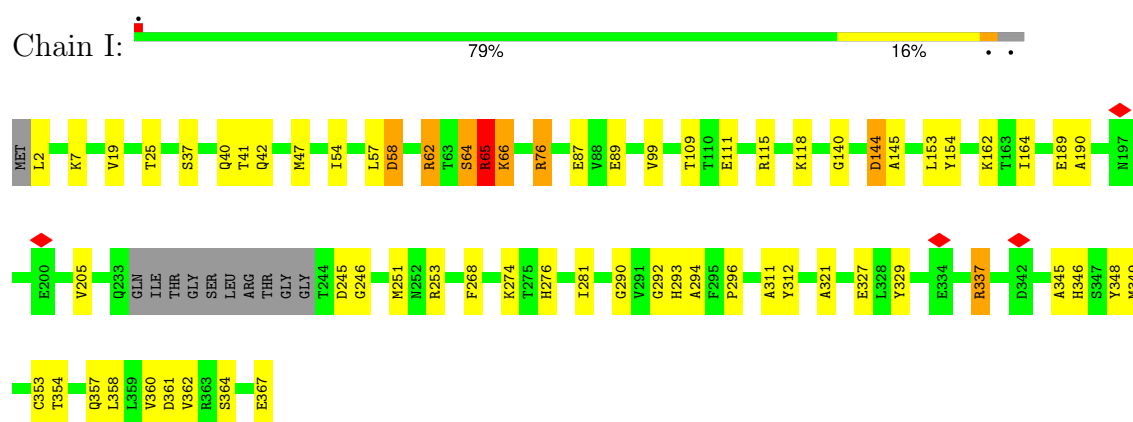
- Molecule 1: Major capsid protein



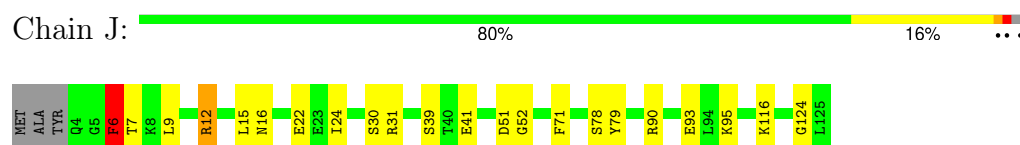
- Molecule 1: Major capsid protein




- Molecule 1: Major capsid protein

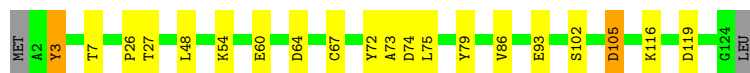


- Molecule 2: Structural protein




- Molecule 2: Structural protein

Chain K:  82% 14% ..




• Molecule 2: Structural protein

Chain L:  86% 10% ..



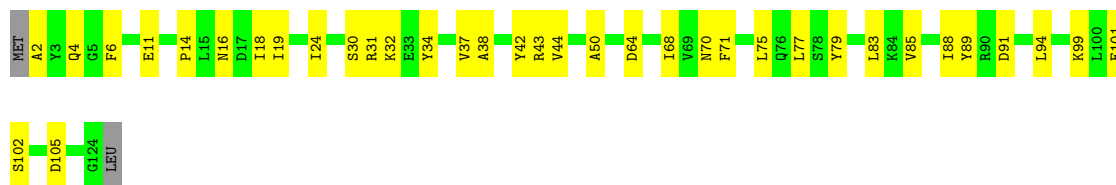
• Molecule 2: Structural protein

Chain M:  82% 16% .




• Molecule 2: Structural protein

Chain N:  70% 29% .




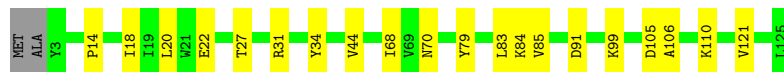
• Molecule 2: Structural protein

Chain O:  86% 12% ..




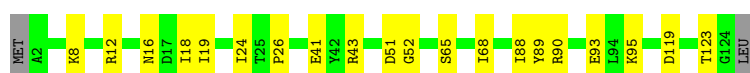
• Molecule 2: Structural protein

Chain P:  82% 16% .

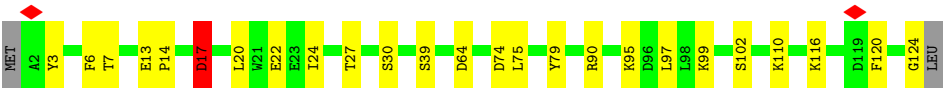
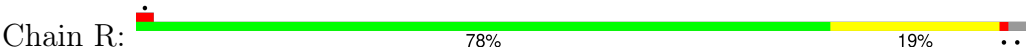


• Molecule 2: Structural protein

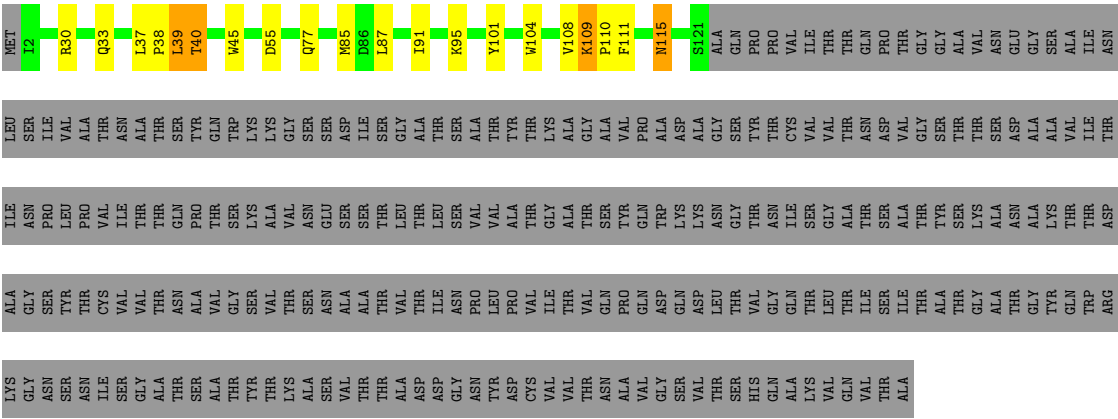
Chain Q:  82% 16% .



● Molecule 2: Structural protein



● Molecule 3: Tail protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	42269	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.255	Depositor
Minimum map value	-1.867	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.197	Depositor
Recommended contour level	0.58	Depositor
Map size (\AA)	1224.0, 1224.0, 1224.0	wwPDB
Map dimensions	1000, 1000, 1000	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.224, 1.224, 1.224	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	A	0.32	1/2967 (0.0%)	0.50	0/4016
1	B	0.30	0/2951	0.53	0/3996
1	C	0.33	0/2956	0.55	0/4001
1	D	0.36	0/2904	0.60	2/3934 (0.1%)
1	E	0.34	0/2938	0.53	0/3979
1	F	0.29	0/2959	0.51	0/4005
1	G	0.30	0/2964	0.55	2/4012 (0.0%)
1	H	0.29	0/2971	0.51	1/4021 (0.0%)
1	I	0.31	0/2877	0.51	0/3896
2	J	0.31	0/932	0.55	0/1261
2	K	0.28	0/955	0.53	1/1292 (0.1%)
2	L	0.29	0/951	0.50	0/1287
2	M	0.27	0/955	0.50	0/1292
2	N	0.30	0/953	0.55	0/1289
2	O	0.29	0/959	0.50	0/1298
2	P	0.29	0/941	0.51	0/1273
2	Q	0.29	0/951	0.52	0/1287
2	R	0.29	0/955	0.52	1/1292 (0.1%)
3	S	0.29	0/994	0.48	0/1355
All	All	0.31	1/36033 (0.0%)	0.53	7/48786 (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
1	C	0	2
1	D	0	3
1	E	0	1
1	F	0	1
1	G	0	3
1	H	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	5
2	J	0	1
2	L	0	1
2	Q	0	1
3	S	0	1
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	SER	CA-CB	-8.18	1.40	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	229	PRO	N-CA-CB	-9.93	91.39	103.30
1	G	229	PRO	N-CD-CG	-6.16	93.96	103.20
1	D	10	PHE	CB-CA-C	6.06	122.52	110.40
2	K	105	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	11	PHE	C-N-CA	-5.49	107.98	121.70
1	H	361	ASP	CB-CG-OD2	5.11	122.90	118.30
2	R	17	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	51	ASP	Mainchain
1	C	69	THR	Mainchain
1	D	337	ARG	Sidechain
1	D	65	ARG	Sidechain
1	D	76	ARG	Sidechain
1	E	76	ARG	Sidechain
1	F	337	ARG	Sidechain
1	G	207	ARG	Sidechain
1	G	337	ARG	Sidechain
1	G	9	ARG	Sidechain
1	H	62	ARG	Sidechain
1	H	76	ARG	Sidechain
1	I	253	ARG	Sidechain
1	I	337	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	62	ARG	Sidechain
1	I	65	ARG	Sidechain
1	I	76	ARG	Sidechain
2	J	12	ARG	Sidechain
2	L	12	ARG	Sidechain
2	Q	12	ARG	Sidechain
3	S	109	LYS	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	A	2906	0	2849	62	0
1	B	2890	0	2822	67	0
1	C	2895	0	2837	59	0
1	D	2845	0	2740	77	0
1	E	2877	0	2799	79	0
1	F	2898	0	2834	77	0
1	G	2903	0	2838	68	0
1	H	2910	0	2851	50	0
1	I	2817	0	2734	40	0
2	J	917	0	909	14	0
2	K	939	0	938	14	0
2	L	935	0	932	11	0
2	M	939	0	938	13	0
2	N	937	0	933	26	0
2	O	943	0	945	7	0
2	P	926	0	917	10	0
2	Q	935	0	934	19	0
2	R	939	0	938	16	0
3	S	965	0	916	16	0
All	All	35316	0	34604	618	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 9.

All (618) 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:G:337:ARG:NH2	2:Q:26:PRO:HD3	1.00	1.31
1:G:337:ARG:NH2	2:Q:26:PRO:CD	1.93	1.30
1:G:337:ARG:HH22	2:Q:26:PRO:CD	1.51	1.22
1:I:337:ARG:NH2	2:L:26:PRO:HD3	1.68	1.09
1:G:337:ARG:HH21	2:Q:26:PRO:HD3	1.29	0.92
1:I:337:ARG:HH22	2:L:26:PRO:HD3	1.30	0.90
1:E:40:GLN:HE22	1:E:45:PHE:HB3	1.38	0.89
1:D:243:GLY:HA2	1:D:249:ALA:O	1.74	0.88
1:E:53:ASP:HA	1:F:23:PRO:HG3	1.58	0.85
1:C:52:TRP:HB3	1:C:73:GLU:HG3	1.61	0.82
1:H:74:ARG:HH12	1:H:76:ARG:NH2	1.78	0.81
1:B:51:ASP:HB3	1:C:21:SER:HB3	1.64	0.79
1:B:307:ILE:HD12	1:B:353:CYS:SG	2.25	0.77
1:I:337:ARG:NH2	2:L:26:PRO:CD	2.48	0.76
1:D:36:ARG:NH1	1:D:309:GLU:OE2	2.18	0.76
1:I:190:ALA:HB2	1:I:358:LEU:HD21	1.68	0.75
1:C:181:ASP:OD1	1:D:207:ARG:NH2	2.20	0.74
1:D:187:GLU:HA	1:D:196:ILE:HD11	1.70	0.74
1:E:240:ARG:HG3	1:E:252:ASN:HB3	1.68	0.74
1:D:92:THR:HG22	1:D:94:ASP:H	1.53	0.73
1:H:200:GLU:HG2	1:H:299:ALA:HB3	1.69	0.73
1:C:52:TRP:O	1:C:54:ILE:N	2.22	0.72
1:H:92:THR:HG22	1:H:94:ASP:H	1.55	0.72
1:H:144:ASP:OD1	1:H:145:ALA:N	2.23	0.72
1:G:337:ARG:HH21	2:Q:26:PRO:CD	1.90	0.72
1:D:67:ALA:HB1	1:E:88:VAL:HG12	1.72	0.72
1:A:184:MET:SD	1:B:207:ARG:NH1	2.64	0.71
1:B:206:ASP:OD1	1:B:207:ARG:N	2.24	0.70
1:E:355:ARG:NH2	1:F:20:GLN:O	2.24	0.70
1:C:53:ASP:HA	1:D:23:PRO:HG3	1.72	0.70
1:C:62:ARG:CD	1:D:316:PRO:HG3	2.23	0.69
1:A:139:LYS:NZ	1:A:278:LEU:O	2.23	0.69
1:A:183:ARG:HD2	1:A:199:GLU:HG2	1.73	0.69
2:M:34:TYR:HB2	2:M:85:VAL:HG13	1.75	0.69
1:A:159:VAL:HG11	1:A:357:GLN:HB3	1.73	0.68
1:I:290:GLY:H	1:I:364:SER:HB3	1.58	0.68
2:O:100:LEU:HD11	2:O:109:VAL:HG21	1.74	0.68
1:A:158:ASP:OD2	2:M:8:LYS:NZ	2.27	0.67
1:A:84:TYR:OH	1:A:346:HIS:ND1	2.25	0.67
1:A:111:GLU:OE2	1:A:115:ARG:NH1	2.27	0.67
1:G:334:GLU:N	1:G:334:GLU:OE2	2.27	0.67
1:H:74:ARG:NH1	1:H:76:ARG:NH2	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:ASP:OD1	1:E:207:ARG:NH1	2.28	0.66
1:G:67:ALA:HB2	1:H:86:LYS:HE3	1.76	0.66
1:A:94:ASP:OD2	2:J:16:ASN:ND2	2.28	0.66
1:G:156:GLN:HG2	2:N:6:PHE:HB2	1.78	0.66
1:E:183:ARG:HD3	1:E:199:GLU:HG3	1.78	0.66
1:D:74:ARG:NH1	1:D:76:ARG:NH2	2.45	0.65
1:D:74:ARG:HH11	1:D:76:ARG:HD3	1.60	0.65
1:E:60:VAL:HA	1:F:85:PHE:HB3	1.79	0.65
1:I:153:LEU:HD21	1:I:353:CYS:H	1.61	0.65
1:B:152:ASP:O	1:B:154:TYR:N	2.28	0.64
1:A:355:ARG:NH2	1:B:20:GLN:O	2.30	0.64
2:L:49:LYS:NZ	2:L:53:SER:OG	2.31	0.64
1:B:55:SER:O	1:B:56:LEU:HD22	1.98	0.64
1:H:79:SER:O	1:H:156:GLN:NE2	2.31	0.64
1:A:20:GLN:O	1:F:355:ARG:NH2	2.31	0.63
1:G:229:PRO:O	1:G:231:ALA:N	2.31	0.63
1:H:317:LYS:HE3	1:H:346:HIS:HE1	1.63	0.63
1:G:60:VAL:HG22	1:H:85:PHE:HA	1.79	0.63
1:A:187:GLU:OE2	1:B:240:ARG:NH1	2.32	0.63
1:G:51:ASP:HB3	1:H:21:SER:HB2	1.81	0.63
1:C:317:LYS:HE2	1:C:346:HIS:HE1	1.64	0.62
1:C:9:ARG:O	1:H:100:ARG:NH1	2.31	0.62
1:E:104:THR:HG21	1:E:107:GLU:HB2	1.80	0.62
1:C:88:VAL:HG12	1:C:344:GLU:HG2	1.81	0.62
2:K:60:GLU:OE1	2:K:60:GLU:N	2.28	0.61
2:R:30:SER:HA	2:R:90:ARG:HB2	1.81	0.61
1:E:287:THR:O	1:E:289:VAL:HG12	1.99	0.61
1:G:4:ASN:HD22	1:G:11:PHE:HB2	1.65	0.61
1:F:78:ILE:HD12	1:F:156:GLN:HG3	1.83	0.61
2:J:22:GLU:OE2	2:J:31:ARG:NH1	2.33	0.61
1:E:183:ARG:NH1	1:E:199:GLU:OE1	2.34	0.61
1:G:225:ALA:O	1:G:227:GLN:N	2.33	0.61
1:A:339:GLU:HG3	2:J:24:ILE:HD12	1.81	0.61
1:E:40:GLN:NE2	1:E:45:PHE:HB3	2.12	0.61
2:M:34:TYR:OH	2:M:64:ASP:OD1	2.11	0.61
2:N:70:ASN:HB2	2:N:79:TYR:HB2	1.83	0.60
2:M:30:SER:HA	2:M:90:ARG:HB2	1.83	0.60
1:A:243:GLY:HA3	1:A:250:HIS:HA	1.82	0.60
1:A:243:GLY:HA2	1:A:251:MET:HG3	1.84	0.60
1:B:322:ASN:ND2	1:H:96:ILE:O	2.33	0.60
1:B:84:TYR:OH	1:B:346:HIS:ND1	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:GLU:HB2	1:F:300:MET:HB2	1.84	0.59
1:G:355:ARG:NH2	1:H:20:GLN:O	2.34	0.59
1:E:54:ILE:O	1:F:121:LYS:NZ	2.34	0.59
1:G:81:PRO:HG3	2:N:2:ALA:HA	1.83	0.59
1:A:86:LYS:HD3	1:F:67:ALA:HB2	1.84	0.59
1:F:282:ASP:OD2	1:F:282:ASP:N	2.35	0.59
1:G:4:ASN:OD1	1:G:5:SER:N	2.31	0.59
1:G:48:ASP:OD2	1:H:100:ARG:NH2	2.36	0.59
1:A:236:THR:OG1	1:F:226:GLN:NE2	2.34	0.59
1:C:64:SER:O	1:C:66:LYS:N	2.36	0.59
1:B:7:LYS:HZ1	2:K:75:LEU:HB2	1.68	0.58
1:E:306:ASN:O	1:E:308:PHE:N	2.36	0.58
2:M:96:ASP:OD1	2:M:110:LYS:NZ	2.36	0.58
2:P:18:ILE:HD11	2:P:68:ILE:HG22	1.85	0.58
2:R:95:LYS:HB3	2:R:97:LEU:HD12	1.86	0.58
1:A:313:ALA:HB3	1:A:348:TYR:HD2	1.68	0.58
1:G:5:SER:C	1:G:7:LYS:H	2.07	0.58
1:B:181:ASP:OD1	1:C:207:ARG:NH2	2.37	0.58
1:I:87:GLU:HB3	1:I:345:ALA:HB3	1.84	0.58
1:I:111:GLU:OE2	1:I:115:ARG:NH2	2.36	0.58
1:E:144:ASP:OD1	1:E:145:ALA:N	2.36	0.58
2:Q:41:GLU:OE1	2:Q:43:ARG:NH1	2.35	0.57
1:E:4:ASN:O	1:E:13:ALA:N	2.30	0.57
1:G:289:VAL:HG12	1:G:365:ASP:HB3	1.87	0.57
1:F:84:TYR:OH	1:F:346:HIS:ND1	2.32	0.57
1:H:252:ASN:ND2	1:H:263:GLN:OE1	2.33	0.57
2:K:48:LEU:HD11	2:K:67:CYS:HB2	1.85	0.57
2:N:34:TYR:HB2	2:N:85:VAL:HG13	1.86	0.57
1:B:159:VAL:HG21	1:B:356:PRO:HG2	1.86	0.57
1:C:96:ILE:O	1:G:322:ASN:ND2	2.37	0.57
1:E:187:GLU:OE2	1:F:240:ARG:NH1	2.37	0.57
1:G:123:ARG:HG3	1:G:123:ARG:HH11	1.69	0.57
1:G:185:HIS:CE1	1:G:189:GLU:HG3	2.40	0.57
1:B:329:TYR:HB2	1:B:346:HIS:HB2	1.86	0.56
1:C:253:ARG:NH2	1:C:255:TYR:OH	2.39	0.56
1:D:199:GLU:OE1	1:E:238:SER:OG	2.20	0.56
1:B:51:ASP:N	1:B:51:ASP:OD1	2.38	0.56
1:E:225:ALA:O	1:F:227:GLN:NE2	2.32	0.56
2:R:14:PRO:HG3	2:R:99:LYS:HE2	1.87	0.56
1:D:238:SER:O	1:D:240:ARG:N	2.38	0.56
1:G:144:ASP:OD1	1:G:145:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:SER:OG	1:C:6:GLU:N	2.39	0.56
1:D:200:GLU:O	1:D:200:GLU:HG3	2.06	0.56
1:A:320:TYR:O	1:A:323:THR:OG1	2.23	0.56
1:F:154:TYR:CZ	1:F:161:LYS:HD3	2.41	0.56
2:K:64:ASP:O	2:K:116:LYS:NZ	2.39	0.56
1:A:313:ALA:HB3	1:A:348:TYR:CD2	2.41	0.56
1:H:40:GLN:HE22	1:H:45:PHE:HB3	1.70	0.56
1:C:70:SER:HB2	1:D:121:LYS:HE2	1.87	0.55
2:Q:51:ASP:OD1	2:Q:52:GLY:N	2.39	0.55
2:K:7:THR:O	2:K:7:THR:HG22	2.06	0.55
1:B:135:MET:HG2	1:B:278:LEU:HB3	1.89	0.55
1:E:193:GLY:HA3	1:F:22:ILE:HD12	1.88	0.55
1:E:287:THR:O	1:E:289:VAL:N	2.39	0.55
1:H:301:LEU:HD13	1:H:307:ILE:HD11	1.89	0.55
1:A:14:ASP:O	1:F:46:LEU:N	2.35	0.55
1:E:240:ARG:HA	1:E:252:ASN:HA	1.88	0.55
1:G:286:ASP:HB3	1:G:289:VAL:HG22	1.88	0.55
1:G:329:TYR:HB2	1:G:346:HIS:HB2	1.88	0.55
1:B:83:MET:HE2	1:B:150:TYR:CD1	2.42	0.55
1:E:166:PHE:HB3	1:E:168:LEU:HD13	1.88	0.55
1:G:135:MET:HG2	1:G:278:LEU:HB3	1.89	0.55
1:E:155:LYS:O	1:E:157:PHE:N	2.40	0.55
1:G:230:LEU:O	1:G:234:GLN:HG3	2.06	0.55
1:G:94:ASP:HB3	2:Q:16:ASN:HB3	1.89	0.54
2:R:74:ASP:OD1	2:R:75:LEU:N	2.40	0.54
1:C:336:ASP:HB2	2:R:24:ILE:HD11	1.89	0.54
1:D:334:GLU:HG2	1:D:341:ILE:HG22	1.90	0.54
1:F:90:SER:HA	1:F:342:ASP:HA	1.89	0.54
1:F:363:ARG:NH2	1:F:365:ASP:OD2	2.30	0.54
1:I:162:LYS:HB3	1:I:360:VAL:HG12	1.89	0.54
1:H:253:ARG:NH2	1:H:255:TYR:OH	2.41	0.54
1:I:57:LEU:HD23	1:I:57:LEU:H	1.71	0.54
1:F:115:ARG:NH2	1:F:332:GLU:OE2	2.39	0.54
1:F:183:ARG:NH1	1:F:199:GLU:OE2	2.40	0.54
1:G:164:ILE:HD12	1:G:360:VAL:HG11	1.88	0.54
1:D:49:LEU:HD13	1:D:76:ARG:NH1	2.23	0.54
1:F:229:PRO:C	1:F:231:ALA:H	2.12	0.54
2:N:32:LYS:HD3	2:N:34:TYR:CZ	2.43	0.54
1:B:83:MET:CE	1:B:150:TYR:CD1	2.91	0.54
1:E:119:LEU:O	1:E:123:ARG:HG3	2.08	0.54
1:F:227:GLN:C	1:F:229:PRO:HD3	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:HG12	1:A:344:GLU:HG2	1.89	0.53
1:G:339:GLU:HG3	2:Q:24:ILE:HD12	1.90	0.53
1:G:183:ARG:NH1	1:G:199:GLU:OE1	2.41	0.53
3:S:30:ARG:HD3	3:S:85:MET:HG3	1.89	0.53
1:B:150:TYR:CZ	2:N:83:LEU:HD11	2.42	0.53
1:C:119:LEU:O	1:C:123:ARG:NH1	2.42	0.53
2:O:22:GLU:OE1	2:O:31:ARG:NH1	2.41	0.53
1:B:245:ASP:HB3	1:B:251:MET:SD	2.49	0.53
3:S:38:PRO:O	3:S:108:VAL:HG21	2.09	0.53
1:B:2:LEU:N	1:B:13:ALA:O	2.42	0.53
1:F:332:GLU:HG3	1:F:341:ILE:HD11	1.91	0.53
2:N:75:LEU:HD12	2:R:7:THR:HG21	1.90	0.53
1:B:150:TYR:CE2	2:N:83:LEU:HD11	2.44	0.53
1:C:57:LEU:HB2	1:D:129:THR:HG23	1.90	0.53
1:D:187:GLU:OE2	1:E:240:ARG:NH1	2.40	0.53
1:E:192:THR:HG21	1:E:301:LEU:HD23	1.90	0.53
1:F:190:ALA:HB2	1:F:358:LEU:HD21	1.91	0.53
1:G:175:ILE:HG21	1:G:219:ILE:HD11	1.90	0.53
1:C:253:ARG:HG2	1:C:262:VAL:HG22	1.91	0.53
1:D:49:LEU:CD1	1:D:76:ARG:NH1	2.72	0.53
1:F:69:THR:HG21	2:J:95:LYS:HG2	1.91	0.53
1:F:143:ILE:HG22	1:F:149:LEU:HA	1.90	0.53
1:I:245:ASP:OD1	1:I:246:GLY:N	2.41	0.53
1:I:245:ASP:HB2	1:I:251:MET:SD	2.49	0.52
1:A:51:ASP:HB3	1:B:21:SER:HB2	1.90	0.52
2:J:30:SER:HA	2:J:90:ARG:HB2	1.91	0.52
1:D:239:LEU:O	1:D:240:ARG:C	2.48	0.52
1:G:227:GLN:O	1:G:228:THR:C	2.47	0.52
1:D:4:ASN:OD1	1:D:5:SER:N	2.41	0.52
1:D:239:LEU:CB	1:D:253:ARG:HB2	2.39	0.52
1:G:229:PRO:O	1:G:232:TRP:N	2.41	0.52
1:E:52:TRP:O	1:E:53:ASP:C	2.48	0.52
2:P:27:THR:HG22	2:P:27:THR:O	2.10	0.52
1:D:205:VAL:HG12	1:D:292:GLY:HA3	1.90	0.52
1:H:174:ASP:OD1	1:H:174:ASP:N	2.42	0.52
1:I:189:GLU:HB3	1:I:357:GLN:HG3	1.91	0.52
2:K:119:ASP:OD2	2:L:90:ARG:NH2	2.42	0.52
2:Q:95:LYS:HB3	2:Q:123:THR:HG21	1.92	0.52
1:C:70:SER:CB	1:D:121:LYS:HE2	2.41	0.51
1:D:237:GLY:C	1:D:239:LEU:H	2.13	0.51
1:E:4:ASN:N	1:E:4:ASN:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ILE:HD11	1:E:125:LYS:HB2	1.91	0.51
1:F:307:ILE:HG13	1:F:355:ARG:HB2	1.92	0.51
1:D:245:ASP:O	1:D:247:VAL:N	2.43	0.51
2:M:60:GLU:OE1	2:M:60:GLU:N	2.42	0.51
1:B:2:LEU:HD23	1:B:14:ASP:HA	1.92	0.51
2:N:101:GLU:HA	2:N:101:GLU:OE2	2.10	0.51
2:Q:93:GLU:OE2	2:R:27:THR:OG1	2.27	0.51
1:E:253:ARG:NH2	1:E:255:TYR:OH	2.44	0.51
1:C:230:LEU:O	1:C:234:GLN:HG2	2.10	0.51
1:D:67:ALA:HB1	1:E:86:LYS:O	2.11	0.51
1:D:365:ASP:OD1	1:D:365:ASP:N	2.43	0.51
2:N:32:LYS:HB3	2:N:89:TYR:CD1	2.45	0.51
1:I:140:GLY:HA3	1:I:154:TYR:CE2	2.46	0.51
1:B:192:THR:HG23	1:B:194:THR:H	1.74	0.51
1:A:49:LEU:HD11	1:A:78:ILE:HD13	1.93	0.50
1:B:48:ASP:OD2	1:C:103:GLY:N	2.44	0.50
1:H:50:THR:HG22	1:H:75:VAL:HG13	1.91	0.50
1:B:41:THR:HG22	1:B:324:LEU:HD22	1.93	0.50
1:D:2:LEU:O	1:D:12:LEU:HB2	2.12	0.50
2:P:106:ALA:O	2:P:110:LYS:HG2	2.11	0.50
1:A:180:GLU:OE1	1:B:240:ARG:NH2	2.42	0.50
1:A:326:GLN:HB2	1:A:329:TYR:CZ	2.46	0.50
1:B:83:MET:HE2	1:B:150:TYR:CG	2.46	0.50
1:C:249:ALA:O	1:C:250:HIS:ND1	2.44	0.50
1:H:162:LYS:HB3	1:H:360:VAL:HG22	1.94	0.50
1:I:144:ASP:OD1	1:I:145:ALA:N	2.44	0.50
2:P:83:LEU:H	2:P:83:LEU:HD23	1.76	0.50
1:E:164:ILE:HD13	1:E:182:LEU:HB2	1.93	0.50
2:L:41:GLU:OE2	2:L:43:ARG:NH2	2.42	0.50
1:D:123:ARG:HG2	1:D:123:ARG:HH11	1.75	0.50
1:E:3:THR:HG22	1:E:12:LEU:HB3	1.94	0.50
1:E:281:ILE:HD11	1:E:361:ASP:HB3	1.93	0.50
1:F:2:LEU:HB3	1:F:14:ASP:HA	1.94	0.50
1:G:162:LYS:HB3	1:G:360:VAL:HG22	1.93	0.50
1:G:164:ILE:HD13	1:G:182:LEU:HB2	1.92	0.50
2:Q:65:SER:HB3	2:Q:89:TYR:HB3	1.94	0.50
1:D:86:LYS:HD2	1:D:346:HIS:CE1	2.47	0.50
1:C:187:GLU:HA	1:C:196:ILE:HG21	1.94	0.50
1:E:287:THR:OG1	1:E:288:ASN:N	2.45	0.50
1:G:337:ARG:NH2	2:Q:26:PRO:CG	2.68	0.50
1:G:337:ARG:HH22	2:Q:26:PRO:HD3	0.67	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:3:TYR:OH	2:R:6:PHE:HA	2.12	0.50
1:B:24:ASN:HB3	1:B:247:VAL:HG11	1.94	0.49
1:A:124:THR:O	1:A:128:ILE:HG23	2.12	0.49
1:E:221:ASP:OD1	3:S:77:GLN:NE2	2.44	0.49
1:H:200:GLU:HB3	1:H:297:ASN:HB3	1.94	0.49
2:P:22:GLU:OE1	2:P:31:ARG:NH1	2.45	0.49
1:B:92:THR:O	1:B:95:GLU:HG2	2.11	0.49
1:D:7:LYS:CB	1:D:10:PHE:HB2	2.42	0.49
1:D:82:MET:HB3	1:D:350:LEU:HB2	1.94	0.49
1:B:47:MET:HG3	1:C:17:GLY:HA2	1.95	0.49
1:B:297:ASN:OD1	1:B:298:VAL:N	2.44	0.49
1:C:241:THR:OG1	1:C:242:GLY:N	2.36	0.49
1:C:329:TYR:HB2	1:C:346:HIS:HB2	1.93	0.49
1:D:245:ASP:O	1:D:247:VAL:HG23	2.12	0.49
1:E:60:VAL:HG21	1:F:83:MET:HB2	1.94	0.49
2:K:72:TYR:O	2:K:74:ASP:N	2.45	0.49
1:H:228:THR:HG23	1:H:231:ALA:H	1.78	0.49
3:S:33:GLN:NE2	3:S:110:PRO:HA	2.28	0.49
1:E:227:GLN:HG2	1:F:227:GLN:CG	2.43	0.49
1:E:277:THR:HG23	1:E:280:SER:HB3	1.94	0.49
1:F:337:ARG:O	1:F:338:ASP:C	2.50	0.49
2:L:42:TYR:O	2:L:43:ARG:NH1	2.45	0.49
1:B:6:GLU:HG3	2:K:75:LEU:HD21	1.95	0.49
2:Q:18:ILE:HD11	2:Q:68:ILE:HG22	1.94	0.49
1:B:205:VAL:HG13	1:B:209:PHE:HB3	1.95	0.49
1:E:296:PRO:HB3	1:E:300:MET:SD	2.53	0.49
1:F:229:PRO:HD2	1:F:232:TRP:CE2	2.48	0.49
1:G:5:SER:C	1:G:7:LYS:N	2.65	0.49
2:L:34:TYR:OH	2:L:64:ASP:OD2	2.18	0.49
1:D:24:ASN:HB3	1:D:247:VAL:CG2	2.43	0.48
1:G:94:ASP:OD2	2:Q:16:ASN:ND2	2.43	0.48
1:H:185:HIS:CE1	1:H:189:GLU:HG3	2.47	0.48
1:A:144:ASP:OD2	1:A:145:ALA:N	2.45	0.48
1:G:8:SER:HB2	1:G:10:PHE:H	1.77	0.48
1:H:307:ILE:CG2	1:H:355:ARG:H	2.26	0.48
1:B:252:ASN:HB2	1:B:263:GLN:HB3	1.95	0.48
1:B:339:GLU:HG3	2:M:24:ILE:HD13	1.95	0.48
1:C:200:GLU:HG3	1:C:297:ASN:HD22	1.78	0.48
1:F:135:MET:HG2	1:F:278:LEU:HB3	1.95	0.48
1:I:164:ILE:HB	1:I:362:VAL:HG12	1.94	0.48
2:N:37:VAL:HG23	2:N:38:ALA:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:VAL:HG12	1:B:344:GLU:HG2	1.94	0.48
1:D:69:THR:HA	1:E:88:VAL:O	2.13	0.48
1:F:218:LYS:HD2	3:S:104:TRP:CG	2.48	0.48
1:I:329:TYR:HB2	1:I:346:HIS:HB2	1.96	0.48
1:A:243:GLY:HA2	1:A:251:MET:H	1.79	0.48
1:C:90:SER:O	1:C:118:LYS:NZ	2.47	0.48
1:F:183:ARG:HD3	1:F:199:GLU:HG3	1.95	0.48
1:A:281:ILE:HD11	1:A:361:ASP:OD2	2.13	0.48
1:E:52:TRP:C	1:E:52:TRP:CD1	2.87	0.48
1:E:174:ASP:OD1	1:E:174:ASP:N	2.39	0.48
1:B:6:GLU:OE1	1:B:6:GLU:N	2.46	0.48
1:A:280:SER:HA	1:A:291:VAL:HG21	1.96	0.48
1:C:189:GLU:O	1:C:357:GLN:NE2	2.47	0.48
1:D:238:SER:C	1:D:240:ARG:H	2.17	0.48
1:F:27:GLY:O	1:F:264:TYR:OH	2.31	0.48
1:F:227:GLN:O	1:F:228:THR:C	2.52	0.48
1:I:293:HIS:ND1	1:I:361:ASP:OD1	2.40	0.48
1:A:40:GLN:HE22	1:B:14:ASP:HB2	1.77	0.47
1:A:135:MET:HG2	1:A:278:LEU:HB3	1.96	0.47
1:A:236:THR:OG1	1:A:236:THR:O	2.30	0.47
1:C:312:TYR:CD1	1:C:349:MET:HB3	2.49	0.47
2:P:14:PRO:HG3	2:P:99:LYS:HE3	1.96	0.47
1:D:311:ALA:O	1:D:349:MET:HA	2.15	0.47
1:F:210:PHE:O	1:F:214:ILE:HG12	2.14	0.47
3:S:33:GLN:HG3	3:S:37:LEU:HD12	1.95	0.47
1:B:41:THR:OG1	1:B:42:GLN:OE1	2.33	0.47
1:F:101:GLN:O	1:F:104:THR:OG1	2.31	0.47
1:G:228:THR:CB	1:G:229:PRO:HD3	2.44	0.47
1:B:40:GLN:HE22	1:B:45:PHE:HB3	1.78	0.47
1:I:65:ARG:HA	1:I:65:ARG:HD3	1.37	0.47
1:A:40:GLN:HE22	1:A:45:PHE:HB3	1.79	0.47
1:C:82:MET:HB2	1:C:348:TYR:CE1	2.50	0.47
1:E:79:SER:OG	1:E:80:PHE:N	2.47	0.47
1:E:168:LEU:HB3	1:E:212:LYS:HB3	1.97	0.47
1:E:306:ASN:O	1:E:307:ILE:C	2.53	0.47
1:G:229:PRO:HD2	1:G:230:LEU:H	1.80	0.47
1:H:305:ASN:O	1:H:306:ASN:C	2.52	0.47
1:I:66:LYS:HD2	1:I:66:LYS:HA	1.59	0.47
2:P:20:LEU:HD12	2:P:121:VAL:HG21	1.95	0.47
3:S:101:TYR:HD2	3:S:115:ASN:HB3	1.80	0.47
1:B:161:LYS:NZ	1:B:359:LEU:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:LYS:C	1:E:157:PHE:H	2.18	0.47
1:B:56:LEU:HG	2:R:124:GLY:HA3	1.97	0.47
1:C:61:ASP:HB3	1:C:64:SER:OG	2.15	0.47
1:E:301:LEU:HD13	1:E:307:ILE:HD11	1.97	0.47
1:G:69:THR:OG1	1:G:70:SER:N	2.47	0.47
1:C:161:LYS:NZ	1:C:359:LEU:O	2.48	0.47
1:D:244:THR:C	1:D:246:GLY:H	2.17	0.47
1:F:307:ILE:HG12	1:F:353:CYS:SG	2.55	0.47
1:H:74:ARG:NH1	1:H:76:ARG:HH21	2.13	0.47
2:N:18:ILE:HG23	2:N:94:LEU:HD22	1.97	0.47
1:D:74:ARG:NH1	1:D:76:ARG:HD3	2.26	0.46
1:E:155:LYS:C	1:E:157:PHE:N	2.68	0.46
1:E:166:PHE:HB3	1:E:168:LEU:CD1	2.44	0.46
1:F:205:VAL:HG12	1:F:292:GLY:HA3	1.96	0.46
1:H:85:PHE:HE1	1:H:347:SER:HB3	1.79	0.46
1:H:135:MET:HG2	1:H:278:LEU:HB3	1.96	0.46
2:N:14:PRO:HG2	2:N:44:VAL:HG22	1.96	0.46
3:S:37:LEU:HD23	3:S:45:TRP:CZ3	2.50	0.46
1:E:48:ASP:OD2	1:F:15:LEU:HD11	2.15	0.46
1:C:297:ASN:OD1	1:C:298:VAL:N	2.47	0.46
1:E:101:GLN:O	1:E:104:THR:HG22	2.16	0.46
1:C:62:ARG:CZ	1:D:316:PRO:HB3	2.45	0.46
1:E:245:ASP:OD1	1:E:248:GLN:HG2	2.16	0.46
1:D:290:GLY:N	1:D:364:SER:OG	2.45	0.46
1:B:34:LEU:H	1:B:34:LEU:HD23	1.79	0.46
1:C:189:GLU:HB3	1:C:357:GLN:HG3	1.97	0.46
1:E:307:ILE:H	1:E:307:ILE:HG12	1.48	0.46
2:Q:19:ILE:HD11	2:Q:88:ILE:HG13	1.96	0.46
1:A:241:THR:HG1	1:A:253:ARG:HE	1.58	0.46
1:A:245:ASP:OD1	1:A:246:GLY:N	2.44	0.46
1:D:336:ASP:O	1:D:337:ARG:C	2.54	0.46
1:H:85:PHE:CE1	1:H:347:SER:HB3	2.51	0.46
1:I:25:THR:O	1:I:25:THR:OG1	2.30	0.46
1:I:89:GLU:HG2	1:I:118:LYS:HD2	1.97	0.46
1:I:37:SER:HB2	1:I:312:TYR:HE2	1.81	0.46
1:A:63:THR:O	2:N:31:ARG:NH1	2.49	0.46
1:C:64:SER:O	1:C:65:ARG:C	2.53	0.46
1:D:7:LYS:CB	1:D:11:PHE:HD2	2.29	0.46
2:M:51:ASP:OD2	2:M:51:ASP:N	2.47	0.46
2:N:19:ILE:HD11	2:N:88:ILE:CD1	2.45	0.46
2:O:36:PRO:HG3	2:O:85:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:HE3	1:A:361:ASP:HB2	1.99	0.46
1:C:3:THR:HG23	1:C:4:ASN:H	1.79	0.46
1:A:192:THR:HG21	1:A:301:LEU:HD22	1.98	0.45
1:F:171:PRO:HG2	3:S:101:TYR:CD1	2.51	0.45
1:G:229:PRO:C	1:G:231:ALA:N	2.69	0.45
3:S:87:LEU:O	3:S:91:ILE:HD12	2.15	0.45
1:A:249:ALA:O	1:A:250:HIS:ND1	2.48	0.45
1:B:337:ARG:HB3	1:B:338:ASP:H	1.65	0.45
1:D:24:ASN:HB3	1:D:247:VAL:HG21	1.98	0.45
1:D:175:ILE:HD12	1:D:175:ILE:N	2.31	0.45
1:E:216:HIS:HE1	1:E:218:LYS:HD2	1.81	0.45
3:S:33:GLN:HE22	3:S:110:PRO:HA	1.80	0.45
1:C:41:THR:HG22	1:C:324:LEU:HD22	1.97	0.45
1:I:205:VAL:HG12	1:I:292:GLY:HA3	1.98	0.45
3:S:109:LYS:O	3:S:111:PHE:N	2.49	0.45
1:A:40:GLN:NE2	1:A:45:PHE:HB3	2.30	0.45
1:A:365:ASP:OD1	1:A:365:ASP:N	2.50	0.45
1:C:56:LEU:O	1:C:57:LEU:HB3	2.17	0.45
2:N:68:ILE:HD13	2:N:88:ILE:HG13	1.98	0.45
1:B:8:SER:HB2	1:B:11:PHE:HD2	1.81	0.45
1:C:73:GLU:HG2	1:C:74:ARG:H	1.82	0.45
1:B:48:ASP:OD1	1:B:48:ASP:N	2.47	0.45
1:H:223:TYR:OH	1:H:255:TYR:O	2.24	0.45
2:M:22:GLU:OE1	2:M:31:ARG:NH1	2.50	0.45
1:A:97:GLN:HB2	1:I:321:ALA:HB1	1.98	0.45
1:C:42:GLN:HG3	1:D:13:ALA:HA	1.99	0.45
1:D:85:PHE:CZ	1:D:133:LEU:HD11	2.52	0.45
1:D:221:ASP:OD1	1:D:222:ALA:N	2.50	0.45
1:D:239:LEU:C	1:D:241:THR:N	2.65	0.45
1:E:100:ARG:NH1	1:E:104:THR:O	2.50	0.45
1:F:240:ARG:HD2	1:F:250:HIS:O	2.17	0.45
3:S:39:LEU:O	3:S:40:THR:OG1	2.28	0.45
1:E:363:ARG:NH2	1:E:365:ASP:OD2	2.40	0.45
1:F:185:HIS:NE2	1:F:357:GLN:O	2.40	0.45
1:A:332:GLU:OE2	1:A:332:GLU:HA	2.16	0.44
1:D:329:TYR:HB2	1:D:346:HIS:HB2	1.98	0.44
1:G:30:SER:HB3	1:G:131:GLU:HG2	1.99	0.44
2:J:116:LYS:HB3	2:J:116:LYS:HE3	1.63	0.44
1:A:249:ALA:N	1:F:196:ILE:O	2.50	0.44
1:C:51:ASP:OD1	1:C:74:ARG:NH2	2.49	0.44
1:G:123:ARG:HG3	1:G:123:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:LYS:HD3	1:H:185:HIS:ND1	2.32	0.44
2:J:93:GLU:OE2	2:K:27:THR:OG1	2.21	0.44
2:Q:8:LYS:H	2:Q:8:LYS:HG2	1.62	0.44
1:D:185:HIS:HE1	1:D:357:GLN:O	2.00	0.44
1:E:51:ASP:O	1:E:52:TRP:C	2.56	0.44
1:E:100:ARG:HA	1:E:108:LEU:HA	1.98	0.44
1:G:29:ILE:HG13	1:G:135:MET:SD	2.57	0.44
1:H:24:ASN:HB2	1:H:247:VAL:HG22	1.99	0.44
1:H:307:ILE:HG22	1:H:353:CYS:SG	2.58	0.44
1:I:58:ASP:OD1	1:I:58:ASP:N	2.51	0.44
1:C:286:ASP:C	1:C:288:ASN:H	2.21	0.44
1:F:88:VAL:HG12	1:F:344:GLU:HG2	1.99	0.44
1:F:307:ILE:HG12	1:F:307:ILE:O	2.18	0.44
1:C:286:ASP:O	1:C:288:ASN:N	2.41	0.44
1:E:48:ASP:HB2	1:F:18:GLU:HB2	2.00	0.44
1:F:229:PRO:O	1:F:230:LEU:HB2	2.18	0.44
1:H:313:ALA:HB3	1:H:348:TYR:CD2	2.52	0.44
1:B:183:ARG:O	1:B:187:GLU:HG3	2.18	0.44
1:C:140:GLY:HA3	1:C:154:TYR:HE2	1.83	0.44
1:F:63:THR:HG22	2:K:86:VAL:HG11	1.99	0.44
1:G:229:PRO:C	1:G:231:ALA:H	2.20	0.44
2:N:14:PRO:HG3	2:N:99:LYS:HZ1	1.83	0.44
1:B:210:PHE:O	1:B:214:ILE:HG23	2.18	0.44
1:B:230:LEU:O	1:B:234:GLN:HG2	2.17	0.44
1:F:69:THR:O	2:J:124:GLY:N	2.37	0.44
1:F:337:ARG:O	1:F:339:GLU:N	2.51	0.44
2:J:71:PHE:HA	2:J:78:SER:HA	2.00	0.44
2:O:32:LYS:HB2	2:O:89:TYR:CD1	2.52	0.44
1:H:130:ARG:NH1	1:H:312:TYR:OH	2.50	0.43
2:K:3:TYR:CE1	2:M:76:GLN:HG3	2.53	0.43
2:K:93:GLU:HG2	2:K:119:ASP:HB2	2.00	0.43
2:P:44:VAL:HG23	2:P:70:ASN:OD1	2.17	0.43
1:C:86:LYS:HD2	1:C:346:HIS:NE2	2.33	0.43
1:G:191:LYS:HB2	1:G:191:LYS:HE3	1.70	0.43
1:G:296:PRO:HB3	1:G:300:MET:SD	2.58	0.43
1:B:85:PHE:CZ	1:B:133:LEU:HD11	2.54	0.43
1:E:197:ASN:HA	1:F:249:ALA:HB3	2.00	0.43
1:I:294:ALA:HB3	1:I:360:VAL:HG23	2.01	0.43
2:L:39:SER:O	2:L:39:SER:OG	2.33	0.43
1:A:86:LYS:NZ	2:K:26:PRO:O	2.50	0.43
1:B:216:HIS:CD2	1:B:217:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:THR:HG23	1:D:194:THR:H	1.82	0.43
1:D:309:GLU:HB2	1:D:352:TYR:CZ	2.53	0.43
1:F:35:PHE:HB3	1:F:310:VAL:HG23	2.00	0.43
1:A:36:ARG:CZ	1:A:306:ASN:HD22	2.31	0.43
1:C:81:PRO:O	1:C:350:LEU:HD13	2.18	0.43
1:C:269:LYS:HE2	1:C:269:LYS:HB3	1.83	0.43
1:D:12:LEU:HD23	1:D:12:LEU:H	1.84	0.43
1:G:5:SER:HB2	1:G:6:GLU:H	1.52	0.43
1:G:181:ASP:OD1	1:G:182:LEU:N	2.51	0.43
1:E:271:LYS:HB3	1:E:271:LYS:HE2	1.86	0.43
1:E:307:ILE:HG22	1:E:353:CYS:SG	2.59	0.43
1:A:52:TRP:HB3	1:A:73:GLU:HG2	2.01	0.43
1:F:79:SER:HB3	2:J:7:THR:OG1	2.19	0.43
1:F:126:PHE:HA	1:F:129:THR:HG22	2.01	0.43
1:C:123:ARG:HG3	1:C:124:THR:HG23	2.01	0.43
1:I:274:LYS:HE3	1:I:276:HIS:NE2	2.34	0.43
2:L:18:ILE:HD11	2:L:68:ILE:HG22	2.01	0.43
1:A:164:ILE:HD13	1:A:182:LEU:HB2	2.00	0.43
1:B:40:GLN:NE2	1:B:45:PHE:HB3	2.33	0.43
1:F:56:LEU:HD12	1:F:56:LEU:HA	1.92	0.43
2:N:42:TYR:HB2	2:N:71:PHE:HB3	2.00	0.43
1:A:240:ARG:NH2	1:A:248:GLN:OE1	2.51	0.42
1:B:153:LEU:HD13	1:B:353:CYS:H	1.84	0.42
1:D:242:GLY:C	1:D:244:THR:H	2.21	0.42
1:F:140:GLY:HA3	1:F:154:TYR:CE2	2.54	0.42
1:I:99:VAL:O	1:I:109:THR:HG22	2.19	0.42
2:P:84:LYS:HD3	2:P:84:LYS:HA	1.80	0.42
1:A:6:GLU:CD	1:A:6:GLU:H	2.16	0.42
1:E:337:ARG:O	1:E:338:ASP:C	2.56	0.42
1:H:201:ILE:HD13	1:H:201:ILE:HA	1.84	0.42
2:N:16:ASN:ND2	2:N:16:ASN:O	2.52	0.42
1:C:239:LEU:HD23	1:C:239:LEU:HA	1.83	0.42
1:D:139:LYS:O	1:D:161:LYS:NZ	2.52	0.42
1:F:128:ILE:HG13	1:F:129:THR:N	2.33	0.42
1:H:155:LYS:HZ2	1:H:155:LYS:HG3	1.75	0.42
1:I:64:SER:O	1:I:65:ARG:HB2	2.19	0.42
2:M:18:ILE:HG22	2:M:97:LEU:HD12	2.02	0.42
2:N:42:TYR:O	2:N:43:ARG:HD3	2.19	0.42
2:R:110:LYS:HD3	2:R:120:PHE:CD2	2.54	0.42
1:B:224:LEU:HD12	1:B:224:LEU:HA	1.79	0.42
2:O:16:ASN:HB2	2:O:79:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:22:GLU:HG3	2:R:24:ILE:HG22	2.01	0.42
1:B:81:PRO:O	1:B:350:LEU:HD13	2.19	0.42
1:F:77:GLN:HB3	2:J:9:LEU:HB2	2.01	0.42
1:D:48:ASP:HB2	1:E:18:GLU:HB2	2.02	0.42
1:D:242:GLY:HA3	1:D:251:MET:HB2	2.01	0.42
1:G:229:PRO:CD	1:G:230:LEU:H	2.32	0.42
1:H:270:ASP:OD2	1:H:272:ARG:NH2	2.47	0.42
2:J:6:PHE:CG	2:J:6:PHE:O	2.73	0.42
2:N:83:LEU:HD22	2:R:3:TYR:CD2	2.53	0.42
2:P:34:TYR:N	2:P:85:VAL:O	2.39	0.42
1:A:240:ARG:O	1:A:250:HIS:HB3	2.19	0.42
1:D:89:GLU:HB3	1:D:343:PHE:HB2	2.01	0.42
2:N:30:SER:HB2	2:N:88:ILE:HG23	2.01	0.42
3:S:95:LYS:HE3	3:S:95:LYS:HB3	1.68	0.42
1:C:183:ARG:HE	1:C:199:GLU:HG3	1.85	0.42
1:G:46:LEU:N	1:H:14:ASP:O	2.48	0.42
1:G:88:VAL:HG12	1:G:344:GLU:HG2	2.02	0.42
1:G:200:GLU:HB2	1:G:300:MET:HB3	2.02	0.42
1:G:229:PRO:HD2	1:G:230:LEU:N	2.34	0.42
1:H:154:TYR:CZ	1:H:161:LYS:HG3	2.54	0.42
1:I:41:THR:O	1:I:42:GLN:NE2	2.53	0.42
1:I:281:ILE:HD11	1:I:361:ASP:HB3	2.01	0.42
1:E:40:GLN:NE2	1:F:14:ASP:OD1	2.53	0.42
1:F:317:LYS:HD3	1:F:317:LYS:HA	1.93	0.42
2:K:54:LYS:H	2:K:54:LYS:HG2	1.71	0.42
1:A:50:THR:HA	1:A:74:ARG:O	2.20	0.41
1:A:281:ILE:HB	1:A:284:VAL:HG22	2.01	0.41
1:B:54:ILE:HA	1:C:23:PRO:HB3	2.02	0.41
1:E:252:ASN:ND2	1:E:263:GLN:OE1	2.46	0.41
1:G:9:ARG:H	1:G:9:ARG:HG2	1.34	0.41
1:H:88:VAL:HG12	1:H:344:GLU:HG2	2.02	0.41
1:I:47:MET:HE1	1:I:354:THR:HG23	2.01	0.41
2:M:15:LEU:HD23	2:M:15:LEU:HA	1.84	0.41
1:B:305:ASN:O	1:B:306:ASN:C	2.58	0.41
1:D:7:LYS:CB	1:D:11:PHE:H	2.33	0.41
2:N:24:ILE:O	2:N:24:ILE:HG22	2.20	0.41
2:O:60:GLU:OE2	2:O:60:GLU:N	2.52	0.41
1:A:6:GLU:O	1:A:7:LYS:HB2	2.20	0.41
1:A:218:LYS:HA	1:A:218:LYS:HD2	1.94	0.41
1:B:296:PRO:HG2	1:B:307:ILE:HD11	2.01	0.41
1:C:185:HIS:HE1	1:C:357:GLN:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:LEU:HD21	1:E:152:ASP:HB2	2.02	0.41
1:E:332:GLU:HG3	1:E:343:PHE:CE1	2.55	0.41
1:F:14:ASP:OD1	1:F:14:ASP:N	2.52	0.41
1:H:40:GLN:NE2	1:H:45:PHE:HB3	2.34	0.41
1:I:2:LEU:HD12	1:I:2:LEU:HA	1.92	0.41
1:I:312:TYR:CD1	1:I:349:MET:HB3	2.54	0.41
1:C:270:ASP:OD1	1:C:271:LYS:N	2.52	0.41
1:C:367:GLU:HA	1:C:367:GLU:OE1	2.20	0.41
1:E:186:MET:SD	1:E:201:ILE:HG21	2.61	0.41
1:G:86:LYS:HG3	1:G:346:HIS:CD2	2.56	0.41
1:I:296:PRO:HG3	1:I:358:LEU:HD13	2.02	0.41
1:A:253:ARG:HA	1:A:261:PHE:O	2.21	0.41
1:D:6:GLU:O	1:D:7:LYS:C	2.58	0.41
1:E:287:THR:C	1:E:289:VAL:H	2.24	0.41
1:F:226:GLN:HG2	1:F:229:PRO:HB3	2.02	0.41
1:G:24:ASN:HB3	1:G:247:VAL:HG21	2.02	0.41
1:H:197:ASN:ND2	1:H:200:GLU:OE1	2.54	0.41
1:A:174:ASP:HB3	1:A:177:ALA:HB3	2.03	0.41
1:A:222:ALA:HB2	1:B:220:ARG:NH2	2.36	0.41
1:C:174:ASP:OD1	1:C:174:ASP:N	2.53	0.41
1:D:57:LEU:HB2	1:E:129:THR:HG21	2.03	0.41
1:F:186:MET:HG3	1:F:201:ILE:HG21	2.03	0.41
1:F:245:ASP:OD1	1:F:248:GLN:HB3	2.20	0.41
1:G:49:LEU:HD13	1:G:76:ARG:NH2	2.36	0.41
1:G:92:THR:O	1:G:95:GLU:HG2	2.20	0.41
2:O:105:ASP:OD1	2:O:108:ALA:N	2.47	0.41
1:A:99:VAL:HG21	2:J:15:LEU:HD11	2.02	0.41
1:B:149:LEU:HD21	1:B:152:ASP:HB2	2.02	0.41
1:F:164:ILE:HD12	1:F:360:VAL:HG21	2.03	0.41
1:B:224:LEU:HD13	1:B:235:ILE:HG21	2.02	0.41
1:D:139:LYS:NZ	1:D:280:SER:O	2.42	0.41
1:D:231:ALA:C	1:D:233:GLN:H	2.24	0.41
1:F:329:TYR:HB2	1:F:346:HIS:HB2	2.02	0.41
1:G:202:HIS:HB3	1:G:295:PHE:CE1	2.56	0.41
2:M:62:GLN:H	2:M:62:GLN:HG2	1.72	0.41
2:Q:18:ILE:HA	2:Q:95:LYS:HG3	2.02	0.41
2:R:17:ASP:C	2:R:17:ASP:OD1	2.59	0.41
1:B:141:LYS:HD2	1:B:143:ILE:HD11	2.03	0.41
1:B:154:TYR:HD2	1:B:159:VAL:HG23	1.86	0.41
1:F:240:ARG:HB3	1:F:250:HIS:HB2	2.03	0.41
1:G:85:PHE:CZ	1:G:133:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:307:ILE:O	1:H:353:CYS:HA	2.20	0.41
2:R:20:LEU:HD23	2:R:20:LEU:HA	1.89	0.41
3:S:33:GLN:HG3	3:S:37:LEU:CD1	2.51	0.41
1:A:7:LYS:HA	1:A:7:LYS:HD2	1.77	0.41
1:C:62:ARG:HD2	1:D:316:PRO:HG3	2.03	0.41
1:D:67:ALA:CB	1:E:88:VAL:HG12	2.48	0.41
1:D:164:ILE:HD13	1:D:182:LEU:HB2	2.02	0.41
1:G:187:GLU:OE1	1:H:240:ARG:NH1	2.37	0.41
1:I:268:PHE:O	1:I:276:HIS:N	2.50	0.41
1:D:3:THR:HG23	1:D:8:SER:O	2.21	0.40
1:D:155:LYS:HE3	1:D:155:LYS:HB2	1.39	0.40
1:D:174:ASP:HA	1:D:218:LYS:HD2	2.02	0.40
1:D:305:ASN:O	1:D:306:ASN:C	2.58	0.40
1:E:7:LYS:HE3	1:E:7:LYS:HB2	1.30	0.40
2:J:51:ASP:OD1	2:J:52:GLY:N	2.54	0.40
2:N:16:ASN:OD1	2:N:68:ILE:HB	2.21	0.40
1:D:244:THR:C	1:D:246:GLY:N	2.74	0.40
1:F:144:ASP:OD1	1:F:145:ALA:N	2.53	0.40
1:H:332:GLU:HG3	1:H:343:PHE:CE2	2.55	0.40
1:I:40:GLN:OE1	1:I:311:ALA:HB1	2.20	0.40
2:N:50:ALA:HA	2:N:64:ASP:OD1	2.21	0.40
1:B:190:ALA:HA	1:B:358:LEU:HD21	2.03	0.40
1:E:77:GLN:OE1	1:F:100:ARG:NH2	2.49	0.40
1:E:119:LEU:HD23	1:E:119:LEU:HA	1.93	0.40
1:F:171:PRO:HG2	3:S:101:TYR:CG	2.57	0.40
1:G:256:TYR:HE1	1:H:236:THR:HG22	1.85	0.40
1:H:271:LYS:HB2	1:H:271:LYS:HE2	1.77	0.40
1:I:327:GLU:OE1	1:I:327:GLU:N	2.45	0.40
1:A:128:ILE:HD11	1:F:55:SER:O	2.21	0.40
1:B:100:ARG:NH1	1:B:104:THR:O	2.51	0.40
1:D:188:ASP:N	1:D:188:ASP:OD1	2.55	0.40
1:F:294:ALA:HB3	1:F:360:VAL:HG13	2.03	0.40
1:H:223:TYR:O	1:H:231:ALA:HB1	2.21	0.40
1:I:54:ILE:HD13	1:I:54:ILE:HA	1.93	0.40
2:R:13:GLU:H	2:R:13:GLU:CD	2.25	0.40
1:D:52:TRP:HZ3	1:D:54:ILE:HD13	1.87	0.40
1:E:187:GLU:CD	1:F:240:ARG:HH12	2.24	0.40
1:E:223:TYR:OH	1:E:255:TYR:O	2.25	0.40
1:F:86:LYS:HD2	1:F:346:HIS:CE1	2.57	0.40
1:G:326:GLN:HG3	1:G:329:TYR:CZ	2.56	0.40
2:L:98:LEU:HD23	2:L:98:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:77:LEU:HD23	2:N:77:LEU:HA	1.86	0.40
2:R:64:ASP:O	2:R:116:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/367 (99%)	352 (97%)	11 (3%)	1 (0%)	37	69
1	B	364/367 (99%)	344 (94%)	19 (5%)	1 (0%)	37	69
1	C	364/367 (99%)	341 (94%)	18 (5%)	5 (1%)	9	40
1	D	364/367 (99%)	329 (90%)	29 (8%)	6 (2%)	8	37
1	E	364/367 (99%)	331 (91%)	27 (7%)	6 (2%)	8	37
1	F	364/367 (99%)	350 (96%)	14 (4%)	0	100	100
1	G	364/367 (99%)	342 (94%)	17 (5%)	5 (1%)	9	40
1	H	364/367 (99%)	350 (96%)	13 (4%)	1 (0%)	37	69
1	I	352/367 (96%)	341 (97%)	9 (3%)	2 (1%)	22	57
2	J	120/125 (96%)	111 (92%)	8 (7%)	1 (1%)	16	51
2	K	121/125 (97%)	116 (96%)	4 (3%)	1 (1%)	16	51
2	L	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
2	M	121/125 (97%)	114 (94%)	7 (6%)	0	100	100
2	N	121/125 (97%)	108 (89%)	12 (10%)	1 (1%)	16	51
2	O	122/125 (98%)	122 (100%)	0	0	100	100
2	P	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
2	Q	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
2	R	121/125 (97%)	118 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	118/372 (32%)	109 (92%)	8 (7%)	1 (1%)	16	51
All	All	4471/4800 (93%)	4229 (95%)	211 (5%)	31 (1%)	21	54

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	153	LEU
1	C	53	ASP
1	C	65	ARG
1	E	54	ILE
1	E	288	ASN
1	E	307	ILE
1	G	229	PRO
1	H	305	ASN
1	I	65	ARG
1	D	8	SER
1	D	235	ILE
1	D	239	LEU
1	D	246	GLY
1	E	156	GLN
1	G	230	LEU
1	I	64	SER
2	K	73	ALA
1	D	73	GLU
1	D	305	ASN
1	E	53	ASP
1	G	7	LYS
1	G	226	GLN
1	C	16	THR
1	E	304	ALA
3	S	40	THR
1	C	284	VAL
2	J	6	PHE
1	A	286	ASP
1	C	55	SER
1	G	5	SER
2	N	4	GLN

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	A	313/317 (99%)	308 (98%)	5 (2%)	58	79
1	B	310/317 (98%)	298 (96%)	12 (4%)	27	60
1	C	310/317 (98%)	296 (96%)	14 (4%)	23	56
1	D	297/317 (94%)	289 (97%)	8 (3%)	40	69
1	E	305/317 (96%)	283 (93%)	22 (7%)	12	41
1	F	311/317 (98%)	301 (97%)	10 (3%)	34	65
1	G	312/317 (98%)	297 (95%)	15 (5%)	21	55
1	H	314/317 (99%)	307 (98%)	7 (2%)	47	73
1	I	301/317 (95%)	291 (97%)	10 (3%)	33	64
2	J	93/99 (94%)	88 (95%)	5 (5%)	18	51
2	K	97/99 (98%)	93 (96%)	4 (4%)	26	59
2	L	96/99 (97%)	93 (97%)	3 (3%)	35	66
2	M	97/99 (98%)	95 (98%)	2 (2%)	48	74
2	N	96/99 (97%)	92 (96%)	4 (4%)	25	58
2	O	97/99 (98%)	93 (96%)	4 (4%)	26	59
2	P	94/99 (95%)	91 (97%)	3 (3%)	34	65
2	Q	96/99 (97%)	94 (98%)	2 (2%)	48	74
2	R	97/99 (98%)	93 (96%)	4 (4%)	26	59
3	S	101/307 (33%)	98 (97%)	3 (3%)	36	66
All	All	3737/4051 (92%)	3600 (96%)	137 (4%)	31	62

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	14	ASP
1	A	36	ARG
1	A	90	SER

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Mol	Chain	Res	Type
1	A	120	MET
1	B	54	ILE
1	B	55	SER
1	B	83	MET
1	B	90	SER
1	B	223	TYR
1	B	228	THR
1	B	272	ARG
1	B	301	LEU
1	B	303	GLU
1	B	305	ASN
1	B	337	ARG
1	B	348	TYR
1	C	40	GLN
1	C	48	ASP
1	C	55	SER
1	C	56	LEU
1	C	57	LEU
1	C	62	ARG
1	C	64	SER
1	C	70	SER
1	C	130	ARG
1	C	155	LYS
1	C	265	ASN
1	C	272	ARG
1	C	348	TYR
1	C	364	SER
1	D	65	ARG
1	D	82	MET
1	D	155	LYS
1	D	199	GLU
1	D	238	SER
1	D	307	ILE
1	D	334	GLU
1	D	348	TYR
1	E	5	SER
1	E	7	LYS
1	E	37	SER
1	E	48	ASP
1	E	50	THR
1	E	51	ASP
1	E	52	TRP

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Mol	Chain	Res	Type
1	E	55	SER
1	E	76	ARG
1	E	126	PHE
1	E	155	LYS
1	E	156	GLN
1	E	158	ASP
1	E	271	LYS
1	E	284	VAL
1	E	307	ILE
1	E	317	LYS
1	E	318	MET
1	E	337	ARG
1	E	342	ASP
1	E	348	TYR
1	E	353	CYS
1	F	82	MET
1	F	85	PHE
1	F	146	ASN
1	F	156	GLN
1	F	233	GLN
1	F	282	ASP
1	F	305	ASN
1	F	307	ILE
1	F	336	ASP
1	F	348	TYR
1	G	5	SER
1	G	8	SER
1	G	9	ARG
1	G	115	ARG
1	G	120	MET
1	G	202	HIS
1	G	207	ARG
1	G	224	LEU
1	G	233	GLN
1	G	251	MET
1	G	253	ARG
1	G	272	ARG
1	G	332	GLU
1	G	336	ASP
1	G	348	TYR
1	H	62	ARG
1	H	85	PHE

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Mol	Chain	Res	Type
1	H	155	LYS
1	H	240	ARG
1	H	305	ASN
1	H	348	TYR
1	H	361	ASP
1	I	7	LYS
1	I	19	VAL
1	I	58	ASP
1	I	62	ARG
1	I	65	ARG
1	I	66	LYS
1	I	76	ARG
1	I	144	ASP
1	I	348	TYR
1	I	367	GLU
2	J	6	PHE
2	J	12	ARG
2	J	39	SER
2	J	41	GLU
2	J	79	TYR
2	K	3	TYR
2	K	79	TYR
2	K	102	SER
2	K	105	ASP
2	L	12	ARG
2	L	39	SER
2	L	102	SER
2	M	3	TYR
2	M	14	PRO
2	N	11	GLU
2	N	91	ASP
2	N	102	SER
2	N	105	ASP
2	O	78	SER
2	O	79	TYR
2	O	91	ASP
2	O	102	SER
2	P	79	TYR
2	P	91	ASP
2	P	105	ASP
2	Q	90	ARG
2	Q	119	ASP

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Mol	Chain	Res	Type
2	R	17	ASP
2	R	39	SER
2	R	79	TYR
2	R	102	SER
3	S	39	LEU
3	S	55	ASP
3	S	115	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	B	202	HIS
1	B	305	ASN
1	C	346	HIS
1	D	185	HIS
1	D	265	ASN
1	E	40	GLN
1	G	233	GLN
1	H	77	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

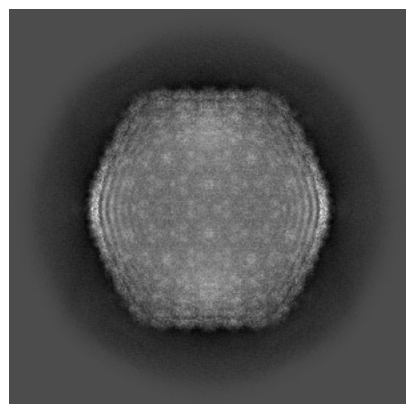
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45155. These allow visual inspection of the internal detail of the map and identification of artifacts.

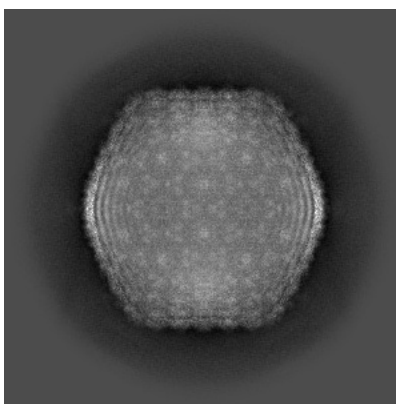
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

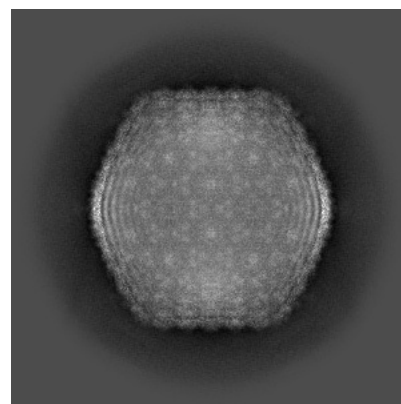
6.1.1 Primary map



X

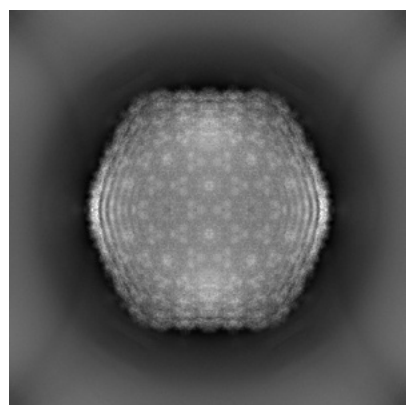


Y

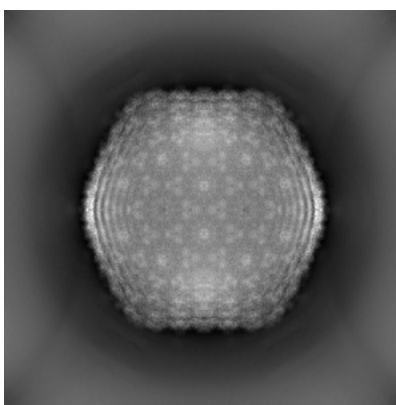


Z

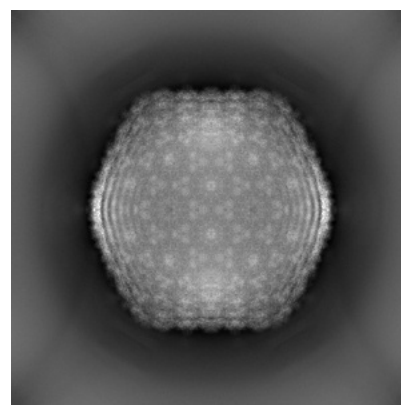
6.1.2 Raw map



X



Y

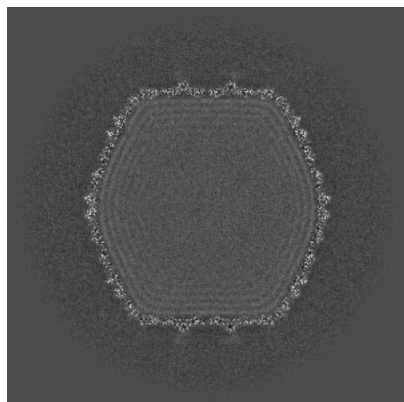


Z

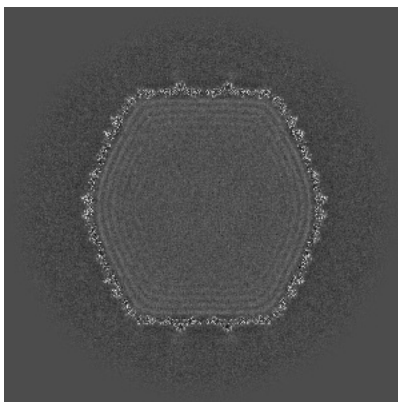
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

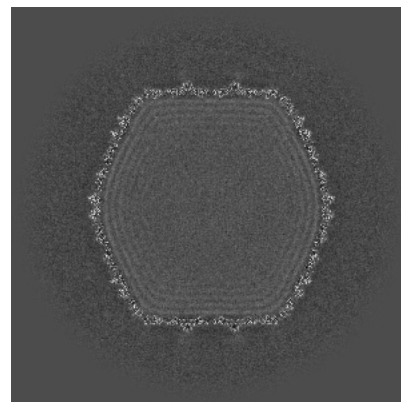
6.2.1 Primary map



X Index: 500

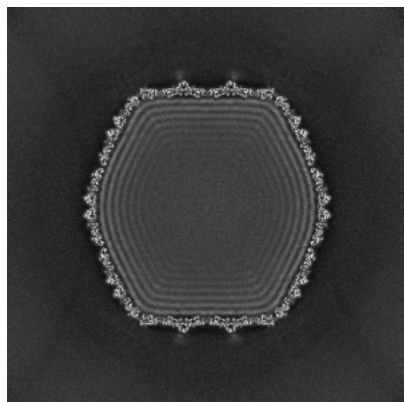


Y Index: 500

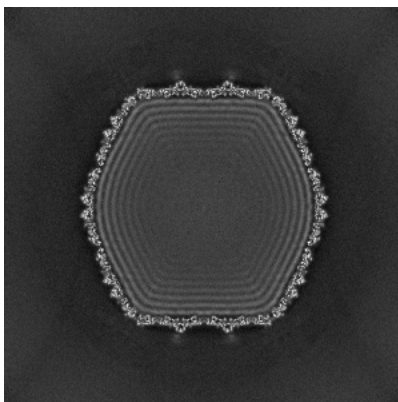


Z Index: 500

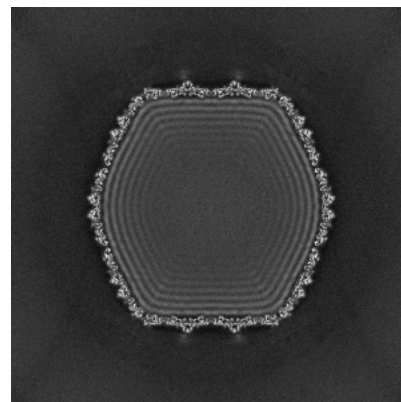
6.2.2 Raw map



X Index: 500



Y Index: 500

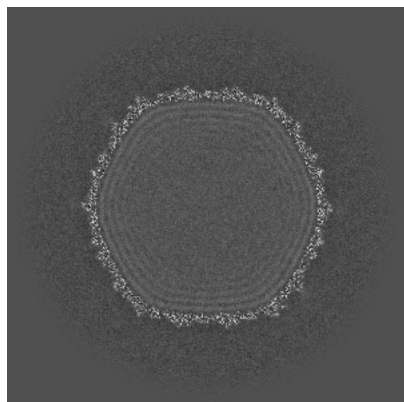


Z Index: 500

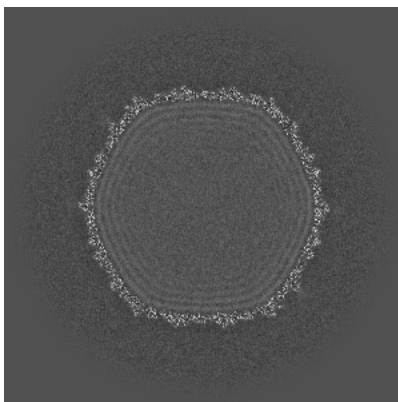
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

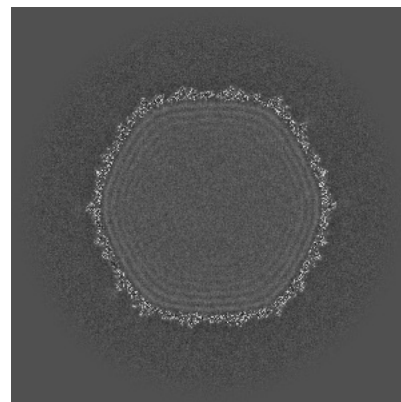
6.3.1 Primary map



X Index: 439

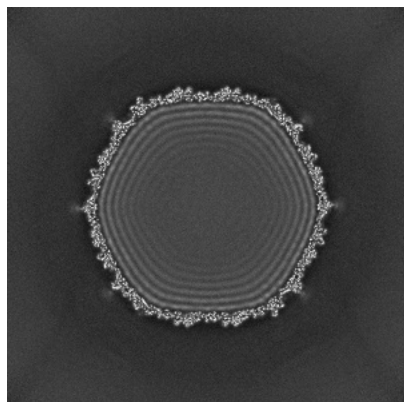


Y Index: 439

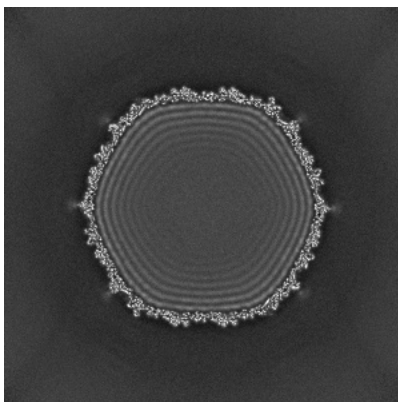


Z Index: 561

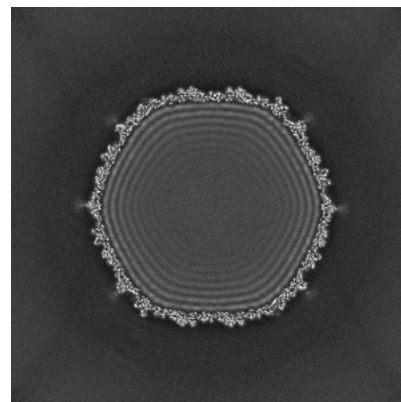
6.3.2 Raw map



X Index: 567



Y Index: 433

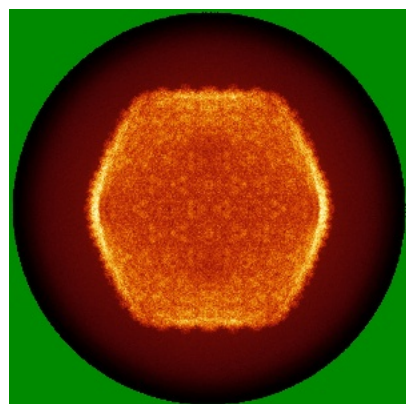


Z Index: 433

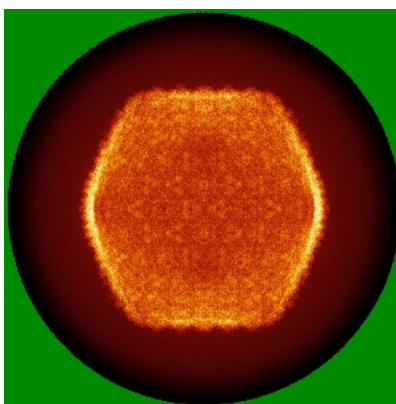
The images above show the largest variance slices of the map in three orthogonal directions.

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

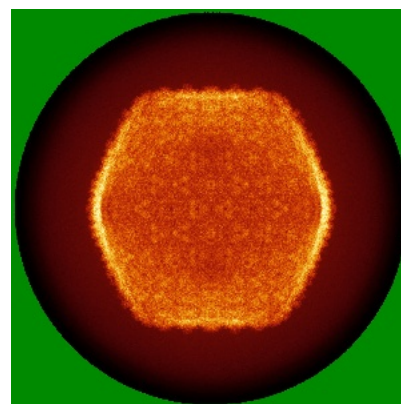
6.4.1 Primary map



X

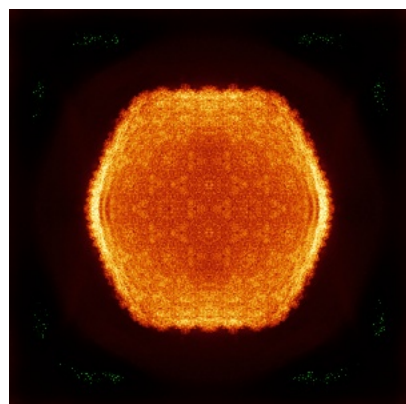


Y

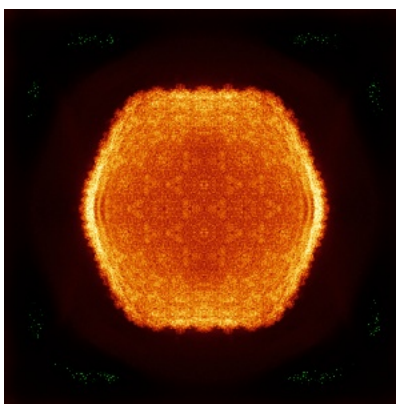


Z

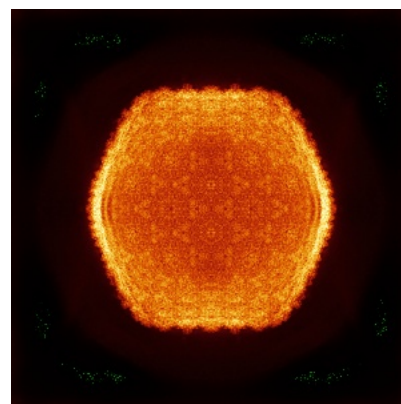
6.4.2 Raw map



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](#)

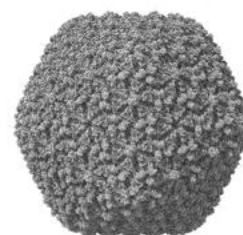
6.5.1 Primary map



X



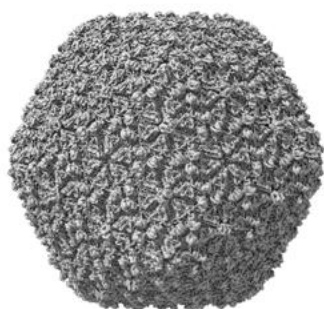
Y



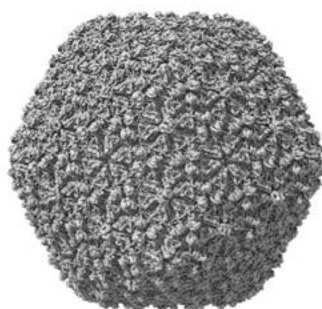
Z

The images above show the 3D surface view of the map at the recommended contour level 0.58. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

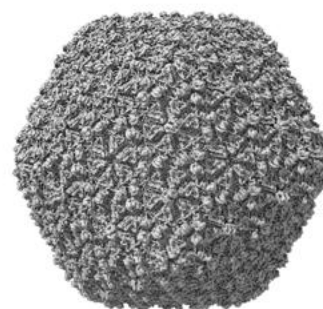
6.5.2 Raw map



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.

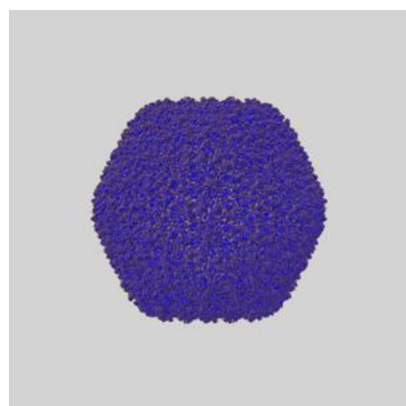
6.6 Mask visualisation [i](#)

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

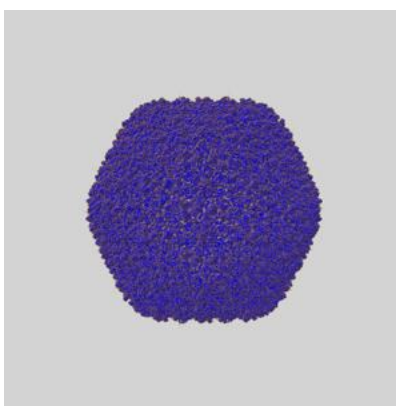
A mask typically either:

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

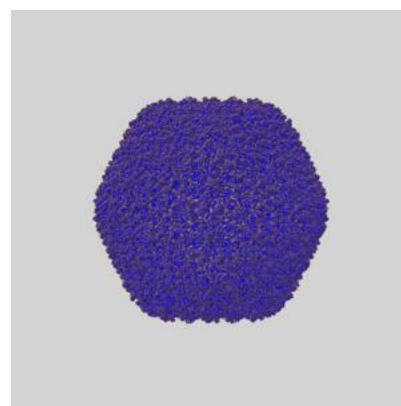
6.6.1 emd_45155_msk_1.map [i](#)



X



Y

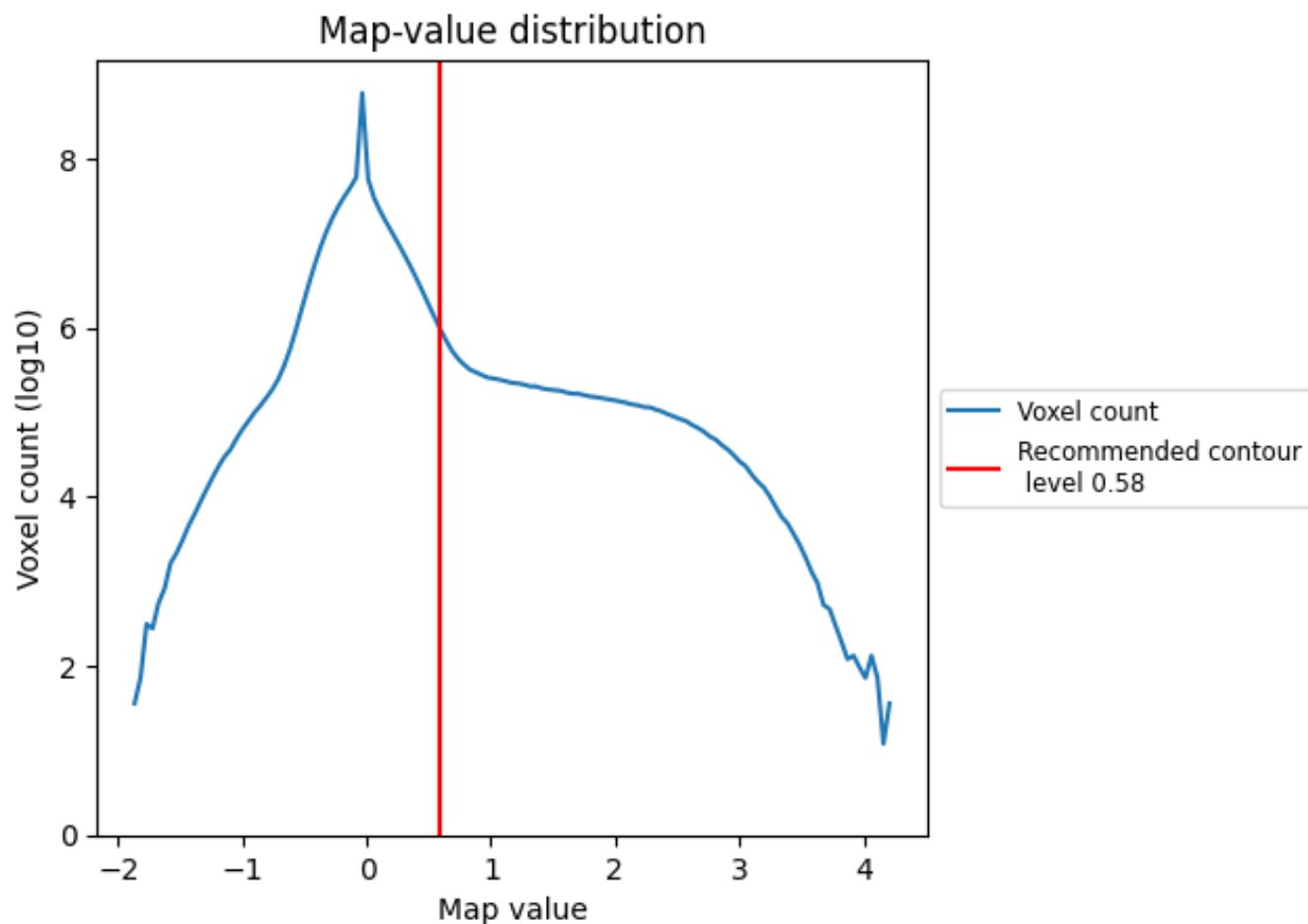


Z

7 Map analysis [i](#)

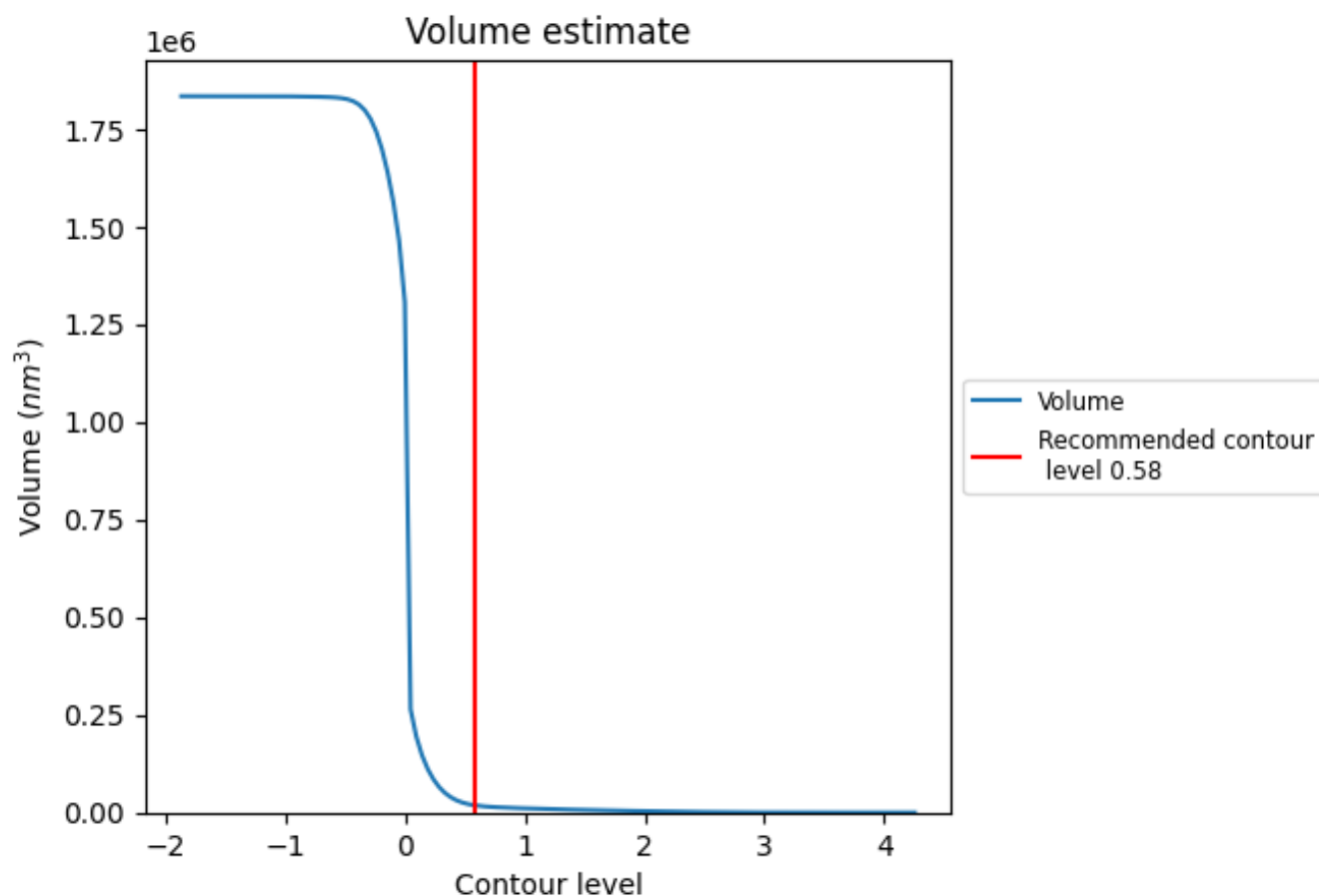
This section contains the results of statistical analysis of the map.

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.

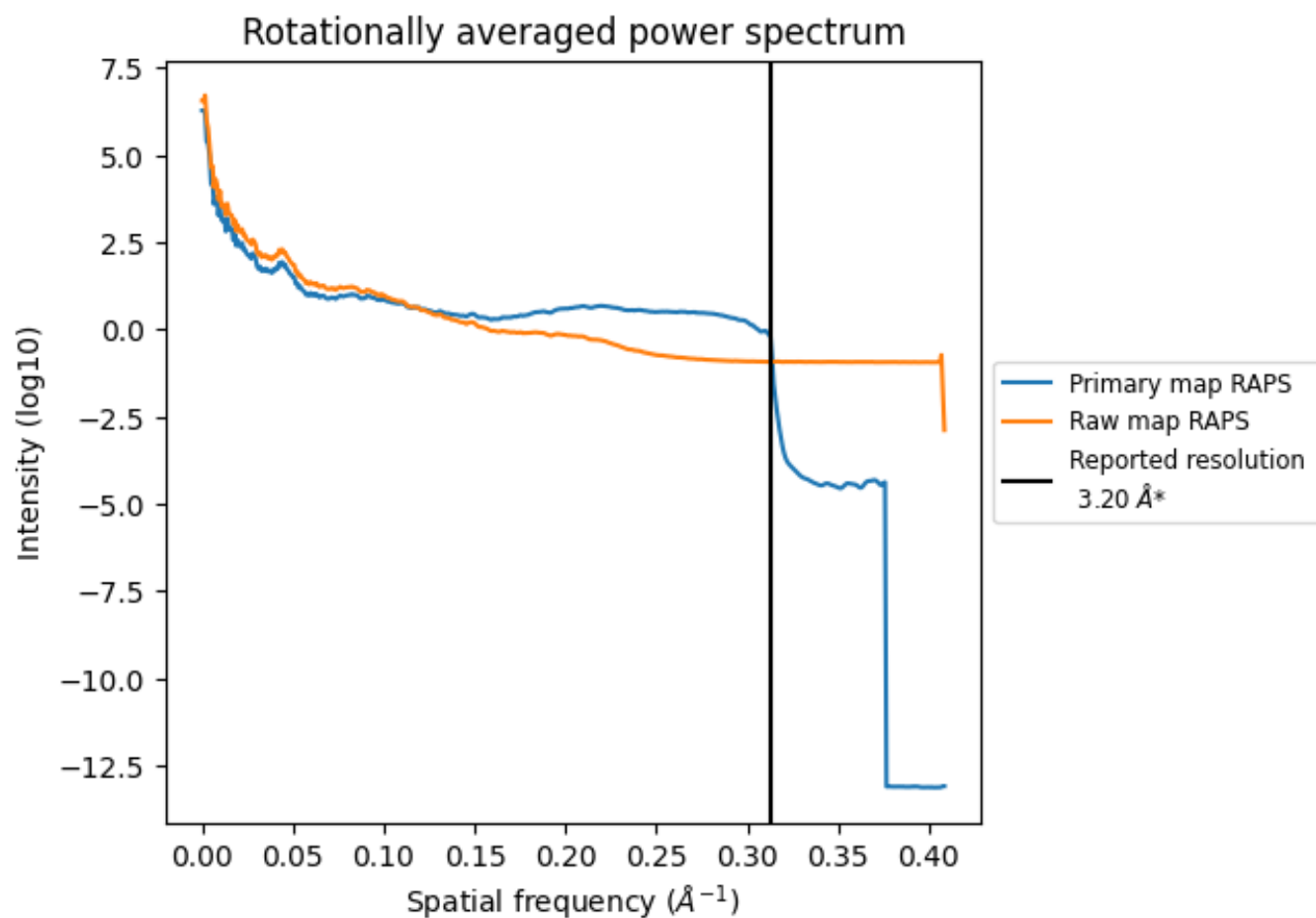
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 18628 nm³; this corresponds to an approximate mass of 16827 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 ⓘ

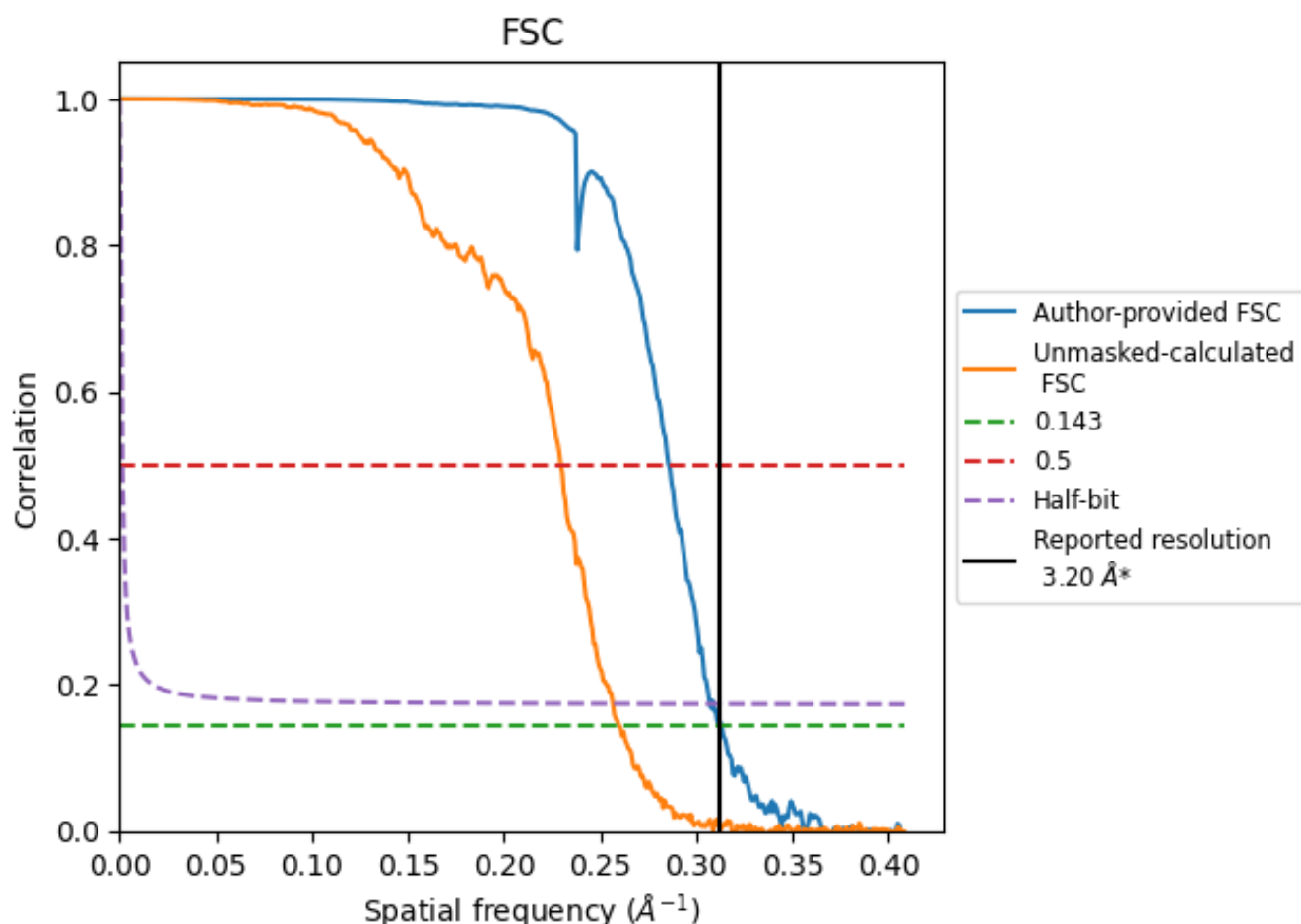


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.50	3.26
Unmasked-calculated*	3.85	4.36	3.90

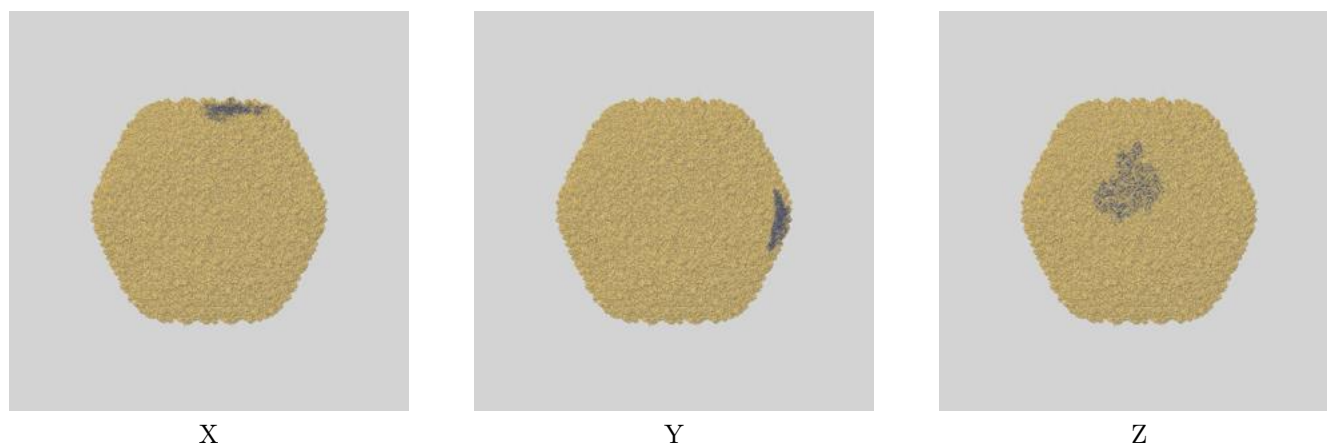
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

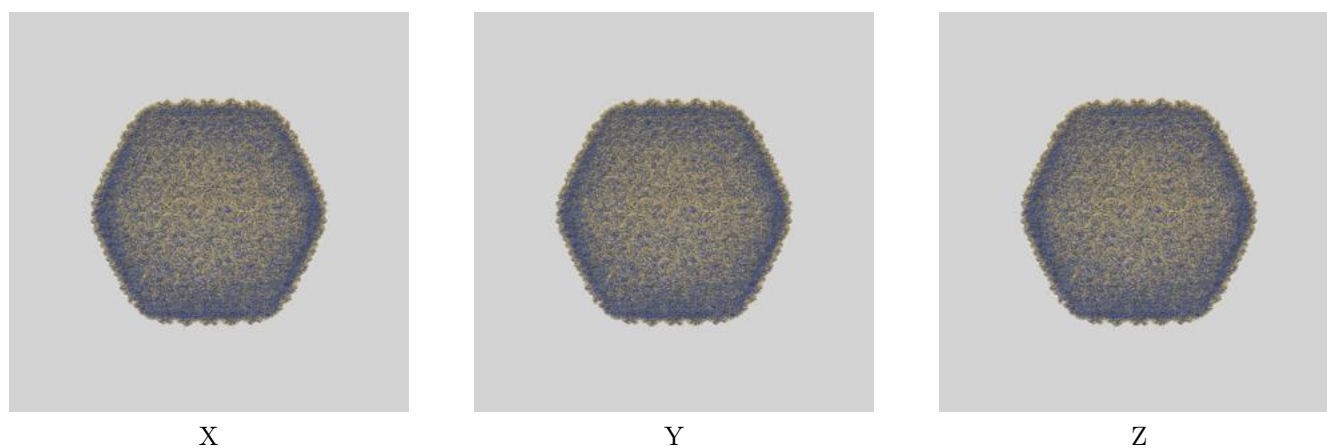
This section contains information regarding the fit between EMDB map EMD-45155 and PDB model 9C2D. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

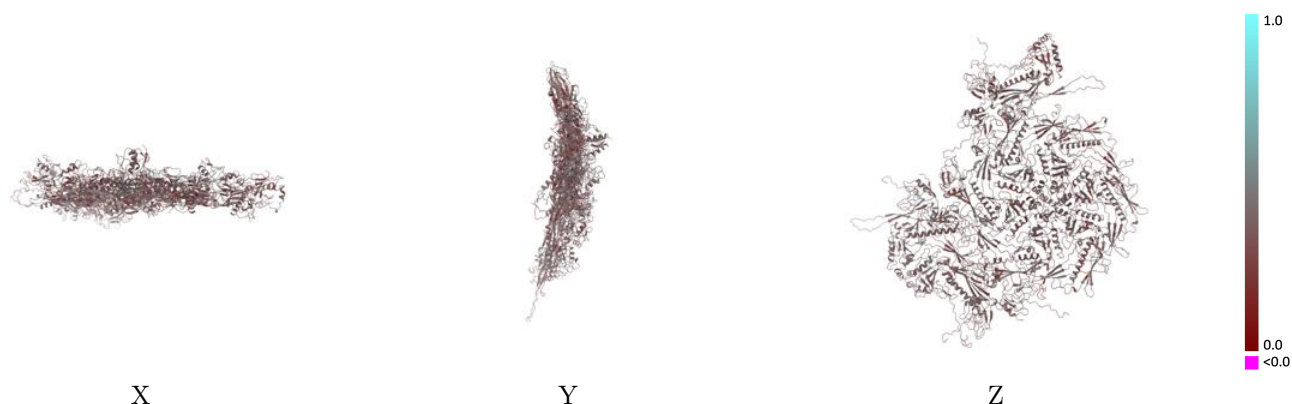


9.1.2 Map-model assembly overlay [i](#)



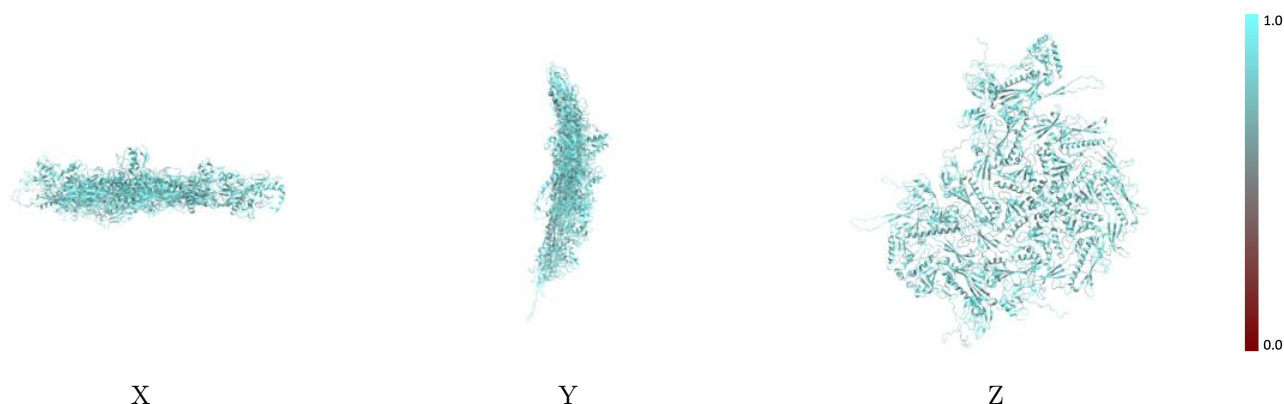
The images above show the 3D surface view of the map at the recommended contour level 0.58 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



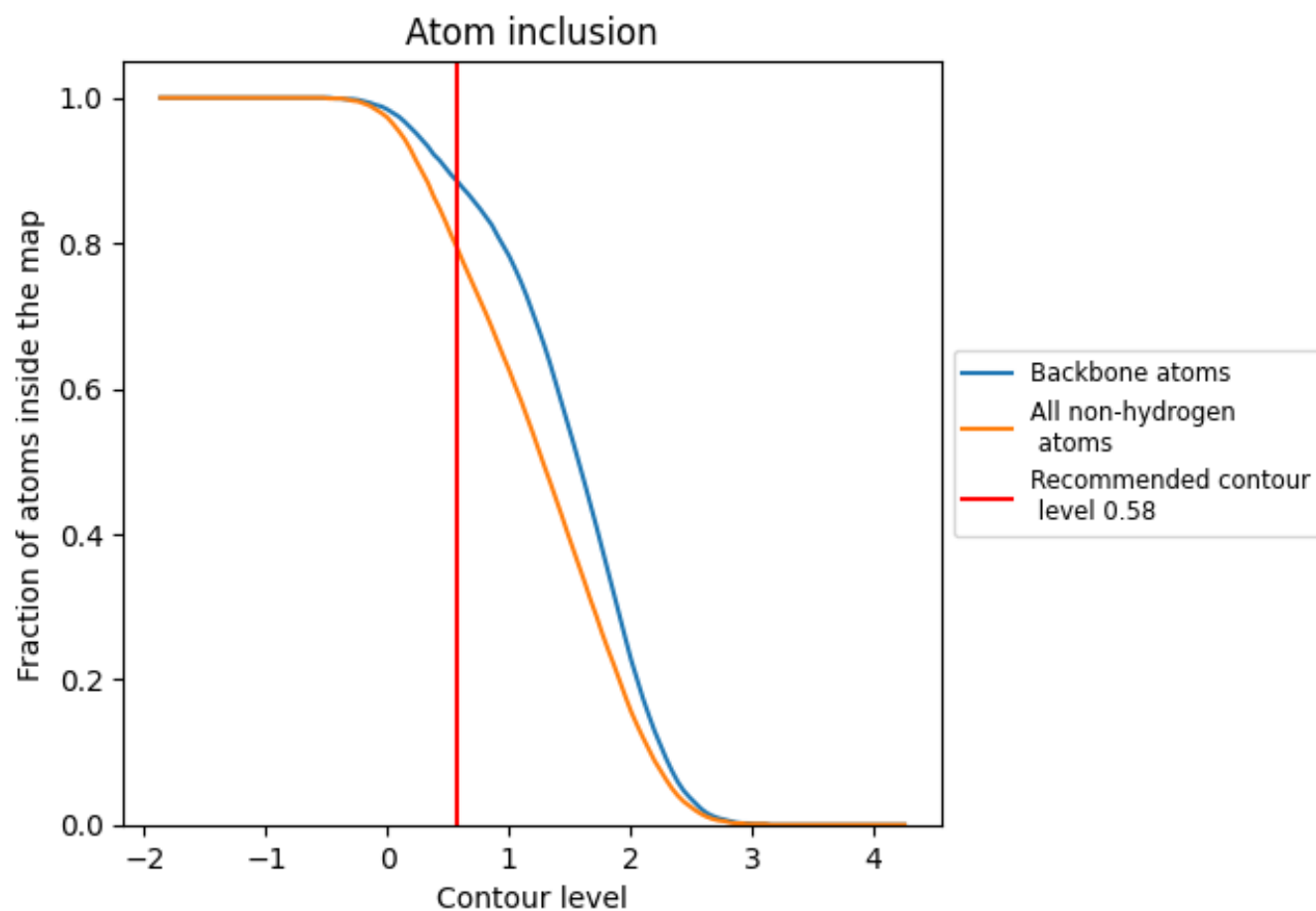
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.58).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 79% 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 (0.58) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.3690
A	 0.7800	 0.3720
B	 0.7950	 0.3660
C	 0.7840	 0.3650
D	 0.7870	 0.3640
E	 0.7950	 0.3660
F	 0.7790	 0.3670
G	 0.7850	 0.3640
H	 0.7780	 0.3690
I	 0.7790	 0.3630
J	 0.8310	 0.4050
K	 0.8120	 0.3790
L	 0.7750	 0.3460
M	 0.8130	 0.3690
N	 0.8160	 0.3880
O	 0.8000	 0.3730
P	 0.8060	 0.3900
Q	 0.8240	 0.3840
R	 0.7860	 0.3410
S	 0.8070	 0.3750

