



Full wwPDB EM Validation Report ⓘ

Mar 22, 2024 – 10:11 AM EDT

PDB ID : 9B42
EMDB ID : EMD-44166
Title : Pseudomonas phage Pa193 neck and extended tail (collar, gateway, tail tube, and sheath proteins)
Deposited on : 2024-03-20
Resolution : 3.50 Å (reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

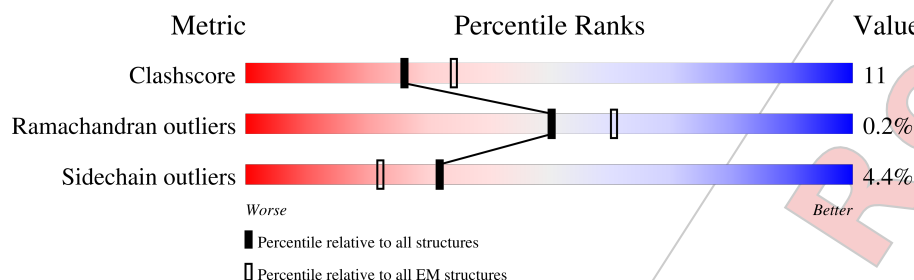
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance [i](#)

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

The reported resolution of this entry is 3.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	S	504	12% 72% 25% .
2	A	132	. 72% 27% .
2	B	132	. 68% 28% .
2	C	132	. 72% 24% .
2	D	132	. 68% 30% .
2	E	132	. 73% 24% .
2	F	132	. 68% 28% .
3	M	150	68% 29% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
3	N	150		•
3	O	150		
3	P	150		•
3	Q	150		•
3	R	150		••
4	G	183		•
4	H	183		•
4	I	183		•
4	J	183		•
4	K	183		•
4	L	183		•

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25948 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 gp32 Sheath.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	504	Total	C	N	O	S	0	0
			3790	2390	641	746	13		

- Molecule 2 is a protein called gp29 Collar.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	132	Total	C	N	O	S	0	0
			1080	694	184	196	6		
2	B	132	Total	C	N	O	S	0	0
			1080	694	184	196	6		
2	C	132	Total	C	N	O	S	0	0
			1080	694	184	196	6		
2	D	132	Total	C	N	O	S	0	0
			1080	694	184	196	6		
2	E	132	Total	C	N	O	S	0	0
			1080	694	184	196	6		
2	F	132	Total	C	N	O	S	0	0
			1080	694	184	196	6		

- Molecule 3 is a protein called gp33 Tail tube.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	150	Total	C	N	O	S	0	0
			1115	700	194	216	5		
3	N	150	Total	C	N	O	S	0	0
			1115	700	194	216	5		
3	O	150	Total	C	N	O	S	0	0
			1115	700	194	216	5		
3	P	150	Total	C	N	O	S	0	0
			1115	700	194	216	5		
3	Q	150	Total	C	N	O	S	0	0
			1115	700	194	216	5		
3	R	150	Total	C	N	O	S	0	0
			1115	700	194	216	5		

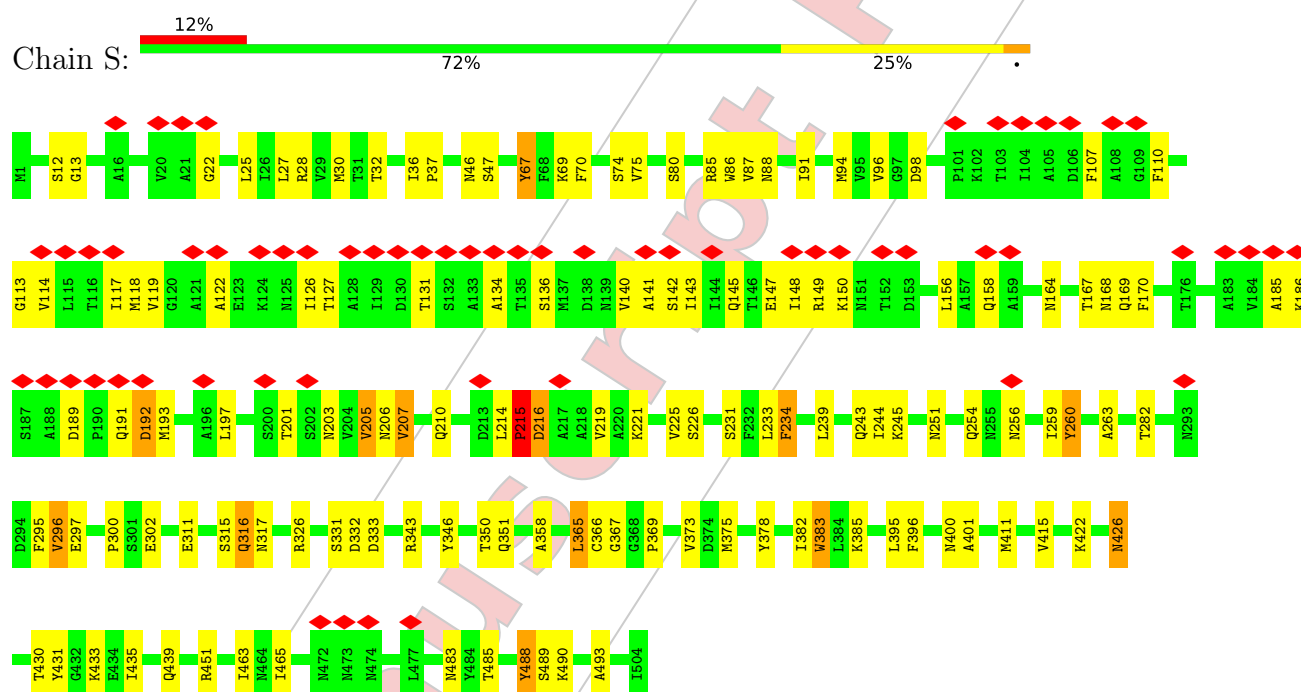
- Molecule 4 is a protein called gp30 Gateway.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	183	Total	C	N	O	S	0	0
			1498	957	253	284	4		
4	G	183	Total	C	N	O	S	0	0
			1498	957	253	284	4		
4	H	183	Total	C	N	O	S	0	0
			1498	957	253	284	4		
4	I	183	Total	C	N	O	S	0	0
			1498	957	253	284	4		
4	K	183	Total	C	N	O	S	0	0
			1498	957	253	284	4		
4	L	183	Total	C	N	O	S	0	0
			1498	957	253	284	4		

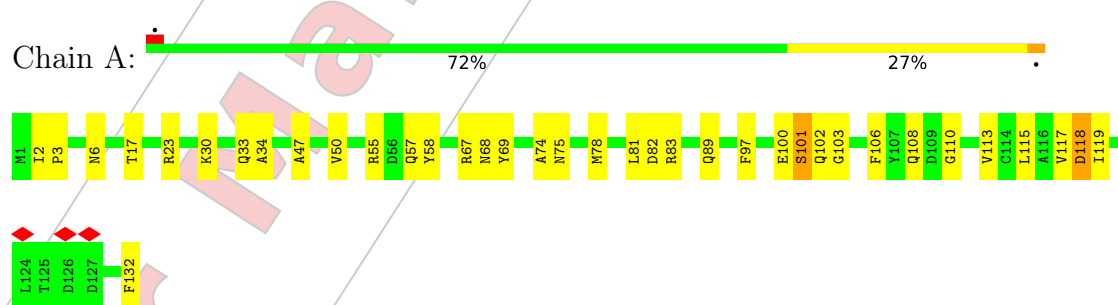
3 Residue-property plots

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: gp32 Sheath

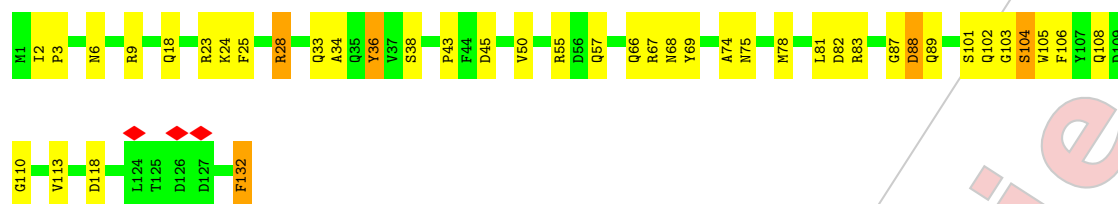


- Molecule 2: gp29 Collar

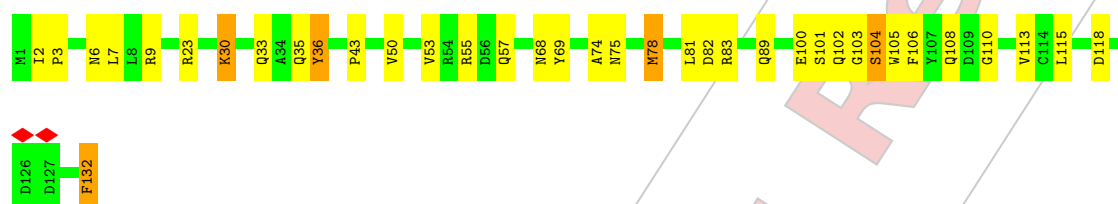


- Molecule 2: gp29 Collar

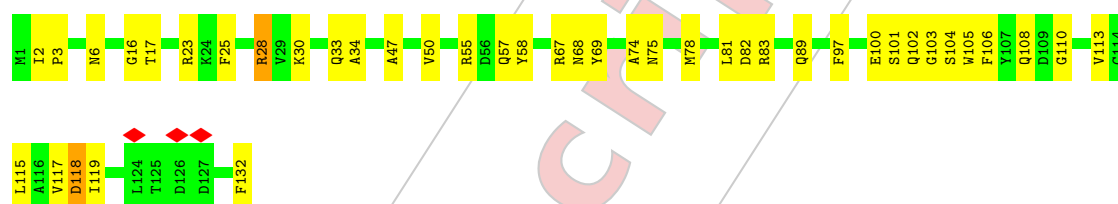




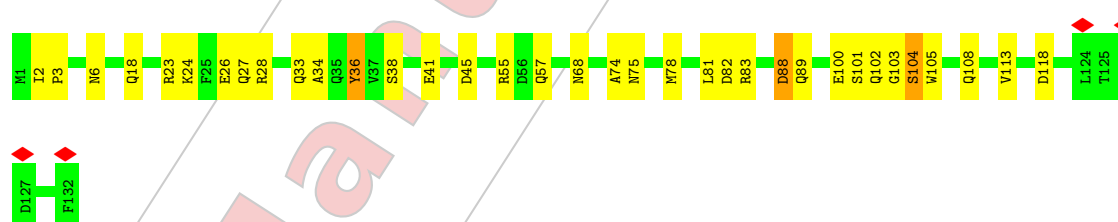
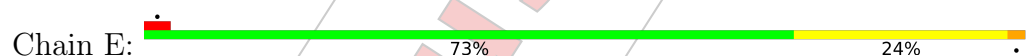
- Molecule 2: gp29 Collar



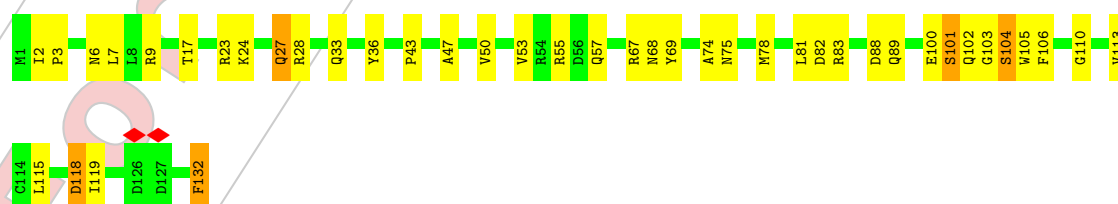
- Molecule 2: gp29 Collar



- Molecule 2: gp29 Collar

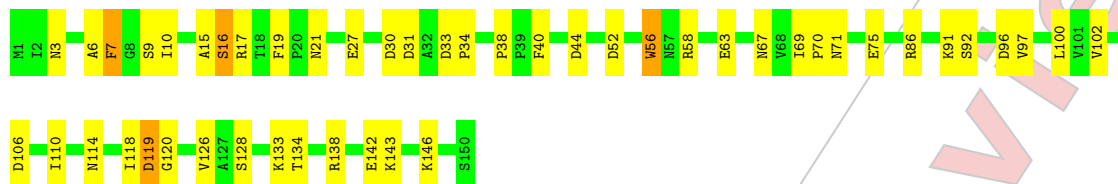


- Molecule 2: gp29 Collar



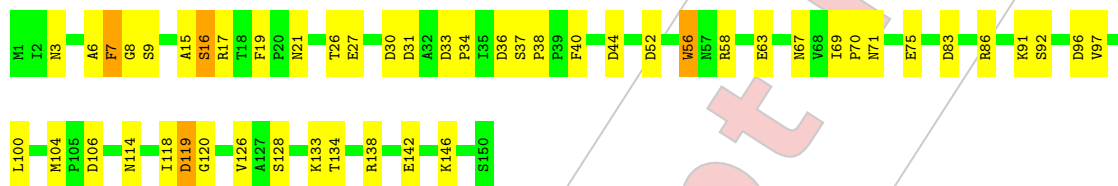
• Molecule 3: gp33 Tail tube

Chain M: 68% 29%



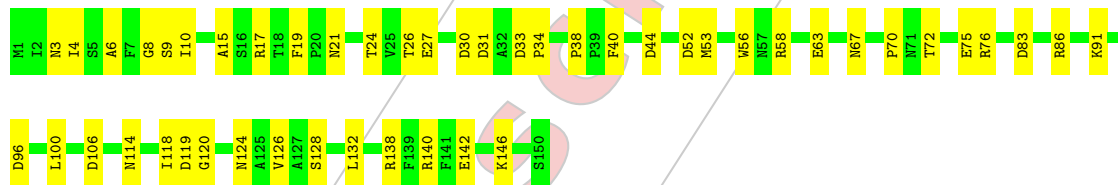
• Molecule 3: gp33 Tail tube

Chain N: 67% 31%



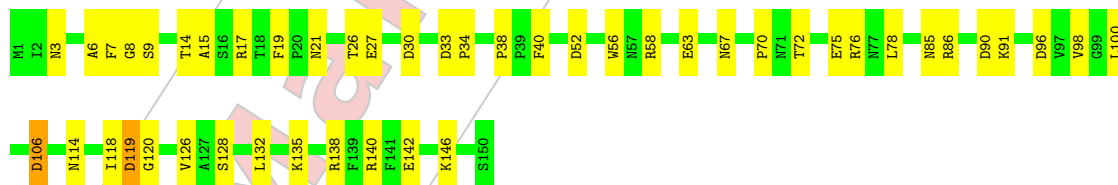
• Molecule 3: gp33 Tail tube

Chain O: 68% 32%



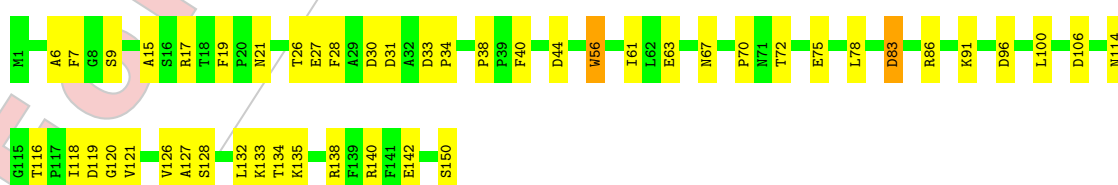
• Molecule 3: gp33 Tail tube

Chain P: 69% 30%

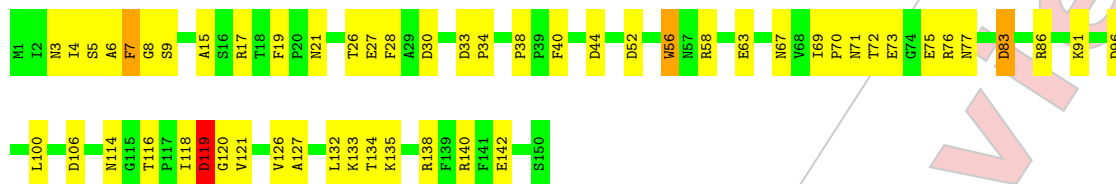


• Molecule 3: gp33 Tail tube

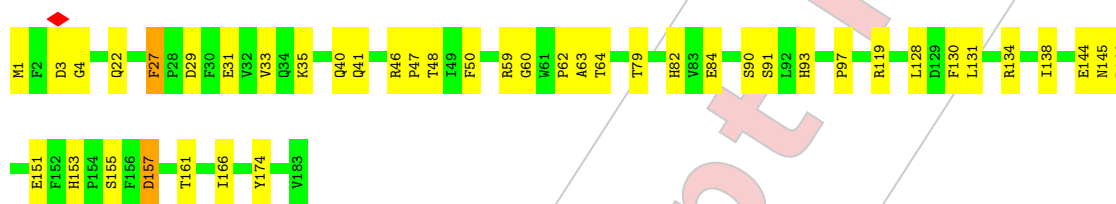
Chain Q: 68% 31%



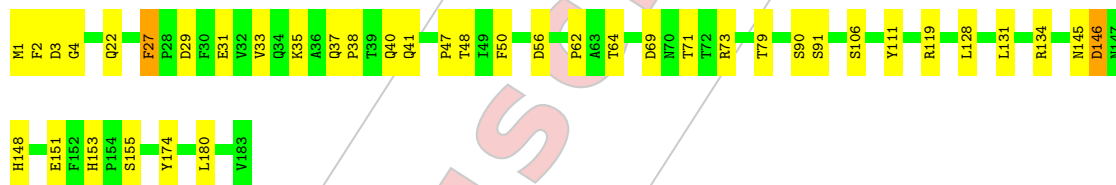
• Molecule 3: gp33 Tail tube

Chain R:  64% 33%

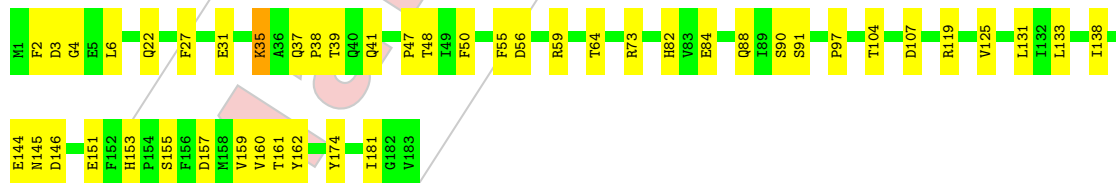
• Molecule 4: gp30 Gateway

Chain J:  77% 22%

• Molecule 4: gp30 Gateway

Chain G:  78% 21%

• Molecule 4: gp30 Gateway

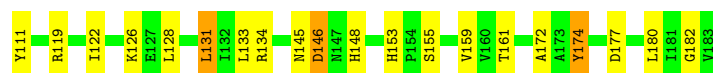
Chain H:  75% 25%

• Molecule 4: gp30 Gateway

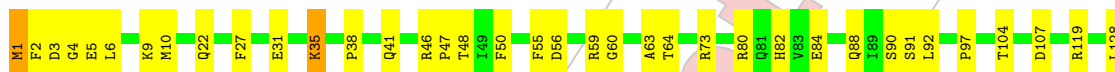
Chain I:  73% 26%



- Molecule 4: gp30 Gateway



- Molecule 4: gp30 Gateway



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	9179	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34.4	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.756	Depositor
Minimum map value	-6.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	S	0.32	0/3861	0.60	2/5270 (0.0%)
2	A	0.33	0/1105	0.64	1/1491 (0.1%)
2	B	0.39	0/1105	0.75	2/1491 (0.1%)
2	C	0.35	0/1105	0.67	1/1491 (0.1%)
2	D	0.34	0/1105	0.64	1/1491 (0.1%)
2	E	0.35	0/1105	0.72	2/1491 (0.1%)
2	F	0.34	0/1105	0.69	1/1491 (0.1%)
3	M	0.34	0/1133	0.63	2/1541 (0.1%)
3	N	0.34	0/1133	0.61	1/1541 (0.1%)
3	O	0.35	0/1133	0.60	1/1541 (0.1%)
3	P	0.35	0/1133	0.64	2/1541 (0.1%)
3	Q	0.36	0/1133	0.59	1/1541 (0.1%)
3	R	0.37	0/1133	0.65	2/1541 (0.1%)
4	G	0.34	0/1536	0.55	0/2091
4	H	0.33	0/1536	0.58	0/2091
4	I	0.34	0/1536	0.57	0/2091
4	J	0.33	0/1536	0.58	1/2091 (0.0%)
4	K	0.36	0/1536	0.60	1/2091 (0.0%)
4	L	0.33	0/1536	0.57	0/2091
All	All	0.34	0/26505	0.62	21/36008 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	118	ASP	CB-CG-OD2	7.21	124.78	118.30
3	R	119	ASP	CB-CG-OD1	6.76	124.38	118.30
3	P	119	ASP	CB-CG-OD1	6.68	124.31	118.30
2	B	118	ASP	CB-CG-OD2	6.58	124.22	118.30
3	M	119	ASP	CB-CG-OD1	6.49	124.14	118.30
2	F	118	ASP	CB-CG-OD1	6.34	124.00	118.30
2	C	118	ASP	CB-CG-OD2	6.14	123.83	118.30
2	B	45	ASP	CB-CG-OD2	6.11	123.80	118.30
3	M	100	LEU	CA-CB-CG	6.11	129.35	115.30
1	S	411	MET	CA-CB-CG	5.91	123.34	113.30
2	A	118	ASP	CB-CG-OD2	5.89	123.61	118.30
2	D	118	ASP	CB-CG-OD2	5.74	123.47	118.30
4	J	3	ASP	CB-CG-OD1	5.50	123.25	118.30
3	N	100	LEU	CA-CB-CG	5.50	127.95	115.30
3	O	100	LEU	CA-CB-CG	5.35	127.60	115.30
1	S	214	LEU	CA-CB-CG	5.29	127.46	115.30
4	K	131	LEU	CB-CG-CD1	5.28	119.98	111.00
2	E	45	ASP	CB-CG-OD2	5.22	123.00	118.30
3	Q	100	LEU	CA-CB-CG	5.17	127.20	115.30
3	P	100	LEU	CA-CB-CG	5.14	127.12	115.30
3	R	100	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	205	VAL	Peptide
1	S	365	LEU	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	S	3790	0	3719	84	0
2	A	1080	0	1043	27	0
2	B	1080	0	1043	30	0
2	C	1080	0	1043	25	0
2	D	1080	0	1043	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1080	0	1043	26	0
2	F	1080	0	1043	26	0
3	M	1115	0	1123	31	0
3	N	1115	0	1123	33	0
3	O	1115	0	1123	36	0
3	P	1115	0	1123	34	0
3	Q	1115	0	1123	33	0
3	R	1115	0	1123	41	0
4	G	1498	0	1438	30	0
4	H	1498	0	1438	37	0
4	I	1498	0	1438	39	0
4	J	1498	0	1438	37	0
4	K	1498	0	1438	50	0
4	L	1498	0	1438	40	0
All	All	25948	0	25343	574	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 11.

All (574) 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:S:451:ARG:NH2	3:R:77:ASN:OD1	2.17	0.78
1:S:91:ILE:HB	1:S:210:GLN:H	1.51	0.75
3:P:70:PRO:HA	3:P:75:GLU:HG2	1.69	0.74
3:O:70:PRO:HA	3:O:75:GLU:HG2	1.69	0.74
4:L:31:GLU:HB2	4:L:48:THR:HG22	1.71	0.73
4:L:1:MET:SD	4:L:1:MET:N	2.57	0.72
2:A:83:ARG:NH1	4:J:146:ASP:OD1	2.23	0.72
3:O:53:MET:HG3	3:Q:61:ILE:HD13	1.71	0.71
1:S:117:ILE:HD11	1:S:148:ILE:HD12	1.73	0.70
3:O:10:ILE:HD11	3:O:24:THR:HB	1.74	0.70
2:A:50:VAL:O	2:B:108:GLN:NE2	2.25	0.69
2:D:83:ARG:NH1	4:I:146:ASP:OD1	2.25	0.69
3:N:3:ASN:HD21	4:K:131:LEU:HD12	1.58	0.69
2:E:57:GLN:NE2	2:F:100:GLU:OE2	2.27	0.68
2:F:83:ARG:NH1	4:L:146:ASP:OD1	2.27	0.67
3:R:86:ARG:O	3:R:91:LYS:NZ	2.27	0.67
3:Q:26:THR:OG1	4:I:119:ARG:NH2	2.27	0.67
3:P:146:LYS:NZ	3:R:83:ASP:OD2	2.27	0.67
3:O:30:ASP:O	3:Q:128:SER:OG	2.13	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:108:GLN:NE2	2:F:50:VAL:O	2.27	0.66
2:F:27:GLN:OE1	2:F:28:ARG:N	2.26	0.66
4:H:31:GLU:HB2	4:H:48:THR:HG22	1.76	0.66
2:B:50:VAL:O	2:C:108:GLN:NE2	2.26	0.66
2:C:83:ARG:NH1	4:H:146:ASP:OD1	2.29	0.66
1:S:164:ASN:O	1:S:168:ASN:N	2.29	0.66
1:S:126:ILE:HG21	1:S:148:ILE:HD13	1.78	0.65
3:N:71:ASN:N	3:N:75:GLU:OE2	2.28	0.65
4:I:82:HIS:HE1	4:I:161:THR:HB	1.60	0.65
3:M:71:ASN:N	3:M:75:GLU:OE2	2.28	0.65
3:O:27:GLU:HG3	3:O:72:THR:HG21	1.79	0.64
3:R:3:ASN:OD1	3:R:4:ILE:N	2.30	0.64
1:S:422:LYS:O	1:S:426:ASN:HB2	1.97	0.64
4:H:64:THR:HG21	4:I:119:ARG:HG2	1.79	0.64
2:A:100:GLU:OE1	4:J:40:GLN:NE2	2.31	0.64
2:E:28:ARG:HG3	2:E:36:TYR:CE1	2.33	0.64
3:O:146:LYS:NZ	3:Q:83:ASP:OD2	2.30	0.64
1:S:367:GLY:HA3	1:S:373:VAL:HG12	1.80	0.64
2:B:57:GLN:NE2	2:C:100:GLU:OE2	2.31	0.64
1:S:215:PRO:HB3	1:S:243:GLN:HB2	1.80	0.63
1:S:385:LYS:HG2	4:K:180:LEU:HD12	1.80	0.63
2:E:28:ARG:HE	4:K:41:GLN:HG2	1.63	0.63
3:M:86:ARG:O	3:M:91:LYS:NZ	2.32	0.63
2:D:100:GLU:OE1	4:I:40:GLN:NE2	2.31	0.63
1:S:74:SER:OG	1:S:75:VAL:N	2.32	0.62
3:Q:86:ARG:O	3:Q:91:LYS:NZ	2.32	0.62
2:B:28:ARG:HG3	2:B:36:TYR:CE1	2.35	0.62
2:D:57:GLN:NE2	2:E:100:GLU:OE2	2.33	0.61
3:Q:27:GLU:HG3	3:Q:72:THR:HG21	1.82	0.61
4:J:1:MET:SD	4:J:1:MET:N	2.73	0.61
2:B:82:ASP:OD1	2:B:83:ARG:N	2.34	0.61
2:E:57:GLN:HB2	2:F:81:LEU:HD23	1.81	0.61
4:G:146:ASP:OD1	4:G:146:ASP:N	2.33	0.61
3:M:118:ILE:HB	3:M:138:ARG:HG2	1.83	0.61
3:P:86:ARG:O	3:P:91:LYS:NZ	2.34	0.61
1:S:430:THR:HG21	1:S:433:LYS:HE3	1.82	0.61
3:O:27:GLU:OE1	3:O:27:GLU:N	2.33	0.61
4:K:146:ASP:N	4:K:146:ASP:OD1	2.32	0.61
2:E:82:ASP:OD1	2:E:83:ARG:N	2.34	0.60
3:N:86:ARG:O	3:N:91:LYS:NZ	2.33	0.60
4:K:31:GLU:HB2	4:K:48:THR:HG22	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ARG:HH21	4:G:41:GLN:HB3	1.66	0.60
4:G:31:GLU:HB2	4:G:48:THR:HG22	1.83	0.60
3:N:27:GLU:N	3:N:27:GLU:OE1	2.34	0.60
3:O:70:PRO:HG2	3:O:132:LEU:HB3	1.84	0.60
3:P:38:PRO:HD2	3:P:63:GLU:HB3	1.84	0.60
1:S:365:LEU:HD13	1:S:375:MET:HG2	1.83	0.60
3:M:38:PRO:HD2	3:M:63:GLU:HB3	1.84	0.60
3:N:38:PRO:HD2	3:N:63:GLU:HB3	1.84	0.60
4:J:82:HIS:HE1	4:J:161:THR:HB	1.67	0.60
2:E:28:ARG:HB2	2:E:38:SER:HA	1.84	0.59
3:N:118:ILE:HB	3:N:138:ARG:HG2	1.84	0.59
3:P:70:PRO:HG2	3:P:132:LEU:HB3	1.84	0.59
3:P:27:GLU:N	3:P:27:GLU:OE1	2.35	0.59
3:R:38:PRO:HD2	3:R:63:GLU:HB3	1.85	0.59
2:B:87:GLY:HA3	4:G:40:GLN:HE21	1.67	0.59
3:Q:38:PRO:HD2	3:Q:63:GLU:HB3	1.85	0.59
3:O:86:ARG:O	3:O:91:LYS:NZ	2.34	0.59
3:O:3:ASN:HD21	4:H:131:LEU:HD12	1.68	0.59
4:K:1:MET:SD	4:K:1:MET:N	2.64	0.59
3:M:146:LYS:NZ	3:O:83:ASP:OD2	2.32	0.59
3:R:118:ILE:HB	3:R:138:ARG:HG2	1.85	0.59
3:P:27:GLU:HG3	3:P:72:THR:HG21	1.84	0.58
2:D:82:ASP:OD1	2:D:83:ARG:N	2.36	0.58
1:S:94:MET:HB2	1:S:207:VAL:HG11	1.85	0.58
2:E:2:ILE:HG23	2:E:3:PRO:HD3	1.85	0.58
2:F:23:ARG:NH2	2:F:89:GLN:OE1	2.36	0.58
2:F:82:ASP:OD1	2:F:83:ARG:N	2.37	0.58
3:Q:27:GLU:N	3:Q:27:GLU:OE1	2.35	0.58
2:B:23:ARG:NH2	2:B:89:GLN:OE1	2.37	0.58
3:N:15:ALA:HB3	3:N:19:PHE:H	1.69	0.57
3:M:7:PHE:HE2	4:G:134:ARG:HG3	1.69	0.57
3:N:120:GLY:O	3:Q:40:PHE:N	2.37	0.57
2:C:23:ARG:NH2	2:C:89:GLN:OE1	2.37	0.57
3:O:38:PRO:HD2	3:O:63:GLU:HB3	1.85	0.57
1:S:110:PHE:HB2	1:S:131:THR:HB	1.86	0.57
2:A:34:ALA:HB1	4:J:33:VAL:HA	1.87	0.57
2:B:101:SER:OG	2:B:102:GLN:N	2.38	0.57
2:F:104:SER:OG	2:F:105:TRP:N	2.37	0.57
3:R:15:ALA:HB3	3:R:19:PHE:H	1.69	0.57
4:K:27:PHE:HB3	4:K:47:PRO:HG3	1.86	0.57
2:C:33:GLN:NE2	4:H:4:GLY:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:15:ALA:HB3	3:Q:19:PHE:H	1.69	0.57
3:O:119:ASP:OD1	3:O:138:ARG:N	2.38	0.57
2:A:82:ASP:OD1	2:A:83:ARG:N	2.38	0.57
2:B:57:GLN:HB2	2:C:81:LEU:HD23	1.86	0.57
2:D:50:VAL:O	2:E:108:GLN:NE2	2.38	0.57
2:B:43:PRO:HG3	2:B:132:PHE:HE1	1.70	0.56
1:S:343:ARG:NH2	1:S:366:CYS:O	2.36	0.56
2:B:33:GLN:NE2	4:G:4:GLY:O	2.38	0.56
3:M:15:ALA:HB3	3:M:19:PHE:H	1.68	0.56
4:K:84:GLU:HG2	4:K:161:THR:HG22	1.88	0.56
1:S:36:ILE:HD12	1:S:37:PRO:HD2	1.86	0.56
1:S:451:ARG:NH1	3:R:73:GLU:OE2	2.35	0.56
2:C:82:ASP:OD1	2:C:83:ARG:N	2.38	0.56
1:S:205:VAL:HG13	1:S:206:ASN:H	1.70	0.56
3:P:114:ASN:HB2	3:P:142:GLU:HB3	1.88	0.56
3:Q:118:ILE:HB	3:Q:138:ARG:HG2	1.88	0.56
4:H:27:PHE:HB3	4:H:47:PRO:HG3	1.88	0.56
3:O:26:THR:OG1	4:H:119:ARG:NH1	2.31	0.56
3:R:3:ASN:ND2	4:J:131:LEU:HB2	2.21	0.56
1:S:193:MET:HB3	1:S:197:LEU:HD13	1.87	0.56
3:R:70:PRO:HD3	3:R:134:THR:HA	1.88	0.56
2:C:104:SER:OG	2:C:105:TRP:N	2.38	0.55
3:P:106:ASP:N	3:P:106:ASP:OD1	2.38	0.55
2:D:104:SER:OG	2:D:105:TRP:N	2.39	0.55
1:S:12:SER:OG	1:S:13:GLY:N	2.39	0.55
3:Q:6:ALA:O	3:Q:9:SER:OG	2.22	0.55
3:Q:33:ASP:O	3:Q:67:ASN:ND2	2.40	0.55
1:S:256:ASN:HB3	1:S:385:LYS:HD3	1.88	0.55
3:N:114:ASN:HB2	3:N:142:GLU:HB3	1.89	0.55
2:A:101:SER:OG	2:A:102:GLN:N	2.40	0.55
2:F:43:PRO:HG3	2:F:132:PHE:HE1	1.71	0.55
4:G:145:ASN:ND2	4:G:151:GLU:OE1	2.40	0.55
4:H:145:ASN:ND2	4:H:151:GLU:OE1	2.40	0.55
2:A:55:ARG:NH1	2:A:68:ASN:OD1	2.40	0.55
3:P:118:ILE:HB	3:P:138:ARG:HG2	1.87	0.55
3:R:33:ASP:O	3:R:67:ASN:ND2	2.40	0.55
3:R:27:GLU:OE1	3:R:27:GLU:N	2.40	0.55
3:R:106:ASP:OD1	3:R:106:ASP:N	2.39	0.55
2:E:55:ARG:NH1	2:E:68:ASN:OD1	2.40	0.54
3:N:33:ASP:O	3:N:67:ASN:ND2	2.40	0.54
3:M:27:GLU:OE1	3:M:27:GLU:N	2.34	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:82:HIS:HE1	4:H:161:THR:HB	1.72	0.54
4:I:22:GLN:NE2	4:I:27:PHE:O	2.37	0.54
2:D:6:ASN:OD1	2:D:75:ASN:ND2	2.40	0.54
2:D:55:ARG:NH1	2:D:68:ASN:OD1	2.40	0.54
2:C:6:ASN:OD1	2:C:75:ASN:ND2	2.41	0.54
2:E:23:ARG:NH2	2:E:89:GLN:OE1	2.40	0.54
4:J:119:ARG:HG2	4:L:64:THR:HG21	1.90	0.54
2:A:6:ASN:OD1	2:A:75:ASN:ND2	2.40	0.54
2:F:101:SER:OG	2:F:102:GLN:N	2.41	0.54
4:G:22:GLN:NE2	4:G:27:PHE:O	2.38	0.54
3:P:3:ASN:HA	4:L:82:HIS:HE1	1.72	0.54
3:Q:106:ASP:OD1	3:Q:106:ASP:N	2.40	0.54
3:R:6:ALA:O	3:R:9:SER:OG	2.24	0.54
4:G:1:MET:SD	4:G:1:MET:N	2.77	0.54
1:S:148:ILE:HG22	1:S:156:LEU:HB3	1.89	0.53
1:S:490:LYS:HE3	4:K:182:GLY:HA3	1.90	0.53
2:C:57:GLN:HB2	2:D:81:LEU:HD23	1.90	0.53
3:O:3:ASN:HA	4:H:82:HIS:NE2	2.23	0.53
4:I:35:LYS:HG3	4:I:50:PHE:HB3	1.90	0.53
4:L:27:PHE:HB3	4:L:47:PRO:HG3	1.89	0.53
1:S:70:PHE:CD2	1:S:302:GLU:HB3	2.44	0.53
3:O:118:ILE:HB	3:O:138:ARG:HG2	1.90	0.53
3:R:26:THR:O	4:J:119:ARG:NH2	2.42	0.53
3:R:71:ASN:OD1	3:R:76:ARG:NH1	2.41	0.53
4:I:27:PHE:HB3	4:I:47:PRO:HG3	1.90	0.53
4:K:22:GLN:NE2	4:K:27:PHE:O	2.38	0.53
4:J:145:ASN:ND2	4:J:151:GLU:OE1	2.42	0.53
4:L:145:ASN:ND2	4:L:151:GLU:OE1	2.41	0.53
1:S:142:SER:HA	1:S:145:GLN:HE21	1.73	0.53
1:S:296:VAL:HG13	1:S:297:GLU:H	1.74	0.53
3:O:15:ALA:HB3	3:O:19:PHE:H	1.73	0.53
4:J:22:GLN:NE2	4:J:27:PHE:O	2.36	0.53
2:C:55:ARG:NH1	2:C:68:ASN:OD1	2.41	0.53
1:S:118:MET:HB2	1:S:185:ALA:HB2	1.90	0.53
2:C:43:PRO:HG3	2:C:132:PHE:HE1	1.74	0.53
1:S:186:LYS:NZ	1:S:192:ASP:OD2	2.34	0.53
2:E:104:SER:OG	2:E:105:TRP:N	2.37	0.53
3:R:3:ASN:HD21	4:J:131:LEU:HB2	1.74	0.53
1:S:114:VAL:HG13	1:S:127:THR:HG22	1.90	0.53
2:E:101:SER:OG	2:E:102:GLN:N	2.42	0.53
4:L:84:GLU:HG2	4:L:161:THR:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:ARG:NH1	2:F:68:ASN:OD1	2.43	0.52
3:P:15:ALA:HB3	3:P:19:PHE:H	1.73	0.52
2:F:6:ASN:OD1	2:F:75:ASN:ND2	2.42	0.52
3:O:40:PHE:N	3:Q:120:GLY:O	2.36	0.52
2:D:101:SER:OG	2:D:102:GLN:N	2.42	0.52
2:E:33:GLN:NE2	4:K:4:GLY:O	2.42	0.52
4:G:27:PHE:HB3	4:G:47:PRO:HG3	1.92	0.52
2:B:104:SER:OG	2:B:105:TRP:N	2.38	0.52
1:S:350:THR:OG1	1:S:351:GLN:N	2.42	0.52
2:A:81:LEU:HD23	2:F:57:GLN:HB2	1.92	0.52
2:B:6:ASN:OD1	2:B:75:ASN:ND2	2.43	0.52
3:M:27:GLU:HB3	4:J:63:ALA:HB2	1.91	0.52
3:Q:17:ARG:HB2	3:Q:96:ASP:HB3	1.92	0.52
3:Q:119:ASP:OD1	3:Q:138:ARG:N	2.40	0.52
4:I:145:ASN:ND2	4:I:151:GLU:OE1	2.42	0.52
2:E:6:ASN:OD1	2:E:75:ASN:ND2	2.42	0.52
3:P:6:ALA:O	3:P:9:SER:OG	2.27	0.52
1:S:483:ASN:ND2	4:K:177:ASP:OD1	2.43	0.52
3:O:124:ASN:HB3	3:O:132:LEU:HD11	1.92	0.52
3:M:33:ASP:O	3:M:67:ASN:ND2	2.43	0.52
3:O:17:ARG:HB2	3:O:96:ASP:HB3	1.92	0.52
3:P:40:PHE:N	3:R:120:GLY:O	2.38	0.52
3:M:120:GLY:O	3:R:40:PHE:N	2.39	0.51
2:C:55:ARG:NH2	2:C:69:TYR:O	2.33	0.51
2:D:25:PHE:HZ	2:D:28:ARG:HG2	1.75	0.51
2:D:16:GLY:H	2:E:3:PRO:HD2	1.75	0.51
3:R:17:ARG:HB2	3:R:96:ASP:HB3	1.92	0.51
2:A:103:GLY:HA3	2:A:113:VAL:HG13	1.93	0.51
4:H:133:LEU:HB2	4:H:159:VAL:HB	1.93	0.51
4:L:35:LYS:HG3	4:L:50:PHE:HB3	1.92	0.51
4:I:31:GLU:HB2	4:I:48:THR:HG22	1.92	0.51
4:K:3:ASP:OD1	4:K:4:GLY:N	2.43	0.51
2:A:55:ARG:NH2	2:A:69:TYR:O	2.33	0.51
1:S:131:THR:HA	1:S:134:ALA:HB2	1.93	0.51
1:S:28:ARG:NH2	1:S:226:SER:OG	2.42	0.51
2:A:69:TYR:HB3	2:A:115:LEU:HD11	1.93	0.50
3:N:106:ASP:N	3:N:106:ASP:OD1	2.44	0.50
4:I:146:ASP:OD1	4:I:146:ASP:N	2.37	0.50
4:K:133:LEU:HB2	4:K:159:VAL:HB	1.94	0.50
1:S:85:ARG:HH22	1:S:88:ASN:H	1.59	0.50
2:C:50:VAL:O	2:D:108:GLN:NE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:17:ARG:HB2	3:M:96:ASP:HB3	1.94	0.50
2:A:67:ARG:HH21	4:G:148:HIS:CD2	2.28	0.50
2:B:103:GLY:HA3	2:B:113:VAL:HG13	1.93	0.50
2:E:103:GLY:HA3	2:E:113:VAL:HG13	1.94	0.50
3:Q:127:ALA:HB2	3:Q:133:LYS:HG2	1.94	0.50
4:I:90:SER:HG	4:I:153:HIS:CD2	2.28	0.50
2:D:23:ARG:NH2	2:D:89:GLN:OE1	2.45	0.50
4:I:1:MET:SD	4:I:1:MET:N	2.74	0.50
4:I:104:THR:HG22	4:I:106:SER:H	1.75	0.50
2:D:67:ARG:HH21	4:K:148:HIS:CD2	2.29	0.50
3:Q:70:PRO:HD3	3:Q:134:THR:HA	1.93	0.50
1:S:25:LEU:HD11	1:S:383:TRP:HB3	1.93	0.50
1:S:30:MET:HE1	1:S:219:VAL:HA	1.94	0.50
1:S:67:TYR:OH	1:S:80:SER:O	2.30	0.50
1:S:239:LEU:HB2	1:S:244:ILE:HG13	1.93	0.50
3:N:3:ASN:HA	4:K:82:HIS:NE2	2.27	0.50
4:G:35:LYS:HG3	4:G:50:PHE:HB3	1.93	0.50
2:D:69:TYR:HB3	2:D:115:LEU:HD11	1.93	0.50
2:D:2:ILE:HG23	2:D:3:PRO:HD3	1.94	0.50
3:P:17:ARG:HB2	3:P:96:ASP:HB3	1.94	0.49
4:L:3:ASP:OD1	4:L:4:GLY:N	2.45	0.49
4:L:22:GLN:NE2	4:L:27:PHE:O	2.36	0.49
1:S:119:VAL:HB	1:S:122:ALA:HB3	1.93	0.49
3:P:8:GLY:HA2	4:L:119:ARG:HD2	1.93	0.49
3:O:106:ASP:OD1	3:O:106:ASP:N	2.44	0.49
4:H:39:THR:OG1	4:H:41:GLN:OE1	2.25	0.49
4:K:35:LYS:HG3	4:K:50:PHE:HB3	1.94	0.49
2:A:100:GLU:N	2:A:115:LEU:O	2.40	0.49
2:D:100:GLU:N	2:D:115:LEU:O	2.39	0.49
3:Q:75:GLU:OE2	3:Q:135:LYS:HD3	2.13	0.49
4:I:90:SER:OG	4:I:91:SER:N	2.45	0.49
4:K:104:THR:N	4:K:107:ASP:OD2	2.45	0.49
3:N:17:ARG:HB2	3:N:96:ASP:HB3	1.94	0.49
4:J:138:ILE:HB	4:L:56:ASP:HB3	1.95	0.49
4:H:35:LYS:HG3	4:H:50:PHE:HB3	1.95	0.49
3:N:27:GLU:HB3	4:I:63:ALA:HB2	1.95	0.49
4:J:90:SER:HG	4:J:153:HIS:CD2	2.31	0.49
4:H:90:SER:HG	4:H:153:HIS:CD2	2.31	0.49
1:S:167:THR:OG1	1:S:169:GLN:HB2	2.12	0.48
1:S:400:ASN:O	4:K:75:TYR:OH	2.31	0.48
3:N:40:PHE:N	3:P:120:GLY:O	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:317:ASN:HD22	1:S:493:ALA:HB3	1.77	0.48
2:F:33:GLN:NE2	4:L:4:GLY:O	2.45	0.48
1:S:465:ILE:HA	1:S:483:ASN:O	2.13	0.48
3:N:126:VAL:HB	3:Q:34:PRO:HG2	1.95	0.48
4:J:47:PRO:HB3	4:J:93:HIS:CG	2.48	0.48
4:J:35:LYS:HG3	4:J:50:PHE:HB3	1.95	0.48
4:H:22:GLN:NE2	4:H:27:PHE:O	2.36	0.48
4:K:126:LYS:HB2	4:K:131:LEU:HD21	1.96	0.48
2:D:33:GLN:NE2	4:I:4:GLY:O	2.46	0.48
3:P:3:ASN:OD1	4:L:131:LEU:HB2	2.13	0.48
3:O:44:ASP:HB3	3:O:56:TRP:HE3	1.79	0.48
3:M:34:PRO:HG2	3:O:126:VAL:HB	1.96	0.48
4:K:68:LEU:HG	4:K:75:TYR:CE1	2.48	0.48
1:S:396:PHE:CE2	4:K:174:TYR:HA	2.48	0.48
3:M:106:ASP:OD1	3:M:106:ASP:N	2.44	0.48
3:N:7:PHE:HE2	4:K:134:ARG:HG3	1.78	0.48
2:F:74:ALA:HB3	2:F:78:MET:SD	2.54	0.47
3:N:16:SER:HB2	3:N:97:VAL:HG22	1.95	0.47
4:J:27:PHE:HB3	4:J:47:PRO:HG3	1.96	0.47
2:A:23:ARG:NH2	2:A:89:GLN:OE1	2.46	0.47
2:E:24:LYS:HA	2:E:88:ASP:OD1	2.15	0.47
2:F:106:PHE:O	2:F:110:GLY:N	2.46	0.47
3:M:126:VAL:HB	3:R:34:PRO:HG2	1.96	0.47
2:C:101:SER:OG	2:C:102:GLN:N	2.47	0.47
3:R:27:GLU:HG3	3:R:72:THR:HG21	1.95	0.47
4:L:90:SER:HG	4:L:153:HIS:CD2	2.31	0.47
4:J:64:THR:HG21	4:G:119:ARG:HD2	1.97	0.47
2:F:2:ILE:HG23	2:F:3:PRO:HD3	1.96	0.47
3:P:3:ASN:HA	4:L:82:HIS:CE1	2.49	0.47
1:S:36:ILE:HG23	1:S:85:ARG:HG2	1.96	0.47
2:D:30:LYS:HZ1	4:I:32:VAL:H	1.62	0.47
1:S:170:PHE:CD2	1:S:197:LEU:HG	2.50	0.47
1:S:201:THR:OG1	1:S:203:ASN:OD1	2.28	0.47
3:M:44:ASP:HB3	3:M:56:TRP:CE3	2.49	0.47
3:N:119:ASP:OD1	3:N:138:ARG:N	2.48	0.47
3:R:114:ASN:HB2	3:R:142:GLU:HB3	1.96	0.47
4:J:90:SER:OG	4:J:91:SER:N	2.47	0.47
4:G:128:LEU:HD23	4:G:128:LEU:HA	1.78	0.47
2:F:55:ARG:NH2	2:F:69:TYR:O	2.34	0.47
1:S:113:GLY:HA2	1:S:191:GLN:HG3	1.95	0.47
1:S:401:ALA:O	4:K:75:TYR:OH	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:GLU:HB2	2:E:41:GLU:HG2	1.97	0.47
4:H:6:LEU:HD21	4:H:160:VAL:HG11	1.96	0.47
4:L:5:GLU:HG2	4:L:9:LYS:HE3	1.97	0.47
3:R:75:GLU:OE2	3:R:135:LYS:HD3	2.15	0.47
4:L:90:SER:OG	4:L:91:SER:N	2.48	0.47
1:S:331:SER:O	1:S:331:SER:OG	2.27	0.46
3:N:30:ASP:OD1	3:N:31:ASP:N	2.49	0.46
4:G:90:SER:OG	4:G:91:SER:N	2.47	0.46
3:M:30:ASP:OD2	4:J:60:GLY:N	2.45	0.46
3:M:30:ASP:OD1	3:M:31:ASP:N	2.48	0.46
3:N:34:PRO:HG2	3:P:126:VAL:HB	1.97	0.46
3:R:8:GLY:HA2	4:J:119:ARG:HD2	1.96	0.46
4:H:59:ARG:NE	4:H:84:GLU:OE2	2.31	0.46
4:H:90:SER:OG	4:H:91:SER:N	2.47	0.46
4:K:90:SER:OG	4:K:91:SER:N	2.48	0.46
1:S:46:ASN:OD1	1:S:47:SER:N	2.48	0.46
1:S:254:GLN:O	1:S:256:ASN:N	2.44	0.46
2:F:7:LEU:HD12	2:F:7:LEU:HA	1.77	0.46
3:M:114:ASN:HB2	3:M:142:GLU:HB3	1.97	0.46
3:Q:26:THR:O	4:I:119:ARG:NH2	2.48	0.46
2:B:25:PHE:CZ	2:B:28:ARG:HB3	2.51	0.46
2:B:28:ARG:HB2	2:B:38:SER:HA	1.97	0.46
3:M:44:ASP:HB3	3:M:56:TRP:HE3	1.80	0.46
3:M:16:SER:HB2	3:M:97:VAL:HG22	1.96	0.46
3:P:72:THR:O	3:P:76:ARG:N	2.31	0.46
4:L:90:SER:HB2	4:L:155:SER:HB3	1.97	0.46
3:R:69:ILE:HG13	4:L:60:GLY:HA3	1.98	0.46
2:C:30:LYS:HA	2:C:36:TYR:HA	1.98	0.46
2:C:74:ALA:HB3	2:C:78:MET:SD	2.55	0.46
4:J:128:LEU:HD23	4:J:128:LEU:HA	1.80	0.46
1:S:30:MET:HB2	1:S:234:PHE:HA	1.97	0.46
1:S:136:SER:O	1:S:140:VAL:HG23	2.16	0.46
3:M:40:PHE:N	3:O:120:GLY:O	2.43	0.46
4:I:90:SER:HB2	4:I:155:SER:HB3	1.97	0.46
4:L:145:ASN:OD1	4:L:145:ASN:N	2.49	0.46
2:B:24:LYS:HA	2:B:88:ASP:OD1	2.16	0.46
3:N:36:ASP:OD1	3:N:37:SER:N	2.49	0.46
1:S:91:ILE:N	1:S:210:GLN:O	2.48	0.45
2:D:118:ASP:OD2	2:D:119:ILE:N	2.49	0.45
4:H:56:ASP:HB3	4:I:138:ILE:HB	1.97	0.45
2:D:106:PHE:O	2:D:110:GLY:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:316:GLN:N	1:S:316:GLN:HE21	2.14	0.45
2:B:34:ALA:HB1	4:G:33:VAL:HA	1.98	0.45
2:C:106:PHE:O	2:C:110:GLY:N	2.47	0.45
3:O:6:ALA:O	3:O:9:SER:OG	2.33	0.45
3:O:72:THR:O	3:O:76:ARG:N	2.31	0.45
2:E:36:TYR:C	4:K:41:GLN:HE22	2.15	0.45
4:H:38:PRO:HG2	4:I:97:PRO:HG3	1.98	0.45
4:H:90:SER:HB2	4:H:155:SER:HB3	1.98	0.45
2:B:55:ARG:NH1	2:B:68:ASN:OD1	2.49	0.45
4:H:84:GLU:HG2	4:H:161:THR:HG22	1.98	0.45
3:P:63:GLU:HG3	3:P:140:ARG:HG2	1.98	0.45
4:L:80:ARG:HD2	4:L:163:ASN:ND2	2.31	0.45
1:S:98:ASP:H	1:S:203:ASN:HB2	1.82	0.45
1:S:149:ARG:HE	1:S:158:GLN:HA	1.80	0.45
3:N:58:ARG:HA	3:N:58:ARG:HD2	1.83	0.45
3:P:75:GLU:OE1	3:P:135:LYS:HD3	2.16	0.45
2:A:17:THR:HG21	2:A:47:ALA:HB1	1.97	0.45
2:D:34:ALA:HB1	4:I:33:VAL:HA	1.98	0.45
3:O:34:PRO:HG2	3:Q:126:VAL:HB	1.98	0.45
4:K:64:THR:HG21	4:L:119:ARG:HG2	1.99	0.45
1:S:141:ALA:O	1:S:145:GLN:HG2	2.16	0.45
2:D:103:GLY:HA3	2:D:113:VAL:HG13	1.99	0.45
2:F:17:THR:HG21	2:F:47:ALA:HB1	1.98	0.45
3:N:70:PRO:HD3	3:N:134:THR:HA	1.99	0.45
1:S:145:GLN:HA	1:S:148:ILE:HG12	1.99	0.45
2:E:74:ALA:HB3	2:E:78:MET:SD	2.57	0.45
4:L:128:LEU:HD23	4:L:128:LEU:HA	1.81	0.45
2:C:7:LEU:HD12	2:C:7:LEU:HA	1.75	0.44
4:I:47:PRO:HB3	4:I:93:HIS:CG	2.52	0.44
4:I:50:PHE:HE1	4:I:92:LEU:HB2	1.81	0.44
4:K:59:ARG:NE	4:K:84:GLU:OE2	2.30	0.44
3:M:70:PRO:HD3	3:M:134:THR:HA	2.00	0.44
4:K:56:ASP:HB3	4:L:138:ILE:HB	1.99	0.44
2:D:119:ILE:HD13	2:D:119:ILE:HA	1.81	0.44
4:G:62:PRO:HB2	4:G:79:THR:HG23	2.00	0.44
1:S:91:ILE:HD12	1:S:210:GLN:HB2	1.99	0.44
2:A:2:ILE:HG23	2:A:3:PRO:HD3	1.98	0.44
3:M:10:ILE:O	3:M:102:VAL:HA	2.17	0.44
3:O:58:ARG:HA	3:O:58:ARG:HD2	1.81	0.44
4:G:90:SER:HB2	4:G:155:SER:HB3	1.99	0.44
4:H:104:THR:N	4:H:107:ASP:OD1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:33:GLN:NE2	4:J:4:GLY:O	2.50	0.44
2:B:33:GLN:HE22	4:G:4:GLY:C	2.21	0.44
4:I:130:PHE:O	4:I:131:LEU:HD12	2.17	0.44
4:K:122:ILE:HG23	4:K:131:LEU:HD22	2.00	0.44
1:S:215:PRO:HB2	1:S:216:ASP:OD1	2.17	0.44
2:E:26:GLU:CD	2:E:27:GLN:HG3	2.38	0.44
4:J:166:ILE:HD12	4:G:111:TYR:CE1	2.52	0.44
4:I:59:ARG:NE	4:I:84:GLU:OE2	2.32	0.44
1:S:164:ASN:O	1:S:168:ASN:CA	2.66	0.44
1:S:231:SER:HB3	1:S:259:ILE:HG23	1.98	0.44
2:B:74:ALA:HB3	2:B:78:MET:SD	2.57	0.44
4:K:90:SER:HB2	4:K:155:SER:HB3	2.00	0.44
2:D:55:ARG:NH2	2:D:69:TYR:O	2.34	0.44
4:H:6:LEU:HD12	4:H:6:LEU:HA	1.85	0.44
4:L:6:LEU:HD21	4:L:160:VAL:HG11	2.00	0.44
1:S:147:GLU:HA	1:S:150:LYS:HG3	2.00	0.43
2:B:2:ILE:HG23	2:B:3:PRO:HD3	1.98	0.43
2:B:106:PHE:O	2:B:110:GLY:N	2.47	0.43
3:Q:63:GLU:OE2	3:Q:140:ARG:NE	2.51	0.43
3:R:7:PHE:HE2	4:J:134:ARG:HG3	1.83	0.43
4:L:59:ARG:NE	4:L:84:GLU:OE2	2.30	0.43
1:S:435:ILE:HG23	1:S:439:GLN:HB2	1.99	0.43
1:S:463:ILE:HA	1:S:485:THR:O	2.18	0.43
2:D:17:THR:HG21	2:D:47:ALA:HB1	1.99	0.43
4:G:56:ASP:HB3	4:H:138:ILE:HB	2.00	0.43
4:L:133:LEU:HB2	4:L:159:VAL:HB	2.00	0.43
3:O:33:ASP:O	3:O:67:ASN:ND2	2.51	0.43
3:P:58:ARG:HD2	3:P:58:ARG:HA	1.79	0.43
3:Q:114:ASN:HB2	3:Q:142:GLU:HB3	2.01	0.43
4:I:40:GLN:O	4:I:41:GLN:HG3	2.19	0.43
1:S:251:ASN:HB3	1:S:260:TYR:CE2	2.53	0.43
2:C:103:GLY:HA3	2:C:113:VAL:HG13	2.01	0.43
2:F:103:GLY:HA3	2:F:113:VAL:HG13	2.00	0.43
4:I:166:ILE:HD12	4:K:111:TYR:CE1	2.53	0.43
3:P:6:ALA:HB2	3:R:132:LEU:CD1	2.48	0.43
3:P:34:PRO:HG2	3:R:126:VAL:HB	2.00	0.43
4:K:145:ASN:OD1	4:K:145:ASN:N	2.49	0.43
1:S:86:TRP:HD1	1:S:86:TRP:O	2.01	0.43
1:S:245:LYS:HE3	1:S:245:LYS:HB3	1.85	0.43
2:B:6:ASN:HB3	2:B:9:ARG:HB3	2.00	0.43
3:P:26:THR:OG1	4:L:119:ARG:NH1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:33:ASP:O	3:P:67:ASN:ND2	2.50	0.43
3:M:102:VAL:HG22	3:M:110:ILE:HB	2.01	0.43
3:N:3:ASN:ND2	4:K:131:LEU:HD12	2.30	0.43
3:N:70:PRO:HG3	3:N:133:LYS:O	2.19	0.43
3:O:30:ASP:OD1	3:O:31:ASP:N	2.52	0.43
1:S:37:PRO:HG3	1:S:96:VAL:HG11	2.00	0.43
2:D:58:TYR:HE2	2:D:67:ARG:HG3	1.84	0.43
2:D:58:TYR:OH	2:D:67:ARG:NH1	2.51	0.43
3:N:44:ASP:HB3	3:N:56:TRP:HE3	1.83	0.43
3:Q:121:VAL:HB	3:Q:135:LYS:HE3	2.01	0.43
3:R:58:ARG:HD2	3:R:58:ARG:HA	1.82	0.43
4:I:92:LEU:HD12	4:I:92:LEU:HA	1.89	0.43
2:A:106:PHE:O	2:A:110:GLY:N	2.46	0.42
2:A:118:ASP:OD2	2:A:119:ILE:N	2.52	0.42
2:D:97:PHE:HA	2:D:117:VAL:O	2.19	0.42
3:M:6:ALA:O	3:M:9:SER:OG	2.37	0.42
3:R:70:PRO:HG3	3:R:133:LYS:O	2.19	0.42
3:R:116:THR:HG23	3:R:118:ILE:HD11	2.00	0.42
3:R:119:ASP:OD2	3:R:138:ARG:NH1	2.52	0.42
4:G:131:LEU:HD23	4:G:131:LEU:HA	1.76	0.42
4:H:145:ASN:OD1	4:H:145:ASN:N	2.50	0.42
2:A:97:PHE:HA	2:A:117:VAL:O	2.19	0.42
3:N:104:MET:HE2	3:N:104:MET:HB2	1.94	0.42
4:I:128:LEU:HD23	4:I:128:LEU:HA	1.80	0.42
1:S:378:TYR:O	1:S:382:ILE:HG13	2.20	0.42
4:I:145:ASN:OD1	4:I:145:ASN:N	2.46	0.42
4:L:92:LEU:HD12	4:L:92:LEU:HA	1.92	0.42
1:S:221:LYS:O	1:S:225:VAL:HG23	2.20	0.42
1:S:395:LEU:HD13	1:S:415:VAL:HG21	2.00	0.42
4:J:40:GLN:O	4:J:41:GLN:HG3	2.19	0.42
4:J:145:ASN:OD1	4:J:145:ASN:N	2.46	0.42
4:K:82:HIS:HE1	4:K:161:THR:HB	1.84	0.42
4:L:90:SER:HG	4:L:153:HIS:CE1	2.37	0.42
1:S:488:TYR:HD1	1:S:489:SER:H	1.67	0.42
2:A:119:ILE:HD13	2:A:119:ILE:HA	1.81	0.42
3:N:44:ASP:HB3	3:N:56:TRP:CE3	2.54	0.42
3:Q:78:LEU:HD23	3:Q:78:LEU:HA	1.92	0.42
4:J:97:PRO:HG3	4:L:38:PRO:HG2	2.00	0.42
1:S:143:ILE:O	1:S:147:GLU:HG2	2.20	0.42
1:S:401:ALA:HB1	4:K:172:ALA:HB1	2.02	0.42
2:B:67:ARG:HH22	4:H:144:GLU:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:63:GLU:HG3	3:O:140:ARG:HG2	2.02	0.42
3:R:127:ALA:HB2	3:R:133:LYS:HG2	2.01	0.42
4:J:59:ARG:NE	4:J:84:GLU:OE2	2.32	0.42
4:J:90:SER:HB2	4:J:155:SER:HB3	2.01	0.42
4:H:90:SER:HG	4:H:153:HIS:CE1	2.37	0.42
2:D:16:GLY:H	2:E:3:PRO:CD	2.33	0.42
2:F:24:LYS:HA	2:F:88:ASP:OD1	2.20	0.42
3:O:3:ASN:ND2	4:H:131:LEU:HD12	2.35	0.42
3:R:28:PHE:HB3	3:R:34:PRO:HB3	2.01	0.42
3:R:44:ASP:HB3	3:R:56:TRP:CE3	2.54	0.42
4:J:130:PHE:O	4:J:131:LEU:HD12	2.19	0.42
4:I:7:ILE:HG12	4:I:51:PHE:HE2	1.84	0.42
4:K:128:LEU:HD23	4:K:128:LEU:HA	1.80	0.42
2:A:58:TYR:OH	2:A:67:ARG:NH1	2.52	0.42
2:F:67:ARG:HH22	4:J:144:GLU:HB2	1.84	0.42
3:P:63:GLU:OE2	3:P:140:ARG:NE	2.53	0.42
3:Q:44:ASP:HB3	3:Q:56:TRP:CE3	2.54	0.42
2:A:57:GLN:HB2	2:B:81:LEU:HD23	2.01	0.42
2:E:34:ALA:HB1	4:K:33:VAL:HA	2.00	0.42
3:M:3:ASN:HD21	4:G:131:LEU:HD12	1.84	0.42
4:K:62:PRO:HB2	4:K:79:THR:HG23	2.01	0.42
2:C:53:VAL:HG21	2:C:115:LEU:HD13	2.01	0.42
3:N:69:ILE:HD13	3:N:69:ILE:HA	1.84	0.42
3:P:85:ASN:ND2	3:P:96:ASP:OD1	2.47	0.42
1:S:260:TYR:CE1	1:S:282:THR:HB	2.55	0.41
3:M:70:PRO:HG3	3:M:133:LYS:O	2.19	0.41
4:G:37:GLN:HG2	4:G:41:GLN:HB2	2.02	0.41
4:L:31:GLU:OE1	4:L:46:ARG:HB2	2.20	0.41
2:A:58:TYR:HE2	2:A:67:ARG:HG3	1.84	0.41
2:C:35:GLN:HE21	2:C:35:GLN:HB2	1.68	0.41
4:J:146:ASP:OD1	4:J:146:ASP:N	2.38	0.41
2:C:6:ASN:HB3	2:C:9:ARG:HB3	2.02	0.41
2:D:57:GLN:HB2	2:E:81:LEU:HD23	2.01	0.41
3:M:143:LYS:HE2	3:M:143:LYS:HB2	1.85	0.41
4:G:38:PRO:HG2	4:H:97:PRO:HG3	2.03	0.41
4:I:46:ARG:O	4:I:48:THR:HG23	2.20	0.41
4:K:38:PRO:HG2	4:L:97:PRO:HG3	2.02	0.41
2:C:33:GLN:HE22	4:H:4:GLY:C	2.24	0.41
2:F:6:ASN:HB3	2:F:9:ARG:HB3	2.03	0.41
3:R:30:ASP:OD2	4:L:59:ARG:HD3	2.21	0.41
4:K:6:LEU:HD12	4:K:6:LEU:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:PHE:CZ	2:D:28:ARG:HG2	2.55	0.41
2:F:118:ASP:OD1	2:F:119:ILE:N	2.53	0.41
3:M:58:ARG:HA	3:M:58:ARG:HD2	1.84	0.41
3:N:6:ALA:O	3:N:9:SER:OG	2.37	0.41
3:P:14:THR:O	3:P:98:VAL:HA	2.21	0.41
4:I:53:LYS:HE3	4:I:85:THR:OG1	2.21	0.41
1:S:32:THR:HG22	1:S:86:TRP:HE3	1.85	0.41
1:S:251:ASN:HA	1:S:254:GLN:HB2	2.01	0.41
2:C:2:ILE:HG23	2:C:3:PRO:HD3	2.02	0.41
3:N:8:GLY:HA2	4:K:119:ARG:HG3	2.03	0.41
3:Q:30:ASP:OD1	3:Q:31:ASP:N	2.54	0.41
4:J:31:GLU:HB2	4:J:48:THR:HG22	2.02	0.41
4:J:62:PRO:HB2	4:J:79:THR:HG23	2.03	0.41
4:K:180:LEU:HD23	4:K:180:LEU:HA	1.77	0.41
2:E:18:GLN:N	2:E:18:GLN:OE1	2.54	0.41
4:I:62:PRO:HB2	4:I:79:THR:HG23	2.03	0.41
2:A:74:ALA:HB3	2:A:78:MET:SD	2.60	0.41
2:B:18:GLN:OE1	2:B:18:GLN:N	2.54	0.41
2:B:55:ARG:HB2	2:B:66:GLN:HE21	1.86	0.41
3:N:26:THR:HB	4:K:119:ARG:NH1	2.36	0.41
3:O:26:THR:HG21	4:G:64:THR:H	1.86	0.41
3:P:26:THR:HG21	4:K:64:THR:H	1.85	0.41
3:P:78:LEU:HD23	3:P:78:LEU:HA	1.94	0.41
3:Q:70:PRO:HG3	3:Q:133:LYS:O	2.21	0.41
3:Q:116:THR:HG23	3:Q:118:ILE:HD11	2.02	0.41
3:R:63:GLU:OE2	3:R:140:ARG:NE	2.53	0.41
3:R:121:VAL:HB	3:R:135:LYS:HE3	2.03	0.41
4:J:46:ARG:O	4:J:48:THR:HG23	2.20	0.41
4:G:69:ASP:OD2	4:G:71:THR:OG1	2.36	0.41
4:G:180:LEU:HD23	4:G:180:LEU:HA	1.91	0.41
4:I:157:ASP:N	4:I:157:ASP:OD1	2.54	0.41
2:B:55:ARG:NH2	2:B:69:TYR:O	2.35	0.41
2:F:53:VAL:HG21	2:F:115:LEU:HD13	2.03	0.41
3:R:27:GLU:HB3	4:L:63:ALA:HB2	2.02	0.41
1:S:27:LEU:HD11	1:S:233:LEU:HB2	2.03	0.40
1:S:297:GLU:O	1:S:300:PRO:HD2	2.21	0.40
3:R:69:ILE:HD13	3:R:69:ILE:HA	1.83	0.40
4:H:125:VAL:HG12	4:H:131:LEU:HD23	2.02	0.40
4:K:27:PHE:HE1	4:K:103:VAL:HG21	1.87	0.40
4:K:69:ASP:OD2	4:K:71:THR:OG1	2.38	0.40
4:L:157:ASP:N	4:L:157:ASP:OD1	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:8:GLY:HA2	4:H:119:ARG:HG3	2.02	0.40
4:H:6:LEU:HD22	4:H:162:TYR:CE1	2.56	0.40
4:H:157:ASP:N	4:H:157:ASP:OD1	2.54	0.40
4:K:92:LEU:HD12	4:K:92:LEU:HA	1.91	0.40
2:D:74:ALA:HB3	2:D:78:MET:SD	2.61	0.40
3:P:30:ASP:OD2	4:K:59:ARG:HD3	2.21	0.40
3:Q:28:PHE:HB3	3:Q:34:PRO:HB3	2.03	0.40
4:G:145:ASN:N	4:G:145:ASN:OD1	2.48	0.40
4:K:90:SER:HG	4:K:153:HIS:CD2	2.39	0.40
4:L:119:ARG:HA	4:L:119:ARG:HD3	1.90	0.40
3:O:4:ILE:O	3:Q:132:LEU:HD12	2.21	0.40
3:O:114:ASN:HB2	3:O:142:GLU:HB3	2.04	0.40
4:H:181:ILE:HD12	4:H:181:ILE:HA	1.92	0.40
4:I:6:LEU:HD21	4:I:160:VAL:HG11	2.03	0.40
4:I:82:HIS:CE1	4:I:161:THR:HB	2.49	0.40
4:L:104:THR:N	4:L:107:ASP:OD1	2.54	0.40
1:S:263:ALA:HB2	1:S:297:GLU:OE1	2.21	0.40
1:S:332:ASP:OD1	1:S:333:ASP:N	2.55	0.40
3:M:69:ILE:HA	3:M:70:PRO:HD2	1.95	0.40
4:J:157:ASP:OD1	4:J:157:ASP:N	2.55	0.40
4:G:90:SER:HG	4:G:153:HIS:CD2	2.39	0.40
4:H:131:LEU:HD23	4:H:131:LEU:HA	1.60	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	S	502/504 (100%)	401 (80%)	93 (18%)	8 (2%)	9	43
2	A	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
2	B	130/132 (98%)	119 (92%)	11 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	130/132 (98%)	118 (91%)	12 (9%)	0	100	100
2	D	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
2	E	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
2	F	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
3	M	148/150 (99%)	139 (94%)	9 (6%)	0	100	100
3	N	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
3	O	148/150 (99%)	137 (93%)	11 (7%)	0	100	100
3	P	148/150 (99%)	139 (94%)	9 (6%)	0	100	100
3	Q	148/150 (99%)	137 (93%)	11 (7%)	0	100	100
3	R	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
4	G	181/183 (99%)	172 (95%)	9 (5%)	0	100	100
4	H	181/183 (99%)	172 (95%)	9 (5%)	0	100	100
4	I	181/183 (99%)	174 (96%)	7 (4%)	0	100	100
4	J	181/183 (99%)	172 (95%)	9 (5%)	0	100	100
4	K	181/183 (99%)	172 (95%)	9 (5%)	0	100	100
4	L	181/183 (99%)	173 (96%)	8 (4%)	0	100	100
All	All	3256/3294 (99%)	2985 (92%)	263 (8%)	8 (0%)	50	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	296	VAL
1	S	315	SER
1	S	22	GLY
1	S	358	ALA
1	S	369	PRO
1	S	87	VAL
1	S	207	VAL
1	S	215	PRO

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	S	401/401 (100%)	383 (96%)	18 (4%)	27	61
2	A	112/112 (100%)	109 (97%)	3 (3%)	44	73
2	B	112/112 (100%)	107 (96%)	5 (4%)	27	61
2	C	112/112 (100%)	107 (96%)	5 (4%)	27	61
2	D	112/112 (100%)	110 (98%)	2 (2%)	59	81
2	E	112/112 (100%)	109 (97%)	3 (3%)	44	73
2	F	112/112 (100%)	107 (96%)	5 (4%)	27	61
3	M	122/122 (100%)	114 (93%)	8 (7%)	16	49
3	N	122/122 (100%)	112 (92%)	10 (8%)	11	40
3	O	122/122 (100%)	119 (98%)	3 (2%)	47	75
3	P	122/122 (100%)	114 (93%)	8 (7%)	16	49
3	Q	122/122 (100%)	117 (96%)	5 (4%)	30	63
3	R	122/122 (100%)	115 (94%)	7 (6%)	20	53
4	G	163/163 (100%)	155 (95%)	8 (5%)	25	59
4	H	163/163 (100%)	155 (95%)	8 (5%)	25	59
4	I	163/163 (100%)	159 (98%)	4 (2%)	47	75
4	J	163/163 (100%)	159 (98%)	4 (2%)	47	75
4	K	163/163 (100%)	155 (95%)	8 (5%)	25	59
4	L	163/163 (100%)	154 (94%)	9 (6%)	21	54
All	All	2783/2783 (100%)	2660 (96%)	123 (4%)	32	62

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	67	TYR
1	S	69	LYS
1	S	107	PHE
1	S	189	ASP
1	S	192	ASP
1	S	215	PRO
1	S	216	ASP
1	S	234	PHE
1	S	260	TYR
1	S	295	PHE
1	S	311	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	316	GLN
1	S	326	ARG
1	S	346	TYR
1	S	383	TRP
1	S	426	ASN
1	S	431	TYR
1	S	488	TYR
2	A	30	LYS
2	A	101	SER
2	A	132	PHE
2	B	28	ARG
2	B	36	TYR
2	B	88	ASP
2	B	104	SER
2	B	132	PHE
2	C	30	LYS
2	C	36	TYR
2	C	78	MET
2	C	104	SER
2	C	132	PHE
2	D	28	ARG
2	D	132	PHE
2	E	36	TYR
2	E	88	ASP
2	E	104	SER
2	F	27	GLN
2	F	36	TYR
2	F	101	SER
2	F	104	SER
2	F	132	PHE
3	M	7	PHE
3	M	16	SER
3	M	21	ASN
3	M	52	ASP
3	M	56	TRP
3	M	92	SER
3	M	119	ASP
3	M	128	SER
3	N	7	PHE
3	N	16	SER
3	N	21	ASN
3	N	52	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	56	TRP
3	N	83	ASP
3	N	92	SER
3	N	119	ASP
3	N	128	SER
3	N	146	LYS
3	O	21	ASN
3	O	52	ASP
3	O	128	SER
3	P	7	PHE
3	P	21	ASN
3	P	52	ASP
3	P	56	TRP
3	P	90	ASP
3	P	106	ASP
3	P	119	ASP
3	P	128	SER
3	Q	7	PHE
3	Q	21	ASN
3	Q	56	TRP
3	Q	83	ASP
3	Q	150	SER
3	R	5	SER
3	R	7	PHE
3	R	21	ASN
3	R	52	ASP
3	R	56	TRP
3	R	83	ASP
3	R	119	ASP
4	J	27	PHE
4	J	29	ASP
4	J	157	ASP
4	J	174	TYR
4	G	2	PHE
4	G	3	ASP
4	G	27	PHE
4	G	29	ASP
4	G	73	ARG
4	G	106	SER
4	G	146	ASP
4	G	174	TYR
4	H	2	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	3	ASP
4	H	35	LYS
4	H	37	GLN
4	H	55	PHE
4	H	73	ARG
4	H	88	GLN
4	H	174	TYR
4	I	3	ASP
4	I	29	ASP
4	I	157	ASP
4	I	174	TYR
4	K	1	MET
4	K	2	PHE
4	K	3	ASP
4	K	29	ASP
4	K	73	ARG
4	K	75	TYR
4	K	146	ASP
4	K	174	TYR
4	L	1	MET
4	L	2	PHE
4	L	10	MET
4	L	35	LYS
4	L	41	GLN
4	L	55	PHE
4	L	73	ARG
4	L	88	GLN
4	L	174	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	145	GLN
1	S	473	ASN
2	A	33	GLN
2	B	57	GLN
2	D	33	GLN
2	E	57	GLN
2	E	98	GLN
3	N	3	ASN
3	P	3	ASN
4	J	40	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	148	HIS
4	I	40	GLN
4	I	163	ASN
4	K	40	GLN
4	K	148	HIS
4	L	40	GLN
4	L	82	HIS

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 monosaccharides 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](#)

There are no chain breaks in this entry.

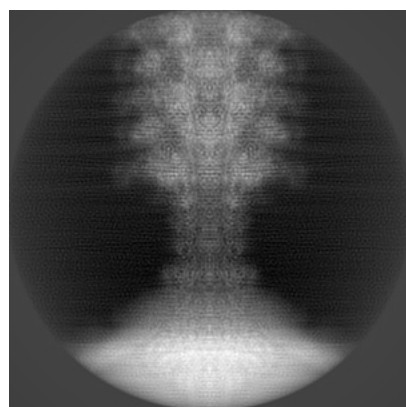
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44166. These allow visual inspection of the internal detail of the map and identification of artifacts.

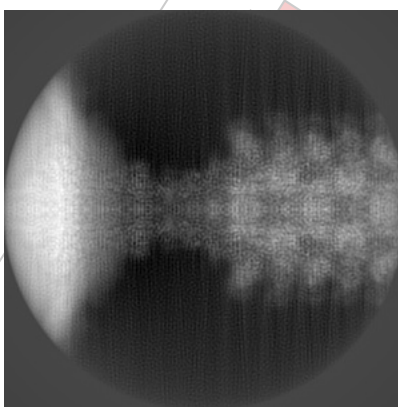
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

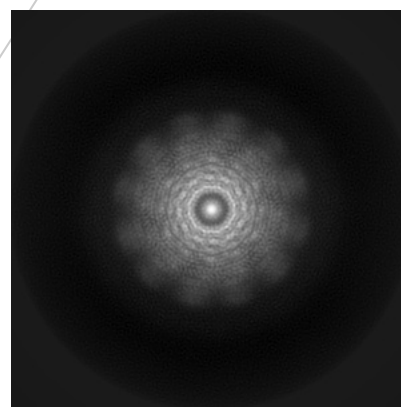
6.1.1 Primary map



X

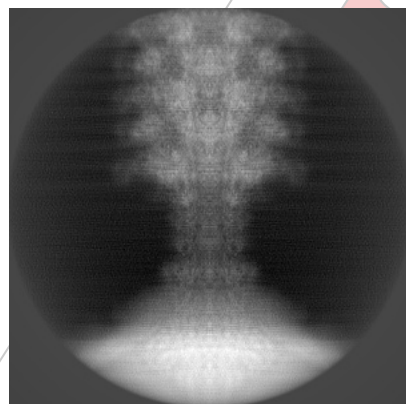


Y

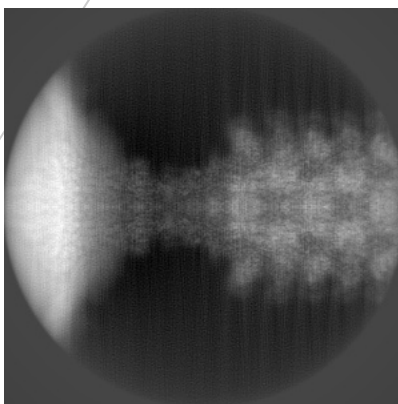


Z

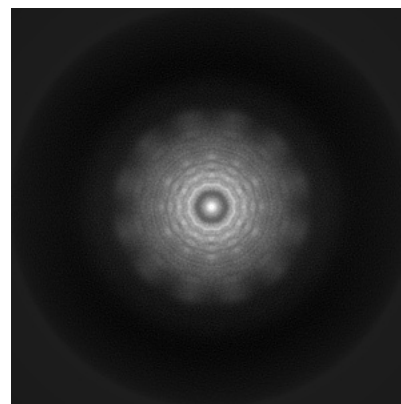
6.1.2 Raw map



X



Y

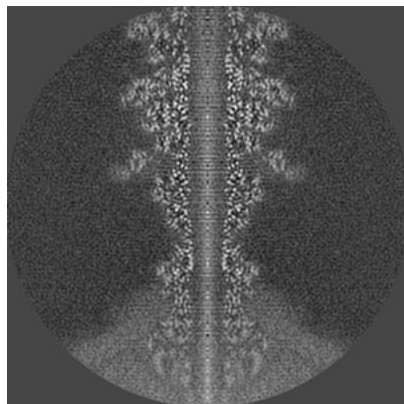


Z

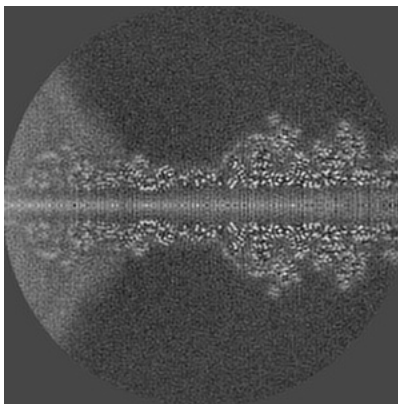
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

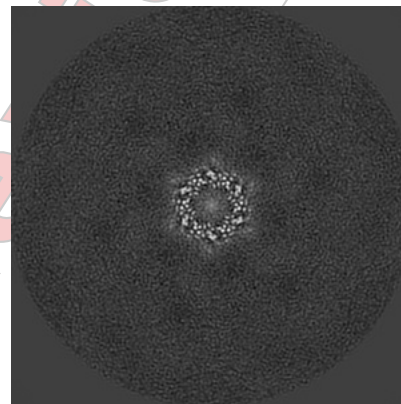
6.2.1 Primary map



X Index: 160

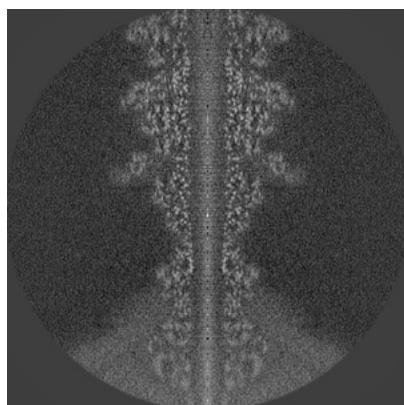


Y Index: 160

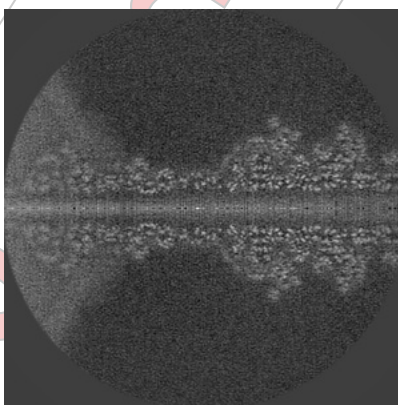


Z Index: 160

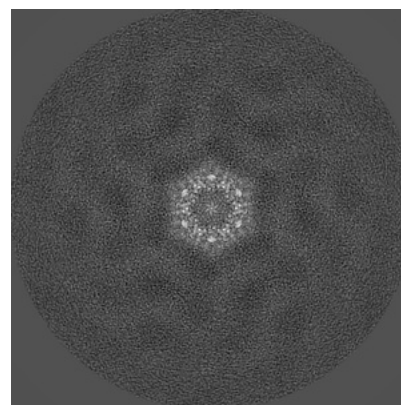
6.2.2 Raw map



X Index: 160



Y Index: 160

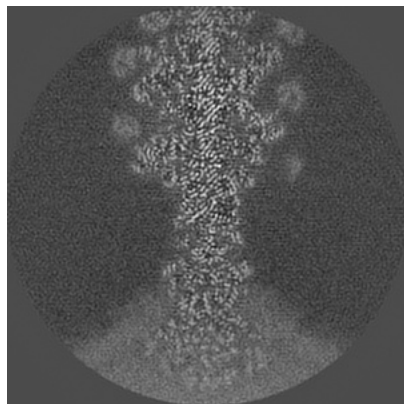


Z Index: 160

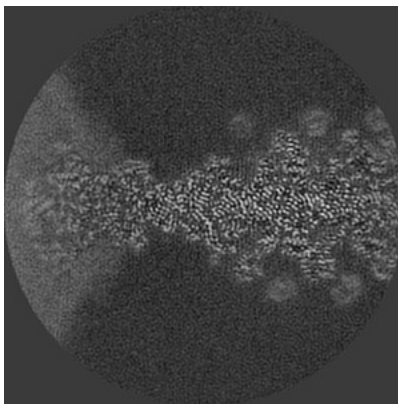
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

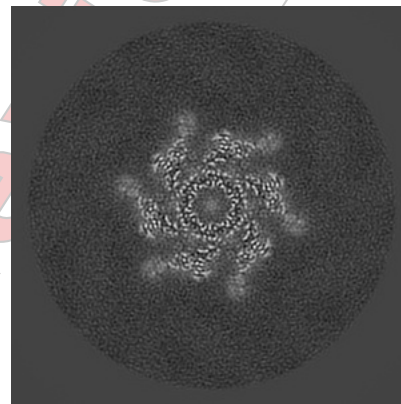
6.3.1 Primary map



X Index: 178

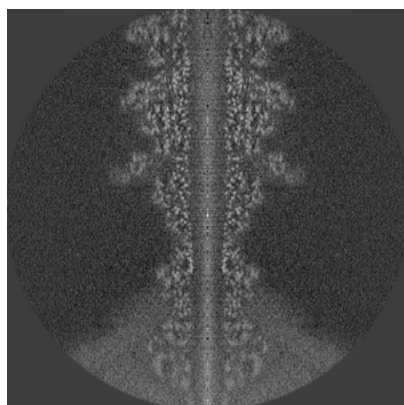


Y Index: 177

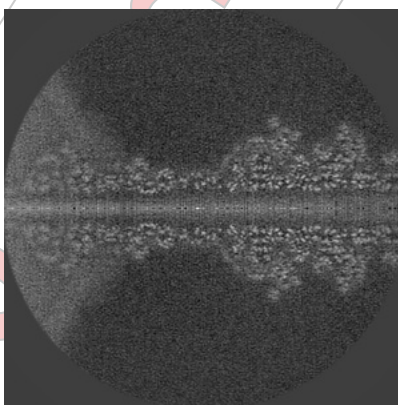


Z Index: 228

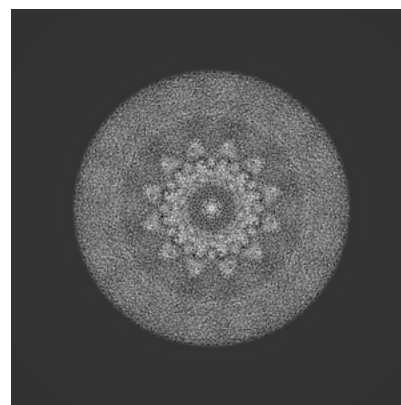
6.3.2 Raw map



X Index: 160



Y Index: 160

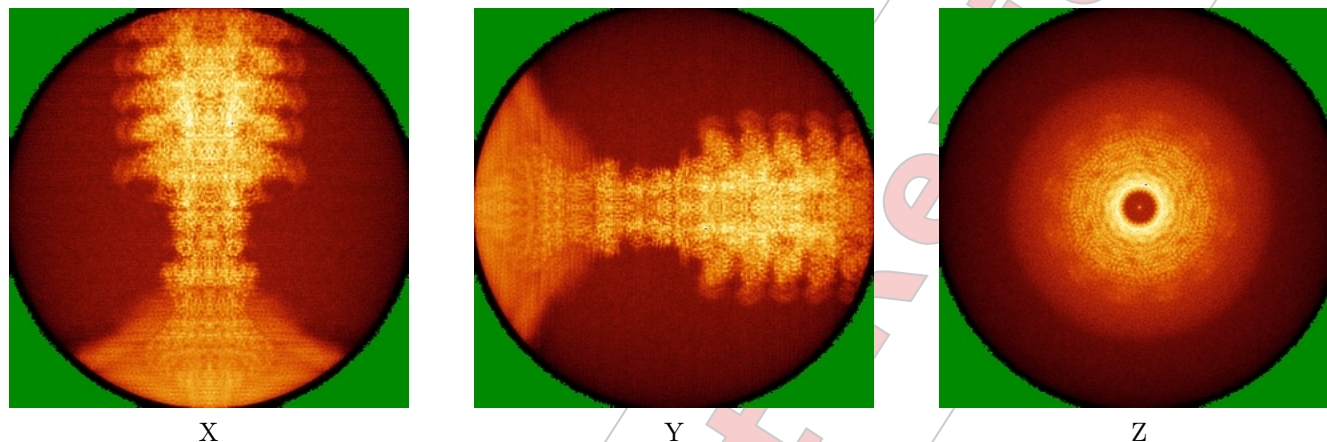


Z Index: 42

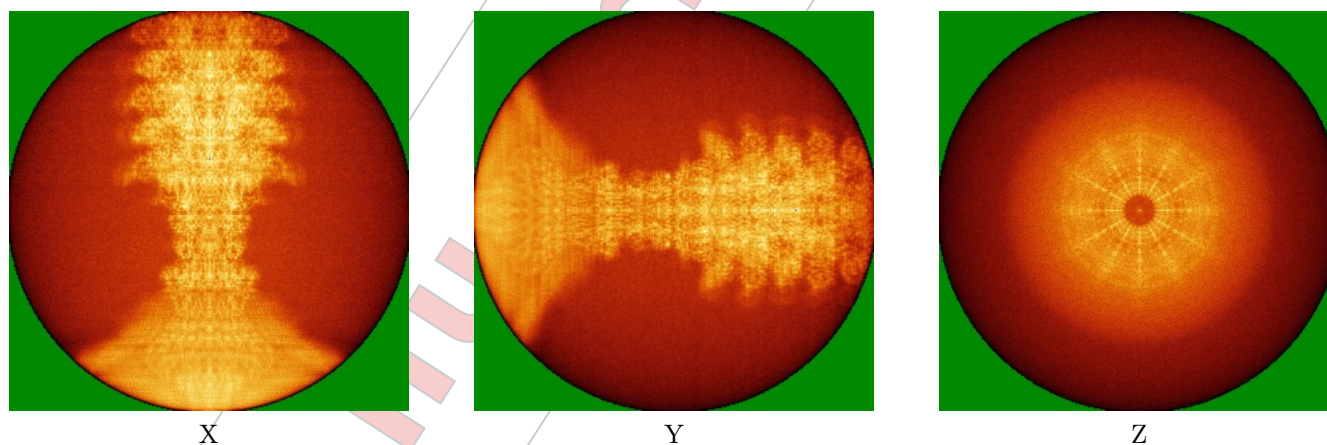
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



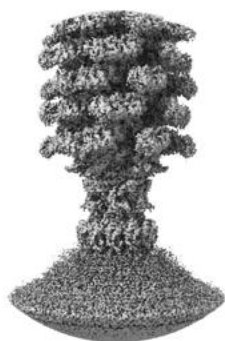
6.4.2 Raw map



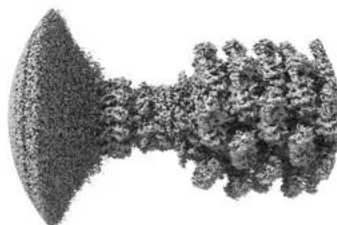
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

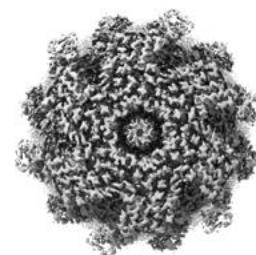
6.5.1 Primary map



X



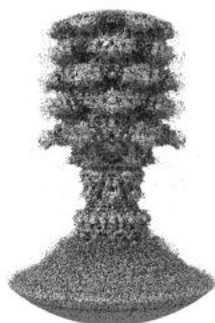
Y



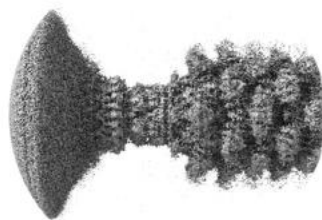
Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

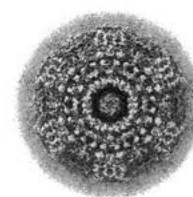
6.5.2 Raw map



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.

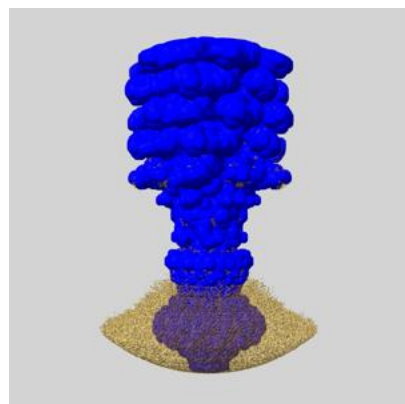
6.6 Mask visualisation [i](#)

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

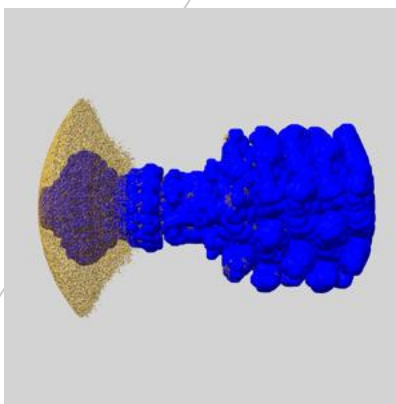
A mask typically either:

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

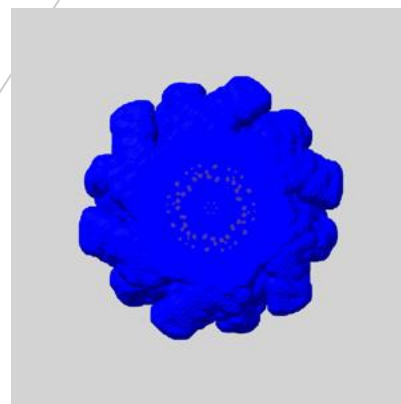
6.6.1 D_1000282513_em-mask-volume_P1.map.V2 [i](#)



X



Y

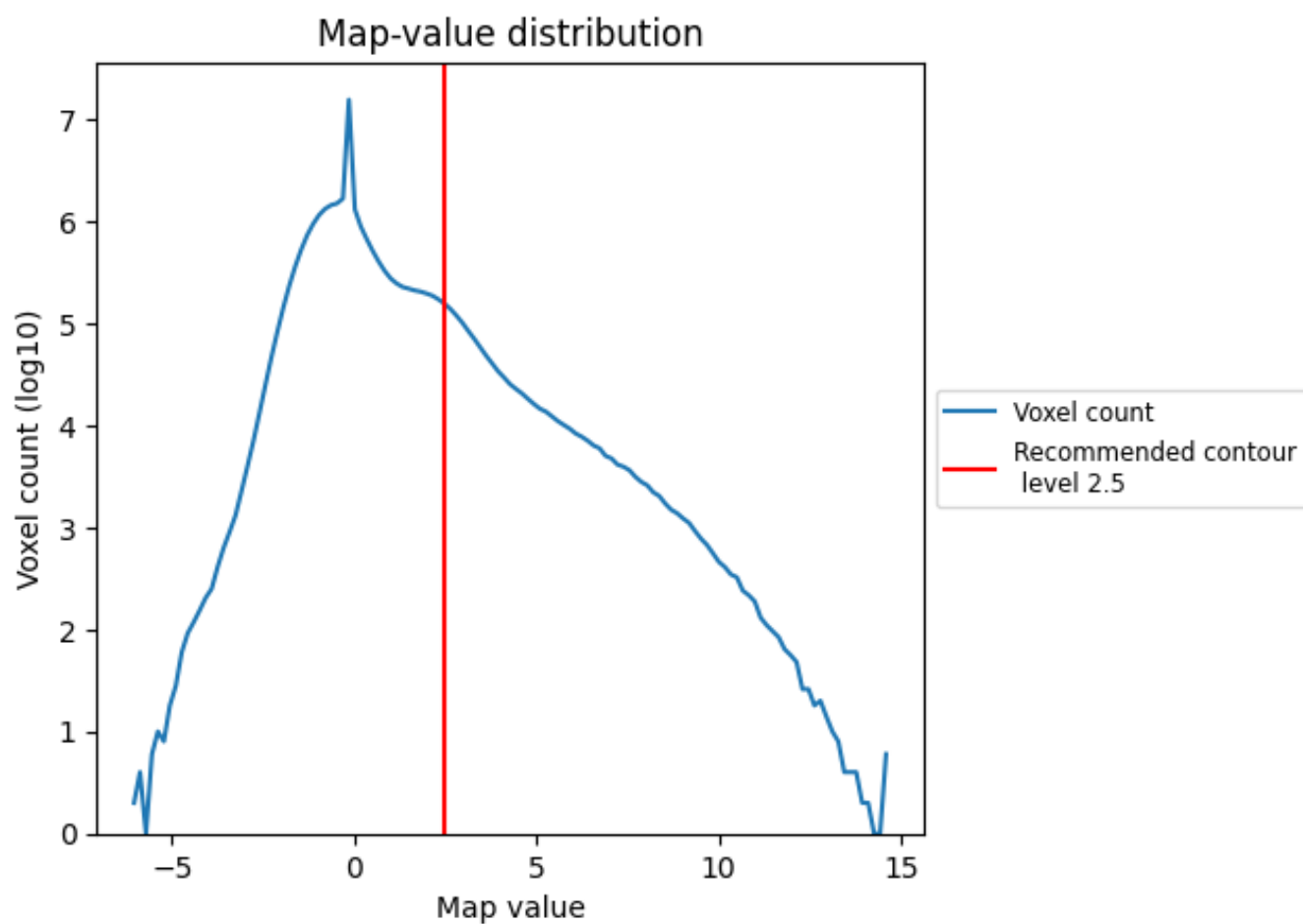


Z

7 Map analysis ⓘ

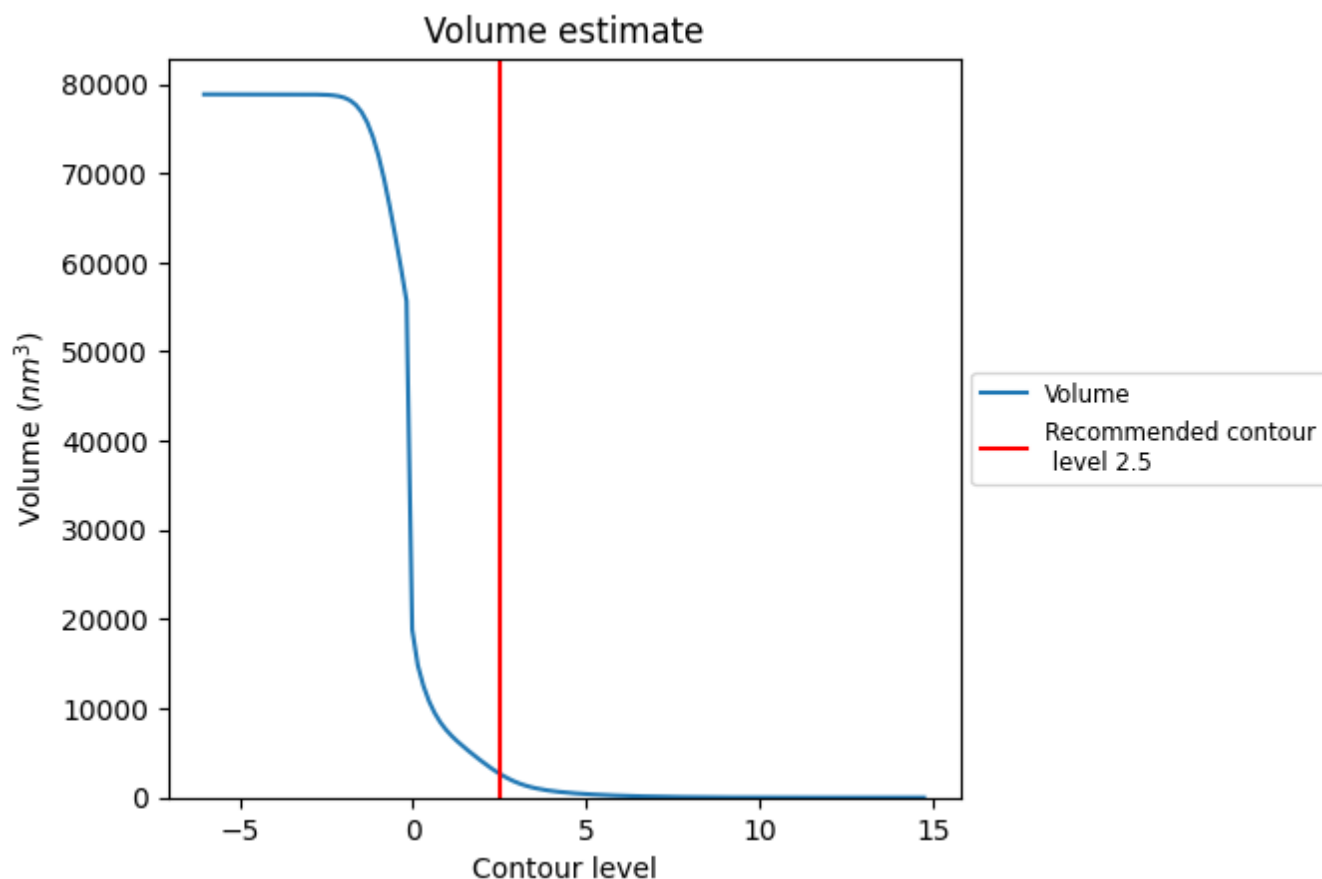
This section contains the results of statistical analysis of the map.

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.

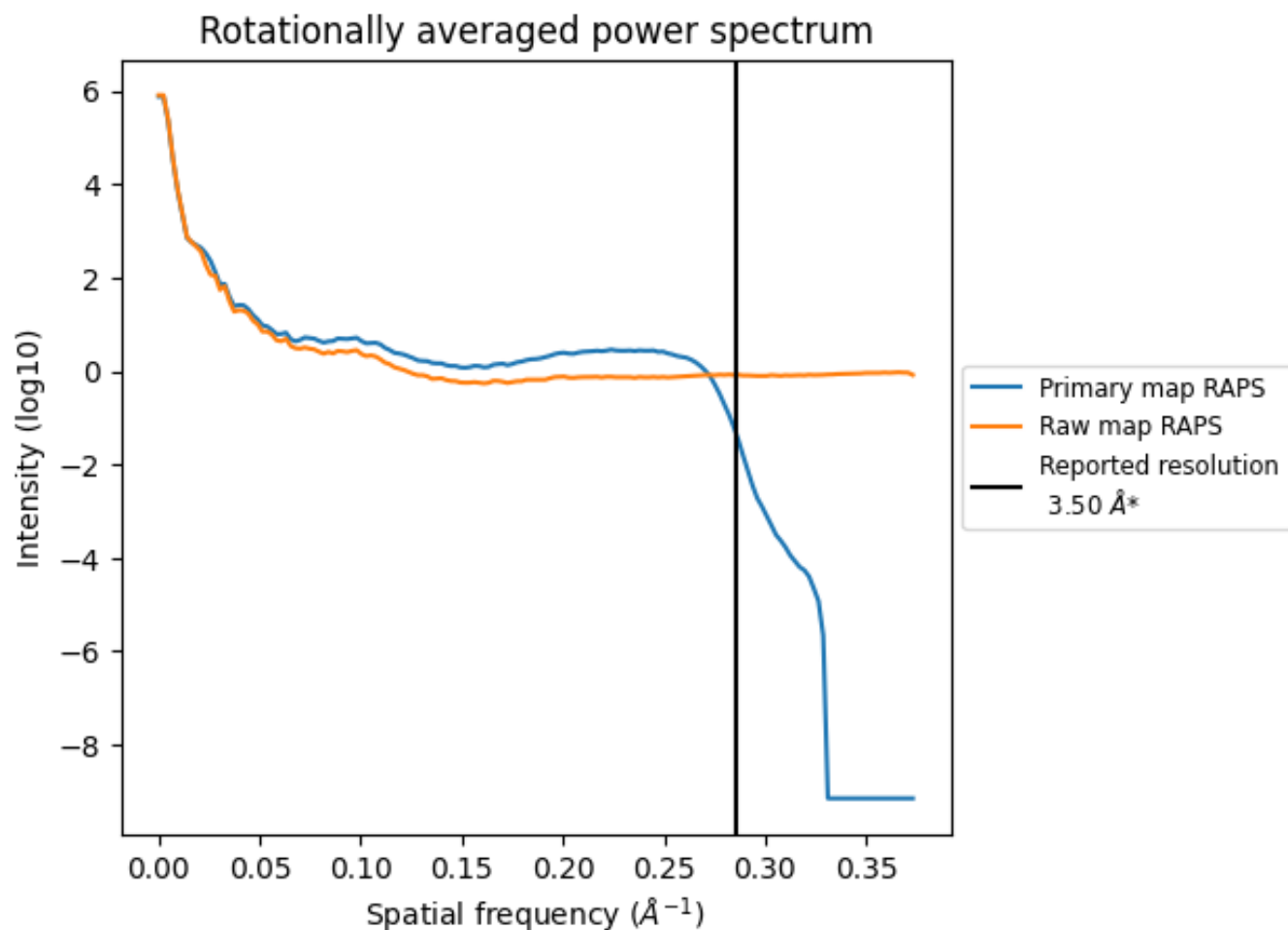
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2681 nm^3 ; this corresponds to an approximate mass of 2422 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 ⓘ

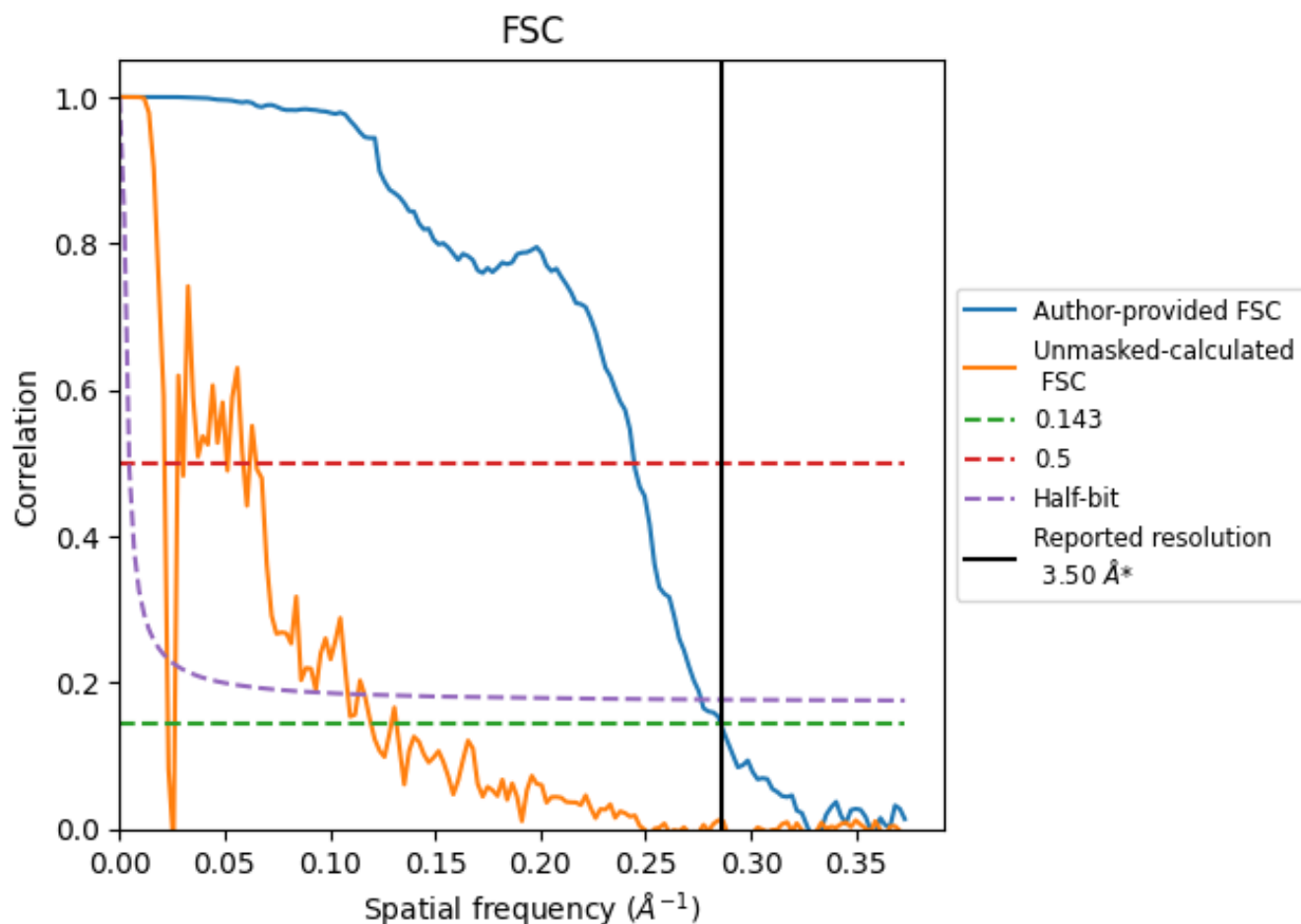


*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

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 0.286 Å⁻¹

8.2 Resolution estimates ⓘ

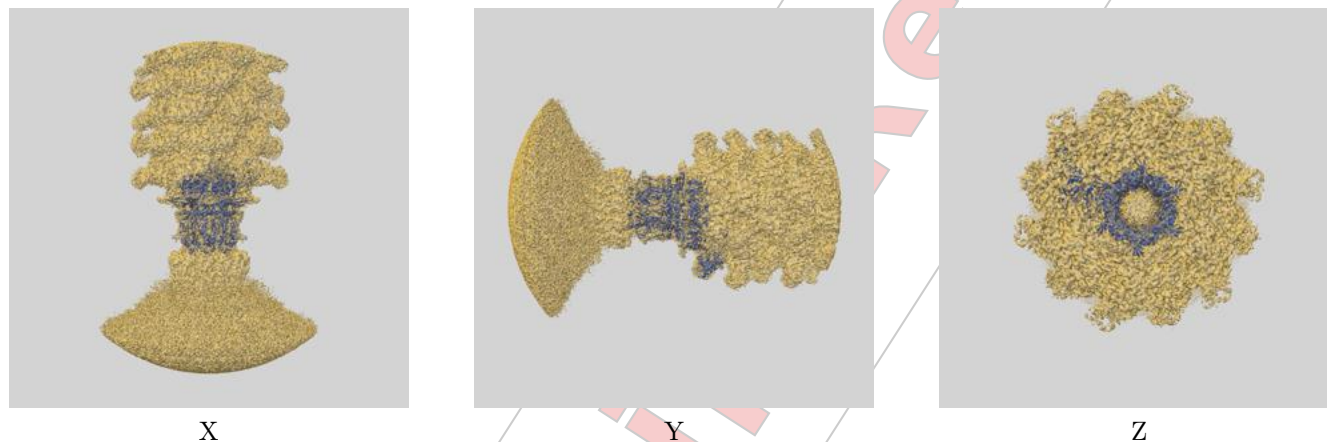
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.09	3.62
Unmasked-calculated*	43.48	46.73	44.25

*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 43.48 differs from the reported value 3.5 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-44166 and PDB model 9B42. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ



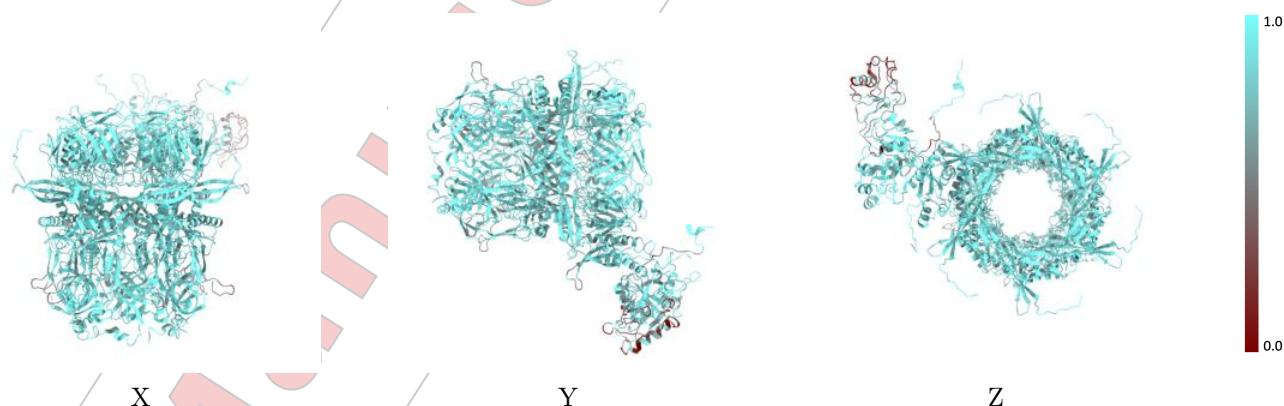
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



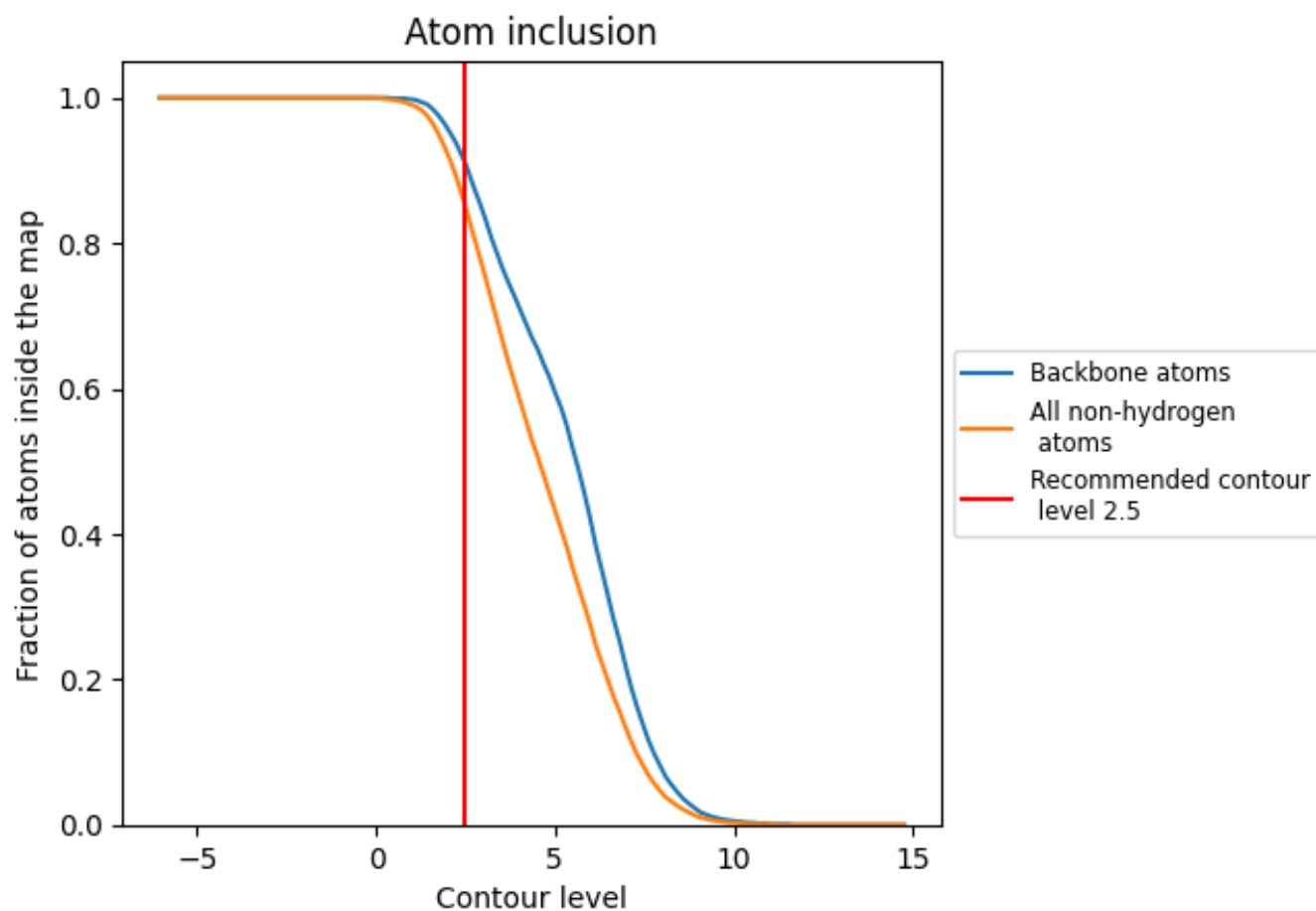
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.4920
A	 0.8540	 0.5040
B	 0.8420	 0.5000
C	 0.8440	 0.5040
D	 0.8570	 0.5040
E	 0.8430	 0.5000
F	 0.8430	 0.5030
G	 0.8750	 0.5040
H	 0.8800	 0.5040
I	 0.8720	 0.5030
J	 0.8730	 0.5050
K	 0.8700	 0.5030
L	 0.8780	 0.5060
M	 0.8810	 0.5110
N	 0.8860	 0.5140
O	 0.8850	 0.5120
P	 0.8850	 0.5140
Q	 0.8880	 0.5130
R	 0.8900	 0.5120
S	 0.7410	 0.4060

