



## Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 03:59 AM EST

PDB ID : 6B0X  
EMDB ID : EMD-7030  
Title : Capsid protein and C-terminal part of scaffolding protein in the Staphylococcus aureus phage 80alpha procapsid  
Authors : Kizziah, J.L.; Dearborn, A.D.; Dokland, T.  
Deposited on : 2017-09-15  
Resolution : 3.72 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

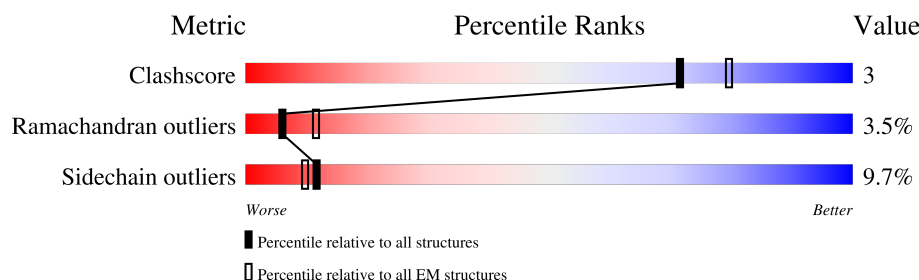
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.72 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  $\geq 3$ , 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	324	<div> <div>42%</div> <div>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div>
1	B	324	<div> <div>19%</div> <div>73%</div> <div>13%</div> <div>•</div> <div>12%</div> </div>
1	C	324	<div> <div>21%</div> <div>73%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>
1	D	324	<div> <div>17%</div> <div>68%</div> <div>18%</div> <div>•</div> <div>12%</div> </div>
1	E	324	<div> <div>22%</div> <div>77%</div> <div>9%</div> <div>•</div> <div>12%</div> </div>
1	F	324	<div> <div>21%</div> <div>73%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>
1	G	324	<div> <div>20%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>12%</div> </div>
2	a	206	<div> <div>7%</div> <div>93%</div> </div>

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Mol	Chain	Length	Quality of chain	
2	b	206	<div><div></div><div>5%</div><div>7%</div></div>	92%
2	c	206	<div><div></div><div>6%</div><div>7%</div></div>	93%
2	d	206	<div><div></div><div>7%</div><div>8%</div></div>	92%
2	e	206	<div><div></div><div>8%</div></div>	92%
2	f	206	<div><div></div><div>5%</div><div>7%</div></div>	92%
2	g	206	<div><div></div><div>6%</div><div>7%</div></div>	92%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16791 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 head protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	284	Total	C	N	O	S	0	0
			2270	1446	370	443	11		
1	B	284	Total	C	N	O	S	0	0
			2270	1446	370	443	11		
1	C	284	Total	C	N	O	S	0	0
			2270	1446	370	443	11		
1	D	284	Total	C	N	O	S	0	0
			2270	1446	370	443	11		
1	E	284	Total	C	N	O	S	0	0
			2270	1446	370	443	11		
1	F	284	Total	C	N	O	S	0	0
			2270	1446	370	443	11		
1	G	284	Total	C	N	O	S	0	0
			2270	1446	370	443	11		

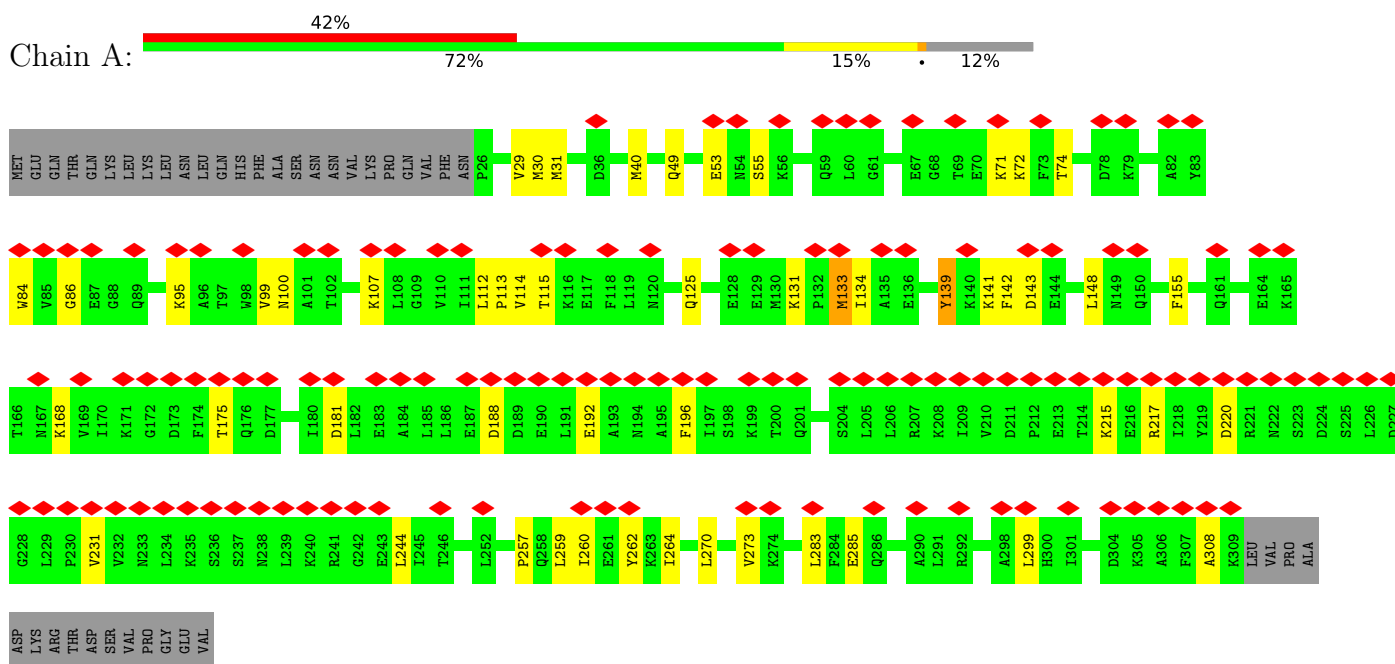
- Molecule 2 is a protein called Scaffold protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	a	14	Total	C	N	O	0	0
			116	72	25	19		
2	b	16	Total	C	N	O	0	0
			132	82	28	22		
2	c	15	Total	C	N	O	0	0
			125	77	27	21		
2	d	16	Total	C	N	O	0	0
			132	82	28	22		
2	e	16	Total	C	N	O	0	0
			132	82	28	22		
2	f	16	Total	C	N	O	0	0
			132	82	28	22		
2	g	16	Total	C	N	O	0	0
			132	82	28	22		

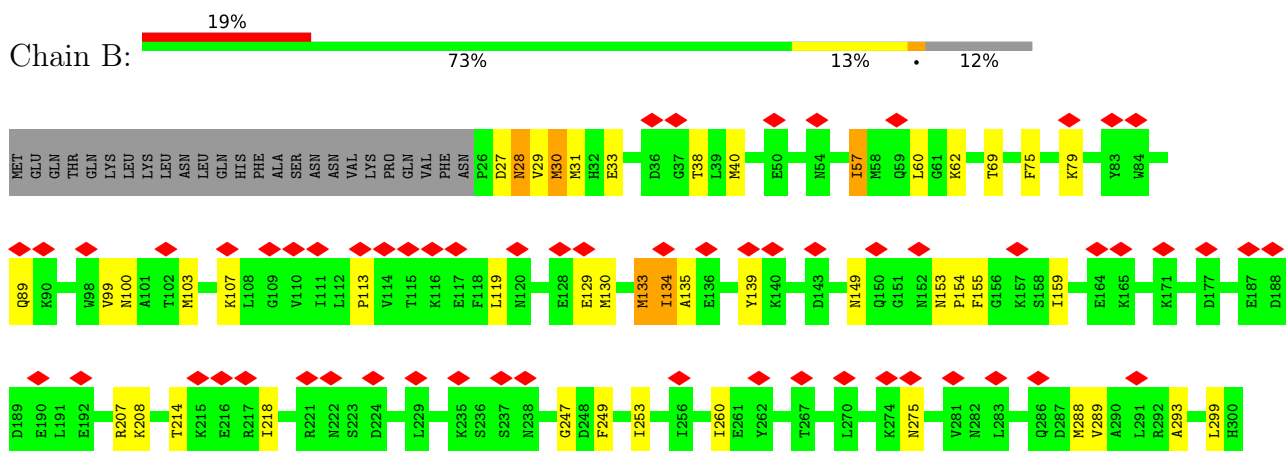
### 3 Residue-property plots

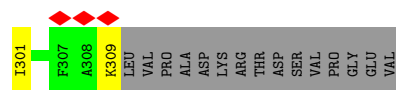
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 head protein

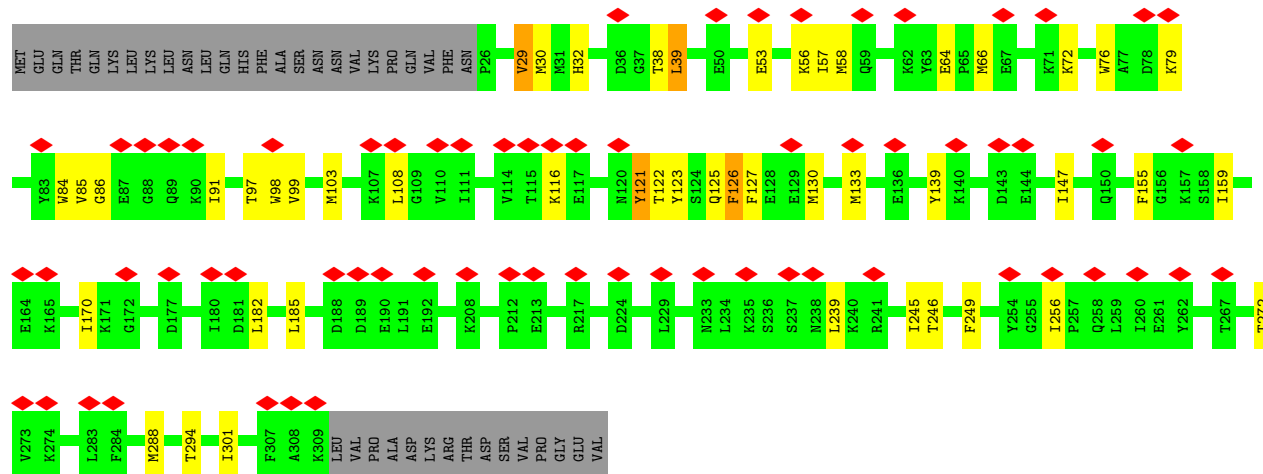
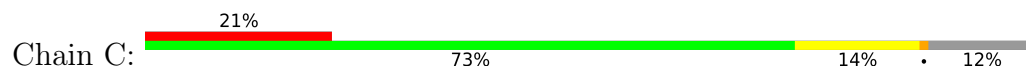


#### • Molecule 1: Major head protein

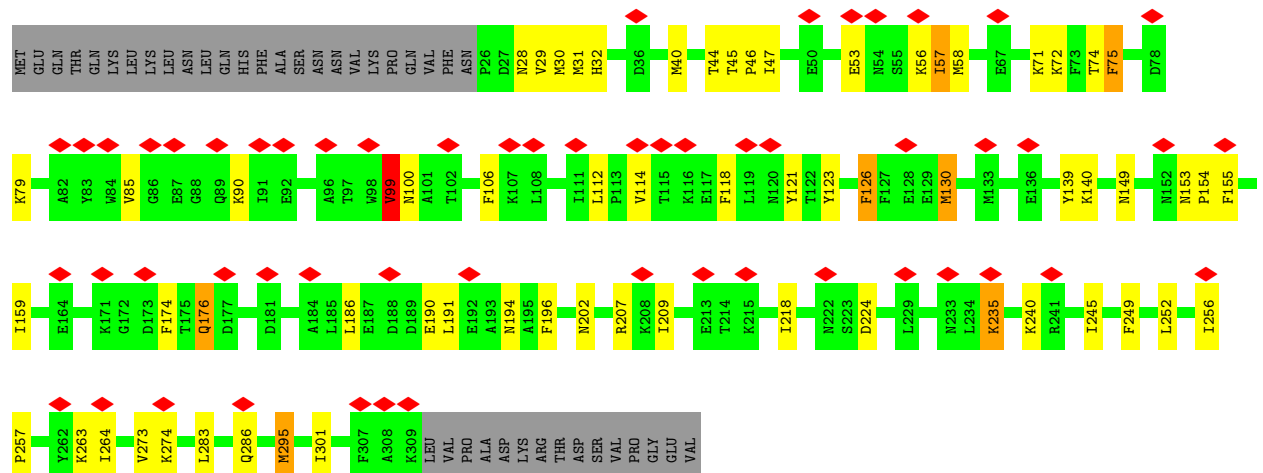




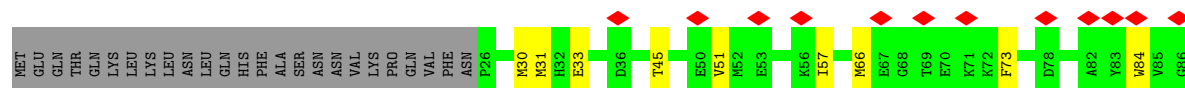
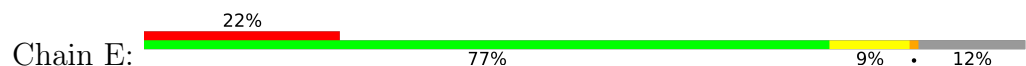
• Molecule 1: Major head protein



• Molecule 1: Major head protein



• Molecule 1: Major head protein







MET	GLU	ALA	GLU	ASN	LYS	LEU	LYS	PHE	GLN	PHE	LYS	PHE	ALA	ASP	GLN	SER	ASP	ASP	PRO	ASP	GLU	PRO	GLY	GLY	GLY	LYS	LYS	GLY	ASN	PRO	ASP	LYS	LYS	GLU	ASN	ASN	ASP	GLU	GLU	GLY	THR	GLU	ILE	THR	PHE	THR	THR	PRO	GLU	GLN	GLN	LYS	VAL	ASP	GLU	ILE	LEU	GLU	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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- Molecule 2: Scaffold protein



MET	GLU	ALA	GLU	ASN	LYS	LEU	LYS	PHE	GLN	PHE	LYS	PHE	ALA	ASP	GLN	SER	ASP	ASP	ASP	GLU	GLU	PRO	GLY	GLY	ASP	GLY	LYS	LYS	GLY	ASN	PRO	ASP	LYS	LYS	GLU	GLY	THR	ILE	THR	PHE	THR	PRO	GLU	GLN	GLN	LYS	VAL	ASP	GLU	ILE	LEU	GLU	ARG		
VAL	ALA	HIS	GLU	LYS	LYS	LYS	LYS	LYS	TYR	ALA	LYS	GLU	LYS	ASP	GLN	ALA	ALA	GLU	ALA	LYS	GLU	ALA	ALA	GLY	GLY	ASP	LYS	LYS	ASN	LYS	ASP	GLN	LYS	ASP	GLU	TYR	GLU	ARG	GLY	LEU	GLU	GLN	GLN	LEU	ARG	GLY	VAL	GLN	GLN	ASN	ILE	GLU	MET	ARG	
GLU	ALA	ARG	LYS	MET	LYS	LEU	SER	GLU	VAL	ASP	SER	SER	ASP	GLU	VAL	VAL	VAL	ASN	LEU	VAL	THR	THR	THR	THR	GLN	GLU	LYS	LYS	SER	ASN	VAL	VAL	VAL	ASN	ALA	ALA	ALA	GLU	VAL	VAL	ASN	GLU	VAL	VAL	VAL	GLN	GLN	GLN	ARG	ALA	ALA	ASN	THR	GLY	
ASP	SER	PHE	ASN	HIS	SER	SER	THR	LYS	GLN	P191	Q192	N193	E196	R199	Q200	K201	R202	I203	I204	K205	N206																																		

- Molecule 2: Scaffold protein



ASP	PHE	ASN	HIS	SER	THR	LYS	ASN	LYS	PRO	Q192	N193	L194	A195	E196	R199	Q200	K201	R202	I203	I204	K205	N206																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
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- Molecule 2: Scaffold protein



MET	GLU	ALA	GLU	ASN	LYS	LEU	LYS	PHE	GLN	PHE	LYS	PHE	ALA	ASP	GLN	SER	ASP	PRO	ASP	GLU	PRO	GLY	GLY	ASP	GLY	LYS	LYS	GLY	ASN	PRO	ASP	LYS	LYS	GLU	GLY	THR	ILE	THR	PHE	THR	PRO	GLU	GLN	GLN	LYS	VAL	GLN	ASP	ILE	LEU	GLU	ARG	GLY
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ASP	SER	PHE	ASN	HIS	THR	LYS	ASN	LYS	P191	Q192	N193	L194	A195	E196	R199	Q200	K201	R202	I203	I204	K205	N206
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10557	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00705	Depositor
Map size ( $\text{\AA}$ )	580.80005, 580.80005, 290.40002	wwPDB
Map dimensions	480, 480, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2100002, 1.2100002, 1.2100002	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	A	0.42	0/2312	0.59	0/3116
1	B	0.40	0/2312	0.56	0/3116
1	C	0.39	0/2312	0.58	0/3116
1	D	0.40	0/2312	0.58	0/3116
1	E	0.40	0/2312	0.58	0/3116
1	F	0.40	0/2312	0.57	0/3116
1	G	0.39	0/2312	0.58	0/3116
2	a	0.42	0/115	0.51	0/151
2	b	0.35	0/132	0.60	0/174
2	c	0.38	0/124	0.51	0/163
2	d	0.32	0/132	0.54	0/174
2	e	0.33	0/132	0.53	0/174
2	f	0.36	0/132	0.51	0/174
2	g	0.34	0/132	0.54	0/174
All	All	0.40	0/17083	0.57	0/22996

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2270	0	2261	5	0
1	B	2270	0	2261	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2270	0	2261	32	0
1	D	2270	0	2261	19	0
1	E	2270	0	2261	6	0
1	F	2270	0	2261	17	0
1	G	2270	0	2261	30	0
2	a	116	0	131	0	0
2	b	132	0	147	0	0
2	c	125	0	139	0	0
2	d	132	0	147	0	0
2	e	132	0	147	0	0
2	f	132	0	147	0	0
2	g	132	0	147	0	0
All	All	16791	0	16832	112	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 3.

All (112) 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:39:LEU:HD21	1:G:127:PHE:CE2	1.76	1.21
1:C:126:PHE:CD1	1:C:130:MET:HG3	1.78	1.16
1:G:39:LEU:HD21	1:G:127:PHE:HE2	1.13	1.01
1:C:126:PHE:CE1	1:C:130:MET:CG	2.44	1.00
1:C:126:PHE:CD1	1:C:130:MET:CG	2.53	0.91
1:C:126:PHE:CE1	1:C:130:MET:SD	2.65	0.89
1:C:126:PHE:HD1	1:C:130:MET:HG3	1.38	0.82
1:G:39:LEU:CD2	1:G:127:PHE:CE2	2.61	0.81
1:C:39:LEU:CD2	1:C:127:PHE:HE2	1.98	0.76
1:C:121:TYR:O	1:C:125:GLN:HB2	1.87	0.73
1:G:121:TYR:O	1:G:125:GLN:HB2	1.93	0.68
1:C:39:LEU:HD23	1:C:127:PHE:CE2	2.29	0.67
1:G:108:LEU:HD21	1:G:126:PHE:CE2	2.30	0.66
1:F:163:ILE:HD13	1:F:303:ASP:HB2	1.79	0.64
1:G:108:LEU:HD21	1:G:126:PHE:HE2	1.63	0.62
1:C:126:PHE:CE1	1:C:130:MET:HG2	2.33	0.62
1:G:57:ILE:HB	1:G:147:ILE:HD11	1.80	0.62
1:C:126:PHE:O	1:C:130:MET:HG3	2.00	0.62
1:C:126:PHE:CE1	1:C:130:MET:HG3	2.17	0.60
1:C:182:LEU:HD21	1:C:245:ILE:HD11	1.84	0.59
1:C:32:HIS:HD2	1:C:123:TYR:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LEU:HD22	1:C:127:PHE:HE2	1.70	0.57
1:C:39:LEU:CD2	1:C:127:PHE:CE2	2.82	0.57
1:C:126:PHE:HE1	1:C:130:MET:HG2	1.69	0.57
1:D:45:THR:HG23	1:D:46:PRO:HD3	1.86	0.57
1:B:134:ILE:HD12	1:B:289:VAL:HG21	1.87	0.56
1:C:159:ILE:HG23	1:C:301:ILE:HG21	1.88	0.56
1:G:45:THR:HG23	1:G:46:PRO:HD3	1.86	0.56
1:E:99:VAL:HG21	1:E:155:PHE:HB3	1.87	0.55
1:A:264:ILE:HG21	1:G:264:ILE:HG22	1.89	0.55
1:G:108:LEU:CD2	1:G:126:PHE:CE2	2.90	0.55
1:A:55:SER:HA	1:A:139:TYR:CD1	2.42	0.54
1:D:57:ILE:HD11	1:D:249:PHE:CE1	2.42	0.54
1:D:74:THR:O	1:D:75:PHE:HB2	2.07	0.54
1:F:108:LEU:HG	1:F:112:LEU:HD11	1.89	0.54
1:C:126:PHE:CD1	1:C:130:MET:SD	3.01	0.53
1:G:126:PHE:CZ	1:G:130:MET:CE	2.92	0.53
1:A:133:MET:SD	1:A:134:ILE:N	2.81	0.53
1:C:108:LEU:HD21	1:C:130:MET:HA	1.90	0.53
1:E:176:GLN:HE21	1:E:218:ILE:HD11	1.73	0.52
1:C:108:LEU:HD22	1:C:133:MET:HB2	1.92	0.52
1:B:159:ILE:HG23	1:B:301:ILE:HG21	1.91	0.52
1:D:159:ILE:HG23	1:D:301:ILE:HG21	1.91	0.52
1:G:121:TYR:O	1:G:125:GLN:CG	2.58	0.52
1:F:45:THR:HG23	1:F:46:PRO:HD3	1.92	0.51
1:F:97:THR:HB	1:F:294:THR:HG21	1.92	0.51
1:C:121:TYR:O	1:C:125:GLN:CG	2.59	0.51
1:F:39:LEU:HD13	1:F:127:PHE:CZ	2.45	0.51
1:A:196:PHE:HB2	1:A:231:VAL:HG22	1.93	0.51
1:D:196:PHE:CZ	1:D:245:ILE:HD11	2.46	0.51
1:C:121:TYR:O	1:C:125:GLN:CB	2.57	0.50
1:G:108:LEU:HD22	1:G:130:MET:HE3	1.94	0.49
1:D:196:PHE:CE2	1:D:245:ILE:HD11	2.47	0.49
1:D:121:TYR:CE2	1:D:123:TYR:HA	2.47	0.49
1:D:121:TYR:CZ	1:D:126:PHE:HB3	2.47	0.49
1:C:246:THR:HG23	1:C:249:PHE:CE1	2.47	0.49
1:D:44:THR:HG23	1:D:257:PRO:HD3	1.95	0.48
1:G:121:TYR:O	1:G:125:GLN:CB	2.61	0.48
1:B:260:ILE:HG22	1:B:288:MET:HB3	1.95	0.48
1:G:77:ALA:HB3	1:G:79:LYS:HE3	1.95	0.48
1:G:182:LEU:HD21	1:G:245:ILE:CD1	2.44	0.47
1:F:110:VAL:HG21	1:G:73:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:HG21	1:D:155:PHE:CD1	2.49	0.47
1:D:264:ILE:O	1:D:286:GLN:NE2	2.44	0.47
1:G:102:THR:HG23	1:G:290:ALA:HA	1.96	0.47
1:A:133:MET:SD	1:A:134:ILE:HG23	2.55	0.46
1:C:147:ILE:HA	1:C:159:ILE:HD12	1.97	0.46
1:F:159:ILE:HG23	1:F:301:ILE:HG21	1.96	0.46
1:E:111:ILE:O	1:E:114:VAL:HG22	2.15	0.46
1:D:32:HIS:CE1	1:D:118:PHE:CZ	3.04	0.45
1:F:112:LEU:HD13	1:F:118:PHE:CE1	2.51	0.45
1:G:39:LEU:HD22	1:G:257:PRO:HG2	1.96	0.45
1:F:186:LEU:HD22	1:F:245:ILE:HD13	1.99	0.45
1:G:108:LEU:C	1:G:108:LEU:HD23	2.36	0.45
1:G:126:PHE:HZ	1:G:130:MET:HE1	1.81	0.45
1:E:218:ILE:HD12	1:E:218:ILE:N	2.33	0.44
1:G:43:PHE:CE2	1:G:123:TYR:HE2	2.35	0.44
1:D:174:PHE:HB3	1:D:209:ILE:HD11	1.98	0.44
1:G:182:LEU:HD21	1:G:245:ILE:HD11	1.99	0.44
1:G:128:GLU:OE2	1:G:128:GLU:HA	2.18	0.44
1:D:176:GLN:HG3	1:D:218:ILE:HD11	2.00	0.44
1:F:286:GLN:OE1	1:F:286:GLN:N	2.51	0.43
1:C:126:PHE:CZ	1:C:130:MET:SD	3.09	0.43
1:G:108:LEU:HD21	1:G:118:PHE:CZ	2.54	0.43
1:B:153:ASN:N	1:B:154:PRO:CD	2.81	0.43
1:D:126:PHE:CD2	1:D:130:MET:HG3	2.54	0.43
1:F:57:ILE:HG23	1:F:251:LYS:HD2	2.01	0.43
1:D:112:LEU:HD11	1:D:126:PHE:CD2	2.55	0.42
1:G:44:THR:HG23	1:G:257:PRO:HD3	2.02	0.42
1:G:47:ILE:HD12	1:G:134:ILE:HD12	2.01	0.42
1:D:140:LYS:NZ	1:D:235:LYS:O	2.53	0.42
1:G:214:THR:HG23	1:G:214:THR:O	2.19	0.42
1:E:108:LEU:HD11	1:E:130:MET:HB2	2.02	0.41
1:G:126:PHE:HZ	1:G:130:MET:CE	2.33	0.41
1:D:153:ASN:N	1:D:154:PRO:CD	2.83	0.41
1:C:97:THR:HB	1:C:294:THR:HG21	2.02	0.41
1:B:133:MET:O	1:B:135:ALA:N	2.53	0.41
1:D:295:MET:N	1:D:295:MET:SD	2.93	0.41
1:F:99:VAL:HG21	1:F:155:PHE:CB	2.51	0.41
1:F:108:LEU:HD11	1:F:112:LEU:HD21	2.02	0.41
1:F:200:THR:HG22	1:G:187:GLU:HG2	2.01	0.41
1:C:126:PHE:HD1	1:C:126:PHE:O	2.02	0.41
1:E:196:PHE:HB2	1:E:231:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ILE:HD13	1:B:293:ALA:HB2	2.03	0.41
1:C:32:HIS:HB2	1:C:122:THR:C	2.41	0.41
1:C:170:ILE:HD11	1:C:185:LEU:HD11	2.03	0.41
1:C:39:LEU:HB3	1:C:127:PHE:CZ	2.57	0.40
1:C:182:LEU:HD21	1:C:245:ILE:CD1	2.48	0.40
1:F:153:ASN:N	1:F:154:PRO:CD	2.84	0.40
1:F:170:ILE:HD12	1:F:182:LEU:HD13	2.04	0.40
1:F:249:PHE:CE2	1:F:297:VAL:HG22	2.56	0.40
1:C:38:THR:HG22	1:C:256:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	282/324 (87%)	235 (83%)	32 (11%)	15 (5%)	2	21
1	B	282/324 (87%)	230 (82%)	39 (14%)	13 (5%)	2	23
1	C	282/324 (87%)	236 (84%)	39 (14%)	7 (2%)	5	35
1	D	282/324 (87%)	236 (84%)	36 (13%)	10 (4%)	3	30
1	E	282/324 (87%)	231 (82%)	44 (16%)	7 (2%)	5	35
1	F	282/324 (87%)	239 (85%)	34 (12%)	9 (3%)	4	31
1	G	282/324 (87%)	228 (81%)	43 (15%)	11 (4%)	3	27
2	a	12/206 (6%)	11 (92%)	1 (8%)	0	100	100
2	b	14/206 (7%)	13 (93%)	0	1 (7%)	1	15
2	c	13/206 (6%)	13 (100%)	0	0	100	100
2	d	14/206 (7%)	13 (93%)	1 (7%)	0	100	100
2	e	14/206 (7%)	12 (86%)	2 (14%)	0	100	100
2	f	14/206 (7%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	g	14/206 (7%)	14 (100%)	0	0	100	100
All	All	2069/3710 (56%)	1725 (83%)	271 (13%)	73 (4%)	6	30

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	113	PRO
1	A	114	VAL
1	A	192	GLU
1	B	113	PRO
1	C	85	VAL
1	D	75	PHE
1	D	99	VAL
1	E	99	VAL
1	F	99	VAL
1	G	114	VAL
2	b	205	LYS
1	A	99	VAL
1	A	115	THR
1	A	257	PRO
1	A	283	LEU
1	B	99	VAL
1	C	91	ILE
1	C	99	VAL
1	D	273	VAL
1	E	283	LEU
1	F	122	THR
1	F	273	VAL
1	G	99	VAL
1	G	300	HIS
1	A	188	ASP
1	B	79	LYS
1	C	30	MET
1	D	30	MET
1	D	114	VAL
1	E	274	LYS
1	F	29	VAL
1	F	272	THR
1	G	30	MET
1	G	258	GLN
1	G	283	LEU

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Mol	Chain	Res	Type
1	A	84	TRP
1	A	308	ALA
1	B	29	VAL
1	B	30	MET
1	B	33	GLU
1	D	106	PHE
1	D	224	ASP
1	D	283	LEU
1	E	84	TRP
1	F	28	ASN
1	G	84	TRP
1	A	29	VAL
1	A	131	LYS
1	B	28	ASN
1	B	134	ILE
1	B	214	THR
1	D	28	ASN
1	D	29	VAL
1	E	158	SER
1	E	228	GLY
1	E	258	GLN
1	F	246	THR
1	G	272	THR
1	G	274	LYS
1	A	273	VAL
1	B	57	ILE
1	B	89	GLN
1	B	218	ILE
1	C	272	THR
1	F	153	ASN
1	F	167	ASN
1	B	247	GLY
1	C	86	GLY
1	G	29	VAL
1	G	247	GLY
1	C	29	VAL
1	A	86	GLY

### 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	249/286 (87%)	217 (87%)	32 (13%)	4	23
1	B	249/286 (87%)	222 (89%)	27 (11%)	6	30
1	C	249/286 (87%)	228 (92%)	21 (8%)	11	40
1	D	249/286 (87%)	217 (87%)	32 (13%)	4	23
1	E	249/286 (87%)	228 (92%)	21 (8%)	11	40
1	F	249/286 (87%)	234 (94%)	15 (6%)	19	50
1	G	249/286 (87%)	223 (90%)	26 (10%)	7	31
2	a	12/178 (7%)	12 (100%)	0	100	100
2	b	14/178 (8%)	13 (93%)	1 (7%)	14	45
2	c	13/178 (7%)	13 (100%)	0	100	100
2	d	14/178 (8%)	14 (100%)	0	100	100
2	e	14/178 (8%)	14 (100%)	0	100	100
2	f	14/178 (8%)	13 (93%)	1 (7%)	14	45
2	g	14/178 (8%)	12 (86%)	2 (14%)	3	19
All	All	1838/3248 (57%)	1660 (90%)	178 (10%)	12	33

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	MET
1	A	40	MET
1	A	49	GLN
1	A	53	GLU
1	A	71	LYS
1	A	72	LYS
1	A	74	THR
1	A	95	LYS
1	A	100	ASN
1	A	107	LYS
1	A	112	LEU
1	A	125	GLN
1	A	133	MET
1	A	139	TYR
1	A	141	LYS

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Mol	Chain	Res	Type
1	A	142	PHE
1	A	143	ASP
1	A	148	LEU
1	A	155	PHE
1	A	168	LYS
1	A	175	THR
1	A	181	ASP
1	A	215	LYS
1	A	217	ARG
1	A	220	ASP
1	A	244	LEU
1	A	259	LEU
1	A	260	ILE
1	A	262	TYR
1	A	270	LEU
1	A	285	GLU
1	A	299	LEU
1	B	27	ASP
1	B	28	ASN
1	B	30	MET
1	B	31	MET
1	B	38	THR
1	B	40	MET
1	B	57	ILE
1	B	60	LEU
1	B	62	LYS
1	B	69	THR
1	B	75	PHE
1	B	100	ASN
1	B	103	MET
1	B	107	LYS
1	B	119	LEU
1	B	129	GLU
1	B	130	MET
1	B	133	MET
1	B	139	TYR
1	B	149	ASN
1	B	155	PHE
1	B	207	ARG
1	B	208	LYS
1	B	249	PHE
1	B	275	ASN

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Mol	Chain	Res	Type
1	B	299	LEU
1	B	309	LYS
1	C	29	VAL
1	C	39	LEU
1	C	53	GLU
1	C	56	LYS
1	C	57	ILE
1	C	58	MET
1	C	64	GLU
1	C	66	MET
1	C	72	LYS
1	C	76	TRP
1	C	79	LYS
1	C	84	TRP
1	C	98	TRP
1	C	103	MET
1	C	116	LYS
1	C	121	TYR
1	C	126	PHE
1	C	139	TYR
1	C	155	PHE
1	C	239	LEU
1	C	288	MET
1	D	31	MET
1	D	40	MET
1	D	47	ILE
1	D	53	GLU
1	D	56	LYS
1	D	57	ILE
1	D	58	MET
1	D	71	LYS
1	D	72	LYS
1	D	79	LYS
1	D	85	VAL
1	D	90	LYS
1	D	99	VAL
1	D	100	ASN
1	D	126	PHE
1	D	130	MET
1	D	139	TYR
1	D	149	ASN
1	D	176	GLN

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Mol	Chain	Res	Type
1	D	186	LEU
1	D	190	GLU
1	D	191	LEU
1	D	194	ASN
1	D	202	ASN
1	D	207	ARG
1	D	235	LYS
1	D	240	LYS
1	D	252	LEU
1	D	256	ILE
1	D	263	LYS
1	D	274	LYS
1	D	295	MET
1	E	30	MET
1	E	31	MET
1	E	33	GLU
1	E	45	THR
1	E	51	VAL
1	E	57	ILE
1	E	66	MET
1	E	73	PHE
1	E	90	LYS
1	E	98	TRP
1	E	102	THR
1	E	108	LEU
1	E	120	ASN
1	E	139	TYR
1	E	155	PHE
1	E	157	LYS
1	E	187	GLU
1	E	207	ARG
1	E	208	LYS
1	E	246	THR
1	E	274	LYS
1	F	31	MET
1	F	72	LYS
1	F	87	GLU
1	F	94	SER
1	F	98	TRP
1	F	112	LEU
1	F	126	PHE
1	F	139	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	157	LYS
1	F	200	THR
1	F	201	GLN
1	F	263	LYS
1	F	270	LEU
1	F	274	LYS
1	F	299	LEU
1	G	28	ASN
1	G	31	MET
1	G	45	THR
1	G	53	GLU
1	G	57	ILE
1	G	63	TYR
1	G	64	GLU
1	G	66	MET
1	G	90	LYS
1	G	95	LYS
1	G	98	TRP
1	G	103	MET
1	G	104	ARG
1	G	114	VAL
1	G	153	ASN
1	G	155	PHE
1	G	189	ASP
1	G	226	LEU
1	G	246	THR
1	G	252	LEU
1	G	256	ILE
1	G	259	LEU
1	G	270	LEU
1	G	274	LYS
1	G	295	MET
1	G	299	LEU
2	b	205	LYS
2	f	193	ASN
2	g	202	ARG
2	g	205	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	125	GLN
1	A	149	ASN
1	A	161	GLN
1	A	258	GLN
1	B	49	GLN
1	B	100	ASN
1	B	178	ASN
1	B	202	ASN
1	C	32	HIS
1	C	238	ASN
1	D	59	GLN
1	E	120	ASN
1	E	176	GLN
1	E	202	ASN
1	F	153	ASN
1	G	202	ASN
1	G	286	GLN
2	a	193	ASN
2	f	193	ASN

### 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 ⓘ

There are no chain breaks in this entry.

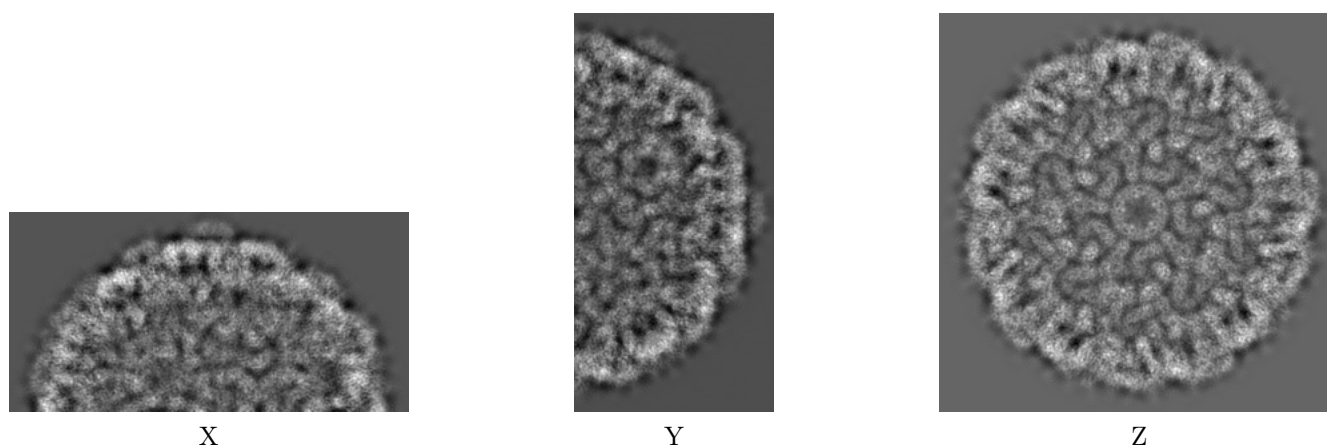
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7030. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

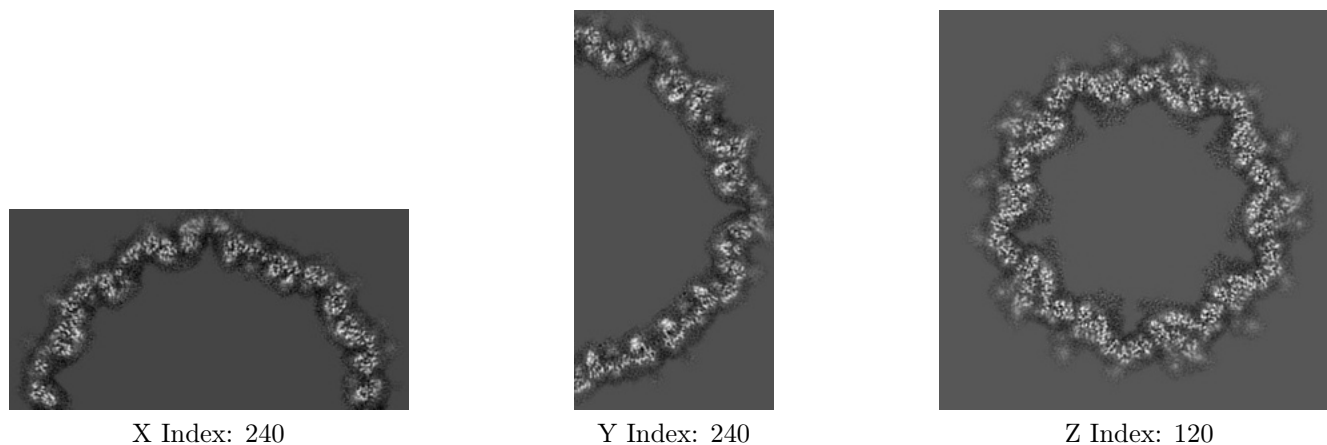
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

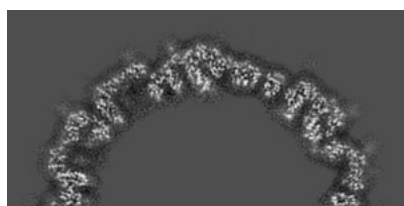
#### 6.2.1 Primary map



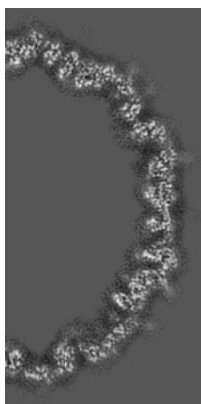
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

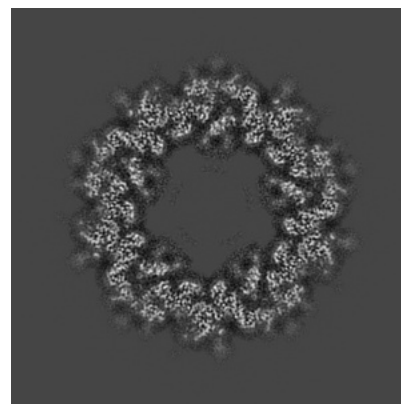
### 6.3.1 Primary map



X Index: 145



Y Index: 196

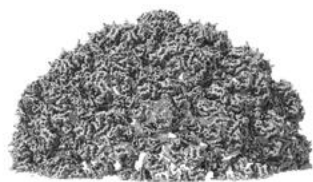


Z Index: 153

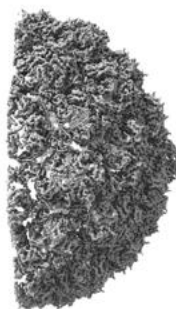
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

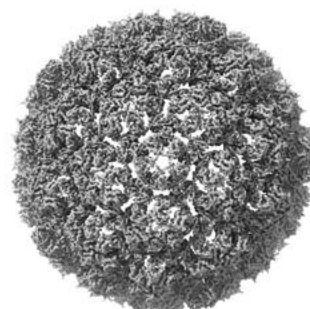
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00705. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

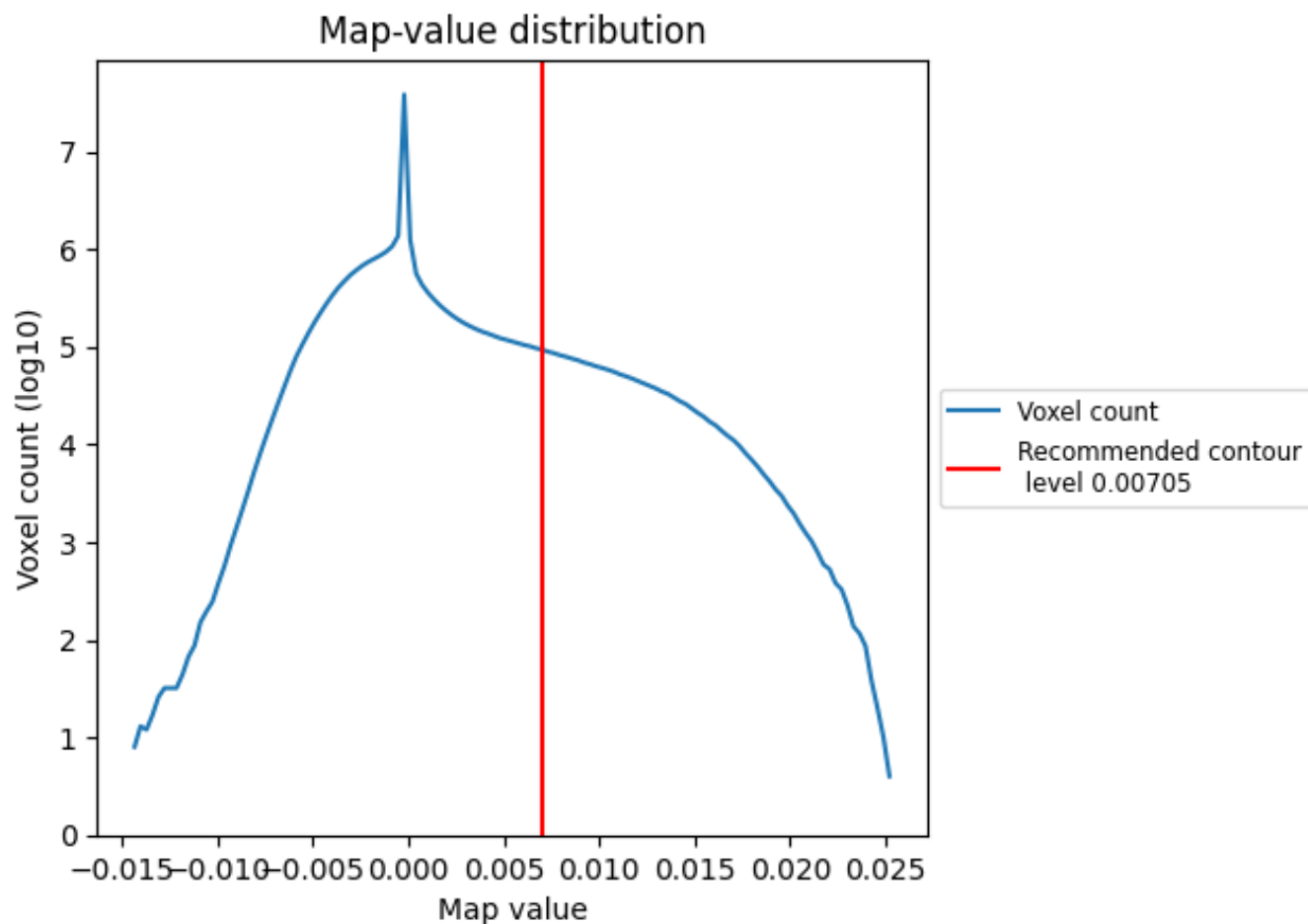
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

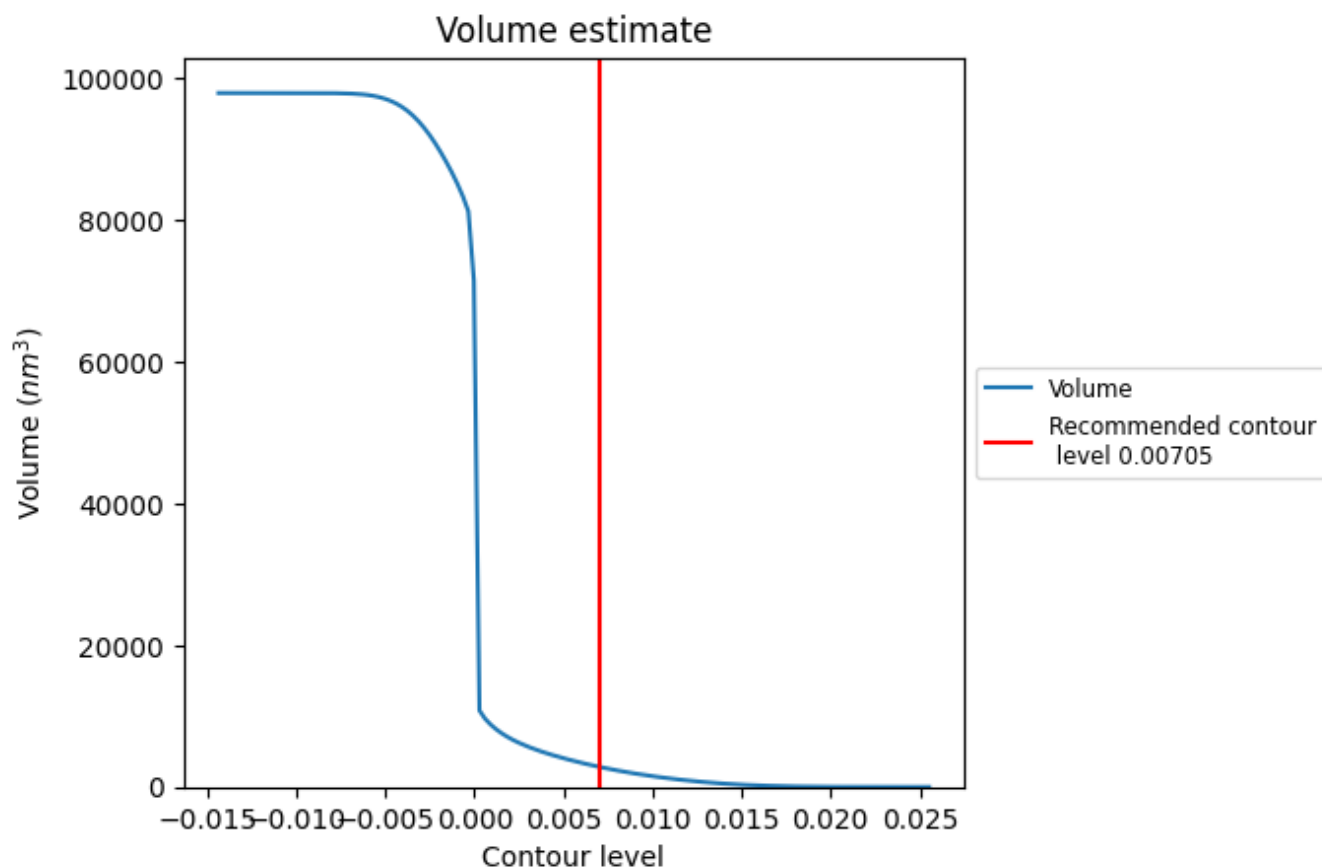
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2818 nm<sup>3</sup>; this corresponds to an approximate mass of 2545 kDa.

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

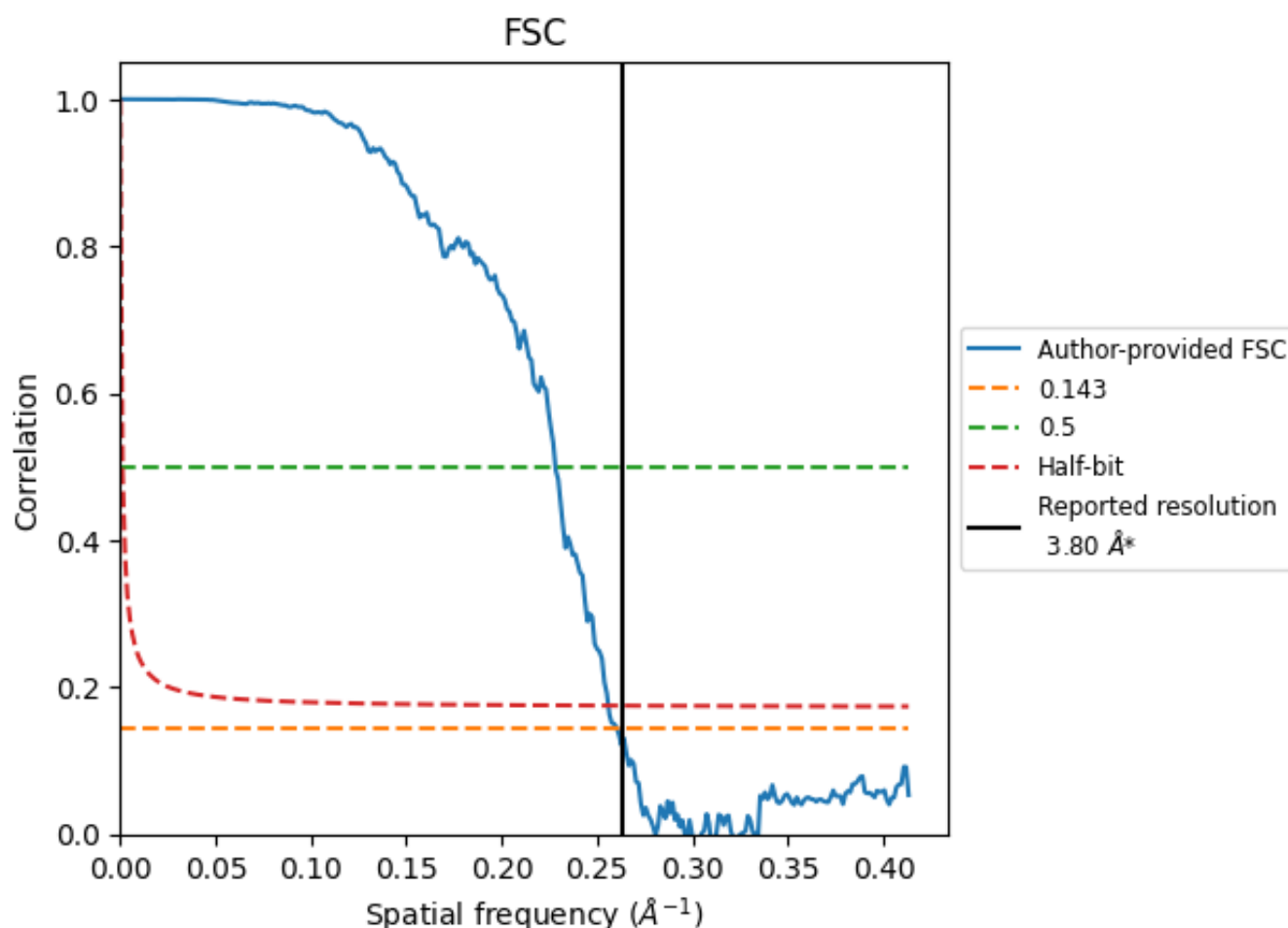
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.84	4.38	3.91
Unmasked-calculated*	-	-	-

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

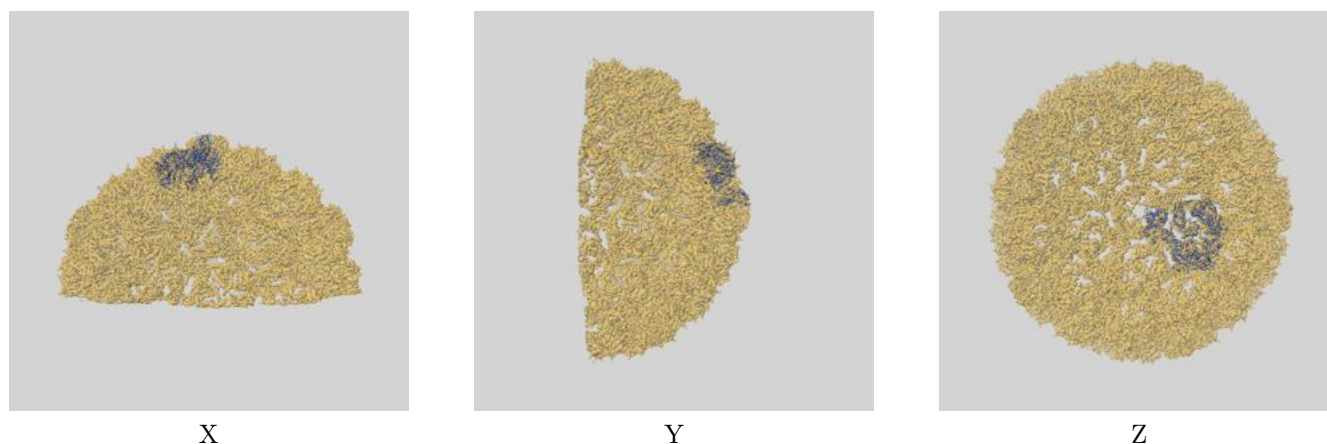


## 9 Map-model fit [i](#)

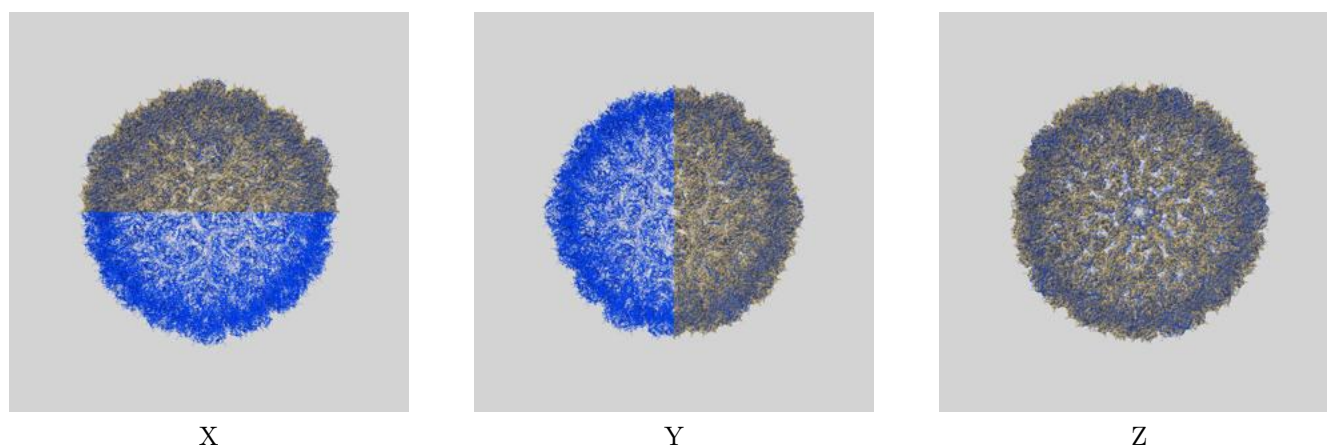
This section contains information regarding the fit between EMDB map EMD-7030 and PDB model 6B0X. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

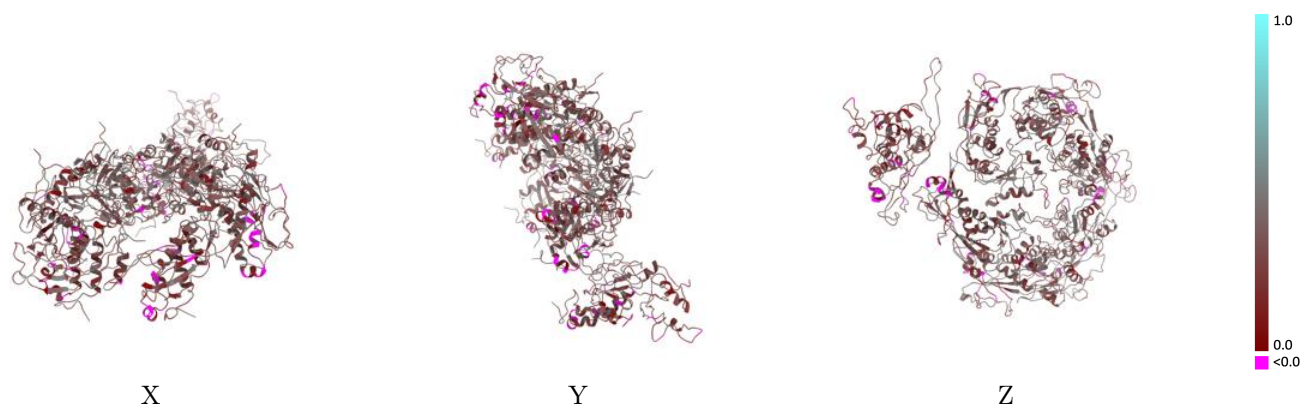


#### 9.1.2 Map-model assembly overlay [i](#)



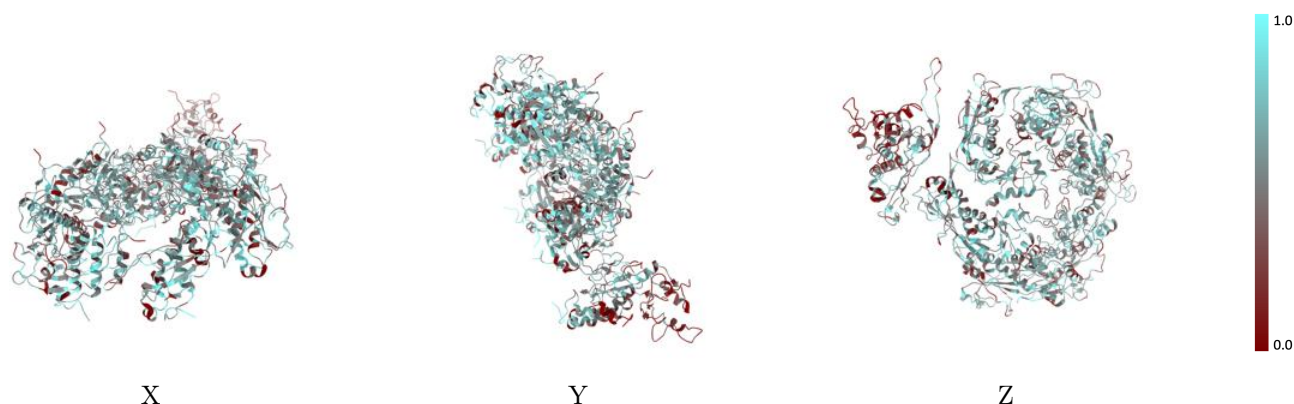
The images above show the 3D surface view of the map at the recommended contour level 0.00705 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



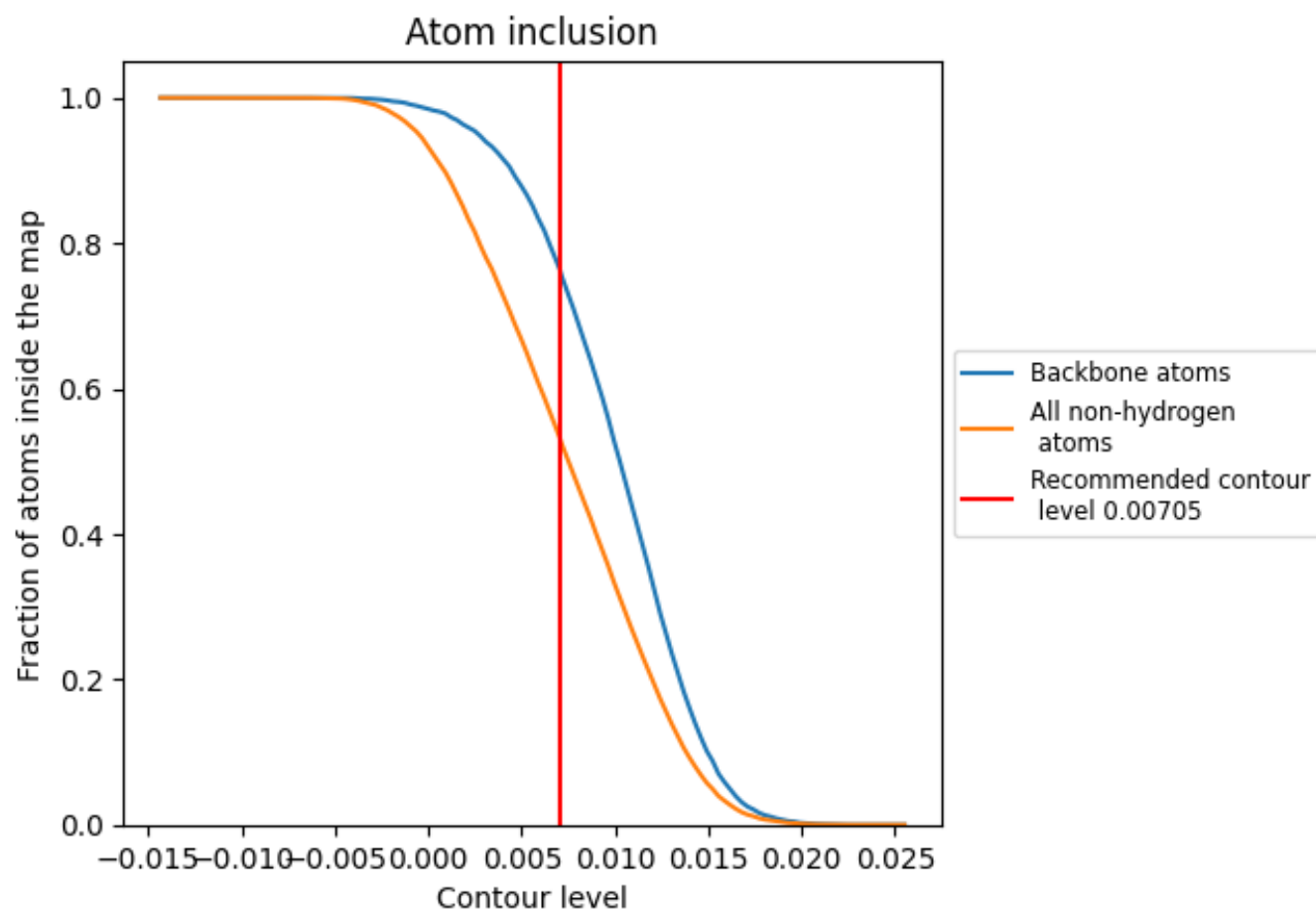
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00705).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 53% 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 (0.00705) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5320	<div></div> 0.2990
A	<div></div> 0.4183	<div></div> 0.2760
B	<div></div> 0.5715	<div></div> 0.3170
C	<div></div> 0.5710	<div></div> 0.3100
D	<div></div> 0.5844	<div></div> 0.2970
E	<div></div> 0.5617	<div></div> 0.2980
F	<div></div> 0.5653	<div></div> 0.3070
G	<div></div> 0.5773	<div></div> 0.3140
a	<div></div> 0.0000	<div></div> 0.1740
b	<div></div> 0.3281	<div></div> 0.2400
c	<div></div> 0.2149	<div></div> 0.2970
d	<div></div> 0.0547	<div></div> 0.2130
e	<div></div> 0.4062	<div></div> 0.2700
f	<div></div> 0.1953	<div></div> 0.2570
g	<div></div> 0.2422	<div></div> 0.2000

1.0

0.0

<0.0