



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 03:48 pm BST

PDB ID : 8ADN  
EMDB ID : EMD-15365  
Title : Vairimorpha necatrix 20S proteasome from spores  
Authors : Jespersen, N.; Ehrenbolger, K.; Winiger, R.; Svedberg, D.; Vossbrinck, C.R.; Barandun, J.  
Deposited on : 2022-07-08  
Resolution : 2.77 Å(reported)  
Based on initial model : 5CZ4

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

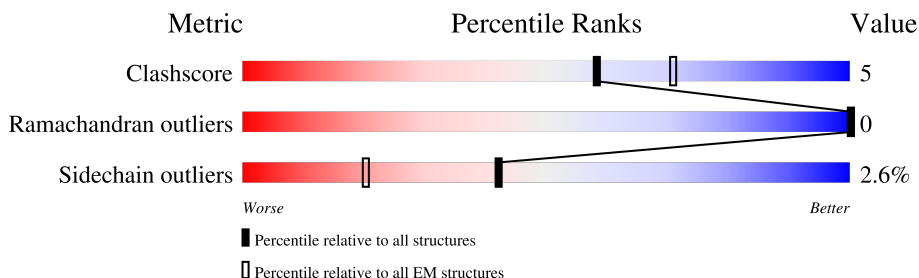
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.77 Å.

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




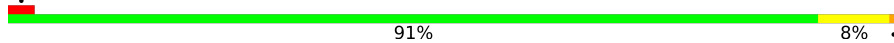


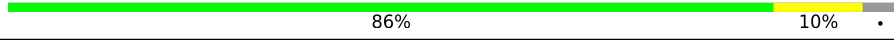


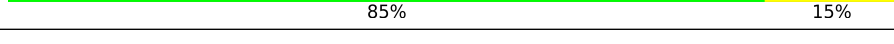
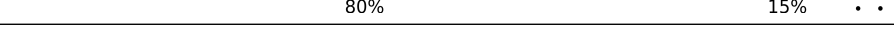
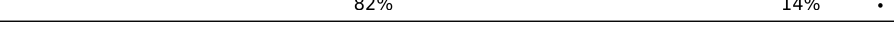
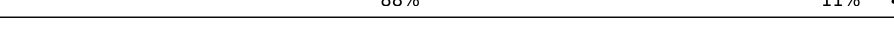

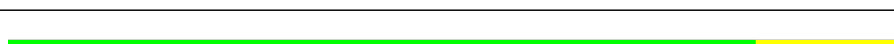




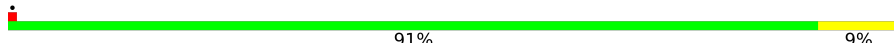
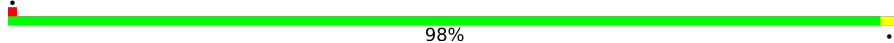



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	3	147	
1	4	147	
2	A	227	
2	O	227	
3	B	231	
3	P	231	
4	C	225	
4	Q	225	

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Mol	Chain	Length	Quality of chain
5	D	234	 81% 18%
5	R	234	 91% 8%
6	E	230	 84% 13%
6	S	230	 86% 12%
7	F	243	 86% 10%
7	T	243	 88% 9%
8	G	234	 86% 12%
8	U	234	 85% 15%
9	H	227	 80% 15%
9	V	227	 82% 14%
10	I	205	 88% 11%
10	W	205	 84% 15%
11	J	193	 92% 8%
11	X	193	 84% 16%
12	K	228	 72% 13% 14%
12	Y	228	 73% 11% 14%
13	L	297	 56% 13% 30%
13	Z	297	 57% 12% 30%
14	M	212	 91% 9%
14	a	212	 98%
15	N	216	 81% 8% 10%
15	b	216	 89% 10%

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 48318 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 Proteasome Inhibitor 31-Like.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	60	Total	C	N	O	0	0
			478	304	78	96		
1	4	60	Total	C	N	O	0	0
			478	304	78	96		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	225	Total	C	N	O	S	0	0
			1686	1063	284	334	5		
2	O	225	Total	C	N	O	S	0	0
			1686	1063	284	334	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	228	Total	C	N	O	S	0	0
			1858	1187	299	362	10		
3	P	228	Total	C	N	O	S	0	0
			1858	1187	299	362	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	219	Total	C	N	O	S	0	0
			1613	1020	275	311	7		
4	Q	219	Total	C	N	O	S	0	0
			1613	1020	275	311	7		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	233	Total	C	N	O	S	0	0
			1853	1174	307	365	7		
5	R	233	Total	C	N	O	S	0	0
			1853	1174	307	365	7		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	225	Total	C	N	O	S	0	0
			1811	1152	308	346	5		
6	S	225	Total	C	N	O	S	0	0
			1811	1152	308	346	5		

- Molecule 7 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	234	Total	C	N	O	S	0	0
			1879	1188	317	365	9		
7	T	234	Total	C	N	O	S	0	0
			1879	1188	317	365	9		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	233	Total	C	N	O	S	0	0
			1843	1186	290	359	8		
8	U	233	Total	C	N	O	S	0	0
			1843	1186	290	359	8		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	218	Total	C	N	O	S	0	0
			1659	1037	293	318	11		
9	V	218	Total	C	N	O	S	0	0
			1659	1037	293	318	11		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	203	Total	C	N	O	S	0	0
			1594	1015	257	308	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	203	Total	C	N	O	S	0	0
			1594	1015	257	308	14		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	193	Total	C	N	O	S	0	0
			1542	983	250	303	6		
11	X	193	Total	C	N	O	S	0	0
			1542	983	250	303	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	195	Total	C	N	O	S	0	0
			1509	961	254	285	9		
12	Y	195	Total	C	N	O	S	0	0
			1509	961	254	285	9		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	208	Total	C	N	O	S	0	0
			1690	1074	280	330	6		
13	Z	208	Total	C	N	O	S	0	0
			1690	1074	280	330	6		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

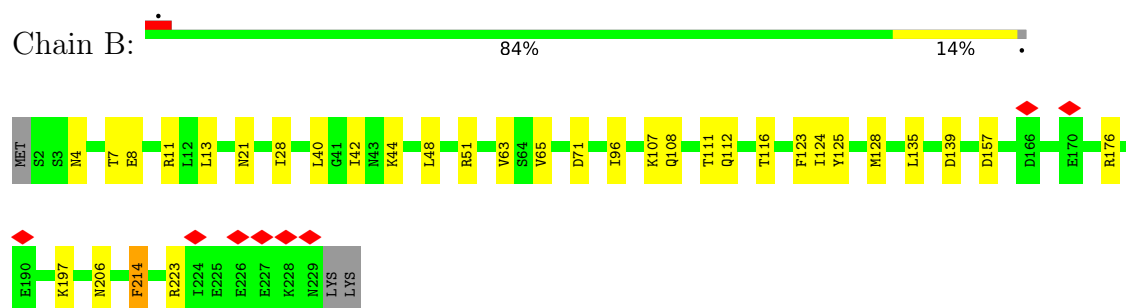
Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	212	Total	C	N	O	S	0	0
			1662	1041	285	323	13		
14	a	212	Total	C	N	O	S	0	0
			1662	1041	285	323	13		

- Molecule 15 is a protein called Proteasome subunit beta type-1.

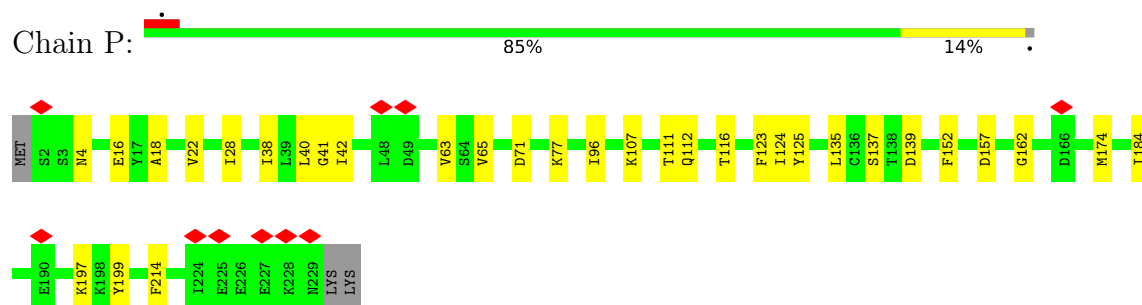
Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	194	Total	C	N	O	S	0	0
			1482	934	249	286	13		
15	b	194	Total	C	N	O	S	0	0
			1482	934	249	286	13		



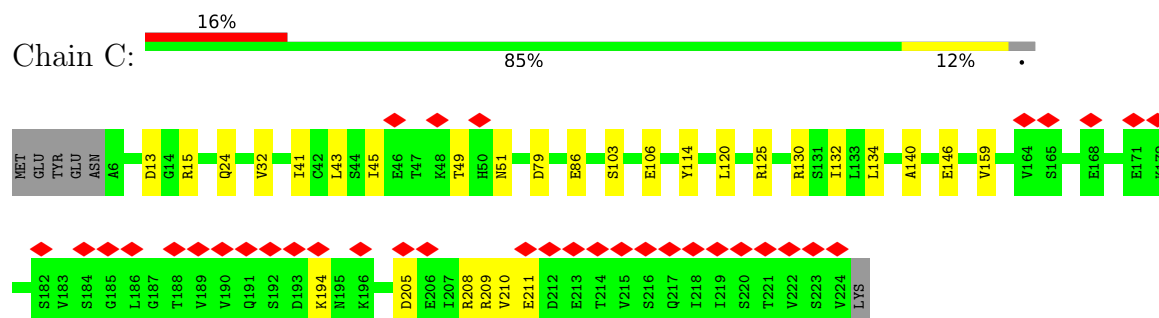
- Molecule 3: Proteasome subunit alpha type-3



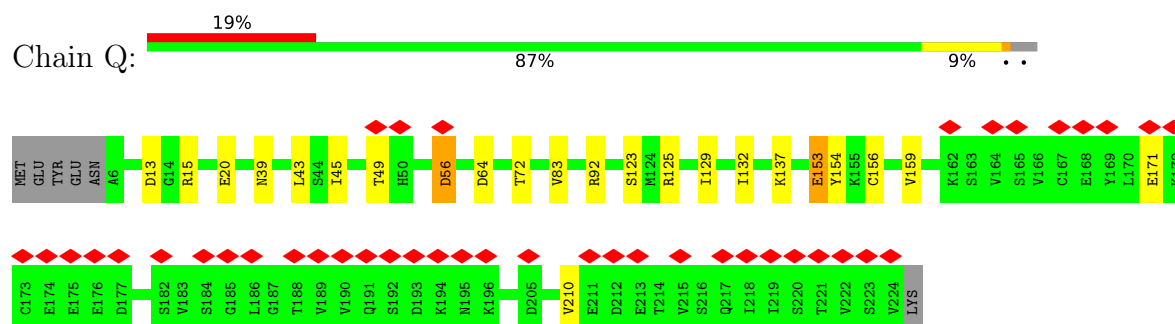
- Molecule 3: Proteasome subunit alpha type-3



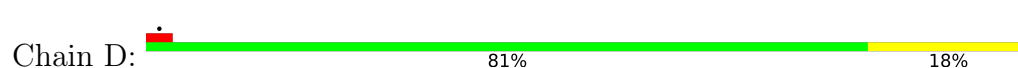
- Molecule 4: Proteasome subunit alpha type-4

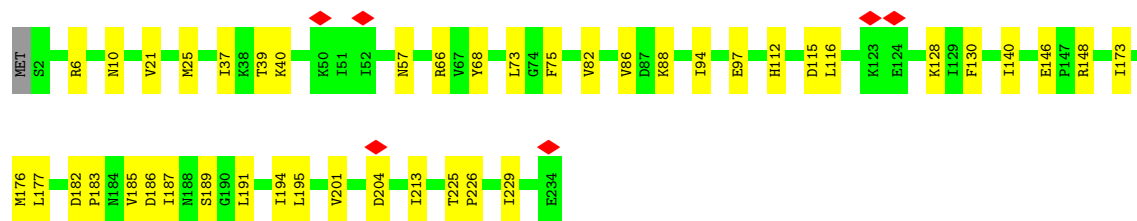


- Molecule 4: Proteasome subunit alpha type-4

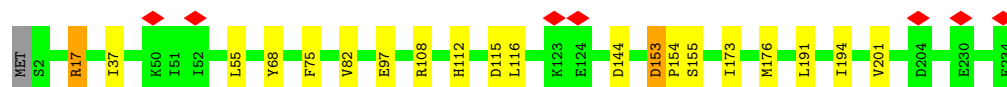
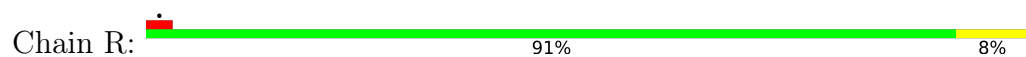


- Molecule 5: Proteasome subunit alpha type-5

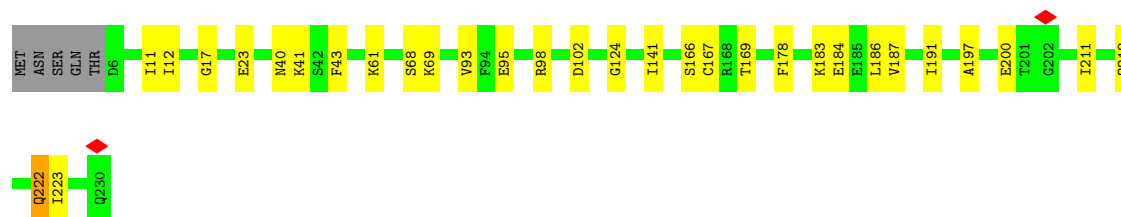
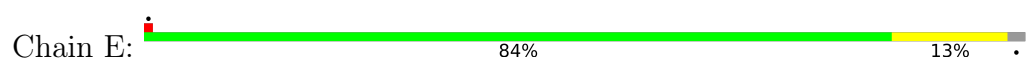




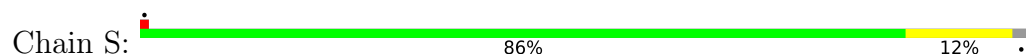
- Molecule 5: Proteasome subunit alpha type-5



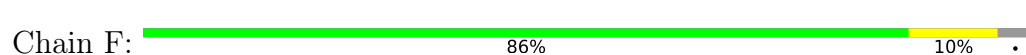
- Molecule 6: Proteasome subunit alpha type-6



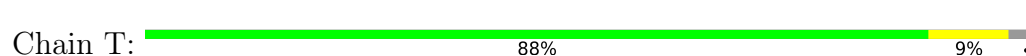
- Molecule 6: Proteasome subunit alpha type-6



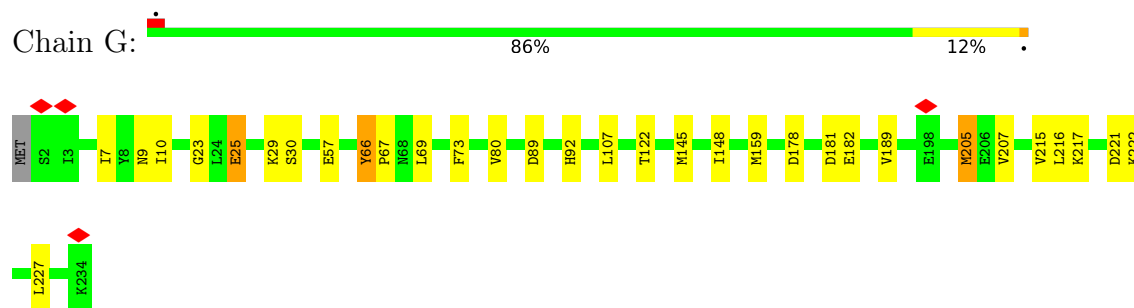
- Molecule 7: Proteasome subunit alpha type-7



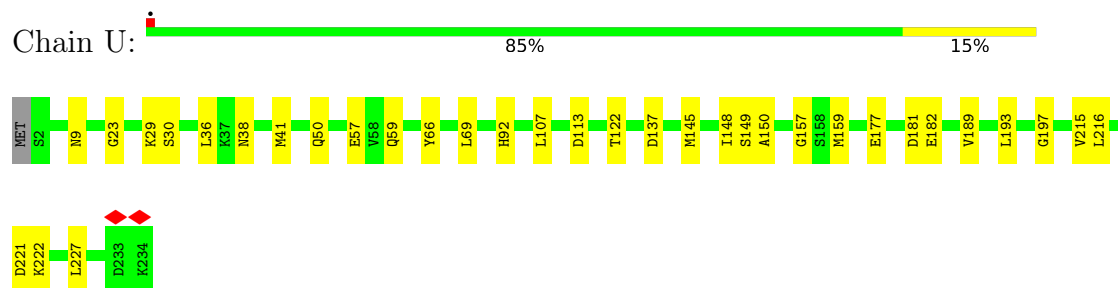
- Molecule 7: Proteasome subunit alpha type-7



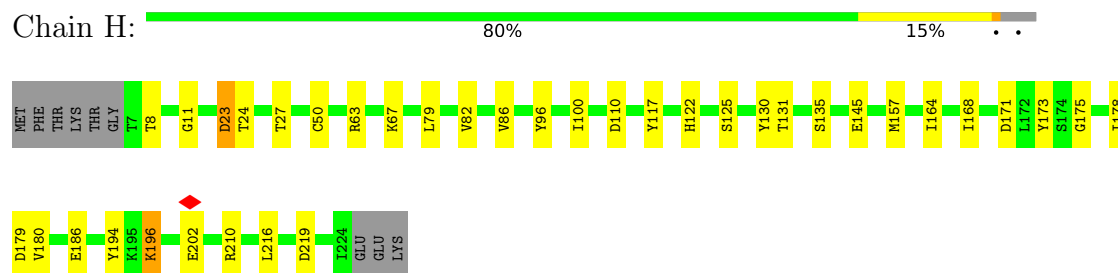
- Molecule 8: Proteasome subunit alpha type-1



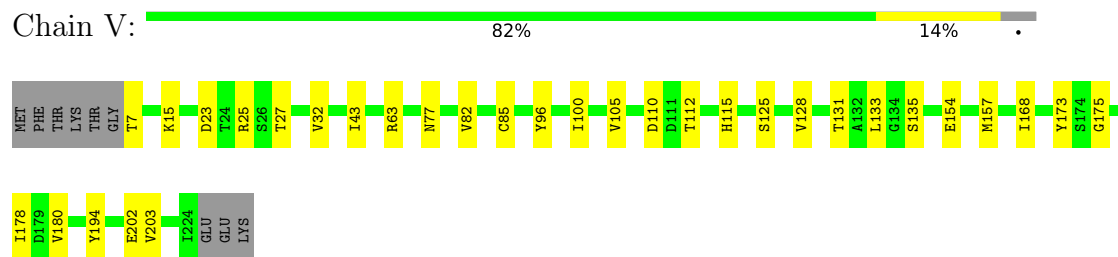
- Molecule 8: Proteasome subunit alpha type-1



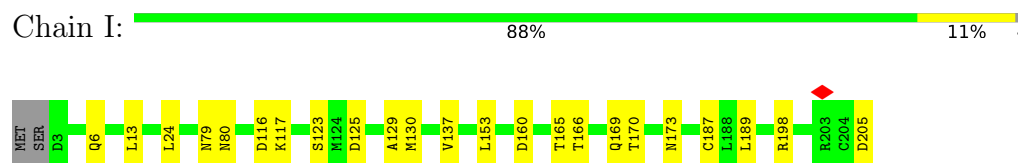
- Molecule 9: Proteasome subunit beta type-2




- Molecule 9: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-3

Chain W:  84% 15% .




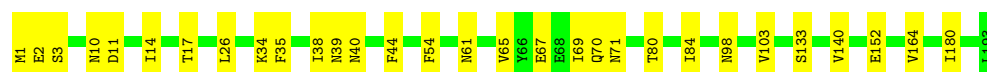
- Molecule 11: Proteasome subunit beta type-4

Chain J:  92% 8%



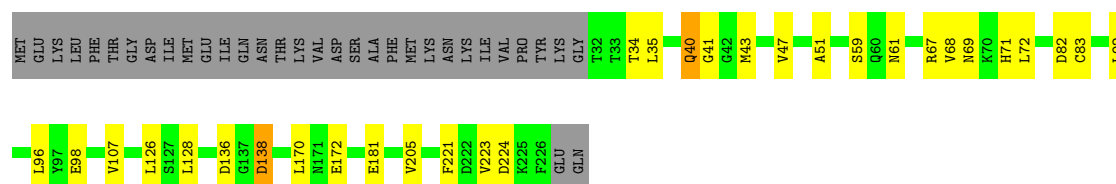
- Molecule 11: Proteasome subunit beta type-4

Chain X:  84% 16%



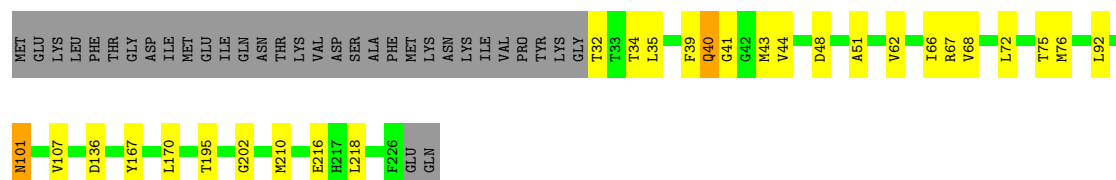
- Molecule 12: Proteasome subunit beta type-5

Chain K:  72% 13% . 14%



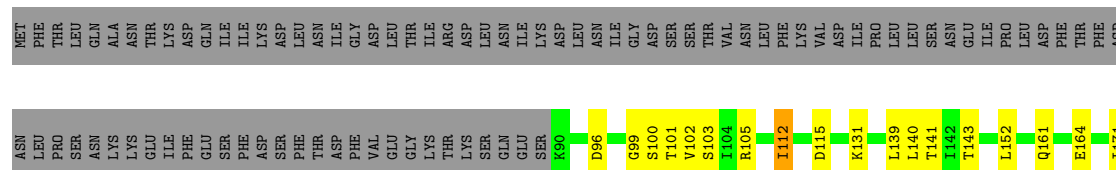
- Molecule 12: Proteasome subunit beta type-5

Chain Y:  73% 11% . 14%

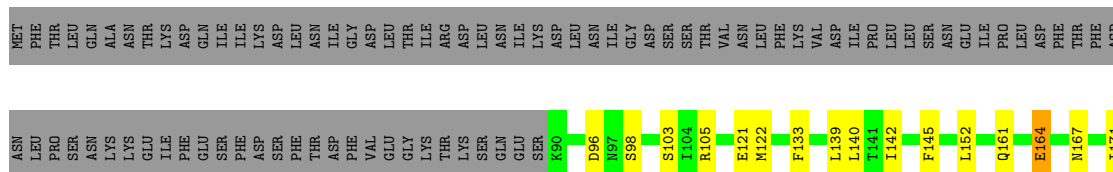


- Molecule 13: Proteasome subunit beta type-6

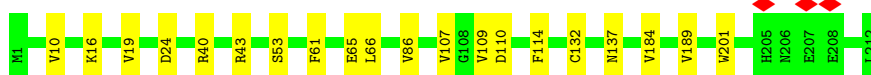
Chain L:  56% 13% . 30%



- Molecule 13: Proteasome subunit beta type-6



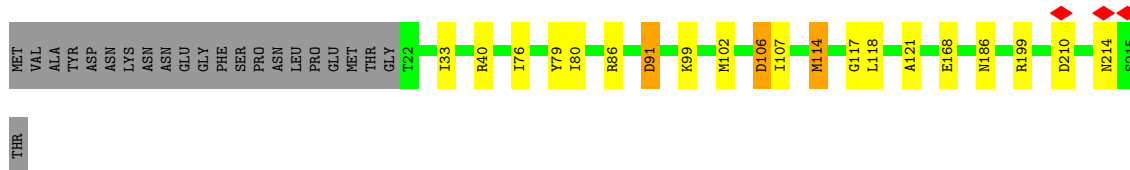
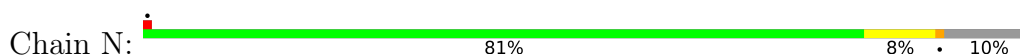
- Molecule 14: Proteasome subunit beta type-7



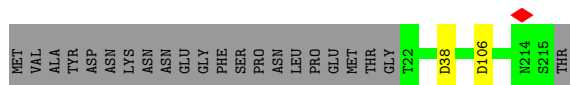
- Molecule 14: Proteasome subunit beta type-7



- Molecule 15: Proteasome subunit beta type-1



- Molecule 15: Proteasome subunit beta type-1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	52679	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 ( $e^-/\text{\AA}^2$ )	35.01, 36.334	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	4.477	Depositor
Minimum map value	-2.358	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.135	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	416.80002, 416.80002, 416.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.042, 1.042, 1.042	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	3	0.25	0/489	0.43	0/653
1	4	0.25	0/489	0.45	0/653
2	A	0.28	0/1711	0.47	0/2316
2	O	0.27	0/1711	0.48	0/2316
3	B	0.27	0/1891	0.47	0/2535
3	P	0.26	0/1891	0.46	0/2535
4	C	0.26	0/1636	0.47	0/2214
4	Q	0.26	0/1636	0.48	0/2214
5	D	0.26	0/1883	0.46	0/2537
5	R	0.26	0/1883	0.48	0/2537
6	E	0.26	0/1841	0.48	0/2478
6	S	0.26	0/1841	0.48	0/2478
7	F	0.26	0/1903	0.47	0/2556
7	T	0.26	0/1903	0.47	0/2556
8	G	0.27	0/1880	0.44	0/2543
8	U	0.27	0/1880	0.44	0/2543
9	H	0.27	0/1687	0.52	0/2280
9	V	0.27	0/1687	0.51	0/2280
10	I	0.28	0/1625	0.48	0/2183
10	W	0.28	0/1625	0.48	0/2183
11	J	0.28	0/1567	0.46	0/2114
11	X	0.28	0/1567	0.47	0/2114
12	K	0.28	0/1542	0.47	0/2078
12	Y	0.27	0/1542	0.47	0/2078
13	L	0.28	0/1727	0.50	0/2332
13	Z	0.28	0/1727	0.50	0/2332
14	M	0.27	0/1684	0.51	0/2279
14	a	0.27	0/1684	0.50	0/2279
15	N	0.28	0/1504	0.50	0/2027
15	b	0.28	0/1504	0.51	0/2027
All	All	0.27	0/49140	0.48	0/66250

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 ⓘ

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	3	478	0	444	8	0
1	4	478	0	444	4	0
2	A	1686	0	1583	14	0
2	O	1686	0	1583	9	0
3	B	1858	0	1827	20	0
3	P	1858	0	1827	25	0
4	C	1613	0	1502	15	0
4	Q	1613	0	1502	15	0
5	D	1853	0	1851	30	0
5	R	1853	0	1851	18	0
6	E	1811	0	1827	17	0
6	S	1811	0	1827	14	0
7	F	1879	0	1919	16	0
7	T	1879	0	1919	11	0
8	G	1843	0	1817	19	0
8	U	1843	0	1817	19	0
9	H	1659	0	1663	23	0
9	V	1659	0	1663	18	0
10	I	1594	0	1574	12	0
10	W	1594	0	1574	16	0
11	J	1542	0	1539	8	0
11	X	1542	0	1539	18	0
12	K	1509	0	1467	20	0
12	Y	1509	0	1467	17	0
13	L	1690	0	1630	20	0
13	Z	1690	0	1630	27	0
14	M	1662	0	1669	11	0
14	a	1662	0	1669	0	0
15	N	1482	0	1493	14	0
15	b	1482	0	1493	0	0
All	All	48318	0	47610	413	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 5.

All (413) 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)
7:F:103:SER:OG	15:N:91:ASP:OD2	1.81	0.98
9:H:186:GLU:OE1	9:H:186:GLU:N	2.09	0.86
9:V:7:THR:N	9:V:135:SER:HG	1.74	0.84
13:Z:96:ASP:OD1	13:Z:98:SER:OG	1.94	0.84
2:O:82:ARG:NH2	8:U:150:ALA:O	2.13	0.82
8:U:177:GLU:OE1	8:U:177:GLU:N	2.13	0.81
5:D:186:ASP:OD1	5:D:187:ILE:N	2.14	0.80
6:E:200:GLU:OE2	6:E:200:GLU:N	2.14	0.80
2:A:216:GLU:N	2:A:216:GLU:OE1	2.15	0.79
1:4:100:ILE:HD11	12:K:51:ALA:HB1	1.67	0.77
11:X:38:ILE:HD11	11:X:44:PHE:HD2	1.49	0.75
2:A:117:GLN:NE2	3:B:71:ASP:OD2	2.20	0.75
10:W:114:THR:OG1	10:W:116:ASP:OD2	2.04	0.75
5:D:73:LEU:HD23	5:D:86:VAL:HG22	1.70	0.74
13:L:115:ASP:OD1	13:L:131:LYS:NZ	2.21	0.73
2:O:110:GLU:OE1	2:O:149:TYR:OH	2.04	0.73
2:O:117:GLN:NE2	3:P:71:ASP:OD1	2.21	0.72
12:K:82:ASP:OD1	12:K:83:CYS:N	2.23	0.71
11:X:38:ILE:HD11	11:X:44:PHE:CD2	2.24	0.71
3:P:40:LEU:HD21	3:P:42:ILE:HD11	1.72	0.71
8:U:221:ASP:OD1	8:U:222:LYS:N	2.24	0.70
10:I:166:THR:O	10:I:170:THR:HG23	1.92	0.70
6:S:93:VAL:HG21	13:Z:161:GLN:OE1	1.91	0.69
10:W:166:THR:O	10:W:170:THR:HG23	1.93	0.69
4:C:130:ARG:NE	4:C:146:GLU:OE1	2.25	0.69
13:L:270:ASP:OD2	13:L:273:THR:OG1	2.11	0.69
15:N:210:ASP:OD1	15:N:214:ASN:ND2	2.26	0.68
11:X:67:GLU:OE2	11:X:71:ASN:ND2	2.23	0.68
1:3:128:ASP:OD1	9:H:122:HIS:ND1	2.27	0.67
8:G:69:LEU:HD21	8:G:107:LEU:HD22	1.77	0.66
7:T:186:GLU:OE2	7:T:233:LYS:NZ	2.27	0.66
11:J:67:GLU:OE1	11:J:71:ASN:ND2	2.27	0.66
8:G:189:VAL:HG21	8:G:227:LEU:HD21	1.78	0.66
10:I:125:ASP:OD1	10:I:129:ALA:N	2.28	0.65
5:R:17:ARG:H	5:R:17:ARG:HD2	1.62	0.65
9:V:105:VAL:HG23	9:V:133:LEU:HD12	1.78	0.65
12:Y:35:LEU:HD13	12:Y:170:LEU:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:40:GLN:OE1	12:Y:41:GLY:N	2.29	0.65
4:C:13:ASP:OD2	4:C:15:ARG:NH1	2.30	0.65
7:F:19:ILE:HG21	7:F:149:THR:HG22	1.78	0.65
9:H:135:SER:OG	9:H:171:ASP:OD2	2.13	0.64
11:X:39:ASN:OD1	11:X:40:ASN:N	2.31	0.64
5:D:195:LEU:HD21	5:D:213:ILE:HD11	1.79	0.64
12:K:35:LEU:HD13	12:K:170:LEU:HD11	1.80	0.64
12:Y:66:ILE:HD11	12:Y:76:MET:SD	2.39	0.63
5:D:66:ARG:NH2	12:K:98:GLU:OE2	2.31	0.63
4:C:43:LEU:HD12	4:C:45:ILE:HD11	1.80	0.63
3:B:40:LEU:HD21	3:B:42:ILE:HD11	1.81	0.62
5:D:88:LYS:NZ	5:D:128:LYS:O	2.29	0.62
7:F:91:LEU:HD22	7:F:102:VAL:HG11	1.81	0.62
3:P:107:LYS:O	3:P:111:THR:HG23	2.00	0.62
6:E:40:ASN:ND2	6:E:178:PHE:O	2.32	0.62
9:H:157:MET:CE	9:H:180:VAL:HG11	2.30	0.61
12:K:40:GLN:OE1	12:K:41:GLY:N	2.33	0.61
1:3:84:ASP:OD2	1:3:99:ALA:HB2	2.00	0.61
3:B:107:LYS:O	3:B:111:THR:HG23	2.00	0.61
10:W:153:LEU:HD12	10:W:170:THR:HG22	1.82	0.61
10:I:169:GLN:O	10:I:173:ASN:ND2	2.35	0.60
4:Q:49:THR:HG23	4:Q:49:THR:O	2.02	0.60
10:W:169:GLN:O	10:W:173:ASN:ND2	2.33	0.60
1:4:100:ILE:CD1	12:K:51:ALA:HB1	2.30	0.60
13:L:293:ARG:NH1	13:L:294:LEU:O	2.34	0.60
7:T:19:ILE:HG21	7:T:149:THR:HG22	1.84	0.60
8:U:189:VAL:HG21	8:U:227:LEU:HD21	1.84	0.59
7:T:207:GLU:OE2	7:T:221:ARG:NH1	2.35	0.59
2:A:207:GLN:OE1	2:A:207:GLN:N	2.30	0.59
5:D:6:ARG:O	5:D:10:ASN:ND2	2.35	0.59
9:H:24:THR:HG22	9:H:179:ASP:OD1	2.03	0.59
10:I:6:GLN:N	10:I:6:GLN:OE1	2.35	0.59
14:M:110:ASP:O	14:M:110:ASP:OD2	2.21	0.59
8:U:69:LEU:HD21	8:U:107:LEU:HD22	1.85	0.58
3:B:4:ASN:ND2	3:B:116:THR:O	2.37	0.58
2:A:19:ASP:OD1	2:A:20:GLN:N	2.37	0.58
7:F:87:LEU:HD11	7:F:111:ILE:HD13	1.86	0.58
13:L:266:ALA:O	13:L:270:ASP:N	2.34	0.58
8:U:69:LEU:HD21	8:U:107:LEU:CD2	2.34	0.58
13:L:152:LEU:HD23	13:L:194:VAL:HG21	1.85	0.58
13:Z:152:LEU:HD23	13:Z:194:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:61:LYS:HG3	6:E:61:LYS:O	2.04	0.57
11:J:177:GLU:OE2	11:J:179:LYS:NZ	2.37	0.57
12:K:223:VAL:HG21	10:W:205:ASP:HB3	1.87	0.57
6:E:191:ILE:HD11	6:E:211:ILE:HD11	1.86	0.57
14:M:24:ASP:O	14:M:40:ARG:NH2	2.37	0.57
3:B:128:MET:SD	3:B:206:ASN:ND2	2.78	0.57
13:Z:270:ASP:OD2	13:Z:273:THR:OG1	2.21	0.57
13:Z:296:GLN:OE1	13:Z:296:GLN:N	2.32	0.57
13:L:296:GLN:OE1	13:L:296:GLN:N	2.34	0.57
3:B:8:GLU:OE1	3:B:8:GLU:O	2.23	0.57
4:C:103:SER:OG	4:C:106:GLU:OE1	2.22	0.56
10:I:153:LEU:HD12	10:I:170:THR:HG22	1.87	0.56
4:Q:132:ILE:HD11	4:Q:159:VAL:HG21	1.86	0.56
9:H:157:MET:HE1	9:H:180:VAL:HG11	1.88	0.56
11:X:140:VAL:HG21	11:X:164:VAL:HG21	1.87	0.56
11:X:80:THR:O	11:X:84:ILE:HG12	2.05	0.56
6:S:191:ILE:HD11	6:S:211:ILE:HD11	1.88	0.56
2:O:19:ASP:OD1	2:O:20:GLN:N	2.37	0.55
11:X:38:ILE:H	11:X:38:ILE:HD12	1.70	0.55
13:L:101:THR:HG23	13:L:143:THR:CG2	2.36	0.55
6:S:98:ARG:N	6:S:98:ARG:HD3	2.21	0.55
13:Z:152:LEU:CD2	13:Z:194:VAL:HG21	2.36	0.55
7:F:47:LYS:NZ	7:F:59:ASN:O	2.31	0.55
3:P:65:VAL:HG22	3:P:123:PHE:CE1	2.41	0.55
7:T:87:LEU:HD11	7:T:111:ILE:HD13	1.87	0.55
3:P:65:VAL:HG22	3:P:123:PHE:HE1	1.72	0.55
3:P:162:GLY:HA3	3:P:184:ILE:HD11	1.87	0.55
8:G:69:LEU:HD21	8:G:107:LEU:CD2	2.36	0.55
9:H:130:TYR:OH	9:H:145:GLU:OE2	2.24	0.54
5:R:144:ASP:OD1	5:R:144:ASP:N	2.39	0.54
8:U:193:LEU:O	8:U:197:GLY:N	2.35	0.54
9:V:157:MET:CE	9:V:180:VAL:HG11	2.38	0.54
2:O:97:ASP:OD1	9:V:63:ARG:NE	2.36	0.54
4:Q:210:VAL:HG12	4:Q:210:VAL:O	2.06	0.54
2:A:174:MET:O	2:A:178:ASN:N	2.39	0.54
5:D:68:TYR:OH	5:D:97:GLU:OE2	2.23	0.54
6:E:40:ASN:OD1	6:E:41:LYS:N	2.42	0.53
10:W:186:GLU:OE2	10:W:197:ARG:NH1	2.39	0.53
3:P:124:ILE:HD11	3:P:152:PHE:HD2	1.73	0.53
8:G:189:VAL:HG21	8:G:227:LEU:CD2	2.38	0.53
13:Z:133:PHE:O	13:Z:140:LEU:N	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:10:ASN:O	11:X:11:ASP:OD2	2.27	0.52
5:R:17:ARG:H	5:R:17:ARG:CD	2.21	0.52
10:I:116:ASP:OD2	10:I:116:ASP:O	2.27	0.52
3:B:65:VAL:HG22	3:B:123:PHE:CE1	2.45	0.52
4:C:43:LEU:CD1	4:C:45:ILE:HD11	2.39	0.52
8:G:66:TYR:CD2	8:G:67:PRO:HD2	2.45	0.52
4:Q:83:VAL:HG21	4:Q:129:ILE:HD11	1.90	0.52
13:Z:140:LEU:HD11	13:Z:194:VAL:CG1	2.40	0.52
5:D:146:GLU:OE1	5:D:148:ARG:NH2	2.41	0.52
9:V:202:GLU:OE1	9:V:203:VAL:N	2.42	0.52
4:Q:171:GLU:HA	5:R:55:LEU:HD21	1.92	0.52
13:L:139:LEU:HD12	13:L:282:ILE:HD11	1.92	0.52
6:E:93:VAL:HG21	13:L:161:GLN:NE2	2.25	0.52
11:J:140:VAL:HG21	11:J:164:VAL:HG21	1.92	0.52
6:S:26:ASN:O	6:S:29:VAL:HG22	2.10	0.52
13:Z:121:GLU:O	13:Z:122:MET:HG2	2.10	0.52
5:D:10:ASN:ND2	6:E:124:GLY:O	2.43	0.52
13:Z:266:ALA:O	13:Z:270:ASP:N	2.36	0.52
11:X:17:THR:HG22	11:X:35:PHE:CE1	2.46	0.51
7:T:15:ASP:OD1	8:U:29:LYS:NZ	2.39	0.51
13:Z:210:ASP:OD2	13:Z:214:HIS:N	2.44	0.51
5:R:68:TYR:OH	5:R:97:GLU:OE1	2.23	0.51
5:D:75:PHE:CD2	5:D:82:VAL:HG21	2.46	0.50
5:D:213:ILE:HD12	5:D:229:ILE:HG12	1.93	0.50
9:H:168:ILE:HG23	9:H:175:GLY:HA2	1.93	0.50
8:U:189:VAL:HG21	8:U:227:LEU:CD2	2.40	0.50
3:B:28:ILE:HD12	3:B:124:ILE:HD12	1.93	0.50
3:B:96:ILE:HD11	3:B:125:TYR:HB2	1.93	0.50
3:P:4:ASN:ND2	3:P:116:THR:O	2.45	0.50
3:B:65:VAL:HG22	3:B:123:PHE:HE1	1.76	0.50
1:3:140:ASP:O	1:3:140:ASP:OD2	2.30	0.50
1:4:85:LEU:HD12	1:4:85:LEU:O	2.11	0.50
12:Y:34:THR:HB	12:Y:75:THR:HG21	1.93	0.50
9:V:25:ARG:HD2	9:V:32:VAL:HG13	1.94	0.50
13:Z:257:ASP:OD1	13:Z:260:ARG:NH2	2.45	0.50
6:S:209:VAL:HG21	6:S:229:LEU:HD21	1.94	0.49
11:X:3:SER:OG	11:X:133:SER:OG	2.22	0.49
1:3:77:PHE:O	13:Z:186:ARG:NH2	2.42	0.49
2:A:105:ILE:O	2:A:109:VAL:HG23	2.12	0.49
4:Q:64:ASP:OD2	4:Q:92:ARG:NH2	2.45	0.49
8:G:221:ASP:OD2	8:G:222:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:48:LEU:HD11	3:B:214:PHE:CE2	2.48	0.49
13:L:152:LEU:CD2	13:L:194:VAL:HG21	2.43	0.49
3:P:137:SER:HG	3:P:152:PHE:HE2	1.58	0.49
5:R:153:ASP:OD1	5:R:155:SER:N	2.44	0.49
11:X:14:ILE:HD13	11:X:180:ILE:HG23	1.94	0.49
4:C:41:ILE:HD11	4:C:140:ALA:HB1	1.95	0.49
8:G:205:MET:HE3	8:G:207:VAL:HG23	1.95	0.49
8:G:89:ASP:OD2	15:N:86:ARG:NH1	2.45	0.48
9:H:8:THR:HG22	9:H:8:THR:O	2.13	0.48
11:X:2:GLU:OE2	11:X:34:LYS:NZ	2.40	0.48
5:R:112:HIS:NE2	5:R:116:LEU:HD11	2.28	0.48
6:S:147:ASP:OD1	6:S:147:ASP:C	2.51	0.48
8:G:23:GLY:HA3	8:G:148:ILE:HD13	1.95	0.48
5:D:94:ILE:HD12	12:K:96:LEU:HD13	1.96	0.48
5:D:185:VAL:HG12	5:D:189:SER:OG	2.13	0.48
9:H:23:ASP:OD2	9:H:23:ASP:C	2.50	0.48
12:Y:101:ASN:OD1	12:Y:101:ASN:N	2.46	0.48
5:R:97:GLU:HG2	12:Y:92:LEU:HD21	1.95	0.48
7:T:91:LEU:HD22	7:T:102:VAL:HG11	1.95	0.48
9:V:96:TYR:CD2	9:V:100:ILE:HD12	2.48	0.48
14:M:109:VAL:HG22	14:M:114:PHE:CD2	2.49	0.48
5:R:173:ILE:HD11	5:R:201:VAL:HG11	1.96	0.48
9:V:157:MET:SD	9:V:180:VAL:HG11	2.54	0.48
8:G:181:ASP:OD1	8:G:182:GLU:N	2.44	0.48
3:P:157:ASP:OD2	3:P:157:ASP:N	2.45	0.48
5:R:37:ILE:CG1	5:R:194:ILE:HD12	2.44	0.48
4:C:86:GLU:HG3	4:C:114:TYR:CZ	2.48	0.47
7:F:91:LEU:HD21	7:F:110:GLN:HG3	1.96	0.47
10:I:13:LEU:HD23	10:I:24:LEU:HD11	1.97	0.47
9:V:23:ASP:OD1	9:V:23:ASP:C	2.52	0.47
5:D:182:ASP:O	5:D:185:VAL:HG23	2.15	0.47
2:A:97:ASP:OD1	9:H:63:ARG:NE	2.40	0.47
8:G:215:VAL:HG22	8:G:216:LEU:N	2.29	0.47
15:N:33:ILE:HG21	15:N:121:ALA:HB1	1.96	0.47
12:Y:195:THR:HB	12:Y:202:GLY:HA2	1.97	0.47
13:L:140:LEU:HD11	13:L:194:VAL:CG1	2.45	0.47
3:P:124:ILE:HD11	3:P:152:PHE:CD2	2.50	0.47
11:X:98:ASN:OD1	11:X:98:ASN:O	2.32	0.47
13:Z:103:SER:OG	13:Z:195:THR:HG21	2.15	0.47
10:I:123:SER:HB3	10:I:137:VAL:HG21	1.96	0.47
10:W:21:VAL:HG13	10:W:190:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:139:LEU:HD12	13:Z:282:ILE:HD11	1.96	0.47
9:V:112:THR:OG1	9:V:115:HIS:NE2	2.45	0.46
12:K:68:VAL:HG22	12:K:72:LEU:O	2.16	0.46
12:K:181:GLU:HA	12:K:181:GLU:OE2	2.15	0.46
11:X:152:GLU:OE1	11:X:152:GLU:N	2.45	0.46
12:Y:51:ALA:CB	12:Y:62:VAL:HG21	2.46	0.46
12:Y:216:GLU:OE1	12:Y:218:LEU:HD21	2.15	0.46
7:F:83:ILE:HG22	7:F:87:LEU:HD12	1.96	0.46
7:F:108:ARG:NH1	8:G:57:GLU:OE1	2.44	0.46
8:U:59:GLN:O	8:U:59:GLN:HG3	2.16	0.46
13:Z:275:ASP:O	13:Z:294:LEU:N	2.39	0.46
9:H:79:LEU:HD23	9:H:79:LEU:H	1.81	0.46
3:P:18:ALA:O	3:P:22:VAL:HG23	2.16	0.46
13:Z:142:ILE:CD1	13:Z:194:VAL:HG22	2.45	0.46
5:R:191:LEU:O	5:R:194:ILE:HG22	2.15	0.46
2:O:97:ASP:OD1	9:V:63:ARG:NH2	2.48	0.46
7:F:37:ASN:OD1	7:F:38:LYS:N	2.49	0.46
4:Q:56:ASP:O	4:Q:56:ASP:OD2	2.34	0.46
13:Z:164:GLU:OE1	13:Z:164:GLU:O	2.33	0.46
3:P:96:ILE:HD11	3:P:125:TYR:HB2	1.97	0.46
11:J:79:VAL:O	11:J:83:VAL:HG23	2.16	0.45
7:T:108:ARG:NH1	8:U:57:GLU:OE2	2.48	0.45
4:C:49:THR:HG22	4:C:194:LYS:O	2.16	0.45
5:R:37:ILE:HG12	5:R:194:ILE:HD12	1.98	0.45
5:D:21:VAL:O	5:D:25:MET:HG2	2.17	0.45
5:D:75:PHE:CG	5:D:82:VAL:HG21	2.51	0.45
5:D:191:LEU:HA	5:D:194:ILE:HG22	1.98	0.45
15:N:40:ARG:NH1	15:N:186:ASN:O	2.46	0.45
6:S:11:ILE:O	6:S:12:ILE:HG23	2.16	0.45
14:M:10:VAL:HG23	14:M:53:SER:HB3	1.99	0.45
3:P:40:LEU:HD21	3:P:42:ILE:CD1	2.45	0.45
6:S:94:PHE:CD1	6:S:94:PHE:C	2.90	0.45
9:V:178:ILE:O	9:V:194:TYR:N	2.48	0.45
10:W:54:PHE:CE1	10:W:108:VAL:HG13	2.52	0.45
11:X:44:PHE:HB2	11:X:103:VAL:HG22	1.99	0.45
13:Z:121:GLU:C	13:Z:122:MET:HG2	2.37	0.45
13:Z:142:ILE:HD13	13:Z:194:VAL:HG22	1.99	0.45
11:J:98:ASN:OD1	11:J:98:ASN:O	2.35	0.45
2:O:38:VAL:HG23	2:O:140:MET:HE3	1.97	0.45
5:D:39:THR:HG23	5:D:183:PRO:O	2.17	0.45
3:P:77:LYS:NZ	10:W:78:ASP:OD1	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:167:CYS:SG	6:S:197:ALA:HB2	2.57	0.45
7:T:47:LYS:NZ	7:T:59:ASN:O	2.41	0.45
13:Z:140:LEU:HD11	13:Z:194:VAL:HG11	1.98	0.45
3:B:108:GLN:NE2	4:C:79:ASP:OD2	2.50	0.45
14:M:66:LEU:HD21	14:M:86:VAL:HG22	1.98	0.45
10:W:138:THR:HG21	10:W:146:LEU:HB3	1.99	0.45
12:K:138:ASP:N	12:K:138:ASP:OD1	2.50	0.45
5:D:73:LEU:HD13	5:D:140:ILE:HG13	1.99	0.44
11:J:11:ASP:N	11:J:11:ASP:OD1	2.50	0.44
8:U:181:ASP:OD1	8:U:182:GLU:N	2.47	0.44
5:D:112:HIS:NE2	5:D:116:LEU:HD11	2.32	0.44
5:D:173:ILE:HD11	5:D:201:VAL:HG11	1.98	0.44
10:I:24:LEU:HB3	10:I:187:CYS:HA	1.99	0.44
14:M:132:CYS:O	14:M:137:ASN:ND2	2.48	0.44
15:N:168:GLU:CD	15:N:168:GLU:H	2.21	0.44
2:O:37:CYS:SG	2:O:182:CYS:CB	3.05	0.44
10:W:123:SER:CB	10:W:137:VAL:HG21	2.48	0.44
15:N:199:ARG:NH1	15:N:199:ARG:HB2	2.33	0.44
7:F:87:LEU:HD11	7:F:111:ILE:CD1	2.48	0.44
9:H:11:GLY:O	9:H:131:THR:N	2.47	0.44
4:Q:13:ASP:O	4:Q:13:ASP:OD2	2.35	0.44
11:J:114:TYR:CD1	11:J:122:LEU:HD11	2.53	0.44
10:W:183:MET:SD	10:W:205:ASP:N	2.91	0.44
10:W:191:ASN:HB2	10:W:192:PRO:HD2	1.98	0.44
9:H:27:THR:HG21	9:H:173:TYR:HD1	1.83	0.44
13:L:171:ILE:HD11	13:L:196:LEU:HG	1.99	0.44
10:I:116:ASP:O	10:I:117:LYS:HB2	2.17	0.44
15:N:80:ILE:HD11	15:N:107:ILE:HD12	1.99	0.44
15:N:102:MET:O	15:N:106:ASP:OD1	2.36	0.44
5:D:225:THR:HG22	5:D:226:PRO:HD2	2.00	0.44
3:P:40:LEU:C	3:P:40:LEU:HD23	2.38	0.44
5:D:37:ILE:HG12	5:D:194:ILE:HD12	2.00	0.43
9:H:82:VAL:HG23	9:H:110:ASP:OD2	2.18	0.43
9:H:96:TYR:CD2	9:H:100:ILE:HD12	2.52	0.43
8:U:23:GLY:HA3	8:U:148:ILE:HD13	1.99	0.43
2:A:37:CYS:SG	2:A:182:CYS:CB	3.06	0.43
13:L:103:SER:OG	13:L:195:THR:HG21	2.18	0.43
15:N:79:TYR:HD2	15:N:107:ILE:HD11	1.82	0.43
10:W:160:ASP:N	10:W:160:ASP:OD2	2.51	0.43
3:B:124:ILE:CG2	3:B:135:LEU:HD11	2.49	0.43
6:E:11:ILE:O	6:E:12:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:41:LEU:O	7:F:211:MET:N	2.48	0.43
8:G:25:GLU:OE2	8:G:25:GLU:HA	2.19	0.43
6:S:210:ASP:OD1	6:S:222:GLN:NE2	2.51	0.43
7:T:42:ILE:HG22	7:T:210:ILE:HG22	2.00	0.43
4:C:210:VAL:HG12	4:C:211:GLU:N	2.33	0.43
9:H:86:VAL:HG21	9:H:117:TYR:CG	2.53	0.43
10:I:79:ASN:O	10:I:80:ASN:HB2	2.19	0.43
8:U:9:ASN:H	8:U:122:THR:HG22	1.84	0.43
6:S:212:TRP:NE1	6:S:222:GLN:OE1	2.52	0.43
8:G:9:ASN:H	8:G:122:THR:HG22	1.84	0.43
13:L:141:THR:HG22	13:L:195:THR:HB	2.01	0.43
15:N:199:ARG:HB2	15:N:199:ARG:HH11	1.84	0.43
2:O:82:ARG:NH1	8:U:113:ASP:OD1	2.52	0.43
9:H:196:LYS:HG3	9:H:196:LYS:O	2.19	0.43
13:Z:145:PHE:N	13:Z:191:TYR:O	2.47	0.43
2:A:9:LEU:HD13	8:G:10:ILE:CG2	2.49	0.43
8:U:215:VAL:HG22	8:U:216:LEU:N	2.34	0.43
13:Z:171:ILE:HD11	13:Z:196:LEU:HG	2.00	0.43
3:B:157:ASP:OD1	3:B:157:ASP:N	2.51	0.42
7:F:15:ASP:OD1	8:G:29:LYS:NZ	2.44	0.42
11:J:23:ASN:OD1	11:J:26:LEU:N	2.46	0.42
7:T:103:SER:O	7:T:107:VAL:HG23	2.19	0.42
9:V:168:ILE:HG23	9:V:175:GLY:O	2.19	0.42
2:A:16:GLY:O	3:B:21:ASN:ND2	2.52	0.42
5:R:108:ARG:NH2	13:Z:167:ASN:OD1	2.52	0.42
9:V:154:GLU:HA	9:V:154:GLU:OE1	2.19	0.42
11:X:61:ASN:O	11:X:65:VAL:HG23	2.19	0.42
13:L:112:ILE:HG23	13:L:280:TRP:HB2	2.00	0.42
13:L:143:THR:O	13:L:192:SER:HA	2.18	0.42
4:Q:156:CYS:SG	5:R:55:LEU:HD22	2.59	0.42
12:Y:68:VAL:HG22	12:Y:72:LEU:O	2.20	0.42
14:M:19:VAL:HG11	14:M:107:VAL:HB	2.02	0.42
3:P:38:ILE:HD11	3:P:174:MET:HG3	2.02	0.42
12:K:107:VAL:HG23	12:K:136:ASP:OD1	2.19	0.42
3:P:112:GLN:NE2	4:Q:125:ARG:O	2.52	0.42
12:K:223:VAL:HG23	12:K:224:ASP:OD1	2.19	0.42
13:L:105:ARG:HB3	13:L:206:VAL:HG23	2.02	0.42
14:M:43:ARG:HG3	14:M:189:VAL:HG11	2.02	0.42
12:Y:39:PHE:CE1	12:Y:44:VAL:HG23	2.54	0.42
12:K:181:GLU:OE2	12:K:181:GLU:CA	2.68	0.42
15:N:91:ASP:OD1	15:N:99:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:115:ASP:OD2	5:R:115:ASP:C	2.58	0.42
4:C:132:ILE:HD11	4:C:159:VAL:HG21	2.01	0.42
13:L:102:VAL:HG23	13:L:222:CYS:SG	2.59	0.42
11:X:26:LEU:HD21	12:Y:167:TYR:CE2	2.54	0.42
6:E:167:CYS:SG	6:E:197:ALA:HB2	2.60	0.42
15:N:117:GLY:C	15:N:118:LEU:HD12	2.40	0.42
8:U:38:ASN:OD1	8:U:41:MET:N	2.46	0.42
1:3:100:ILE:CD1	12:Y:51:ALA:HB1	2.50	0.42
1:3:100:ILE:HD11	12:Y:51:ALA:HB1	2.02	0.42
4:C:120:LEU:HD22	5:D:130:PHE:CD1	2.55	0.42
12:K:51:ALA:HB3	12:K:59:SER:HB3	2.01	0.42
12:K:69:ASN:OD1	12:K:71:HIS:N	2.43	0.42
13:L:96:ASP:OD2	13:L:191:TYR:OH	2.23	0.42
3:P:124:ILE:CG2	3:P:135:LEU:HD11	2.50	0.42
5:D:115:ASP:OD1	5:D:115:ASP:C	2.59	0.41
5:R:153:ASP:HB2	5:R:154:PRO:HD2	2.01	0.41
5:D:97:GLU:HG2	12:K:92:LEU:HD21	2.02	0.41
6:E:17:GLY:O	7:F:25:ALA:HB2	2.20	0.41
6:E:183:LYS:HG2	6:E:184:GLU:N	2.35	0.41
9:H:8:THR:O	9:H:164:ILE:HD13	2.20	0.41
3:P:16:GLU:OE1	3:P:16:GLU:HA	2.20	0.41
12:K:34:THR:HG22	12:K:47:VAL:HG12	2.01	0.41
3:P:28:ILE:HD12	3:P:124:ILE:HD12	2.03	0.41
6:S:183:LYS:HG2	6:S:184:GLU:N	2.35	0.41
10:W:123:SER:HB2	10:W:137:VAL:HG21	2.02	0.41
2:A:3:LEU:HD21	8:G:7:ILE:CG2	2.50	0.41
12:K:82:ASP:OD2	12:K:126:LEU:HD12	2.20	0.41
3:P:42:ILE:HD12	3:P:199:TYR:CE1	2.56	0.41
3:P:63:VAL:HA	3:P:124:ILE:O	2.20	0.41
8:U:149:SER:O	8:U:150:ALA:HB3	2.21	0.41
3:B:63:VAL:HG12	3:B:125:TYR:CD1	2.55	0.41
9:H:178:ILE:O	9:H:194:TYR:N	2.54	0.41
4:Q:72:THR:HG23	4:Q:132:ILE:HB	2.03	0.41
13:Z:218:VAL:HG21	13:Z:221:VAL:HB	2.02	0.41
6:E:43:PHE:HA	6:E:141:ILE:HG13	2.02	0.41
4:Q:13:ASP:OD2	4:Q:13:ASP:C	2.58	0.41
4:Q:153:GLU:OE1	4:Q:154:TYR:N	2.54	0.41
11:X:69:ILE:HG23	11:X:70:GLN:N	2.35	0.41
4:C:32:VAL:HG22	4:C:45:ILE:HG23	2.02	0.41
14:M:61:PHE:O	14:M:65:GLU:HG2	2.19	0.41
9:V:82:VAL:HG23	9:V:110:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:37:ILE:HD11	5:D:177:LEU:HD21	2.02	0.41
6:E:222:GLN:OE1	6:E:223:ILE:N	2.54	0.41
7:F:108:ARG:O	7:F:112:VAL:HG23	2.21	0.41
15:N:76:ILE:HD11	15:N:114:MET:HE3	2.03	0.41
4:Q:43:LEU:CD1	4:Q:45:ILE:HD11	2.50	0.41
5:R:75:PHE:CD2	5:R:82:VAL:HG21	2.55	0.41
7:F:4:LEU:HD22	8:G:7:ILE:HD11	2.02	0.41
7:F:42:ILE:HG22	7:F:210:ILE:HG22	2.02	0.41
8:G:73:PHE:HB2	8:G:80:VAL:HG13	2.03	0.41
9:H:210:ARG:HA	10:I:165:THR:HG21	2.01	0.41
3:P:40:LEU:HD23	3:P:41:GLY:N	2.36	0.41
3:P:197:LYS:HG3	3:P:214:PHE:CD2	2.56	0.41
7:T:87:LEU:HD11	7:T:111:ILE:CD1	2.51	0.41
9:V:43:ILE:HD13	9:V:85:CYS:SG	2.61	0.41
12:Y:107:VAL:HG23	12:Y:136:ASP:OD1	2.21	0.41
6:E:166:SER:O	6:E:169:THR:HG22	2.20	0.41
6:S:183:LYS:O	6:S:187:VAL:HG23	2.21	0.41
5:D:82:VAL:O	5:D:86:VAL:HG23	2.21	0.40
4:Q:15:ARG:HB3	4:Q:15:ARG:NH1	2.36	0.40
1:3:84:ASP:OD1	1:3:84:ASP:O	2.39	0.40
1:3:84:ASP:OD1	12:Y:32:THR:N	2.55	0.40
2:A:112:PHE:O	2:A:116:ILE:HG12	2.21	0.40
14:M:110:ASP:OD2	14:M:110:ASP:C	2.59	0.40
2:A:65:GLN:NE2	2:A:209:PHE:O	2.54	0.40
3:B:63:VAL:HA	3:B:124:ILE:O	2.21	0.40
3:B:112:GLN:NE2	4:C:125:ARG:O	2.54	0.40
6:E:43:PHE:CE1	6:E:186:LEU:HD12	2.57	0.40
6:E:183:LYS:O	6:E:187:VAL:HG23	2.20	0.40
9:H:23:ASP:OD2	9:H:23:ASP:O	2.39	0.40
13:L:99:GLY:HA3	13:L:224:GLY:HA3	2.04	0.40
14:M:184:VAL:HG23	14:M:189:VAL:HG22	2.03	0.40
6:S:116:ALA:O	6:S:120:THR:HG23	2.21	0.40
9:V:27:THR:HG21	9:V:173:TYR:HD1	1.86	0.40
13:Z:280:TRP:CZ2	13:Z:289:LYS:HE2	2.57	0.40
1:4:103:PRO:O	1:4:104:GLU:HG2	2.22	0.40
2:A:97:ASP:OD2	9:H:67:LYS:CE	2.69	0.40
3:B:7:THR:HG21	3:B:13:LEU:HD23	2.03	0.40
3:B:8:GLU:O	4:C:24:GLN:OE1	2.40	0.40
5:D:57:ASN:O	5:D:57:ASN:OD1	2.39	0.40
5:D:204:ASP:OD1	5:D:204:ASP:N	2.54	0.40
6:E:68:SER:O	6:E:69:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:12:LEU:HB2	10:W:109:ILE:HD12	2.02	0.40
12:K:205:VAL:N	12:K:221:PHE:O	2.51	0.40
5:R:153:ASP:OD1	5:R:153:ASP:C	2.60	0.40
8:U:36:LEU:HD23	8:U:157:GLY:HA3	2.03	0.40
9:V:128:VAL:HG21	9:V:131:THR:HG21	2.04	0.40
12:Y:51:ALA:HB2	12:Y:62:VAL:HG21	2.03	0.40
13:Z:105:ARG:HB3	13:Z:206:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	54/147 (37%)	53 (98%)	1 (2%)	0	100	100
1	4	54/147 (37%)	51 (94%)	3 (6%)	0	100	100
2	A	223/227 (98%)	221 (99%)	2 (1%)	0	100	100
2	O	223/227 (98%)	219 (98%)	4 (2%)	0	100	100
3	B	226/231 (98%)	223 (99%)	3 (1%)	0	100	100
3	P	226/231 (98%)	222 (98%)	4 (2%)	0	100	100
4	C	217/225 (96%)	212 (98%)	5 (2%)	0	100	100
4	Q	217/225 (96%)	211 (97%)	6 (3%)	0	100	100
5	D	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
5	R	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
6	E	223/230 (97%)	220 (99%)	3 (1%)	0	100	100
6	S	223/230 (97%)	221 (99%)	2 (1%)	0	100	100
7	F	232/243 (96%)	224 (97%)	8 (3%)	0	100	100
7	T	232/243 (96%)	229 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	231/234 (99%)	228 (99%)	3 (1%)	0	100	100
8	U	231/234 (99%)	225 (97%)	6 (3%)	0	100	100
9	H	216/227 (95%)	211 (98%)	5 (2%)	0	100	100
9	V	216/227 (95%)	212 (98%)	4 (2%)	0	100	100
10	I	201/205 (98%)	195 (97%)	6 (3%)	0	100	100
10	W	201/205 (98%)	197 (98%)	4 (2%)	0	100	100
11	J	191/193 (99%)	191 (100%)	0	0	100	100
11	X	191/193 (99%)	188 (98%)	3 (2%)	0	100	100
12	K	193/228 (85%)	191 (99%)	2 (1%)	0	100	100
12	Y	193/228 (85%)	189 (98%)	4 (2%)	0	100	100
13	L	206/297 (69%)	202 (98%)	4 (2%)	0	100	100
13	Z	206/297 (69%)	204 (99%)	2 (1%)	0	100	100
14	M	210/212 (99%)	200 (95%)	10 (5%)	0	100	100
14	a	210/212 (99%)	196 (93%)	14 (7%)	0	100	100
15	N	192/216 (89%)	188 (98%)	4 (2%)	0	100	100
15	b	192/216 (89%)	188 (98%)	4 (2%)	0	100	100
All	All	6092/6698 (91%)	5954 (98%)	138 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	3	52/135 (38%)	50 (96%)	2 (4%)	28	59
1	4	52/135 (38%)	49 (94%)	3 (6%)	17	42
2	A	172/206 (84%)	168 (98%)	4 (2%)	45	75
2	O	172/206 (84%)	168 (98%)	4 (2%)	45	75
3	B	206/209 (99%)	198 (96%)	8 (4%)	27	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	206/209 (99%)	205 (100%)	1 (0%)	86	95
4	C	157/207 (76%)	152 (97%)	5 (3%)	34	65
4	Q	157/207 (76%)	151 (96%)	6 (4%)	28	59
5	D	208/209 (100%)	206 (99%)	2 (1%)	73	89
5	R	208/209 (100%)	205 (99%)	3 (1%)	62	85
6	E	204/209 (98%)	198 (97%)	6 (3%)	37	68
6	S	204/209 (98%)	199 (98%)	5 (2%)	42	73
7	F	215/223 (96%)	213 (99%)	2 (1%)	75	91
7	T	215/223 (96%)	212 (99%)	3 (1%)	62	85
8	G	200/201 (100%)	191 (96%)	9 (4%)	23	52
8	U	200/201 (100%)	193 (96%)	7 (4%)	31	62
9	H	182/190 (96%)	175 (96%)	7 (4%)	28	59
9	V	182/190 (96%)	179 (98%)	3 (2%)	58	83
10	I	179/181 (99%)	174 (97%)	5 (3%)	38	69
10	W	179/181 (99%)	172 (96%)	7 (4%)	27	58
11	J	177/177 (100%)	176 (99%)	1 (1%)	84	94
11	X	177/177 (100%)	175 (99%)	2 (1%)	70	88
12	K	157/187 (84%)	150 (96%)	7 (4%)	23	52
12	Y	157/187 (84%)	151 (96%)	6 (4%)	28	59
13	L	186/271 (69%)	175 (94%)	11 (6%)	16	41
13	Z	186/271 (69%)	181 (97%)	5 (3%)	40	71
14	M	195/195 (100%)	193 (99%)	2 (1%)	73	89
14	a	195/195 (100%)	190 (97%)	5 (3%)	41	72
15	N	159/178 (89%)	156 (98%)	3 (2%)	52	79
15	b	159/178 (89%)	157 (99%)	2 (1%)	65	86
All	All	5298/5956 (89%)	5162 (97%)	136 (3%)	42	72

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	128	ASP
1	3	141	ASP
1	4	128	ASP

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Mol	Chain	Res	Type
1	4	140	ASP
1	4	141	ASP
2	A	198	ASP
2	A	200	ASP
2	A	207	GLN
2	A	214	LYS
3	B	11	ARG
3	B	44	LYS
3	B	51	ARG
3	B	139	ASP
3	B	176	ARG
3	B	197	LYS
3	B	214	PHE
3	B	223	ARG
4	C	51	ASN
4	C	134	LEU
4	C	205	ASP
4	C	208	ARG
4	C	209	ARG
5	D	40	LYS
5	D	176	MET
6	E	23	GLU
6	E	95	GLU
6	E	98	ARG
6	E	102	ASP
6	E	218	GLN
6	E	222	GLN
7	F	194	LYS
7	F	200	LYS
8	G	25	GLU
8	G	30	SER
8	G	66	TYR
8	G	92	HIS
8	G	145	MET
8	G	159	MET
8	G	178	ASP
8	G	205	MET
8	G	217	LYS
9	H	23	ASP
9	H	50	CYS
9	H	125	SER
9	H	196	LYS

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Mol	Chain	Res	Type
9	H	202	GLU
9	H	216	LEU
9	H	219	ASP
10	I	130	MET
10	I	160	ASP
10	I	189	LEU
10	I	198	ARG
10	I	205	ASP
11	J	54	PHE
12	K	40	GLN
12	K	43	MET
12	K	61	ASN
12	K	67	ARG
12	K	128	LEU
12	K	138	ASP
12	K	172	GLU
13	L	100	SER
13	L	112	ILE
13	L	164	GLU
13	L	188	PHE
13	L	192	SER
13	L	202	ASP
13	L	241	LYS
13	L	253	GLU
13	L	257	ASP
13	L	268	GLU
13	L	275	ASP
14	M	16	LYS
14	M	201	TRP
15	N	91	ASP
15	N	106	ASP
15	N	114	MET
2	O	17	LYS
2	O	139	LYS
2	O	144	ASP
2	O	214	LYS
3	P	139	ASP
4	Q	20	GLU
4	Q	39	ASN
4	Q	56	ASP
4	Q	123	SER
4	Q	137	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	Q	153	GLU
5	R	17	ARG
5	R	153	ASP
5	R	176	MET
6	S	43	PHE
6	S	89	LYS
6	S	102	ASP
6	S	174	GLU
6	S	218	GLN
7	T	86	ASN
7	T	165	ARG
7	T	182	ARG
8	U	30	SER
8	U	50	GLN
8	U	66	TYR
8	U	92	HIS
8	U	137	ASP
8	U	145	MET
8	U	159	MET
9	V	15	LYS
9	V	77	ASN
9	V	125	SER
10	W	23	PHE
10	W	80	ASN
10	W	132	GLU
10	W	158	MET
10	W	160	ASP
10	W	203	ARG
10	W	204	CYS
11	X	1	MET
11	X	54	PHE
12	Y	40	GLN
12	Y	43	MET
12	Y	48	ASP
12	Y	67	ARG
12	Y	101	ASN
12	Y	210	MET
13	Z	164	GLU
13	Z	191	TYR
13	Z	241	LYS
13	Z	246	GLU
13	Z	275	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	a	16	LYS
14	a	151	ASP
14	a	186	LYS
14	a	201	TRP
14	a	202	GLN
15	b	38	ASP
15	b	106	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	D	64	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

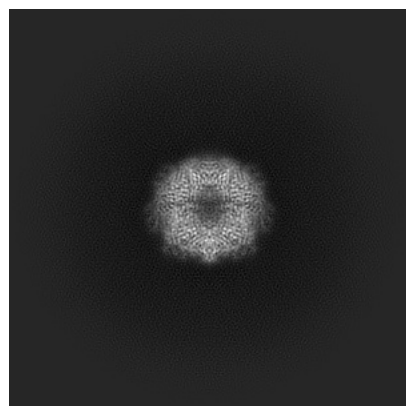
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15365. These allow visual inspection of the internal detail of the map and identification of artifacts.

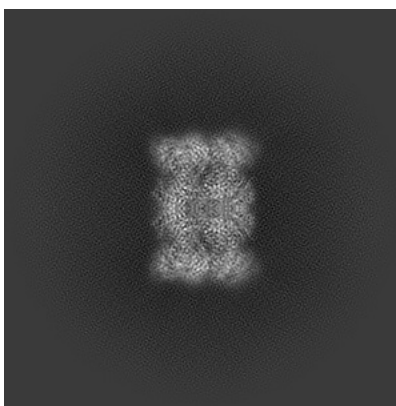
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

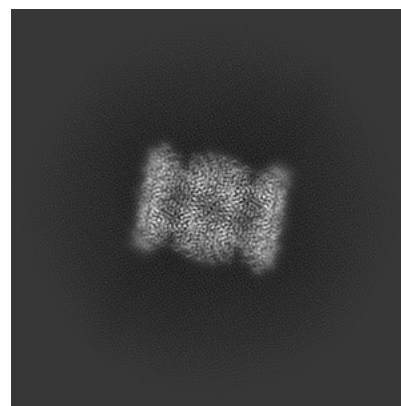
#### 6.1.1 Primary map



X

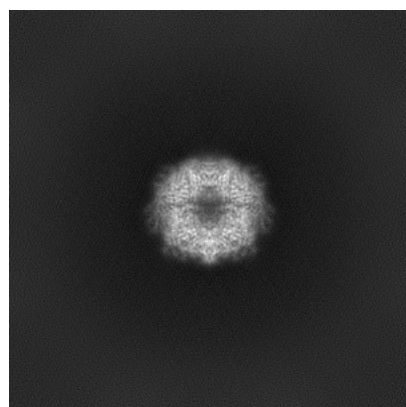


Y

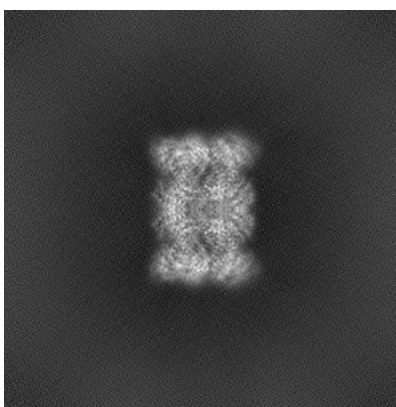


Z

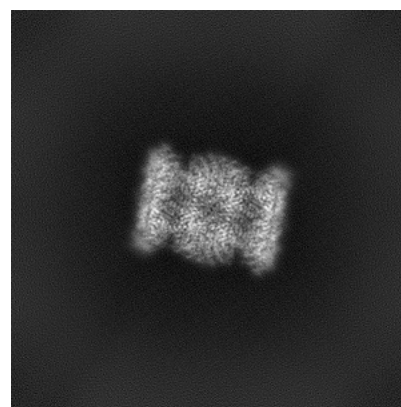
#### 6.1.2 Raw map



X



Y

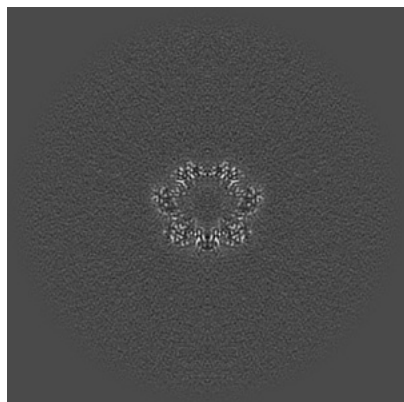


Z

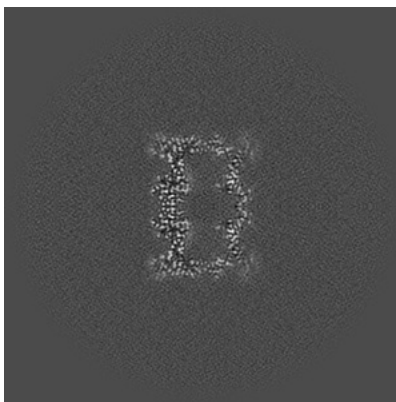
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

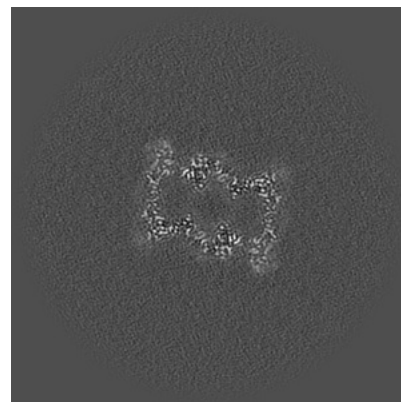
### 6.2.1 Primary map



X Index: 200

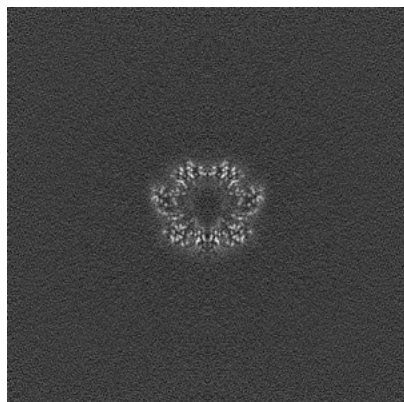


Y Index: 200

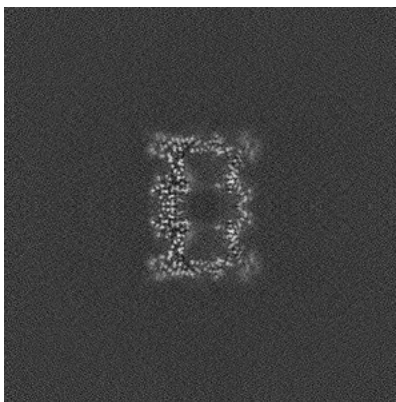


Z Index: 200

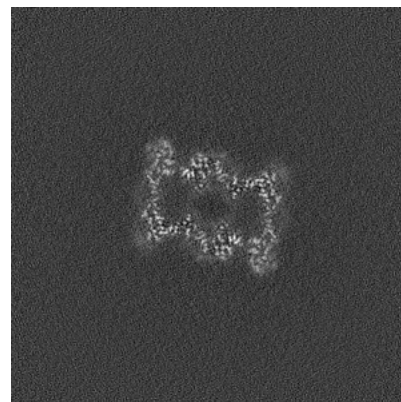
### 6.2.2 Raw map



X Index: 200



Y Index: 200

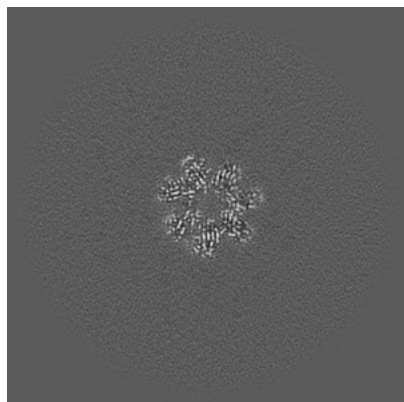


Z Index: 200

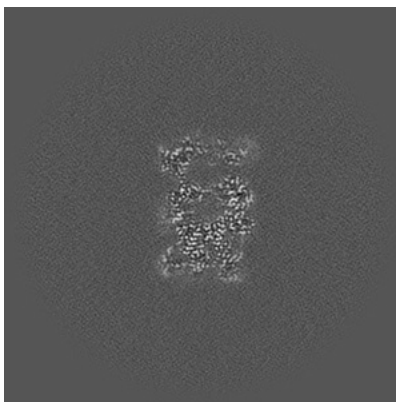
The images above show central slices of the map in three orthogonal directions.

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

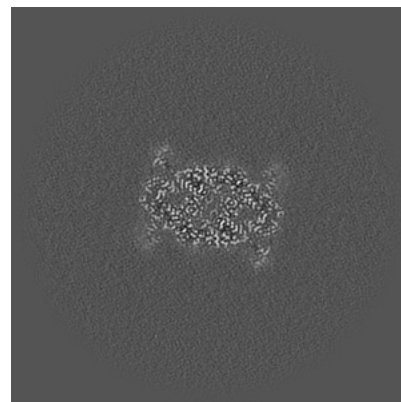
### 6.3.1 Primary map



X Index: 182

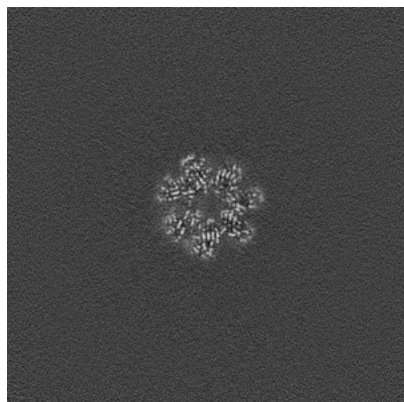


Y Index: 182

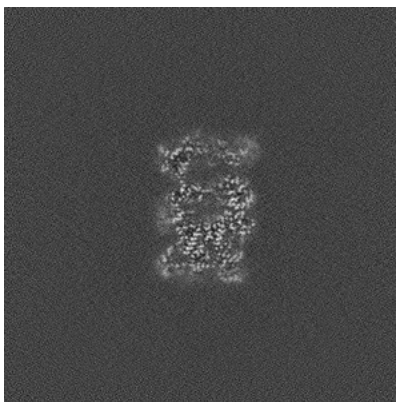


Z Index: 179

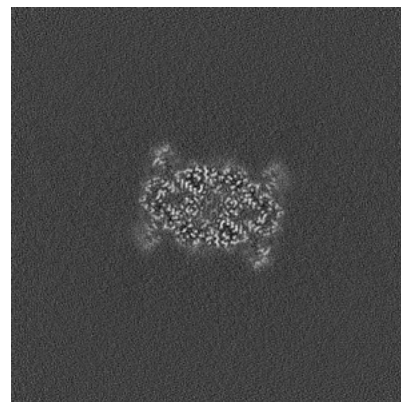
### 6.3.2 Raw map



X Index: 182



Y Index: 182

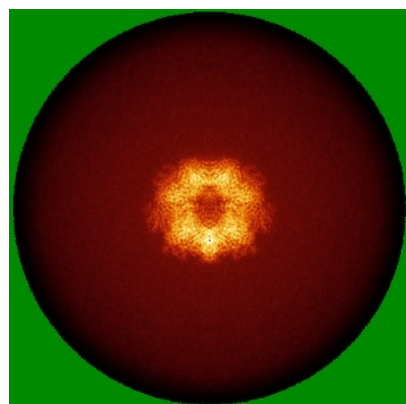


Z Index: 179

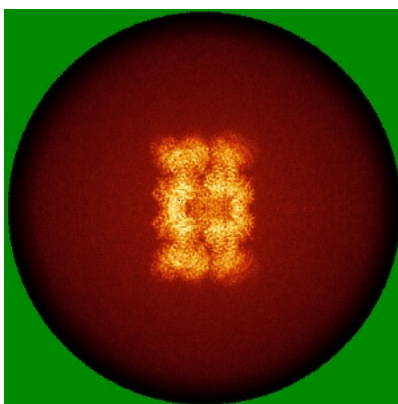
The images above show the largest variance slices of the map in three orthogonal directions.

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

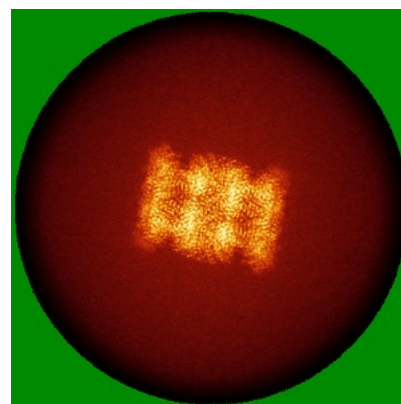
### 6.4.1 Primary map



X

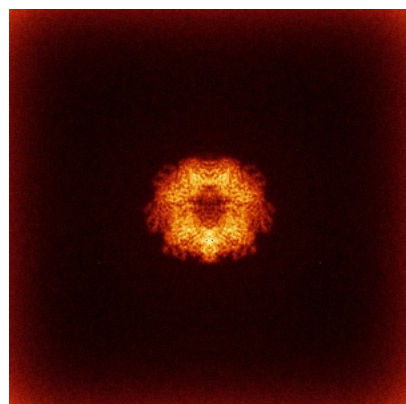


Y

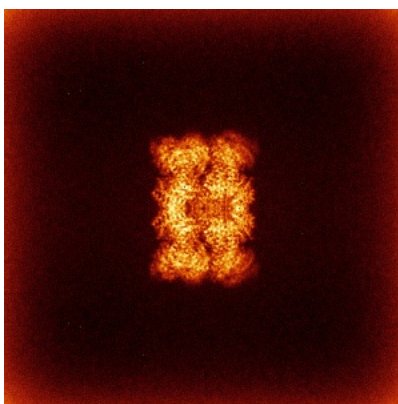


Z

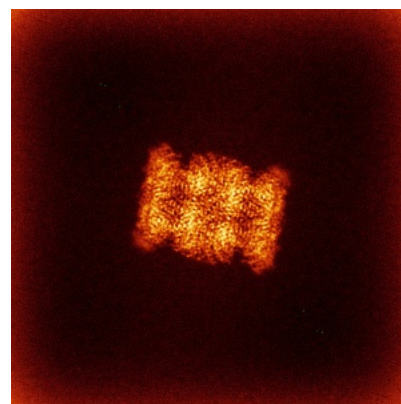
### 6.4.2 Raw map



X



Y

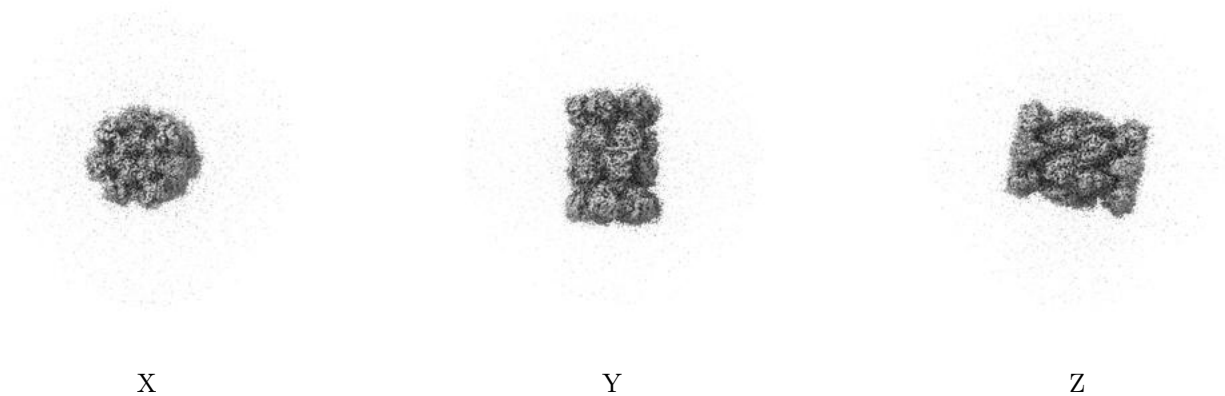


Z

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

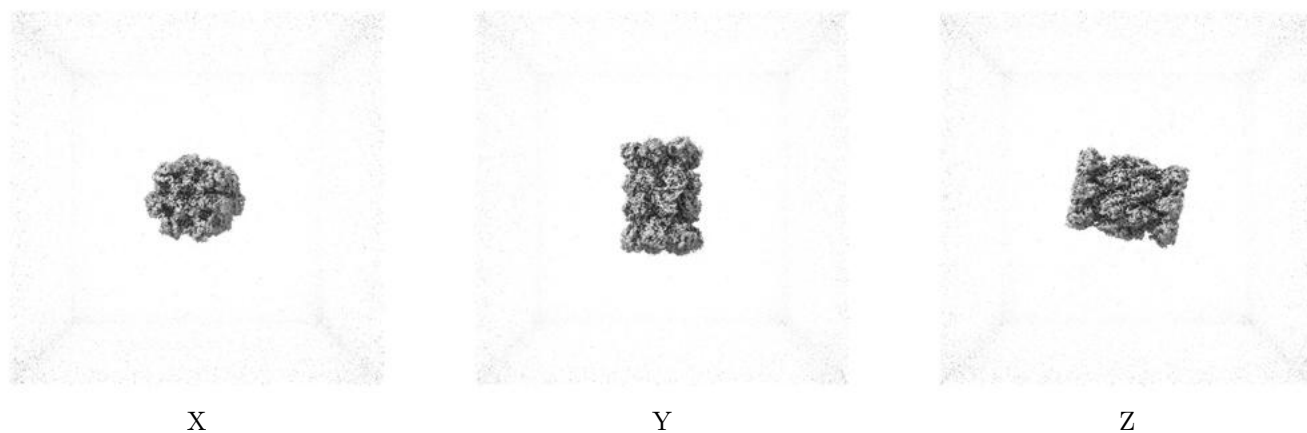
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



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.

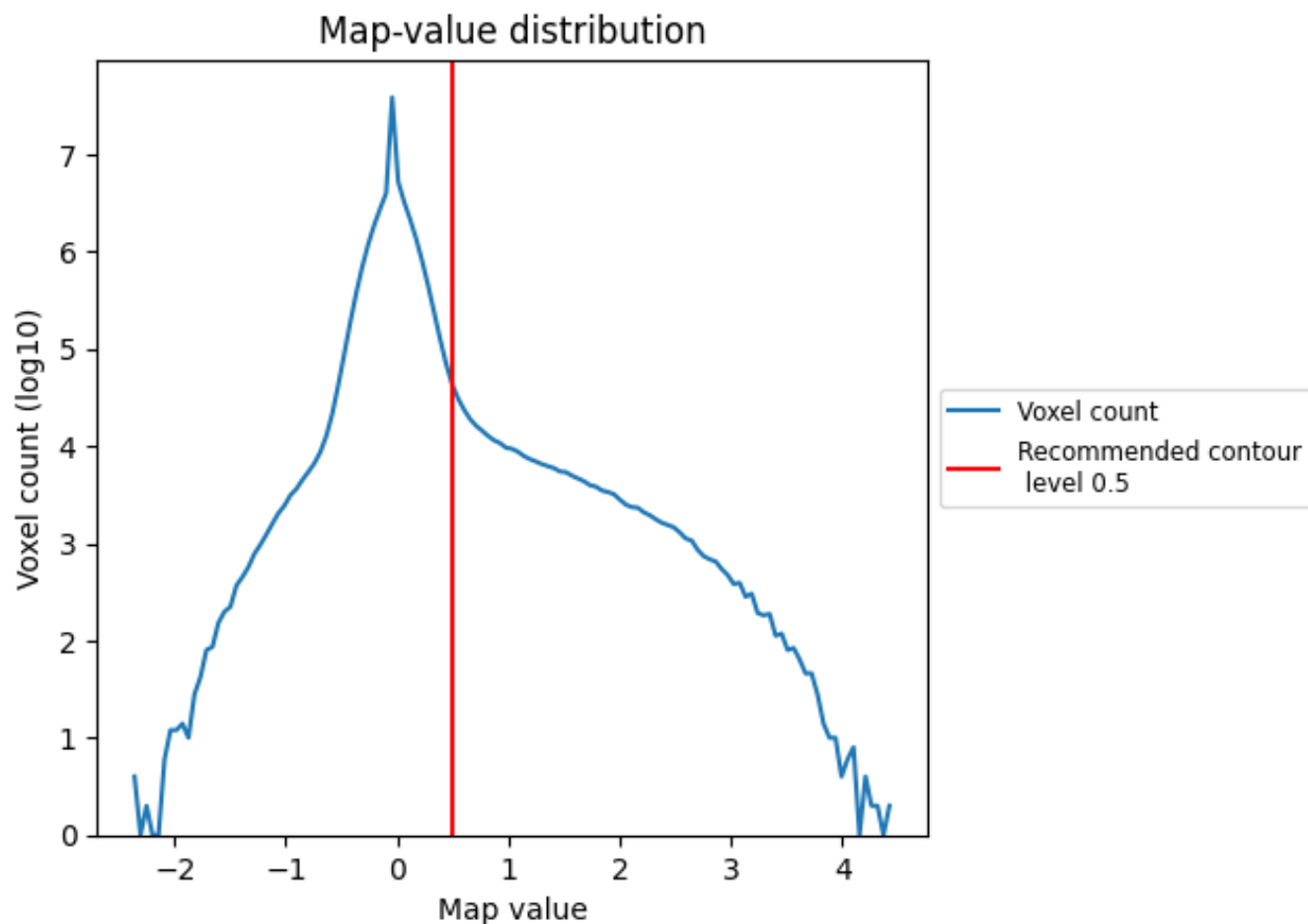
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

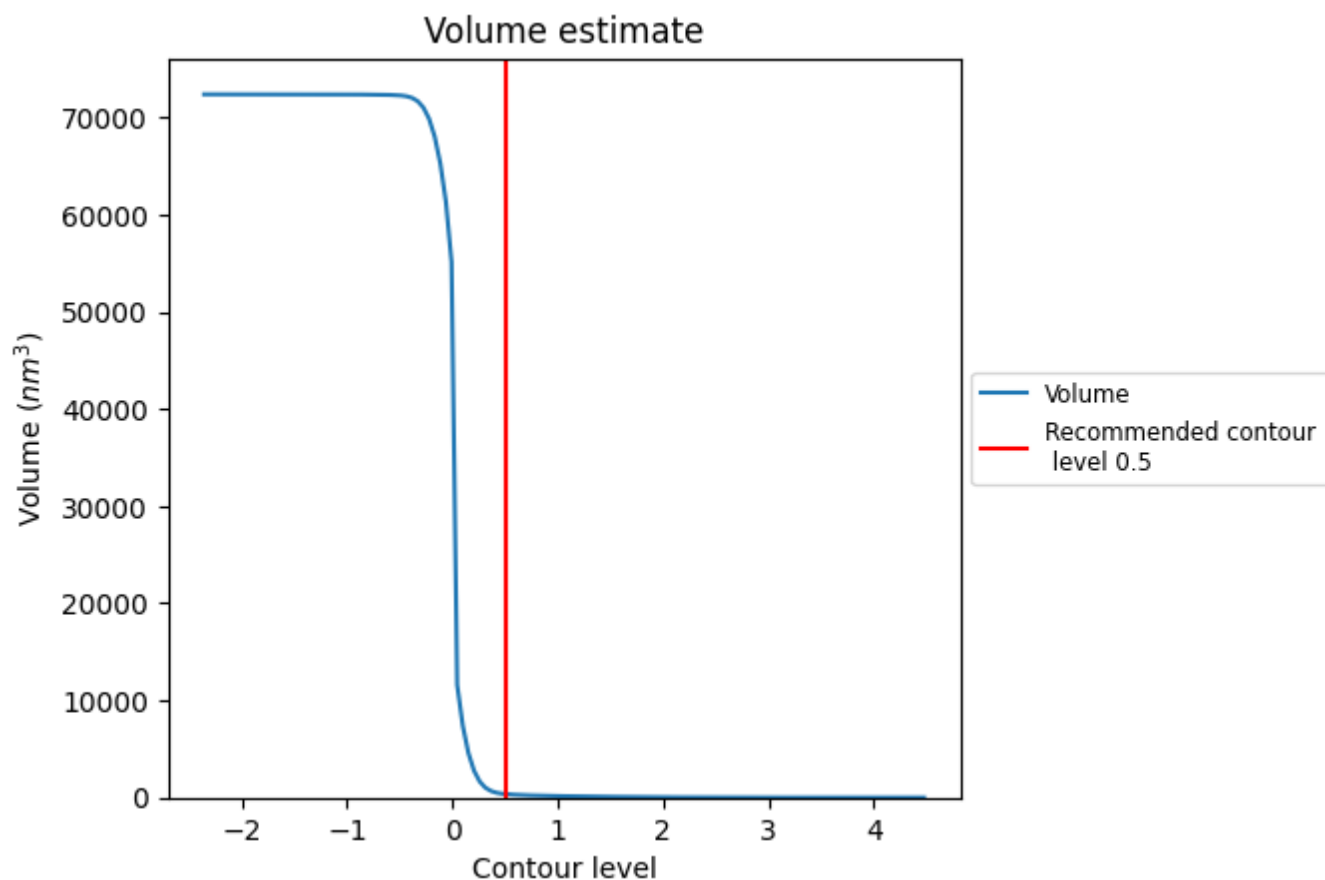
This section contains the results of statistical analysis of the map.

### 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.

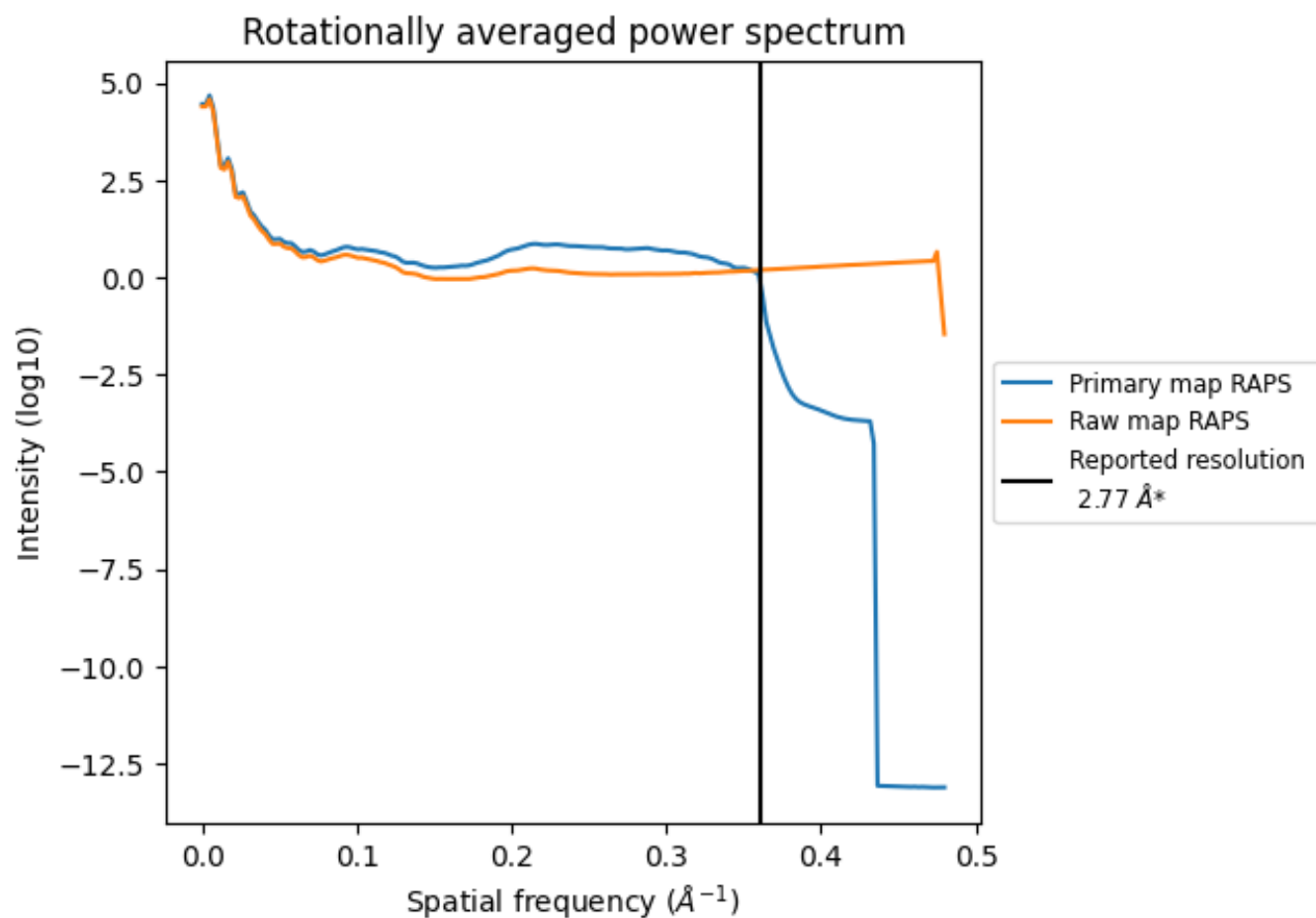
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 364 nm<sup>3</sup>; this corresponds to an approximate mass of 329 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 ⓘ

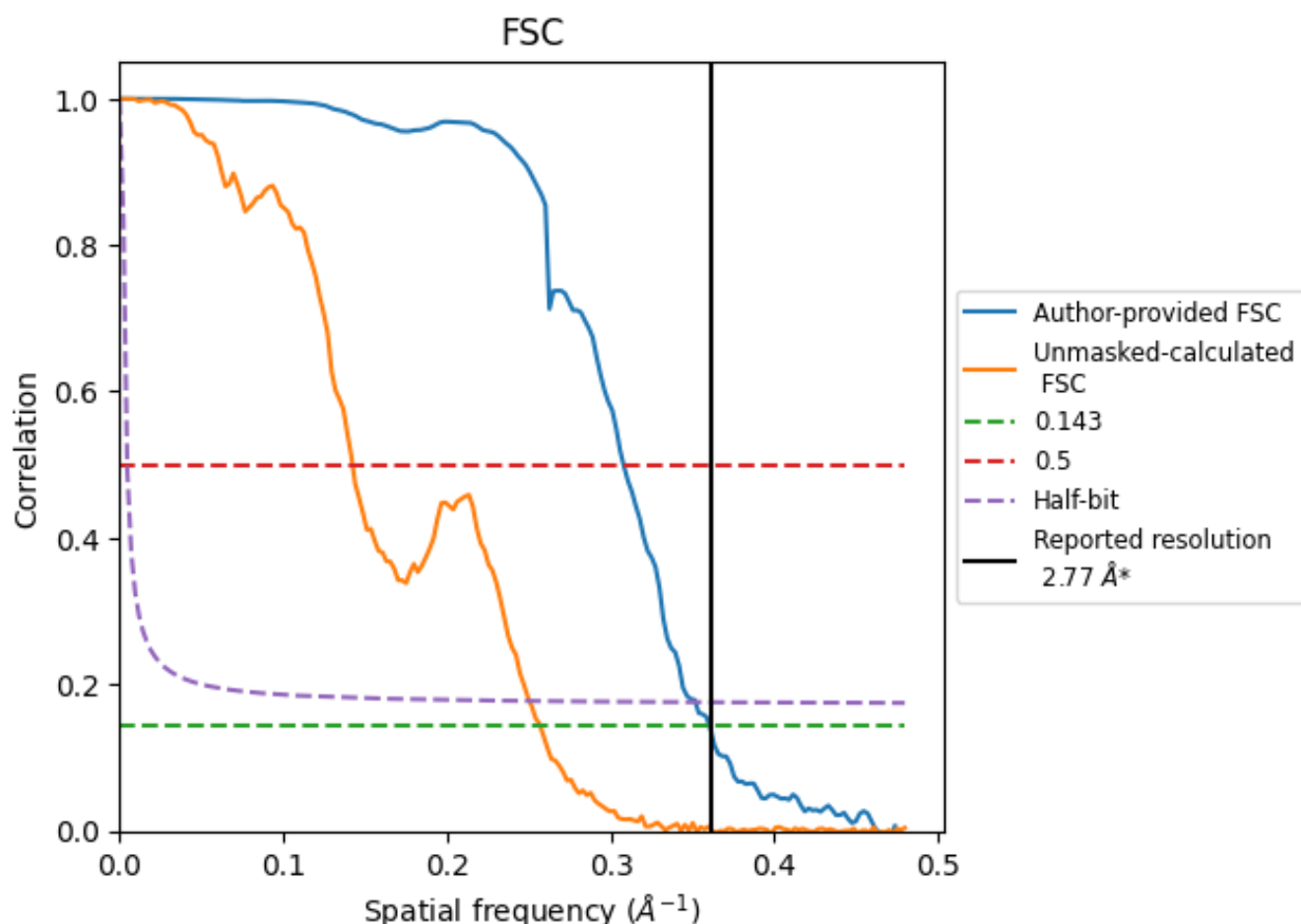


\*Reported resolution corresponds to spatial frequency of 0.361 Å<sup>-1</sup>

## 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 0.361 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

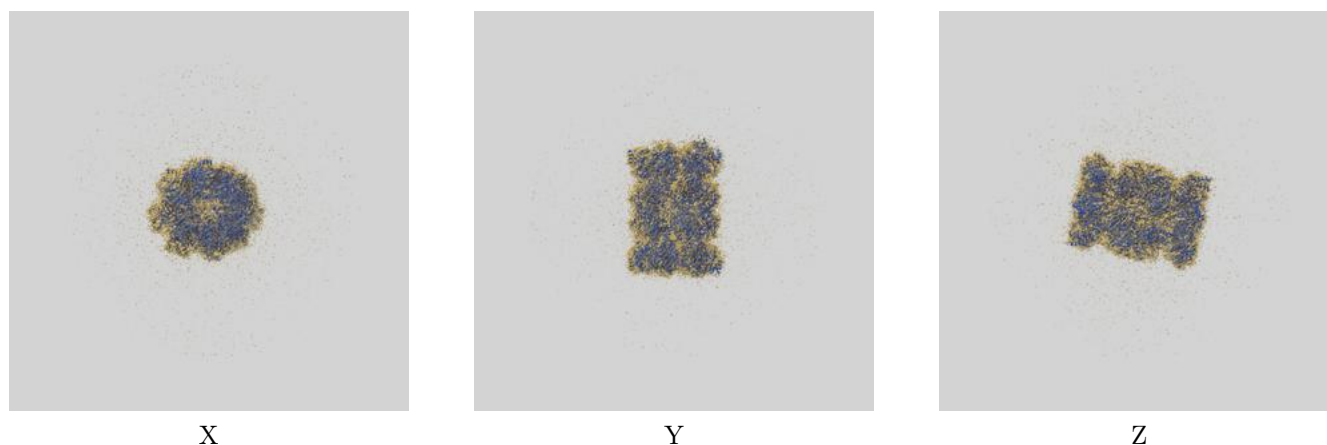
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.25	2.84
Unmasked-calculated*	3.89	7.03	3.99

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 2.77 by more than 10 %

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

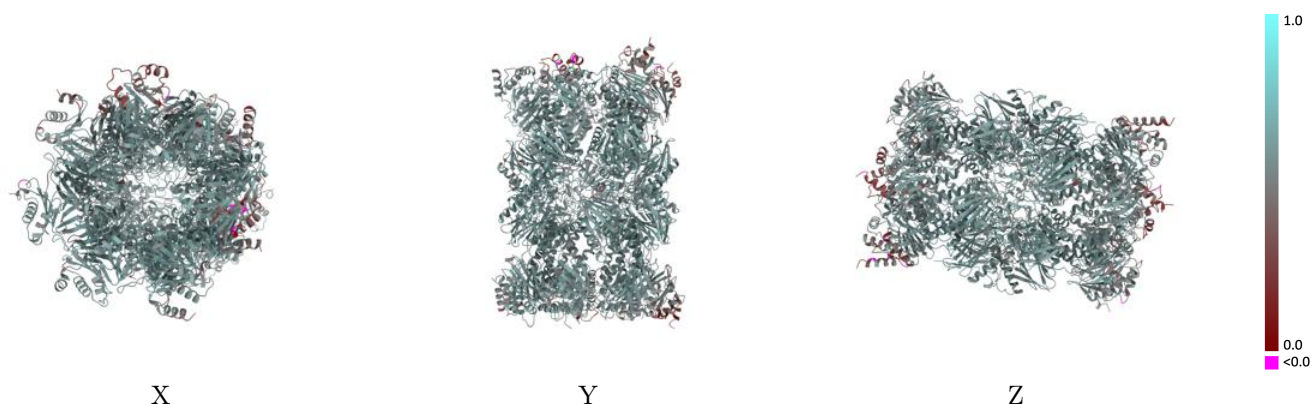
This section contains information regarding the fit between EMDB map EMD-15365 and PDB model 8ADN. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



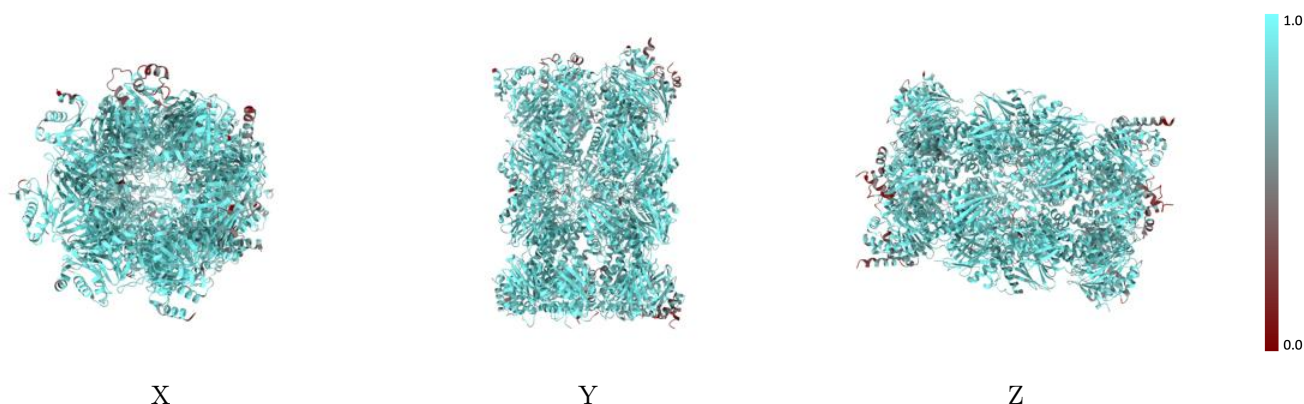
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



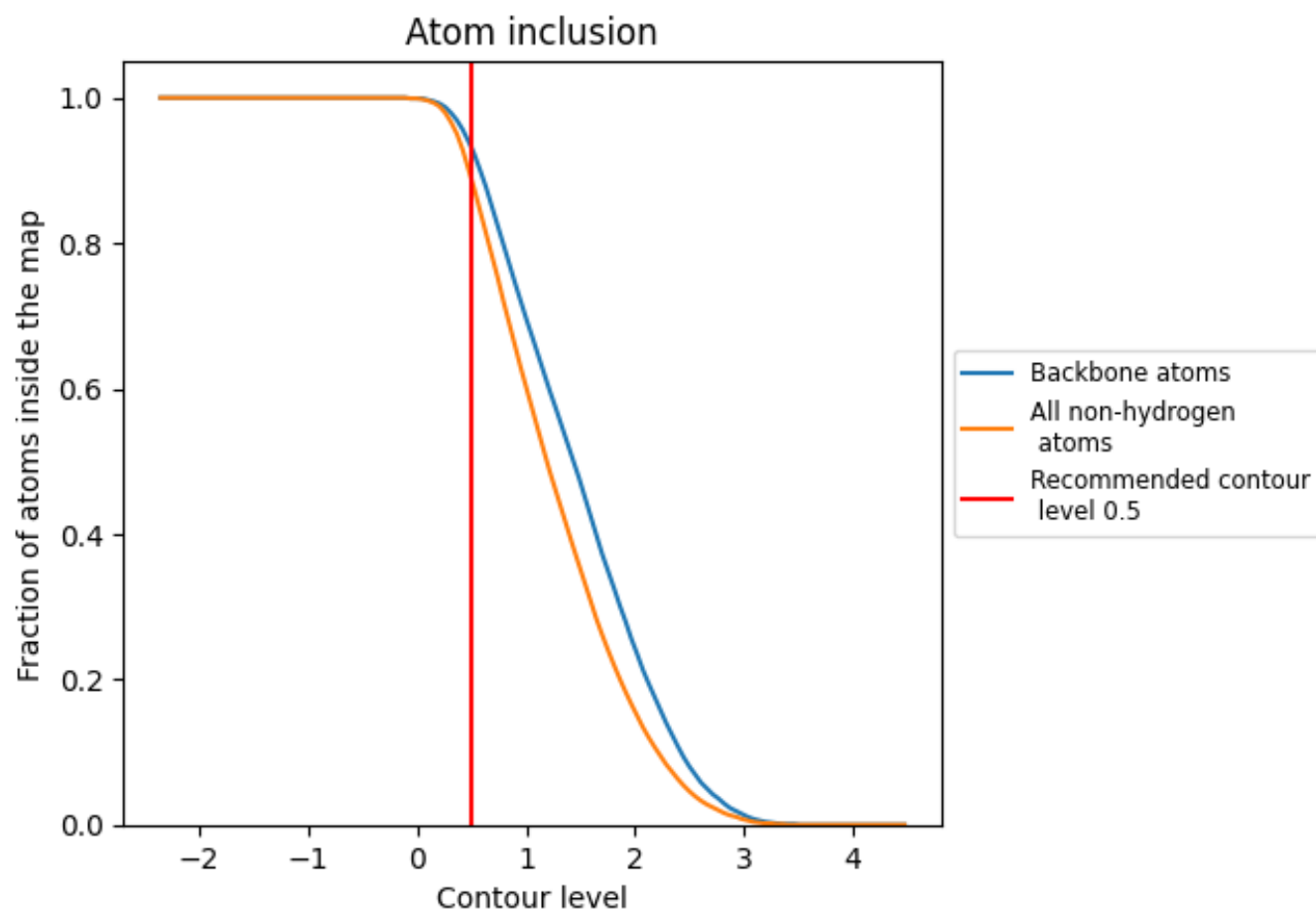
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.5660
3	 0.7120	 0.5340
4	 0.7160	 0.5310
A	 0.8370	 0.5280
B	 0.8560	 0.5340
C	 0.7940	 0.5180
D	 0.8390	 0.5430
E	 0.8830	 0.5510
F	 0.9030	 0.5700
G	 0.8870	 0.5670
H	 0.9190	 0.5890
I	 0.9430	 0.5970
J	 0.9310	 0.5950
K	 0.9360	 0.5910
L	 0.9110	 0.5820
M	 0.9240	 0.5880
N	 0.9300	 0.5920
O	 0.8440	 0.5320
P	 0.8480	 0.5350
Q	 0.7930	 0.5130
R	 0.8390	 0.5350
S	 0.8820	 0.5560
T	 0.8960	 0.5700
U	 0.8950	 0.5690
V	 0.9170	 0.5900
W	 0.9440	 0.5980
X	 0.9310	 0.5910
Y	 0.9360	 0.5930
Z	 0.9090	 0.5830
a	 0.9210	 0.5860
b	 0.9380	 0.5960

