



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:20 PM UTC

PDB ID : 6RGQ / pdb_00006rgq
EMDB ID : EMD-4877
Title : Human 20S Proteasome
Authors : Toste Rego, A.; da Fonseca, P.C.A.
Deposited on : 2019-04-17
Resolution : 2.60 Å(reported)
Based on initial model : 5LE5

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

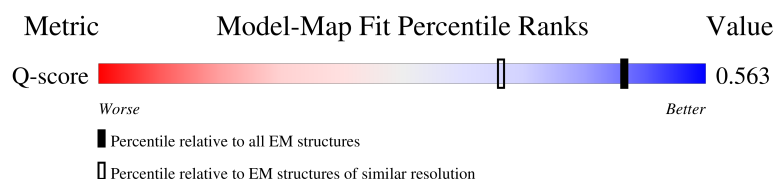
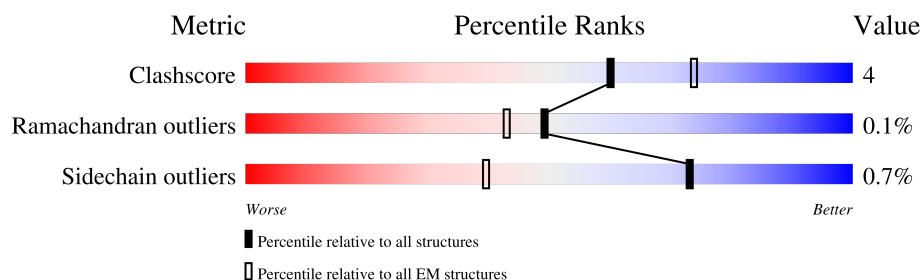
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



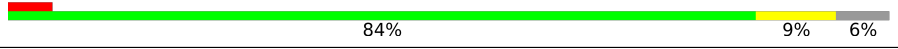
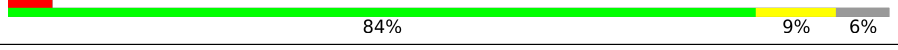
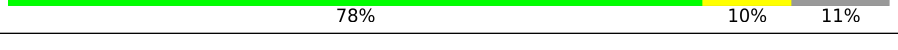
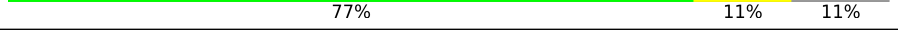
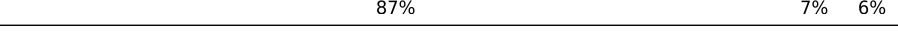
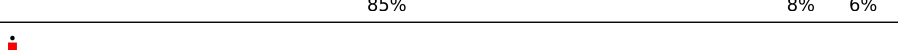
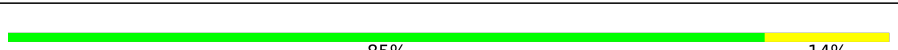
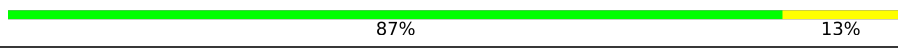
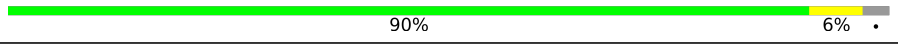
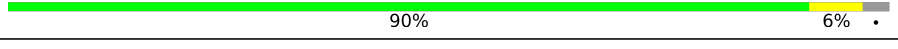
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	
1	O	246	
2	B	234	
2	P	234	

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Mol	Chain	Length	Quality of chain
3	C	261	
3	Q	261	
4	D	248	
4	R	248	
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	205	
10	X	205	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	M	213	
13	a	213	
14	N	219	
14	b	219	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 45340 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 subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		
1	O	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		
2	P	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		
3	Q	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		
4	R	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		
5	S	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		
6	T	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		
7	U	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		
8	V	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		
9	W	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		
11	Y	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		
12	Z	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		
13	a	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		

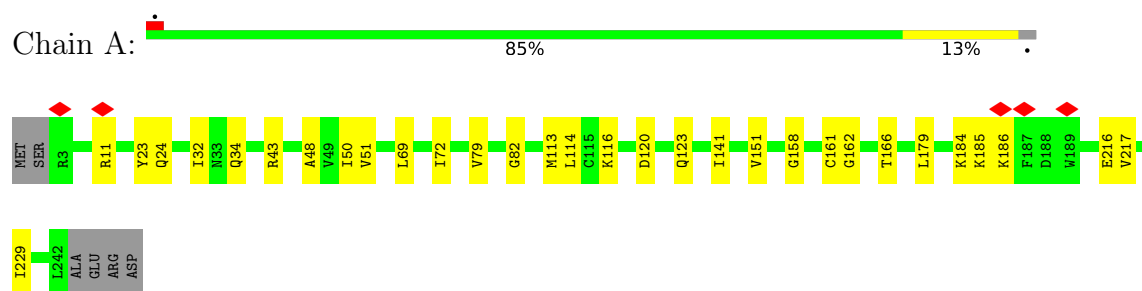
- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		
14	b	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		

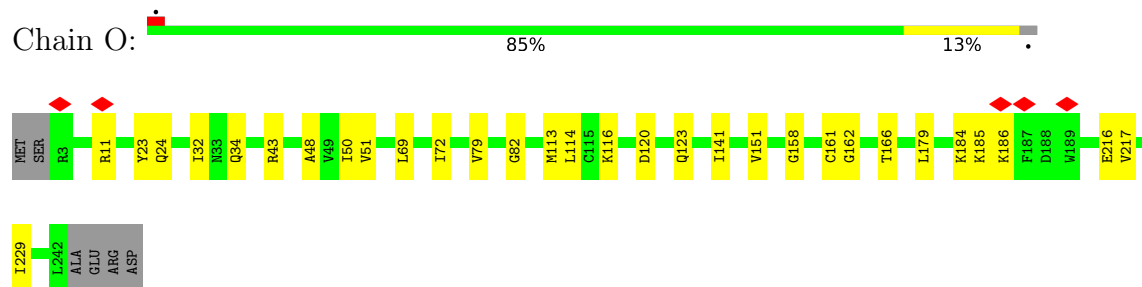
3 Residue-property plots [i](#)

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

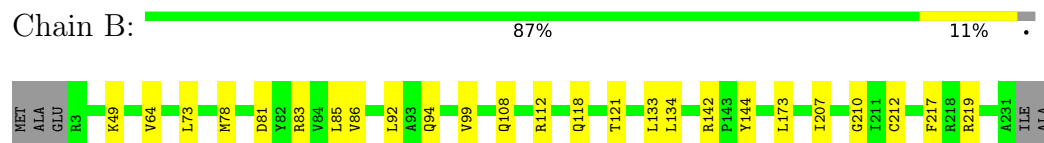
- Molecule 1: Proteasome subunit alpha type-6



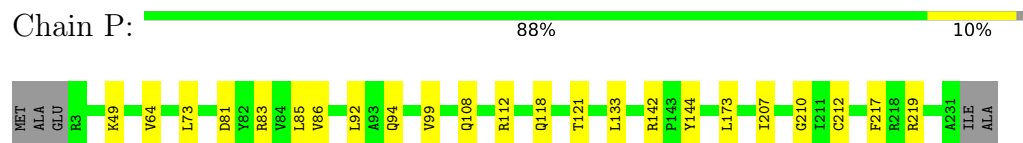
- Molecule 1: Proteasome subunit alpha type-6



- Molecule 2: Proteasome subunit alpha type-2

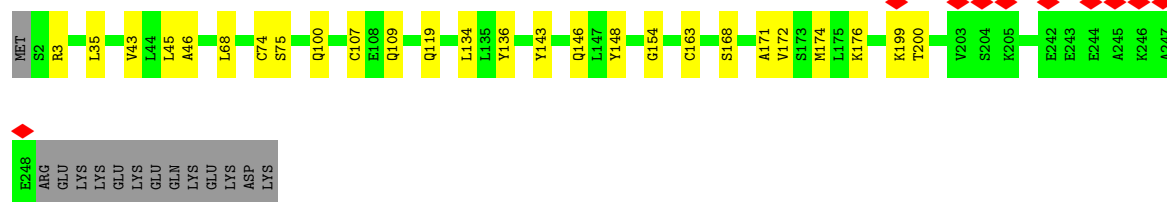


- Molecule 2: Proteasome subunit alpha type-2



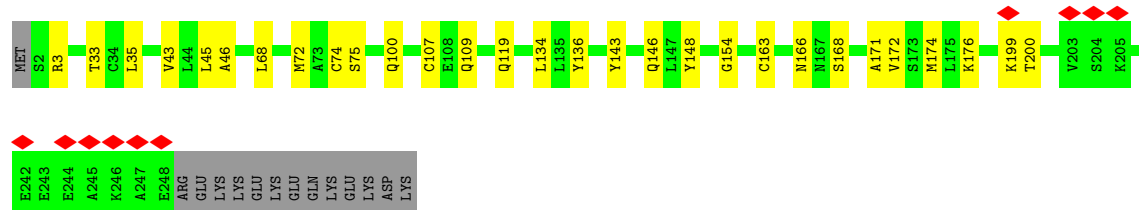
- Molecule 3: Proteasome subunit alpha type-4

Chain C: 



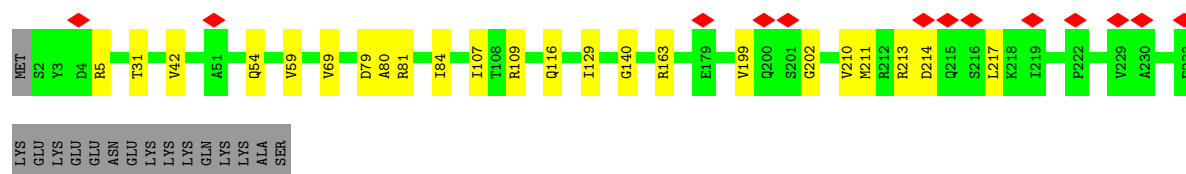
- Molecule 3: Proteasome subunit alpha type-4

Chain Q: 



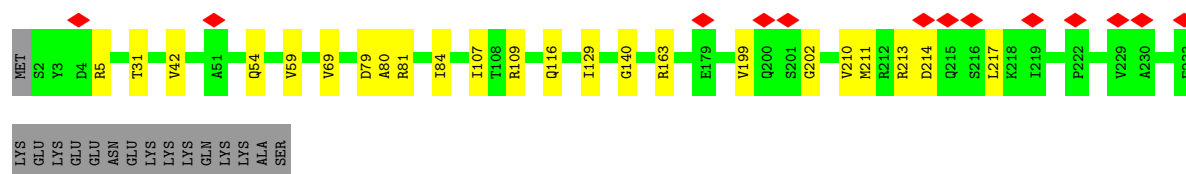
- Molecule 4: Proteasome subunit alpha type-7

Chain D: 



- Molecule 4: Proteasome subunit alpha type-7

Chain R: 



- Molecule 5: Proteasome subunit alpha type-5

Chain E: 





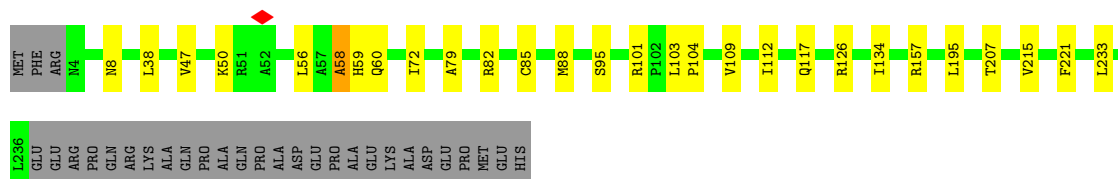
- Molecule 5: Proteasome subunit alpha type-5

Chain S: 86% 10%



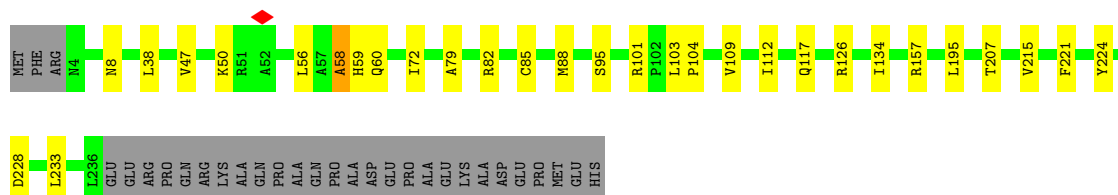
- Molecule 6: Proteasome subunit alpha type-1

Chain F: 78% 10% 11%



- Molecule 6: Proteasome subunit alpha type-1

Chain T: 77% 11% 11%



- Molecule 7: Proteasome subunit alpha type-3

Chain G: 87% 7% 6%

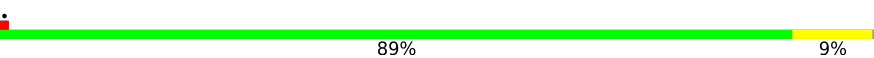


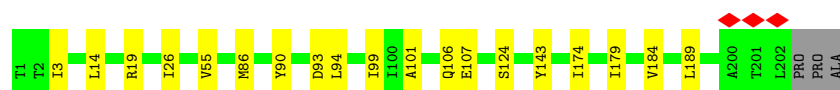
- Molecule 7: Proteasome subunit alpha type-3

Chain U: 85% 8% 6%

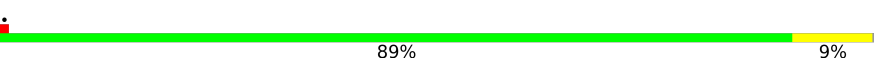


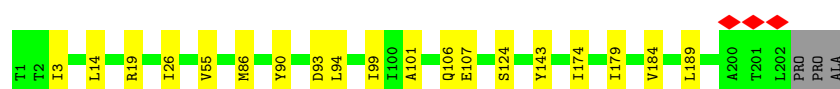
- Molecule 8: Proteasome subunit beta type-6

Chain H:  89% 9%



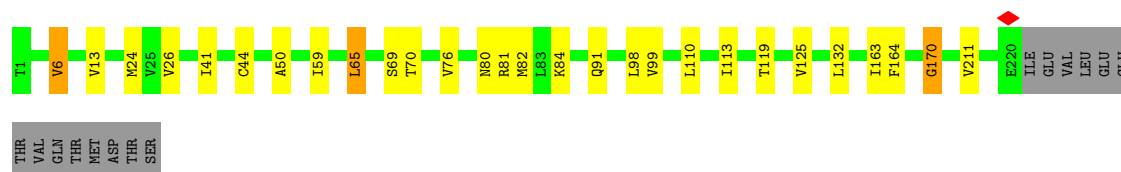
- Molecule 8: Proteasome subunit beta type-6

Chain V:  89% 9%



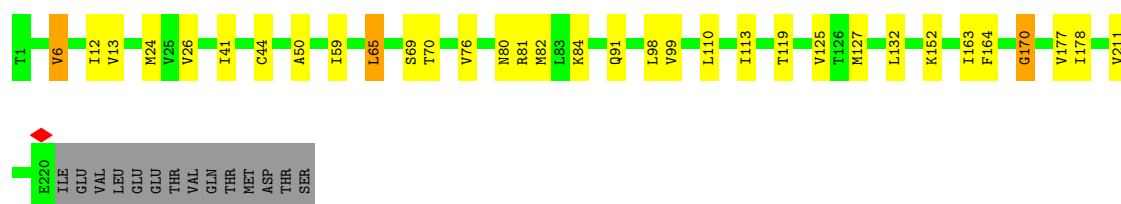
- Molecule 9: Proteasome subunit beta type-7

Chain I:  82% 11% 6%



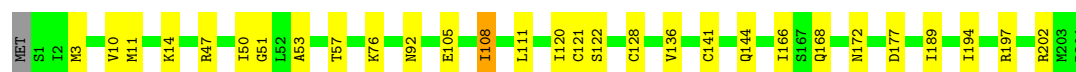
- Molecule 9: Proteasome subunit beta type-7

Chain W:  80% 13% 6%



- Molecule 10: Proteasome subunit beta type-3

Chain J:  85% 14%

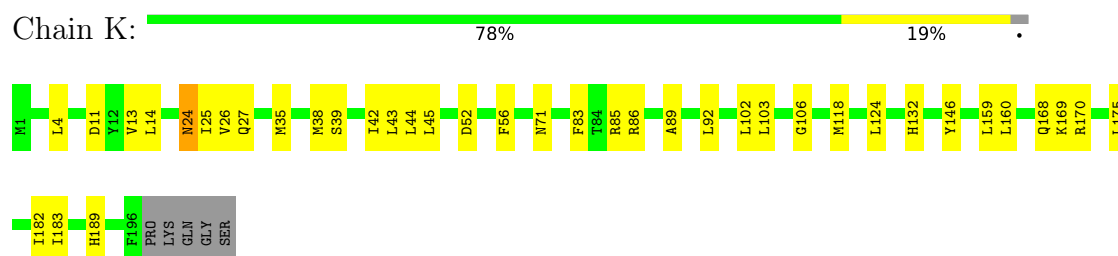


- Molecule 10: Proteasome subunit beta type-3

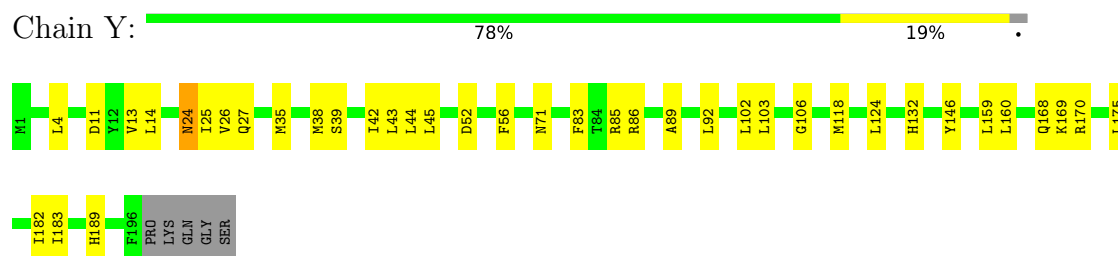
Chain X:  85% 14%



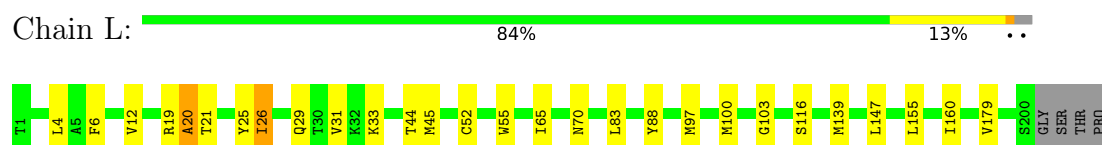
- Molecule 11: Proteasome subunit beta type-2



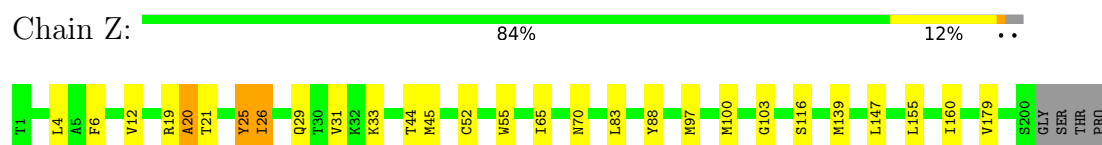
- Molecule 11: Proteasome subunit beta type-2



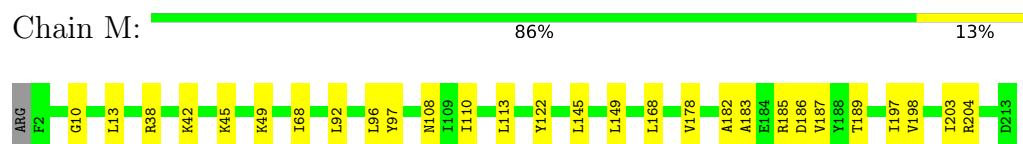
- Molecule 12: Proteasome subunit beta type-5



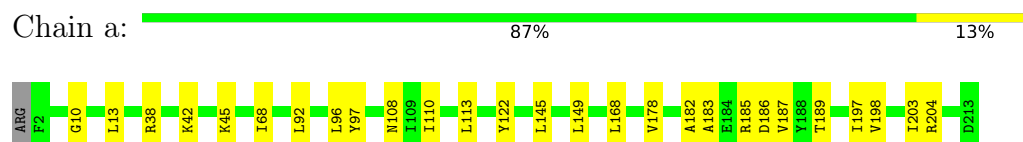
- Molecule 12: Proteasome subunit beta type-5



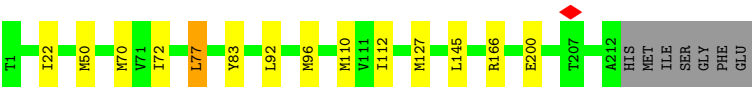
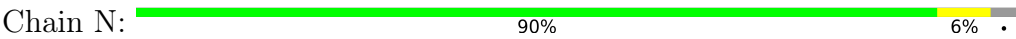
- Molecule 13: Proteasome subunit beta type-1



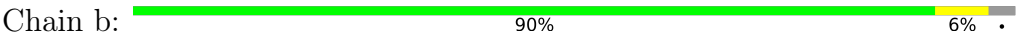
- Molecule 13: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	50885	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	95000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	18.005	Depositor
Minimum map value	-9.676	Depositor
Average map value	-0.019	Depositor
Map value standard deviation	0.769	Depositor
Recommended contour level	2.6	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	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	0.39	0/1763	0.62	0/2393
1	O	0.39	0/1763	0.62	0/2393
2	B	0.41	0/1701	0.53	0/2318
2	P	0.41	0/1701	0.53	0/2318
3	C	0.37	0/1815	0.58	0/2466
3	Q	0.37	0/1815	0.58	0/2466
4	D	0.34	0/1657	0.55	0/2261
4	R	0.34	0/1657	0.55	0/2261
5	E	0.36	0/1685	0.52	0/2290
5	S	0.35	0/1685	0.52	0/2290
6	F	0.39	0/1738	0.54	0/2364
6	T	0.38	0/1738	0.54	0/2364
7	G	0.38	0/1795	0.51	0/2434
7	U	0.38	0/1795	0.51	0/2434
8	H	0.42	0/1491	0.53	0/2021
8	V	0.42	0/1491	0.53	0/2021
9	I	0.42	0/1603	0.63	2/2180 (0.1%)
9	W	0.41	0/1603	0.63	2/2180 (0.1%)
10	J	0.42	0/1563	0.62	0/2113
10	X	0.42	0/1563	0.62	0/2113
11	K	0.44	0/1538	0.62	0/2088
11	Y	0.44	0/1538	0.62	0/2088
12	L	0.56	3/1531 (0.2%)	0.67	0/2076
12	Z	0.56	3/1531 (0.2%)	0.67	0/2076
13	M	0.41	0/1613	0.61	0/2178
13	a	0.41	0/1613	0.61	0/2178
14	N	0.43	0/1598	0.60	0/2170
14	b	0.42	0/1598	0.60	0/2170
All	All	0.41	6/46182 (0.0%)	0.58	4/62704 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	O	0	2
4	D	0	1
4	R	0	1
6	F	0	2
6	T	0	2
11	K	0	1
11	Y	0	1
All	All	0	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	25	TYR	C-O	-6.08	1.16	1.24
12	Z	25	TYR	C-O	-6.08	1.16	1.24
12	L	26	ILE	C-O	-5.96	1.17	1.24
12	Z	26	ILE	C-O	-5.95	1.17	1.24
12	Z	20	ALA	C-O	-5.87	1.17	1.24
12	L	20	ALA	C-O	-5.79	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	170	GLY	CA-C-N	6.71	134.35	121.54
9	I	170	GLY	C-N-CA	6.71	134.35	121.54
9	W	170	GLY	CA-C-N	6.69	134.32	121.54
9	W	170	GLY	C-N-CA	6.69	134.32	121.54

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	LYS	Peptide
1	A	186	LYS	Peptide
4	D	214	ASP	Peptide
6	F	58	ALA	Peptide
6	F	60	GLN	Peptide
11	K	24	ASN	Peptide
1	O	185	LYS	Peptide
1	O	186	LYS	Peptide
4	R	214	ASP	Peptide
6	T	58	ALA	Peptide

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Mol	Chain	Res	Type	Group
6	T	60	GLN	Peptide
11	Y	24	ASN	Peptide

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	A	1734	0	1652	19	0
1	O	1734	0	1652	18	0
2	B	1662	0	1590	19	0
2	P	1662	0	1590	17	0
3	C	1786	0	1717	16	0
3	Q	1786	0	1717	18	0
4	D	1633	0	1518	13	0
4	R	1633	0	1518	13	0
5	E	1659	0	1589	17	0
5	S	1659	0	1589	17	0
6	F	1704	0	1638	17	0
6	T	1704	0	1638	18	0
7	G	1760	0	1680	13	0
7	U	1760	0	1680	14	0
8	H	1465	0	1419	10	0
8	V	1465	0	1419	11	0
9	I	1576	0	1558	20	0
9	W	1576	0	1558	23	0
10	J	1534	0	1539	19	0
10	X	1534	0	1539	19	0
11	K	1506	0	1475	28	0
11	Y	1506	0	1475	28	0
12	L	1500	0	1441	19	0
12	Z	1500	0	1441	20	0
13	M	1583	0	1579	18	0
13	a	1583	0	1579	17	0
14	N	1568	0	1513	10	0
14	b	1568	0	1513	10	0
All	All	45340	0	43816	400	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (400) 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)
12:L:21:THR:HG22	12:L:26:ILE:HA	1.57	0.86
12:Z:21:THR:HG22	12:Z:26:ILE:HA	1.57	0.86
14:b:22:ILE:HG12	14:b:50:MET:HE2	1.71	0.73
14:N:22:ILE:HG12	14:N:50:MET:HE2	1.71	0.72
12:Z:19:ARG:HG2	12:Z:21:THR:HG23	1.73	0.69
12:L:19:ARG:HG2	12:L:21:THR:HG23	1.73	0.69
13:a:168:LEU:HD11	13:a:197:ILE:HD11	1.76	0.66
13:M:168:LEU:HD11	13:M:197:ILE:HD11	1.76	0.65
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.78	0.65
2:P:108:GLN:HE22	10:X:76:LYS:HG2	1.61	0.65
2:B:108:GLN:HE22	10:J:76:LYS:HG2	1.61	0.65
8:H:106:GLN:HG2	8:H:107:GLU:HG3	1.80	0.64
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.78	0.63
8:V:106:GLN:HG2	8:V:107:GLU:HG3	1.80	0.63
1:O:158:GLY:O	2:P:83:ARG:NH2	2.33	0.62
10:X:121:CYS:SG	10:X:122:SER:N	2.72	0.62
10:J:121:CYS:SG	10:J:122:SER:N	2.72	0.62
1:A:158:GLY:O	2:B:83:ARG:NH2	2.33	0.62
5:E:121:LEU:HD12	6:F:79:ALA:HB3	1.81	0.62
4:R:199:VAL:HG12	4:R:202:GLY:H	1.65	0.62
9:I:164:PHE:O	13:a:38:ARG:NH2	2.32	0.61
13:M:38:ARG:NH2	9:W:164:PHE:O	2.32	0.61
5:S:121:LEU:HD12	6:T:79:ALA:HB3	1.81	0.61
4:D:199:VAL:HG12	4:D:202:GLY:H	1.65	0.60
13:M:13:LEU:HD11	13:M:149:LEU:HD11	1.83	0.60
13:a:13:LEU:HD11	13:a:149:LEU:HD11	1.83	0.59
6:F:50:LYS:HB3	6:F:59:HIS:HB2	1.84	0.59
6:T:50:LYS:HB3	6:T:59:HIS:HB2	1.84	0.59
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.85	0.59
6:T:47:VAL:HG12	6:T:195:LEU:HD22	1.85	0.59
6:F:47:VAL:HG12	6:F:195:LEU:HD22	1.85	0.58
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.85	0.58
2:P:210:GLY:HA2	2:P:219:ARG:HA	1.85	0.58
12:L:26:ILE:O	12:L:26:ILE:HG22	2.04	0.58
13:a:145:LEU:HD21	13:a:182:ALA:HB2	1.86	0.58
14:N:166:ARG:NH2	14:N:200:GLU:OE1	2.38	0.57
2:B:210:GLY:HA2	2:B:219:ARG:HA	1.85	0.57
13:M:145:LEU:HD21	13:M:182:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LEU:HD21	2:B:133:LEU:HD11	1.87	0.57
3:C:119:GLN:NE2	4:D:79:ASP:OD1	2.37	0.57
13:M:10:GLY:HA3	13:M:42:LYS:HE2	1.87	0.57
8:H:3:ILE:HD12	8:H:99:ILE:HG22	1.87	0.56
2:P:85:LEU:HD21	2:P:133:LEU:HD11	1.87	0.56
4:R:109:ARG:NH2	12:Z:70:ASN:OD1	2.38	0.56
3:Q:119:GLN:NE2	4:R:79:ASP:OD1	2.37	0.56
8:V:3:ILE:HD12	8:V:99:ILE:HG22	1.88	0.56
12:Z:26:ILE:O	12:Z:26:ILE:HG22	2.04	0.56
14:b:166:ARG:NH2	14:b:200:GLU:OE1	2.38	0.56
2:P:99:VAL:HG13	10:X:92:ASN:HD22	1.71	0.56
9:I:80:ASN:HD21	9:I:119:THR:HG21	1.70	0.56
6:T:72:ILE:HG22	6:T:134:ILE:HG12	1.88	0.56
1:A:116:LYS:NZ	9:I:69:SER:OG	2.39	0.55
14:N:92:LEU:HD23	14:N:112:ILE:HD11	1.88	0.55
9:W:80:ASN:HD21	9:W:119:THR:HG21	1.70	0.55
6:F:72:ILE:HG22	6:F:134:ILE:HG12	1.88	0.55
4:D:109:ARG:NH2	12:L:70:ASN:OD1	2.38	0.55
4:R:211:MET:HB2	4:R:217:LEU:HD23	1.88	0.55
14:b:92:LEU:HD23	14:b:112:ILE:HD11	1.88	0.55
13:a:10:GLY:HA3	13:a:42:LYS:HE2	1.87	0.55
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.88	0.55
11:Y:42:ILE:HG22	11:Y:106:GLY:HA3	1.89	0.55
11:K:42:ILE:HG22	11:K:106:GLY:HA3	1.89	0.54
11:K:169:LYS:O	11:Y:27:GLN:NE2	2.40	0.54
2:B:99:VAL:HG13	10:J:92:ASN:HD22	1.71	0.54
3:C:3:ARG:HG2	4:D:5:ARG:HE	1.73	0.54
4:R:80:ALA:HA	4:R:129:ILE:HD13	1.90	0.54
5:E:13:ASN:HB3	6:F:126:ARG:HB3	1.89	0.54
11:K:27:GLN:NE2	11:Y:169:LYS:O	2.41	0.54
1:O:116:LYS:NZ	9:W:69:SER:OG	2.39	0.54
3:Q:109:GLN:NE2	11:Y:71:ASN:OD1	2.41	0.54
11:Y:4:LEU:HD22	11:Y:45:LEU:HB3	1.90	0.54
4:D:80:ALA:HA	4:D:129:ILE:HD13	1.90	0.54
4:D:211:MET:HB2	4:D:217:LEU:HD23	1.89	0.54
5:E:41:GLN:NE2	5:E:151:PRO:O	2.41	0.54
3:Q:3:ARG:HG2	4:R:5:ARG:HE	1.73	0.54
5:S:41:GLN:NE2	5:S:151:PRO:O	2.41	0.54
11:K:4:LEU:HD22	11:K:45:LEU:HB3	1.90	0.54
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.88	0.54
5:E:195:ILE:HG23	5:E:217:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:195:ILE:HG23	5:S:217:LEU:HD11	1.90	0.53
12:Z:45:MET:HG2	12:Z:52:CYS:HB2	1.90	0.53
3:C:109:GLN:NE2	11:K:71:ASN:OD1	2.41	0.53
6:F:117:GLN:NE2	7:G:83:ASP:OD1	2.42	0.53
5:S:13:ASN:HB3	6:T:126:ARG:HB3	1.89	0.53
12:L:45:MET:HG2	12:L:52:CYS:HB2	1.90	0.53
7:G:35:THR:HA	7:G:166:GLY:HA3	1.91	0.53
5:E:167:ALA:HB3	6:F:56:LEU:HD13	1.90	0.53
5:E:10:ARG:NH1	6:F:8:ASN:OD1	2.43	0.52
5:S:10:ARG:NH1	6:T:8:ASN:OD1	2.43	0.52
11:Y:35:MET:HG2	11:Y:45:LEU:HG	1.91	0.52
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.90	0.52
7:U:35:THR:HA	7:U:166:GLY:HA3	1.91	0.52
11:K:102:LEU:O	11:K:132:HIS:NE2	2.43	0.52
2:P:83:ARG:HA	2:P:86:VAL:HG12	1.91	0.52
1:A:72:ILE:HG21	1:A:114:LEU:HD21	1.92	0.52
9:W:6:VAL:HG12	9:W:13:VAL:HB	1.92	0.52
10:J:3:MET:HE1	10:J:105:GLU:HG3	1.92	0.52
1:O:72:ILE:HG21	1:O:114:LEU:HD21	1.92	0.52
11:Y:38:MET:HB2	11:Y:42:ILE:HG13	1.91	0.52
12:Z:33:LYS:HG2	12:Z:45:MET:HE3	1.92	0.52
6:T:117:GLN:NE2	7:U:83:ASP:OD1	2.42	0.51
11:Y:52:ASP:OD1	12:Z:88:TYR:OH	2.25	0.51
9:I:6:VAL:HG12	9:I:13:VAL:HB	1.92	0.51
11:K:38:MET:HB2	11:K:42:ILE:HG13	1.91	0.51
12:L:97:MET:HB3	12:L:116:SER:HB3	1.92	0.51
1:A:34:GLN:NE2	7:G:17:ASP:O	2.44	0.51
11:K:35:MET:HG2	11:K:45:LEU:HG	1.91	0.51
1:O:34:GLN:NE2	7:U:17:ASP:O	2.44	0.51
7:U:50:GLU:OE2	7:U:201:HIS:ND1	2.34	0.51
11:Y:102:LEU:O	11:Y:132:HIS:NE2	2.43	0.51
11:K:52:ASP:OD1	12:L:88:TYR:OH	2.25	0.51
2:B:83:ARG:HA	2:B:86:VAL:HG12	1.91	0.51
12:Z:97:MET:HB3	12:Z:116:SER:HB3	1.92	0.51
14:N:92:LEU:HD21	14:N:110:MET:HG2	1.93	0.50
12:L:33:LYS:HG2	12:L:45:MET:HE3	1.92	0.50
5:S:41:GLN:HA	5:S:46:VAL:HG12	1.94	0.50
10:X:47:ARG:HD3	10:X:111:LEU:HD12	1.93	0.50
2:B:94:GLN:HG3	9:I:65:LEU:HD22	1.94	0.50
2:P:94:GLN:HG3	9:W:65:LEU:HD22	1.94	0.50
3:Q:45:LEU:HD13	3:Q:75:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:50:ALA:HB2	10:X:128:CYS:HB2	1.94	0.50
11:Y:45:LEU:HB2	11:Y:103:LEU:HB3	1.94	0.50
7:U:108:LEU:HD21	7:U:137:LEU:HB3	1.94	0.50
10:X:3:MET:HE1	10:X:105:GLU:HG3	1.92	0.50
7:G:108:LEU:HD21	7:G:137:LEU:HB3	1.94	0.50
10:J:47:ARG:HD3	10:J:111:LEU:HD12	1.93	0.50
1:O:51:VAL:HG22	1:O:217:VAL:HG22	1.94	0.50
2:P:73:LEU:HD13	2:P:133:LEU:HD22	1.94	0.50
9:I:41:ILE:HG12	9:I:76:VAL:HG22	1.94	0.49
11:K:45:LEU:HB2	11:K:103:LEU:HB3	1.94	0.49
1:O:161:CYS:SG	1:O:162:GLY:N	2.85	0.49
9:I:50:ALA:HB2	10:J:128:CYS:HB2	1.94	0.49
12:L:6:PHE:HB3	12:L:139:MET:HE2	1.93	0.49
5:S:164:GLN:HB3	6:T:58:ALA:HB3	1.94	0.49
3:C:100:GLN:HA	11:K:86:ARG:HG3	1.94	0.49
9:I:24:MET:HE3	13:a:187:VAL:HG21	1.94	0.49
9:W:110:LEU:HD21	9:W:125:VAL:HG22	1.93	0.49
12:L:83:LEU:HD11	12:L:97:MET:HE1	1.94	0.49
14:b:92:LEU:HD21	14:b:110:MET:HG2	1.93	0.49
11:K:182:ILE:HG22	11:K:189:HIS:HB2	1.95	0.49
13:M:187:VAL:HG21	9:W:24:MET:HE3	1.94	0.49
2:B:73:LEU:HD13	2:B:133:LEU:HD22	1.94	0.49
3:C:45:LEU:HD13	3:C:75:SER:HB2	1.94	0.49
5:E:41:GLN:HA	5:E:46:VAL:HG12	1.94	0.49
9:I:110:LEU:HD21	9:I:125:VAL:HG22	1.94	0.49
12:Z:6:PHE:HB3	12:Z:139:MET:HE2	1.93	0.49
10:J:11:MET:HE3	10:J:166:ILE:HG13	1.95	0.49
11:Y:168:GLN:NE2	11:Y:175:LEU:O	2.46	0.49
1:A:51:VAL:HG22	1:A:217:VAL:HG22	1.95	0.49
1:A:161:CYS:SG	1:A:162:GLY:N	2.85	0.49
10:J:50:ILE:HG13	10:J:108:ILE:HG22	1.95	0.49
13:M:197:ILE:HD13	13:M:204:ARG:HH21	1.78	0.49
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.95	0.49
5:S:199:LEU:HD12	5:S:210:LEU:HD21	1.95	0.49
10:X:189:ILE:HG12	10:X:194:ILE:HD12	1.95	0.49
9:W:41:ILE:HG12	9:W:76:VAL:HG22	1.94	0.48
8:V:124:SER:OG	8:V:143:TYR:OH	2.31	0.48
12:Z:83:LEU:HD11	12:Z:97:MET:HE1	1.95	0.48
5:E:164:GLN:HB3	6:F:58:ALA:HB3	1.94	0.48
11:K:43:LEU:HD12	11:K:183:ILE:HD11	1.95	0.48
10:X:50:ILE:HG13	10:X:108:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:44:CYS:HB2	9:I:99:VAL:HB	1.96	0.48
13:a:197:ILE:HD13	13:a:204:ARG:HH21	1.78	0.48
5:E:31:ILE:HD13	5:E:140:ALA:HB2	1.95	0.48
9:I:59:ILE:HD12	9:I:82:MET:HB3	1.96	0.48
10:J:189:ILE:HG12	10:J:194:ILE:HD12	1.95	0.48
3:Q:100:GLN:HA	11:Y:86:ARG:HG3	1.94	0.48
9:I:211:VAL:HG11	10:J:197:ARG:HD3	1.96	0.48
11:K:89:ALA:HA	11:K:92:LEU:HD23	1.96	0.48
12:L:4:LEU:HB2	12:L:160:ILE:HD11	1.95	0.48
10:X:11:MET:HE3	10:X:166:ILE:HG13	1.95	0.48
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.96	0.48
9:W:44:CYS:HB2	9:W:99:VAL:HB	1.96	0.48
1:A:11:ARG:HG2	1:A:23:TYR:HE2	1.79	0.47
5:E:199:LEU:HD12	5:E:210:LEU:HD21	1.95	0.47
11:Y:182:ILE:HG22	11:Y:189:HIS:HB2	1.95	0.47
1:A:24:GLN:NE2	7:G:14:PHE:H	2.12	0.47
7:G:50:GLU:OE2	7:G:201:HIS:ND1	2.34	0.47
3:Q:163:CYS:O	3:Q:168:SER:OG	2.32	0.47
10:X:141:CYS:HB2	10:X:144:GLN:HB2	1.96	0.47
11:Y:43:LEU:HD12	11:Y:183:ILE:HD11	1.95	0.47
10:J:141:CYS:HB2	10:J:144:GLN:HB2	1.96	0.47
11:K:56:PHE:HE2	11:K:102:LEU:HD21	1.80	0.47
1:O:123:GLN:NE2	2:P:81:ASP:OD1	2.32	0.47
3:C:143:TYR:HB2	3:C:146:GLN:HE21	1.80	0.47
12:Z:19:ARG:HD3	12:Z:26:ILE:HG12	1.96	0.47
11:K:168:GLN:NE2	11:K:175:LEU:O	2.46	0.47
1:O:11:ARG:HG2	1:O:23:TYR:HE2	1.79	0.47
12:Z:4:LEU:HB2	12:Z:160:ILE:HD11	1.95	0.47
11:K:102:LEU:HB2	11:K:118:MET:HG2	1.97	0.47
11:K:170:ARG:HA	11:Y:27:GLN:HE21	1.80	0.47
12:L:19:ARG:HD3	12:L:26:ILE:HG12	1.97	0.47
8:V:179:ILE:HG12	8:V:184:VAL:HG22	1.96	0.47
11:Y:102:LEU:HB2	11:Y:118:MET:HG2	1.97	0.47
8:H:124:SER:OG	8:H:143:TYR:OH	2.31	0.47
8:V:55:VAL:HG13	8:V:86:MET:HG2	1.96	0.47
9:W:59:ILE:HD12	9:W:82:MET:HB3	1.96	0.47
9:W:211:VAL:HG11	10:X:197:ARG:HD3	1.96	0.47
11:Y:56:PHE:HE2	11:Y:102:LEU:HD21	1.80	0.47
6:F:95:SER:HB3	6:F:103:LEU:HD12	1.97	0.47
3:Q:143:TYR:HB2	3:Q:146:GLN:HE21	1.80	0.47
6:T:95:SER:HB3	6:T:103:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:90:TYR:HB3	8:H:94:LEU:HD23	1.97	0.47
8:H:179:ILE:HG12	8:H:184:VAL:HG22	1.96	0.47
3:C:68:LEU:HD11	3:C:74:CYS:HB3	1.97	0.46
1:O:24:GLN:NE2	7:U:14:PHE:H	2.12	0.46
11:Y:89:ALA:HA	11:Y:92:LEU:HD23	1.96	0.46
5:E:69:GLU:HG2	5:E:226:PHE:CD2	2.50	0.46
8:H:55:VAL:HG13	8:H:86:MET:HG2	1.96	0.46
11:Y:118:MET:HE2	11:Y:124:LEU:HD13	1.98	0.46
12:L:29:GLN:OE1	10:X:202:ARG:NH1	2.38	0.46
4:R:31:THR:OG1	4:R:163:ARG:O	2.27	0.46
10:X:57:THR:O	11:Y:85:ARG:NH2	2.49	0.46
11:K:118:MET:HE2	11:K:124:LEU:HD13	1.98	0.46
8:V:90:TYR:HB3	8:V:94:LEU:HD23	1.97	0.46
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.96	0.46
13:a:45:LYS:HE3	13:a:203:ILE:HD12	1.97	0.46
13:a:68:ILE:HD11	13:a:92:LEU:HD13	1.97	0.46
11:K:27:GLN:HE21	11:Y:170:ARG:HA	1.80	0.46
12:L:147:LEU:HD21	12:L:155:LEU:HD21	1.98	0.46
10:J:57:THR:O	11:K:85:ARG:NH2	2.49	0.46
9:W:81:ARG:HA	9:W:84:LYS:HG2	1.98	0.46
9:W:127:MET:HE2	9:W:127:MET:HB3	1.83	0.46
3:Q:68:LEU:HD11	3:Q:74:CYS:HB3	1.97	0.46
5:S:69:GLU:HG2	5:S:226:PHE:CD2	2.50	0.46
6:F:101:ARG:HH22	6:F:104:PRO:HD3	1.81	0.46
6:F:215:VAL:HB	6:F:221:PHE:HD1	1.81	0.46
9:I:81:ARG:HA	9:I:84:LYS:HG2	1.98	0.46
8:V:93:ASP:OD2	9:W:91:GLN:NE2	2.49	0.46
6:T:215:VAL:HB	6:T:221:PHE:HD1	1.81	0.45
10:X:10:VAL:HG23	10:X:53:ALA:HB2	1.98	0.45
7:U:148:LEU:HD22	7:U:160:TYR:HB2	1.98	0.45
8:H:93:ASP:OD2	9:I:91:GLN:NE2	2.49	0.45
5:S:97:GLN:HG3	12:Z:65:ILE:HG13	1.97	0.45
7:G:148:LEU:HD22	7:G:160:TYR:HB2	1.98	0.45
10:J:10:VAL:HG23	10:J:53:ALA:HB2	1.98	0.45
13:M:68:ILE:HD11	13:M:92:LEU:HD13	1.96	0.45
1:O:69:LEU:HD13	1:O:216:GLU:HG3	1.98	0.45
2:B:118:GLN:O	2:B:121:THR:OG1	2.34	0.45
2:P:49:LYS:H	2:P:207:ILE:HA	1.82	0.45
6:F:88:MET:HE3	6:F:112:ILE:HD11	1.99	0.45
6:T:101:ARG:HH22	6:T:104:PRO:HD3	1.81	0.45
4:R:42:VAL:HG13	4:R:210:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:110:ILE:HB	13:a:122:TYR:HB2	1.97	0.45
3:C:163:CYS:O	3:C:168:SER:OG	2.32	0.45
4:D:42:VAL:HG13	4:D:210:VAL:HG22	1.99	0.45
13:M:110:ILE:HB	13:M:122:TYR:HB2	1.97	0.45
12:Z:147:LEU:HD21	12:Z:155:LEU:HD21	1.98	0.45
13:M:45:LYS:HE3	13:M:203:ILE:HD12	1.97	0.45
10:J:122:SER:HB2	10:J:136:VAL:HB	2.00	0.44
6:T:88:MET:HE3	6:T:112:ILE:HD11	1.99	0.44
10:X:14:LYS:HE3	10:X:120:ILE:HG12	1.99	0.44
10:X:141:CYS:HB3	10:X:177:ASP:HB2	2.00	0.44
1:A:24:GLN:HE22	7:G:14:PHE:H	1.65	0.44
2:B:49:LYS:H	2:B:207:ILE:HA	1.82	0.44
5:E:97:GLN:HG3	12:L:65:ILE:HG13	1.98	0.44
12:Z:25:TYR:O	12:Z:25:TYR:CG	2.70	0.44
6:T:109:VAL:HA	6:T:112:ILE:HD12	2.00	0.44
13:a:186:ASP:HB3	13:a:189:THR:HG22	1.99	0.44
8:H:174:ILE:HB	8:H:189:LEU:HB2	1.99	0.44
13:M:186:ASP:HB3	13:M:189:THR:HG22	1.99	0.44
1:O:24:GLN:HE22	7:U:14:PHE:H	1.65	0.44
3:Q:171:ALA:HB2	3:Q:200:THR:HG21	2.00	0.44
4:R:140:GLY:O	4:R:213:ARG:NH1	2.51	0.44
8:V:174:ILE:HB	8:V:189:LEU:HB2	1.99	0.44
10:J:14:LYS:HE3	10:J:120:ILE:HG12	1.99	0.44
4:D:140:GLY:O	4:D:213:ARG:NH1	2.51	0.44
10:J:202:ARG:NH1	12:Z:29:GLN:OE1	2.38	0.44
2:P:73:LEU:HD11	2:P:86:VAL:HG23	2.00	0.44
10:X:122:SER:HB2	10:X:136:VAL:HB	2.00	0.44
1:A:69:LEU:HD13	1:A:216:GLU:HG3	1.98	0.43
8:H:19:ARG:HG3	8:H:26:ILE:HG23	2.00	0.43
9:I:26:VAL:HB	13:a:185:ARG:HA	2.00	0.43
2:P:92:LEU:HD13	2:P:112:ARG:HB3	2.00	0.43
3:Q:136:TYR:HB2	3:Q:148:TYR:HB2	2.00	0.43
4:R:116:GLN:NE2	5:S:84:ASP:OD1	2.46	0.43
5:S:74:ILE:HG12	5:S:109:VAL:HG22	2.00	0.43
14:b:96:MET:HE3	14:b:127:MET:HA	2.00	0.43
1:A:113:MET:HE3	9:I:70:THR:HA	2.00	0.43
10:J:141:CYS:HB3	10:J:177:ASP:HB2	2.00	0.43
13:a:96:LEU:HD11	13:a:108:ASN:HD22	1.83	0.43
3:C:35:LEU:HG	3:C:46:ALA:HB3	2.00	0.43
12:L:44:THR:HG21	12:L:100:MET:HE3	2.01	0.43
3:Q:174:MET:HE1	3:Q:199:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:69:VAL:HG11	4:R:107:ILE:HG21	2.00	0.43
3:C:136:TYR:HB2	3:C:148:TYR:HB2	2.00	0.43
5:E:51:GLU:HG3	5:E:206:MET:HE3	2.01	0.43
13:a:113:LEU:HD23	13:a:198:VAL:HG12	2.00	0.43
14:b:96:MET:HE2	14:b:110:MET:HE1	1.99	0.43
4:D:31:THR:OG1	4:D:163:ARG:O	2.27	0.43
5:E:74:ILE:HG12	5:E:109:VAL:HG22	2.00	0.43
13:M:185:ARG:HA	9:W:26:VAL:HB	2.00	0.43
14:N:96:MET:HE2	14:N:110:MET:HE1	1.99	0.43
8:V:19:ARG:HG3	8:V:26:ILE:HG23	2.00	0.43
3:C:174:MET:HE1	3:C:199:LYS:HG3	2.01	0.43
2:B:92:LEU:HD13	2:B:112:ARG:HB3	2.00	0.43
6:F:109:VAL:HA	6:F:112:ILE:HD12	2.00	0.43
9:I:132:LEU:HB3	14:b:145:LEU:HD12	2.01	0.43
3:Q:154:GLY:O	4:R:81:ARG:NH2	2.42	0.43
11:K:146:TYR:HB2	11:K:159:LEU:HD13	2.01	0.43
5:S:51:GLU:HG3	5:S:206:MET:HE3	2.01	0.43
12:Z:44:THR:HG21	12:Z:100:MET:HE3	2.01	0.43
3:C:171:ALA:HB2	3:C:200:THR:HG21	2.00	0.43
7:G:206:ASP:OD1	7:G:206:ASP:N	2.44	0.43
3:Q:100:GLN:HE21	11:Y:83:PHE:HE1	1.67	0.43
14:b:110:MET:HB2	14:b:110:MET:HE2	1.80	0.43
3:C:100:GLN:HE21	11:K:83:PHE:HE1	1.67	0.42
4:D:116:GLN:NE2	5:E:84:ASP:OD1	2.46	0.42
7:G:50:GLU:HB2	7:G:197:ILE:HG23	2.01	0.42
14:N:77:LEU:H	14:N:77:LEU:HG	1.65	0.42
14:N:96:MET:HE3	14:N:127:MET:HA	2.00	0.42
2:B:73:LEU:HD11	2:B:86:VAL:HG23	2.00	0.42
4:D:69:VAL:HG11	4:D:107:ILE:HG21	2.00	0.42
9:I:98:LEU:HB2	9:I:113:ILE:HB	2.01	0.42
11:K:14:LEU:HD21	11:K:160:LEU:HD22	2.02	0.42
13:M:113:LEU:HD23	13:M:198:VAL:HG12	2.00	0.42
2:P:64:VAL:HG11	2:P:210:GLY:HA3	2.01	0.42
11:Y:146:TYR:HB2	11:Y:159:LEU:HD13	2.01	0.42
10:X:168:GLN:O	10:X:172:ASN:ND2	2.52	0.42
6:F:207:THR:HG22	6:F:233:LEU:HD12	2.02	0.42
3:Q:35:LEU:HG	3:Q:46:ALA:HB3	2.00	0.42
2:B:64:VAL:HG11	2:B:210:GLY:HA3	2.02	0.42
1:O:50:ILE:HD12	1:O:79:VAL:HB	2.01	0.42
2:P:212:CYS:HB2	2:P:217:PHE:HD1	1.85	0.42
11:Y:11:ASP:OD1	11:Y:11:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:14:LEU:HD21	11:Y:160:LEU:HD22	2.02	0.42
1:A:120:ASP:OD1	2:B:83:ARG:NH1	2.53	0.42
2:B:78:MET:HE2	2:B:78:MET:HB3	1.90	0.42
11:K:24:ASN:O	11:K:26:VAL:N	2.53	0.42
12:L:103:GLY:HA2	12:L:179:VAL:HG11	2.02	0.42
7:U:21:PHE:O	7:U:25:TYR:N	2.49	0.42
3:C:154:GLY:O	4:D:81:ARG:NH2	2.42	0.42
5:E:195:ILE:HD11	5:E:219:THR:HG21	2.01	0.42
7:G:181:MET:SD	7:G:181:MET:N	2.90	0.42
10:J:168:GLN:O	10:J:172:ASN:ND2	2.52	0.42
13:M:96:LEU:HD11	13:M:108:ASN:HD22	1.84	0.42
1:O:113:MET:HE3	9:W:70:THR:HA	2.00	0.42
4:R:54:GLN:HE21	4:R:59:VAL:HG21	1.85	0.42
7:G:72:HIS:CE1	7:G:105:ASN:HB3	2.55	0.42
14:b:77:LEU:H	14:b:77:LEU:HG	1.65	0.42
14:N:145:LEU:HD12	9:W:132:LEU:HB3	2.01	0.41
1:O:69:LEU:HD23	1:O:229:ILE:HG12	2.02	0.41
1:O:120:ASP:OD1	2:P:83:ARG:NH1	2.53	0.41
2:P:118:GLN:O	2:P:121:THR:OG1	2.34	0.41
5:S:195:ILE:HD11	5:S:219:THR:HG21	2.02	0.41
9:W:98:LEU:HB2	9:W:113:ILE:HB	2.01	0.41
2:B:212:CYS:HB2	2:B:217:PHE:HD1	1.85	0.41
11:K:39:SER:HB2	11:K:42:ILE:HG12	2.02	0.41
13:M:145:LEU:HD22	13:M:178:VAL:HG22	2.02	0.41
1:A:123:GLN:NE2	2:B:81:ASP:OD1	2.32	0.41
6:F:157:ARG:NH1	7:G:58:TYR:O	2.53	0.41
11:K:11:ASP:OD1	11:K:11:ASP:N	2.52	0.41
12:L:55:TRP:NE1	13:M:97:TYR:OH	2.51	0.41
13:M:183:ALA:HA	13:M:189:THR:HG23	2.03	0.41
1:O:43:ARG:HA	1:O:48:ALA:HA	2.02	0.41
3:Q:107:CYS:HB2	3:Q:146:GLN:OE1	2.20	0.41
13:a:145:LEU:HD22	13:a:178:VAL:HG22	2.02	0.41
1:O:32:ILE:HA	1:O:82:GLY:HA2	2.03	0.41
11:Y:24:ASN:O	11:Y:26:VAL:N	2.53	0.41
5:E:86:LYS:HA	5:E:89:ILE:HG12	2.02	0.41
3:Q:172:VAL:HG12	3:Q:176:LYS:HE2	2.03	0.41
4:D:54:GLN:HE21	4:D:59:VAL:HG21	1.85	0.41
6:T:157:ARG:NH1	7:U:58:TYR:O	2.53	0.41
1:A:50:ILE:HD12	1:A:79:VAL:HB	2.01	0.41
1:A:113:MET:HG3	9:I:70:THR:HG22	2.03	0.41
3:Q:72:MET:HE3	3:Q:72:MET:HB2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:72:HIS:CE1	7:U:105:ASN:HB3	2.55	0.41
3:C:107:CYS:HB2	3:C:146:GLN:OE1	2.20	0.41
6:T:82:ARG:HA	6:T:85:CYS:HB3	2.03	0.41
11:Y:39:SER:HB2	11:Y:42:ILE:HG12	2.02	0.41
1:A:32:ILE:HA	1:A:82:GLY:HA2	2.03	0.41
2:B:142:ARG:HD3	2:B:144:TYR:CZ	2.56	0.41
3:Q:33:THR:OG1	3:Q:166:ASN:O	2.33	0.41
5:S:86:LYS:HA	5:S:89:ILE:HG12	2.03	0.41
6:T:207:THR:HG22	6:T:233:LEU:HD12	2.02	0.41
7:U:50:GLU:HB2	7:U:197:ILE:HG23	2.01	0.41
7:U:161:TRP:CE2	7:U:182:LYS:HE2	2.56	0.41
10:X:10:VAL:HG11	10:X:51:GLY:HA3	2.03	0.41
12:Z:103:GLY:HA2	12:Z:179:VAL:HG11	2.02	0.41
14:b:70:MET:HG2	14:b:83:TYR:HE2	1.85	0.41
2:B:134:LEU:HD23	2:B:134:LEU:HA	1.80	0.41
11:K:38:MET:SD	11:K:44:LEU:HB2	2.61	0.41
9:W:12:ILE:HG23	9:W:178:ILE:HB	2.03	0.41
11:Y:38:MET:SD	11:Y:44:LEU:HB2	2.61	0.41
8:V:124:SER:HG	8:V:143:TYR:HH	1.68	0.40
3:C:172:VAL:HG12	3:C:176:LYS:HE2	2.03	0.40
6:F:82:ARG:HA	6:F:85:CYS:HB3	2.03	0.40
14:N:70:MET:HG2	14:N:83:TYR:HE2	1.85	0.40
2:P:142:ARG:HD3	2:P:144:TYR:CZ	2.56	0.40
9:W:152:LYS:HD3	9:W:177:VAL:HG21	2.03	0.40
9:W:163:ILE:HG12	9:W:170:GLY:HA2	2.04	0.40
1:A:43:ARG:HA	1:A:48:ALA:HA	2.02	0.40
13:M:49:LYS:HB2	13:M:113:LEU:HB2	2.03	0.40
14:N:110:MET:HE2	14:N:110:MET:HB2	1.80	0.40
6:T:224:TYR:HD1	6:T:228:ASP:HB3	1.87	0.40
7:U:181:MET:SD	7:U:181:MET:N	2.90	0.40
12:Z:55:TRP:NE1	13:a:97:TYR:OH	2.51	0.40
13:a:183:ALA:HA	13:a:189:THR:HG23	2.03	0.40
1:A:69:LEU:HD23	1:A:229:ILE:HG12	2.02	0.40
10:J:10:VAL:HG11	10:J:51:GLY:HA3	2.03	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	238/246 (97%)	224 (94%)	13 (6%)	1 (0%)	30	51
1	O	238/246 (97%)	224 (94%)	13 (6%)	1 (0%)	30	51
2	B	227/234 (97%)	220 (97%)	7 (3%)	0	100	100
2	P	227/234 (97%)	220 (97%)	7 (3%)	0	100	100
3	C	245/261 (94%)	232 (95%)	13 (5%)	0	100	100
3	Q	245/261 (94%)	232 (95%)	13 (5%)	0	100	100
4	D	230/248 (93%)	219 (95%)	11 (5%)	0	100	100
4	R	230/248 (93%)	219 (95%)	11 (5%)	0	100	100
5	E	231/241 (96%)	220 (95%)	11 (5%)	0	100	100
5	S	231/241 (96%)	220 (95%)	11 (5%)	0	100	100
6	F	231/263 (88%)	222 (96%)	9 (4%)	0	100	100
6	T	231/263 (88%)	222 (96%)	9 (4%)	0	100	100
7	G	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
7	U	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
8	H	200/205 (98%)	194 (97%)	6 (3%)	0	100	100
8	V	200/205 (98%)	194 (97%)	6 (3%)	0	100	100
9	I	218/234 (93%)	206 (94%)	12 (6%)	0	100	100
9	W	218/234 (93%)	206 (94%)	12 (6%)	0	100	100
10	J	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
10	X	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
11	K	194/201 (96%)	179 (92%)	14 (7%)	1 (0%)	24	46
11	Y	194/201 (96%)	179 (92%)	14 (7%)	1 (0%)	24	46
12	L	198/204 (97%)	189 (96%)	9 (4%)	0	100	100
12	Z	198/204 (97%)	189 (96%)	9 (4%)	0	100	100
13	M	210/213 (99%)	198 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	210/213 (99%)	198 (94%)	12 (6%)	0	100	100
14	N	210/219 (96%)	196 (93%)	14 (7%)	0	100	100
14	b	210/219 (96%)	196 (93%)	14 (7%)	0	100	100
All	All	6142/6458 (95%)	5836 (95%)	302 (5%)	4 (0%)	49	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	25	ILE
11	Y	25	ILE
1	A	184	LYS
1	O	184	LYS

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	163/210 (78%)	161 (99%)	2 (1%)	63	83
1	O	163/210 (78%)	161 (99%)	2 (1%)	63	83
2	B	150/191 (78%)	149 (99%)	1 (1%)	76	89
2	P	150/191 (78%)	149 (99%)	1 (1%)	76	89
3	C	160/221 (72%)	158 (99%)	2 (1%)	61	82
3	Q	160/221 (72%)	158 (99%)	2 (1%)	61	82
4	D	136/211 (64%)	135 (99%)	1 (1%)	76	89
4	R	136/211 (64%)	135 (99%)	1 (1%)	76	89
5	E	158/203 (78%)	158 (100%)	0	100	100
5	S	158/203 (78%)	158 (100%)	0	100	100
6	F	160/224 (71%)	159 (99%)	1 (1%)	78	91
6	T	160/224 (71%)	159 (99%)	1 (1%)	78	91
7	G	162/212 (76%)	161 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	162/212 (76%)	161 (99%)	1 (1%)	78	91
8	H	140/159 (88%)	140 (100%)	0	100	100
8	V	140/159 (88%)	140 (100%)	0	100	100
9	I	157/195 (80%)	155 (99%)	2 (1%)	61	82
9	W	157/195 (80%)	155 (99%)	2 (1%)	61	82
10	J	155/174 (89%)	154 (99%)	1 (1%)	78	91
10	X	155/174 (89%)	154 (99%)	1 (1%)	78	91
11	K	148/171 (86%)	147 (99%)	1 (1%)	76	89
11	Y	148/171 (86%)	147 (99%)	1 (1%)	76	89
12	L	138/159 (87%)	137 (99%)	1 (1%)	76	89
12	Z	138/159 (87%)	137 (99%)	1 (1%)	76	89
13	M	158/178 (89%)	158 (100%)	0	100	100
13	a	158/178 (89%)	158 (100%)	0	100	100
14	N	149/181 (82%)	147 (99%)	2 (1%)	61	82
14	b	149/181 (82%)	147 (99%)	2 (1%)	61	82
All	All	4268/5378 (79%)	4238 (99%)	30 (1%)	73	89

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	THR
1	A	179	LEU
2	B	173	LEU
3	C	43	VAL
3	C	134	LEU
4	D	84	ILE
6	F	38	LEU
7	G	53	VAL
9	I	6	VAL
9	I	65	LEU
10	J	108	ILE
11	K	13	VAL
12	L	12	VAL
14	N	72	ILE
14	N	77	LEU
1	O	166	THR
1	O	179	LEU

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Mol	Chain	Res	Type
2	P	173	LEU
3	Q	43	VAL
3	Q	134	LEU
4	R	84	ILE
6	T	38	LEU
7	U	53	VAL
9	W	6	VAL
9	W	65	LEU
10	X	108	ILE
11	Y	13	VAL
12	Z	12	VAL
14	b	72	ILE
14	b	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	34	GLN
1	A	75	ASN
1	A	92	GLN
1	A	238	HIS
2	B	87	HIS
2	B	94	GLN
2	B	108	GLN
2	B	188	HIS
3	C	40	ASN
3	C	88	ASN
3	C	109	GLN
3	C	240	HIS
4	D	54	GLN
4	D	154	HIS
4	D	175	ASN
5	E	41	GLN
5	E	155	HIS
6	F	16	GLN
6	F	20	HIS
6	F	43	HIS
8	H	66	HIS
8	H	158	ASN
9	I	80	ASN

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Mol	Chain	Res	Type
9	I	116	HIS
9	I	165	ASN
10	J	71	ASN
10	J	92	ASN
11	K	27	GLN
11	K	63	ASN
11	K	71	ASN
11	K	82	ASN
11	K	189	HIS
13	M	58	HIS
13	M	108	ASN
13	M	157	ASN
1	O	24	GLN
1	O	33	ASN
1	O	75	ASN
1	O	92	GLN
1	O	238	HIS
2	P	87	HIS
2	P	94	GLN
2	P	108	GLN
2	P	188	HIS
3	Q	40	ASN
3	Q	88	ASN
3	Q	240	HIS
4	R	54	GLN
4	R	154	HIS
4	R	175	ASN
5	S	41	GLN
5	S	155	HIS
6	T	16	GLN
6	T	20	HIS
6	T	43	HIS
8	V	66	HIS
8	V	158	ASN
9	W	80	ASN
9	W	165	ASN
10	X	92	ASN
11	Y	27	GLN
11	Y	63	ASN
11	Y	82	ASN
11	Y	189	HIS
13	a	58	HIS

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Mol	Chain	Res	Type
13	a	157	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 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.

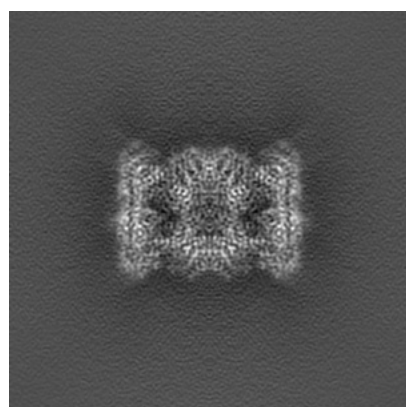
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4877. These allow visual inspection of the internal detail of the map and identification of artifacts.

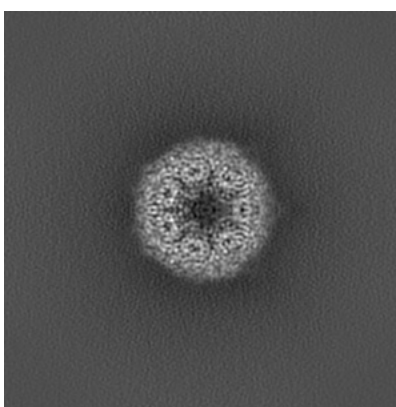
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

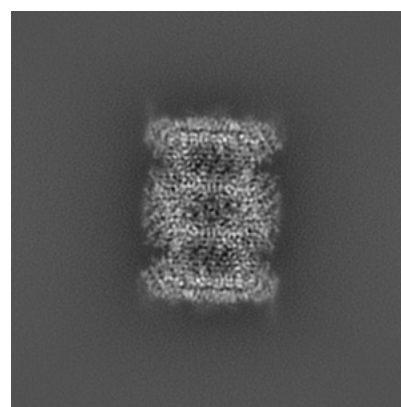
6.1.1 Primary map



X



Y

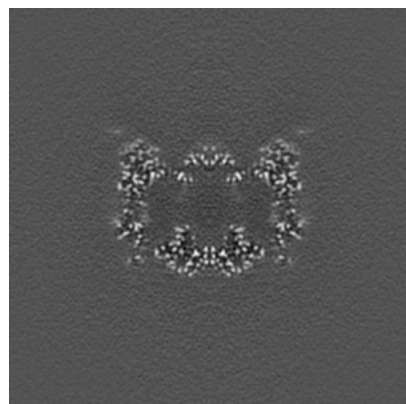


Z

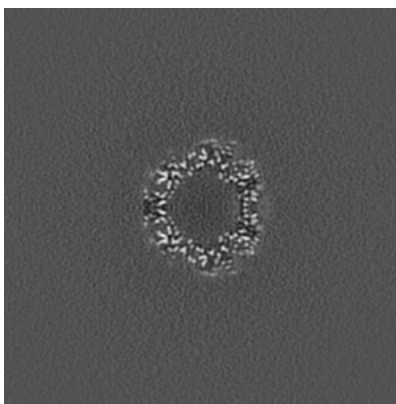
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

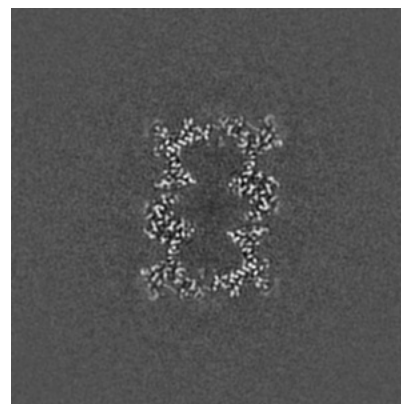
6.2.1 Primary map



X Index: 200



Y Index: 200

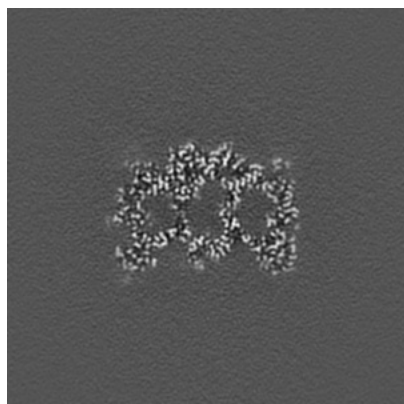


Z Index: 200

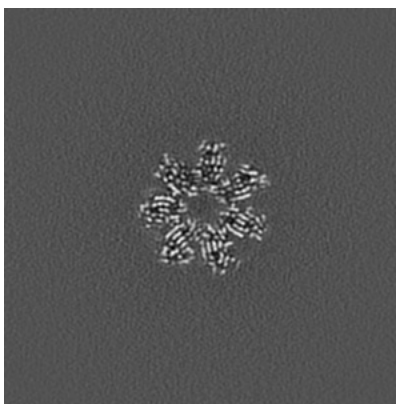
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

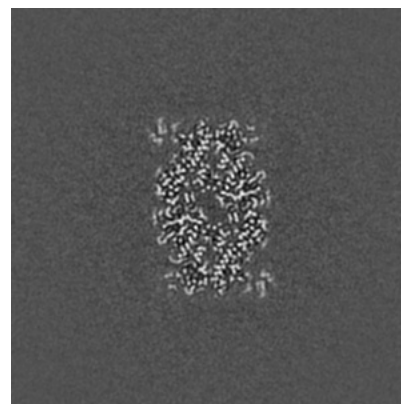
6.3.1 Primary map



X Index: 224



Y Index: 224

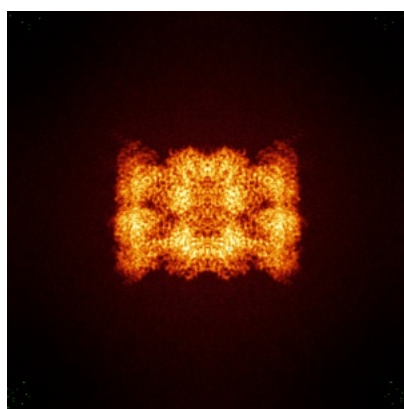


Z Index: 167

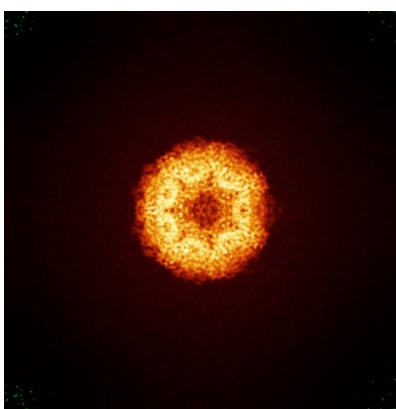
The images above show the largest variance slices of the map in three orthogonal directions.

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

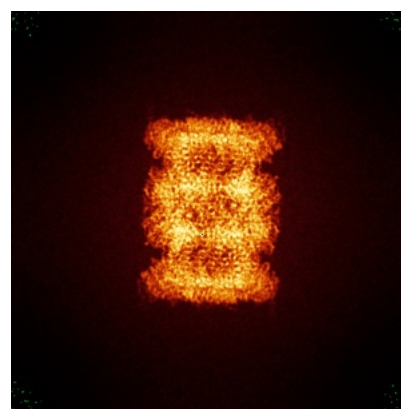
6.4.1 Primary map



X



Y

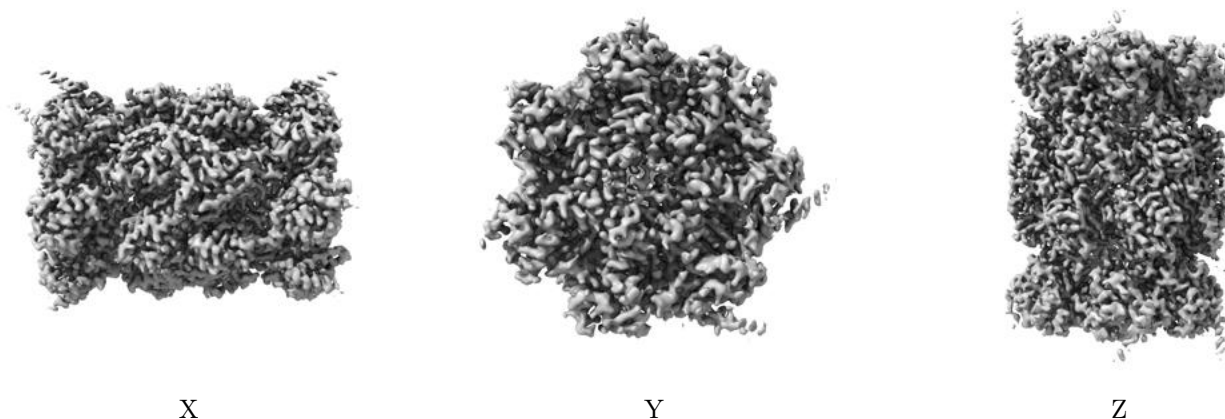


Z

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 2.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

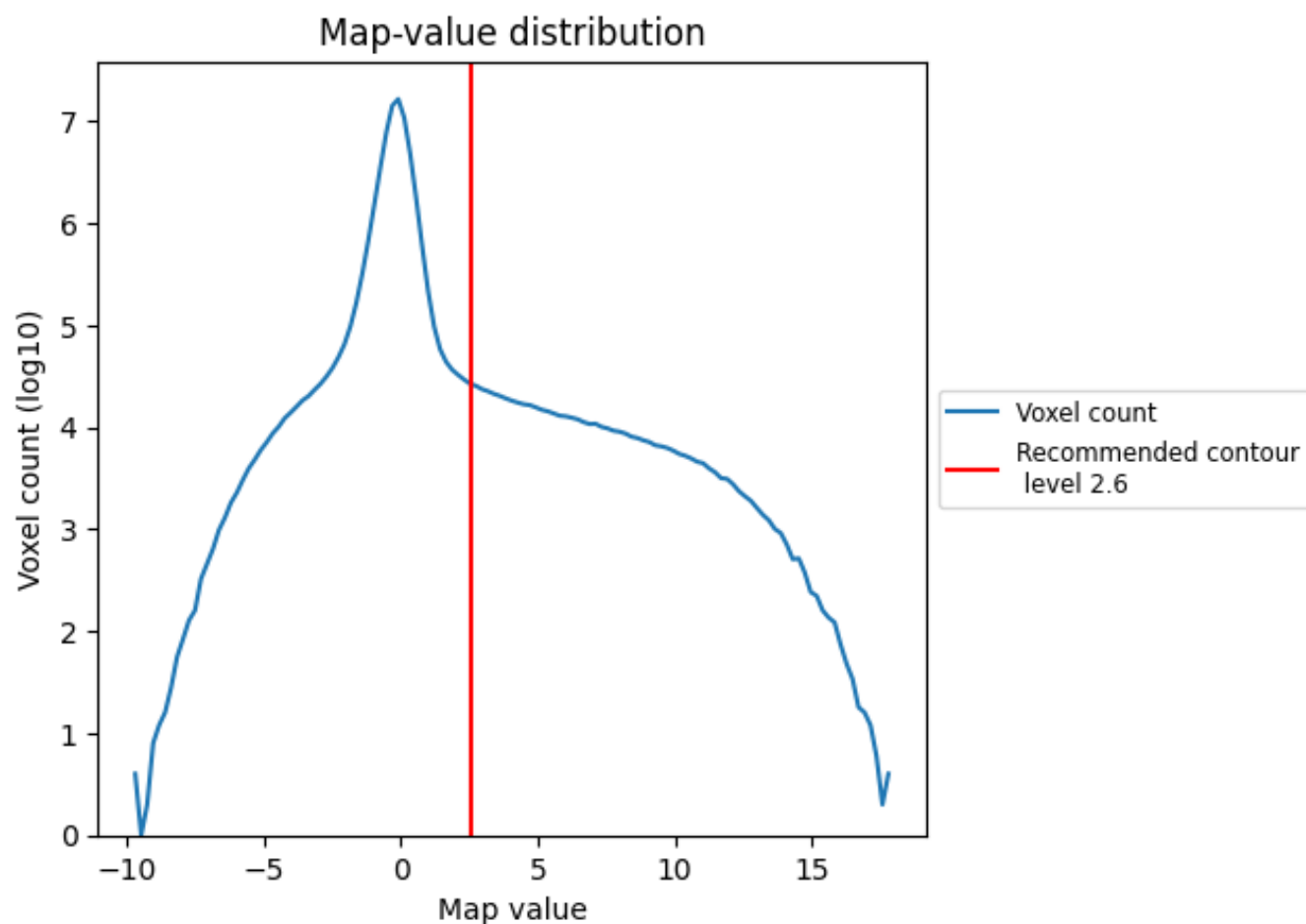
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

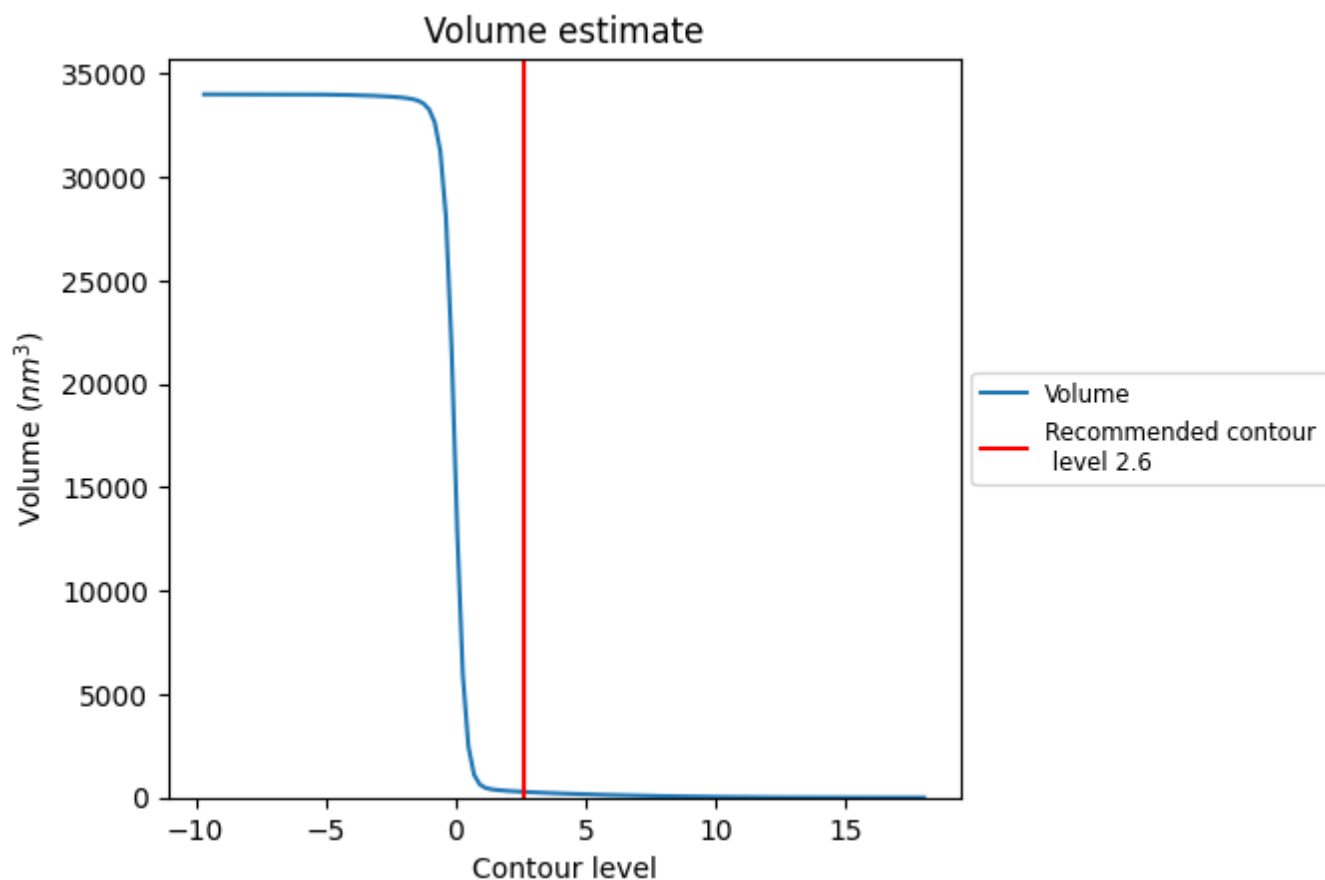
This section contains the results of statistical analysis of the map.

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.

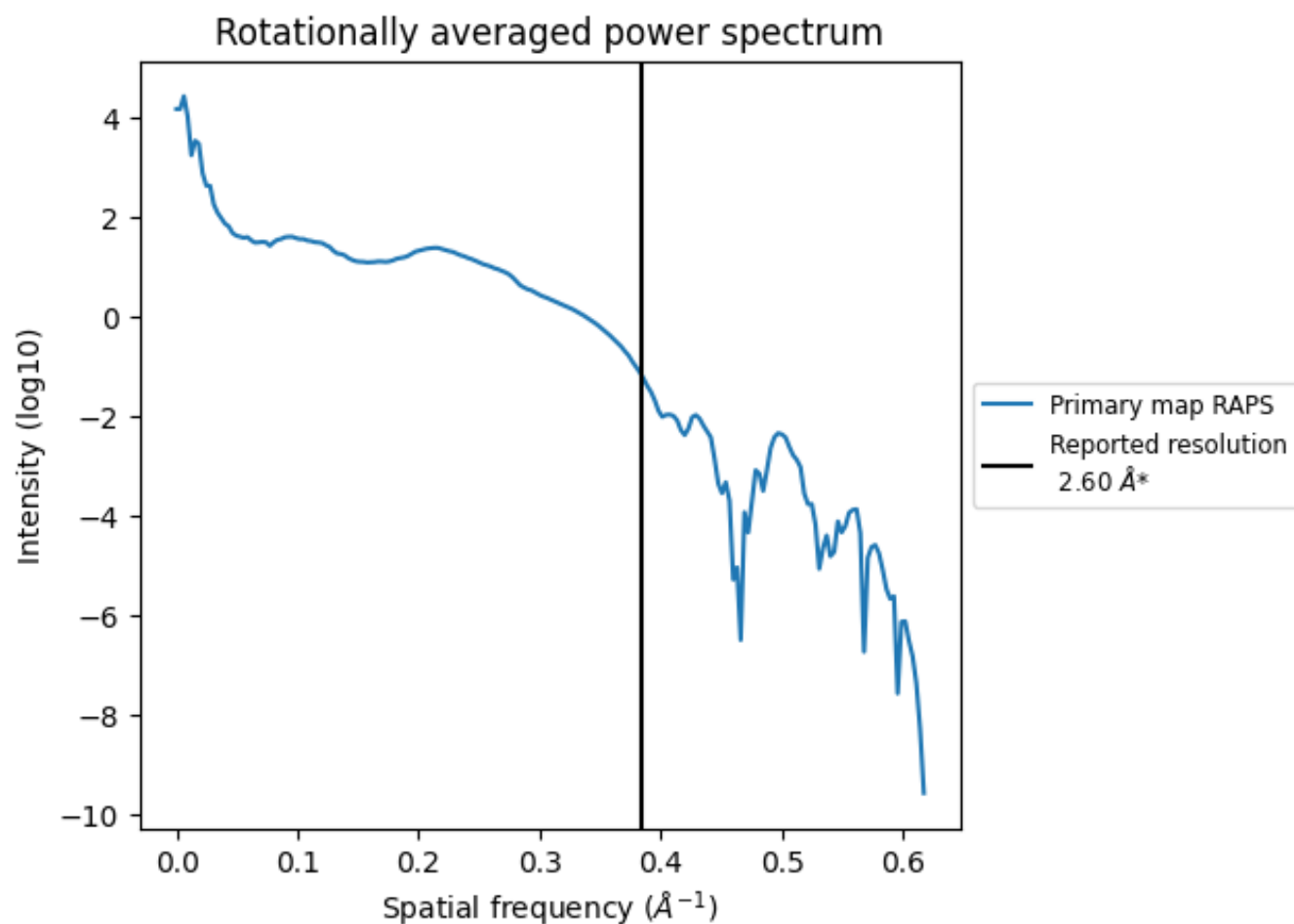
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm³; this corresponds to an approximate mass of 250 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 ⓘ

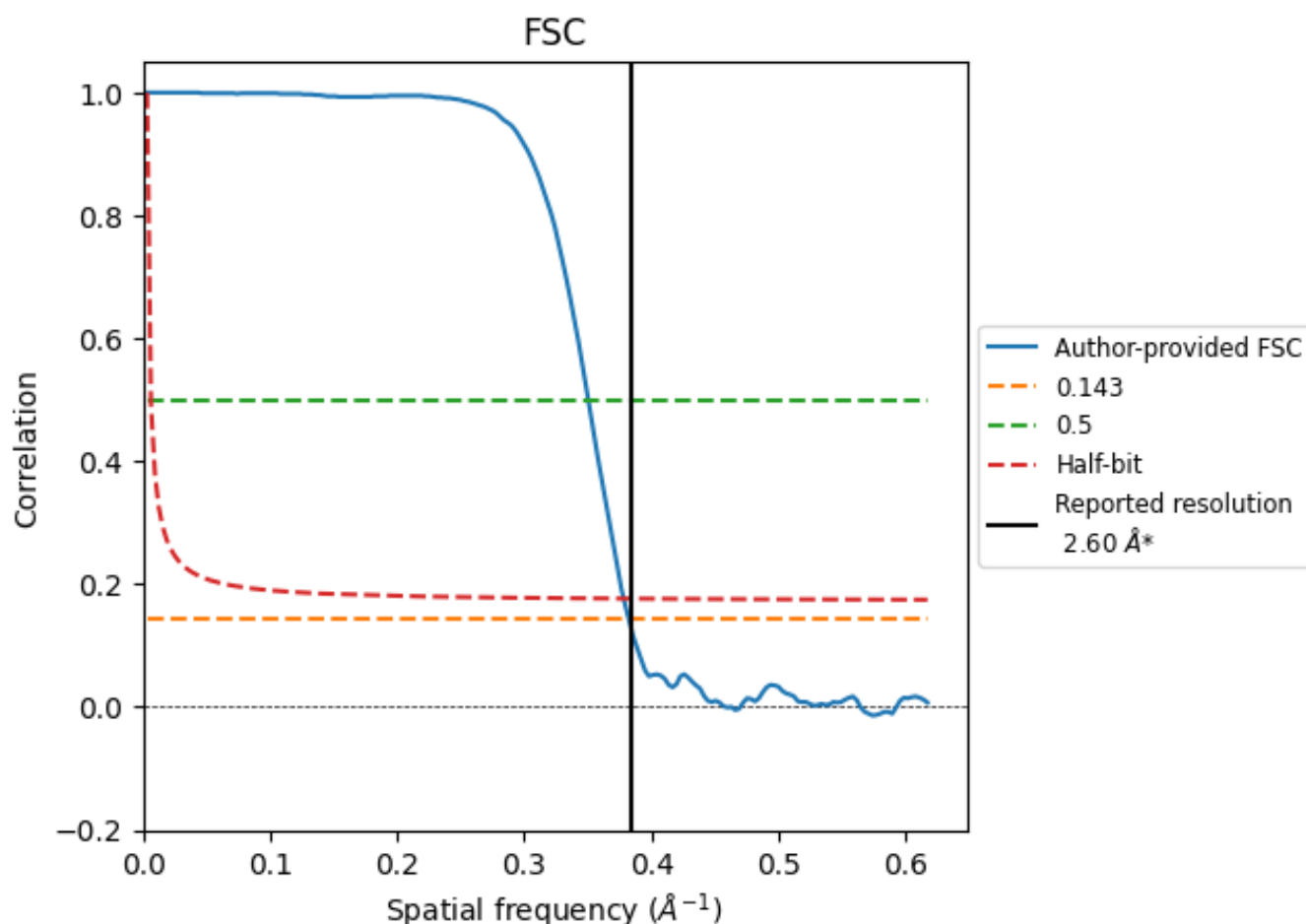


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

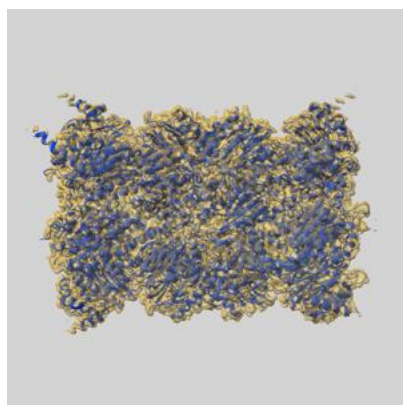
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	2.85	2.64
Unmasked-calculated*	-	-	-

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

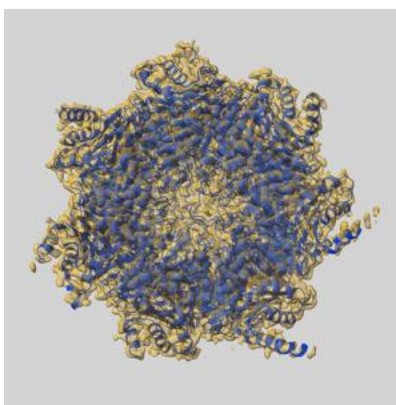
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4877 and PDB model 6RGQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

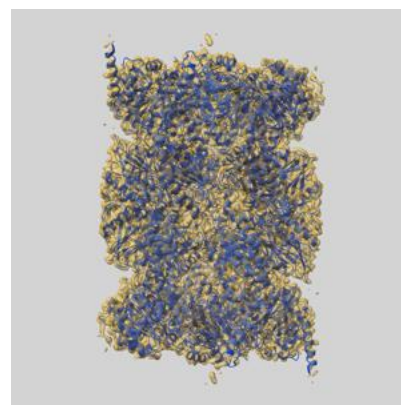
9.1 Map-model overlay [i](#)



X



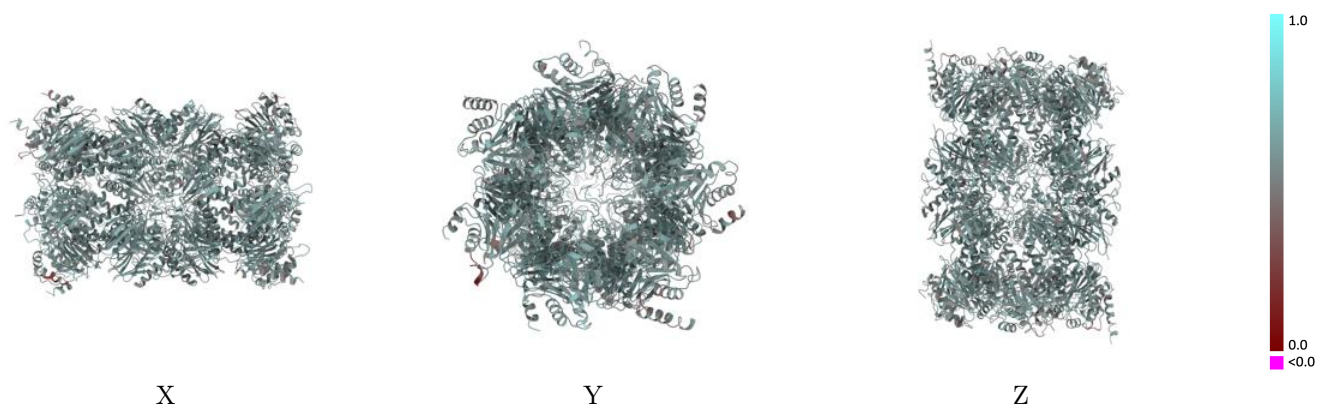
Y



Z

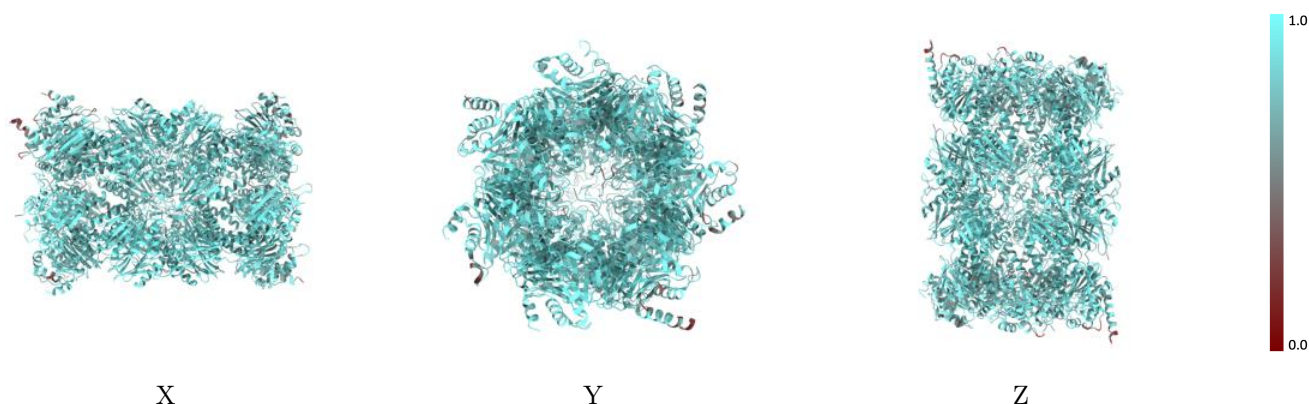
The images above show the 3D surface view of the map at the recommended contour level 2.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



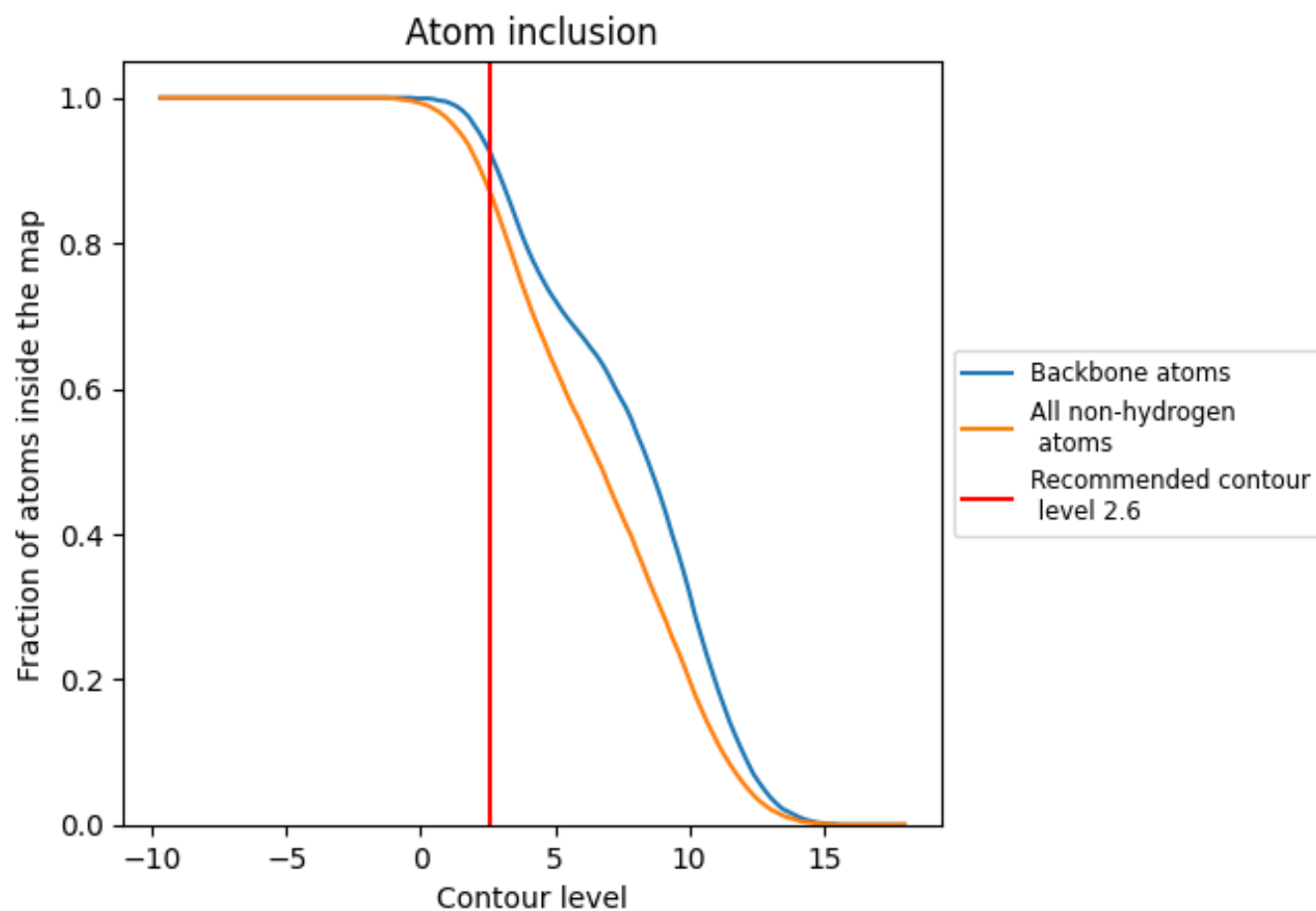
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.5630
A	 0.8490	 0.5530
B	 0.8950	 0.5720
C	 0.8250	 0.5520
D	 0.8090	 0.5460
E	 0.8080	 0.5540
F	 0.8660	 0.5590
G	 0.8650	 0.5600
H	 0.8990	 0.5670
I	 0.8850	 0.5680
J	 0.8960	 0.5740
K	 0.8990	 0.5730
L	 0.9030	 0.5690
M	 0.8840	 0.5710
N	 0.9090	 0.5760
O	 0.8480	 0.5530
P	 0.8940	 0.5730
Q	 0.8240	 0.5500
R	 0.8100	 0.5470
S	 0.8080	 0.5550
T	 0.8660	 0.5580
U	 0.8650	 0.5590
V	 0.8990	 0.5670
W	 0.8850	 0.5690
X	 0.8960	 0.5750
Y	 0.8980	 0.5710
Z	 0.9020	 0.5690
a	 0.8840	 0.5690
b	 0.9090	 0.5750

