



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:39 AM UTC

PDB ID : 7NAP / pdb_00007nap
EMDB ID : EMD-24277
Title : Human PA28-20S-PA28 proteasome complex
Authors : Zhao, J.; Makhija, S.; Huang, B.; Cheng, Y.
Deposited on : 2021-06-22
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

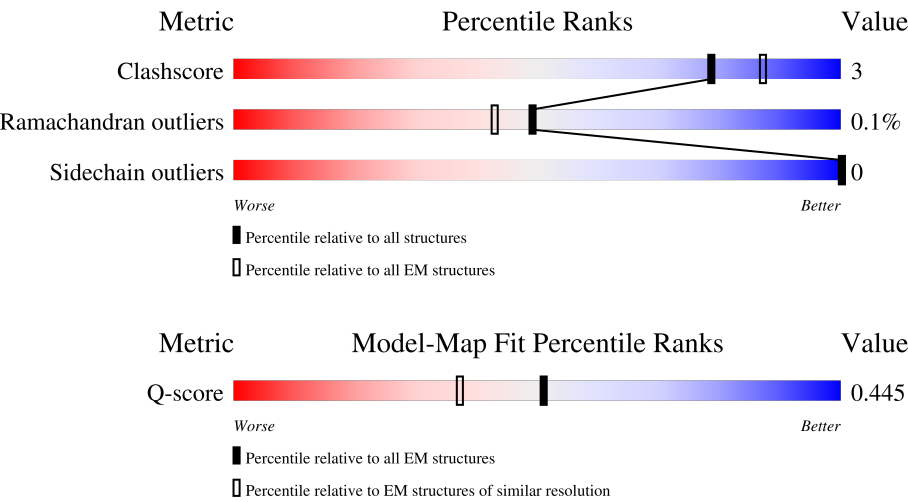
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	234	90% 8% .
1	O	234	89% 9% .
2	B	261	91% . 5%
2	P	261	92% . 5%

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Mol	Chain	Length	Quality of chain
3	C	248	
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	263	
11	Y	263	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	239	
14	b	239	
15	d	239	

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Mol	Chain	Length	Quality of chain
15	f	239	 82%6%12%
15	h	239	 84%7%10%
15	i	239	 85%6%9%
15	k	239	 86%5%9%
15	m	239	 82%6%12%
15	o	239	 85%6%10%
15	p	239	 85%6%9%
16	c	249	 80%5%15%
16	e	249	 82%•15%
16	g	249	 82%•15%
16	j	249	 81%•15%
16	l	249	 82%•15%
16	n	249	 82%•15%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 69762 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-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	229	Total	C	N	O	S	0	0
			1696	1101	294	295	6		
1	A	229	Total	C	N	O	S	0	0
			1696	1101	294	295	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	249	Total	C	N	O	S	0	0
			1793	1146	318	319	10		
2	B	249	Total	C	N	O	S	0	0
			1793	1146	318	319	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	235	Total	C	N	O	S	0	0
			1703	1082	314	302	5		
3	C	235	Total	C	N	O	S	0	0
			1703	1082	314	302	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	241	Total	C	N	O	S	0	0
			1751	1116	301	322	12		
4	D	241	Total	C	N	O	S	0	0
			1751	1116	301	322	12		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	239	Total	C	N	O	S	0	0
			1810	1144	331	324	11		
5	E	239	Total	C	N	O	S	0	0
			1810	1144	331	324	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	240	Total	C	N	O	S	0	0
			1785	1145	313	316	11		
6	F	240	Total	C	N	O	S	0	0
			1785	1145	313	316	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	239	Total	C	N	O	S	0	0
			1769	1133	305	319	12		
7	G	239	Total	C	N	O	S	0	0
			1769	1133	305	319	12		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	222	Total	C	N	O	S	0	0
			1609	1023	276	299	11		
8	H	222	Total	C	N	O	S	0	0
			1609	1023	276	299	11		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	204	Total	C	N	O	S	0	0
			1564	1003	264	278	19		
9	I	204	Total	C	N	O	S	0	0
			1564	1003	264	278	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	197	Total	C	N	O	S	0	0
			1544	998	265	272	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	197	Total	C	N	O	S	0	0
			1544	998	265	272	9		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	200	Total	C	N	O	S	0	0
			1525	968	273	275	9		
11	K	200	Total	C	N	O	S	0	0
			1525	968	273	275	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	213	Total	C	N	O	S	0	0
			1599	1022	279	288	10		
12	L	213	Total	C	N	O	S	0	0
			1599	1022	279	288	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	215	Total	C	N	O	S	0	0
			1643	1043	289	299	12		
13	M	215	Total	C	N	O	S	0	0
			1643	1043	289	299	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	202	Total	C	N	O	S	0	0
			1491	939	258	282	12		
14	N	202	Total	C	N	O	S	0	0
			1491	939	258	282	12		

- Molecule 15 is a protein called Proteasome activator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	217	Total	C	N	O	S	0	0
			1686	1094	284	304	4		
15	m	211	Total	C	N	O	S	0	0
			1648	1069	279	297	3		

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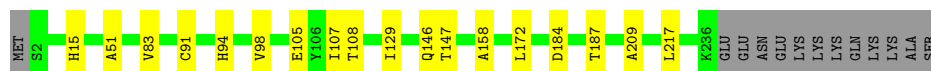
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Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	216	Total	C	N	O	S	0	0
			1677	1087	285	301	4		
15	p	217	Total	C	N	O	S	0	0
			1695	1099	287	305	4		
15	d	217	Total	C	N	O	S	0	0
			1686	1094	284	304	4		
15	f	211	Total	C	N	O	S	0	0
			1648	1069	279	297	3		
15	h	216	Total	C	N	O	S	0	0
			1677	1087	285	301	4		
15	i	217	Total	C	N	O	S	0	0
			1695	1099	287	305	4		

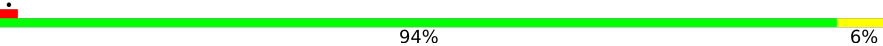
- Molecule 16 is a protein called Proteasome activator complex subunit 1.

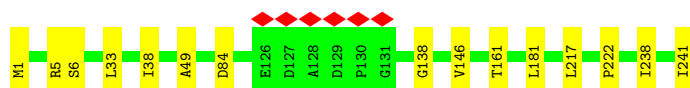
Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	212	Total	C	N	O	S	0	0
			1626	1049	282	291	4		
16	l	211	Total	C	N	O	S	0	0
			1641	1059	282	295	5		
16	n	211	Total	C	N	O	S	0	0
			1626	1050	281	289	6		
16	c	212	Total	C	N	O	S	0	0
			1626	1049	282	291	4		
16	e	211	Total	C	N	O	S	0	0
			1641	1059	282	295	5		
16	g	211	Total	C	N	O	S	0	0
			1626	1050	281	289	6		

Chain C:  88% 7% 5%

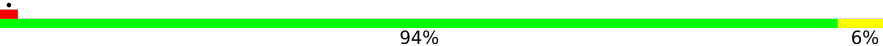


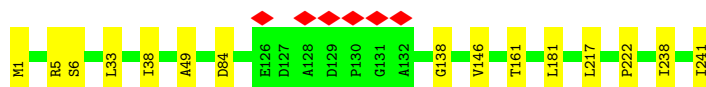
- Molecule 4: Proteasome subunit alpha type-5

Chain R:  94% 6%



- Molecule 4: Proteasome subunit alpha type-5

Chain D:  94% 6%



- Molecule 5: Proteasome subunit alpha type-1

Chain S:  86% 5% 9%



- Molecule 5: Proteasome subunit alpha type-1

Chain E:  86% 5% 9%



- Molecule 6: Proteasome subunit alpha type-3

Chain T:  90% 6%



- Molecule 6: Proteasome subunit alpha type-3

Chain F:  89% 5% 6%



- Molecule 7: Proteasome subunit alpha type-6

Chain U:  91% 6%



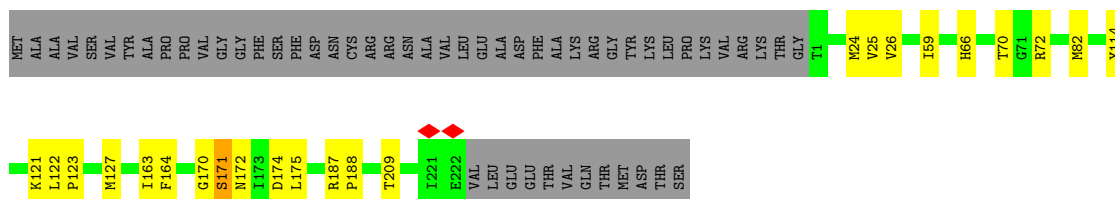
- Molecule 7: Proteasome subunit alpha type-6

Chain G:  91% 6%



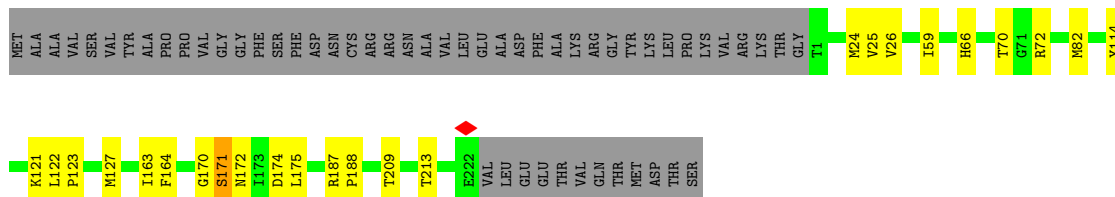
- Molecule 8: Proteasome subunit beta type-7

Chain V:  72% 8% 20%



- Molecule 8: Proteasome subunit beta type-7

Chain H:  71% 8% 20%



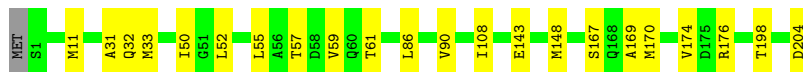
- Molecule 9: Proteasome subunit beta type-3

Chain W:  90% 10%



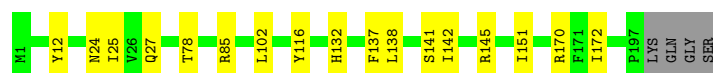
- Molecule 9: Proteasome subunit beta type-3

Chain I:  89% 11%



- Molecule 10: Proteasome subunit beta type-2

Chain X:  90% 8%



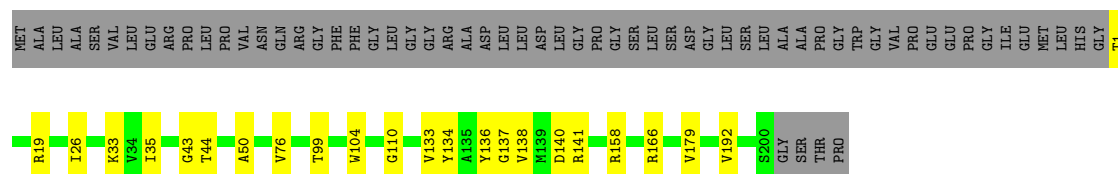
- Molecule 10: Proteasome subunit beta type-2

Chain J:  89% 9%



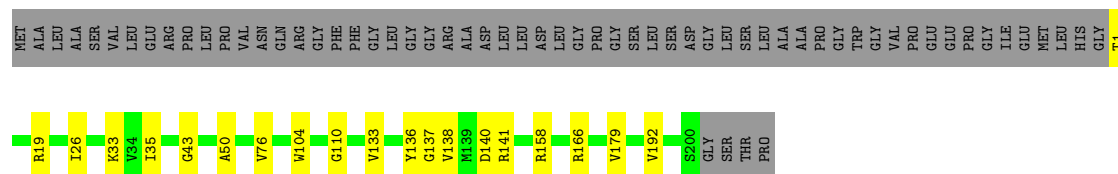
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  67% 9% 24%



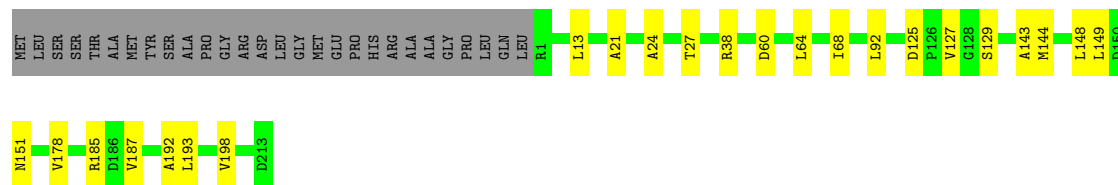
- Molecule 11: Proteasome subunit beta type-5

Chain K:  68% 8% 24%



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  79% 10% 12%



- Molecule 12: Proteasome subunit beta type-1

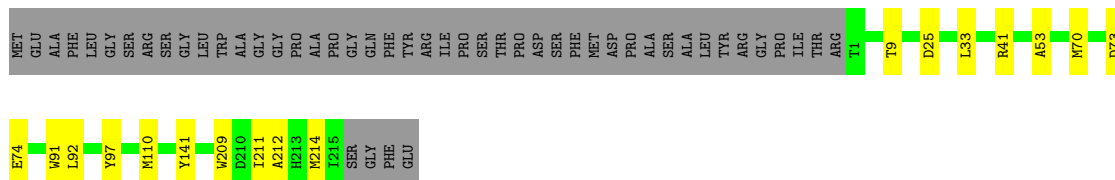
Chain L:  80% 9% 12%





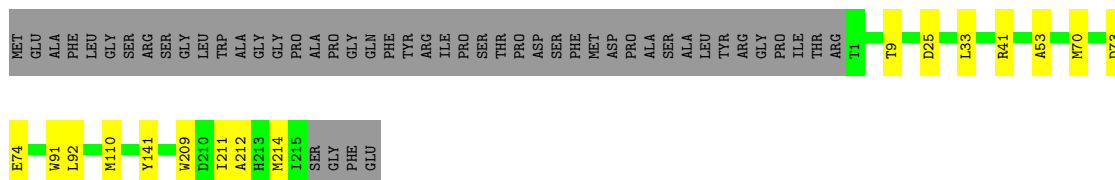
- Molecule 13: Proteasome subunit beta type-4

Chain a: 75% 6% 19%



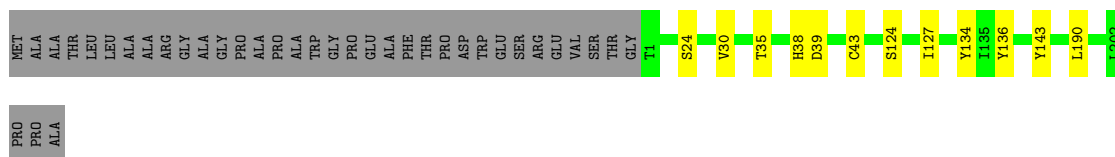
- Molecule 13: Proteasome subunit beta type-4

Chain M: 75% 6% 19%



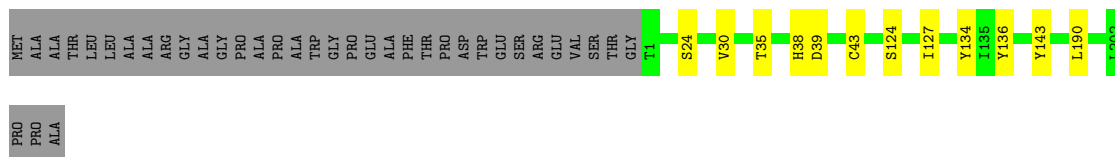
- Molecule 14: Proteasome subunit beta type-6

Chain b: 79% 5% 15%



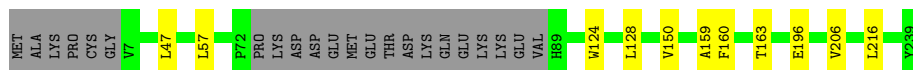
- Molecule 14: Proteasome subunit beta type-6

Chain N: 79% 5% 15%



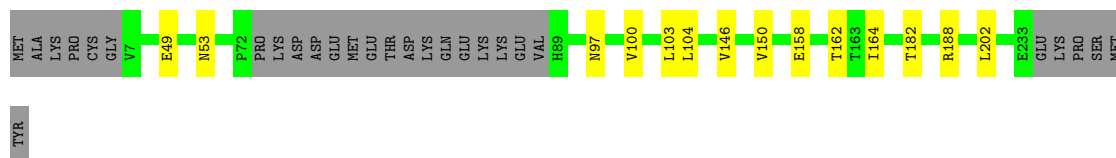
- Molecule 15: Proteasome activator complex subunit 2

Chain k: 86% 5% 9%



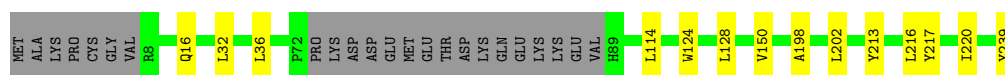
- Molecule 15: Proteasome activator complex subunit 2

Chain m:  82% 6% 12%



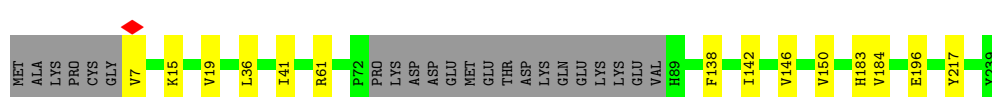
- Molecule 15: Proteasome activator complex subunit 2

Chain o:  85% 6% 10%



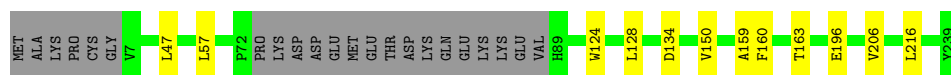
- Molecule 15: Proteasome activator complex subunit 2

Chain p:  85% 6% 9%



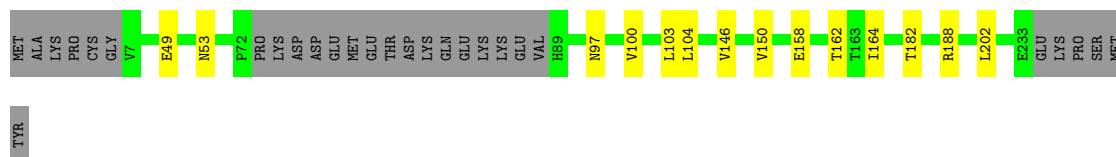
- Molecule 15: Proteasome activator complex subunit 2

Chain d:  86% 5% 9%



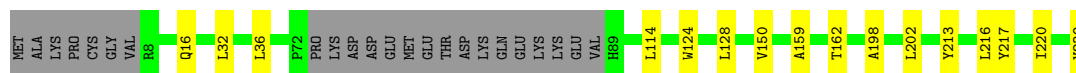
- Molecule 15: Proteasome activator complex subunit 2

Chain f:  82% 6% 12%



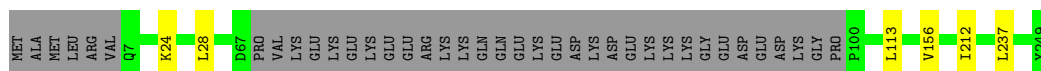
- Molecule 15: Proteasome activator complex subunit 2

Chain h:  84% 7% 10%

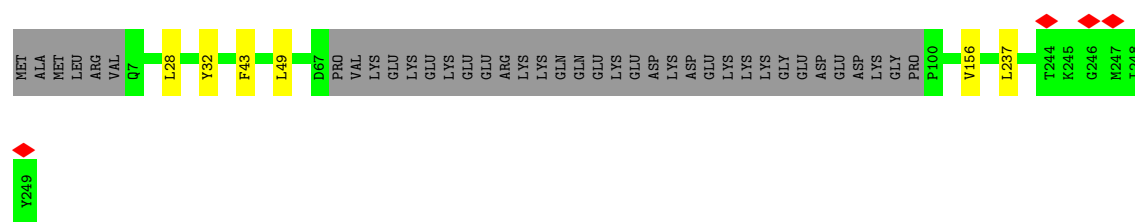


- Molecule 15: Proteasome activator complex subunit 2

Chain i:  85% 6% 9%



Chain g: 82% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22946	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	24.562	Depositor
Minimum map value	-12.511	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	466.7904, 466.7904, 466.7904	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	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	0.25	0/1735	0.43	0/2362
1	O	0.25	0/1735	0.43	0/2362
2	B	0.22	0/1821	0.39	0/2477
2	P	0.22	0/1821	0.39	0/2477
3	C	0.24	0/1729	0.42	0/2356
3	Q	0.24	0/1729	0.42	0/2356
4	D	0.25	0/1780	0.42	0/2417
4	R	0.25	0/1780	0.42	0/2417
5	E	0.25	0/1845	0.43	0/2504
5	S	0.25	0/1845	0.44	0/2504
6	F	0.25	0/1820	0.41	0/2464
6	T	0.25	0/1820	0.40	0/2464
7	G	0.24	0/1802	0.43	0/2449
7	U	0.24	0/1802	0.43	0/2449
8	H	0.26	0/1636	0.41	0/2223
8	V	0.26	0/1636	0.41	0/2223
9	I	0.27	0/1593	0.45	0/2149
9	W	0.27	0/1593	0.45	0/2149
10	J	0.26	0/1577	0.43	0/2138
10	X	0.26	0/1577	0.43	0/2138
11	K	0.25	0/1556	0.39	0/2104
11	Y	0.25	0/1556	0.39	0/2104
12	L	0.26	0/1629	0.40	0/2201
12	Z	0.26	0/1629	0.40	0/2201
13	M	0.26	0/1676	0.44	0/2272
13	a	0.26	0/1676	0.44	0/2272
14	N	0.27	0/1517	0.39	0/2056
14	b	0.27	0/1517	0.39	0/2056
15	d	0.23	0/1720	0.43	0/2338
15	f	0.22	0/1680	0.40	0/2281
15	h	0.22	0/1710	0.42	0/2322
15	i	0.23	0/1729	0.41	0/2349
15	k	0.23	0/1720	0.43	0/2338
15	m	0.23	0/1680	0.40	0/2281

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	o	0.22	0/1710	0.42	0/2322
15	p	0.23	0/1729	0.41	0/2349
16	c	0.23	0/1657	0.41	0/2250
16	e	0.23	0/1672	0.42	0/2265
16	g	0.23	0/1657	0.41	0/2247
16	j	0.23	0/1657	0.41	0/2250
16	l	0.23	0/1672	0.43	0/2265
16	n	0.23	0/1657	0.41	0/2247
All	All	0.24	0/71082	0.42	0/96448

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
4	D	0	1
4	R	0	1
8	H	0	1
8	V	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	5	ARG	Peptide
8	H	187	ARG	Peptide
4	R	5	ARG	Peptide
8	V	187	ARG	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	1696	0	1647	11	0
1	O	1696	0	1647	12	0
2	B	1793	0	1704	8	0
2	P	1793	0	1704	7	0
3	C	1703	0	1616	11	0
3	Q	1703	0	1616	11	0
4	D	1751	0	1707	10	0
4	R	1751	0	1707	10	0
5	E	1810	0	1759	7	0
5	S	1810	0	1759	8	0
6	F	1785	0	1717	8	0
6	T	1785	0	1717	6	0
7	G	1769	0	1730	10	0
7	U	1769	0	1730	9	0
8	H	1609	0	1609	16	0
8	V	1609	0	1609	15	0
9	I	1564	0	1587	22	0
9	W	1564	0	1587	19	0
10	J	1544	0	1537	27	0
10	X	1544	0	1537	24	0
11	K	1525	0	1490	22	0
11	Y	1525	0	1490	25	0
12	L	1599	0	1582	18	0
12	Z	1599	0	1582	20	0
13	M	1643	0	1611	14	0
13	a	1643	0	1611	15	0
14	N	1491	0	1458	12	0
14	b	1491	0	1458	12	0
15	d	1686	0	1677	8	0
15	f	1648	0	1657	8	0
15	h	1677	0	1679	11	0
15	i	1695	0	1689	8	0
15	k	1686	0	1677	7	0
15	m	1648	0	1657	8	0
15	o	1677	0	1679	10	0
15	p	1695	0	1689	8	0
16	c	1626	0	1608	8	0
16	e	1641	0	1643	3	0
16	g	1626	0	1623	3	0
16	j	1626	0	1608	7	0
16	l	1641	0	1643	3	0
16	n	1626	0	1623	4	0
All	All	69762	0	68660	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (380) 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)
14:b:30:VAL:CG1	13:M:212:ALA:HA	1.96	0.95
13:a:212:ALA:HA	14:N:30:VAL:CG1	1.97	0.95
13:a:212:ALA:HA	14:N:30:VAL:HG11	1.59	0.83
14:b:30:VAL:HG11	13:M:212:ALA:HA	1.58	0.83
12:Z:185:ARG:NH1	8:H:26:VAL:O	2.12	0.82
8:V:26:VAL:O	12:L:185:ARG:NH1	2.13	0.81
12:L:148:LEU:HD23	12:L:178:VAL:HG12	1.68	0.75
12:Z:148:LEU:HD23	12:Z:178:VAL:HG12	1.68	0.74
8:V:123:PRO:HB3	13:M:214:MET:SD	2.31	0.70
13:a:9:THR:O	13:a:41:ARG:NH2	2.24	0.70
13:M:9:THR:O	13:M:41:ARG:NH2	2.24	0.70
13:a:214:MET:SD	8:H:123:PRO:HB3	2.32	0.69
10:X:170:ARG:NE	11:K:136:TYR:CD1	2.63	0.67
6:T:227:VAL:O	6:T:232:ARG:NH1	2.28	0.67
9:W:143:GLU:HG3	12:L:144:MET:HG3	1.75	0.67
9:W:11:MET:HE1	9:W:169:ALA:HB3	1.77	0.67
12:Z:187:VAL:HG21	8:H:24:MET:HE3	1.76	0.67
6:F:227:VAL:O	6:F:232:ARG:NH1	2.28	0.67
8:V:24:MET:HE3	12:L:187:VAL:HG21	1.76	0.66
11:Y:136:TYR:CD1	10:J:170:ARG:NE	2.63	0.66
12:Z:144:MET:HG3	9:I:143:GLU:HG3	1.75	0.66
9:I:57:THR:O	10:J:85:ARG:NH2	2.29	0.66
9:W:57:THR:O	10:X:85:ARG:NH2	2.29	0.66
9:I:11:MET:HE1	9:I:169:ALA:HB3	1.77	0.66
8:H:213:THR:HG1	9:I:198:THR:HG1	1.30	0.65
9:W:32:GLN:NE2	9:W:33:MET:O	2.30	0.65
16:l:156:VAL:HG21	16:l:237:LEU:HD21	1.79	0.65
9:I:32:GLN:NE2	9:I:33:MET:O	2.30	0.64
14:b:35:THR:OG1	14:b:43:CYS:SG	2.56	0.64
16:e:156:VAL:HG21	16:e:237:LEU:HD21	1.78	0.64
14:N:35:THR:OG1	14:N:43:CYS:SG	2.56	0.64
5:E:88:MET:HE3	5:E:112:ILE:HD11	1.81	0.62
5:S:88:MET:HE3	5:S:112:ILE:HD11	1.81	0.62
11:Y:138:VAL:HG23	10:J:141:SER:OG	2.00	0.62
9:W:32:GLN:NE2	11:K:166:ARG:HH11	1.98	0.62
3:Q:146:GLN:NE2	3:Q:147:THR:O	2.32	0.62
3:C:146:GLN:NE2	3:C:147:THR:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:166:ARG:HH11	9:I:32:GLN:NE2	1.97	0.61
10:X:141:SER:OG	11:K:138:VAL:HG23	2.01	0.61
10:X:172:ILE:HG23	10:J:25:ILE:C	2.26	0.60
11:Y:76:VAL:HG21	11:Y:110:GLY:HA3	1.83	0.60
10:X:25:ILE:C	10:J:172:ILE:HG23	2.26	0.60
14:b:30:VAL:HG21	13:M:211:ILE:HG13	1.83	0.60
2:P:90:LEU:HD11	2:P:114:LEU:HD22	1.82	0.60
2:B:90:LEU:HD11	2:B:114:LEU:HD22	1.82	0.60
1:O:81:ASP:OD1	7:U:123:GLN:NE2	2.34	0.60
13:a:211:ILE:HG13	14:N:30:VAL:HG21	1.84	0.60
1:A:81:ASP:OD1	7:G:123:GLN:NE2	2.34	0.59
11:K:76:VAL:HG21	11:K:110:GLY:HA3	1.83	0.59
15:k:159:ALA:O	15:k:163:THR:HG23	2.03	0.59
12:L:27:THR:OG1	12:L:192:ALA:HB3	2.03	0.59
12:Z:27:THR:OG1	12:Z:192:ALA:HB3	2.03	0.59
15:d:159:ALA:O	15:d:163:THR:HG23	2.03	0.58
9:W:204:ASP:HB3	11:K:192:VAL:HG11	1.86	0.57
9:W:52:LEU:HB3	9:W:59:VAL:HG22	1.86	0.57
12:Z:24:ALA:HB1	12:Z:193:LEU:HD11	1.86	0.57
15:h:16:GLN:HG2	15:i:41:ILE:HG21	1.87	0.57
11:Y:192:VAL:HG11	9:I:204:ASP:HB3	1.85	0.57
12:L:24:ALA:HB1	12:L:193:LEU:HD11	1.86	0.57
1:O:118:GLN:O	1:O:121:THR:HG22	2.05	0.57
7:G:121:ILE:O	7:G:124:VAL:HG22	2.05	0.57
9:I:52:LEU:HB3	9:I:59:VAL:HG22	1.86	0.57
7:U:121:ILE:O	7:U:124:VAL:HG22	2.05	0.56
14:N:124:SER:OG	14:N:143:TYR:OH	2.09	0.56
15:o:16:GLN:HG2	15:p:41:ILE:HG21	1.87	0.56
2:P:76:VAL:HG11	2:P:83:ALA:CB	2.35	0.56
9:W:143:GLU:OE2	12:L:144:MET:SD	2.63	0.56
9:W:176:ARG:NH2	11:K:26:ILE:O	2.39	0.56
12:Z:144:MET:SD	9:I:143:GLU:OE2	2.63	0.56
1:A:118:GLN:O	1:A:121:THR:HG22	2.05	0.56
2:B:76:VAL:HG11	2:B:83:ALA:CB	2.35	0.56
7:G:125:TYR:HA	7:G:131:MET:HE3	1.87	0.56
11:Y:26:ILE:O	9:I:176:ARG:NH2	2.39	0.55
14:b:30:VAL:HG13	13:M:212:ALA:HA	1.85	0.55
15:k:47:LEU:HD21	15:k:206:VAL:HG13	1.88	0.55
15:d:47:LEU:HD21	15:d:206:VAL:HG13	1.88	0.55
15:d:57:LEU:HD23	15:d:196:GLU:HG2	1.88	0.55
10:X:145:ARG:NH1	11:K:158:ARG:NH1	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:133:VAL:HG11	10:J:137:PHE:HB3	1.89	0.55
16:g:28:LEU:HD12	16:g:32:TYR:HB3	1.87	0.55
3:Q:158:ALA:HB3	3:Q:172:LEU:HD21	1.88	0.55
7:U:125:TYR:HA	7:U:131:MET:HE3	1.87	0.55
8:V:66:HIS:O	8:V:70:THR:HG22	2.07	0.55
10:X:137:PHE:HB3	11:K:133:VAL:HG11	1.89	0.55
15:k:57:LEU:HD23	15:k:196:GLU:HG2	1.88	0.55
8:H:66:HIS:O	8:H:70:THR:HG22	2.07	0.55
5:S:47:VAL:HG12	5:S:212:ILE:HG12	1.89	0.55
13:M:25:ASP:OD1	13:M:41:ARG:NH2	2.39	0.55
11:Y:158:ARG:NH1	10:J:145:ARG:NH1	2.55	0.54
13:a:25:ASP:OD1	13:a:41:ARG:NH2	2.39	0.54
16:n:28:LEU:HD12	16:n:32:TYR:HB3	1.87	0.54
3:C:158:ALA:HB3	3:C:172:LEU:HD21	1.88	0.54
11:Y:44:THR:O	11:Y:99:THR:OG1	2.09	0.54
5:E:47:VAL:HG12	5:E:212:ILE:HG12	1.89	0.54
6:F:120:HIS:O	6:F:123:THR:HG22	2.08	0.54
12:Z:125:ASP:OD1	12:Z:129:SER:N	2.41	0.54
14:b:127:ILE:HD11	14:b:136:TYR:CD1	2.43	0.54
4:R:161:THR:HG22	5:S:78:THR:OG1	2.08	0.53
14:b:124:SER:OG	14:b:143:TYR:OH	2.09	0.53
14:N:127:ILE:HD11	14:N:136:TYR:CD1	2.43	0.53
9:I:50:ILE:HG13	9:I:108:ILE:HD13	1.89	0.53
4:D:161:THR:HG22	5:E:78:THR:OG1	2.08	0.53
9:W:50:ILE:HG13	9:W:108:ILE:HD13	1.89	0.53
13:M:41:ARG:NH1	13:M:53:ALA:O	2.41	0.53
8:V:114:TYR:CZ	8:V:127:MET:HE1	2.44	0.53
13:a:212:ALA:HA	14:N:30:VAL:HG13	1.86	0.53
8:H:114:TYR:CZ	8:H:127:MET:HE1	2.44	0.53
6:T:120:HIS:O	6:T:123:THR:HG22	2.08	0.53
2:B:76:VAL:HG11	2:B:83:ALA:HB1	1.91	0.53
12:L:125:ASP:OD1	12:L:129:SER:N	2.41	0.53
13:a:41:ARG:NH1	13:a:53:ALA:O	2.41	0.53
12:Z:38:ARG:NH2	8:H:164:PHE:O	2.42	0.53
5:S:109:VAL:HA	5:S:112:ILE:HD12	1.91	0.52
8:V:164:PHE:O	12:L:38:ARG:NH2	2.42	0.52
10:X:172:ILE:HD13	10:J:24:ASN:O	2.10	0.52
16:j:231:LEU:HD11	15:p:7:VAL:HG12	1.91	0.52
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.91	0.52
7:G:72:ILE:HG21	7:G:114:LEU:HD21	1.92	0.52
16:c:231:LEU:HD11	15:i:7:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:150:VAL:HG12	15:o:216:LEU:CD2	2.40	0.52
2:P:76:VAL:HG11	2:P:83:ALA:HB1	1.91	0.52
11:Y:137:GLY:C	10:J:142:ILE:HD11	2.35	0.52
9:W:61:THR:OG1	10:X:85:ARG:NH2	2.40	0.52
10:X:142:ILE:HD11	11:K:137:GLY:C	2.35	0.52
15:m:103:LEU:HB3	15:m:202:LEU:HD23	1.92	0.52
9:I:86:LEU:O	9:I:90:VAL:HG23	2.09	0.52
15:h:150:VAL:HG12	15:h:216:LEU:CD2	2.40	0.52
7:G:190:THR:O	7:G:194:THR:OG1	2.21	0.52
9:W:11:MET:HE2	9:W:170:MET:HG2	1.92	0.51
5:E:109:VAL:HA	5:E:112:ILE:HD12	1.91	0.51
7:G:153:LYS:HE3	7:G:166:THR:HG21	1.91	0.51
15:f:103:LEU:HB3	15:f:202:LEU:HD23	1.92	0.51
2:B:133:SER:OG	2:B:150:SER:O	2.28	0.51
9:I:11:MET:HE2	9:I:170:MET:HG2	1.92	0.51
11:K:50:ALA:HB2	12:L:127:VAL:HG13	1.93	0.51
7:U:153:LYS:HE3	7:U:166:THR:HG21	1.91	0.51
9:W:86:LEU:O	9:W:90:VAL:HG23	2.09	0.51
11:Y:50:ALA:HB2	12:Z:127:VAL:HG13	1.93	0.51
15:m:104:LEU:HG	15:m:202:LEU:HD21	1.92	0.51
15:m:146:VAL:O	15:m:150:VAL:HG23	2.11	0.51
10:X:24:ASN:O	10:J:172:ILE:HD13	2.10	0.51
3:C:209:ALA:HB1	3:C:217:LEU:HD11	1.92	0.51
12:Z:143:ALA:HB3	9:I:143:GLU:HG2	1.92	0.50
15:f:104:LEU:HG	15:f:202:LEU:HD21	1.92	0.50
15:f:146:VAL:O	15:f:150:VAL:HG23	2.11	0.50
8:H:70:THR:HG23	8:H:72:ARG:H	1.76	0.50
11:Y:166:ARG:HH11	9:I:32:GLN:HE21	1.57	0.50
7:U:190:THR:O	7:U:194:THR:OG1	2.21	0.50
11:Y:19:ARG:O	11:Y:33:LYS:NZ	2.45	0.50
11:K:19:ARG:O	11:K:33:LYS:NZ	2.45	0.50
3:Q:209:ALA:HB1	3:Q:217:LEU:HD11	1.92	0.50
8:V:70:THR:HG23	8:V:72:ARG:H	1.76	0.50
11:Y:141:ARG:HG3	10:J:142:ILE:HD12	1.93	0.50
9:I:61:THR:OG1	10:J:85:ARG:NH2	2.40	0.49
12:L:13:LEU:HD11	12:L:149:LEU:HD11	1.94	0.49
16:c:113:LEU:HD23	16:c:212:ILE:HD11	1.94	0.49
9:W:32:GLN:HE21	11:K:166:ARG:HH11	1.58	0.49
15:m:158:GLU:O	15:m:162:THR:HG23	2.12	0.49
15:o:150:VAL:HG12	15:o:216:LEU:HD23	1.94	0.49
8:V:114:TYR:CE2	8:V:127:MET:HE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:143:GLU:HG2	12:L:143:ALA:HB3	1.93	0.49
12:Z:13:LEU:HD11	12:Z:149:LEU:HD11	1.94	0.49
13:a:33:LEU:HD13	14:N:134:TYR:CE1	2.48	0.49
8:H:114:TYR:CE2	8:H:127:MET:HE1	2.48	0.49
15:h:150:VAL:HG12	15:h:216:LEU:HD23	1.94	0.49
2:P:133:SER:OG	2:P:150:SER:O	2.28	0.49
4:R:238:ILE:HA	4:R:241:ILE:HD12	1.94	0.49
15:f:158:GLU:O	15:f:162:THR:HG23	2.12	0.49
10:X:142:ILE:HD12	11:K:141:ARG:HG3	1.94	0.49
4:D:238:ILE:HA	4:D:241:ILE:HD12	1.94	0.48
16:j:113:LEU:HD23	16:j:212:ILE:HD11	1.94	0.48
14:N:38:HIS:ND1	14:N:39:ASP:OD1	2.44	0.48
11:Y:133:VAL:CG1	10:J:137:PHE:HB3	2.44	0.48
13:M:92:LEU:HD21	13:M:110:MET:HE2	1.95	0.48
12:Z:60:ASP:OD1	13:a:97:TYR:OH	2.22	0.48
15:o:198:ALA:O	15:o:202:LEU:HD13	2.14	0.48
16:g:43:PHE:CZ	16:g:49:LEU:HD13	2.49	0.48
1:O:85:LEU:HD13	1:O:133:LEU:HD11	1.96	0.48
14:b:134:TYR:CE1	13:M:33:LEU:HD13	2.48	0.48
11:Y:104:TRP:CD1	11:Y:179:VAL:HG12	2.48	0.48
10:X:172:ILE:HG12	10:J:25:ILE:HA	1.96	0.48
16:n:43:PHE:CZ	16:n:49:LEU:HD13	2.49	0.48
4:D:38:ILE:HD11	4:D:181:LEU:HD21	1.95	0.48
1:O:173:LEU:O	1:O:177:TYR:N	2.48	0.47
10:X:137:PHE:HB3	11:K:133:VAL:CG1	2.44	0.47
16:l:24:LYS:O	16:l:28:LEU:HD13	2.13	0.47
8:H:59:ILE:HD12	8:H:82:MET:HB3	1.96	0.47
11:K:104:TRP:CD1	11:K:179:VAL:HG12	2.48	0.47
12:L:68:ILE:HD11	12:L:92:LEU:HD13	1.95	0.47
16:e:24:LYS:O	16:e:28:LEU:HD13	2.13	0.47
2:P:16:GLY:O	15:o:239:TYR:OH	2.32	0.47
15:k:150:VAL:HG12	15:k:216:LEU:CD2	2.44	0.47
6:F:69:VAL:HG23	6:F:73:VAL:HG13	1.96	0.47
8:V:59:ILE:HD12	8:V:82:MET:HB3	1.97	0.47
12:Z:68:ILE:HD11	12:Z:92:LEU:HD13	1.95	0.47
13:a:141:TYR:CE2	14:N:24:SER:HB2	2.49	0.47
14:b:24:SER:HB2	13:M:141:TYR:CE2	2.49	0.47
14:b:38:HIS:ND1	14:b:39:ASP:OD1	2.44	0.47
15:m:182:THR:OG1	15:m:188:ARG:NH2	2.48	0.47
4:D:161:THR:HG21	16:c:247:MET:O	2.14	0.47
15:d:150:VAL:HG12	15:d:216:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:38:ILE:HD11	4:R:181:LEU:HD21	1.95	0.47
13:a:92:LEU:HD21	13:a:110:MET:HE2	1.95	0.47
8:H:209:THR:HG21	9:I:167:SER:OG	2.14	0.47
11:Y:140:ASP:OD2	10:J:170:ARG:NE	2.48	0.47
4:R:161:THR:HG21	16:j:247:MET:O	2.14	0.47
8:V:209:THR:HG21	9:W:167:SER:OG	2.14	0.47
1:A:173:LEU:O	1:A:177:TYR:N	2.48	0.47
15:h:198:ALA:O	15:h:202:LEU:HD13	2.14	0.47
15:f:182:THR:OG1	15:f:188:ARG:NH2	2.48	0.47
13:a:73:ASP:OD1	13:a:74:GLU:N	2.49	0.46
10:J:78:THR:HG22	10:J:116:TYR:OH	2.16	0.46
6:T:69:VAL:HG23	6:T:73:VAL:HG13	1.96	0.46
10:X:170:ARG:NE	11:K:140:ASP:OD2	2.48	0.46
15:d:160:PHE:O	15:d:163:THR:OG1	2.30	0.46
15:i:36:LEU:HD13	15:i:217:TYR:HB2	1.97	0.46
8:V:25:VAL:HG23	12:L:185:ARG:O	2.16	0.46
16:j:181:ARG:O	16:j:185:VAL:HG23	2.16	0.46
1:A:85:LEU:HD13	1:A:133:LEU:HD11	1.96	0.46
9:W:55:LEU:O	9:W:59:VAL:HG23	2.15	0.46
15:o:36:LEU:HD13	15:o:217:TYR:HB2	1.98	0.46
15:p:36:LEU:HD13	15:p:217:TYR:HB2	1.97	0.46
13:M:73:ASP:OD1	13:M:74:GLU:N	2.49	0.46
9:I:55:LEU:O	9:I:59:VAL:HG23	2.15	0.46
15:h:36:LEU:HD13	15:h:217:TYR:HB2	1.98	0.46
10:X:78:THR:HG22	10:X:116:TYR:OH	2.16	0.45
10:X:25:ILE:HA	10:J:172:ILE:HG12	1.96	0.45
16:c:181:ARG:O	16:c:185:VAL:HG23	2.16	0.45
3:Q:94:HIS:O	3:Q:98:VAL:HG22	2.16	0.45
1:A:195:LYS:NZ	1:A:202:MET:SD	2.86	0.45
11:Y:134:TYR:HH	10:J:137:PHE:HD1	1.62	0.45
1:O:195:LYS:NZ	1:O:202:MET:SD	2.86	0.45
12:Z:127:VAL:HG22	12:Z:127:VAL:O	2.17	0.45
5:S:70:ILE:HD13	5:S:108:LEU:HD23	1.99	0.45
3:Q:184:ASP:O	3:Q:187:THR:OG1	2.33	0.45
1:O:134:LEU:HD21	1:O:160:THR:CG2	2.47	0.45
5:E:70:ILE:HD13	5:E:108:LEU:HD23	1.99	0.45
12:L:127:VAL:HG22	12:L:127:VAL:O	2.17	0.45
13:a:209:TRP:HB2	14:N:190:LEU:HD12	1.98	0.45
4:D:146:VAL:HG11	4:D:222:PRO:HA	1.99	0.45
2:P:35:LEU:N	2:P:46:ALA:O	2.49	0.44
8:V:171:SER:OG	8:V:172:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:97:ASN:HB3	15:f:100:VAL:HG22	1.99	0.44
13:a:70:MET:HE1	13:a:91:TRP:CE2	2.52	0.44
15:m:97:ASN:HB3	15:m:100:VAL:HG22	2.00	0.44
15:m:104:LEU:HD22	15:m:164:ILE:HG23	1.98	0.44
13:M:70:MET:HE1	13:M:91:TRP:CE2	2.52	0.44
10:X:141:SER:OG	11:K:138:VAL:CG2	2.66	0.44
12:Z:185:ARG:O	8:H:25:VAL:HG23	2.16	0.44
8:H:174:ASP:O	8:H:175:LEU:HD22	2.17	0.44
1:A:134:LEU:HD21	1:A:160:THR:CG2	2.47	0.44
3:C:94:HIS:O	3:C:98:VAL:HG22	2.16	0.44
15:h:124:TRP:CE2	15:h:128:LEU:HD11	2.52	0.44
4:R:146:VAL:HG11	4:R:222:PRO:HA	1.99	0.44
14:b:190:LEU:HD12	13:M:209:TRP:HB2	1.98	0.44
15:o:124:TRP:CE2	15:o:128:LEU:HD11	2.52	0.44
1:A:67:ILE:HG21	1:A:109:LEU:HD21	1.99	0.44
2:B:35:LEU:N	2:B:46:ALA:O	2.49	0.44
15:f:49:GLU:O	15:f:53:ASN:ND2	2.51	0.44
15:f:104:LEU:HD22	15:f:164:ILE:HG23	1.98	0.44
4:D:1:MET:HE3	16:c:142:ILE:HD11	1.99	0.44
11:K:1:THR:CB	11:K:33:LYS:HZ3	2.31	0.44
11:K:35:ILE:N	11:K:43:GLY:O	2.49	0.44
4:R:1:MET:HE3	16:j:142:ILE:HD11	1.99	0.44
11:Y:1:THR:CB	11:Y:33:LYS:HZ3	2.30	0.44
15:m:49:GLU:O	15:m:53:ASN:ND2	2.51	0.44
1:A:83:ARG:HA	1:A:86:VAL:HG12	2.00	0.44
1:O:83:ARG:HA	1:O:86:VAL:HG12	2.00	0.44
7:U:72:ILE:HD11	7:U:78:CYS:SG	2.58	0.44
9:I:170:MET:O	9:I:174:VAL:HG22	2.18	0.44
6:T:27:MET:O	6:T:30:VAL:HG12	2.18	0.43
8:V:174:ASP:O	8:V:175:LEU:HD22	2.17	0.43
9:W:170:MET:O	9:W:174:VAL:HG22	2.18	0.43
11:Y:50:ALA:CB	12:Z:127:VAL:HG13	2.48	0.43
2:B:16:GLY:O	15:h:239:TYR:OH	2.32	0.43
6:F:27:MET:O	6:F:30:VAL:HG12	2.18	0.43
15:p:61:ARG:NH2	15:p:196:GLU:OE2	2.51	0.43
12:L:21:ALA:HB3	12:L:198:VAL:CG1	2.49	0.43
15:i:61:ARG:NH2	15:i:196:GLU:OE2	2.51	0.43
11:Y:138:VAL:CG2	10:J:141:SER:OG	2.65	0.43
15:o:114:LEU:HD13	15:o:213:TYR:CE1	2.54	0.43
11:K:50:ALA:CB	12:L:127:VAL:HG13	2.48	0.43
2:P:176:LYS:NZ	3:Q:51:ALA:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:158:ALA:CB	3:Q:172:LEU:HD21	2.48	0.43
4:D:49:ALA:HB2	4:D:217:LEU:CD1	2.48	0.43
7:G:72:ILE:HD11	7:G:78:CYS:SG	2.58	0.43
8:H:171:SER:OG	8:H:172:ASN:N	2.50	0.43
1:O:67:ILE:HG21	1:O:109:LEU:HD21	2.00	0.43
1:A:211:ILE:HD11	1:A:218:ARG:NH2	2.34	0.43
15:h:114:LEU:HD13	15:h:213:TYR:CE1	2.54	0.43
5:S:9:ASP:OD2	5:S:11:THR:HG22	2.19	0.43
6:F:120:HIS:NE2	7:G:86:ASP:OD1	2.52	0.43
1:O:211:ILE:HD11	1:O:218:ARG:NH2	2.34	0.43
15:o:32:LEU:HA	15:o:36:LEU:HD12	2.01	0.43
3:C:83:VAL:HG21	3:C:129:ILE:HD11	2.01	0.43
15:d:150:VAL:HG12	15:d:216:LEU:HD23	2.01	0.43
10:X:102:LEU:O	10:X:132:HIS:NE2	2.52	0.42
15:p:146:VAL:O	15:p:150:VAL:HG13	2.19	0.42
5:E:9:ASP:OD2	5:E:11:THR:HG22	2.19	0.42
14:N:30:VAL:HG12	14:N:30:VAL:O	2.18	0.42
16:c:156:VAL:HG22	16:c:229:ILE:CG2	2.48	0.42
15:i:146:VAL:O	15:i:150:VAL:HG13	2.19	0.42
15:i:183:HIS:CE1	15:i:184:VAL:HG23	2.54	0.42
4:R:84:ASP:OD2	4:R:138:GLY:N	2.52	0.42
8:V:121:LYS:C	8:V:122:LEU:HD22	2.44	0.42
14:b:30:VAL:HG12	14:b:30:VAL:O	2.18	0.42
15:k:150:VAL:HG12	15:k:216:LEU:HD23	2.01	0.42
3:Q:83:VAL:HG21	3:Q:129:ILE:HD11	2.01	0.42
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.02	0.42
9:W:11:MET:HE1	9:W:169:ALA:CB	2.46	0.42
3:C:158:ALA:CB	3:C:172:LEU:HD21	2.48	0.42
16:g:156:VAL:HG21	16:g:237:LEU:HD21	2.01	0.42
4:R:49:ALA:HB2	4:R:217:LEU:HD12	2.01	0.42
10:X:27:GLN:HB3	10:J:170:ARG:O	2.19	0.42
5:E:26:MET:O	5:E:29:VAL:HG12	2.19	0.42
15:i:15:LYS:O	15:i:19:VAL:HG23	2.19	0.42
12:Z:21:ALA:HB3	12:Z:198:VAL:CG1	2.49	0.42
16:j:156:VAL:HG22	16:j:229:ILE:CG2	2.48	0.42
15:p:183:HIS:CE1	15:p:184:VAL:HG23	2.54	0.42
4:D:84:ASP:OD2	4:D:138:GLY:N	2.52	0.42
8:H:121:LYS:C	8:H:122:LEU:HD22	2.44	0.42
16:n:156:VAL:HG21	16:n:237:LEU:HD21	2.01	0.42
15:p:15:LYS:O	15:p:19:VAL:HG23	2.19	0.42
3:C:15:HIS:CE1	4:D:33:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:15:HIS:CE1	4:R:33:LEU:HD21	2.54	0.42
3:Q:105:GLU:HA	3:Q:108:THR:HG22	2.02	0.42
4:R:49:ALA:HB2	4:R:217:LEU:CD1	2.49	0.42
10:X:12:TYR:OH	10:X:151:ILE:HG23	2.20	0.42
11:Y:35:ILE:N	11:Y:43:GLY:O	2.49	0.42
8:H:163:ILE:HG23	8:H:170:GLY:HA2	2.02	0.42
9:I:11:MET:HE1	9:I:169:ALA:CB	2.46	0.42
10:J:102:LEU:O	10:J:132:HIS:NE2	2.52	0.42
6:T:53:VAL:O	6:T:53:VAL:HG13	2.20	0.42
10:X:170:ARG:O	10:J:27:GLN:HB3	2.19	0.42
1:A:78:MET:HE1	7:G:22:LEU:HD12	2.01	0.42
1:O:78:MET:HE1	7:U:22:LEU:HD12	2.02	0.42
5:S:26:MET:O	5:S:29:VAL:HG12	2.19	0.42
10:X:138:LEU:CD2	11:K:133:VAL:HG23	2.49	0.42
1:A:202:MET:HE2	1:A:229:LEU:HD21	2.02	0.42
6:F:53:VAL:HG13	6:F:53:VAL:O	2.20	0.42
2:B:97:TYR:OH	10:J:67:TYR:OH	2.34	0.42
2:B:176:LYS:NZ	3:C:51:ALA:O	2.52	0.42
10:J:12:TYR:OH	10:J:151:ILE:HG23	2.19	0.42
10:J:78:THR:O	10:J:82:ASN:ND2	2.53	0.42
11:Y:133:VAL:HG23	10:J:138:LEU:CD2	2.50	0.41
4:D:49:ALA:HB2	4:D:217:LEU:HD12	2.01	0.41
3:C:105:GLU:HA	3:C:108:THR:HG22	2.02	0.41
15:h:32:LEU:HA	15:h:36:LEU:HD12	2.00	0.41
12:Z:64:LEU:HD21	12:Z:92:LEU:HD11	2.03	0.41
3:C:91:CYS:SG	3:C:107:ILE:HD13	2.61	0.41
15:k:124:TRP:CE2	15:k:128:LEU:HD11	2.55	0.41
15:d:124:TRP:CE2	15:d:128:LEU:HD11	2.55	0.41
16:c:198:ARG:O	16:c:201:VAL:HG22	2.21	0.41
16:e:113:LEU:HD23	16:e:212:ILE:HG21	2.03	0.41
1:O:39:ALA:N	1:O:42:GLY:O	2.54	0.41
1:O:202:MET:HE2	1:O:229:LEU:HD21	2.02	0.41
10:X:142:ILE:HD11	11:K:137:GLY:CA	2.51	0.41
16:j:198:ARG:O	16:j:201:VAL:HG22	2.21	0.41
16:l:113:LEU:HD23	16:l:212:ILE:HG21	2.03	0.41
7:G:166:THR:HG22	7:G:167:ALA:N	2.36	0.41
15:i:138:PHE:CE2	15:i:142:ILE:HD11	2.56	0.41
7:U:166:THR:HG22	7:U:167:ALA:N	2.36	0.40
11:Y:166:ARG:HA	9:I:33:MET:HG3	2.02	0.40
15:p:138:PHE:CE2	15:p:142:ILE:HD11	2.56	0.40
3:C:184:ASP:O	3:C:187:THR:OG1	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:64:LEU:HD21	12:L:92:LEU:HD11	2.03	0.40
15:h:159:ALA:O	15:h:162:THR:OG1	2.32	0.40
5:S:164:ARG:O	5:S:198:THR:HG22	2.22	0.40
15:k:160:PHE:O	15:k:163:THR:OG1	2.30	0.40
6:F:139:SER:HA	6:F:216:VAL:HG11	2.03	0.40
3:Q:91:CYS:SG	3:Q:107:ILE:HD13	2.61	0.40
12:Z:151:ASN:HD22	9:I:148:MET:CE	2.35	0.40
15:d:134:ASP:N	15:d:134:ASP:OD1	2.55	0.40
15:h:32:LEU:HD21	15:h:220:ILE:HD13	2.03	0.40
6:T:70:ASP:HB3	6:T:73:VAL:HG12	2.03	0.40
11:Y:137:GLY:CA	10:J:142:ILE:HD11	2.51	0.40
15:o:32:LEU:HD21	15:o:220:ILE:HD13	2.03	0.40
16:n:35:LYS:O	16:n:38:SER:OG	2.33	0.40
6:F:70:ASP:HB3	6:F:73:VAL:HG12	2.03	0.40
16:c:35:LYS:O	16:c:38:SER:OG	2.31	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	227/234 (97%)	225 (99%)	2 (1%)	0	100	100
1	O	227/234 (97%)	225 (99%)	2 (1%)	0	100	100
2	B	247/261 (95%)	244 (99%)	3 (1%)	0	100	100
2	P	247/261 (95%)	244 (99%)	3 (1%)	0	100	100
3	C	233/248 (94%)	228 (98%)	5 (2%)	0	100	100
3	Q	233/248 (94%)	228 (98%)	5 (2%)	0	100	100
4	D	239/241 (99%)	232 (97%)	6 (2%)	1 (0%)	30	62
4	R	239/241 (99%)	232 (97%)	6 (2%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	237/263 (90%)	233 (98%)	4 (2%)	0	100	100
5	S	237/263 (90%)	233 (98%)	4 (2%)	0	100	100
6	F	238/255 (93%)	237 (100%)	1 (0%)	0	100	100
6	T	238/255 (93%)	237 (100%)	1 (0%)	0	100	100
7	G	237/246 (96%)	234 (99%)	3 (1%)	0	100	100
7	U	237/246 (96%)	234 (99%)	3 (1%)	0	100	100
8	H	220/277 (79%)	215 (98%)	3 (1%)	2 (1%)	14	47
8	V	220/277 (79%)	215 (98%)	3 (1%)	2 (1%)	14	47
9	I	202/205 (98%)	198 (98%)	3 (2%)	1 (0%)	24	59
9	W	202/205 (98%)	198 (98%)	3 (2%)	1 (0%)	24	59
10	J	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
10	X	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
11	K	198/263 (75%)	197 (100%)	1 (0%)	0	100	100
11	Y	198/263 (75%)	197 (100%)	1 (0%)	0	100	100
12	L	211/241 (88%)	208 (99%)	3 (1%)	0	100	100
12	Z	211/241 (88%)	208 (99%)	3 (1%)	0	100	100
13	M	213/264 (81%)	210 (99%)	3 (1%)	0	100	100
13	a	213/264 (81%)	210 (99%)	3 (1%)	0	100	100
14	N	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
14	b	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
15	d	213/239 (89%)	211 (99%)	2 (1%)	0	100	100
15	f	207/239 (87%)	205 (99%)	2 (1%)	0	100	100
15	h	212/239 (89%)	210 (99%)	2 (1%)	0	100	100
15	i	213/239 (89%)	210 (99%)	3 (1%)	0	100	100
15	k	213/239 (89%)	211 (99%)	2 (1%)	0	100	100
15	m	207/239 (87%)	205 (99%)	2 (1%)	0	100	100
15	o	212/239 (89%)	210 (99%)	2 (1%)	0	100	100
15	p	213/239 (89%)	210 (99%)	3 (1%)	0	100	100
16	c	208/249 (84%)	207 (100%)	1 (0%)	0	100	100
16	e	207/249 (83%)	205 (99%)	2 (1%)	0	100	100
16	g	207/249 (83%)	206 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	j	208/249 (84%)	207 (100%)	1 (0%)	0	100	100
16	l	207/249 (83%)	206 (100%)	1 (0%)	0	100	100
16	n	207/249 (83%)	206 (100%)	1 (0%)	0	100	100
All	All	9128/10282 (89%)	9007 (99%)	113 (1%)	8 (0%)	49	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	W	31	ALA
9	I	31	ALA
4	R	6	SER
8	V	171	SER
4	D	6	SER
8	H	171	SER
8	V	188	PRO
8	H	188	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/191 (83%)	158 (100%)	0	100	100
1	O	158/191 (83%)	158 (100%)	0	100	100
2	B	159/221 (72%)	159 (100%)	0	100	100
2	P	159/221 (72%)	159 (100%)	0	100	100
3	C	152/211 (72%)	152 (100%)	0	100	100
3	Q	152/211 (72%)	152 (100%)	0	100	100
4	D	173/203 (85%)	173 (100%)	0	100	100
4	R	173/203 (85%)	173 (100%)	0	100	100
5	E	181/224 (81%)	181 (100%)	0	100	100
5	S	181/224 (81%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	167/212 (79%)	167 (100%)	0	100	100
6	T	167/212 (79%)	167 (100%)	0	100	100
7	G	175/210 (83%)	175 (100%)	0	100	100
7	U	175/210 (83%)	175 (100%)	0	100	100
8	H	165/228 (72%)	165 (100%)	0	100	100
8	V	165/228 (72%)	165 (100%)	0	100	100
9	I	164/174 (94%)	164 (100%)	0	100	100
9	W	164/174 (94%)	164 (100%)	0	100	100
10	J	156/171 (91%)	156 (100%)	0	100	100
10	X	156/171 (91%)	156 (100%)	0	100	100
11	K	146/202 (72%)	146 (100%)	0	100	100
11	Y	146/202 (72%)	146 (100%)	0	100	100
12	L	161/199 (81%)	161 (100%)	0	100	100
12	Z	161/199 (81%)	161 (100%)	0	100	100
13	M	166/215 (77%)	166 (100%)	0	100	100
13	a	166/215 (77%)	166 (100%)	0	100	100
14	N	149/181 (82%)	149 (100%)	0	100	100
14	b	149/181 (82%)	149 (100%)	0	100	100
15	d	174/212 (82%)	174 (100%)	0	100	100
15	f	172/212 (81%)	172 (100%)	0	100	100
15	h	173/212 (82%)	173 (100%)	0	100	100
15	i	175/212 (82%)	175 (100%)	0	100	100
15	k	174/212 (82%)	174 (100%)	0	100	100
15	m	172/212 (81%)	172 (100%)	0	100	100
15	o	173/212 (82%)	173 (100%)	0	100	100
15	p	175/212 (82%)	175 (100%)	0	100	100
16	c	165/224 (74%)	165 (100%)	0	100	100
16	e	170/224 (76%)	170 (100%)	0	100	100
16	g	167/224 (75%)	167 (100%)	0	100	100
16	j	165/224 (74%)	165 (100%)	0	100	100
16	l	170/224 (76%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	n	167/224 (75%)	167 (100%)	0	100	100
All	All	6936/8724 (80%)	6936 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	102	GLN
2	P	146	GLN
3	Q	15	HIS
4	R	41	GLN
4	R	164	GLN
4	R	227	HIS
5	S	60	GLN
5	S	183	ASN
6	T	110	HIS
7	U	100	ASN
7	U	150	GLN
9	W	17	ASN
9	W	32	GLN
10	X	24	ASN
10	X	63	ASN
12	Z	151	ASN
12	Z	159	GLN
14	b	110	GLN
14	b	123	GLN
15	k	161	GLN
16	j	27	ASN
16	j	164	HIS
16	j	173	GLN
16	j	191	GLN
16	l	147	ASN
15	o	38	GLN
15	o	136	ASN
16	n	27	ASN
16	n	173	GLN
16	n	191	GLN
15	p	53	ASN
15	p	183	HIS
2	B	102	GLN

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Mol	Chain	Res	Type
2	B	146	GLN
3	C	15	HIS
4	D	41	GLN
4	D	164	GLN
4	D	227	HIS
5	E	60	GLN
6	F	110	HIS
7	G	100	ASN
7	G	150	GLN
9	I	32	GLN
9	I	168	GLN
10	J	24	ASN
12	L	151	ASN
12	L	159	GLN
14	N	110	GLN
14	N	123	GLN
15	d	53	ASN
15	d	161	GLN
15	d	183	HIS
16	c	27	ASN
16	c	164	HIS
16	c	173	GLN
16	c	191	GLN
16	e	147	ASN
15	h	38	GLN
15	h	136	ASN
16	g	27	ASN
16	g	173	GLN
16	g	191	GLN
15	i	53	ASN
15	i	183	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

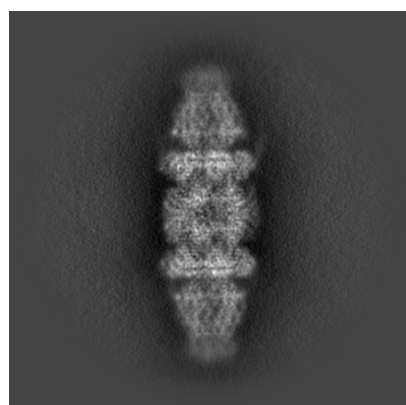
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24277. These allow visual inspection of the internal detail of the map and identification of artifacts.

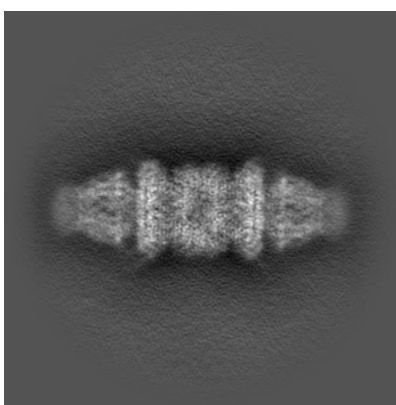
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

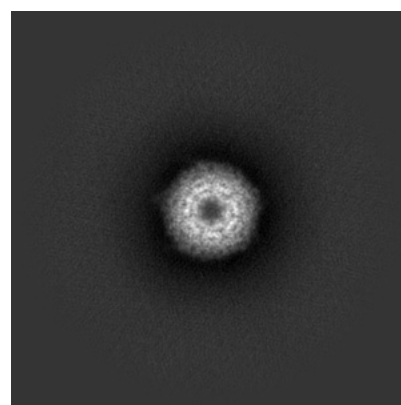
6.1.1 Primary map



X



Y

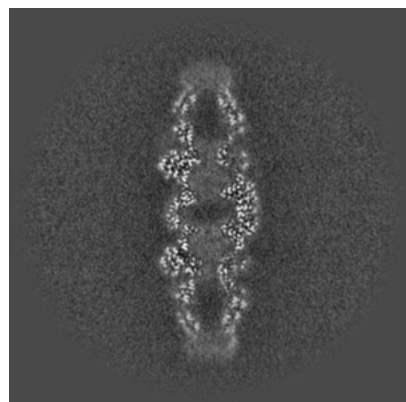


Z

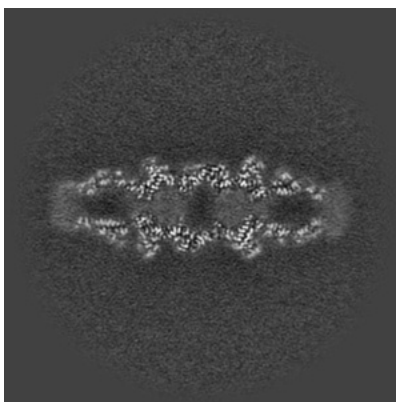
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

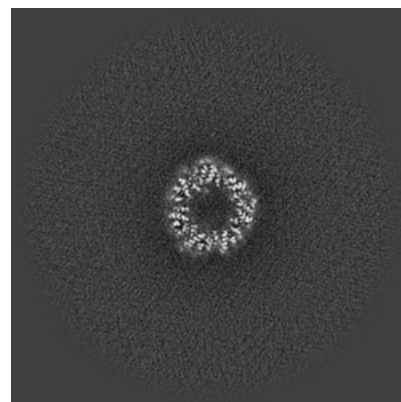
6.2.1 Primary map



X Index: 192



Y Index: 192

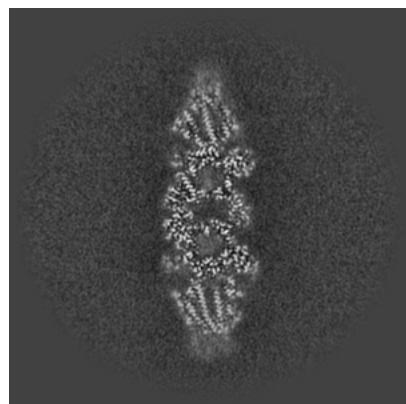


Z Index: 192

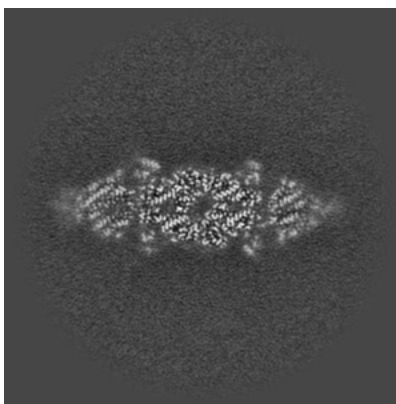
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

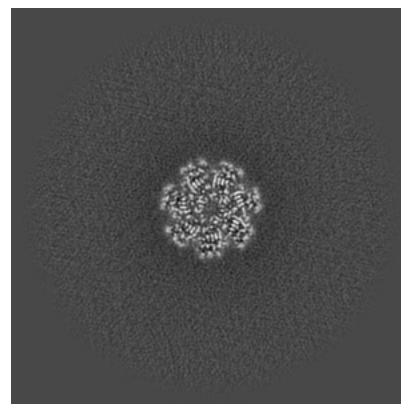
6.3.1 Primary map



X Index: 207



Y Index: 211

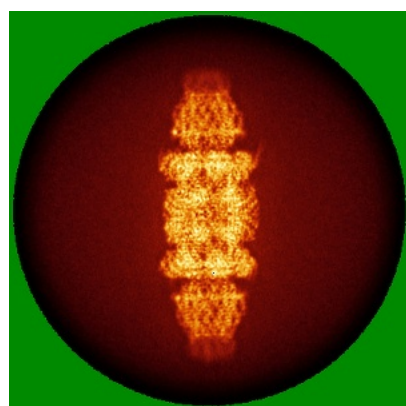


Z Index: 235

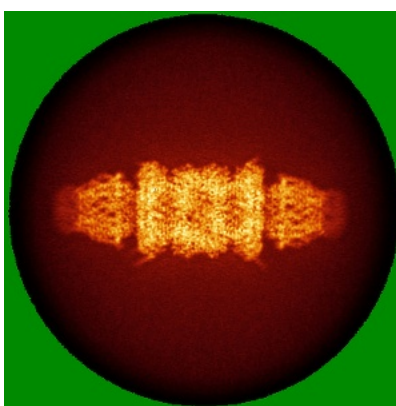
The images above show the largest variance slices of the map in three orthogonal directions.

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

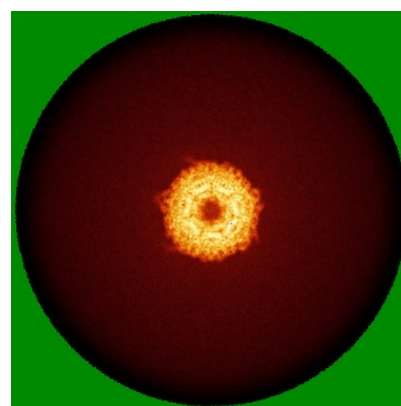
6.4.1 Primary map



X



Y

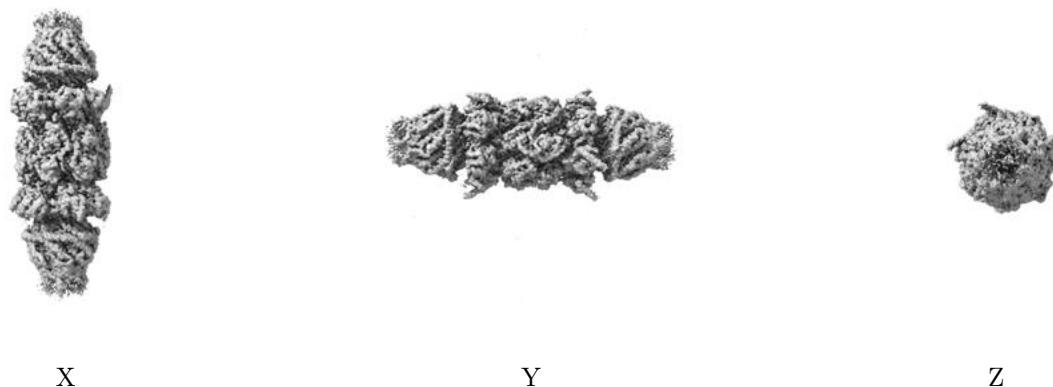


Z

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

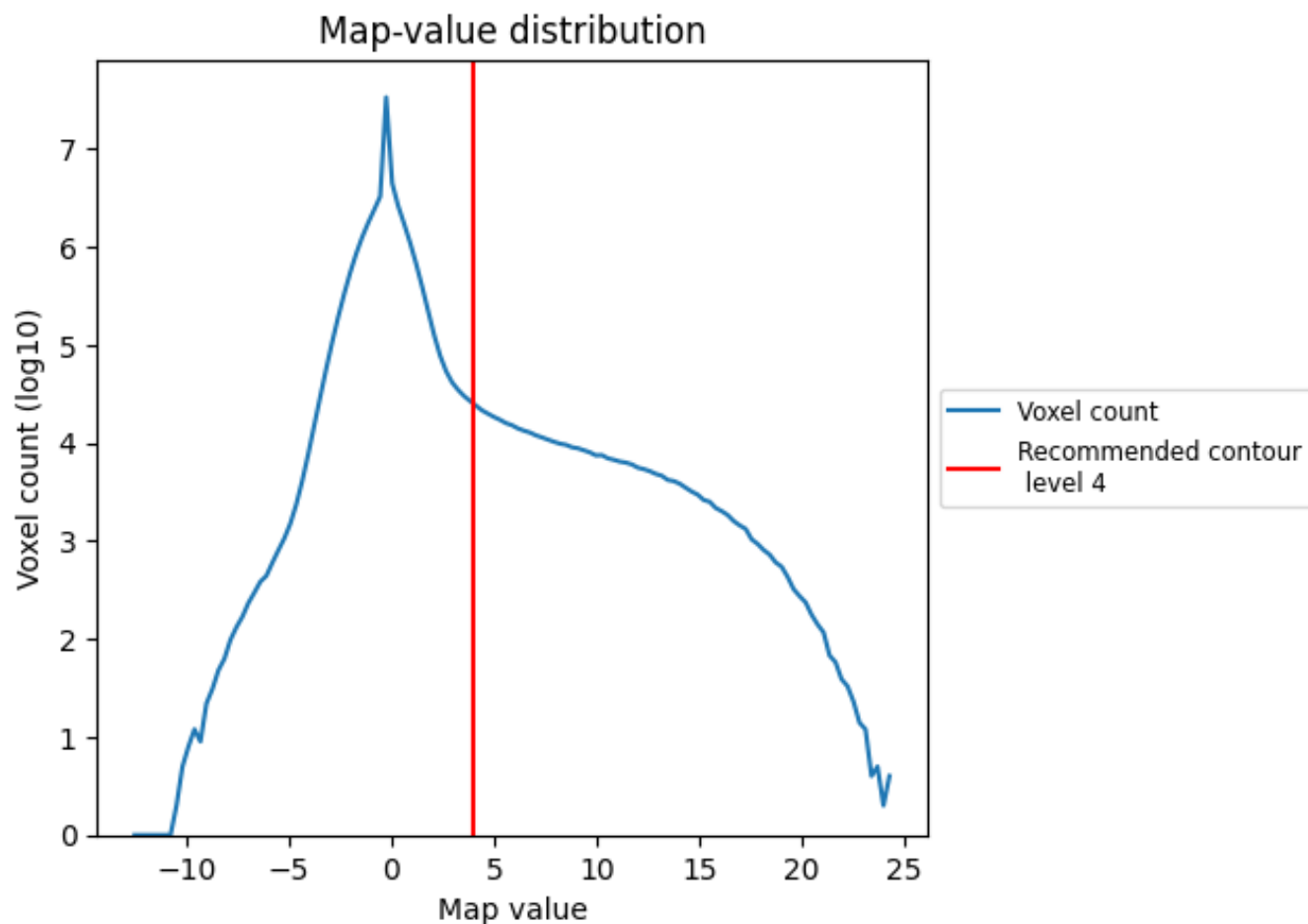
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

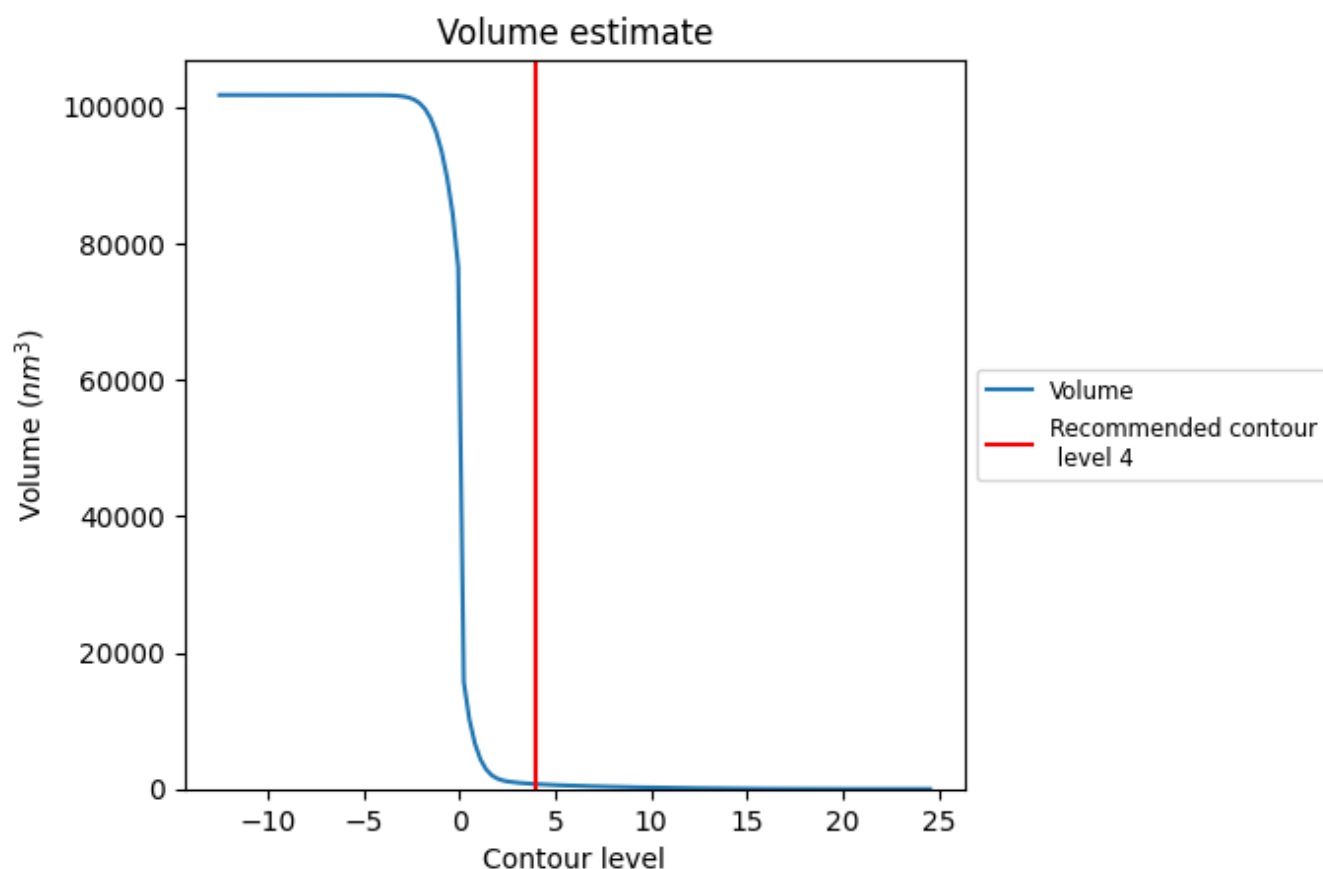
This section contains the results of statistical analysis of the map.

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.

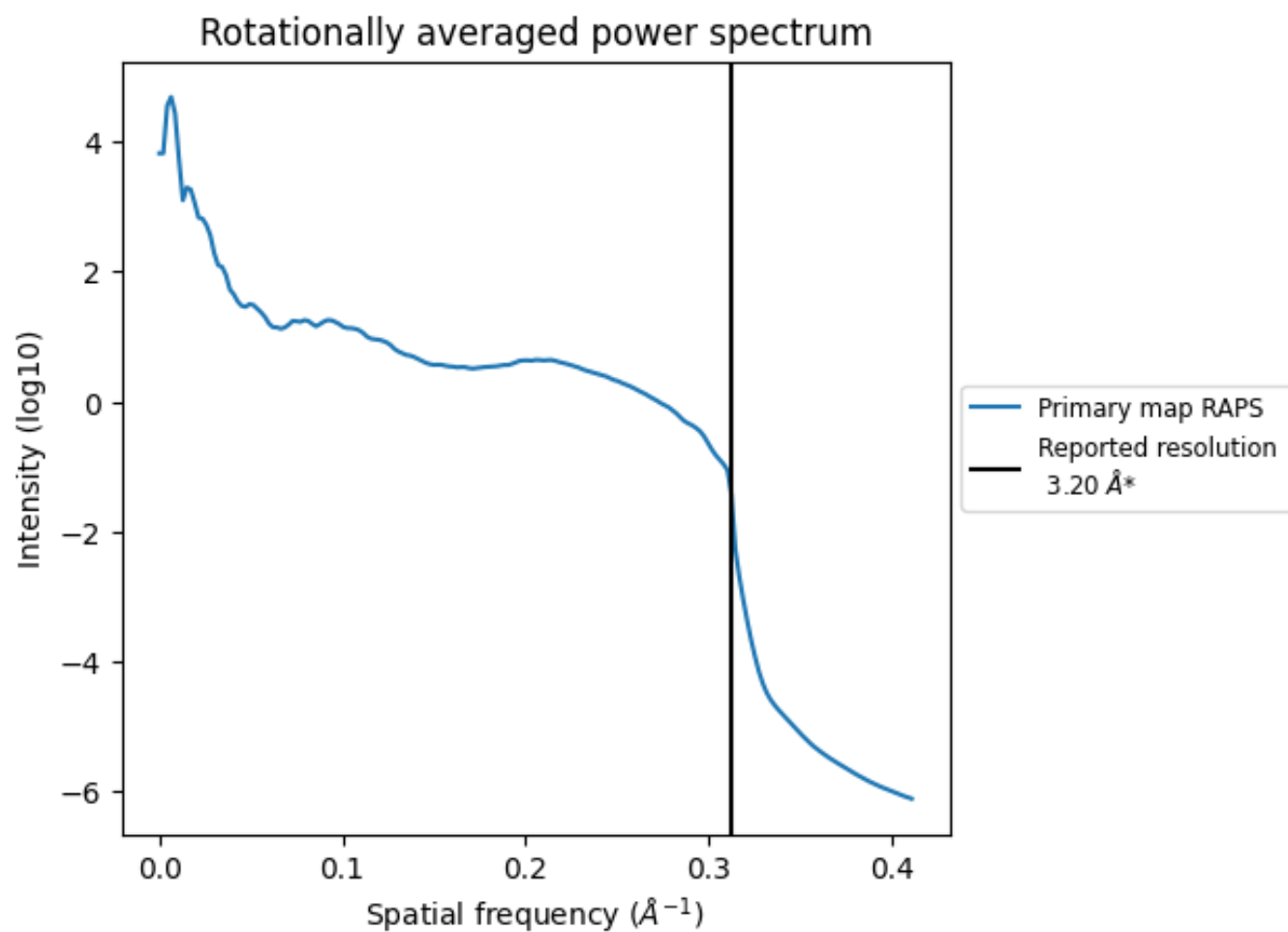
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 718 nm³; this corresponds to an approximate mass of 648 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

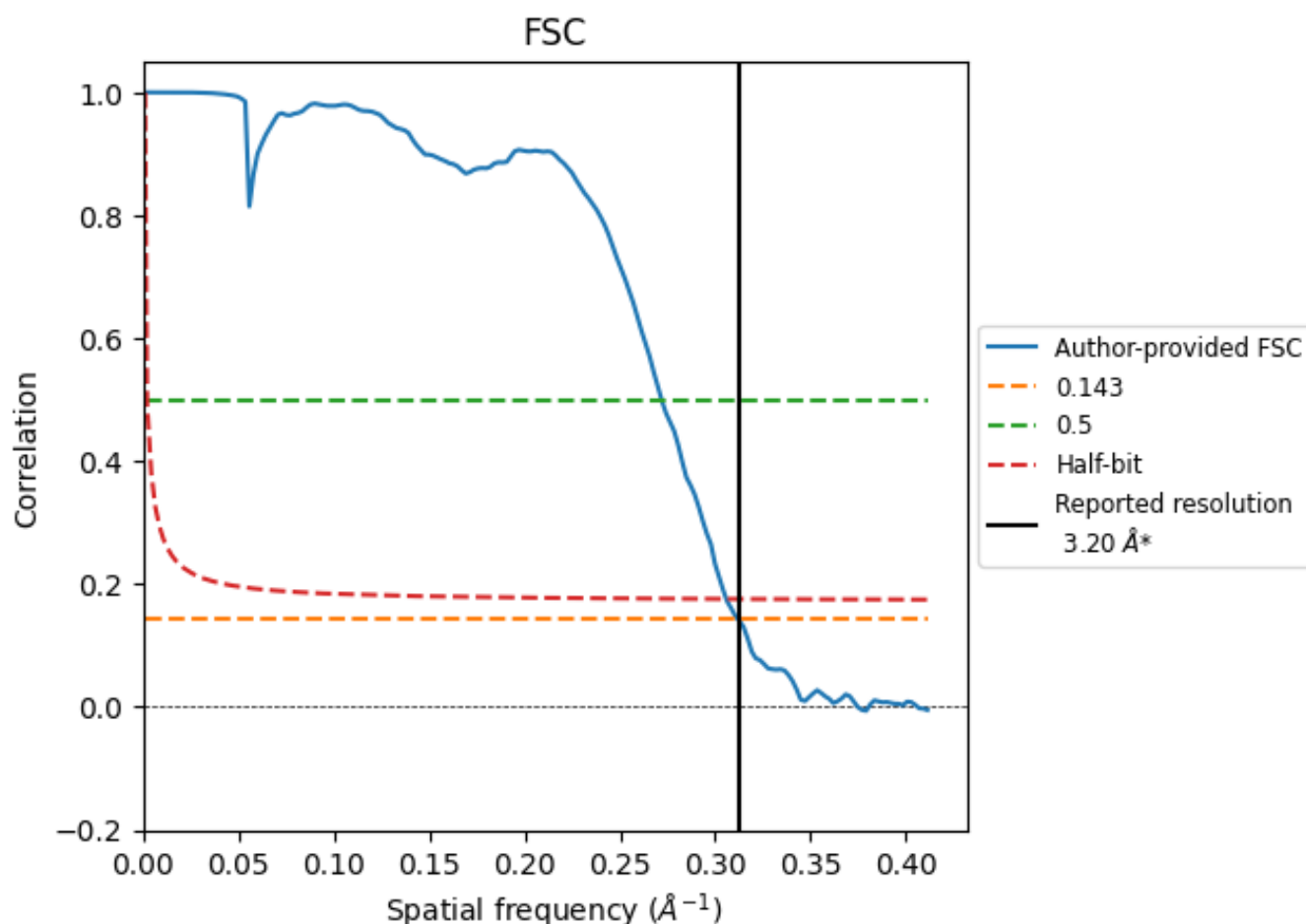


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

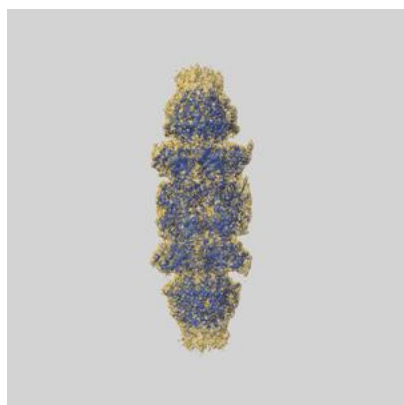
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.68	3.27
Unmasked-calculated*	-	-	-

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

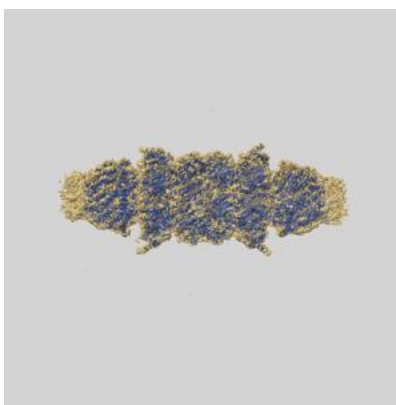
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24277 and PDB model 7NAP. Per-residue inclusion information can be found in section [3](#) on page [9](#).

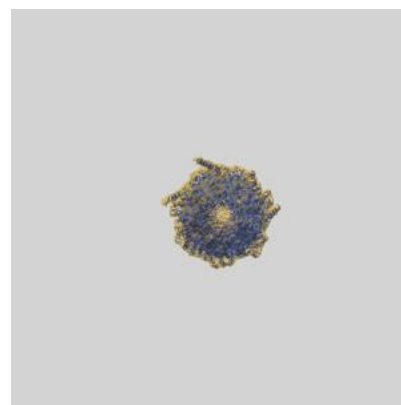
9.1 Map-model overlay [i](#)



X



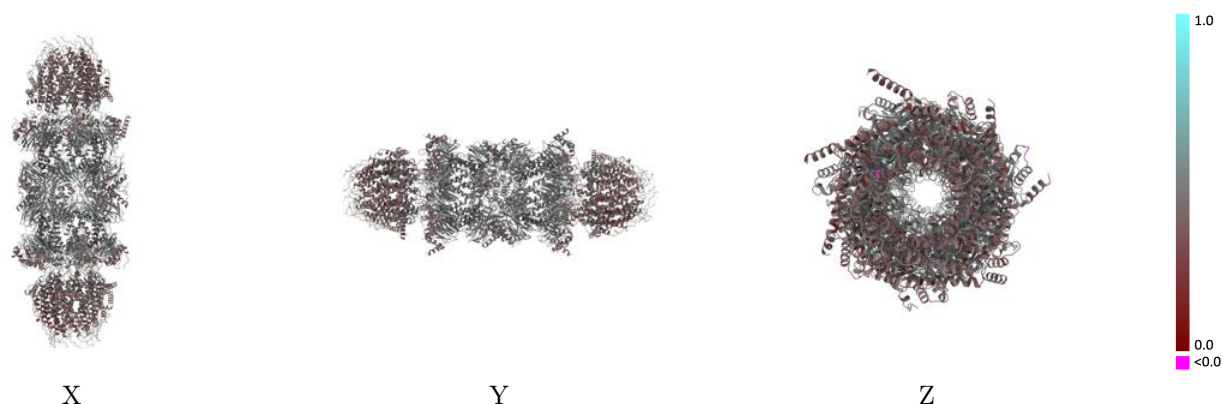
Y



Z

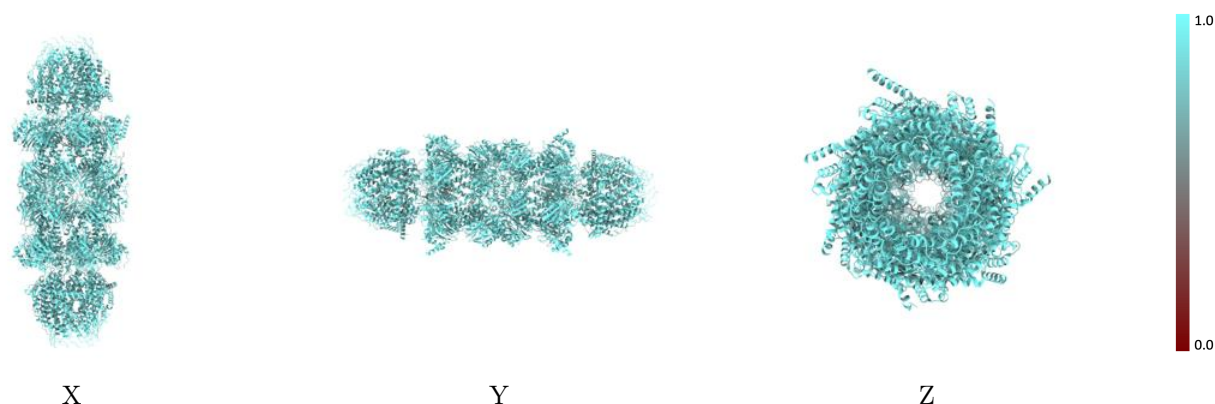
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



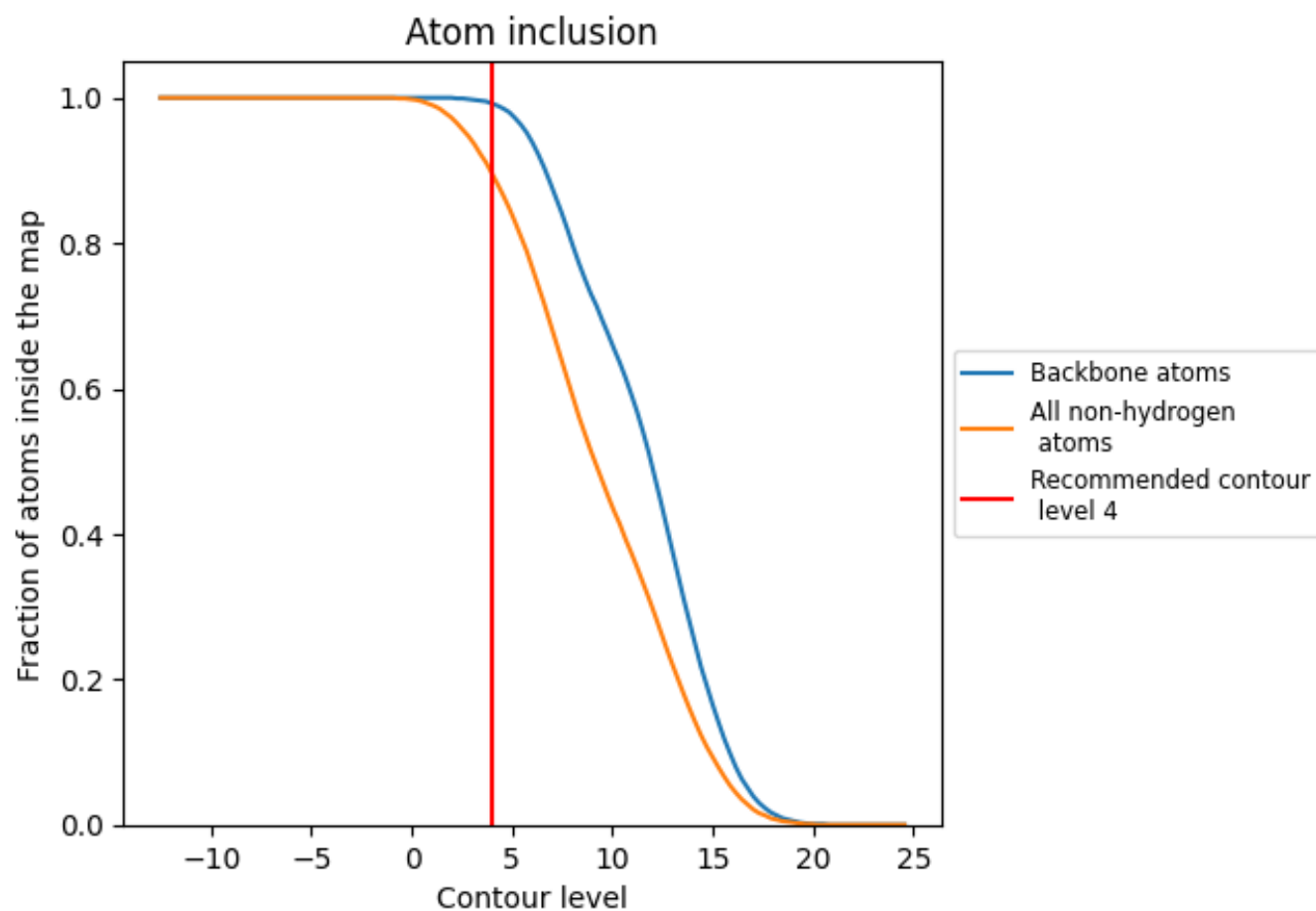
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 90% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.4450
A	 0.9070	 0.4620
B	 0.9080	 0.4650
C	 0.9140	 0.4560
D	 0.8840	 0.4470
E	 0.9060	 0.4610
F	 0.9120	 0.4600
G	 0.9060	 0.4600
H	 0.9150	 0.4740
I	 0.8980	 0.4750
J	 0.9020	 0.4850
K	 0.9290	 0.4740
L	 0.9010	 0.4740
M	 0.9140	 0.4750
N	 0.9150	 0.4780
O	 0.9050	 0.4590
P	 0.9110	 0.4630
Q	 0.9130	 0.4560
R	 0.8920	 0.4520
S	 0.9110	 0.4550
T	 0.9070	 0.4610
U	 0.9110	 0.4590
V	 0.9100	 0.4720
W	 0.9050	 0.4750
X	 0.9050	 0.4800
Y	 0.9190	 0.4680
Z	 0.9020	 0.4770
a	 0.9160	 0.4800
b	 0.9090	 0.4740
c	 0.8660	 0.3960
d	 0.8850	 0.4090
e	 0.8830	 0.4140
f	 0.8910	 0.4060
g	 0.8660	 0.3960
h	 0.8710	 0.3970



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Chain	Atom inclusion	Q-score
i	 0.8670	 0.3860
j	 0.8600	 0.4020
k	 0.8890	 0.4160
l	 0.8790	 0.4060
m	 0.8830	 0.3980
n	 0.8540	 0.3920
o	 0.8600	 0.3880
p	 0.8750	 0.3990