



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:31 PM UTC

PDB ID : 9F9P / pdb_00009f9p
EMDB ID : EMD-50258
Title : CryoEM structure of recombinant Trypanosoma cruzi apo proteasome 20S subunit
Authors : Rowland, P.
Deposited on : 2024-05-08
Resolution : 2.25 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:

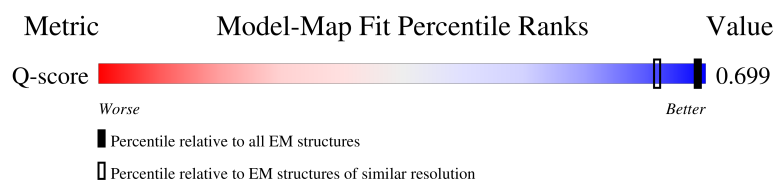
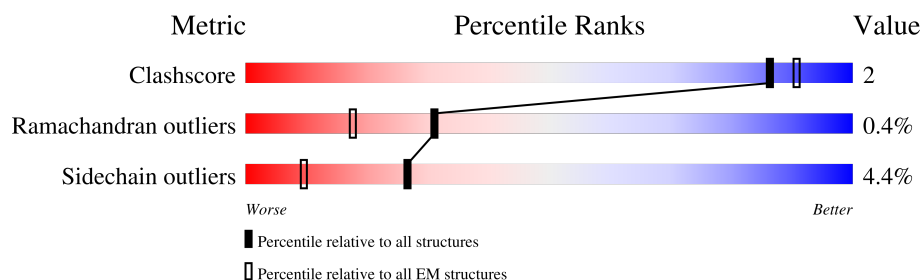
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.25 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.



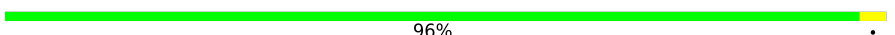
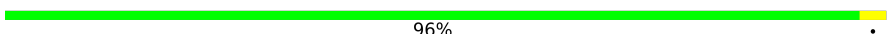
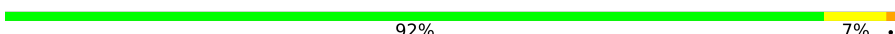
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3458 (1.75 - 2.75)

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	268	
1	O	268	
2	B	231	
2	P	231	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	286	 82% 12% • 5%
3	Q	286	 82% 12% • 5%
4	D	247	 84% 10% • 5%
4	R	247	 83% 9% • 5%
5	E	245	 81% 11% • 7%
5	S	245	 81% 11% • 7%
6	F	265	 74% 8% • 17%
6	T	265	 74% 8% • 17%
7	G	237	 86% 9% • •
7	U	237	 86% 9% • •
8	H	284	 77% • 20%
8	V	284	 77% • 20%
9	I	292	 65% 9% • 25%
9	W	292	 66% 9% • 25%
10	J	205	 96% •
10	X	205	 96% •
11	K	206	 92% 7% •
11	Y	206	 91% 7% •
12	L	311	 59% 5% 35%
12	Z	311	 59% 5% 35%
13	M	246	 78% 6% • 15%
13	a	246	 77% 6% • 15%
14	N	218	 91% 9%
14	b	218	 91% 8% •

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 49596 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1884	1190	328	353	13		
1	O	244	Total	C	N	O	S	0	0
			1884	1190	328	353	13		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ALA	-	expression tag	UNP A0A2V2W7U6
A	252	GLU	-	expression tag	UNP A0A2V2W7U6
A	253	ASN	-	expression tag	UNP A0A2V2W7U6
A	254	LEU	-	expression tag	UNP A0A2V2W7U6
A	255	TYR	-	expression tag	UNP A0A2V2W7U6
A	256	PHE	-	expression tag	UNP A0A2V2W7U6
A	257	GLN	-	expression tag	UNP A0A2V2W7U6
A	258	SER	-	expression tag	UNP A0A2V2W7U6
A	259	HIS	-	expression tag	UNP A0A2V2W7U6
A	260	HIS	-	expression tag	UNP A0A2V2W7U6
A	261	HIS	-	expression tag	UNP A0A2V2W7U6
A	262	HIS	-	expression tag	UNP A0A2V2W7U6
A	263	HIS	-	expression tag	UNP A0A2V2W7U6
A	264	HIS	-	expression tag	UNP A0A2V2W7U6
A	265	HIS	-	expression tag	UNP A0A2V2W7U6
A	266	HIS	-	expression tag	UNP A0A2V2W7U6
A	267	HIS	-	expression tag	UNP A0A2V2W7U6
A	268	HIS	-	expression tag	UNP A0A2V2W7U6
O	251	ALA	-	expression tag	UNP A0A2V2W7U6
O	252	GLU	-	expression tag	UNP A0A2V2W7U6
O	253	ASN	-	expression tag	UNP A0A2V2W7U6
O	254	LEU	-	expression tag	UNP A0A2V2W7U6
O	255	TYR	-	expression tag	UNP A0A2V2W7U6
O	256	PHE	-	expression tag	UNP A0A2V2W7U6
O	257	GLN	-	expression tag	UNP A0A2V2W7U6
O	258	SER	-	expression tag	UNP A0A2V2W7U6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	259	HIS	-	expression tag	UNP A0A2V2W7U6
O	260	HIS	-	expression tag	UNP A0A2V2W7U6
O	261	HIS	-	expression tag	UNP A0A2V2W7U6
O	262	HIS	-	expression tag	UNP A0A2V2W7U6
O	263	HIS	-	expression tag	UNP A0A2V2W7U6
O	264	HIS	-	expression tag	UNP A0A2V2W7U6
O	265	HIS	-	expression tag	UNP A0A2V2W7U6
O	266	HIS	-	expression tag	UNP A0A2V2W7U6
O	267	HIS	-	expression tag	UNP A0A2V2W7U6
O	268	HIS	-	expression tag	UNP A0A2V2W7U6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	228	Total	C	N	O	S	0	0
			1737	1095	292	342	8		
2	P	228	Total	C	N	O	S	0	0
			1737	1095	292	342	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2126	1338	367	413	8		
3	Q	271	Total	C	N	O	S	0	0
			2126	1338	367	413	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	234	Total	C	N	O	S	0	0
			1864	1173	329	355	7		
4	R	234	Total	C	N	O	S	0	0
			1864	1173	329	355	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	223	ARG	HIS	conflict	UNP A0A2V2WZ04
R	223	ARG	HIS	conflict	UNP A0A2V2WZ04

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	227	Total	C	N	O	S	0	0
			1757	1102	302	344	9		
5	S	227	Total	C	N	O	S	0	0
			1757	1102	302	344	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	221	Total	C	N	O	S	0	0
			1722	1095	298	320	9		
6	T	221	Total	C	N	O	S	0	0
			1722	1095	298	320	9		

- Molecule 7 is a protein called Putative proteasome alpha 7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	227	Total	C	N	O	S	0	0
			1724	1078	297	336	13		
7	U	227	Total	C	N	O	S	0	0
			1724	1078	297	336	13		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	228	Total	C	N	O	S	0	0
			1723	1081	290	339	13		
8	V	228	Total	C	N	O	S	0	0
			1723	1081	290	339	13		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1663	1043	294	315	11		
9	W	219	Total	C	N	O	S	0	0
			1663	1043	294	315	11		

- Molecule 10 is a protein called Putative proteasome beta 3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1555	976	265	299	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1555	976	265	299	15		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1586	995	275	299	17		
11	Y	206	Total	C	N	O	S	0	0
			1586	995	275	299	17		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total	C	N	O	S	0	0
			1578	995	274	300	9		
12	Z	201	Total	C	N	O	S	0	0
			1578	995	274	300	9		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	208	Total	C	N	O	S	0	0
			1647	1042	279	314	12		
13	a	208	Total	C	N	O	S	0	0
			1647	1042	279	314	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	245	ASN	LYS	conflict	UNP A0A2V2VW62
a	245	ASN	LYS	conflict	UNP A0A2V2VW62

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total	C	N	O	S	0	0
			1695	1075	290	313	17		
14	b	218	Total	C	N	O	S	0	0
			1695	1075	290	313	17		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	39	Total 39	O 39	0
15	B	33	Total 33	O 33	0
15	C	33	Total 33	O 33	0
15	D	21	Total 21	O 21	0
15	E	22	Total 22	O 22	0
15	F	26	Total 26	O 26	0
15	G	33	Total 33	O 33	0
15	H	52	Total 52	O 52	0
15	I	44	Total 44	O 44	0
15	J	50	Total 50	O 50	0
15	K	37	Total 37	O 37	0
15	L	29	Total 29	O 29	0
15	M	48	Total 48	O 48	0
15	N	69	Total 69	O 69	0
15	O	39	Total 39	O 39	0
15	P	33	Total 33	O 33	0
15	Q	33	Total 33	O 33	0
15	R	21	Total 21	O 21	0
15	S	22	Total 22	O 22	0
15	T	26	Total 26	O 26	0
15	U	33	Total 33	O 33	0
15	V	52	Total 52	O 52	0

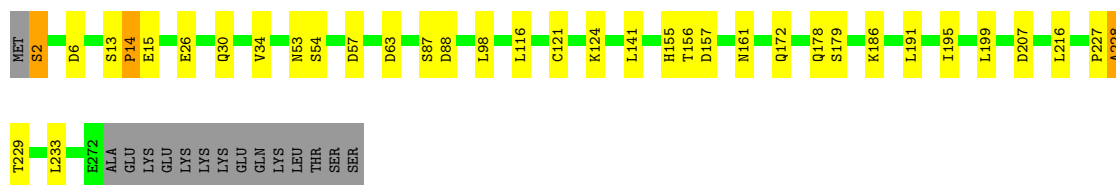
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
15	W	45	Total 45	O 45	0
15	X	50	Total 50	O 50	0
15	Y	37	Total 37	O 37	0
15	Z	29	Total 29	O 29	0
15	a	48	Total 48	O 48	0
15	b	70	Total 70	O 70	0

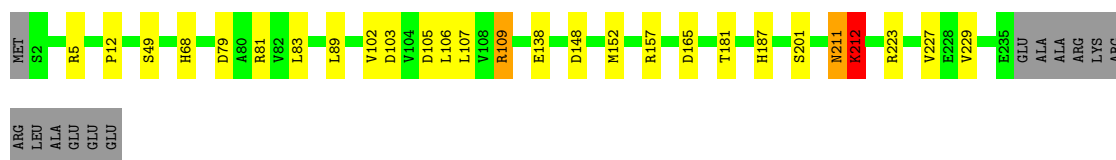
- Molecule 3: Proteasome subunit alpha type

Chain Q:  82% 12% • 5%



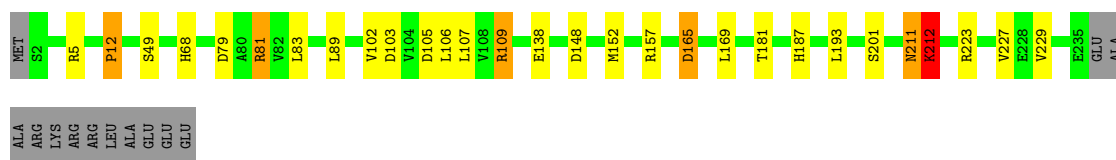
- Molecule 4: Proteasome subunit alpha type

Chain D:  84% 10% • 5%



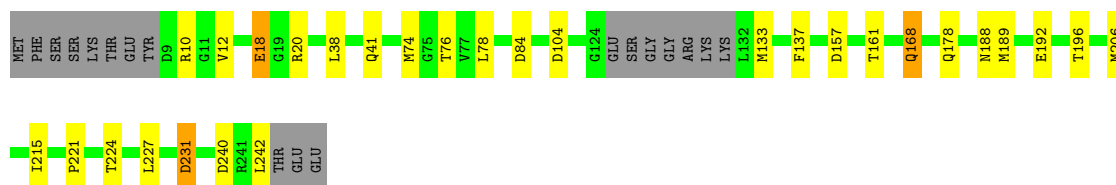
- Molecule 4: Proteasome subunit alpha type

Chain R:  83% 9% • 5%



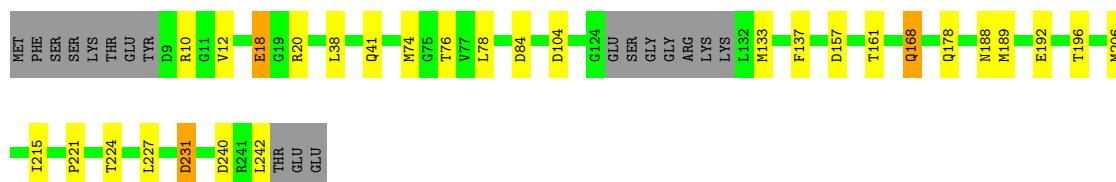
- Molecule 5: Proteasome subunit alpha type

Chain E:  81% 11% • 7%



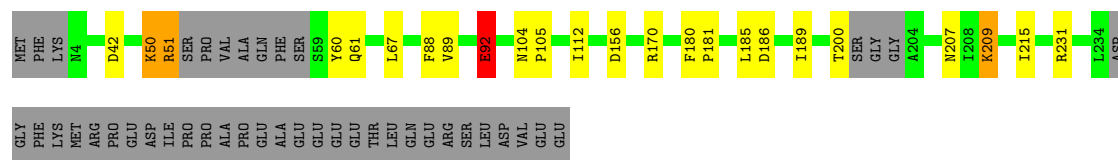
- Molecule 5: Proteasome subunit alpha type

Chain S:  81% 11% • 7%



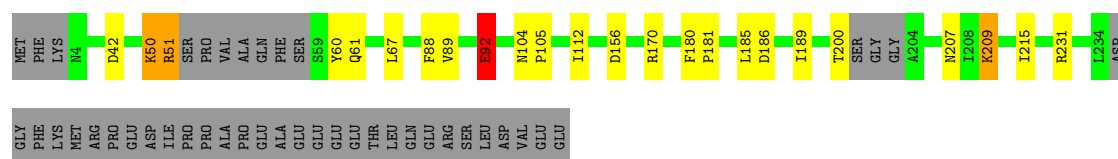
- Molecule 6: Proteasome subunit alpha type

Chain F: 



- Molecule 6: Proteasome subunit alpha type

Chain T: 



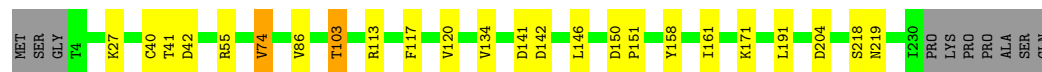
- Molecule 7: Putative proteasome alpha 7 subunit

Chain G: 



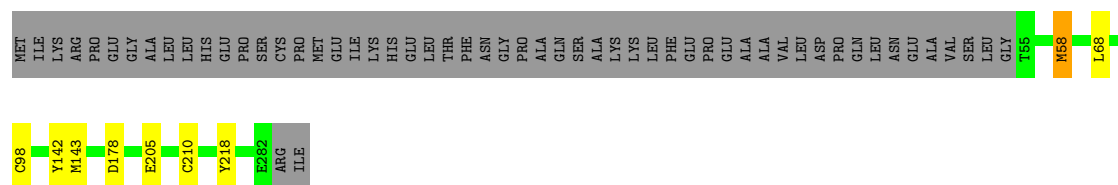
- Molecule 7: Putative proteasome alpha 7 subunit

Chain U: 



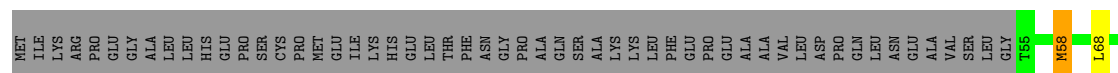
- Molecule 8: Proteasome subunit beta

Chain H: 



- Molecule 8: Proteasome subunit beta

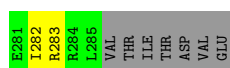
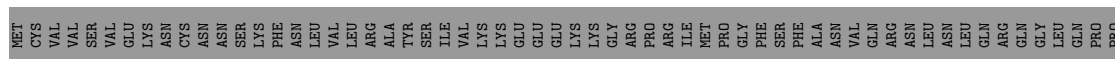
Chain V: 





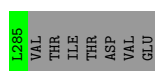
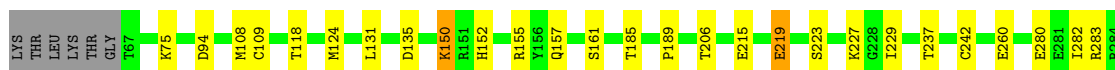
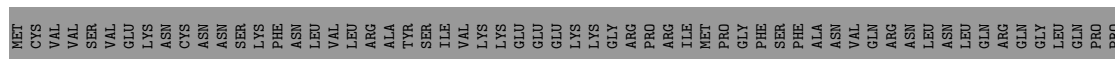
- Molecule 9: Proteasome subunit beta

Chain I: 65% 9% 25%



- Molecule 9: Proteasome subunit beta

Chain W: 66% 9% 25%



- Molecule 10: Putative proteasome beta 3 subunit

Chain J: 96%



- Molecule 10: Putative proteasome beta 3 subunit

Chain X: 96%



- Molecule 11: Proteasome subunit beta

Chain K: 92% 7%



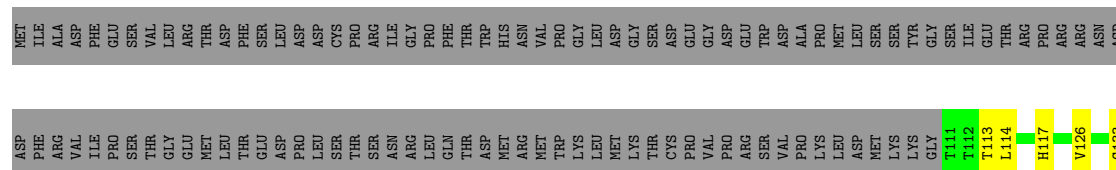
- Molecule 11: Proteasome subunit beta

Chain Y:  91% 7% •



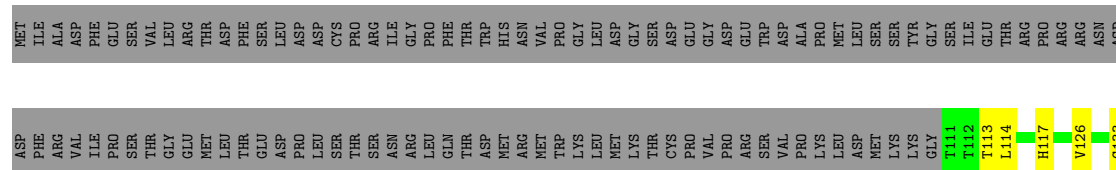
• Molecule 12: Proteasome subunit beta

Chain L:  59% 5% 35%



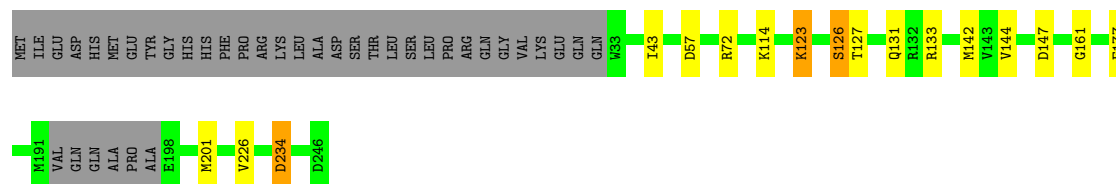
• Molecule 12: Proteasome subunit beta

Chain Z:  59% 5% 35%



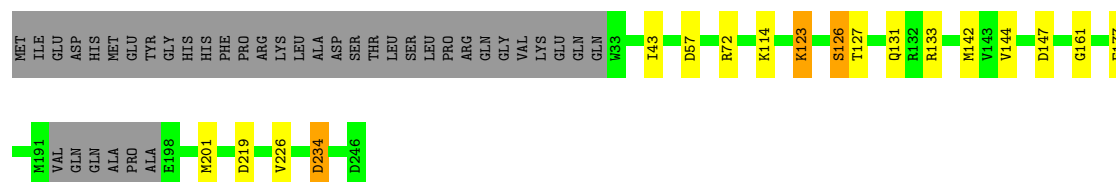
• Molecule 13: Proteasome subunit beta

Chain M:  78% 6% 15%

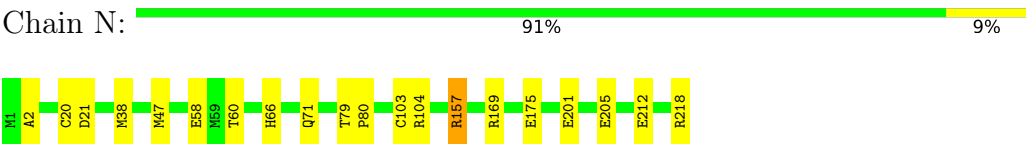


• Molecule 13: Proteasome subunit beta

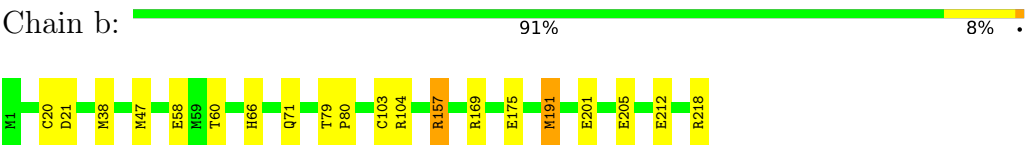
Chain a:  77% 6% 15%



● Molecule 14: Proteasome subunit beta



● Molecule 14: Proteasome subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92013	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 ($e^-/\text{\AA}^2$)	1.05	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

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	0.76	0/1922	1.17	6/2605 (0.2%)
1	O	0.76	0/1922	1.17	6/2605 (0.2%)
2	B	0.79	0/1770	1.15	2/2398 (0.1%)
2	P	0.79	0/1770	1.15	2/2398 (0.1%)
3	C	0.70	0/2168	1.07	5/2939 (0.2%)
3	Q	0.70	0/2168	1.07	5/2939 (0.2%)
4	D	0.64	0/1894	1.12	3/2549 (0.1%)
4	R	0.64	0/1894	1.12	3/2549 (0.1%)
5	E	0.66	0/1783	1.06	2/2417 (0.1%)
5	S	0.66	0/1783	1.06	2/2417 (0.1%)
6	F	0.74	0/1757	1.13	2/2375 (0.1%)
6	T	0.74	0/1757	1.13	2/2375 (0.1%)
7	G	0.76	0/1755	1.14	4/2379 (0.2%)
7	U	0.76	0/1755	1.14	4/2379 (0.2%)
8	H	0.81	0/1757	1.17	0/2380
8	V	0.81	0/1757	1.17	0/2380
9	I	0.84	0/1690	1.24	6/2286 (0.3%)
9	W	0.83	0/1690	1.24	6/2286 (0.3%)
10	J	0.82	0/1580	1.17	1/2131 (0.0%)
10	X	0.82	0/1580	1.17	1/2131 (0.0%)
11	K	0.80	0/1612	1.16	4/2177 (0.2%)
11	Y	0.80	0/1612	1.16	4/2177 (0.2%)
12	L	0.81	0/1611	1.08	2/2178 (0.1%)
12	Z	0.81	0/1611	1.08	2/2178 (0.1%)
13	M	0.79	0/1682	1.17	2/2270 (0.1%)
13	a	0.79	0/1682	1.17	2/2270 (0.1%)
14	N	0.88	0/1733	1.18	3/2344 (0.1%)
14	b	0.88	0/1733	1.17	3/2344 (0.1%)
All	All	0.77	0/49428	1.14	84/66856 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
4	R	0	2
5	E	0	1
5	S	0	1
7	G	0	2
7	U	0	2
11	K	0	2
11	Y	0	2
12	L	0	1
12	Z	0	1
13	M	0	1
13	a	0	1
14	N	0	2
14	b	0	2
All	All	0	22

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	48	LYS	CB-CA-C	-9.92	97.02	111.70
2	B	48	LYS	CB-CA-C	-9.90	97.05	111.70
13	a	177	PHE	CB-CA-C	-7.44	98.29	110.79
13	M	177	PHE	CB-CA-C	-7.43	98.31	110.79
7	G	142	ASP	CA-CB-CG	7.36	119.96	112.60
7	U	142	ASP	CA-CB-CG	7.31	119.91	112.60
3	C	6	ASP	CA-CB-CG	7.06	119.66	112.60
4	D	12	PRO	N-CA-C	7.06	127.02	112.47
11	K	155	ASP	CA-CB-CG	7.06	119.66	112.60
3	Q	6	ASP	CA-CB-CG	7.05	119.65	112.60
4	R	12	PRO	N-CA-C	7.04	126.97	112.47
11	Y	155	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	144	ASP	CA-CB-CG	7.01	119.61	112.60
1	O	144	ASP	CA-CB-CG	6.96	119.56	112.60
1	O	117	ASP	CB-CA-C	-6.74	99.40	110.85
4	R	79	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	117	ASP	CB-CA-C	-6.62	99.59	110.85
4	D	79	ASP	CA-CB-CG	6.60	119.20	112.60
12	L	117	HIS	CA-CB-CG	6.56	120.36	113.80
12	Z	117	HIS	CA-CB-CG	6.53	120.33	113.80
5	E	84	ASP	CA-CB-CG	6.50	119.09	112.60
5	S	84	ASP	CA-CB-CG	6.49	119.09	112.60
9	W	94	ASP	CA-CB-CG	6.45	119.05	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	94	ASP	CA-CB-CG	6.42	119.02	112.60
6	T	156	ASP	CA-CB-CG	6.40	119.00	112.60
1	O	75	THR	CB-CA-C	-6.39	96.74	109.33
1	A	75	THR	CB-CA-C	-6.38	96.76	109.33
6	F	156	ASP	CA-CB-CG	6.38	118.98	112.60
1	O	59	ARG	CB-CA-C	6.35	116.16	110.44
11	K	9	ARG	CG-CD-NE	-6.35	98.03	112.00
13	M	147	ASP	CA-CB-CG	6.33	118.93	112.60
11	Y	9	ARG	CG-CD-NE	-6.32	98.11	112.00
1	A	59	ARG	CB-CA-C	6.28	116.09	110.44
13	a	147	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	75	THR	CA-CB-OG1	6.26	118.99	109.60
1	O	75	THR	CA-CB-OG1	6.24	118.95	109.60
14	b	103	CYS	CB-CA-C	-6.16	96.53	110.07
14	N	103	CYS	CB-CA-C	-6.15	96.55	110.07
9	W	135	ASP	CA-CB-CG	6.15	118.75	112.60
9	I	135	ASP	CA-CB-CG	6.09	118.69	112.60
14	b	175	GLU	CB-CG-CD	5.94	122.70	112.60
14	N	175	GLU	CB-CG-CD	5.91	122.66	112.60
4	D	165	ASP	CA-CB-CG	5.72	118.32	112.60
4	R	165	ASP	CA-CB-CG	5.67	118.27	112.60
9	I	189	PRO	N-CA-C	5.65	121.90	114.27
9	W	189	PRO	N-CA-C	5.63	121.87	114.27
1	O	83	ASP	CA-CB-CG	5.60	118.20	112.60
3	Q	88	ASP	CA-CB-CG	5.53	118.12	112.60
12	L	117	HIS	N-CA-CB	-5.52	101.88	110.55
1	A	83	ASP	CA-CB-CG	5.52	118.12	112.60
12	Z	117	HIS	N-CA-CB	-5.52	101.89	110.55
3	C	88	ASP	CA-CB-CG	5.50	118.10	112.60
3	Q	14	PRO	N-CA-C	5.50	123.79	112.47
11	Y	138	VAL	O-C-N	-5.49	117.88	121.72
3	C	14	PRO	N-CA-C	5.48	123.76	112.47
10	X	135	ASP	CA-CB-CG	5.41	118.01	112.60
14	N	66	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
10	J	135	ASP	CA-CB-CG	5.37	117.97	112.60
14	b	66	HIS	CE1-NE2-CD2	-5.37	103.64	109.00
11	K	138	VAL	O-C-N	-5.36	117.97	121.72
2	P	163	LYS	CB-CA-C	-5.35	102.41	110.92
3	Q	63	ASP	CA-CB-CG	5.32	117.92	112.60
2	B	163	LYS	CB-CA-C	-5.31	102.47	110.92
3	C	63	ASP	CA-CB-CG	5.31	117.91	112.60
7	U	103	THR	CA-CB-OG1	5.29	117.53	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	103	THR	CA-CB-OG1	5.27	117.51	109.60
9	W	155	ARG	CB-CA-C	-5.17	101.06	110.63
9	I	155	ARG	CB-CA-C	-5.17	101.07	110.63
7	U	146	LEU	N-CA-CB	-5.16	102.66	110.77
11	Y	78	ARG	CB-CA-C	-5.16	100.04	109.54
7	G	146	LEU	N-CA-CB	-5.16	102.67	110.77
11	K	78	ARG	CB-CA-C	-5.14	100.08	109.54
3	C	161	ASN	CA-CB-CG	-5.09	107.51	112.60
7	G	141	ASP	CA-CB-CG	5.09	117.69	112.60
9	W	219	GLU	CB-CG-CD	5.09	121.25	112.60
6	F	92	GLU	CB-CG-CD	5.08	121.24	112.60
5	E	74	MET	CB-CA-C	-5.06	99.11	109.38
9	I	219	GLU	CB-CG-CD	5.06	121.20	112.60
3	Q	161	ASN	CA-CB-CG	-5.06	107.54	112.60
9	I	227	LYS	CB-CA-C	-5.06	102.39	110.79
6	T	92	GLU	CB-CG-CD	5.05	121.18	112.60
5	S	74	MET	CB-CA-C	-5.04	99.16	109.38
9	W	227	LYS	CB-CA-C	-5.02	102.45	110.79
7	U	141	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	109	ARG	Sidechain
4	D	157	ARG	Sidechain
5	E	10	ARG	Sidechain
7	G	113	ARG	Sidechain
7	G	42	ASP	Peptide
11	K	78	ARG	Sidechain
11	K	9	ARG	Sidechain
12	L	183	ARG	Sidechain
13	M	72	ARG	Sidechain
14	N	104	ARG	Sidechain
14	N	157	ARG	Sidechain
4	R	109	ARG	Sidechain
4	R	157	ARG	Sidechain
5	S	10	ARG	Sidechain
7	U	113	ARG	Sidechain
7	U	42	ASP	Peptide
11	Y	78	ARG	Sidechain
11	Y	9	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
12	Z	183	ARG	Sidechain
13	a	72	ARG	Sidechain
14	b	104	ARG	Sidechain
14	b	157	ARG	Sidechain

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	1884	0	1874	4	0
1	O	1884	0	1874	4	0
2	B	1737	0	1716	5	0
2	P	1737	0	1716	5	0
3	C	2126	0	2090	15	0
3	Q	2126	0	2090	15	0
4	D	1864	0	1861	10	0
4	R	1864	0	1861	13	0
5	E	1757	0	1755	12	0
5	S	1757	0	1755	12	0
6	F	1722	0	1703	9	0
6	T	1722	0	1703	9	0
7	G	1724	0	1691	8	0
7	U	1724	0	1691	8	0
8	H	1723	0	1694	3	0
8	V	1723	0	1694	3	0
9	I	1663	0	1698	9	0
9	W	1663	0	1698	8	0
10	J	1555	0	1549	5	0
10	X	1555	0	1549	5	0
11	K	1586	0	1573	6	0
11	Y	1586	0	1573	6	0
12	L	1578	0	1526	10	0
12	Z	1578	0	1526	10	0
13	M	1647	0	1594	4	0
13	a	1647	0	1594	5	0
14	N	1695	0	1654	8	0
14	b	1695	0	1654	8	0
15	A	39	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	B	33	0	0	0	0
15	C	33	0	0	0	0
15	D	21	0	0	0	0
15	E	22	0	0	2	0
15	F	26	0	0	1	0
15	G	33	0	0	0	0
15	H	52	0	0	0	0
15	I	44	0	0	1	0
15	J	50	0	0	0	0
15	K	37	0	0	2	0
15	L	29	0	0	1	0
15	M	48	0	0	0	0
15	N	69	0	0	2	0
15	O	39	0	0	0	0
15	P	33	0	0	0	0
15	Q	33	0	0	0	0
15	R	21	0	0	0	0
15	S	22	0	0	2	0
15	T	26	0	0	1	0
15	U	33	0	0	0	0
15	V	52	0	0	0	0
15	W	45	0	0	1	0
15	X	50	0	0	0	0
15	Y	37	0	0	2	0
15	Z	29	0	0	1	0
15	a	48	0	0	1	0
15	b	70	0	0	1	0
All	All	49596	0	47956	203	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 2.

All (203) 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:N:157:ARG:HD3	15:N:348:HOH:O	1.60	0.98
14:b:157:ARG:HD3	15:b:348:HOH:O	1.62	0.96
9:I:124:MET:HE1	9:I:152:HIS:ND1	2.05	0.72
11:Y:22:ASN:ND2	11:Y:33:GLU:OE1	2.21	0.72
9:W:124:MET:HE1	9:W:152:HIS:ND1	2.05	0.70
10:X:12:LEU:C	10:X:12:LEU:HD23	2.18	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:12:LEU:C	10:J:12:LEU:HD23	2.18	0.69
6:F:189:ILE:HD11	6:F:215:ILE:HD11	1.75	0.67
6:F:209:LYS:HG2	15:F:319:HOH:O	1.95	0.67
6:T:189:ILE:HD11	6:T:215:ILE:HD11	1.75	0.67
6:T:209:LYS:HG2	15:T:319:HOH:O	1.95	0.66
11:K:22:ASN:ND2	11:K:33:GLU:OE1	2.21	0.66
11:Y:88:ASN:HB2	15:Y:317:HOH:O	1.96	0.66
11:K:88:ASN:HB2	15:K:317:HOH:O	1.96	0.65
10:J:125:ASP:OD2	10:J:129:ALA:HB3	1.98	0.64
8:V:58:MET:HE2	8:V:210:CYS:SG	2.38	0.64
10:X:125:ASP:OD2	10:X:129:ALA:HB3	1.97	0.63
8:H:58:MET:HE2	8:H:210:CYS:SG	2.38	0.63
4:R:148:ASP:OD1	4:R:152:MET:HB3	1.99	0.62
4:D:148:ASP:OD1	4:D:152:MET:HB3	1.99	0.61
14:b:169:ARG:HD3	14:b:201:GLU:O	2.01	0.60
5:S:20:ARG:NH1	15:S:302:HOH:O	2.35	0.60
6:F:92:GLU:HG2	6:F:112:ILE:HD13	1.83	0.60
3:C:121:CYS:SG	3:C:156:THR:HG23	2.42	0.60
3:Q:121:CYS:SG	3:Q:156:THR:HG23	2.42	0.59
14:N:169:ARG:HD3	14:N:201:GLU:O	2.01	0.59
4:D:89:LEU:HD23	11:K:67:LEU:HD21	1.85	0.59
6:T:92:GLU:HG2	6:T:112:ILE:HD13	1.83	0.58
5:E:20:ARG:NH1	15:E:302:HOH:O	2.35	0.58
4:R:89:LEU:HD23	11:Y:67:LEU:HD21	1.85	0.58
11:K:3:GLU:HG2	11:K:35:LYS:NZ	2.19	0.57
7:G:150:ASP:HB2	7:G:151:PRO:CD	2.35	0.57
12:L:310:VAL:O	12:L:310:VAL:CG1	2.51	0.57
12:Z:310:VAL:CG1	12:Z:310:VAL:O	2.51	0.57
14:N:21:ASP:OD1	14:N:21:ASP:C	2.48	0.57
11:Y:3:GLU:HG2	11:Y:35:LYS:NZ	2.19	0.57
3:C:157:ASP:C	3:C:157:ASP:OD1	2.48	0.57
3:Q:199:LEU:HD23	3:Q:216:LEU:HD23	1.87	0.57
7:U:150:ASP:HB2	7:U:151:PRO:CD	2.35	0.57
4:D:223:ARG:O	4:D:227:VAL:HG23	2.05	0.56
12:L:268:ARG:HE	12:L:272:HIS:HE1	1.53	0.56
3:Q:157:ASP:OD1	3:Q:157:ASP:C	2.47	0.56
4:R:223:ARG:O	4:R:227:VAL:HG23	2.05	0.56
4:D:68:HIS:HE1	4:D:102:VAL:O	1.88	0.56
12:L:277:ASP:O	15:L:401:HOH:O	2.18	0.56
4:R:68:HIS:HE1	4:R:102:VAL:O	1.88	0.56
12:L:310:VAL:O	12:L:310:VAL:HG13	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:268:ARG:HE	12:Z:272:HIS:HE1	1.53	0.56
12:Z:277:ASP:O	15:Z:401:HOH:O	2.18	0.55
12:Z:310:VAL:O	12:Z:310:VAL:HG13	2.06	0.55
7:G:117:PHE:O	7:G:120:VAL:HG12	2.07	0.55
3:C:199:LEU:HD23	3:C:216:LEU:HD23	1.87	0.55
12:L:114:LEU:C	12:L:114:LEU:HD12	2.32	0.55
14:b:21:ASP:OD1	14:b:21:ASP:C	2.47	0.55
7:U:117:PHE:O	7:U:120:VAL:HG12	2.07	0.55
4:D:211:ASN:O	4:D:212:LYS:HB2	2.07	0.55
3:Q:124:LYS:NZ	3:Q:156:THR:HG22	2.22	0.55
12:Z:114:LEU:C	12:Z:114:LEU:HD12	2.32	0.55
5:E:221:PRO:HG2	5:E:224:THR:HG22	1.89	0.54
4:R:211:ASN:O	4:R:212:LYS:HB2	2.07	0.54
3:C:124:LYS:NZ	3:C:156:THR:HG22	2.22	0.54
5:S:221:PRO:HG2	5:S:224:THR:HG22	1.89	0.53
13:M:43:ILE:HG13	13:M:142:MET:HE2	1.91	0.53
11:K:1:MET:HE3	11:K:145:TYR:CD1	2.44	0.53
11:Y:1:MET:HE3	11:Y:145:TYR:CD1	2.44	0.52
13:M:234:ASP:OD1	13:M:234:ASP:N	2.42	0.52
5:S:18:GLU:HG3	15:S:302:HOH:O	2.10	0.51
9:W:229:ILE:O	15:W:301:HOH:O	2.19	0.51
1:O:75:THR:HG23	1:O:137:PHE:CD1	2.46	0.51
13:a:43:ILE:HG13	13:a:142:MET:HE2	1.91	0.51
5:E:18:GLU:HG3	15:E:302:HOH:O	2.09	0.50
5:E:206:MET:HE1	5:E:215:ILE:CG2	2.41	0.50
9:I:150:LYS:HE2	9:I:185:THR:CG2	2.42	0.50
5:S:231:ASP:N	5:S:231:ASP:OD1	2.44	0.50
14:b:20:CYS:SG	14:b:38:MET:HE3	2.51	0.50
1:A:75:THR:HG23	1:A:137:PHE:CD1	2.46	0.50
5:E:157:ASP:OD1	5:E:157:ASP:C	2.55	0.50
9:W:150:LYS:HE2	9:W:185:THR:CG2	2.42	0.50
5:S:206:MET:HE1	5:S:215:ILE:CG2	2.41	0.50
9:I:124:MET:HE1	9:I:152:HIS:CG	2.47	0.50
5:S:157:ASP:C	5:S:157:ASP:OD1	2.55	0.50
2:B:187:HIS:CE1	2:B:231:ILE:HG22	2.47	0.50
5:E:231:ASP:N	5:E:231:ASP:OD1	2.44	0.49
14:N:20:CYS:SG	14:N:38:MET:HE3	2.51	0.49
2:P:187:HIS:CE1	2:P:231:ILE:HG22	2.48	0.49
9:W:124:MET:HE1	9:W:152:HIS:CG	2.47	0.49
3:C:124:LYS:HZ2	3:C:156:THR:HG22	1.77	0.49
7:U:150:ASP:HB2	7:U:151:PRO:HD2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TRP:CH2	1:A:163:GLY:HA3	2.48	0.49
5:E:38:LEU:C	5:E:38:LEU:HD12	2.38	0.49
9:I:271:PRO:O	9:I:274:THR:OG1	2.25	0.49
3:Q:199:LEU:CD2	3:Q:216:LEU:HD23	2.43	0.49
3:C:199:LEU:CD2	3:C:216:LEU:HD23	2.43	0.48
5:S:38:LEU:C	5:S:38:LEU:HD12	2.38	0.48
7:G:150:ASP:HB2	7:G:151:PRO:HD2	1.94	0.48
9:I:280:GLU:OE1	10:J:198:ARG:NE	2.40	0.48
1:O:161:TRP:CH2	1:O:163:GLY:HA3	2.48	0.48
9:I:229:ILE:O	15:I:301:HOH:O	2.20	0.48
13:a:234:ASP:OD1	13:a:234:ASP:N	2.42	0.48
3:C:34:VAL:HG12	3:C:141:LEU:HD12	1.97	0.47
2:B:6:TYR:OH	3:C:2:SER:O	2.28	0.47
3:C:233:LEU:HD23	10:J:186:VAL:HG11	1.96	0.47
3:Q:233:LEU:HD23	10:X:186:VAL:HG11	1.96	0.47
12:L:233:HIS:HE1	15:Y:329:HOH:O	1.98	0.47
9:W:280:GLU:OE1	10:X:198:ARG:NE	2.40	0.47
3:Q:228:ALA:HB2	9:W:283:ARG:HD3	1.96	0.47
5:E:168:GLN:HE21	5:E:168:GLN:HA	1.80	0.47
3:Q:34:VAL:HG12	3:Q:141:LEU:HD12	1.96	0.47
3:Q:124:LYS:HZ2	3:Q:156:THR:HG22	1.79	0.47
3:Q:116:LEU:C	3:Q:116:LEU:HD13	2.40	0.46
3:C:228:ALA:HB2	9:I:283:ARG:HD3	1.97	0.46
2:P:162:GLY:O	2:P:165:SER:HB3	2.14	0.46
12:Z:154:THR:O	12:Z:209:THR:HG23	2.16	0.46
2:B:162:GLY:O	2:B:165:SER:HB3	2.15	0.46
7:G:74:VAL:HG13	7:G:134:VAL:HG13	1.98	0.46
2:P:6:TYR:OH	3:Q:2:SER:O	2.28	0.46
6:F:88:PHE:CE2	6:F:112:ILE:HD12	2.51	0.46
12:L:154:THR:O	12:L:209:THR:HG23	2.16	0.45
7:U:55:ARG:HH11	7:U:55:ARG:HG3	1.81	0.45
6:F:180:PHE:N	6:F:181:PRO:CD	2.79	0.45
5:S:168:GLN:HE21	5:S:168:GLN:HA	1.81	0.45
2:B:37:LYS:HE2	3:C:57:ASP:OD2	2.17	0.45
3:C:116:LEU:C	3:C:116:LEU:HD13	2.40	0.45
6:T:88:PHE:CE2	6:T:112:ILE:HD12	2.51	0.45
7:G:55:ARG:HG3	7:G:55:ARG:HH11	1.81	0.45
6:T:180:PHE:N	6:T:181:PRO:CD	2.79	0.45
7:U:74:VAL:HG13	7:U:134:VAL:HG13	1.98	0.45
2:P:37:LYS:HE2	3:Q:57:ASP:OD2	2.17	0.45
3:Q:191:LEU:O	3:Q:195:ILE:HG13	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:47:MET:HE2	14:N:60:THR:HG22	1.99	0.44
10:X:12:LEU:HD23	10:X:12:LEU:O	2.17	0.44
14:b:79:THR:HB	14:b:80:PRO:HD2	2.00	0.44
10:J:12:LEU:HD23	10:J:12:LEU:O	2.17	0.44
15:K:327:HOH:O	12:Z:233:HIS:HE1	1.99	0.44
12:Z:113:THR:HG22	12:Z:126:VAL:HG12	2.00	0.44
6:T:104:ASN:HD22	6:T:105:PRO:HD2	1.82	0.44
5:E:133:MET:HE1	5:E:137:PHE:CE2	2.53	0.44
6:F:185:LEU:O	6:F:189:ILE:HG13	2.18	0.44
4:R:68:HIS:CE1	4:R:102:VAL:O	2.70	0.44
12:Z:225:ASP:OD1	12:Z:225:ASP:C	2.61	0.44
13:a:219:ASP:O	15:a:301:HOH:O	2.21	0.44
6:F:104:ASN:HD22	6:F:105:PRO:HD2	1.82	0.43
14:b:47:MET:HE2	14:b:60:THR:HG22	1.99	0.43
12:L:113:THR:HG22	12:L:126:VAL:HG12	2.00	0.43
5:S:133:MET:HE1	5:S:137:PHE:CE2	2.53	0.43
13:M:126:SER:OG	13:M:161:GLY:O	2.36	0.43
14:N:79:THR:HB	14:N:80:PRO:HD2	2.00	0.43
4:D:68:HIS:CE1	4:D:102:VAL:O	2.70	0.43
3:C:191:LEU:O	3:C:195:ILE:HG13	2.18	0.43
3:Q:13:SER:HB3	3:Q:14:PRO:CD	2.48	0.43
12:L:225:ASP:OD1	12:L:225:ASP:C	2.61	0.43
4:D:211:ASN:O	4:D:212:LYS:CB	2.67	0.43
5:E:240:ASP:C	5:E:242:LEU:H	2.27	0.43
6:T:185:LEU:O	6:T:189:ILE:HG13	2.18	0.43
13:a:126:SER:OG	13:a:161:GLY:O	2.36	0.43
3:C:53:ASN:OD1	3:C:54:SER:N	2.52	0.43
7:G:218:SER:O	7:G:219:ASN:HB2	2.19	0.43
3:C:13:SER:HB3	3:C:14:PRO:CD	2.48	0.43
4:R:187:HIS:CE1	4:R:229:VAL:HG22	2.54	0.42
14:b:191:MET:HE3	14:b:191:MET:HB2	1.95	0.42
2:P:37:LYS:NZ	2:P:142:ASN:O	2.50	0.42
9:W:108:MET:HG3	9:W:242:CYS:SG	2.59	0.42
8:H:68:LEU:HD23	8:H:98:CYS:SG	2.59	0.42
3:Q:53:ASN:OD1	3:Q:54:SER:N	2.52	0.42
4:D:187:HIS:CE1	4:D:229:VAL:HG22	2.54	0.42
11:K:3:GLU:HG2	11:K:35:LYS:HZ3	1.83	0.42
9:I:108:MET:HG3	9:I:242:CYS:SG	2.59	0.42
4:R:193:LEU:HD23	4:R:193:LEU:HA	1.89	0.42
6:F:67:LEU:HD13	6:F:89:VAL:HG11	2.02	0.42
4:R:107:LEU:C	4:R:107:LEU:HD13	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:104:ASP:HB2	13:a:123:LYS:HG2	2.01	0.42
6:T:67:LEU:HD13	6:T:89:VAL:HG11	2.02	0.42
4:D:107:LEU:C	4:D:107:LEU:HD13	2.44	0.42
5:E:104:ASP:HB2	13:M:123:LYS:HG2	2.01	0.42
4:R:211:ASN:O	4:R:212:LYS:CB	2.67	0.42
5:S:240:ASP:C	5:S:242:LEU:H	2.27	0.42
7:U:218:SER:O	7:U:219:ASN:HB2	2.19	0.42
12:Z:268:ARG:HE	12:Z:272:HIS:CE1	2.37	0.42
8:V:68:LEU:HD23	8:V:98:CYS:SG	2.59	0.41
4:D:106:LEU:HD13	4:D:109:ARG:HH12	1.84	0.41
8:V:142:TYR:CE2	14:b:58:GLU:HG3	2.56	0.41
6:T:50:LYS:O	6:T:51:ARG:C	2.64	0.41
7:G:86:VAL:HG11	7:G:134:VAL:HG21	2.02	0.41
4:R:81:ARG:HH21	4:R:81:ARG:HD3	1.69	0.41
4:R:106:LEU:HD13	4:R:109:ARG:HH12	1.84	0.41
5:E:78:LEU:HD12	5:E:78:LEU:C	2.46	0.41
9:I:150:LYS:HE2	9:I:185:THR:HG23	2.02	0.41
6:F:50:LYS:O	6:F:51:ARG:C	2.63	0.41
7:U:86:VAL:HG11	7:U:134:VAL:HG21	2.02	0.41
7:U:158:TYR:CE1	7:U:161:ILE:HD13	2.56	0.41
4:R:165:ASP:O	4:R:169:LEU:HB2	2.21	0.41
5:S:78:LEU:C	5:S:78:LEU:HD12	2.46	0.41
8:H:142:TYR:CE2	14:N:58:GLU:HG3	2.56	0.41
9:W:150:LYS:HE2	9:W:185:THR:HG23	2.03	0.41
11:Y:54:ARG:HH21	11:Y:54:ARG:HD2	1.73	0.41
12:L:268:ARG:HE	12:L:272:HIS:CE1	2.37	0.40
14:N:2:ALA:N	15:N:306:HOH:O	2.54	0.40
7:G:158:TYR:CE1	7:G:161:ILE:HD13	2.56	0.40
1:A:81:ALA:N	1:A:82:PRO:HD2	2.36	0.40
1:O:81:ALA:N	1:O:82:PRO:HD2	2.37	0.40
1:O:75:THR:HG23	1:O:137:PHE:CE1	2.56	0.40
1:A:75:THR:HG23	1:A:137:PHE:CE1	2.56	0.40
2:B:58:LEU:HD23	2:B:58:LEU:HA	1.92	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	242/268 (90%)	237 (98%)	4 (2%)	1 (0%)	30	31
1	O	242/268 (90%)	237 (98%)	4 (2%)	1 (0%)	30	31
2	B	226/231 (98%)	222 (98%)	4 (2%)	0	100	100
2	P	226/231 (98%)	222 (98%)	4 (2%)	0	100	100
3	C	269/286 (94%)	257 (96%)	8 (3%)	4 (2%)	8	4
3	Q	269/286 (94%)	257 (96%)	8 (3%)	4 (2%)	8	4
4	D	232/247 (94%)	220 (95%)	8 (3%)	4 (2%)	7	3
4	R	232/247 (94%)	220 (95%)	8 (3%)	4 (2%)	7	3
5	E	223/245 (91%)	214 (96%)	9 (4%)	0	100	100
5	S	223/245 (91%)	214 (96%)	9 (4%)	0	100	100
6	F	215/265 (81%)	209 (97%)	6 (3%)	0	100	100
6	T	215/265 (81%)	209 (97%)	6 (3%)	0	100	100
7	G	225/237 (95%)	219 (97%)	6 (3%)	0	100	100
7	U	225/237 (95%)	218 (97%)	7 (3%)	0	100	100
8	H	226/284 (80%)	222 (98%)	4 (2%)	0	100	100
8	V	226/284 (80%)	222 (98%)	4 (2%)	0	100	100
9	I	217/292 (74%)	208 (96%)	8 (4%)	1 (0%)	24	24
9	W	217/292 (74%)	208 (96%)	8 (4%)	1 (0%)	24	24
10	J	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	X	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
11	K	204/206 (99%)	200 (98%)	3 (2%)	1 (0%)	24	24
11	Y	204/206 (99%)	200 (98%)	3 (2%)	1 (0%)	24	24
12	L	199/311 (64%)	191 (96%)	7 (4%)	1 (0%)	24	24
12	Z	199/311 (64%)	191 (96%)	7 (4%)	1 (0%)	24	24
13	M	204/246 (83%)	199 (98%)	4 (2%)	1 (0%)	24	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	204/246 (83%)	199 (98%)	4 (2%)	1 (0%)	24	24
14	N	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
14	b	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	6200/7082 (88%)	6011 (97%)	163 (3%)	26 (0%)	31	31

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	212	LYS
4	R	212	LYS
3	C	172	GLN
3	Q	172	GLN
3	C	227	PRO
4	D	201	SER
11	K	72	GLU
3	Q	227	PRO
4	R	201	SER
11	Y	72	GLU
4	D	49	SER
4	D	211	ASN
4	R	49	SER
4	R	211	ASN
1	A	145	ALA
3	C	207	ASP
9	I	237	THR
13	M	133	ARG
1	O	145	ALA
3	Q	207	ASP
3	Q	228	ALA
9	W	237	THR
13	a	133	ARG
3	C	228	ALA
12	L	133	GLY
12	Z	133	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/221 (90%)	190 (96%)	9 (4%)	24	29
1	O	199/221 (90%)	190 (96%)	9 (4%)	24	29
2	B	187/190 (98%)	180 (96%)	7 (4%)	30	37
2	P	187/190 (98%)	180 (96%)	7 (4%)	30	37
3	C	225/239 (94%)	214 (95%)	11 (5%)	22	24
3	Q	225/239 (94%)	214 (95%)	11 (5%)	22	24
4	D	201/211 (95%)	193 (96%)	8 (4%)	28	34
4	R	201/211 (95%)	192 (96%)	9 (4%)	24	29
5	E	191/207 (92%)	178 (93%)	13 (7%)	14	14
5	S	191/207 (92%)	178 (93%)	13 (7%)	14	14
6	F	179/217 (82%)	167 (93%)	12 (7%)	15	14
6	T	179/217 (82%)	167 (93%)	12 (7%)	15	14
7	G	188/196 (96%)	180 (96%)	8 (4%)	26	31
7	U	188/196 (96%)	180 (96%)	8 (4%)	26	31
8	H	187/234 (80%)	182 (97%)	5 (3%)	39	49
8	V	187/234 (80%)	182 (97%)	5 (3%)	39	49
9	I	179/246 (73%)	166 (93%)	13 (7%)	13	12
9	W	179/246 (73%)	166 (93%)	13 (7%)	13	12
10	J	166/167 (99%)	164 (99%)	2 (1%)	63	74
10	X	166/167 (99%)	164 (99%)	2 (1%)	63	74
11	K	168/168 (100%)	162 (96%)	6 (4%)	31	39
11	Y	168/168 (100%)	163 (97%)	5 (3%)	36	45
12	L	164/265 (62%)	159 (97%)	5 (3%)	36	45
12	Z	164/265 (62%)	159 (97%)	5 (3%)	36	45
13	M	175/208 (84%)	165 (94%)	10 (6%)	18	19
13	a	175/208 (84%)	165 (94%)	10 (6%)	18	19
14	N	177/177 (100%)	173 (98%)	4 (2%)	44	55
14	b	177/177 (100%)	172 (97%)	5 (3%)	38	48
All	All	5172/5892 (88%)	4945 (96%)	227 (4%)	27	29

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	57	LEU
1	A	75	THR
1	A	146	ASP
1	A	164	SER
1	A	193	LEU
1	A	233	ARG
1	A	241	GLU
1	A	244	THR
2	B	13	PRO
2	B	39	MET
2	B	52	SER
2	B	90	LYS
2	B	183	GLU
2	B	215	LYS
2	B	218	LEU
3	C	2	SER
3	C	15	GLU
3	C	26	GLU
3	C	30	GLN
3	C	87	SER
3	C	98	LEU
3	C	155	HIS
3	C	178	GLN
3	C	179	SER
3	C	186	LYS
3	C	229	THR
4	D	5	ARG
4	D	81	ARG
4	D	83	LEU
4	D	103	ASP
4	D	105	ASP
4	D	138	GLU
4	D	181	THR
4	D	212	LYS
5	E	12	VAL
5	E	18	GLU
5	E	41	GLN
5	E	76	THR
5	E	161	THR
5	E	168	GLN
5	E	178	GLN
5	E	188	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	189	MET
5	E	192	GLU
5	E	196	THR
5	E	227	LEU
5	E	231	ASP
6	F	42	ASP
6	F	50	LYS
6	F	51	ARG
6	F	60	TYR
6	F	61	GLN
6	F	92	GLU
6	F	170	ARG
6	F	186	ASP
6	F	200	THR
6	F	207	ASN
6	F	209	LYS
6	F	231	ARG
7	G	27	LYS
7	G	40	CYS
7	G	41	THR
7	G	74	VAL
7	G	103	THR
7	G	171	LYS
7	G	191	LEU
7	G	204	ASP
8	H	58	MET
8	H	143	MET
8	H	178	ASP
8	H	205	GLU
8	H	218	TYR
9	I	75	LYS
9	I	109	CYS
9	I	118	THR
9	I	131	LEU
9	I	150	LYS
9	I	157	GLN
9	I	161	SER
9	I	206	THR
9	I	215	GLU
9	I	219	GLU
9	I	223	SER
9	I	260	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	282	ILE
10	J	12	LEU
10	J	131	CYS
11	K	9	ARG
11	K	63	CYS
11	K	67	LEU
11	K	75	ARG
11	K	77	ILE
11	K	201	ILE
12	L	142	MET
12	L	220	SER
12	L	302	GLN
12	L	304	LYS
12	L	310	VAL
13	M	57	ASP
13	M	114	LYS
13	M	123	LYS
13	M	126	SER
13	M	127	THR
13	M	131	GLN
13	M	144	VAL
13	M	201	MET
13	M	226	VAL
13	M	234	ASP
14	N	71	GLN
14	N	205	GLU
14	N	212	GLU
14	N	218	ARG
1	O	40	ARG
1	O	57	LEU
1	O	75	THR
1	O	146	ASP
1	O	164	SER
1	O	193	LEU
1	O	233	ARG
1	O	241	GLU
1	O	244	THR
2	P	13	PRO
2	P	39	MET
2	P	52	SER
2	P	90	LYS
2	P	183	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	215	LYS
2	P	218	LEU
3	Q	2	SER
3	Q	15	GLU
3	Q	26	GLU
3	Q	30	GLN
3	Q	87	SER
3	Q	98	LEU
3	Q	155	HIS
3	Q	178	GLN
3	Q	179	SER
3	Q	186	LYS
3	Q	229	THR
4	R	5	ARG
4	R	12	PRO
4	R	81	ARG
4	R	83	LEU
4	R	103	ASP
4	R	105	ASP
4	R	138	GLU
4	R	181	THR
4	R	212	LYS
5	S	12	VAL
5	S	18	GLU
5	S	41	GLN
5	S	76	THR
5	S	161	THR
5	S	168	GLN
5	S	178	GLN
5	S	188	ASN
5	S	189	MET
5	S	192	GLU
5	S	196	THR
5	S	227	LEU
5	S	231	ASP
6	T	42	ASP
6	T	50	LYS
6	T	51	ARG
6	T	60	TYR
6	T	61	GLN
6	T	92	GLU
6	T	170	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	186	ASP
6	T	200	THR
6	T	207	ASN
6	T	209	LYS
6	T	231	ARG
7	U	27	LYS
7	U	40	CYS
7	U	41	THR
7	U	74	VAL
7	U	103	THR
7	U	171	LYS
7	U	191	LEU
7	U	204	ASP
8	V	58	MET
8	V	143	MET
8	V	178	ASP
8	V	205	GLU
8	V	218	TYR
9	W	75	LYS
9	W	109	CYS
9	W	118	THR
9	W	131	LEU
9	W	150	LYS
9	W	157	GLN
9	W	161	SER
9	W	206	THR
9	W	215	GLU
9	W	219	GLU
9	W	223	SER
9	W	260	GLU
9	W	282	ILE
10	X	12	LEU
10	X	131	CYS
11	Y	63	CYS
11	Y	67	LEU
11	Y	75	ARG
11	Y	77	ILE
11	Y	201	ILE
12	Z	142	MET
12	Z	220	SER
12	Z	302	GLN
12	Z	304	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	310	VAL
13	a	57	ASP
13	a	114	LYS
13	a	123	LYS
13	a	126	SER
13	a	127	THR
13	a	131	GLN
13	a	144	VAL
13	a	201	MET
13	a	226	VAL
13	a	234	ASP
14	b	71	GLN
14	b	191	MET
14	b	205	GLU
14	b	212	GLU
14	b	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
2	B	107	GLN
2	B	142	ASN
2	B	178	ASN
2	B	223	GLN
3	C	94	ASN
3	C	149	HIS
3	C	230	GLN
4	D	68	HIS
4	D	92	GLN
4	D	97	ASN
4	D	143	HIS
5	E	41	GLN
5	E	155	GLN
5	E	168	GLN
5	E	188	ASN
6	F	104	ASN
7	G	223	GLN
8	H	112	GLN
8	H	115	ASN
8	H	129	ASN
8	H	196	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	211	GLN
9	I	139	GLN
10	J	26	ASN
11	K	11	ASN
11	K	73	HIS
11	K	136	GLN
12	L	233	HIS
12	L	272	HIS
14	N	90	HIS
14	N	203	ASN
1	O	89	GLN
2	P	107	GLN
2	P	142	ASN
2	P	178	ASN
2	P	223	GLN
3	Q	94	ASN
3	Q	149	HIS
3	Q	230	GLN
4	R	68	HIS
4	R	92	GLN
4	R	143	HIS
5	S	41	GLN
5	S	155	GLN
5	S	168	GLN
5	S	188	ASN
5	S	204	GLN
6	T	104	ASN
7	U	223	GLN
8	V	112	GLN
8	V	115	ASN
8	V	129	ASN
8	V	196	ASN
8	V	211	GLN
9	W	259	ASN
10	X	26	ASN
11	Y	11	ASN
11	Y	73	HIS
11	Y	136	GLN
12	Z	233	HIS
12	Z	272	HIS
14	b	81	ASN
14	b	90	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	b	203	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.

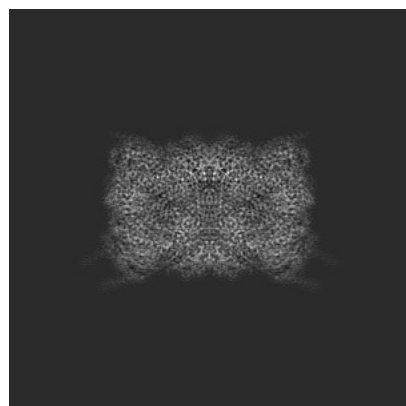
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50258. These allow visual inspection of the internal detail of the map and identification of artifacts.

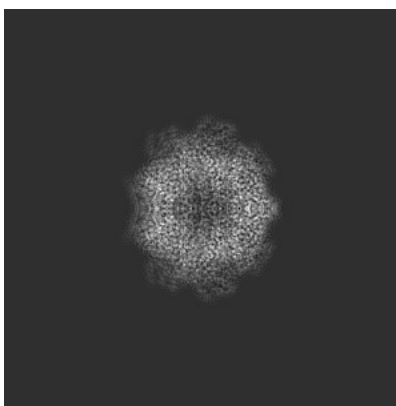
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

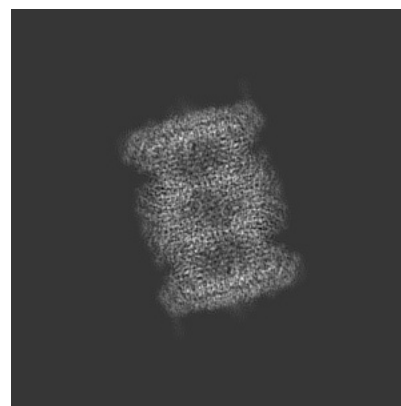
6.1.1 Primary map



X

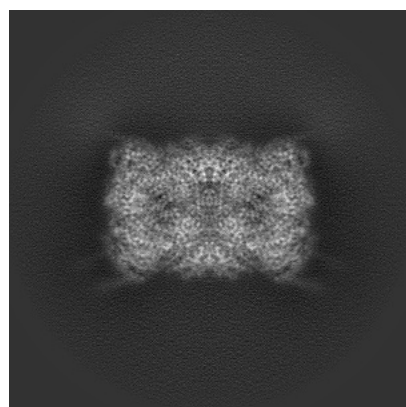


Y

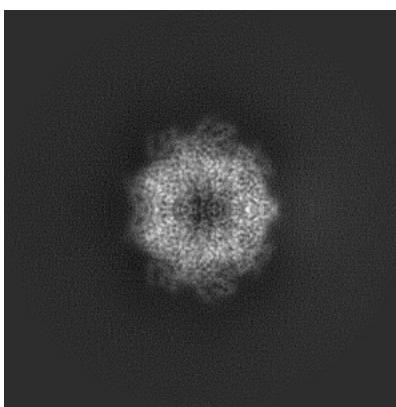


Z

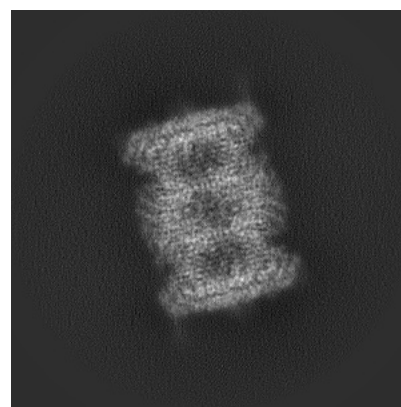
6.1.2 Raw map



X



Y

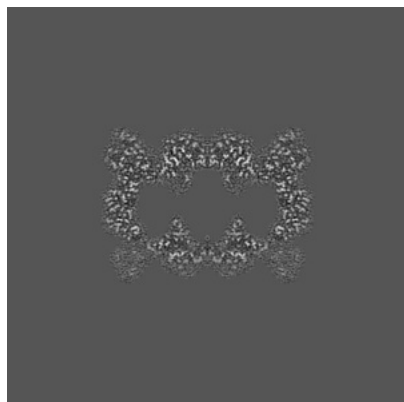


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

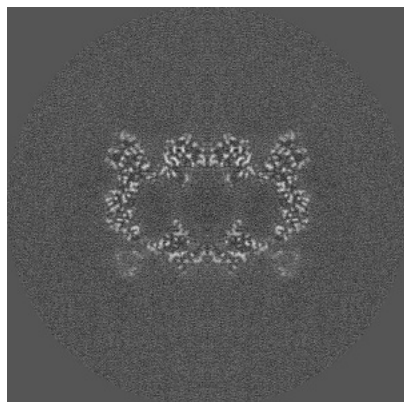


Y Index: 240

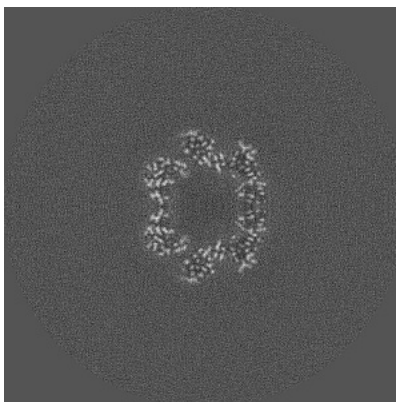


Z Index: 240

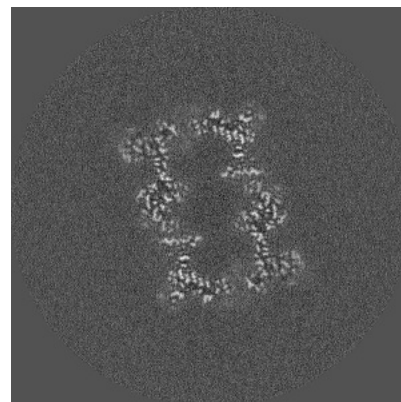
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

6.3 Largest variance slices [i](#)

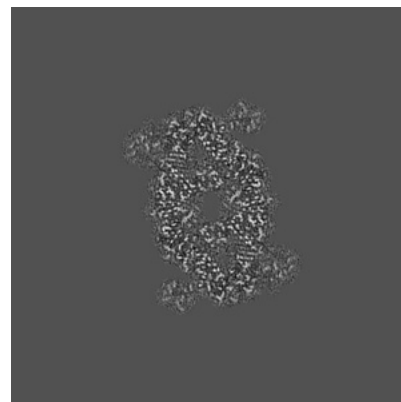
6.3.1 Primary map



X Index: 212

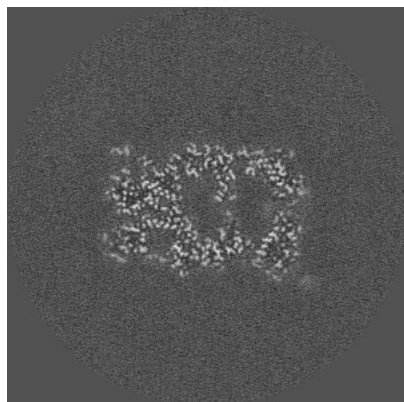


Y Index: 271

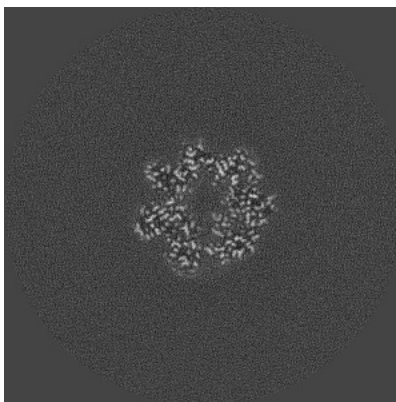


Z Index: 277

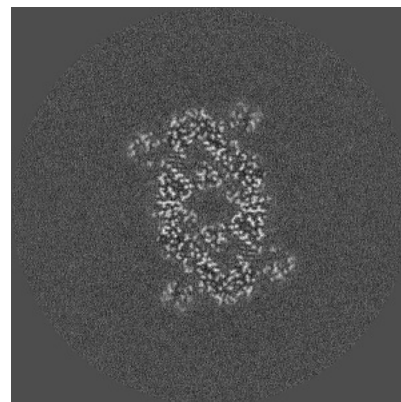
6.3.2 Raw map



X Index: 212



Y Index: 209

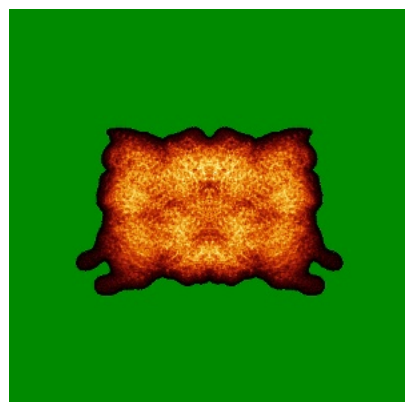


Z Index: 276

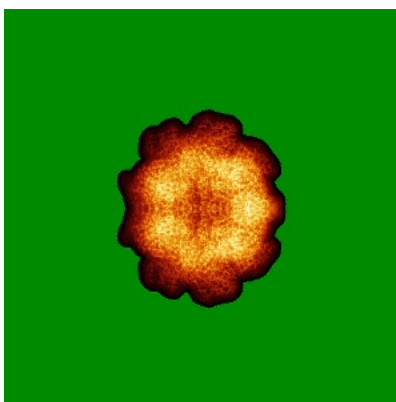
The images above show the largest variance slices of the map in three orthogonal directions.

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

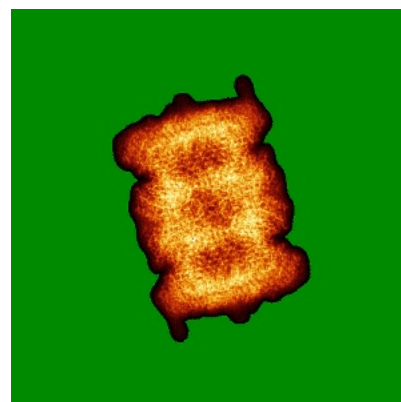
6.4.1 Primary map



X

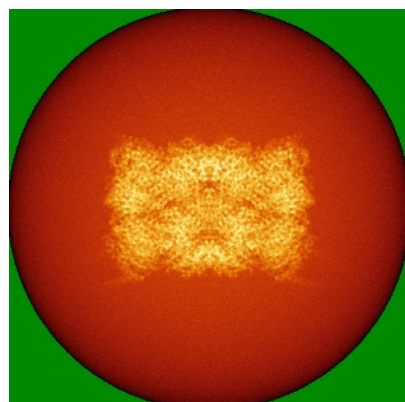


Y

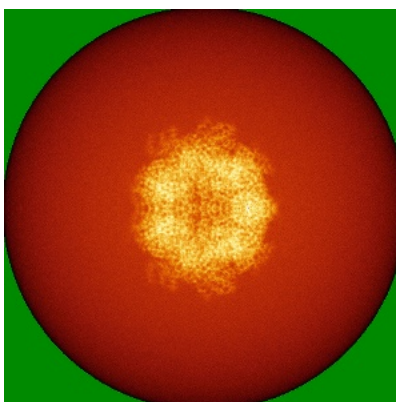


Z

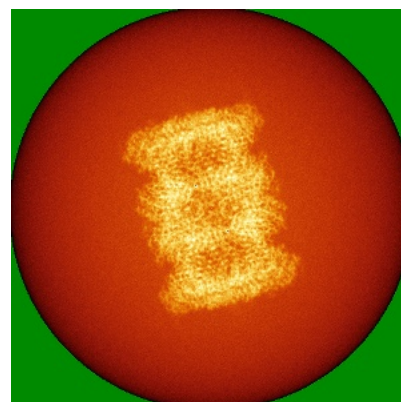
6.4.2 Raw map



X



Y

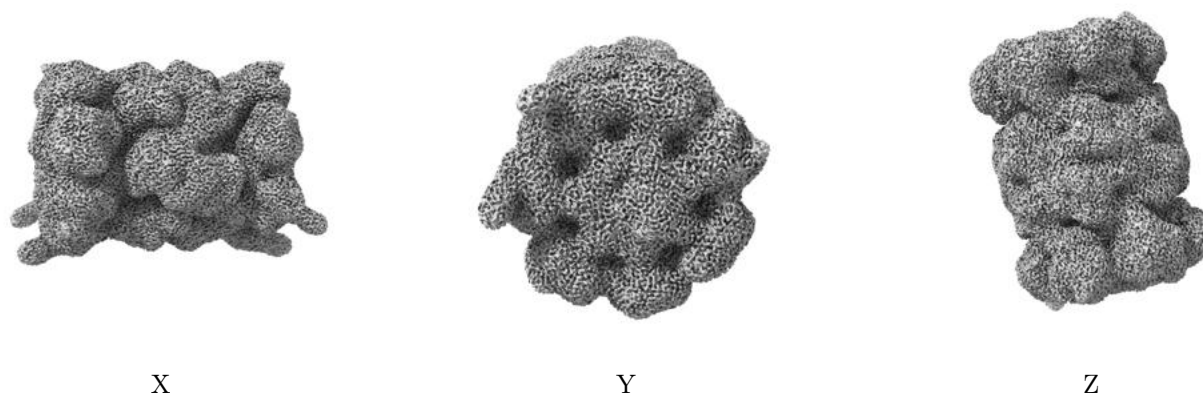


Z

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

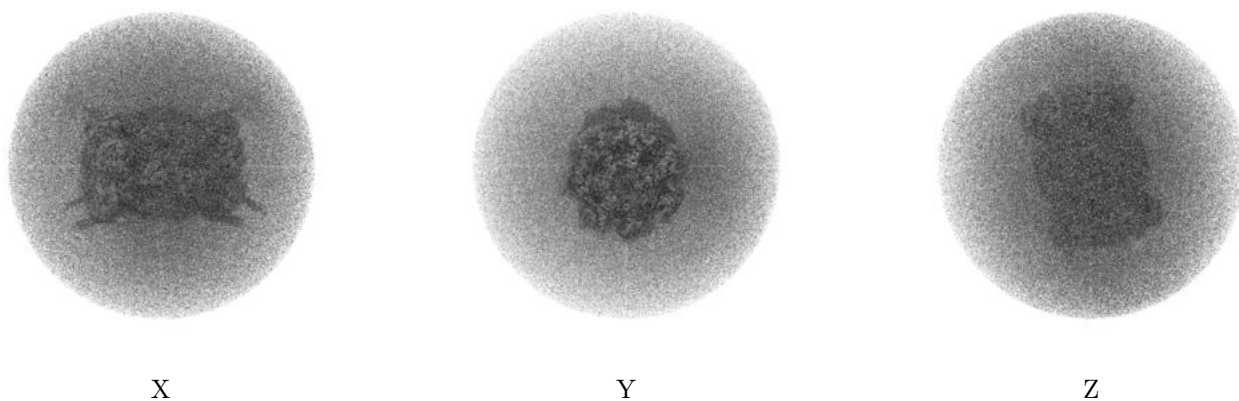
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

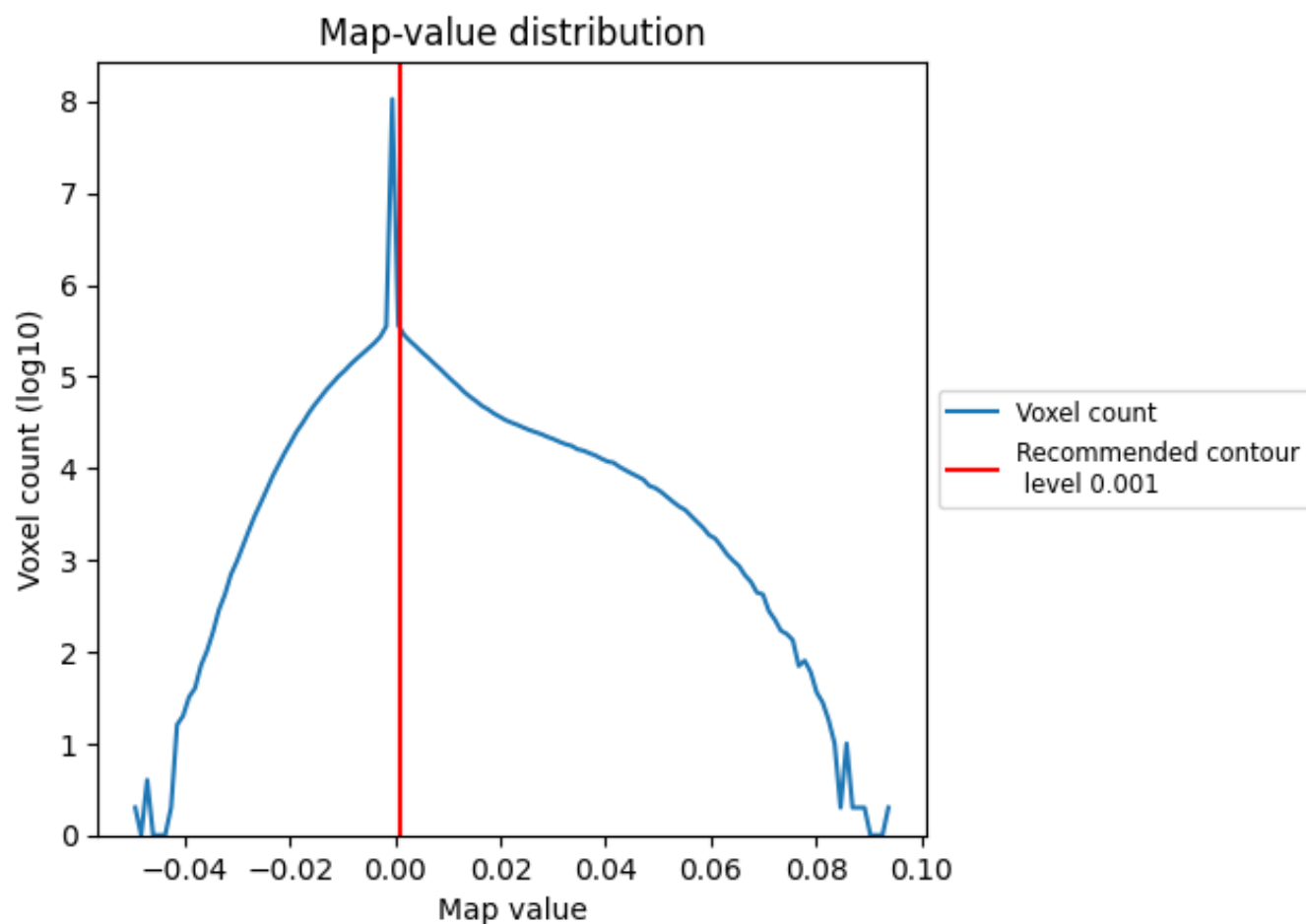
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

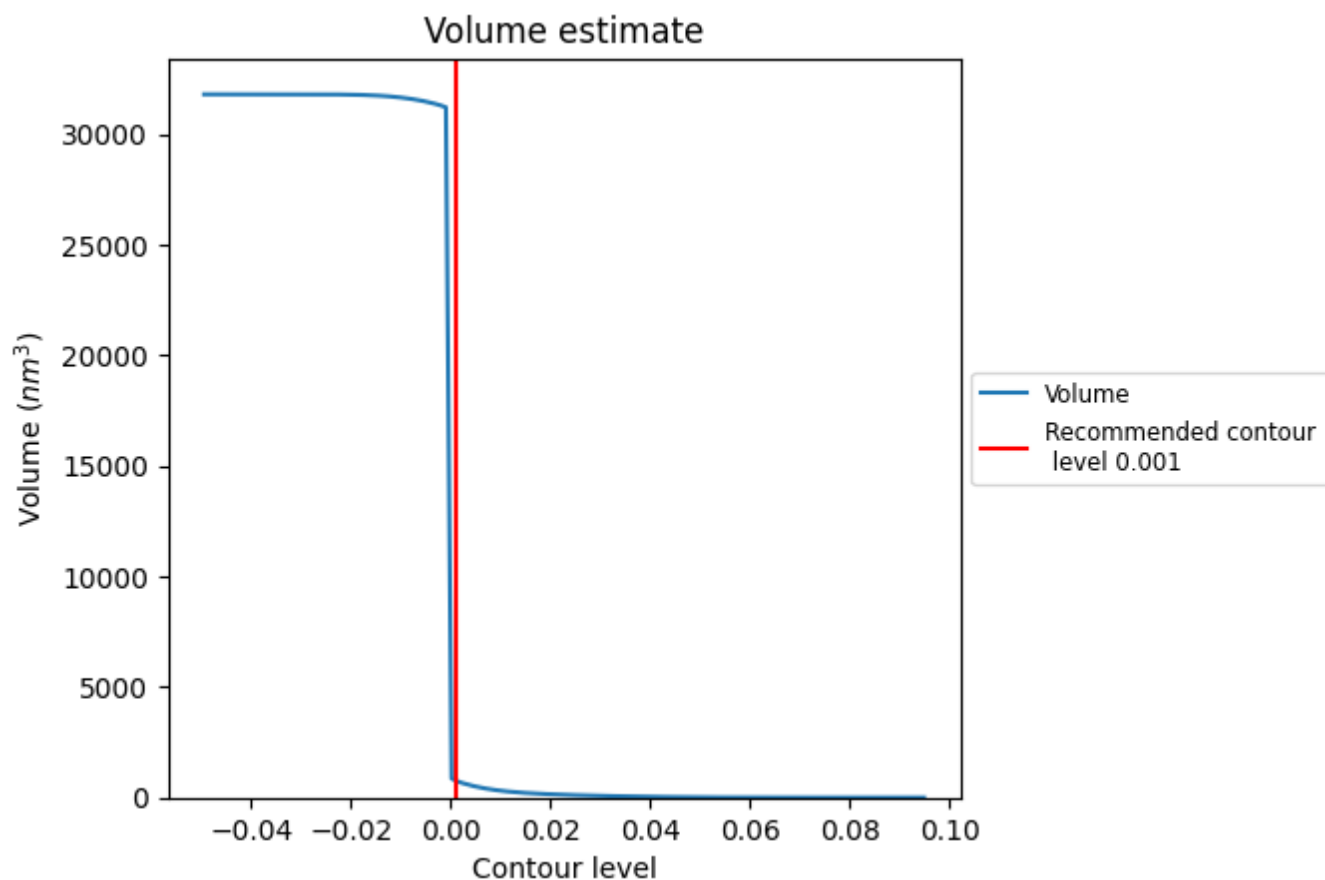
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

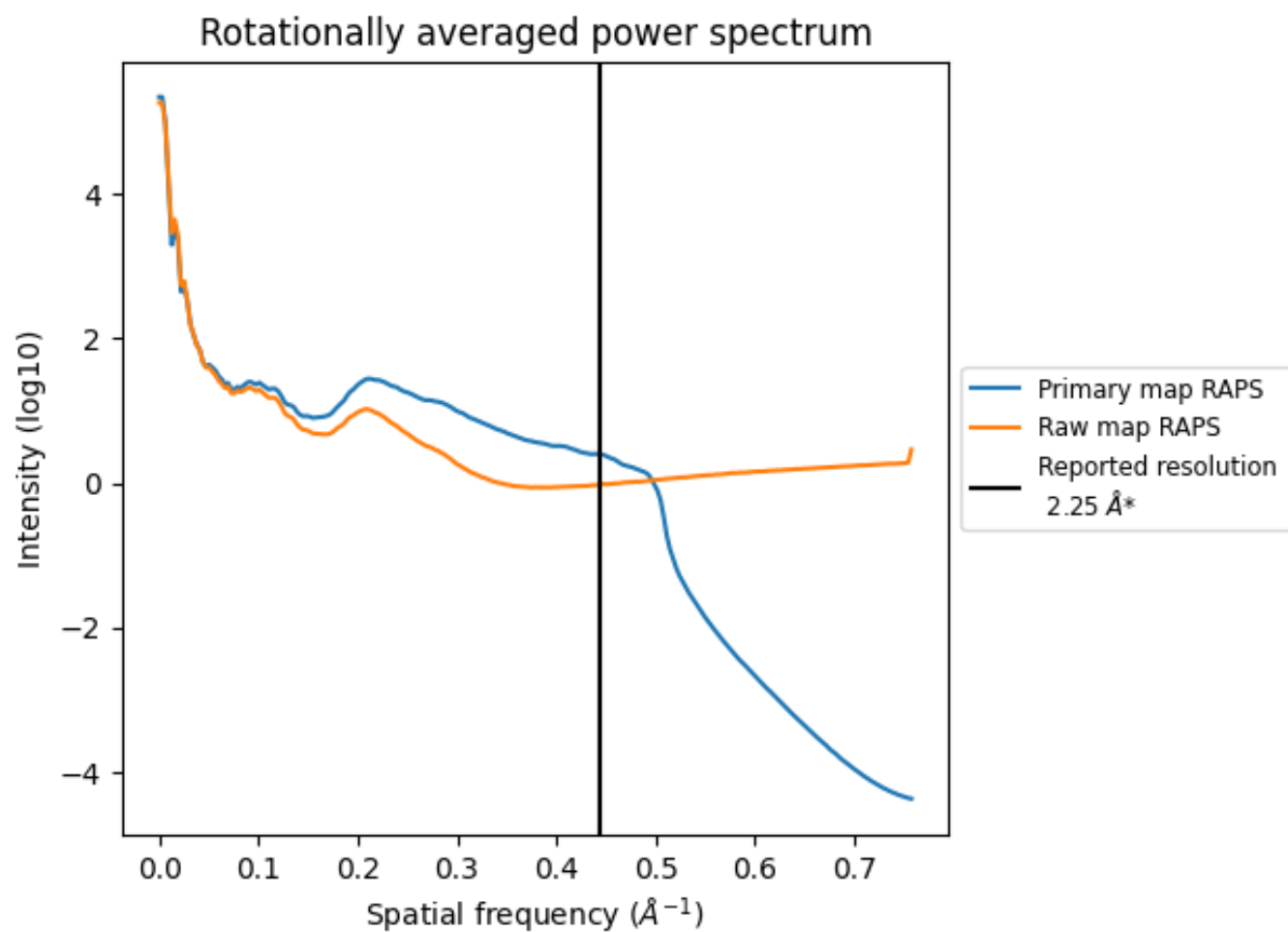
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 771 nm^3 ; this corresponds to an approximate mass of 696 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 ⓘ

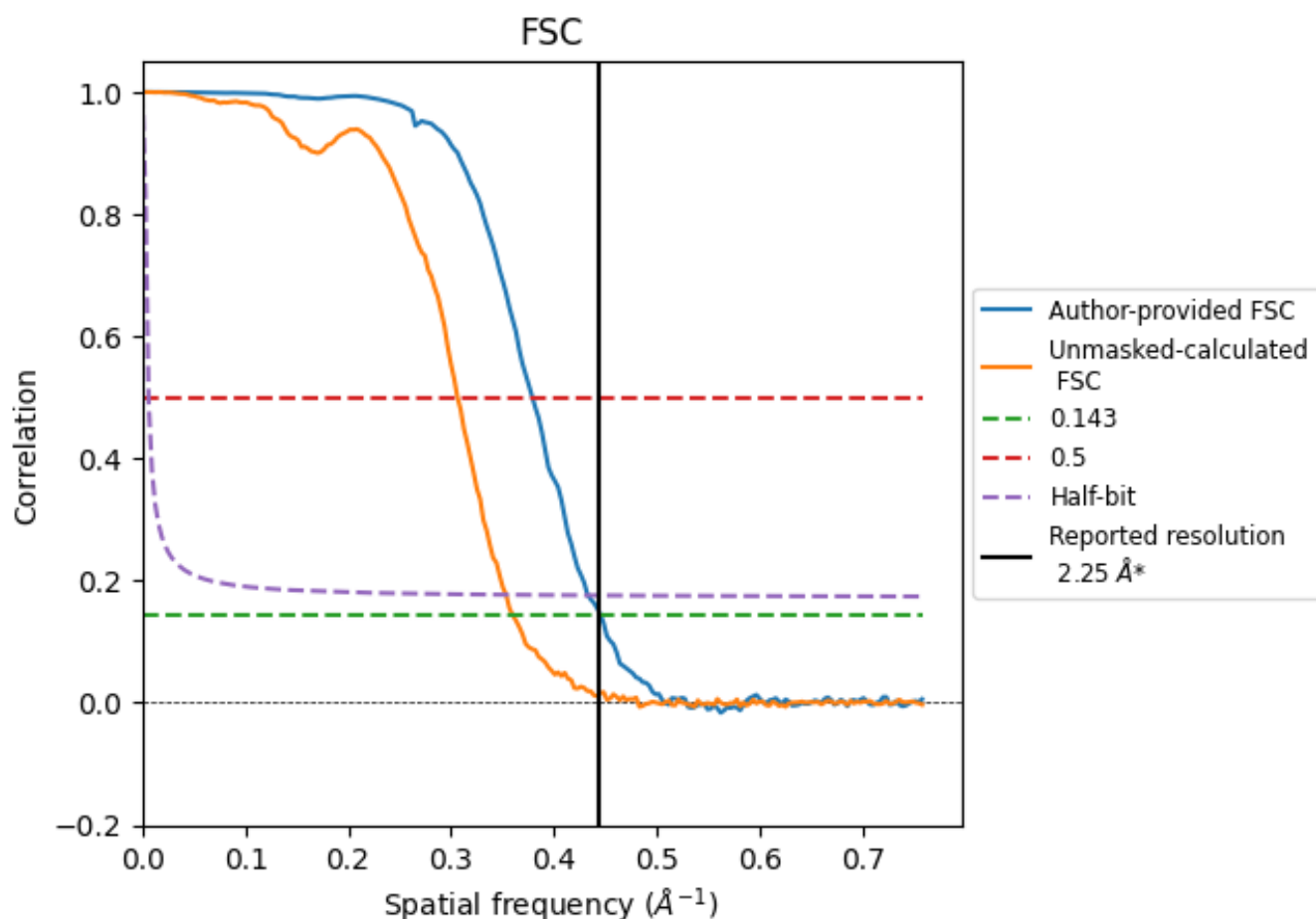


*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

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 $0.444 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

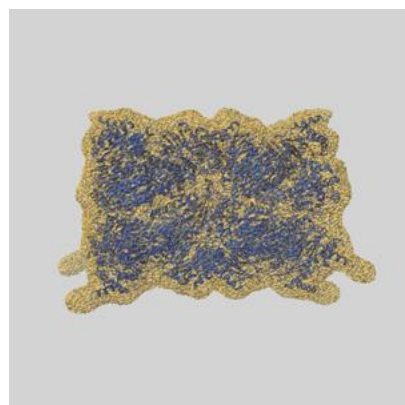
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.64	2.31
Unmasked-calculated*	2.78	3.27	2.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.78 differs from the reported value 2.25 by more than 10 %

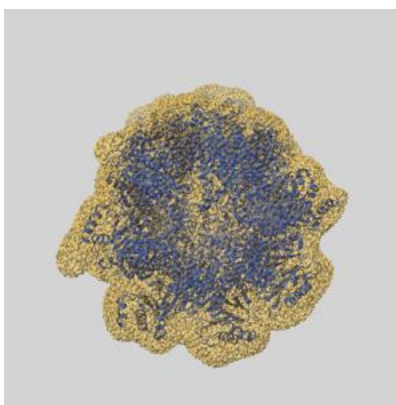
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50258 and PDB model 9F9P. Per-residue inclusion information can be found in section [3](#) on page [10](#).

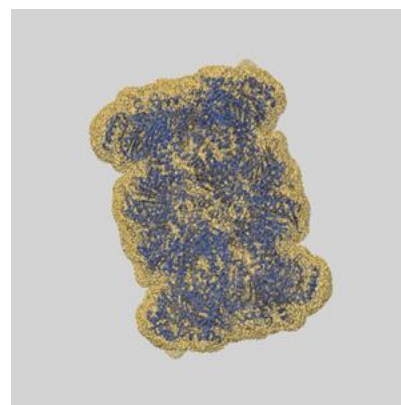
9.1 Map-model overlay [i](#)



X



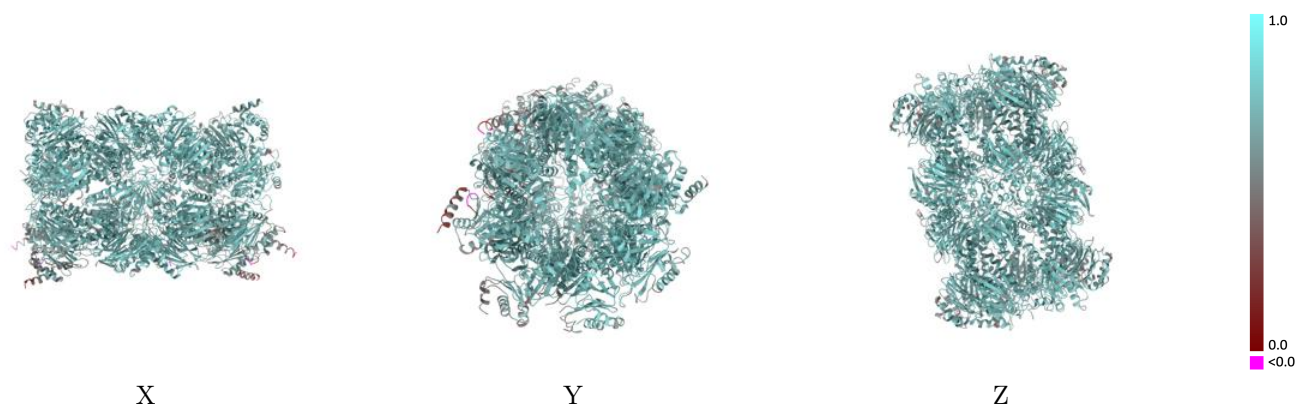
Y



Z

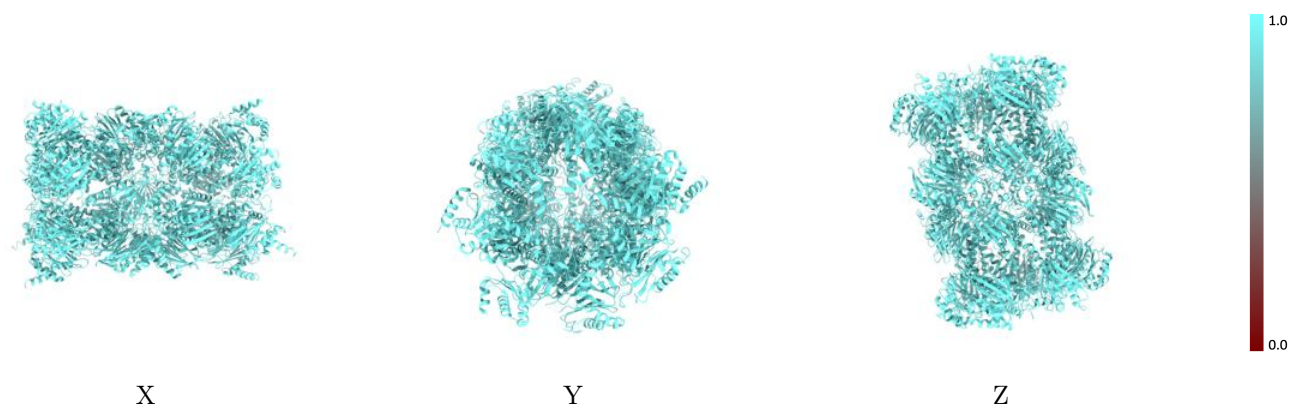
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



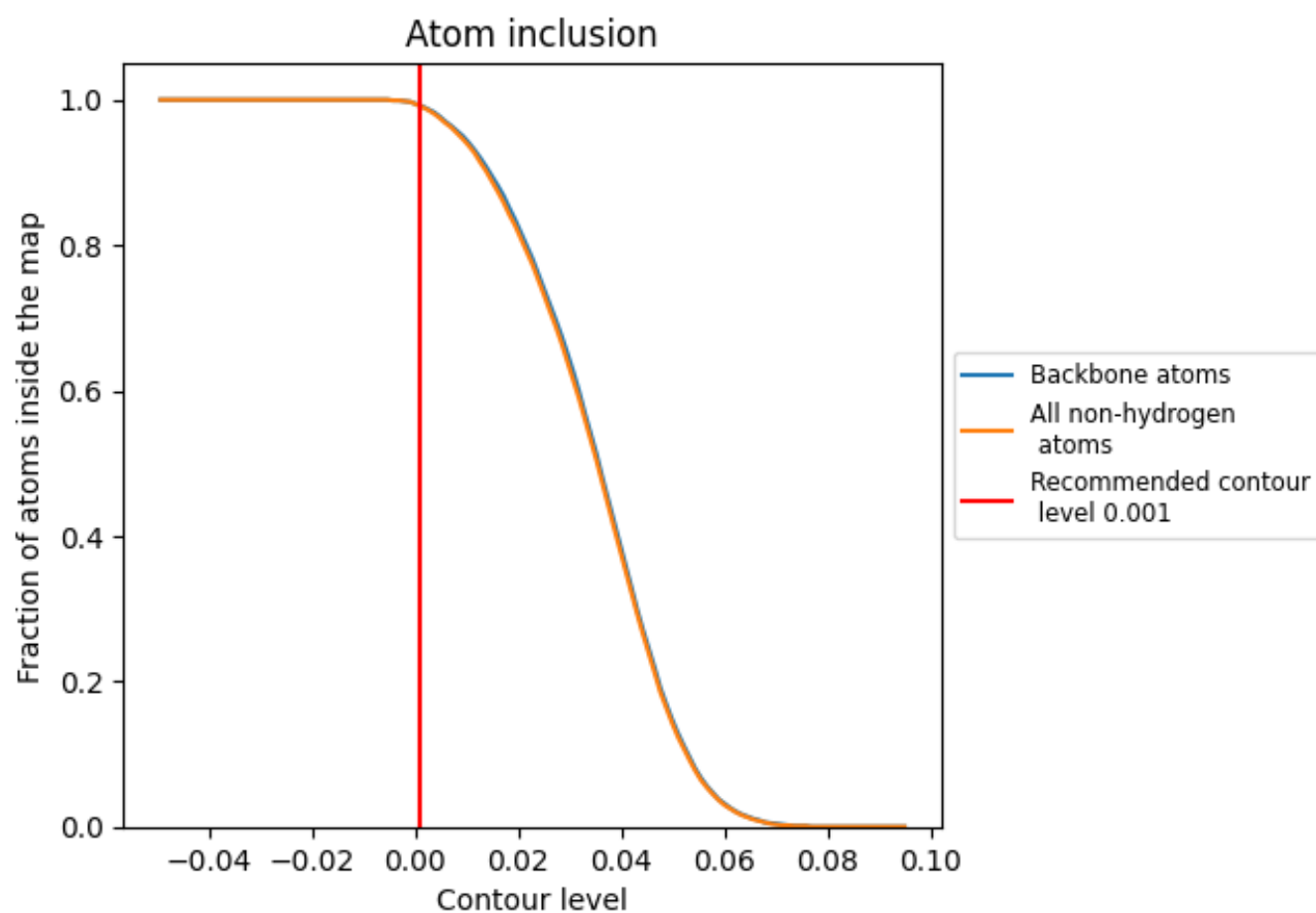
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.001).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9910	 0.6990
A	 0.9940	 0.7080
B	 0.9920	 0.7050
C	 0.9810	 0.6550
D	 0.9770	 0.6310
E	 0.9970	 0.6420
F	 0.9880	 0.6900
G	 0.9920	 0.7040
H	 0.9930	 0.7380
I	 0.9930	 0.7090
J	 0.9990	 0.7360
K	 0.9960	 0.7150
L	 0.9950	 0.7230
M	 0.9950	 0.7230
N	 0.9920	 0.7390
O	 0.9940	 0.7080
P	 0.9920	 0.7040
Q	 0.9810	 0.6560
R	 0.9770	 0.6280
S	 0.9970	 0.6430
T	 0.9880	 0.6900
U	 0.9920	 0.7020
V	 0.9930	 0.7370
W	 0.9940	 0.7110
X	 0.9990	 0.7350
Y	 0.9960	 0.7150
Z	 0.9950	 0.7240
a	 0.9950	 0.7220
b	 0.9920	 0.7370

