



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:59 PM UTC

PDB ID : 8T0M / pdb_00008t0m
EMDB ID : EMD-40944
Title : Proteasome 20S core particle from Pre1-1 Pre4-1 Double mutant
Authors : Walsh Jr., R.M.; Rawson, S.; Schnell, H.; Velez, B.; Hanna, J.
Deposited on : 2023-06-01
Resolution : 2.40 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

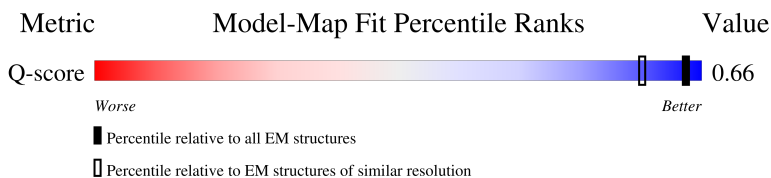
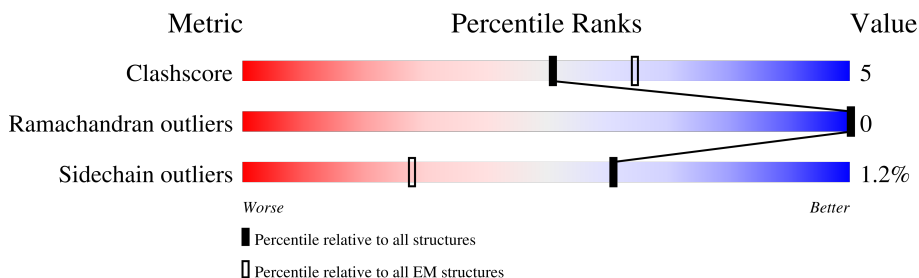
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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.



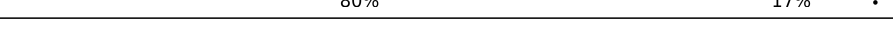
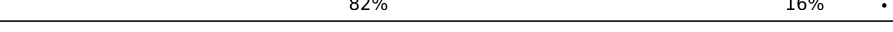
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	252	
1	O	252	
2	B	250	
2	P	250	

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Mol	Chain	Length	Quality of chain
3	C	258	
3	Q	258	
4	D	254	
4	R	254	
5	E	260	
5	S	260	
6	F	234	
6	T	234	
7	G	288	
7	U	288	
8	H	215	
8	V	215	
9	I	261	
9	W	261	
10	J	205	
10	X	205	
11	K	198	
11	Y	198	
12	L	287	
12	Z	287	
13	M	241	
13	a	241	
14	N	251	
14	b	251	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 47538 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1805	1152	301	344	8		
1	O	229	Total	C	N	O	S	0	0
			1805	1152	301	344	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	248	Total	C	N	O	S	0	0
			1900	1210	313	374	3		
2	P	248	Total	C	N	O	S	0	0
			1900	1210	313	374	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	237	Total	C	N	O	S	0	0
			1861	1177	313	368	3		
3	Q	237	Total	C	N	O	S	0	0
			1861	1177	313	368	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	221	Total	C	N	O	S	0	0
			1727	1084	298	341	4		
4	R	221	Total	C	N	O	S	0	0
			1727	1084	298	341	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	227	Total	C	N	O	S	0	0
			1750	1097	294	352	7		
5	S	227	Total	C	N	O	S	0	0
			1750	1097	294	352	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	230	Total	C	N	O	S	0	0
			1765	1110	305	346	4		
6	T	230	Total	C	N	O	S	0	0
			1765	1110	305	346	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	U	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	183	Total	C	N	O	S	0	0
			1424	905	234	278	7		
8	V	183	Total	C	N	O	S	0	0
			1424	905	234	278	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	202	Total	C	N	O	S	0	0
			1550	985	266	293	6		
9	W	202	Total	C	N	O	S	0	0
			1550	985	266	293	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	200	Total	C	N	O	S	0	0
			1551	991	254	298	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	200	Total	C	N	O	S	0	0
			1551	991	254	298	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	194	Total	C	N	O	S	0	0
			1558	993	263	297	5		
11	Y	194	Total	C	N	O	S	0	0
			1558	993	263	297	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	conflict	UNP P22141
Y	142	PHE	SER	conflict	UNP P22141

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	207	Total	C	N	O	S	0	0
			1617	1029	275	306	7		
12	Z	207	Total	C	N	O	S	0	0
			1617	1029	275	306	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	220	Total	C	N	O	S	0	0
			1737	1101	300	332	4		
13	a	220	Total	C	N	O	S	0	0
			1737	1101	300	332	4		

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

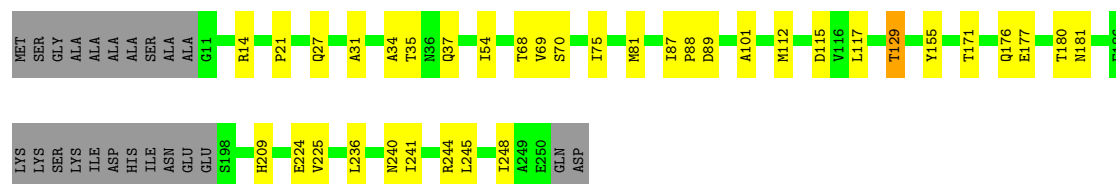
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	211	Total	C	N	O	S	0	0
			1639	1037	281	315	6		
14	b	211	Total	C	N	O	S	0	0
			1639	1037	281	315	6		

3 Residue-property plots

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

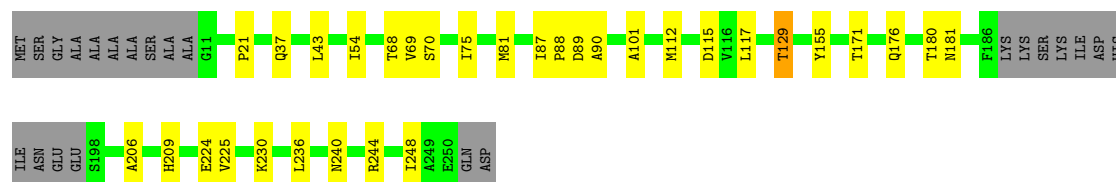
• Molecule 1: Proteasome subunit alpha type-1

Chain A: 



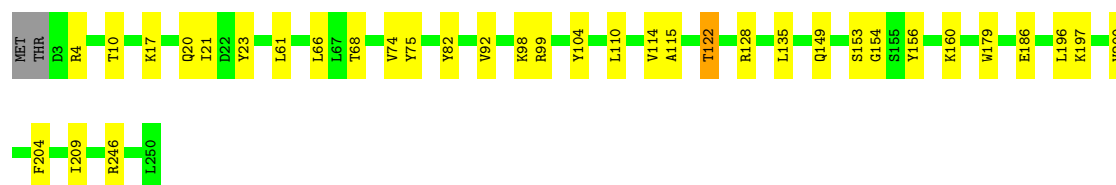
• Molecule 1: Proteasome subunit alpha type-1

Chain O: 



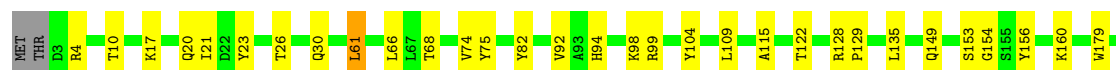
• Molecule 2: Proteasome subunit alpha type-2

Chain B: 



• Molecule 2: Proteasome subunit alpha type-2

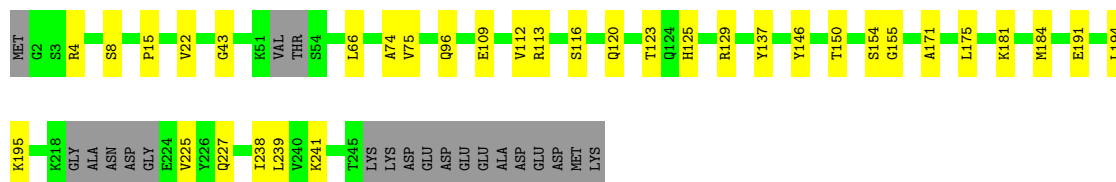
Chain P: 





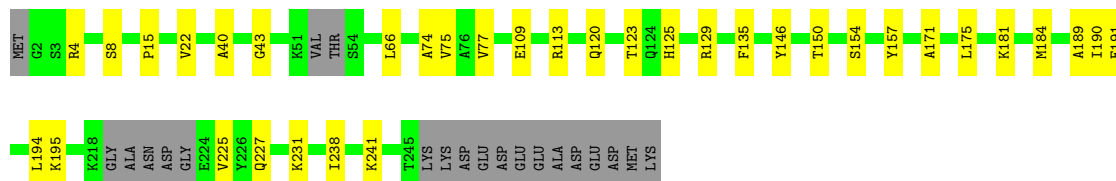
• Molecule 3: Proteasome subunit alpha type-3

Chain C: 79% 13% 8%



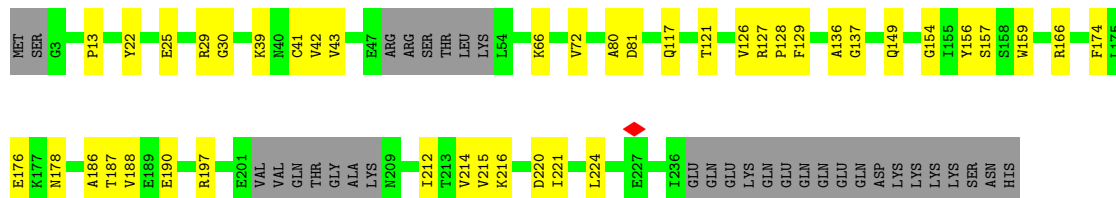
• Molecule 3: Proteasome subunit alpha type-3

Chain Q: 78% 14% 8%



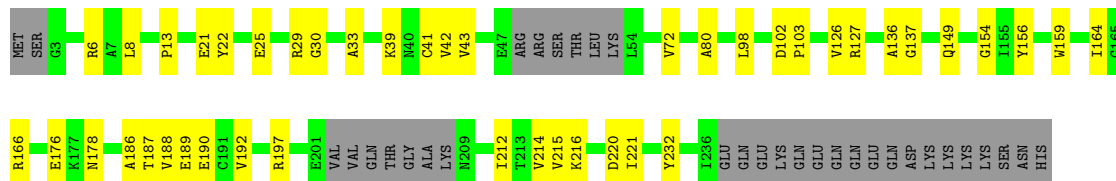
• Molecule 4: Proteasome subunit alpha type-4

Chain D: 70% 17% 13%



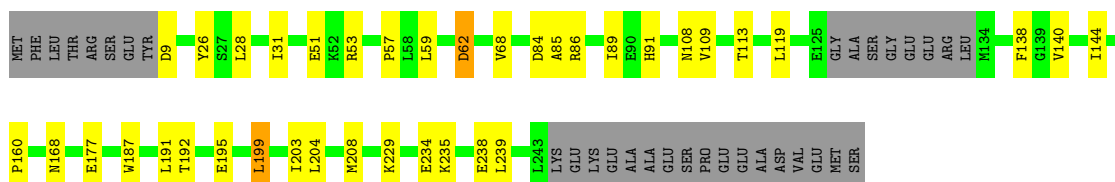
• Molecule 4: Proteasome subunit alpha type-4

Chain R: 70% 17% 13%



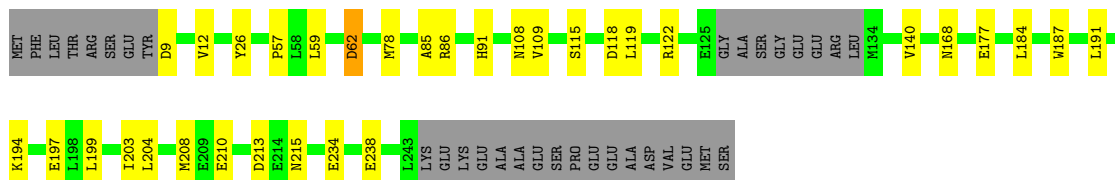
• Molecule 5: Proteasome subunit alpha type-5

Chain E: 73% 14% 13%



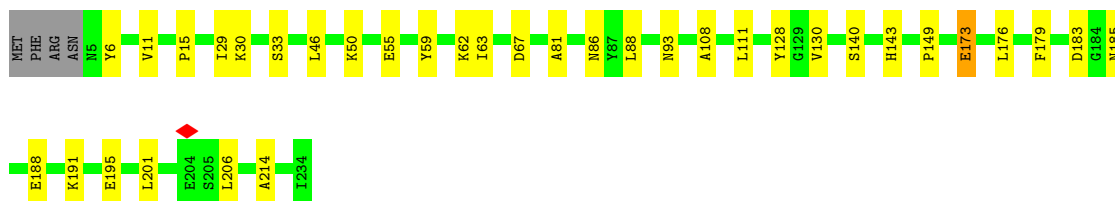
• Molecule 5: Proteasome subunit alpha type-5

Chain S: 75% 12% 13%



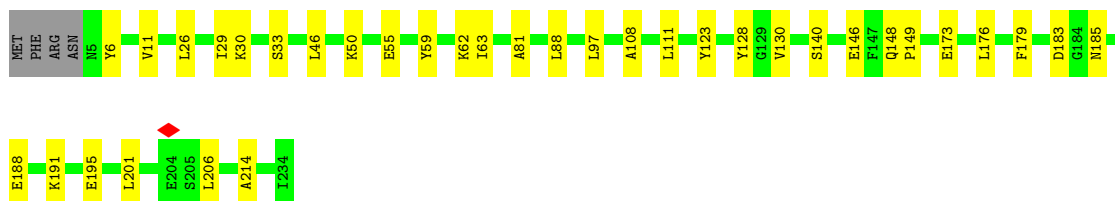
• Molecule 6: Proteasome subunit alpha type-6

Chain F: 83% 15%



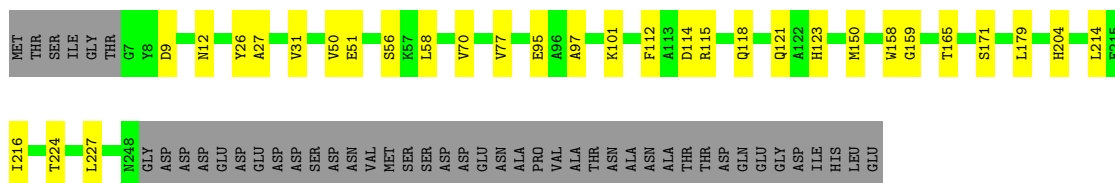
• Molecule 6: Proteasome subunit alpha type-6

Chain T: 83% 15%



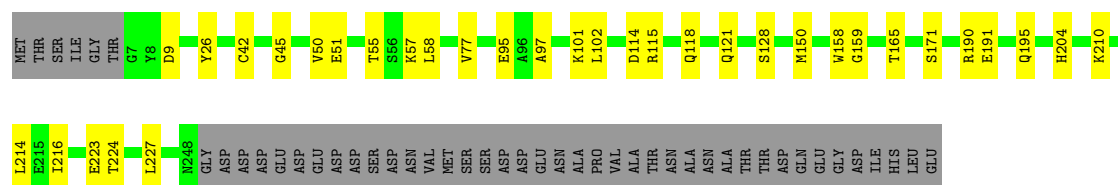
• Molecule 7: Proteasome subunit alpha type-7

Chain G: 73% 11% 16%



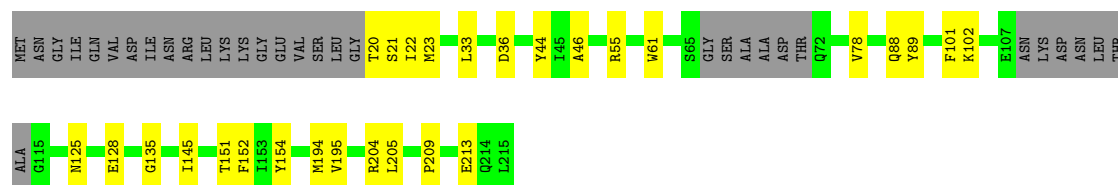
• Molecule 7: Proteasome subunit alpha type-7

Chain U:  72% 12% 16%



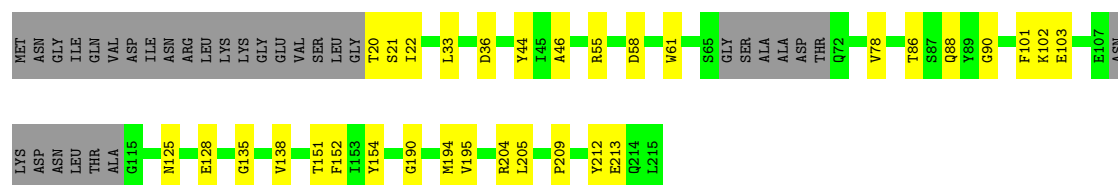
• Molecule 8: Proteasome subunit beta type-1

Chain H:  72% 13% 15%



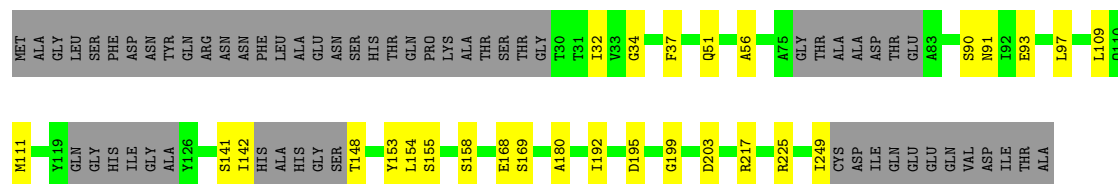
• Molecule 8: Proteasome subunit beta type-1

Chain V:  70% 15% 15%



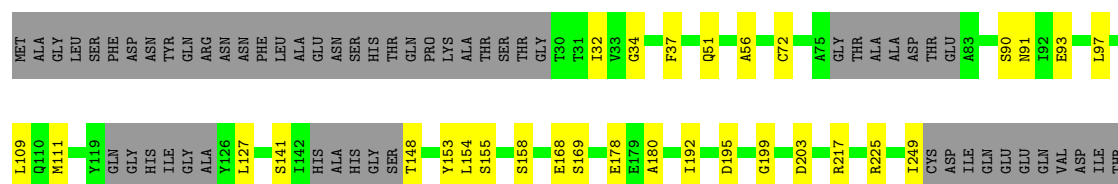
• Molecule 9: Proteasome subunit beta type-2

Chain I:  67% 11% 23%



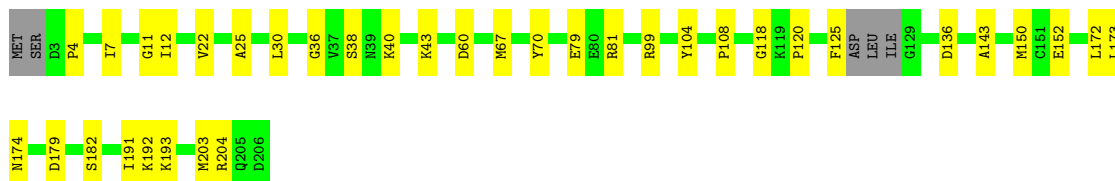
• Molecule 9: Proteasome subunit beta type-2

Chain W:  66% 11% 23%

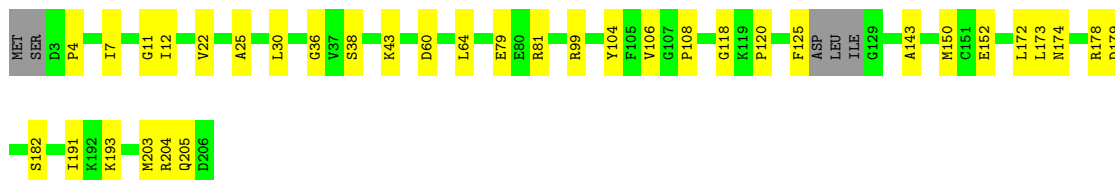


ALA

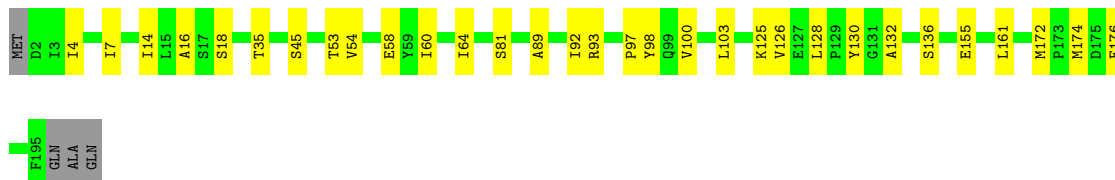
• Molecule 10: Proteasome subunit beta type-3

Chain J:  80% 18%

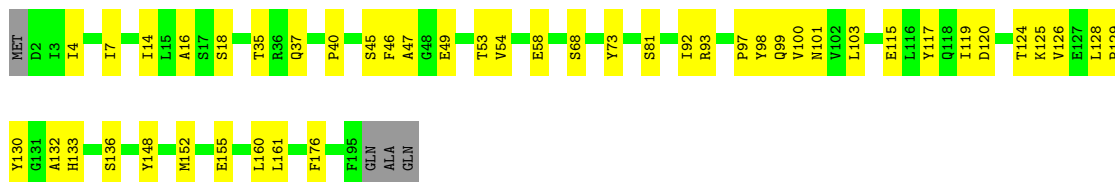
• Molecule 10: Proteasome subunit beta type-3

Chain X:  80% 17%

• Molecule 11: Proteasome subunit beta type-4

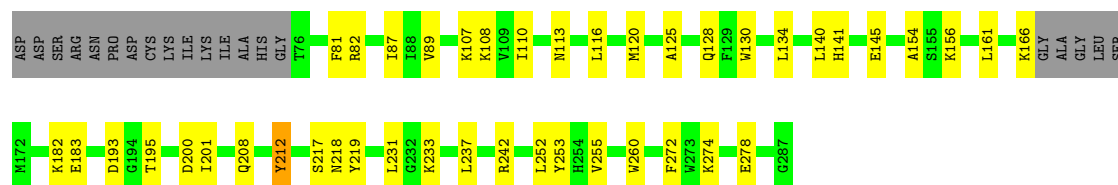
Chain K:  82% 16%

• Molecule 11: Proteasome subunit beta type-4

Chain Y:  75% 23%

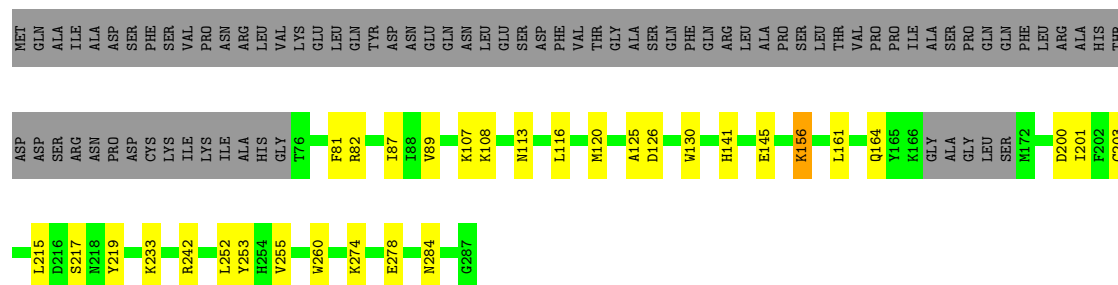
• Molecule 12: Proteasome subunit beta type-5

Chain L:  57% 15% 28%



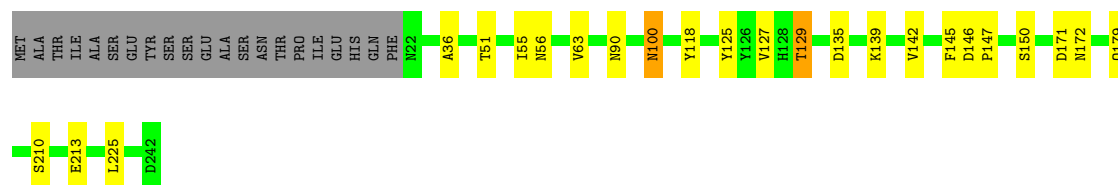
- Molecule 12: Proteasome subunit beta type-5

Chain Z: 61% 11% 28%



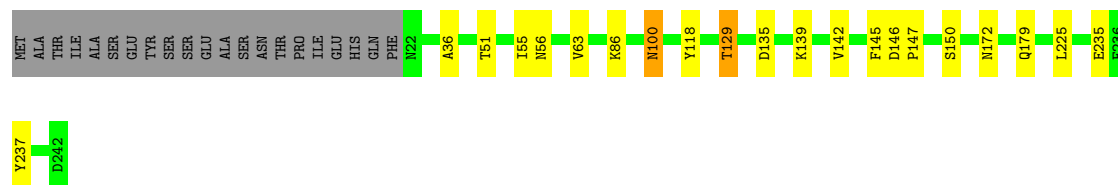
- Molecule 13: Proteasome subunit beta type-6

Chain M: 81% 9% 9%



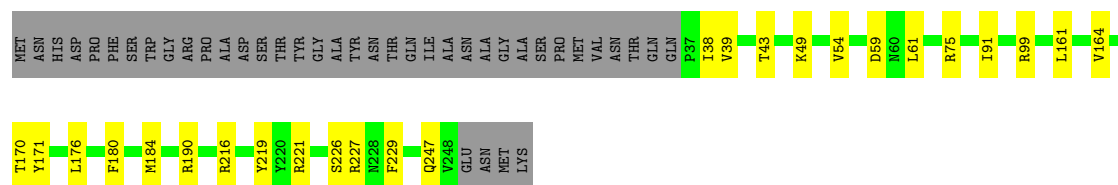
- Molecule 13: Proteasome subunit beta type-6

Chain a: 83% 8% 9%



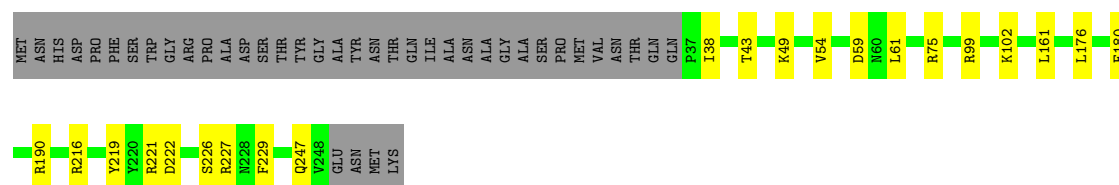
- Molecule 14: Proteasome subunit beta type-7

Chain N: 74% 10% 16%



- Molecule 14: Proteasome subunit beta type-7

Response	Percentage
Yes, the U.S. is a democracy	76%
No, the U.S. is not a democracy	8%
Don't know	16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	766100	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 ($e^-/\text{\AA}^2$)	54.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.963	Depositor
Minimum map value	-4.126	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.426	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.17	0/1841	0.37	0/2495
1	O	0.16	0/1841	0.35	0/2495
2	B	0.16	0/1937	0.33	0/2622
2	P	0.14	0/1937	0.32	0/2622
3	C	0.15	0/1889	0.31	0/2553
3	Q	0.14	0/1889	0.30	0/2553
4	D	0.15	0/1754	0.36	0/2376
4	R	0.14	0/1754	0.34	0/2376
5	E	0.12	0/1774	0.31	0/2392
5	S	0.11	0/1774	0.30	0/2392
6	F	0.15	0/1792	0.39	1/2422 (0.0%)
6	T	0.14	0/1792	0.37	1/2422 (0.0%)
7	G	0.15	0/1925	0.31	0/2599
7	U	0.14	0/1925	0.31	0/2599
8	H	0.14	0/1451	0.32	0/1961
8	V	0.13	0/1451	0.29	0/1961
9	I	0.16	0/1575	0.35	0/2131
9	W	0.15	0/1575	0.33	0/2131
10	J	0.16	0/1580	0.33	0/2130
10	X	0.15	0/1580	0.32	0/2130
11	K	0.18	0/1587	0.37	0/2140
11	Y	0.13	0/1587	0.34	0/2140
12	L	0.14	0/1653	0.32	0/2235
12	Z	0.12	0/1653	0.29	0/2235
13	M	0.14	0/1774	0.34	0/2392
13	a	0.14	0/1774	0.34	0/2392
14	N	0.16	0/1666	0.38	0/2262
14	b	0.15	0/1666	0.37	0/2262
All	All	0.15	0/48396	0.33	2/65420 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	183	ASP	CB-CA-C	-5.50	110.25	116.63
6	T	183	ASP	CB-CA-C	-5.48	110.28	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1805	0	1797	22	0
1	O	1805	0	1797	19	0
2	B	1900	0	1910	22	0
2	P	1900	0	1910	27	0
3	C	1861	0	1862	19	0
3	Q	1861	0	1862	19	0
4	D	1727	0	1723	30	0
4	R	1727	0	1723	29	0
5	E	1750	0	1729	26	0
5	S	1750	0	1729	20	0
6	F	1765	0	1769	21	0
6	T	1765	0	1769	24	0
7	G	1885	0	1876	22	0
7	U	1885	0	1876	23	0
8	H	1424	0	1395	18	0
8	V	1424	0	1395	21	0
9	I	1550	0	1572	16	0
9	W	1550	0	1572	18	0
10	J	1551	0	1539	23	0
10	X	1551	0	1539	23	0
11	K	1558	0	1561	19	0
11	Y	1558	0	1561	25	0
12	L	1617	0	1564	29	0
12	Z	1617	0	1564	21	0
13	M	1737	0	1691	19	0
13	a	1737	0	1691	14	0
14	N	1639	0	1650	18	0
14	b	1639	0	1650	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	47538	0	47276	518	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (518) 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)
11:K:172:MET:HE2	11:K:174:MET:HE3	1.58	0.83
12:L:208:GLN:O	12:L:212:TYR:HB2	1.83	0.78
7:G:95:GLU:HG3	7:G:115:ARG:HH11	1.49	0.76
7:U:190:ARG:NH1	7:U:223:GLU:OE1	2.21	0.74
4:D:154:GLY:O	5:E:86:ARG:NH2	2.20	0.73
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.70	0.73
7:U:95:GLU:HG3	7:U:115:ARG:HH11	1.53	0.72
9:I:51:GLN:HG2	9:I:56:ALA:HB2	1.72	0.72
5:E:85:ALA:HB2	5:E:140:VAL:HG21	1.73	0.71
10:J:60:ASP:OD1	11:K:93:ARG:NH2	2.24	0.71
1:O:129:THR:HG22	2:P:128:ARG:HH21	1.55	0.71
6:F:93:ASN:OD1	13:M:90:ASN:ND2	2.22	0.69
3:Q:123:THR:HG22	4:R:127:ARG:HH21	1.57	0.68
9:W:51:GLN:HG2	9:W:56:ALA:HB2	1.74	0.67
13:M:129:THR:HG23	13:M:145:PHE:HB2	1.77	0.67
4:R:154:GLY:O	5:S:86:ARG:NH2	2.22	0.67
12:Z:233:LYS:HG3	12:Z:252:LEU:HD11	1.77	0.66
10:X:22:VAL:HG13	10:X:120:PRO:HB3	1.78	0.66
10:J:22:VAL:HG13	10:J:120:PRO:HB3	1.78	0.66
13:a:129:THR:HG23	13:a:145:PHE:HB2	1.76	0.65
12:L:233:LYS:HG3	12:L:252:LEU:HD11	1.78	0.65
4:R:187:THR:HG22	4:R:189:GLU:H	1.61	0.65
2:B:98:LYS:HD3	2:B:99:ARG:HH22	1.60	0.65
13:a:146:ASP:OD1	13:a:147:PRO:HD2	1.97	0.65
11:K:16:ALA:HB2	11:K:161:LEU:HD21	1.79	0.65
2:P:98:LYS:HD3	2:P:99:ARG:HH22	1.61	0.65
3:Q:109:GLU:OE2	3:Q:113:ARG:NH2	2.29	0.65
1:A:176:GLN:O	1:A:180:THR:HG23	1.97	0.64
8:H:20:THR:HG23	8:H:36:ASP:OD1	1.97	0.64
6:F:88:LEU:HD11	6:F:108:ALA:HB1	1.79	0.64
8:H:102:LYS:HE3	14:N:99:ARG:HH12	1.61	0.64
4:R:39:LYS:HG3	4:R:186:ALA:HA	1.79	0.64
7:U:95:GLU:HG2	7:U:115:ARG:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:GLU:OE2	3:C:113:ARG:NH2	2.29	0.64
13:M:146:ASP:OD1	13:M:147:PRO:HD2	1.98	0.64
8:V:20:THR:HG23	8:V:36:ASP:OD1	1.98	0.63
11:Y:16:ALA:HB2	11:Y:161:LEU:HD21	1.80	0.63
14:b:102:LYS:HA	14:b:102:LYS:HE2	1.81	0.63
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.81	0.63
10:J:25:ALA:HB1	10:J:172:LEU:HD22	1.81	0.63
14:N:216:ARG:HH22	9:W:169:SER:HA	1.63	0.62
1:A:129:THR:HG22	2:B:128:ARG:HH21	1.64	0.62
5:S:85:ALA:HB2	5:S:140:VAL:HG21	1.82	0.62
13:M:100:ASN:ND2	13:M:100:ASN:O	2.30	0.62
13:a:100:ASN:O	13:a:100:ASN:ND2	2.32	0.61
14:b:49:LYS:HB3	14:b:54:VAL:HG12	1.82	0.61
10:X:25:ALA:HB1	10:X:172:LEU:HD22	1.82	0.61
9:I:169:SER:HA	14:b:216:ARG:HH22	1.65	0.61
1:O:54:ILE:HD12	1:O:225:VAL:HG22	1.83	0.61
10:X:79:GLU:OE1	10:X:81:ARG:NH1	2.34	0.61
14:b:161:LEU:HG	14:b:176:LEU:HD12	1.82	0.61
5:E:234:GLU:O	5:E:238:GLU:HG2	2.00	0.61
10:J:11:GLY:HA3	10:J:43:LYS:HE2	1.83	0.61
11:K:172:MET:CE	11:K:174:MET:HE3	2.29	0.60
2:P:98:LYS:HD3	2:P:99:ARG:NH2	2.16	0.60
10:X:12:ILE:HG21	10:X:143:ALA:HB3	1.83	0.60
9:I:203:ASP:OD2	9:I:217:ARG:NH1	2.34	0.60
10:X:11:GLY:HA3	10:X:43:LYS:HE2	1.84	0.60
14:N:161:LEU:HG	14:N:176:LEU:HD12	1.83	0.60
1:A:54:ILE:HD12	1:A:225:VAL:HG22	1.82	0.59
4:D:39:LYS:NZ	4:D:186:ALA:O	2.35	0.59
6:F:191:LYS:O	6:F:195:GLU:HG2	2.02	0.59
10:J:150:MET:HE2	10:J:174:ASN:HB2	1.82	0.59
2:B:98:LYS:HD3	2:B:99:ARG:NH2	2.16	0.59
8:V:102:LYS:HE3	14:b:99:ARG:HH12	1.65	0.59
4:D:186:ALA:N	4:D:190:GLU:OE1	2.33	0.59
6:F:176:LEU:HD13	7:G:58:LEU:HD23	1.85	0.59
14:N:49:LYS:HB3	14:N:54:VAL:HG12	1.83	0.59
5:E:62:ASP:OD1	5:E:62:ASP:N	2.35	0.59
9:W:203:ASP:OD2	9:W:217:ARG:NH1	2.32	0.58
10:X:118:GLY:HA2	10:X:193:LYS:HE3	1.85	0.58
5:E:68:VAL:HG21	5:E:89:ILE:HG13	1.85	0.58
10:J:12:ILE:HG21	10:J:143:ALA:HB3	1.84	0.58
2:B:4:ARG:HD2	2:B:4:ARG:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:GLU:OE1	10:J:81:ARG:NH1	2.37	0.58
14:N:221:ARG:NH1	9:W:168:GLU:OE1	2.30	0.58
10:J:173:LEU:HD23	10:J:203:MET:HE2	1.86	0.57
12:Z:82:ARG:NH1	12:Z:200:ASP:OD2	2.37	0.57
12:L:242:ARG:NH1	10:X:36:GLY:O	2.37	0.57
13:M:63:VAL:HG12	13:M:225:LEU:HD22	1.85	0.57
2:P:122:THR:HG22	3:Q:129:ARG:HH21	1.69	0.57
12:Z:108:LYS:HA	12:Z:120:MET:HE3	1.85	0.57
12:L:166:LYS:HD2	12:L:193:ASP:HA	1.87	0.57
14:b:227:ARG:NH2	14:b:247:GLN:OE1	2.37	0.57
5:E:235:LYS:HD2	5:E:239:LEU:HD23	1.86	0.56
11:Y:155:GLU:CD	11:Y:155:GLU:H	2.13	0.56
9:I:109:LEU:HD21	9:I:148:THR:HG21	1.88	0.56
4:R:216:LYS:HB2	4:R:220:ASP:HB3	1.87	0.56
6:T:55:GLU:CD	6:T:55:GLU:H	2.12	0.56
12:L:125:ALA:HA	13:M:150:SER:HB2	1.87	0.56
4:D:43:VAL:HG22	4:D:214:VAL:HG22	1.88	0.56
5:S:177:GLU:OE2	5:S:177:GLU:N	2.22	0.56
5:S:187:TRP:HA	5:S:191:LEU:HD11	1.86	0.56
9:W:91:ASN:HB2	9:W:111:MET:HE1	1.87	0.56
11:Y:18:SER:HB2	11:Y:176:PHE:HB2	1.88	0.56
10:J:118:GLY:HA2	10:J:193:LYS:HE3	1.86	0.56
12:L:130:TRP:CE2	12:L:161:LEU:HD11	2.40	0.56
6:T:176:LEU:HD13	7:U:58:LEU:HD23	1.88	0.56
2:P:186:GLU:OE1	2:P:246:ARG:NH1	2.39	0.55
8:V:135:GLY:HA2	14:b:38:ILE:HD13	1.88	0.55
10:J:36:GLY:O	12:Z:242:ARG:NH1	2.38	0.55
14:b:59:ASP:HA	14:b:229:PHE:HA	1.89	0.55
13:a:63:VAL:HG12	13:a:225:LEU:HD22	1.87	0.55
1:O:101:ALA:HA	1:O:112:MET:HE2	1.89	0.55
3:Q:190:ILE:O	3:Q:194:LEU:HD12	2.07	0.55
10:X:173:LEU:HD23	10:X:203:MET:HE2	1.89	0.55
12:L:110:ILE:HG12	12:L:120:MET:HE2	1.88	0.55
6:F:55:GLU:H	6:F:55:GLU:CD	2.15	0.54
5:S:62:ASP:OD1	5:S:62:ASP:N	2.34	0.54
3:C:191:GLU:O	3:C:195:LYS:HG2	2.08	0.54
14:N:59:ASP:HA	14:N:229:PHE:HA	1.90	0.54
4:R:43:VAL:HG22	4:R:214:VAL:HG22	1.88	0.54
4:D:216:LYS:HB2	4:D:220:ASP:HB3	1.88	0.54
2:B:122:THR:HG22	3:C:129:ARG:HH21	1.72	0.54
9:W:109:LEU:HD21	9:W:148:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:235:GLU:OE1	13:a:237:TYR:OH	2.23	0.54
10:X:60:ASP:OD1	11:Y:93:ARG:NH2	2.41	0.53
13:M:51:THR:HG1	13:M:56:ASN:HD21	1.53	0.53
1:A:89:ASP:OD1	7:G:121:GLN:NE2	2.40	0.53
3:C:120:GLN:HG3	4:D:80:ALA:HB1	1.90	0.53
5:E:177:GLU:H	5:E:177:GLU:CD	2.15	0.53
9:I:168:GLU:OE2	14:b:221:ARG:NH1	2.35	0.53
2:B:186:GLU:OE1	2:B:246:ARG:NH1	2.41	0.53
2:P:4:ARG:HD3	7:U:128:SER:HB3	1.90	0.53
2:B:75:TYR:HB3	2:B:82:TYR:CD1	2.44	0.53
8:V:195:VAL:HG22	8:V:204:ARG:HD3	1.90	0.53
11:K:18:SER:HB2	11:K:176:PHE:HB2	1.91	0.53
8:V:20:THR:HG22	8:V:22:ILE:HG23	1.91	0.53
4:D:81:ASP:HB3	4:D:129:PHE:HD1	1.75	0.52
1:O:75:ILE:HD11	1:O:81:MET:HE2	1.92	0.52
7:U:51:GLU:OE2	7:U:204:HIS:ND1	2.32	0.52
10:X:150:MET:HE2	10:X:174:ASN:HB2	1.91	0.52
1:A:236:LEU:HB3	1:A:240:ASN:HB2	1.92	0.52
7:G:97:ALA:O	7:G:101:LYS:HE2	2.09	0.52
12:L:108:LYS:HA	12:L:120:MET:HE3	1.91	0.52
1:O:89:ASP:OD1	7:U:121:GLN:NE2	2.39	0.52
5:E:177:GLU:OE2	5:E:177:GLU:N	2.32	0.52
8:H:20:THR:HG22	8:H:22:ILE:HG23	1.91	0.52
8:H:195:VAL:HG22	8:H:204:ARG:HD3	1.90	0.52
9:I:91:ASN:HB2	9:I:111:MET:HE1	1.91	0.52
5:E:187:TRP:HA	5:E:191:LEU:HD11	1.90	0.52
9:I:37:PHE:HB3	9:I:180:ALA:HB2	1.92	0.52
4:R:178:ASN:OD1	4:R:197:ARG:NH2	2.43	0.52
1:A:115:ASP:HB3	1:A:155:TYR:CZ	2.44	0.52
2:P:75:TYR:HB3	2:P:82:TYR:CD1	2.45	0.52
12:Z:130:TRP:CE2	12:Z:161:LEU:HD11	2.45	0.52
1:O:115:ASP:HB3	1:O:155:TYR:CZ	2.45	0.51
1:O:181:ASN:CG	1:O:209:HIS:HD1	2.17	0.51
7:G:50:VAL:HB	7:G:77:VAL:HG21	1.93	0.51
6:F:29:ILE:HD11	6:F:149:PRO:HD3	1.92	0.51
4:R:42:VAL:HG11	4:R:136:ALA:HB1	1.93	0.51
10:X:99:ARG:HG3	10:X:104:TYR:CE2	2.46	0.51
11:K:54:VAL:O	11:K:58:GLU:HG3	2.10	0.51
6:T:88:LEU:HD11	6:T:108:ALA:HB1	1.91	0.51
8:V:125:ASN:ND2	8:V:128:GLU:OE1	2.44	0.51
10:J:22:VAL:HG23	10:J:191:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:81:SER:HB2	11:K:125:LYS:HD2	1.92	0.51
12:L:82:ARG:O	12:L:219:TYR:OH	2.18	0.51
12:L:193:ASP:OD1	12:L:195:THR:OG1	2.26	0.51
11:K:155:GLU:H	11:K:155:GLU:CD	2.18	0.51
11:K:53:THR:HG22	11:K:100:VAL:HG13	1.92	0.51
7:U:50:VAL:HB	7:U:77:VAL:HG21	1.93	0.51
4:D:178:ASN:OD1	4:D:197:ARG:NH2	2.44	0.50
1:A:75:ILE:HD11	1:A:81:MET:HE2	1.92	0.50
1:A:101:ALA:HA	1:A:112:MET:HE2	1.92	0.50
3:C:123:THR:HG22	4:D:127:ARG:HH21	1.76	0.50
4:D:42:VAL:HG11	4:D:136:ALA:HB1	1.91	0.50
4:R:98:LEU:O	12:Z:156:LYS:NZ	2.44	0.50
4:R:188:VAL:O	4:R:192:VAL:HG23	2.11	0.50
8:V:194:MET:HB2	8:V:205:LEU:HB2	1.93	0.50
9:W:72:CYS:SG	9:W:127:LEU:HD22	2.52	0.50
1:O:176:GLN:O	1:O:180:THR:HG23	2.11	0.50
7:G:51:GLU:OE2	7:G:204:HIS:ND1	2.33	0.50
5:S:108:ASN:OD1	5:S:109:VAL:N	2.45	0.50
1:A:181:ASN:CG	1:A:209:HIS:HD1	2.16	0.50
2:B:200:VAL:HG21	2:B:209:ILE:HD11	1.94	0.50
8:H:135:GLY:HA2	14:N:38:ILE:HD13	1.94	0.50
11:K:126:VAL:HG13	11:K:128:LEU:HG	1.93	0.50
5:S:184:LEU:HD11	6:T:55:GLU:HG2	1.94	0.50
14:b:219:TYR:CZ	14:b:227:ARG:HG3	2.47	0.50
5:E:91:HIS:CG	5:E:119:LEU:HD11	2.46	0.50
5:S:91:HIS:CG	5:S:119:LEU:HD11	2.47	0.50
7:G:95:GLU:HG2	7:G:115:ARG:HB3	1.93	0.50
9:W:141:SER:HB3	9:W:154:LEU:HD13	1.94	0.50
3:Q:74:ALA:HB2	3:Q:227:GLN:NE2	2.27	0.49
11:Y:7:ILE:HG23	11:Y:14:ILE:HB	1.94	0.49
12:L:134:LEU:HD21	12:L:154:ALA:HB1	1.92	0.49
14:N:180:PHE:HZ	8:V:44:TYR:HD1	1.60	0.49
14:N:219:TYR:CZ	14:N:227:ARG:HG3	2.47	0.49
11:Y:126:VAL:HG13	11:Y:128:LEU:HG	1.93	0.49
8:H:194:MET:HB2	8:H:205:LEU:HB2	1.93	0.49
9:I:192:ILE:HG23	9:I:199:GLY:HA2	1.94	0.49
1:O:69:VAL:HA	7:U:158:TRP:CZ3	2.48	0.49
6:F:108:ALA:HA	6:F:111:LEU:HD12	1.94	0.49
10:J:99:ARG:HG3	10:J:104:TYR:CE2	2.47	0.49
11:K:7:ILE:HG23	11:K:14:ILE:HB	1.94	0.49
3:C:74:ALA:HB2	3:C:227:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:151:THR:HA	8:H:154:TYR:HD2	1.76	0.49
14:N:227:ARG:NH2	14:N:247:GLN:OE1	2.45	0.49
1:A:70:SER:OG	1:A:224:GLU:OE2	2.27	0.49
4:R:187:THR:HG22	4:R:189:GLU:N	2.28	0.49
10:X:22:VAL:HG23	10:X:191:ILE:HB	1.93	0.49
12:Z:161:LEU:HD22	12:Z:164:GLN:NE2	2.28	0.49
5:E:108:ASN:OD1	5:E:109:VAL:N	2.46	0.49
6:F:176:LEU:HA	6:F:179:PHE:CE2	2.48	0.49
8:H:125:ASN:ND2	8:H:128:GLU:OE1	2.45	0.49
3:Q:238:ILE:HD12	3:Q:241:LYS:HD3	1.94	0.49
13:a:172:ASN:O	13:a:179:GLN:NE2	2.46	0.49
3:Q:109:GLU:OE1	3:Q:157:TYR:OH	2.26	0.48
4:R:25:GLU:OE1	4:R:29:ARG:NH1	2.46	0.48
4:D:72:VAL:HG13	4:D:221:ILE:HD13	1.95	0.48
13:M:51:THR:OG1	13:M:56:ASN:ND2	2.36	0.48
1:A:69:VAL:HA	7:G:158:TRP:CZ3	2.48	0.48
6:F:6:TYR:OH	7:G:9:ASP:OD2	2.25	0.48
13:a:51:THR:OG1	13:a:56:ASN:ND2	2.35	0.48
6:T:176:LEU:HD23	7:U:57:LYS:HE3	1.94	0.48
7:G:115:ARG:NH2	8:H:89:TYR:OH	2.34	0.48
5:S:234:GLU:O	5:S:238:GLU:HG2	2.14	0.48
6:T:26:LEU:HD23	6:T:149:PRO:HD2	1.96	0.48
6:T:191:LYS:O	6:T:195:GLU:HG2	2.14	0.48
12:Z:125:ALA:HA	13:a:150:SER:HB2	1.95	0.48
3:C:4:ARG:HG2	3:C:4:ARG:HH11	1.79	0.48
6:F:185:ASN:ND2	6:F:188:GLU:HB2	2.29	0.48
8:H:209:PRO:O	8:H:213:GLU:HB2	2.14	0.48
9:I:141:SER:HB3	9:I:154:LEU:HD13	1.94	0.48
6:F:33:SER:O	6:F:62:LYS:NZ	2.45	0.48
7:G:214:LEU:HD21	7:G:216:ILE:HD11	1.94	0.48
4:R:72:VAL:HG13	4:R:221:ILE:HD13	1.95	0.48
8:V:209:PRO:O	8:V:213:GLU:HB2	2.14	0.48
7:U:214:LEU:HD21	7:U:216:ILE:HD11	1.94	0.48
2:B:99:ARG:CZ	9:I:90:SER:HB2	2.44	0.47
5:E:199:LEU:O	5:E:203:ILE:HG12	2.14	0.47
8:H:44:TYR:HD1	14:b:180:PHE:HZ	1.61	0.47
10:X:4:PRO:HA	10:X:7:ILE:HG13	1.95	0.47
1:A:88:PRO:HB2	7:G:121:GLN:HG3	1.95	0.47
13:M:135:ASP:OD1	13:M:139:LYS:N	2.47	0.47
6:F:30:LYS:HA	6:F:30:LYS:HD2	1.60	0.47
7:U:97:ALA:O	7:U:101:LYS:HE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:54:VAL:O	11:Y:58:GLU:HG3	2.15	0.47
4:D:188:VAL:HG21	4:D:216:LYS:HE2	1.95	0.47
9:W:37:PHE:HB3	9:W:180:ALA:HB2	1.96	0.47
5:E:84:ASP:HB3	5:E:138:PHE:HD1	1.79	0.47
6:T:108:ALA:HA	6:T:111:LEU:HD12	1.95	0.47
10:X:64:LEU:HD11	10:X:106:VAL:HG21	1.96	0.47
2:P:241:GLN:NE2	2:P:245:ASP:OD1	2.47	0.47
4:R:187:THR:HB	4:R:190:GLU:HG3	1.95	0.47
5:S:213:ASP:OD1	5:S:215:ASN:ND2	2.37	0.47
6:T:29:ILE:HD11	6:T:149:PRO:HD3	1.97	0.47
12:L:113:ASN:ND2	12:L:116:LEU:HB2	2.30	0.47
3:Q:4:ARG:NH1	6:T:123:TYR:OH	2.47	0.47
10:X:179:ASP:OD2	10:X:182:SER:OG	2.30	0.47
4:D:25:GLU:OE1	4:D:29:ARG:NH1	2.48	0.46
10:J:143:ALA:HB2	10:J:179:ASP:HB2	1.97	0.46
13:M:210:SER:HB3	10:X:152:GLU:HB3	1.98	0.46
2:P:179:TRP:HA	2:P:183:LEU:HD11	1.97	0.46
11:Y:92:ILE:HA	11:Y:97:PRO:HB3	1.97	0.46
11:K:92:ILE:HA	11:K:97:PRO:HB3	1.98	0.46
1:O:236:LEU:HB3	1:O:240:ASN:HB2	1.97	0.46
8:H:151:THR:O	8:V:152:PHE:HA	2.15	0.46
10:X:143:ALA:HB2	10:X:179:ASP:HB2	1.97	0.46
2:B:104:TYR:OH	9:I:93:GLU:OE2	2.34	0.46
3:Q:191:GLU:O	3:Q:195:LYS:HG2	2.16	0.46
8:V:190:GLY:O	8:V:212:TYR:OH	2.20	0.46
10:J:4:PRO:HA	10:J:7:ILE:HG13	1.98	0.46
12:L:130:TRP:NE1	13:M:118:TYR:OH	2.49	0.46
1:O:43:LEU:HD11	1:O:206:ALA:HB1	1.96	0.46
1:A:34:ALA:O	1:A:37:GLN:HG2	2.15	0.46
6:F:63:ILE:HG21	6:F:214:ALA:HB2	1.98	0.46
11:K:132:ALA:HB1	11:K:136:SER:HB3	1.98	0.46
12:L:110:ILE:CD1	12:L:128:GLN:HA	2.46	0.46
1:O:70:SER:OG	1:O:224:GLU:OE2	2.28	0.46
6:T:185:ASN:ND2	6:T:188:GLU:HB2	2.31	0.46
12:Z:274:LYS:O	12:Z:278:GLU:HG2	2.15	0.46
3:C:22:VAL:HG11	3:C:154:SER:HB3	1.98	0.45
6:F:46:LEU:HB2	6:F:214:ALA:HB3	1.98	0.45
8:H:23:MET:HB2	8:H:145:ILE:HG22	1.98	0.45
12:L:87:ILE:HB	12:L:255:VAL:HB	1.99	0.45
6:T:50:LYS:HB3	6:T:59:TYR:HB3	1.98	0.45
2:B:21:ILE:HG21	2:B:153:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:10:THR:HG23	2:P:20:GLN:HB2	1.97	0.45
2:P:61:LEU:HD23	2:P:61:LEU:HA	1.82	0.45
2:P:104:TYR:OH	9:W:93:GLU:OE2	2.33	0.45
6:T:63:ILE:HG21	6:T:214:ALA:HB2	1.97	0.45
11:K:98:TYR:HB3	11:K:100:VAL:HG23	1.98	0.45
6:T:46:LEU:HB2	6:T:214:ALA:HB3	1.98	0.45
6:T:201:LEU:HD11	6:T:206:LEU:HG	1.98	0.45
8:H:46:ALA:O	14:b:221:ARG:NH2	2.48	0.45
12:Z:113:ASN:ND2	12:Z:116:LEU:HB2	2.31	0.45
1:A:177:GLU:OE1	1:A:177:GLU:N	2.48	0.45
4:R:30:GLY:O	4:R:166:ARG:HG3	2.17	0.45
13:a:55:ILE:O	14:b:190:ARG:NH2	2.39	0.45
1:A:244:ARG:O	1:A:248:ILE:HG13	2.16	0.45
5:E:168:ASN:HB3	5:E:187:TRP:CZ2	2.52	0.45
8:V:55:ARG:HG3	8:V:61:TRP:CE2	2.52	0.45
12:Z:87:ILE:HB	12:Z:255:VAL:HB	1.99	0.45
14:N:184:MET:HE2	14:N:184:MET:HB3	1.90	0.45
8:V:151:THR:HA	8:V:154:TYR:HD2	1.82	0.45
11:Y:35:THR:HG22	11:Y:45:SER:HB3	1.99	0.45
3:C:181:LYS:HE2	3:C:181:LYS:HB2	1.86	0.45
6:F:50:LYS:HB3	6:F:59:TYR:HB3	1.98	0.45
13:M:55:ILE:O	14:N:190:ARG:NH2	2.46	0.45
9:W:192:ILE:HG23	9:W:199:GLY:HA2	1.99	0.45
1:A:75:ILE:HG21	1:A:117:LEU:HD21	1.99	0.44
3:C:171:ALA:O	3:C:175:LEU:HD23	2.17	0.44
6:F:140:SER:OG	6:F:143:HIS:NE2	2.47	0.44
1:O:244:ARG:O	1:O:248:ILE:HG13	2.17	0.44
6:T:128:TYR:O	6:T:149:PRO:HB3	2.18	0.44
7:U:224:THR:OG1	7:U:227:LEU:O	2.35	0.44
11:Y:49:GLU:HB2	11:Y:99:GLN:HB3	1.99	0.44
13:a:135:ASP:OD1	13:a:139:LYS:N	2.48	0.44
10:J:179:ASP:OD2	10:J:182:SER:OG	2.31	0.44
2:P:160:LYS:HB3	2:P:179:TRP:CZ2	2.53	0.44
5:S:194:LYS:HA	5:S:197:GLU:HG3	1.99	0.44
7:U:9:ASP:HB2	7:U:26:TYR:CE2	2.52	0.44
1:A:21:PRO:HA	2:B:23:TYR:CD1	2.53	0.44
3:C:181:LYS:O	3:C:184:MET:HG2	2.18	0.44
7:G:27:ALA:O	7:G:31:VAL:HG23	2.18	0.44
6:T:6:TYR:OH	7:U:9:ASP:OD2	2.26	0.44
2:B:115:ALA:HB1	2:B:154:GLY:O	2.18	0.44
4:D:149:GLN:O	4:D:156:TYR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:201:LEU:HD11	6:F:206:LEU:HG	1.99	0.44
6:T:33:SER:O	6:T:62:LYS:NZ	2.44	0.44
7:G:12:ASN:ND2	7:G:123:HIS:O	2.44	0.44
11:K:4:ILE:HG22	11:K:103:LEU:HD12	2.00	0.44
1:O:87:ILE:HA	1:O:90:ALA:HB3	1.98	0.44
4:R:149:GLN:O	4:R:156:TYR:HA	2.17	0.44
8:V:20:THR:HG22	8:V:21:SER:N	2.32	0.44
5:E:229:LYS:HB3	5:E:229:LYS:HE3	1.78	0.44
13:M:172:ASN:O	13:M:179:GLN:NE2	2.50	0.44
5:S:78:MET:HE2	5:S:78:MET:HB3	1.91	0.44
11:Y:132:ALA:HB1	11:Y:136:SER:HB3	1.98	0.44
9:I:225:ARG:NH1	10:J:152:GLU:HG3	2.33	0.44
3:Q:40:ALA:HB2	3:Q:189:ALA:HB2	2.00	0.44
11:Y:4:ILE:HG22	11:Y:103:LEU:HD12	2.00	0.44
12:L:156:LYS:HD2	12:L:156:LYS:HA	1.84	0.44
1:O:75:ILE:HG21	1:O:117:LEU:HD21	2.00	0.44
2:P:200:VAL:HG21	2:P:209:ILE:HD11	1.99	0.44
11:K:89:ALA:O	11:K:92:ILE:HG22	2.17	0.43
1:A:31:ALA:O	1:A:35:THR:HG23	2.18	0.43
2:B:196:LEU:HD12	2:B:196:LEU:HA	1.86	0.43
2:B:197:LYS:HG3	2:B:204:PHE:CD2	2.53	0.43
7:G:114:ASP:O	7:G:118:GLN:HG2	2.18	0.43
3:Q:171:ALA:O	3:Q:175:LEU:HD23	2.18	0.43
4:R:159:TRP:CE2	5:S:59:LEU:HD23	2.53	0.43
2:B:10:THR:HG23	2:B:20:GLN:HB2	1.99	0.43
2:B:66:LEU:HD22	9:I:97:LEU:HD21	2.01	0.43
4:D:66:LYS:HB3	4:D:66:LYS:HE2	1.51	0.43
8:H:20:THR:HG22	8:H:21:SER:N	2.31	0.43
2:P:99:ARG:CZ	9:W:90:SER:HB2	2.48	0.43
12:Z:107:LYS:HA	12:Z:107:LYS:HD2	1.82	0.43
8:H:55:ARG:HG3	8:H:61:TRP:CE2	2.53	0.43
2:B:74:VAL:HG12	2:B:135:LEU:HB2	2.00	0.43
4:D:30:GLY:O	4:D:166:ARG:HG3	2.18	0.43
10:J:136:ASP:OD1	10:J:136:ASP:N	2.51	0.43
4:R:189:GLU:HG2	4:R:232:TYR:HE1	1.83	0.43
5:S:168:ASN:HB3	5:S:187:TRP:CZ2	2.53	0.43
6:T:176:LEU:HA	6:T:179:PHE:CE2	2.54	0.43
4:D:13:PRO:HA	5:E:26:TYR:CD1	2.53	0.43
5:E:85:ALA:O	5:E:89:ILE:HG12	2.17	0.43
13:M:213:GLU:CG	9:W:225:ARG:HD2	2.48	0.43
2:P:17:LYS:HD2	2:P:17:LYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:150:MET:SD	7:U:165:THR:HG23	2.58	0.43
2:B:160:LYS:HB3	2:B:179:TRP:CZ2	2.53	0.43
11:K:7:ILE:HD13	11:K:130:TYR:HB3	2.01	0.43
11:K:60:ILE:O	11:K:64:ILE:HG12	2.19	0.43
2:P:21:ILE:HG21	2:P:153:SER:HB3	2.01	0.43
7:G:150:MET:SD	7:G:165:THR:HG23	2.58	0.43
10:J:203:MET:HG3	10:J:204:ARG:O	2.19	0.43
12:L:201:ILE:HD11	12:L:219:TYR:CD2	2.54	0.43
4:R:137:GLY:HA2	4:R:215:VAL:HG11	2.00	0.43
4:D:25:GLU:O	4:D:29:ARG:HD3	2.18	0.43
12:L:125:ALA:CA	13:M:150:SER:HB2	2.49	0.43
1:A:14:ARG:O	1:A:27:GLN:NE2	2.43	0.43
4:D:43:VAL:HG13	4:D:212:ILE:HG23	2.00	0.43
2:P:74:VAL:HG12	2:P:135:LEU:HB2	2.00	0.43
5:S:204:LEU:O	5:S:208:MET:HG3	2.19	0.43
8:V:102:LYS:HG3	8:V:138:VAL:HG23	2.00	0.43
4:D:137:GLY:HA2	4:D:215:VAL:HG11	2.01	0.42
4:D:174:PHE:O	4:D:178:ASN:ND2	2.40	0.42
5:E:31:ILE:HD11	5:E:160:PRO:HG2	2.01	0.42
5:S:118:ASP:O	5:S:122:ARG:HG3	2.19	0.42
9:W:34:GLY:O	9:W:153:TYR:HA	2.19	0.42
8:H:78:VAL:HG11	8:H:101:PHE:CE2	2.54	0.42
12:L:255:VAL:HA	12:L:260:TRP:HA	2.01	0.42
3:C:15:PRO:HA	4:D:22:TYR:CD1	2.54	0.42
4:D:121:THR:HG22	4:D:128:PRO:HB3	2.00	0.42
1:O:21:PRO:HA	2:P:23:TYR:CD1	2.54	0.42
2:P:66:LEU:HD22	9:W:97:LEU:HD21	2.01	0.42
11:Y:81:SER:HB2	11:Y:125:LYS:HD2	2.00	0.42
4:R:13:PRO:HA	5:S:26:TYR:CD1	2.54	0.42
7:U:191:GLU:O	7:U:195:GLN:HG2	2.18	0.42
12:Z:201:ILE:HD11	12:Z:219:TYR:CD2	2.55	0.42
4:D:159:TRP:CE2	5:E:59:LEU:HD23	2.54	0.42
12:L:107:LYS:HA	12:L:107:LYS:HD2	1.78	0.42
2:P:128:ARG:NH1	2:P:129:PRO:O	2.52	0.42
9:W:32:ILE:O	9:W:155:SER:HA	2.20	0.42
10:X:99:ARG:HG3	10:X:104:TYR:HE2	1.85	0.42
12:Z:126:ASP:OD1	13:a:118:TYR:OH	2.35	0.42
12:L:274:LYS:O	12:L:278:GLU:HG2	2.19	0.42
11:Y:7:ILE:HD13	11:Y:130:TYR:HB3	2.02	0.42
12:Z:255:VAL:HA	12:Z:260:TRP:HA	2.02	0.42
6:F:173:GLU:OE1	7:G:56:SER:OG	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:152:PHE:HA	8:V:151:THR:O	2.19	0.42
9:I:32:ILE:O	9:I:155:SER:HA	2.19	0.42
13:M:36:ALA:HB2	13:M:142:VAL:HG23	2.01	0.42
13:M:125:TYR:HB3	13:M:127:VAL:HG22	2.01	0.42
2:P:115:ALA:HB1	2:P:154:GLY:O	2.20	0.42
7:G:70:VAL:HG11	7:G:112:PHE:CE1	2.54	0.42
12:L:89:VAL:HB	12:L:253:TYR:HB2	2.02	0.42
12:L:140:LEU:HD23	12:L:140:LEU:HA	1.90	0.42
10:X:30:LEU:HB3	10:X:38:SER:HB3	2.02	0.42
11:Y:101:ASN:HB3	11:Y:133:HIS:CE1	2.55	0.42
3:C:194:LEU:HD23	3:C:239:LEU:HD23	2.02	0.42
9:I:34:GLY:O	9:I:153:TYR:HA	2.19	0.42
12:L:141:HIS:CE1	12:L:145:GLU:HG3	2.54	0.42
2:P:26:THR:O	2:P:30:GLN:HG2	2.20	0.42
3:Q:22:VAL:HG11	3:Q:154:SER:HB3	2.01	0.42
3:Q:181:LYS:O	3:Q:184:MET:HG2	2.20	0.42
7:U:55:THR:HA	7:U:210:LYS:HE3	2.02	0.42
1:A:68:THR:HG21	7:G:159:GLY:HA3	2.01	0.42
7:G:179:LEU:HD12	7:G:179:LEU:HA	1.82	0.42
12:L:237:LEU:HD21	12:L:272:PHE:HA	2.02	0.42
13:M:171:ASP:OD2	10:X:178:ARG:NH2	2.49	0.42
9:W:158:SER:OG	9:W:195:ASP:OD2	2.30	0.42
5:E:51:GLU:OE2	5:E:53:ARG:HD3	2.19	0.41
1:O:87:ILE:N	1:O:88:PRO:HD2	2.35	0.41
2:P:94:HIS:O	2:P:99:ARG:HG2	2.19	0.41
2:P:196:LEU:HD12	2:P:196:LEU:HA	1.89	0.41
11:Y:37:GLN:HE21	11:Y:40:PRO:HA	1.85	0.41
14:b:43:THR:O	14:b:75:ARG:NH1	2.53	0.41
10:J:30:LEU:HB3	10:J:38:SER:HB3	2.01	0.41
12:L:182:LYS:HD3	12:L:183:GLU:HG2	2.02	0.41
5:E:192:THR:HG23	5:E:195:GLU:H	1.86	0.41
4:R:6:ARG:HG2	4:R:8:LEU:HD23	2.01	0.41
4:R:25:GLU:O	4:R:29:ARG:HD3	2.19	0.41
4:R:192:VAL:HG13	4:R:212:ILE:HG21	2.03	0.41
11:Y:98:TYR:HB3	11:Y:100:VAL:HG23	2.01	0.41
14:b:180:PHE:CD2	14:b:222:ASP:HB2	2.55	0.41
5:E:113:THR:HG23	5:E:144:ILE:HD12	2.03	0.41
9:I:158:SER:OG	9:I:195:ASP:OD2	2.29	0.41
12:L:81:PHE:HA	12:L:200:ASP:O	2.20	0.41
1:O:68:THR:HG21	7:U:159:GLY:HA3	2.02	0.41
12:Z:203:CYS:SG	12:Z:215:LEU:HD12	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:HIS:HB3	4:D:126:VAL:HG12	2.01	0.41
4:D:166:ARG:HG3	4:D:166:ARG:H	1.65	0.41
6:F:128:TYR:O	6:F:149:PRO:HB3	2.19	0.41
11:K:35:THR:HG22	11:K:45:SER:HB3	2.02	0.41
14:N:39:VAL:HG12	14:N:91:ILE:HG13	2.02	0.41
14:N:61:LEU:HB2	14:N:226:SER:HB2	2.03	0.41
7:U:102:LEU:HA	8:V:103:GLU:HG3	2.01	0.41
10:X:203:MET:HG3	10:X:204:ARG:O	2.20	0.41
11:Y:46:PHE:HD2	11:Y:53:THR:HB	1.86	0.41
3:C:96:GLN:HB3	10:J:70:TYR:CD2	2.55	0.41
1:O:230:LYS:H	1:O:230:LYS:HE2	1.86	0.41
4:D:176:GLU:HG2	5:E:57:PRO:HG2	2.01	0.41
5:E:28:LEU:HA	5:E:31:ILE:HD12	2.02	0.41
5:E:204:LEU:O	5:E:208:MET:HG3	2.21	0.41
14:N:43:THR:O	14:N:75:ARG:NH1	2.53	0.41
2:P:109:LEU:HD23	2:P:109:LEU:HA	1.87	0.41
3:Q:120:GLN:HG3	4:R:80:ALA:HB1	2.01	0.41
11:Y:129:PRO:HB2	11:Y:148:TYR:CZ	2.56	0.41
12:Z:141:HIS:CE1	12:Z:145:GLU:HG3	2.55	0.41
1:A:87:ILE:N	1:A:88:PRO:HD2	2.36	0.41
9:W:178:GLU:N	9:W:178:GLU:CD	2.79	0.41
11:Y:68:SER:HA	11:Y:73:TYR:O	2.21	0.41
12:Z:81:PHE:HA	12:Z:200:ASP:O	2.21	0.41
13:a:36:ALA:HB2	13:a:142:VAL:HG23	2.01	0.41
1:A:241:ILE:O	1:A:245:LEU:HG	2.20	0.41
3:C:43:GLY:HA2	3:C:146:TYR:CE1	2.55	0.41
10:J:192:LYS:HE2	10:J:192:LYS:HB2	1.73	0.41
12:L:218:ASN:HB2	12:L:231:LEU:HD13	2.03	0.41
14:N:164:VAL:HG23	14:N:170:THR:HG22	2.03	0.41
3:Q:125:HIS:HB3	4:R:126:VAL:HG12	2.02	0.41
5:S:168:ASN:HB3	5:S:187:TRP:CE2	2.56	0.41
6:T:97:LEU:O	13:a:86:LYS:NZ	2.37	0.41
6:T:146:GLU:OE1	6:T:148:GLN:NE2	2.54	0.41
8:V:58:ASP:OD1	8:V:58:ASP:N	2.54	0.41
13:M:56:ASN:HB3	14:N:171:TYR:CE1	2.56	0.41
3:Q:43:GLY:HA2	3:Q:146:TYR:CE1	2.56	0.41
6:T:173:GLU:HG3	7:U:58:LEU:HG	2.03	0.41
11:Y:115:GLU:HB3	11:Y:117:TYR:CE2	2.56	0.41
12:Z:89:VAL:HB	12:Z:253:TYR:HB2	2.03	0.41
2:B:110:LEU:O	2:B:114:VAL:HG23	2.21	0.40
4:D:157:SER:HB2	5:E:59:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:224:THR:OG1	7:G:227:LEU:O	2.35	0.40
10:J:40:LYS:NZ	12:Z:284:ASN:O	2.50	0.40
4:R:33:ALA:HB3	4:R:164:ILE:CG1	2.51	0.40
14:b:61:LEU:HB2	14:b:226:SER:HB2	2.02	0.40
12:L:272:PHE:CE1	10:X:205:GLN:HG3	2.57	0.40
14:N:221:ARG:NH2	8:V:46:ALA:O	2.54	0.40
11:Y:4:ILE:HG13	11:Y:47:ALA:HB2	2.03	0.40
11:Y:119:ILE:HA	11:Y:124:THR:O	2.21	0.40
4:D:212:ILE:HG21	4:D:224:LEU:HD22	2.02	0.40
3:Q:238:ILE:HD12	3:Q:238:ILE:HA	1.97	0.40
7:U:114:ASP:O	7:U:118:GLN:HG2	2.22	0.40
8:V:78:VAL:HG11	8:V:101:PHE:CE2	2.57	0.40
10:X:108:PRO:HD2	10:X:125:PHE:HB2	2.02	0.40
11:Y:120:ASP:OD1	11:Y:120:ASP:C	2.65	0.40
2:B:149:GLN:O	2:B:156:TYR:HA	2.21	0.40
3:C:112:VAL:HG22	3:C:137:TYR:CG	2.57	0.40
3:C:238:ILE:HD12	3:C:241:LYS:HE3	2.03	0.40
6:F:15:PRO:HA	7:G:26:TYR:CD1	2.56	0.40
10:J:108:PRO:HD2	10:J:125:PHE:HB2	2.03	0.40
2:P:149:GLN:O	2:P:156:TYR:HA	2.22	0.40
3:Q:15:PRO:HA	4:R:22:TYR:CD1	2.55	0.40
3:Q:77:VAL:HG22	3:Q:135:PHE:HE1	1.86	0.40
6:T:30:LYS:HA	6:T:30:LYS:HD2	1.76	0.40
11:Y:152:MET:HE1	11:Y:160:LEU:HD22	2.03	0.40
2:B:17:LYS:HD2	2:B:17:LYS:N	2.35	0.40
3:C:116:SER:HB3	3:C:155:GLY:O	2.22	0.40
4:D:117:GLN:O	4:D:121:THR:HG23	2.21	0.40
4:R:102:ASP:OD1	4:R:103:PRO:HD2	2.22	0.40
4:R:176:GLU:HG2	5:S:57:PRO:HG2	2.04	0.40
5:S:199:LEU:O	5:S:203:ILE:HG12	2.22	0.40
7:U:42:CYS:SG	7:U:45:GLY:N	2.95	0.40
8:V:86:THR:HA	8:V:90:GLY:O	2.21	0.40
12:Z:274:LYS:HE2	12:Z:274:LYS:HB2	1.78	0.40
13:a:51:THR:HG1	13:a:56:ASN:HD21	1.65	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	225/252 (89%)	223 (99%)	2 (1%)	0	100	100
1	O	225/252 (89%)	224 (100%)	1 (0%)	0	100	100
2	B	246/250 (98%)	243 (99%)	3 (1%)	0	100	100
2	P	246/250 (98%)	245 (100%)	1 (0%)	0	100	100
3	C	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
3	Q	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
4	D	215/254 (85%)	209 (97%)	6 (3%)	0	100	100
4	R	215/254 (85%)	208 (97%)	7 (3%)	0	100	100
5	E	223/260 (86%)	221 (99%)	2 (1%)	0	100	100
5	S	223/260 (86%)	221 (99%)	2 (1%)	0	100	100
6	F	228/234 (97%)	223 (98%)	5 (2%)	0	100	100
6	T	228/234 (97%)	225 (99%)	3 (1%)	0	100	100
7	G	240/288 (83%)	238 (99%)	2 (1%)	0	100	100
7	U	240/288 (83%)	238 (99%)	2 (1%)	0	100	100
8	H	177/215 (82%)	176 (99%)	1 (1%)	0	100	100
8	V	177/215 (82%)	176 (99%)	1 (1%)	0	100	100
9	I	194/261 (74%)	192 (99%)	2 (1%)	0	100	100
9	W	194/261 (74%)	192 (99%)	2 (1%)	0	100	100
10	J	196/205 (96%)	190 (97%)	6 (3%)	0	100	100
10	X	196/205 (96%)	192 (98%)	4 (2%)	0	100	100
11	K	192/198 (97%)	190 (99%)	2 (1%)	0	100	100
11	Y	192/198 (97%)	188 (98%)	4 (2%)	0	100	100
12	L	203/287 (71%)	201 (99%)	2 (1%)	0	100	100
12	Z	203/287 (71%)	200 (98%)	3 (2%)	0	100	100
13	M	218/241 (90%)	213 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	218/241 (90%)	214 (98%)	4 (2%)	0	100	100
14	N	209/251 (83%)	204 (98%)	5 (2%)	0	100	100
14	b	209/251 (83%)	204 (98%)	5 (2%)	0	100	100
All	All	5994/6908 (87%)	5908 (99%)	86 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/210 (92%)	192 (99%)	2 (1%)	68	84
1	O	194/210 (92%)	191 (98%)	3 (2%)	57	77
2	B	207/209 (99%)	203 (98%)	4 (2%)	50	71
2	P	207/209 (99%)	204 (99%)	3 (1%)	59	79
3	C	199/216 (92%)	194 (98%)	5 (2%)	42	64
3	Q	199/216 (92%)	193 (97%)	6 (3%)	36	58
4	D	195/226 (86%)	193 (99%)	2 (1%)	68	84
4	R	195/226 (86%)	193 (99%)	2 (1%)	68	84
5	E	188/215 (87%)	185 (98%)	3 (2%)	55	76
5	S	188/215 (87%)	183 (97%)	5 (3%)	39	62
6	F	189/193 (98%)	185 (98%)	4 (2%)	47	69
6	T	189/193 (98%)	187 (99%)	2 (1%)	65	82
7	G	200/239 (84%)	199 (100%)	1 (0%)	81	91
7	U	200/239 (84%)	199 (100%)	1 (0%)	81	91
8	H	153/178 (86%)	151 (99%)	2 (1%)	61	80
8	V	153/178 (86%)	151 (99%)	2 (1%)	61	80
9	I	169/214 (79%)	167 (99%)	2 (1%)	63	81
9	W	169/214 (79%)	168 (99%)	1 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	168/173 (97%)	167 (99%)	1 (1%)	78	89
10	X	168/173 (97%)	168 (100%)	0	100	100
11	K	172/175 (98%)	172 (100%)	0	100	100
11	Y	172/175 (98%)	172 (100%)	0	100	100
12	L	167/235 (71%)	165 (99%)	2 (1%)	63	81
12	Z	167/235 (71%)	165 (99%)	2 (1%)	63	81
13	M	183/201 (91%)	181 (99%)	2 (1%)	65	82
13	a	183/201 (91%)	181 (99%)	2 (1%)	65	82
14	N	180/212 (85%)	180 (100%)	0	100	100
14	b	180/212 (85%)	180 (100%)	0	100	100
All	All	5128/5792 (88%)	5069 (99%)	59 (1%)	61	81

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	171	THR
2	B	61	LEU
2	B	68	THR
2	B	92	VAL
2	B	122	THR
3	C	8	SER
3	C	66	LEU
3	C	75	VAL
3	C	150	THR
3	C	225	VAL
4	D	41	CYS
4	D	187	THR
5	E	9	ASP
5	E	62	ASP
5	E	199	LEU
6	F	11	VAL
6	F	67	ASP
6	F	86	ASN
6	F	173	GLU
7	G	171	SER
8	H	33	LEU
8	H	88	GLN

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Mol	Chain	Res	Type
9	I	142	ILE
9	I	249	ILE
10	J	67	MET
12	L	212	TYR
12	L	217	SER
13	M	100	ASN
13	M	129	THR
1	O	37	GLN
1	O	129	THR
1	O	171	THR
2	P	61	LEU
2	P	68	THR
2	P	92	VAL
3	Q	8	SER
3	Q	66	LEU
3	Q	75	VAL
3	Q	150	THR
3	Q	225	VAL
3	Q	231	LYS
4	R	21	GLU
4	R	41	CYS
5	S	9	ASP
5	S	12	VAL
5	S	62	ASP
5	S	115	SER
5	S	210	GLU
6	T	11	VAL
6	T	140	SER
7	U	171	SER
8	V	33	LEU
8	V	88	GLN
9	W	249	ILE
12	Z	156	LYS
12	Z	217	SER
13	a	100	ASN
13	a	129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
2	B	241	GLN

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Mol	Chain	Res	Type
4	D	118	GLN
4	D	122	GLN
4	D	167	ASN
5	E	100	ASN
5	E	168	ASN
6	F	31	GLN
6	F	166	GLN
6	F	185	ASN
7	G	207	ASN
8	H	160	ASN
10	J	65	ASN
10	J	170	GLN
11	K	55	GLN
11	K	118	GLN
11	K	166	GLN
12	L	160	ASN
12	L	265	ASN
13	M	178	ASN
13	M	217	GLN
14	N	71	ASN
14	N	183	HIS
1	O	175	GLN
3	Q	96	GLN
4	R	94	GLN
4	R	167	ASN
5	S	91	HIS
5	S	100	ASN
5	S	168	ASN
5	S	206	GLN
6	T	148	GLN
6	T	152	ASN
6	T	166	GLN
6	T	185	ASN
7	U	207	ASN
8	V	160	ASN
10	X	65	ASN
10	X	73	ASN
10	X	170	GLN
10	X	174	ASN
11	Y	63	ASN
11	Y	118	GLN
12	Z	164	GLN

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Mol	Chain	Res	Type
12	Z	265	ASN
13	a	178	ASN
13	a	217	GLN
14	b	71	ASN
14	b	183	HIS
14	b	228	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.

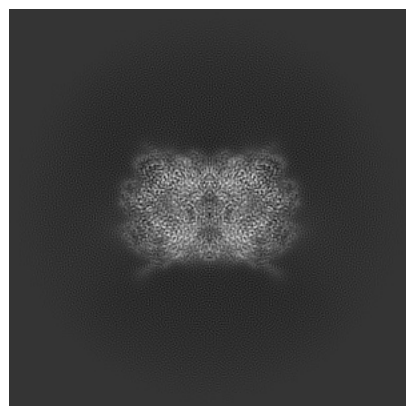
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40944. These allow visual inspection of the internal detail of the map and identification of artifacts.

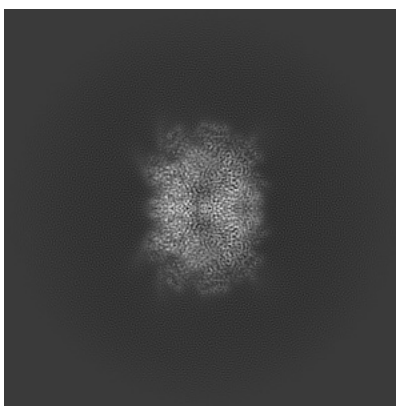
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

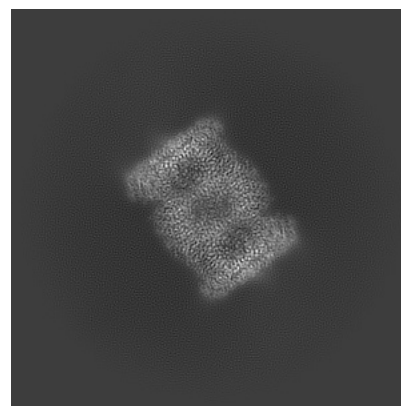
6.1.1 Primary map



X

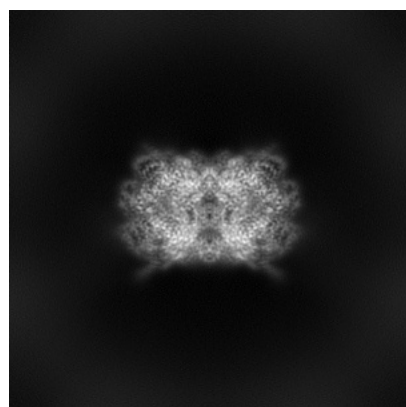


Y

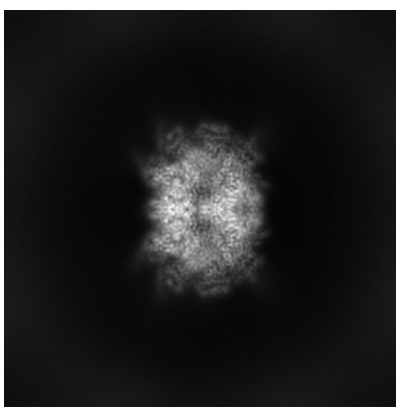


Z

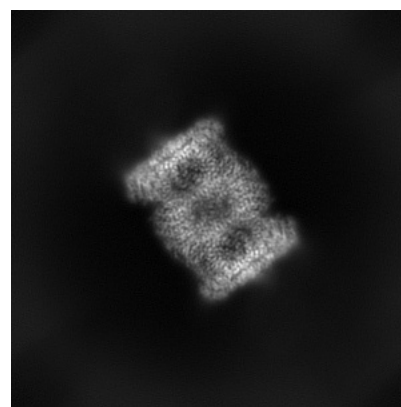
6.1.2 Raw map



X



Y

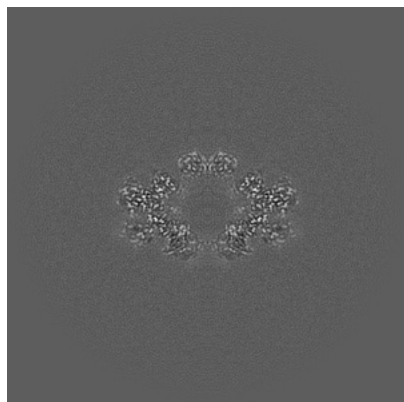


Z

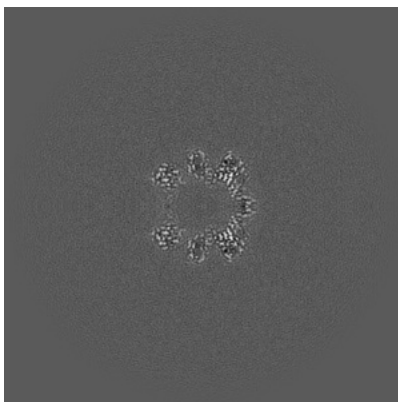
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

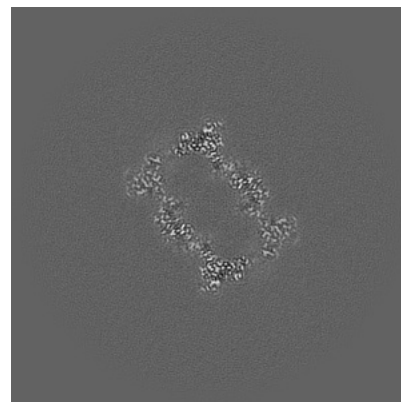
6.2.1 Primary map



X Index: 180

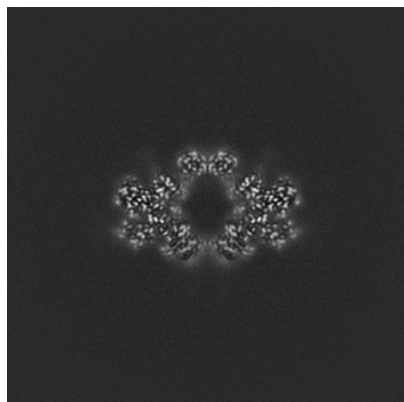


Y Index: 180

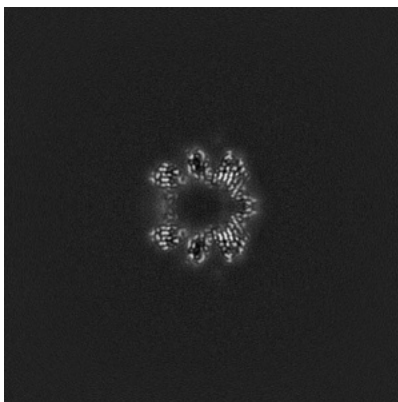


Z Index: 180

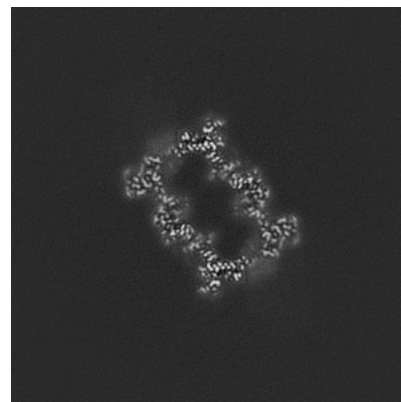
6.2.2 Raw map



X Index: 180



Y Index: 180

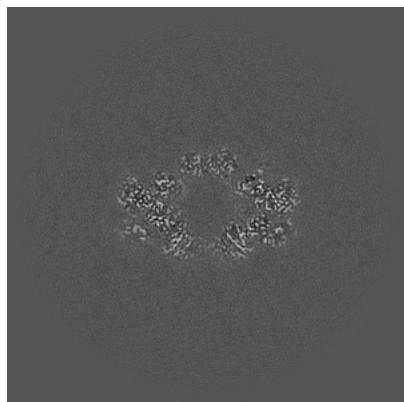


Z Index: 180

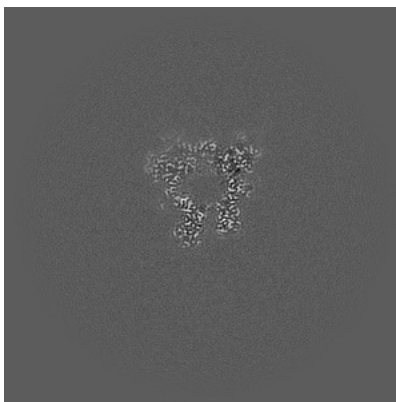
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

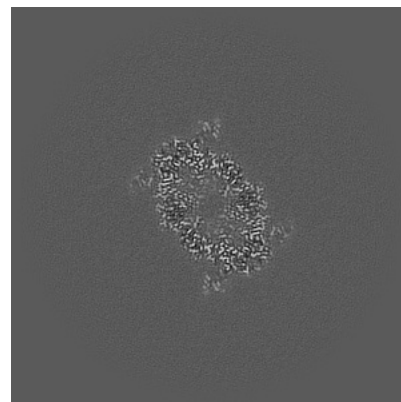
6.3.1 Primary map



X Index: 178

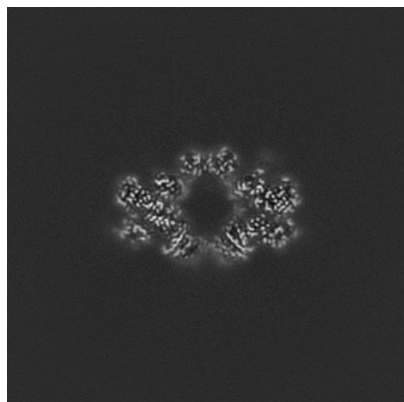


Y Index: 140

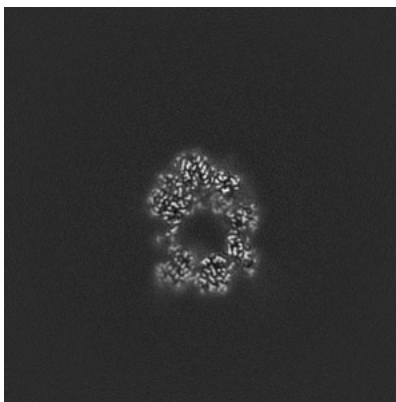


Z Index: 203

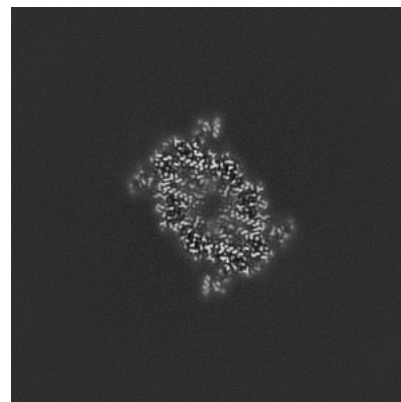
6.3.2 Raw map



X Index: 178



Y Index: 204

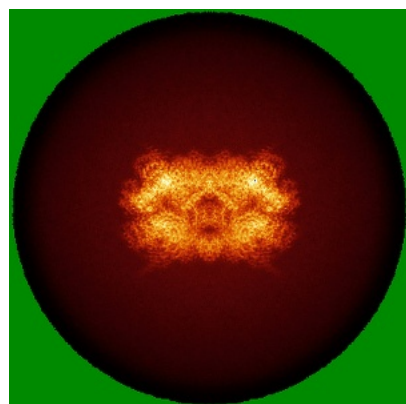


Z Index: 203

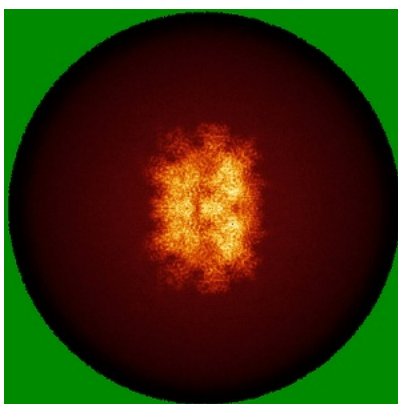
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

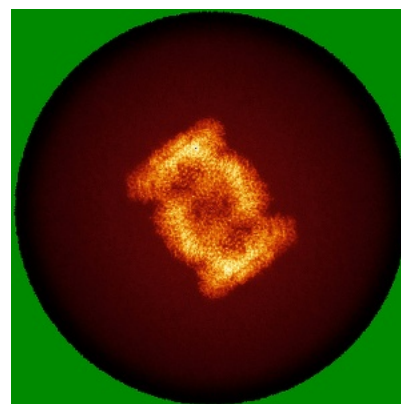
6.4.1 Primary map



X

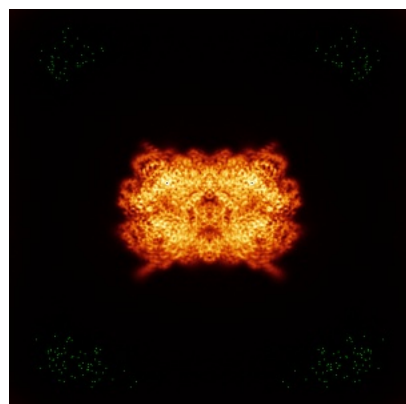


Y

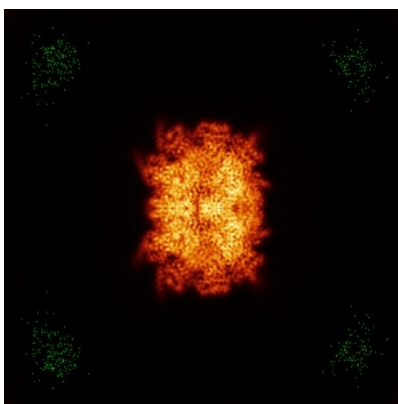


Z

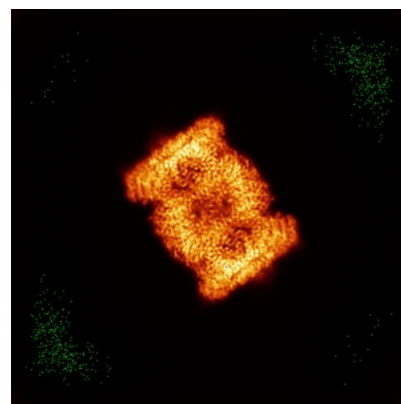
6.4.2 Raw map



X



Y

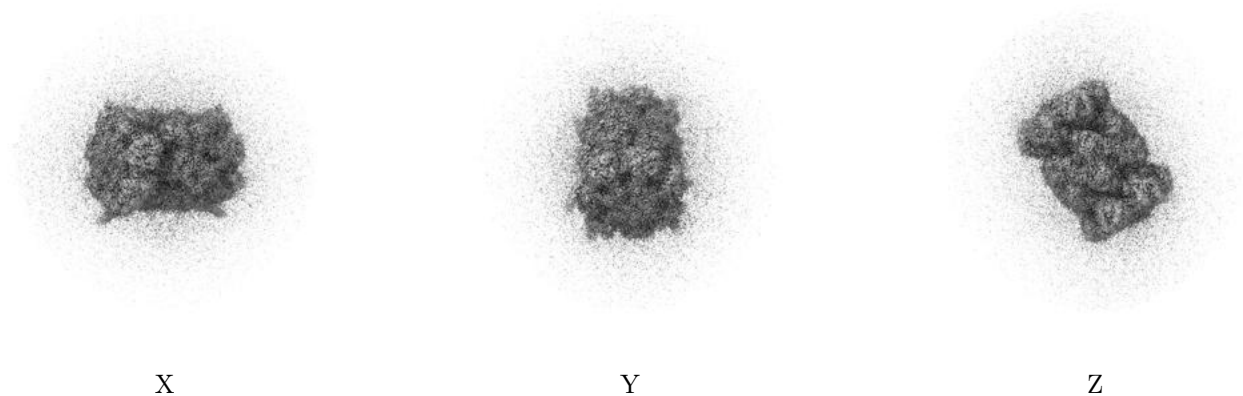


Z

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.

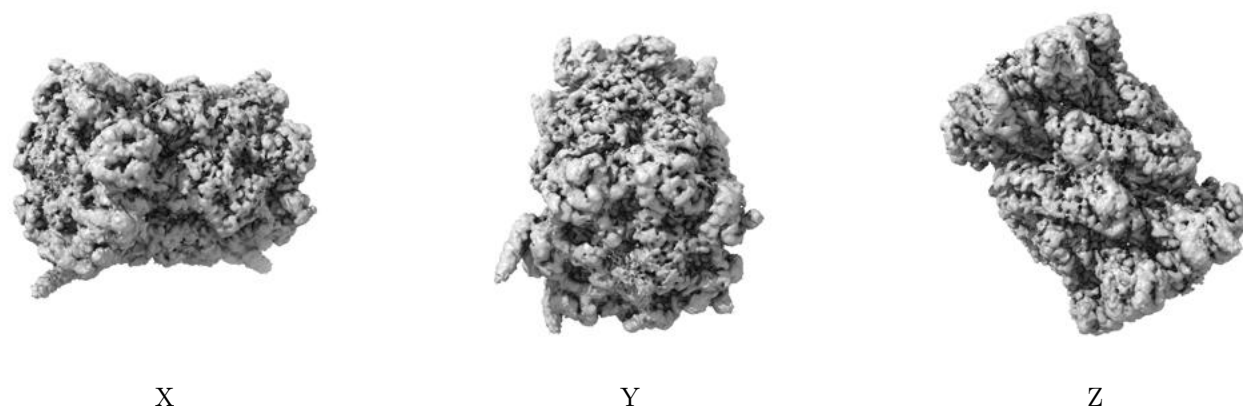
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.426. 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.

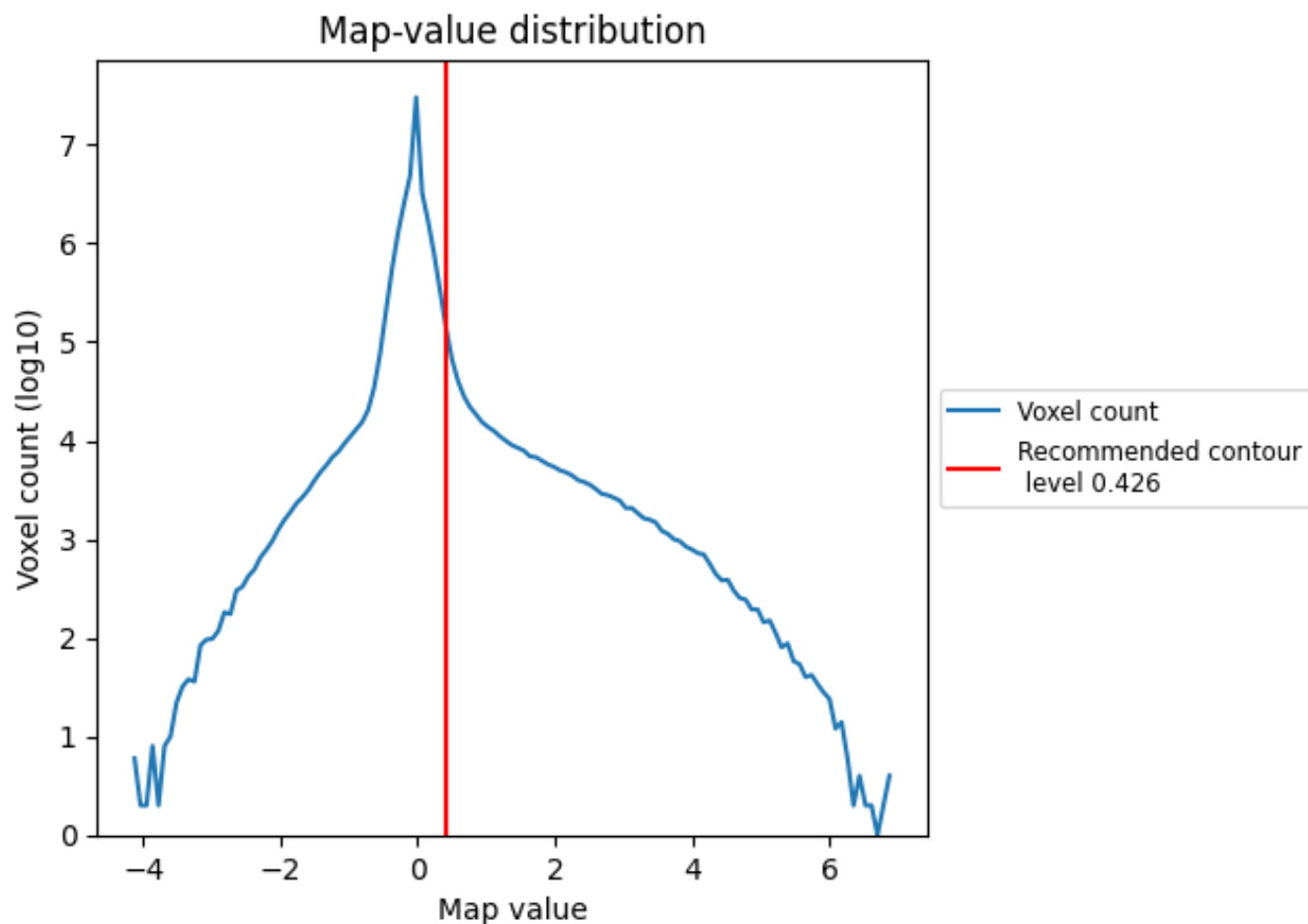
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

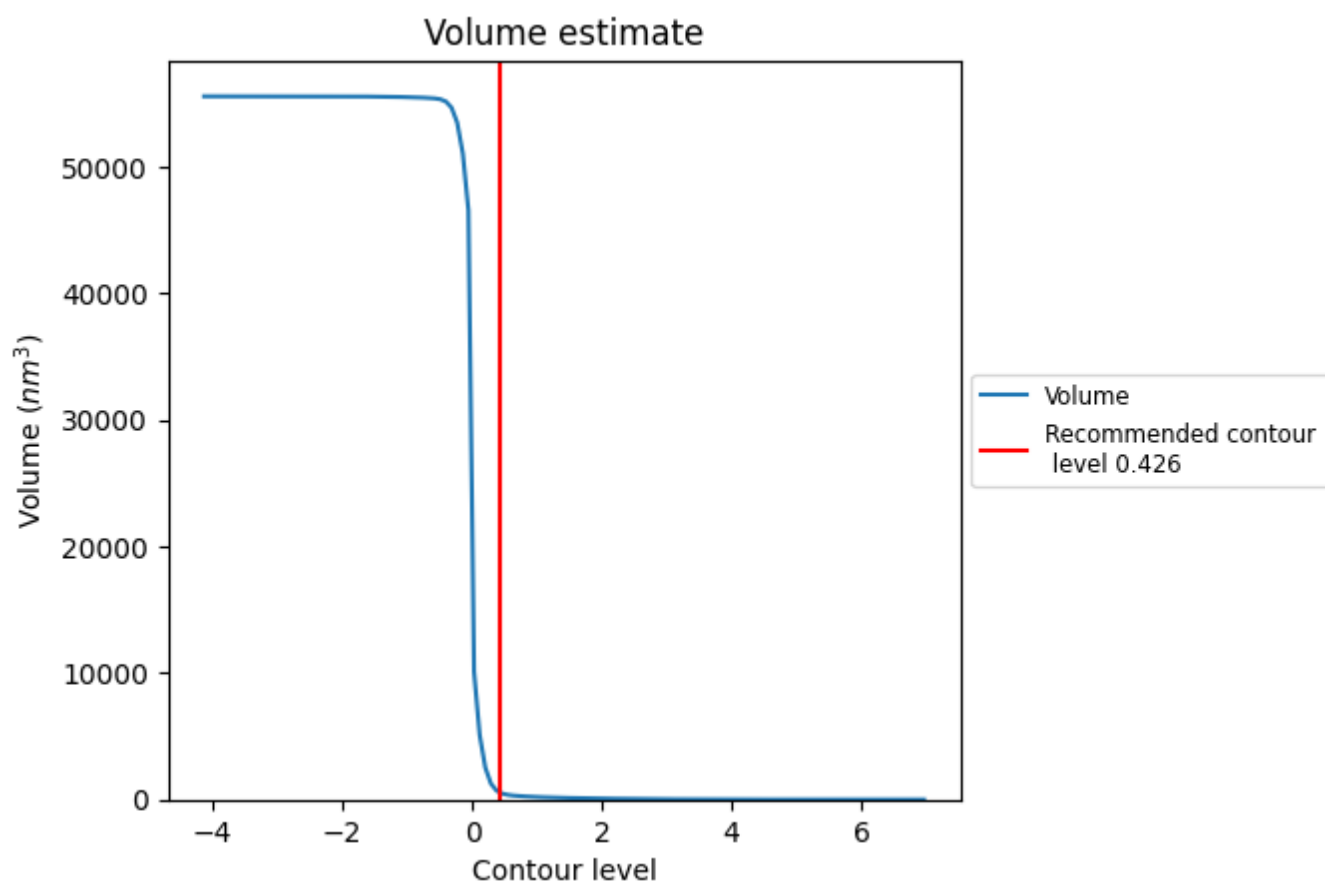
This section contains the results of statistical analysis of the map.

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.

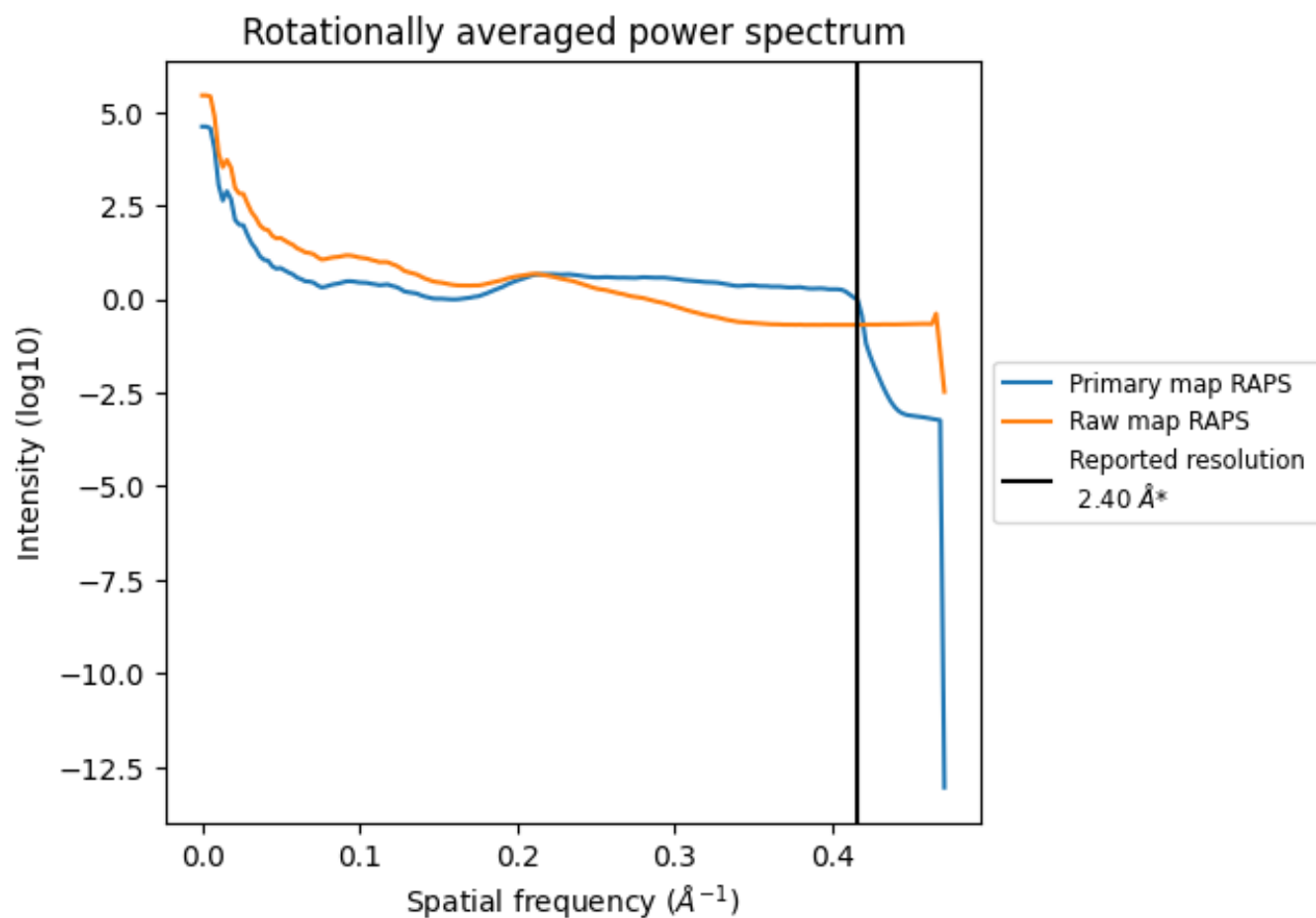
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 579 nm³; this corresponds to an approximate mass of 523 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 ⓘ

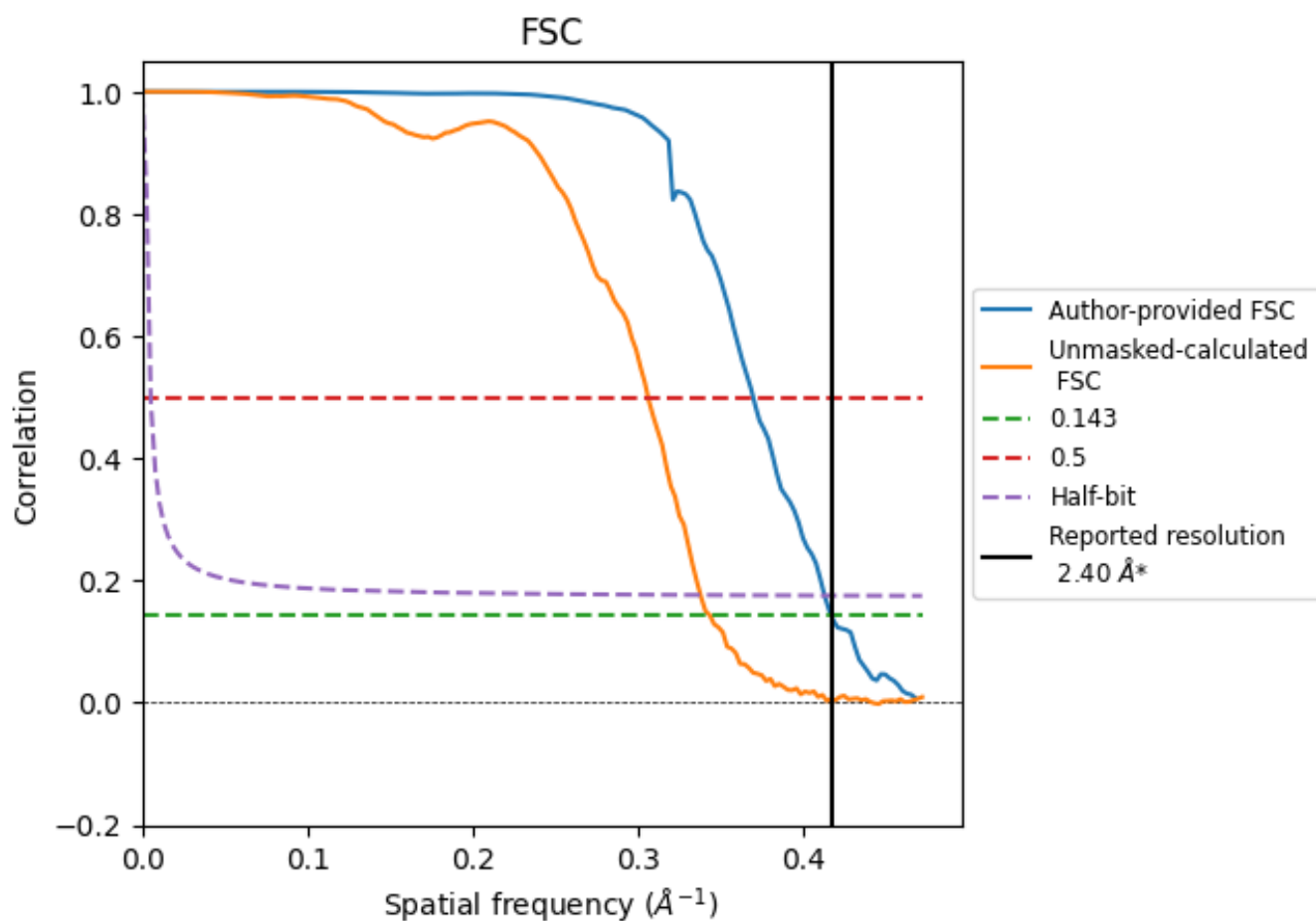


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 $0.417 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

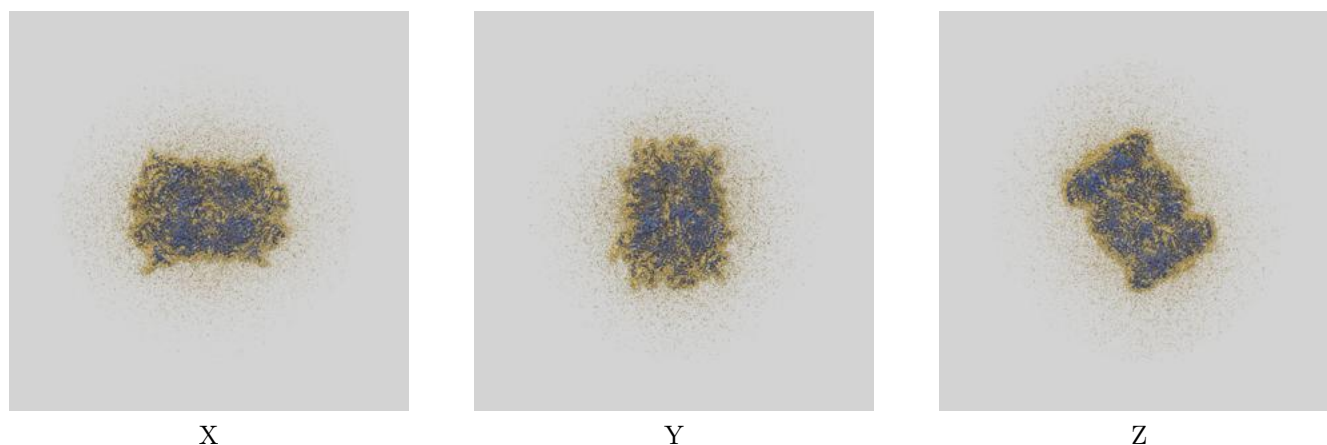
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.71	2.42
Unmasked-calculated*	2.91	3.27	2.96

*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 2.91 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

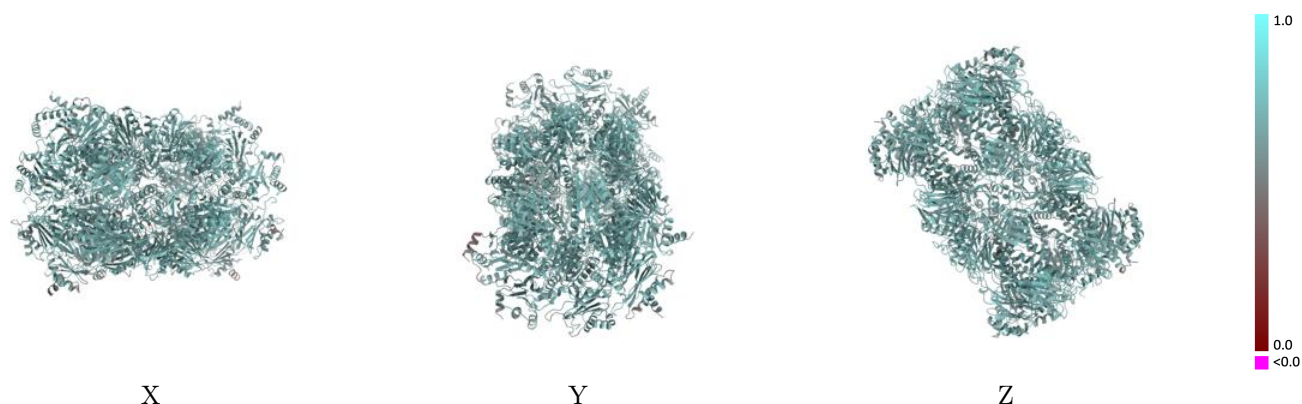
This section contains information regarding the fit between EMDB map EMD-40944 and PDB model 8T0M. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.426 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](#)

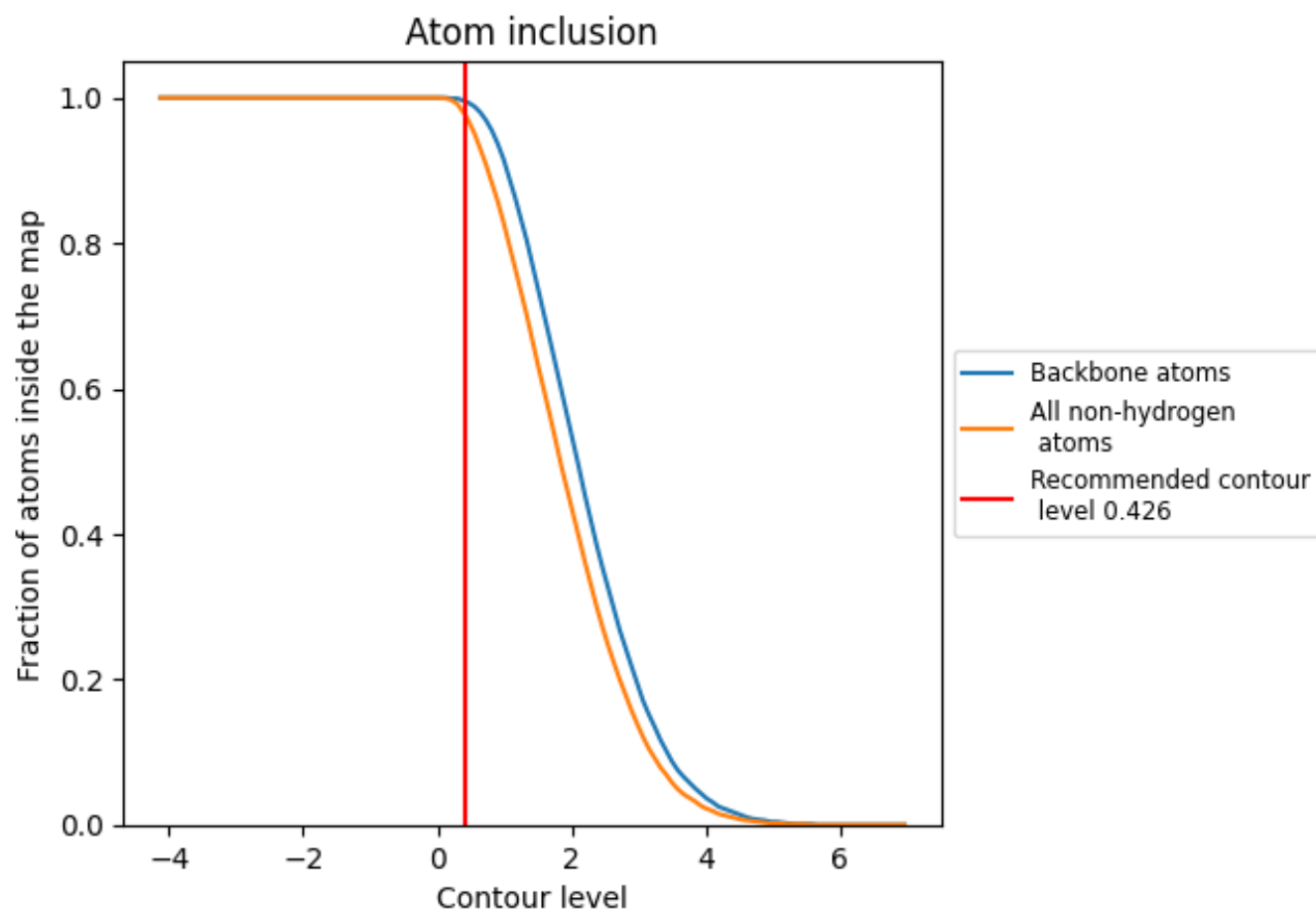


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.426) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.6600
A	 0.9890	 0.6690
B	 0.9780	 0.6680
C	 0.9700	 0.6520
D	 0.9590	 0.6190
E	 0.9590	 0.6270
F	 0.9720	 0.6520
G	 0.9700	 0.6610
H	 0.9800	 0.6610
I	 0.9820	 0.6730
J	 0.9840	 0.6840
K	 0.9690	 0.6520
L	 0.9810	 0.6690
M	 0.9770	 0.6680
N	 0.9830	 0.6780
O	 0.9880	 0.6710
P	 0.9800	 0.6710
Q	 0.9730	 0.6550
R	 0.9600	 0.6200
S	 0.9600	 0.6300
T	 0.9710	 0.6520
U	 0.9710	 0.6600
V	 0.9790	 0.6600
W	 0.9810	 0.6730
X	 0.9840	 0.6840
Y	 0.9690	 0.6540
Z	 0.9800	 0.6710
a	 0.9740	 0.6700
b	 0.9830	 0.6790

