



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:22 PM UTC

PDB ID : 8RVQ / pdb_00008rvq
EMDB ID : EMD-19529
Title : 20S proteasome from pre1-1
Authors : Mark, E.; Ramos, P.C.; Kayser, F.; Hoeckendorff, J.; Dohmen, R.J.; Wendler, P.
Deposited on : 2024-02-01
Resolution : 2.02 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:

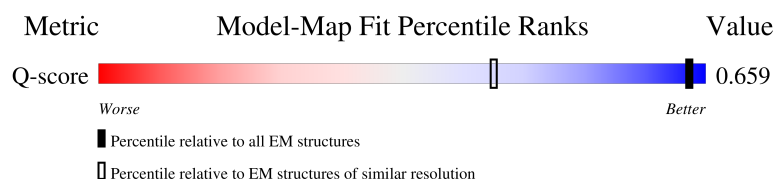
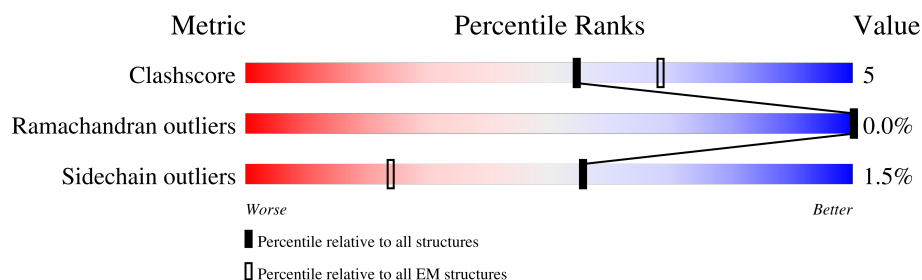
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.02 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	1728 (1.52 - 2.52)

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	1	222	
1	M	222	
2	2	233	
2	N	233	

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Mol	Chain	Length	Quality of chain
3	D	254	
3	R	254	
4	F	234	
4	T	234	
5	G	288	
5	U	288	
6	H	196	
6	V	196	
7	I	232	
7	W	232	
8	J	205	
8	X	205	
9	L	212	
9	Z	212	
10	A	252	
10	O	252	
11	B	250	
11	P	250	
12	C	258	
12	Q	258	
13	E	260	
13	S	260	
14	K	212	
14	Y	212	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 51191 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 beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	222	Total	C	N	O	S	0	0
			1756	1115	303	334	4		
1	M	222	Total	C	N	O	S	0	0
			1756	1115	303	334	4		

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		
2	N	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
3	R	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	231	Total	C	N	O	S	0	0
			1772	1114	307	347	4		
4	T	231	Total	C	N	O	S	0	0
			1772	1114	307	347	4		

- Molecule 5 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	240	Total	C	N	O	S	0	0
			1867	1188	325	350	4		
5	U	240	Total	C	N	O	S	0	0
			1867	1188	325	350	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	196	Total	C	N	O	S	0	0
			1511	955	250	299	7		
6	V	196	Total	C	N	O	S	0	0
			1511	955	250	299	7		

- Molecule 7 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	220	Total	C	N	O	S	0	0
			1670	1054	291	319	6		
7	W	220	Total	C	N	O	S	0	0
			1670	1054	291	319	6		

- Molecule 8 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	203	Total	C	N	O	S	0	0
			1574	1007	257	302	8		
8	X	203	Total	C	N	O	S	0	0
			1574	1007	257	302	8		

- Molecule 9 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	212	Total	C	N	O	S	0	0
			1643	1045	280	311	7		
9	Z	212	Total	C	N	O	S	0	0
			1643	1045	280	311	7		

- Molecule 10 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	228	Total	C	N	O	S	0	0
			1814	1155	305	346	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	228	Total	C	N	O	S	0	0
			1814	1155	305	346	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	245	Total	C	N	O	S	0	0
			1875	1194	309	369	3		
11	P	245	Total	C	N	O	S	0	0
			1875	1194	309	369	3		

- Molecule 12 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	240	Total	C	N	O	S	0	0
			1882	1189	318	372	3		
12	Q	243	Total	C	N	O	S	0	0
			1900	1200	321	376	3		

- Molecule 13 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	238	Total	C	N	O	S	0	0
			1829	1145	310	367	7		
13	S	237	Total	C	N	O	S	0	0
			1821	1140	309	365	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	187	Total	C	N	O	S	0	0
			1495	952	252	287	4		
14	Y	187	Total	C	N	O	S	0	0
			1496	952	252	288	4		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	engineered mutation	UNP P22141
K	199	ASP	-	expression tag	UNP P22141
K	200	TYR	-	expression tag	UNP P22141
K	201	LYS	-	expression tag	UNP P22141

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Chain	Residue	Modelled	Actual	Comment	Reference
K	202	ASP	-	expression tag	UNP P22141
K	203	ASP	-	expression tag	UNP P22141
K	204	ASP	-	expression tag	UNP P22141
K	205	ASP	-	expression tag	UNP P22141
K	206	LYS	-	expression tag	UNP P22141
K	207	HIS	-	expression tag	UNP P22141
K	208	HIS	-	expression tag	UNP P22141
K	209	HIS	-	expression tag	UNP P22141
K	210	HIS	-	expression tag	UNP P22141
K	211	HIS	-	expression tag	UNP P22141
K	212	HIS	-	expression tag	UNP P22141
Y	142	PHE	SER	engineered mutation	UNP P22141
Y	199	ASP	-	expression tag	UNP P22141
Y	200	TYR	-	expression tag	UNP P22141
Y	201	LYS	-	expression tag	UNP P22141
Y	202	ASP	-	expression tag	UNP P22141
Y	203	ASP	-	expression tag	UNP P22141
Y	204	ASP	-	expression tag	UNP P22141
Y	205	ASP	-	expression tag	UNP P22141
Y	206	LYS	-	expression tag	UNP P22141
Y	207	HIS	-	expression tag	UNP P22141
Y	208	HIS	-	expression tag	UNP P22141
Y	209	HIS	-	expression tag	UNP P22141
Y	210	HIS	-	expression tag	UNP P22141
Y	211	HIS	-	expression tag	UNP P22141
Y	212	HIS	-	expression tag	UNP P22141

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	AltConf
15	1	95	Total O 95 95	0
15	2	97	Total O 97 97	0
15	D	95	Total O 95 95	0
15	F	92	Total O 92 92	0
15	G	74	Total O 74 74	0
15	H	72	Total O 72 72	0

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Mol	Chain	Residues	Atoms		AltConf
15	I	101	Total 101	O 101	0
15	J	72	Total 72	O 72	0
15	L	80	Total 80	O 80	0
15	M	99	Total 99	O 99	0
15	N	99	Total 99	O 99	0
15	R	100	Total 100	O 100	0
15	T	86	Total 86	O 86	0
15	U	76	Total 76	O 76	0
15	V	68	Total 68	O 68	0
15	W	100	Total 100	O 100	0
15	X	76	Total 76	O 76	0
15	Z	81	Total 81	O 81	0
15	A	91	Total 91	O 91	0
15	B	83	Total 83	O 83	0
15	C	73	Total 73	O 73	0
15	E	103	Total 103	O 103	0
15	K	73	Total 73	O 73	0
15	O	91	Total 91	O 91	0
15	P	85	Total 85	O 85	0
15	Q	78	Total 78	O 78	0
15	S	102	Total 102	O 102	0

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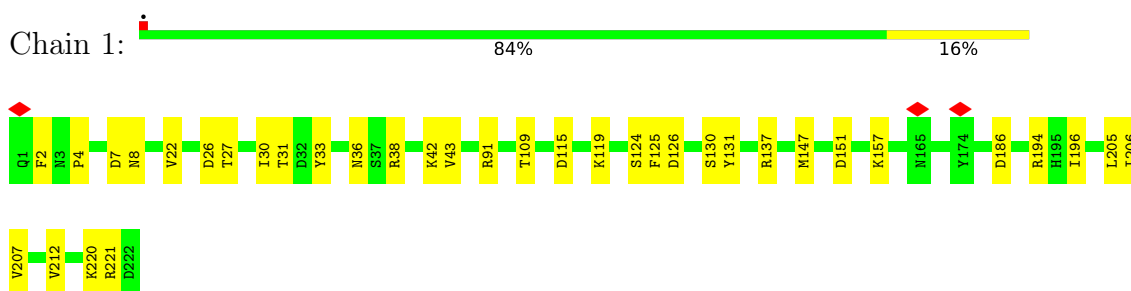
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Mol	Chain	Residues	Atoms		AltConf
15	Y	70	Total	O	0
			70	70	

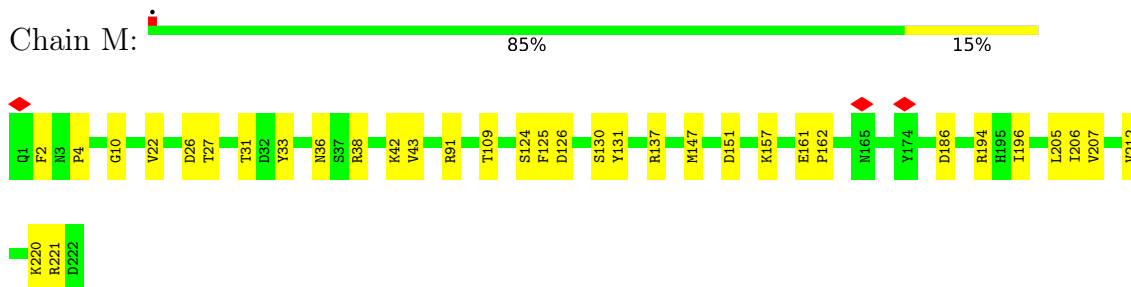
3 Residue-property plots

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.

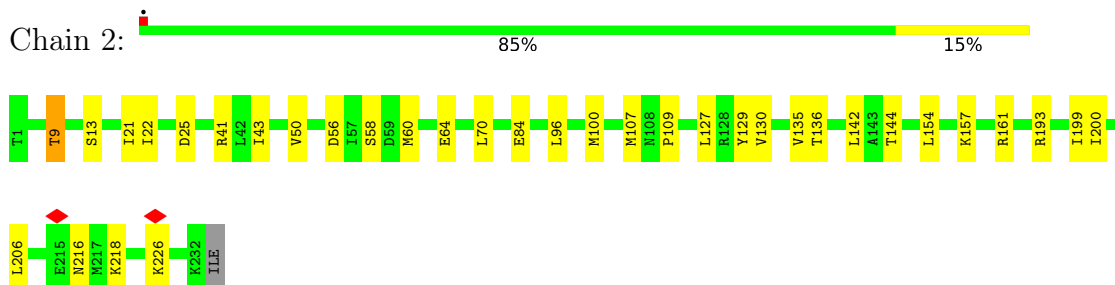
- Molecule 1: Proteasome subunit beta type-6



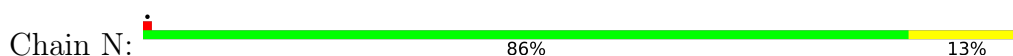
- Molecule 1: Proteasome subunit beta type-6

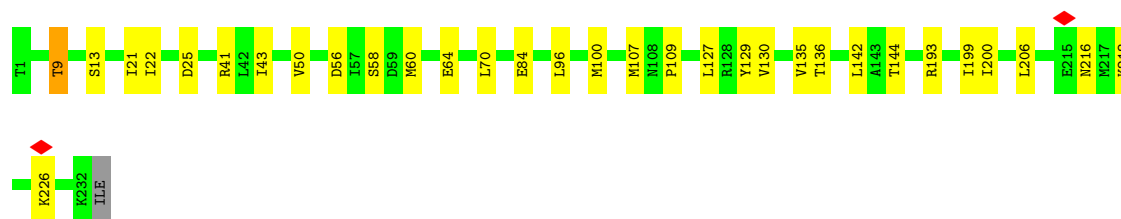


- Molecule 2: Proteasome subunit beta type-7

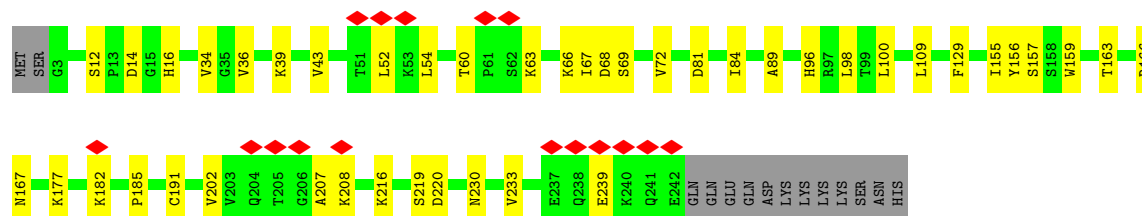
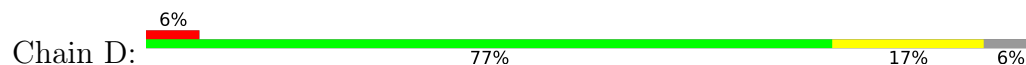


- Molecule 2: Proteasome subunit beta type-7

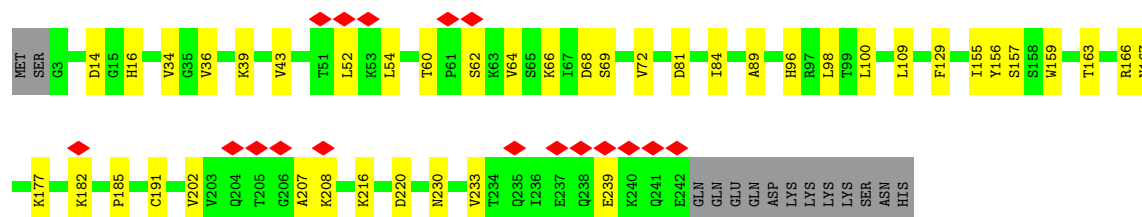
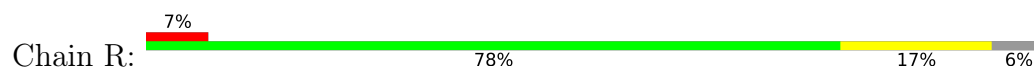




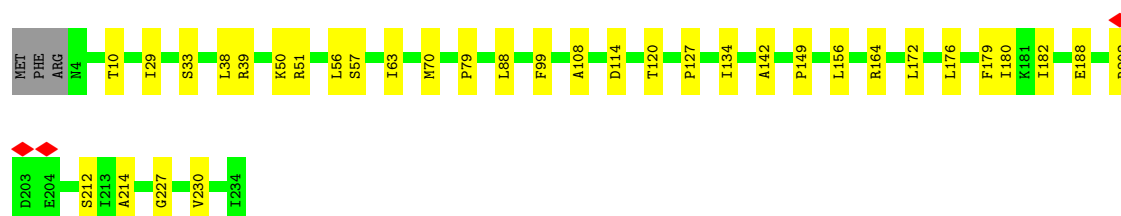
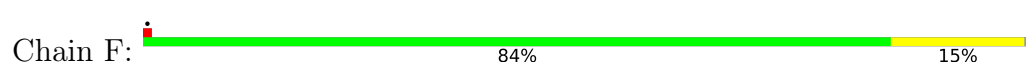
• Molecule 3: Proteasome subunit alpha type-4



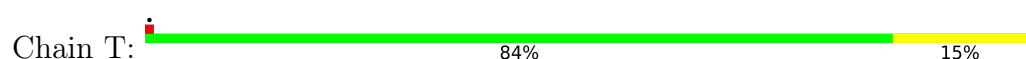
• Molecule 3: Proteasome subunit alpha type-4

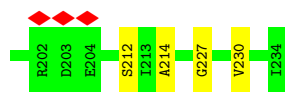


• Molecule 4: Proteasome subunit alpha type-6

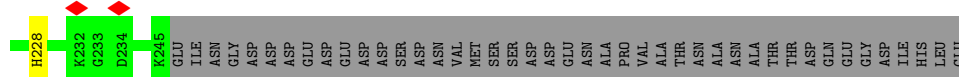
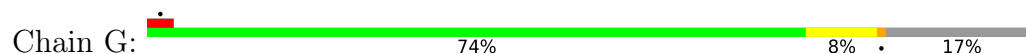


• Molecule 4: Proteasome subunit alpha type-6

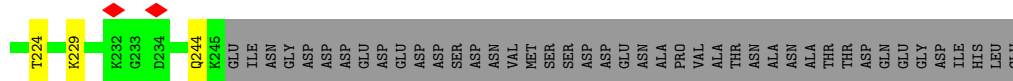
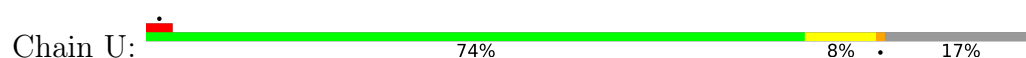




- Molecule 5: Probable proteasome subunit alpha type-7



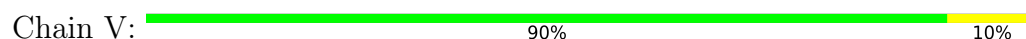
- Molecule 5: Probable proteasome subunit alpha type-7



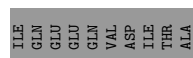
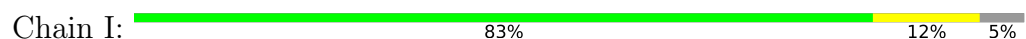
- Molecule 6: Proteasome subunit beta type-1



- Molecule 6: Proteasome subunit beta type-1

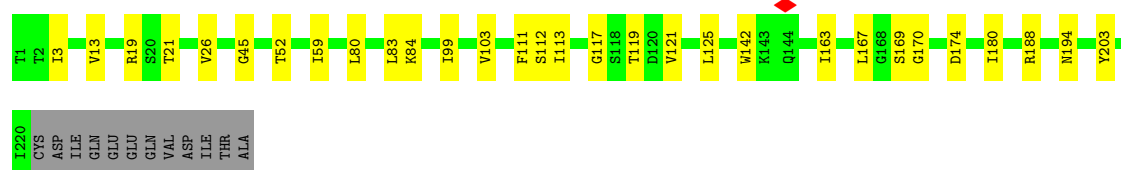


- Molecule 7: Proteasome subunit beta type-2



- Molecule 7: Proteasome subunit beta type-2

Chain W:  82% 13% 5%



- Molecule 8: Proteasome subunit beta type-3

Chain J:  90% 9% .



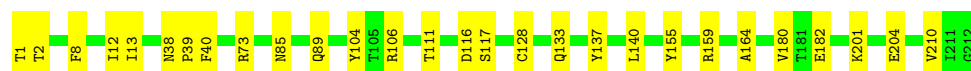
- Molecule 8: Proteasome subunit beta type-3

Chain X:  89% 9% .



- Molecule 9: Proteasome subunit beta type-5

Chain L:  87% 13%



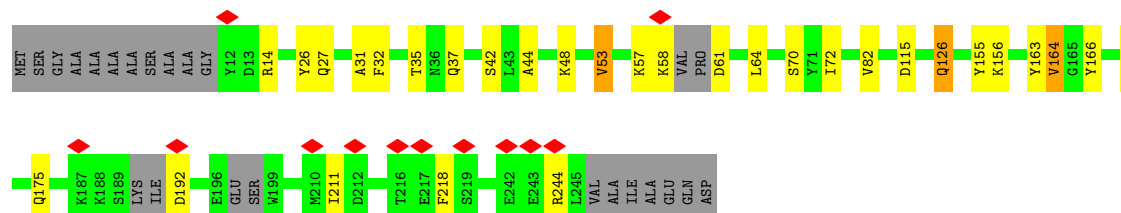
- Molecule 9: Proteasome subunit beta type-5

Chain Z:  87% 13%



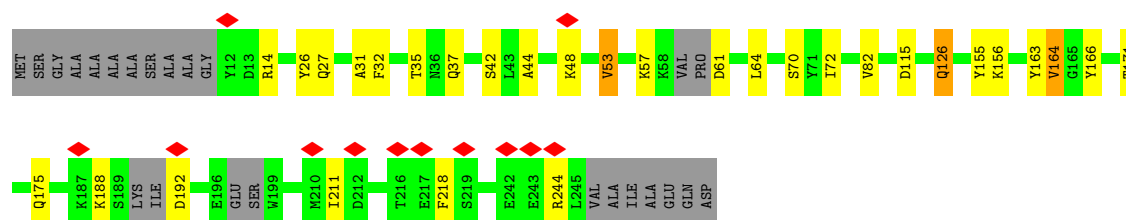
- Molecule 10: Proteasome subunit alpha type-1

Chain A:  5% 78% 11% 10%



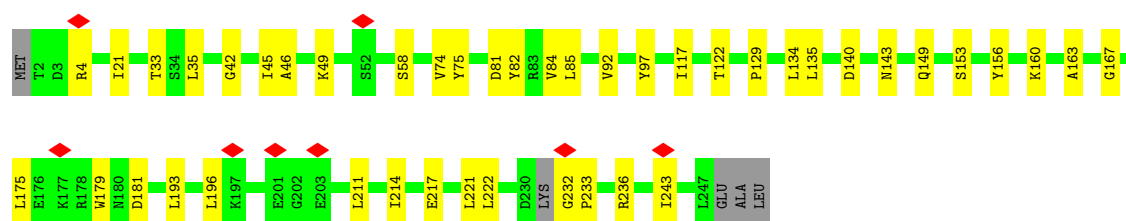
- Molecule 10: Proteasome subunit alpha type-1

Chain O: 



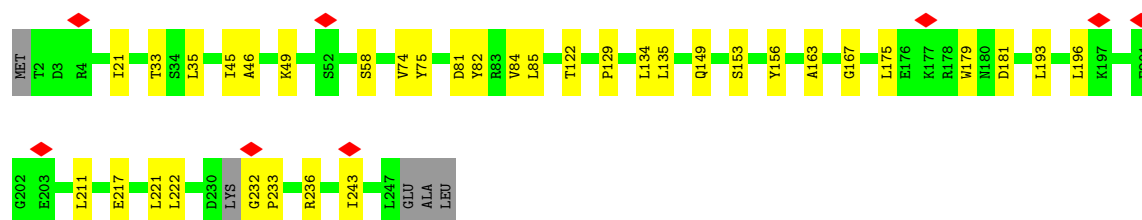
- Molecule 11: Proteasome subunit alpha type-2

Chain B: 



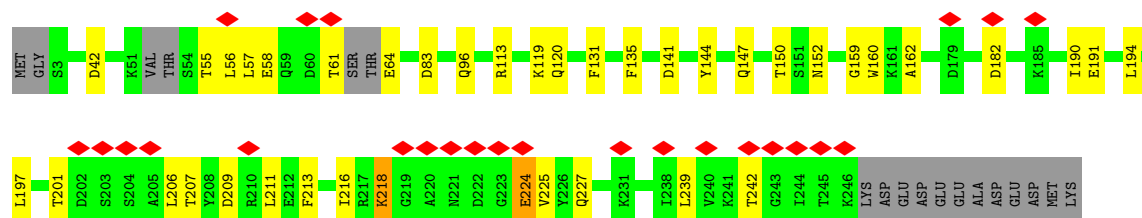
- Molecule 11: Proteasome subunit alpha type-2

Chain P: 



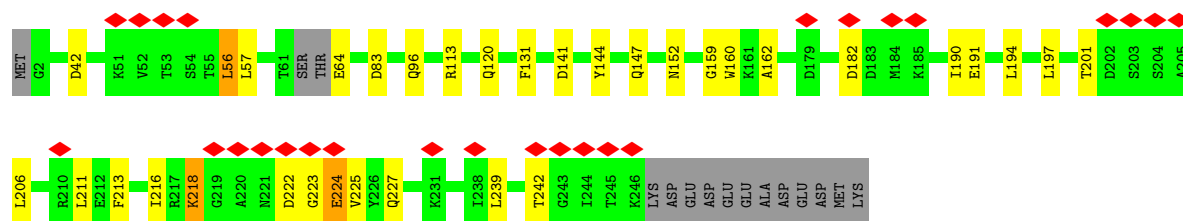
- Molecule 12: Proteasome subunit alpha type-3

Chain C: 

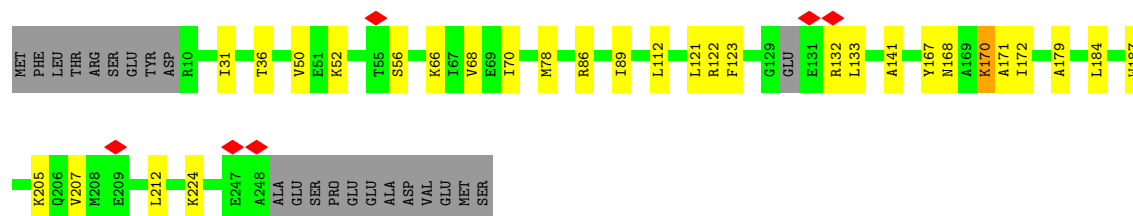
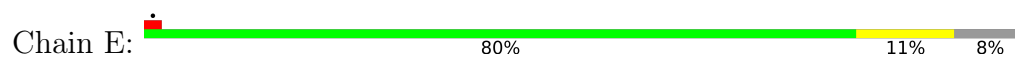


- Molecule 12: Proteasome subunit alpha type-3

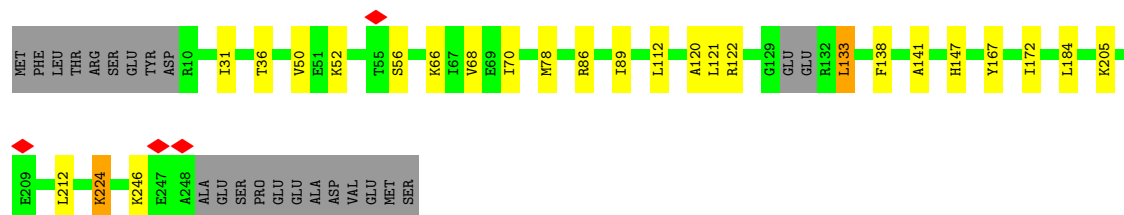
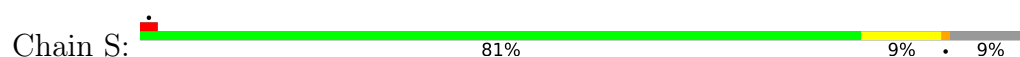
Chain Q: 



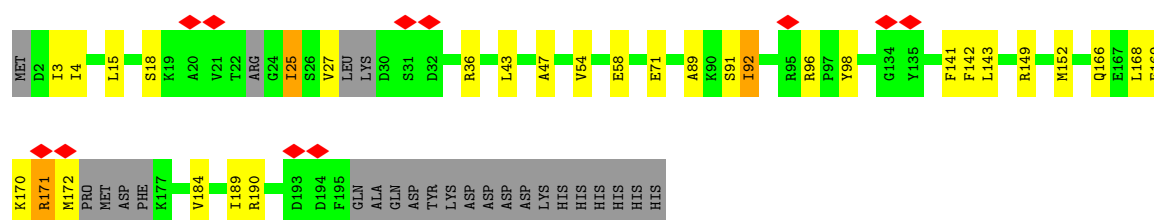
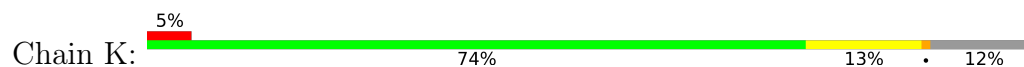
- Molecule 13: Proteasome subunit alpha type-5



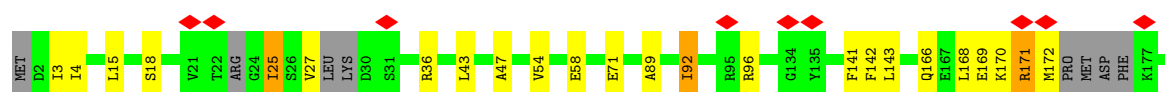
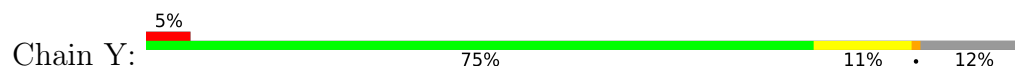
- Molecule 13: Proteasome subunit alpha type-5

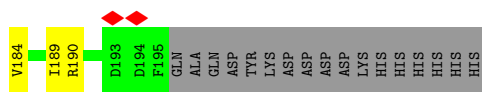


- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	341154	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.948	Depositor
Minimum map value	-1.197	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.276	Depositor
Map size ($\text{\AA}$)	500.4, 500.4, 500.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.834, 0.834, 0.834	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	1	0.11	0/1794	0.31	0/2420
1	M	0.11	0/1794	0.30	0/2420
2	2	0.12	0/1846	0.31	0/2503
2	N	0.12	0/1846	0.31	0/2503
3	D	0.11	0/1910	0.29	0/2586
3	R	0.11	0/1910	0.29	0/2586
4	F	0.11	0/1799	0.28	0/2433
4	T	0.11	0/1799	0.28	0/2433
5	G	0.11	0/1907	0.28	0/2575
5	U	0.10	0/1907	0.27	0/2575
6	H	0.11	0/1540	0.29	0/2087
6	V	0.11	0/1540	0.29	0/2087
7	I	0.11	0/1701	0.29	0/2307
7	W	0.11	0/1701	0.29	0/2307
8	J	0.12	0/1604	0.33	0/2166
8	X	0.12	0/1604	0.33	0/2166
9	L	0.11	0/1680	0.29	0/2274
9	Z	0.11	0/1680	0.29	0/2274
10	A	0.11	0/1848	0.29	0/2497
10	O	0.11	0/1848	0.29	0/2497
11	B	0.11	0/1911	0.27	0/2588
11	P	0.11	0/1911	0.29	0/2588
12	C	0.10	0/1910	0.26	0/2580
12	Q	0.10	0/1929	0.26	0/2608
13	E	0.10	0/1853	0.26	0/2494
13	S	0.10	0/1845	0.26	0/2484
14	K	0.10	0/1519	0.29	0/2044
14	Y	0.10	0/1520	0.29	0/2046
All	All	0.11	0/49656	0.29	0/67128

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1756	0	1711	26	0
1	M	1756	0	1711	24	0
2	2	1815	0	1821	25	0
2	N	1815	0	1821	23	0
3	D	1881	0	1892	27	0
3	R	1881	0	1892	24	0
4	F	1772	0	1775	23	0
4	T	1772	0	1775	25	0
5	G	1867	0	1860	17	0
5	U	1867	0	1860	17	0
6	H	1511	0	1481	10	0
6	V	1511	0	1481	10	0
7	I	1670	0	1679	19	0
7	W	1670	0	1679	20	0
8	J	1574	0	1566	13	0
8	X	1574	0	1566	13	0
9	L	1643	0	1595	17	0
9	Z	1643	0	1595	16	0
10	A	1814	0	1800	19	0
10	O	1814	0	1800	19	0
11	B	1875	0	1881	24	0
11	P	1875	0	1881	19	0
12	C	1882	0	1881	27	0
12	Q	1900	0	1901	24	0
13	E	1829	0	1814	20	0
13	S	1821	0	1808	18	0
14	K	1495	0	1492	22	0
14	Y	1496	0	1492	18	0
15	1	95	0	0	2	0
15	2	97	0	0	2	0
15	A	91	0	0	3	0
15	B	83	0	0	1	0
15	C	73	0	0	2	0
15	D	95	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	103	0	0	1	0
15	F	92	0	0	0	0
15	G	74	0	0	1	0
15	H	72	0	0	0	0
15	I	101	0	0	1	0
15	J	72	0	0	2	0
15	K	73	0	0	3	0
15	L	80	0	0	2	0
15	M	99	0	0	2	0
15	N	99	0	0	1	0
15	O	91	0	0	3	0
15	P	85	0	0	1	0
15	Q	78	0	0	2	0
15	R	100	0	0	1	0
15	S	102	0	0	1	0
15	T	86	0	0	0	0
15	U	76	0	0	2	0
15	V	68	0	0	0	0
15	W	100	0	0	1	0
15	X	76	0	0	2	0
15	Y	70	0	0	2	0
15	Z	81	0	0	1	0
All	All	51191	0	48510	493	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 (493) 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:B:160:LYS:HB2	12:C:57:LEU:HD12	1.68	0.75
1:M:196:ILE:HD11	7:W:21:THR:HG21	1.73	0.70
1:1:196:ILE:HD11	7:I:21:THR:HG21	1.73	0.70
1:M:151:ASP:HB3	1:M:157:LYS:HD2	1.75	0.69
1:1:151:ASP:HB3	1:1:157:LYS:HD2	1.75	0.68
4:T:114:ASP:OD1	5:U:86:ARG:NH1	2.27	0.68
4:F:114:ASP:OD1	5:G:86:ARG:NH1	2.27	0.67
13:S:122:ARG:HH21	13:S:133:LEU:HD23	1.59	0.67
4:T:88:LEU:HD11	4:T:108:ALA:HB1	1.75	0.66
4:F:88:LEU:HD11	4:F:108:ALA:HB1	1.76	0.66
12:C:42:ASP:HB3	12:C:218:LYS:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:171:ARG:NH2	14:Y:172:MET:SD	2.68	0.65
14:Y:3:ILE:HB	14:Y:18:SER:HB3	1.78	0.65
12:C:216:ILE:HG12	12:C:227:GLN:HG2	1.79	0.65
12:Q:216:ILE:HG12	12:Q:227:GLN:HG2	1.79	0.64
5:U:38:ILE:HD11	5:U:176:LEU:HD21	1.79	0.64
12:Q:42:ASP:HB3	12:Q:218:LYS:HE2	1.79	0.64
14:K:36:ARG:HH21	14:K:54:VAL:HG13	1.62	0.64
14:K:171:ARG:NH2	14:K:172:MET:SD	2.70	0.64
4:F:39:ARG:NH1	4:F:142:ALA:O	2.31	0.63
5:G:38:ILE:HD11	5:G:176:LEU:HD21	1.79	0.63
7:I:3:ILE:HG22	7:I:99:ILE:HD12	1.80	0.63
4:T:39:ARG:NH1	4:T:142:ALA:O	2.31	0.63
14:K:3:ILE:HB	14:K:18:SER:HB3	1.79	0.62
2:N:127:LEU:HG	2:N:142:LEU:HD12	1.81	0.62
12:C:197:LEU:O	12:C:201:THR:OG1	2.14	0.62
7:I:112:SER:HB3	7:I:125:LEU:HD13	1.80	0.62
10:O:175:GLN:NE2	15:O:303:HOH:O	2.33	0.62
9:L:201:LYS:NZ	9:L:210:VAL:O	2.32	0.62
7:W:3:ILE:HG22	7:W:99:ILE:HD12	1.80	0.61
10:A:175:GLN:NE2	15:A:304:HOH:O	2.33	0.61
8:J:13:VAL:HG13	8:J:138:VAL:HG12	1.83	0.61
7:W:112:SER:HB3	7:W:125:LEU:HD13	1.81	0.61
1:1:207:VAL:HG22	1:1:212:VAL:HG22	1.83	0.61
8:X:21:VAL:HG12	8:X:190:ILE:HB	1.82	0.61
2:2:127:LEU:HG	2:2:142:LEU:HD12	1.82	0.60
11:B:179:TRP:NE1	11:B:181:ASP:OD1	2.34	0.60
12:Q:113:ARG:NH2	14:Y:71:GLU:OE2	2.34	0.60
8:X:13:VAL:HG13	8:X:138:VAL:HG12	1.82	0.60
2:2:25:ASP:OD1	2:2:41:ARG:NH2	2.31	0.60
3:D:14:ASP:OD2	3:D:16:HIS:ND1	2.35	0.60
8:J:21:VAL:HG12	8:J:190:ILE:HB	1.83	0.60
13:E:66:LYS:HA	13:E:78:MET:HE2	1.84	0.60
5:G:9:ASP:N	5:G:9:ASP:OD1	2.35	0.60
3:R:54:LEU:HD13	12:Q:162:ALA:HB3	1.84	0.60
10:A:42:SER:OG	10:A:171:THR:OG1	2.20	0.60
13:S:66:LYS:HA	13:S:78:MET:HE2	1.84	0.60
1:M:31:THR:HG23	1:M:36:ASN:HD21	1.67	0.59
1:1:109:THR:HB	1:1:125:PHE:HB2	1.85	0.59
3:R:14:ASP:OD2	3:R:16:HIS:ND1	2.35	0.59
1:M:207:VAL:HG22	1:M:212:VAL:HG22	1.83	0.59
10:O:72:ILE:HG12	10:O:82:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:50:VAL:HG21	13:S:66:LYS:HB2	1.83	0.59
1:M:194:ARG:HG2	8:X:151:GLU:HG3	1.85	0.58
12:C:113:ARG:NH2	14:K:71:GLU:OE2	2.34	0.58
10:A:72:ILE:HG12	10:A:82:VAL:HG22	1.83	0.58
5:U:9:ASP:N	5:U:9:ASP:OD1	2.35	0.58
13:E:50:VAL:HG21	13:E:66:LYS:HB2	1.84	0.58
10:O:42:SER:OG	10:O:171:THR:OG1	2.20	0.58
1:1:194:ARG:HG2	8:J:151:GLU:HG3	1.85	0.58
7:W:103:VAL:HG11	7:W:180:ILE:HA	1.86	0.58
10:A:192:ASP:N	15:A:305:HOH:O	2.36	0.58
14:Y:96:ARG:NH1	15:Y:306:HOH:O	2.36	0.58
1:M:109:THR:HB	1:M:125:PHE:HB2	1.85	0.58
10:O:192:ASP:N	15:O:304:HOH:O	2.36	0.58
14:Y:36:ARG:HH21	14:Y:54:VAL:HG13	1.68	0.58
14:K:96:ARG:NH1	15:K:306:HOH:O	2.36	0.58
7:I:103:VAL:HG11	7:I:180:ILE:HA	1.86	0.57
12:C:64:GLU:N	15:C:305:HOH:O	2.38	0.57
13:E:170:LYS:HD3	13:E:171:ALA:H	1.69	0.57
1:M:4:PRO:HG3	2:N:107:MET:HE1	1.86	0.57
9:L:38:ASN:HD22	9:L:40:PHE:H	1.53	0.57
2:2:218:LYS:NZ	7:I:142:TRP:O	2.37	0.57
4:F:70:MET:HE1	4:F:108:ALA:HB3	1.87	0.57
12:C:141:ASP:OD1	12:C:147:GLN:NE2	2.38	0.57
10:O:61:ASP:HB2	10:O:64:LEU:HD13	1.87	0.57
12:Q:64:GLU:N	15:Q:305:HOH:O	2.38	0.56
4:T:70:MET:HE1	4:T:108:ALA:HB3	1.87	0.56
3:D:54:LEU:HD13	12:C:162:ALA:HB3	1.85	0.56
3:R:98:LEU:HD11	14:Y:58:GLU:HB3	1.86	0.56
1:1:4:PRO:HG3	2:2:107:MET:HE1	1.87	0.56
12:Q:197:LEU:O	12:Q:201:THR:OG1	2.14	0.56
1:M:38:ARG:NH1	15:M:305:HOH:O	2.39	0.56
1:M:221:ARG:NH2	15:M:304:HOH:O	2.38	0.56
14:Y:190:ARG:NH1	15:Y:307:HOH:O	2.39	0.56
1:1:38:ARG:NH1	15:1:304:HOH:O	2.38	0.56
11:P:236:ARG:NH1	15:P:303:HOH:O	2.39	0.56
2:N:25:ASP:OD1	2:N:41:ARG:NH2	2.31	0.56
12:Q:141:ASP:OD1	12:Q:147:GLN:NE2	2.38	0.56
12:C:58:GLU:OE2	12:C:61:THR:OG1	2.23	0.56
1:1:221:ARG:NH2	15:1:305:HOH:O	2.39	0.56
7:I:21:THR:HG22	7:I:26:VAL:HA	1.88	0.56
2:N:218:LYS:NZ	7:W:142:TRP:O	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:60:THR:HG22	12:Q:159:GLY:H	1.71	0.55
3:R:81:ASP:OD1	12:Q:120:GLN:NE2	2.36	0.55
9:Z:159:ARG:NH1	9:Z:204:GLU:OE1	2.40	0.55
9:Z:38:ASN:HD22	9:Z:40:PHE:H	1.55	0.55
2:2:154:LEU:O	2:2:157:LYS:HB2	2.07	0.55
10:A:61:ASP:HB2	10:A:64:LEU:HD13	1.88	0.55
14:K:190:ARG:NH1	15:K:308:HOH:O	2.39	0.55
5:G:63:LYS:NZ	15:G:303:HOH:O	2.39	0.55
8:J:135:ASP:OD1	8:J:135:ASP:N	2.39	0.55
11:P:179:TRP:NE1	11:P:181:ASP:OD1	2.38	0.55
5:U:244:GLN:NE2	15:U:305:HOH:O	2.39	0.55
12:Q:144:TYR:HB2	12:Q:147:GLN:HE21	1.72	0.54
7:W:21:THR:HG22	7:W:26:VAL:HA	1.88	0.54
1:1:7:ASP:OD1	1:1:8:ASN:N	2.40	0.54
3:D:81:ASP:OD1	12:C:120:GLN:NE2	2.36	0.54
11:B:149:GLN:O	11:B:156:TYR:HA	2.07	0.54
12:C:144:TYR:HB2	12:C:147:GLN:HE21	1.72	0.54
12:Q:182:ASP:OD1	12:Q:182:ASP:N	2.41	0.54
9:Z:12:ILE:HB	9:Z:180:VAL:HB	1.89	0.54
11:B:236:ARG:NH1	15:B:303:HOH:O	2.39	0.54
8:X:11:ILE:HG21	8:X:142:ALA:HB3	1.89	0.54
5:U:19:GLY:O	10:O:37:GLN:NE2	2.41	0.54
8:X:34:LEU:HD21	14:Y:141:PHE:HE2	1.72	0.54
10:O:57:LYS:HD3	10:O:70:SER:HA	1.89	0.54
12:Q:206:LEU:HD11	12:Q:211:LEU:HD21	1.89	0.54
12:Q:194:LEU:HD12	12:Q:242:THR:HG21	1.90	0.54
11:P:149:GLN:O	11:P:156:TYR:HA	2.08	0.53
5:U:63:LYS:NZ	15:U:304:HOH:O	2.39	0.53
12:C:194:LEU:HD12	12:C:242:THR:HG21	1.90	0.53
12:C:206:LEU:HD11	12:C:211:LEU:HD21	1.90	0.53
9:L:12:ILE:HB	9:L:180:VAL:HB	1.88	0.53
10:A:14:ARG:O	10:A:27:GLN:NE2	2.42	0.53
10:O:126:GLN:NE2	11:P:81:ASP:OD1	2.41	0.53
8:J:34:LEU:HD21	14:K:141:PHE:HE2	1.73	0.53
9:Z:106:ARG:NH1	15:Z:307:HOH:O	2.39	0.53
1:1:31:THR:HG23	1:1:36:ASN:HD21	1.73	0.53
8:J:11:ILE:HG21	8:J:142:ALA:HB3	1.88	0.53
1:M:137:ARG:HA	1:M:147:MET:HE1	1.90	0.53
3:D:98:LEU:HD11	14:K:58:GLU:HB3	1.91	0.53
11:B:33:THR:HG22	11:B:167:GLY:H	1.74	0.53
12:C:224:GLU:OE1	12:C:225:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:14:ARG:O	10:O:27:GLN:NE2	2.41	0.53
1:1:137:ARG:HA	1:1:147:MET:HE1	1.91	0.52
12:C:182:ASP:OD1	12:C:182:ASP:N	2.40	0.52
1:M:220:LYS:HD2	7:W:194:ASN:HB3	1.91	0.52
13:E:52:LYS:NZ	15:E:302:HOH:O	2.43	0.52
12:Q:224:GLU:OE1	12:Q:225:VAL:N	2.42	0.52
2:N:129:TYR:O	2:N:136:THR:HA	2.09	0.52
3:R:62:SER:O	3:R:64:VAL:N	2.43	0.52
4:T:182:ILE:HD13	4:T:188:GLU:HG2	1.91	0.52
13:E:123:PHE:O	13:E:132:ARG:NH1	2.43	0.52
9:L:73:ARG:NH2	15:L:304:HOH:O	2.35	0.52
11:P:35:LEU:HG	11:P:163:ALA:HB2	1.91	0.52
1:1:220:LYS:HD2	7:I:194:ASN:HB3	1.91	0.52
1:M:2:PHE:CE1	2:N:109:PRO:HG3	2.45	0.52
8:X:135:ASP:OD1	8:X:135:ASP:N	2.39	0.52
2:2:129:TYR:O	2:2:136:THR:HA	2.09	0.52
2:N:129:TYR:HE2	2:N:144:THR:HB	1.75	0.52
11:P:46:ALA:HB1	11:P:196:LEU:HD11	1.92	0.52
3:D:12:SER:OG	3:D:14:ASP:OD1	2.22	0.51
2:N:56:ASP:OD2	2:N:58:SER:OG	2.24	0.51
10:A:126:GLN:NE2	11:B:81:ASP:OD1	2.41	0.51
4:F:182:ILE:HD13	4:F:188:GLU:HG2	1.91	0.51
11:B:46:ALA:HB1	11:B:196:LEU:HD11	1.92	0.51
13:S:52:LYS:NZ	15:S:301:HOH:O	2.43	0.51
3:D:60:THR:HG22	12:C:159:GLY:H	1.75	0.51
11:P:33:THR:HG22	11:P:167:GLY:H	1.76	0.51
1:1:2:PHE:CE1	2:2:109:PRO:HG3	2.45	0.51
7:I:19:ARG:NH2	7:I:169:SER:O	2.44	0.51
3:R:216:LYS:HB2	3:R:220:ASP:HB3	1.92	0.51
4:T:79:PRO:HB3	13:S:121:LEU:HD11	1.93	0.51
11:B:49:LYS:HD3	11:B:58:SER:HB2	1.92	0.51
2:2:161:ARG:NH1	15:2:312:HOH:O	2.44	0.51
7:I:19:ARG:NH2	15:I:302:HOH:O	2.44	0.51
9:L:159:ARG:NH1	9:L:204:GLU:OE1	2.43	0.51
3:R:68:ASP:OD1	3:R:69:SER:N	2.41	0.51
3:D:216:LYS:HB2	3:D:220:ASP:HB3	1.93	0.51
4:T:29:ILE:HD11	4:T:149:PRO:HD3	1.93	0.51
7:W:45:GLY:HA3	7:W:52:THR:HG21	1.93	0.51
3:D:157:SER:OG	3:D:159:TRP:NE1	2.44	0.50
3:D:63:LYS:NZ	15:D:306:HOH:O	2.43	0.50
5:U:214:LEU:HD21	5:U:216:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:19:ARG:NH2	7:W:169:SER:O	2.43	0.50
9:Z:73:ARG:NH2	9:Z:104:TYR:O	2.44	0.50
11:P:211:LEU:HD12	11:P:243:ILE:HG12	1.92	0.50
11:B:35:LEU:HG	11:B:163:ALA:HB2	1.92	0.50
1:M:26:ASP:OD1	1:M:27:THR:N	2.44	0.50
3:R:230:ASN:ND2	15:R:308:HOH:O	2.42	0.50
4:F:79:PRO:HB3	13:E:121:LEU:HD11	1.93	0.50
7:I:174:ASP:OD2	7:I:188:ARG:NH1	2.44	0.50
3:R:157:SER:OG	3:R:159:TRP:NE1	2.44	0.50
4:T:50:LYS:HE3	4:T:212:SER:HB2	1.94	0.50
11:P:74:VAL:HG12	11:P:135:LEU:HB2	1.94	0.50
1:I:186:ASP:OD2	7:I:203:TYR:OH	2.27	0.50
2:2:96:LEU:O	2:2:100:MET:HG2	2.12	0.50
8:J:134:LYS:NZ	15:J:310:HOH:O	2.45	0.50
5:G:193:VAL:HG13	5:G:216:ILE:HG21	1.93	0.49
9:L:106:ARG:NH1	15:L:306:HOH:O	2.36	0.49
7:W:19:ARG:NH2	15:W:302:HOH:O	2.43	0.49
9:Z:201:LYS:NZ	9:Z:210:VAL:O	2.32	0.49
12:Q:152:ASN:ND2	15:Q:306:HOH:O	2.39	0.49
2:2:50:VAL:HG23	2:2:200:ILE:HD11	1.94	0.49
7:I:45:GLY:HA3	7:I:52:THR:HG21	1.94	0.49
7:W:174:ASP:OD2	7:W:188:ARG:NH1	2.44	0.49
13:E:70:ILE:HG21	13:E:112:LEU:HD21	1.94	0.49
11:P:49:LYS:HD3	11:P:58:SER:HB2	1.94	0.49
5:G:214:LEU:HD21	5:G:216:ILE:HD11	1.94	0.49
5:U:193:VAL:HG13	5:U:216:ILE:HG21	1.94	0.49
8:X:134:LYS:NZ	15:X:312:HOH:O	2.45	0.49
10:A:156:LYS:O	10:A:163:TYR:HA	2.12	0.49
11:B:193:LEU:HD21	11:B:211:LEU:HD11	1.94	0.49
4:F:50:LYS:HE3	4:F:212:SER:HB2	1.94	0.49
3:R:66:LYS:HG2	3:R:72:VAL:HG12	1.94	0.49
13:S:70:ILE:HG21	13:S:112:LEU:HD21	1.94	0.49
2:2:21:ILE:HG12	2:2:199:ILE:HG12	1.95	0.49
11:B:211:LEU:HD12	11:B:243:ILE:HG12	1.93	0.49
4:F:29:ILE:HD11	4:F:149:PRO:HD3	1.93	0.49
8:J:107:PRO:HG2	8:J:124:PHE:HB2	1.95	0.49
10:A:57:LYS:HD3	10:A:70:SER:HA	1.95	0.49
10:O:156:LYS:O	10:O:163:TYR:HA	2.12	0.49
5:G:19:GLY:O	10:A:37:GLN:NE2	2.43	0.49
11:B:74:VAL:HG12	11:B:135:LEU:HB2	1.94	0.49
6:H:148:LYS:NZ	6:H:184:GLU:OE1	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:96:LEU:O	2:N:100:MET:HG2	2.12	0.49
8:X:107:PRO:HG2	8:X:124:PHE:HB2	1.95	0.48
14:K:4:ILE:HG13	14:K:47:ALA:HB2	1.94	0.48
11:P:193:LEU:HD21	11:P:211:LEU:HD11	1.94	0.48
9:Z:38:ASN:HB2	9:Z:39:PRO:HD2	1.94	0.48
14:K:15:LEU:HD12	14:K:43:LEU:HD23	1.96	0.48
14:Y:4:ILE:HG13	14:Y:47:ALA:HB2	1.95	0.48
3:D:230:ASN:ND2	15:D:307:HOH:O	2.43	0.48
2:N:50:VAL:HG23	2:N:200:ILE:HD11	1.95	0.48
3:D:68:ASP:OD1	3:D:69:SER:N	2.43	0.48
4:F:33:SER:OG	4:F:51:ARG:NE	2.47	0.48
1:1:26:ASP:OD1	1:1:27:THR:N	2.46	0.48
10:O:126:GLN:HG2	11:P:84:VAL:HG21	1.96	0.48
2:2:56:ASP:OD2	2:2:58:SER:OG	2.24	0.48
13:S:205:LYS:HB2	13:S:212:LEU:HD22	1.96	0.48
1:1:126:ASP:OD1	1:1:130:SER:N	2.47	0.47
2:N:21:ILE:HG12	2:N:199:ILE:HG12	1.95	0.47
14:K:166:GLN:O	14:K:170:LYS:HG2	2.14	0.47
3:D:34:VAL:HG23	3:D:163:THR:HG22	1.95	0.47
14:Y:166:GLN:O	14:Y:170:LYS:HG2	2.14	0.47
3:D:66:LYS:HG2	3:D:72:VAL:HG12	1.95	0.47
5:G:52:LYS:HG2	5:G:66:LYS:HD2	1.96	0.47
9:Z:116:ASP:OD1	9:Z:117:SER:N	2.48	0.47
13:E:205:LYS:HB2	13:E:212:LEU:HD22	1.95	0.47
4:T:33:SER:OG	4:T:51:ARG:NE	2.47	0.47
1:M:126:ASP:OD1	1:M:130:SER:N	2.47	0.47
13:S:31:ILE:HD13	13:S:141:ALA:HB2	1.96	0.47
9:L:38:ASN:HB2	9:L:39:PRO:HD2	1.95	0.47
3:R:96:HIS:NE2	3:R:100:LEU:HD12	2.30	0.47
10:A:32:PHE:O	10:A:35:THR:OG1	2.25	0.47
3:D:96:HIS:NE2	3:D:100:LEU:HD12	2.30	0.47
7:W:113:ILE:HG12	7:W:119:THR:HG22	1.97	0.47
14:Y:184:VAL:HG22	14:Y:189:ILE:HG12	1.97	0.47
8:J:178:ASP:O	15:J:301:HOH:O	2.20	0.47
12:Q:194:LEU:HD13	12:Q:239:LEU:HD23	1.97	0.47
14:Y:15:LEU:HD12	14:Y:43:LEU:HD23	1.96	0.47
4:F:57:SER:HB2	13:E:167:TYR:CE2	2.50	0.47
9:L:155:TYR:OH	9:L:204:GLU:OE2	2.30	0.47
7:W:111:PHE:CD1	7:W:121:VAL:HG22	2.50	0.47
5:G:6:THR:OG1	5:G:7:GLY:N	2.46	0.46
8:J:69:TYR:CD2	12:C:96:GLN:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:133:GLN:HG3	14:K:25:ILE:HD12	1.97	0.46
5:U:52:LYS:HG2	5:U:66:LYS:HD2	1.96	0.46
10:O:32:PHE:O	10:O:35:THR:OG1	2.25	0.46
7:I:113:ILE:HG12	7:I:119:THR:HG22	1.98	0.46
10:A:126:GLN:HG2	11:B:84:VAL:HG21	1.96	0.46
12:C:207:THR:OG1	12:C:209:ASP:OD1	2.28	0.46
12:C:194:LEU:HD13	12:C:239:LEU:HD23	1.97	0.46
12:Q:191:GLU:HG2	12:Q:242:THR:HG22	1.97	0.46
2:N:226:LYS:NZ	15:N:310:HOH:O	2.44	0.46
1:M:22:VAL:HG22	1:M:206:ILE:HG12	1.98	0.46
3:R:185:PRO:HB2	3:R:191:CYS:SG	2.56	0.46
7:I:111:PHE:CD1	7:I:121:VAL:HG22	2.50	0.46
9:L:116:ASP:OD1	9:L:117:SER:N	2.48	0.46
3:R:34:VAL:HG23	3:R:163:THR:HG22	1.97	0.46
4:T:57:SER:HB2	13:S:167:TYR:CE2	2.51	0.46
7:W:111:PHE:HD1	7:W:121:VAL:HG22	1.81	0.46
13:E:31:ILE:HD13	13:E:141:ALA:HB2	1.96	0.46
11:P:221:LEU:O	11:P:233:PRO:HG3	2.16	0.46
10:A:44:ALA:HB2	10:A:53:VAL:HG13	1.98	0.46
6:V:163:ILE:HG23	6:V:170:GLY:HA2	1.98	0.46
6:H:45:ARG:HD2	6:H:52:THR:HB	1.98	0.45
1:M:10:GLY:HA3	1:M:42:LYS:HZ3	1.81	0.45
7:I:111:PHE:HD1	7:I:121:VAL:HG22	1.81	0.45
8:X:69:TYR:CD2	12:Q:96:GLN:HB3	2.50	0.45
12:C:152:ASN:ND2	15:C:306:HOH:O	2.39	0.45
3:D:185:PRO:HB2	3:D:191:CYS:SG	2.56	0.45
1:I:22:VAL:HG22	1:I:206:ILE:HG12	1.98	0.45
9:Z:104:TYR:CZ	9:Z:182:GLU:HG2	2.52	0.45
5:U:70:VAL:HB	5:U:74:ILE:HB	1.98	0.45
10:O:44:ALA:HB2	10:O:53:VAL:HG13	1.98	0.45
5:G:70:VAL:HB	5:G:74:ILE:HB	1.98	0.45
9:L:137:TYR:CG	14:K:25:ILE:HG23	2.52	0.45
1:M:124:SER:O	1:M:131:TYR:HA	2.17	0.45
6:V:45:ARG:HD2	6:V:52:THR:HB	1.98	0.45
6:V:148:LYS:NZ	6:V:184:GLU:OE1	2.34	0.45
12:C:119:LYS:HZ1	12:C:135:PHE:HD2	1.65	0.45
14:K:89:ALA:O	14:K:92:ILE:HG22	2.17	0.45
14:K:184:VAL:HG22	14:K:189:ILE:HG12	1.98	0.45
3:D:52:LEU:HB2	12:C:160:TRP:HZ3	1.82	0.45
3:D:89:ALA:HB1	3:D:109:LEU:HD11	1.99	0.45
13:E:179:ALA:HB2	13:E:207:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:3:ILE:HD13	14:Y:168:LEU:HD13	1.98	0.45
14:Y:89:ALA:O	14:Y:92:ILE:HG22	2.16	0.45
3:R:52:LEU:HB2	12:Q:160:TRP:HZ3	1.82	0.45
4:T:156:LEU:HG	5:U:59:LEU:HD23	1.99	0.45
7:I:163:ILE:HG23	7:I:170:GLY:HA2	1.99	0.45
8:J:11:ILE:HD11	8:J:175:ALA:HB2	1.98	0.45
9:L:104:TYR:CZ	9:L:182:GLU:HG2	2.52	0.45
3:R:167:ASN:HB2	3:R:202:VAL:HG11	1.99	0.45
10:O:164:VAL:HG23	10:O:166:TYR:CE1	2.52	0.45
9:Z:137:TYR:CG	14:Y:25:ILE:HG23	2.52	0.44
4:F:156:LEU:HG	5:G:59:LEU:HD23	1.99	0.44
3:D:167:ASN:HB2	3:D:202:VAL:HG11	2.00	0.44
4:F:176:LEU:HA	4:F:179:PHE:CZ	2.53	0.44
3:R:89:ALA:HB1	3:R:109:LEU:HD11	1.99	0.44
5:U:38:ILE:HG13	5:U:176:LEU:HD11	2.00	0.44
6:V:18:SER:HB2	6:V:31:THR:H	1.82	0.44
2:2:70:LEU:HD11	4:T:99:PHE:HE2	1.83	0.44
2:2:226:LYS:NZ	15:2:313:HOH:O	2.44	0.44
4:F:227:GLY:O	4:F:230:VAL:HG22	2.18	0.44
7:W:163:ILE:HG23	7:W:170:GLY:HA2	1.99	0.44
9:Z:133:GLN:HG3	14:Y:25:ILE:HD12	2.00	0.44
14:K:91:SER:HG	14:K:98:TYR:H	1.64	0.44
2:2:129:TYR:HE2	2:2:144:THR:HB	1.82	0.44
6:V:14:LEU:HD23	6:V:44:CYS:SG	2.58	0.44
11:B:42:GLY:HA2	11:B:214:ILE:O	2.17	0.44
11:B:221:LEU:O	11:B:233:PRO:HG3	2.17	0.44
10:O:244:ARG:NH1	15:O:314:HOH:O	2.50	0.44
11:P:85:LEU:HD23	11:P:134:LEU:HD11	1.99	0.44
6:H:14:LEU:HD23	6:H:44:CYS:SG	2.58	0.44
6:H:163:ILE:HG23	6:H:170:GLY:HA2	1.98	0.44
9:L:38:ASN:ND2	9:L:40:PHE:H	2.16	0.44
2:N:130:VAL:HB	2:N:136:THR:HG22	2.00	0.44
4:T:227:GLY:O	4:T:230:VAL:HG22	2.18	0.44
14:K:171:ARG:NH1	15:K:307:HOH:O	2.39	0.44
12:Q:83:ASP:HB3	12:Q:131:PHE:HD1	1.82	0.44
1:1:124:SER:O	1:1:131:TYR:HA	2.17	0.44
2:N:43:ILE:HG12	2:N:64:GLU:HG2	1.99	0.44
10:A:164:VAL:HG23	10:A:166:TYR:CE1	2.52	0.44
13:E:36:THR:HA	13:E:172:ILE:O	2.17	0.44
13:E:170:LYS:HD3	13:E:171:ALA:N	2.33	0.44
2:2:43:ILE:HG12	2:2:64:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:99:PHE:HE2	2:N:70:LEU:HD11	1.83	0.43
1:M:43:VAL:HG12	1:M:205:LEU:HD12	2.00	0.43
7:I:59:ILE:HG13	7:I:83:LEU:HD23	2.00	0.43
4:T:176:LEU:HA	4:T:179:PHE:CZ	2.53	0.43
12:Q:144:TYR:HB2	12:Q:147:GLN:NE2	2.34	0.43
1:I:42:LYS:HB2	1:I:42:LYS:HE3	1.73	0.43
2:2:130:VAL:HB	2:2:136:THR:HG22	2.00	0.43
6:H:55:ILE:HD11	6:H:93:LEU:HD13	2.00	0.43
8:X:178:ASP:O	15:X:301:HOH:O	2.20	0.43
9:Z:2:THR:HG21	9:Z:164:ALA:HB1	2.01	0.43
4:F:120:THR:HG22	4:F:127:PRO:HB3	2.01	0.43
4:T:63:ILE:HG21	4:T:214:ALA:HB2	2.00	0.43
4:F:63:ILE:HG21	4:F:214:ALA:HB2	2.01	0.43
10:A:211:ILE:HG12	10:A:218:PHE:HD2	1.83	0.43
12:C:191:GLU:HG2	12:C:242:THR:HG22	1.99	0.43
1:M:194:ARG:HD3	1:M:194:ARG:HA	1.88	0.43
14:K:149:ARG:HB2	14:K:152:MET:HG3	2.01	0.43
13:S:36:THR:HA	13:S:172:ILE:O	2.19	0.43
1:I:33:TYR:HA	7:I:167:LEU:HD12	2.00	0.43
2:2:200:ILE:HG12	2:2:206:LEU:HD13	2.01	0.43
3:D:159:TRP:CZ3	13:E:56:SER:HB3	2.54	0.43
6:H:18:SER:HB2	6:H:31:THR:H	1.82	0.43
1:M:33:TYR:HA	7:W:167:LEU:HD12	2.01	0.43
12:C:144:TYR:HB2	12:C:147:GLN:NE2	2.33	0.43
4:T:120:THR:HG22	4:T:127:PRO:HB3	2.01	0.43
10:A:14:ARG:HG2	10:A:26:TYR:CD2	2.54	0.43
14:K:3:ILE:HD13	14:K:168:LEU:HD13	2.00	0.43
5:G:38:ILE:HG13	5:G:176:LEU:HD11	2.00	0.43
8:X:11:ILE:HD11	8:X:175:ALA:HB2	1.99	0.43
12:C:83:ASP:HB3	12:C:131:PHE:HD1	1.83	0.43
13:E:68:VAL:HG21	13:E:89:ILE:HD13	2.01	0.43
3:D:69:SER:O	3:D:219:SER:OG	2.34	0.42
4:T:10:THR:HG21	4:T:127:PRO:HD3	2.01	0.42
10:A:244:ARG:NH1	15:A:313:HOH:O	2.51	0.42
11:B:85:LEU:HD23	11:B:134:LEU:HD11	2.00	0.42
4:F:38:LEU:HD13	4:F:172:LEU:HD22	2.01	0.42
9:L:8:PHE:CE1	9:L:13:ILE:HG12	2.54	0.42
6:V:55:ILE:HD11	6:V:93:LEU:HD13	2.00	0.42
3:D:159:TRP:HZ3	13:E:56:SER:HB3	1.84	0.42
7:I:80:LEU:HD12	7:I:113:ILE:HD11	2.00	0.42
2:N:9:THR:O	2:N:41:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:169:LYS:HE3	4:T:169:LYS:HB2	1.84	0.42
11:P:21:ILE:HG21	11:P:153:SER:HB3	2.02	0.42
1:1:8:ASN:HA	1:1:30:ILE:O	2.20	0.42
1:1:194:ARG:HD3	1:1:194:ARG:HA	1.88	0.42
2:2:84:GLU:CD	2:2:84:GLU:H	2.28	0.42
1:M:186:ASP:OD2	7:W:203:TYR:OH	2.27	0.42
2:N:193:ARG:NH1	6:V:194:GLU:OE1	2.52	0.42
1:1:43:VAL:HG12	1:1:205:LEU:HD12	2.00	0.42
5:G:151:LEU:HG	5:G:157:TYR:HB3	2.02	0.42
14:Y:169:GLU:HA	14:Y:172:MET:HG2	2.01	0.42
4:F:70:MET:HE2	4:F:134:ILE:HG21	2.02	0.42
11:B:122:THR:HG22	11:B:129:PRO:HB3	2.02	0.42
13:S:68:VAL:HG21	13:S:89:ILE:HD13	2.01	0.42
4:F:10:THR:HG21	4:F:127:PRO:HD3	2.02	0.42
4:F:56:LEU:HG	13:E:184:LEU:HD23	2.02	0.42
9:L:2:THR:HG21	9:L:164:ALA:HB1	2.01	0.42
4:T:70:MET:HE2	4:T:134:ILE:HG21	2.02	0.42
12:C:150:THR:HG22	12:C:160:TRP:HE1	1.85	0.42
3:R:159:TRP:HZ3	13:S:56:SER:HB3	1.84	0.42
5:U:151:LEU:HG	5:U:157:TYR:HB3	2.02	0.42
7:W:80:LEU:HD12	7:W:113:ILE:HD11	2.00	0.42
10:O:14:ARG:HG2	10:O:26:TYR:CD2	2.54	0.42
3:R:36:VAL:HG22	3:R:43:VAL:HB	2.02	0.42
3:R:81:ASP:HB3	3:R:129:PHE:HD2	1.84	0.42
2:2:9:THR:O	2:2:41:ARG:NH1	2.53	0.42
2:N:130:VAL:HA	2:N:135:VAL:O	2.20	0.42
3:D:166:ARG:HB3	3:D:167:ASN:H	1.64	0.41
3:R:159:TRP:CZ3	13:S:56:SER:HB3	2.54	0.41
3:R:166:ARG:HB3	3:R:167:ASN:H	1.64	0.41
11:B:35:LEU:HD23	11:B:175:LEU:HD11	2.01	0.41
12:Q:56:LEU:HD23	12:Q:56:LEU:H	1.85	0.41
3:D:81:ASP:HB3	3:D:129:PHE:HD2	1.84	0.41
8:J:78:GLU:OE2	11:B:97:TYR:OH	2.26	0.41
7:W:59:ILE:HG13	7:W:83:LEU:HD23	2.00	0.41
3:D:36:VAL:HG22	3:D:43:VAL:HB	2.02	0.41
4:T:38:LEU:HD13	4:T:172:LEU:HD22	2.01	0.41
8:X:17:GLY:HA3	8:X:163:LEU:HD22	2.02	0.41
9:Z:8:PHE:CE1	9:Z:13:ILE:HG12	2.55	0.41
10:A:115:ASP:HB3	10:A:155:TYR:CZ	2.56	0.41
2:2:60:MET:O	2:2:64:GLU:HG3	2.20	0.41
6:H:132:THR:HA	6:H:135:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:161:GLU:HA	1:M:162:PRO:HD3	1.93	0.41
2:N:200:ILE:HG12	2:N:206:LEU:HD13	2.01	0.41
4:T:38:LEU:HD11	4:T:179:PHE:CE1	2.56	0.41
6:V:104:ASP:O	6:V:107:LYS:NZ	2.48	0.41
9:Z:13:ILE:HG13	9:Z:153:ALA:HB1	2.03	0.41
2:2:70:LEU:HD11	4:T:99:PHE:CE2	2.56	0.41
11:B:75:TYR:HB3	11:B:82:TYR:CD1	2.55	0.41
12:C:190:ILE:HG23	12:C:213:PHE:CZ	2.56	0.41
11:P:217:GLU:HB3	11:P:232:GLY:HA3	2.01	0.41
3:D:156:TYR:OH	13:E:86:ARG:NH2	2.54	0.41
9:L:128:CYS:SG	9:L:140:LEU:HD12	2.60	0.41
6:V:171:GLY:O	6:V:193:TYR:OH	2.31	0.41
14:Y:142:PHE:CG	14:Y:143:LEU:N	2.89	0.41
2:2:13:SER:HB3	2:2:22:ILE:HG13	2.02	0.41
4:F:99:PHE:CE2	2:N:70:LEU:HD11	2.56	0.41
3:R:207:ALA:HB2	3:R:233:VAL:HG11	2.02	0.41
5:U:114:ASP:O	5:U:118:GLN:HG2	2.21	0.41
9:Z:155:TYR:OH	9:Z:204:GLU:OE2	2.30	0.41
13:E:168:ASN:HB3	13:E:187:TRP:CE2	2.55	0.41
14:K:169:GLU:HA	14:K:172:MET:HG2	2.02	0.41
12:Q:190:ILE:HG23	12:Q:213:PHE:CZ	2.56	0.41
4:F:164:ARG:HH11	4:F:202:ARG:HD2	1.86	0.41
8:J:88:THR:HG23	8:J:124:PHE:CZ	2.56	0.41
2:N:60:MET:O	2:N:64:GLU:HG3	2.20	0.41
2:N:84:GLU:H	2:N:84:GLU:CD	2.28	0.41
12:Q:222:ASP:OD1	12:Q:223:GLY:N	2.46	0.41
2:2:193:ARG:NH1	6:H:194:GLU:OE1	2.53	0.41
3:D:207:ALA:HB2	3:D:233:VAL:HG11	2.01	0.41
4:F:38:LEU:HD11	4:F:179:PHE:CE1	2.56	0.41
5:G:150:MET:HB3	5:G:160:TYR:CE1	2.56	0.41
9:Z:128:CYS:SG	9:Z:140:LEU:HD12	2.60	0.41
10:A:31:ALA:O	10:A:35:THR:HG23	2.21	0.41
11:B:92:VAL:HG21	11:B:117:ILE:HD11	2.03	0.41
11:B:217:GLU:HB3	11:B:232:GLY:HA3	2.02	0.41
13:E:122:ARG:HH21	13:E:133:LEU:HG	1.86	0.41
10:O:115:ASP:HB3	10:O:155:TYR:CZ	2.56	0.41
10:O:211:ILE:HG12	10:O:218:PHE:HD2	1.86	0.41
11:P:35:LEU:HD23	11:P:175:LEU:HD11	2.01	0.41
11:P:75:TYR:HB3	11:P:82:TYR:CD1	2.55	0.41
13:S:120:ALA:HA	13:S:138:PHE:HE2	1.86	0.41
13:S:147:HIS:NE2	13:S:224:LYS:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:26:ASP:O	1:1:42:LYS:HE2	2.21	0.41
5:G:69:VAL:HG22	5:G:228:HIS:ND1	2.36	0.41
5:G:114:ASP:O	5:G:118:GLN:HG2	2.21	0.41
1:M:26:ASP:O	1:M:42:LYS:HE2	2.21	0.41
3:R:156:TYR:OH	13:S:86:ARG:NH2	2.54	0.41
5:U:38:ILE:HG12	5:U:39:GLY:N	2.36	0.41
8:X:88:THR:HG23	8:X:124:PHE:CZ	2.56	0.41
13:S:246:LYS:HE2	13:S:246:LYS:HB3	1.96	0.41
1:1:125:PHE:CD2	1:1:131:TYR:HB3	2.56	0.40
4:T:56:LEU:HG	13:S:184:LEU:HD23	2.03	0.40
6:V:132:THR:HA	6:V:135:TYR:HD2	1.85	0.40
11:B:21:ILE:HG21	11:B:153:SER:HB3	2.02	0.40
2:2:130:VAL:HA	2:2:135:VAL:O	2.20	0.40
6:H:59:VAL:HG11	6:H:82:PHE:CE2	2.56	0.40
1:M:125:PHE:CD2	1:M:131:TYR:HB3	2.56	0.40
5:U:150:MET:HB3	5:U:160:TYR:CE1	2.56	0.40
9:L:85:ASN:O	9:L:89:GLN:HG3	2.22	0.40
2:N:13:SER:HB3	2:N:22:ILE:HG13	2.02	0.40
11:B:140:ASP:OD1	11:B:143:ASN:HB2	2.21	0.40
14:K:168:LEU:O	14:K:171:ARG:NE	2.50	0.40
1:1:115:ASP:OD1	1:1:119:LYS:N	2.54	0.40
3:D:67:ILE:HG21	3:D:109:LEU:HD21	2.04	0.40
4:T:70:MET:HE3	4:T:105:VAL:HG13	2.03	0.40
14:K:142:PHE:CG	14:K:143:LEU:N	2.89	0.40
11:P:122:THR:HG22	11:P:129:PRO:HB3	2.03	0.40
5:G:38:ILE:HG12	5:G:39:GLY:N	2.35	0.40
6:H:83:LYS:HE2	6:H:83:LYS:HB3	1.89	0.40
4:T:38:LEU:HD12	4:T:38:LEU:HA	1.89	0.40
5:U:224:THR:HG22	5:U:229:LYS:HD2	2.04	0.40
7:W:84:LYS:HG3	7:W:117:GLY:O	2.22	0.40
10:O:31:ALA:O	10:O:35:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
1	M	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
2	2	230/233 (99%)	218 (95%)	12 (5%)	0	100	100
2	N	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
3	D	238/254 (94%)	229 (96%)	9 (4%)	0	100	100
3	R	238/254 (94%)	230 (97%)	8 (3%)	0	100	100
4	F	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
4	T	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
5	G	238/288 (83%)	235 (99%)	3 (1%)	0	100	100
5	U	238/288 (83%)	235 (99%)	3 (1%)	0	100	100
6	H	194/196 (99%)	192 (99%)	2 (1%)	0	100	100
6	V	194/196 (99%)	192 (99%)	2 (1%)	0	100	100
7	I	218/232 (94%)	217 (100%)	1 (0%)	0	100	100
7	W	218/232 (94%)	217 (100%)	1 (0%)	0	100	100
8	J	201/205 (98%)	192 (96%)	9 (4%)	0	100	100
8	X	201/205 (98%)	191 (95%)	10 (5%)	0	100	100
9	L	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
9	Z	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
10	A	220/252 (87%)	214 (97%)	6 (3%)	0	100	100
10	O	220/252 (87%)	214 (97%)	6 (3%)	0	100	100
11	B	241/250 (96%)	234 (97%)	7 (3%)	0	100	100
11	P	241/250 (96%)	234 (97%)	7 (3%)	0	100	100
12	C	234/258 (91%)	226 (97%)	8 (3%)	0	100	100
12	Q	239/258 (93%)	231 (97%)	8 (3%)	0	100	100
13	E	234/260 (90%)	229 (98%)	5 (2%)	0	100	100
13	S	233/260 (90%)	230 (99%)	3 (1%)	0	100	100
14	K	179/212 (84%)	175 (98%)	3 (2%)	1 (1%)	21	12
14	Y	179/212 (84%)	175 (98%)	3 (2%)	1 (1%)	21	12
All	All	6176/6616 (93%)	6011 (97%)	163 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	K	25	ILE
14	Y	25	ILE

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	1	185/185 (100%)	184 (100%)	1 (0%)	81	81
1	M	185/185 (100%)	184 (100%)	1 (0%)	81	81
2	2	198/199 (100%)	196 (99%)	2 (1%)	68	71
2	N	198/199 (100%)	196 (99%)	2 (1%)	68	71
3	D	212/226 (94%)	205 (97%)	7 (3%)	33	29
3	R	212/226 (94%)	205 (97%)	7 (3%)	33	29
4	F	190/193 (98%)	189 (100%)	1 (0%)	81	81
4	T	190/193 (98%)	189 (100%)	1 (0%)	81	81
5	G	198/239 (83%)	193 (98%)	5 (2%)	42	40
5	U	198/239 (83%)	192 (97%)	6 (3%)	36	32
6	H	162/162 (100%)	162 (100%)	0	100	100
6	V	162/162 (100%)	162 (100%)	0	100	100
7	I	179/190 (94%)	178 (99%)	1 (1%)	78	79
7	W	179/190 (94%)	178 (99%)	1 (1%)	78	79
8	J	171/173 (99%)	168 (98%)	3 (2%)	51	52
8	X	171/173 (99%)	168 (98%)	3 (2%)	51	52
9	L	169/169 (100%)	167 (99%)	2 (1%)	63	65
9	Z	169/169 (100%)	167 (99%)	2 (1%)	63	65
10	A	196/210 (93%)	191 (97%)	5 (3%)	40	38
10	O	196/210 (93%)	191 (97%)	5 (3%)	40	38
11	B	205/209 (98%)	202 (98%)	3 (2%)	57	59
11	P	205/209 (98%)	203 (99%)	2 (1%)	68	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	C	200/216 (93%)	196 (98%)	4 (2%)	48	48
12	Q	202/216 (94%)	198 (98%)	4 (2%)	48	48
13	E	195/215 (91%)	193 (99%)	2 (1%)	68	71
13	S	194/215 (90%)	192 (99%)	2 (1%)	68	71
14	K	165/189 (87%)	162 (98%)	3 (2%)	51	52
14	Y	165/189 (87%)	162 (98%)	3 (2%)	51	52
All	All	5251/5550 (95%)	5173 (98%)	78 (2%)	55	59

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	91	ARG
2	2	9	THR
2	2	216	ASN
3	D	39	LYS
3	D	84	ILE
3	D	155	ILE
3	D	177	LYS
3	D	182	LYS
3	D	208	LYS
3	D	239	GLU
4	F	180	ILE
5	G	9	ASP
5	G	12	ASN
5	G	38	ILE
5	G	51	GLU
5	G	151	LEU
7	I	13	VAL
8	J	13	VAL
8	J	121	ILE
8	J	183	TRP
9	L	1	THR
9	L	111	THR
1	M	91	ARG
2	N	9	THR
2	N	216	ASN
3	R	39	LYS
3	R	84	ILE
3	R	155	ILE
3	R	177	LYS

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Mol	Chain	Res	Type
3	R	182	LYS
3	R	208	LYS
3	R	239	GLU
4	T	180	ILE
5	U	9	ASP
5	U	12	ASN
5	U	38	ILE
5	U	51	GLU
5	U	121	GLN
5	U	151	LEU
7	W	13	VAL
8	X	13	VAL
8	X	121	ILE
8	X	183	TRP
9	Z	1	THR
9	Z	111	THR
10	A	48	LYS
10	A	53	VAL
10	A	58	LYS
10	A	126	GLN
10	A	164	VAL
11	B	4	ARG
11	B	45	ILE
11	B	222	LEU
12	C	55	THR
12	C	56	LEU
12	C	218	LYS
12	C	224	GLU
13	E	170	LYS
13	E	224	LYS
14	K	27	VAL
14	K	92	ILE
14	K	171	ARG
10	O	48	LYS
10	O	53	VAL
10	O	126	GLN
10	O	164	VAL
10	O	188	LYS
11	P	45	ILE
11	P	222	LEU
12	Q	56	LEU
12	Q	57	LEU

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Mol	Chain	Res	Type
12	Q	218	LYS
12	Q	224	GLU
13	S	133	LEU
13	S	224	LYS
14	Y	27	VAL
14	Y	92	ILE
14	Y	171	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	158	ASN
2	2	216	ASN
3	D	94	GLN
4	F	119	ASN
4	F	148	GLN
5	G	62	GLN
6	H	161	GLN
7	I	141	HIS
8	J	169	GLN
8	J	204	GLN
9	L	143	ASN
9	L	176	ASN
1	M	197	GLN
3	R	94	GLN
4	T	91	GLN
4	T	93	ASN
4	T	119	ASN
4	T	148	GLN
6	V	161	GLN
7	W	141	HIS
8	X	169	GLN
9	Z	66	HIS
9	Z	143	ASN
9	Z	176	ASN
10	A	126	GLN
10	A	240	ASN
12	C	147	GLN
12	C	227	GLN
13	E	114	GLN
14	K	41	HIS
14	K	118	GLN

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Mol	Chain	Res	Type
10	O	126	GLN
12	Q	227	GLN
14	Y	41	HIS
14	Y	118	GLN

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.

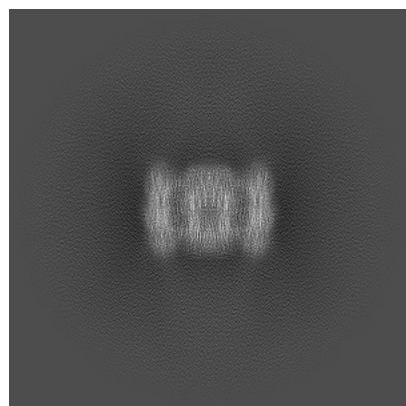
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19529. These allow visual inspection of the internal detail of the map and identification of artifacts.

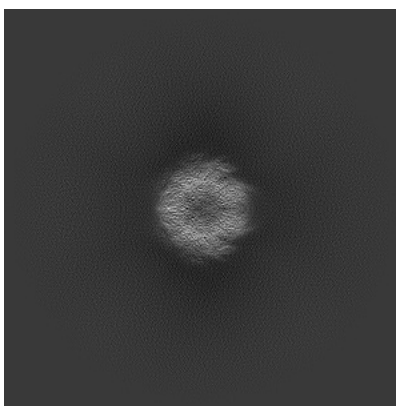
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

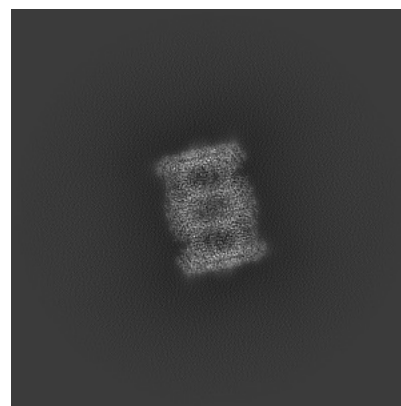
6.1.1 Primary map



X

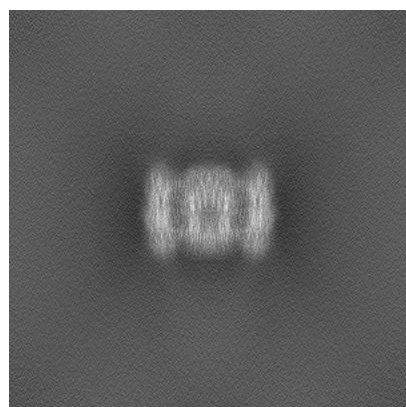


Y

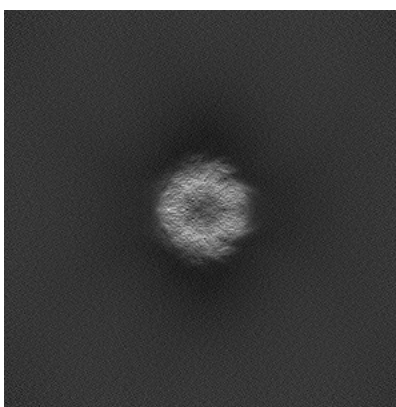


Z

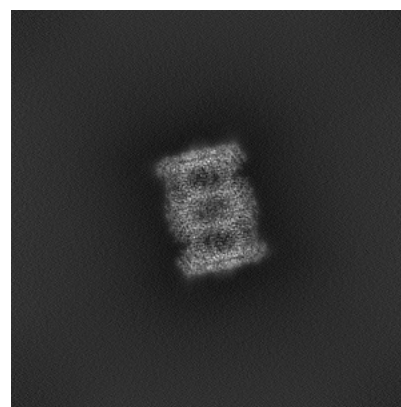
6.1.2 Raw map



X



Y

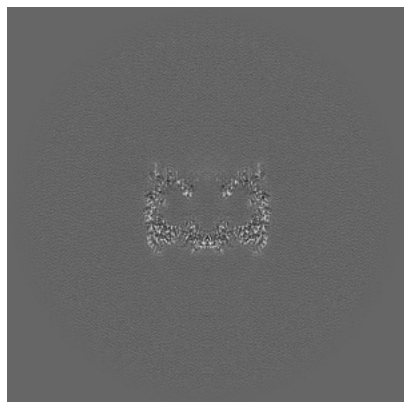


Z

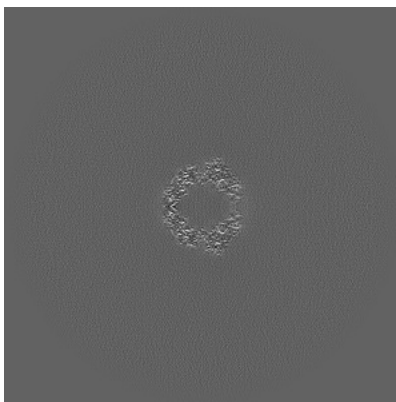
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

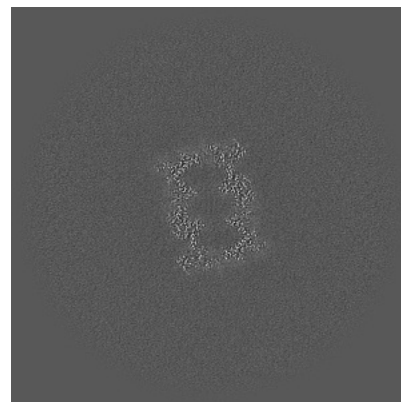
6.2.1 Primary map



X Index: 300



Y Index: 300

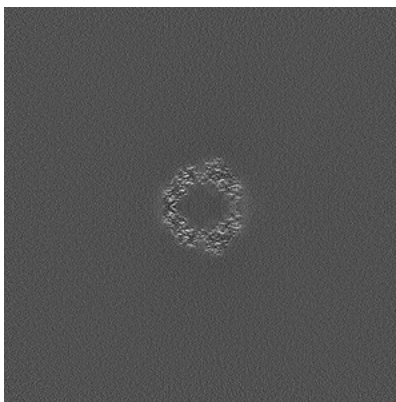


Z Index: 300

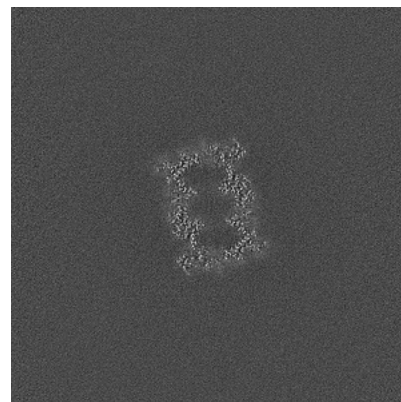
6.2.2 Raw map



X Index: 300



Y Index: 300

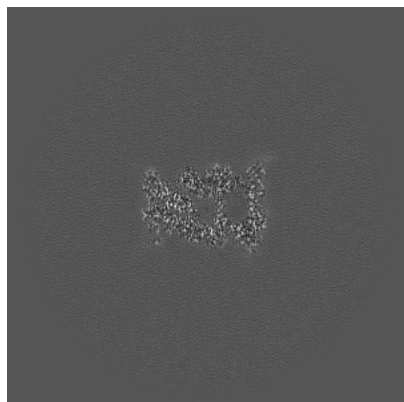


Z Index: 300

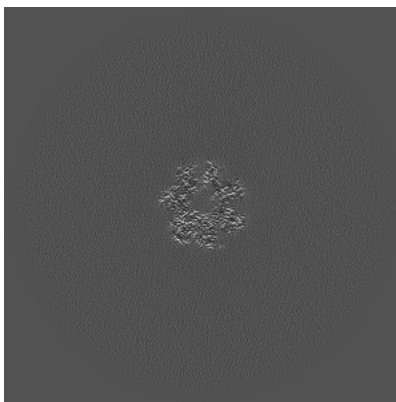
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

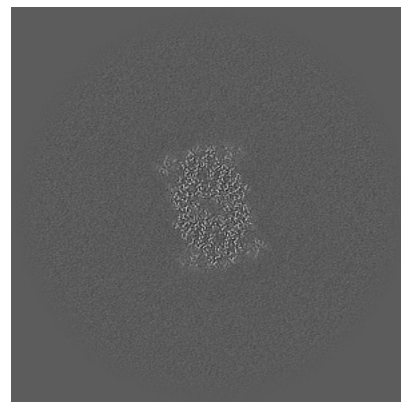
6.3.1 Primary map



X Index: 273

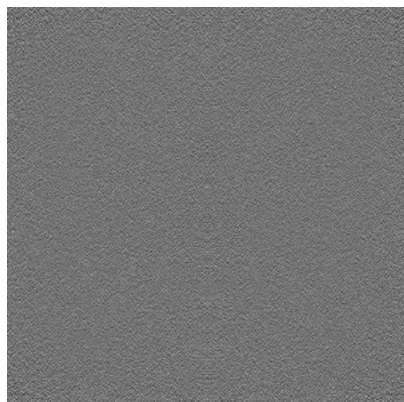


Y Index: 273

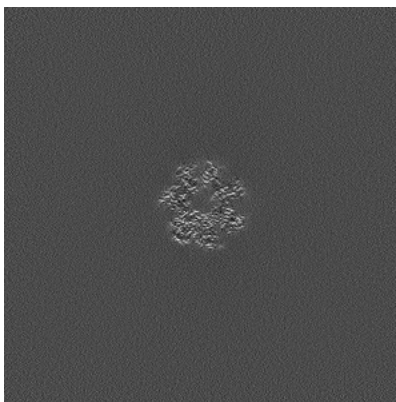


Z Index: 268

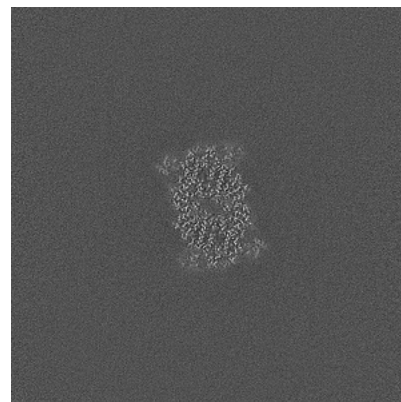
6.3.2 Raw map



X Index: 0



Y Index: 273

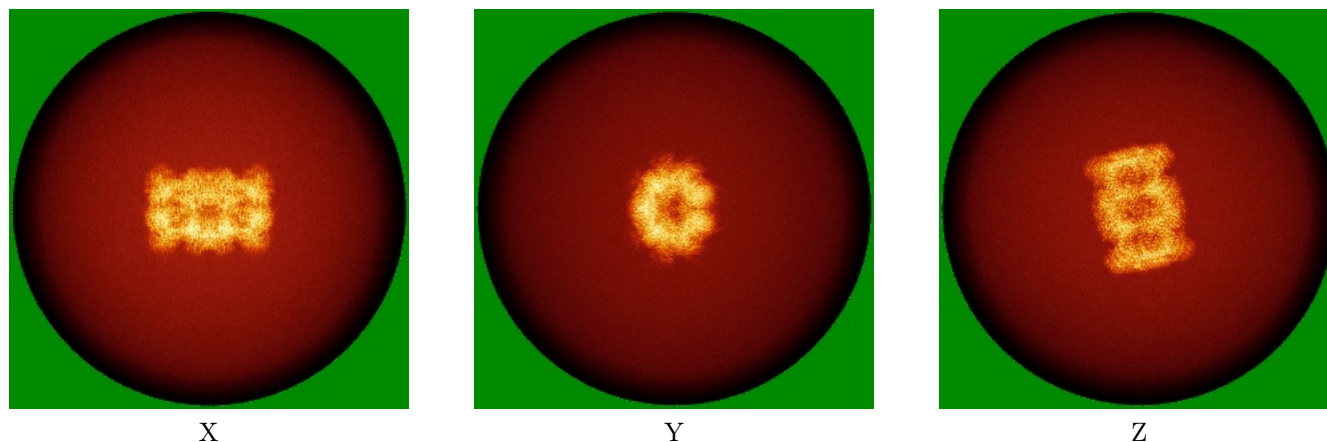


Z Index: 268

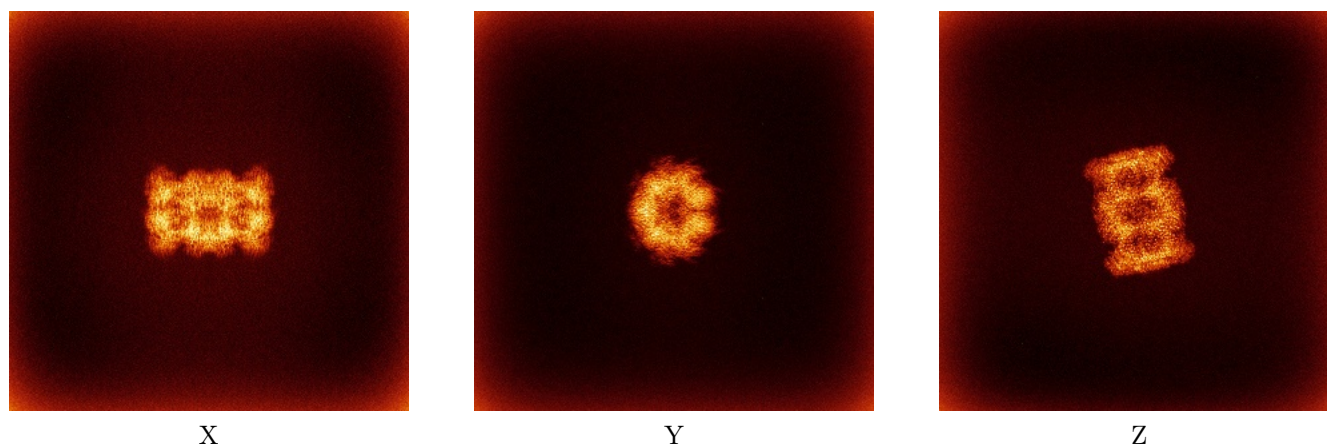
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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



X



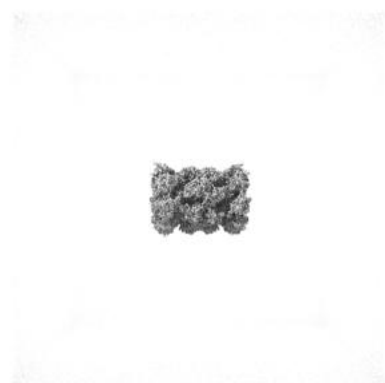
Y



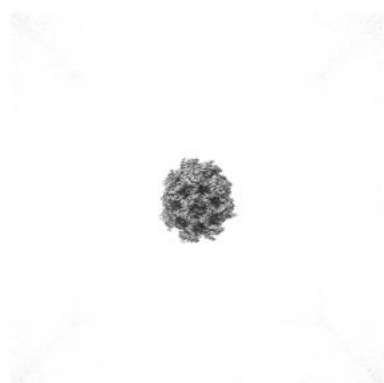
Z

The images above show the 3D surface view of the map at the recommended contour level 0.276. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

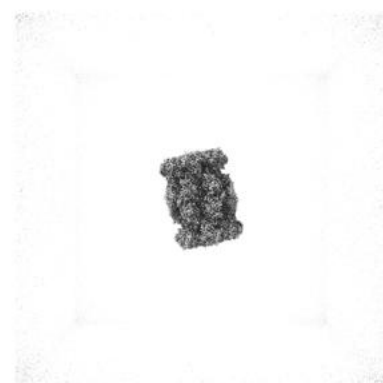
6.5.2 Raw map



X



Y



Z

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.

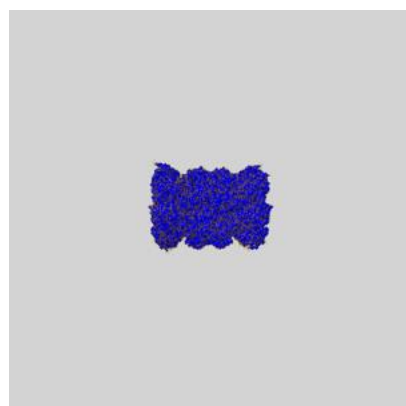
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

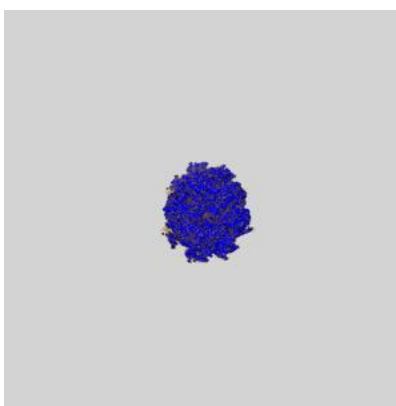
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

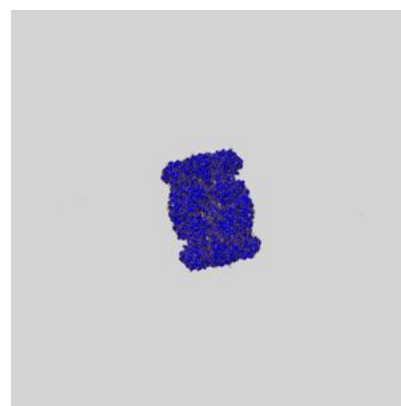
6.6.1 emd_19529_msk_1.map [i](#)



X



Y

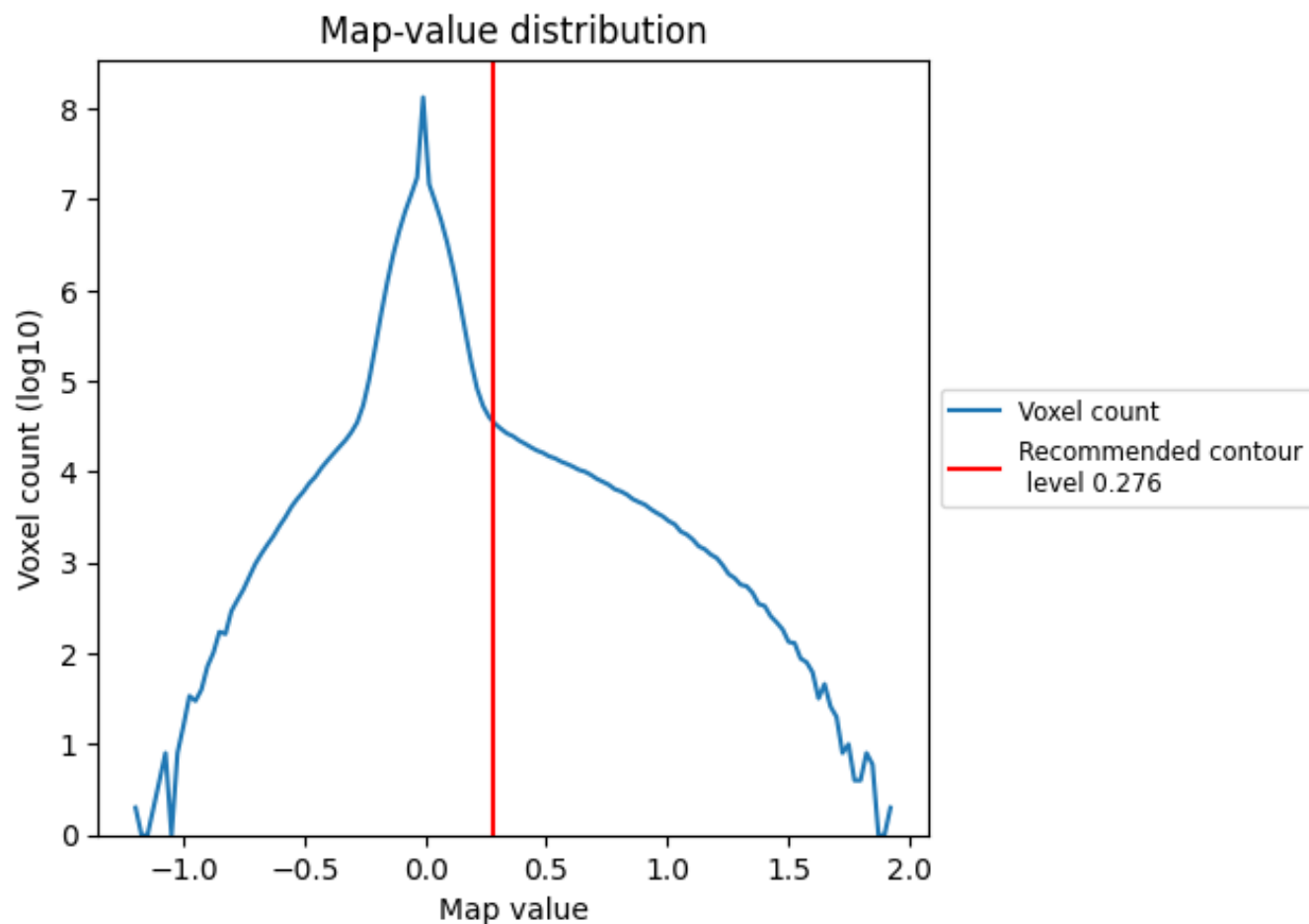


Z

7 Map analysis [i](#)

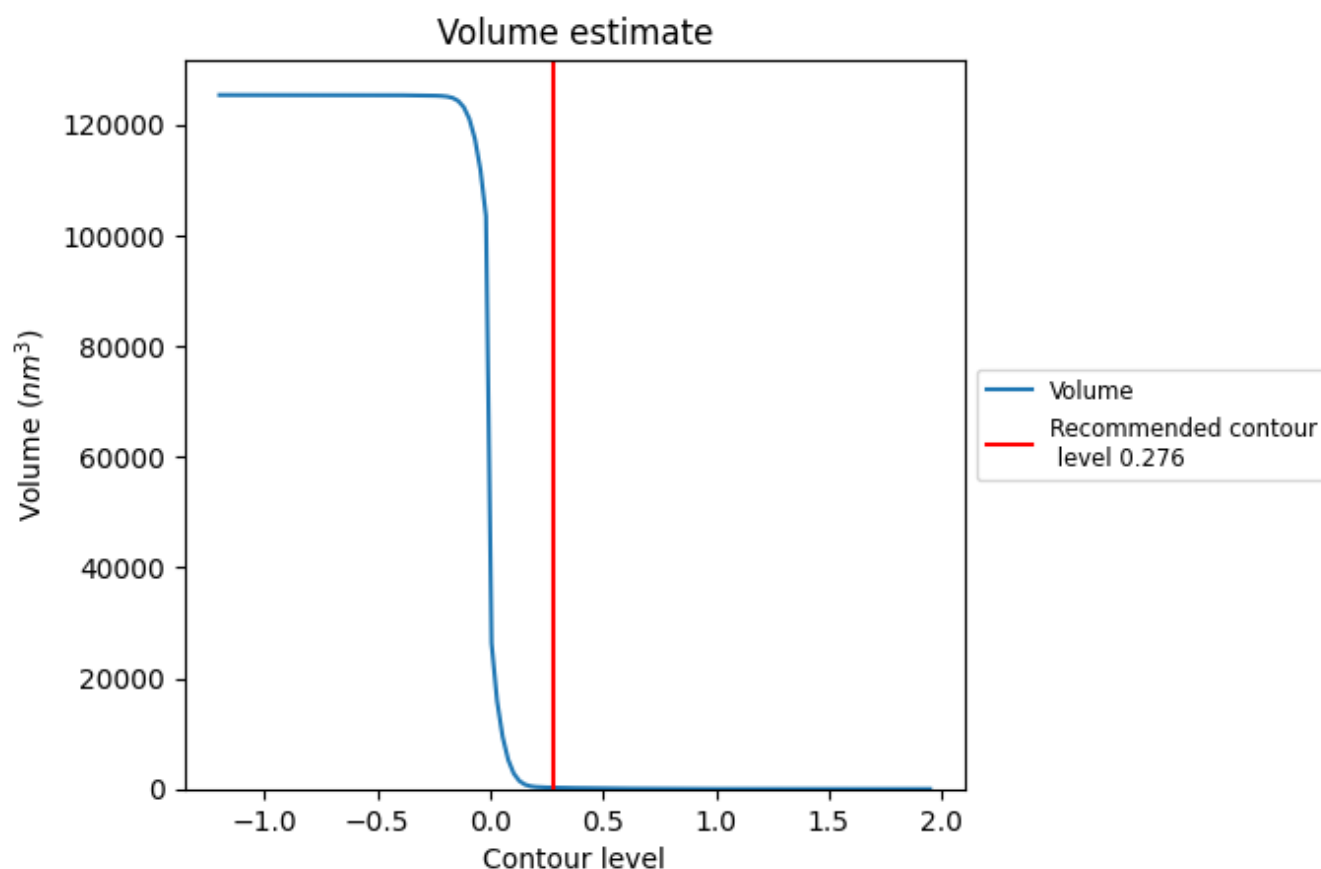
This section contains the results of statistical analysis of the map.

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.

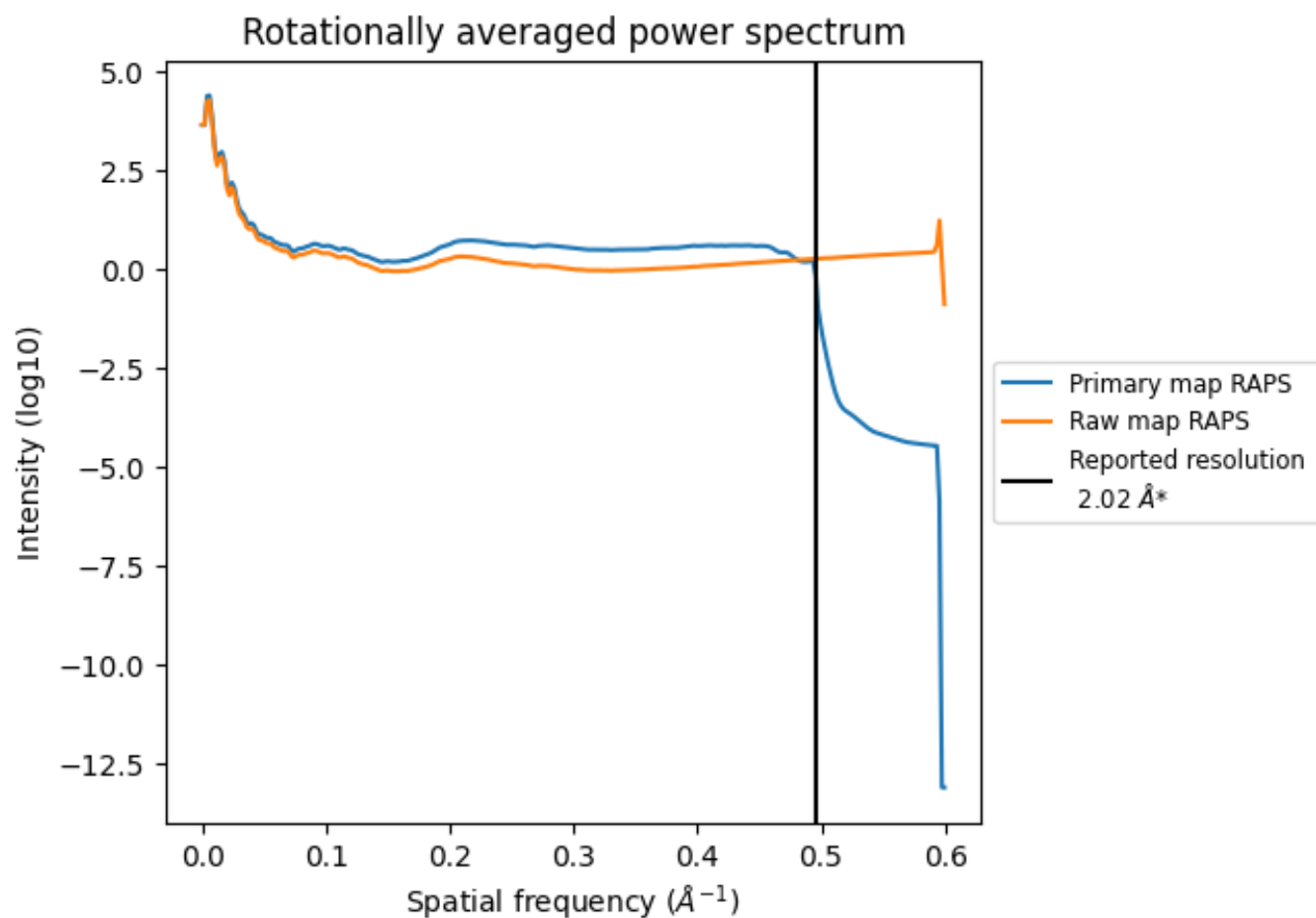
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm³; this corresponds to an approximate mass of 217 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 ⓘ

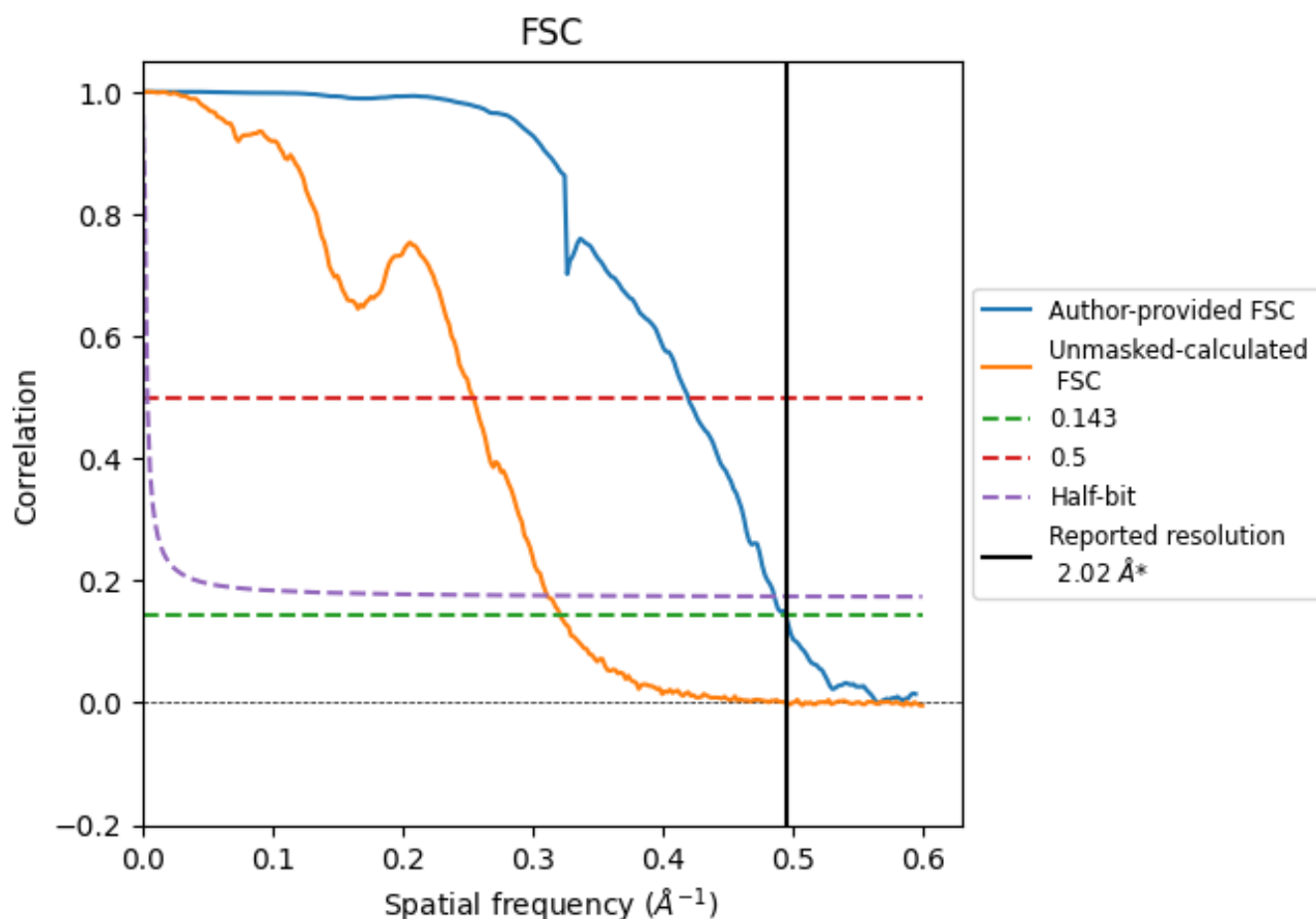


*Reported resolution corresponds to spatial frequency of 0.495 Å⁻¹

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 0.495 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

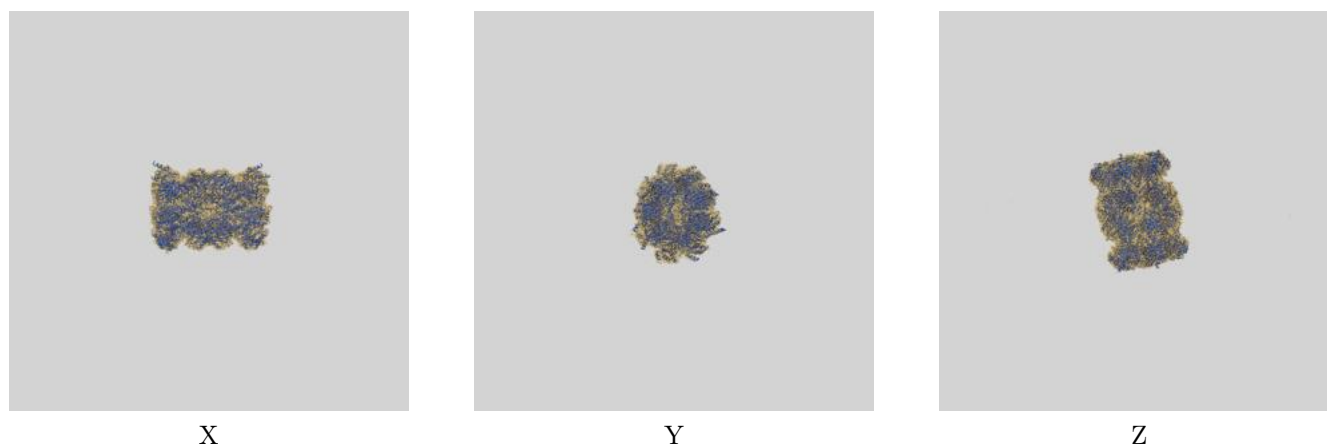
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.02	-	-
Author-provided FSC curve	2.02	2.38	2.06
Unmasked-calculated*	3.11	3.93	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.02 by more than 10 %

9 Map-model fit [i](#)

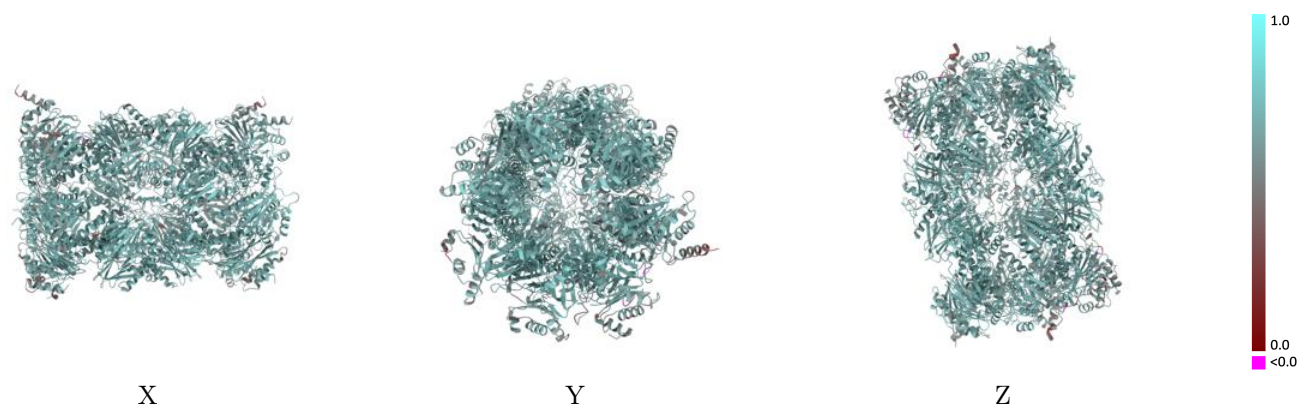
This section contains information regarding the fit between EMDB map EMD-19529 and PDB model 8RVQ. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



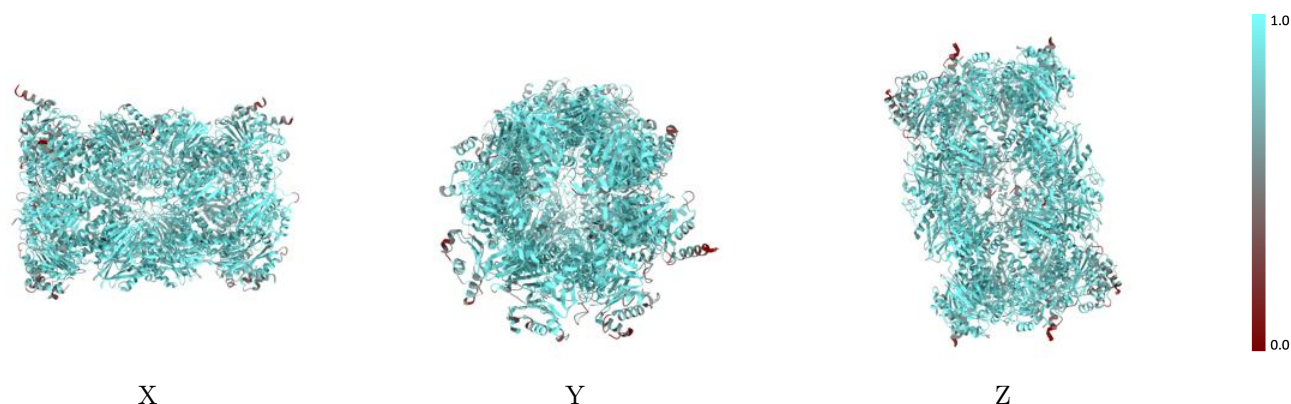
The images above show the 3D surface view of the map at the recommended contour level 0.276 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



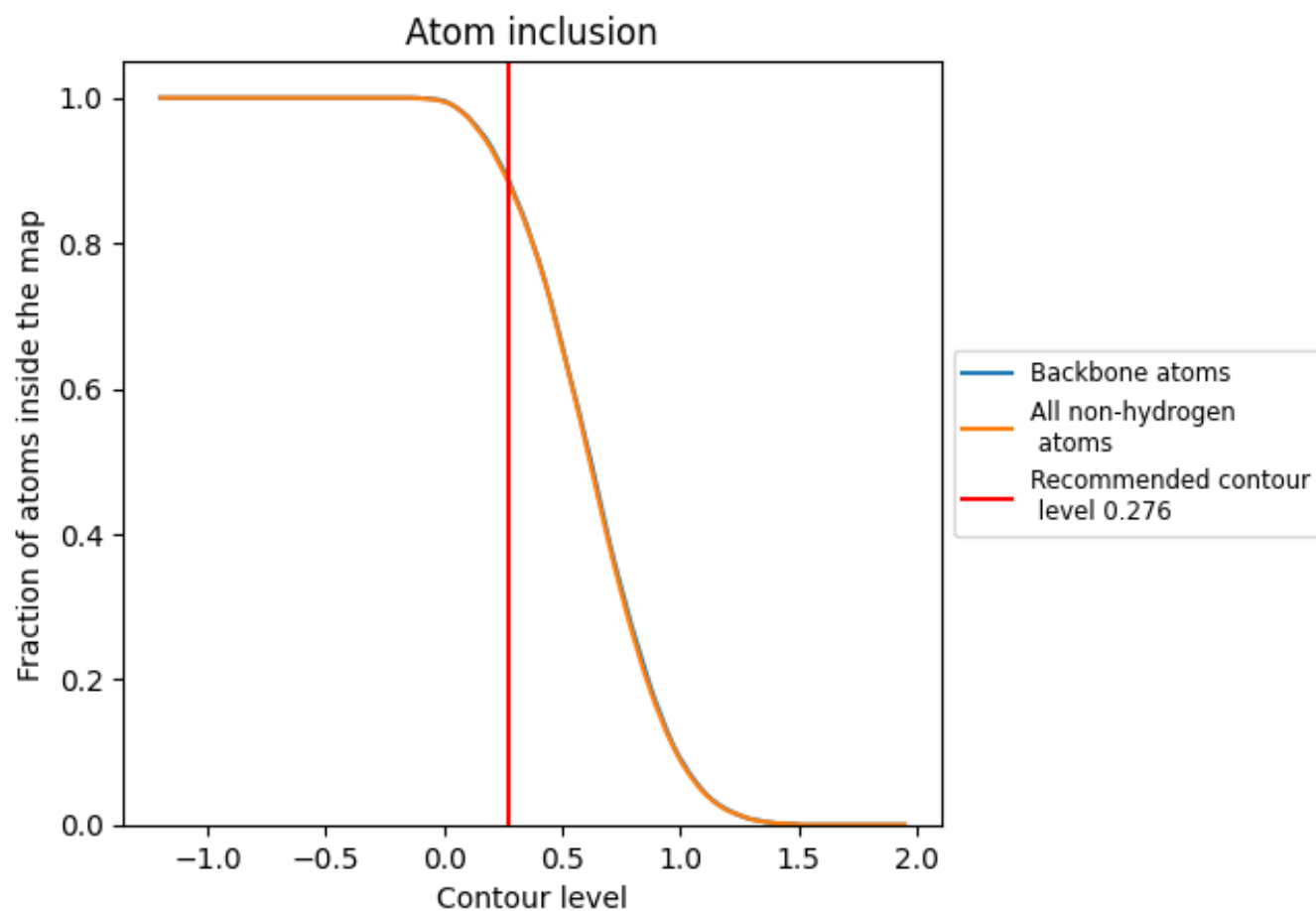
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.276).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.276) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.6590
1	 0.9210	 0.6720
2	 0.9320	 0.6820
A	 0.8340	 0.6460
B	 0.8630	 0.6430
C	 0.7960	 0.6180
D	 0.8120	 0.6160
E	 0.8890	 0.6580
F	 0.9220	 0.6730
G	 0.8720	 0.6570
H	 0.9410	 0.6910
I	 0.9370	 0.6820
J	 0.9300	 0.6760
K	 0.8440	 0.6420
L	 0.9250	 0.6780
M	 0.9200	 0.6730
N	 0.9330	 0.6820
O	 0.8320	 0.6410
P	 0.8630	 0.6410
Q	 0.7900	 0.6180
R	 0.8090	 0.6200
S	 0.8910	 0.6620
T	 0.9220	 0.6750
U	 0.8720	 0.6570
V	 0.9410	 0.6900
W	 0.9370	 0.6810
X	 0.9290	 0.6750
Y	 0.8440	 0.6410
Z	 0.9250	 0.6790

