



Full wwPDB EM Validation Report ⓘ

Sep 29, 2026 – 06:26 PM JST

PDB ID : 9X4E / pdb_00009x4e
EMDB ID : EMD-66543
Title : Structure of the old Killifish Proteasome
Authors : Kim, J.; Song, J.J.; Kim, Y.
Deposited on : 2025-10-10
Resolution : 3.26 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.dev133
MolProbity : 4-5-2 with Phenix2.2
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) : 2.51

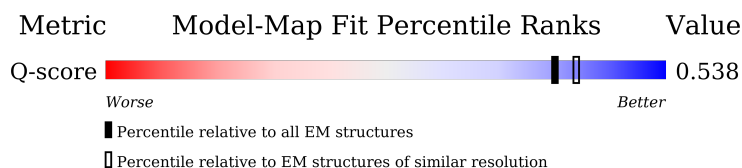
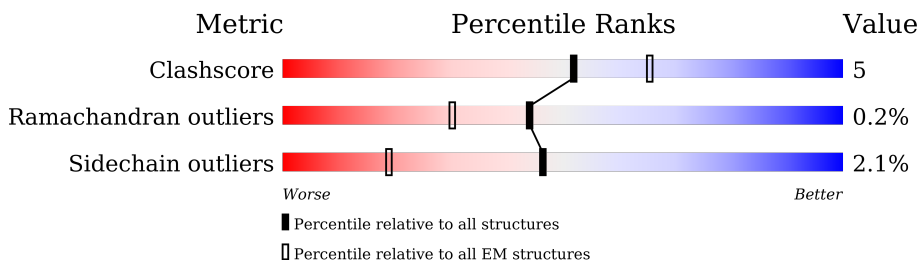
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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	14557 (2.76 - 3.76)

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

Mol	Chain	Length	Quality of chain
1	A	234	
1	O	234	
2	B	261	
2	P	261	

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Mol	Chain	Length	Quality of chain
3	C	251	
3	Q	251	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	233	
8	X	233	
9	I	205	
9	W	205	
10	J	277	
10	V	277	
11	K	293	
11	Z	293	
12	L	212	
12	Y	212	
13	M	254	
13	a	254	
14	N	237	
14	b	237	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 48247 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	228	Total	C	N	O	S	0	0
			1777	1137	296	338	6		
1	O	228	Total	C	N	O	S	0	0
			1777	1137	296	338	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	247	Total	C	N	O	S	0	0
			1935	1223	328	373	11		
2	P	246	Total	C	N	O	S	0	0
			1926	1218	327	370	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	228	Total	C	N	O	S	0	0
			1792	1129	323	336	4		
3	Q	231	Total	C	N	O	S	0	0
			1814	1143	326	341	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	235	Total	C	N	O	S	0	0
			1798	1127	295	365	11		
4	R	235	Total	C	N	O	S	0	0
			1798	1127	295	365	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	228	Total	C	N	O	S	0	0
			1789	1122	321	335	11		
5	S	228	Total	C	N	O	S	0	0
			1793	1124	321	337	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	240	Total	C	N	O	S	0	0
			1879	1190	317	362	10		
6	T	239	Total	C	N	O	S	0	0
			1872	1186	316	360	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	241	Total	C	N	O	S	0	0
			1877	1188	312	363	14		
7	U	235	Total	C	N	O	S	0	0
			1827	1152	307	354	14		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	199	Total	C	N	O	S	0	0
			1496	937	260	289	10		
8	X	199	Total	C	N	O	S	0	0
			1496	937	260	289	10		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1596	1012	266	299	19		
9	W	204	Total	C	N	O	S	0	0
			1596	1012	266	299	19		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	224	Total	C	N	O	S	0	0
			1683	1050	296	324	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	221	Total	C	N	O	S	0	0
			1660	1038	289	320	13		

- Molecule 11 is a protein called Proteasome subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	200	Total	C	N	O	S	0	0
			1553	976	275	290	12		
11	Z	200	Total	C	N	O	S	0	0
			1553	976	275	290	12		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	209	Total	C	N	O	S	0	0
			1664	1072	273	309	10		
12	Y	209	Total	C	N	O	S	0	0
			1664	1072	273	309	10		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	215	Total	C	N	O	S	0	0
			1690	1076	288	318	8		
13	a	214	Total	C	N	O	S	0	0
			1682	1070	287	317	8		

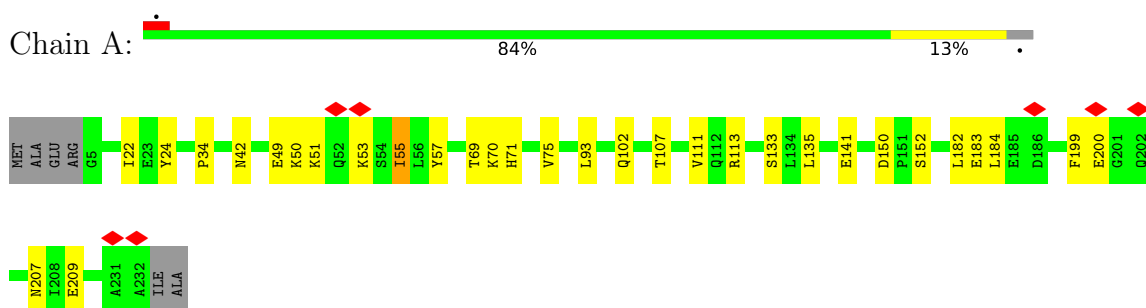
- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1630	1034	274	313	9		
14	b	212	Total	C	N	O	S	0	0
			1630	1034	274	313	9		

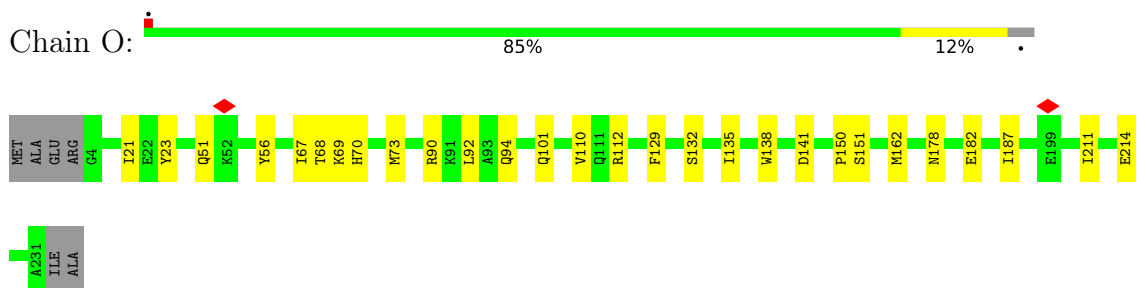
3 Residue-property plots

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.

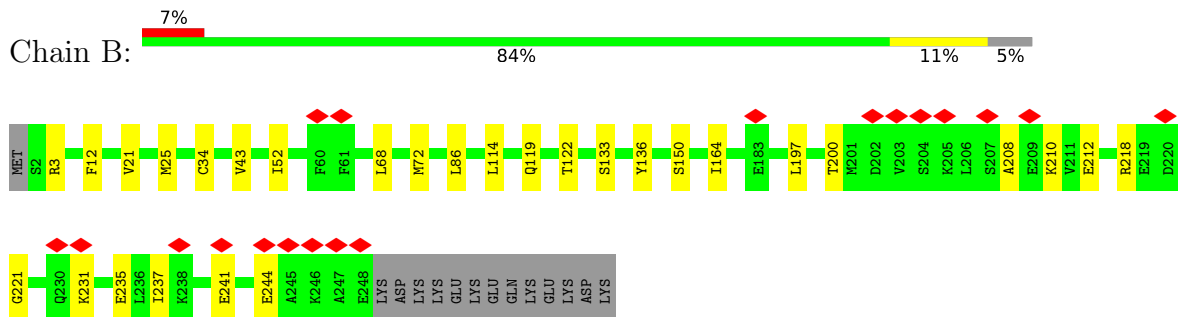
- Molecule 1: Proteasome subunit alpha type



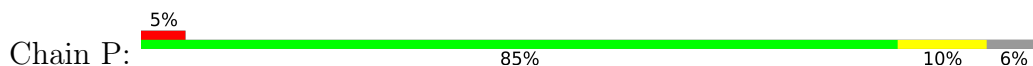
- Molecule 1: Proteasome subunit alpha type

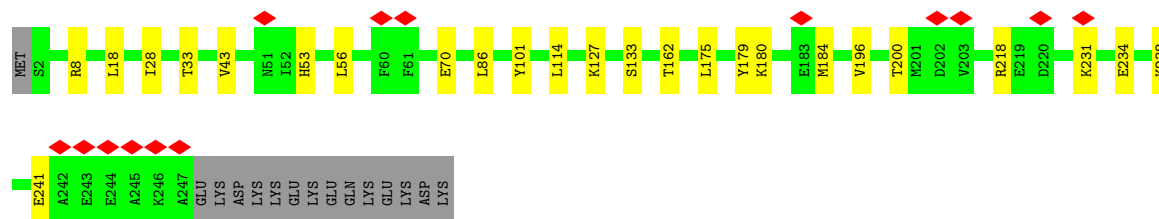


- Molecule 2: Proteasome subunit alpha type

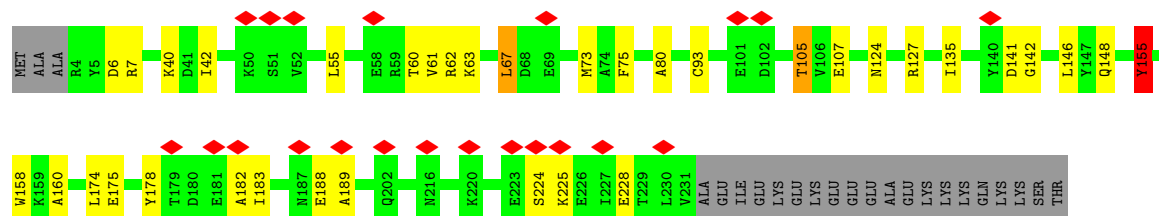
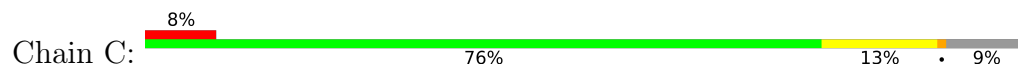


- Molecule 2: Proteasome subunit alpha type

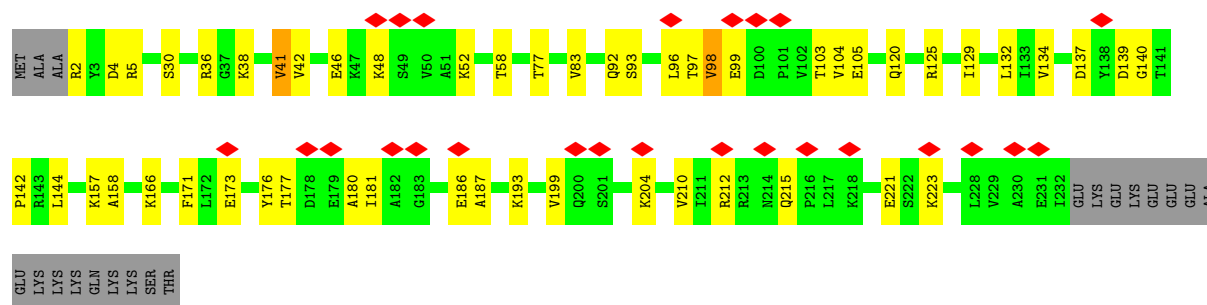




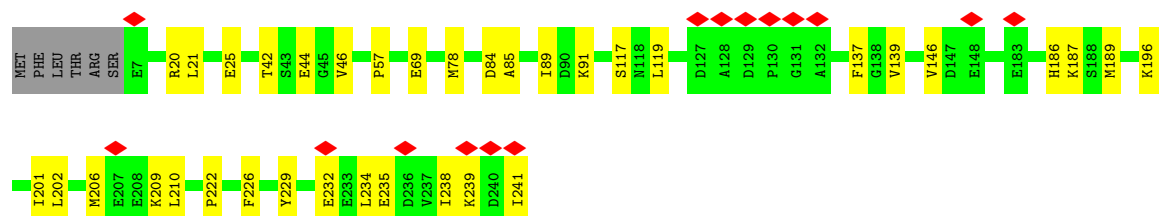
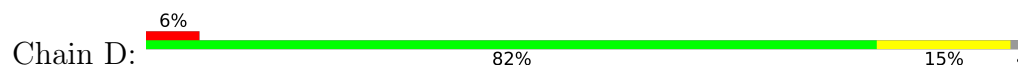
• Molecule 3: Proteasome subunit alpha type



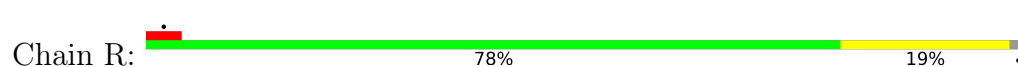
• Molecule 3: Proteasome subunit alpha type

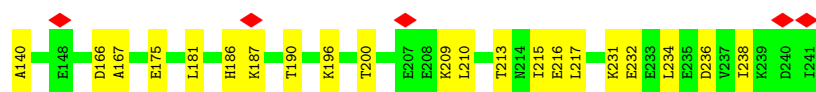


• Molecule 4: Proteasome subunit alpha type

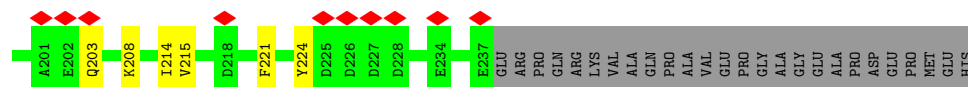
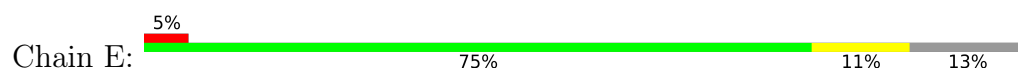


• Molecule 4: Proteasome subunit alpha type

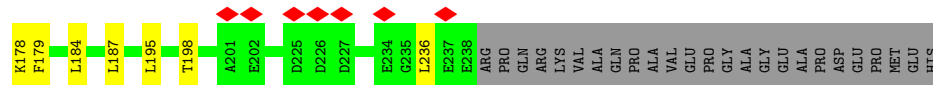
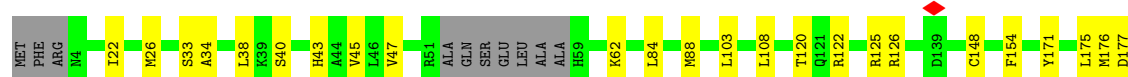




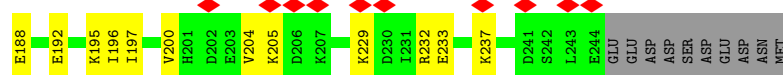
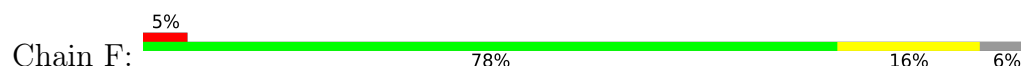
- Molecule 5: Proteasome subunit alpha type



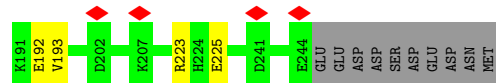
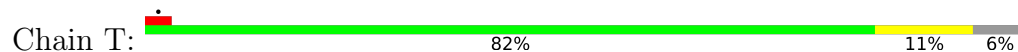
- Molecule 5: Proteasome subunit alpha type



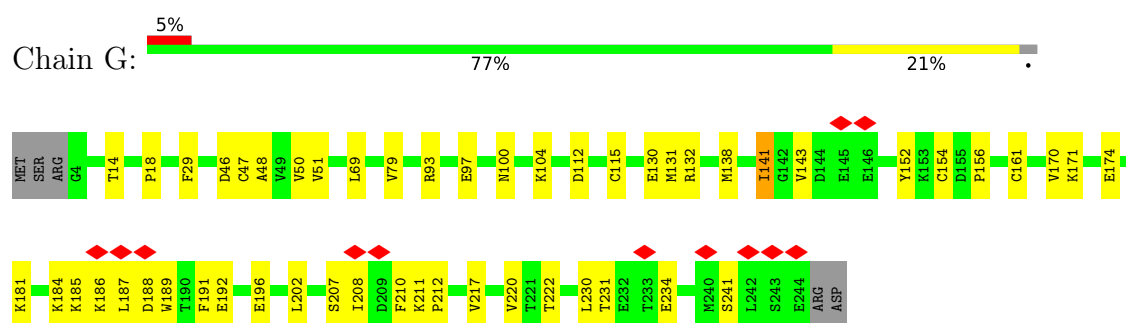
- Molecule 6: Proteasome subunit alpha type



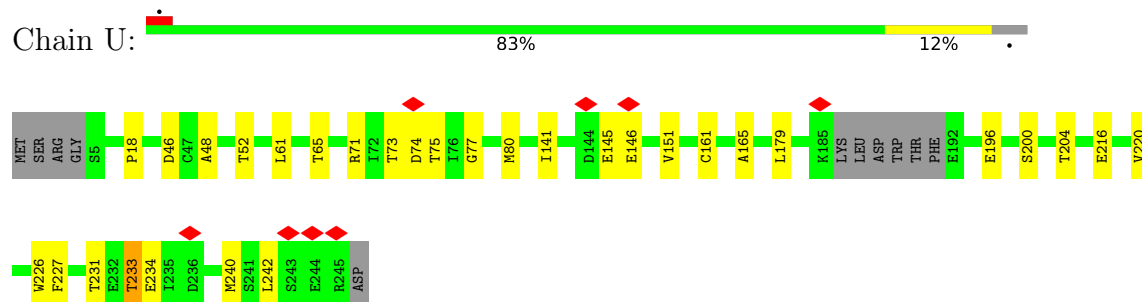
- Molecule 6: Proteasome subunit alpha type



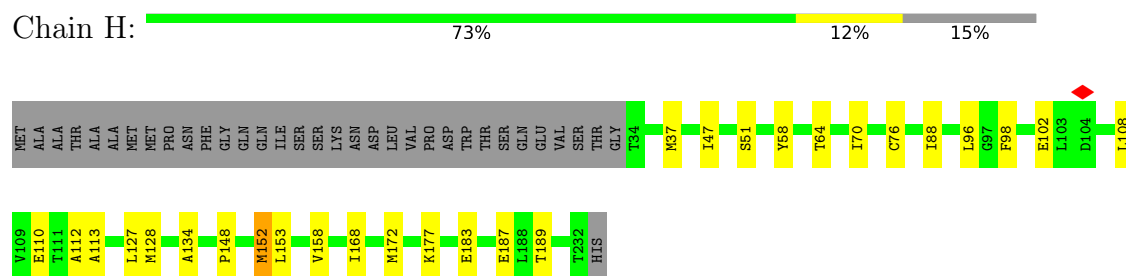
- Molecule 7: Proteasome subunit alpha type



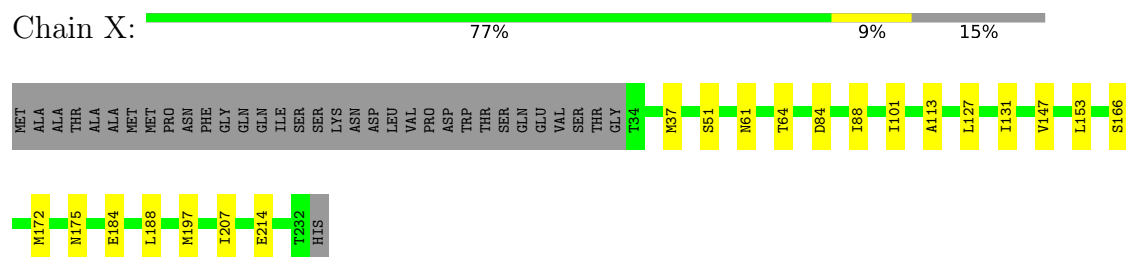
- Molecule 7: Proteasome subunit alpha type



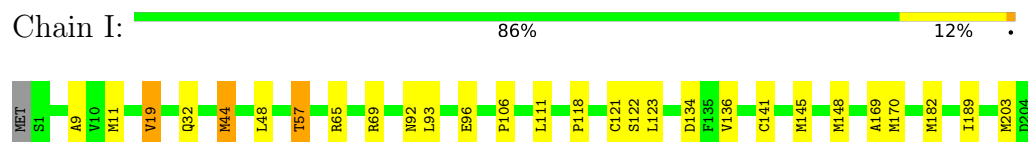
- Molecule 8: Proteasome subunit beta



- Molecule 8: Proteasome subunit beta

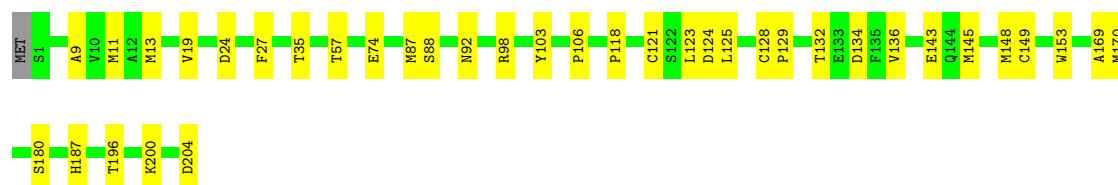


- Molecule 9: Proteasome subunit beta



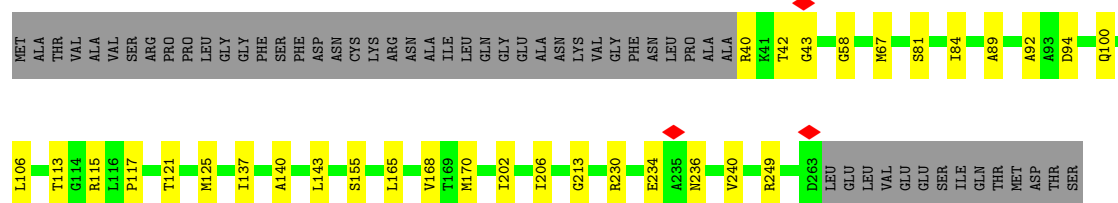
- Molecule 9: Proteasome subunit beta

Chain W:  81% 18%



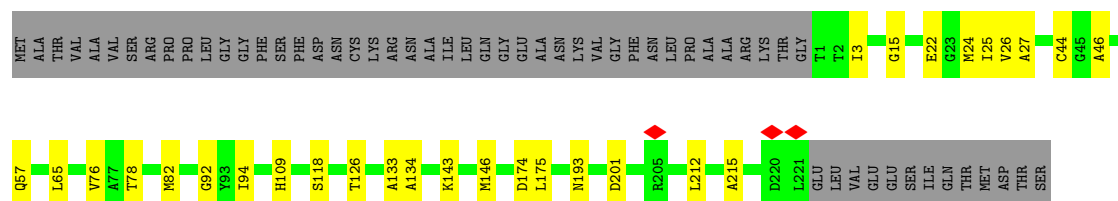
• Molecule 10: Proteasome subunit beta

Chain J:  69% 12% 19%



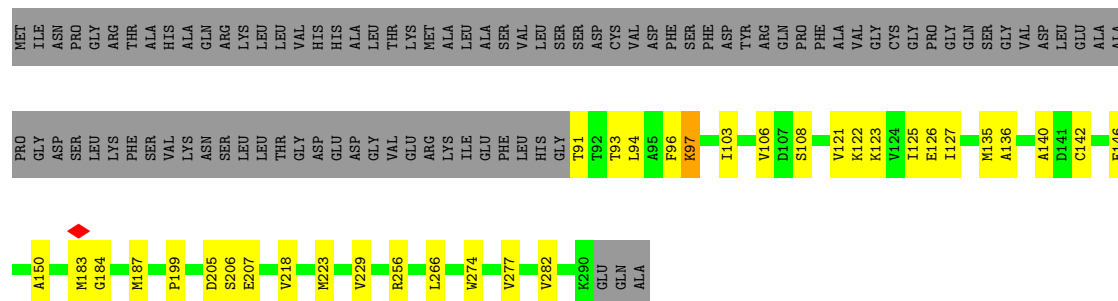
• Molecule 10: Proteasome subunit beta

Chain V:  69% 10% 20%



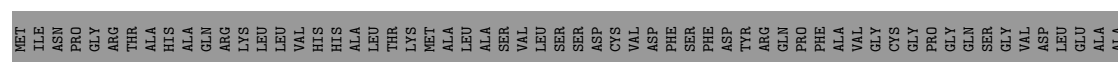
• Molecule 11: Proteasome subunit 5

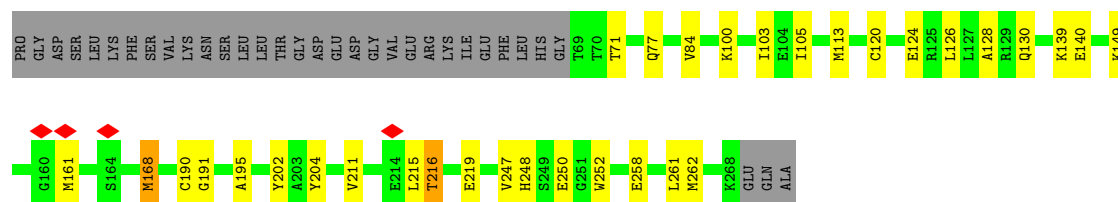
Chain K:  56% 12% 32%



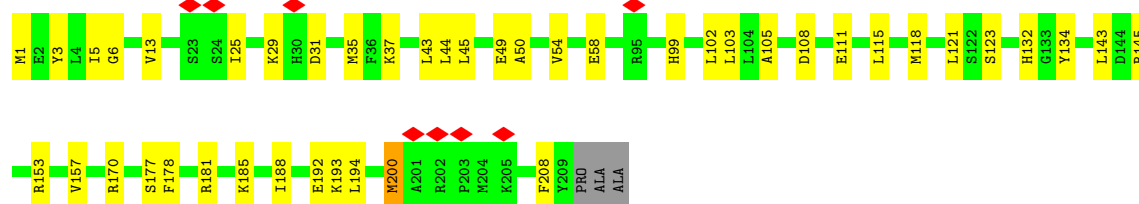
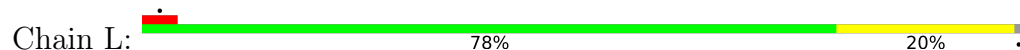
• Molecule 11: Proteasome subunit 5

Chain Z:  57% 11% 32%

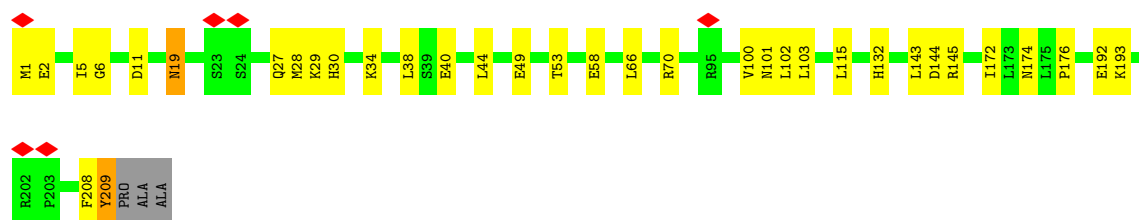
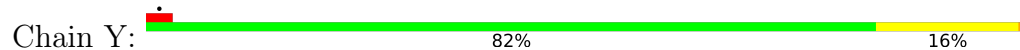




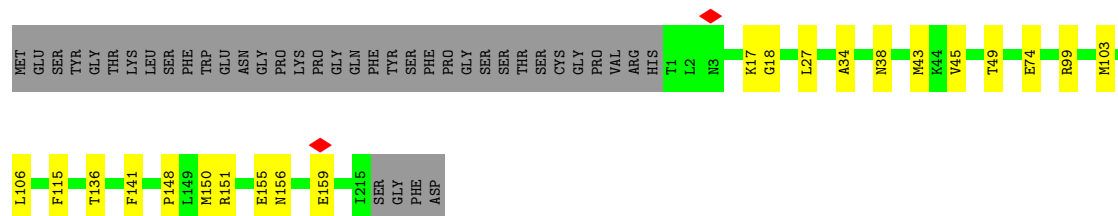
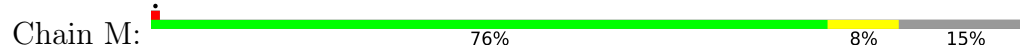
• Molecule 12: Proteasome subunit beta



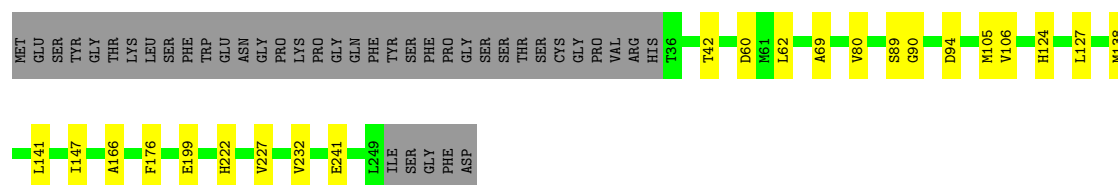
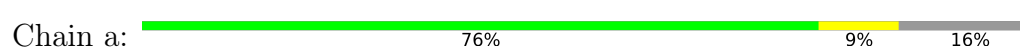
• Molecule 12: Proteasome subunit beta



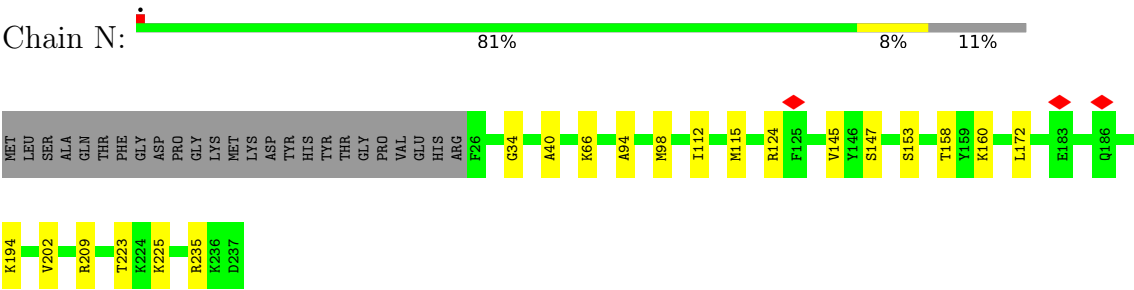
• Molecule 13: Proteasome subunit beta



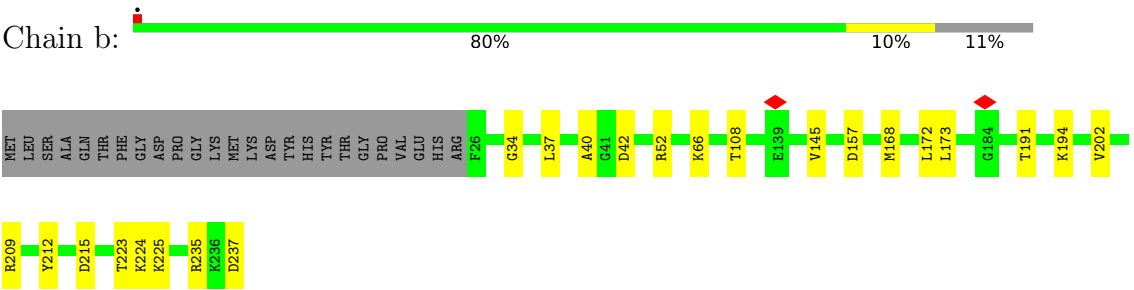
• Molecule 13: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	121745	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.23	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/1816	0.37	0/2460
1	O	0.18	0/1816	0.44	0/2460
2	B	0.18	0/1965	0.41	0/2646
2	P	0.17	0/1956	0.41	0/2634
3	C	0.20	0/1818	0.44	1/2455 (0.0%)
3	Q	0.17	0/1840	0.39	0/2485
4	D	0.17	0/1826	0.41	0/2468
4	R	0.18	0/1826	0.42	0/2468
5	E	0.17	0/1821	0.39	0/2460
5	S	0.18	0/1825	0.42	0/2465
6	F	0.16	0/1915	0.40	0/2578
6	T	0.15	0/1908	0.35	0/2568
7	G	0.18	0/1913	0.45	0/2591
7	U	0.18	0/1859	0.39	0/2515
8	H	0.17	0/1520	0.35	0/2057
8	X	0.19	0/1520	0.36	0/2057
9	I	0.17	0/1624	0.36	0/2187
9	W	0.20	0/1624	0.44	0/2187
10	J	0.18	0/1711	0.38	0/2315
10	V	0.18	0/1688	0.39	0/2286
11	K	0.18	0/1582	0.38	0/2135
11	Z	0.18	0/1582	0.41	0/2135
12	L	0.17	0/1699	0.37	0/2294
12	Y	0.18	0/1699	0.39	0/2294
13	M	0.18	0/1723	0.39	0/2334
13	a	0.18	0/1715	0.41	0/2323
14	N	0.18	0/1661	0.39	0/2242
14	b	0.18	0/1661	0.37	0/2242
All	All	0.18	0/49113	0.40	1/66341 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	Q	0	1
10	J	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	61	VAL	N-CA-C	-5.62	107.26	112.43

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	230	ARG	Peptide
3	Q	2	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1777	0	1763	21	0
1	O	1777	0	1763	20	0
2	B	1935	0	1949	23	0
2	P	1926	0	1943	14	0
3	C	1792	0	1835	29	0
3	Q	1814	0	1857	32	0
4	D	1798	0	1774	24	0
4	R	1798	0	1774	31	0
5	E	1789	0	1780	16	0
5	S	1793	0	1781	19	0
6	F	1879	0	1851	22	0
6	T	1872	0	1844	18	0
7	G	1877	0	1862	36	0
7	U	1827	0	1817	21	0
8	H	1496	0	1492	20	0
8	X	1496	0	1492	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1596	0	1606	15	0
9	W	1596	0	1606	25	0
10	J	1683	0	1683	21	0
10	V	1660	0	1661	20	0
11	K	1553	0	1527	23	0
11	Z	1553	0	1527	19	0
12	L	1664	0	1668	24	0
12	Y	1664	0	1668	23	0
13	M	1690	0	1687	13	0
13	a	1682	0	1673	11	0
14	N	1630	0	1624	14	0
14	b	1630	0	1624	12	0
All	All	48247	0	48131	520	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 (520) 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:187:MET:HB2	11:K:206:SER:HB2	1.42	0.99
14:N:194:LYS:HE2	14:N:194:LYS:H	1.43	0.81
5:E:120:THR:HG22	6:F:129:ARG:HH12	1.45	0.80
4:R:59:MET:HE2	4:R:64:ILE:HD11	1.64	0.79
4:D:146:VAL:HG11	4:D:222:PRO:HA	1.66	0.77
11:K:125:ILE:HD12	11:K:146:GLU:HG3	1.67	0.76
3:C:67:LEU:HD11	3:C:73:MET:HE1	1.67	0.75
3:Q:181:ILE:HG23	3:Q:187:ALA:HB2	1.69	0.74
14:b:34:GLY:HA3	14:b:66:LYS:HE3	1.70	0.73
11:Z:139:LYS:HE2	11:Z:139:LYS:HA	1.71	0.72
10:J:94:ASP:HB3	10:J:137:ILE:HG23	1.72	0.72
14:N:147:SER:HB3	14:N:160:LYS:HG2	1.72	0.72
7:G:50:VAL:HG13	7:G:141:ILE:HD12	1.72	0.71
1:A:199:PHE:HZ	1:A:207:ASN:HB3	1.55	0.71
7:G:69:LEU:HG	7:G:79:VAL:HG22	1.73	0.70
8:H:51:SER:HB2	8:H:64:THR:H	1.56	0.70
1:O:68:THR:HG23	1:O:70:HIS:H	1.57	0.69
2:P:28:ILE:HD13	2:P:133:SER:HB2	1.72	0.69
3:C:63:LYS:HD2	3:C:75:PHE:H	1.56	0.69
8:X:197:MET:HE1	8:X:207:ILE:HG12	1.75	0.69
7:G:51:VAL:HG22	7:G:217:VAL:HG12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:172:LEU:HD23	14:N:202:VAL:HG12	1.73	0.68
3:Q:212:ARG:HD3	3:Q:215:GLN:HE21	1.58	0.68
11:K:207:GLU:HB3	12:L:50:ALA:HB3	1.77	0.67
13:M:136:THR:HB	13:M:150:MET:HE3	1.76	0.67
11:Z:103:ILE:HD13	11:Z:124:GLU:HG3	1.77	0.66
7:G:143:VAL:HG23	7:G:220:VAL:HG13	1.78	0.65
12:Y:1:MET:HG2	12:Y:2:GLU:H	1.60	0.65
12:L:44:LEU:HD11	12:L:102:LEU:HD23	1.79	0.65
12:L:177:SER:HB3	12:L:193:LYS:HZ1	1.61	0.65
4:R:31:ILE:HD13	4:R:140:ALA:HB2	1.79	0.65
14:b:223:THR:HG23	14:b:225:LYS:H	1.62	0.64
10:J:249:ARG:HG3	10:J:249:ARG:HH11	1.62	0.64
7:G:211:LYS:HE2	7:G:212:PRO:HD2	1.80	0.64
12:L:200:MET:HE3	12:Y:176:PRO:HA	1.78	0.64
14:N:194:LYS:HE2	14:N:194:LYS:N	2.12	0.64
2:B:241:GLU:HA	2:B:244:GLU:HG3	1.79	0.64
8:H:148:PRO:HG2	8:H:152:MET:HE3	1.80	0.64
5:S:40:SER:HB2	5:S:187:LEU:HD11	1.79	0.64
7:G:187:LEU:HD12	7:G:188:ASP:H	1.64	0.63
5:S:38:LEU:HD21	5:S:179:PHE:CE1	2.32	0.63
6:F:204:VAL:HG23	6:F:205:LYS:HG3	1.80	0.63
10:J:43:GLY:HA3	10:J:89:ALA:HA	1.81	0.63
6:F:123:THR:HG22	7:G:132:ARG:HH21	1.63	0.63
12:Y:5:ILE:HD11	12:Y:143:LEU:HD11	1.80	0.63
9:W:11:MET:HE3	9:W:170:MET:HG2	1.81	0.62
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.82	0.62
1:A:69:THR:HG23	1:A:71:HIS:H	1.65	0.62
7:U:141:ILE:HG22	7:U:151:VAL:HG22	1.80	0.61
10:V:25:ILE:HD12	9:W:143:GLU:OE2	2.01	0.61
2:B:86:LEU:HD22	2:B:114:LEU:HD11	1.82	0.61
9:I:122:SER:HB2	9:I:136:VAL:HG13	1.82	0.61
5:S:34:ALA:HB2	5:S:198:THR:HG21	1.83	0.61
6:T:184:MET:HE3	6:T:184:MET:H	1.66	0.61
3:Q:38:LYS:HE2	3:Q:181:ILE:HB	1.83	0.60
8:H:113:ALA:HB1	8:H:153:LEU:HD11	1.84	0.60
7:U:48:ALA:HB3	7:U:220:VAL:HG12	1.82	0.60
8:X:88:ILE:HD11	8:X:127:LEU:HD13	1.83	0.60
11:Z:71:THR:HG23	11:Z:84:VAL:HG12	1.84	0.60
14:b:172:LEU:HD23	14:b:202:VAL:HG22	1.84	0.60
1:A:34:PRO:HG2	1:A:49:GLU:HG2	1.83	0.59
6:F:34:SER:HB2	6:F:65:ARG:HH12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD13	1:A:113:ARG:HB3	1.83	0.59
9:I:19:VAL:HG22	9:I:118:PRO:HB3	1.84	0.59
3:Q:171:PHE:HZ	3:Q:193:LYS:HD2	1.66	0.59
7:U:141:ILE:HD11	7:U:227:PHE:HE1	1.67	0.59
9:I:9:ALA:HB1	9:I:145:MET:HE1	1.84	0.59
10:J:113:THR:HG22	10:J:115:ARG:HG3	1.85	0.59
10:V:126:THR:HG21	10:V:134:ALA:HB3	1.84	0.59
4:R:175:GLU:CD	4:R:175:GLU:H	2.11	0.59
6:F:23:VAL:HG11	6:F:123:THR:HG23	1.83	0.59
3:Q:97:THR:O	3:Q:97:THR:HG22	2.03	0.58
14:N:209:ARG:HA	10:V:26:VAL:HB	1.85	0.58
5:S:176:MET:O	5:S:179:PHE:HB2	2.04	0.58
8:X:84:ASP:HB3	8:X:127:LEU:HD22	1.86	0.58
13:a:94:ASP:HB3	13:a:141:LEU:HD22	1.84	0.58
6:T:49:VAL:HG11	6:T:65:ARG:HB2	1.84	0.58
8:X:51:SER:HB2	8:X:64:THR:H	1.68	0.58
7:G:192:GLU:O	7:G:196:GLU:HG2	2.04	0.57
12:L:49:GLU:HG2	12:L:99:HIS:HB3	1.85	0.57
1:O:94:GLN:HG3	10:V:65:LEU:HG	1.87	0.57
2:P:180:LYS:H	2:P:184:MET:HE1	1.68	0.57
8:X:37:MET:HE1	8:X:172:MET:SD	2.44	0.57
2:B:122:THR:HG22	3:C:127:ARG:HH21	1.69	0.57
8:H:96:LEU:HD11	8:H:112:ALA:HB2	1.87	0.57
5:S:178:LYS:HD2	5:S:178:LYS:O	2.05	0.57
4:R:167:ALA:HB1	4:R:181:LEU:HD22	1.86	0.57
1:O:56:TYR:HE2	7:U:161:CYS:HB3	1.69	0.57
3:Q:98:VAL:HG12	3:Q:99:GLU:H	1.69	0.57
4:R:13:ASN:HB3	5:S:126:ARG:HB3	1.86	0.57
2:B:3:ARG:HB3	3:C:7:ARG:HH21	1.70	0.56
12:L:5:ILE:HD11	12:L:143:LEU:HD11	1.88	0.56
12:L:29:LYS:HG2	12:L:31:ASP:H	1.70	0.56
14:N:112:ILE:HA	14:N:115:MET:HE2	1.87	0.56
7:U:71:ARG:HH12	7:U:74:ASP:HA	1.70	0.56
9:W:87:MET:SD	9:W:129:PRO:HB3	2.45	0.56
3:C:225:LYS:HA	3:C:225:LYS:HE2	1.88	0.56
14:b:168:MET:HE1	14:b:209:ARG:HB2	1.86	0.56
2:B:52:ILE:HG21	2:B:210:LYS:HG2	1.87	0.56
3:C:67:LEU:HD11	3:C:73:MET:CE	2.35	0.56
12:L:177:SER:HB3	12:L:193:LYS:NZ	2.21	0.56
3:C:63:LYS:O	3:C:63:LYS:HD3	2.06	0.56
2:P:86:LEU:HD22	2:P:114:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:182:MET:HE2	9:I:203:MET:HE3	1.88	0.56
3:Q:38:LYS:HD3	3:Q:38:LYS:N	2.20	0.56
9:W:124:ASP:HB3	9:W:128:CYS:H	1.71	0.56
8:H:127:LEU:C	8:H:128:MET:HE2	2.30	0.55
3:Q:30:SER:HA	3:Q:48:LYS:NZ	2.21	0.55
9:I:92:ASN:O	9:I:96:GLU:HG3	2.06	0.55
6:T:108:LEU:HD13	6:T:139:SER:HB3	1.89	0.55
7:G:202:LEU:HB3	7:G:210:PHE:HE1	1.71	0.55
3:C:182:ALA:O	3:C:188:GLU:HG2	2.06	0.55
9:I:69:ARG:HE	9:I:93:LEU:HD12	1.71	0.55
12:Y:29:LYS:HE2	11:Z:191:GLY:HA2	1.89	0.55
3:C:148:GLN:O	3:C:155:TYR:HA	2.06	0.55
14:N:40:ALA:HB2	14:N:145:VAL:HG23	1.89	0.55
2:P:33:THR:HG21	2:P:200:THR:HG21	1.86	0.54
7:G:217:VAL:HG23	7:G:230:LEU:HB2	1.89	0.54
4:D:187:LYS:HE2	4:D:187:LYS:HA	1.89	0.54
7:G:174:GLU:CD	7:G:174:GLU:H	2.16	0.54
7:G:187:LEU:HD12	7:G:188:ASP:N	2.22	0.54
8:X:131:ILE:HG12	8:X:147:VAL:HB	1.89	0.54
5:E:43:HIS:CE1	5:E:184:LEU:HD21	2.43	0.54
11:K:266:LEU:HB3	11:K:277:VAL:HB	1.90	0.54
10:V:215:ALA:HB3	9:W:196:THR:HG23	1.89	0.54
4:D:235:GLU:O	4:D:239:LYS:HG2	2.08	0.54
3:C:224:SER:O	3:C:228:GLU:HG2	2.08	0.54
12:Y:101:ASN:HB3	12:Y:132:HIS:CE1	2.42	0.54
10:J:236:ASN:HB3	14:b:235:ARG:NH2	2.22	0.53
3:Q:103:THR:HG22	3:Q:105:GLU:H	1.72	0.53
3:Q:212:ARG:HB2	3:Q:215:GLN:HG2	1.90	0.53
7:U:200:SER:O	7:U:204:THR:HG23	2.08	0.53
12:Y:44:LEU:HD21	12:Y:102:LEU:HD23	1.89	0.53
5:E:103:LEU:HD23	5:E:108:LEU:HG	1.89	0.53
6:F:49:VAL:HG11	6:F:65:ARG:HB2	1.90	0.53
11:Z:258:GLU:HG2	11:Z:262:MET:HE3	1.91	0.53
10:J:42:THR:HG23	10:J:92:ALA:HB2	1.90	0.53
6:T:94:GLU:OE1	6:T:114:ARG:HB2	2.08	0.53
5:E:64:LEU:HD13	5:E:74:ILE:HD12	1.90	0.53
10:J:58:GLY:HA3	10:J:202:ILE:HD11	1.90	0.53
13:a:138:MET:HE3	13:a:138:MET:HA	1.91	0.53
12:L:3:TYR:HD2	12:L:178:PHE:HE2	1.57	0.53
4:D:91:LYS:HD2	4:D:119:LEU:HD22	1.91	0.53
2:B:119:GLN:HG3	3:C:80:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:19:ARG:HH21	6:F:21:PHE:HE1	1.56	0.53
9:W:9:ALA:HB1	9:W:145:MET:HE1	1.91	0.53
8:H:88:ILE:HD11	8:H:127:LEU:HD13	1.91	0.53
10:J:67:MET:HE2	14:b:212:TYR:CE2	2.44	0.52
3:Q:42:VAL:HG22	3:Q:210:VAL:HG12	1.92	0.52
9:W:106:PRO:HD2	9:W:123:LEU:HB2	1.91	0.52
7:G:48:ALA:HB1	7:G:141:ILE:HD13	1.90	0.52
4:R:108:THR:HG23	4:R:111:SER:H	1.74	0.52
5:S:22:ILE:HD11	5:S:120:THR:HG23	1.90	0.52
7:U:52:THR:HG22	7:U:216:GLU:HB2	1.92	0.52
14:b:37:LEU:HD11	14:b:173:LEU:HD11	1.91	0.52
8:H:183:GLU:O	8:H:187:GLU:HG3	2.09	0.52
9:I:106:PRO:HD2	9:I:123:LEU:HB2	1.91	0.52
10:J:155:SER:HB2	10:J:168:VAL:HG11	1.92	0.52
13:M:17:LYS:HD3	13:M:159:GLU:HG2	1.92	0.52
14:N:235:ARG:HG2	10:V:193:ASN:HB3	1.91	0.52
3:Q:5:ARG:HB3	3:Q:5:ARG:NH1	2.24	0.52
2:B:3:ARG:HB3	3:C:7:ARG:NH2	2.25	0.52
2:B:21:VAL:O	2:B:25:MET:HG2	2.09	0.52
11:K:135:MET:HG3	11:K:142:CYS:CB	2.40	0.52
6:F:229:LYS:HD2	6:F:232:ARG:HH21	1.74	0.52
10:J:121:THR:HG22	10:J:125:MET:HE3	1.92	0.51
12:L:153:ARG:O	12:L:157:VAL:HG23	2.10	0.51
9:W:24:ASP:OD2	9:W:180:SER:HB3	2.10	0.51
4:R:232:GLU:CD	4:R:232:GLU:H	2.18	0.51
3:C:73:MET:HE3	3:C:135:ILE:HD12	1.91	0.51
10:J:165:LEU:HD21	8:X:61:ASN:OD1	2.10	0.51
12:Y:192:GLU:HB3	12:Y:208:PHE:HD2	1.76	0.51
3:C:67:LEU:HD12	3:C:67:LEU:H	1.75	0.51
9:W:124:ASP:OD2	9:W:125:LEU:N	2.44	0.51
14:N:223:THR:HG23	14:N:225:LYS:H	1.75	0.51
11:Z:120:CYS:O	11:Z:124:GLU:HG2	2.10	0.51
6:T:41:CYS:HB2	6:T:189:LEU:HD11	1.91	0.51
3:Q:46:GLU:HG3	3:Q:199:VAL:HG22	1.92	0.50
5:E:72:ILE:HG22	5:E:134:ILE:HG12	1.92	0.50
6:T:83:ASP:HB3	6:T:131:PHE:HD1	1.76	0.50
1:O:187:ILE:HD11	1:O:211:ILE:HD11	1.93	0.50
10:J:40:ARG:NH1	10:J:42:THR:HG21	2.27	0.50
6:T:188:GLU:O	6:T:192:GLU:HG2	2.12	0.50
13:a:60:ASP:HA	13:a:222:HIS:HA	1.93	0.50
3:Q:120:GLN:NE2	4:R:133:MET:HE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:100:LYS:NZ	11:Z:100:LYS:HB3	2.26	0.50
11:K:256:ARG:HD2	12:Y:144:ASP:OD2	2.12	0.49
6:T:23:VAL:O	6:T:27:MET:HG2	2.12	0.49
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.93	0.49
4:R:66:LYS:HA	4:R:78:MET:HE2	1.94	0.49
3:C:160:ALA:HB1	3:C:174:LEU:HD13	1.94	0.49
9:I:148:MET:HE3	9:I:169:ALA:HA	1.95	0.49
5:E:33:SER:HB2	5:E:62:LYS:NZ	2.28	0.49
6:F:185:THR:HG22	6:F:187:ARG:H	1.78	0.49
4:D:186:HIS:HB2	4:D:189:MET:HG3	1.95	0.49
4:R:50:VAL:HG12	4:R:216:GLU:HB2	1.94	0.49
9:W:200:LYS:NZ	9:W:200:LYS:HB2	2.28	0.49
1:A:199:PHE:O	1:A:200:GLU:HG3	2.12	0.49
12:L:54:VAL:O	12:L:58:GLU:HG2	2.13	0.49
10:V:76:VAL:HG11	10:V:109:HIS:HB2	1.94	0.49
9:W:19:VAL:HG13	9:W:118:PRO:HB3	1.95	0.49
1:A:53:LYS:HD2	1:A:53:LYS:N	2.27	0.49
1:O:69:LYS:NZ	1:O:69:LYS:HB3	2.28	0.49
4:R:53:ARG:O	4:R:53:ARG:HG2	2.12	0.49
10:V:78:THR:HG22	10:V:82:MET:HE3	1.95	0.49
3:C:73:MET:HE3	3:C:135:ILE:HG23	1.95	0.49
4:D:197:SER:O	4:D:201:ILE:HG12	2.13	0.49
4:D:202:LEU:HG	4:D:206:MET:HE2	1.95	0.49
5:S:120:THR:HG22	6:T:129:ARG:HH12	1.78	0.49
7:G:138:MET:HB3	7:G:154:CYS:HB2	1.95	0.48
8:H:158:VAL:HG21	8:H:172:MET:HE2	1.95	0.48
8:H:168:ILE:O	8:H:172:MET:HG2	2.13	0.48
10:J:140:ALA:HB1	10:J:170:MET:SD	2.53	0.48
4:R:68:VAL:HG21	4:R:89:ILE:HD13	1.95	0.48
12:Y:2:GLU:HG3	12:Y:34:LYS:NZ	2.28	0.48
9:I:57:THR:HB	12:L:121:LEU:O	2.12	0.48
3:Q:157:LYS:HE2	4:R:58:LEU:HA	1.94	0.48
14:b:191:THR:HG23	14:b:194:LYS:H	1.77	0.48
6:F:87:LEU:HD13	6:F:135:PHE:HE2	1.79	0.48
7:G:50:VAL:HB	7:G:79:VAL:HG21	1.95	0.48
7:G:231:THR:HG22	7:G:234:GLU:HG3	1.94	0.48
4:R:65:GLU:HA	4:R:65:GLU:OE1	2.13	0.48
5:S:43:HIS:CE1	5:S:184:LEU:HD11	2.49	0.48
11:K:140:ALA:HA	14:N:153:SER:HB3	1.95	0.48
14:N:34:GLY:HA3	14:N:66:LYS:HE3	1.95	0.48
9:W:148:MET:HE2	9:W:169:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:LEU:HA	2:B:200:THR:HG22	1.95	0.48
8:H:58:TYR:HB2	13:M:141:PHE:HZ	1.77	0.48
3:Q:137:ASP:HB2	3:Q:140:GLY:O	2.13	0.48
4:D:209:LYS:HE3	4:D:210:LEU:H	1.77	0.48
4:R:217:LEU:HB2	4:R:234:LEU:HD21	1.95	0.48
6:F:237:LYS:HA	6:F:237:LYS:HE2	1.95	0.48
8:H:37:MET:HG2	8:H:189:THR:HG23	1.95	0.48
5:S:38:LEU:HD21	5:S:179:PHE:CD1	2.49	0.48
6:T:190:VAL:HA	6:T:193:VAL:HG22	1.96	0.48
12:Y:6:GLY:HA3	12:Y:115:LEU:HD11	1.96	0.48
12:Y:11:ASP:O	12:Y:11:ASP:OD2	2.32	0.48
3:C:42:ILE:HD11	3:C:189:ALA:HB3	1.95	0.47
2:P:234:GLU:O	2:P:238:LYS:HG3	2.13	0.47
5:S:122:ARG:HB3	5:S:125:ARG:HG3	1.96	0.47
9:W:103:TYR:HA	9:W:125:LEU:HD21	1.96	0.47
11:Z:195:ALA:HB3	11:Z:204:TYR:CE2	2.49	0.47
3:C:105:THR:HG22	3:C:107:GLU:OE1	2.14	0.47
7:G:184:LYS:NZ	7:G:185:LYS:HD2	2.29	0.47
1:O:67:ILE:HD11	1:O:73:MET:HE2	1.95	0.47
2:P:18:LEU:HD21	3:Q:125:ARG:HH11	1.78	0.47
1:A:50:LYS:HD2	1:A:209:GLU:HG3	1.97	0.47
7:G:185:LYS:O	7:G:186:LYS:HG3	2.14	0.47
11:K:135:MET:HG3	11:K:142:CYS:HB2	1.96	0.47
12:L:108:ASP:HB3	12:L:111:GLU:HB3	1.95	0.47
5:S:26:MET:HE2	5:S:148:CYS:SG	2.54	0.47
6:F:192:GLU:O	6:F:196:ILE:HG12	2.14	0.47
8:X:113:ALA:HB1	8:X:153:LEU:HD11	1.94	0.47
7:G:187:LEU:HD12	7:G:189:TRP:H	1.78	0.47
12:L:178:PHE:HB2	12:L:194:LEU:HB3	1.96	0.47
1:O:138:TRP:NE1	1:O:141:ASP:HA	2.29	0.47
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.97	0.47
7:U:165:ALA:HB1	7:U:179:LEU:HD13	1.96	0.47
3:C:63:LYS:HD2	3:C:75:PHE:N	2.27	0.47
5:E:215:VAL:HB	5:E:221:PHE:HD1	1.80	0.47
11:K:108:SER:HB2	11:K:121:VAL:H	1.80	0.47
12:L:6:GLY:HA3	12:L:115:LEU:HD11	1.97	0.47
14:N:94:ALA:O	14:N:98:MET:HG3	2.15	0.47
1:O:101:GLN:HE22	10:V:57:GLN:CD	2.23	0.47
6:T:184:MET:HB2	6:T:188:GLU:HB2	1.97	0.47
3:Q:221:GLU:OE1	3:Q:223:LYS:HG2	2.14	0.46
4:D:85:ALA:HB2	4:D:139:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:99:ARG:HD3	13:M:106:LEU:HG	1.97	0.46
3:Q:92:GLN:HG3	12:Y:66:LEU:HD12	1.97	0.46
3:Q:96:LEU:HD11	12:Y:58:GLU:HB3	1.98	0.46
2:B:208:ALA:HB2	2:B:237:ILE:HD12	1.96	0.46
1:O:92:LEU:HD13	1:O:112:ARG:HB3	1.98	0.46
11:Z:77:GLN:CD	11:Z:77:GLN:H	2.22	0.46
13:a:62:LEU:HD11	13:a:69:ALA:HB1	1.97	0.46
3:Q:83:VAL:HG21	3:Q:129:ILE:HD11	1.98	0.46
3:Q:158:ALA:HB3	4:R:58:LEU:HD22	1.97	0.46
7:G:211:LYS:HE2	7:G:212:PRO:CD	2.44	0.46
11:K:126:GLU:HG2	11:K:274:TRP:CZ2	2.51	0.46
7:G:104:LYS:NZ	7:G:104:LYS:HB3	2.31	0.46
7:G:130:GLU:HG2	7:G:131:MET:HG2	1.98	0.46
7:G:187:LEU:CD1	7:G:189:TRP:H	2.29	0.46
2:P:179:TYR:CD1	2:P:184:MET:HE3	2.50	0.46
6:F:185:THR:H	6:F:188:GLU:HB2	1.81	0.46
7:G:47:CYS:SG	7:G:191:PHE:HA	2.56	0.46
8:X:175:ASN:HB3	8:X:188:LEU:HD11	1.98	0.46
7:G:207:SER:C	7:G:208:ILE:HD13	2.40	0.46
10:J:106:LEU:HD22	10:J:117:PRO:HB3	1.98	0.46
2:P:218:ARG:HH11	2:P:218:ARG:HG3	1.81	0.46
5:E:33:SER:HB2	5:E:62:LYS:HZ2	1.80	0.45
6:F:41:CYS:SG	6:F:42:LYS:N	2.88	0.45
2:P:175:LEU:HD13	2:P:196:VAL:HG21	1.98	0.45
10:V:22:GLU:HG2	10:V:27:ALA:HB2	1.97	0.45
9:I:65:ARG:HG3	9:I:65:ARG:HH11	1.80	0.45
13:a:80:VAL:HG12	13:a:106:VAL:HG21	1.97	0.45
3:C:146:LEU:HD22	3:C:158:TRP:HB2	1.98	0.45
6:F:108:LEU:HD13	6:F:139:SER:HB2	1.99	0.45
7:G:181:LYS:HE2	7:G:181:LYS:HA	1.99	0.45
5:S:154:PHE:HE1	6:T:63:ASN:HD21	1.64	0.45
4:D:78:MET:SD	4:D:89:ILE:HD11	2.57	0.45
8:H:47:ILE:HD11	8:H:134:ALA:HB3	1.97	0.45
10:J:81:SER:HB2	10:J:84:ILE:HB	1.97	0.45
13:M:151:ARG:O	13:M:155:GLU:HG2	2.16	0.45
4:D:42:THR:HG23	4:D:44:GLU:H	1.82	0.45
4:R:121:LEU:HD23	4:R:123:PHE:CE1	2.51	0.45
12:Y:66:LEU:O	12:Y:70:ARG:HG3	2.16	0.45
2:B:52:ILE:HD13	2:B:210:LYS:HD3	1.99	0.45
2:B:68:LEU:HD12	2:B:72:MET:HE2	1.98	0.45
8:H:70:ILE:HD11	8:H:76:CYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:132:SER:HB3	1:O:162:MET:HE3	1.97	0.45
10:V:212:LEU:HD21	9:W:200:LYS:NZ	2.32	0.45
9:W:132:THR:HG22	9:W:134:ASP:H	1.81	0.45
13:a:241:GLU:N	13:a:241:GLU:OE1	2.50	0.45
2:B:34:CYS:HB2	2:B:164:ILE:HG12	1.99	0.45
7:G:46:ASP:HB2	7:G:222:THR:HG22	1.98	0.45
8:H:37:MET:HE1	8:H:172:MET:SD	2.57	0.45
12:L:118:MET:HA	12:L:123:SER:O	2.17	0.45
10:V:143:LYS:O	10:V:146:MET:HG3	2.17	0.45
9:I:44:MET:O	9:I:48:LEU:HB3	2.17	0.44
1:O:214:GLU:N	1:O:214:GLU:OE1	2.51	0.44
5:S:33:SER:H	5:S:62:LYS:HZ3	1.64	0.44
2:B:133:SER:HB3	2:B:164:ILE:HD12	1.99	0.44
10:J:234:GLU:O	10:J:234:GLU:HG2	2.17	0.44
11:K:183:MET:HE2	11:K:184:GLY:N	2.32	0.44
12:L:37:LYS:HD2	12:L:188:ILE:HD12	2.00	0.44
9:W:13:MET:HE3	9:W:153:TRP:HD1	1.82	0.44
2:B:3:ARG:HG3	5:E:123:TYR:OH	2.17	0.44
8:H:108:LEU:HB3	8:H:110:GLU:OE1	2.17	0.44
4:R:119:LEU:HD23	4:R:119:LEU:HA	1.83	0.44
2:B:218:ARG:HH12	2:B:221:GLY:HA2	1.82	0.44
7:G:93:ARG:O	7:G:97:GLU:HG2	2.17	0.44
4:R:215:ILE:HD11	4:R:238:ILE:HD11	1.99	0.44
7:U:77:GLY:HA3	7:U:227:PHE:CE1	2.53	0.44
9:W:13:MET:HE3	9:W:153:TRP:CD1	2.52	0.44
11:Z:126:LEU:O	11:Z:130:GLN:HG2	2.17	0.44
11:Z:168:MET:HB2	11:Z:168:MET:HE2	1.71	0.44
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.85	0.44
2:B:241:GLU:HA	2:B:244:GLU:CG	2.46	0.44
13:M:156:ASN:OD1	13:M:156:ASN:C	2.60	0.44
7:U:240:MET:HE2	7:U:240:MET:HA	2.00	0.44
1:A:55:ILE:HD12	1:A:55:ILE:H	1.83	0.44
3:C:175:GLU:OE1	4:D:57:PRO:HD2	2.18	0.44
12:L:43:LEU:HD11	12:L:181:ARG:HD3	2.00	0.44
1:O:51:GLN:HG2	1:O:56:TYR:CG	2.53	0.44
2:P:70:GLU:H	2:P:70:GLU:CD	2.25	0.44
2:P:231:LYS:HD3	2:P:231:LYS:N	2.32	0.44
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.98	0.44
6:T:158:TYR:HB3	7:U:61:LEU:HD11	2.00	0.44
1:A:70:LYS:NZ	1:A:70:LYS:HB3	2.33	0.44
1:A:150:ASP:C	1:A:150:ASP:OD1	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:GLU:OE1	3:C:107:GLU:N	2.50	0.44
1:O:182:GLU:OE1	1:O:182:GLU:HA	2.18	0.44
3:Q:5:ARG:HB3	3:Q:5:ARG:CZ	2.47	0.44
11:Z:140:GLU:OE1	11:Z:140:GLU:HA	2.18	0.44
4:D:232:GLU:H	4:D:232:GLU:CD	2.26	0.44
9:I:111:LEU:HD12	9:I:189:ILE:HG22	2.00	0.44
7:U:73:THR:HG23	7:U:75:THR:H	1.83	0.44
10:V:3:ILE:HG21	10:V:44:CYS:HB2	2.00	0.44
11:Z:250:GLU:CD	11:Z:250:GLU:H	2.26	0.44
10:J:121:THR:O	10:J:125:MET:HG3	2.18	0.43
11:K:122:LYS:NZ	11:K:122:LYS:HB3	2.32	0.43
11:K:127:ILE:HG23	11:K:150:ALA:HA	2.00	0.43
5:S:171:TYR:CZ	5:S:175:LEU:HD21	2.53	0.43
6:T:87:LEU:HD13	6:T:135:PHE:HE2	1.83	0.43
6:T:223:ARG:HD2	6:T:225:GLU:OE2	2.18	0.43
10:V:92:GLY:C	10:V:94:ILE:H	2.25	0.43
12:Y:19:ASN:HD21	12:Y:193:LYS:HZ3	1.65	0.43
1:A:57:TYR:CE2	7:G:161:CYS:HB3	2.53	0.43
5:E:208:LYS:NZ	5:E:208:LYS:HB3	2.33	0.43
13:M:103:MET:HE3	13:M:103:MET:HB3	1.82	0.43
1:O:21:ILE:HG21	1:O:151:SER:HB3	2.01	0.43
14:b:40:ALA:HB2	14:b:145:VAL:HG23	1.99	0.43
3:Q:132:LEU:HD22	3:Q:144:LEU:HD11	2.00	0.43
4:R:210:LEU:HG	4:R:238:ILE:HD12	2.00	0.43
7:U:71:ARG:HB3	7:U:71:ARG:CZ	2.49	0.43
12:L:35:MET:HE2	12:L:45:LEU:HD21	2.01	0.43
3:Q:36:ARG:HD2	3:Q:142:PRO:O	2.18	0.43
4:D:137:PHE:HB3	4:D:139:VAL:HG22	1.99	0.43
6:F:23:VAL:O	6:F:27:MET:HG2	2.18	0.43
1:A:107:THR:O	1:A:111:VAL:HG23	2.19	0.43
8:H:128:MET:HE2	8:H:128:MET:N	2.34	0.43
11:K:266:LEU:HD12	11:K:266:LEU:HA	1.91	0.43
14:N:124:ARG:HD2	14:N:124:ARG:O	2.18	0.43
4:R:44:GLU:N	4:R:44:GLU:OE1	2.52	0.43
7:U:146:GLU:N	7:U:146:GLU:OE2	2.51	0.43
10:V:175:LEU:HD23	10:V:175:LEU:HA	1.87	0.43
10:V:212:LEU:HD21	9:W:200:LYS:HZ3	1.82	0.43
4:D:21:LEU:HD23	4:D:21:LEU:HA	1.83	0.43
11:K:282:VAL:HG11	9:W:204:ASP:HB3	2.00	0.43
13:M:18:GLY:HA2	13:M:115:PHE:CE2	2.54	0.43
3:Q:157:LYS:HD2	3:Q:176:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:166:LYS:NZ	3:Q:166:LYS:HB3	2.32	0.43
13:a:227:VAL:HG22	13:a:232:VAL:HG22	2.01	0.43
1:A:22:ILE:HG21	1:A:152:SER:HB3	1.99	0.43
4:D:84:ASP:HB3	4:D:137:PHE:HD1	1.83	0.43
13:M:45:VAL:HB	13:M:49:THR:HB	2.00	0.43
2:B:136:TYR:HE1	2:B:150:SER:HB2	1.84	0.43
3:C:67:LEU:HD11	3:C:73:MET:SD	2.58	0.43
1:A:53:LYS:HD2	1:A:53:LYS:H	1.83	0.42
8:H:177:LYS:HE2	8:H:177:LYS:HB2	1.84	0.42
11:K:96:PHE:CE2	11:K:103:ILE:HD12	2.54	0.42
12:L:200:MET:HE1	12:Y:174:ASN:OD1	2.19	0.42
9:W:87:MET:HG3	9:W:121:CYS:SG	2.59	0.42
3:C:141:ASP:CG	3:C:142:GLY:N	2.76	0.42
5:E:107:ARG:HH12	13:M:74:GLU:CD	2.26	0.42
5:S:177:ASP:OD2	5:S:177:ASP:N	2.51	0.42
7:U:196:GLU:OE1	7:U:242:LEU:HB2	2.18	0.42
12:Y:29:LYS:HG3	12:Y:30:HIS:O	2.19	0.42
14:b:224:LYS:NZ	14:b:224:LYS:HB3	2.32	0.42
4:R:98:ASN:O	4:R:102:THR:HG22	2.19	0.42
13:a:124:HIS:NE2	13:a:166:ALA:HB1	2.34	0.42
1:A:184:LEU:HD12	1:A:184:LEU:HA	1.90	0.42
2:B:231:LYS:NZ	2:B:231:LYS:HB2	2.33	0.42
12:L:192:GLU:HB2	12:L:208:PHE:CD2	2.55	0.42
12:Y:53:THR:HG22	12:Y:100:VAL:HG12	2.00	0.42
7:U:71:ARG:HH22	7:U:74:ASP:HA	1.84	0.42
7:G:115:CYS:SG	7:G:152:TYR:HB3	2.60	0.42
11:K:97:LYS:HD2	11:K:199:PRO:HB2	2.00	0.42
1:O:23:TYR:CD1	7:U:18:PRO:HA	2.55	0.42
1:O:90:ARG:HB3	10:V:65:LEU:HD21	2.02	0.42
2:P:241:GLU:OE1	2:P:241:GLU:HA	2.19	0.42
4:R:196:LYS:O	4:R:200:THR:HG23	2.19	0.42
10:V:15:GLY:HA2	10:V:174:ASP:O	2.20	0.42
3:C:178:TYR:O	3:C:178:TYR:CG	2.72	0.42
5:E:182:CYS:SG	5:E:186:ASP:HB2	2.59	0.42
4:R:133:MET:HE3	4:R:133:MET:HA	2.01	0.42
5:S:84:LEU:O	5:S:88:MET:HG3	2.20	0.42
4:D:235:GLU:HA	4:D:235:GLU:OE2	2.20	0.42
9:W:143:GLU:OE2	9:W:143:GLU:HA	2.20	0.42
11:Z:105:ILE:HG23	11:Z:128:ALA:HA	2.01	0.42
3:C:6:ASP:HA	3:C:124:ASN:HB3	2.01	0.42
2:P:8:ARG:HH12	3:Q:5:ARG:CZ	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:38:LEU:HD11	12:Y:44:LEU:HD12	2.02	0.42
12:Y:103:LEU:HD23	12:Y:115:LEU:HD21	2.02	0.42
11:Z:215:LEU:HD22	11:Z:219:GLU:HB2	2.02	0.42
1:A:102:GLN:HE22	10:J:100:GLN:CD	2.27	0.42
10:J:40:ARG:HD3	10:J:92:ALA:CB	2.50	0.42
5:S:103:LEU:HD23	5:S:108:LEU:HG	2.01	0.42
10:J:206:ILE:HG23	10:J:213:GLY:HA2	2.02	0.41
12:L:1:MET:N	12:L:134:TYR:HD1	2.18	0.41
7:U:141:ILE:HD11	7:U:227:PHE:CE1	2.51	0.41
9:W:27:PHE:HB3	9:W:35:THR:HG22	2.02	0.41
13:a:105:MET:HE2	13:a:105:MET:HB3	1.88	0.41
2:B:12:PHE:CE2	3:C:127:ARG:HD2	2.55	0.41
4:D:117:SER:HB3	5:E:82:ARG:NH2	2.35	0.41
8:H:98:PHE:O	8:H:102:GLU:HG3	2.20	0.41
11:K:94:LEU:HD11	11:K:229:VAL:HG21	2.01	0.41
11:K:136:ALA:HB3	11:K:218:VAL:HG13	2.02	0.41
11:K:223:MET:H	11:K:223:MET:HG2	1.63	0.41
12:L:13:VAL:HG11	12:L:105:ALA:HB1	2.02	0.41
6:T:27:MET:SD	6:T:153:PRO:HG2	2.60	0.41
11:K:93:THR:HG22	11:K:106:VAL:HG12	2.01	0.41
7:U:145:GLU:OE1	7:U:145:GLU:HA	2.21	0.41
9:I:134:ASP:OD2	9:I:134:ASP:N	2.54	0.41
2:P:53:HIS:HB3	2:P:56:LEU:HD12	2.01	0.41
3:Q:4:ASP:HB3	4:R:126:GLU:HA	2.02	0.41
9:W:74:GLU:OE1	9:W:74:GLU:HA	2.19	0.41
1:A:51:LYS:HE2	1:A:51:LYS:HB2	1.94	0.41
2:B:231:LYS:O	2:B:235:GLU:HG2	2.21	0.41
6:F:40:ARG:HB2	6:F:45:VAL:HG12	2.02	0.41
11:K:91:THR:HG22	11:K:123:LYS:NZ	2.35	0.41
3:Q:180:ALA:O	3:Q:186:GLU:HB3	2.20	0.41
4:D:196:LYS:HG3	4:D:241:ILE:HG21	2.02	0.41
4:D:229:TYR:HB3	4:D:234:LEU:HG	2.02	0.41
9:I:32:GLN:HG3	11:Z:202:TYR:OH	2.20	0.41
13:M:148:PRO:HG2	10:V:133:ALA:HA	2.02	0.41
6:T:187:ARG:O	6:T:190:VAL:HG22	2.21	0.41
7:U:231:THR:HG23	7:U:233:THR:H	1.85	0.41
9:W:187:HIS:CD2	9:W:196:THR:HB	2.55	0.41
12:Y:103:LEU:HD12	12:Y:132:HIS:HD2	1.86	0.41
14:b:168:MET:HE2	14:b:168:MET:HB3	1.77	0.41
1:A:24:TYR:CD1	7:G:18:PRO:HA	2.56	0.41
3:C:183:ILE:HD12	3:C:183:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:GLU:OE2	4:D:44:GLU:N	2.53	0.41
5:E:40:SER:HB2	5:E:187:LEU:HD11	2.03	0.41
13:M:43:MET:HE2	13:M:43:MET:HB3	1.90	0.41
13:a:42:THR:HA	13:a:90:GLY:O	2.21	0.41
13:a:127:LEU:HD23	13:a:147:ILE:HD11	2.01	0.41
8:H:110:GLU:CD	8:H:110:GLU:H	2.28	0.41
11:K:183:MET:HE3	14:N:124:ARG:NH1	2.36	0.41
4:R:236:ASP:OD1	4:R:236:ASP:N	2.52	0.41
11:Z:216:THR:HB	11:Z:219:GLU:HG2	2.03	0.41
2:B:241:GLU:CD	2:B:241:GLU:H	2.29	0.41
4:D:210:LEU:HG	4:D:238:ILE:HD11	2.03	0.41
7:G:170:VAL:HG13	7:G:171:LYS:HG2	2.03	0.41
1:O:67:ILE:HD13	1:O:73:MET:HG3	2.03	0.41
4:R:21:LEU:O	4:R:25:GLU:HG3	2.21	0.41
4:R:78:MET:HE3	4:R:78:MET:HB2	1.91	0.41
4:R:209:LYS:HE2	4:R:209:LYS:HA	2.03	0.41
12:Y:193:LYS:HE3	12:Y:209:TYR:HE2	1.86	0.41
3:C:62:ARG:HH11	3:C:62:ARG:HG2	1.86	0.41
5:E:146:GLN:O	5:E:153:TYR:HA	2.21	0.41
5:E:214:ILE:HD12	5:E:224:TYR:HE2	1.86	0.41
6:F:65:ARG:HH21	6:F:78:ALA:HA	1.86	0.41
6:F:195:LYS:HB3	6:F:195:LYS:HE2	1.86	0.41
8:H:152:MET:HE3	8:H:152:MET:HB3	1.89	0.41
6:T:150:MET:HE2	6:T:150:MET:HB3	1.86	0.41
8:X:214:GLU:OE1	8:X:214:GLU:N	2.53	0.41
2:B:72:MET:HE2	2:B:72:MET:HB3	1.79	0.40
4:D:69:GLU:HB2	4:D:226:PHE:CD2	2.56	0.40
12:L:25:ILE:HA	12:Y:172:ILE:HD11	2.02	0.40
13:M:27:LEU:HD11	13:M:34:ALA:HB1	2.03	0.40
1:O:101:GLN:HG3	9:W:88:SER:OG	2.22	0.40
1:O:129:PHE:O	1:O:150:PRO:HB3	2.21	0.40
7:U:80:MET:HE2	7:U:80:MET:HB3	1.87	0.40
1:A:75:VAL:HG12	1:A:135:LEU:HB2	2.03	0.40
7:G:184:LYS:HE3	7:G:184:LYS:HB3	1.90	0.40
7:G:202:LEU:HB3	7:G:210:PHE:CE1	2.54	0.40
9:I:11:MET:HE3	9:I:170:MET:HG2	2.02	0.40
10:V:3:ILE:HD12	10:V:46:ALA:HB2	2.02	0.40
14:b:52:ARG:HH22	14:b:237:ASP:C	2.30	0.40
6:F:37:ILE:HG23	6:F:176:ILE:HD11	2.03	0.40
7:G:29:PHE:CE1	7:G:156:PRO:HD2	2.56	0.40
10:J:40:ARG:HH11	10:J:92:ALA:HB1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:261:LEU:HD12	11:Z:261:LEU:HA	1.89	0.40
4:D:20:ARG:HB3	4:D:25:GLU:OE2	2.21	0.40
4:R:44:GLU:OE2	4:R:190:THR:HA	2.21	0.40
1:A:57:TYR:HE2	7:G:161:CYS:HB3	1.87	0.40
6:F:37:ILE:HD12	6:F:197:ILE:HG13	2.04	0.40
3:Q:173:GLU:CD	4:R:57:PRO:HD2	2.47	0.40
11:Z:247:VAL:HA	11:Z:252:TRP:HA	2.03	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	A	226/234 (97%)	219 (97%)	6 (3%)	1 (0%)	30	59
1	O	226/234 (97%)	222 (98%)	4 (2%)	0	100	100
2	B	245/261 (94%)	236 (96%)	9 (4%)	0	100	100
2	P	244/261 (94%)	230 (94%)	14 (6%)	0	100	100
3	C	226/251 (90%)	214 (95%)	11 (5%)	1 (0%)	30	59
3	Q	229/251 (91%)	218 (95%)	10 (4%)	1 (0%)	30	59
4	D	233/241 (97%)	228 (98%)	5 (2%)	0	100	100
4	R	233/241 (97%)	221 (95%)	10 (4%)	2 (1%)	14	42
5	E	224/263 (85%)	213 (95%)	10 (4%)	1 (0%)	30	59
5	S	224/263 (85%)	213 (95%)	10 (4%)	1 (0%)	30	59
6	F	238/255 (93%)	232 (98%)	4 (2%)	2 (1%)	16	44
6	T	237/255 (93%)	232 (98%)	5 (2%)	0	100	100
7	G	239/246 (97%)	231 (97%)	8 (3%)	0	100	100
7	U	231/246 (94%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	197/233 (84%)	194 (98%)	3 (2%)	0	100	100
8	X	197/233 (84%)	194 (98%)	3 (2%)	0	100	100
9	I	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
9	W	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
10	J	222/277 (80%)	213 (96%)	9 (4%)	0	100	100
10	V	219/277 (79%)	210 (96%)	9 (4%)	0	100	100
11	K	198/293 (68%)	192 (97%)	6 (3%)	0	100	100
11	Z	198/293 (68%)	191 (96%)	7 (4%)	0	100	100
12	L	207/212 (98%)	202 (98%)	5 (2%)	0	100	100
12	Y	207/212 (98%)	200 (97%)	7 (3%)	0	100	100
13	M	213/254 (84%)	208 (98%)	5 (2%)	0	100	100
13	a	212/254 (84%)	209 (99%)	3 (1%)	0	100	100
14	N	210/237 (89%)	204 (97%)	6 (3%)	0	100	100
14	b	210/237 (89%)	207 (99%)	2 (1%)	1 (0%)	24	55
All	All	6149/6924 (89%)	5941 (97%)	198 (3%)	10 (0%)	44	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
3	Q	98	VAL
4	R	187	LYS
3	C	155	TYR
6	F	184	MET
5	S	236	LEU
14	b	215	ASP
5	E	203	GLN
6	F	183	ASP
4	R	56	SER

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	187/191 (98%)	183 (98%)	4 (2%)	47	66
1	O	187/191 (98%)	186 (100%)	1 (0%)	81	82
2	B	206/220 (94%)	204 (99%)	2 (1%)	68	75
2	P	205/220 (93%)	201 (98%)	4 (2%)	48	66
3	C	190/209 (91%)	183 (96%)	7 (4%)	30	55
3	Q	192/209 (92%)	183 (95%)	9 (5%)	23	51
4	D	198/204 (97%)	197 (100%)	1 (0%)	81	82
4	R	198/204 (97%)	193 (98%)	5 (2%)	42	63
5	E	195/222 (88%)	191 (98%)	4 (2%)	47	66
5	S	196/222 (88%)	195 (100%)	1 (0%)	81	82
6	F	199/213 (93%)	194 (98%)	5 (2%)	42	63
6	T	198/213 (93%)	195 (98%)	3 (2%)	57	71
7	G	207/212 (98%)	202 (98%)	5 (2%)	43	64
7	U	202/212 (95%)	197 (98%)	5 (2%)	42	63
8	H	157/185 (85%)	156 (99%)	1 (1%)	78	81
8	X	157/185 (85%)	154 (98%)	3 (2%)	50	67
9	I	175/176 (99%)	170 (97%)	5 (3%)	37	60
9	W	175/176 (99%)	170 (97%)	5 (3%)	37	60
10	J	180/223 (81%)	178 (99%)	2 (1%)	65	75
10	V	178/223 (80%)	175 (98%)	3 (2%)	53	69
11	K	160/235 (68%)	158 (99%)	2 (1%)	61	73
11	Z	160/235 (68%)	152 (95%)	8 (5%)	22	49
12	L	177/178 (99%)	171 (97%)	6 (3%)	32	57
12	Y	177/178 (99%)	170 (96%)	7 (4%)	28	54
13	M	180/213 (84%)	179 (99%)	1 (1%)	78	81
13	a	179/213 (84%)	176 (98%)	3 (2%)	53	69
14	N	175/196 (89%)	174 (99%)	1 (1%)	78	81
14	b	175/196 (89%)	172 (98%)	3 (2%)	53	69
All	All	5165/5754 (90%)	5059 (98%)	106 (2%)	46	66

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	133	SER
1	A	141	GLU
1	A	183	GLU
2	B	43	VAL
2	B	212	GLU
3	C	40	LYS
3	C	55	LEU
3	C	60	THR
3	C	67	LEU
3	C	93	CYS
3	C	105	THR
3	C	155	TYR
4	D	46	VAL
5	E	9	ASP
5	E	23	GLU
5	E	117	GLN
5	E	175	LEU
6	F	35	THR
6	F	53	VAL
6	F	144	ASP
6	F	200	VAL
6	F	233	GLU
7	G	14	THR
7	G	100	ASN
7	G	112	ASP
7	G	141	ILE
7	G	241	SER
8	H	152	MET
9	I	19	VAL
9	I	44	MET
9	I	57	THR
9	I	121	CYS
9	I	141	CYS
10	J	143	LEU
10	J	240	VAL
11	K	97	LYS
11	K	205	ASP
12	L	103	LEU
12	L	132	HIS
12	L	145	ARG
12	L	170	ARG
12	L	185	LYS

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Mol	Chain	Res	Type
12	L	200	MET
13	M	38	ASN
14	N	158	THR
1	O	178	ASN
2	P	43	VAL
2	P	101	TYR
2	P	127	LYS
2	P	162	THR
3	Q	41	VAL
3	Q	52	LYS
3	Q	58	THR
3	Q	77	THR
3	Q	93	SER
3	Q	104	VAL
3	Q	139	ASP
3	Q	177	THR
3	Q	204	LYS
4	R	56	SER
4	R	166	ASP
4	R	186	HIS
4	R	213	THR
4	R	231	LYS
5	S	45	VAL
6	T	17	ASP
6	T	33	SER
6	T	139	SER
7	U	46	ASP
7	U	65	THR
7	U	226	TRP
7	U	233	THR
7	U	234	GLU
10	V	24	MET
10	V	118	SER
10	V	201	ASP
9	W	57	THR
9	W	92	ASN
9	W	98	ARG
9	W	136	VAL
9	W	149	CYS
8	X	101	ILE
8	X	166	SER
8	X	184	GLU

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Mol	Chain	Res	Type
12	Y	19	ASN
12	Y	27	GLN
12	Y	28	MET
12	Y	40	GLU
12	Y	49	GLU
12	Y	145	ARG
12	Y	209	TYR
11	Z	113	MET
11	Z	149	LYS
11	Z	161	MET
11	Z	168	MET
11	Z	190	CYS
11	Z	211	VAL
11	Z	216	THR
11	Z	248	HIS
13	a	89	SER
13	a	176	PHE
13	a	199	GLU
14	b	42	ASP
14	b	108	THR
14	b	157	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	96	GLN
1	A	102	GLN
1	A	109	GLN
2	B	40	ASN
2	B	109	GLN
2	B	146	GLN
2	B	198	ASN
3	C	122	GLN
3	C	124	ASN
3	C	207	ASN
4	D	97	GLN
5	E	59	HIS
5	E	117	GLN
5	E	121	GLN
5	E	203	GLN
7	G	127	GLN

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Mol	Chain	Res	Type
12	L	19	ASN
12	L	101	ASN
14	N	155	GLN
14	N	181	ASN
1	O	94	GLN
1	O	101	GLN
2	P	20	GLN
2	P	102	GLN
4	R	99	HIS
4	R	214	ASN
5	S	146	GLN
6	T	201	HIS
7	U	34	GLN
10	V	30	ASN
10	V	57	GLN
10	V	156	HIS
10	V	189	HIS
9	W	172	ASN
9	W	187	HIS
8	X	143	GLN
12	Y	19	ASN
12	Y	82	ASN
12	Y	101	ASN
12	Y	132	HIS
11	Z	97	GLN
13	a	243	ASN
13	a	248	HIS
14	b	32	ASN
14	b	155	GLN
14	b	181	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

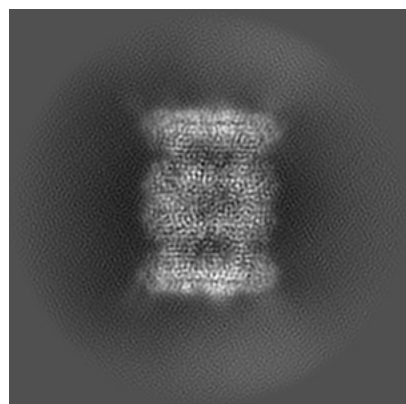
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66543. These allow visual inspection of the internal detail of the map and identification of artifacts.

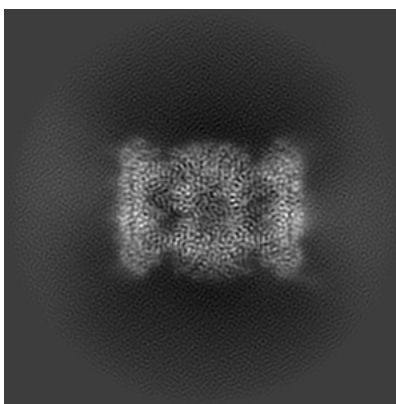
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

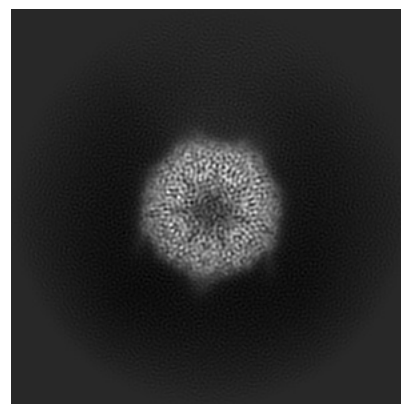
6.1.1 Primary map



X

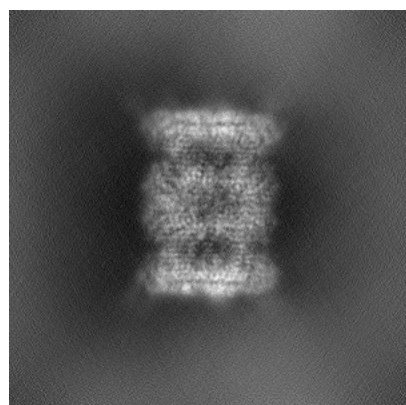


Y

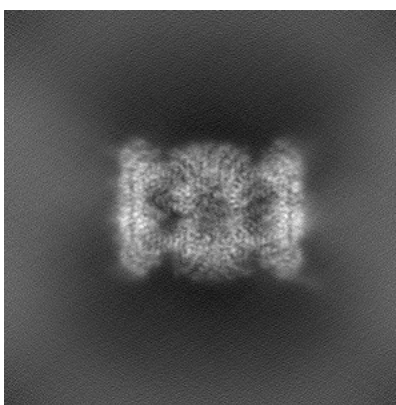


Z

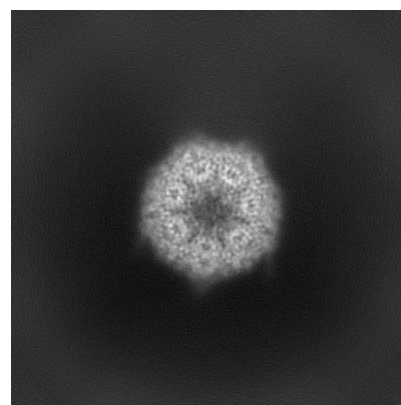
6.1.2 Raw map



X



Y

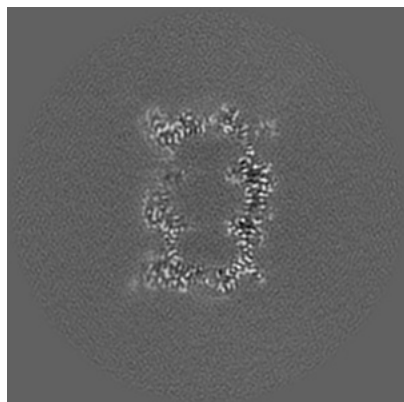


Z

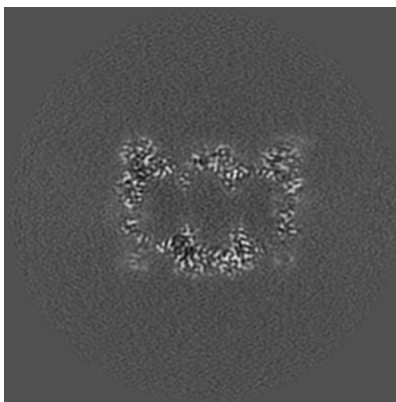
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

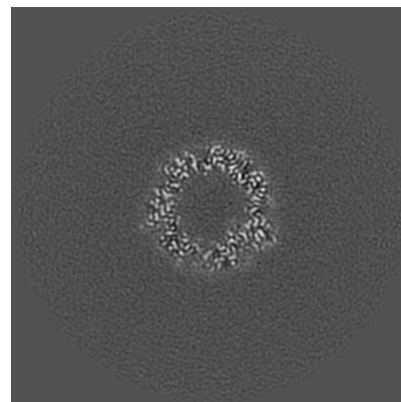
6.2.1 Primary map



X Index: 200

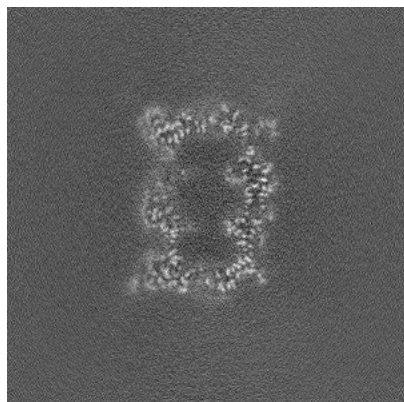


Y Index: 200

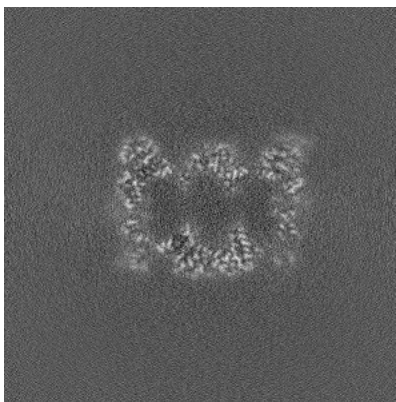


Z Index: 200

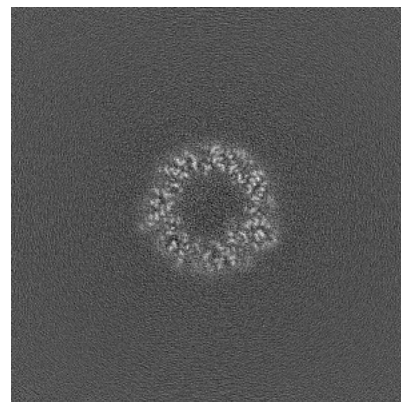
6.2.2 Raw map



X Index: 200



Y Index: 200

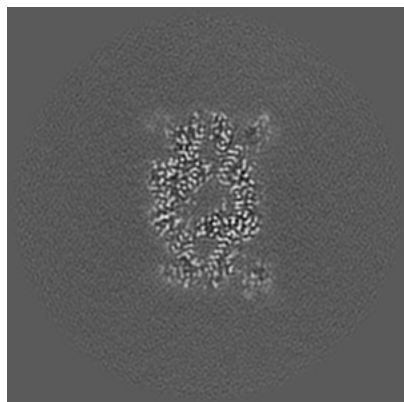


Z Index: 200

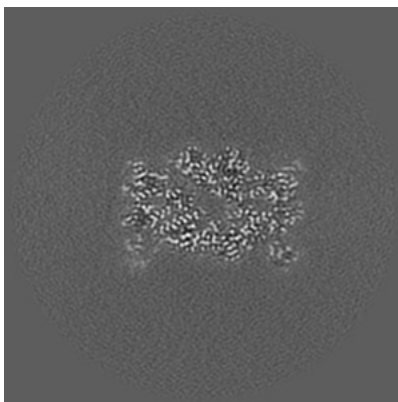
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

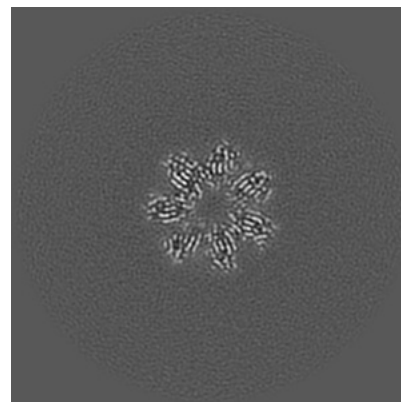
6.3.1 Primary map



X Index: 170

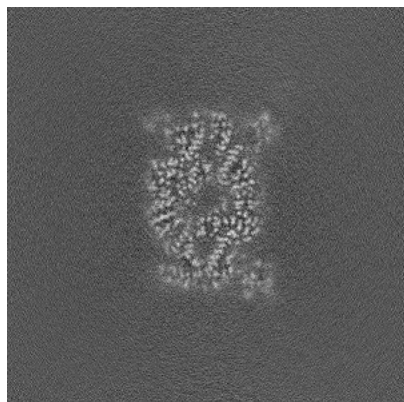


Y Index: 232

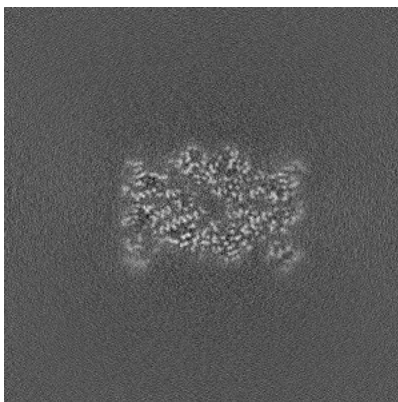


Z Index: 183

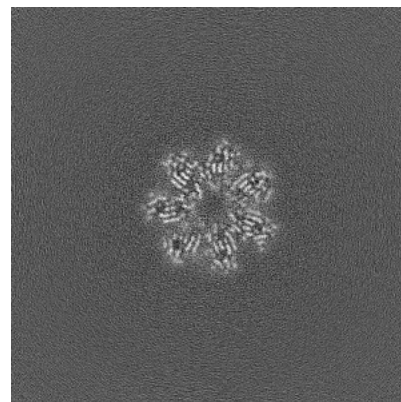
6.3.2 Raw map



X Index: 170



Y Index: 232

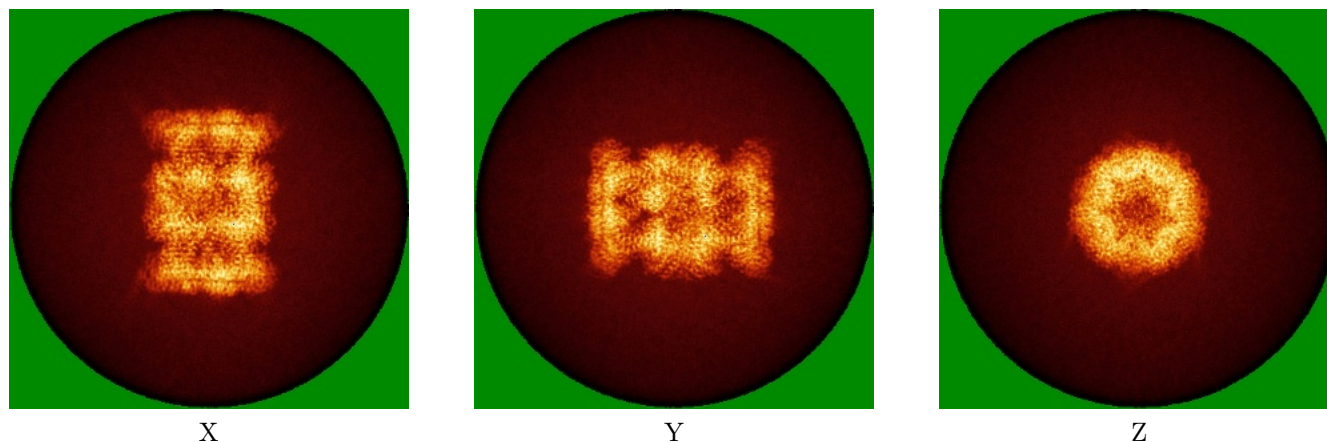


Z Index: 183

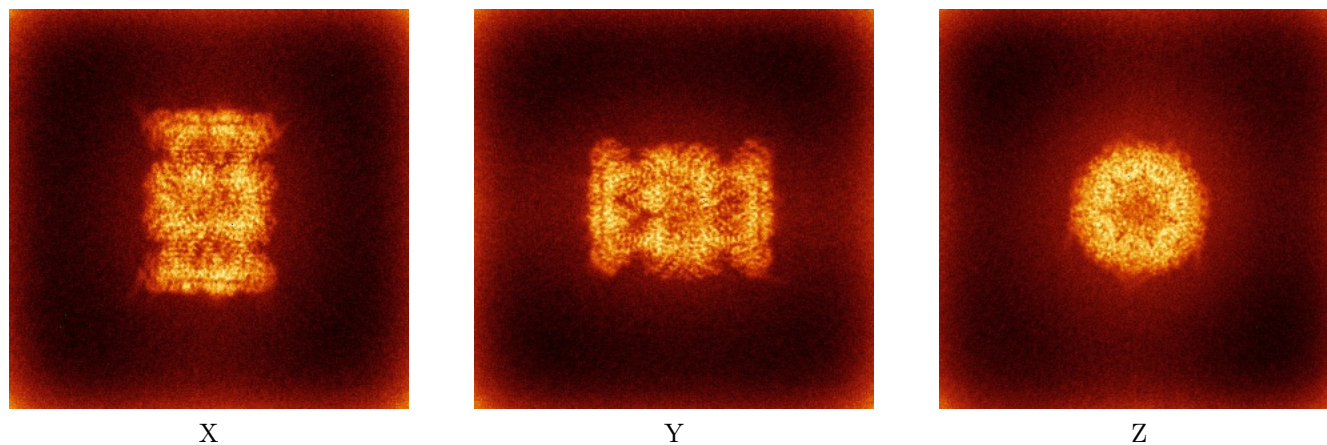
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



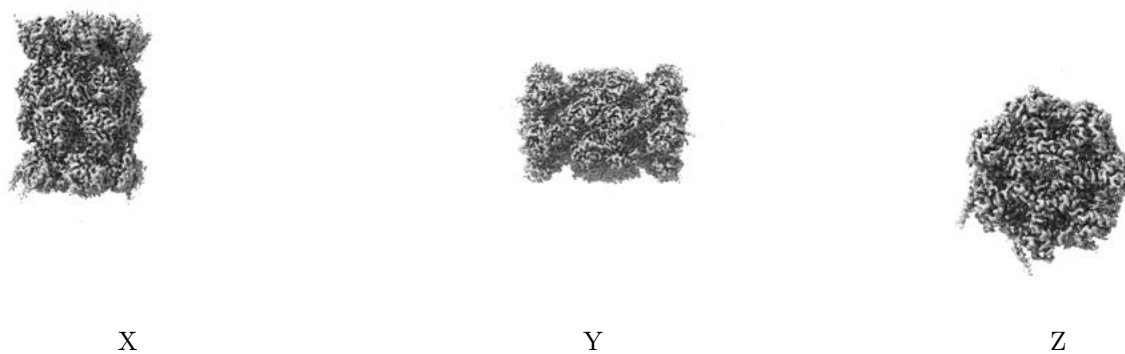
6.4.2 Raw map



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.

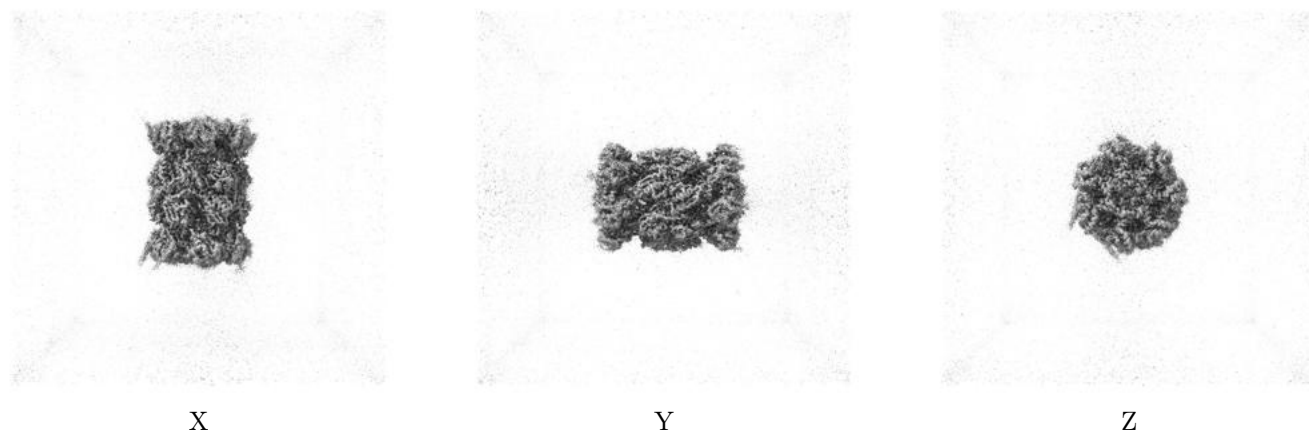
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. 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.

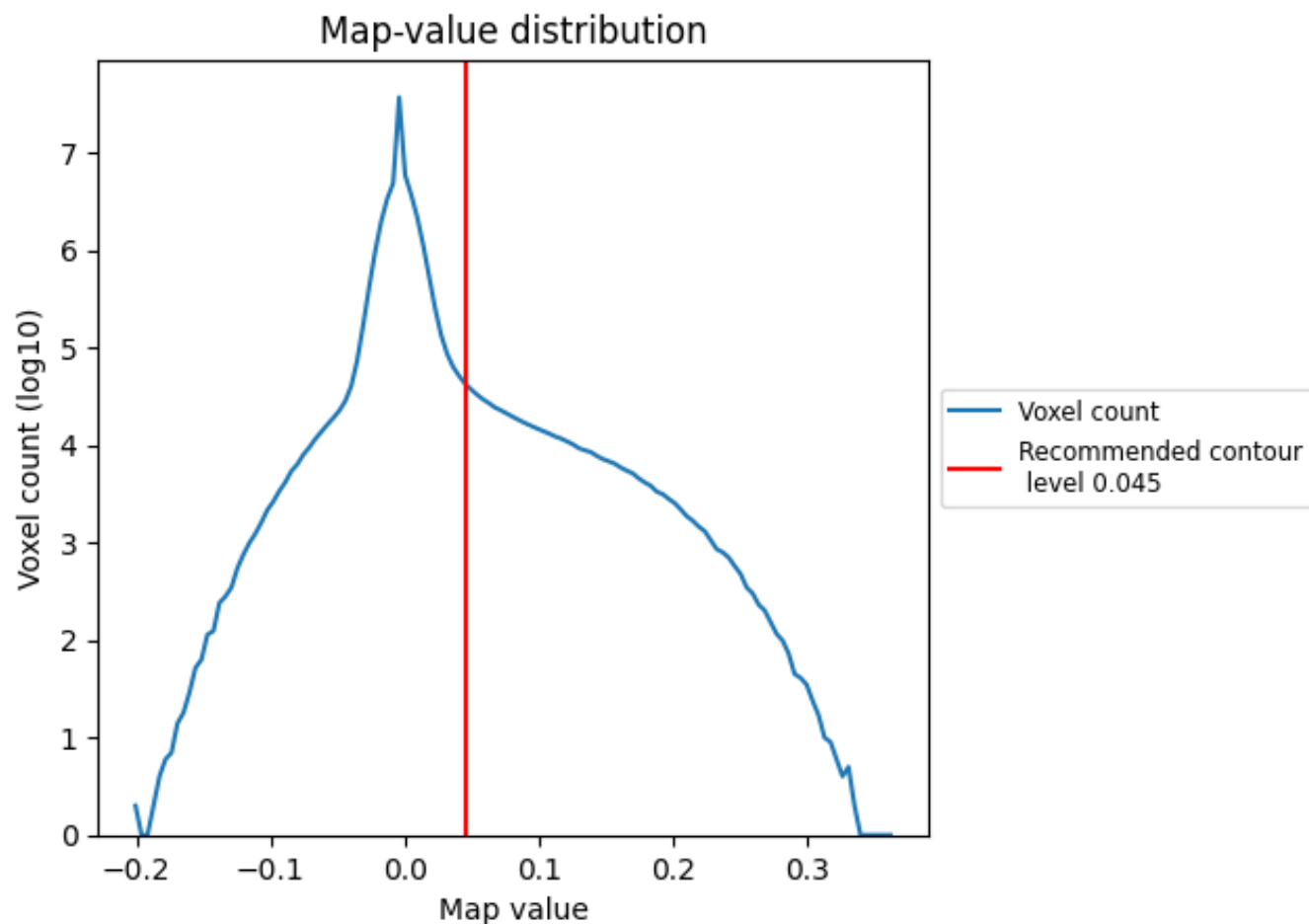
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

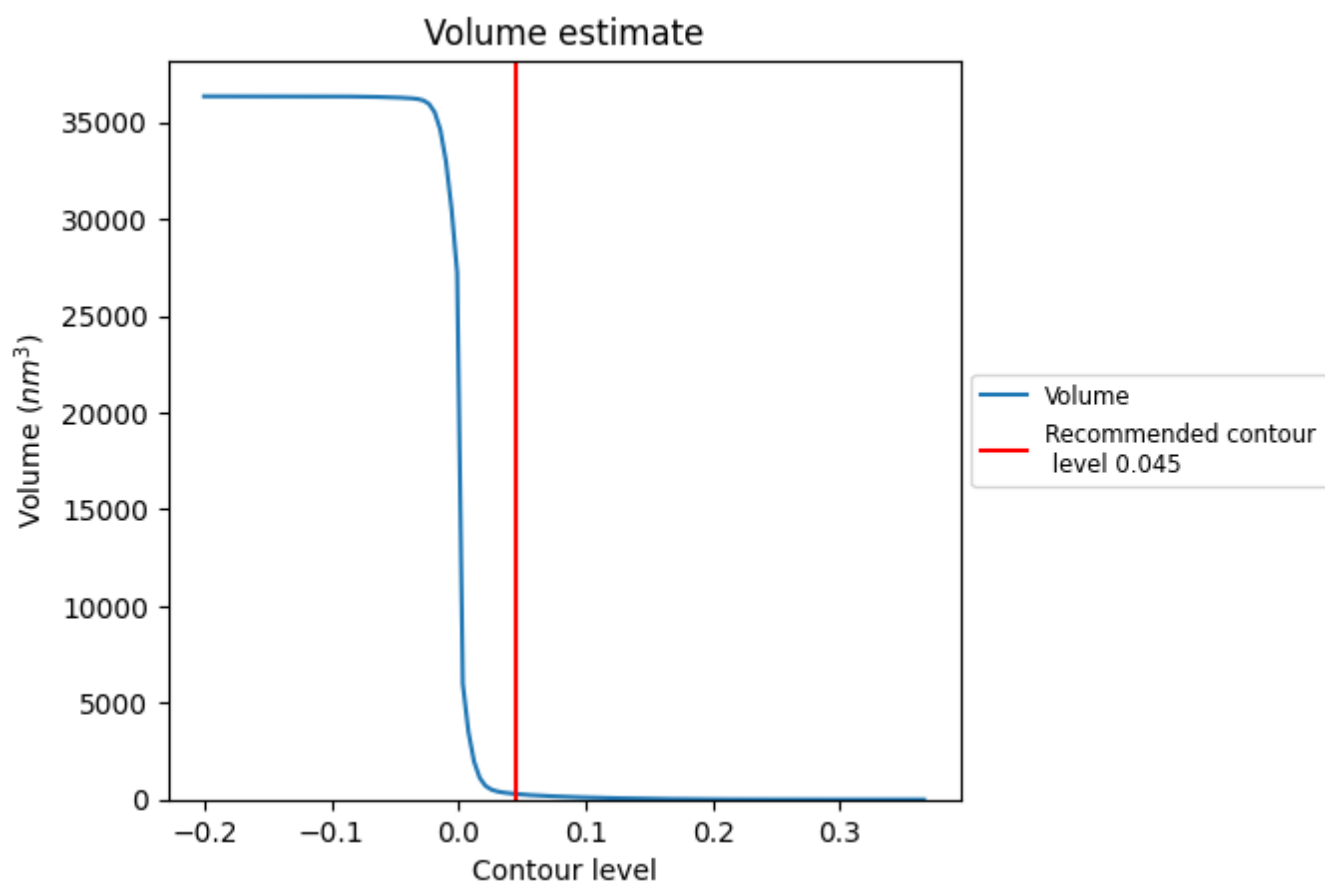
This section contains the results of statistical analysis of the map.

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.

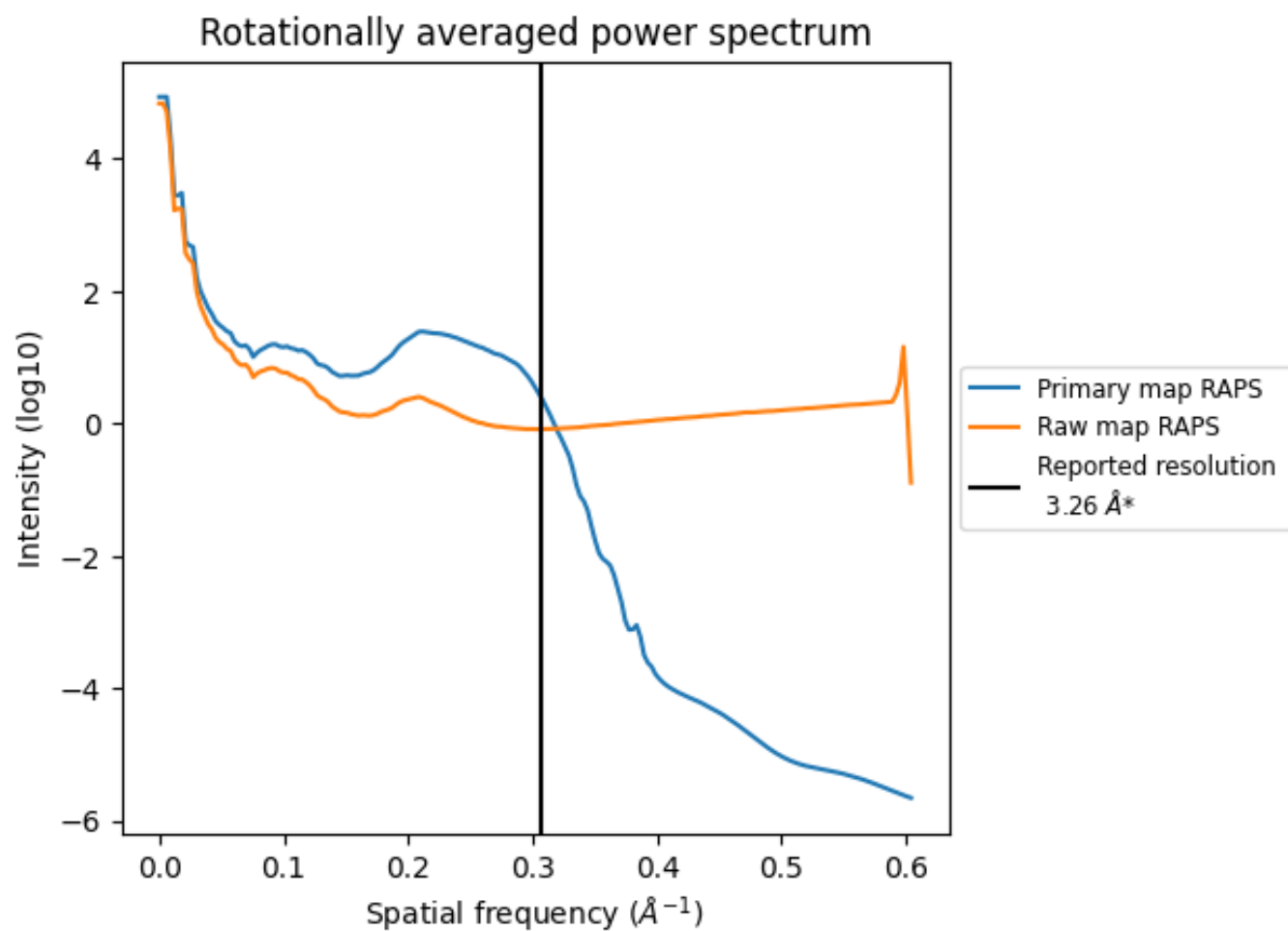
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287 nm³; this corresponds to an approximate mass of 259 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 ⓘ

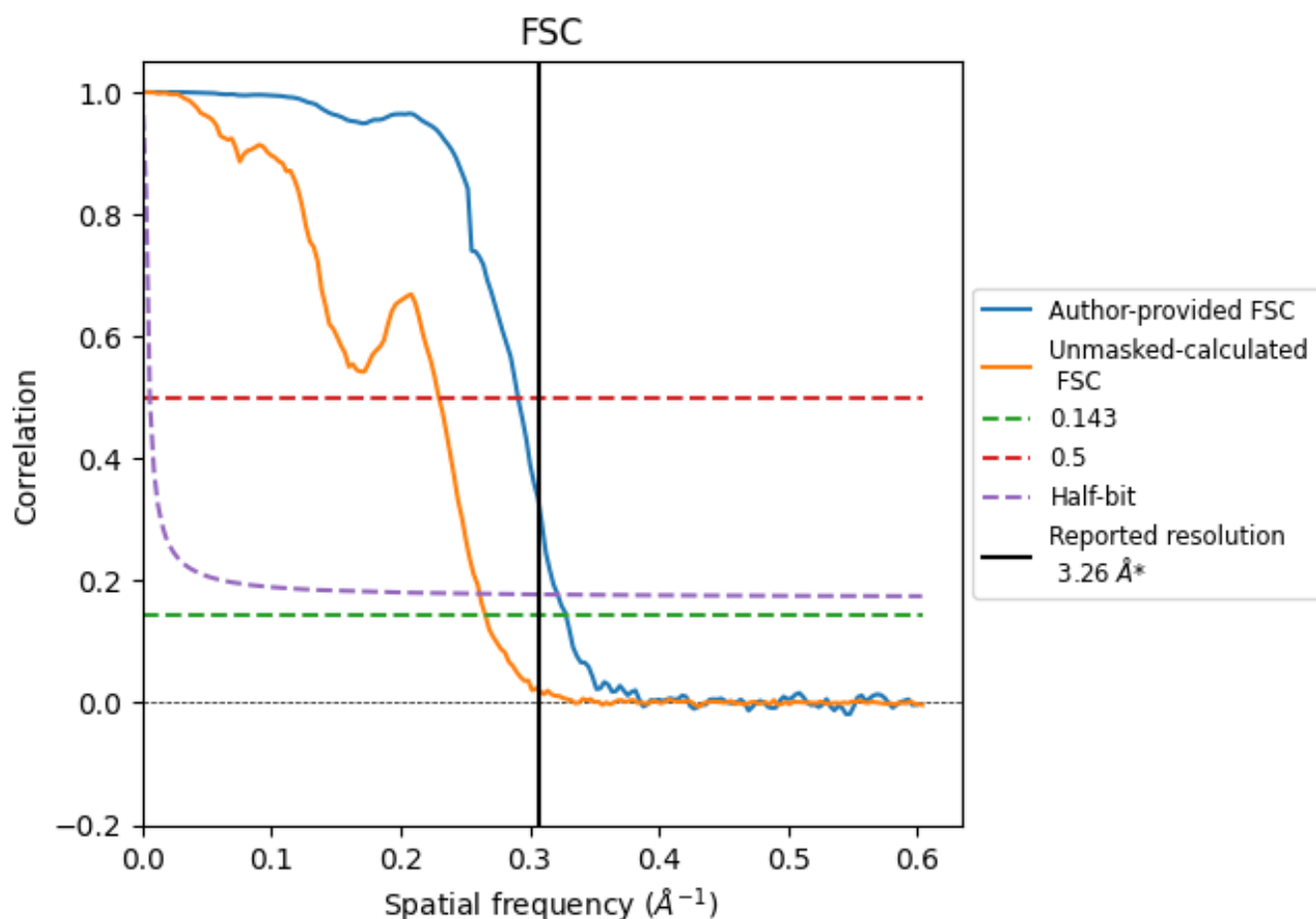


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

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 0.307 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

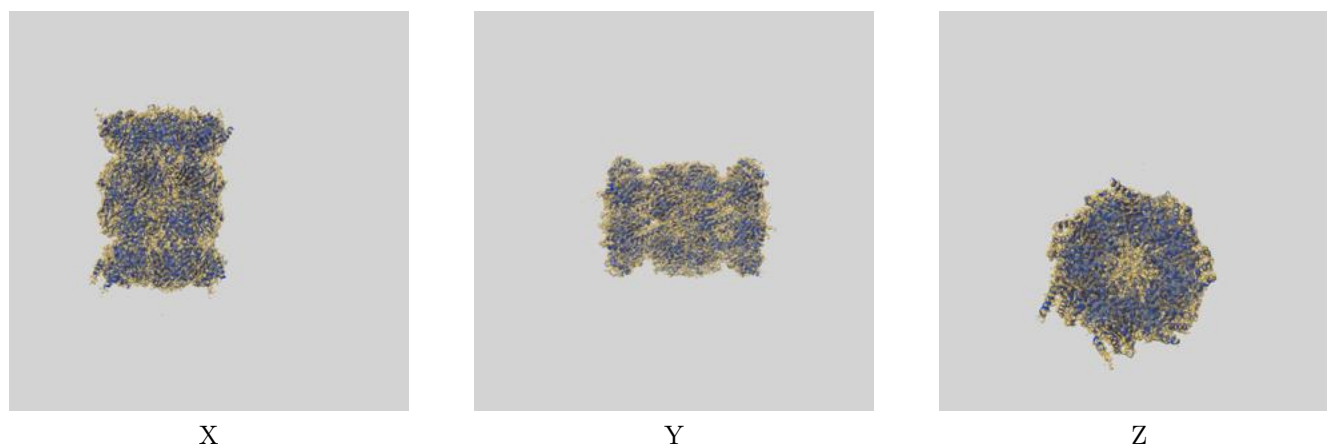
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.05	3.44	3.11
Unmasked-calculated*	3.76	4.36	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

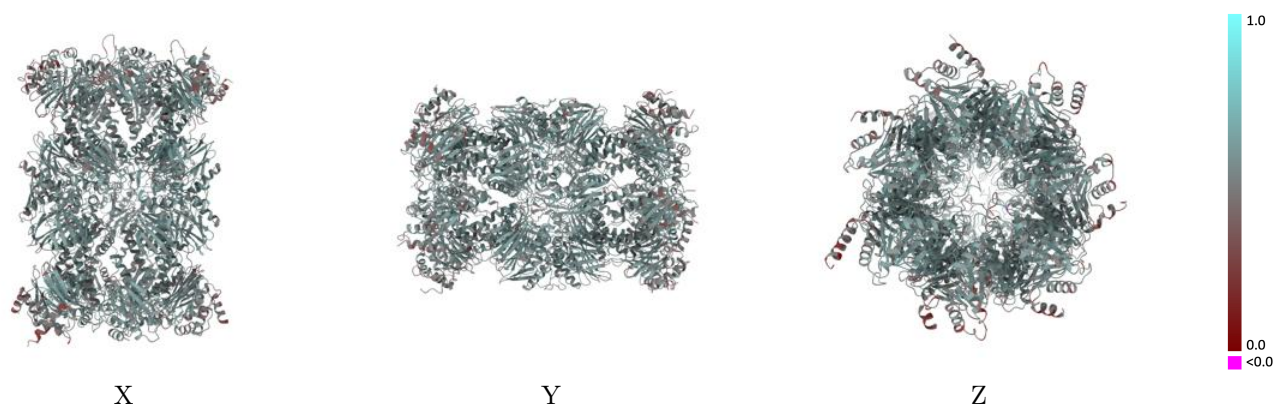
This section contains information regarding the fit between EMDB map EMD-66543 and PDB model 9X4E. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



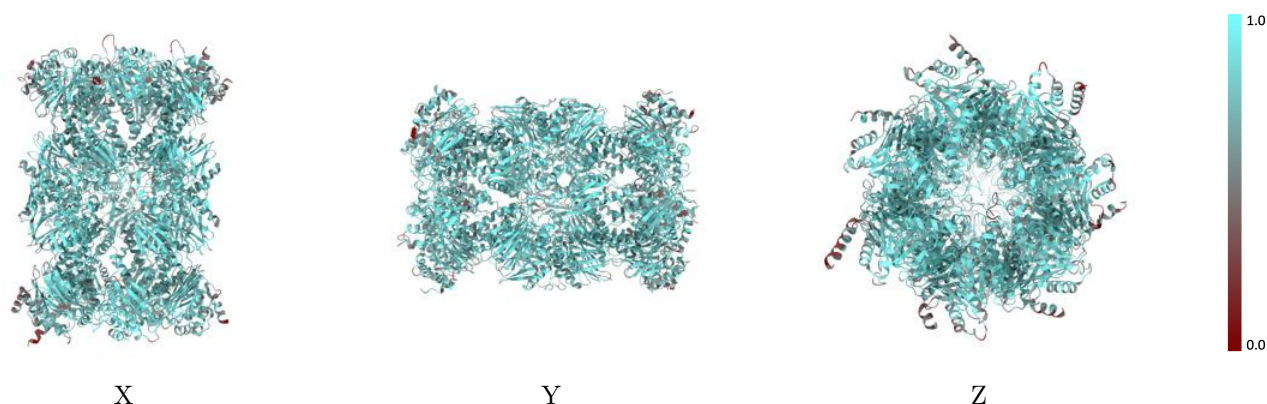
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



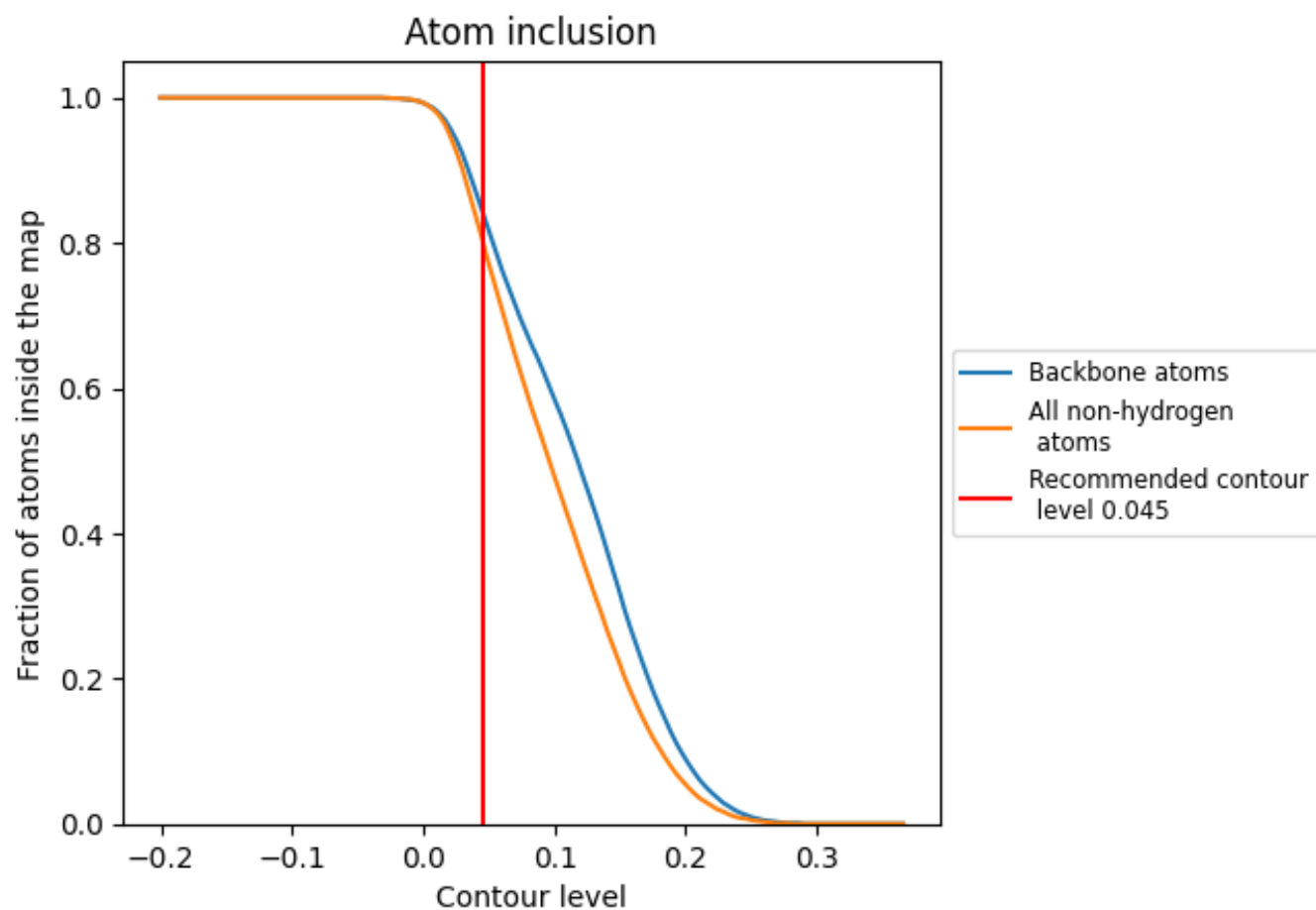
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.5380
A	 0.8050	 0.5380
B	 0.7680	 0.5280
C	 0.7420	 0.4940
D	 0.7410	 0.5160
E	 0.7720	 0.5170
F	 0.7850	 0.5300
G	 0.7710	 0.5250
H	 0.8510	 0.5650
I	 0.8430	 0.5630
J	 0.8380	 0.5580
K	 0.8100	 0.5380
L	 0.7980	 0.5490
M	 0.8520	 0.5670
N	 0.8220	 0.5500
O	 0.8330	 0.5470
P	 0.7830	 0.5230
Q	 0.7480	 0.4990
R	 0.7740	 0.5190
S	 0.8030	 0.5130
T	 0.8020	 0.5340
U	 0.7850	 0.5280
V	 0.8310	 0.5570
W	 0.8470	 0.5580
X	 0.8580	 0.5690
Y	 0.8140	 0.5430
Z	 0.8120	 0.5370
a	 0.8570	 0.5690
b	 0.8340	 0.5550

