



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:14 AM UTC

PDB ID : 6R70 / pdb_00006r70
EMDB ID : EMD-4738
Title : Endogeneous native human 20S proteasome
Authors : Schmidli, C.; Albiez, S.; Rima, L.; Righetto, R.; Mohammed, I.; Oliva, P.; Kovacik, L.; Stahlberg, H.; Braun, T.
Deposited on : 2019-03-28
Resolution : 3.50 Å(reported)
Based on initial model : 5LE5

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

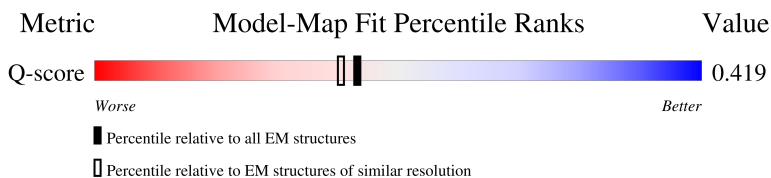
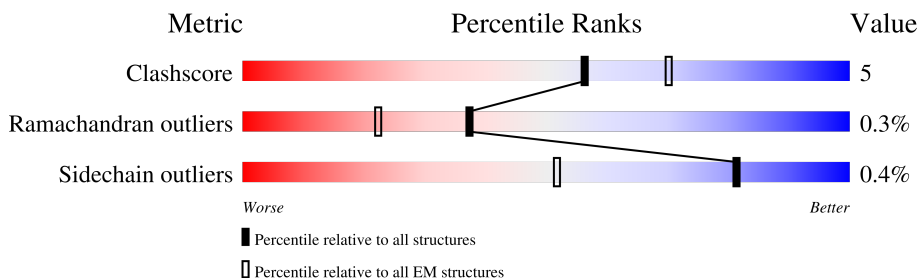
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	M	216	
1	a	216	
2	A	230	
2	O	230	

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Mol	Chain	Length	Quality of chain
3	B	248	
3	P	248	
4	C	237	
4	Q	237	
5	D	233	
5	R	233	
6	E	238	
6	S	238	
7	F	240	
7	T	240	
8	G	244	
8	U	244	
9	H	220	
9	V	220	
10	I	204	
10	W	204	
11	J	196	
11	X	196	
12	K	201	
12	Y	201	
13	L	213	
13	Z	213	
14	N	203	
14	b	203	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 48581 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-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		
1	a	216	Total	C	N	O	S	1	0
			1692	1067	291	322	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	230	Total	C	N	O	S	2	0
			1811	1158	308	339	6		
2	O	230	Total	C	N	O	S	0	0
			1798	1150	305	337	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	248	Total	C	N	O	S	1	0
			1958	1238	336	373	11		
3	P	247	Total	C	N	O	S	2	0
			1950	1234	332	373	11		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	236	Total	C	N	O	S	0	0
			1864	1171	330	359	4		
4	Q	231	Total	C	N	O	S	0	0
			1832	1153	323	352	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	233	Total	C	N	O	S	2	0
			1791	1124	296	360	11		
5	R	233	Total	C	N	O	S	1	0
			1783	1119	295	358	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	233	Total	C	N	O	S	0	0
			1831	1148	328	345	10		
6	S	237	Total	C	N	O	S	3	0
			1888	1184	341	353	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	239	Total	C	N	O	S	4	0
			1894	1202	323	357	12		
7	T	240	Total	C	N	O	S	1	0
			1884	1195	321	356	12		

- Molecule 8 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	241	Total	C	N	O	S	2	0
			1892	1203	317	362	10		
8	U	232	Total	C	N	O	S	0	0
			1798	1138	304	346	10		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	220	Total	C	N	O	S	2	0
			1672	1053	286	320	13		
9	V	220	Total	C	N	O	S	2	0
			1669	1051	283	322	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	204	Total	C	N	O	S	6	0
			1633	1039	274	301	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	204	Total	C	N	O	S	2	0
			1608	1024	270	295	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	195	Total	C	N	O	S	2	0
			1580	1013	269	289	9		
11	X	195	Total	C	N	O	S	2	0
			1575	1010	268	288	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
12	Y	199	Total	C	N	O	S	3	0
			1570	991	278	291	10		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	213	Total	C	N	O	S	2	0
			1660	1051	284	314	11		
13	Z	213	Total	C	N	O	S	1	0
			1657	1049	284	313	11		

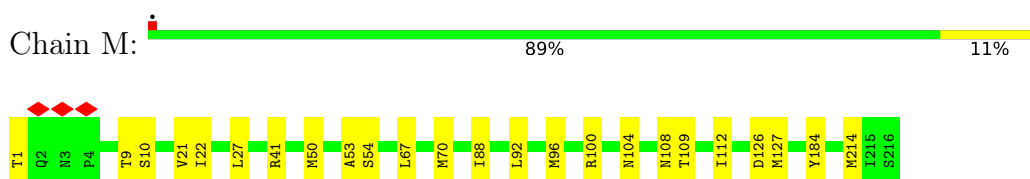
- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	1	0
			1519	953	258	295	13		
14	b	203	Total	C	N	O	S	1	0
			1526	958	259	296	13		

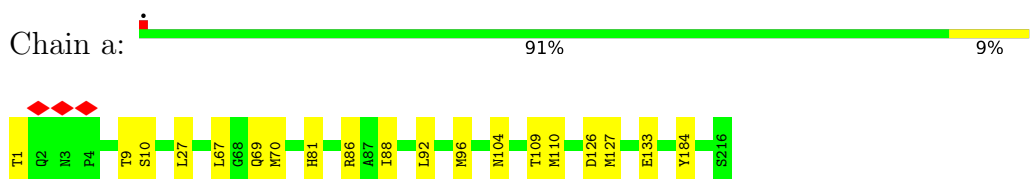
3 Residue-property plots

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.

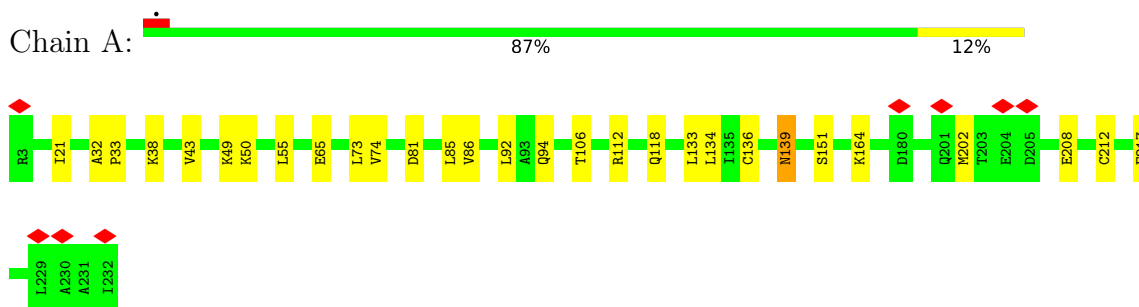
- Molecule 1: Proteasome subunit beta type-4



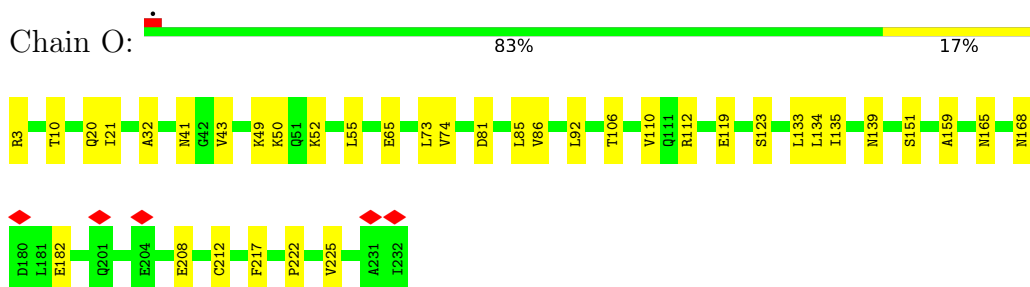
- Molecule 1: Proteasome subunit beta type-4



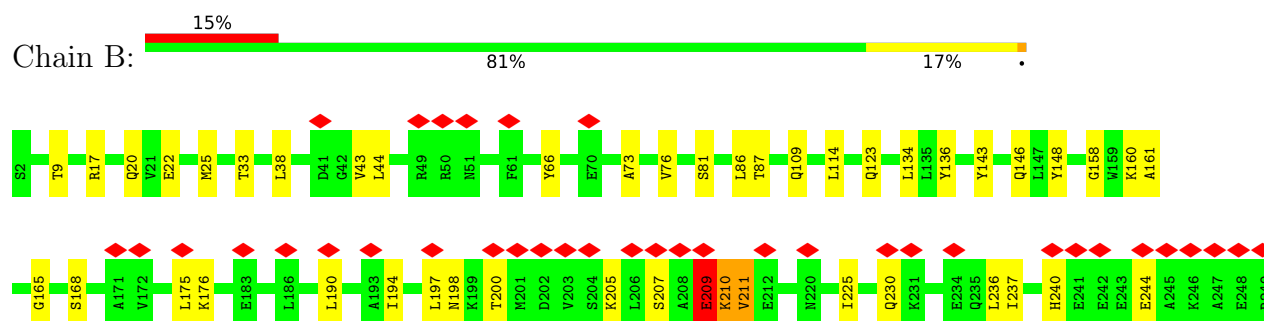
- Molecule 2: Proteasome subunit alpha type-2



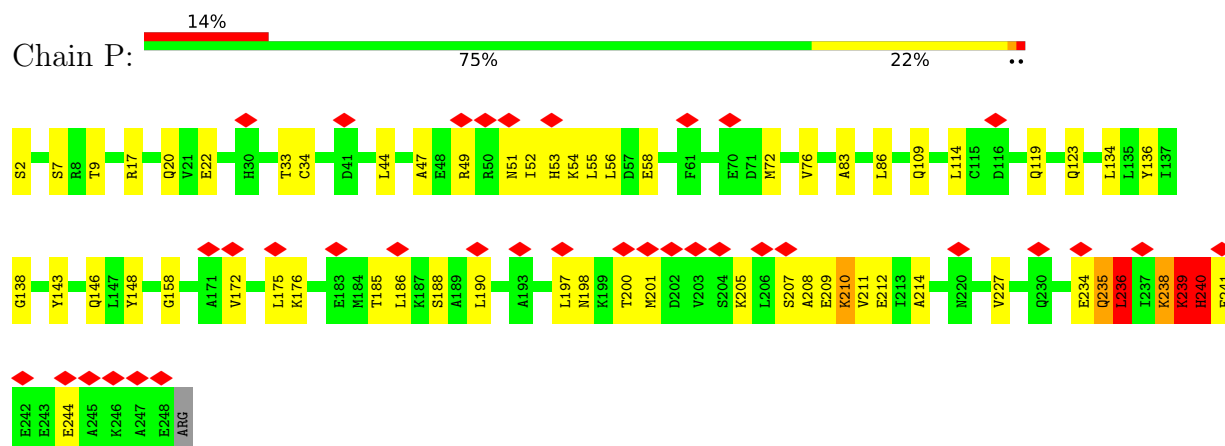
- Molecule 2: Proteasome subunit alpha type-2



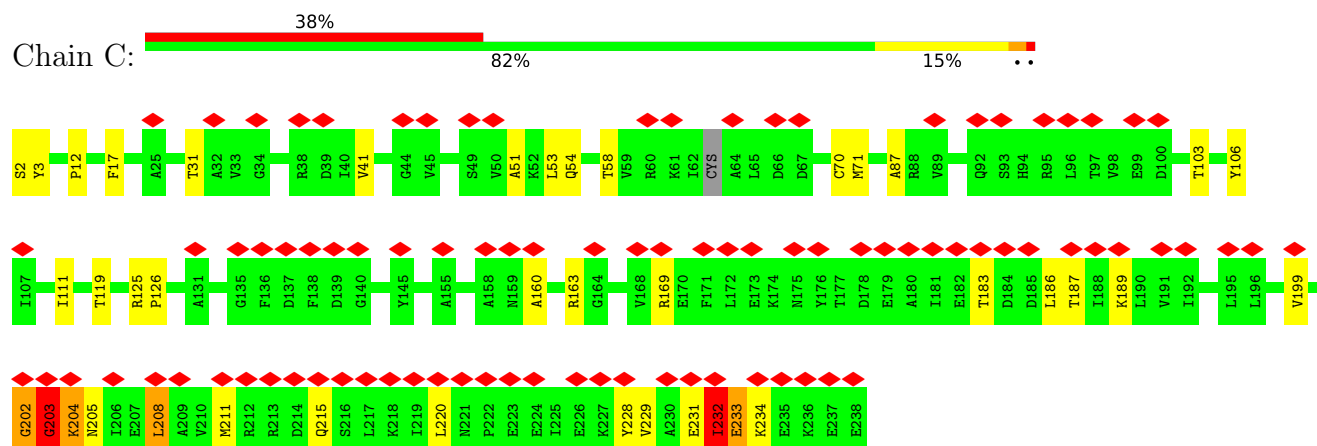
- Molecule 3: Proteasome subunit alpha type-4



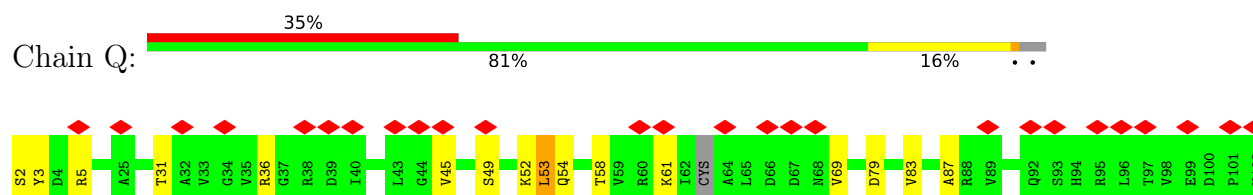
- Molecule 3: Proteasome subunit alpha type-4

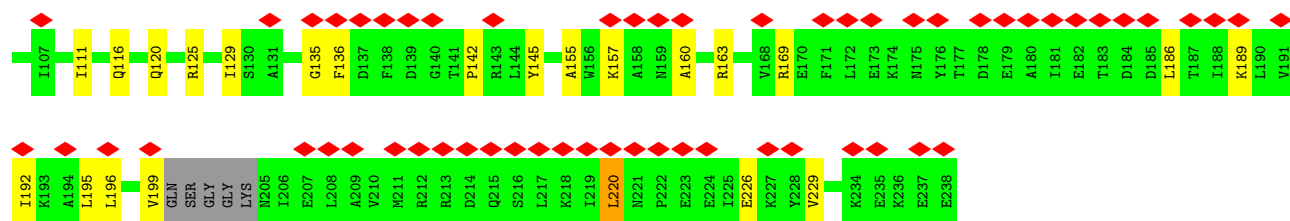


- Molecule 4: Proteasome subunit alpha type-7

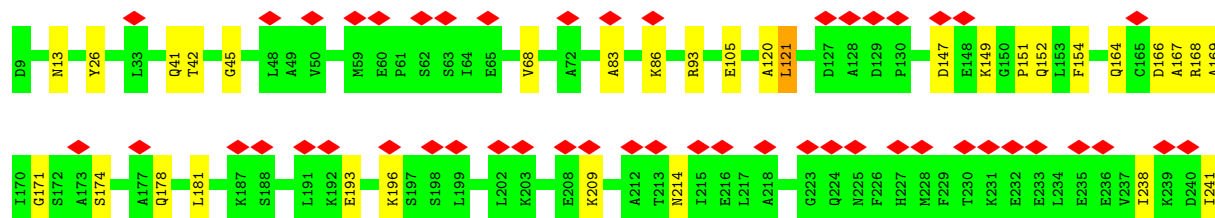
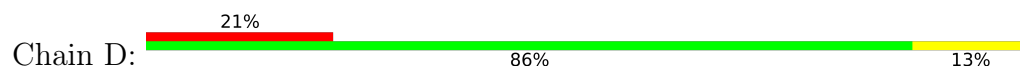


- Molecule 4: Proteasome subunit alpha type-7

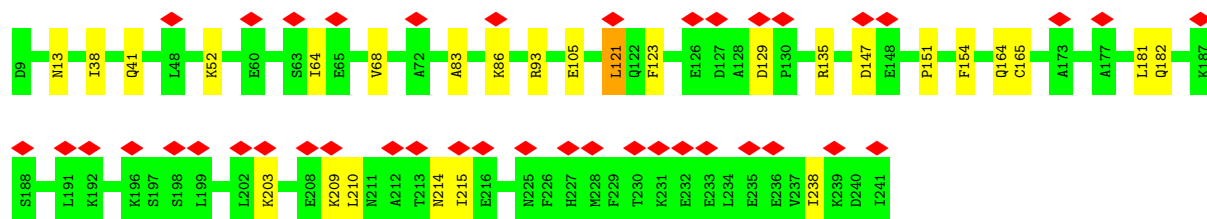
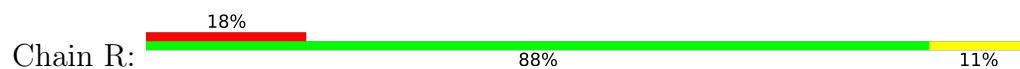




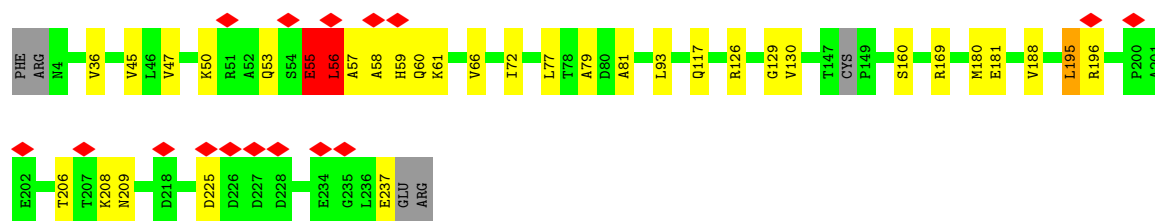
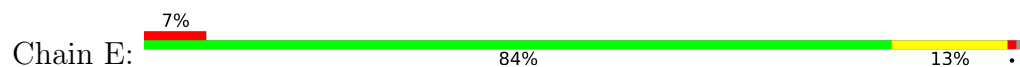
• Molecule 5: Proteasome subunit alpha type-5



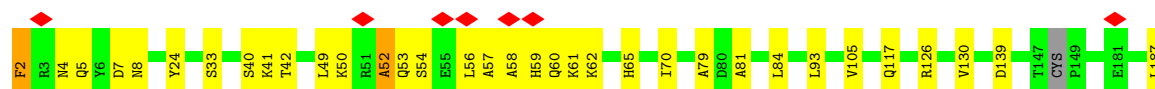
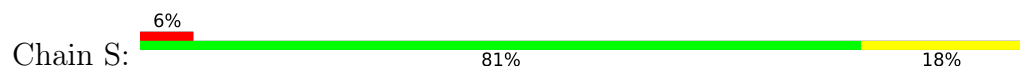
• Molecule 5: Proteasome subunit alpha type-5

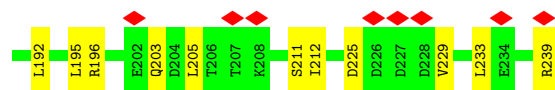


• Molecule 6: Proteasome subunit alpha type-1

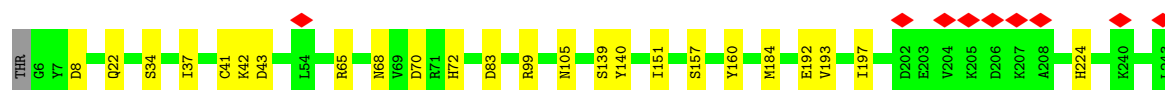


• Molecule 6: Proteasome subunit alpha type-1

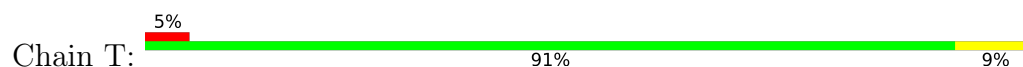




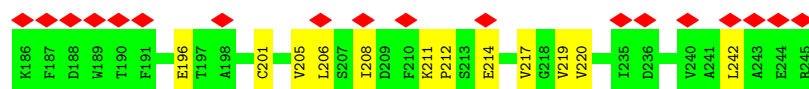
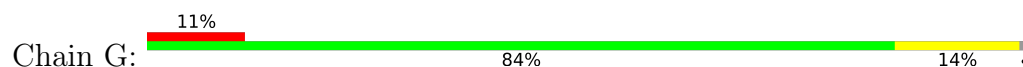
• Molecule 7: Proteasome subunit alpha type-3



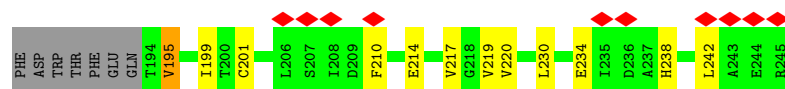
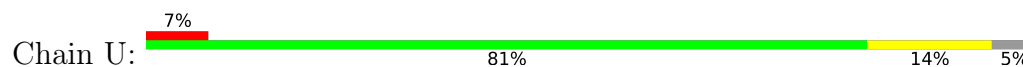
• Molecule 7: Proteasome subunit alpha type-3



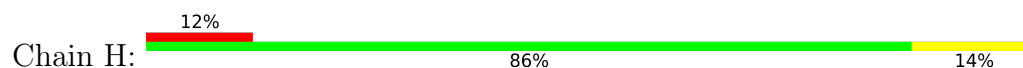
• Molecule 8: Proteasome subunit alpha type-6

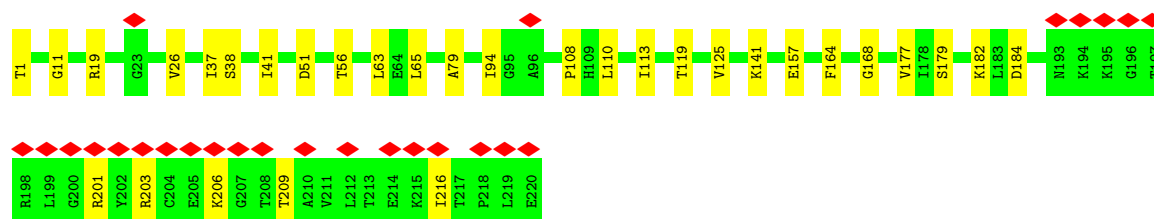


• Molecule 8: Proteasome subunit alpha type-6

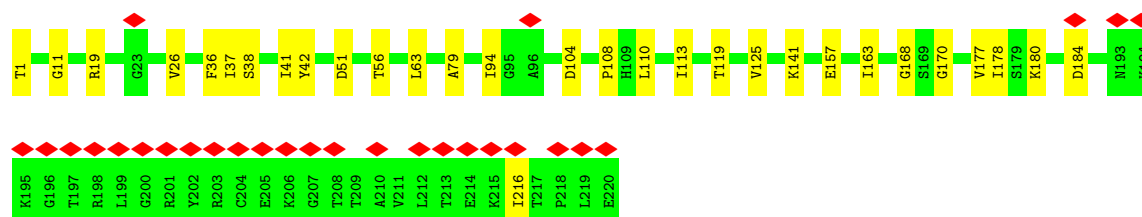
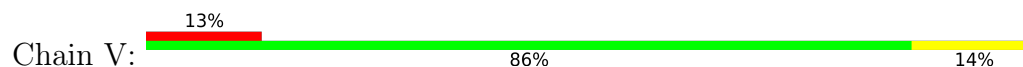


• Molecule 9: Proteasome subunit beta type-7

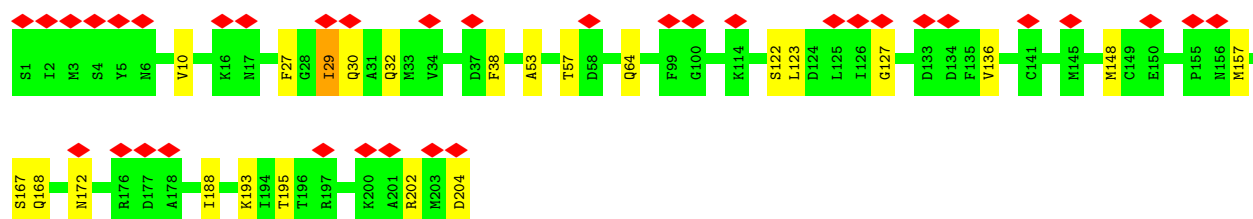
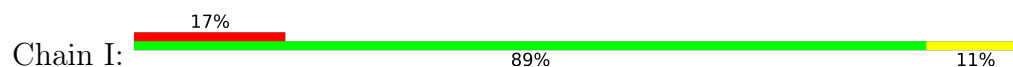




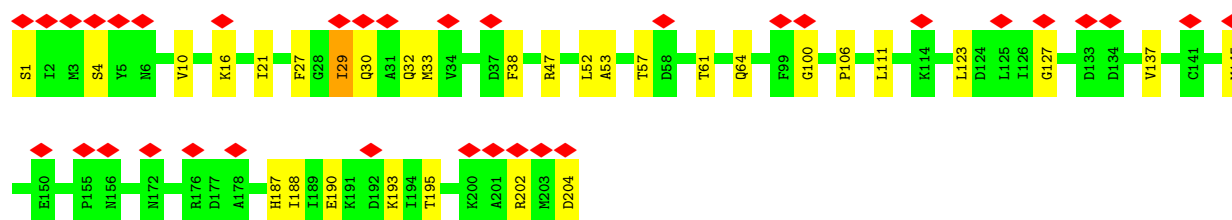
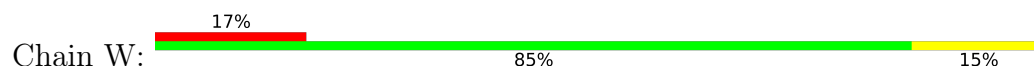
• Molecule 9: Proteasome subunit beta type-7



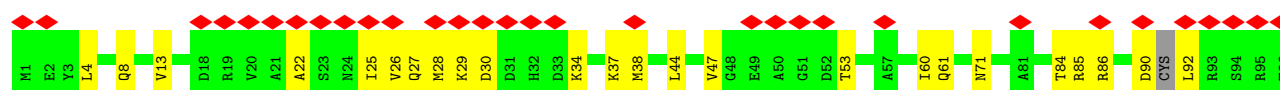
• Molecule 10: Proteasome subunit beta type-3

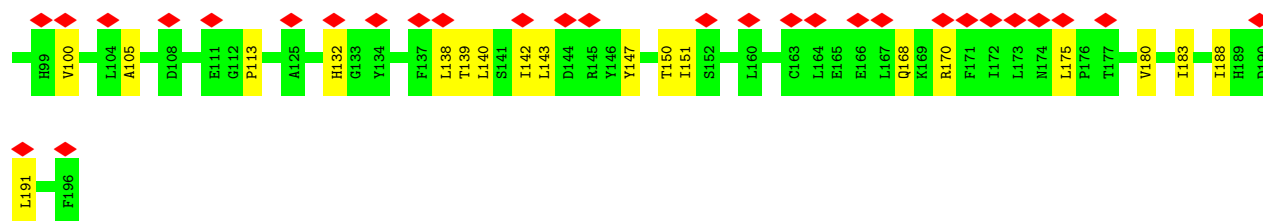


• Molecule 10: Proteasome subunit beta type-3

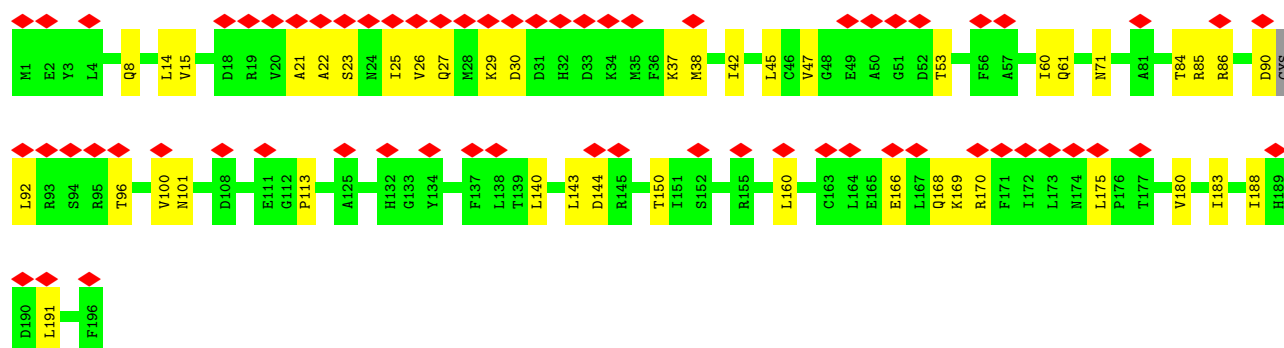
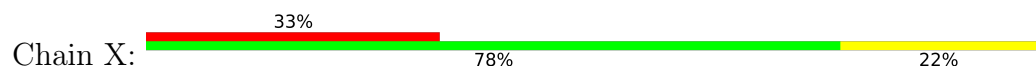


• Molecule 11: Proteasome subunit beta type-2

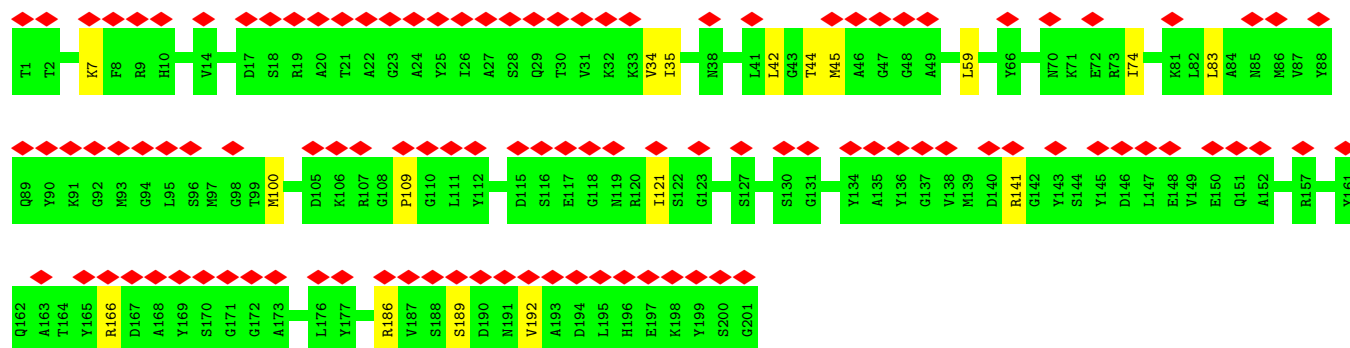




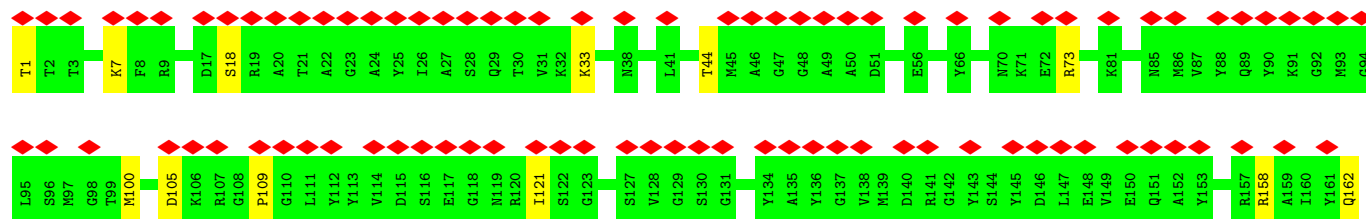
• Molecule 11: Proteasome subunit beta type-2

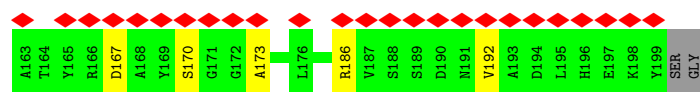


• Molecule 12: Proteasome subunit beta type-5

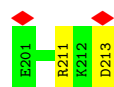
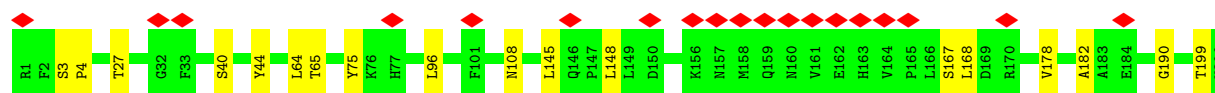
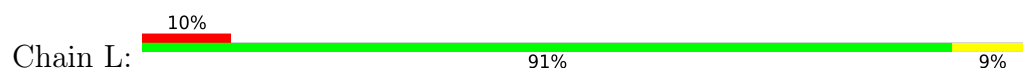


• Molecule 12: Proteasome subunit beta type-5

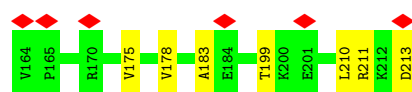
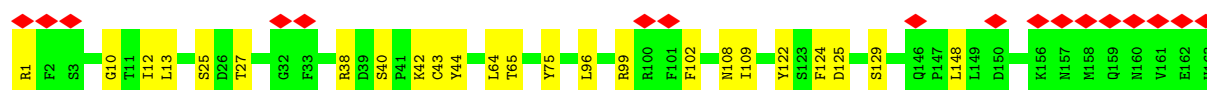
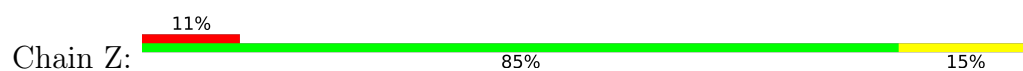




• Molecule 13: Proteasome subunit beta type-1



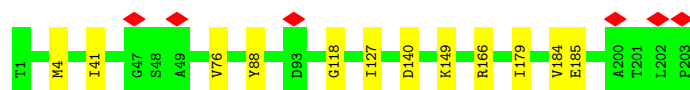
• Molecule 13: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-6



• Molecule 14: Proteasome subunit beta type-6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	16015	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	389.76, 389.76, 389.76	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.015, 1.015, 1.015	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	M	0.41	0/1720	0.53	0/2328
1	a	0.42	0/1728	0.58	0/2339
2	A	0.39	0/1856	0.58	0/2514
2	O	0.39	0/1837	0.61	1/2488 (0.0%)
3	B	0.36	0/1991	0.69	3/2681 (0.1%)
3	P	0.60	6/1986 (0.3%)	0.99	15/2675 (0.6%)
4	C	0.37	0/1889	0.82	6/2547 (0.2%)
4	Q	0.31	0/1856	0.72	2/2503 (0.1%)
5	D	0.33	0/1818	0.66	4/2456 (0.2%)
5	R	0.32	0/1810	0.63	0/2444
6	E	0.38	0/1864	0.67	2/2517 (0.1%)
6	S	0.39	0/1932	0.67	2/2607 (0.1%)
7	F	0.39	0/1941	0.56	0/2612
7	T	0.40	0/1922	0.63	0/2588
8	G	0.38	0/1929	0.53	0/2602
8	U	0.38	0/1824	0.57	2/2459 (0.1%)
9	H	0.33	0/1705	0.55	0/2307
9	V	0.36	0/1702	0.60	2/2303 (0.1%)
10	I	0.25	0/1668	0.51	0/2247
10	W	0.26	0/1640	0.60	4/2209 (0.2%)
11	J	0.23	0/1615	0.55	0/2182
11	X	0.23	0/1613	0.56	2/2180 (0.1%)
12	K	0.23	0/1590	0.50	0/2147
12	Y	0.22	0/1610	0.53	0/2172
13	L	0.31	0/1696	0.58	2/2285 (0.1%)
13	Z	0.31	0/1690	0.56	0/2276
14	N	0.43	0/1548	0.55	0/2095
14	b	0.43	0/1556	0.53	0/2107
All	All	0.36	6/49536 (0.0%)	0.62	47/66870 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	4
3	P	0	7
4	C	0	4
4	Q	0	2
5	R	0	1
6	E	0	3
6	S	0	2
8	U	0	1
10	I	0	1
10	W	0	2
13	Z	0	1
All	All	0	28

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	239	LYS	CG-CD	7.78	1.75	1.52
3	P	239	LYS	CB-CG	6.66	1.72	1.52
3	P	240	HIS	N-CA	6.04	1.53	1.46
3	P	235	GLN	CB-CG	-5.75	1.35	1.52
3	P	239	LYS	CD-CE	5.31	1.68	1.52
3	P	239	LYS	CE-NZ	5.05	1.64	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	239	LYS	CA-C-N	16.73	153.50	121.54
3	P	239	LYS	C-N-CA	16.73	153.50	121.54
3	P	240	HIS	N-CA-C	8.55	129.00	110.80
4	C	204	LYS	N-CA-C	7.78	127.37	110.80
3	P	54	LYS	N-CA-C	-7.72	99.61	108.49
3	P	239	LYS	CB-CG-CD	7.28	128.04	111.30
8	U	145	GLU	CA-C-N	7.24	135.37	121.54
8	U	145	GLU	C-N-CA	7.24	135.37	121.54
4	Q	220	LEU	CA-C-N	7.12	134.51	121.70
4	Q	220	LEU	C-N-CA	7.12	134.51	121.70
3	P	236	LEU	CA-CB-CG	6.66	139.60	116.30
3	P	234	GLU	CA-CB-CG	6.65	127.40	114.10
4	C	202	GLY	CA-C-N	6.33	133.81	121.41
4	C	202	GLY	C-N-CA	6.33	133.81	121.41
11	X	23	SER	CA-C-N	6.31	133.59	121.54
11	X	23	SER	C-N-CA	6.31	133.59	121.54
3	P	239	LYS	CD-CE-NZ	6.12	131.47	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	52	LYS	N-CA-C	-6.12	100.74	108.45
3	P	240	HIS	CB-CA-C	-6.11	98.25	110.42
4	C	232	ILE	CG1-CB-CG2	-5.92	92.95	110.70
6	S	225	ASP	CA-C-N	5.80	130.41	121.19
6	S	225	ASP	C-N-CA	5.80	130.41	121.19
10	W	16[A]	LYS	CA-C-N	5.61	132.26	121.54
10	W	16[A]	LYS	C-N-CA	5.61	132.26	121.54
10	W	16[B]	LYS	CA-C-N	5.61	132.26	121.54
10	W	16[B]	LYS	C-N-CA	5.61	132.26	121.54
9	V	180	LYS	CA-C-N	5.52	132.09	121.54
9	V	180	LYS	C-N-CA	5.52	132.09	121.54
3	P	239	LYS	CA-CB-CG	5.52	125.14	114.10
3	B	209	GLU	CA-C-N	5.50	132.03	121.54
3	B	209	GLU	C-N-CA	5.50	132.03	121.54
13	L	190	GLY	CA-C-N	5.41	131.87	121.54
13	L	190	GLY	C-N-CA	5.41	131.87	121.54
5	D	120[A]	ALA	CA-C-N	5.39	131.84	121.54
5	D	120[A]	ALA	C-N-CA	5.39	131.84	121.54
5	D	120[B]	ALA	CA-C-N	5.39	131.84	121.54
5	D	120[B]	ALA	C-N-CA	5.39	131.84	121.54
4	C	231	GLU	CA-C-N	5.39	131.67	121.97
4	C	231	GLU	C-N-CA	5.39	131.67	121.97
3	P	235	GLN	CA-C-O	-5.22	115.52	120.90
3	B	211	VAL	CB-CA-C	-5.18	106.87	111.74
3	P	239	LYS	CA-C-O	-5.16	113.13	120.51
3	P	53	HIS	CA-C-N	5.09	129.11	120.81
3	P	53	HIS	C-N-CA	5.09	129.11	120.81
3	P	210	LYS	CB-CA-C	5.04	120.46	110.42
6	E	225	ASP	CA-C-N	5.03	129.19	121.19
6	E	225	ASP	C-N-CA	5.03	129.19	121.19

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	205	LYS	Peptide
3	B	207	SER	Peptide
3	B	209	GLU	Peptide
3	B	211	VAL	Peptide
4	C	199	VAL	Peptide
4	C	203	GLY	Peptide
4	C	232	ILE	Peptide

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Mol	Chain	Res	Type	Group
4	C	233	GLU	Peptide
6	E	53	GLN	Peptide
6	E	55	GLU	Peptide
6	E	56	LEU	Peptide
10	I	29	ILE	Peptide
3	P	205	LYS	Peptide
3	P	209	GLU	Peptide
3	P	236	LEU	Mainchain
3	P	238	LYS	Mainchain,Peptide
3	P	240	HIS	Peptide
3	P	52	ILE	Peptide
4	Q	220	LEU	Peptide
4	Q	49	SER	Peptide
5	R	129	ASP	Peptide
6	S	2	PHE	Peptide
6	S	52	ALA	Peptide
8	U	55	LYS	Peptide
10	W	100	GLY	Peptide
10	W	29	ILE	Peptide
13	Z	1	ARG	Peptide

5.2 Too-close contacts [i](#)

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	M	1687	0	1666	13	0
1	a	1692	0	1670	12	0
2	A	1811	0	1812	21	0
2	O	1798	0	1795	21	0
3	B	1958	0	1982	28	0
3	P	1950	0	1974	36	0
4	C	1864	0	1887	23	0
4	Q	1832	0	1854	25	0
5	D	1791	0	1773	20	0
5	R	1783	0	1768	22	0
6	E	1831	0	1821	20	0
6	S	1888	0	1880	30	0
7	F	1894	0	1890	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	1884	0	1873	14	0
8	G	1892	0	1907	22	0
8	U	1798	0	1813	20	0
9	H	1672	0	1703	24	0
9	V	1669	0	1694	17	0
10	I	1633	0	1660	15	0
10	W	1608	0	1637	19	0
11	J	1580	0	1582	27	0
11	X	1575	0	1579	28	0
12	K	1559	0	1523	12	0
12	Y	1570	0	1550	11	0
13	L	1660	0	1666	11	0
13	Z	1657	0	1661	18	0
14	N	1519	0	1496	7	0
14	b	1526	0	1503	7	0
All	All	48581	0	48619	472	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 (472) 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)
3:P:239:LYS:CD	3:P:239:LYS:CG	1.75	1.56
3:P:235:GLN:O	3:P:239:LYS:HB2	1.65	0.97
3:B:210:LYS:HE3	3:B:237:ILE:HD13	1.75	0.68
3:P:143:TYR:HB2	3:P:146:GLN:HE21	1.57	0.68
3:B:143:TYR:HB2	3:B:146:GLN:HE21	1.58	0.68
11:J:22:ALA:HA	11:J:27:GLN:HA	1.76	0.67
11:X:22:ALA:HA	11:X:27:GLN:HA	1.77	0.67
8:U:49:VAL:HG11	8:U:195:VAL:HG12	1.76	0.66
3:P:236:LEU:O	3:P:239:LYS:O	2.13	0.66
5:R:164:GLN:HB3	6:S:58:ALA:HB3	1.77	0.66
9:H:51:ASP:HB3	9:H:94:ILE:HG23	1.76	0.65
8:G:49[B]:VAL:HG22	8:G:219:VAL:HG12	1.79	0.65
11:X:25:ILE:HG13	11:X:26:VAL:HG13	1.79	0.65
9:V:51:ASP:HB3	9:V:94:ILE:HG23	1.79	0.64
4:C:203:GLY:HA2	4:C:205:ASN:H	1.62	0.64
6:E:50:LYS:HB3	6:E:59:HIS:HB3	1.80	0.64
13:L:145:LEU:HD21	13:L:182:ALA:HB2	1.79	0.64
4:C:228:TYR:O	4:C:232:ILE:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:60:GLN:NE2	6:E:61:LYS:O	2.32	0.63
3:P:198:ASN:ND2	3:P:241:GLU:OE2	2.31	0.63
11:J:25:ILE:HG13	11:J:26:VAL:HG13	1.80	0.62
5:D:83:ALA:HA	5:D:86:LYS:HG3	1.80	0.61
6:E:81:ALA:HB2	6:E:130:VAL:HG21	1.82	0.61
2:O:165:ASN:HD21	2:O:168:ASN:HD22	1.49	0.61
10:I:57:THR:O	11:J:85:ARG:NH2	2.33	0.61
2:O:49:LYS:HE2	2:O:208:GLU:HB2	1.81	0.61
5:R:41:GLN:NE2	5:R:151:PRO:O	2.34	0.61
1:M:92:LEU:HD23	1:M:112:ILE:HD11	1.81	0.61
13:L:27:THR:HB	13:L:40:SER:H	1.66	0.61
6:S:81:ALA:HB2	6:S:130:VAL:HG21	1.83	0.60
3:P:51:ASN:ND2	3:P:58:GLU:OE2	2.35	0.60
10:I:64:GLN:OE1	11:J:86:ARG:NH2	2.35	0.60
2:O:110:VAL:HG22	2:O:135:ILE:HD12	1.84	0.60
2:A:49:LYS:HE2	2:A:208:GLU:HB2	1.83	0.60
12:Y:18:SER:HB2	12:Y:173:ALA:H	1.67	0.60
8:U:49:VAL:HG12	8:U:219:VAL:HG12	1.84	0.59
11:X:53:THR:HG22	11:X:100:VAL:HG13	1.83	0.59
5:D:41:GLN:NE2	5:D:151:PRO:O	2.34	0.59
3:P:210:LYS:H	3:P:211:VAL:HG22	1.65	0.59
3:P:109:GLN:NE2	11:X:71:ASN:OD1	2.34	0.59
10:W:57:THR:O	11:X:85:ARG:NH2	2.35	0.59
10:W:64:GLN:OE1	11:X:86:ARG:NH2	2.36	0.59
3:B:109:GLN:NE2	11:J:71:ASN:OD1	2.36	0.59
9:H:203:ARG:NH1	10:I:157:MET:SD	2.75	0.59
13:Z:27:THR:HB	13:Z:40:SER:H	1.67	0.58
5:R:83:ALA:HA	5:R:86:LYS:HG3	1.85	0.58
8:U:112:ASP:N	8:U:112:ASP:OD1	2.36	0.58
4:C:51:ALA:HB1	4:C:54:GLN:HB2	1.84	0.58
5:D:166:ASP:HB2	6:E:56:LEU:HB3	1.85	0.57
1:M:9:THR:OG1	1:M:10:SER:N	2.38	0.57
7:T:70:ASP:OD1	7:T:99:ARG:NH2	2.38	0.57
2:A:81:ASP:OD1	8:G:123:GLN:NE2	2.37	0.57
6:S:60:GLN:NE2	6:S:61:LYS:O	2.36	0.56
8:U:11:ARG:O	8:U:24:GLN:NE2	2.38	0.56
6:E:47:VAL:HG12	6:E:195:LEU:HD12	1.87	0.56
4:Q:116:GLN:HG3	5:R:83:ALA:HB1	1.87	0.56
5:R:165:CYS:HA	6:S:57:ALA:HA	1.87	0.56
11:J:138:LEU:HD21	11:J:170:ARG:HB3	1.88	0.56
2:O:106:THR:H	2:O:139:ASN:HD21	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:148:LEU:HD23	13:Z:178:VAL:HG12	1.87	0.56
11:J:90:ASP:O	11:J:92:LEU:N	2.39	0.56
2:O:41:ASN:ND2	2:O:182:GLU:OE1	2.39	0.56
11:J:168:GLN:NE2	11:J:175:LEU:O	2.38	0.56
2:A:212:CYS:HB2	2:A:217:PHE:HD1	1.71	0.56
11:X:168:GLN:NE2	11:X:175:LEU:O	2.37	0.56
1:a:86:ARG:NH1	1:a:133:GLU:OE2	2.39	0.56
12:K:141:ARG:NH1	11:X:166:GLU:OE2	2.39	0.55
2:A:139:ASN:OD1	2:A:139:ASN:N	2.37	0.55
5:D:154:PHE:HD1	5:D:164:GLN:HA	1.72	0.55
2:O:32:ALA:HB2	2:O:50:LYS:HE3	1.89	0.55
1:a:27:LEU:HD22	1:a:184:TYR:HB2	1.88	0.55
11:J:53:THR:HG22	11:J:100:VAL:HG13	1.87	0.55
3:B:73:ALA:HB2	3:B:225:ILE:HD13	1.89	0.55
5:D:168:ARG:HA	5:D:178:GLN:HE22	1.72	0.55
4:C:160:ALA:O	4:C:169:ARG:NH2	2.40	0.55
8:G:11:ARG:O	8:G:24:GLN:NE2	2.40	0.55
11:X:37:LYS:O	11:X:61:GLN:NE2	2.40	0.55
3:B:198:ASN:ND2	3:B:244:GLU:OE2	2.40	0.54
7:F:139[B]:SER:OG	7:F:140:TYR:N	2.40	0.54
10:I:10[A]:VAL:HG23	10:I:53:ALA:HB2	1.89	0.54
12:K:192:VAL:HG11	10:W:204:ASP:HB3	1.89	0.54
1:M:27:LEU:HD22	1:M:184:TYR:HB2	1.89	0.54
11:X:90:ASP:O	11:X:92:LEU:N	2.40	0.54
5:D:147:ASP:OD1	5:D:147:ASP:N	2.41	0.54
8:U:6:SER:OG	8:U:11:ARG:NH1	2.40	0.54
7:F:70:ASP:OD1	7:F:99:ARG:NH2	2.39	0.54
2:O:74:VAL:HG12	2:O:134:LEU:HB2	1.89	0.54
3:P:136:TYR:HB2	3:P:148:TYR:HB2	1.89	0.54
9:V:63:LEU:HD11	9:V:79:ALA:HB2	1.89	0.54
4:C:2:SER:OG	4:C:3:TYR:N	2.41	0.54
9:H:201:ARG:HH21	9:H:203:ARG:HD2	1.73	0.54
7:T:179:LEU:HD11	7:T:196:ILE:HD11	1.89	0.54
9:H:38:SER:HB3	9:H:41:ILE:HB	1.89	0.54
7:F:43:ASP:OD1	7:F:43:ASP:N	2.39	0.54
6:S:41:LYS:HG3	6:S:42:THR:HG23	1.89	0.54
9:V:38:SER:HB3	9:V:41:ILE:HB	1.88	0.54
9:H:209:THR:HG21	10:I:167:SER:HB2	1.90	0.53
12:K:7:LYS:HD2	12:K:109:PRO:HB2	1.89	0.53
6:S:33:SER:OG	6:S:62:LYS:NZ	2.41	0.53
8:U:165:ALA:HB1	8:U:179:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:136:TYR:HB2	3:B:148:TYR:HB2	1.90	0.53
10:I:204:ASP:HB3	12:Y:192:VAL:HG11	1.89	0.53
5:R:105:GLU:OE2	13:Z:75:TYR:OH	2.26	0.53
2:A:92:LEU:HD13	2:A:112:ARG:HB3	1.90	0.53
3:P:51:ASN:HB2	3:P:56:LEU:HD13	1.91	0.53
1:M:96:MET:HE3	1:M:127:MET:HA	1.90	0.53
6:E:160:SER:O	6:E:169:ARG:NH1	2.41	0.53
2:O:92:LEU:HD13	2:O:112:ARG:HB3	1.88	0.53
6:S:50:LYS:HE3	6:S:211:SER:HB3	1.90	0.53
5:D:149:LYS:HD2	5:D:152:GLN:HE21	1.72	0.53
1:M:1:THR:N	1:M:104:ASN:OD1	2.42	0.53
2:A:43:VAL:HG21	2:A:136:CYS:HB2	1.91	0.53
11:J:140:LEU:HD23	11:J:143:LEU:HD12	1.90	0.53
2:O:10:THR:HG23	2:O:20:GLN:HB2	1.90	0.53
13:Z:96:LEU:HD11	13:Z:108:ASN:HD22	1.74	0.53
13:L:148:LEU:HD23	13:L:178:VAL:HG12	1.91	0.52
3:B:197:LEU:HA	3:B:200:THR:HG22	1.90	0.52
9:H:177:VAL:HB	9:H:184:ASP:HB2	1.91	0.52
4:C:208:LEU:HD22	4:C:220:LEU:HD22	1.91	0.52
3:P:49:ARG:HE	3:P:212:GLU:HG2	1.73	0.52
1:a:67:LEU:HD11	1:a:88:ILE:HD12	1.92	0.52
12:Y:158:ARG:HE	12:Y:162:GLN:HE21	1.58	0.52
1:a:9:THR:OG1	1:a:10:SER:N	2.42	0.52
9:V:1:THR:N	9:V:168:GLY:O	2.43	0.52
9:H:209:THR:OG1	10:I:168:GLN:NE2	2.43	0.52
1:M:67:LEU:HD11	1:M:88:ILE:HD12	1.91	0.51
6:S:50:LYS:HB3	6:S:59:HIS:HB3	1.90	0.51
1:a:96:MET:HE3	1:a:127:MET:HA	1.91	0.51
5:D:121:LEU:HD12	6:E:79:ALA:HB3	1.91	0.51
9:H:1:THR:N	9:H:168:GLY:O	2.43	0.51
3:P:185:THR:HG23	3:P:188:SER:H	1.75	0.51
9:V:141:LYS:NZ	9:V:157:GLU:OE2	2.42	0.51
1:a:92:LEU:HD22	1:a:110:MET:HE1	1.91	0.51
9:H:141:LYS:NZ	9:H:157:GLU:OE2	2.42	0.51
2:O:222:PRO:HA	2:O:225:VAL:HG12	1.92	0.51
5:R:164:GLN:O	6:S:58:ALA:N	2.38	0.51
11:J:8:GLN:HE21	11:J:113:PRO:HG2	1.76	0.51
3:P:197:LEU:HA	3:P:200:THR:HG22	1.92	0.51
9:V:113:ILE:HG12	9:V:119:THR:HG22	1.92	0.51
8:G:54:LYS:N	8:G:214:GLU:O	2.43	0.51
11:J:37:LYS:O	11:J:61:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:211:ARG:NH2	13:L:213:ASP:OD2	2.44	0.51
6:S:4:ASN:O	6:S:8:ASN:ND2	2.44	0.51
6:S:52:ALA:O	6:S:54:SER:N	2.41	0.51
10:W:52:LEU:HG	10:W:106:PRO:HB3	1.93	0.51
13:Z:25:SER:HG	13:Z:43[A]:CYS:HG	1.57	0.51
11:J:170:ARG:HA	11:X:27:GLN:HE21	1.75	0.50
14:b:149:LYS:NZ	14:b:185:GLU:OE1	2.44	0.50
4:Q:160:ALA:O	4:Q:169:ARG:NH2	2.44	0.50
5:D:193:GLU:HA	5:D:196:LYS:HG2	1.93	0.50
3:P:190:LEU:HD13	3:P:236:LEU:HD11	1.92	0.50
13:L:96:LEU:HD11	13:L:108:ASN:HD22	1.77	0.50
3:P:176:LYS:HG2	4:Q:53:LEU:HD11	1.92	0.50
5:R:182:GLN:HE22	6:S:56:LEU:H	1.58	0.50
2:O:81:ASP:OD1	8:U:123:GLN:NE2	2.45	0.50
5:R:68:VAL:HB	5:R:93:ARG:HH21	1.77	0.50
2:O:159:ALA:HB3	3:P:55:LEU:HD22	1.94	0.50
10:W:137:VAL:HG11	10:W:145:MET:HB3	1.92	0.50
4:Q:45:VAL:HG21	4:Q:61:LYS:HB2	1.94	0.50
14:b:88:TYR:HB2	14:b:118:GLY:HA3	1.94	0.50
4:C:183:THR:O	4:C:187:THR:OG1	2.27	0.50
5:D:164:GLN:O	6:E:58:ALA:N	2.29	0.50
7:F:34:SER:HB2	7:F:65:ARG:HH12	1.77	0.49
9:H:19:ARG:HH21	13:Z:211:ARG:HH21	1.60	0.49
11:J:27:GLN:HE21	11:X:170:ARG:HA	1.76	0.49
11:X:15:VAL:HB	11:X:45:LEU:HD11	1.94	0.49
13:Z:211:ARG:NH2	13:Z:213:ASP:OD2	2.45	0.49
5:D:68:VAL:HB	5:D:93:ARG:HH21	1.76	0.49
3:P:86:LEU:HD22	3:P:114:LEU:HD11	1.95	0.49
5:R:209:LYS:O	5:R:214:ASN:ND2	2.40	0.49
11:X:30:ASP:OD1	11:X:30:ASP:N	2.42	0.49
2:O:212:CYS:HB2	2:O:217:PHE:HD1	1.77	0.49
8:U:43:ARG:HA	8:U:48:ALA:HA	1.94	0.49
3:B:161:ALA:HB3	4:C:53:LEU:HD22	1.95	0.49
8:G:165:ALA:HB1	8:G:179:LEU:HD13	1.95	0.49
10:I:122:SER:HB3	10:I:136:VAL:HB	1.95	0.49
11:J:4:LEU:HB2	11:J:132:HIS:HB2	1.94	0.49
9:V:37:ILE:HD11	9:V:56:THR:HB	1.95	0.49
2:A:202:MET:SD	2:A:202:MET:N	2.84	0.49
7:F:37:ILE:HG12	7:F:197:ILE:HD11	1.94	0.49
8:G:206:LEU:HB3	8:G:208:ILE:HG12	1.94	0.49
14:N:88:TYR:HB2	14:N:118:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:207:SER:OG	3:P:208:ALA:N	2.46	0.49
5:D:105:GLU:OE2	13:L:75:TYR:OH	2.31	0.49
7:F:157:SER:O	8:G:88:ARG:NH2	2.40	0.49
14:N:179:ILE:HG12	14:N:184:VAL:HG22	1.95	0.49
9:H:19:ARG:HG3	9:H:26:VAL:HG13	1.94	0.48
13:L:211:ARG:HH21	9:V:19:ARG:HH21	1.61	0.48
6:S:117:GLN:NE2	7:T:83:ASP:OD1	2.46	0.48
11:X:14:LEU:HD21	11:X:160:LEU:HD22	1.95	0.48
6:S:139:ASP:HB3	1:a:81:HIS:HE1	1.78	0.48
8:U:210:PHE:HB3	8:U:214:GLU:HB3	1.95	0.48
12:Y:7:LYS:HD2	12:Y:109:PRO:HB2	1.95	0.48
6:S:2:PHE:N	6:S:5:GLN:H	2.11	0.48
6:E:196:ARG:HH22	6:E:237:GLU:HG2	1.79	0.48
7:F:8:ASP:O	7:F:22:GLN:NE2	2.38	0.48
10:W:123:LEU:HD23	10:W:127:GLY:HA2	1.96	0.48
2:A:73:LEU:HD21	2:A:86:VAL:HG22	1.95	0.48
7:F:160:TYR:HE1	8:G:61:LEU:HD23	1.79	0.48
14:b:179:ILE:HG12	14:b:184:VAL:HG22	1.96	0.48
8:G:143:ILE:HG12	8:G:220:VAL:HG12	1.96	0.48
13:L:167:SER:OG	13:L:168:LEU:N	2.47	0.48
4:C:70:CYS:SG	4:C:71:MET:N	2.87	0.47
9:H:63:LEU:HD11	9:H:79:ALA:HB2	1.95	0.47
3:P:201:MET:SD	3:P:210:LYS:NZ	2.87	0.47
6:S:40:SER:HB3	6:S:187:LEU:HD22	1.95	0.47
10:W:29:ILE:O	10:W:32:GLN:N	2.47	0.47
4:Q:226:GLU:HA	4:Q:229:VAL:HG12	1.95	0.47
7:T:8:ASP:O	7:T:22:GLN:NE2	2.38	0.47
7:F:41:CYS:SG	7:F:42:LYS:N	2.87	0.47
5:R:203:LYS:HB2	5:R:210:LEU:HD13	1.97	0.47
11:X:183:ILE:HD12	11:X:188:ILE:HG22	1.97	0.47
3:B:190:LEU:HB3	3:B:236:LEU:HD21	1.96	0.47
10:I:29:ILE:O	10:I:32:GLN:N	2.48	0.47
7:T:43:ASP:OD1	7:T:43:ASP:N	2.48	0.47
9:V:19:ARG:HG3	9:V:26:VAL:HG13	1.96	0.47
2:A:33:PRO:HG3	2:A:164:LYS:HB2	1.96	0.47
6:E:50:LYS:HB2	6:E:209:ASN:HA	1.95	0.47
9:H:37:ILE:HD11	9:H:56:THR:HB	1.96	0.47
9:H:201:ARG:HE	9:H:203:ARG:HB2	1.78	0.47
11:J:180:VAL:HG13	11:J:191:LEU:HB2	1.96	0.47
9:V:110:LEU:HD21	9:V:125:VAL:HG22	1.97	0.47
13:Z:183:ALA:HB2	13:Z:210:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:151:ILE:HG13	7:F:157:SER:HB2	1.95	0.47
11:X:38:MET:HB2	11:X:42:ILE:HG23	1.96	0.47
12:Y:1:THR:HG22	12:Y:33:LYS:HZ3	1.80	0.47
4:C:103:THR:HG23	4:C:106:TYR:H	1.80	0.47
11:J:30:ASP:OD1	11:J:30:ASP:N	2.40	0.47
2:O:73:LEU:HD12	2:O:86:VAL:HG22	1.96	0.47
12:Y:44:THR:OG1	12:Y:100:MET:N	2.44	0.47
1:a:1:THR:N	1:a:104:ASN:OD1	2.48	0.47
1:M:41:ARG:NH1	1:M:53:ALA:O	2.48	0.46
6:E:77:LEU:HD12	6:E:129:GLY:HA3	1.97	0.46
5:R:121:LEU:HD12	6:S:79:ALA:HB3	1.97	0.46
9:H:113:ILE:HG12	9:H:119:THR:HG22	1.97	0.46
9:V:177:VAL:HB	9:V:184:ASP:HB2	1.96	0.46
11:X:140:LEU:HD23	11:X:143:LEU:HD12	1.97	0.46
5:D:238:ILE:HA	5:D:241:ILE:HD12	1.97	0.46
4:C:41:VAL:HG23	4:C:211:MET:HB3	1.97	0.46
8:G:175:SER:OG	8:G:201:CYS:SG	2.67	0.46
8:G:196:GLU:HB3	8:G:242:LEU:HD21	1.98	0.46
11:J:29:LYS:HD2	12:K:121:ILE:HB	1.97	0.46
2:O:178:ASN:OD1	2:O:178:ASN:N	2.46	0.46
8:U:175:SER:OG	8:U:201:CYS:SG	2.68	0.46
6:E:66:VAL:HG21	6:E:72:ILE:HG23	1.98	0.46
9:H:11:GLY:HA2	9:H:108:PRO:HB3	1.97	0.46
3:P:44:LEU:HD22	3:P:190:LEU:HD23	1.98	0.46
6:S:203:GLN:O	6:S:239:ARG:NH1	2.39	0.46
7:T:37:ILE:HG12	7:T:197:ILE:HD11	1.97	0.46
11:X:96:THR:O	11:X:96:THR:OG1	2.33	0.46
9:H:179:SER:HG	9:H:182:LYS:H	1.63	0.46
3:P:172:VAL:HA	3:P:175:LEU:HB2	1.97	0.46
6:S:196:ARG:HB2	6:S:205:LEU:HD11	1.98	0.46
3:B:33:THR:HG21	3:B:200:THR:HG21	1.98	0.46
3:B:209:GLU:HA	3:B:230:GLN:HE22	1.81	0.46
6:E:55:GLU:O	6:E:57:ALA:N	2.49	0.46
12:K:59:LEU:HD22	12:K:83:LEU:HB2	1.98	0.46
13:Z:12:ILE:HG22	13:Z:25:SER:HB3	1.96	0.46
7:F:37:ILE:HD11	7:F:193:VAL:HG13	1.98	0.46
11:J:139:THR:HA	11:J:142:ILE:HD12	1.98	0.46
12:K:186:ARG:NH1	12:K:189:SER:OG	2.49	0.46
6:S:229:VAL:HG22	6:S:233:LEU:HG	1.98	0.46
11:X:180:VAL:HG13	11:X:191:LEU:HB2	1.97	0.46
10:W:202:ARG:NH2	10:W:204:ASP:OD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:13:LEU:HD23	13:Z:175:VAL:HG13	1.97	0.46
12:Y:167:ASP:HB3	12:Y:170:SER:HB3	1.98	0.45
7:F:68:ASN:OD1	7:F:224:HIS:ND1	2.49	0.45
8:G:51:VAL:HG22	8:G:217:VAL:HG22	1.98	0.45
8:U:112:ASP:HB3	8:U:152:TYR:CZ	2.52	0.45
2:A:32:ALA:HB2	2:A:50:LYS:HE3	1.98	0.45
11:X:29:LYS:HD2	12:Y:121:ILE:HB	1.98	0.45
4:C:87:ALA:HB2	4:C:111:ILE:HD11	1.98	0.45
5:R:182:GLN:HE22	6:S:56:LEU:N	2.14	0.45
2:A:73:LEU:HD12	2:A:133:LEU:HD22	1.99	0.45
3:P:17:ARG:NH2	3:P:22:GLU:OE1	2.46	0.45
5:R:52:LYS:HZ2	5:R:64:ILE:HG22	1.81	0.45
9:H:216:ILE:HG23	10:I:193:LYS:HD2	1.97	0.45
12:K:44:THR:OG1	12:K:100:MET:N	2.44	0.45
12:K:166:ARG:NE	11:X:144:ASP:OD2	2.36	0.45
2:O:85:LEU:HD13	2:O:133:LEU:HD11	1.98	0.45
4:Q:2:SER:OG	4:Q:3:TYR:N	2.47	0.45
4:Q:87:ALA:HB2	4:Q:111:ILE:HD11	1.99	0.45
1:M:100:ARG:NH1	13:L:4:PRO:O	2.33	0.45
2:A:21:ILE:HG21	2:A:151:SER:HB3	1.98	0.45
14:N:140:ASP:OD2	14:b:166:ARG:NE	2.39	0.45
4:C:12:PRO:HG3	5:D:26:TYR:CZ	2.52	0.45
14:N:166:ARG:NE	14:b:140:ASP:OD2	2.39	0.45
6:S:7:ASP:HB2	6:S:24:TYR:HE2	1.82	0.45
8:G:50:ILE:HD12	8:G:79:VAL:HB	1.99	0.45
3:P:185:THR:OG1	3:P:186:LEU:N	2.48	0.45
2:A:118:GLN:HG3	3:B:81:SER:HB2	1.98	0.45
3:B:25[B]:MET:HE3	3:B:25[B]:MET:HB3	1.88	0.45
3:B:194:ILE:HD13	3:B:236:LEU:HG	1.99	0.45
4:C:189:LYS:HZ2	4:C:232:ILE:HD12	1.82	0.45
8:G:112:ASP:N	8:G:112:ASP:OD1	2.48	0.45
3:P:158:GLY:O	4:Q:54:GLN:NE2	2.48	0.45
7:T:68:ASN:OD1	7:T:224:HIS:ND1	2.49	0.45
6:E:93:LEU:HD23	6:E:93:LEU:HA	1.86	0.44
11:J:147:TYR:HA	11:J:151:ILE:HD11	1.98	0.44
6:S:52:ALA:HB2	6:S:59:HIS:HA	1.99	0.44
8:U:54:LYS:N	8:U:214:GLU:O	2.44	0.44
9:V:42:TYR:HB2	9:V:178:ILE:HD11	1.99	0.44
1:M:214:MET:HE3	1:M:214:MET:HB3	1.88	0.44
3:B:123:GLN:HG3	4:C:125:ARG:HG2	2.00	0.44
11:J:60:ILE:HG13	11:J:84:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:64:LEU:HD21	13:L:108:ASN:HD21	1.83	0.44
14:N:169:SER:O	14:N:169:SER:OG	2.31	0.44
5:R:215:ILE:HD11	5:R:238:ILE:HD11	1.98	0.44
10:W:10:VAL:HG23	10:W:53:ALA:HB2	1.98	0.44
2:A:106:THR:H	2:A:139:ASN:HD21	1.65	0.44
11:J:13:VAL:HG21	11:J:105:ALA:HB1	2.00	0.44
12:K:35:ILE:HD11	12:K:45:MET:HE3	1.98	0.44
10:I:202:ARG:NH2	10:I:204:ASP:OD2	2.40	0.44
4:Q:120:GLN:HG3	5:R:135:ARG:HG2	1.99	0.44
12:Y:105:ASP:OD2	12:Y:105:ASP:N	2.50	0.44
2:A:74:VAL:HG12	2:A:134:LEU:HB2	1.99	0.44
2:O:65:GLU:HG2	2:O:86:VAL:HG11	1.99	0.44
2:A:38:LYS:HA	2:A:43:VAL:HG12	2.00	0.44
3:B:44:LEU:HD22	3:B:190:LEU:HD23	2.00	0.44
9:H:164:PHE:O	13:Z:38:ARG:NH2	2.41	0.44
11:J:34:LYS:HD3	11:J:47:VAL:HG12	2.00	0.44
11:X:8:GLN:HE21	11:X:113:PRO:HG2	1.82	0.44
10:W:27:PHE:HB2	10:W:38:PHE:HB2	1.99	0.44
3:B:17:ARG:NH2	3:B:22:GLU:OE1	2.47	0.44
11:X:21:ALA:HB3	11:X:29:LYS:HB3	1.99	0.44
5:D:167:ALA:HB1	5:D:181:LEU:HD22	1.99	0.44
6:E:206:THR:OG1	6:E:208:LYS:O	2.35	0.44
8:G:53:GLN:NE2	8:G:206:LEU:HD21	2.33	0.44
11:J:183:ILE:HG13	11:J:188:ILE:HG22	2.00	0.44
2:O:159:ALA:HB1	2:O:173:LEU:HD13	2.00	0.44
4:Q:69:VAL:HG22	4:Q:135:GLY:HA3	2.00	0.44
8:G:211:LYS:HE3	8:G:212:PRO:HD2	1.99	0.43
2:O:55:LEU:HD22	8:U:165:ALA:HB3	2.00	0.43
4:Q:145:TYR:HA	4:Q:155:ALA:HA	2.00	0.43
1:a:92:LEU:HD23	1:a:92:LEU:HA	1.84	0.43
2:A:55:LEU:HD22	8:G:165:ALA:HB3	1.99	0.43
3:B:76:VAL:HG12	3:B:134:LEU:HG	2.00	0.43
14:N:41:ILE:HG12	14:N:76:VAL:HG22	1.99	0.43
4:Q:31:THR:OG1	4:Q:163:ARG:O	2.33	0.43
6:S:49:LEU:HG	6:S:195:LEU:HD11	2.00	0.43
13:Z:125:ASP:OD2	13:Z:129:SER:N	2.51	0.43
2:A:85:LEU:HD13	2:A:133:LEU:HD11	1.99	0.43
5:D:171:GLY:N	5:D:174:SER:HB2	2.34	0.43
5:R:147:ASP:OD1	5:R:147:ASP:N	2.49	0.43
8:U:199:ILE:HG23	8:U:242:LEU:HD11	1.99	0.43
10:I:123:LEU:HD23	10:I:127:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:198:ASN:ND2	3:P:244:GLU:OE2	2.52	0.43
6:S:70:ILE:HD11	6:S:105:VAL:HG22	2.00	0.43
10:W:61:THR:HG23	11:X:86:ARG:HH12	1.83	0.43
11:X:60:ILE:HG13	11:X:84:THR:HG23	2.00	0.43
10:I:188:ILE:HB	10:I:195:THR:HB	2.00	0.43
12:K:34:VAL:HG12	12:K:42:LEU:HD12	2.01	0.43
7:T:179:LEU:HD22	7:T:192:GLU:HG2	1.99	0.43
8:U:14:THR:O	8:U:14:THR:OG1	2.36	0.43
10:W:21:ILE:HG23	10:W:187:HIS:HB2	2.00	0.43
1:M:54:SER:O	1:M:108:ASN:ND2	2.43	0.43
4:C:31:THR:OG1	4:C:163:ARG:O	2.29	0.43
7:T:87:LEU:HD23	7:T:87:LEU:HA	1.89	0.43
3:P:72:MET:HG2	3:P:138:GLY:HA3	2.01	0.43
5:R:13:ASN:HB3	6:S:126:ARG:HB3	2.00	0.43
8:U:155:ASP:OD1	8:U:155:ASP:N	2.51	0.43
8:U:234:GLU:O	8:U:238:HIS:ND1	2.38	0.43
1:a:109:THR:HA	1:a:126:ASP:HA	2.01	0.43
3:B:66:TYR:HD2	3:B:87:THR:HG21	1.84	0.43
8:G:166:THR:OG1	8:G:167:ALA:N	2.50	0.43
11:X:47:VAL:HG23	11:X:101:ASN:HB2	2.01	0.43
11:J:38:MET:HE3	11:J:44:LEU:HB3	2.00	0.43
6:S:50:LYS:HD3	6:S:59:HIS:HB3	2.00	0.43
8:U:143:ILE:HG12	8:U:220:VAL:HG12	2.01	0.43
4:C:119:THR:HG22	4:C:126:PRO:HB3	2.00	0.42
5:D:42:THR:OG1	5:D:45:GLY:O	2.28	0.42
5:D:209:LYS:O	5:D:214:ASN:ND2	2.45	0.42
3:P:76:VAL:HG11	3:P:83:ALA:HB1	2.01	0.42
6:S:93:LEU:HD23	6:S:93:LEU:HA	1.90	0.42
13:Z:122:TYR:HB3	13:Z:124:PHE:HE1	1.84	0.42
3:B:175:LEU:HD23	3:B:175:LEU:HA	1.91	0.42
3:P:119:GLN:NE2	4:Q:79:ASP:OD1	2.52	0.42
5:R:38:ILE:HG23	5:R:181:LEU:HD11	2.01	0.42
13:Z:10:GLY:HA3	13:Z:42:LYS:HE2	2.01	0.42
7:T:167:LYS:NZ	7:T:206:ASP:OD2	2.52	0.42
4:C:229:VAL:O	4:C:232:ILE:N	2.53	0.42
7:F:184:MET:HE1	7:F:192:GLU:HG3	2.01	0.42
8:G:43:ARG:HA	8:G:48:ALA:HA	2.00	0.42
11:J:28[B]:MET:HE3	11:J:28[B]:MET:HB2	1.91	0.42
4:Q:36:ARG:HD2	4:Q:142:PRO:HG2	2.02	0.42
1:M:22:ILE:HG23	1:M:50:MET:HE3	2.01	0.42
3:B:158:GLY:N	4:C:58:THR:OG1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:36:ARG:HG3	4:Q:142:PRO:HB2	2.01	0.42
12:Y:186[A]:ARG:HE	12:Y:186[A]:ARG:HB2	1.63	0.42
3:B:86:LEU:HD23	3:B:86:LEU:HA	1.86	0.42
3:P:214:ALA:HB2	3:P:227:VAL:HG22	2.02	0.42
5:R:121:LEU:HA	5:R:123:PHE:HD1	1.85	0.42
9:V:216:ILE:HG23	10:W:193:LYS:HD2	2.02	0.42
10:W:190:GLU:OE1	10:W:193:LYS:NZ	2.35	0.42
2:A:85:LEU:HA	2:A:85:LEU:HD23	1.91	0.42
11:J:27:GLN:NE2	11:X:169:LYS:O	2.53	0.42
12:K:166:ARG:NH1	10:W:33:MET:O	2.50	0.42
13:L:44:TYR:CD2	13:L:65:THR:HG21	2.55	0.42
5:R:121:LEU:HD22	5:R:123:PHE:HE1	1.85	0.42
7:T:34:SER:HB2	7:T:65:ARG:HH12	1.83	0.42
9:V:163:ILE:HG23	9:V:170:GLY:HA2	2.01	0.42
13:Z:44:TYR:CD2	13:Z:65:THR:HG21	2.55	0.42
3:B:86:LEU:HD22	3:B:114:LEU:HD11	2.01	0.42
8:G:42:VAL:HG23	8:G:165:ALA:HB2	2.02	0.42
4:Q:195:LEU:HD23	4:Q:195:LEU:HA	1.82	0.42
5:R:154:PHE:HD1	5:R:164:GLN:HA	1.84	0.42
13:Z:64:LEU:HD21	13:Z:108:ASN:HD21	1.85	0.42
9:H:206:LYS:HA	9:H:206:LYS:HD2	1.93	0.41
4:Q:196:LEU:HA	4:Q:199:VAL:HG12	2.02	0.41
3:B:38:LEU:HD23	3:B:160:LYS:HG2	2.02	0.41
9:H:63:LEU:HD23	9:H:63:LEU:HA	1.84	0.41
3:P:76:VAL:HG12	3:P:134:LEU:HG	2.02	0.41
8:U:50:ILE:HD12	8:U:79:VAL:HB	2.01	0.41
9:V:11:GLY:HA2	9:V:108:PRO:HB3	2.02	0.41
3:B:176:LYS:HA	4:C:53:LEU:HD11	2.02	0.41
4:C:234:LYS:HA	4:C:234:LYS:HD3	1.72	0.41
7:F:72:HIS:CE1	7:F:105:ASN:HB3	2.55	0.41
14:b:41:ILE:HG12	14:b:76:VAL:HG22	2.02	0.41
1:M:109:THR:HA	1:M:126:ASP:HA	2.01	0.41
14:N:4:MET:HG3	14:N:127:ILE:HG22	2.03	0.41
3:P:9:THR:HB	3:P:20:GLN:HG3	2.02	0.41
3:P:123:GLN:HG3	4:Q:125:ARG:HG2	2.02	0.41
3:P:158:GLY:N	4:Q:58:THR:OG1	2.54	0.41
6:S:192:LEU:HD21	6:S:212:ILE:HD11	2.02	0.41
2:A:94:GLN:HG3	9:H:65:LEU:HD22	2.03	0.41
4:Q:186:LEU:HD12	4:Q:189:LYS:HB3	2.03	0.41
8:U:217:VAL:HB	8:U:230:LEU:HD12	2.03	0.41
10:W:188:ILE:HB	10:W:195:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:240:HIS:NE2	3:B:244:GLU:OE2	2.54	0.41
4:Q:36:ARG:HH21	4:Q:157:LYS:HG2	1.86	0.41
10:W:47:ARG:HB3	10:W:111:LEU:HB2	2.03	0.41
1:M:70:MET:HE2	1:M:70:MET:HB3	1.75	0.41
5:D:169:ALA:O	5:D:174:SER:OG	2.30	0.41
6:E:36:VAL:HG23	6:E:47:VAL:HB	2.01	0.41
8:G:153:LYS:HE2	8:G:163:PHE:HE2	1.86	0.41
10:I:148:MET:HE2	10:I:172:ASN:HD22	1.85	0.41
2:O:119:GLU:O	2:O:123:SER:OG	2.29	0.41
3:P:33:THR:HG21	3:P:200:THR:HG21	2.03	0.41
3:P:34:CYS:HA	3:P:47:ALA:HA	2.02	0.41
9:H:110:LEU:HD21	9:H:125:VAL:HG22	2.01	0.41
3:P:2:SER:OG	4:Q:5:ARG:NH2	2.54	0.41
4:Q:192:ILE:O	4:Q:196:LEU:HB2	2.21	0.41
7:T:99:ARG:NH1	1:a:69:GLN:OE1	2.51	0.41
14:b:4:MET:HG3	14:b:127:ILE:HG22	2.02	0.41
3:B:165:GLY:O	3:B:168:SER:OG	2.36	0.41
4:C:186:LEU:HA	4:C:189:LYS:HB2	2.03	0.41
9:V:63:LEU:HA	9:V:63:LEU:HD23	1.85	0.41
12:Y:73:ARG:HH12	12:Y:105:ASP:HA	1.85	0.41
13:Z:99:ARG:HH21	13:Z:102:PHE:HD2	1.69	0.41
2:A:65:GLU:HG2	2:A:86:VAL:HG11	2.03	0.41
3:B:9:THR:HB	3:B:20:GLN:HG3	2.03	0.41
5:D:13:ASN:HB3	6:E:126:ARG:HB3	2.03	0.41
6:E:45:VAL:HG11	6:E:188:VAL:HA	2.03	0.41
6:E:117:GLN:NE2	7:F:83:ASP:OD1	2.54	0.41
10:I:27:PHE:HB2	10:I:38:PHE:HB2	2.03	0.41
4:Q:136:PHE:HE1	4:Q:142:PRO:HB3	1.86	0.41
10:W:1:SER:HB2	10:W:4:SER:HB3	2.02	0.41
8:G:205:VAL:HG23	8:G:206:LEU:HD12	2.03	0.40
6:S:84:LEU:HD12	6:S:84:LEU:HA	1.93	0.40
7:T:72:HIS:CE1	7:T:105:ASN:HB3	2.55	0.40
9:V:36:PHE:HD1	9:V:42:TYR:HE1	1.69	0.40
10:W:4:SER:O	10:W:4:SER:OG	2.36	0.40
4:C:17:PHE:HD1	4:C:17:PHE:HA	1.79	0.40
2:O:21:ILE:HG21	2:O:151:SER:HB3	2.02	0.40
1:a:70:MET:HB3	1:a:70:MET:HE2	1.75	0.40
6:E:180:MET:HG2	6:E:181:GLU:HG2	2.04	0.40
12:K:74:ILE:HD12	12:K:74:ILE:HA	1.94	0.40
7:F:160:TYR:HD1	7:F:160:TYR:HA	1.77	0.40
9:H:201:ARG:HD2	9:H:201:ARG:HA	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:83:VAL:HG21	4:Q:129:ILE:HD11	2.04	0.40
7:T:66:LEU:HD12	7:T:212:GLU:HG2	2.02	0.40
13:Z:12:ILE:HG13	13:Z:109:ILE:HD12	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	M	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
1	a	215/216 (100%)	207 (96%)	8 (4%)	0	100	100
2	A	230/230 (100%)	221 (96%)	9 (4%)	0	100	100
2	O	228/230 (99%)	219 (96%)	9 (4%)	0	100	100
3	B	247/248 (100%)	237 (96%)	9 (4%)	1 (0%)	30	62
3	P	247/248 (100%)	234 (95%)	10 (4%)	3 (1%)	10	41
4	C	232/237 (98%)	215 (93%)	12 (5%)	5 (2%)	5	30
4	Q	225/237 (95%)	212 (94%)	12 (5%)	1 (0%)	30	62
5	D	233/233 (100%)	221 (95%)	11 (5%)	1 (0%)	30	62
5	R	232/233 (100%)	221 (95%)	10 (4%)	1 (0%)	30	62
6	E	229/238 (96%)	215 (94%)	12 (5%)	2 (1%)	14	47
6	S	236/238 (99%)	227 (96%)	8 (3%)	1 (0%)	30	62
7	F	241/240 (100%)	237 (98%)	4 (2%)	0	100	100
7	T	239/240 (100%)	231 (97%)	8 (3%)	0	100	100
8	G	235/244 (96%)	230 (98%)	5 (2%)	0	100	100
8	U	222/244 (91%)	215 (97%)	6 (3%)	1 (0%)	24	57
9	H	220/220 (100%)	217 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	220/220 (100%)	215 (98%)	5 (2%)	0	100	100
10	I	208/204 (102%)	202 (97%)	5 (2%)	1 (0%)	24	57
10	W	204/204 (100%)	195 (96%)	8 (4%)	1 (0%)	24	57
11	J	193/196 (98%)	179 (93%)	14 (7%)	0	100	100
11	X	193/196 (98%)	186 (96%)	7 (4%)	0	100	100
12	K	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
12	Y	200/201 (100%)	194 (97%)	6 (3%)	0	100	100
13	L	213/213 (100%)	204 (96%)	9 (4%)	0	100	100
13	Z	212/213 (100%)	203 (96%)	9 (4%)	0	100	100
14	N	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
14	b	202/203 (100%)	193 (96%)	9 (4%)	0	100	100
All	All	6170/6246 (99%)	5923 (96%)	229 (4%)	18 (0%)	37	67

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	203	GLY
4	C	204	LYS
4	C	233	GLU
6	E	56	LEU
3	P	239	LYS
6	S	53	GLN
3	P	238	LYS
3	B	210	LYS
6	E	55	GLU
5	D	121	LEU
10	I	30	GLN
3	P	240	HIS
4	C	202	GLY
4	Q	52	LYS
5	R	121	LEU
10	W	30	GLN
8	U	57	PRO
4	C	232	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	M	179/179 (100%)	178 (99%)	1 (1%)	78	79
1	a	180/179 (101%)	180 (100%)	0	100	100
2	A	191/189 (101%)	190 (100%)	1 (0%)	81	80
2	O	189/189 (100%)	187 (99%)	2 (1%)	65	74
3	B	209/208 (100%)	208 (100%)	1 (0%)	81	80
3	P	209/208 (100%)	207 (99%)	2 (1%)	68	75
4	C	200/201 (100%)	198 (99%)	2 (1%)	68	75
4	Q	197/201 (98%)	196 (100%)	1 (0%)	81	80
5	D	196/195 (100%)	196 (100%)	0	100	100
5	R	195/195 (100%)	195 (100%)	0	100	100
6	E	199/204 (98%)	198 (100%)	1 (0%)	81	80
6	S	206/204 (101%)	204 (99%)	2 (1%)	68	75
7	F	201/198 (102%)	201 (100%)	0	100	100
7	T	199/198 (100%)	199 (100%)	0	100	100
8	G	207/208 (100%)	207 (100%)	0	100	100
8	U	196/208 (94%)	194 (99%)	2 (1%)	68	75
9	H	183/181 (101%)	183 (100%)	0	100	100
9	V	183/181 (101%)	181 (99%)	2 (1%)	65	74
10	I	178/173 (103%)	178 (100%)	0	100	100
10	W	175/173 (101%)	175 (100%)	0	100	100
11	J	168/167 (101%)	167 (99%)	1 (1%)	78	79
11	X	168/167 (101%)	167 (99%)	1 (1%)	78	79
12	K	156/156 (100%)	156 (100%)	0	100	100
12	Y	158/156 (101%)	158 (100%)	0	100	100
13	L	180/178 (101%)	177 (98%)	3 (2%)	53	70
13	Z	179/178 (101%)	178 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	158/158 (100%)	158 (100%)	0	100	100
14	b	159/158 (101%)	159 (100%)	0	100	100
All	All	5198/5190 (100%)	5175 (100%)	23 (0%)	81	81

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	21	VAL
2	A	139	ASN
3	B	43	VAL
4	C	208	LEU
4	C	215	GLN
6	E	195	LEU
11	J	150	THR
13	L	3[A]	SER
13	L	3[B]	SER
13	L	199	THR
2	O	3	ARG
2	O	43	VAL
3	P	7[A]	SER
3	P	7[B]	SER
4	Q	53	LEU
6	S	65[A]	HIS
6	S	65[B]	HIS
8	U	87	SER
8	U	195	VAL
9	V	104[A]	ASP
9	V	104[B]	ASP
11	X	150	THR
13	Z	199	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	81	HIS
2	A	108	GLN
2	A	188	HIS
3	B	146	GLN
3	B	155	ASN
3	B	230	GLN

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Mol	Chain	Res	Type
5	D	152	GLN
5	D	182	GLN
7	F	72	HIS
8	G	33	ASN
8	G	92	GLN
8	G	128	ASN
9	H	153	ASN
10	I	168	GLN
10	I	187	HIS
11	J	8	GLN
11	J	27	GLN
11	J	55	GLN
12	K	70	ASN
12	K	85	ASN
12	K	175	ASN
13	L	79	ASN
13	L	80	ASN
13	L	108	ASN
14	N	66	HIS
14	N	158	ASN
2	O	139	ASN
2	O	147	GLN
2	O	165	ASN
3	P	40	ASN
3	P	146	GLN
3	P	155	ASN
3	P	240	HIS
4	Q	18	GLN
4	Q	122	ASN
4	Q	175	ASN
5	R	104	ASN
5	R	182	GLN
5	R	186	HIS
5	R	227	HIS
6	S	31	GLN
7	T	72	HIS
8	U	90	GLN
8	U	150	GLN
10	W	156	ASN
10	W	187	HIS
11	X	8	GLN
11	X	27	GLN

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Mol	Chain	Res	Type
11	X	63	ASN
11	X	132	HIS
12	Y	70	ASN
12	Y	162	GLN
13	Z	79	ASN
13	Z	80	ASN
13	Z	108	ASN
13	Z	157	ASN
1	a	81	HIS
14	b	66	HIS
14	b	158	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

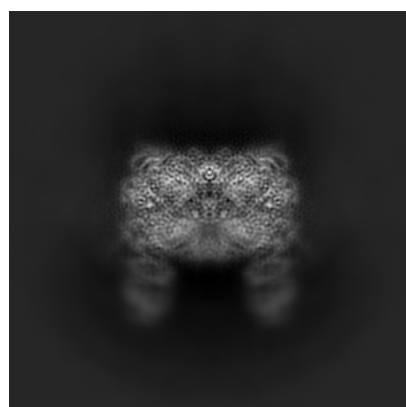
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4738. These allow visual inspection of the internal detail of the map and identification of artifacts.

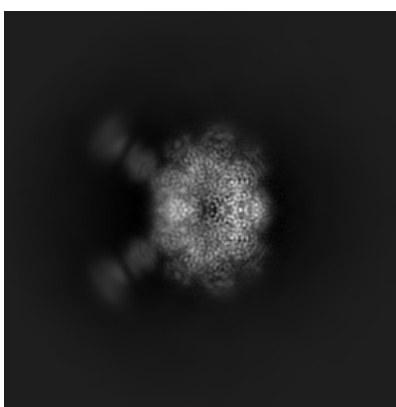
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

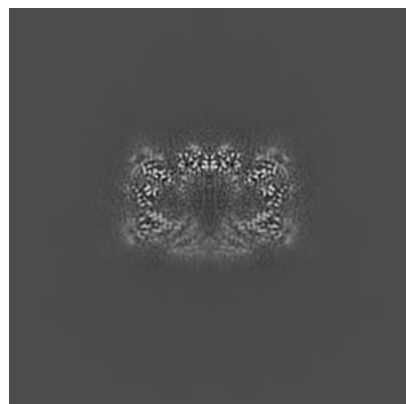


Z

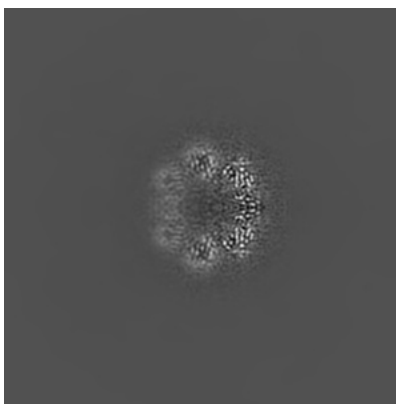
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

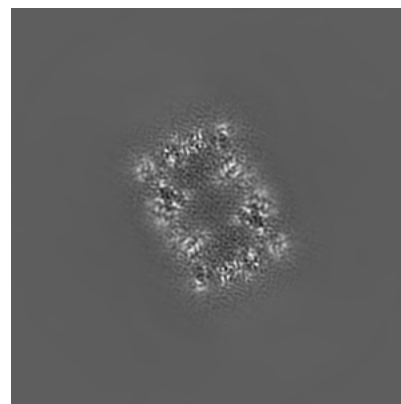
6.2.1 Primary map



X Index: 192



Y Index: 192

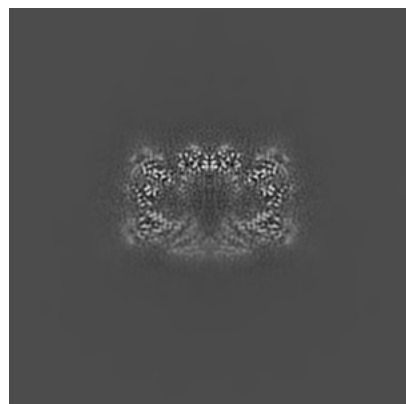


Z Index: 192

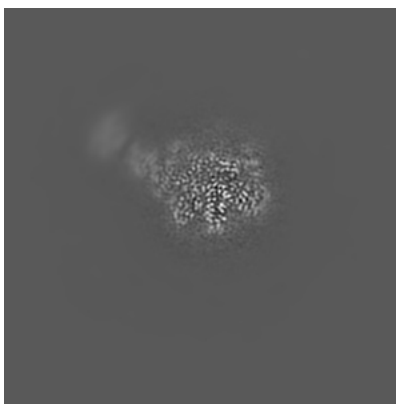
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

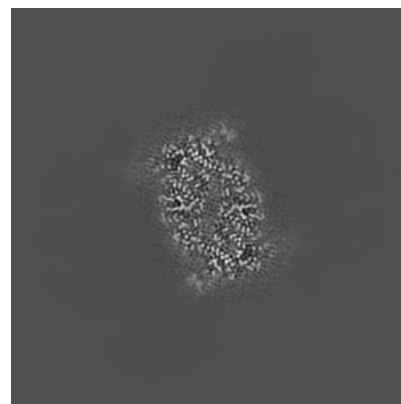
6.3.1 Primary map



X Index: 192



Y Index: 135

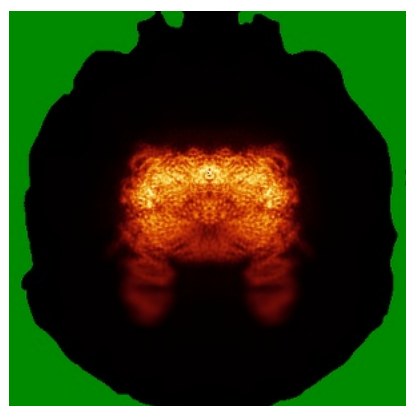


Z Index: 223

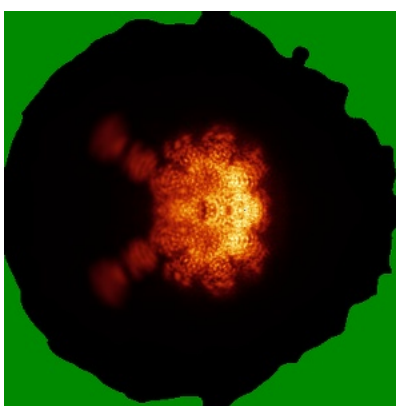
The images above show the largest variance slices of the map in three orthogonal directions.

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

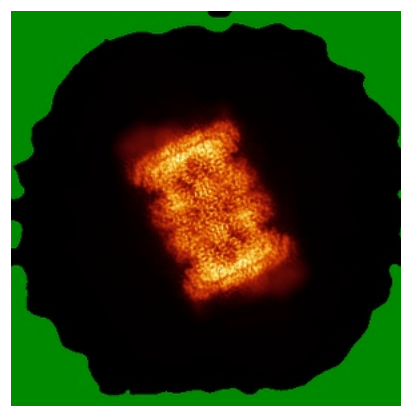
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

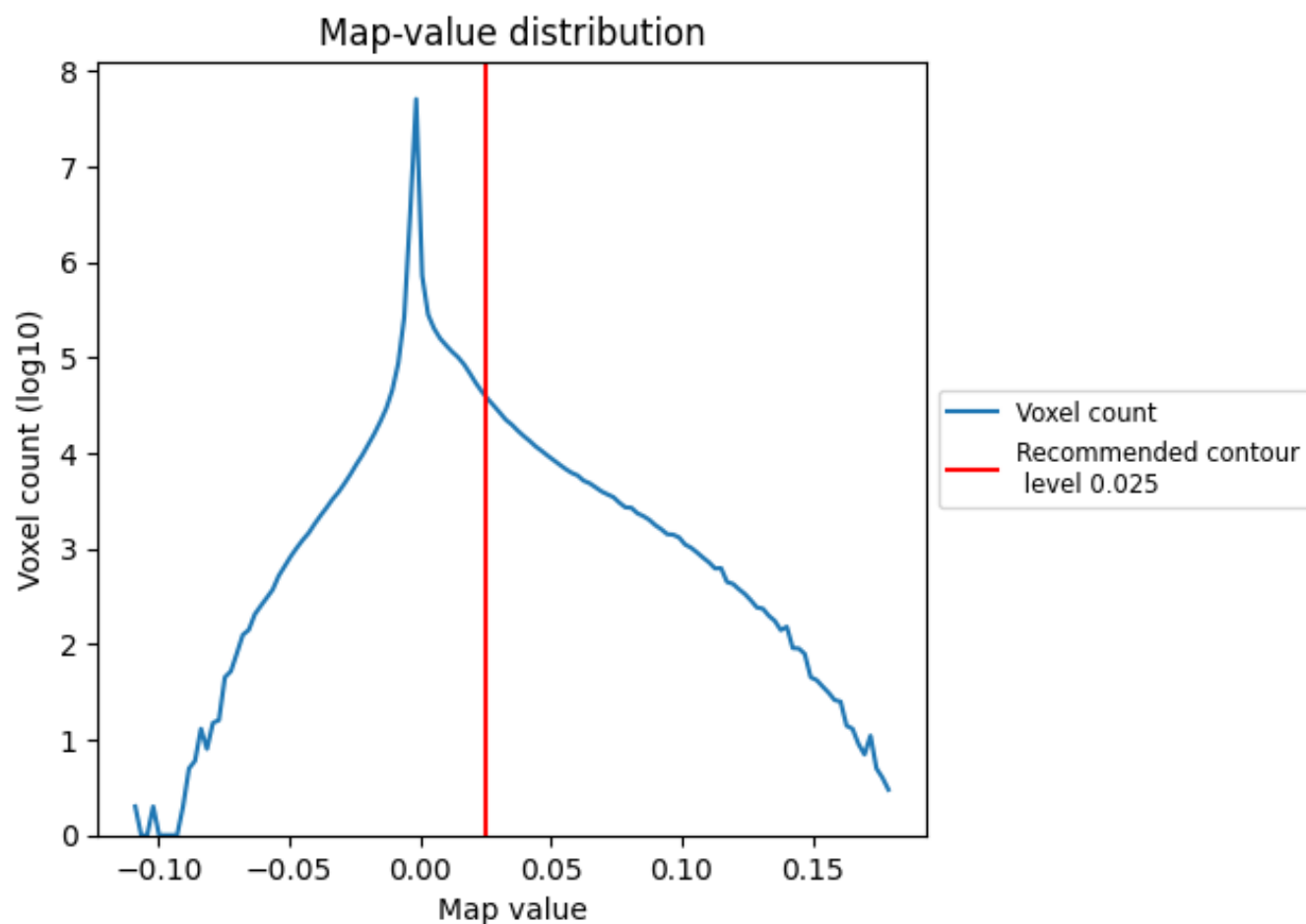
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

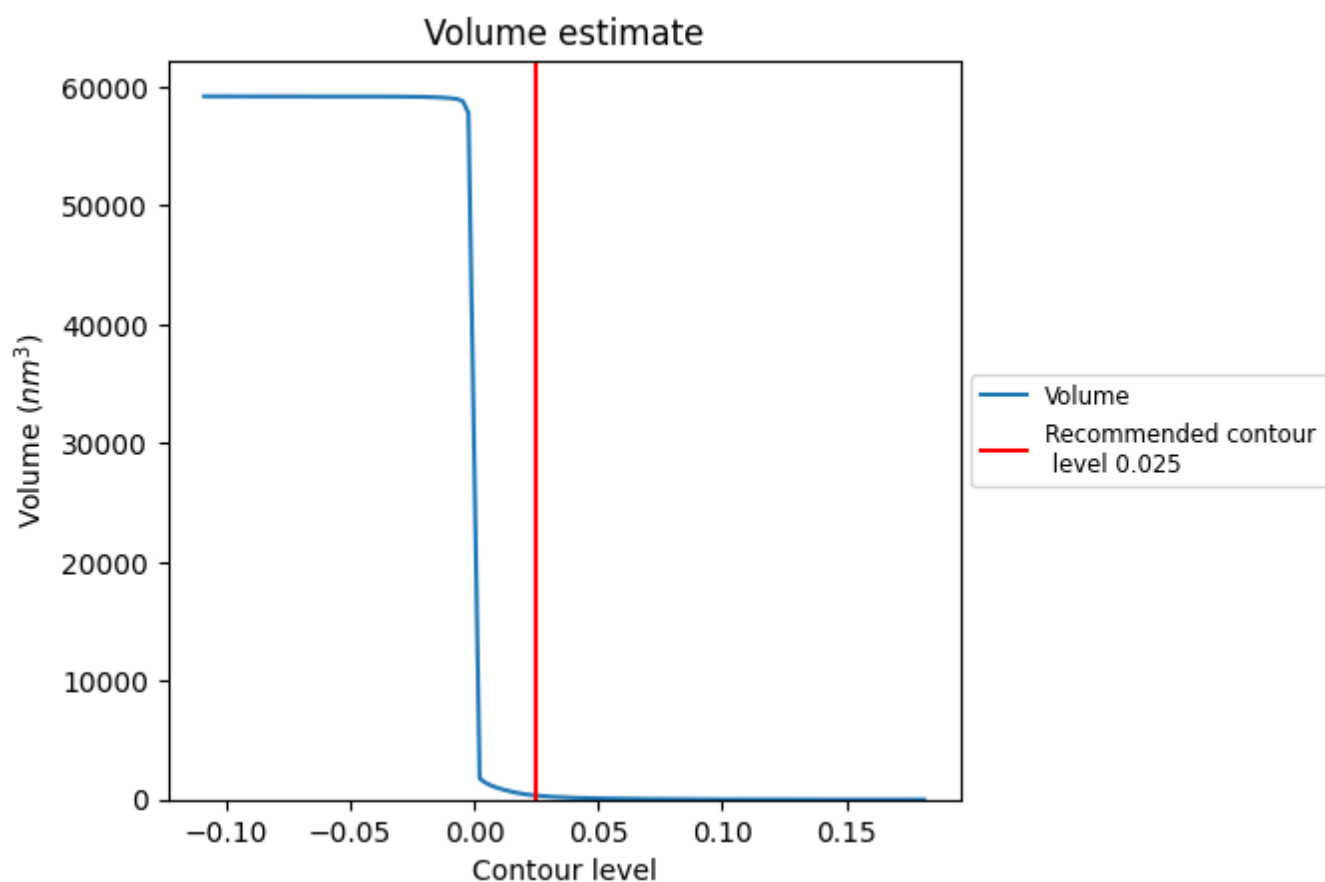
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

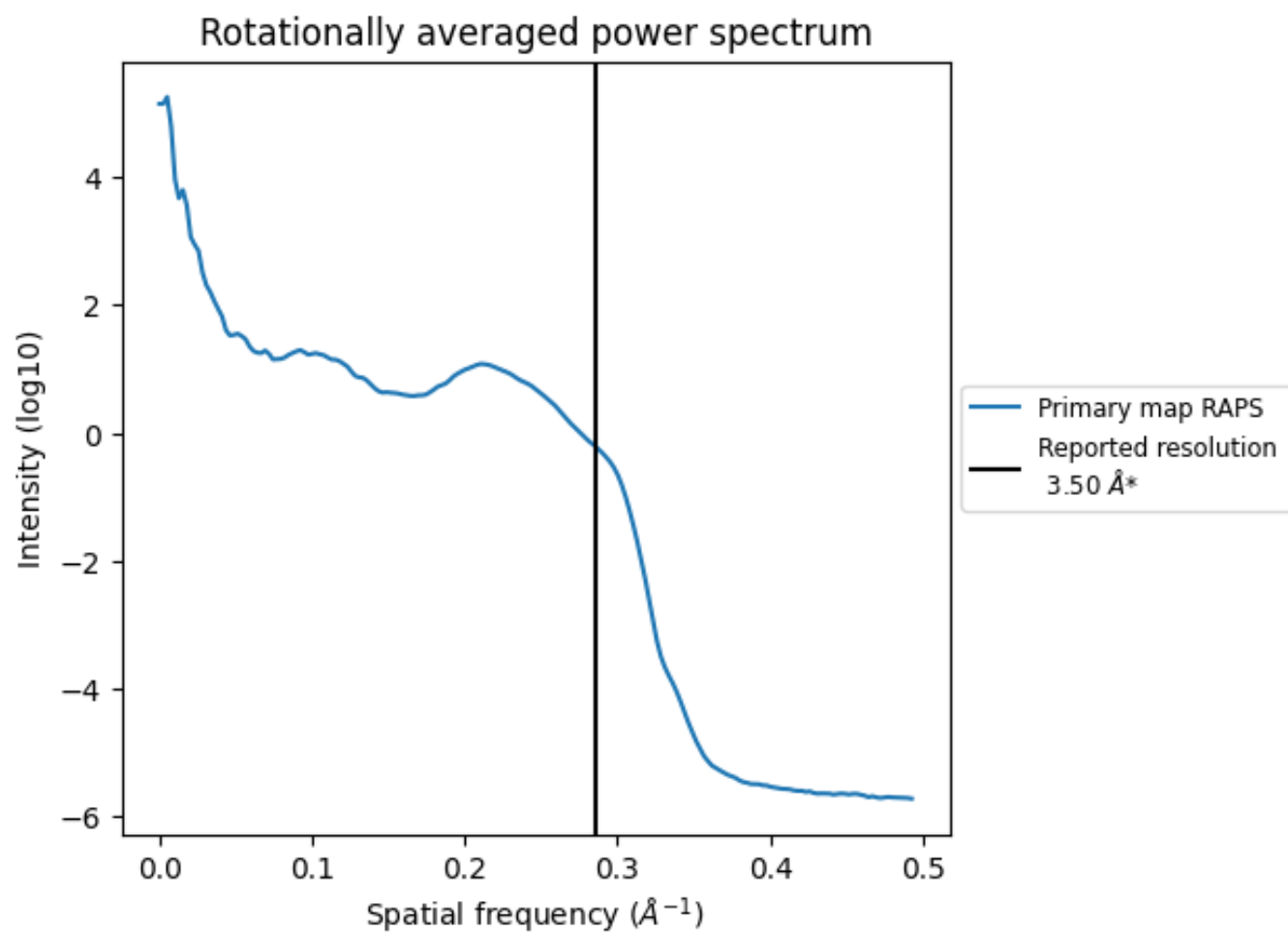
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm³; this corresponds to an approximate mass of 304 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 ⓘ

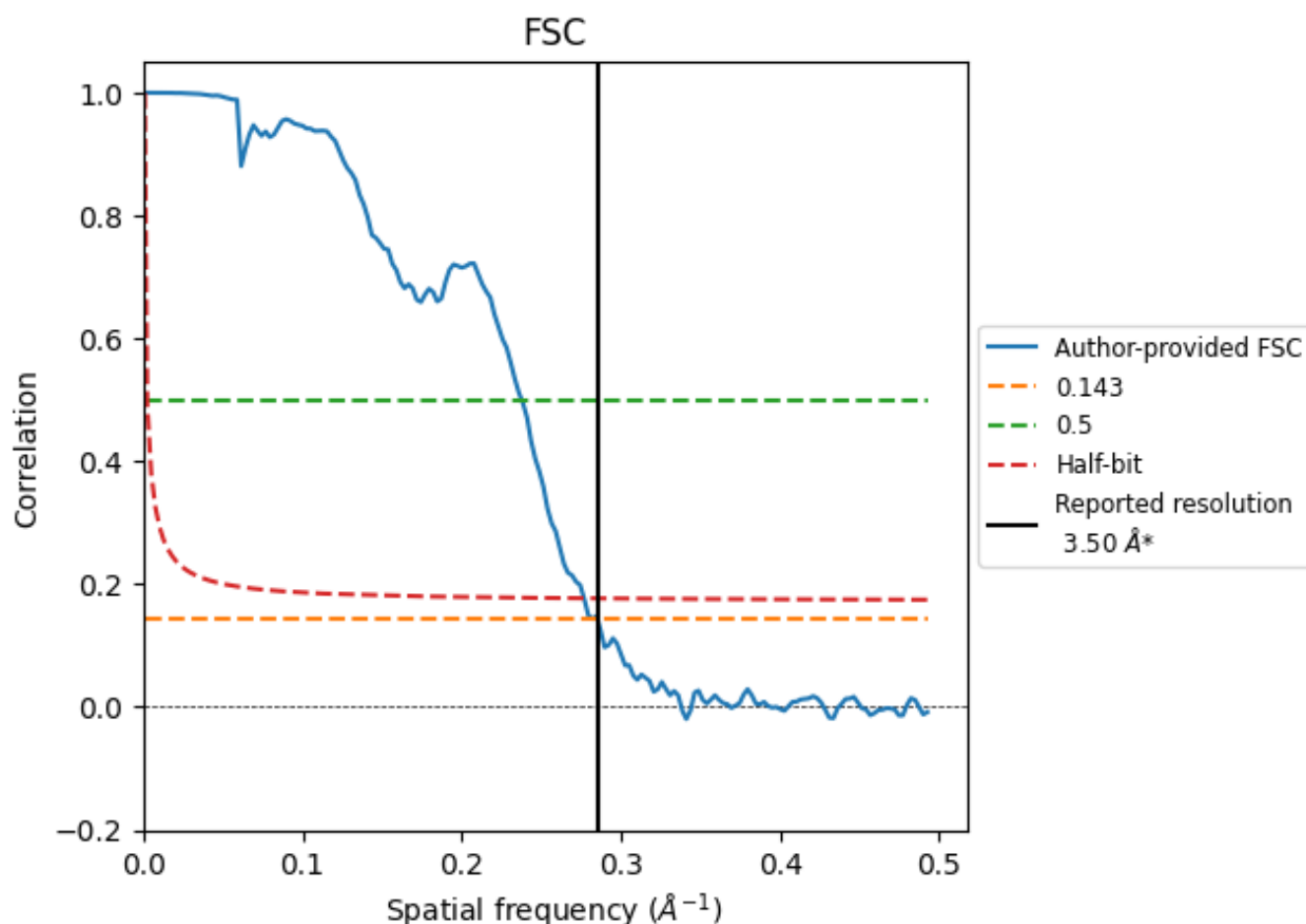


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	4.21	3.61
Unmasked-calculated*	-	-	-

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

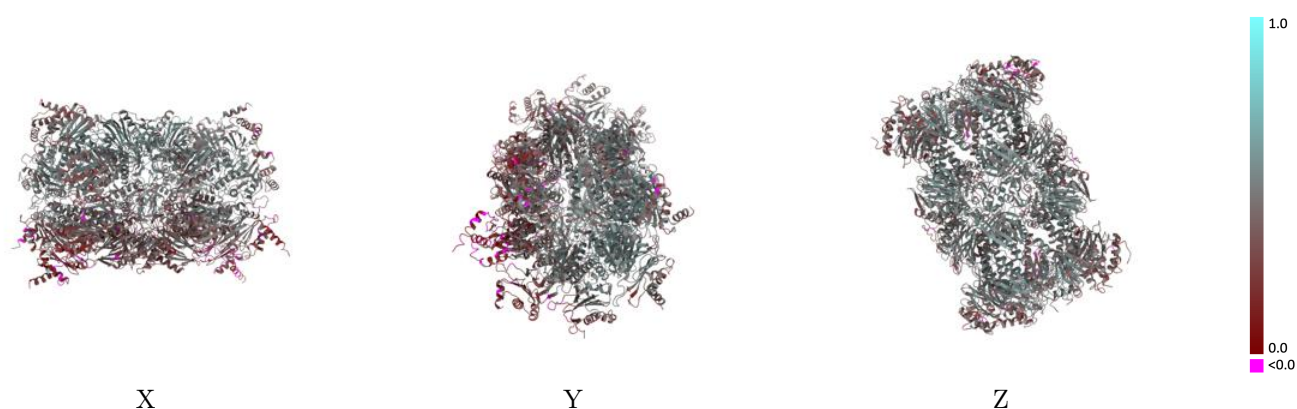
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4738 and PDB model 6R70. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

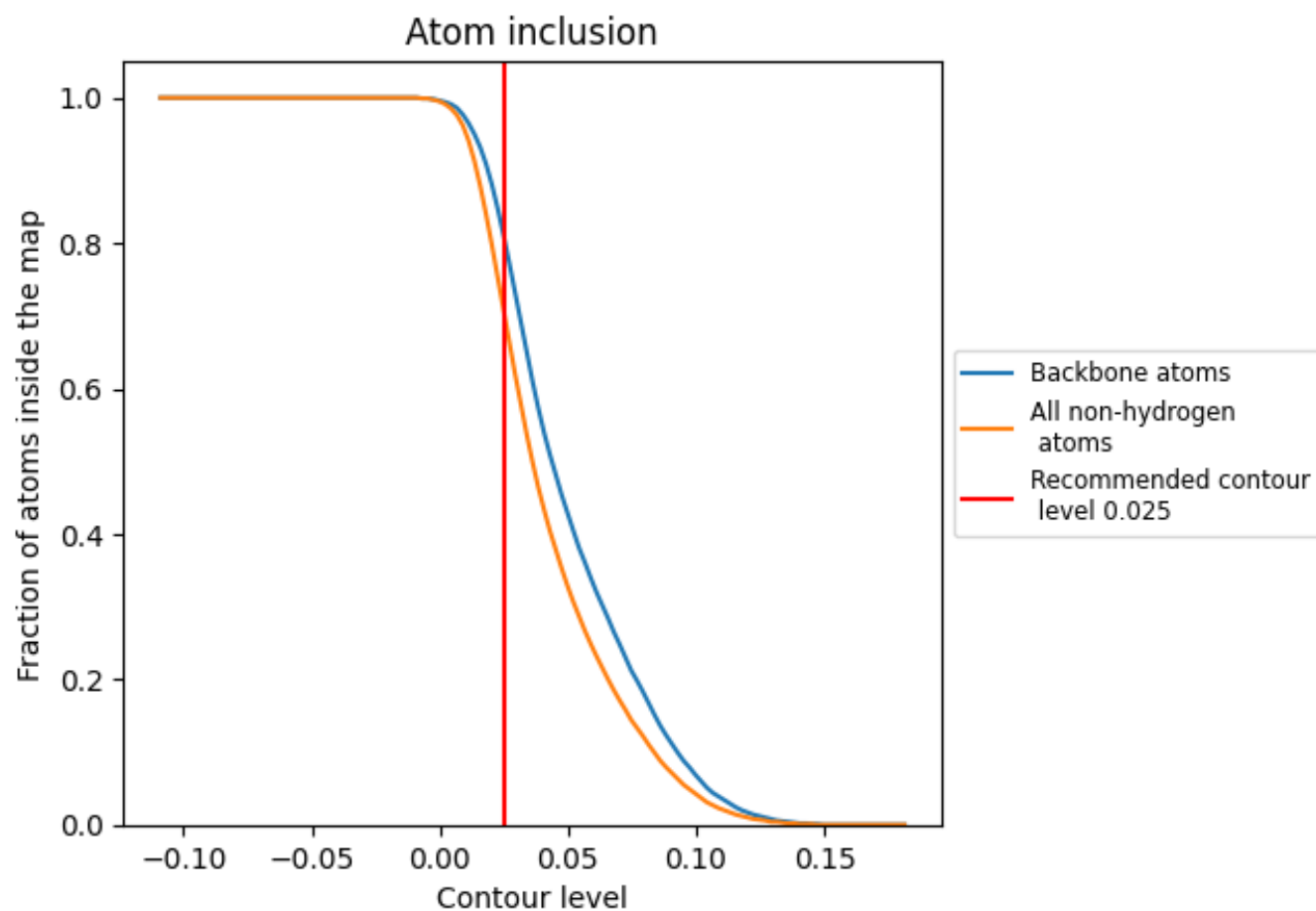


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 71% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7060	 0.4190
A	 0.8140	 0.4670
B	 0.7100	 0.3890
C	 0.5190	 0.2580
D	 0.6520	 0.3420
E	 0.7930	 0.4180
F	 0.8120	 0.4710
G	 0.7730	 0.4540
H	 0.7260	 0.4450
I	 0.6570	 0.4190
J	 0.5220	 0.3580
K	 0.3960	 0.3450
L	 0.7080	 0.4380
M	 0.8790	 0.5220
N	 0.8720	 0.5080
O	 0.8210	 0.4740
P	 0.7100	 0.3960
Q	 0.5410	 0.2760
R	 0.6700	 0.3560
S	 0.7810	 0.4220
T	 0.8160	 0.4700
U	 0.8200	 0.4770
V	 0.7330	 0.4550
W	 0.6600	 0.4210
X	 0.4930	 0.3600
Y	 0.3660	 0.3400
Z	 0.7060	 0.4400
a	 0.8710	 0.5120
b	 0.8680	 0.5050

