



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:04 AM UTC

PDB ID : 6QM8 / pdb_00006qm8
EMDB ID : EMD-4591
Title : Leishmania tarentolae proteasome 20S subunit apo structure
Authors : Rowland, P.; Goswami, P.
Deposited on : 2019-02-01
Resolution : 3.30 Å(reported)
Based on initial model : 4R3O

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:

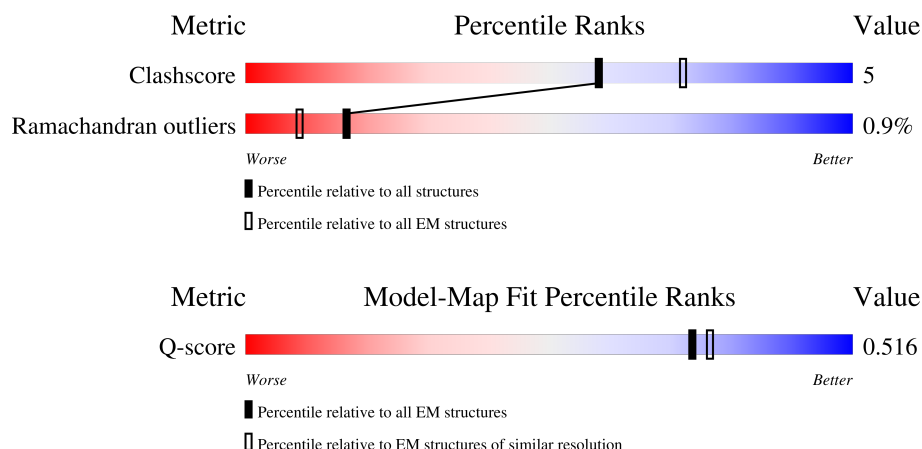
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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.



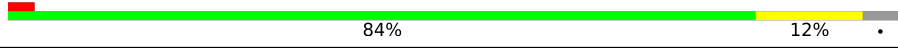
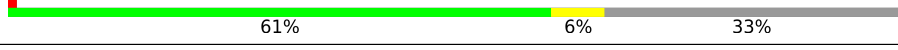
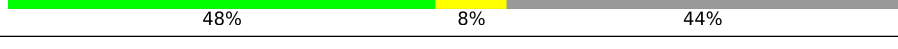
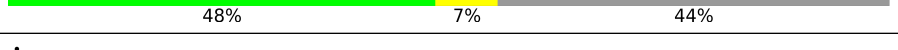
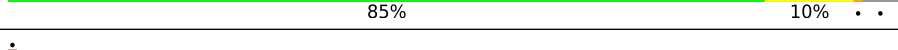
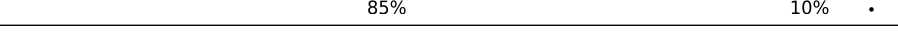
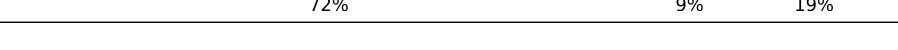
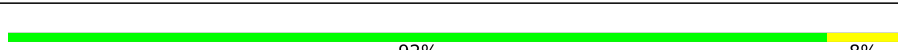
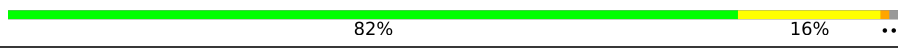
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	250	
1	O	250	
2	B	231	
2	P	231	
3	C	285	

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Mol	Chain	Length	Quality of chain
3	Q	285	
4	D	248	
4	R	248	
5	E	344	
5	S	344	
6	F	428	
6	T	428	
7	G	238	
7	U	238	
8	H	283	
8	V	283	
9	I	254	
9	W	254	
10	J	205	
10	X	205	
11	K	206	
11	Y	206	
12	L	302	
12	Z	302	
13	M	339	
13	a	339	
14	N	220	
14	b	220	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 49124 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 alpha1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1857	1169	323	353	12		
1	O	244	Total	C	N	O	S	0	0
			1857	1169	323	353	12		

- Molecule 2 is a protein called Proteasome alpha2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1754	1112	292	342	8		
2	P	229	Total	C	N	O	S	0	0
			1754	1112	292	342	8		

- Molecule 3 is a protein called Proteasome alpha3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	276	Total	C	N	O	S	0	0
			2195	1379	382	422	12		
3	Q	276	Total	C	N	O	S	0	0
			2195	1379	382	422	12		

- Molecule 4 is a protein called Proteasome alpha4 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	239	Total	C	N	O	S	0	0
			1873	1180	322	363	8		
4	R	239	Total	C	N	O	S	0	0
			1873	1180	322	363	8		

- Molecule 5 is a protein called Proteasome alpha5 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	229	Total	C	N	O	S	0	0
			1756	1094	302	347	13		
5	S	229	Total	C	N	O	S	0	0
			1756	1094	302	347	13		

- Molecule 6 is a protein called Proteasome alpha6 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		
6	T	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		

- Molecule 7 is a protein called Proteasome alpha7 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	228	Total	C	N	O	S	0	0
			1727	1077	306	334	10		
7	U	228	Total	C	N	O	S	0	0
			1727	1077	306	334	10		

- Molecule 8 is a protein called Proteasome beta1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total	C	N	O	S	0	0
			1710	1062	295	341	12		
8	V	229	Total	C	N	O	S	0	0
			1710	1062	295	341	12		

- Molecule 9 is a protein called Proteasome beta2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		
9	W	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		

- Molecule 10 is a protein called Proteasome beta3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

- Molecule 11 is a protein called Proteasome beta4 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		
11	Y	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		

- Molecule 12 is a protein called Proteasome beta5 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	202	Total	C	N	O	S	0	0
			1579	998	277	297	7		
12	Z	202	Total	C	N	O	S	0	0
			1579	998	277	297	7		

- Molecule 13 is a protein called Proteasome beta6 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		
13	a	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		

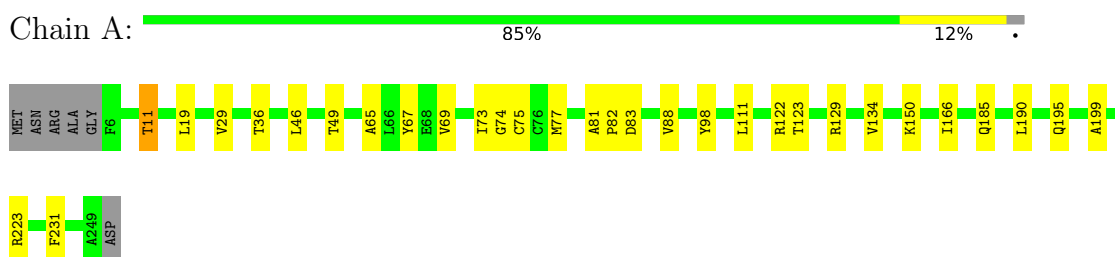
- Molecule 14 is a protein called Proteasome beta7 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		
14	b	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		

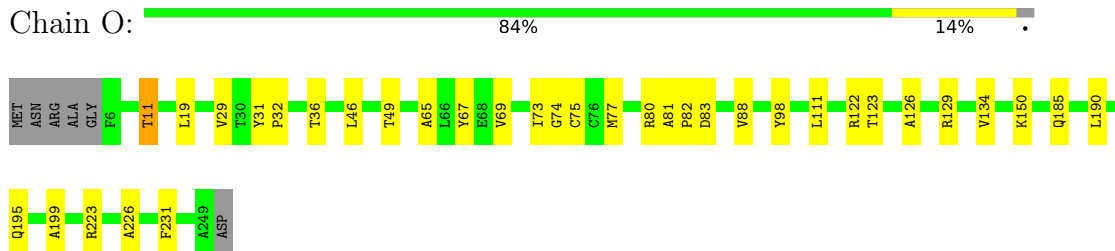
3 Residue-property plots [i](#)

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.

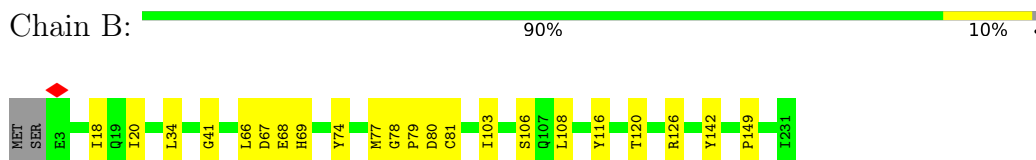
- Molecule 1: Proteasome alpha1 chain



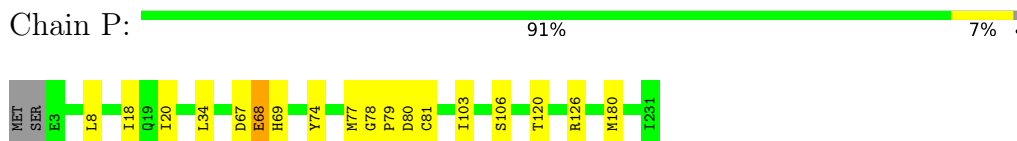
- Molecule 1: Proteasome alpha1 chain



- Molecule 2: Proteasome alpha2 chain

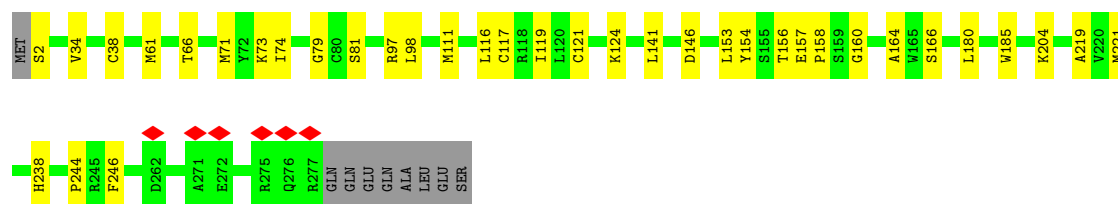


- Molecule 2: Proteasome alpha2 chain



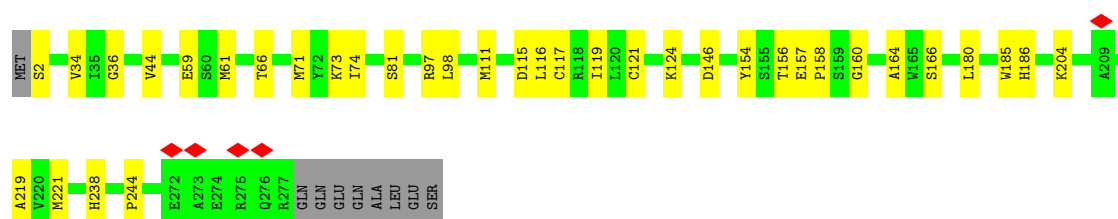
- Molecule 3: Proteasome alpha3 chain

Chain C:  84% 13% .



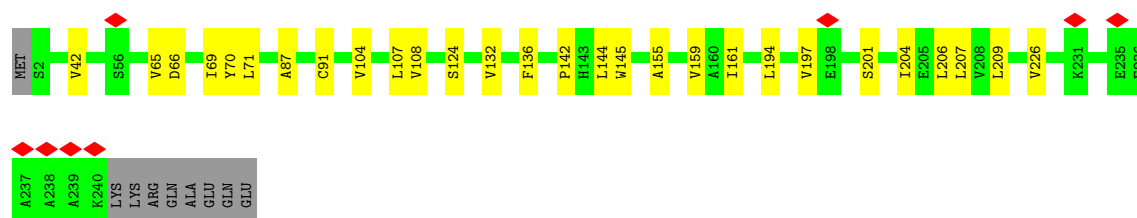
- Molecule 3: Proteasome alpha3 chain

Chain Q:  84% 13% .



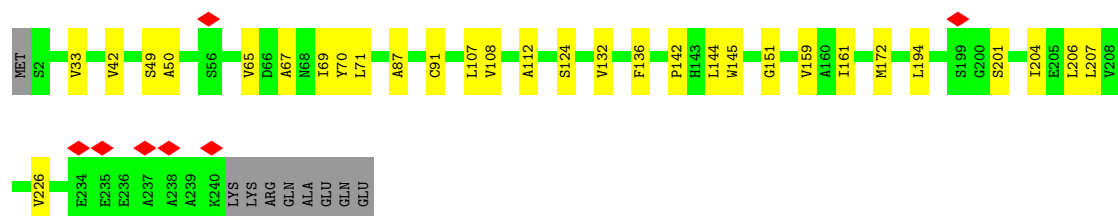
- Molecule 4: Proteasome alpha4 chain

Chain D:  85% 11% .



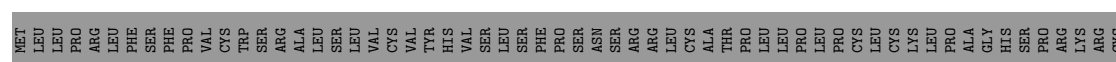
- Molecule 4: Proteasome alpha4 chain

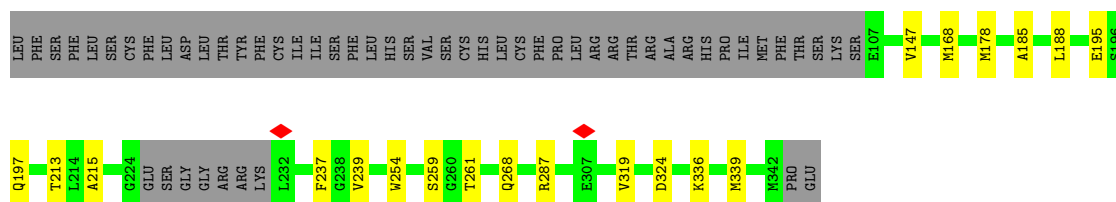
Chain R:  84% 12% .



- Molecule 5: Proteasome alpha5 chain

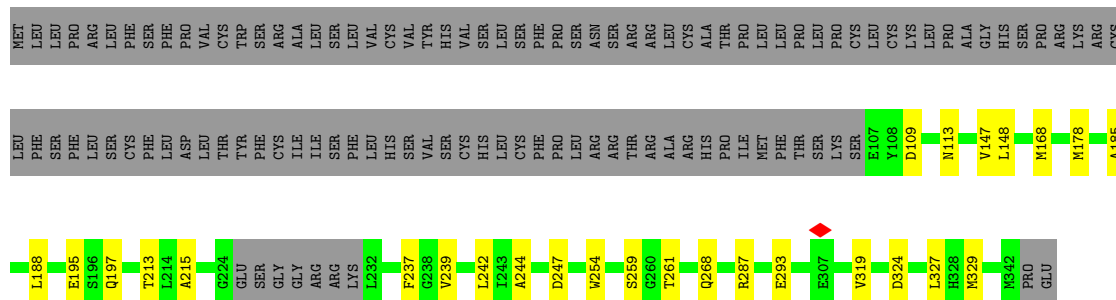
Chain E:  61% 6% 33%





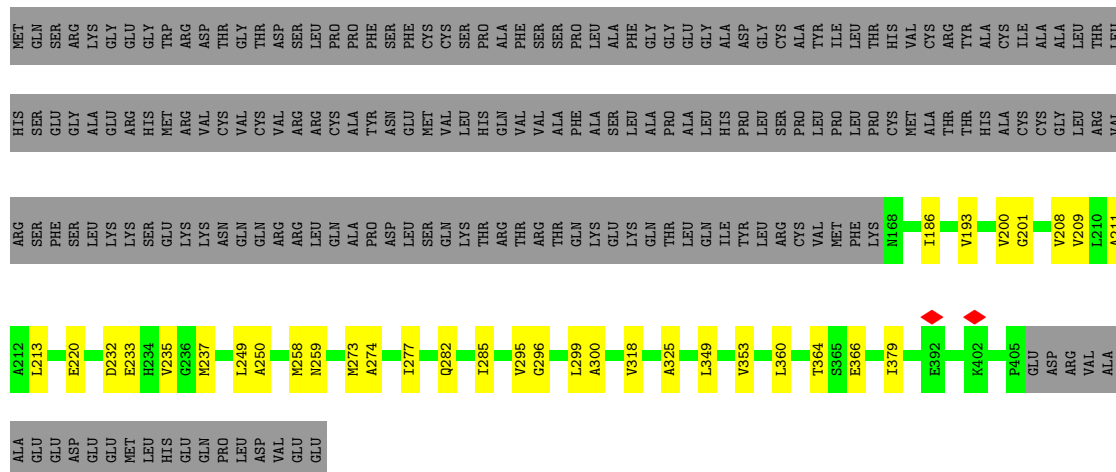
• Molecule 5: Proteasome alpha5 chain

Chain S: 59% 8% 33%



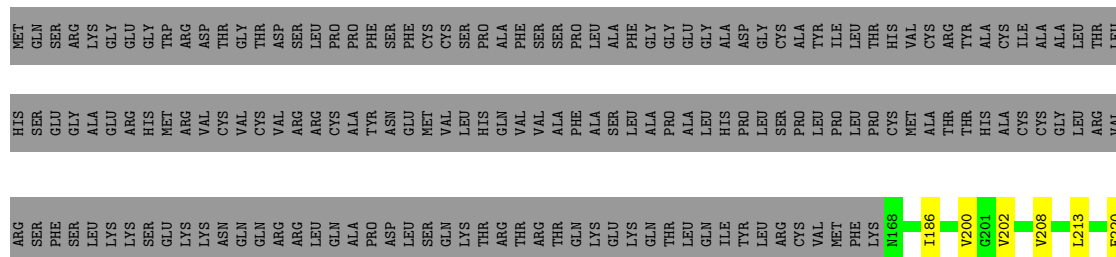
• Molecule 6: Proteasome alpha6 chain

Chain F: 48% 8% 44%



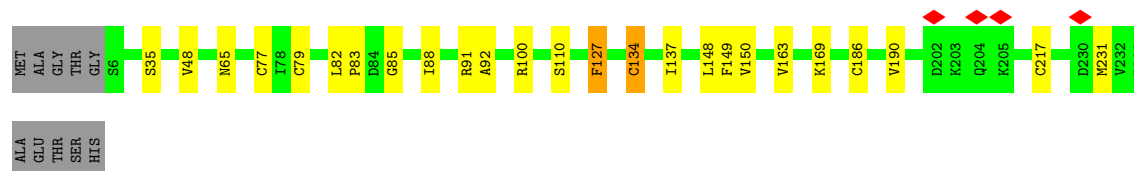
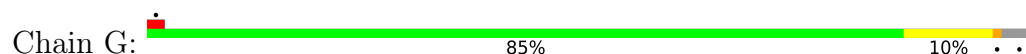
• Molecule 6: Proteasome alpha6 chain

Chain T: 48% 7% 44%

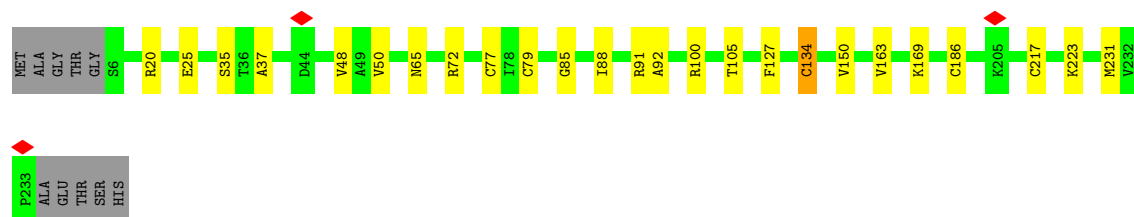
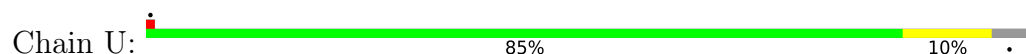




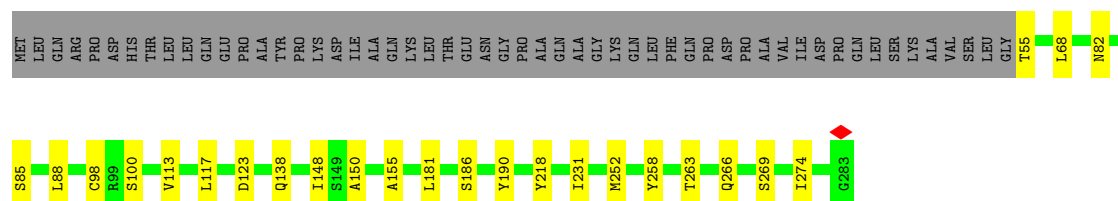
• Molecule 7: Proteasome alpha7 chain



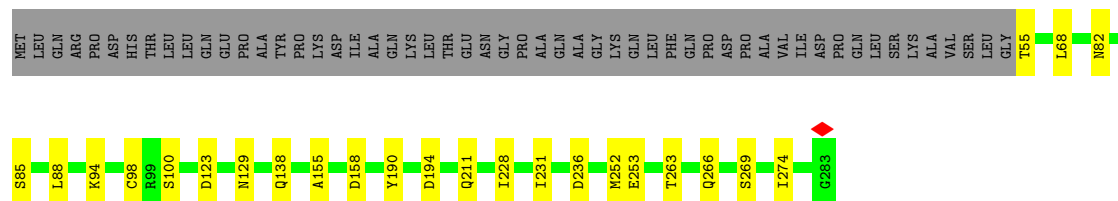
• Molecule 7: Proteasome alpha7 chain



• Molecule 8: Proteasome beta1 chain

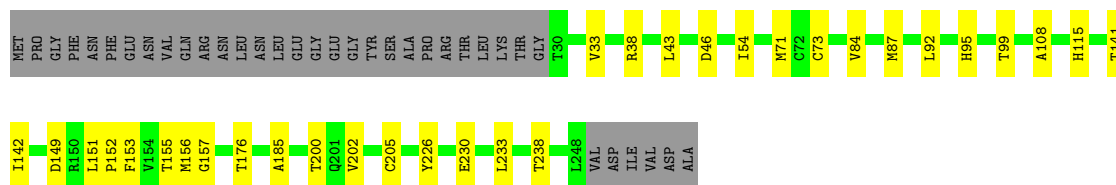


• Molecule 8: Proteasome beta1 chain



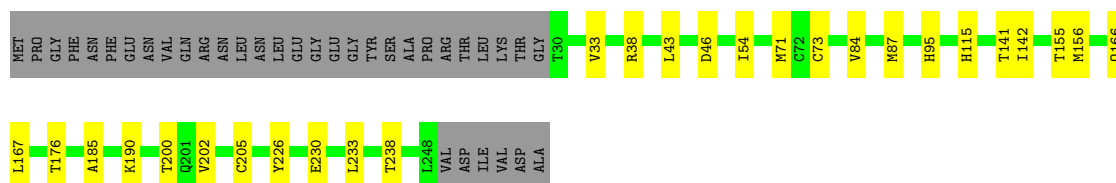
• Molecule 9: Proteasome beta2 chain

Chain I:  74% 13% 14%



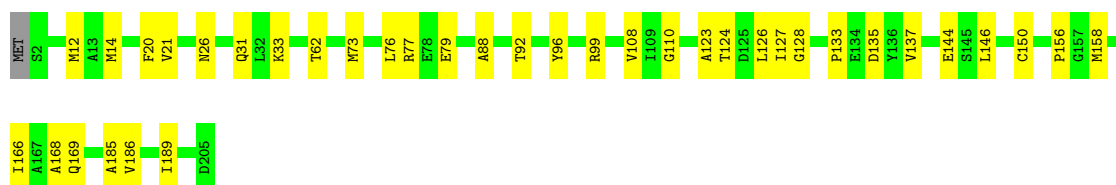
• Molecule 9: Proteasome beta2 chain

Chain W:  76% 11% 14%



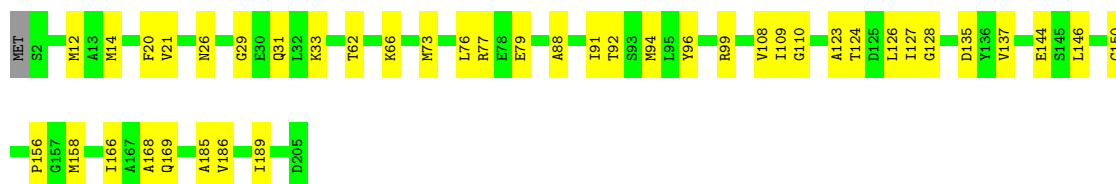
• Molecule 10: Proteasome beta3 chain

Chain J:  81% 18%

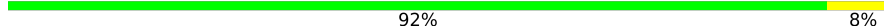


• Molecule 10: Proteasome beta3 chain

Chain X:  80% 20%



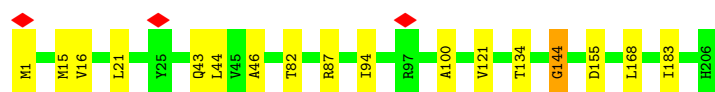
• Molecule 11: Proteasome beta4 chain

Chain K:  92% 8%



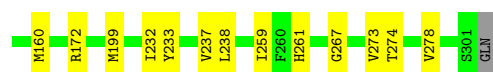
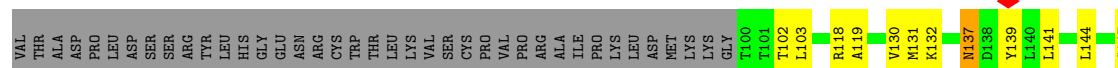
• Molecule 11: Proteasome beta4 chain

Chain Y:  92% 8%



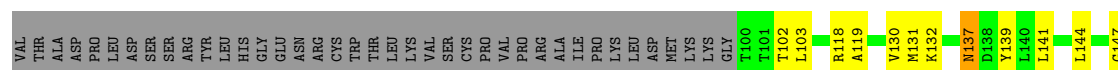
• Molecule 12: Proteasome beta5 chain

Chain L: 59% 8% 33%



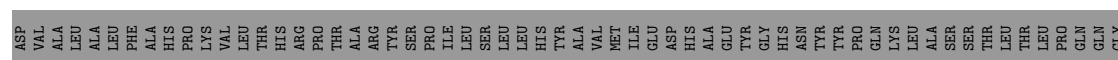
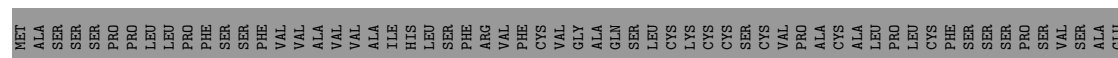
• Molecule 12: Proteasome beta5 chain

Chain Z: 58% 9% 33%



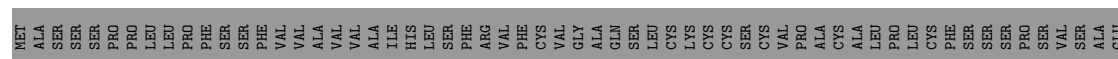
• Molecule 13: Proteasome beta6 chain

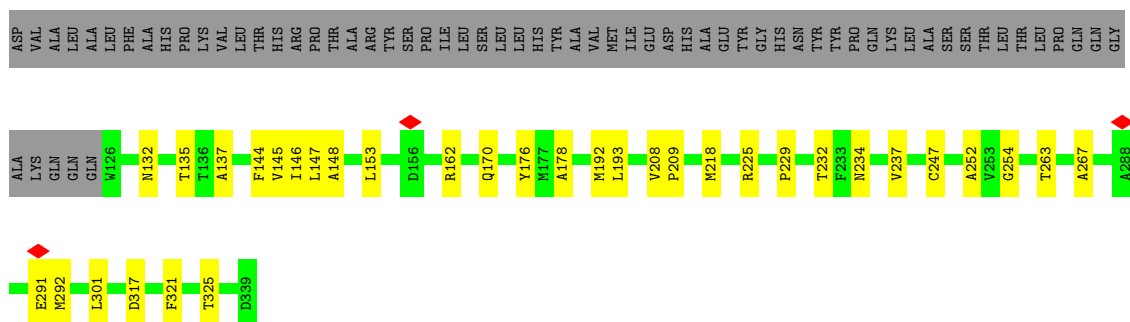
Chain M: 53% 10% 37%



• Molecule 13: Proteasome beta6 chain

Chain a: 53% 10% 37%





● Molecule 14: Proteasome beta7 chain

Chain N: 82% 16% ..



● Molecule 14: Proteasome beta7 chain

Chain b: 83% 15% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97438	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.515	Depositor
Minimum map value	-0.311	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0545	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	1.00	0/1889	1.52	2/2562 (0.1%)
1	O	0.98	0/1889	1.53	4/2562 (0.2%)
2	B	0.98	0/1787	1.55	2/2421 (0.1%)
2	P	0.96	0/1787	1.52	2/2421 (0.1%)
3	C	1.00	0/2242	1.52	3/3034 (0.1%)
3	Q	0.99	0/2242	1.52	6/3034 (0.2%)
4	D	1.02	0/1902	1.58	0/2562
4	R	1.02	0/1902	1.59	0/2562
5	E	1.03	0/1784	1.55	1/2414 (0.0%)
5	S	1.01	0/1784	1.54	4/2414 (0.2%)
6	F	1.00	0/1907	1.49	0/2575
6	T	0.98	0/1907	1.47	2/2575 (0.1%)
7	G	0.98	0/1759	1.54	6/2379 (0.3%)
7	U	0.98	0/1759	1.52	2/2379 (0.1%)
8	H	0.95	0/1742	1.52	0/2359
8	V	0.95	0/1742	1.53	1/2359 (0.0%)
9	I	0.98	0/1685	1.52	2/2284 (0.1%)
9	W	0.97	0/1685	1.51	0/2284
10	J	0.94	0/1583	1.51	3/2135 (0.1%)
10	X	0.93	0/1583	1.50	1/2135 (0.0%)
11	K	0.96	0/1643	1.51	0/2222
11	Y	0.96	0/1643	1.51	2/2222 (0.1%)
12	L	0.95	0/1613	1.51	2/2183 (0.1%)
12	Z	0.95	0/1613	1.51	3/2183 (0.1%)
13	M	0.98	0/1743	1.52	5/2354 (0.2%)
13	a	0.97	0/1743	1.52	1/2354 (0.0%)
14	N	0.94	0/1748	1.47	1/2363 (0.0%)
14	b	0.94	0/1748	1.48	1/2363 (0.0%)
All	All	0.98	0/50054	1.52	56/67694 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
4	R	0	1
7	G	0	1
7	U	0	1
10	X	0	1
14	N	0	1
14	b	0	1
All	All	0	7

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	137	ASN	CA-CB-CG	9.95	122.55	112.60
12	Z	137	ASN	CA-CB-CG	9.68	122.28	112.60
12	Z	137	ASN	CB-CA-C	9.32	128.96	110.42
12	L	137	ASN	CB-CA-C	8.69	127.72	110.42
10	J	135	ASP	CA-CB-CG	6.84	119.44	112.60
14	b	21	ASP	CA-CB-CG	6.68	119.28	112.60
14	N	21	ASP	CA-CB-CG	6.60	119.20	112.60
7	G	231	MET	CA-C-N	6.33	125.39	120.33
7	G	231	MET	C-N-CA	6.33	125.39	120.33
7	U	231	MET	CA-C-N	6.11	125.21	120.33
7	U	231	MET	C-N-CA	6.11	125.21	120.33
10	X	135	ASP	CA-CB-CG	5.94	118.54	112.60
6	T	288	SER	CA-C-N	5.80	126.41	119.98
6	T	288	SER	C-N-CA	5.80	126.41	119.98
3	C	156	THR	CB-CA-C	5.66	121.51	110.30
11	Y	155	ASP	CA-CB-CG	5.64	118.25	112.60
2	B	34	LEU	CA-C-N	5.58	126.03	122.18
2	B	34	LEU	C-N-CA	5.58	126.03	122.18
11	Y	144	GLY	CA-C-O	-5.52	118.47	122.45
13	M	276	ASP	CA-CB-CG	5.52	118.12	112.60
3	Q	156	THR	CB-CA-C	5.51	121.22	110.30
1	A	11	THR	CB-CA-C	5.49	120.62	111.83
2	P	34	LEU	CA-C-N	5.47	125.82	121.61
2	P	34	LEU	C-N-CA	5.47	125.82	121.61
7	G	127	PHE	CA-C-N	5.44	127.57	120.28
7	G	127	PHE	C-N-CA	5.44	127.57	120.28
10	J	133	PRO	CA-C-N	5.42	127.81	120.38
10	J	133	PRO	C-N-CA	5.42	127.81	120.38
3	C	158	PRO	CA-C-N	5.30	128.12	120.38
3	C	158	PRO	C-N-CA	5.30	128.12	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	157	GLY	CA-C-O	-5.26	118.37	122.52
5	S	293	GLU	CA-C-N	5.24	125.80	119.98
5	S	293	GLU	C-N-CA	5.24	125.80	119.98
3	Q	115	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	150	LYS	CB-CA-C	5.21	116.45	109.42
5	S	324	ASP	CA-CB-CG	5.20	117.80	112.60
8	V	158	ASP	CB-CA-C	5.20	117.04	109.08
1	O	11	THR	CB-CA-C	5.19	120.12	112.03
3	Q	158	PRO	CA-C-N	5.19	127.95	120.38
3	Q	158	PRO	C-N-CA	5.19	127.95	120.38
5	E	324	ASP	CA-CB-CG	5.18	117.78	112.60
1	O	150	LYS	CB-CA-C	5.18	116.41	109.42
12	Z	215	ASP	CA-CB-CG	5.16	117.76	112.60
5	S	109	ASP	CA-CB-CG	5.13	117.73	112.60
7	G	190	VAL	CA-C-N	5.12	125.67	119.98
7	G	190	VAL	C-N-CA	5.12	125.67	119.98
13	M	293	THR	CA-C-N	5.11	127.39	120.38
13	M	293	THR	C-N-CA	5.11	127.39	120.38
1	O	226	ALA	CA-C-N	5.07	127.34	120.44
1	O	226	ALA	C-N-CA	5.07	127.34	120.44
13	M	159	LEU	CA-C-N	5.05	127.31	120.44
13	M	159	LEU	C-N-CA	5.05	127.31	120.44
3	Q	186	HIS	CA-C-N	5.04	127.03	120.28
3	Q	186	HIS	C-N-CA	5.04	127.03	120.28
9	I	149	ASP	CA-CB-CG	5.01	117.61	112.60
13	a	162	ARG	NE-CZ-NH2	5.01	123.71	119.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	124	SER	Peptide
7	G	134	CYS	Peptide
14	N	49	ALA	Peptide
4	R	124	SER	Peptide
7	U	134	CYS	Peptide
10	X	29	GLY	Peptide
14	b	49	ALA	Peptide

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	1857	0	1871	19	0
1	O	1857	0	1871	20	0
2	B	1754	0	1741	14	0
2	P	1754	0	1741	13	0
3	C	2195	0	2142	24	0
3	Q	2195	0	2142	22	0
4	D	1873	0	1868	20	0
4	R	1873	0	1868	18	0
5	E	1756	0	1736	11	0
5	S	1756	0	1736	16	0
6	F	1869	0	1823	20	0
6	T	1869	0	1823	19	0
7	G	1727	0	1691	16	0
7	U	1727	0	1691	16	0
8	H	1710	0	1665	18	0
8	V	1710	0	1665	17	0
9	I	1659	0	1684	19	0
9	W	1659	0	1684	16	0
10	J	1557	0	1552	25	0
10	X	1557	0	1552	27	0
11	K	1612	0	1571	14	0
11	Y	1612	0	1571	12	0
12	L	1579	0	1538	16	0
12	Z	1579	0	1538	17	0
13	M	1702	0	1638	18	0
13	a	1702	0	1638	18	0
14	N	1712	0	1668	22	0
14	b	1712	0	1668	21	0
All	All	49124	0	48376	458	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 (458) 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:Y:15:MET:HE1	11:Y:168:LEU:HD23	1.57	0.86
7:U:150:VAL:HG21	7:U:163:VAL:HG21	1.60	0.82
1:A:36:THR:HG22	1:A:49:THR:HG23	1.61	0.80
8:V:68:LEU:HD23	8:V:98:CYS:SG	2.21	0.80
11:K:15:MET:HE1	11:K:168:LEU:HD23	1.64	0.79
3:Q:111:MET:HE1	3:Q:119:ILE:HD12	1.65	0.78
7:G:150:VAL:HG21	7:G:163:VAL:HG21	1.65	0.77
3:C:111:MET:HE1	3:C:119:ILE:HD12	1.67	0.77
1:O:36:THR:HG22	1:O:49:THR:HG23	1.66	0.76
4:R:70:TYR:CD2	4:R:209:LEU:HD21	2.21	0.75
6:T:235:VAL:HG21	6:T:273:MET:HE1	1.68	0.75
6:F:235:VAL:HG21	6:F:273:MET:HE1	1.69	0.73
8:H:68:LEU:HD23	8:H:98:CYS:SG	2.28	0.73
4:D:70:TYR:CD2	4:D:209:LEU:HD21	2.23	0.72
13:M:237:VAL:HG22	13:M:247:CYS:HB3	1.70	0.71
9:I:238:THR:HG21	10:J:168:ALA:HB1	1.73	0.71
6:F:200:VAL:HG22	6:F:325:ALA:HB2	1.73	0.70
9:W:33:VAL:HG22	9:W:155:THR:HG22	1.73	0.69
8:H:88:LEU:HD13	8:H:231:ILE:HG22	1.75	0.69
1:A:123:THR:O	2:B:126:ARG:NH1	2.26	0.68
9:I:71:MET:HG3	9:I:205:CYS:SG	2.34	0.68
1:O:67:TYR:CD2	1:O:88:VAL:HG21	2.28	0.68
5:E:185:ALA:HB2	5:E:239:VAL:HG21	1.76	0.68
1:A:67:TYR:CD2	1:A:88:VAL:HG21	2.28	0.67
7:G:88:ILE:HD12	7:G:134:CYS:SG	2.34	0.67
11:K:15:MET:HE1	11:K:168:LEU:CD2	2.25	0.67
13:a:147:LEU:HD11	13:a:178:ALA:HB2	1.78	0.66
1:O:69:VAL:HG11	1:O:111:LEU:HD21	1.77	0.66
13:a:145:VAL:HG11	13:a:237:VAL:HG13	1.78	0.66
1:A:49:THR:HG21	1:A:65:ALA:CB	2.26	0.65
7:G:100:ARG:NH1	8:V:269:SER:O	2.28	0.65
5:S:185:ALA:HB2	5:S:239:VAL:HG21	1.78	0.65
9:W:238:THR:HG21	10:X:168:ALA:HB1	1.78	0.65
6:T:200:VAL:HG22	6:T:325:ALA:HB2	1.76	0.65
1:O:75:CYS:SG	1:O:77:MET:HE2	2.37	0.65
13:M:147:LEU:HD11	13:M:178:ALA:HB2	1.78	0.64
13:M:137:ALA:HB2	13:M:263:THR:HG23	1.80	0.64
3:C:97:ARG:HD2	10:J:76:LEU:HD13	1.79	0.64
11:Y:43:GLN:OE1	11:Y:82:THR:HG21	1.98	0.64
14:b:38:ILE:HG21	14:b:187:ALA:HB2	1.79	0.64
13:M:232:THR:HG23	13:M:234:ASN:HD21	1.61	0.64
9:I:33:VAL:HG22	9:I:155:THR:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:123:THR:O	2:P:126:ARG:NH1	2.32	0.62
11:Y:15:MET:HE1	11:Y:168:LEU:CD2	2.27	0.62
1:O:49:THR:HG21	1:O:65:ALA:CB	2.29	0.62
7:U:88:ILE:HD12	7:U:134:CYS:SG	2.40	0.62
8:V:88:LEU:HD13	8:V:231:ILE:HG22	1.82	0.62
11:K:183:ILE:HG22	11:Y:21:LEU:HD11	1.82	0.62
3:Q:124:LYS:NZ	3:Q:157:GLU:O	2.33	0.62
13:M:145:VAL:HG11	13:M:237:VAL:HG13	1.81	0.62
13:a:146:ILE:CG2	13:a:301:LEU:HD12	2.29	0.62
8:H:269:SER:O	7:U:100:ARG:NH1	2.34	0.61
9:W:71:MET:HG3	9:W:205:CYS:SG	2.40	0.61
14:N:38:ILE:HG21	14:N:187:ALA:HB2	1.82	0.60
3:Q:66:THR:OG1	10:X:79:GLU:HG2	2.01	0.60
13:a:237:VAL:HG22	13:a:247:CYS:HB3	1.82	0.59
3:Q:97:ARG:HD2	10:X:76:LEU:HD13	1.83	0.59
13:a:232:THR:HG23	13:a:234:ASN:HD21	1.67	0.59
3:C:34:VAL:HG11	3:C:81:SER:HB3	1.85	0.59
3:C:34:VAL:HG11	3:C:81:SER:CB	2.33	0.59
3:Q:34:VAL:HG11	3:Q:81:SER:HB3	1.85	0.59
6:T:274:ALA:HB1	6:T:318:VAL:HG11	1.84	0.58
9:W:185:ALA:HA	9:W:202:VAL:HG11	1.85	0.58
3:Q:73:LYS:O	3:Q:97:ARG:NH1	2.32	0.58
3:C:66:THR:OG1	10:J:79:GLU:HG2	2.03	0.58
2:P:80:ASP:OD2	2:P:126:ARG:NH2	2.37	0.58
8:V:68:LEU:HD11	8:V:155:ALA:HB3	1.86	0.58
10:X:14:MET:HE3	10:X:150:CYS:SG	2.43	0.58
11:K:21:LEU:HD11	11:Y:183:ILE:HG22	1.85	0.58
3:C:124:LYS:NZ	3:C:157:GLU:O	2.36	0.58
8:H:68:LEU:N	8:H:68:LEU:HD12	2.19	0.58
13:a:137:ALA:HB2	13:a:263:THR:HG23	1.85	0.58
1:A:75:CYS:SG	1:A:77:MET:HE2	2.44	0.57
9:I:185:ALA:HA	9:I:202:VAL:HG11	1.86	0.57
13:M:146:ILE:CG2	13:M:301:LEU:HD12	2.34	0.57
14:N:59:MET:HE1	14:N:95:LYS:HD2	1.86	0.57
9:I:92:LEU:HD11	9:I:108:ALA:HB2	1.85	0.57
8:V:263:THR:HG21	8:V:274:ILE:HG23	1.86	0.57
8:H:68:LEU:HD11	8:H:155:ALA:HB3	1.87	0.56
3:Q:154:TYR:CE1	3:Q:164:ALA:HB2	2.39	0.56
9:W:142:ILE:N	9:W:142:ILE:HD12	2.20	0.56
2:B:106:SER:HB3	3:C:61:MET:HE1	1.86	0.56
10:J:123:ALA:HB2	10:J:137:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:141:THR:HB	9:I:156:MET:HE3	1.88	0.56
1:A:69:VAL:HG11	1:A:111:LEU:HD21	1.86	0.56
3:Q:34:VAL:HG11	3:Q:81:SER:CB	2.35	0.56
3:C:71:MET:HG3	3:C:219:ALA:HB2	1.87	0.56
9:I:142:ILE:N	9:I:142:ILE:HD12	2.21	0.55
13:a:135:THR:HG21	13:a:267:ALA:HB3	1.89	0.55
14:b:59:MET:HE1	14:b:95:LYS:HD2	1.88	0.55
6:F:237:MET:HE1	6:F:250:ALA:HB2	1.89	0.55
1:O:122:ARG:NH1	1:O:129:ARG:O	2.39	0.55
1:O:195:GLN:OE1	1:O:223:ARG:NH1	2.38	0.55
4:R:71:LEU:HD12	4:R:71:LEU:C	2.31	0.55
1:A:122:ARG:NH1	1:A:129:ARG:O	2.39	0.54
7:G:48:VAL:HG11	7:G:77:CYS:CB	2.37	0.54
12:Z:131:MET:HE1	12:Z:274:THR:HG21	1.89	0.54
1:A:195:GLN:OE1	1:A:223:ARG:NH1	2.40	0.54
3:Q:71:MET:HG3	3:Q:219:ALA:HB2	1.89	0.54
12:Z:141:LEU:HD12	12:Z:278:VAL:HG22	1.89	0.54
3:C:117:CYS:O	3:C:121:CYS:SG	2.66	0.54
5:E:147:VAL:HG22	5:E:319:VAL:HG12	1.89	0.54
9:W:84:VAL:HG22	9:W:115:HIS:CD2	2.43	0.54
10:X:62:THR:OG1	11:Y:87:ARG:NH2	2.41	0.54
4:R:206:LEU:C	4:R:206:LEU:HD12	2.33	0.54
8:V:94:LYS:NZ	8:V:236:ASP:O	2.41	0.54
14:N:102:CYS:SG	14:N:104:CYS:SG	3.03	0.53
12:Z:103:LEU:C	12:Z:103:LEU:HD12	2.33	0.53
1:A:74:GLY:HA3	1:A:231:PHE:CD1	2.43	0.53
11:K:94:ILE:HG22	11:K:100:ALA:HB2	1.89	0.53
10:X:124:THR:HG22	10:X:128:GLY:HA2	1.90	0.53
12:L:103:LEU:HD12	12:L:103:LEU:C	2.33	0.53
10:X:123:ALA:HB2	10:X:137:VAL:HB	1.90	0.53
8:V:190:TYR:CE2	14:b:29:LEU:HD21	2.42	0.53
5:S:147:VAL:HG22	5:S:319:VAL:HG12	1.91	0.53
4:D:194:LEU:HD13	4:D:204:ILE:HD11	1.90	0.53
3:C:121:CYS:HB3	3:C:160:GLY:O	2.09	0.53
4:D:91:CYS:SG	4:D:107:LEU:HD13	2.48	0.53
14:N:56:PHE:HD1	14:N:106:MET:HE3	1.73	0.53
11:Y:16:VAL:CG1	11:Y:46:ALA:HB2	2.38	0.53
14:N:33:PRO:HB3	8:V:252:MET:HE3	1.91	0.53
2:P:67:ASP:O	2:P:69:HIS:N	2.42	0.53
4:D:201:SER:HB3	4:D:226:VAL:HG11	1.90	0.53
3:C:166:SER:HB3	3:C:185:TRP:CZ2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:277:ILE:HD11	6:F:299:LEU:HD12	1.92	0.52
11:K:43:GLN:OE1	11:K:82:THR:HG21	2.09	0.52
2:P:20:ILE:HD11	2:P:120:THR:HB	1.92	0.52
4:R:201:SER:HB3	4:R:226:VAL:HG11	1.92	0.52
1:A:73:ILE:HG21	1:A:111:LEU:HD23	1.91	0.52
13:M:192:MET:HA	13:M:192:MET:HE3	1.90	0.52
13:a:146:ILE:HG21	13:a:301:LEU:HD12	1.92	0.52
2:B:67:ASP:O	2:B:69:HIS:N	2.43	0.52
12:L:119:ALA:HB2	12:L:130:VAL:HG21	1.92	0.52
9:W:141:THR:HB	9:W:156:MET:HE3	1.91	0.52
3:C:154:TYR:CE1	3:C:164:ALA:HB2	2.45	0.51
8:H:263:THR:HG21	8:H:274:ILE:HG23	1.92	0.51
1:O:73:ILE:HG21	1:O:111:LEU:HD23	1.92	0.51
12:L:131:MET:HE1	12:L:274:THR:HG21	1.90	0.51
8:V:55:THR:HG21	8:V:100:SER:HA	1.91	0.51
4:D:65:VAL:HG21	4:D:71:LEU:HD23	1.93	0.51
10:J:124:THR:HG22	10:J:128:GLY:HA2	1.92	0.51
4:D:132:VAL:HG23	4:D:161:ILE:HD13	1.91	0.51
3:C:73:LYS:O	3:C:97:ARG:NH1	2.40	0.51
4:D:87:ALA:HB1	4:D:107:LEU:HD11	1.93	0.51
1:O:46:LEU:HD21	1:O:199:ALA:HB2	1.91	0.51
8:V:138:GLN:HG2	14:b:58:MET:HE1	1.93	0.51
2:B:80:ASP:OD2	2:B:126:ARG:NH2	2.44	0.51
10:J:26:ASN:HD21	10:J:186:VAL:HG23	1.75	0.51
9:I:233:LEU:HD13	10:J:169:GLN:HG3	1.93	0.51
10:J:62:THR:OG1	11:K:87:ARG:NH2	2.44	0.51
4:R:91:CYS:SG	4:R:107:LEU:HD13	2.51	0.51
7:U:20:ARG:NH1	7:U:25:GLU:OE2	2.44	0.51
10:X:31:GLN:HA	10:X:31:GLN:HE21	1.75	0.51
10:X:88:ALA:O	10:X:92:THR:HG23	2.10	0.51
4:R:144:LEU:HD21	4:R:159:VAL:HG12	1.93	0.50
10:X:126:LEU:HD12	10:X:127:ILE:HG23	1.93	0.50
12:L:237:VAL:HG21	12:L:261:HIS:HB2	1.93	0.50
4:D:42:VAL:HG13	4:D:206:LEU:HD13	1.92	0.50
3:Q:121:CYS:HB3	3:Q:160:GLY:O	2.11	0.50
2:P:67:ASP:O	2:P:68:GLU:C	2.53	0.50
1:A:46:LEU:HD21	1:A:199:ALA:HB2	1.94	0.50
4:R:65:VAL:HG11	4:R:107:LEU:HD21	1.94	0.50
7:U:35:SER:O	7:U:79:CYS:SG	2.69	0.50
5:S:197:GLN:HB3	12:Z:160:MET:HG3	1.92	0.50
7:U:186:CYS:SG	7:U:217:CYS:HB3	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:21:ASP:O	14:b:37:ARG:HD3	2.12	0.50
6:F:186:ILE:HD11	6:F:285:ILE:HB	1.94	0.50
9:I:54:ILE:HD11	10:J:144:GLU:HG2	1.94	0.50
1:A:185:GLN:HG3	1:A:190:LEU:HD22	1.94	0.49
14:N:21:ASP:O	14:N:37:ARG:HD3	2.11	0.49
13:a:170:GLN:NE2	13:a:176:TYR:OH	2.44	0.49
5:E:168:MET:SD	5:E:178:MET:HE1	2.52	0.49
4:D:71:LEU:C	4:D:71:LEU:HD12	2.37	0.49
14:b:24:LEU:HD21	14:b:53:TYR:CG	2.47	0.49
6:F:282:GLN:HA	6:F:285:ILE:HG12	1.94	0.49
11:K:16:VAL:CG1	11:K:46:ALA:HB2	2.42	0.49
1:O:83:ASP:OD2	1:O:129:ARG:NH1	2.46	0.49
13:a:144:PHE:HB3	13:a:325:THR:HG22	1.95	0.49
1:A:19:LEU:HG	2:B:77:MET:HE1	1.94	0.49
4:R:194:LEU:HD13	4:R:204:ILE:HD11	1.95	0.49
13:a:192:MET:HE3	13:a:192:MET:HA	1.94	0.49
13:M:170:GLN:NE2	13:M:176:TYR:OH	2.45	0.49
4:R:65:VAL:HG21	4:R:71:LEU:HD23	1.95	0.49
5:E:197:GLN:HB3	12:L:160:MET:HG3	1.94	0.49
9:I:238:THR:HG21	10:J:168:ALA:CB	2.42	0.49
12:L:144:LEU:C	12:L:144:LEU:HD12	2.38	0.49
6:T:277:ILE:HD11	6:T:299:LEU:CD1	2.43	0.49
3:C:141:LEU:HG	3:C:153:LEU:HD11	1.95	0.49
7:U:48:VAL:HG11	7:U:77:CYS:HB3	1.94	0.49
1:A:98:TYR:HH	9:I:95:HIS:CE1	2.31	0.48
3:Q:166:SER:HB3	3:Q:185:TRP:CZ2	2.49	0.48
7:U:88:ILE:CD1	7:U:134:CYS:SG	3.00	0.48
8:V:68:LEU:HD12	8:V:68:LEU:N	2.28	0.48
9:I:87:MET:HE1	9:I:115:HIS:CE1	2.48	0.48
12:L:118:ARG:O	12:L:132:LYS:NZ	2.45	0.48
6:T:213:LEU:HD11	6:T:364:THR:HG22	1.94	0.48
12:L:118:ARG:NH1	12:L:267:GLY:O	2.47	0.48
12:Z:144:LEU:C	12:Z:144:LEU:HD12	2.38	0.48
9:I:84:VAL:HG22	9:I:115:HIS:CD2	2.49	0.48
10:J:14:MET:HE3	10:J:150:CYS:SG	2.53	0.48
11:K:16:VAL:HG21	11:K:44:LEU:HD11	1.96	0.48
4:R:33:VAL:HG13	4:R:172:MET:HE1	1.96	0.48
4:R:132:VAL:HG23	4:R:161:ILE:HD13	1.96	0.48
14:b:56:PHE:HD1	14:b:106:MET:HE3	1.78	0.48
4:D:206:LEU:C	4:D:206:LEU:HD12	2.38	0.48
7:G:48:VAL:HG11	7:G:77:CYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:135:THR:HG21	13:M:267:ALA:HB3	1.96	0.48
14:b:23:LEU:HD11	14:b:30:ALA:HB1	1.95	0.48
14:N:24:LEU:HD21	14:N:53:TYR:CG	2.49	0.48
3:C:74:ILE:HG21	3:C:116:LEU:HD21	1.96	0.47
7:G:35:SER:O	7:G:79:CYS:SG	2.71	0.47
6:T:232:ASP:O	6:T:233:GLU:C	2.57	0.47
9:W:233:LEU:HD13	10:X:169:GLN:HG3	1.95	0.47
4:D:108:VAL:HG21	4:D:145:TRP:CG	2.50	0.47
8:H:252:MET:HE3	14:b:33:PRO:HB3	1.95	0.47
11:K:1:MET:HA	11:K:144:GLY:HA2	1.95	0.47
11:Y:94:ILE:HG22	11:Y:100:ALA:HB2	1.95	0.47
3:C:238:HIS:HB2	11:K:121:VAL:HG13	1.96	0.47
13:M:144:PHE:HB3	13:M:325:THR:HG22	1.97	0.47
10:J:88:ALA:O	10:J:92:THR:HG23	2.15	0.47
14:N:19:ALA:HB2	14:N:186:VAL:HG22	1.97	0.47
4:R:206:LEU:HD12	4:R:207:LEU:N	2.29	0.47
12:Z:237:VAL:HG21	12:Z:261:HIS:HB2	1.96	0.47
4:D:145:TRP:CE2	4:D:155:ALA:HB2	2.49	0.47
6:F:249:LEU:HD12	6:F:295:VAL:HG11	1.96	0.47
2:B:20:ILE:HD11	2:B:120:THR:HB	1.97	0.47
8:H:55:THR:HG21	8:H:100:SER:HA	1.97	0.47
10:J:96:TYR:CE1	10:J:99:ARG:HG3	2.49	0.47
12:L:102:THR:HG22	12:L:199:MET:HE2	1.96	0.47
14:N:46:ALA:HB2	14:N:194:VAL:HG11	1.97	0.47
14:N:174:PHE:CE2	14:N:204:THR:HG21	2.49	0.47
5:S:168:MET:SD	5:S:178:MET:HE1	2.55	0.47
8:V:123:ASP:OD1	8:V:123:ASP:C	2.57	0.47
8:H:82:ASN:ND2	8:H:85:SER:HB3	2.30	0.47
10:J:92:THR:HG22	10:J:124:THR:HG21	1.97	0.47
4:R:108:VAL:HG21	4:R:145:TRP:CG	2.50	0.47
10:X:26:ASN:HD21	10:X:186:VAL:HG23	1.80	0.47
2:B:67:ASP:O	2:B:68:GLU:C	2.58	0.47
5:E:287:ARG:NH2	6:F:220:GLU:O	2.48	0.47
14:N:5:GLY:O	14:N:50:THR:HG23	2.14	0.47
13:a:225:ARG:O	13:a:229:PRO:HA	2.15	0.47
10:X:92:THR:HG22	10:X:124:THR:HG21	1.97	0.46
9:I:43:LEU:HB3	9:I:73:CYS:SG	2.55	0.46
10:J:73:MET:HE3	10:J:77:ARG:HH21	1.80	0.46
12:L:259:ILE:HG21	12:L:273:VAL:HG13	1.97	0.46
7:G:85:GLY:O	7:G:88:ILE:HB	2.16	0.46
11:Y:16:VAL:HG21	11:Y:44:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:102:THR:HG22	12:Z:199:MET:HE2	1.97	0.46
12:Z:118:ARG:O	12:Z:132:LYS:NZ	2.47	0.46
5:E:268:GLN:HE21	5:E:268:GLN:HA	1.80	0.46
9:W:43:LEU:HB3	9:W:73:CYS:SG	2.55	0.46
13:a:146:ILE:HG22	13:a:301:LEU:HD12	1.97	0.46
14:N:21:ASP:OD1	14:N:21:ASP:N	2.47	0.46
10:X:91:ILE:HD12	10:X:109:ILE:HD11	1.98	0.46
6:F:232:ASP:O	6:F:233:GLU:C	2.58	0.46
3:C:180:LEU:HD21	3:C:204:LYS:HG2	1.98	0.46
5:E:259:SER:HB2	5:E:261:THR:HG23	1.98	0.46
6:F:211:ALA:HB1	6:F:360:LEU:HD22	1.98	0.46
1:O:74:GLY:HA3	1:O:231:PHE:CD1	2.51	0.46
4:D:144:LEU:HD21	4:D:159:VAL:HG12	1.97	0.46
4:D:206:LEU:HD12	4:D:207:LEU:N	2.31	0.46
3:Q:238:HIS:HB2	11:Y:121:VAL:HG13	1.97	0.46
4:R:136:PHE:CE1	4:R:142:PRO:HB3	2.50	0.46
13:a:208:VAL:HG22	13:a:209:PRO:HD2	1.98	0.46
4:R:42:VAL:HG13	4:R:206:LEU:HD13	1.98	0.46
4:R:112:ALA:HB1	4:R:151:GLY:O	2.15	0.46
10:J:20:PHE:CE1	10:J:110:GLY:HA3	2.50	0.46
10:J:33:LYS:HB2	12:Z:233:TYR:OH	2.16	0.46
9:W:38:ARG:NH1	9:W:176:THR:HG22	2.31	0.46
8:H:138:GLN:HG2	14:N:58:MET:HE1	1.98	0.45
13:M:146:ILE:HG22	13:M:301:LEU:HD12	1.97	0.45
1:O:19:LEU:HG	2:P:77:MET:HE1	1.98	0.45
6:F:349:LEU:HD11	6:F:379:ILE:HD13	1.99	0.45
12:Z:119:ALA:HB2	12:Z:130:VAL:HG21	1.98	0.45
4:D:69:ILE:HG12	4:D:104:VAL:HG22	1.98	0.45
4:D:136:PHE:CE1	4:D:142:PRO:HB3	2.50	0.45
6:T:186:ILE:HD11	6:T:285:ILE:HB	1.98	0.45
6:T:202:VAL:HG12	6:T:323:ALA:HB1	1.98	0.45
1:A:29:VAL:HG21	1:A:134:VAL:HG23	1.99	0.45
3:Q:2:SER:HB2	7:U:127:PHE:CD1	2.51	0.45
2:P:78:GLY:N	2:P:79:PRO:CD	2.80	0.45
3:Q:238:HIS:CB	11:Y:121:VAL:HG13	2.46	0.45
6:T:277:ILE:HD11	6:T:299:LEU:HD12	1.99	0.45
6:F:274:ALA:HB1	6:F:318:VAL:HG11	1.98	0.45
2:B:41:GLY:HA2	2:B:142:TYR:CD1	2.51	0.45
5:E:195:GLU:HG3	5:E:215:ALA:HB1	1.99	0.45
10:J:31:GLN:HE21	10:J:31:GLN:HA	1.82	0.45
14:N:23:LEU:HD11	14:N:30:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:106:SER:HB3	3:Q:61:MET:HE1	1.97	0.45
10:X:108:VAL:HG13	10:X:137:VAL:HG23	1.99	0.45
2:B:116:TYR:CD1	2:B:149:PRO:HA	2.52	0.45
9:I:151:LEU:HB3	9:I:152:PRO:HD2	1.99	0.45
10:X:158:MET:HE1	10:X:166:ILE:HG12	1.99	0.45
14:b:46:ALA:HB3	14:b:109:ILE:HG12	1.98	0.45
7:U:65:ASN:HD22	7:U:65:ASN:HA	1.68	0.45
11:Y:1:MET:HA	11:Y:144:GLY:HA2	1.99	0.45
13:M:148:ALA:HB2	13:M:321:PHE:CD1	2.51	0.44
5:S:268:GLN:HE21	5:S:268:GLN:HA	1.81	0.44
12:Z:259:ILE:HG21	12:Z:273:VAL:HG13	1.99	0.44
12:L:141:LEU:HD12	12:L:278:VAL:HG22	1.98	0.44
5:S:113:ASN:HB3	6:T:291:ARG:HB3	1.99	0.44
6:T:285:ILE:HG22	6:T:292:PRO:HB3	1.99	0.44
7:U:48:VAL:HG11	7:U:77:CYS:CB	2.47	0.44
1:A:83:ASP:OD2	1:A:129:ARG:NH1	2.51	0.44
3:C:146:ASP:OD1	3:C:146:ASP:N	2.50	0.44
3:Q:117:CYS:O	3:Q:121:CYS:SG	2.72	0.44
10:X:73:MET:HE3	10:X:77:ARG:HH21	1.83	0.44
12:Z:118:ARG:NH1	12:Z:267:GLY:O	2.49	0.44
13:a:193:LEU:HD11	13:a:218:MET:SD	2.57	0.44
14:b:108:PHE:C	14:b:108:PHE:CD2	2.95	0.44
12:L:259:ILE:CG2	12:L:273:VAL:HG13	2.48	0.44
14:N:108:PHE:C	14:N:108:PHE:CD2	2.95	0.44
4:R:87:ALA:HB1	4:R:107:LEU:HD11	2.00	0.44
7:U:91:ARG:O	7:U:92:ALA:C	2.60	0.44
14:b:21:ASP:OD1	14:b:21:ASP:N	2.48	0.44
8:H:123:ASP:C	8:H:123:ASP:OD1	2.61	0.44
13:M:148:ALA:HB2	13:M:321:PHE:CE1	2.52	0.44
5:S:148:LEU:HD11	5:S:244:ALA:HB3	1.99	0.44
14:b:88:LEU:HD11	14:b:106:MET:HE2	2.00	0.44
4:D:66:ASP:O	4:D:69:ILE:N	2.50	0.44
5:E:213:THR:HG21	5:E:254:TRP:HB3	2.00	0.44
12:L:233:TYR:OH	10:X:33:LYS:HB2	2.16	0.44
10:X:21:VAL:HG22	10:X:189:ILE:HG12	1.99	0.44
14:b:24:LEU:HD21	14:b:53:TYR:CD2	2.53	0.44
4:D:194:LEU:HA	4:D:197:VAL:HG12	2.00	0.44
6:F:277:ILE:HD11	6:F:299:LEU:CD1	2.48	0.44
6:T:249:LEU:HD12	6:T:295:VAL:HG11	1.98	0.44
7:G:88:ILE:CD1	7:G:134:CYS:SG	3.05	0.44
1:O:185:GLN:HG3	1:O:190:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:10:ILE:HD12	14:b:146:LEU:HD22	2.00	0.44
1:O:98:TYR:HH	9:W:95:HIS:CE1	2.34	0.44
10:J:21:VAL:HG22	10:J:189:ILE:HG12	1.99	0.43
12:L:103:LEU:HD22	12:L:238:LEU:HD22	2.00	0.43
13:M:311:ARG:HD3	13:M:311:ARG:HA	1.89	0.43
1:O:81:ALA:N	1:O:82:PRO:HD2	2.33	0.43
3:Q:221:MET:HE2	3:Q:244:PRO:HB2	2.00	0.43
7:U:85:GLY:O	7:U:88:ILE:HB	2.18	0.43
14:b:174:PHE:CE2	14:b:204:THR:HG21	2.53	0.43
6:F:213:LEU:HD11	6:F:364:THR:HG22	2.00	0.43
3:C:98:LEU:HG	10:J:73:MET:HE2	2.01	0.43
5:E:336:LYS:HA	5:E:339:MET:HE3	2.00	0.43
9:I:95:HIS:O	9:I:99:THR:HG23	2.17	0.43
4:R:69:ILE:HG21	4:R:107:LEU:CD2	2.48	0.43
5:S:213:THR:HG21	5:S:254:TRP:HB3	2.00	0.43
9:W:54:ILE:HD11	10:X:144:GLU:HG2	1.99	0.43
12:Z:259:ILE:CG2	12:Z:273:VAL:HG13	2.48	0.43
2:B:18:ILE:HD13	2:B:18:ILE:HA	1.93	0.43
6:T:208:VAL:HG11	6:T:300:ALA:HB1	1.99	0.43
1:A:81:ALA:N	1:A:82:PRO:HD2	2.33	0.43
7:G:91:ARG:O	7:G:92:ALA:C	2.62	0.43
7:G:110:SER:HA	7:G:149:PHE:CE2	2.53	0.43
3:Q:146:ASP:OD1	3:Q:146:ASP:N	2.51	0.43
8:V:82:ASN:ND2	8:V:85:SER:HB3	2.34	0.43
7:G:186:CYS:SG	7:G:217:CYS:HB3	2.59	0.43
3:Q:98:LEU:HG	10:X:73:MET:HE2	2.01	0.43
2:B:66:LEU:HD12	2:B:108:LEU:HD21	2.00	0.43
2:P:18:ILE:HD13	2:P:18:ILE:HA	1.96	0.43
3:Q:36:GLY:HA2	3:Q:44:VAL:O	2.19	0.43
8:H:113:VAL:HG12	8:H:117:LEU:HD22	2.00	0.42
1:O:29:VAL:HG21	1:O:134:VAL:HG23	2.01	0.42
7:U:72:ARG:HG2	7:U:223:LYS:HG2	2.01	0.42
7:U:105:THR:HG21	8:V:129:ASN:HD22	1.84	0.42
13:a:148:ALA:HB2	13:a:321:PHE:CE1	2.53	0.42
13:a:148:ALA:HB2	13:a:321:PHE:CD1	2.54	0.42
8:H:190:TYR:CE2	14:N:29:LEU:HD21	2.53	0.42
8:H:258:TYR:OH	8:V:194:ASP:OD2	2.36	0.42
9:I:43:LEU:HD12	9:I:71:MET:HB2	2.02	0.42
6:T:398:LEU:HD12	6:T:398:LEU:HA	1.93	0.42
14:b:186:VAL:HG23	14:b:200:PHE:HE2	1.84	0.42
2:B:78:GLY:N	2:B:79:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:HIS:CB	11:K:121:VAL:HG13	2.49	0.42
2:P:74:TYR:HB3	2:P:81:CYS:SG	2.59	0.42
9:W:87:MET:HE1	9:W:115:HIS:CE1	2.54	0.42
9:I:152:PRO:HG2	9:I:153:PHE:CD2	2.54	0.42
5:S:287:ARG:NH2	6:T:220:GLU:O	2.52	0.42
6:F:208:VAL:HG11	6:F:300:ALA:HB1	2.02	0.42
7:G:137:ILE:CG2	7:G:148:LEU:HD11	2.50	0.42
11:K:106:LEU:HD11	11:K:142:CYS:HA	2.02	0.42
6:T:299:LEU:HD23	6:T:299:LEU:HA	1.91	0.42
9:W:238:THR:HG21	10:X:168:ALA:CB	2.47	0.42
2:B:69:HIS:NE2	2:B:103:ILE:O	2.51	0.42
8:H:218:TYR:HD1	8:H:218:TYR:C	2.28	0.42
12:L:137:ASN:OD1	12:L:139:TYR:N	2.48	0.42
13:M:309:ALA:HB2	13:M:336:LEU:HD13	2.02	0.42
3:Q:180:LEU:HD21	3:Q:204:LYS:HG2	2.00	0.42
1:A:166:ILE:HG22	1:A:190:LEU:HD23	2.02	0.42
3:C:2:SER:HB2	7:G:127:PHE:CD1	2.55	0.42
1:O:31:TYR:N	1:O:32:PRO:HD2	2.35	0.42
10:X:20:PHE:CE1	10:X:110:GLY:HA3	2.55	0.42
14:b:9:ALA:HA	14:b:17:LEU:O	2.20	0.42
7:G:110:SER:HA	7:G:149:PHE:CZ	2.55	0.41
12:L:137:ASN:HD21	12:L:172:ARG:CD	2.33	0.41
13:M:263:THR:HG21	13:M:271:VAL:HB	2.02	0.41
1:O:126:ALA:HB2	2:P:8:LEU:HD21	2.02	0.41
6:T:237:MET:HE1	6:T:250:ALA:HB2	2.02	0.41
14:b:122:ASP:HB2	14:b:126:THR:HB	2.01	0.41
3:C:38:CYS:N	3:C:166:SER:O	2.49	0.41
9:I:38:ARG:NH1	9:I:176:THR:HG22	2.35	0.41
10:J:92:THR:HG22	10:J:124:THR:CG2	2.50	0.41
5:S:259:SER:HB2	5:S:261:THR:HG23	2.02	0.41
5:S:327:LEU:HD21	5:S:329:MET:HE2	2.03	0.41
6:T:282:GLN:HA	6:T:285:ILE:HG12	2.02	0.41
14:b:46:ALA:HB2	14:b:194:VAL:HG11	2.02	0.41
5:E:188:LEU:HD21	5:E:237:PHE:CD2	2.56	0.41
6:F:193:VAL:HG22	6:F:296:GLY:N	2.36	0.41
14:N:162:ALA:HA	14:N:165:ILE:HG22	2.02	0.41
2:P:69:HIS:NE2	2:P:103:ILE:O	2.52	0.41
10:X:96:TYR:CE1	10:X:99:ARG:HG3	2.54	0.41
12:Z:137:ASN:HD21	12:Z:172:ARG:CD	2.33	0.41
14:b:109:ILE:HG22	14:b:118:LEU:HD13	2.03	0.41
8:H:181:LEU:HB3	8:H:186:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:126:LEU:HD12	10:J:127:ILE:HG23	2.01	0.41
14:N:9:ALA:HA	14:N:17:LEU:O	2.21	0.41
1:O:11:THR:HG23	1:O:11:THR:O	2.19	0.41
10:X:92:THR:HG22	10:X:124:THR:CG2	2.50	0.41
10:J:108:VAL:HG13	10:J:137:VAL:HG23	2.03	0.41
11:K:44:LEU:HD12	11:K:44:LEU:C	2.45	0.41
13:M:146:ILE:HG21	13:M:301:LEU:HD12	2.02	0.41
5:S:178:MET:HE2	5:S:178:MET:HB3	1.87	0.41
5:S:195:GLU:HG3	5:S:215:ALA:HB1	2.03	0.41
7:G:65:ASN:HD22	7:G:65:ASN:HA	1.66	0.41
8:H:148:ILE:HD12	8:H:150:ALA:HB3	2.01	0.41
13:M:301:LEU:HD23	13:M:301:LEU:HA	1.88	0.41
3:Q:74:ILE:HG21	3:Q:116:LEU:HD21	2.02	0.41
12:Z:157:VAL:O	12:Z:158:LEU:C	2.63	0.41
13:a:132:ASN:HB3	13:a:153:LEU:CD1	2.51	0.41
3:C:79:GLY:HA3	3:C:246:PHE:CE1	2.56	0.41
3:C:221:MET:HE2	3:C:244:PRO:HB2	2.02	0.41
4:D:69:ILE:HG21	4:D:107:LEU:HD22	2.03	0.41
8:H:218:TYR:C	8:H:218:TYR:CD1	2.98	0.41
9:W:167:LEU:HD12	9:W:167:LEU:HA	1.88	0.41
2:B:74:TYR:HB3	2:B:81:CYS:SG	2.61	0.41
10:J:12:MET:HG3	10:J:146:LEU:HD22	2.03	0.41
10:J:158:MET:HE1	10:J:166:ILE:HG12	2.03	0.41
14:N:88:LEU:HD11	14:N:106:MET:HE2	2.03	0.41
14:N:89:HIS:CD2	14:N:125:GLY:O	2.74	0.41
4:D:65:VAL:HG11	4:D:107:LEU:HD21	2.02	0.40
6:F:201:GLY:HA2	6:F:209:VAL:O	2.20	0.40
2:P:74:TYR:CB	2:P:81:CYS:SG	3.10	0.40
5:S:188:LEU:HD21	5:S:237:PHE:CD2	2.56	0.40
6:T:258:MET:O	6:T:259:ASN:C	2.64	0.40
1:A:11:THR:HG23	1:A:11:THR:O	2.21	0.40
7:G:82:LEU:N	7:G:83:PRO:CD	2.84	0.40
7:U:37:ALA:HB2	7:U:50:VAL:HG23	2.02	0.40
5:S:242:LEU:HD23	5:S:242:LEU:HA	1.88	0.40
5:S:247:ASP:OD1	5:S:247:ASP:N	2.55	0.40
8:V:253:GLU:OE1	8:V:253:GLU:N	2.54	0.40
9:W:166:GLN:HE21	9:W:190:LYS:HE2	1.86	0.40
12:Z:141:LEU:HD12	12:Z:278:VAL:CG2	2.52	0.40
6:F:299:LEU:HD23	6:F:299:LEU:HA	1.91	0.40
6:F:349:LEU:O	6:F:353:VAL:HG23	2.22	0.40
14:N:23:LEU:HB2	14:N:181:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:12:MET:HG3	10:X:146:LEU:HD22	2.02	0.40
12:Z:137:ASN:OD1	12:Z:139:TYR:N	2.50	0.40
6:F:258:MET:O	6:F:259:ASN:C	2.63	0.40
14:N:46:ALA:HB3	14:N:109:ILE:HG12	2.04	0.40
8:V:211:GLN:HA	8:V:228:ILE:HG21	2.03	0.40
10:X:66:LYS:HB3	10:X:94:MET:CE	2.51	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	O	242/250 (97%)	227 (94%)	14 (6%)	1 (0%)	30	60
2	P	227/231 (98%)	208 (92%)	17 (8%)	2 (1%)	14	43
3	Q	274/285 (96%)	257 (94%)	16 (6%)	1 (0%)	30	60
4	D	60/248 (24%)	59 (98%)	1 (2%)	0	100	100
4	R	237/248 (96%)	225 (95%)	9 (4%)	3 (1%)	9	35
5	E	225/344 (65%)	215 (96%)	10 (4%)	0	100	100
5	S	225/344 (65%)	213 (95%)	12 (5%)	0	100	100
6	F	132/428 (31%)	122 (92%)	9 (7%)	1 (1%)	16	45
6	T	236/428 (55%)	216 (92%)	18 (8%)	2 (1%)	16	45
7	G	211/238 (89%)	198 (94%)	12 (6%)	1 (0%)	24	55
7	U	226/238 (95%)	211 (93%)	14 (6%)	1 (0%)	30	60
8	H	200/283 (71%)	180 (90%)	19 (10%)	1 (0%)	24	55
8	V	227/283 (80%)	204 (90%)	22 (10%)	1 (0%)	30	60
9	I	217/254 (85%)	194 (89%)	19 (9%)	4 (2%)	6	29
9	W	217/254 (85%)	197 (91%)	16 (7%)	4 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	202/205 (98%)	183 (91%)	17 (8%)	2 (1%)	12	40
10	X	202/205 (98%)	184 (91%)	16 (8%)	2 (1%)	12	40
11	K	137/206 (66%)	125 (91%)	12 (9%)	0	100	100
11	Y	204/206 (99%)	185 (91%)	18 (9%)	1 (0%)	24	55
12	L	200/302 (66%)	175 (88%)	23 (12%)	2 (1%)	12	40
12	Z	186/302 (62%)	159 (86%)	25 (13%)	2 (1%)	11	39
13	M	212/339 (62%)	195 (92%)	11 (5%)	6 (3%)	4	21
13	a	171/339 (50%)	159 (93%)	7 (4%)	5 (3%)	3	21
14	N	216/220 (98%)	190 (88%)	23 (11%)	3 (1%)	9	33
14	b	216/220 (98%)	191 (88%)	22 (10%)	3 (1%)	9	33
All	All	5102/6900 (74%)	4672 (92%)	382 (8%)	48 (1%)	16	43

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	156	PRO
2	P	68	GLU
4	R	49	SER
10	X	156	PRO
11	Y	134	THR
7	G	169	LYS
12	L	147	GLY
13	M	205	GLY
13	M	292	MET
14	N	52	SER
14	N	115	GLU
4	R	67	ALA
9	W	46	ASP
12	Z	147	GLY
13	a	291	GLU
13	a	292	MET
14	b	5	GLY
14	b	52	SER
14	b	115	GLU
9	I	200	THR
10	J	185	ALA
12	L	232	ILE
13	M	291	GLU

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Mol	Chain	Res	Type
14	N	5	GLY
2	P	180	MET
3	Q	59	GLU
7	U	169	LYS
9	W	200	THR
10	X	185	ALA
6	F	366	GLU
8	H	266	GLN
9	I	46	ASP
9	I	226	TYR
9	I	230	GLU
13	M	317	ASP
1	O	80	ARG
4	R	50	ALA
6	T	366	GLU
8	V	266	GLN
9	W	226	TYR
9	W	230	GLU
13	a	252	ALA
13	a	317	ASP
13	M	252	ALA
12	Z	232	ILE
6	T	259	ASN
13	a	254	GLY
13	M	254	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

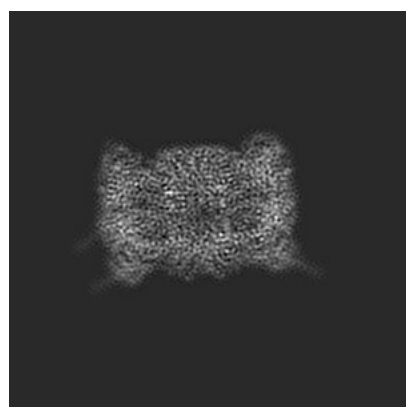
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4591. These allow visual inspection of the internal detail of the map and identification of artifacts.

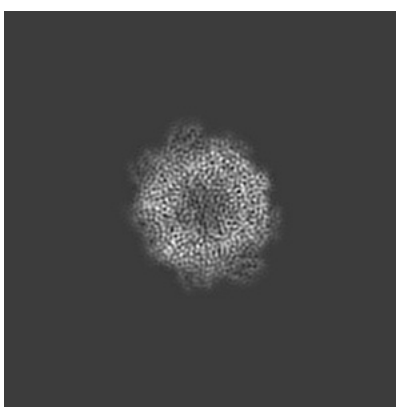
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

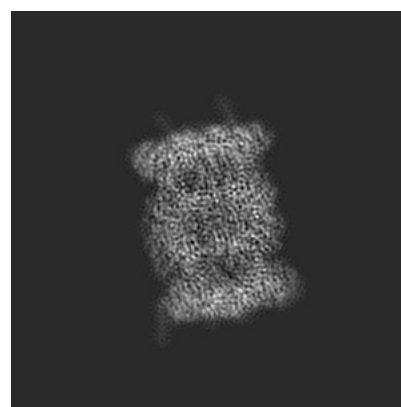
6.1.1 Primary map



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: 150



Y Index: 150



Z Index: 150

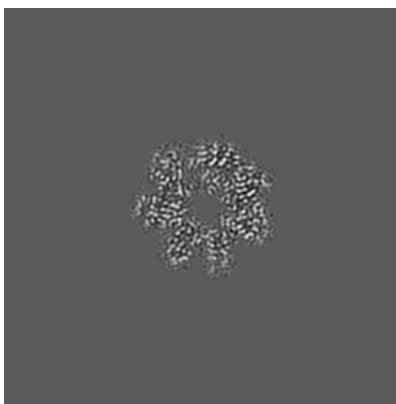
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 167



Y Index: 159

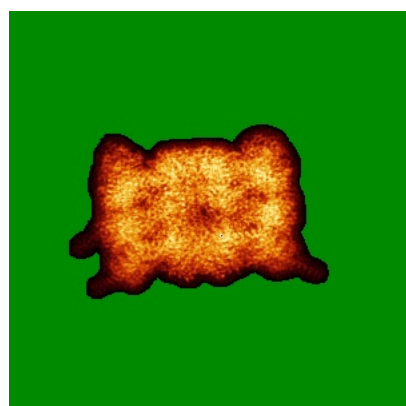


Z Index: 178

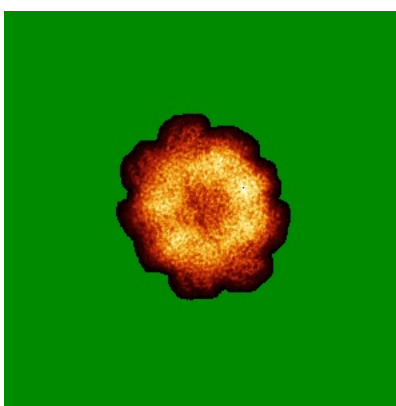
The images above show the largest variance slices of the map in three orthogonal directions.

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

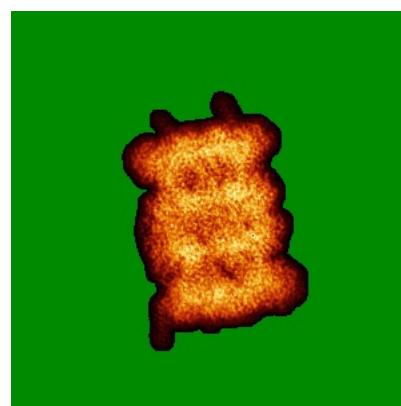
6.4.1 Primary map



X



Y

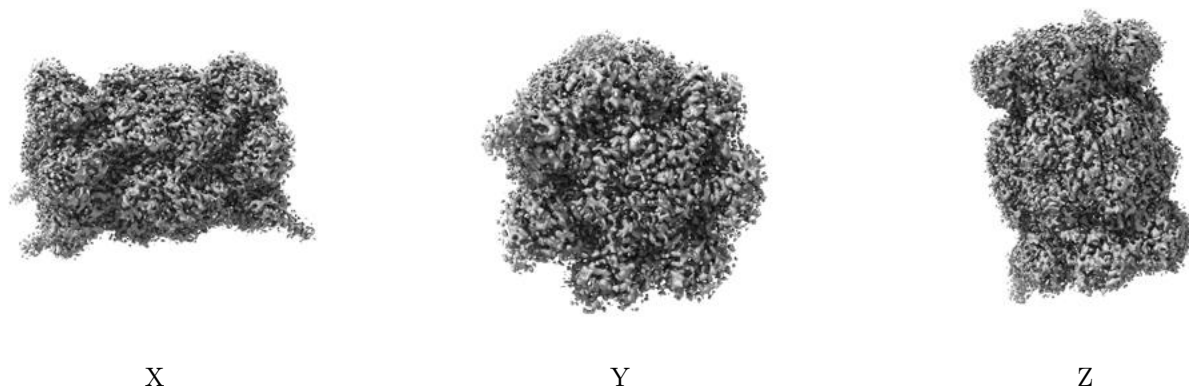


Z

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 0.0545. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

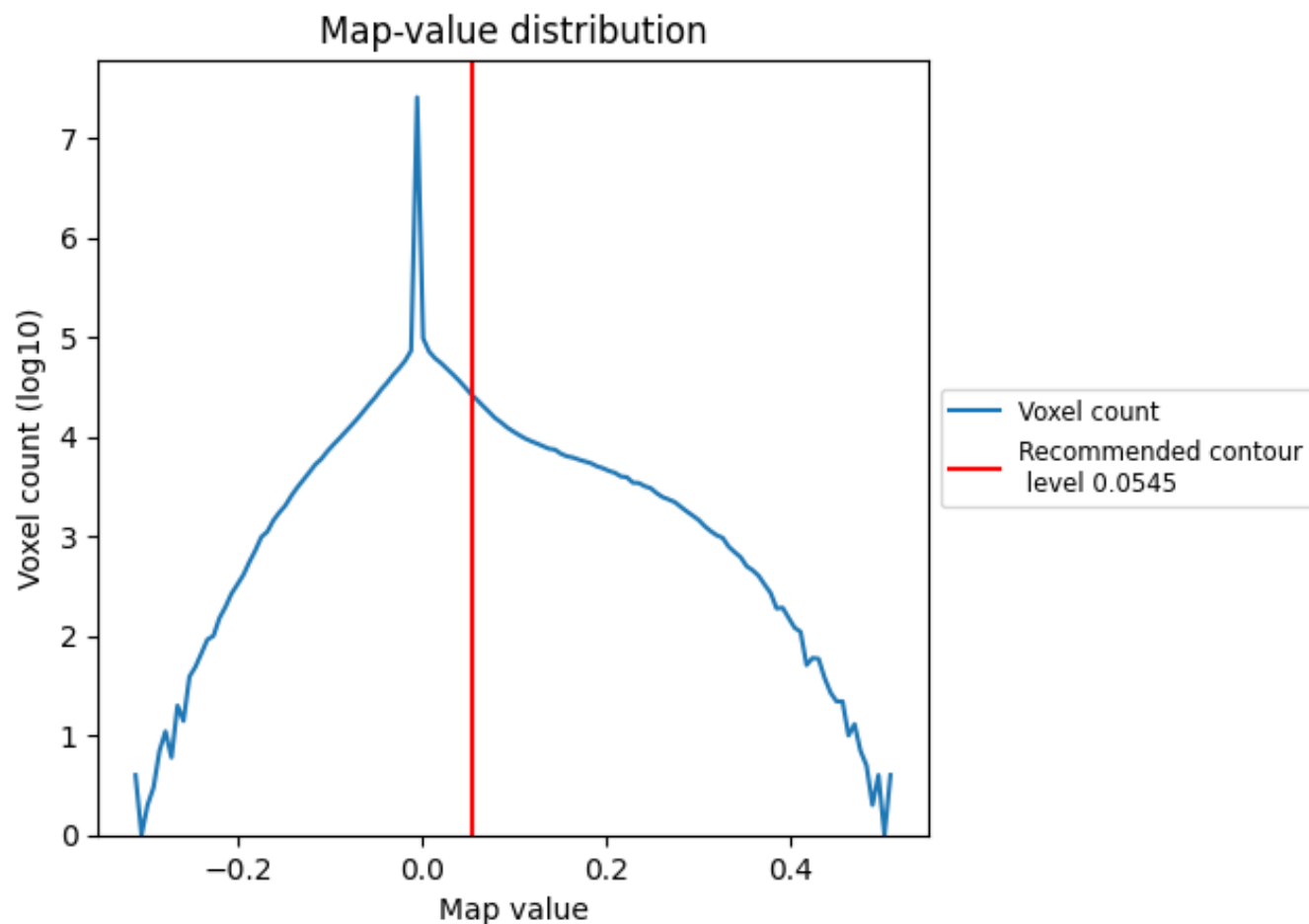
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

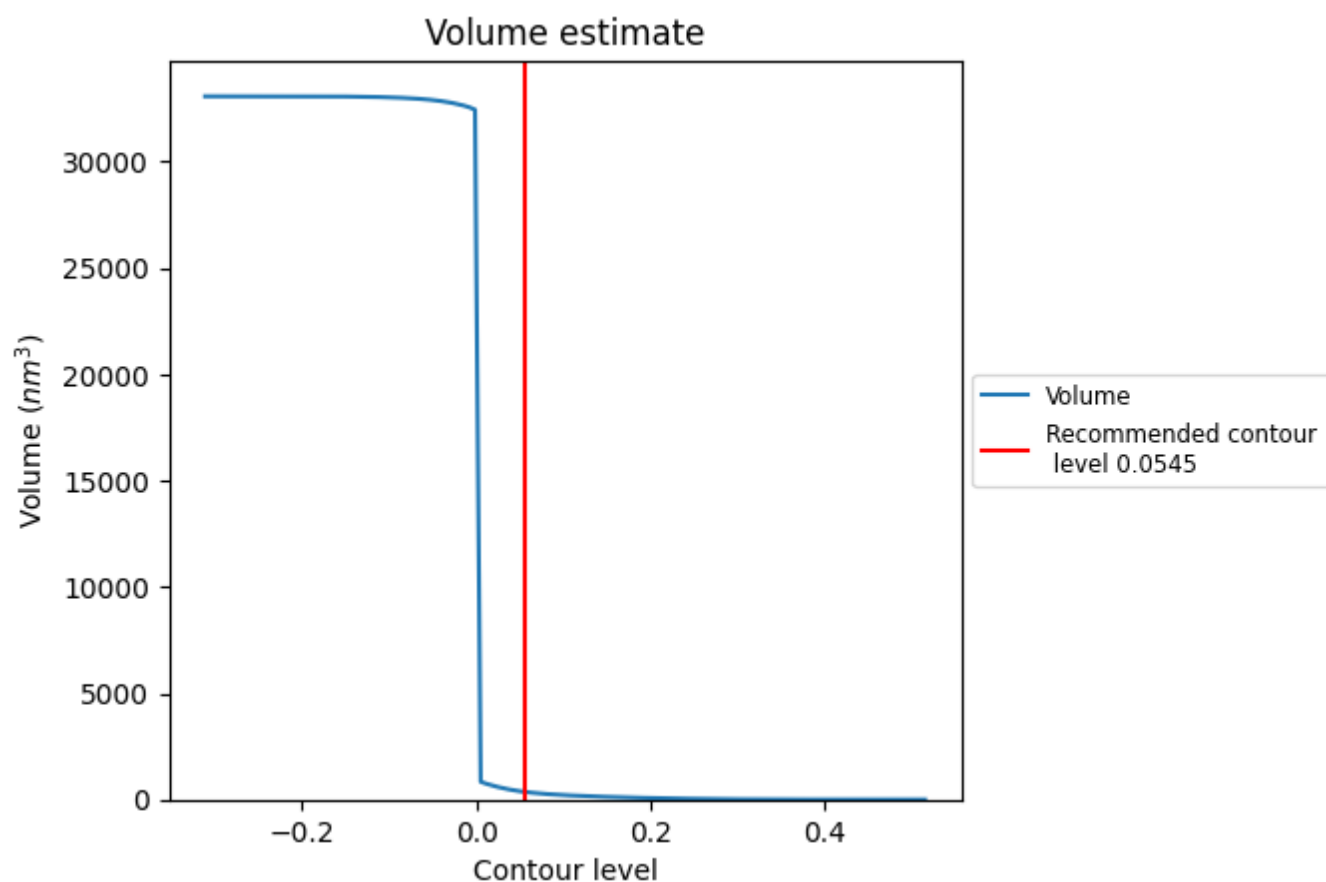
This section contains the results of statistical analysis of the map.

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.

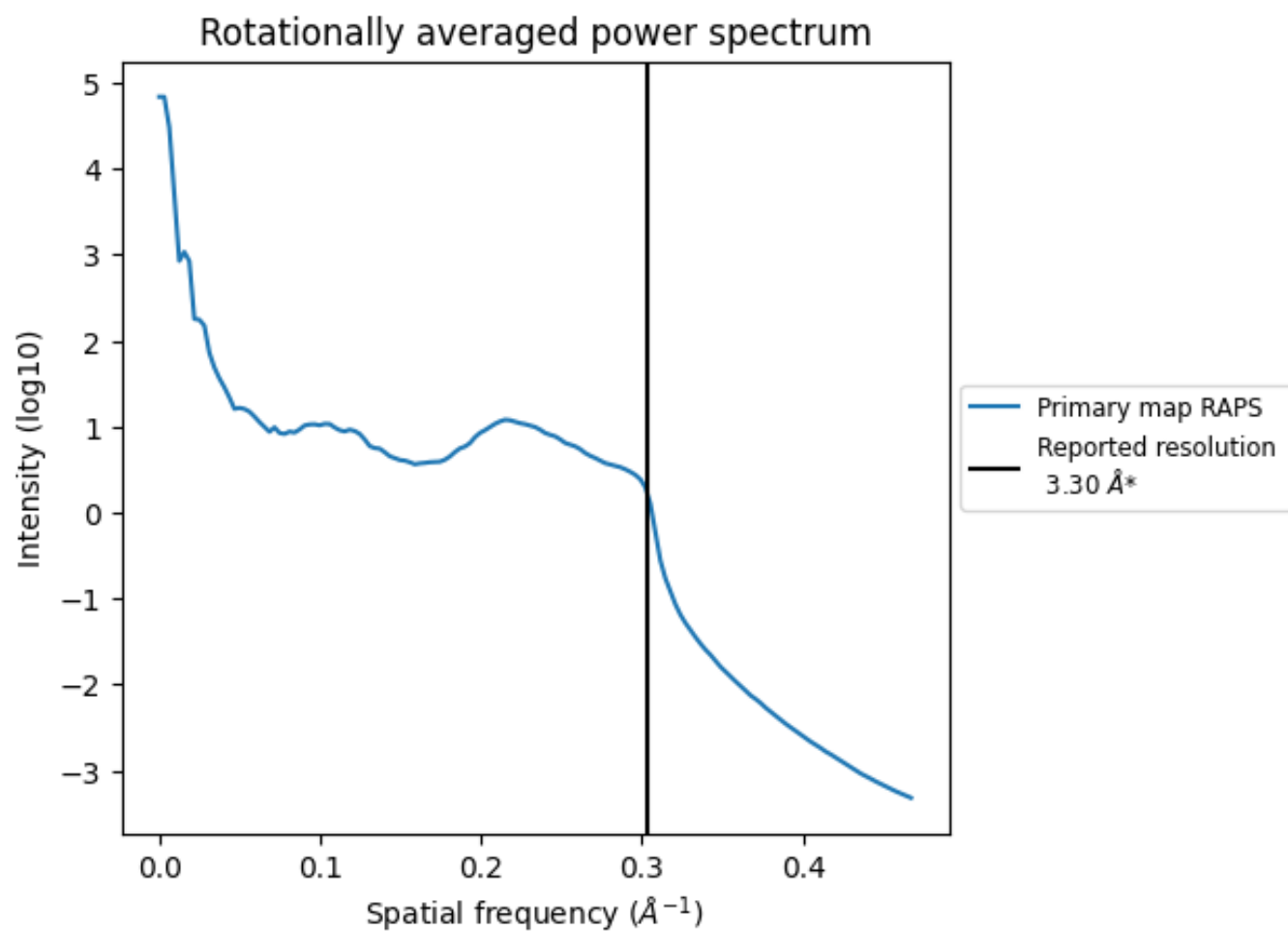
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365 nm³; this corresponds to an approximate mass of 330 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 0.303 Å⁻¹

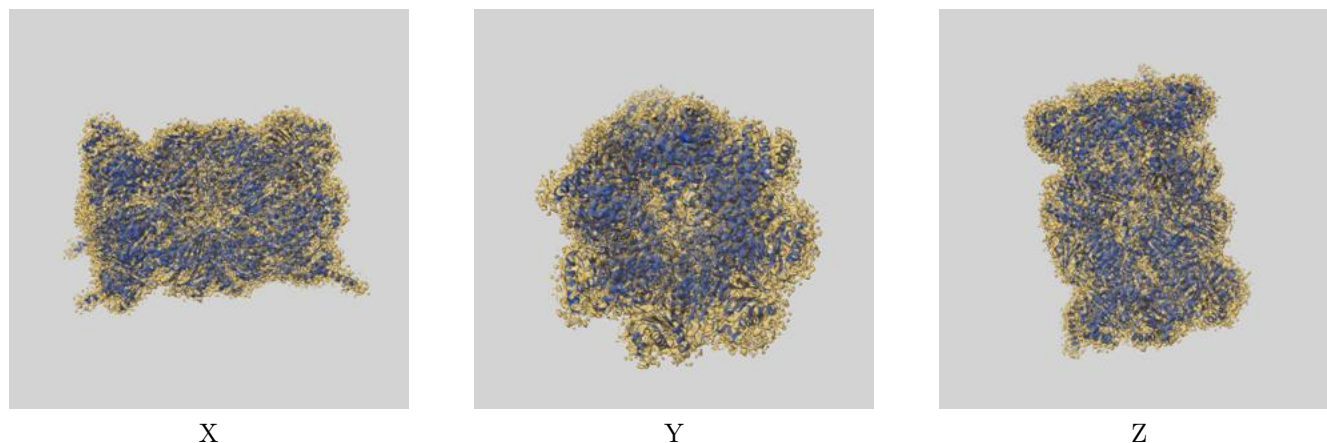
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

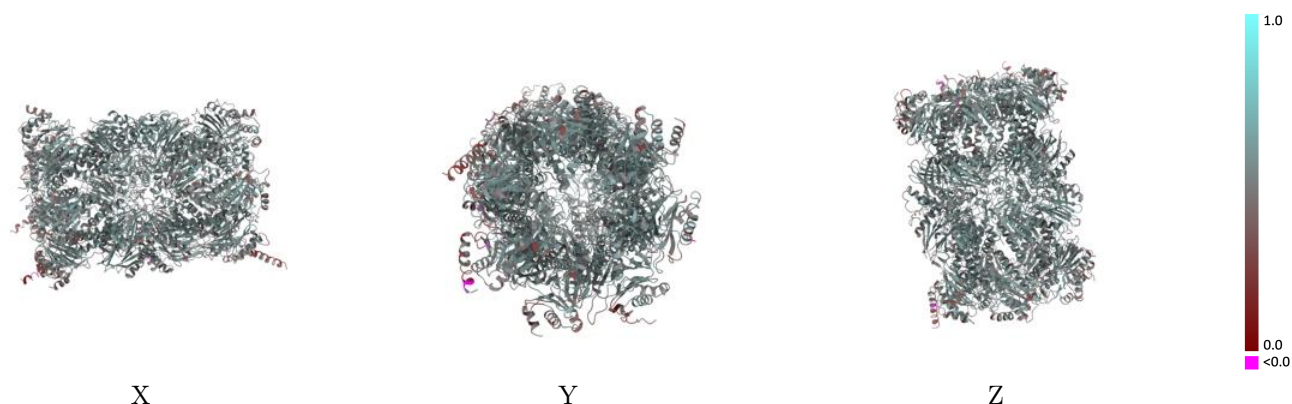
This section contains information regarding the fit between EMDB map EMD-4591 and PDB model 6QM8. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



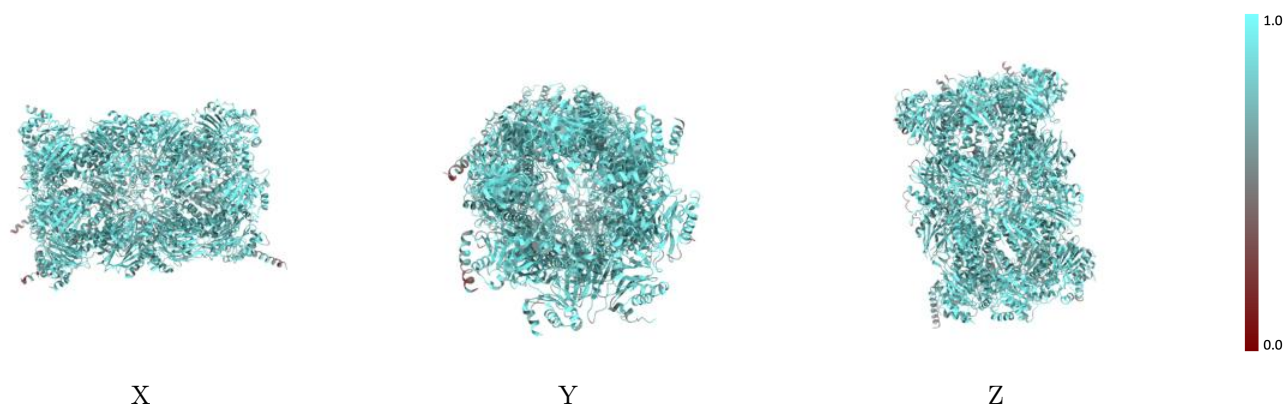
The images above show the 3D surface view of the map at the recommended contour level 0.0545 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



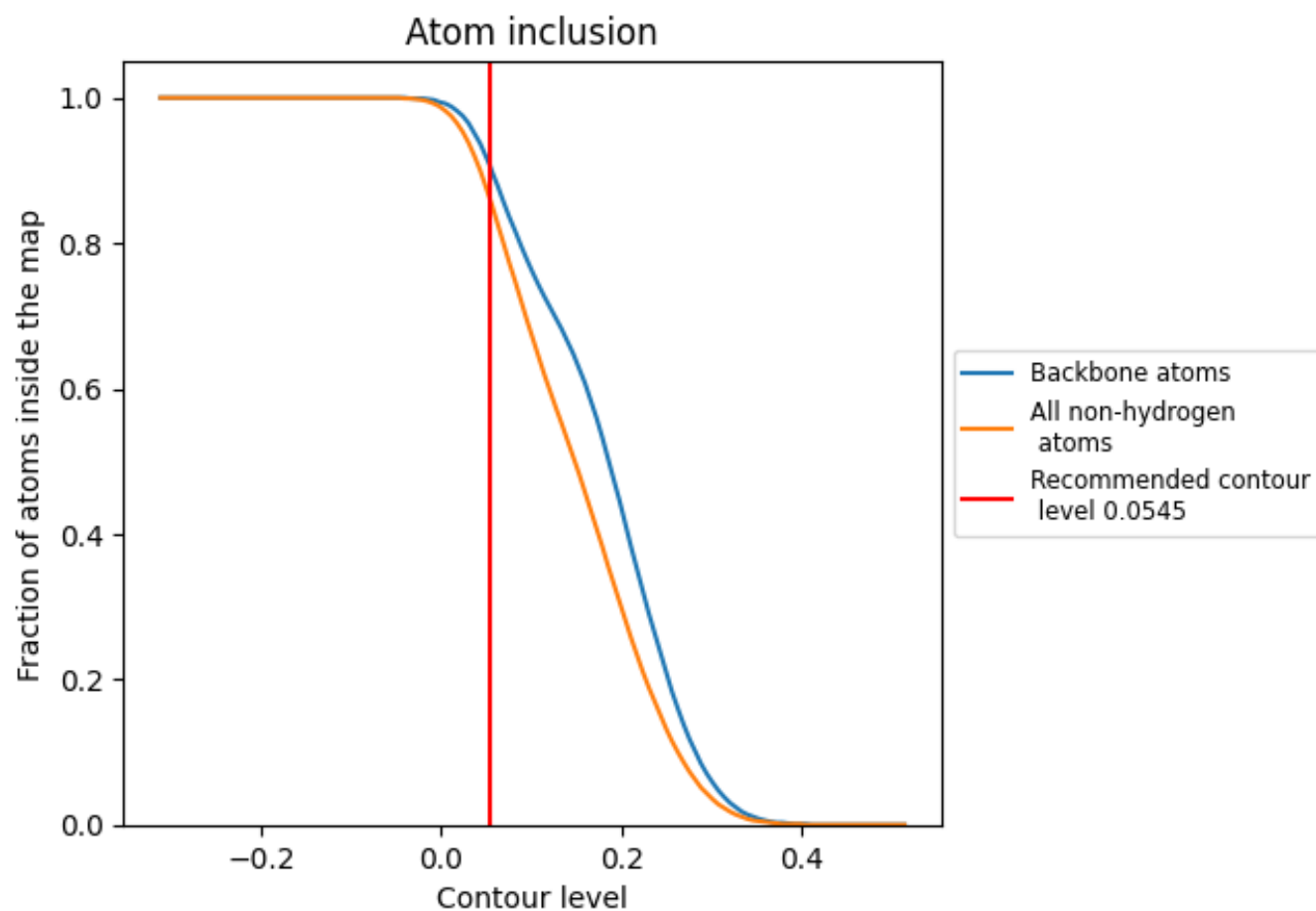
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0545).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.0545) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.5160
A	 0.8640	 0.5160
B	 0.8630	 0.5230
C	 0.8310	 0.4880
D	 0.8130	 0.4750
E	 0.8330	 0.4920
F	 0.8500	 0.5060
G	 0.8510	 0.5050
H	 0.9010	 0.5480
I	 0.8640	 0.5260
J	 0.8690	 0.5310
K	 0.8580	 0.5230
L	 0.8600	 0.5270
M	 0.8520	 0.5140
N	 0.8780	 0.5420
O	 0.8700	 0.5190
P	 0.8790	 0.5240
Q	 0.8500	 0.4960
R	 0.8100	 0.4740
S	 0.8500	 0.4930
T	 0.8590	 0.5130
U	 0.8660	 0.5140
V	 0.9040	 0.5480
W	 0.8610	 0.5190
X	 0.8810	 0.5360
Y	 0.8620	 0.5220
Z	 0.8830	 0.5290
a	 0.8490	 0.5220
b	 0.8950	 0.5410

