



Full wwPDB EM Validation Report ⓘ

Jan 15, 2025 – 08:34 PM JST

PDB ID : 8YIX
EMDB ID : EMD-39332
Title : Cryo-EM structure of human proteasome assembly intermediate half-proteasome
Authors : Han, Y.; Han, Q.; Tang, Q.; Zhang, Y.; Liu, K.
Deposited on : 2024-02-29
Resolution : 2.91 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

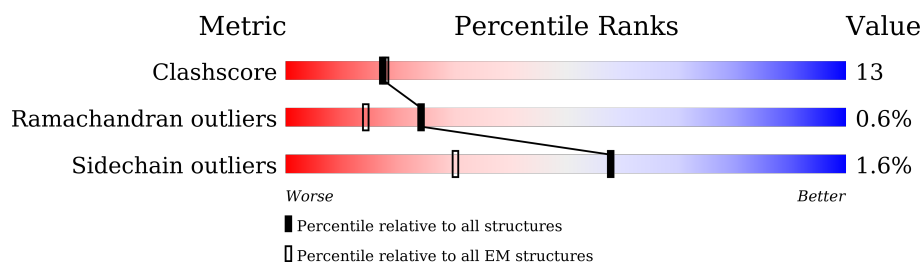
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	234	 76% 21% ..
2	B	261	 72% 23% 6%
3	C	248	 75% 20% 5%
4	D	241	 77% 23%
5	E	263	 73% 17% 9%
6	F	255	 77% 17% 5%
7	G	246	 76% 23%
8	H	277	 64% 21% 14%

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Mol	Chain	Length	Quality of chain
9	I	205	
10	J	201	
11	K	263	
12	L	241	
13	M	253	
14	N	239	
15	f	288	
16	g	264	
17	h	141	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 29572 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	232	Total	C	N	O	S	0	0
			1797	1146	304	340	7		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	246	Total	C	N	O	S	0	0
			1903	1202	323	368	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	236	Total	C	N	O	S	0	0
			1827	1148	322	352	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	241	Total	C	N	O	S	0	0
			1844	1161	305	366	12		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	239	Total	C	N	O	S	1	0
			1879	1179	339	349	12		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	241	Total	C	N	O	S	1	0
			1873	1189	321	351	12		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	245	Total	C	N	O	S	0	0
			1899	1204	320	361	14		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	238	Total	C	N	O	S	1	0
			1807	1147	307	341	12		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	200	Total	C	N	O	S	1	0
			1568	999	262	289	18		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	2	0
			1581	1013	269	289	10		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	2	0
			1764	1117	312	323	12		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	197	Total	C	N	O	S	1	0
			1514	960	260	283	11		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	205	Total	C	N	O	S	1	0
			1597	1008	275	303	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	188	Total	C	N	O	S	1	0
			1434	904	239	278	13		

- Molecule 15 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	277	Total	C	N	O	S	0	0
			2217	1412	372	414	19		

- Molecule 16 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	264	Total	C	N	O	S	0	0
			2062	1323	336	388	15		

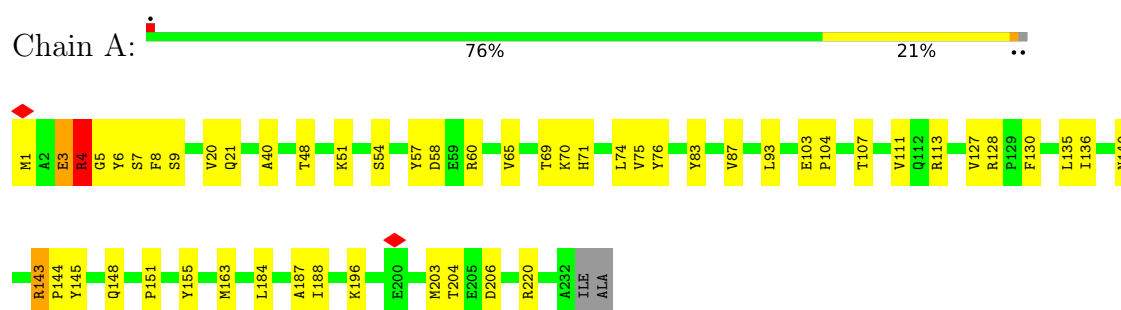
- Molecule 17 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	127	Total	C	N	O	S	0	0
			1006	638	168	195	5		

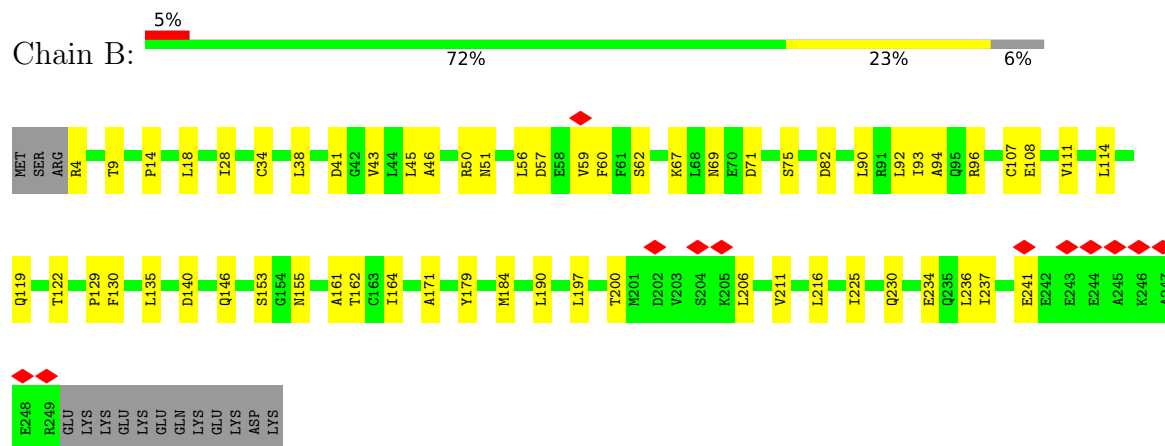
3 Residue-property plots [i](#)

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.

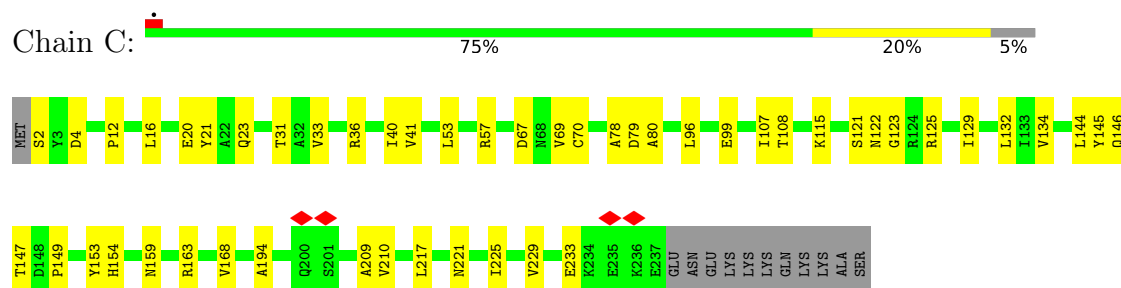
- Molecule 1: Proteasome subunit alpha type-2




- Molecule 2: Proteasome subunit alpha type-4

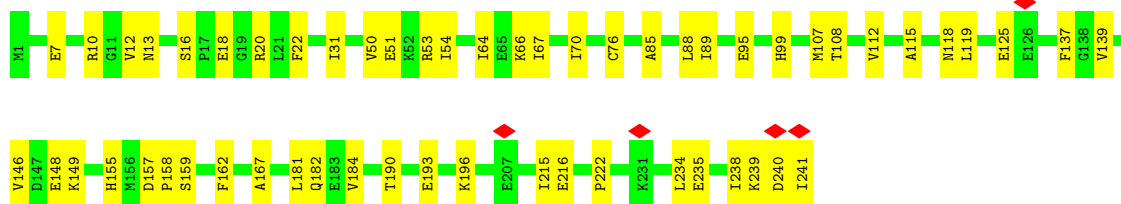


- Molecule 3: Proteasome subunit alpha type-7



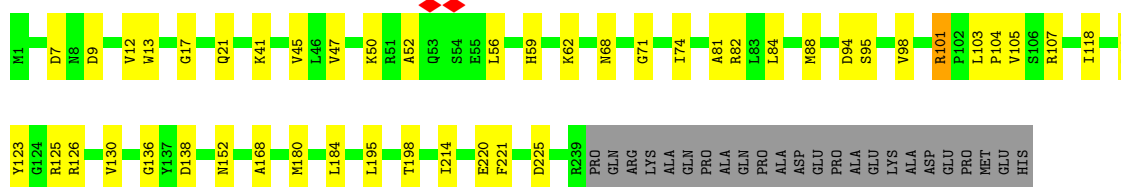
- Molecule 4: Proteasome subunit alpha type-5

Chain D:  77% 23%




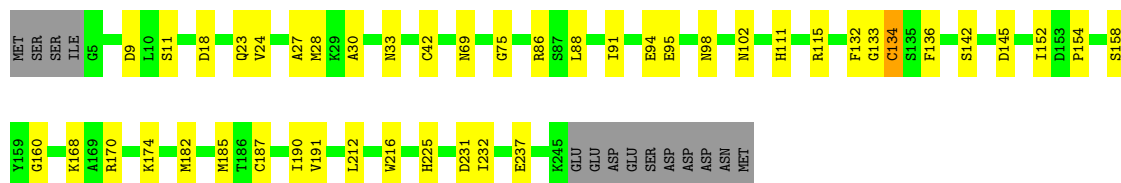
• Molecule 5: Proteasome subunit alpha type-1

Chain E:  73% 17% 9%




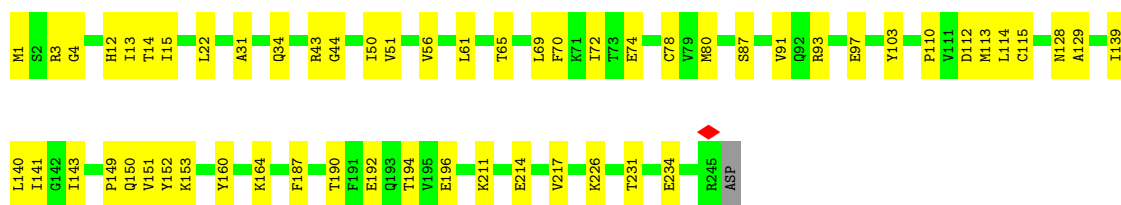
• Molecule 6: Proteasome subunit alpha type-3

Chain F:  77% 17% 5%



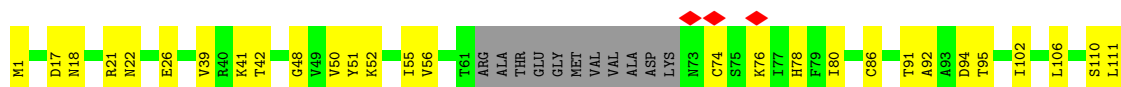
• Molecule 7: Proteasome subunit alpha type-6

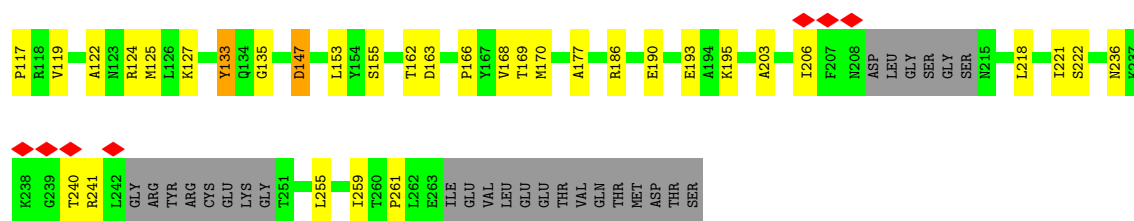
Chain G:  76% 23%



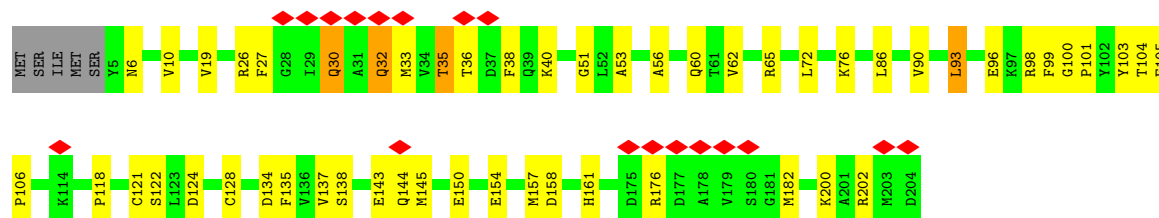
• Molecule 8: Proteasome subunit beta type-7

Chain H:  64% 21% 14%

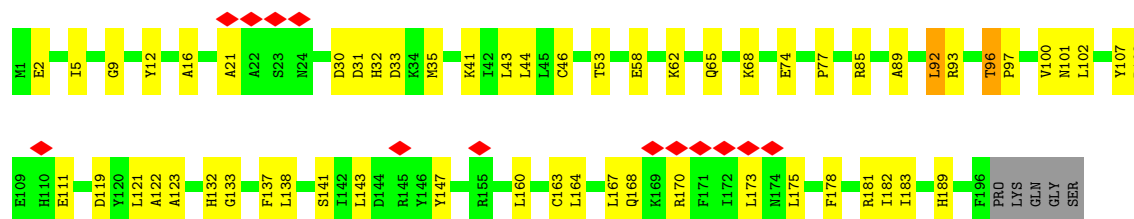




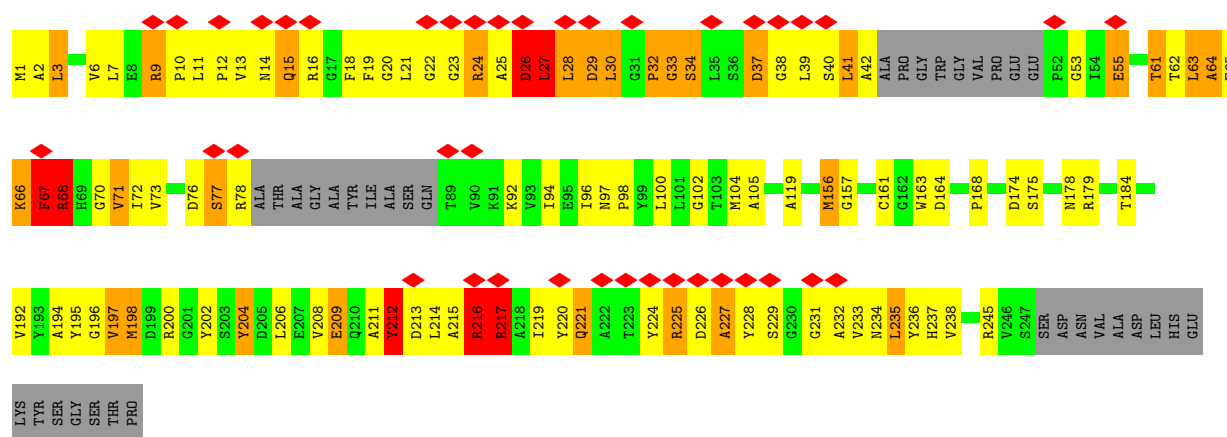
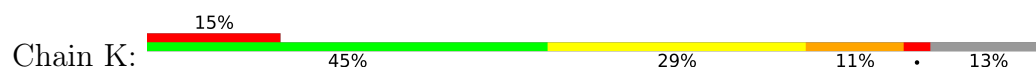
• Molecule 9: Proteasome subunit beta type-3



• Molecule 10: Proteasome subunit beta type-2

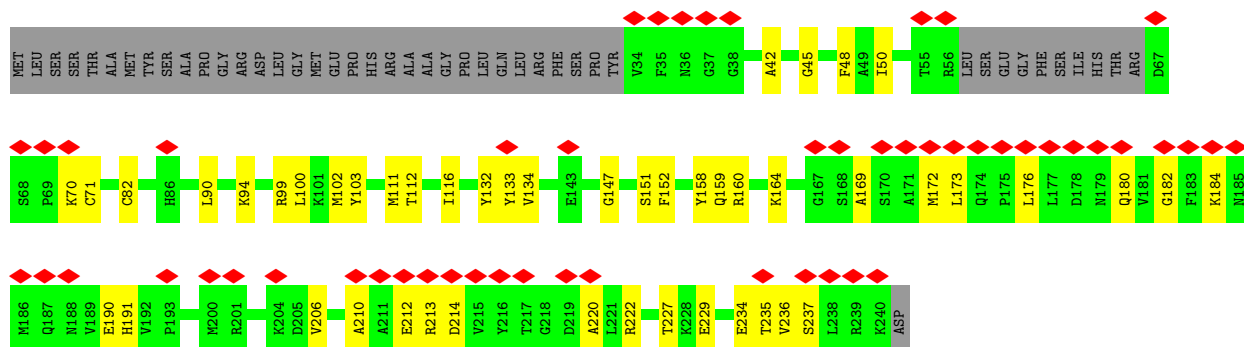


• Molecule 11: Proteasome subunit beta type-5

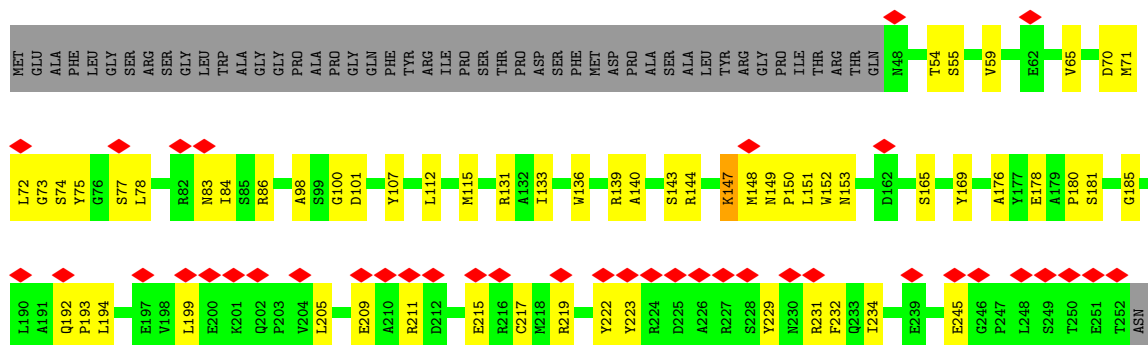


• Molecule 12: Proteasome subunit beta type-1

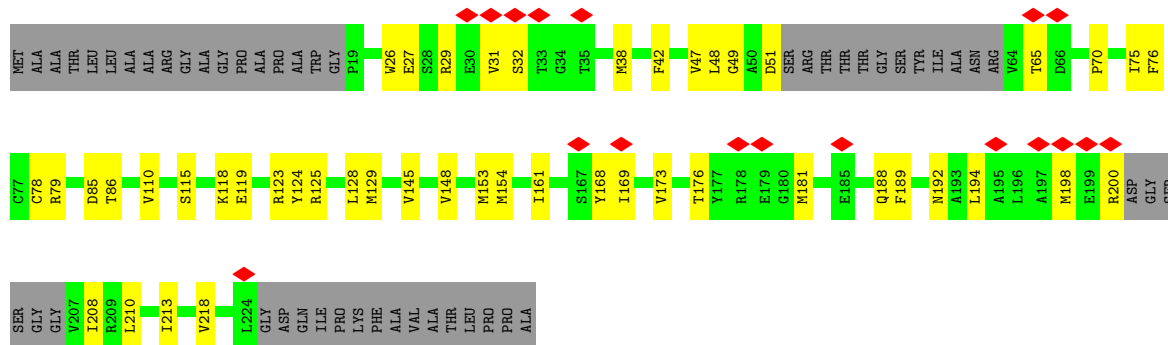




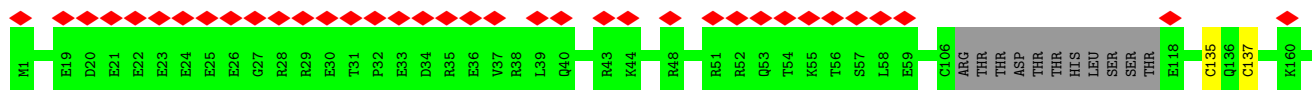
• Molecule 13: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-6

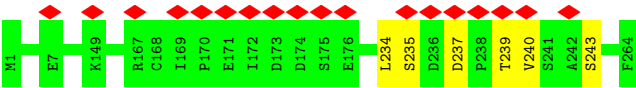


• Molecule 15: Proteasome assembly chaperone 1

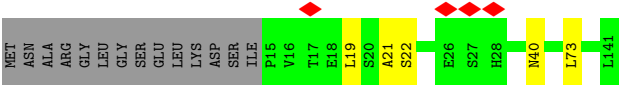
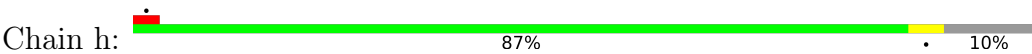




• Molecule 16: Proteasome assembly chaperone 2



• Molecule 17: Proteasome maturation protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	310562	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.128	Depositor
Minimum map value	-3.506	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.161	Depositor
Recommended contour level	0.592	Depositor
Map size (\AA)	316.49997, 316.49997, 316.49997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.055, 1.055, 1.055	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	0/1836	0.60	0/2489
2	B	0.65	0/1933	0.58	0/2613
3	C	0.62	0/1853	0.55	0/2509
4	D	0.57	0/1873	0.59	0/2528
5	E	0.62	0/1917	0.59	0/2589
6	F	0.63	0/1911	0.54	0/2575
7	G	0.65	0/1933	0.55	0/2613
8	H	0.56	0/1841	0.60	1/2492 (0.0%)
9	I	0.56	0/1597	0.59	1/2154 (0.0%)
10	J	0.53	0/1620	0.54	1/2191 (0.0%)
11	K	0.68	0/1803	1.05	8/2428 (0.3%)
12	L	0.43	0/1541	0.53	0/2075
13	M	0.42	0/1630	0.53	0/2205
14	N	0.46	0/1463	0.55	0/1979
15	f	0.54	1/2262 (0.0%)	0.62	1/3061 (0.0%)
16	g	0.58	0/2108	0.59	0/2858
17	h	0.61	0/1025	0.73	2/1381 (0.1%)
All	All	0.59	1/30146 (0.0%)	0.62	14/40740 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
8	H	0	1
9	I	0	1
10	J	0	1
11	K	0	5
13	M	0	1
15	f	0	1
17	h	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	135	CYS	CB-SG	5.18	1.91	1.82

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	67	PHE	CB-CA-C	-19.09	72.21	110.40
11	K	212	TYR	CB-CG-CD2	-14.32	112.41	121.00
11	K	212	TYR	CB-CG-CD1	12.74	128.65	121.00
15	f	135	CYS	CA-CB-SG	7.77	127.98	114.00
11	K	67	PHE	N-CA-CB	-7.53	97.05	110.60
8	H	111	LEU	CA-CB-CG	6.67	130.63	115.30
11	K	212	TYR	CA-CB-CG	6.63	126.00	113.40
10	J	92	LEU	CB-CG-CD1	-6.33	100.24	111.00
11	K	212	TYR	OH-CZ-CE2	-6.13	103.53	120.10
17	h	40	ASN	O-C-N	-5.76	113.48	122.70
11	K	212	TYR	CD1-CE1-CZ	-5.58	114.78	119.80
17	h	73	LEU	CB-CG-CD2	-5.52	101.61	111.00
9	I	93	LEU	CA-CB-CG	5.12	127.07	115.30
11	K	68	ARG	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ARG	Sidechain
8	H	133	TYR	Peptide
9	I	99	PHE	Peptide
10	J	96	THR	Peptide
11	K	216	ARG	Sidechain
11	K	217	ARG	Sidechain
11	K	225	ARG	Sidechain
11	K	68	ARG	Sidechain
11	K	9	ARG	Peptide
13	M	147	LYS	Peptide
15	f	137	CYS	Peptide
17	h	22	SER	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	1797	0	1770	35	0
2	B	1903	0	1876	39	0
3	C	1827	0	1812	34	0
4	D	1844	0	1832	53	0
5	E	1879	0	1872	33	0
6	F	1873	0	1855	48	0
7	G	1899	0	1902	33	0
8	H	1807	0	1828	40	0
9	I	1568	0	1580	39	0
10	J	1581	0	1585	41	0
11	K	1764	0	1758	223	0
12	L	1514	0	1527	38	0
13	M	1597	0	1580	66	0
14	N	1434	0	1395	32	0
15	f	2217	0	2227	0	0
16	g	2062	0	2092	0	0
17	h	1006	0	1003	0	0
All	All	29572	0	29494	641	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 13.

All (641) 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)
4:D:107:MET:CE	11:K:39:LEU:HD21	1.21	1.63
6:F:132:PHE:CZ	11:K:1:MET:CE	2.12	1.33
4:D:107:MET:HE3	11:K:39:LEU:CD2	1.59	1.32
4:D:107:MET:CE	11:K:39:LEU:CD2	2.10	1.30
6:F:132:PHE:CZ	11:K:1:MET:HE1	1.71	1.25
11:K:200:ARG:HB3	11:K:212:TYR:CE2	1.72	1.23
11:K:28:LEU:HD11	13:M:107:TYR:CE2	1.74	1.22
6:F:132:PHE:CE1	11:K:1:MET:HE1	1.74	1.21
6:F:132:PHE:CE1	11:K:1:MET:CE	2.27	1.16
11:K:28:LEU:HD11	13:M:107:TYR:HE2	1.01	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:107:MET:HE1	11:K:39:LEU:HD21	1.19	1.11
11:K:21:LEU:HD22	14:N:124:TYR:CE1	1.85	1.11
11:K:21:LEU:HD22	14:N:124:TYR:HE1	0.98	1.10
6:F:132:PHE:CZ	11:K:1:MET:HE2	1.80	1.09
6:F:132:PHE:HZ	11:K:1:MET:CE	1.56	1.08
11:K:197:VAL:HG21	11:K:219:ILE:HG21	1.34	1.06
11:K:200:ARG:HB3	11:K:212:TYR:HE2	0.88	1.05
5:E:94:ASP:OD1	11:K:32:PRO:HB3	1.59	1.01
11:K:30:LEU:CD2	13:M:140:ALA:HA	1.88	1.01
11:K:21:LEU:CD2	14:N:124:TYR:HE1	1.77	0.97
11:K:72:ILE:HG13	11:K:209:GLU:HG3	1.47	0.97
11:K:200:ARG:CB	11:K:212:TYR:HE2	1.79	0.96
11:K:63:LEU:HD11	11:K:194:ALA:HB1	1.49	0.94
11:K:66:LYS:HB3	11:K:67:PHE:HD1	1.33	0.93
11:K:12:PRO:O	11:K:18:PHE:CD1	2.24	0.91
13:M:71:MET:HB2	13:M:231:ARG:HB3	1.52	0.89
11:K:13:VAL:HG22	11:K:18:PHE:CZ	2.09	0.87
11:K:197:VAL:HG12	11:K:216:ARG:HD2	1.55	0.86
9:I:65:ARG:NH2	9:I:96:GLU:OE2	2.09	0.86
11:K:28:LEU:CD1	13:M:107:TYR:CE2	2.59	0.86
4:D:107:MET:HE3	11:K:39:LEU:HD21	0.86	0.84
11:K:30:LEU:HD22	13:M:140:ALA:HA	1.60	0.83
11:K:30:LEU:CD1	13:M:136:TRP:NE1	2.43	0.81
4:D:107:MET:HE2	11:K:39:LEU:HD11	1.63	0.81
6:F:132:PHE:HE1	11:K:1:MET:CE	1.89	0.81
11:K:23:GLY:O	13:M:107:TYR:OH	1.97	0.81
11:K:67:PHE:CE2	11:K:168:PRO:HG2	2.15	0.80
3:C:31:THR:OG1	3:C:163:ARG:O	1.99	0.80
11:K:9:ARG:CG	11:K:14:ASN:HD21	1.94	0.80
11:K:9:ARG:HG3	11:K:14:ASN:ND2	1.96	0.80
9:I:27:PHE:HD2	9:I:200:LYS:HZ1	1.30	0.80
6:F:98:ASN:ND2	11:K:18:PHE:O	2.15	0.79
4:D:118:ASN:OD1	5:E:82:ARG:NH2	2.16	0.79
11:K:11:LEU:O	11:K:14:ASN:OD1	1.99	0.79
11:K:19:PHE:HZ	13:M:107:TYR:CE1	2.01	0.78
1:A:143:ARG:NH1	1:A:144:PRO:O	2.16	0.78
11:K:198:MET:HA	11:K:212:TYR:CE1	2.19	0.77
11:K:67:PHE:HB3	11:K:70:GLY:O	1.84	0.77
12:L:70:LYS:HG3	12:L:71[B]:CYS:H	1.50	0.77
12:L:70:LYS:HG3	12:L:71[A]:CYS:H	1.50	0.77
11:K:66:LYS:HB3	11:K:67:PHE:CD1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:21:LEU:CD2	14:N:124:TYR:CE1	2.61	0.76
4:D:107:MET:CE	11:K:39:LEU:CG	2.63	0.76
11:K:9:ARG:CG	11:K:14:ASN:ND2	2.49	0.76
3:C:154:HIS:HD2	4:D:64:ILE:HG22	1.50	0.76
7:G:141:ILE:HG22	7:G:151:VAL:HG12	1.69	0.75
11:K:67:PHE:CD2	11:K:168:PRO:HG2	2.21	0.75
11:K:11:LEU:HG	11:K:14:ASN:OD1	1.87	0.75
13:M:131:ARG:NH2	13:M:178:GLU:OE2	2.19	0.75
3:C:146:GLN:OE1	3:C:159:ASN:ND2	2.19	0.75
8:H:21:ARG:HH21	8:H:22:ASN:HD21	1.36	0.74
4:D:146:VAL:HG11	4:D:222:PRO:HA	1.69	0.74
11:K:71:VAL:HG13	11:K:238:VAL:HB	1.69	0.74
11:K:30:LEU:CD2	13:M:140:ALA:CA	2.65	0.74
8:H:186:ARG:NH2	8:H:193:GLU:OE1	2.20	0.73
4:D:107:MET:CE	11:K:39:LEU:HD11	2.17	0.73
4:D:107:MET:HE1	11:K:39:LEU:CD2	1.96	0.73
6:F:42:CYS:HB3	6:F:190:ILE:HG13	1.70	0.73
11:K:30:LEU:HD22	13:M:140:ALA:CA	2.18	0.73
11:K:53:GLY:H	12:L:133:TYR:HB2	1.54	0.73
7:G:3:ARG:HE	7:G:4:GLY:H	1.37	0.73
4:D:7:GLU:OE1	4:D:10:ARG:NH1	2.21	0.73
1:A:7:SER:O	1:A:21:GLN:NE2	2.22	0.72
11:K:198:MET:HA	11:K:212:TYR:CZ	2.24	0.72
2:B:140:ASP:OD1	2:B:146:GLN:NE2	2.23	0.72
1:A:3:GLU:O	1:A:5:GLY:N	2.22	0.72
2:B:69:ASN:HD21	2:B:94:ALA:HB1	1.53	0.72
11:K:71:VAL:HG21	11:K:161:CYS:HB2	1.70	0.71
13:M:70:ASP:HA	13:M:232:PHE:HA	1.71	0.71
3:C:154:HIS:CD2	4:D:64:ILE:HG22	2.25	0.71
3:C:115:LYS:NZ	3:C:147:THR:OG1	2.23	0.71
11:K:67:PHE:CZ	11:K:168:PRO:HG2	2.26	0.70
11:K:197:VAL:CG1	11:K:216:ARG:HD2	2.21	0.70
2:B:119:GLN:NE2	3:C:79:ASP:OD1	2.25	0.70
6:F:11:SER:HA	7:G:1:MET:HG3	1.72	0.70
7:G:43:ARG:HG3	7:G:149:PRO:HB2	1.74	0.70
5:E:104:PRO:HG2	5:E:107:ARG:HG3	1.72	0.70
11:K:9:ARG:HG3	11:K:14:ASN:HD21	1.54	0.69
7:G:72:ILE:HG21	7:G:114:LEU:HD21	1.73	0.69
13:M:101:ASP:OD2	14:N:125:ARG:NH1	2.27	0.68
11:K:221:GLN:HG2	11:K:224:TYR:HB2	1.74	0.68
9:I:32:GLN:HG2	10:J:137:PHE:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:103:TYR:O	8:H:124:ARG:NH1	2.26	0.68
11:K:216:ARG:HD3	11:K:216:ARG:N	2.09	0.68
7:G:192:GLU:O	7:G:196:GLU:HG2	1.94	0.67
6:F:94:GLU:CD	11:K:16:ARG:HG2	2.14	0.67
10:J:21:ALA:HB2	10:J:32:HIS:CG	2.29	0.67
8:H:195:LYS:HG2	8:H:218:LEU:HD13	1.76	0.67
11:K:30:LEU:HD12	13:M:136:TRP:NE1	2.10	0.67
8:H:169:THR:HG21	8:H:177:ALA:HB3	1.77	0.67
14:N:79:ARG:HB3	14:N:86:THR:HG21	1.77	0.67
8:H:26:GLU:OE2	9:I:103:TYR:OH	2.11	0.66
12:L:220:ALA:HA	12:L:237:SER:HA	1.78	0.66
6:F:132:PHE:HZ	11:K:1:MET:HE2	1.35	0.66
4:D:70:ILE:HD11	4:D:76:CYS:HB2	1.78	0.66
9:I:35:THR:HG23	9:I:56:ALA:HB3	1.78	0.66
4:D:95:GLU:OE1	11:K:39:LEU:O	2.13	0.66
11:K:61:THR:HB	11:K:76:ASP:HB3	1.78	0.65
11:K:19:PHE:CZ	13:M:107:TYR:CE1	2.85	0.65
5:E:122:ARG:NH1	5:E:123:TYR:O	2.29	0.65
11:K:19:PHE:CZ	13:M:107:TYR:HE1	2.13	0.65
13:M:180:PRO:HB2	13:M:199:LEU:HD13	1.78	0.65
3:C:69:VAL:HG11	3:C:107:ILE:HG21	1.78	0.65
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.79	0.64
9:I:93:LEU:O	9:I:96:GLU:HG3	1.97	0.64
9:I:6:ASN:OD1	9:I:26:ARG:NH2	2.29	0.64
11:K:13:VAL:HG22	11:K:18:PHE:CE2	2.32	0.64
13:M:73:GLY:HA2	13:M:84:ILE:HD11	1.78	0.64
14:N:173:VAL:HG13	14:N:189:PHE:HZ	1.62	0.64
2:B:108:GLU:OE2	3:C:57:ARG:NH1	2.30	0.64
4:D:50:VAL:HG11	4:D:66:LYS:HB2	1.78	0.64
10:J:138:LEU:HD22	10:J:170:ARG:HD3	1.80	0.64
12:L:173:LEU:HD23	12:L:206:VAL:HG12	1.79	0.64
6:F:212:LEU:HD12	6:F:237:GLU:HG2	1.80	0.63
2:B:69:ASN:HD21	2:B:94:ALA:CB	2.10	0.63
11:K:19:PHE:HZ	13:M:107:TYR:HE1	1.47	0.63
3:C:99:GLU:OE1	11:K:179:ARG:NH2	2.28	0.62
11:K:30:LEU:HD11	13:M:136:TRP:NE1	2.14	0.62
11:K:71:VAL:C	11:K:72:ILE:HD13	2.19	0.62
5:E:50:LYS:HB3	5:E:59:HIS:HB3	1.82	0.62
9:I:154:GLU:H	9:I:157:MET:HE2	1.64	0.62
13:M:86:ARG:NH2	13:M:100:GLY:O	2.32	0.62
11:K:53:GLY:H	12:L:133:TYR:CB	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:31:VAL:HG23	14:N:32:SER:H	1.65	0.61
11:K:204:TYR:HE2	11:K:212:TYR:HD2	1.48	0.61
11:K:195:TYR:O	11:K:198:MET:HB2	2.00	0.61
4:D:107:MET:CE	11:K:39:LEU:CD1	2.78	0.61
8:H:259:ILE:HG22	8:H:261:PRO:HD3	1.81	0.61
9:I:158:ASP:OD1	9:I:161:HIS:ND1	2.29	0.61
14:N:173:VAL:HG13	14:N:189:PHE:CZ	2.34	0.61
11:K:196:GLY:C	11:K:198:MET:H	2.03	0.61
11:K:21:LEU:HD12	11:K:21:LEU:H	1.66	0.60
6:F:132:PHE:CE1	11:K:1:MET:HE2	2.19	0.60
13:M:181:SER:HB3	13:M:199:LEU:HD11	1.84	0.60
8:H:133:TYR:O	8:H:135:GLY:N	2.35	0.60
11:K:30:LEU:HD21	13:M:140:ALA:HA	1.79	0.60
11:K:212:TYR:HD1	11:K:216:ARG:HG2	1.67	0.60
9:I:35:THR:HG23	9:I:56:ALA:CB	2.31	0.60
8:H:155:SER:HB3	8:H:168:VAL:HG21	1.83	0.60
8:H:50:VAL:HG12	8:H:55:ILE:HG22	1.84	0.59
9:I:10:VAL:HG11	9:I:51:GLY:HA3	1.83	0.59
13:M:77:SER:OG	14:N:27:GLU:HB2	2.02	0.59
12:L:112:THR:O	12:L:116:ILE:HG13	2.03	0.59
1:A:74:LEU:HD12	1:A:87:VAL:HG22	1.83	0.59
11:K:67:PHE:CE2	11:K:168:PRO:CG	2.86	0.59
11:K:208:VAL:O	11:K:211:ALA:HB3	2.02	0.59
11:K:214:LEU:HD23	11:K:233:VAL:HG11	1.85	0.59
14:N:75:ILE:HG12	14:N:110:VAL:HG22	1.85	0.59
13:M:83:ASN:H	13:M:231:ARG:CZ	2.14	0.59
4:D:107:MET:HE2	11:K:39:LEU:CD1	2.33	0.58
4:D:85:ALA:O	4:D:89:ILE:HG12	2.03	0.58
6:F:9:ASP:O	6:F:23:GLN:NE2	2.36	0.58
9:I:100:GLY:H	9:I:101:PRO:HD3	1.67	0.58
11:K:28:LEU:HD12	13:M:107:TYR:OH	2.03	0.58
11:K:156[A]:MET:HB2	11:K:175:SER:HB3	1.85	0.58
11:K:156[B]:MET:HB2	11:K:175:SER:HB3	1.85	0.58
13:M:71:MET:N	13:M:231:ARG:O	2.36	0.58
11:K:30:LEU:HD11	13:M:136:TRP:CE2	2.39	0.58
13:M:83:ASN:H	13:M:231:ARG:NE	2.01	0.58
6:F:75:GLY:HA3	6:F:225:HIS:CE1	2.38	0.58
11:K:72:ILE:HG13	11:K:209:GLU:CG	2.28	0.58
10:J:168:GLN:HB2	10:J:175:LEU:HD22	1.86	0.58
11:K:197:VAL:O	11:K:216:ARG:NH1	2.35	0.58
1:A:127:VAL:HG22	1:A:128:ARG:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:132:PHE:HE1	11:K:1:MET:HE1	1.46	0.58
7:G:231:THR:OG1	7:G:234:GLU:OE2	2.18	0.58
6:F:102:ASN:OD1	11:K:19:PHE:O	2.22	0.58
6:F:132:PHE:O	6:F:154:PRO:HB3	2.04	0.58
9:I:35:THR:CG2	10:J:123:ALA:HB3	2.34	0.57
4:D:85:ALA:HB2	4:D:139:VAL:HG21	1.86	0.57
11:K:9:ARG:HB2	11:K:10:PRO:HA	1.85	0.57
11:K:27:LEU:O	11:K:29:ASP:N	2.31	0.57
9:I:19:VAL:HG22	9:I:118:PRO:HB3	1.86	0.57
9:I:62:VAL:HG21	9:I:104:THR:HG21	1.85	0.57
9:I:144:GLN:OE1	9:I:176:ARG:NH2	2.37	0.57
5:E:62:LYS:NZ	5:E:74:ILE:O	2.31	0.57
5:E:98:VAL:HA	13:M:139:ARG:HG3	1.85	0.57
10:J:92:LEU:HD11	10:J:121:LEU:HA	1.87	0.57
2:B:4:ARG:HA	2:B:14:PRO:HD3	1.86	0.57
4:D:215:ILE:HD11	4:D:238:ILE:HD11	1.86	0.57
11:K:32:PRO:C	11:K:34:SER:H	2.07	0.57
11:K:235:LEU:HD23	11:K:236:TYR:H	1.68	0.57
12:L:103:TYR:CD1	12:L:111:MET:HB2	2.40	0.56
14:N:48:LEU:HD23	14:N:78:CYS:SG	2.45	0.56
14:N:38:MET:HG3	14:N:161:ILE:HG22	1.87	0.56
5:E:50:LYS:NZ	5:E:225:ASP:OD1	2.38	0.56
11:K:77:SER:HB3	11:K:232:ALA:N	2.20	0.56
11:K:212:TYR:HA	11:K:216:ARG:HH21	1.69	0.56
14:N:188:GLN:NE2	14:N:192:ASN:OD1	2.39	0.56
1:A:65:VAL:O	1:A:220:ARG:NH1	2.34	0.56
8:H:42:THR:HG23	8:H:92:ALA:HB2	1.88	0.56
11:K:72:ILE:HD12	11:K:237:HIS:HD2	1.70	0.56
3:C:67:ASP:OD2	10:J:65:GLN:NE2	2.37	0.56
3:C:80:ALA:HA	3:C:129:ILE:HD13	1.88	0.56
11:K:28:LEU:HD11	13:M:107:TYR:CZ	2.35	0.56
1:A:3:GLU:O	1:A:4:ARG:C	2.43	0.56
6:F:231:ASP:OD1	6:F:232:ILE:N	2.40	0.55
9:I:135:PHE:HZ	9:I:150:GLU:HG2	1.71	0.55
11:K:30:LEU:HD23	11:K:30:LEU:H	1.70	0.55
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.88	0.55
6:F:94:GLU:OE1	11:K:16:ARG:HG2	2.07	0.55
5:E:68:ASN:ND2	5:E:220:GLU:OE1	2.40	0.55
9:I:35:THR:HG22	10:J:123:ALA:HB3	1.89	0.55
9:I:134:ASP:OD1	9:I:135:PHE:N	2.39	0.55
10:J:138:LEU:HD23	10:J:167:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:95:SER:OG	5:E:101:ARG:NH2	2.40	0.55
10:J:43:LEU:HD12	10:J:183:ILE:HD11	1.87	0.55
11:K:67:PHE:CG	11:K:168:PRO:HG2	2.41	0.55
11:K:66:LYS:HD2	11:K:67:PHE:CE1	2.41	0.55
11:K:206:LEU:HD11	11:K:237:HIS:NE2	2.22	0.55
4:D:157:ASP:O	4:D:159:SER:N	2.33	0.55
5:E:17:GLY:O	6:F:33:ASN:ND2	2.40	0.55
11:K:67:PHE:CE1	11:K:168:PRO:HG2	2.41	0.55
12:L:212:GLU:HG3	12:L:213:ARG:HD2	1.89	0.55
11:K:32:PRO:O	11:K:34:SER:N	2.35	0.55
4:D:99:HIS:ND1	11:K:39:LEU:HG	2.22	0.55
5:E:184:LEU:HD11	5:E:214:ILE:HG12	1.89	0.55
8:H:127:LYS:HE3	8:H:162:THR:HG23	1.89	0.54
11:K:30:LEU:HD12	13:M:136:TRP:HE1	1.71	0.54
4:D:99:HIS:HB2	11:K:39:LEU:HG	1.89	0.54
5:E:52:ALA:HB2	5:E:59:HIS:CG	2.42	0.54
8:H:52:LYS:NZ	8:H:190:GLU:HG3	2.22	0.54
11:K:67:PHE:CE1	11:K:202:TYR:CE2	2.95	0.54
2:B:45:LEU:HD13	2:B:75:SER:HB2	1.89	0.54
2:B:171:ALA:HB2	2:B:200:THR:HG21	1.89	0.54
1:A:48:THR:HB	1:A:75:VAL:HG21	1.90	0.54
11:K:65:PHE:HE1	11:K:213:ASP:HB3	1.73	0.54
11:K:76:ASP:O	11:K:92:LYS:NZ	2.41	0.54
12:L:227:THR:HG23	12:L:229:GLU:H	1.72	0.54
2:B:161:ALA:HB3	3:C:53:LEU:HD13	1.90	0.53
8:H:51:TYR:OH	8:H:222:SER:OG	2.23	0.53
8:H:94:ASP:OD2	9:I:98:ARG:NH2	2.39	0.53
4:D:196:LYS:NZ	4:D:240:ASP:O	2.41	0.53
11:K:233:VAL:O	11:K:234:ASN:C	2.47	0.53
5:E:105:VAL:HG21	5:E:136:GLY:HA3	1.90	0.53
11:K:9:ARG:HB2	11:K:10:PRO:CA	2.38	0.53
3:C:209:ALA:HB1	3:C:217:LEU:HD11	1.91	0.53
4:D:181:LEU:HA	4:D:184:VAL:HG22	1.89	0.53
9:I:121:CYS:SG	9:I:122:SER:N	2.81	0.53
11:K:28:LEU:CD1	13:M:107:TYR:CZ	2.91	0.53
11:K:28:LEU:HD23	11:K:28:LEU:O	2.08	0.53
11:K:30:LEU:HD23	11:K:30:LEU:N	2.24	0.53
6:F:24:VAL:O	6:F:28:MET:HG3	2.09	0.53
2:B:216:LEU:HD12	2:B:225:ILE:HG12	1.90	0.53
10:J:168:GLN:NE2	10:J:173:LEU:O	2.41	0.53
11:K:9:ARG:CB	11:K:14:ASN:HD21	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:212:TYR:CD1	11:K:216:ARG:HG2	2.43	0.52
1:A:130:PHE:O	1:A:151:PRO:HB3	2.09	0.52
3:C:229:VAL:O	3:C:233:GLU:HG2	2.09	0.52
5:E:84:LEU:O	5:E:88:MET:HG3	2.09	0.52
11:K:174:ASP:HB3	11:K:178:ASN:HB2	1.90	0.52
13:M:59:VAL:HG12	13:M:181:SER:HB2	1.91	0.52
11:K:30:LEU:HD22	13:M:140:ALA:N	2.25	0.52
11:K:30:LEU:HD21	13:M:140:ALA:CB	2.40	0.52
11:K:67:PHE:CD1	11:K:168:PRO:HG2	2.44	0.52
12:L:45:GLY:HA3	12:L:48:PHE:CE1	2.44	0.52
13:M:222:TYR:HB2	13:M:229:TYR:HD2	1.74	0.52
14:N:85:ASP:HB3	14:N:128:LEU:HD22	1.91	0.52
3:C:132:LEU:HD22	3:C:144:LEU:HD11	1.92	0.52
11:K:21:LEU:HD13	14:N:123:ARG:HG3	1.91	0.52
4:D:196:LYS:NZ	4:D:241:ILE:O	2.26	0.52
8:H:102:ILE:HD12	8:H:125:MET:HB3	1.91	0.52
1:A:74:LEU:CD2	1:A:136:ILE:HG13	2.40	0.52
11:K:197:VAL:CG2	11:K:219:ILE:HG21	2.24	0.52
4:D:88:LEU:HD23	4:D:119:LEU:HD23	1.92	0.52
4:D:31:ILE:HD11	4:D:158:PRO:HG3	1.90	0.51
11:K:206:LEU:HD11	11:K:237:HIS:CE1	2.45	0.51
6:F:88:LEU:HD12	6:F:134[A]:CYS:SG	2.51	0.51
11:K:198:MET:HG2	11:K:212:TYR:HE1	1.76	0.51
11:K:28:LEU:CD1	13:M:107:TYR:OH	2.59	0.51
10:J:30:ASP:O	10:J:32:HIS:N	2.43	0.51
4:D:235:GLU:O	4:D:239:LYS:HD3	2.10	0.51
7:G:78:CYS:HB3	7:G:140:LEU:HD23	1.92	0.51
7:G:112:ASP:HB3	7:G:152:TYR:CZ	2.46	0.51
11:K:27:LEU:HD12	11:K:30:LEU:HD12	1.92	0.51
2:B:92:LEU:O	2:B:96:ARG:HG3	2.11	0.51
6:F:88:LEU:HD12	6:F:134[B]:CYS:SG	2.51	0.51
9:I:35:THR:HG21	10:J:123:ALA:CB	2.40	0.51
9:I:86:LEU:O	9:I:90:VAL:HG23	2.10	0.51
12:L:70:LYS:HG2	12:L:82:CYS:H	1.75	0.51
11:K:9:ARG:HA	11:K:9:ARG:HH21	1.76	0.51
9:I:10:VAL:HG23	9:I:53:ALA:HB2	1.92	0.51
11:K:24:ARG:NH2	13:M:115:MET:HG3	2.25	0.51
6:F:191:VAL:HG21	6:F:216:TRP:CZ3	2.46	0.50
2:B:122:THR:HG22	2:B:129:PRO:HB3	1.93	0.50
2:B:135:LEU:HD11	2:B:162:THR:HG23	1.93	0.50
11:K:41:LEU:O	11:K:42:ALA:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:ILE:HG22	4:D:64:ILE:HD11	1.94	0.50
11:K:30:LEU:CD1	13:M:136:TRP:CD1	2.95	0.50
12:L:111:MET:CE	12:L:116:ILE:HG12	2.42	0.50
2:B:107:CYS:O	2:B:111:VAL:HG23	2.11	0.50
9:I:72:LEU:O	9:I:76:LYS:HG3	2.11	0.50
5:E:81:ALA:HB2	5:E:130:VAL:HG21	1.93	0.50
11:K:12:PRO:O	11:K:18:PHE:CE1	2.65	0.50
11:K:29:ASP:HB3	13:M:143:SER:OG	2.11	0.50
11:K:197:VAL:O	11:K:216:ARG:NE	2.44	0.50
13:M:144:ARG:NE	13:M:149:ASN:O	2.38	0.50
14:N:145:VAL:HG12	14:N:145:VAL:O	2.12	0.50
4:D:51:GLU:HG2	4:D:53:ARG:HG3	1.92	0.50
8:H:106:LEU:HD11	8:H:122:ALA:HB2	1.92	0.50
12:L:222:ARG:HA	12:L:235:THR:HG22	1.93	0.50
13:M:144:ARG:HG3	13:M:151:LEU:HD12	1.93	0.50
8:H:203:ALA:HA	8:H:206:ILE:HG12	1.94	0.49
9:I:35:THR:CG2	10:J:123:ALA:CB	2.89	0.49
11:K:67:PHE:CD1	11:K:67:PHE:N	2.79	0.49
11:K:13:VAL:HG22	11:K:18:PHE:CE1	2.46	0.49
11:K:197:VAL:HG12	11:K:216:ARG:CD	2.36	0.49
11:K:67:PHE:CD2	11:K:168:PRO:CG	2.94	0.49
4:D:125:GLU:HG3	5:E:125:ARG:CZ	2.42	0.49
11:K:72:ILE:HD12	11:K:209:GLU:OE2	2.11	0.49
11:K:198:MET:CA	11:K:212:TYR:CZ	2.94	0.49
5:E:7:ASP:O	5:E:21:GLN:NE2	2.42	0.49
7:G:12:HIS:HB3	7:G:15:ILE:HG12	1.95	0.49
11:K:28:LEU:O	11:K:29:ASP:HB2	2.13	0.49
14:N:176:THR:HG23	14:N:189:PHE:HE1	1.78	0.49
2:B:46:ALA:HB1	2:B:197:LEU:HD22	1.95	0.49
11:K:33:GLY:O	11:K:34:SER:CB	2.60	0.49
13:M:219:ARG:HB3	13:M:223:TYR:CE2	2.48	0.49
8:H:21:ARG:HH21	8:H:22:ASN:ND2	2.07	0.49
2:B:230:GLN:NE2	2:B:234:GLU:OE2	2.38	0.48
3:C:108:THR:HG21	3:C:145:TYR:HB3	1.95	0.48
7:G:13:ILE:HG23	7:G:14:THR:HG23	1.94	0.48
10:J:46[A]:CYS:SG	10:J:100:VAL:HG13	2.53	0.48
4:D:13:ASN:HA	5:E:126:ARG:HD3	1.96	0.48
7:G:51:VAL:HG22	7:G:217:VAL:HG22	1.95	0.48
10:J:101:ASN:HB3	10:J:132:HIS:CE1	2.47	0.48
11:K:30:LEU:HD21	13:M:140:ALA:CA	2.41	0.48
2:B:14:PRO:HB3	3:C:21:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:70:LYS:CG	12:L:71[B]:CYS:H	2.22	0.48
13:M:211:ARG:O	13:M:215:GLU:HG2	2.13	0.48
14:N:169:ILE:O	14:N:173:VAL:HG23	2.12	0.48
12:L:70:LYS:CG	12:L:71[A]:CYS:H	2.22	0.48
11:K:11:LEU:HG	11:K:14:ASN:CG	2.34	0.48
11:K:29:ASP:HB3	13:M:147:LYS:NZ	2.29	0.48
11:K:226:ASP:CG	11:K:231:GLY:HA2	2.34	0.48
4:D:155:HIS:O	4:D:162:PHE:HA	2.14	0.48
8:H:78:HIS:N	8:H:86:CYS:O	2.41	0.48
6:F:142:SER:HB3	6:F:145:ASP:HB2	1.94	0.48
11:K:198:MET:CG	11:K:212:TYR:HE1	2.27	0.48
11:K:217:ARG:HE	11:K:233:VAL:HG12	1.79	0.48
13:M:150:PRO:HB2	13:M:152:TRP:NE1	2.29	0.48
8:H:55:ILE:HD11	8:H:221:ILE:HD13	1.96	0.48
9:I:30:GLN:HE21	10:J:141:SER:HA	1.79	0.48
9:I:154:GLU:H	9:I:157:MET:CE	2.25	0.48
11:K:3:LEU:O	11:K:7:LEU:HG	2.14	0.48
11:K:196:GLY:C	11:K:198:MET:N	2.66	0.48
13:M:192:GLN:HB3	13:M:193:PRO:HD3	1.96	0.48
14:N:26:TRP:HA	14:N:29:ARG:HE	1.79	0.48
1:A:184:LEU:O	1:A:188:ILE:HG13	2.14	0.48
3:C:2:SER:HA	3:C:12:PRO:HD3	1.94	0.48
12:L:172:MET:O	12:L:213:ARG:NH2	2.47	0.48
14:N:148:VAL:HA	14:N:153:MET:O	2.14	0.48
7:G:44:GLY:HA3	7:G:194:THR:HG21	1.95	0.47
10:J:68:LYS:HD3	10:J:74:GLU:HG2	1.96	0.47
11:K:220:TYR:CE2	11:K:221:GLN:HG3	2.49	0.47
10:J:108:ASP:HB3	10:J:111:GLU:HB2	1.96	0.47
13:M:65:VAL:HG23	13:M:165:SER:HB2	1.95	0.47
11:K:94:ILE:N	11:K:102:GLY:O	2.47	0.47
11:K:96:ILE:HG21	11:K:100:LEU:HD23	1.96	0.47
14:N:51:ASP:HB2	14:N:198:MET:CE	2.44	0.47
1:A:140:ASN:HB2	1:A:145:TYR:HE2	1.79	0.47
5:E:122:ARG:HD3	5:E:125:ARG:HG3	1.95	0.47
5:E:123:TYR:HE1	11:K:6:VAL:HG13	1.78	0.47
1:A:40:ALA:HB2	1:A:187:ALA:HB2	1.97	0.47
3:C:225:ILE:O	3:C:229:VAL:HG23	2.14	0.47
4:D:16:SER:C	4:D:18:GLU:H	2.18	0.47
8:H:153:LEU:HD21	8:H:168:VAL:HG12	1.96	0.47
9:I:56:ALA:O	9:I:60:GLN:HG3	2.14	0.47
10:J:89:ALA:O	10:J:93:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:184:THR:HG22	11:K:195:TYR:CE1	2.49	0.47
1:A:107:THR:O	1:A:111:VAL:HG23	2.15	0.47
4:D:137:PHE:O	4:D:158:PRO:HB3	2.15	0.47
8:H:110:SER:OG	8:H:117:PRO:HG3	2.15	0.47
9:I:35:THR:HG21	10:J:123:ALA:HB1	1.97	0.47
11:K:94:ILE:HD11	11:K:104:MET:HG2	1.97	0.46
13:M:98:ALA:HB1	13:M:153:ASN:HD21	1.80	0.46
11:K:21:LEU:HD12	11:K:21:LEU:N	2.30	0.46
11:K:38:GLY:C	11:K:40:SER:N	2.69	0.46
11:K:105:ALA:HB3	11:K:157:GLY:HA3	1.96	0.46
12:L:169:ALA:HB1	12:L:173:LEU:HD13	1.98	0.46
13:M:72:LEU:HA	13:M:231:ARG:HH12	1.80	0.46
3:C:168:VAL:HG13	3:C:194:ALA:HB1	1.97	0.46
7:G:80:MET:HB3	7:G:87:SER:HB3	1.97	0.46
13:M:215:GLU:O	13:M:219:ARG:HG3	2.14	0.46
14:N:29:ARG:NH1	14:N:129:MET:HE1	2.30	0.46
12:L:234:GLU:O	12:L:234:GLU:HG2	2.15	0.46
10:J:35:MET:SD	10:J:181:ARG:HD2	2.56	0.46
11:K:156[A]:MET:H	11:K:175:SER:HB3	1.81	0.46
11:K:156[B]:MET:H	11:K:175:SER:HB3	1.81	0.46
11:K:197:VAL:HG21	11:K:219:ILE:CG2	2.25	0.46
11:K:229:SER:O	11:K:229:SER:OG	2.30	0.46
10:J:33:ASP:OD2	10:J:181:ARG:NH2	2.48	0.46
10:J:164:LEU:HD21	10:J:178:PHE:CD2	2.51	0.46
13:M:169:TYR:O	13:M:176:ALA:HA	2.15	0.46
14:N:213:ILE:HG12	14:N:218:VAL:HG22	1.98	0.46
8:H:119:VAL:HG23	8:H:147[A]:ASP:OD1	2.16	0.46
11:K:198:MET:HB3	11:K:212:TYR:OH	2.15	0.46
12:L:99:ARG:HA	12:L:102:MET:HE3	1.97	0.46
2:B:9:THR:HG21	2:B:129:PRO:HD3	1.97	0.45
1:A:204:THR:HG22	1:A:206:ASP:H	1.81	0.45
2:B:57:ASP:O	2:B:59:VAL:HG13	2.16	0.45
2:B:90:LEU:HG	2:B:114:LEU:HD13	1.97	0.45
5:E:103:LEU:HD12	5:E:104:PRO:HD2	1.98	0.45
11:K:9:ARG:NE	11:K:11:LEU:HD23	2.31	0.45
11:K:67:PHE:CZ	11:K:168:PRO:HD2	2.52	0.45
12:L:147:GLY:O	12:L:160:ARG:NH2	2.48	0.45
12:L:176:LEU:O	12:L:180:GLN:HB2	2.16	0.45
2:B:34:CYS:HB2	2:B:164:ILE:HG13	1.98	0.45
11:K:67:PHE:CD2	11:K:68:ARG:CA	2.99	0.45
12:L:70:LYS:CG	12:L:82:CYS:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:55:SER:HA	13:M:185:GLY:HA3	1.97	0.45
3:C:40:ILE:HD11	3:C:210:VAL:HB	1.98	0.45
5:E:45:VAL:HG12	5:E:214:ILE:HG13	1.99	0.45
6:F:18:ASP:OD1	6:F:18:ASP:N	2.48	0.45
11:K:70:GLY:HA2	11:K:163:TRP:CZ3	2.51	0.45
9:I:143:GLU:HG2	9:I:144:GLN:H	1.80	0.45
11:K:9:ARG:HB2	11:K:14:ASN:HD21	1.82	0.45
13:M:148:MET:HG3	13:M:150:PRO:HD3	1.98	0.45
2:B:206:LEU:HD11	2:B:211:VAL:HG11	1.98	0.45
6:F:30:ALA:O	6:F:33:ASN:HB2	2.16	0.45
7:G:139:ILE:HG12	7:G:153:LYS:HG3	1.99	0.45
7:G:143:ILE:HD13	7:G:149:PRO:HA	1.99	0.45
10:J:5:ILE:HG21	10:J:160:LEU:HD11	1.98	0.45
11:K:96:ILE:HG23	11:K:119:ALA:HB2	1.99	0.45
4:D:50:VAL:HG12	4:D:216:GLU:HB3	1.99	0.45
7:G:115:CYS:SG	7:G:160:TYR:HB2	2.57	0.45
11:K:37:ASP:OD1	11:K:37:ASP:N	2.45	0.45
11:K:164:ASP:OD1	11:K:164:ASP:N	2.47	0.45
2:B:82:ASP:HB3	2:B:130:PHE:HD1	1.81	0.45
3:C:146:GLN:O	3:C:153:TYR:HA	2.17	0.45
9:I:124:ASP:OD1	9:I:128:CYS:HB3	2.16	0.45
11:K:217:ARG:O	11:K:220:TYR:HB3	2.16	0.45
4:D:99:HIS:CB	11:K:39:LEU:HG	2.47	0.45
10:J:101:ASN:HB3	10:J:132:HIS:ND1	2.32	0.45
11:K:194:ALA:O	11:K:198:MET:HG3	2.17	0.45
13:M:194:LEU:HD22	13:M:217:CYS:SG	2.57	0.45
2:B:93:ILE:HG23	8:H:1:MET:N	2.32	0.44
4:D:20:ARG:HH21	4:D:22:PHE:HZ	1.64	0.44
10:J:85:ARG:NH1	10:J:122:ALA:O	2.50	0.44
11:K:77:SER:HB3	11:K:231:GLY:CA	2.47	0.44
14:N:49:GLY:HA2	14:N:210:LEU:HA	1.99	0.44
7:G:141:ILE:HA	7:G:150:GLN:O	2.18	0.44
10:J:53:THR:HG22	10:J:100:VAL:HG22	1.98	0.44
11:K:217:ARG:HG2	11:K:233:VAL:HG12	1.99	0.44
12:L:42:ALA:HA	12:L:50:ILE:O	2.17	0.44
4:D:12:VAL:HG12	4:D:13:ASN:N	2.33	0.44
4:D:234:LEU:O	4:D:238:ILE:HD12	2.17	0.44
11:K:156[A]:MET:HE3	11:K:156[A]:MET:HB3	1.90	0.44
1:A:70:LYS:HE2	8:H:236:ASN:HB3	1.99	0.44
8:H:39:VAL:HG23	8:H:41:LYS:HE3	2.00	0.44
11:K:156[B]:MET:HE3	11:K:156[B]:MET:HB3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ASN:CB	2:B:71:ASP:H	2.31	0.44
3:C:33:VAL:HG22	3:C:168:VAL:HG11	2.00	0.44
6:F:191:VAL:HG21	6:F:216:TRP:CE3	2.53	0.44
11:K:32:PRO:C	11:K:34:SER:N	2.69	0.44
1:A:143:ARG:HD2	1:A:145:TYR:CZ	2.53	0.44
2:B:41:ASP:OD1	2:B:41:ASP:N	2.51	0.44
3:C:23:GLN:HG2	3:C:149:PRO:HD2	1.99	0.44
5:E:71:GLY:HA3	5:E:221:PHE:CZ	2.53	0.44
4:D:67:ILE:HA	4:D:76:CYS:O	2.18	0.43
11:K:53:GLY:HA2	12:L:133:TYR:HD1	1.83	0.43
13:M:98:ALA:HB1	13:M:153:ASN:ND2	2.33	0.43
10:J:58:GLU:O	10:J:62:LYS:HG2	2.18	0.43
12:L:190:GLU:O	12:L:191:HIS:ND1	2.50	0.43
1:A:128:ARG:HD2	7:G:22:LEU:HD21	2.00	0.43
2:B:51:ASN:HB3	2:B:56:LEU:CD1	2.49	0.43
11:K:216:ARG:N	11:K:216:ARG:CD	2.76	0.43
13:M:54:THR:HA	13:M:75:TYR:HE1	1.82	0.43
1:A:58:ASP:OD1	1:A:60:ARG:HG2	2.18	0.43
1:A:135:LEU:HG	1:A:163:MET:CE	2.49	0.43
2:B:67:LYS:HE2	2:B:69:ASN:O	2.18	0.43
4:D:95:GLU:HG3	4:D:115:ALA:HB1	2.00	0.43
4:D:99:HIS:ND1	11:K:39:LEU:CD1	2.81	0.43
6:F:27:ALA:O	6:F:30:ALA:HB3	2.18	0.43
6:F:42:CYS:HB2	6:F:185:MET:O	2.18	0.43
7:G:31:ALA:HA	7:G:34:GLN:HG2	2.00	0.43
7:G:128:ASN:OD1	7:G:129:ALA:N	2.50	0.43
8:H:52:LYS:HZ2	8:H:190:GLU:HG3	1.83	0.43
10:J:119:ASP:OD1	10:J:123:ALA:HB3	2.18	0.43
11:K:27:LEU:HD13	11:K:27:LEU:HA	1.75	0.43
12:L:234:GLU:O	12:L:236:VAL:HG23	2.18	0.43
13:M:72:LEU:HD12	13:M:231:ARG:HH12	1.83	0.43
13:M:234:ILE:HB	13:M:245:GLU:OE2	2.18	0.43
2:B:18:LEU:HD21	3:C:125:ARG:HD2	1.99	0.43
6:F:136:PHE:CE2	6:F:152:ILE:HD13	2.53	0.43
7:G:50:ILE:HD12	7:G:69:LEU:HD22	2.01	0.43
9:I:105:GLU:HG3	9:I:138:SER:OG	2.18	0.43
1:A:74:LEU:HD23	1:A:136:ILE:HG13	1.99	0.43
2:B:179:TYR:CE1	2:B:184:MET:HG3	2.53	0.43
4:D:107:MET:HE2	11:K:39:LEU:CG	2.45	0.43
11:K:226:ASP:O	11:K:227:ALA:HB2	2.19	0.43
1:A:54:SER:HG	1:A:57:TYR:HE1	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:THR:O	4:D:112:VAL:HG23	2.19	0.43
4:D:190:THR:HG23	4:D:193:GLU:H	1.83	0.43
8:H:80:ILE:HG22	8:H:106:LEU:HD12	1.99	0.43
9:I:137:VAL:HG11	9:I:145:MET:HB3	2.01	0.43
10:J:44:LEU:HD11	10:J:102:LEU:HD22	2.01	0.43
11:K:15:GLN:HB3	11:K:16:ARG:H	1.44	0.43
14:N:168:TYR:CD1	14:N:200:ARG:HD3	2.53	0.43
1:A:111:VAL:HG22	1:A:136:ILE:HD13	2.01	0.43
5:E:9:ASP:HB3	5:E:12:VAL:HG23	2.00	0.43
5:E:152:ASN:HA	6:F:86:ARG:HH12	1.83	0.43
11:K:184:THR:HG23	11:K:198:MET:SD	2.59	0.43
7:G:74:GLU:OE2	7:G:226:LYS:HE2	2.18	0.43
12:L:90:LEU:O	12:L:94:LYS:HG3	2.19	0.43
3:C:4:ASP:N	3:C:4:ASP:OD1	2.48	0.42
3:C:221:ASN:OD1	3:C:221:ASN:N	2.52	0.42
4:D:107:MET:HE1	11:K:39:LEU:HD11	2.00	0.42
6:F:94:GLU:OE1	11:K:16:ARG:CG	2.67	0.42
7:G:70:PHE:CD2	7:G:91:VAL:HG21	2.55	0.42
8:H:255:LEU:HD13	9:I:202:ARG:HH22	1.84	0.42
10:J:143:LEU:O	10:J:147:TYR:N	2.47	0.42
11:K:27:LEU:HB3	11:K:30:LEU:O	2.18	0.42
3:C:96:LEU:HD12	3:C:96:LEU:HA	1.82	0.42
11:K:215:ALA:HB3	11:K:216:ARG:HH21	1.83	0.42
12:L:212:GLU:C	12:L:213:ARG:HD2	2.40	0.42
3:C:16:LEU:O	3:C:20:GLU:HG3	2.19	0.42
3:C:41:VAL:HG21	3:C:134:VAL:HB	2.01	0.42
6:F:69:ASN:OD1	6:F:225:HIS:HD2	2.03	0.42
6:F:94:GLU:OE1	11:K:16:ARG:HD3	2.18	0.42
14:N:42:PHE:CE2	14:N:47:VAL:HG23	2.54	0.42
6:F:152:ILE:HG13	6:F:158:SER:CB	2.50	0.42
7:G:110:PRO:HD2	7:G:113:MET:HB2	2.02	0.42
10:J:77:PRO:HD2	10:J:108:ASP:HB2	2.01	0.42
11:K:13:VAL:CG2	11:K:18:PHE:CZ	2.93	0.42
3:C:36:ARG:HA	3:C:41:VAL:HG23	2.02	0.42
6:F:170:ARG:NH1	6:F:174:LYS:HE3	2.34	0.42
11:K:38:GLY:O	11:K:39:LEU:HB3	2.20	0.42
11:K:63:LEU:HB3	11:K:64:ALA:H	1.58	0.42
11:K:72:ILE:HD12	11:K:237:HIS:CD2	2.54	0.42
2:B:122:THR:HG21	2:B:153:SER:HA	2.02	0.42
6:F:187:CYS:O	6:F:191:VAL:HG23	2.19	0.42
10:J:9:GLY:HA3	10:J:12:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:182:ILE:HG22	10:J:189:HIS:HB2	2.02	0.42
11:K:198:MET:SD	11:K:212:TYR:CE1	3.13	0.42
11:K:200:ARG:HA	11:K:204:TYR:CZ	2.54	0.42
1:A:20:VAL:O	1:A:20:VAL:HG13	2.19	0.42
9:I:154:GLU:O	9:I:157:MET:HG3	2.20	0.42
11:K:97:ASN:HB2	11:K:98:PRO:HD2	2.02	0.42
12:L:111:MET:HE2	12:L:116:ILE:HG12	2.01	0.42
14:N:118:LYS:HD3	14:N:154:MET:HE2	2.02	0.42
6:F:152:ILE:HG13	6:F:158:SER:HB3	2.01	0.42
7:G:110:PRO:HB2	7:G:112:ASP:OD1	2.20	0.42
8:H:91:THR:O	8:H:95:THR:HG23	2.20	0.42
10:J:96:THR:OG1	10:J:97:PRO:HD3	2.20	0.42
12:L:100:LEU:HD12	12:L:111:MET:HE1	2.02	0.42
14:N:194:LEU:HB3	14:N:208:ILE:HD12	2.02	0.42
1:A:103:GLU:HG2	1:A:104:PRO:HD2	2.02	0.41
2:B:50:ARG:HA	2:B:50:ARG:HD3	1.73	0.41
5:E:138:ASP:OD1	5:E:138:ASP:N	2.51	0.41
6:F:111:HIS:O	6:F:115:ARG:HG3	2.20	0.41
11:K:26:ASP:O	11:K:27:LEU:HB2	2.19	0.41
12:L:210:ALA:O	12:L:213:ARG:HB2	2.20	0.41
8:H:163:ASP:OD1	14:N:65:THR:OG1	2.31	0.41
11:K:212:TYR:O	11:K:216:ARG:HD3	2.19	0.41
12:L:152:PHE:CD2	12:L:158:TYR:HB3	2.55	0.41
2:B:28:ILE:HD12	2:B:28:ILE:H	1.85	0.41
6:F:91:ILE:O	6:F:95:GLU:HG2	2.20	0.41
10:J:16:ALA:HB2	10:J:160:LEU:HD21	2.02	0.41
11:K:38:GLY:O	11:K:39:LEU:CB	2.68	0.41
11:K:39:LEU:O	11:K:39:LEU:HD23	2.20	0.41
14:N:115:SER:O	14:N:119:GLU:HG3	2.20	0.41
4:D:167:ALA:HB1	4:D:181:LEU:HD22	2.01	0.41
6:F:168:LYS:HE3	6:F:168:LYS:HB2	1.83	0.41
11:K:25:ALA:O	11:K:26:ASP:C	2.58	0.41
12:L:111:MET:HE3	12:L:116:ILE:HA	2.02	0.41
12:L:151:SER:HB3	12:L:164:LYS:HG2	2.01	0.41
12:L:213:ARG:HB3	12:L:214:ASP:H	1.72	0.41
1:A:8:PHE:O	7:G:15:ILE:HD12	2.21	0.41
6:F:170:ARG:HH21	6:F:170:ARG:HG3	1.86	0.41
9:I:26:ARG:NE	9:I:182:MET:SD	2.93	0.41
11:K:20:GLY:C	11:K:22:GLY:H	2.22	0.41
11:K:24:ARG:HE	11:K:24:ARG:HB2	1.36	0.41
11:K:39:LEU:CD2	11:K:39:LEU:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ILE:O	2:B:241:GLU:HG3	2.21	0.41
8:H:240:THR:O	8:H:241:ARG:HB2	2.21	0.41
11:K:12:PRO:O	11:K:18:PHE:HD1	1.92	0.41
1:A:51:LYS:HE3	1:A:51:LYS:HB2	1.83	0.41
8:H:17:ASP:O	8:H:18:ASN:HB2	2.21	0.41
9:I:105:GLU:HA	9:I:106:PRO:HD3	1.83	0.41
11:K:33:GLY:O	11:K:34:SER:HB3	2.20	0.41
14:N:70:PRO:HB3	14:N:76:PHE:CZ	2.56	0.41
1:A:69:THR:HG1	1:A:71:HIS:CE1	2.39	0.41
3:C:70:CYS:SG	3:C:217:LEU:HD13	2.60	0.41
5:E:168:ALA:HB2	5:E:198:THR:CG2	2.51	0.41
11:K:30:LEU:HD21	13:M:140:ALA:HB2	2.03	0.41
12:L:132:TYR:HB3	12:L:134:VAL:HG22	2.03	0.41
1:A:4:ARG:C	1:A:6:TYR:H	2.25	0.41
1:A:148:GLN:O	1:A:155:TYR:HA	2.20	0.41
1:A:196:LYS:HG3	1:A:203:MET:HE2	2.02	0.41
3:C:121:SER:O	3:C:123:GLY:N	2.54	0.41
8:H:74:CYS:HB3	8:H:76:LYS:NZ	2.36	0.41
11:K:1:MET:HG2	11:K:2:ALA:H	1.86	0.41
1:A:76:TYR:HB3	1:A:83:TYR:CD1	2.55	0.40
2:B:67:LYS:HE3	2:B:225:ILE:HD12	2.03	0.40
4:D:182:GLN:HA	5:E:56:LEU:HD11	2.03	0.40
5:E:13:TRP:CH2	6:F:133:GLY:HA3	2.56	0.40
5:E:41:LYS:HG3	5:E:180:MET:HB3	2.02	0.40
6:F:160:GLY:HA3	7:G:65:THR:HG21	2.03	0.40
7:G:164:LYS:HB3	7:G:187:PHE:CE1	2.57	0.40
7:G:211:LYS:HB2	7:G:214:GLU:HG3	2.01	0.40
8:H:48:GLY:HA2	8:H:56:VAL:O	2.21	0.40
8:H:155:SER:HB2	8:H:170:MET:HE3	2.03	0.40
10:J:41:LYS:HD2	10:J:107:TYR:HB3	2.04	0.40
11:K:41:LEU:H	11:K:41:LEU:HG	1.65	0.40
11:K:214:LEU:HD23	11:K:233:VAL:HG21	2.03	0.40
2:B:60:PHE:O	2:B:62:SER:N	2.54	0.40
5:E:118:ILE:HG12	11:K:1:MET:HA	2.03	0.40
8:H:50:VAL:HG22	8:H:166:PRO:O	2.21	0.40
11:K:14:ASN:OD1	11:K:14:ASN:N	2.49	0.40
13:M:74:SER:HB3	13:M:78:LEU:HB2	2.02	0.40
13:M:112:LEU:HD11	13:M:133:ILE:HG23	2.02	0.40
2:B:38:LEU:HD12	2:B:43:VAL:HG22	2.03	0.40
2:B:190:LEU:HD22	2:B:236:LEU:HD21	2.03	0.40
4:D:148:GLU:HG3	4:D:149:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:86:ARG:HH11	6:F:86:ARG:HD2	1.73	0.40
7:G:93:ARG:O	7:G:97:GLU:HG2	2.20	0.40
9:I:38:PHE:CE2	9:I:40:LYS:HG2	2.56	0.40
10:J:2:GLU:O	10:J:133:GLY:HA3	2.21	0.40
12:L:182:GLY:C	12:L:184:LYS:H	2.25	0.40
1:A:93:LEU:HD13	1:A:113:ARG:HB3	2.03	0.40
1:A:140:ASN:HB2	1:A:145:TYR:CE2	2.56	0.40
7:G:56:VAL:HG13	7:G:61:LEU:HD22	2.03	0.40
10:J:21:ALA:HB2	10:J:32:HIS:CD2	2.56	0.40
10:J:163:CYS:O	10:J:167:LEU:HD23	2.22	0.40
1:A:4:ARG:O	1:A:6:TYR:N	2.55	0.40
11:K:66:LYS:HD2	11:K:67:PHE:HE1	1.83	0.40
11:K:67:PHE:HD2	11:K:68:ARG:CA	2.34	0.40
13:M:205:LEU:HD23	13:M:209:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/234 (98%)	218 (95%)	11 (5%)	1 (0%)	30	59
2	B	244/261 (94%)	233 (96%)	11 (4%)	0	100	100
3	C	234/248 (94%)	223 (95%)	10 (4%)	1 (0%)	30	59
4	D	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
5	E	238/263 (90%)	228 (96%)	10 (4%)	0	100	100
6	F	240/255 (94%)	235 (98%)	5 (2%)	0	100	100
7	G	243/246 (99%)	231 (95%)	11 (4%)	1 (0%)	30	59
8	H	231/277 (83%)	209 (90%)	22 (10%)	0	100	100
9	I	199/205 (97%)	182 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	196/201 (98%)	178 (91%)	17 (9%)	1 (0%)	25	55
11	K	224/263 (85%)	181 (81%)	28 (12%)	15 (7%)	1	2
12	L	194/241 (80%)	173 (89%)	21 (11%)	0	100	100
13	M	204/253 (81%)	193 (95%)	11 (5%)	0	100	100
14	N	183/239 (77%)	162 (88%)	21 (12%)	0	100	100
15	f	273/288 (95%)	242 (89%)	31 (11%)	0	100	100
16	g	262/264 (99%)	235 (90%)	24 (9%)	3 (1%)	12	36
17	h	125/141 (89%)	110 (88%)	14 (11%)	1 (1%)	16	44
All	All	3759/4120 (91%)	3457 (92%)	279 (7%)	23 (1%)	24	51

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
11	K	61	THR
11	K	64	ALA
11	K	67	PHE
11	K	197	VAL
11	K	227	ALA
16	g	234	LEU
17	h	21	ALA
11	K	26	ASP
11	K	28	LEU
11	K	32	PRO
11	K	34	SER
11	K	55	GLU
3	C	122	ASN
11	K	29	ASP
11	K	37	ASP
7	G	190	THR
11	K	27	LEU
11	K	66	LYS
10	J	31	ASP
16	g	235	SER
11	K	33	GLY
16	g	240	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/191 (97%)	181 (97%)	5 (3%)	40	72
2	B	198/221 (90%)	197 (100%)	1 (0%)	86	95
3	C	191/211 (90%)	191 (100%)	0	100	100
4	D	201/203 (99%)	201 (100%)	0	100	100
5	E	203/224 (91%)	202 (100%)	1 (0%)	86	95
6	F	195/212 (92%)	192 (98%)	3 (2%)	60	84
7	G	206/210 (98%)	206 (100%)	0	100	100
8	H	196/228 (86%)	194 (99%)	2 (1%)	73	90
9	I	169/174 (97%)	164 (97%)	5 (3%)	36	69
10	J	169/171 (99%)	169 (100%)	0	100	100
11	K	179/202 (89%)	148 (83%)	31 (17%)	1	4
12	L	162/199 (81%)	161 (99%)	1 (1%)	84	94
13	M	169/206 (82%)	169 (100%)	0	100	100
14	N	150/181 (83%)	148 (99%)	2 (1%)	65	86
15	f	251/262 (96%)	249 (99%)	2 (1%)	79	92
16	g	237/237 (100%)	234 (99%)	3 (1%)	65	86
17	h	117/128 (91%)	116 (99%)	1 (1%)	75	91
All	All	3179/3460 (92%)	3122 (98%)	57 (2%)	58	81

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU
1	A	4	ARG
1	A	9	SER
1	A	143	ARG
2	B	155	ASN
5	E	101	ARG

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Mol	Chain	Res	Type
6	F	134[A]	CYS
6	F	134[B]	CYS
6	F	182	MET
8	H	147[A]	ASP
8	H	147[B]	ASP
9	I	30	GLN
9	I	32	GLN
9	I	33	MET
9	I	35	THR
9	I	36	THR
11	K	3	LEU
11	K	15	GLN
11	K	24	ARG
11	K	26	ASP
11	K	27	LEU
11	K	30	LEU
11	K	41	LEU
11	K	55	GLU
11	K	62	THR
11	K	63	LEU
11	K	67	PHE
11	K	68	ARG
11	K	71	VAL
11	K	73	VAL
11	K	77	SER
11	K	78	ARG
11	K	156[A]	MET
11	K	156[B]	MET
11	K	192	VAL
11	K	198	MET
11	K	204	TYR
11	K	209	GLU
11	K	212	TYR
11	K	216	ARG
11	K	217	ARG
11	K	221	GLN
11	K	225	ARG
11	K	228	TYR
11	K	235	LEU
11	K	245[A]	ARG
11	K	245[B]	ARG
12	L	159	GLN

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Mol	Chain	Res	Type
14	N	181[A]	MET
14	N	181[B]	MET
15	f	285	ASN
15	f	288	THR
16	g	237	ASP
16	g	239	THR
16	g	243	SER
17	h	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	69	ASN
3	C	154	HIS
6	F	225	HIS
8	H	22	ASN
9	I	30	GLN
11	K	15	GLN
11	K	234	ASN
11	K	237	HIS
13	M	153	ASN
15	f	280	ASN
17	h	80	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

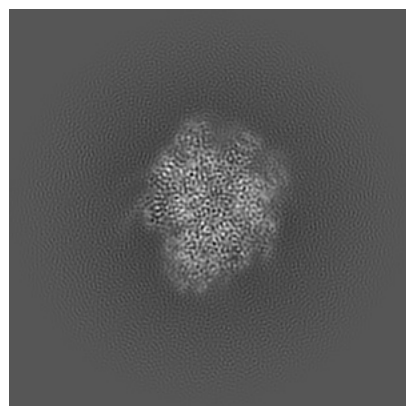
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39332. These allow visual inspection of the internal detail of the map and identification of artifacts.

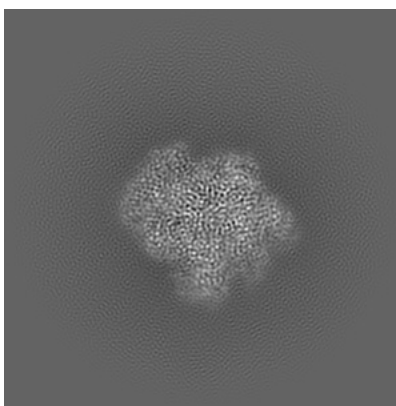
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

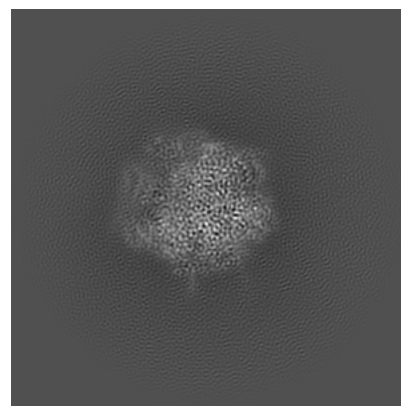
6.1.1 Primary map



X

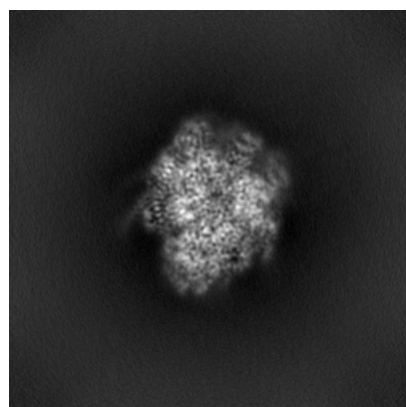


Y

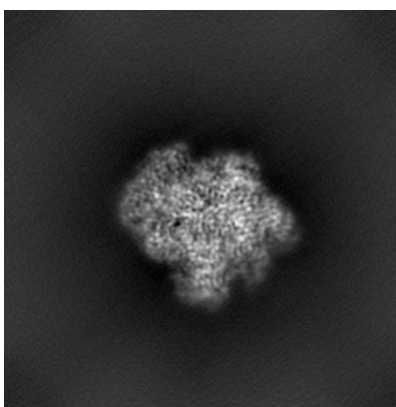


Z

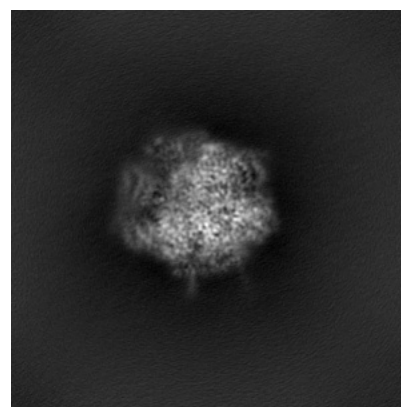
6.1.2 Raw map



X



Y

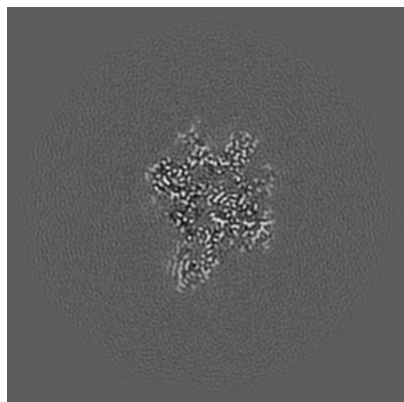


Z

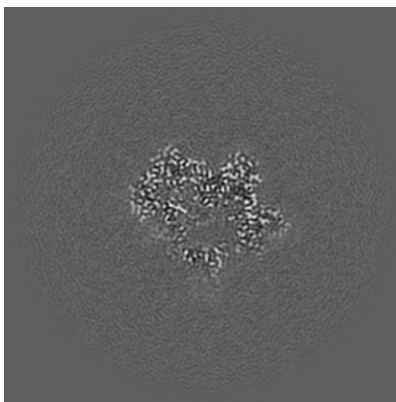
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

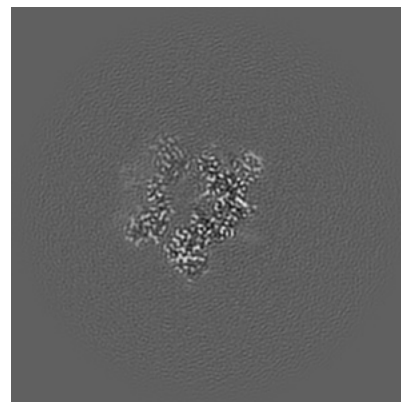
6.2.1 Primary map



X Index: 150

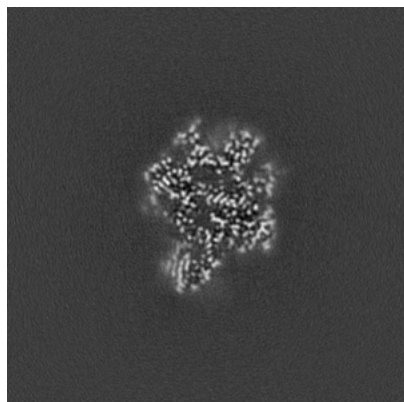


Y Index: 150

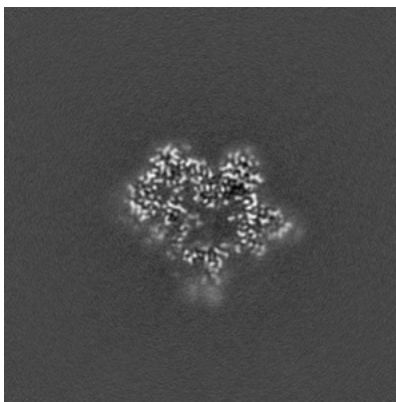


Z Index: 150

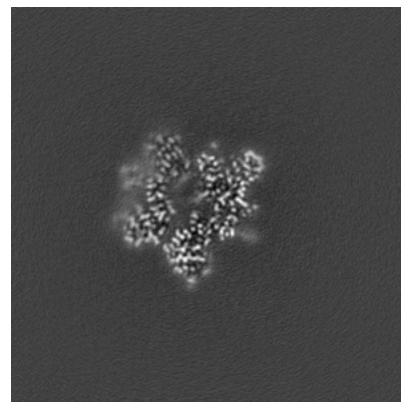
6.2.2 Raw map



X Index: 150



Y Index: 150

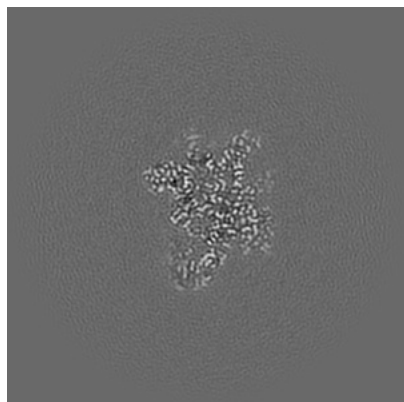


Z Index: 150

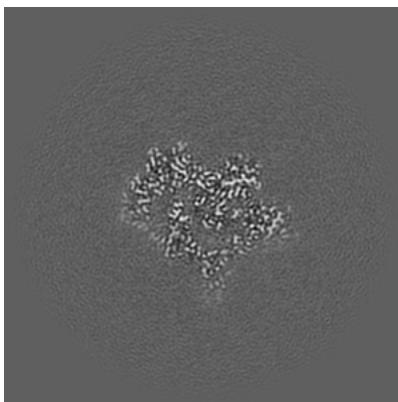
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

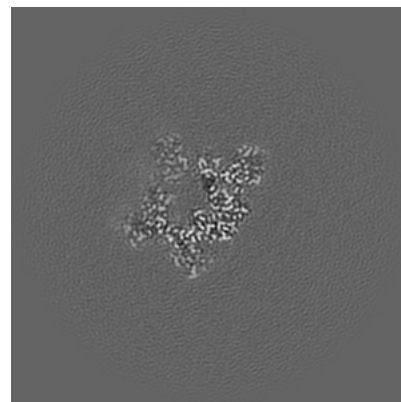
6.3.1 Primary map



X Index: 153

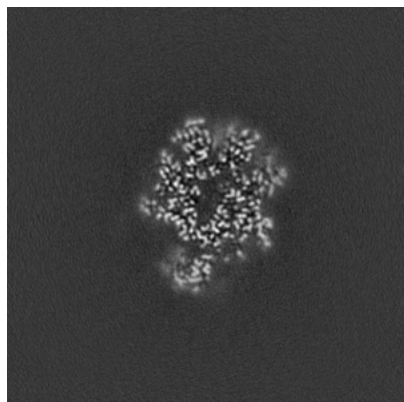


Y Index: 143

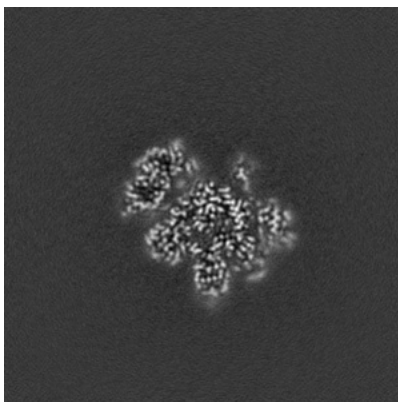


Z Index: 156

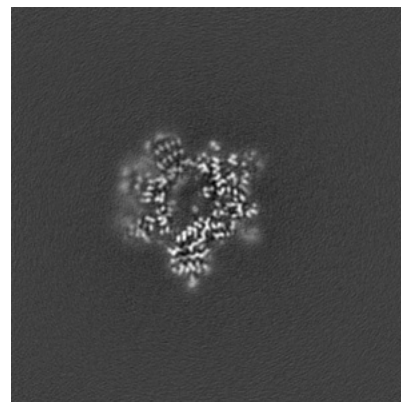
6.3.2 Raw map



X Index: 146



Y Index: 134

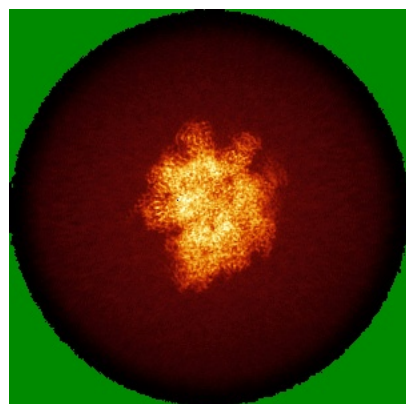


Z Index: 147

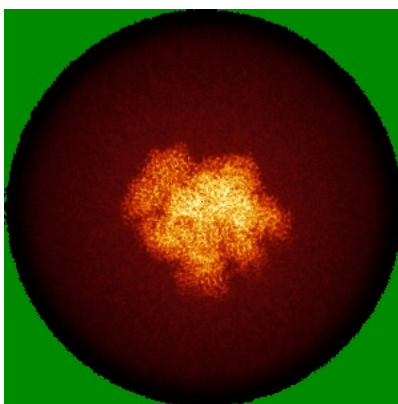
The images above show the largest variance slices of the map in three orthogonal directions.

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

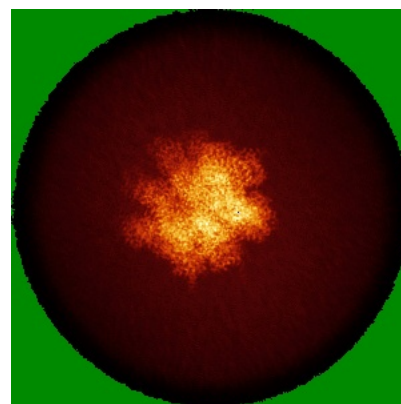
6.4.1 Primary map



X

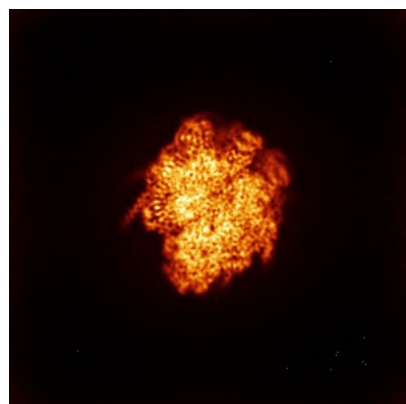


Y

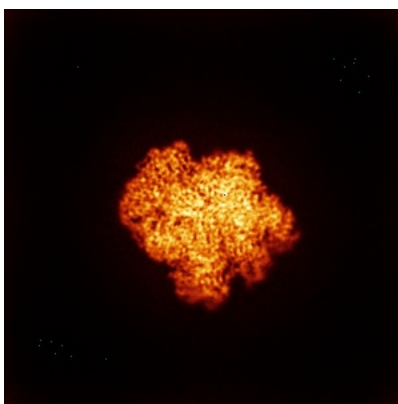


Z

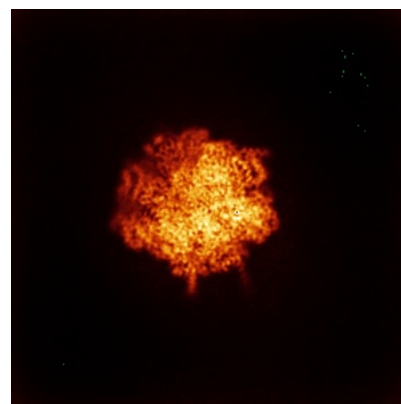
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

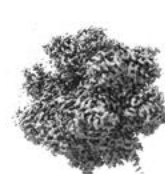
6.5.1 Primary map



X



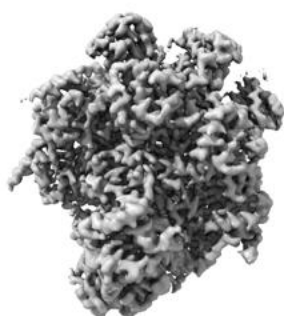
Y



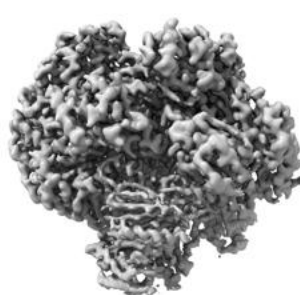
Z

The images above show the 3D surface view of the map at the recommended contour level 0.592. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

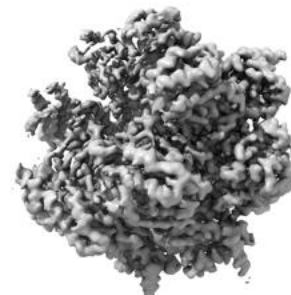
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

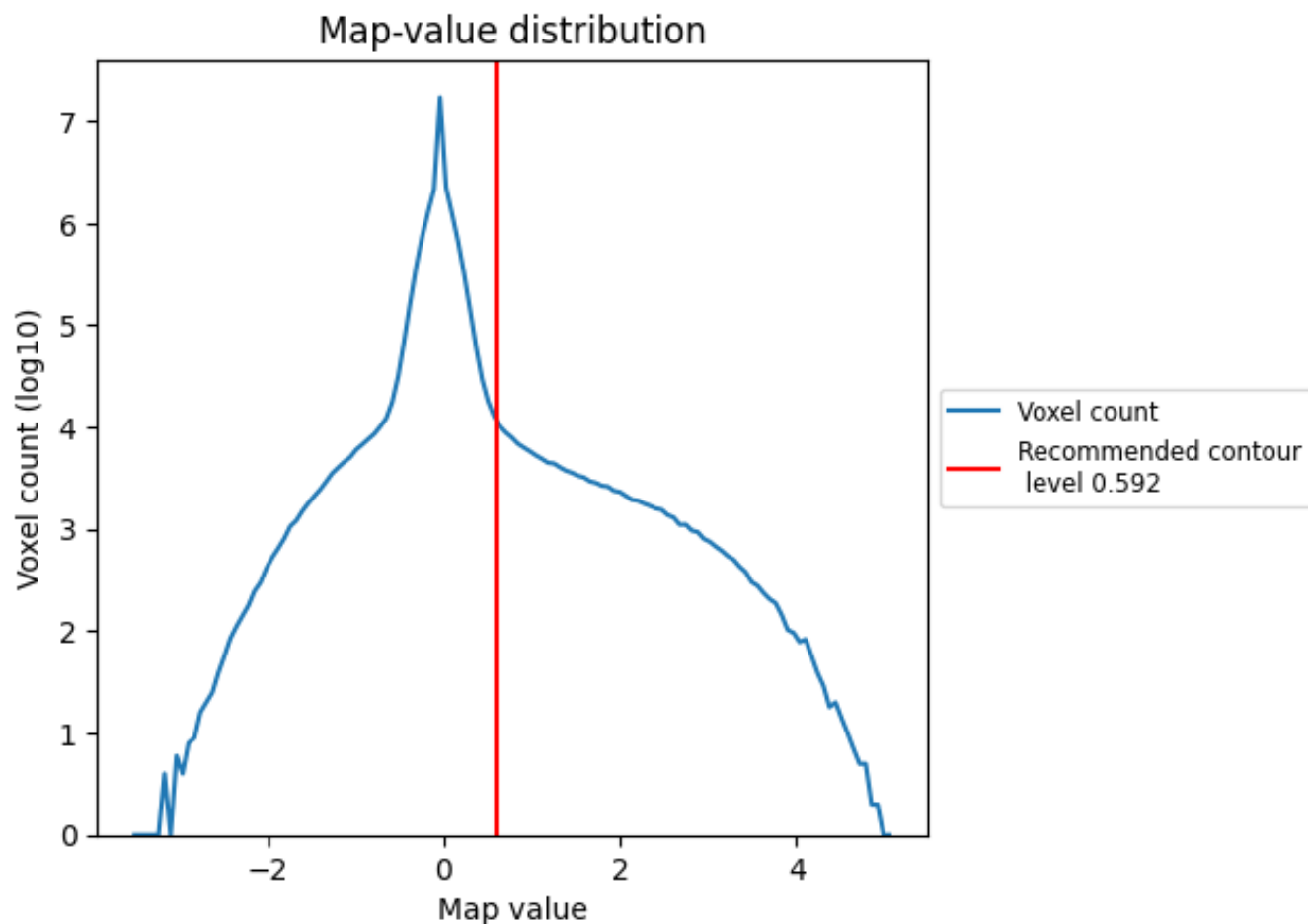
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

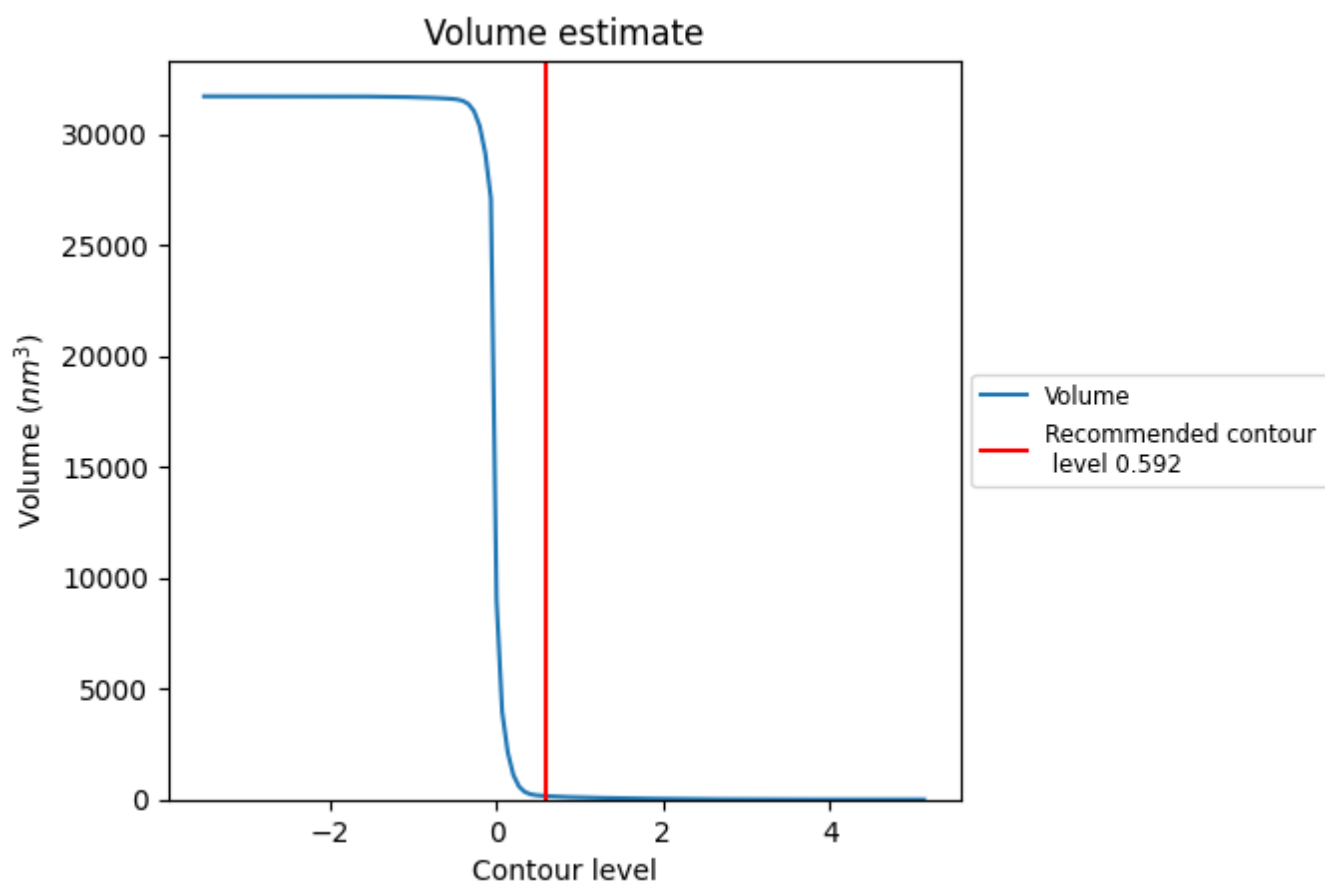
This section contains the results of statistical analysis of the map.

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.

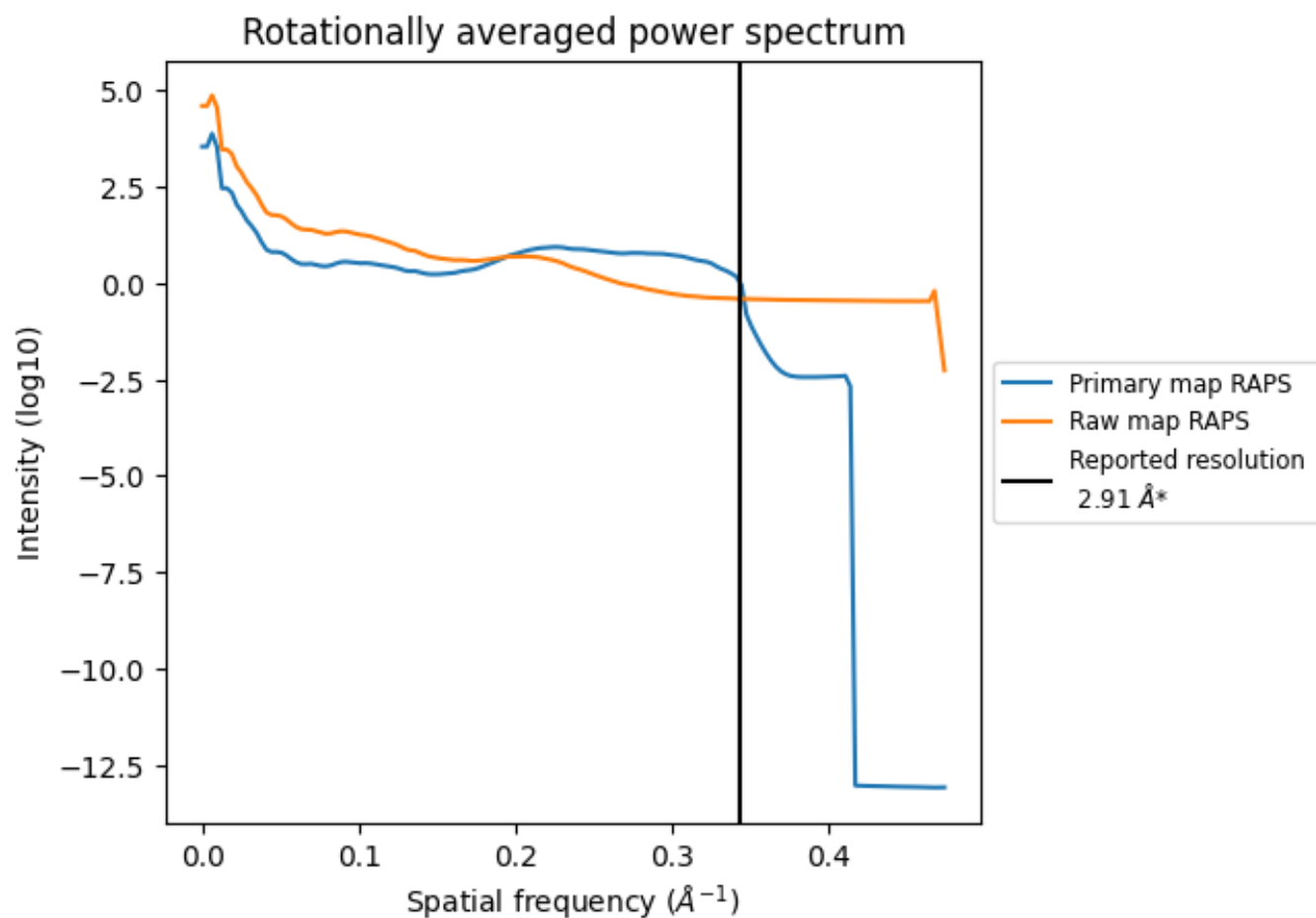
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 142 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 ⓘ

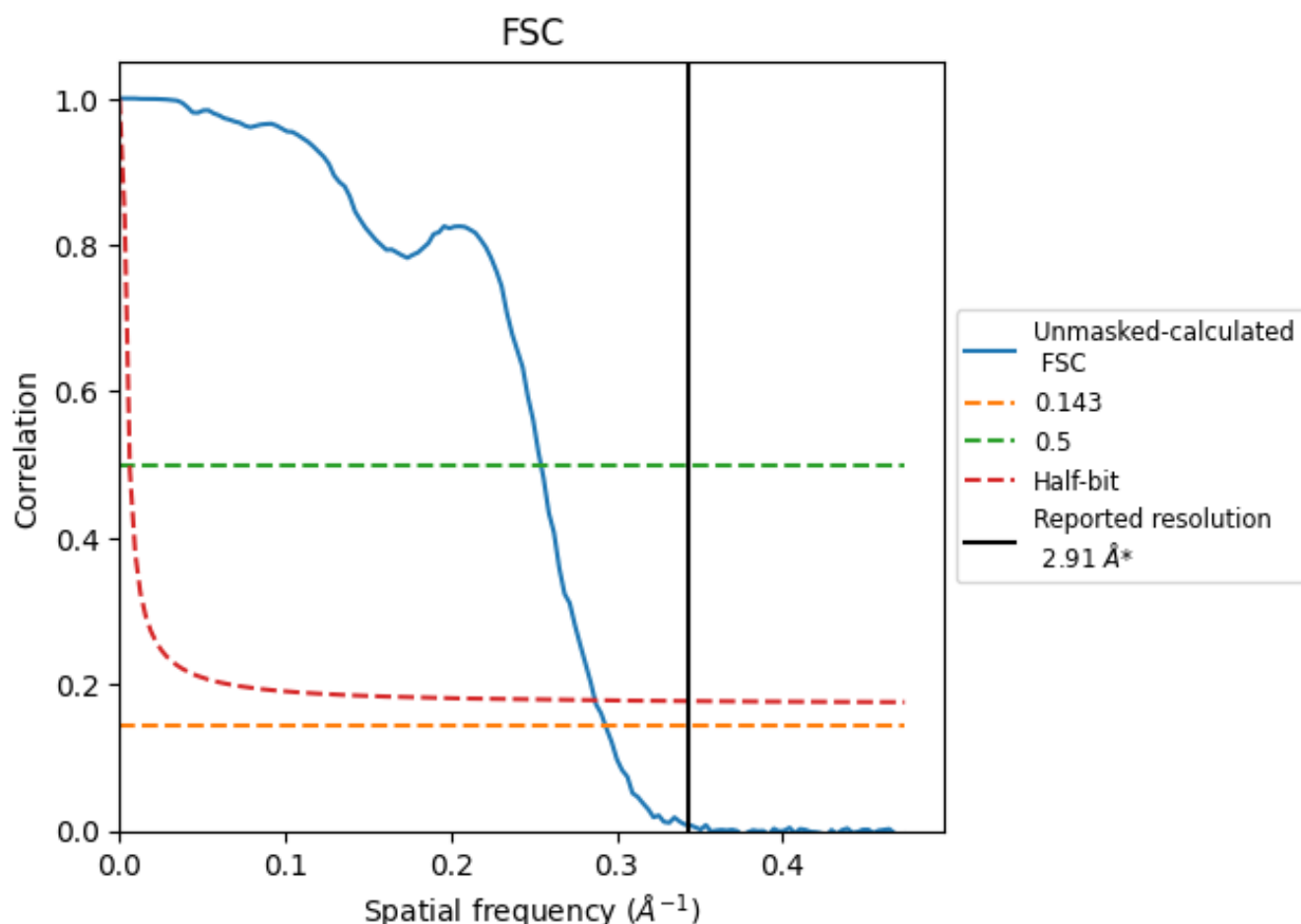


*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

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 0.344 \AA^{-1}

8.2 Resolution estimates [i](#)

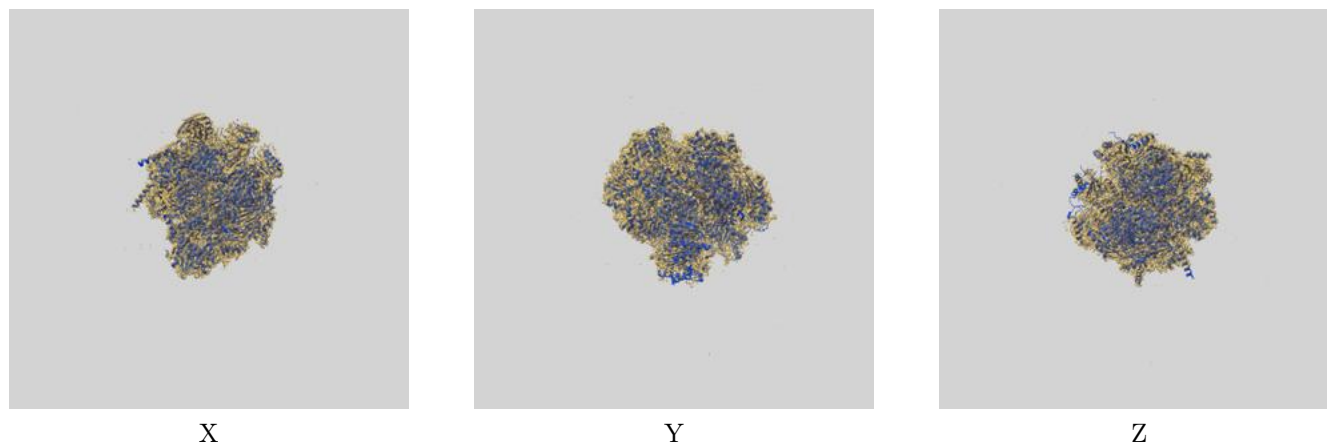
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.41	3.93	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

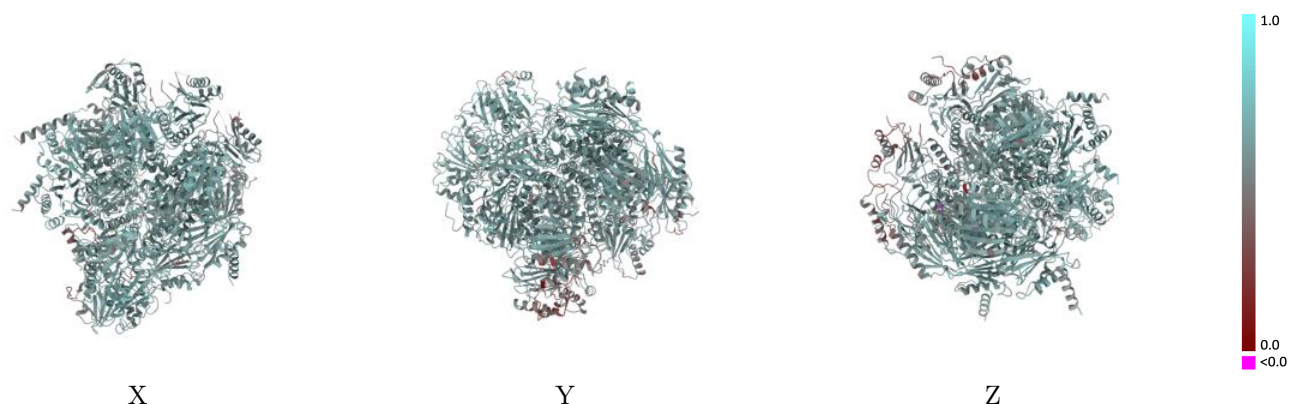
This section contains information regarding the fit between EMDB map EMD-39332 and PDB model 8YIX. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



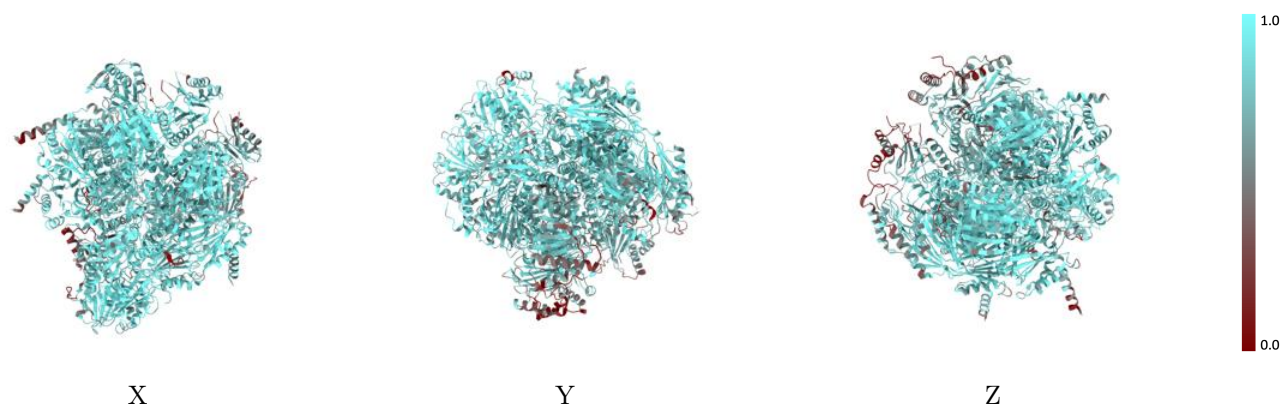
The images above show the 3D surface view of the map at the recommended contour level 0.592 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



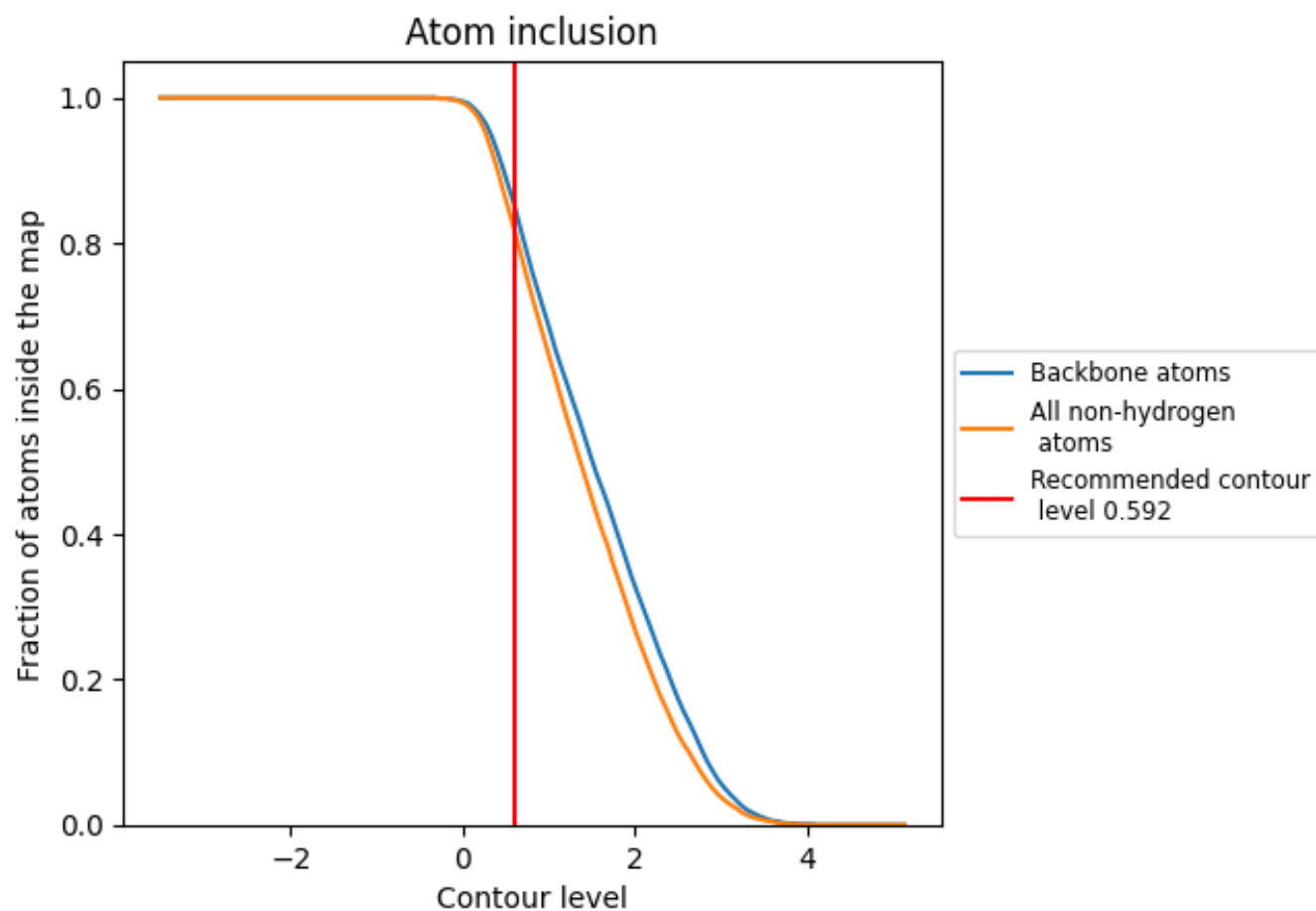
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.592).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.592) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8220	<div><div></div></div> 0.5890
A	<div><div></div></div> 0.9190	<div><div></div></div> 0.6170
B	<div><div></div></div> 0.8690	<div><div></div></div> 0.6090
C	<div><div></div></div> 0.9000	<div><div></div></div> 0.6210
D	<div><div></div></div> 0.8570	<div><div></div></div> 0.5980
E	<div><div></div></div> 0.9090	<div><div></div></div> 0.6190
F	<div><div></div></div> 0.8990	<div><div></div></div> 0.6140
G	<div><div></div></div> 0.9090	<div><div></div></div> 0.6170
H	<div><div></div></div> 0.8470	<div><div></div></div> 0.5970
I	<div><div></div></div> 0.8200	<div><div></div></div> 0.5840
J	<div><div></div></div> 0.8040	<div><div></div></div> 0.5820
K	<div><div></div></div> 0.7200	<div><div></div></div> 0.5520
L	<div><div></div></div> 0.6010	<div><div></div></div> 0.5050
M	<div><div></div></div> 0.6420	<div><div></div></div> 0.5430
N	<div><div></div></div> 0.7310	<div><div></div></div> 0.5630
f	<div><div></div></div> 0.7540	<div><div></div></div> 0.5610
g	<div><div></div></div> 0.8550	<div><div></div></div> 0.6000
h	<div><div></div></div> 0.8710	<div><div></div></div> 0.6030

1.0

0.0

<0.0