



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 07:24 PM UTC

PDB ID : 8AZK / pdb_00008azk
EMDB ID : EMD-15767
Title : Bovine 20S proteasome, untreated
Authors : Szenkier, N.; Arie, M.; Matzov, D.; Sertchook, R.; Carmeli, R.; Cascio, P.; Stanhill, A.; Shalev Benami, M.; Navon, A.
Deposited on : 2022-09-06
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

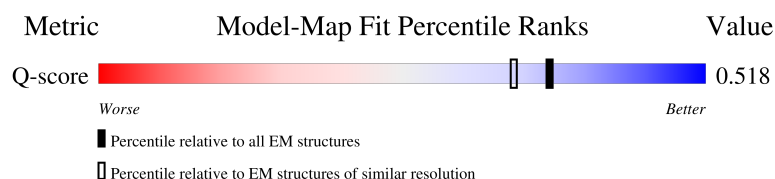
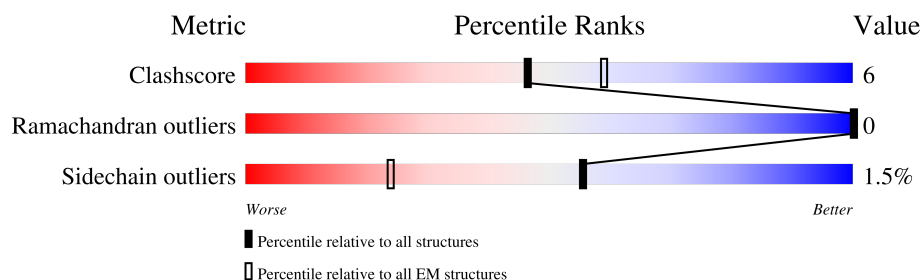
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



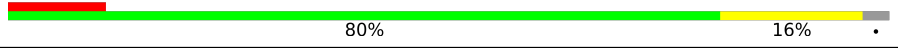
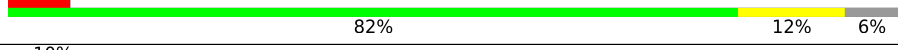
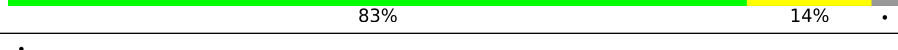
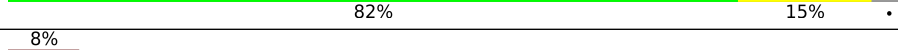
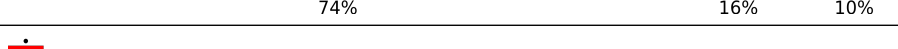
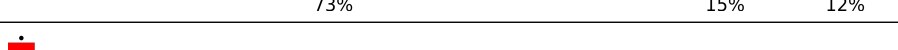
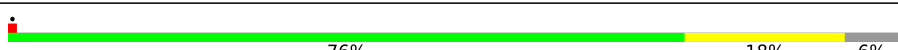
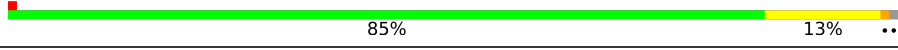
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	J	205	 87% 12%
1	X	205	 84% 16%
2	A	246	 80% 15%
2	O	246	 75% 21%

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Mol	Chain	Length	Quality of chain
3	B	233	
3	P	233	
4	C	261	
4	Q	261	
5	D	248	
5	R	248	
6	E	241	
6	S	241	
7	F	263	
7	T	263	
8	G	254	
8	U	254	
9	H	205	
9	V	205	
10	I	234	
10	W	234	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	1	213	
13	M	213	
14	2	219	
14	N	219	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 46965 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	204	Total	C	N	O	S	0	0
			1588	1013	265	292	18		
1	X	204	Total	C	N	O	S	0	0
			1587	1011	264	294	18		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	34	LEU	MET	conflict	UNP P33672
J	143	ALA	THR	conflict	UNP P33672
J	161	ASP	GLU	conflict	UNP P33672
X	34	LEU	MET	conflict	UNP P33672
X	143	ALA	THR	conflict	UNP P33672
X	161	ASP	GLU	conflict	UNP P33672

- Molecule 2 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	237	Total	C	N	O	S	0	0
			1783	1135	301	334	13		
2	O	240	Total	C	N	O	S	0	0
			1817	1157	307	340	13		

- Molecule 3 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	228	Total	C	N	O	S	0	0
			1727	1110	287	324	6		
3	P	228	Total	C	N	O	S	0	0
			1720	1103	290	321	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	253	Total	C	N	O	S	0	0
			1887	1193	324	360	10		
4	Q	246	Total	C	N	O	S	0	0
			1819	1157	319	334	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	241	Total	C	N	O	S	0	0
			1774	1114	324	331	5		
5	R	242	Total	C	N	O	S	0	0
			1765	1112	316	332	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	38	ARG	LYS	conflict	UNP Q3ZBG0
D	216	SER	PRO	conflict	UNP Q3ZBG0
R	38	ARG	LYS	conflict	UNP Q3ZBG0
R	216	SER	PRO	conflict	UNP Q3ZBG0

- Molecule 6 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	233	Total	C	N	O	S	0	0
			1732	1089	288	344	11		
6	S	232	Total	C	N	O	S	0	0
			1735	1090	290	345	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	27	ASP	ALA	conflict	UNP Q5E987
E	184	LEU	VAL	conflict	UNP Q5E987
S	27	ASP	ALA	conflict	UNP Q5E987
S	184	LEU	VAL	conflict	UNP Q5E987

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	237	Total	C	N	O	S	0	0
			1795	1131	322	333	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	231	Total	C	N	O	S	0	0
			1749	1103	318	318	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	247	ALA	THR	conflict	UNP Q3T0X5
T	247	ALA	THR	conflict	UNP Q3T0X5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	241	Total	C	N	O	S	0	0
			1844	1169	314	350	11		
8	U	241	Total	C	N	O	S	0	0
			1819	1150	311	347	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	189	ILE	VAL	conflict	UNP Q58DU5
G	219	LEU	ILE	conflict	UNP Q58DU5
G	231	ILE	VAL	conflict	UNP Q58DU5
U	189	ILE	VAL	conflict	UNP Q58DU5
U	219	LEU	ILE	conflict	UNP Q58DU5
U	231	ILE	VAL	conflict	UNP Q58DU5

- Molecule 9 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	202	Total	C	N	O	S	0	0
			1485	934	254	285	12		
9	V	199	Total	C	N	O	S	0	0
			1456	915	254	277	10		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	124	SER	PRO	conflict	UNP Q3MHN0
H	182	SER	PRO	conflict	UNP Q3MHN0
H	198	ALA	THR	conflict	UNP Q3MHN0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	199	VAL	ILE	conflict	UNP Q3MHN0
H	205	ALA	LEU	conflict	UNP Q3MHN0
V	124	SER	PRO	conflict	UNP Q3MHN0
V	182	SER	PRO	conflict	UNP Q3MHN0
V	198	ALA	THR	conflict	UNP Q3MHN0
V	199	VAL	ILE	conflict	UNP Q3MHN0
V	205	ALA	LEU	conflict	UNP Q3MHN0

- Molecule 10 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	220	Total	C	N	O	S	0	0
			1617	1023	269	313	12		
10	W	220	Total	C	N	O	S	0	0
			1612	1018	268	314	12		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	91	ARG	GLN	conflict	UNP Q2TBP0
I	153	ASN	LYS	conflict	UNP Q2TBP0
I	181	ASN	SER	conflict	UNP Q2TBP0
I	190	THR	SER	conflict	UNP Q2TBP0
I	199	LEU	PHE	conflict	UNP Q2TBP0
I	209	THR	ASN	conflict	UNP Q2TBP0
I	216	ILE	VAL	conflict	UNP Q2TBP0
I	218	PRO	THR	conflict	UNP Q2TBP0
W	91	ARG	GLN	conflict	UNP Q2TBP0
W	153	ASN	LYS	conflict	UNP Q2TBP0
W	181	ASN	SER	conflict	UNP Q2TBP0
W	190	THR	SER	conflict	UNP Q2TBP0
W	199	LEU	PHE	conflict	UNP Q2TBP0
W	209	THR	ASN	conflict	UNP Q2TBP0
W	216	ILE	VAL	conflict	UNP Q2TBP0
W	218	PRO	THR	conflict	UNP Q2TBP0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	198	Total	C	N	O	S	0	0
			1565	1004	265	287	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	197	Total	C	N	O	S	0	0
			1553	998	262	284	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	91	CYS	TYR	conflict	UNP Q5E9K0
K	155	ARG	LYS	conflict	UNP Q5E9K0
K	185	LYS	ARG	conflict	UNP Q5E9K0
Y	91	CYS	TYR	conflict	UNP Q5E9K0
Y	155	ARG	LYS	conflict	UNP Q5E9K0
Y	185	LYS	ARG	conflict	UNP Q5E9K0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total	C	N	O	S	0	0
			1538	971	270	288	9		
12	Z	200	Total	C	N	O	S	0	0
			1540	972	272	287	9		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	151	GLN	GLU	conflict	UNP Q32KL2
L	173	ALA	SER	conflict	UNP Q32KL2
L	175	ASN	SER	conflict	UNP Q32KL2
L	197	GLU	ASP	conflict	UNP Q32KL2
L	204	PRO	HIS	conflict	UNP Q32KL2
Z	151	GLN	GLU	conflict	UNP Q32KL2
Z	173	ALA	SER	conflict	UNP Q32KL2
Z	175	ASN	SER	conflict	UNP Q32KL2
Z	197	GLU	ASP	conflict	UNP Q32KL2
Z	204	PRO	HIS	conflict	UNP Q32KL2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	211	Total	C	N	O	S	0	0
			1601	1014	272	305	10		
13	1	212	Total	C	N	O	S	0	0
			1615	1026	276	303	10		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	6	VAL	ALA	conflict	UNP Q2TBX6
M	12	ILE	VAL	conflict	UNP Q2TBX6
M	21	ALA	SER	conflict	UNP Q2TBX6
M	194	ARG	LYS	conflict	UNP Q2TBX6
M	195	ILE	VAL	conflict	UNP Q2TBX6
M	205	GLU	GLY	conflict	UNP Q2TBX6
M	209	SER	PRO	conflict	UNP Q2TBX6
1	6	VAL	ALA	conflict	UNP Q2TBX6
1	12	ILE	VAL	conflict	UNP Q2TBX6
1	21	ALA	SER	conflict	UNP Q2TBX6
1	194	ARG	LYS	conflict	UNP Q2TBX6
1	195	ILE	VAL	conflict	UNP Q2TBX6
1	205	GLU	GLY	conflict	UNP Q2TBX6
1	209	SER	PRO	conflict	UNP Q2TBX6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1617	1023	285	297	12		
14	2	212	Total	C	N	O	S	0	0
			1625	1029	285	299	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	14	VAL	LEU	conflict	UNP Q3T108
N	86	ARG	LYS	conflict	UNP Q3T108
N	167	ASP	GLU	conflict	UNP Q3T108
N	189	THR	ILE	conflict	UNP Q3T108
N	205	THR	ALA	conflict	UNP Q3T108
2	14	VAL	LEU	conflict	UNP Q3T108
2	86	ARG	LYS	conflict	UNP Q3T108
2	167	ASP	GLU	conflict	UNP Q3T108
2	189	THR	ILE	conflict	UNP Q3T108
2	205	THR	ALA	conflict	UNP Q3T108

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

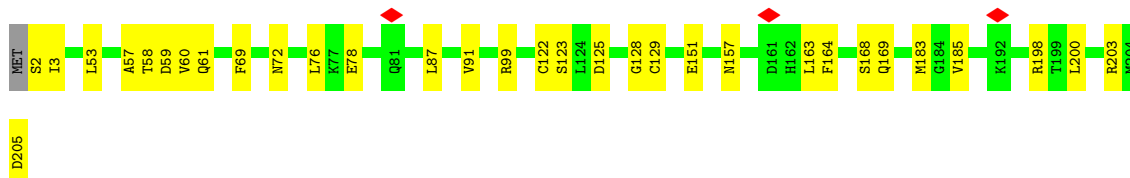
- Molecule 1: Proteasome subunit beta type-3

Chain J: 



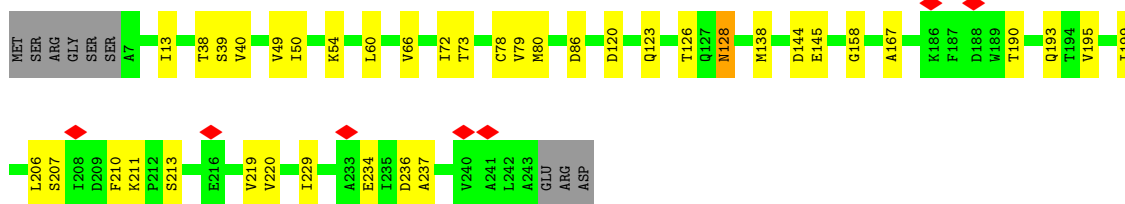
- Molecule 1: Proteasome subunit beta type-3

Chain X: 



- Molecule 2: Proteasome subunit alpha type-6

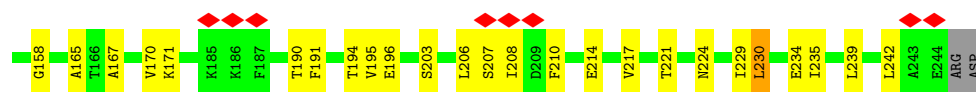
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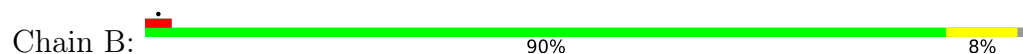
- Molecule 2: Proteasome subunit alpha type-6

Chain O: 

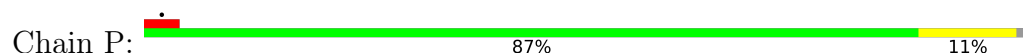




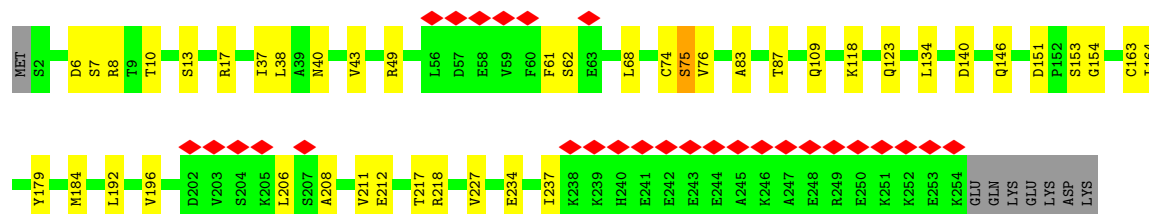
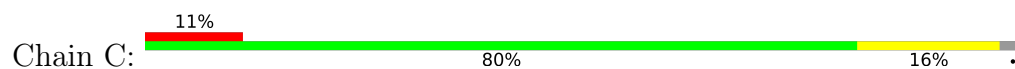
• Molecule 3: Proteasome subunit alpha type-2



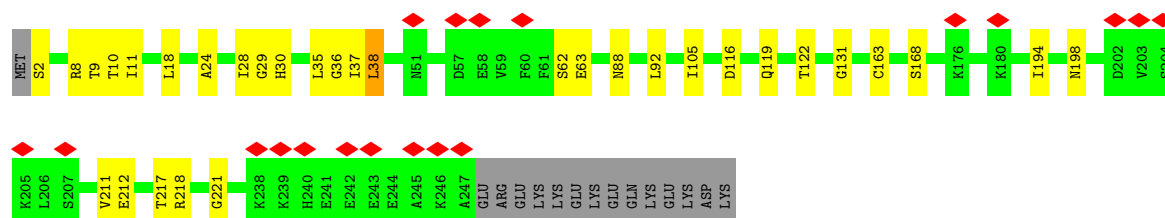
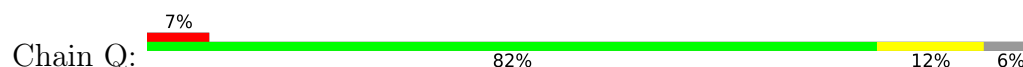
• Molecule 3: Proteasome subunit alpha type-2



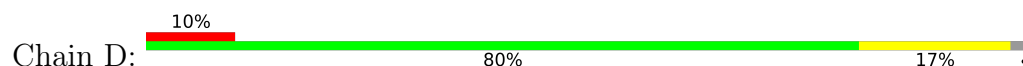
• Molecule 4: Proteasome subunit alpha type-4

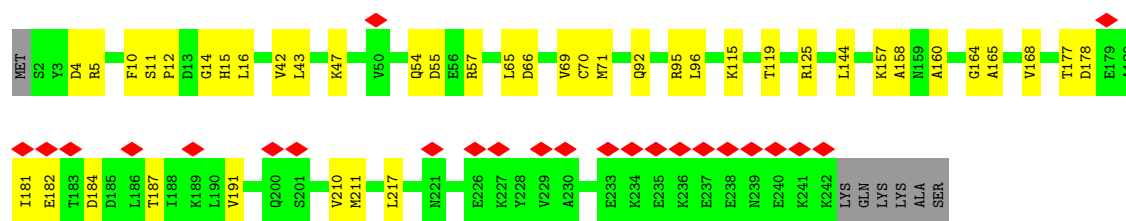


• Molecule 4: Proteasome subunit alpha type-4

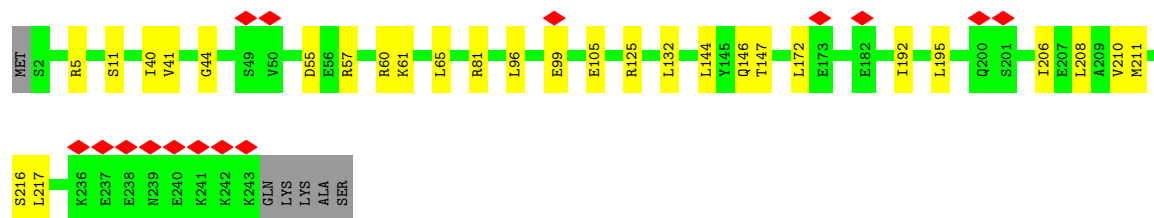
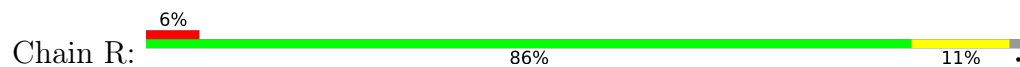


• Molecule 5: Proteasome subunit alpha type-7

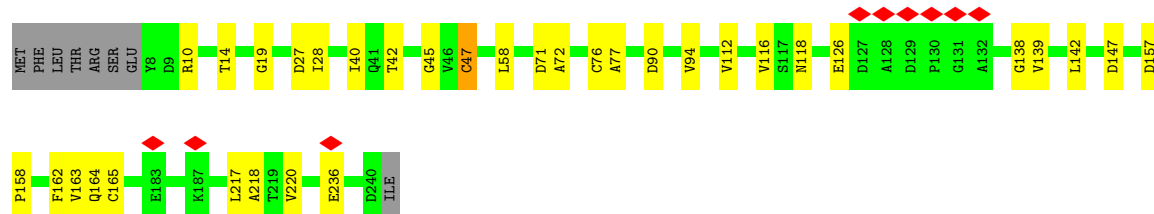
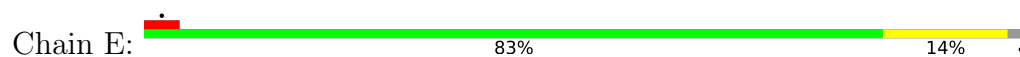




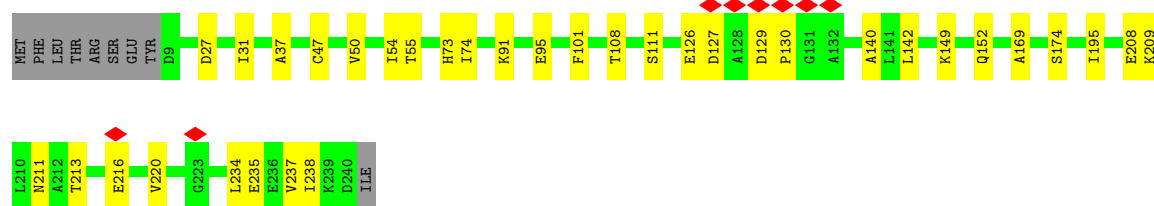
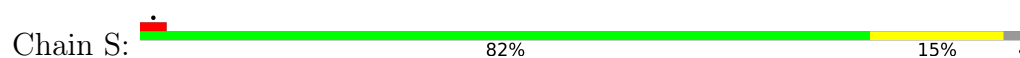
• Molecule 5: Proteasome subunit alpha type-7



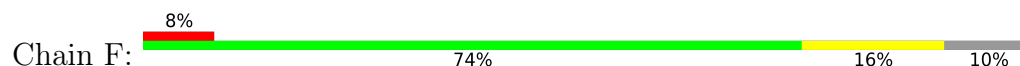
• Molecule 6: Proteasome subunit alpha type-5

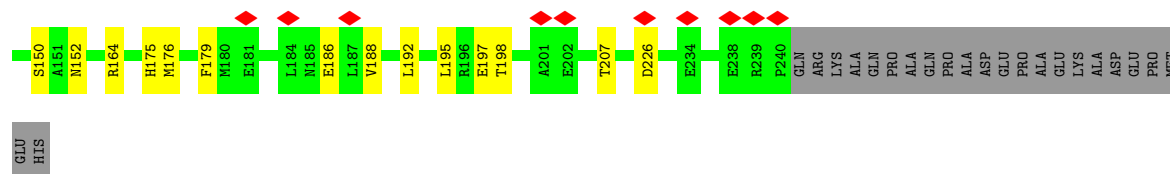


• Molecule 6: Proteasome subunit alpha type-5

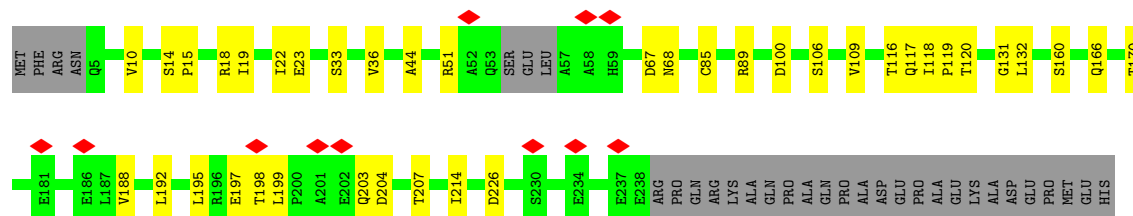


• Molecule 7: Proteasome subunit alpha type-1

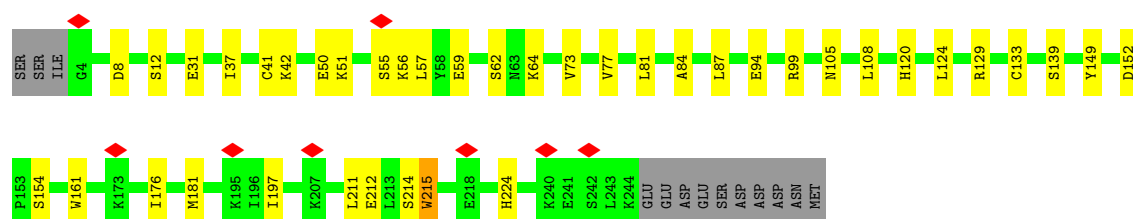
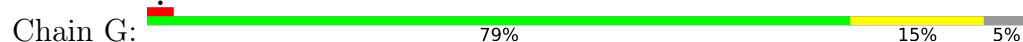




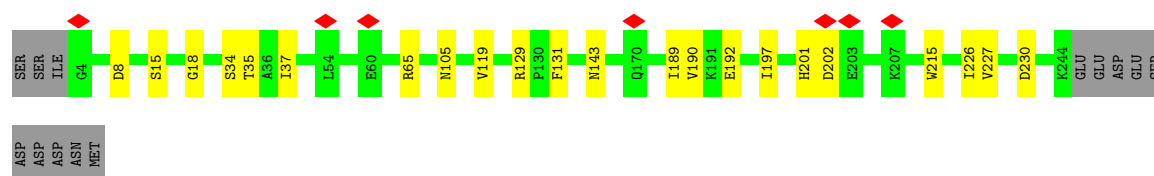
• Molecule 7: Proteasome subunit alpha type-1



• Molecule 8: Proteasome subunit alpha type-3



• Molecule 8: Proteasome subunit alpha type-3



• Molecule 9: Proteasome subunit beta type-6

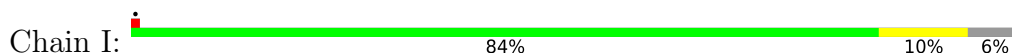


• Molecule 9: Proteasome subunit beta type-6

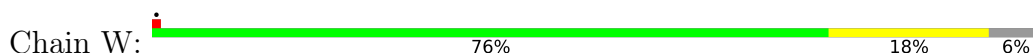




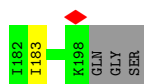
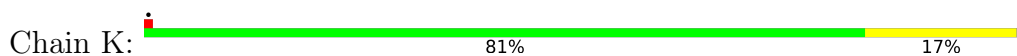
- Molecule 10: Proteasome subunit beta type-7



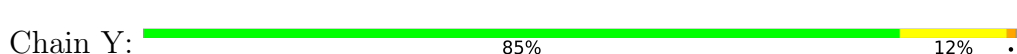
- Molecule 10: Proteasome subunit beta type-7



- Molecule 11: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-2

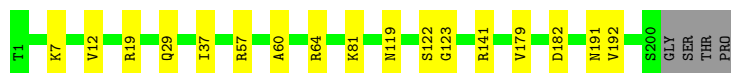


- Molecule 12: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-5

Chain Z:  90% 8% .



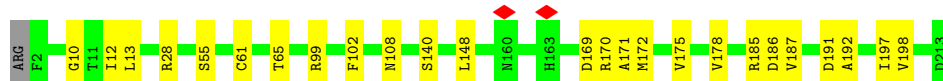
• Molecule 13: Proteasome subunit beta type-1

Chain M:  85% 13% ..



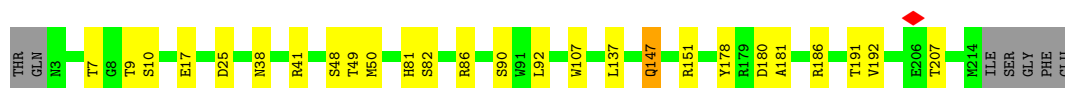
• Molecule 13: Proteasome subunit beta type-1

Chain 1:  88% 12%



• Molecule 14: Proteasome subunit beta type-4

Chain N:  85% 11% .



• Molecule 14: Proteasome subunit beta type-4

Chain 2:  87% 10% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	346962	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.699	Depositor
Minimum map value	-0.415	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	378.4, 378.4, 378.4	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	J	0.26	0/1617	0.35	0/2181
1	X	0.26	0/1616	0.36	0/2181
2	A	0.23	0/1816	0.33	0/2468
2	O	0.23	0/1850	0.34	0/2508
3	B	0.23	0/1766	0.40	2/2400 (0.1%)
3	P	0.26	0/1759	0.33	0/2392
4	C	0.23	0/1917	0.35	0/2601
4	Q	0.25	0/1849	0.41	0/2510
5	D	0.23	0/1799	0.42	2/2445 (0.1%)
5	R	0.29	0/1791	0.40	0/2437
6	E	0.21	0/1759	0.31	0/2384
6	S	0.21	0/1762	0.33	0/2387
7	F	0.20	0/1830	0.34	0/2484
7	T	0.20	0/1781	0.33	0/2415
8	G	0.21	0/1879	0.33	0/2538
8	U	0.21	0/1854	0.32	0/2509
9	H	0.26	0/1511	0.34	0/2048
9	V	0.40	0/1482	0.44	2/2010 (0.1%)
10	I	0.24	0/1644	0.33	0/2231
10	W	0.25	0/1639	0.34	0/2226
11	K	0.28	0/1598	0.34	0/2166
11	Y	0.27	0/1586	0.36	0/2151
12	L	0.25	0/1569	0.32	0/2122
12	Z	0.25	0/1571	0.33	0/2124
13	1	0.25	0/1645	0.33	0/2220
13	M	0.23	0/1629	0.34	0/2198
14	2	0.25	0/1658	0.36	0/2247
14	N	0.26	0/1650	0.36	0/2237
All	All	0.25	0/47827	0.35	6/64820 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	39	ALA	CA-C-N	8.10	131.13	120.28
3	B	39	ALA	C-N-CA	8.10	131.13	120.28
5	D	47	LYS	CA-C-N	6.24	131.13	120.72
5	D	47	LYS	C-N-CA	6.24	131.13	120.72
9	V	95	MET	N-CA-C	-5.37	105.51	111.36
9	V	96	ALA	CB-CA-C	-5.26	110.53	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1588	0	1609	18	0
1	X	1587	0	1600	19	0
2	A	1783	0	1747	30	0
2	O	1817	0	1791	38	0
3	B	1727	0	1686	12	0
3	P	1720	0	1658	16	0
4	C	1887	0	1802	26	0
4	Q	1819	0	1762	33	0
5	D	1774	0	1696	29	0
5	R	1765	0	1664	27	0
6	E	1732	0	1680	25	0
6	S	1735	0	1692	21	0
7	F	1795	0	1742	29	0
7	T	1749	0	1709	28	0
8	G	1844	0	1789	29	0
8	U	1819	0	1724	13	0
9	H	1485	0	1441	12	0
9	V	1456	0	1405	13	0
10	I	1617	0	1605	18	0
10	W	1612	0	1594	36	0
11	K	1565	0	1552	27	0
11	Y	1553	0	1534	19	0
12	L	1538	0	1491	13	0
12	Z	1540	0	1499	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	1615	0	1594	12	0
13	M	1601	0	1575	26	0
14	2	1625	0	1590	14	0
14	N	1617	0	1575	17	0
All	All	46965	0	45806	566	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 6.

All (566) 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)
7:F:117:GLN:O	7:F:120:THR:HG22	1.39	1.23
5:R:40:ILE:HD11	5:R:210:VAL:CG2	1.68	1.22
10:W:213:THR:HG22	10:W:214:GLU:H	1.09	1.16
5:R:40:ILE:HD11	5:R:210:VAL:HG21	1.24	1.14
11:K:4:LEU:HD11	11:K:47:VAL:CG2	1.85	1.07
11:K:25:ILE:HG23	11:K:26:VAL:HG23	1.35	1.06
11:K:4:LEU:HD11	11:K:47:VAL:HG23	1.40	1.01
10:W:213:THR:HG22	10:W:214:GLU:N	1.78	0.95
10:W:213:THR:CG2	10:W:214:GLU:H	1.82	0.92
14:N:25:ASP:OD1	14:N:41:ARG:NH1	2.05	0.90
1:J:58:THR:HG21	11:K:121:LEU:O	1.74	0.88
2:A:120:ASP:OD1	3:B:83:ARG:NH1	2.08	0.87
14:2:25:ASP:OD1	14:2:41:ARG:NH1	2.10	0.85
1:J:58:THR:CG2	11:K:121:LEU:O	2.24	0.85
2:A:211:LYS:NZ	2:A:213:SER:OG	2.08	0.83
4:C:179:TYR:O	4:C:184:MET:SD	2.36	0.83
13:M:176:LYS:O	13:M:180:ILE:HG12	1.79	0.83
7:F:67:ASP:OD2	7:F:96:ARG:NH2	2.12	0.83
6:E:90:ASP:O	6:E:94:VAL:HG23	1.78	0.83
13:M:26:ASP:OD2	13:M:189:THR:HG23	1.79	0.81
4:Q:2:SER:OG	5:R:5:ARG:NH2	2.13	0.81
11:Y:96:THR:HG23	11:Y:96:THR:O	1.80	0.81
6:E:118:ASN:OD1	7:F:82:ARG:NH1	2.13	0.81
5:R:40:ILE:CD1	5:R:210:VAL:CG2	2.58	0.81
3:P:64:VAL:O	3:P:219:ARG:NH1	2.14	0.81
11:K:4:LEU:HD11	11:K:47:VAL:HG21	1.63	0.80
14:N:38:ASN:OD1	14:N:186:ARG:NH1	2.15	0.80
13:M:28:ARG:NH2	13:M:187:VAL:O	2.15	0.80
4:C:13:SER:OG	4:C:17:ARG:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:51:LYS:NZ	8:G:62:SER:O	2.13	0.79
2:O:97:GLU:OE1	2:O:117:ARG:NH1	2.16	0.79
1:J:169:GLN:OE1	10:I:209:THR:OG1	2.01	0.79
8:G:152:ASP:OD2	8:G:154:SER:OG	2.01	0.79
8:G:31:GLU:N	8:G:31:GLU:OE1	2.16	0.78
4:Q:218:ARG:NH1	4:Q:221:GLY:O	2.17	0.78
2:A:38:THR:HG22	2:A:39:SER:H	1.49	0.77
9:H:110:GLN:OE1	9:H:112:TYR:OH	2.01	0.77
10:W:129:SER:OG	10:W:166:ASP:OD2	2.03	0.76
4:Q:217:THR:HG22	4:Q:218:ARG:N	2.01	0.76
5:R:40:ILE:HD11	5:R:210:VAL:HG23	1.67	0.75
6:S:108:THR:OG1	6:S:111:SER:OG	2.03	0.75
8:U:34:SER:OG	8:U:65:ARG:NH1	2.19	0.75
7:T:203:GLN:NE2	7:T:204:ASP:O	2.20	0.75
2:A:40:VAL:HG12	2:A:167:ALA:HB2	1.69	0.74
2:A:38:THR:HG22	2:A:39:SER:N	1.99	0.74
4:C:123:GLN:OE1	5:D:125:ARG:NH2	2.21	0.74
13:M:47:THR:HG22	13:M:48:ASP:N	2.02	0.74
7:F:98:VAL:O	14:N:90:SER:OG	2.04	0.74
8:G:197:ILE:HD11	8:G:211:LEU:HD11	1.69	0.74
10:I:14:LEU:HD21	10:I:44:CYS:SG	2.27	0.74
11:K:165:GLU:OE1	12:Z:141:ARG:NH2	2.21	0.73
7:T:197:GLU:N	7:T:197:GLU:OE1	2.21	0.73
7:F:5:GLN:OE1	7:F:5:GLN:N	2.22	0.73
4:Q:163:CYS:O	4:Q:168:SER:OG	2.07	0.72
12:L:91:LYS:NZ	12:L:117:GLU:O	2.23	0.72
13:M:27:THR:O	13:M:27:THR:HG22	1.88	0.72
2:A:49:VAL:HG22	2:A:219:VAL:HG12	1.71	0.72
14:2:9:THR:O	14:2:41:ARG:NH2	2.21	0.72
13:M:27:THR:HB	13:M:192:ALA:HB3	1.72	0.71
6:E:27:ASP:OD1	6:E:28:ILE:N	2.22	0.71
1:J:12:MET:SD	1:J:138:VAL:HG12	2.31	0.71
2:O:120:ASP:OD1	3:P:83:ARG:NH1	2.24	0.71
9:V:88:TYR:OH	14:2:59:ASP:OD1	2.09	0.71
4:Q:2:SER:O	5:R:5:ARG:NH2	2.23	0.70
7:T:100:ASP:OD2	14:2:86:ARG:NH2	2.25	0.70
7:T:188:VAL:O	7:T:192:LEU:HD13	1.92	0.70
13:M:114:ASP:OD1	13:M:115:GLU:N	2.25	0.70
8:G:12:SER:OG	8:G:124:LEU:O	2.07	0.70
13:1:61:CYS:O	13:1:65:THR:HG23	1.92	0.69
2:O:217:VAL:CG2	2:O:230:LEU:HD22	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:197:GLU:OE1	12:L:197:GLU:N	2.25	0.69
4:Q:24:ALA:O	4:Q:28:ILE:HG12	1.92	0.69
7:T:33:SER:OG	7:T:51:ARG:NH1	2.26	0.69
14:N:147:GLN:OE1	14:N:151:ARG:NH1	2.25	0.68
9:V:22:THR:HG22	9:V:22:THR:O	1.91	0.68
11:Y:2:GLU:HB3	11:Y:47:VAL:HG21	1.74	0.68
5:R:99:GLU:OE2	12:Z:81:LYS:NZ	2.18	0.68
13:1:28:ARG:NH2	13:1:191:ASP:OD1	2.26	0.68
13:M:47:THR:HG22	13:M:48:ASP:H	1.58	0.68
11:K:12:TYR:OH	11:K:152:SER:O	2.07	0.68
5:D:66:ASP:OD2	5:D:95:ARG:NH2	2.26	0.67
5:R:96:LEU:HD11	11:Y:58:GLU:HB3	1.75	0.67
11:K:139:THR:HG23	11:K:163:CYS:HB2	1.75	0.67
2:O:230:LEU:HD23	2:O:235:ILE:HG13	1.77	0.67
4:Q:28:ILE:HD11	4:Q:131:GLY:O	1.94	0.67
4:Q:62:SER:OG	4:Q:212:GLU:OE2	2.13	0.66
6:S:211:ASN:ND2	6:S:213:THR:OG1	2.28	0.66
4:Q:116:ASP:OD1	5:R:81:ARG:NH1	2.28	0.66
6:E:28:ILE:HD11	6:E:157:ASP:OD2	1.96	0.66
7:T:117:GLN:O	7:T:120:THR:OG1	2.13	0.66
13:1:169:ASP:OD1	13:1:170:ARG:N	2.28	0.66
10:W:76:VAL:HG11	10:W:109:HIS:HB2	1.78	0.65
4:C:49:ARG:NH1	4:C:211:VAL:O	2.30	0.65
14:N:9:THR:O	14:N:41:ARG:NH2	2.29	0.65
8:G:59:GLU:N	8:G:59:GLU:OE1	2.30	0.65
11:K:3:TYR:OH	11:K:139:THR:HG21	1.97	0.65
3:P:10:THR:OG1	3:P:121:THR:O	2.13	0.65
7:T:10:VAL:O	7:T:10:VAL:HG22	1.96	0.65
1:X:61:GLN:NE2	11:Y:123:ALA:O	2.30	0.64
1:X:78:GLU:OE1	1:X:78:GLU:N	2.29	0.64
8:G:73:VAL:HG12	8:G:139:SER:HB3	1.79	0.64
5:R:192:ILE:CD1	5:R:208:LEU:HD11	2.27	0.64
5:R:99:GLU:N	5:R:99:GLU:OE1	2.30	0.64
3:B:64:VAL:HG22	3:B:64:VAL:O	1.98	0.64
13:M:27:THR:HG22	13:M:39:ASP:HA	1.79	0.64
1:X:125:ASP:OD1	1:X:128:GLY:N	2.31	0.64
6:S:235:GLU:OE1	6:S:235:GLU:N	2.30	0.63
4:C:68:LEU:HD21	4:C:74:CYS:SG	2.38	0.63
6:E:157:ASP:CG	6:E:158:PRO:CD	2.71	0.63
11:K:4:LEU:CD1	11:K:47:VAL:HG21	2.28	0.63
14:2:166:ARG:NH2	14:2:200:GLU:OE2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:234:GLU:OE1	2:O:234:GLU:N	2.31	0.63
4:Q:194:ILE:O	4:Q:198:ASN:ND2	2.32	0.63
10:W:6:VAL:HG21	10:W:138:PHE:CE1	2.34	0.63
13:M:99:ARG:NE	13:M:102:PHE:O	2.32	0.63
11:K:39:SER:OG	11:K:74:GLU:OE1	2.16	0.62
7:F:197:GLU:N	7:F:197:GLU:OE1	2.31	0.62
2:A:38:THR:CG2	2:A:39:SER:H	2.12	0.62
2:O:47:CYS:SG	2:O:194:THR:HG21	2.39	0.62
4:Q:211:VAL:HG22	4:Q:212:GLU:N	2.14	0.62
3:B:67:ILE:HD11	3:B:73:LEU:CD1	2.29	0.62
2:A:40:VAL:HG12	2:A:167:ALA:CB	2.29	0.62
2:A:236:ASP:OD1	2:A:237:ALA:N	2.33	0.62
11:K:35:MET:SD	11:K:181:ARG:NH1	2.71	0.62
8:G:99:ARG:NH1	8:G:105:ASN:OD1	2.33	0.62
7:T:85:CYS:SG	7:T:89:ARG:NH2	2.73	0.62
2:A:72:ILE:O	2:A:73:THR:OG1	2.19	0.61
1:J:58:THR:HG22	11:K:121:LEU:O	2.01	0.61
2:A:234:GLU:OE1	2:A:234:GLU:N	2.34	0.61
4:C:140:ASP:OD2	4:C:146:GLN:NE2	2.34	0.61
6:E:236:GLU:N	6:E:236:GLU:OE1	2.32	0.61
6:S:234:LEU:O	6:S:237:VAL:HG22	2.01	0.61
12:Z:7:LYS:HB2	12:Z:12:VAL:HG22	1.83	0.61
2:O:217:VAL:HG21	2:O:230:LEU:HD22	1.81	0.61
11:Y:108:ASP:OD1	11:Y:109:GLU:N	2.32	0.61
1:J:61:GLN:NE2	11:K:123:ALA:O	2.34	0.61
2:O:208:ILE:HD11	2:O:210:PHE:CE1	2.36	0.60
11:Y:12:TYR:OH	11:Y:152:SER:O	2.17	0.60
2:A:158:GLY:O	3:B:83:ARG:NH2	2.34	0.60
13:M:47:THR:HG21	13:M:49:LYS:NZ	2.17	0.60
4:C:75:SER:O	4:C:75:SER:OG	2.19	0.60
5:D:55:ASP:OD2	5:D:57:ARG:HG3	2.02	0.59
4:C:6:ASP:OD1	4:C:7:SER:N	2.35	0.59
4:C:37:ILE:O	4:C:43:VAL:HG23	2.02	0.59
10:W:30:ASN:O	10:W:187:ARG:NH2	2.35	0.59
8:G:87:LEU:HD12	8:G:133:CYS:SG	2.43	0.59
8:G:108:LEU:HD23	8:G:149:TYR:HD2	1.67	0.59
11:K:108:ASP:OD1	11:K:109:GLU:N	2.34	0.59
2:O:214:GLU:N	2:O:214:GLU:OE1	2.36	0.59
4:Q:217:THR:CG2	4:Q:218:ARG:N	2.66	0.59
5:R:192:ILE:HD12	5:R:208:LEU:HD11	1.84	0.59
7:T:198:THR:O	7:T:199:LEU:HD22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:38:LEU:HD12	7:F:39:LYS:N	2.18	0.58
6:E:157:ASP:OD1	6:E:158:PRO:CD	2.51	0.58
2:A:54:LYS:NZ	2:A:66:VAL:O	2.37	0.58
10:W:14:LEU:HD23	10:W:44:CYS:SG	2.44	0.58
2:O:158:GLY:O	3:P:83:ARG:NH2	2.37	0.57
11:Y:102:LEU:HD11	11:Y:118:MET:SD	2.44	0.57
4:C:118:LYS:NZ	4:C:151:ASP:O	2.30	0.57
5:D:42:VAL:HG11	5:D:191:VAL:HG21	1.85	0.57
4:Q:217:THR:HG22	4:Q:218:ARG:H	1.65	0.57
7:T:36:VAL:HG22	7:T:160:SER:CB	2.35	0.57
6:E:157:ASP:CG	6:E:158:PRO:HD2	2.29	0.57
11:Y:88:LEU:HD23	11:Y:118:MET:CE	2.35	0.57
12:Z:7:LYS:CB	12:Z:12:VAL:HG22	2.35	0.57
7:F:186:GLU:N	7:F:186:GLU:OE1	2.35	0.57
7:F:10:VAL:HG22	7:F:10:VAL:O	2.05	0.57
5:R:206:ILE:CG2	5:R:208:LEU:HG	2.35	0.57
10:W:7:VAL:HG12	10:W:123:PRO:O	2.05	0.57
10:I:99:VAL:HG12	10:I:99:VAL:O	2.05	0.57
11:K:43:LEU:HD12	11:K:183:ILE:HD11	1.86	0.57
13:M:47:THR:CG2	13:M:48:ASP:H	2.18	0.56
5:D:187:THR:O	5:D:191:VAL:HG23	2.05	0.56
2:O:113:MET:SD	2:O:113:MET:N	2.78	0.56
5:D:4:ASP:OD1	5:D:4:ASP:O	2.23	0.56
1:J:135:ASP:OD1	1:J:135:ASP:N	2.38	0.56
4:C:40:ASN:ND2	4:C:184:MET:O	2.39	0.56
6:E:164:GLN:OE1	6:E:165:CYS:N	2.39	0.56
7:F:164:ARG:NE	7:F:198:THR:O	2.37	0.56
10:I:220:GLU:OE1	10:I:220:GLU:N	2.39	0.56
14:N:17:GLU:N	14:N:17:GLU:OE1	2.38	0.56
1:J:59:ASP:O	1:J:63:VAL:HG23	2.06	0.56
8:U:119:VAL:HG13	8:U:131:PHE:CD2	2.41	0.56
4:C:163:CYS:SG	4:C:164:ILE:N	2.78	0.56
2:O:21:ARG:NH2	2:O:26:GLU:OE1	2.39	0.56
5:D:181:ILE:HG22	5:D:182:GLU:H	1.70	0.55
10:W:6:VAL:HG12	10:W:7:VAL:N	2.21	0.55
10:W:213:THR:CG2	10:W:214:GLU:N	2.49	0.55
9:H:40:ARG:NH1	9:H:181:GLU:O	2.39	0.55
10:I:14:LEU:HD23	10:I:15:GLY:N	2.22	0.55
6:S:169:ALA:O	6:S:174:SER:OG	2.24	0.55
10:W:104:ASP:OD1	10:W:106:THR:OG1	2.13	0.55
5:D:43:LEU:N	5:D:43:LEU:HD23	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:203:SER:O	2:O:207:SER:N	2.33	0.55
1:X:125:ASP:OD1	1:X:129:CYS:N	2.39	0.55
8:G:41:CYS:SG	8:G:42:LYS:N	2.80	0.55
4:C:61:PHE:O	4:C:62:SER:OG	2.15	0.55
9:H:14:LEU:HD22	9:H:44:CYS:SG	2.47	0.55
7:T:36:VAL:HG22	7:T:160:SER:HB3	1.89	0.55
12:Z:12:VAL:HB	12:Z:179:VAL:CG1	2.37	0.55
1:J:155:GLU:HB2	1:J:158:MET:HE2	1.89	0.54
1:J:193:ASP:OD1	1:J:193:ASP:N	2.39	0.54
8:G:64:LYS:NZ	8:G:212:GLU:OE2	2.38	0.54
3:B:72:GLY:O	3:B:135:ILE:HG13	2.08	0.54
5:R:216:SER:O	5:R:217:LEU:HB2	2.07	0.54
3:P:214:GLU:O	3:P:214:GLU:HG2	2.07	0.54
7:T:166:GLN:O	7:T:170:THR:HG23	2.07	0.54
14:2:137:LEU:C	14:2:137:LEU:HD12	2.33	0.54
13:M:47:THR:CG2	13:M:48:ASP:N	2.68	0.54
2:A:123:GLN:O	2:A:126:THR:OG1	2.22	0.54
5:D:65:LEU:HD13	5:D:69:VAL:HG12	1.88	0.54
11:K:2:GLU:N	11:K:2:GLU:OE1	2.40	0.54
4:Q:88:ASN:O	4:Q:92:LEU:HD23	2.08	0.54
3:B:149:ASP:OD2	3:B:151:SER:OG	2.23	0.54
6:S:220:VAL:HG12	6:S:220:VAL:O	2.08	0.54
8:G:108:LEU:HD23	8:G:149:TYR:CD2	2.43	0.53
11:Y:35:MET:SD	11:Y:181:ARG:NE	2.81	0.53
12:L:12:VAL:HB	12:L:179:VAL:CG1	2.38	0.53
9:H:190:LEU:HD12	9:H:190:LEU:C	2.33	0.53
2:A:38:THR:CG2	2:A:39:SER:N	2.66	0.53
6:E:76:CYS:SG	6:E:77:ALA:N	2.82	0.53
4:Q:217:THR:CG2	4:Q:218:ARG:H	2.20	0.53
7:F:117:GLN:O	7:F:120:THR:CG2	2.32	0.53
7:T:44:ALA:O	7:T:214:ILE:HD12	2.08	0.53
10:W:6:VAL:CG2	10:W:138:PHE:CE1	2.91	0.53
1:J:49:LEU:HD21	1:J:87:LEU:HD22	1.90	0.53
4:C:192:LEU:O	4:C:196:VAL:HG23	2.08	0.53
11:Y:30:ASP:OD1	11:Y:30:ASP:N	2.41	0.53
7:F:33:SER:O	7:F:62:LYS:NZ	2.41	0.52
2:A:206:LEU:HD12	2:A:210:PHE:HZ	1.75	0.52
4:C:83:ALA:O	4:C:87:THR:HG23	2.10	0.52
2:O:155:ASP:OD1	2:O:155:ASP:N	2.42	0.52
5:R:41:VAL:HG23	5:R:211:MET:HB2	1.91	0.52
6:S:149:LYS:O	6:S:152:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:88:LEU:HD23	11:Y:118:MET:HE2	1.92	0.52
12:Z:37:ILE:HG23	12:Z:60:ALA:HB2	1.91	0.52
7:T:116:THR:HG22	7:T:116:THR:O	2.09	0.52
6:E:157:ASP:OD1	6:E:158:PRO:HD2	2.09	0.52
10:W:172:ASN:OD1	10:W:191:VAL:HG13	2.10	0.51
3:B:178:ASN:HD21	3:B:181:LEU:HD21	1.74	0.51
2:O:242:LEU:O	2:O:242:LEU:HD12	2.09	0.51
3:P:185:ASP:OD1	3:P:185:ASP:N	2.39	0.51
1:J:37:THR:HG22	1:J:37:THR:O	2.09	0.51
8:G:37:ILE:HD12	8:G:176:ILE:HD11	1.93	0.51
10:I:149:GLU:OE1	10:I:149:GLU:N	2.36	0.51
4:Q:38:LEU:C	4:Q:38:LEU:HD23	2.36	0.51
6:E:10:ARG:O	6:E:14:THR:HG21	2.11	0.51
7:F:42:THR:O	7:F:42:THR:OG1	2.29	0.51
12:L:115:ASP:OD2	12:L:119:ASN:ND2	2.41	0.51
13:M:23:VAL:HG21	13:M:51:VAL:CG1	2.40	0.51
10:W:6:VAL:HG21	10:W:138:PHE:HE1	1.74	0.51
13:M:47:THR:HB	13:M:50:THR:HG22	1.92	0.51
12:L:157:ARG:NH1	12:L:190:ASP:OD1	2.44	0.51
5:R:105:GLU:OE2	5:R:105:GLU:N	2.44	0.51
7:T:120:THR:O	8:U:129:ARG:NE	2.42	0.51
6:E:147:ASP:N	6:E:147:ASP:OD1	2.45	0.50
9:H:28:ASN:OD1	10:I:122:LEU:HD21	2.11	0.50
9:H:104:ASP:OD1	9:H:104:ASP:N	2.43	0.50
3:P:109:LEU:HD23	3:P:135:ILE:HD12	1.92	0.50
8:U:230:ASP:OD1	8:U:230:ASP:N	2.43	0.50
4:Q:35:LEU:HD23	4:Q:36:GLY:N	2.27	0.50
5:R:41:VAL:CG2	5:R:211:MET:HB2	2.42	0.50
8:G:214:SER:OG	8:G:224:HIS:NE2	2.39	0.50
10:W:152:LYS:CG	10:W:175:LEU:HD21	2.42	0.50
11:Y:153:ARG:NH2	11:Y:184:ASP:OD2	2.44	0.50
1:J:151:GLU:OE1	13:1:185:ARG:NE	2.40	0.50
6:E:138:GLY:O	6:E:139:VAL:HG13	2.11	0.50
4:Q:35:LEU:HD23	4:Q:35:LEU:C	2.36	0.50
14:N:192:VAL:O	14:N:192:VAL:HG13	2.10	0.50
3:P:47:THR:HG23	3:P:48:GLU:N	2.27	0.50
7:F:46:LEU:HD11	7:F:135:ALA:HB3	1.94	0.50
8:G:77:VAL:HG11	8:G:84:ALA:HB1	1.92	0.50
12:Z:191:ASN:OD1	12:Z:192:VAL:N	2.45	0.50
10:W:187:ARG:HB3	10:W:188:PRO:HD3	1.94	0.49
14:N:178:TYR:HE1	14:N:207:THR:HG23	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:67:ILE:HD11	3:B:73:LEU:HD12	1.94	0.49
4:C:109:GLN:NE2	11:K:71:ASN:OD1	2.46	0.49
6:S:47:CYS:SG	6:S:195:ILE:HG12	2.52	0.49
13:M:23:VAL:HG21	13:M:51:VAL:HG13	1.93	0.49
14:N:180:ASP:OD1	14:N:181:ALA:N	2.45	0.49
4:Q:211:VAL:HG22	4:Q:212:GLU:H	1.76	0.49
12:Z:119:ASN:O	12:Z:119:ASN:ND2	2.46	0.49
11:K:18:ASP:OD1	11:K:19:ARG:N	2.46	0.49
13:M:47:THR:HG21	13:M:49:LYS:HZ2	1.78	0.49
7:T:18:ARG:NH1	7:T:23:GLU:OE2	2.45	0.49
11:Y:37:LYS:O	11:Y:61:GLN:NE2	2.45	0.49
1:X:58:THR:HG23	1:X:59:ASP:OD1	2.13	0.49
9:H:22:THR:O	9:H:22:THR:HG23	2.11	0.49
13:M:145:LEU:HD22	13:M:178:VAL:HG13	1.95	0.49
6:S:91:LYS:NZ	6:S:95:GLU:OE1	2.31	0.49
6:S:101:PHE:O	12:Z:57:ARG:NH1	2.45	0.49
2:A:66:VAL:O	2:A:66:VAL:HG23	2.12	0.49
10:I:40:ASN:OD1	10:I:40:ASN:N	2.44	0.49
12:L:122:SER:OG	12:L:123:GLY:N	2.46	0.49
2:A:86:ASP:OD1	8:G:120:HIS:NE2	2.43	0.49
4:C:212:GLU:OE2	4:C:227:VAL:HG13	2.12	0.49
5:D:42:VAL:CG1	5:D:191:VAL:HG21	2.43	0.48
11:Y:96:THR:O	11:Y:96:THR:CG2	2.54	0.48
11:Y:143:LEU:HD23	11:Y:159:LEU:HD21	1.95	0.48
5:D:181:ILE:HG22	5:D:182:GLU:N	2.28	0.48
6:S:31:ILE:CD1	6:S:140:ALA:HB2	2.43	0.48
12:Z:122:SER:OG	12:Z:123:GLY:N	2.46	0.48
2:A:190:THR:N	2:A:193:GLN:OE1	2.46	0.48
4:C:6:ASP:OD2	5:D:5:ARG:NH1	2.46	0.48
2:O:128:ASN:OD1	2:O:128:ASN:N	2.45	0.48
6:E:19:GLY:CA	7:F:28:ALA:HB2	2.43	0.48
6:E:157:ASP:OD1	6:E:158:PRO:HD3	2.14	0.48
3:P:206:ASN:C	3:P:207:ILE:HG13	2.38	0.48
2:O:115:CYS:HG	2:O:154:CYS:HG	1.61	0.48
2:O:206:LEU:O	2:O:207:SER:OG	2.24	0.48
5:R:192:ILE:HD11	5:R:208:LEU:HD11	1.96	0.48
1:X:72:ASN:O	1:X:76:LEU:HD23	2.14	0.47
1:X:183:MET:HE1	12:L:165:TYR:O	2.13	0.47
2:A:60:LEU:HD12	8:G:161:TRP:HB2	1.96	0.47
5:R:44:GLY:HA2	5:R:208:LEU:HD23	1.96	0.47
9:V:31:THR:HG22	9:V:32:ASP:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:122:CYS:SG	1:X:123:SER:N	2.87	0.47
2:A:229:ILE:O	2:A:229:ILE:HG22	2.14	0.47
2:O:146:GLU:N	2:O:146:GLU:OE1	2.48	0.47
10:W:166:ASP:OD1	10:W:167:LEU:N	2.47	0.47
1:X:203:ARG:NE	1:X:205:ASP:OD2	2.47	0.47
13:M:27:THR:HB	13:M:192:ALA:CB	2.42	0.47
10:W:6:VAL:CG1	10:W:7:VAL:N	2.77	0.47
5:D:157:LYS:HZ2	5:D:158:ALA:HB2	1.79	0.47
7:F:150:SER:O	7:F:152:ASN:N	2.45	0.47
12:L:4:LEU:HD12	12:L:5:ALA:N	2.30	0.47
14:N:48:SER:O	14:N:49:THR:OG1	2.29	0.47
13:1:171:ALA:O	13:1:175:VAL:HG23	2.13	0.47
4:C:6:ASP:OD1	4:C:8:ARG:N	2.48	0.47
4:C:206:LEU:HD12	4:C:208:ALA:H	1.78	0.47
10:I:183:LEU:HD23	10:I:183:LEU:O	2.15	0.47
11:K:19:ARG:O	11:K:20:VAL:HG23	2.13	0.47
2:O:7:ALA:N	2:O:10:ASP:OD2	2.41	0.47
2:O:170:VAL:HG13	2:O:171:LYS:HG2	1.97	0.47
9:V:43:CYS:SG	9:V:98:ILE:HG23	2.54	0.47
10:W:6:VAL:CG2	10:W:138:PHE:CZ	2.97	0.47
14:2:9:THR:OG1	14:2:10:SER:N	2.48	0.47
2:O:5:SER:OG	2:O:6:SER:N	2.48	0.47
5:R:60:ARG:O	5:R:61:LYS:HB2	2.15	0.47
7:T:85:CYS:SG	7:T:89:ARG:NE	2.87	0.47
5:D:69:VAL:HG12	5:D:70:CYS:N	2.30	0.47
6:E:27:ASP:OD1	6:E:27:ASP:C	2.57	0.46
14:N:81:HIS:O	14:N:82:SER:OG	2.33	0.46
3:P:47:THR:HG22	3:P:208:GLU:HB3	1.97	0.46
4:Q:28:ILE:CD1	4:Q:131:GLY:O	2.62	0.46
14:2:165:ALA:O	14:2:169:VAL:HG23	2.15	0.46
4:Q:119:GLN:O	4:Q:122:THR:OG1	2.31	0.46
6:S:50:VAL:HG12	6:S:216:GLU:HB2	1.97	0.46
9:H:30:VAL:HG12	9:H:30:VAL:O	2.15	0.46
11:K:46:CYS:SG	11:K:53:THR:HG23	2.56	0.46
3:B:78:MET:HE2	3:B:81:ASP:CG	2.41	0.46
12:Z:19:ARG:NH2	12:Z:29:GLN:OE1	2.43	0.46
1:J:12:MET:SD	1:J:138:VAL:CG1	3.00	0.46
6:S:108:THR:HG1	6:S:111:SER:HG	1.51	0.46
10:I:3:ILE:HG22	10:I:4:ALA:N	2.30	0.46
10:I:99:VAL:HG13	10:I:125:VAL:CG2	2.45	0.46
14:N:178:TYR:CE1	14:N:207:THR:HG23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:55:ASP:OD2	5:R:57:ARG:NH1	2.49	0.46
8:U:8:ASP:OD1	8:U:8:ASP:N	2.48	0.46
10:W:66:HIS:O	10:W:70:THR:HG22	2.16	0.46
10:I:139:GLU:OE2	14:2:179:ARG:NH2	2.45	0.46
7:T:195:LEU:HD23	7:T:195:LEU:C	2.41	0.46
10:W:153:ASN:O	10:W:157:GLU:HG3	2.16	0.46
3:P:68:THR:HG23	3:P:70:HIS:H	1.81	0.46
10:I:108:PRO:O	10:I:109:HIS:ND1	2.49	0.45
10:I:140:ASP:OD2	14:2:171:ARG:NH2	2.49	0.45
6:S:73:HIS:NE2	6:S:74:ILE:HD11	2.30	0.45
2:A:128:ASN:N	2:A:128:ASN:OD1	2.49	0.45
9:V:173:VAL:HG12	9:V:190:LEU:HB3	1.97	0.45
6:S:54:ILE:HG22	6:S:55:THR:N	2.31	0.45
7:T:36:VAL:HG22	7:T:160:SER:HB2	1.98	0.45
1:X:99:ARG:NH2	10:W:51:ASP:OD2	2.48	0.45
2:O:242:LEU:HD12	2:O:242:LEU:C	2.40	0.45
13:1:148:LEU:HD23	13:1:178:VAL:HG22	1.98	0.45
8:G:8:ASP:OD1	8:G:8:ASP:N	2.42	0.45
5:R:65:LEU:HD12	5:R:65:LEU:N	2.32	0.45
5:D:11:SER:HB3	5:D:12:PRO:HD2	1.98	0.45
6:E:112:VAL:O	6:E:116:VAL:HG23	2.17	0.45
1:X:151:GLU:OE1	13:M:185:ARG:NE	2.37	0.45
8:G:176:ILE:HG22	8:G:176:ILE:O	2.17	0.45
13:M:27:THR:O	13:M:27:THR:CG2	2.61	0.45
2:O:50:ILE:HD12	2:O:79:VAL:CG2	2.46	0.45
4:Q:29:GLY:O	4:Q:30:HIS:ND1	2.48	0.45
10:W:55:THR:O	10:W:59:ILE:HG12	2.17	0.45
13:1:10:GLY:O	13:1:55:SER:OG	2.32	0.45
10:W:121:LYS:CG	10:W:121:LYS:O	2.65	0.45
14:N:9:THR:OG1	14:N:10:SER:N	2.49	0.45
5:R:65:LEU:HD12	5:R:65:LEU:H	1.82	0.45
5:D:16:LEU:HD12	5:D:16:LEU:N	2.33	0.44
13:M:16:ALA:HB2	13:M:121:VAL:HG13	1.99	0.44
2:O:40:VAL:HG12	2:O:167:ALA:CB	2.47	0.44
6:S:152:GLN:N	6:S:152:GLN:OE1	2.50	0.44
10:I:44:CYS:SG	10:I:99:VAL:HB	2.57	0.44
9:V:83:PHE:CE1	9:V:98:ILE:HD13	2.52	0.44
10:W:217:THR:O	10:W:217:THR:OG1	2.34	0.44
5:D:96:LEU:HD11	11:K:58:GLU:CB	2.47	0.44
7:F:207:THR:OG1	7:F:226:ASP:O	2.34	0.44
8:G:55:SER:O	8:G:57:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:214:SER:OG	8:G:215:TRP:N	2.50	0.44
9:H:55:VAL:HG12	9:H:83:PHE:CE1	2.52	0.44
2:O:72:ILE:HD11	2:O:78:CYS:SG	2.57	0.44
11:K:94:SER:OG	11:K:95:ARG:N	2.50	0.44
11:K:135:GLY:O	11:K:139:THR:OG1	2.25	0.44
4:Q:8:ARG:O	4:Q:10:THR:N	2.51	0.44
10:W:37:ILE:HD12	10:W:43:CYS:HB3	1.99	0.44
9:H:6:VAL:HG12	9:H:7:GLN:N	2.33	0.44
14:N:137:LEU:HD12	14:N:137:LEU:C	2.42	0.44
6:E:40:ILE:HG12	6:E:47:CYS:SG	2.58	0.44
7:F:11:THR:HG23	8:G:129:ARG:HB2	2.00	0.44
9:H:51:ASP:O	9:H:55:VAL:HG23	2.17	0.44
3:P:189:THR:O	3:P:193:THR:HG23	2.18	0.44
4:Q:211:VAL:CG2	4:Q:212:GLU:N	2.80	0.44
9:V:17:ASP:OD1	9:V:33:LYS:NZ	2.50	0.44
1:X:185:VAL:HG11	1:X:200:LEU:HD12	1.98	0.44
3:B:203:THR:HG23	3:B:205:ASP:H	1.83	0.44
13:M:123:SER:O	13:M:130:TYR:HA	2.18	0.44
11:Y:160:LEU:O	11:Y:164:LEU:HG	2.17	0.44
1:J:116:THR:O	1:J:118:LYS:N	2.51	0.44
13:M:47:THR:HB	13:M:50:THR:CG2	2.48	0.44
2:O:229:ILE:O	2:O:230:LEU:HB2	2.17	0.44
9:V:18:SER:OG	9:V:173:VAL:HG22	2.18	0.44
6:E:217:LEU:HD23	6:E:218:ALA:N	2.33	0.43
11:K:152:SER:OG	11:K:153:ARG:N	2.51	0.43
3:P:45:LEU:HD11	3:P:136:CYS:SG	2.58	0.43
7:T:106:SER:O	7:T:109:VAL:HG12	2.17	0.43
1:X:164:PHE:O	1:X:168:SER:OG	2.28	0.43
2:O:38:THR:C	2:O:39:SER:HG	2.26	0.43
8:U:119:VAL:HG13	8:U:131:PHE:HD2	1.83	0.43
6:E:162:PHE:C	6:E:163:VAL:HG13	2.43	0.43
10:W:152:LYS:HG3	10:W:175:LEU:HD21	1.99	0.43
13:1:172:MET:SD	13:1:197:ILE:HD11	2.58	0.43
4:C:217:THR:OG1	4:C:218:ARG:N	2.50	0.43
7:F:7:ASP:OD1	7:F:7:ASP:N	2.44	0.43
8:G:73:VAL:HG12	8:G:139:SER:CB	2.47	0.43
5:R:144:LEU:C	5:R:144:LEU:HD23	2.42	0.43
11:Y:47:VAL:HG22	11:Y:48:GLY:N	2.33	0.43
2:A:123:GLN:NE2	3:B:81:ASP:OD1	2.51	0.43
11:K:18:ASP:OD2	11:K:175:LEU:HD22	2.19	0.43
2:O:50:ILE:HG23	2:O:141:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:129:ASP:N	6:S:130:PRO:HD3	2.34	0.43
8:G:81:LEU:N	8:G:81:LEU:HD22	2.33	0.43
2:O:40:VAL:HG12	2:O:167:ALA:HB2	2.00	0.43
2:O:139:ILE:HG12	2:O:153:LYS:HG3	2.00	0.43
10:W:40:ASN:N	10:W:40:ASN:OD1	2.50	0.43
7:F:47:VAL:HG23	7:F:195:LEU:HD23	2.00	0.43
10:I:97:ALA:HB1	10:I:127:MET:SD	2.58	0.43
7:T:10:VAL:O	7:T:10:VAL:CG2	2.66	0.43
7:F:188:VAL:O	7:F:192:LEU:HD12	2.19	0.43
2:A:50:ILE:HG21	2:A:79:VAL:HG11	2.01	0.43
8:U:192:GLU:OE2	8:U:192:GLU:N	2.49	0.43
9:V:1:THR:HG23	9:V:33:LYS:NZ	2.33	0.43
10:W:190:THR:HG22	10:W:191:VAL:N	2.34	0.43
11:Y:45:LEU:N	11:Y:45:LEU:HD12	2.33	0.43
1:X:87:LEU:O	1:X:91:VAL:HG23	2.19	0.43
5:D:177:THR:OG1	5:D:178:ASP:N	2.49	0.43
9:H:104:ASP:O	9:H:107:GLU:O	2.37	0.43
7:T:19:ILE:HB	7:T:22:ILE:HD12	2.00	0.43
9:V:14:LEU:HD23	9:V:44:CYS:SG	2.59	0.43
13:1:12:ILE:HG22	13:1:13:LEU:N	2.33	0.43
13:1:186:ASP:OD1	13:1:187:VAL:N	2.52	0.43
2:A:206:LEU:O	2:A:207:SER:OG	2.28	0.42
13:M:209:SER:O	13:M:210:LEU:HD12	2.19	0.42
1:J:122:CYS:SG	1:J:123:SER:N	2.91	0.42
5:D:10:PHE:CE1	5:D:16:LEU:HD11	2.54	0.42
1:J:154:TRP:O	1:J:154:TRP:CE3	2.71	0.42
4:C:76:VAL:HG11	4:C:83:ALA:HB1	2.02	0.42
5:D:115:LYS:O	5:D:119:THR:OG1	2.31	0.42
5:D:144:LEU:HD23	5:D:144:LEU:C	2.44	0.42
6:E:42:THR:OG1	6:E:45:GLY:O	2.34	0.42
8:G:87:LEU:CD1	8:G:133:CYS:SG	3.08	0.42
12:L:7:LYS:HB3	12:L:12:VAL:HG22	2.01	0.42
7:F:38:LEU:HD13	7:F:179:PHE:HE2	1.83	0.42
7:F:85:CYS:O	7:F:89:ARG:HG3	2.19	0.42
2:O:195:VAL:HG23	2:O:196:GLU:N	2.34	0.42
13:1:191:ASP:O	13:1:192:ALA:HB2	2.20	0.42
5:D:210:VAL:HG22	5:D:211:MET:N	2.34	0.42
2:O:38:THR:HG22	2:O:39:SER:N	2.33	0.42
7:T:207:THR:OG1	7:T:226:ASP:O	2.34	0.42
8:U:105:ASN:OD1	8:U:105:ASN:N	2.53	0.42
2:O:73:THR:HG23	2:O:75:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:32:ALA:O	3:P:33:PRO:C	2.62	0.42
7:T:118:ILE:HB	7:T:119:PRO:CD	2.50	0.42
3:B:43:VAL:HG12	3:B:44:VAL:N	2.34	0.42
5:D:4:ASP:OD2	6:E:126:GLU:C	2.62	0.42
5:D:14:GLY:O	5:D:15:HIS:C	2.63	0.42
5:D:158:ALA:HB3	6:E:58:LEU:HD13	2.01	0.42
12:L:1:THR:HG22	12:L:2:THR:N	2.34	0.42
6:S:234:LEU:O	6:S:238:ILE:HD12	2.20	0.42
7:T:85:CYS:O	7:T:89:ARG:HG3	2.19	0.42
10:W:126:THR:HG21	10:W:134:ALA:HB3	2.00	0.42
11:Y:19:ARG:O	11:Y:20:VAL:HG23	2.19	0.42
4:C:8:ARG:O	4:C:10:THR:N	2.53	0.42
5:D:164:GLY:O	5:D:168:VAL:HG23	2.20	0.42
7:F:175:HIS:CD2	7:F:175:HIS:N	2.87	0.42
12:L:167:ASP:OD2	12:L:170:SER:OG	2.30	0.42
7:T:14:SER:OG	7:T:15:PRO:HD2	2.20	0.42
8:U:35:THR:HG22	8:U:37:ILE:HG23	2.01	0.42
8:U:201:HIS:NE2	8:U:202:ASP:O	2.53	0.42
10:W:96:ALA:O	10:W:98:LEU:HG	2.19	0.42
5:D:65:LEU:HD11	5:D:71:MET:CG	2.50	0.42
4:Q:35:LEU:HD21	4:Q:37:ILE:CD1	2.50	0.42
7:T:131:GLY:O	7:T:132:LEU:HD12	2.20	0.42
14:2:20:VAL:HG12	14:2:21:VAL:N	2.35	0.42
1:X:198:ARG:NE	10:W:214:GLU:OE2	2.45	0.42
7:F:176:MET:HE1	8:G:56:LYS:HZ1	1.85	0.42
3:P:190:ALA:O	3:P:193:THR:OG1	2.38	0.42
8:U:189:ILE:HG23	8:U:190:VAL:N	2.35	0.42
9:V:142:THR:O	9:V:142:THR:HG22	2.20	0.42
5:D:160:ALA:O	5:D:165:ALA:HB1	2.20	0.41
7:F:100:ASP:OD1	14:N:86:ARG:NH2	2.52	0.41
4:Q:10:THR:O	4:Q:11:ILE:HD13	2.20	0.41
9:V:1:THR:HG23	9:V:33:LYS:HZ3	1.85	0.41
13:1:99:ARG:NE	13:1:102:PHE:O	2.52	0.41
14:2:22:ILE:HG22	14:2:23:ALA:N	2.34	0.41
4:C:134:LEU:HD12	4:C:134:LEU:N	2.35	0.41
2:O:42:VAL:HG12	2:O:165:ALA:HB1	2.02	0.41
3:P:113:VAL:O	3:P:117:MET:HG3	2.20	0.41
4:Q:2:SER:OG	4:Q:2:SER:O	2.36	0.41
6:S:37:ALA:HB2	6:S:50:VAL:HG23	2.00	0.41
1:X:2:SER:OG	1:X:3:ILE:N	2.53	0.41
2:A:195:VAL:HG12	2:A:199:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:44:ALA:HB1	7:F:144:ILE:HD11	2.03	0.41
7:F:51:ARG:O	7:F:57:ALA:HB3	2.20	0.41
9:V:6:VAL:HG22	9:V:7:GLN:N	2.35	0.41
2:A:80:MET:HE1	2:A:138:MET:HB2	2.01	0.41
2:O:190:THR:OG1	2:O:191:PHE:N	2.53	0.41
4:Q:62:SER:OG	4:Q:63:GLU:N	2.54	0.41
12:L:4:LEU:HD12	12:L:4:LEU:C	2.46	0.41
12:L:43:GLY:O	12:L:44:THR:OG1	2.35	0.41
14:2:192:VAL:O	14:2:192:VAL:HG13	2.21	0.41
5:D:184:ASP:O	5:D:187:THR:N	2.46	0.41
2:O:56:VAL:O	2:O:56:VAL:HG12	2.21	0.41
2:O:221:THR:HG23	2:O:224:ASN:H	1.84	0.41
10:I:155:VAL:O	10:I:159:ILE:HG12	2.20	0.41
4:Q:10:THR:O	4:Q:10:THR:OG1	2.34	0.41
4:Q:18:LEU:HD21	5:R:125:ARG:HH11	1.85	0.41
1:X:57:ALA:O	1:X:60:VAL:HB	2.20	0.41
1:X:169:GLN:OE1	10:W:209:THR:HG22	2.20	0.41
2:A:229:ILE:O	2:A:229:ILE:CG2	2.68	0.41
5:R:44:GLY:O	5:R:195:LEU:HD11	2.21	0.41
5:R:146:GLN:OE1	5:R:147:THR:N	2.54	0.41
6:S:208:GLU:HG2	6:S:209:LYS:H	1.86	0.41
10:W:18:THR:O	10:W:171:SER:HB2	2.21	0.41
1:X:69:PHE:CD1	1:X:69:PHE:C	2.99	0.41
6:E:71:ASP:OD1	6:E:72:ALA:N	2.48	0.41
13:M:192:ALA:O	13:M:210:LEU:HD22	2.21	0.41
4:Q:105:ILE:O	4:Q:105:ILE:HG23	2.21	0.41
10:W:183:LEU:HG	10:W:183:LEU:O	2.21	0.41
7:F:52:ALA:O	7:F:54:SER:N	2.54	0.41
8:G:181:MET:SD	8:G:181:MET:N	2.89	0.41
14:N:92:LEU:HD23	14:N:92:LEU:HA	1.95	0.41
1:J:12:MET:CG	1:J:138:VAL:HG12	2.50	0.40
2:A:220:VAL:O	2:A:220:VAL:HG13	2.21	0.40
4:C:153:SER:O	4:C:154:GLY:C	2.64	0.40
2:A:144:ASP:OD1	2:A:145:GLU:N	2.54	0.40
4:Q:198:ASN:HD22	4:Q:198:ASN:H	1.69	0.40
7:T:67:ASP:OD1	7:T:68:ASN:N	2.45	0.40
14:2:43:MET:SD	14:2:64:LYS:HG3	2.61	0.40
8:U:15:SER:O	8:U:18:GLY:N	2.52	0.40
8:U:226:ILE:HG22	8:U:227:VAL:N	2.37	0.40
6:S:126:GLU:OE2	6:S:127:ASP:N	2.54	0.40
4:C:234:GLU:HA	4:C:237:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:197:ILE:HD11	8:G:211:LEU:CD1	2.44	0.40
10:I:99:VAL:O	10:I:100:LEU:C	2.64	0.40
14:N:50:MET:HE2	14:N:192:VAL:HG12	2.03	0.40
4:Q:62:SER:HG	4:Q:212:GLU:CD	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	J	202/205 (98%)	181 (90%)	21 (10%)	0	100	100
1	X	202/205 (98%)	182 (90%)	20 (10%)	0	100	100
2	A	235/246 (96%)	212 (90%)	23 (10%)	0	100	100
2	O	238/246 (97%)	216 (91%)	22 (9%)	0	100	100
3	B	226/233 (97%)	204 (90%)	22 (10%)	0	100	100
3	P	226/233 (97%)	203 (90%)	23 (10%)	0	100	100
4	C	251/261 (96%)	223 (89%)	28 (11%)	0	100	100
4	Q	244/261 (94%)	230 (94%)	14 (6%)	0	100	100
5	D	239/248 (96%)	209 (87%)	30 (13%)	0	100	100
5	R	240/248 (97%)	219 (91%)	21 (9%)	0	100	100
6	E	231/241 (96%)	206 (89%)	25 (11%)	0	100	100
6	S	230/241 (95%)	206 (90%)	24 (10%)	0	100	100
7	F	235/263 (89%)	205 (87%)	30 (13%)	0	100	100
7	T	227/263 (86%)	206 (91%)	21 (9%)	0	100	100
8	G	239/254 (94%)	211 (88%)	28 (12%)	0	100	100
8	U	239/254 (94%)	219 (92%)	20 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	200/205 (98%)	187 (94%)	13 (6%)	0	100	100
9	V	197/205 (96%)	184 (93%)	13 (7%)	0	100	100
10	I	218/234 (93%)	194 (89%)	24 (11%)	0	100	100
10	W	218/234 (93%)	199 (91%)	19 (9%)	0	100	100
11	K	196/201 (98%)	178 (91%)	18 (9%)	0	100	100
11	Y	195/201 (97%)	175 (90%)	20 (10%)	0	100	100
12	L	199/204 (98%)	190 (96%)	9 (4%)	0	100	100
12	Z	198/204 (97%)	187 (94%)	11 (6%)	0	100	100
13	1	210/213 (99%)	191 (91%)	19 (9%)	0	100	100
13	M	209/213 (98%)	197 (94%)	12 (6%)	0	100	100
14	2	210/219 (96%)	193 (92%)	17 (8%)	0	100	100
14	N	210/219 (96%)	188 (90%)	22 (10%)	0	100	100
All	All	6164/6454 (96%)	5595 (91%)	569 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	J	172/174 (99%)	167 (97%)	5 (3%)	37	66
1	X	172/174 (99%)	169 (98%)	3 (2%)	53	74
2	A	185/210 (88%)	182 (98%)	3 (2%)	55	75
2	O	189/210 (90%)	183 (97%)	6 (3%)	34	64
3	B	175/190 (92%)	173 (99%)	2 (1%)	65	78
3	P	170/190 (90%)	168 (99%)	2 (1%)	63	78
4	C	184/221 (83%)	182 (99%)	2 (1%)	65	78
4	Q	175/221 (79%)	173 (99%)	2 (1%)	65	78
5	D	169/211 (80%)	166 (98%)	3 (2%)	51	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	165/211 (78%)	162 (98%)	3 (2%)	51	73
6	E	183/204 (90%)	180 (98%)	3 (2%)	55	75
6	S	185/204 (91%)	183 (99%)	2 (1%)	65	78
7	F	185/224 (83%)	185 (100%)	0	100	100
7	T	179/224 (80%)	179 (100%)	0	100	100
8	G	188/211 (89%)	185 (98%)	3 (2%)	55	75
8	U	180/211 (85%)	177 (98%)	3 (2%)	53	74
9	H	148/159 (93%)	146 (99%)	2 (1%)	59	76
9	V	143/159 (90%)	141 (99%)	2 (1%)	59	76
10	I	170/195 (87%)	169 (99%)	1 (1%)	78	83
10	W	170/195 (87%)	169 (99%)	1 (1%)	78	83
11	K	164/171 (96%)	162 (99%)	2 (1%)	63	78
11	Y	161/171 (94%)	159 (99%)	2 (1%)	63	78
12	L	151/159 (95%)	148 (98%)	3 (2%)	48	72
12	Z	152/159 (96%)	150 (99%)	2 (1%)	61	77
13	1	169/178 (95%)	166 (98%)	3 (2%)	51	73
13	M	167/178 (94%)	163 (98%)	4 (2%)	43	69
14	2	166/181 (92%)	164 (99%)	2 (1%)	63	78
14	N	164/181 (91%)	160 (98%)	4 (2%)	43	69
All	All	4781/5376 (89%)	4711 (98%)	70 (2%)	55	75

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	56	LEU
1	J	60	VAL
1	J	124	LEU
1	J	126	LEU
1	J	146	MET
1	X	53	LEU
1	X	157	ASN
1	X	163	LEU
2	A	13	ILE
2	A	78	CYS
2	A	128	ASN

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Mol	Chain	Res	Type
3	B	55	LEU
3	B	115	SER
4	C	38	LEU
4	C	75	SER
5	D	54	GLN
5	D	92	GLN
5	D	217	LEU
6	E	47	CYS
6	E	142	LEU
6	E	220	VAL
8	G	50	GLU
8	G	94	GLU
8	G	215	TRP
9	H	40	ARG
9	H	123	GLN
10	I	43	CYS
11	K	32	HIS
11	K	138	LEU
12	L	4	LEU
12	L	29	GLN
12	L	80	SER
13	M	50	THR
13	M	108	ASN
13	M	191	ASP
13	M	210	LEU
14	N	7	THR
14	N	107	TRP
14	N	147	GLN
14	N	191	THR
2	O	13	ILE
2	O	78	CYS
2	O	115	CYS
2	O	128	ASN
2	O	230	LEU
2	O	239	LEU
3	P	20	GLN
3	P	135	ILE
4	Q	9	THR
4	Q	38	LEU
5	R	11	SER
5	R	132	LEU
5	R	172	LEU

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Mol	Chain	Res	Type
6	S	27	ASP
6	S	142	LEU
8	U	143	ASN
8	U	197	ILE
8	U	215	TRP
9	V	38	HIS
9	V	43	CYS
10	W	126	THR
11	Y	19	ARG
11	Y	102	LEU
12	Z	64	ARG
12	Z	182	ASP
13	1	108	ASN
13	1	140	SER
13	1	198	VAL
14	2	139	THR
14	2	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	81	GLN
1	J	162	HIS
1	J	173	ASN
1	X	31	GLN
1	X	162	HIS
1	X	188	HIS
3	B	188	HIS
4	C	95	GLN
4	C	109	GLN
5	D	54	GLN
5	D	120	GLN
6	E	178	GLN
7	F	31	GLN
7	F	65	HIS
7	F	175	HIS
8	G	147	GLN
8	G	201	HIS
9	H	62	GLN
9	H	77	HIS
12	L	89	GLN
12	L	151	GLN

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Mol	Chain	Res	Type
12	L	162	GLN
13	M	58	HIS
13	M	80	ASN
13	M	108	ASN
14	N	81	HIS
14	N	213	HIS
2	O	150	GLN
3	P	206	ASN
4	Q	84	ASN
4	Q	88	ASN
4	Q	95	GLN
4	Q	100	GLN
4	Q	123	GLN
4	Q	177	GLN
4	Q	198	ASN
5	R	15	HIS
5	R	92	GLN
5	R	175	ASN
6	S	99	HIS
6	S	186	HIS
6	S	211	ASN
6	S	221	GLN
7	T	65	HIS
7	T	166	GLN
8	U	224	HIS
9	V	66	HIS
9	V	110	GLN
11	Y	189	HIS
12	Z	119	ASN
12	Z	175	ASN
12	Z	178	HIS
14	2	3	ASN
14	2	69	GLN
14	2	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

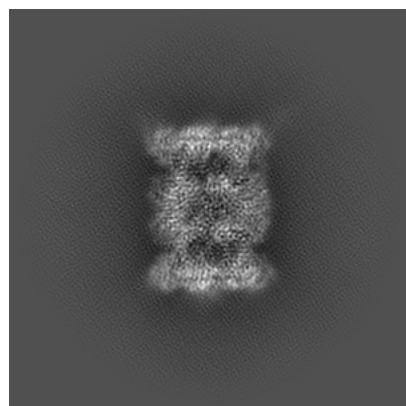
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15767. These allow visual inspection of the internal detail of the map and identification of artifacts.

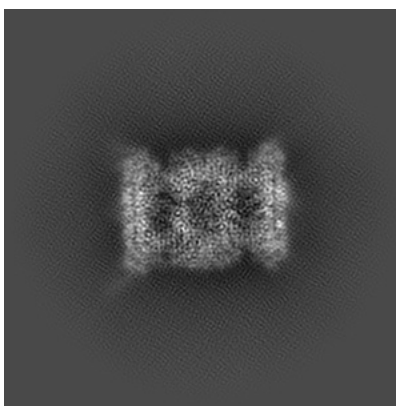
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

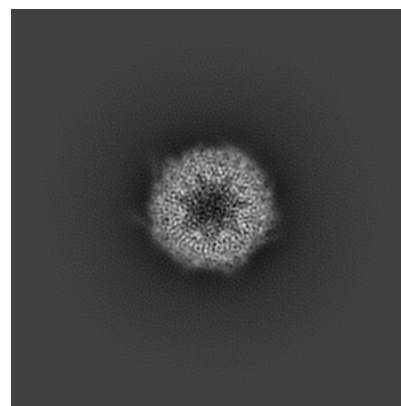
6.1.1 Primary map



X

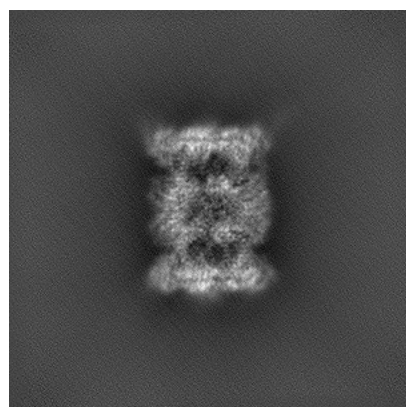


Y

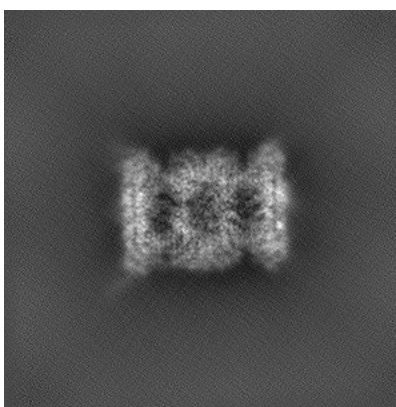


Z

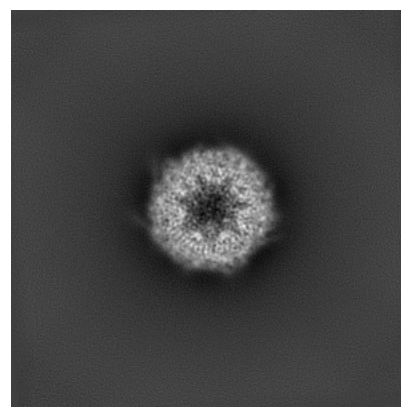
6.1.2 Raw map



X



Y

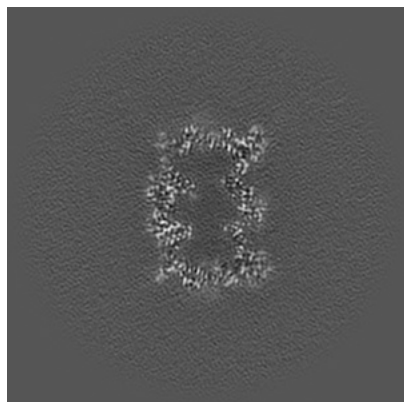


Z

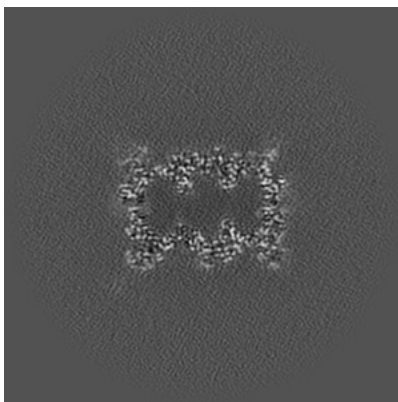
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

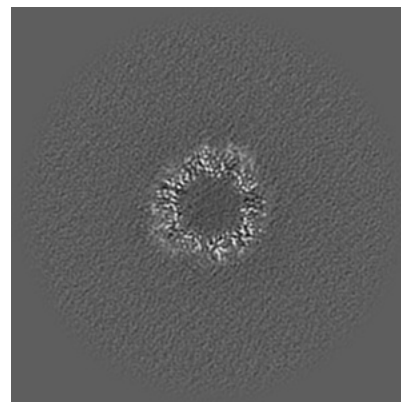
6.2.1 Primary map



X Index: 220

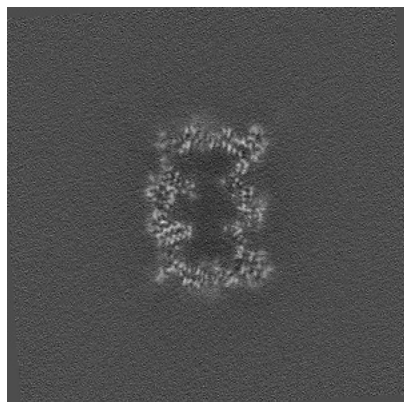


Y Index: 220

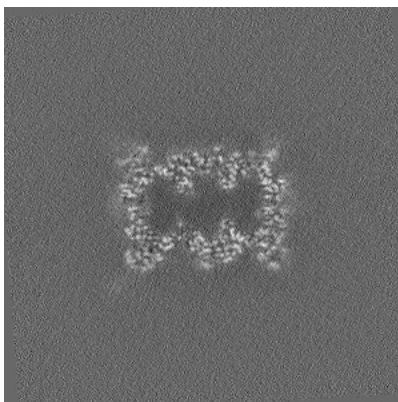


Z Index: 220

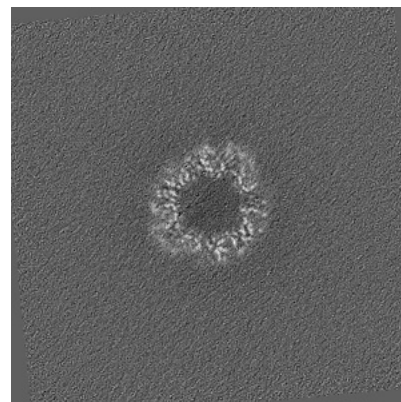
6.2.2 Raw map



X Index: 220



Y Index: 220

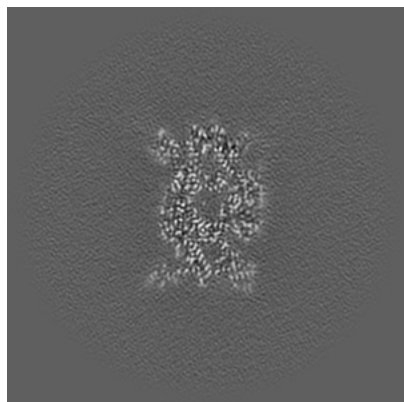


Z Index: 220

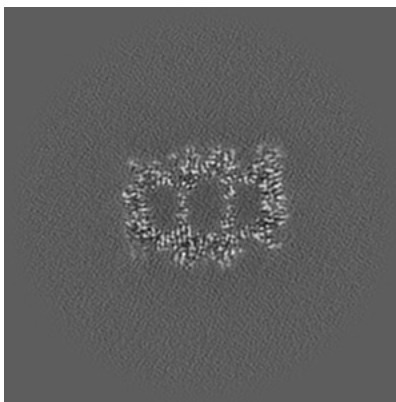
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

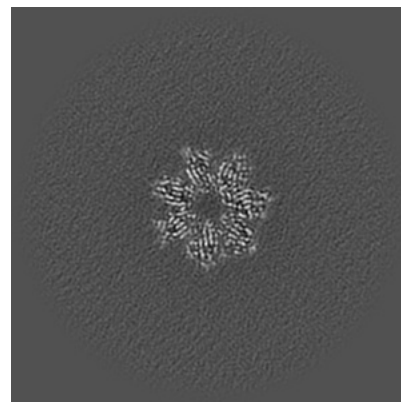
6.3.1 Primary map



X Index: 251

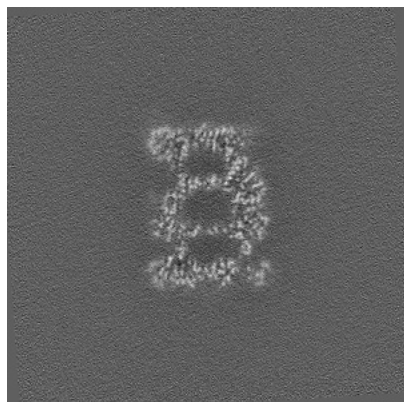


Y Index: 238

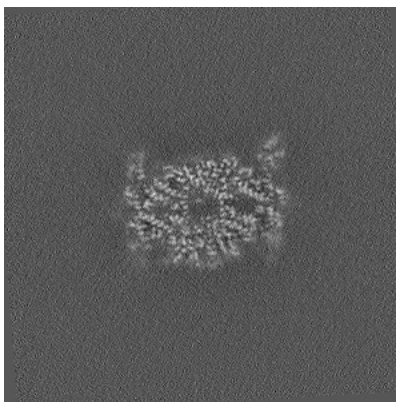


Z Index: 198

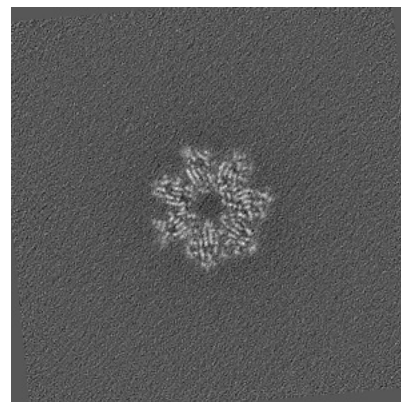
6.3.2 Raw map



X Index: 202



Y Index: 190

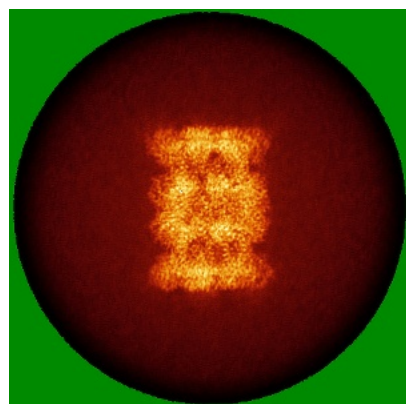


Z Index: 198

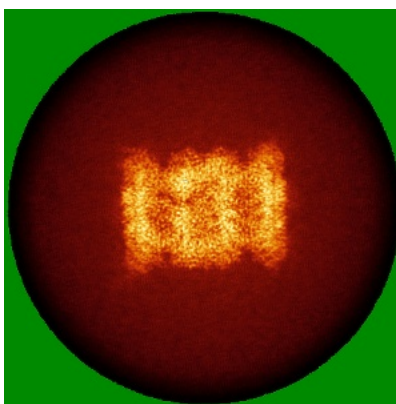
The images above show the largest variance slices of the map in three orthogonal directions.

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

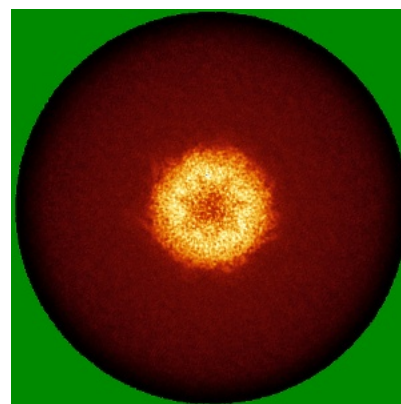
6.4.1 Primary map



X

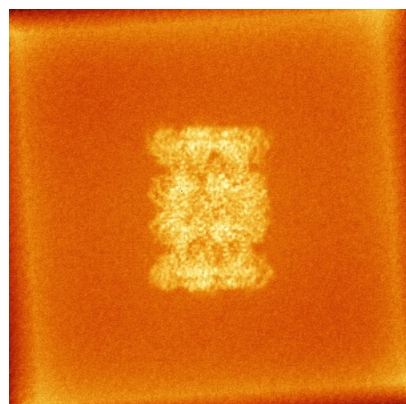


Y

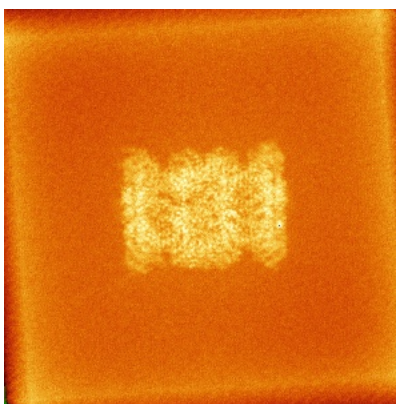


Z

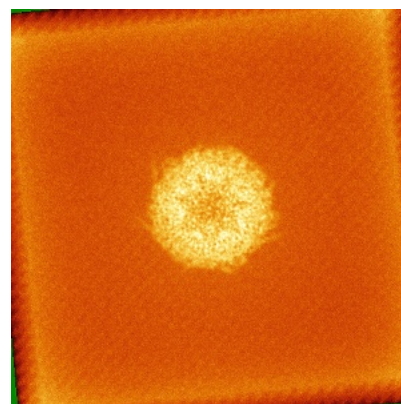
6.4.2 Raw map



X



Y

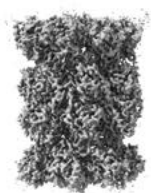


Z

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



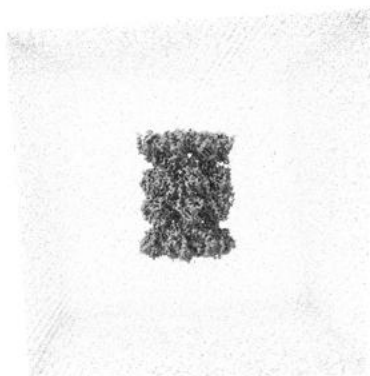
Y



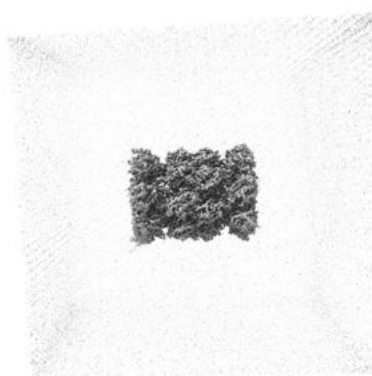
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

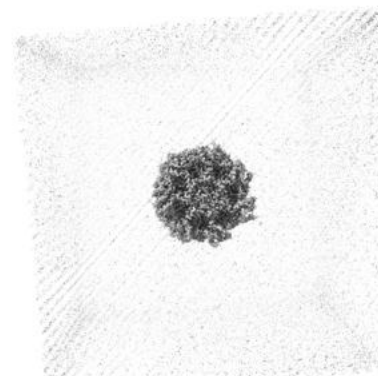
6.5.2 Raw map



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.

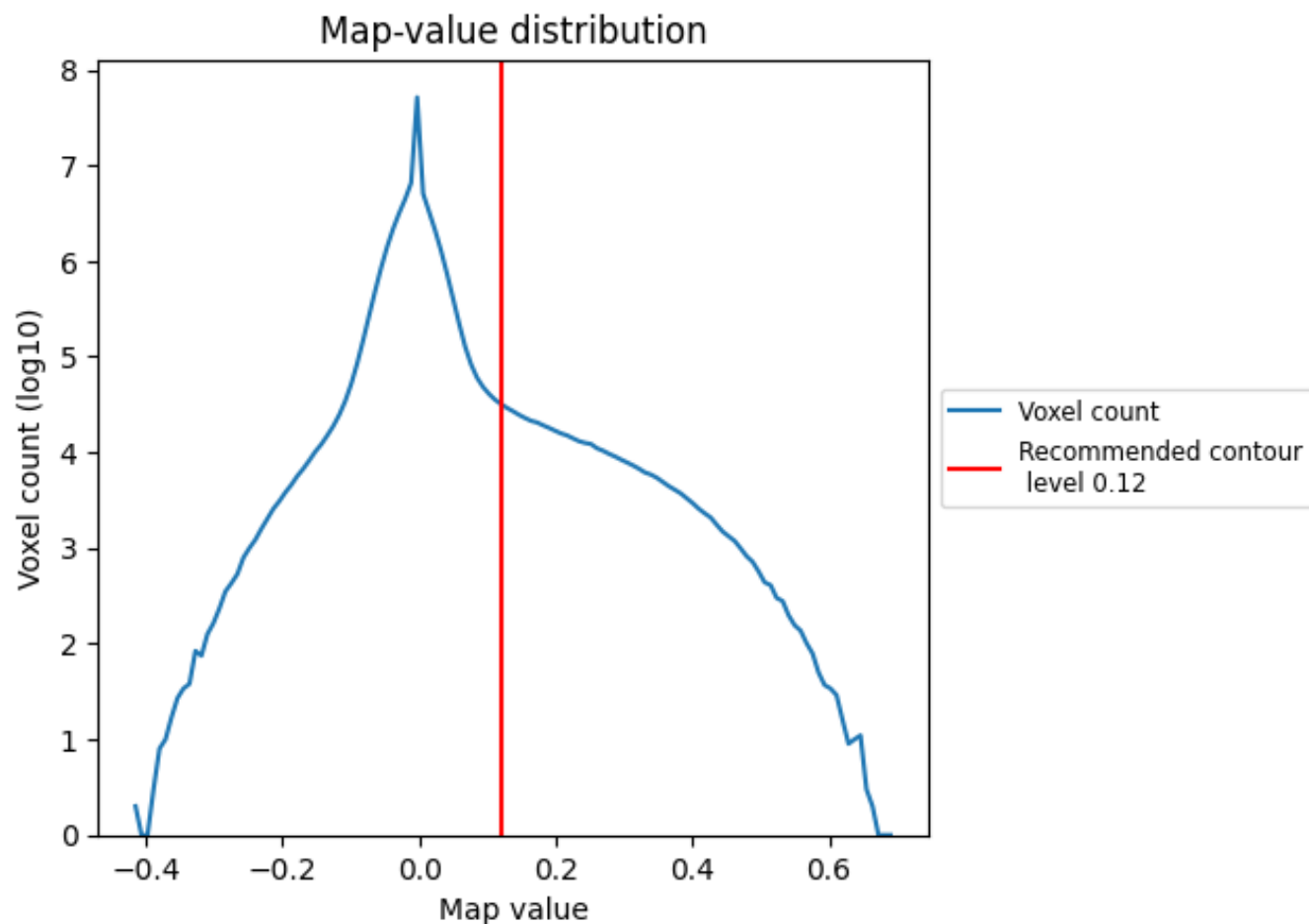
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

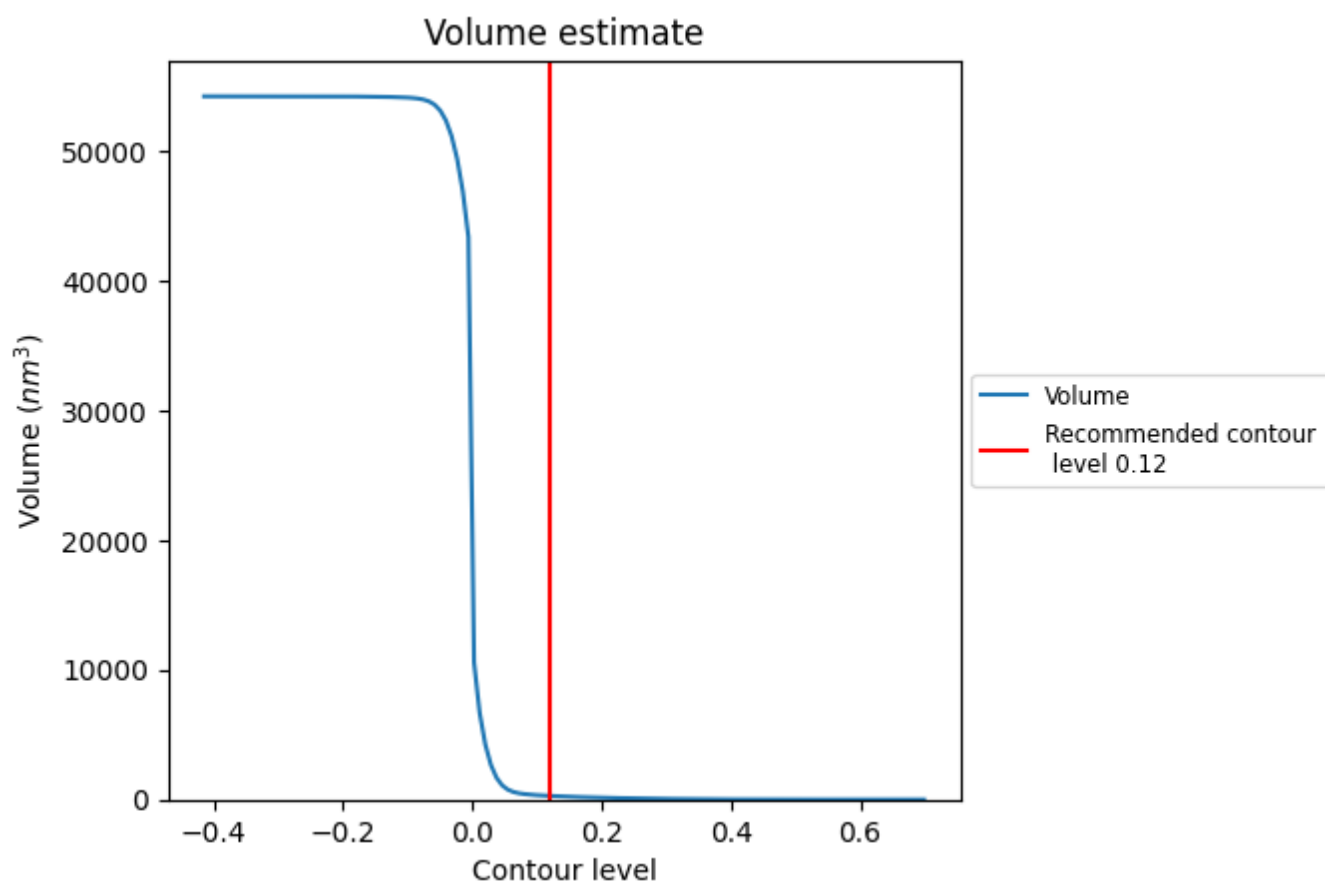
This section contains the results of statistical analysis of the map.

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.

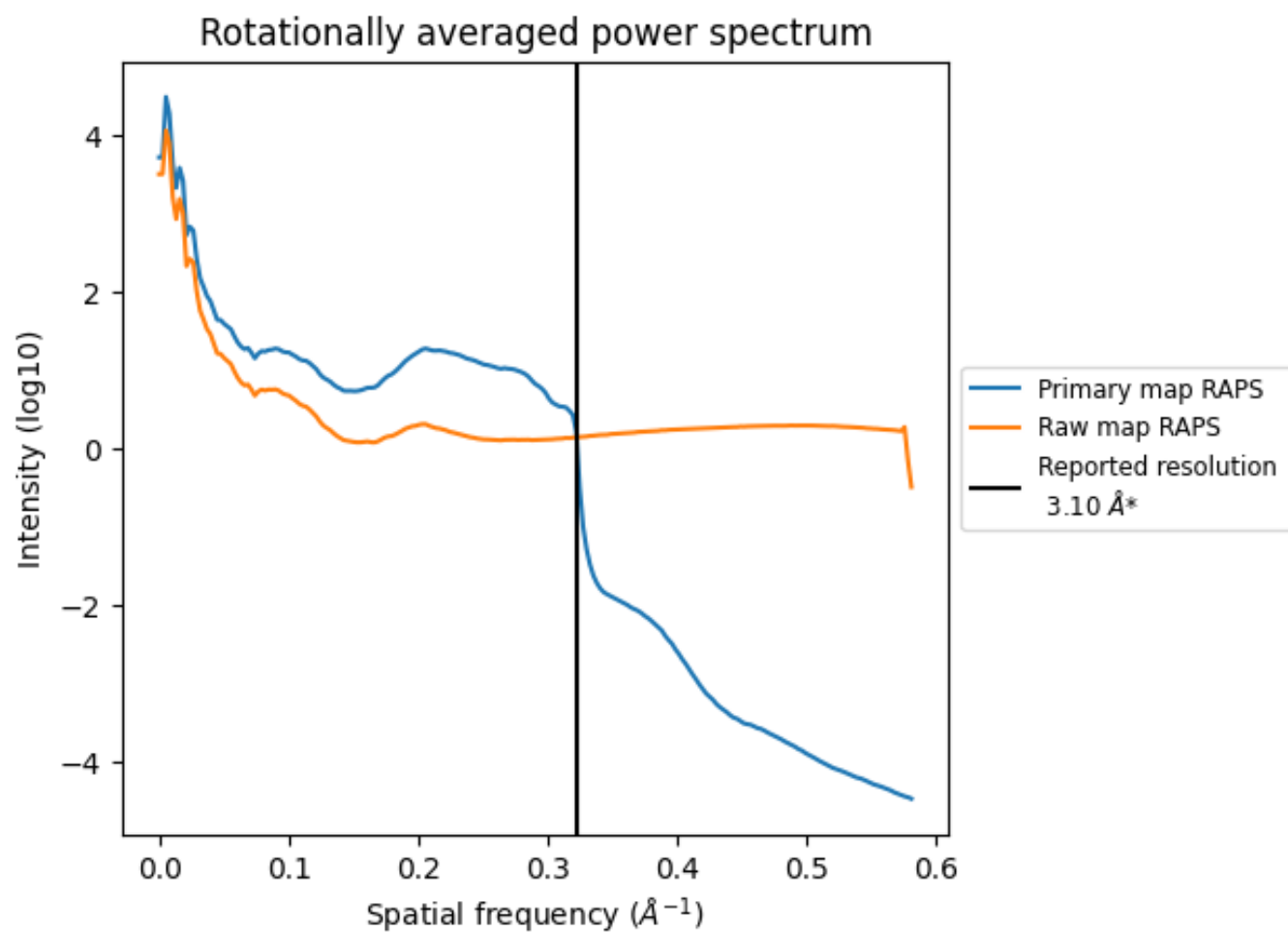
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 283 nm^3 ; this corresponds to an approximate mass of 255 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 ⓘ

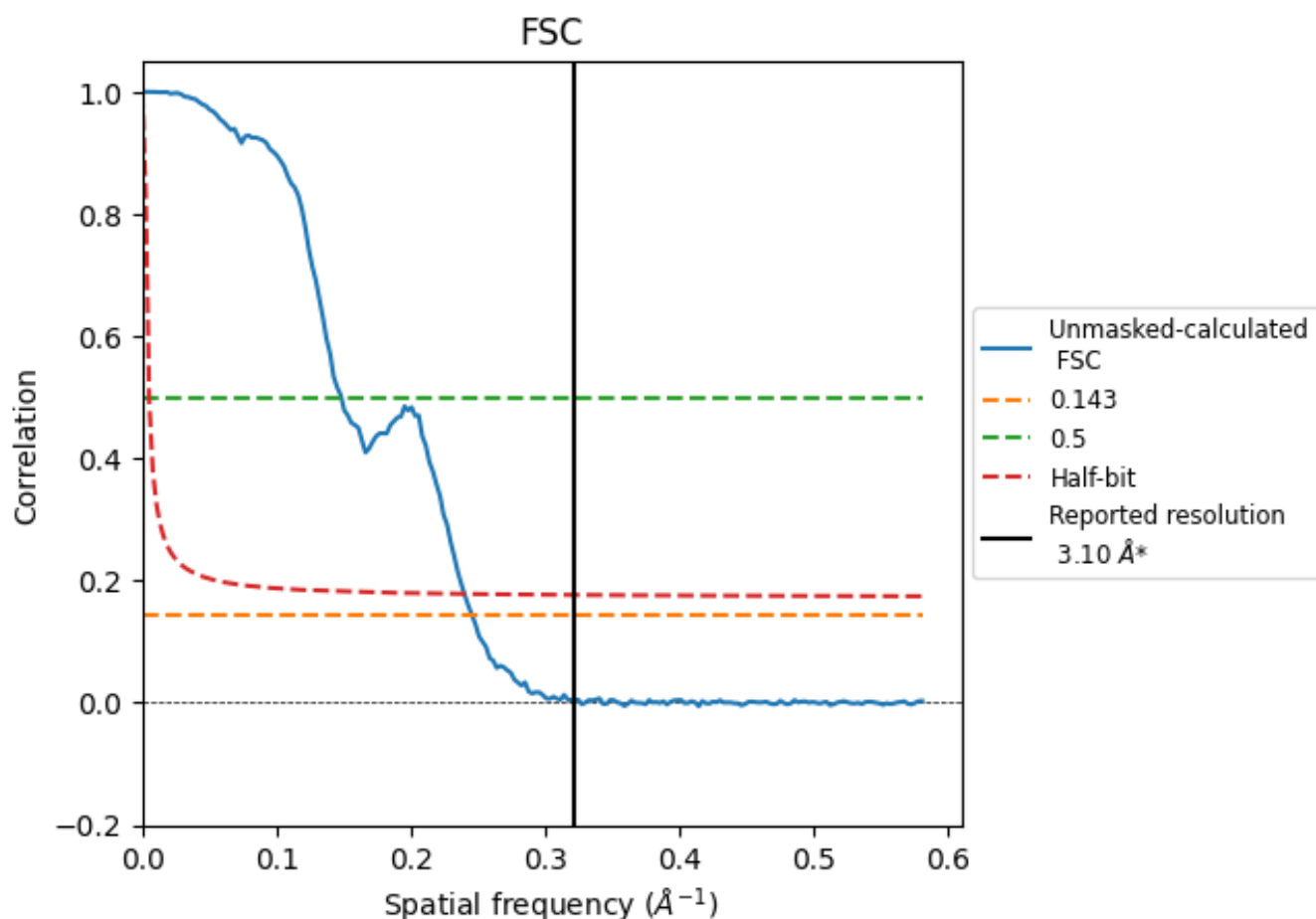


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

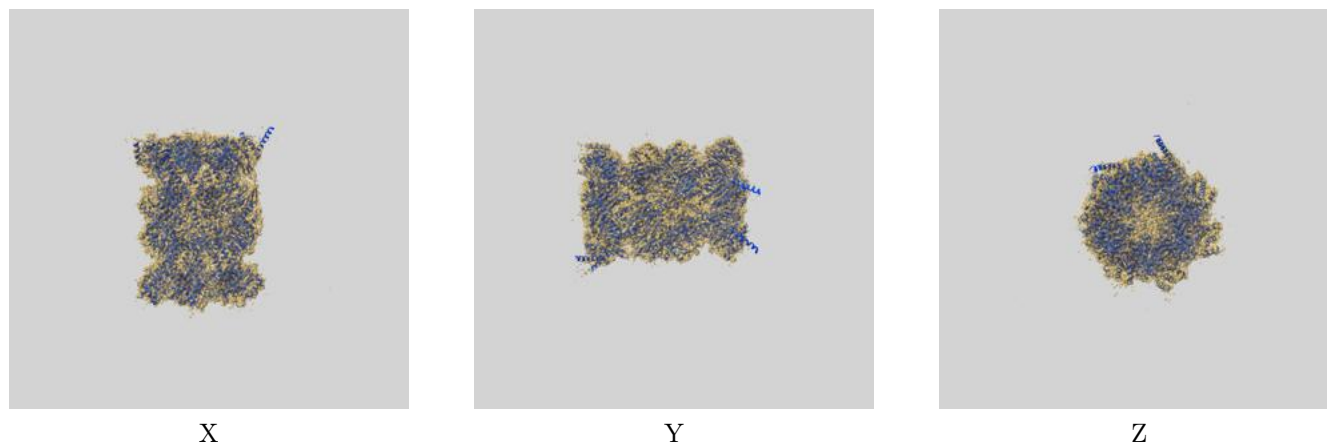
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	6.74	4.16

*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 4.07 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

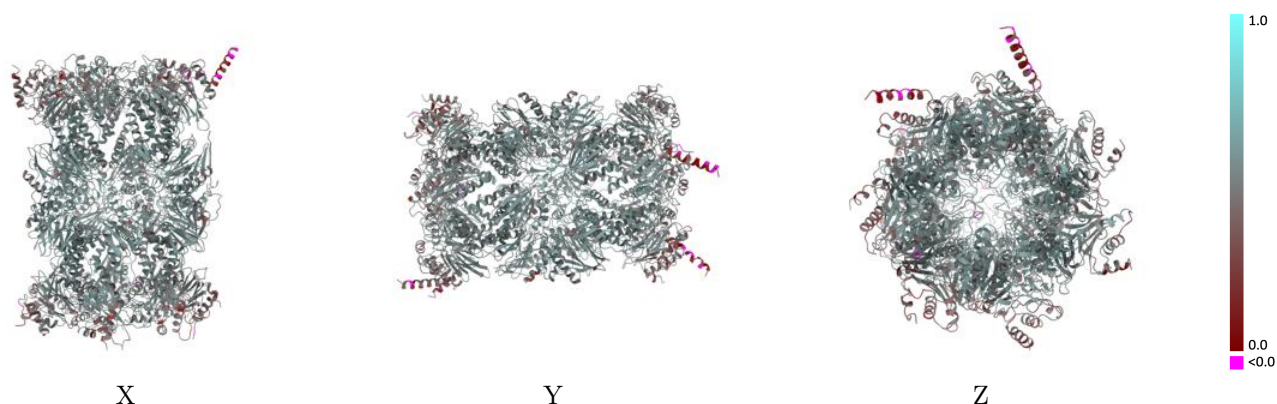
This section contains information regarding the fit between EMDB map EMD-15767 and PDB model 8AZK. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



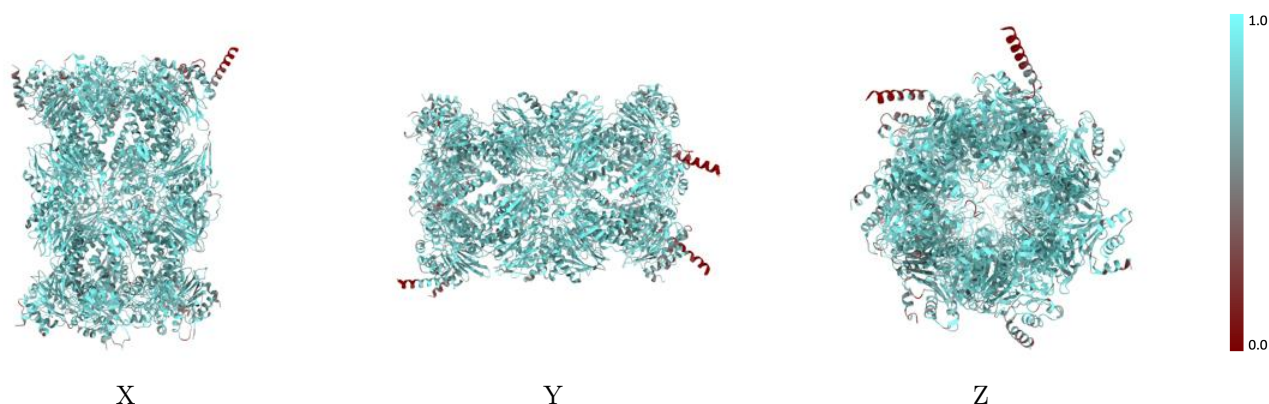
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



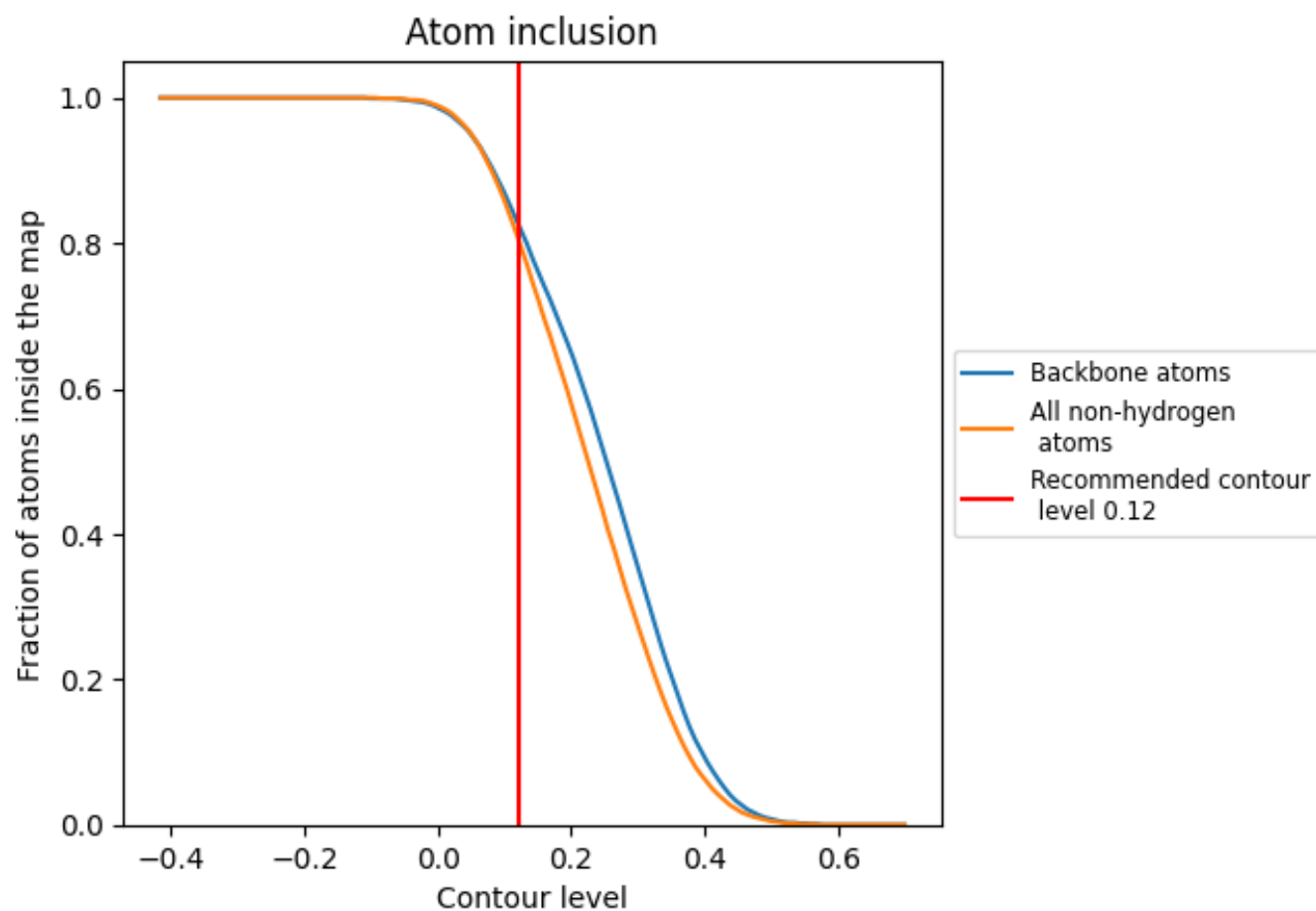
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.5180
1	 0.8260	 0.5350
2	 0.8460	 0.5510
A	 0.8090	 0.5070
B	 0.8070	 0.5050
C	 0.7490	 0.4800
D	 0.7590	 0.4820
E	 0.7830	 0.4960
F	 0.7380	 0.4650
G	 0.7720	 0.4940
H	 0.8630	 0.5580
I	 0.8350	 0.5360
J	 0.8330	 0.5470
K	 0.8570	 0.5620
L	 0.8580	 0.5540
M	 0.8100	 0.5300
N	 0.8590	 0.5490
O	 0.7990	 0.4980
P	 0.8030	 0.5130
Q	 0.7690	 0.4890
R	 0.7700	 0.4940
S	 0.7590	 0.4920
T	 0.7750	 0.4810
U	 0.7860	 0.5000
V	 0.8670	 0.5640
W	 0.8240	 0.5420
X	 0.8200	 0.5390
Y	 0.8500	 0.5470
Z	 0.8620	 0.5500

