



Full wwPDB EM Validation Report ⓘ

Sep 29, 2025 – 01:35 PM EDT

PDB ID : 9Y1O / pdb_00009y1o
EMDB ID : EMD-72400
Title : The structure of the Plasmodium falciparum 20S proteasome
Authors : Zhang, H.; Zhao, J.; Fajtova, P.; O'Donoghue, A.J.
Deposited on : 2025-08-29
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:

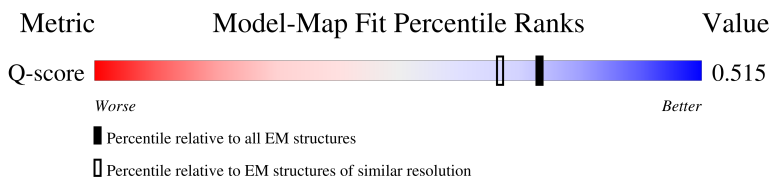
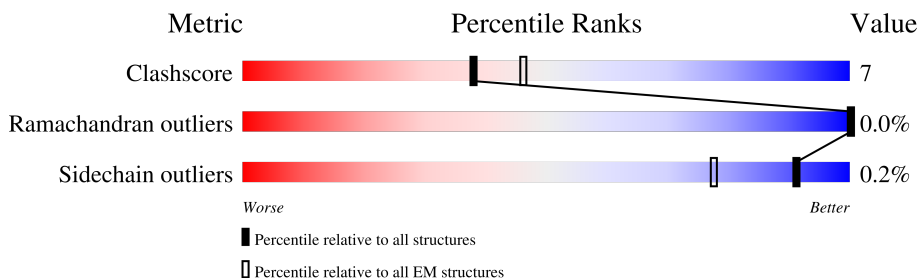
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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.













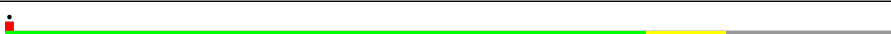



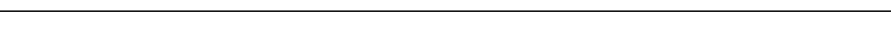
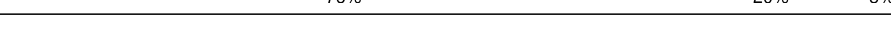








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A	260	 73% 22% 5%
1	O	260	 79% 16% 5%
2	B	235	 79% 17% .
2	P	235	 80% 17% .

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Mol	Chain	Length	Quality of chain
3	C	246	
3	Q	246	
4	D	241	
4	R	241	
5	E	256	
5	S	256	
6	F	254	
6	T	254	
7	G	252	
7	U	252	
8	H	252	
8	V	252	
9	I	229	
9	W	229	
10	J	218	
10	X	218	
11	K	195	
11	Y	195	
12	L	211	
12	Z	211	
13	N	302	
13	b	302	
14	M	240	
14	a	240	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 94870 atoms, of which 46726 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-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	246	Total	C	H	N	O	S	0	0
			3633	1172	1776	313	360	12		
1	O	246	Total	C	H	N	O	S	0	0
			3633	1172	1776	313	360	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	227	Total	C	H	N	O	S	0	0
			3322	1100	1630	278	308	6		
2	P	227	Total	C	H	N	O	S	0	0
			3322	1100	1630	278	308	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	240	Total	C	H	N	O	S	0	0
			3470	1156	1673	296	342	3		
3	Q	240	Total	C	H	N	O	S	0	0
			3470	1156	1673	296	342	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	233	Total	C	H	N	O	S	0	0
			3507	1131	1749	306	313	8		
4	R	233	Total	C	H	N	O	S	0	0
			3507	1131	1749	306	313	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	231	Total	C	H	N	O	S	0	0
			3377	1085	1658	288	336	10		
5	S	231	Total	C	H	N	O	S	0	0
			3377	1085	1658	288	336	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	232	Total	C	H	N	O	S	0	0
			3456	1129	1698	290	329	10		
6	T	232	Total	C	H	N	O	S	0	0
			3456	1129	1698	290	329	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	245	Total	C	H	N	O	S	0	0
			3850	1257	1882	331	368	12		
7	U	245	Total	C	H	N	O	S	0	0
			3850	1257	1882	331	368	12		

- Molecule 8 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	204	Total	C	H	N	O	S	0	0
			3237	1038	1615	280	294	10		
8	V	204	Total	C	H	N	O	S	0	0
			3237	1038	1615	280	294	10		

- Molecule 9 is a protein called Proteasome subunit beta-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	211	Total	C	H	N	O	S	0	0
			3059	980	1514	271	281	13		
9	W	211	Total	C	H	N	O	S	0	0
			3059	980	1514	271	281	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	208	Total	C	H	N	O	S	0	0
			3203	1035	1588	264	304	12		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	X	208	Total	C	H	N	O	S	0	0
			3203	1035	1588	264	304	12		

- Molecule 11 is a protein called Proteasome subunit beta-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	195	Total	C	H	N	O	S	0	0
			3123	1027	1538	264	287	7		
11	Y	195	Total	C	H	N	O	S	0	0
			3123	1027	1538	264	287	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	211	Total	C	H	N	O	S	0	0
			3233	1051	1590	273	312	7		
12	Z	211	Total	C	H	N	O	S	0	0
			3233	1051	1590	273	312	7		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	230	Total	C	H	N	O	S	0	0
			3656	1188	1805	318	338	7		
13	b	230	Total	C	H	N	O	S	0	0
			3656	1188	1805	318	338	7		

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	266	GLU	-	expression tag	UNP A0A0L7LW03
N	267	ASN	-	expression tag	UNP A0A0L7LW03
N	268	LEU	-	expression tag	UNP A0A0L7LW03
N	269	TYR	-	expression tag	UNP A0A0L7LW03
N	270	PHE	-	expression tag	UNP A0A0L7LW03
N	271	GLN	-	expression tag	UNP A0A0L7LW03
N	272	SER	-	expression tag	UNP A0A0L7LW03
N	273	SER	-	expression tag	UNP A0A0L7LW03
N	274	ALA	-	expression tag	UNP A0A0L7LW03
N	275	TRP	-	expression tag	UNP A0A0L7LW03
N	276	SER	-	expression tag	UNP A0A0L7LW03
N	277	HIS	-	expression tag	UNP A0A0L7LW03

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Chain	Residue	Modelled	Actual	Comment	Reference
N	278	PRO	-	expression tag	UNP A0A0L7LW03
N	279	GLN	-	expression tag	UNP A0A0L7LW03
N	280	PHE	-	expression tag	UNP A0A0L7LW03
N	281	GLU	-	expression tag	UNP A0A0L7LW03
N	282	LYS	-	expression tag	UNP A0A0L7LW03
N	283	GLY	-	expression tag	UNP A0A0L7LW03
N	284	GLY	-	expression tag	UNP A0A0L7LW03
N	285	GLY	-	expression tag	UNP A0A0L7LW03
N	286	SER	-	expression tag	UNP A0A0L7LW03
N	287	GLY	-	expression tag	UNP A0A0L7LW03
N	288	GLY	-	expression tag	UNP A0A0L7LW03
N	289	GLY	-	expression tag	UNP A0A0L7LW03
N	290	SER	-	expression tag	UNP A0A0L7LW03
N	291	GLY	-	expression tag	UNP A0A0L7LW03
N	292	GLY	-	expression tag	UNP A0A0L7LW03
N	293	SER	-	expression tag	UNP A0A0L7LW03
N	294	ALA	-	expression tag	UNP A0A0L7LW03
N	295	TRP	-	expression tag	UNP A0A0L7LW03
N	296	SER	-	expression tag	UNP A0A0L7LW03
N	297	HIS	-	expression tag	UNP A0A0L7LW03
N	298	PRO	-	expression tag	UNP A0A0L7LW03
N	299	GLN	-	expression tag	UNP A0A0L7LW03
N	300	PHE	-	expression tag	UNP A0A0L7LW03
N	301	GLU	-	expression tag	UNP A0A0L7LW03
N	302	LYS	-	expression tag	UNP A0A0L7LW03
b	266	GLU	-	expression tag	UNP A0A0L7LW03
b	267	ASN	-	expression tag	UNP A0A0L7LW03
b	268	LEU	-	expression tag	UNP A0A0L7LW03
b	269	TYR	-	expression tag	UNP A0A0L7LW03
b	270	PHE	-	expression tag	UNP A0A0L7LW03
b	271	GLN	-	expression tag	UNP A0A0L7LW03
b	272	SER	-	expression tag	UNP A0A0L7LW03
b	273	SER	-	expression tag	UNP A0A0L7LW03
b	274	ALA	-	expression tag	UNP A0A0L7LW03
b	275	TRP	-	expression tag	UNP A0A0L7LW03
b	276	SER	-	expression tag	UNP A0A0L7LW03
b	277	HIS	-	expression tag	UNP A0A0L7LW03
b	278	PRO	-	expression tag	UNP A0A0L7LW03
b	279	GLN	-	expression tag	UNP A0A0L7LW03
b	280	PHE	-	expression tag	UNP A0A0L7LW03
b	281	GLU	-	expression tag	UNP A0A0L7LW03
b	282	LYS	-	expression tag	UNP A0A0L7LW03

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Chain	Residue	Modelled	Actual	Comment	Reference
b	283	GLY	-	expression tag	UNP A0A0L7LW03
b	284	GLY	-	expression tag	UNP A0A0L7LW03
b	285	GLY	-	expression tag	UNP A0A0L7LW03
b	286	SER	-	expression tag	UNP A0A0L7LW03
b	287	GLY	-	expression tag	UNP A0A0L7LW03
b	288	GLY	-	expression tag	UNP A0A0L7LW03
b	289	GLY	-	expression tag	UNP A0A0L7LW03
b	290	SER	-	expression tag	UNP A0A0L7LW03
b	291	GLY	-	expression tag	UNP A0A0L7LW03
b	292	GLY	-	expression tag	UNP A0A0L7LW03
b	293	SER	-	expression tag	UNP A0A0L7LW03
b	294	ALA	-	expression tag	UNP A0A0L7LW03
b	295	TRP	-	expression tag	UNP A0A0L7LW03
b	296	SER	-	expression tag	UNP A0A0L7LW03
b	297	HIS	-	expression tag	UNP A0A0L7LW03
b	298	PRO	-	expression tag	UNP A0A0L7LW03
b	299	GLN	-	expression tag	UNP A0A0L7LW03
b	300	PHE	-	expression tag	UNP A0A0L7LW03
b	301	GLU	-	expression tag	UNP A0A0L7LW03
b	302	LYS	-	expression tag	UNP A0A0L7LW03

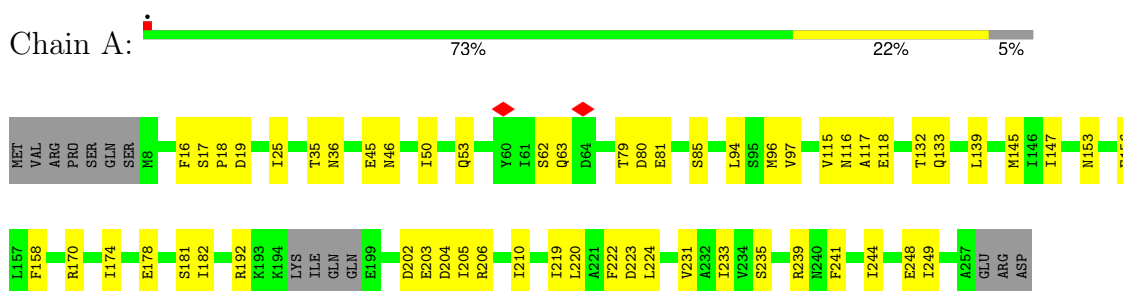
- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	M	212	Total	C	H	N	O	S	0	0
			3309	1064	1647	276	316	6		
14	a	212	Total	C	H	N	O	S	0	0
			3309	1064	1647	276	316	6		

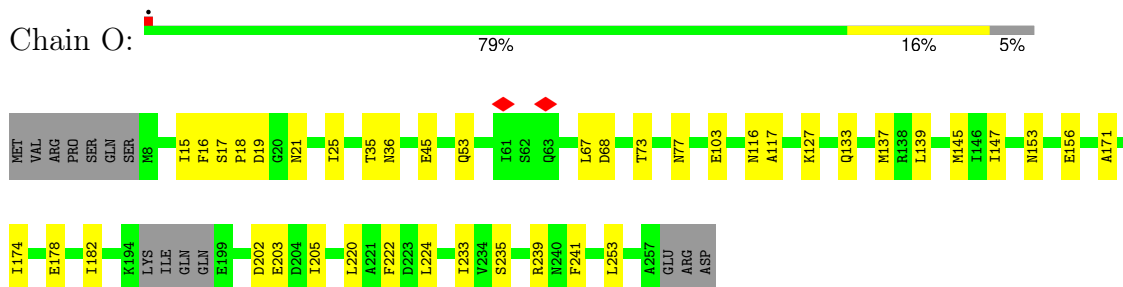
3 Residue-property plots

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

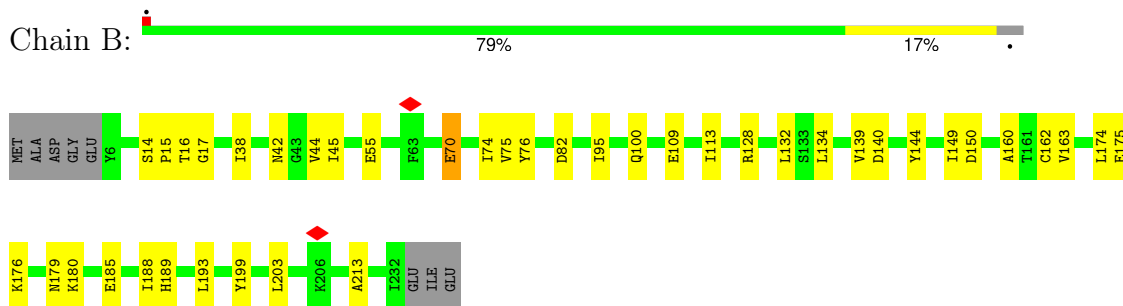
- Molecule 1: Proteasome subunit alpha type-6



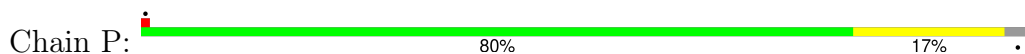
- Molecule 1: Proteasome subunit alpha type-6

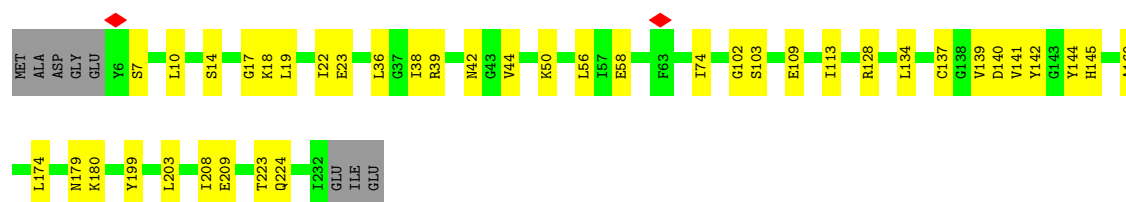


- Molecule 2: Proteasome subunit alpha type-2



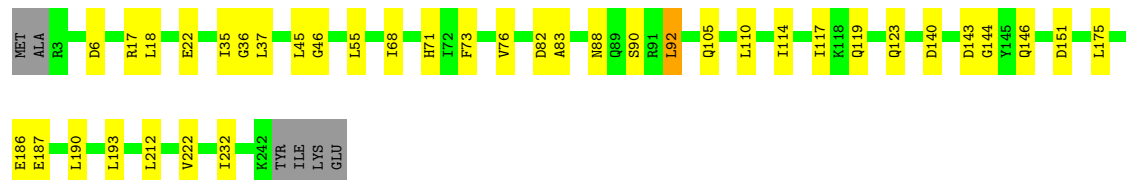
- Molecule 2: Proteasome subunit alpha type-2





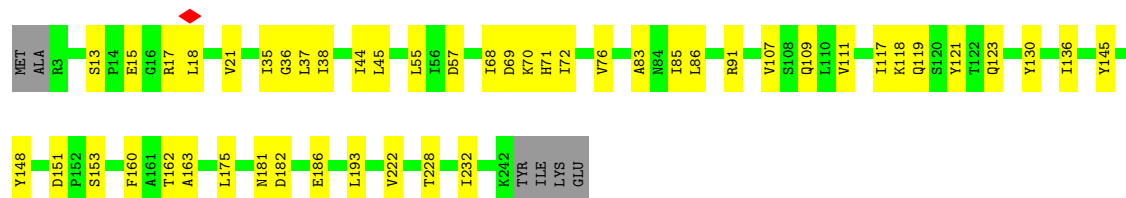
• Molecule 3: Proteasome subunit alpha type-3

Chain C: 82% 15%



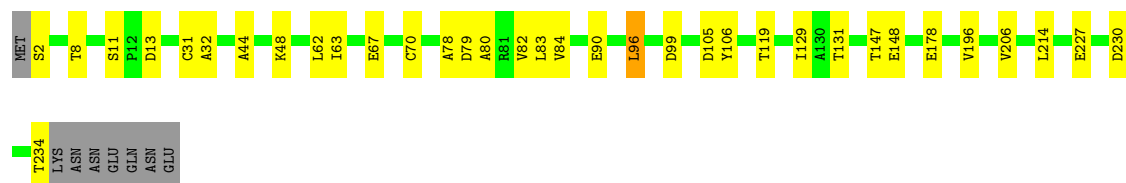
• Molecule 3: Proteasome subunit alpha type-3

Chain Q: 78% 20%



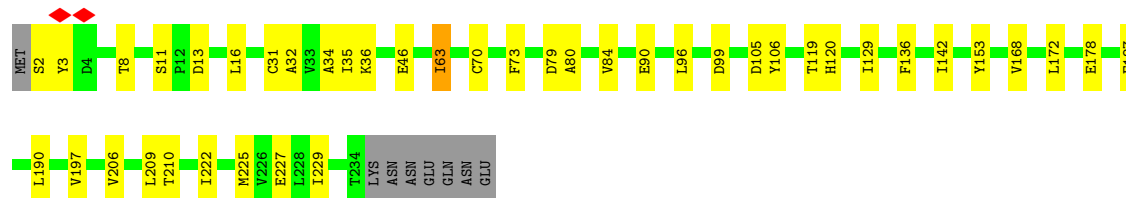
• Molecule 4: Proteasome subunit alpha type-4

Chain D: 82% 14%



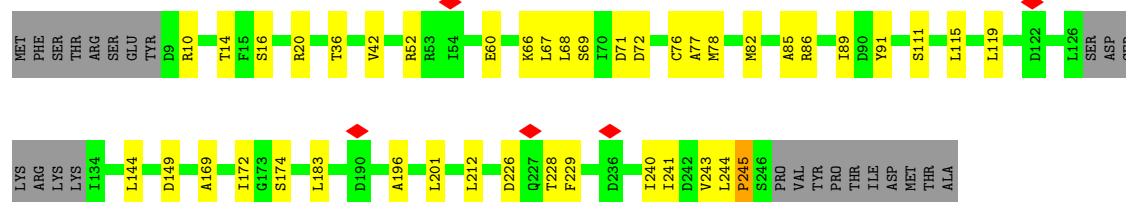
• Molecule 4: Proteasome subunit alpha type-4

Chain R: 79% 17%




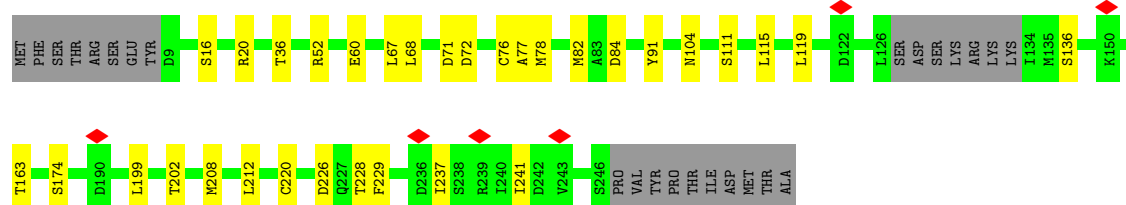
• Molecule 5: Proteasome subunit alpha type-5

Chain E: 




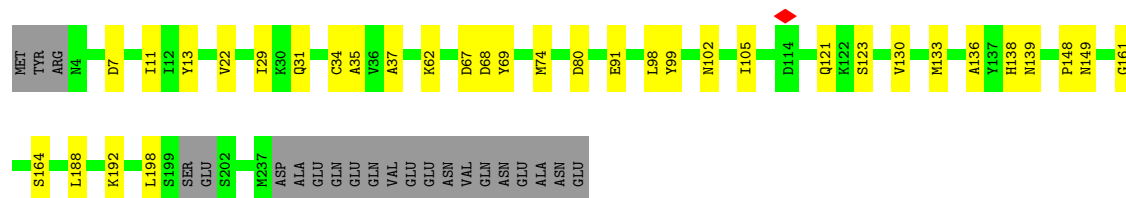
- Molecule 5: Proteasome subunit alpha type-5

Chain S: 




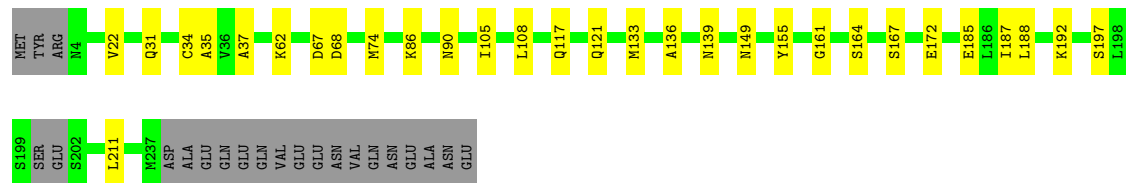
- Molecule 6: Proteasome subunit alpha type-1

Chain F: 




- Molecule 6: Proteasome subunit alpha type-1

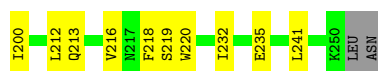
Chain T: 



- Molecule 7: Proteasome subunit alpha type-3

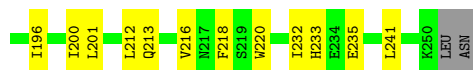
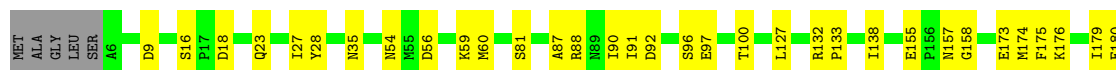
Chain G: 





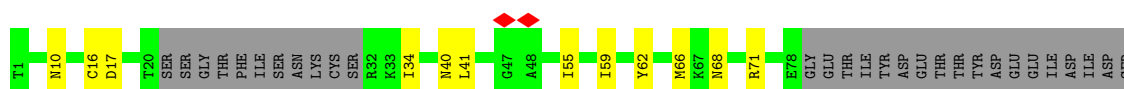
• Molecule 7: Proteasome subunit alpha type-3

Chain U: 79% 18%



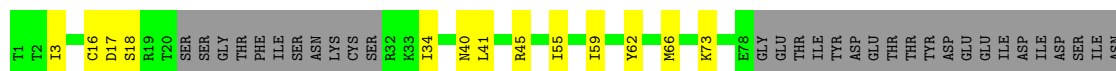
• Molecule 8: Proteasome endopeptidase complex

Chain H: 72% 9% 19%



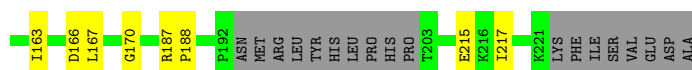
• Molecule 8: Proteasome endopeptidase complex

Chain V: 69% 12% 19%



• Molecule 9: Proteasome subunit beta-2

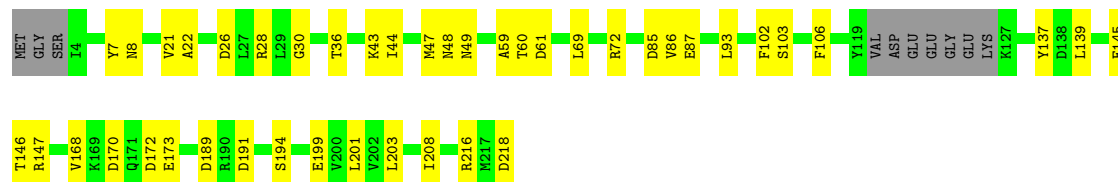
Chain I: 72% 20% 8%



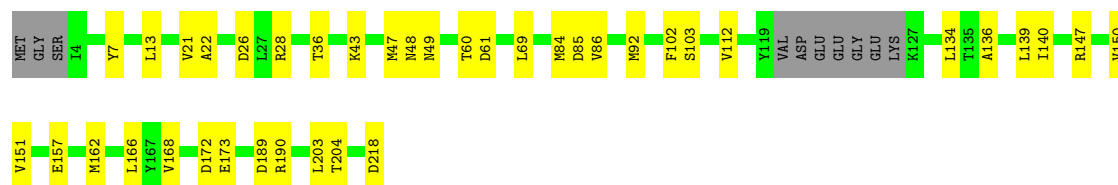
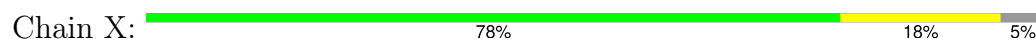
• Molecule 9: Proteasome subunit beta-2

Chain W: 73% 19% 8%

- Molecule 10: Proteasome subunit beta-3



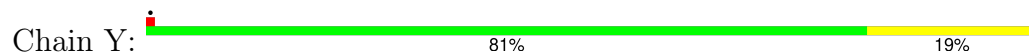
- Molecule 10: Proteasome subunit beta-3



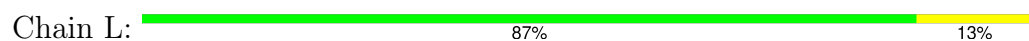
- Molecule 11: Proteasome subunit beta-4



- Molecule 11: Proteasome subunit beta-4



- Molecule 12: Proteasome subunit beta-5

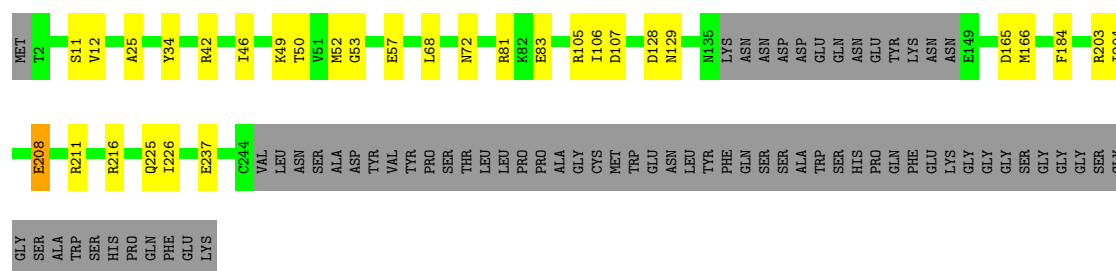




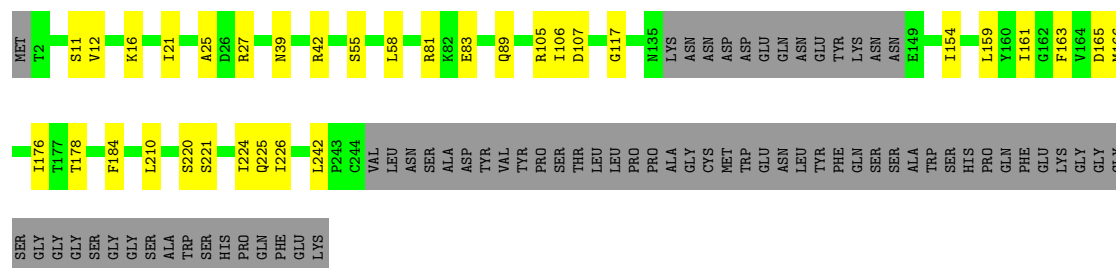
- Molecule 12: Proteasome subunit beta-5



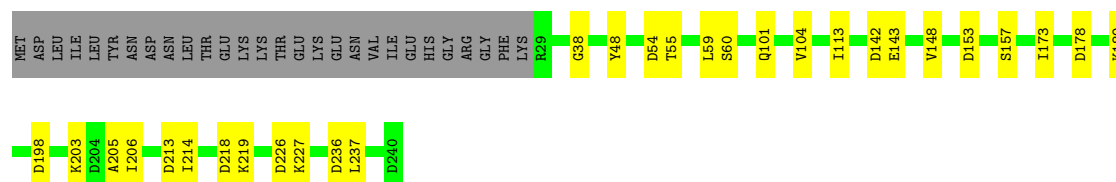
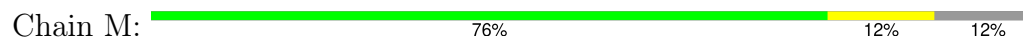
- Molecule 13: Proteasome subunit beta



- Molecule 13: Proteasome subunit beta

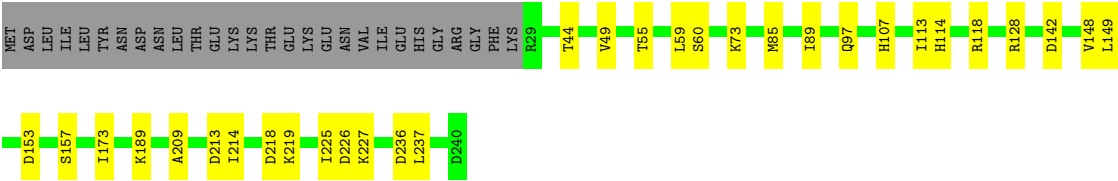


- Molecule 14: Proteasome subunit beta



- Molecule 14: Proteasome subunit beta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166209	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.639	Depositor
Minimum map value	-0.264	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	A	0.13	0/1883	0.33	0/2556
1	O	0.13	0/1883	0.33	0/2556
2	B	0.13	0/1726	0.32	0/2351
2	P	0.13	0/1726	0.32	0/2351
3	C	0.14	0/1832	0.33	0/2506
3	Q	0.14	0/1832	0.32	0/2506
4	D	0.14	0/1788	0.34	0/2424
4	R	0.14	0/1788	0.34	0/2424
5	E	0.21	0/1742	0.52	3/2364 (0.1%)
5	S	0.12	0/1742	0.32	0/2364
6	F	0.14	0/1790	0.32	0/2424
6	T	0.13	0/1790	0.32	0/2424
7	G	0.13	0/2012	0.33	0/2727
7	U	0.13	0/2012	0.34	0/2727
8	H	0.13	0/1649	0.30	0/2215
8	V	0.12	0/1649	0.30	0/2215
9	I	0.16	0/1575	0.36	0/2147
9	W	0.15	0/1575	0.36	0/2147
10	J	0.14	0/1643	0.33	0/2223
10	X	0.15	0/1643	0.33	0/2223
11	K	0.13	0/1620	0.33	0/2188
11	Y	0.14	0/1620	0.35	0/2188
12	L	0.12	0/1677	0.29	0/2263
12	Z	0.12	0/1677	0.28	0/2263
13	N	0.12	0/1890	0.30	0/2555
13	b	0.12	0/1890	0.29	0/2555
14	M	0.12	0/1694	0.29	0/2300
14	a	0.13	0/1694	0.30	0/2300
All	All	0.14	0/49042	0.33	3/66486 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	245	PRO	CA-N-CD	-15.48	90.33	112.00
5	E	245	PRO	N-CA-C	6.92	121.93	111.14
5	E	245	PRO	N-CD-CG	-5.94	94.30	103.20

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	A	1857	1776	1774	39	0
1	O	1857	1776	1774	31	0
2	B	1692	1630	1629	27	0
2	P	1692	1630	1629	30	0
3	C	1797	1673	1672	27	0
3	Q	1797	1673	1672	40	0
4	D	1758	1749	1748	29	0
4	R	1758	1749	1748	32	0
5	E	1719	1658	1656	31	0
5	S	1719	1658	1656	27	0
6	F	1758	1698	1696	26	0
6	T	1758	1698	1696	18	0
7	G	1968	1882	1881	29	0
7	U	1968	1882	1881	33	0
8	H	1622	1615	1613	14	0
8	V	1622	1615	1613	16	0
9	I	1545	1514	1513	30	0
9	W	1545	1514	1513	30	0
10	J	1615	1588	1586	32	0
10	X	1615	1588	1586	28	0
11	K	1585	1538	1538	14	0
11	Y	1585	1538	1538	28	0
12	L	1643	1590	1590	21	0
12	Z	1643	1590	1590	20	0
13	N	1851	1805	1803	21	0
13	b	1851	1805	1803	21	0
14	M	1662	1647	1646	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	a	1662	1647	1646	22	0
All	All	48144	46726	46690	682	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 7.

All (682) 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)
10:J:8:ASN:OD1	11:K:123:ASN:ND2	2.05	0.87
12:Z:125:LEU:HD21	12:Z:139:LEU:HD13	1.56	0.86
5:E:245:PRO:HD2	5:E:245:PRO:O	1.78	0.83
2:B:74:ILE:HD11	2:B:134:LEU:HD13	1.59	0.83
6:F:67:ASP:OD2	6:F:68:ASP:N	2.12	0.83
1:O:103:GLU:OE2	1:O:127:LYS:NZ	2.10	0.83
6:T:67:ASP:OD1	6:T:68:ASP:N	2.12	0.82
10:J:8:ASN:ND2	10:J:30:GLY:O	2.12	0.82
5:S:104:ASN:OD1	14:a:118:ARG:NH1	2.12	0.82
10:J:172:ASP:OD1	10:J:173:GLU:N	2.13	0.80
5:E:60:GLU:OE2	5:E:60:GLU:N	2.14	0.80
12:L:3:THR:OG1	12:L:128:CYS:SG	2.39	0.80
13:N:105:ARG:NH1	13:N:107:ASP:OD1	2.14	0.79
13:b:105:ARG:NH1	13:b:107:ASP:OD2	2.15	0.79
14:a:173:ILE:HD11	14:a:209:ALA:HB2	1.66	0.78
14:M:142:ASP:OD2	14:M:143:GLU:N	2.17	0.78
13:N:83:GLU:N	13:N:83:GLU:OE1	2.17	0.78
10:J:145:GLU:OE2	10:J:147:ARG:N	2.17	0.77
11:Y:18:ASP:OD2	11:Y:175:GLN:NE2	2.16	0.77
1:O:45:GLU:OE2	1:O:45:GLU:N	2.18	0.76
1:A:45:GLU:OE2	1:A:45:GLU:N	2.18	0.76
6:T:105:ILE:HD12	6:T:136:ALA:HB3	1.68	0.75
2:P:10:LEU:HD13	1:O:15:ILE:HD11	1.69	0.74
12:L:63:ILE:HD12	12:L:74:ILE:HG21	1.66	0.74
14:a:55:THR:OG1	14:a:219:LYS:O	2.03	0.74
1:O:145:MET:HG3	1:O:174:ILE:HD12	1.70	0.74
3:Q:151:ASP:OD2	3:Q:153:SER:OG	2.04	0.74
4:R:178:GLU:N	4:R:178:GLU:OE1	2.19	0.74
4:R:225:MET:O	4:R:229:ILE:HG23	1.87	0.73
14:M:219:LYS:NZ	14:M:236:ASP:OD1	2.20	0.73
4:D:67:GLU:OE2	4:D:67:GLU:N	2.21	0.73
12:L:154:GLU:OE1	12:L:200:TYR:OH	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:121:LEU:O	11:Y:122:SER:OG	2.05	0.72
8:H:190:GLN:OE1	13:N:34:TYR:OH	2.06	0.72
13:b:83:GLU:OE2	13:b:83:GLU:N	2.22	0.72
12:Z:4:LEU:CD1	12:Z:139:LEU:HD11	2.20	0.72
14:M:213:ASP:OD1	14:M:214:ILE:N	2.23	0.72
1:A:63:GLN:N	1:A:63:GLN:OE1	2.23	0.72
12:L:4:LEU:CD1	12:L:139:LEU:HD11	2.21	0.71
3:C:45:LEU:HD12	3:C:73:PHE:CE2	2.26	0.71
4:D:178:GLU:OE2	4:D:178:GLU:N	2.23	0.71
2:P:203:LEU:HD23	2:P:208:ILE:HD11	1.72	0.71
3:C:88:ASN:O	3:C:92:LEU:HD22	1.91	0.70
3:C:105:GLN:OE1	3:C:110:LEU:N	2.23	0.70
4:D:105:ASP:OD1	4:D:106:TYR:N	2.24	0.70
3:Q:119:GLN:NE2	4:R:79:ASP:OD1	2.25	0.70
3:Q:181:ASN:OD1	3:Q:182:ASP:N	2.25	0.70
1:A:170:ARG:NH1	2:B:55:GLU:O	2.25	0.69
13:N:165:ASP:OD1	13:N:166:MET:N	2.26	0.69
14:a:213:ASP:OD1	14:a:214:ILE:N	2.25	0.69
13:b:165:ASP:OD1	13:b:166:MET:N	2.25	0.69
10:J:61:ASP:OD2	10:J:106:PHE:N	2.26	0.68
7:G:196:ILE:O	7:G:200:ILE:HG23	1.94	0.68
6:F:105:ILE:HD12	6:F:136:ALA:HB3	1.76	0.67
10:J:48:ASN:OD1	10:J:49:ASN:N	2.26	0.67
1:A:235:SER:O	1:A:239:ARG:N	2.27	0.67
7:U:9:ASP:O	7:U:23:GLN:NE2	2.28	0.67
7:U:233:HIS:ND1	7:U:235:GLU:OE1	2.24	0.67
11:Y:24:SER:OG	11:Y:25:ILE:N	2.27	0.67
10:X:7:TYR:OH	11:Y:119:ASP:OD2	2.11	0.67
4:D:11:SER:OG	4:D:13:ASP:OD1	2.13	0.66
13:N:216:ARG:NE	9:W:139:GLU:OE1	2.28	0.66
3:Q:72:ILE:HG12	3:Q:107:VAL:HG12	1.78	0.66
11:K:24:SER:OG	11:K:25:ILE:N	2.27	0.66
3:Q:76:VAL:HG21	3:Q:83:ALA:HB2	1.77	0.66
11:Y:2:ASP:OD2	11:Y:54:ARG:NH2	2.28	0.66
10:X:157:GLU:OE2	10:X:157:GLU:N	2.26	0.66
3:C:37:LEU:HD21	3:C:175:LEU:HD22	1.77	0.66
13:b:210:LEU:HD13	13:b:224:ILE:HD13	1.77	0.66
12:L:204:GLU:OE2	12:L:205:GLN:N	2.29	0.66
10:X:28:ARG:O	10:X:43:LYS:NZ	2.28	0.66
12:L:1:THR:N	12:L:169:GLY:O	2.28	0.65
12:L:4:LEU:HD13	12:L:139:LEU:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:105:ASP:OD1	4:R:106:TYR:N	2.29	0.65
10:X:48:ASN:OD1	10:X:49:ASN:N	2.28	0.65
3:Q:76:VAL:HG21	3:Q:83:ALA:CB	2.27	0.65
3:Q:15:GLU:OE1	3:Q:15:GLU:N	2.29	0.65
3:Q:228:THR:O	3:Q:232:ILE:HD12	1.97	0.65
1:O:53:GLN:NE2	1:O:220:LEU:HD11	2.12	0.65
1:A:220:LEU:HD12	1:A:224:LEU:HD21	1.77	0.65
11:Y:92:TYR:O	11:Y:96:ASN:N	2.29	0.65
1:O:220:LEU:HD13	1:O:222:PHE:CZ	2.31	0.65
12:L:63:ILE:CD1	12:L:74:ILE:HD13	2.27	0.64
7:U:90:ILE:HG21	7:U:138:ILE:HD12	1.79	0.64
2:B:185:GLU:O	2:B:189:HIS:ND1	2.28	0.64
4:D:96:LEU:HD22	11:K:63:LYS:HD3	1.79	0.64
5:E:91:TYR:CG	5:E:119:LEU:HD22	2.32	0.64
14:a:44:THR:HG22	14:a:149:LEU:HD13	1.81	0.63
4:D:70:CYS:SG	4:D:214:LEU:HD12	2.38	0.63
9:W:12:VAL:HG13	9:W:110:LEU:HD11	1.80	0.63
4:R:2:SER:OG	4:R:3:TYR:N	2.26	0.63
7:U:35:ASN:OD1	7:U:54:ASN:ND2	2.32	0.63
1:A:53:GLN:NE2	1:A:220:LEU:HD11	2.14	0.62
14:M:55:THR:OG1	14:M:219:LYS:O	2.06	0.62
7:G:90:ILE:HG21	7:G:138:ILE:HD13	1.81	0.62
2:P:14:SER:O	2:P:17:GLY:N	2.32	0.62
12:Z:115:ASP:OD1	12:Z:116:ASP:N	2.31	0.62
14:a:219:LYS:NZ	14:a:236:ASP:OD1	2.28	0.62
1:O:25:ILE:HD13	1:O:139:LEU:HD11	1.81	0.62
7:U:28:TYR:OH	7:U:155:GLU:OE2	2.16	0.61
4:R:90:GLU:OE2	4:R:106:TYR:OH	2.16	0.61
1:O:178:GLU:O	1:O:182:ILE:HG23	2.00	0.61
13:N:208:GLU:OE2	13:N:211:ARG:NH1	2.32	0.61
9:W:156:CYS:O	9:W:157:GLU:C	2.44	0.61
3:C:119:GLN:NE2	3:C:123:GLN:OE1	2.33	0.61
11:Y:184:TYR:OH	11:Y:189:GLU:OE1	2.14	0.61
14:M:226:ASP:OD1	14:M:227:LYS:N	2.32	0.61
13:b:81:ARG:NH2	6:T:139:ASN:OD1	2.34	0.61
3:C:140:ASP:OD2	3:C:146:GLN:NE2	2.34	0.61
6:F:62:LYS:NZ	6:F:74:MET:O	2.32	0.61
8:H:55:ILE:O	8:H:59:ILE:HG23	2.01	0.61
11:Y:78:VAL:HG11	11:Y:114:GLN:HG2	1.83	0.61
12:L:180:HIS:NE2	12:L:185:ASP:OD2	2.29	0.60
2:B:100:GLN:OE1	10:J:72:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:156:CYS:O	9:I:157:GLU:C	2.43	0.60
10:X:85:ASP:OD1	10:X:86:VAL:N	2.35	0.60
10:J:85:ASP:OD1	10:J:86:VAL:N	2.35	0.60
14:M:153:ASP:OD1	14:M:157:SER:N	2.35	0.60
3:Q:68:ILE:HD13	3:Q:72:ILE:HG22	1.83	0.60
10:J:93:LEU:HD23	10:J:137:TYR:CE2	2.37	0.59
12:L:37:ILE:HD11	12:L:56:GLU:OE2	2.01	0.59
1:O:153:ASN:OD1	1:O:239:ARG:NH2	2.35	0.59
2:B:132:LEU:HD13	2:B:134:LEU:CD2	2.33	0.59
9:I:144:ASP:OD2	9:I:145:ASN:ND2	2.34	0.59
11:K:139:VAL:HG13	11:K:167:LEU:HD21	1.84	0.59
13:N:225:GLN:OE1	13:N:226:ILE:N	2.35	0.59
6:T:86:LYS:O	6:T:90:ASN:ND2	2.27	0.59
1:O:235:SER:O	1:O:239:ARG:N	2.35	0.59
5:E:68:LEU:HD13	5:E:78:MET:CE	2.32	0.59
1:A:116:ASN:OD1	1:A:117:ALA:N	2.36	0.58
6:F:139:ASN:OD1	13:N:81:ARG:NH2	2.35	0.58
5:S:76:CYS:SG	5:S:77:ALA:N	2.76	0.58
8:H:68:ASN:OD1	8:H:71:ARG:NH1	2.37	0.58
1:O:220:LEU:HD12	1:O:224:LEU:HD21	1.84	0.58
10:X:136:ALA:HB2	10:X:150:VAL:CG2	2.33	0.58
12:L:38:ASN:ND2	12:L:67:GLU:OE1	2.36	0.58
12:Z:4:LEU:HD11	12:Z:139:LEU:HD11	1.84	0.58
8:V:157:ASP:OD2	8:V:158:LYS:N	2.37	0.58
2:P:50:LYS:NZ	2:P:209:GLU:OE1	2.37	0.58
1:A:25:ILE:HD13	1:A:139:LEU:HD11	1.86	0.57
3:C:6:ASP:OD2	4:D:2:SER:OG	2.22	0.57
2:P:140:ASP:OD2	2:P:140:ASP:N	2.37	0.57
10:X:147:ARG:O	10:X:147:ARG:HD3	2.03	0.57
11:Y:152:THR:OG1	11:Y:155:GLU:OE2	2.17	0.57
1:A:153:ASN:OD1	1:A:239:ARG:NH2	2.38	0.57
9:W:30:ASN:OD1	9:W:187:ARG:NH1	2.37	0.57
10:X:218:ASP:OD1	10:X:218:ASP:N	2.34	0.57
1:A:202:ASP:OD1	1:A:203:GLU:N	2.37	0.57
4:D:62:LEU:HD21	4:D:214:LEU:HD11	1.86	0.57
7:G:173:GLU:OE1	7:G:173:GLU:N	2.26	0.57
10:X:172:ASP:OD1	10:X:173:GLU:N	2.37	0.57
1:A:178:GLU:O	1:A:182:ILE:HG23	2.04	0.57
14:a:153:ASP:OD1	14:a:157:SER:N	2.38	0.57
11:K:139:VAL:CG1	11:K:167:LEU:HD21	2.35	0.57
1:A:62:SER:OG	1:A:63:GLN:OE1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:27:ILE:HD11	7:U:133:PRO:HG2	1.86	0.56
13:N:107:ASP:O	13:N:107:ASP:OD2	2.23	0.56
5:E:76:CYS:SG	5:E:77:ALA:N	2.78	0.56
8:H:41:LEU:HD11	8:H:129:VAL:HG23	1.88	0.56
10:J:102:PHE:O	10:J:103:SER:OG	2.20	0.56
11:Y:39:ILE:HG21	11:Y:65:VAL:HG11	1.88	0.56
11:Y:45:LEU:HD11	11:Y:102:CYS:SG	2.44	0.56
1:A:81:GLU:N	1:A:81:GLU:OE2	2.39	0.56
3:C:22:GLU:C	3:C:22:GLU:OE1	2.49	0.56
7:U:196:ILE:O	7:U:200:ILE:HG12	2.05	0.56
2:P:14:SER:OG	2:P:17:GLY:O	2.22	0.56
11:Y:21:SER:OG	11:Y:32:ASP:OD1	2.18	0.56
6:F:34:CYS:SG	6:F:35:ALA:N	2.79	0.55
4:R:206:VAL:HG12	4:R:222:ILE:HD11	1.88	0.55
13:b:161:ILE:HG22	13:b:176:ILE:HD12	1.89	0.55
9:I:166:ASP:OD2	9:I:167:LEU:N	2.40	0.55
11:K:92:TYR:O	11:K:96:ASN:N	2.39	0.55
14:a:44:THR:HG23	14:a:149:LEU:HD22	1.88	0.55
3:C:71:HIS:HB3	3:C:222:VAL:HG11	1.89	0.55
7:G:90:ILE:HG21	7:G:138:ILE:CD1	2.37	0.55
9:I:144:ASP:O	9:I:145:ASN:ND2	2.40	0.55
12:Z:139:LEU:O	12:Z:143:TYR:N	2.38	0.55
7:G:72:VAL:HG23	7:G:76:ILE:HB	1.88	0.54
10:J:218:ASP:OD1	12:Z:164:THR:OG1	2.22	0.54
2:P:179:ASN:OD1	2:P:180:LYS:N	2.41	0.54
12:Z:160:ILE:HG21	12:Z:174:VAL:HG23	1.89	0.54
6:T:34:CYS:SG	6:T:35:ALA:N	2.80	0.54
5:E:82:MET:HA	5:E:82:MET:HE3	1.88	0.54
6:F:7:ASP:OD1	6:F:7:ASP:N	2.39	0.54
10:J:93:LEU:HD23	10:J:137:TYR:HE2	1.73	0.54
5:S:68:LEU:HD11	5:S:78:MET:HE2	1.87	0.54
3:C:17:ARG:C	3:C:18:LEU:HD12	2.32	0.54
8:V:41:LEU:HD11	8:V:129:VAL:HG23	1.90	0.54
4:D:62:LEU:C	4:D:62:LEU:HD23	2.32	0.54
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.88	0.54
12:Z:42:LEU:HD12	12:Z:179:ILE:HD11	1.90	0.54
13:b:220:SER:OG	13:b:221:SER:N	2.40	0.54
5:E:69:SER:OG	5:E:71:ASP:O	2.26	0.54
1:A:192:ARG:NH2	1:A:204:ASP:OD2	2.40	0.54
4:D:63:ILE:CD1	4:D:84:VAL:HG21	2.37	0.54
2:B:38:ILE:HD11	2:B:174:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:226:ASP:O	5:E:228:THR:HG23	2.08	0.54
4:R:63:ILE:CD1	4:R:84:VAL:HG21	2.37	0.54
3:C:76:VAL:HG11	3:C:83:ALA:CB	2.38	0.54
6:F:98:LEU:HD12	6:F:98:LEU:O	2.07	0.54
14:a:114:HIS:NE2	14:a:142:ASP:OD2	2.38	0.54
10:X:139:LEU:HD12	10:X:140:ILE:HD13	1.89	0.54
5:E:52:ARG:HG3	5:E:52:ARG:O	2.08	0.53
5:E:68:LEU:HD13	5:E:78:MET:HE1	1.89	0.53
5:S:91:TYR:CG	5:S:119:LEU:HD22	2.43	0.53
8:V:55:ILE:O	8:V:59:ILE:HG22	2.08	0.53
10:J:189:ASP:O	12:Z:26:ILE:HD11	2.08	0.53
2:B:139:VAL:HG22	2:B:144:TYR:HD1	1.73	0.53
6:F:31:GLN:O	6:F:31:GLN:NE2	2.41	0.53
9:W:79:CYS:O	9:W:83:LEU:HD22	2.09	0.53
13:b:225:GLN:OE1	13:b:226:ILE:N	2.41	0.53
10:X:168:VAL:HG12	10:X:168:VAL:O	2.08	0.53
3:C:186:GLU:OE1	3:C:187:GLU:N	2.41	0.53
1:O:116:ASN:OD1	1:O:117:ALA:N	2.42	0.53
9:W:41:ILE:CG2	9:W:100:LEU:HD21	2.39	0.53
8:V:221:ASP:OD1	8:V:222:ASN:N	2.41	0.53
9:I:17:ASP:OD2	9:I:17:ASP:C	2.52	0.52
3:Q:182:ASP:C	3:Q:182:ASP:OD2	2.52	0.52
4:D:48:LYS:HE2	4:D:48:LYS:HA	1.91	0.52
7:U:97:GLU:OE1	7:U:97:GLU:HA	2.10	0.52
9:I:66:HIS:ND1	9:I:78:MET:HE2	2.24	0.52
8:V:73:LYS:HD2	1:O:73:THR:HG22	1.92	0.52
4:R:11:SER:OG	4:R:13:ASP:OD1	2.27	0.52
2:B:109:GLU:O	2:B:113:ILE:HG12	2.09	0.52
5:S:52:ARG:HG3	5:S:52:ARG:O	2.10	0.52
2:B:14:SER:O	2:B:17:GLY:N	2.33	0.52
5:S:68:LEU:HD11	5:S:78:MET:CE	2.40	0.52
9:W:7:VAL:HG12	9:W:123:PRO:O	2.09	0.52
10:J:168:VAL:HG12	10:J:168:VAL:O	2.10	0.52
2:P:160:ALA:HB1	2:P:174:LEU:HD21	1.92	0.52
5:E:212:LEU:HD21	5:E:241:ILE:HG12	1.91	0.51
7:G:41:GLU:HA	7:G:46:ILE:HD13	1.92	0.51
11:K:59:GLU:OE2	11:K:59:GLU:HA	2.11	0.51
2:P:42:ASN:OD1	2:P:42:ASN:N	2.43	0.51
9:W:64:GLU:OE1	9:W:64:GLU:HA	2.10	0.51
1:A:205:ILE:HG23	1:A:233:ILE:CD1	2.40	0.51
2:B:132:LEU:HD13	2:B:134:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:12:VAL:HG13	9:I:110:LEU:HD11	1.92	0.51
2:P:109:GLU:O	2:P:113:ILE:HG12	2.09	0.51
3:Q:68:ILE:HG23	3:Q:91:ARG:HG3	1.92	0.51
11:K:110:LYS:NZ	11:K:111:ASP:OD1	2.43	0.51
14:M:178:ASP:OD2	10:X:190:ARG:NE	2.43	0.51
6:T:117:GLN:NE2	6:T:121:GLN:OE1	2.43	0.51
1:A:206:ARG:O	1:A:210:ILE:HG12	2.10	0.51
6:F:161:GLY:O	6:F:164:SER:OG	2.18	0.51
5:S:111:SER:HG	14:a:107:HIS:CD2	2.29	0.51
1:A:46:ASN:O	1:A:235:SER:OG	2.22	0.51
1:A:147:ILE:HD11	1:A:241:PHE:HE1	1.75	0.51
14:a:226:ASP:OD1	14:a:227:LYS:N	2.39	0.51
2:B:15:PRO:O	2:B:16:THR:OG1	2.19	0.51
10:J:85:ASP:OD1	10:J:87:GLU:N	2.36	0.51
12:L:26:ILE:HD11	10:X:189:ASP:O	2.10	0.51
12:L:139:LEU:O	12:L:143:TYR:N	2.37	0.51
3:Q:44:ILE:C	3:Q:45:LEU:HD22	2.36	0.51
4:R:70:CYS:SG	4:R:209:LEU:HD12	2.51	0.51
9:I:38:SER:OG	9:I:39:LYS:N	2.45	0.50
8:V:234:THR:HG22	8:V:237:PHE:O	2.12	0.50
13:b:21:ILE:HD11	13:b:117:GLY:HA2	1.92	0.50
7:U:132:ARG:O	6:T:121:GLN:NE2	2.45	0.50
1:A:133:GLN:NE2	2:B:128:ARG:O	2.44	0.50
7:U:60:MET:HE1	6:T:172:GLU:HB3	1.94	0.50
7:G:56:ASP:O	7:G:59:LYS:NZ	2.37	0.50
14:M:113:ILE:HG21	14:M:148:VAL:CG2	2.40	0.50
12:Z:180:HIS:NE2	12:Z:185:ASP:OD2	2.40	0.50
10:X:102:PHE:O	10:X:103:SER:OG	2.19	0.50
2:B:162:CYS:SG	2:B:163:VAL:N	2.84	0.50
4:D:99:ASP:O	4:D:99:ASP:OD2	2.29	0.50
6:F:29:ILE:HD11	6:F:130:VAL:C	2.36	0.50
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.93	0.50
4:D:90:GLU:OE2	4:D:90:GLU:HA	2.11	0.50
7:G:241:LEU:C	7:G:241:LEU:HD23	2.37	0.50
12:L:89:GLN:OE1	12:L:89:GLN:HA	2.12	0.50
12:Z:37:ILE:HD11	12:Z:56:GLU:OE2	2.12	0.50
1:O:202:ASP:OD1	1:O:203:GLU:N	2.45	0.50
1:O:205:ILE:HG23	1:O:233:ILE:CD1	2.42	0.50
2:B:140:ASP:OD1	2:B:140:ASP:N	2.45	0.50
3:Q:37:LEU:HD21	3:Q:175:LEU:HD22	1.94	0.50
11:Y:125:ASP:OD2	11:Y:126:SER:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:191:ASP:OD2	10:J:194:SER:N	2.45	0.49
3:Q:162:THR:HG22	3:Q:163:ALA:N	2.27	0.49
7:U:173:GLU:OE1	7:U:174:MET:N	2.45	0.49
13:b:27:ARG:NH2	13:b:39:ASN:OD1	2.41	0.49
7:U:176:LYS:O	7:U:180:GLU:HG2	2.12	0.49
7:U:213:GLN:N	7:U:213:GLN:OE1	2.44	0.49
4:R:36:LYS:NZ	5:S:60:GLU:OE2	2.31	0.49
13:b:106:ILE:HG22	13:b:106:ILE:O	2.12	0.49
10:J:28:ARG:O	10:J:43:LYS:NZ	2.45	0.49
12:Z:122:GLU:OE1	12:Z:122:GLU:C	2.55	0.49
10:X:84:MET:HE1	10:X:92:MET:SD	2.51	0.49
10:J:87:GLU:HA	10:J:87:GLU:OE1	2.12	0.49
13:N:184:PHE:CD1	9:W:136:ALA:HB2	2.48	0.49
5:E:144:LEU:HD21	5:E:172:ILE:CG2	2.42	0.49
8:H:62:TYR:O	8:H:66:MET:HG2	2.13	0.49
4:R:80:ALA:HB2	4:R:129:ILE:HD12	1.95	0.49
14:a:173:ILE:CD1	14:a:209:ALA:HB2	2.40	0.49
2:B:44:VAL:HG12	2:B:213:ALA:HB3	1.94	0.49
5:E:169:ALA:HB1	5:E:183:LEU:HD13	1.95	0.49
6:T:22:VAL:HG11	6:T:149:ASN:HB3	1.95	0.49
13:N:52:MET:HE3	13:N:53:GLY:O	2.12	0.48
4:R:120:HIS:O	5:S:136:SER:OG	2.22	0.48
1:O:117:ALA:HB3	1:O:156:GLU:OE1	2.13	0.48
6:T:37:ALA:HB2	6:T:133:MET:SD	2.53	0.48
2:P:58:GLU:OE1	2:P:58:GLU:N	2.46	0.48
5:S:226:ASP:O	5:S:228:THR:HG23	2.13	0.48
3:C:76:VAL:HG11	3:C:83:ALA:HB2	1.95	0.48
4:R:168:VAL:O	4:R:172:LEU:HD23	2.13	0.48
9:W:38:SER:OG	9:W:39:LYS:N	2.45	0.48
9:W:144:ASP:OD2	9:W:144:ASP:C	2.56	0.48
5:E:68:LEU:HD12	5:E:68:LEU:N	2.29	0.48
1:A:50:ILE:HD11	1:A:85:SER:HB3	1.95	0.48
14:M:218:ASP:O	14:M:237:LEU:N	2.40	0.48
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.95	0.48
13:b:16:LYS:HA	13:b:21:ILE:HG22	1.95	0.48
7:U:16:SER:OG	7:U:18:ASP:OD1	2.23	0.48
2:B:179:ASN:OD1	2:B:180:LYS:N	2.46	0.48
7:G:93:ARG:O	7:G:93:ARG:HD3	2.14	0.48
13:N:11:SER:O	13:N:42:ARG:NH2	2.46	0.48
13:N:216:ARG:NH1	9:W:135:MET:SD	2.87	0.48
4:R:90:GLU:HA	4:R:90:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:147:ARG:O	10:X:147:ARG:CD	2.61	0.48
6:F:188:LEU:O	6:F:192:LYS:HG2	2.13	0.48
10:J:172:ASP:OD1	10:J:172:ASP:C	2.57	0.48
5:S:71:ASP:OD1	5:S:72:ASP:N	2.40	0.48
11:Y:7:LEU:HD13	11:Y:143:LEU:HD22	1.96	0.48
6:F:29:ILE:HD12	6:F:148:PRO:HG3	1.96	0.48
7:G:213:GLN:OE1	7:G:213:GLN:N	2.46	0.48
10:J:170:ASP:OD2	10:J:170:ASP:C	2.56	0.48
13:b:11:SER:O	13:b:42:ARG:NH2	2.46	0.48
13:b:224:ILE:HD12	13:b:242:LEU:HD13	1.96	0.48
6:T:188:LEU:O	6:T:192:LYS:HG2	2.14	0.48
11:Y:166:GLU:OE2	11:Y:166:GLU:HA	2.14	0.48
9:W:187:ARG:HB3	9:W:188:PRO:CD	2.44	0.48
4:D:227:GLU:C	4:D:227:GLU:OE2	2.57	0.47
2:P:7:SER:O	2:P:7:SER:OG	2.32	0.47
3:Q:21:VAL:HG21	3:Q:153:SER:HB3	1.95	0.47
13:b:89:GLN:OE1	13:b:89:GLN:C	2.58	0.47
9:I:37:ILE:HD11	9:I:43:CYS:SG	2.54	0.47
13:N:106:ILE:O	13:N:106:ILE:HG22	2.13	0.47
2:P:203:LEU:CD2	2:P:208:ILE:HD11	2.41	0.47
10:X:203:LEU:HD12	10:X:204:THR:N	2.30	0.47
8:H:221:ASP:OD1	8:H:222:ASN:N	2.47	0.47
5:S:111:SER:O	5:S:115:LEU:HG	2.15	0.47
14:a:85:MET:O	14:a:89:ILE:HG23	2.14	0.47
5:E:149:ASP:OD2	5:E:149:ASP:N	2.46	0.47
11:Y:114:GLN:N	11:Y:114:GLN:OE1	2.47	0.47
1:A:244:ILE:HG23	1:A:248:GLU:OE1	2.15	0.47
9:I:126:ALA:O	9:I:127:LEU:HD23	2.15	0.47
4:R:46:GLU:OE2	4:R:197:VAL:HG22	2.14	0.47
11:Y:21:SER:HG	11:Y:32:ASP:CG	2.16	0.47
5:E:241:ILE:HA	5:E:244:LEU:HD23	1.97	0.47
13:N:12:VAL:HG12	13:N:25:ALA:HB2	1.96	0.47
3:C:90:SER:OG	3:C:114:ILE:HD11	2.15	0.47
3:C:119:GLN:NE2	4:D:79:ASP:OD2	2.48	0.47
5:E:16:SER:OG	5:E:20:ARG:O	2.31	0.47
5:E:36:THR:OG1	5:E:174:SER:O	2.26	0.47
9:I:136:ALA:HB2	13:b:184:PHE:CD1	2.50	0.47
9:I:187:ARG:HB3	9:I:188:PRO:HD3	1.95	0.47
9:I:215:GLU:OE2	9:I:217:ILE:HD11	2.15	0.47
10:J:7:TYR:OH	11:K:119:ASP:OD1	2.29	0.47
11:K:7:LEU:HD13	11:K:143:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:39:ILE:HG21	11:K:65:VAL:HG11	1.97	0.47
13:N:204:ILE:O	13:N:208:GLU:OE1	2.33	0.47
2:P:128:ARG:O	1:O:133:GLN:NE2	2.48	0.47
4:R:8:THR:CG2	4:R:16:LEU:HD23	2.43	0.47
9:W:48:VAL:HG23	9:W:95:VAL:HG13	1.97	0.47
1:O:137:MET:HE3	1:O:137:MET:HA	1.95	0.47
10:X:47:MET:HE2	10:X:69:LEU:HB3	1.96	0.47
1:A:18:PRO:O	1:A:19:ASP:OD1	2.33	0.47
3:C:144:GLY:O	3:C:146:GLN:NE2	2.48	0.47
7:G:212:LEU:O	7:G:216:VAL:HG12	2.14	0.47
11:K:18:ASP:OD2	11:K:175:GLN:NE2	2.48	0.47
1:O:18:PRO:O	1:O:19:ASP:OD1	2.33	0.47
1:O:35:THR:O	1:O:36:ASN:OD1	2.33	0.47
5:E:201:LEU:HD22	5:E:240:ILE:HG22	1.97	0.47
4:R:73:PHE:HB2	4:R:129:ILE:HD11	1.96	0.47
4:R:206:VAL:CG1	4:R:222:ILE:HD11	2.45	0.47
7:U:90:ILE:HG21	7:U:138:ILE:CD1	2.44	0.47
1:A:118:GLU:HG3	1:A:158:PHE:CZ	2.49	0.47
5:E:244:LEU:C	5:E:244:LEU:HD12	2.40	0.47
1:O:253:LEU:O	1:O:253:LEU:HD23	2.15	0.47
2:B:42:ASN:OD1	2:B:42:ASN:N	2.45	0.46
9:I:42:TRP:O	9:I:100:LEU:HD12	2.15	0.46
4:R:209:LEU:HD23	4:R:210:THR:N	2.30	0.46
13:N:203:ARG:NH2	13:N:237:GLU:OE1	2.48	0.46
4:R:190:LEU:HD22	4:R:225:MET:HB3	1.96	0.46
6:F:37:ALA:HB2	6:F:133:MET:SD	2.55	0.46
7:G:186:ASP:OD2	7:G:186:ASP:N	2.41	0.46
9:I:41:ILE:CG2	9:I:100:LEU:HD11	2.45	0.46
2:P:203:LEU:N	2:P:203:LEU:HD12	2.31	0.46
3:Q:85:ILE:HD11	3:Q:130:TYR:HE1	1.79	0.46
4:R:99:ASP:OD1	4:R:99:ASP:O	2.33	0.46
7:U:241:LEU:C	7:U:241:LEU:HD23	2.40	0.46
8:V:3:ILE:HD11	8:V:45:ARG:O	2.16	0.46
3:C:143:ASP:OD1	3:C:143:ASP:C	2.59	0.46
4:D:196:VAL:O	4:D:196:VAL:CG1	2.63	0.46
7:G:27:ILE:HD11	7:G:133:PRO:HG2	1.98	0.46
2:P:139:VAL:HG22	2:P:144:TYR:HD1	1.80	0.46
3:Q:119:GLN:NE2	3:Q:123:GLN:OE1	2.48	0.46
10:X:21:VAL:HG11	10:X:112:VAL:HG13	1.96	0.46
1:A:16:PHE:O	1:A:17:SER:OG	2.23	0.46
7:G:28:TYR:OH	7:G:155:GLU:OE1	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:69:ASP:OD1	3:Q:70:LYS:N	2.43	0.46
5:S:208:MET:HE1	5:S:212:LEU:HA	1.97	0.46
3:C:186:GLU:O	3:C:190:LEU:HD23	2.16	0.46
8:V:17:ASP:C	8:V:17:ASP:OD2	2.58	0.46
6:T:62:LYS:NZ	6:T:74:MET:O	2.45	0.46
1:A:35:THR:O	1:A:36:ASN:OD1	2.33	0.46
7:G:34:ASN:OD1	7:G:35:ASN:N	2.46	0.46
8:V:62:TYR:O	8:V:66:MET:HG3	2.15	0.46
9:W:159:ILE:HG21	9:W:173:VAL:HG23	1.98	0.46
13:b:154:ILE:HG21	13:b:159:LEU:HD21	1.98	0.46
4:D:31:CYS:SG	4:D:32:ALA:N	2.88	0.46
5:E:144:LEU:HD21	5:E:172:ILE:HG23	1.99	0.46
6:F:98:LEU:HD11	6:F:99:TYR:CE2	2.51	0.46
9:I:35:HIS:HB3	9:I:56:THR:HG21	1.98	0.46
11:Y:113:TYR:C	11:Y:114:GLN:OE1	2.59	0.46
5:E:10:ARG:HB2	5:E:14:THR:HG21	1.98	0.45
5:E:243:VAL:O	5:E:243:VAL:HG12	2.16	0.45
8:H:169:LEU:H	8:H:169:LEU:HD12	1.80	0.45
3:Q:111:VAL:HG12	3:Q:136:ILE:HD13	1.97	0.45
4:R:187:PHE:CZ	4:R:229:ILE:HG22	2.50	0.45
5:S:16:SER:OG	5:S:20:ARG:O	2.32	0.45
5:S:163:THR:O	5:S:163:THR:HG23	2.16	0.45
12:L:160:ILE:HG21	12:L:174:VAL:HG13	1.98	0.45
3:Q:109:GLN:NE2	11:Y:72:ASN:OD1	2.49	0.45
11:Y:13:VAL:HG11	11:Y:105:ALA:HB1	1.98	0.45
3:Q:71:HIS:HB3	3:Q:222:VAL:HG11	1.97	0.45
9:W:59:LEU:HD22	9:W:83:LEU:HD21	1.97	0.45
3:C:82:ASP:N	3:C:82:ASP:OD1	2.49	0.45
12:L:166:ARG:HA	10:X:36:THR:HG22	1.98	0.45
2:P:141:VAL:HG13	2:P:142:TYR:CD1	2.51	0.45
14:a:113:ILE:HG21	14:a:148:VAL:CG2	2.46	0.45
9:W:8:CYS:SG	9:W:9:GLN:N	2.88	0.45
1:O:19:ASP:OD1	1:O:19:ASP:C	2.60	0.45
2:B:45:ILE:HD13	2:B:188:ILE:HG12	1.98	0.45
3:C:17:ARG:O	3:C:18:LEU:HD12	2.16	0.45
7:G:46:ILE:HD12	7:G:151:ILE:HD11	1.98	0.45
2:P:74:ILE:HD11	2:P:134:LEU:HD13	1.99	0.45
4:R:119:THR:O	4:R:119:THR:HG22	2.16	0.45
9:W:76:VAL:HG13	9:W:100:LEU:HD22	1.99	0.45
8:H:10:ASN:ND2	8:H:10:ASN:O	2.50	0.45
1:O:77:ASN:OD1	1:O:77:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:198:LEU:C	6:F:198:LEU:HD23	2.41	0.45
2:P:144:TYR:O	2:P:145:HIS:ND1	2.50	0.45
2:P:223:THR:OG1	2:P:224:GLN:N	2.49	0.45
5:S:36:THR:OG1	5:S:174:SER:O	2.29	0.45
5:S:82:MET:SD	5:S:82:MET:N	2.89	0.45
5:S:199:LEU:O	5:S:202:THR:OG1	2.28	0.45
2:B:70:GLU:O	2:B:70:GLU:HG2	2.17	0.45
3:Q:182:ASP:OD2	3:Q:182:ASP:O	2.35	0.45
9:W:35:HIS:HB3	9:W:56:THR:HG21	1.99	0.45
3:Q:111:VAL:HG11	3:Q:148:TYR:HD1	1.82	0.44
9:W:100:LEU:HD23	9:W:101:GLY:N	2.32	0.44
6:F:11:ILE:HG22	7:G:132:ARG:HB2	1.99	0.44
4:R:96:LEU:HD23	11:Y:63:LYS:HD3	1.98	0.44
7:U:127:LEU:HD23	7:U:127:LEU:N	2.32	0.44
3:Q:13:SER:OG	3:Q:17:ARG:N	2.46	0.44
8:V:128:LEU:HD22	8:V:157:ASP:OD1	2.17	0.44
13:b:163:PHE:HE1	13:b:178:THR:HG22	1.82	0.44
7:U:96:SER:O	7:U:100:THR:HG23	2.17	0.44
6:T:108:LEU:C	6:T:108:LEU:HD23	2.43	0.44
2:P:18:LYS:HB3	2:P:23:GLU:OE2	2.16	0.44
12:Z:38:ASN:OD1	12:Z:39:LYS:N	2.45	0.44
2:B:175:GLU:OE1	2:B:176:LYS:N	2.50	0.44
5:S:84:ASP:OD1	5:S:84:ASP:N	2.49	0.44
12:Z:22:MET:O	12:Z:22:MET:HG3	2.17	0.44
1:A:19:ASP:OD1	1:A:19:ASP:C	2.61	0.44
6:F:22:VAL:HG11	6:F:149:ASN:HB3	1.99	0.44
13:N:57:GLU:OE2	13:N:57:GLU:HA	2.18	0.44
14:a:218:ASP:O	14:a:237:LEU:N	2.46	0.44
1:O:205:ILE:HG23	1:O:233:ILE:HD13	2.00	0.44
1:A:220:LEU:HD13	1:A:222:PHE:CZ	2.53	0.44
3:C:151:ASP:OD2	3:C:151:ASP:C	2.61	0.44
7:G:23:GLN:O	7:G:27:ILE:HG13	2.18	0.44
8:H:128:LEU:HD22	8:H:157:ASP:OD1	2.18	0.44
14:a:113:ILE:HD12	14:a:113:ILE:H	1.81	0.44
2:B:75:VAL:HG22	2:B:76:TYR:N	2.33	0.44
4:D:214:LEU:C	4:D:214:LEU:HD23	2.43	0.44
9:I:30:ASN:OD1	9:I:187:ARG:NH1	2.42	0.44
8:V:189:ILE:HD12	8:V:213:CYS:HB3	1.99	0.44
12:Z:51:ASP:OD2	14:a:128:ARG:NH2	2.41	0.44
7:U:212:LEU:O	7:U:216:VAL:HG12	2.18	0.44
14:M:48:TYR:OH	14:M:198:ASP:OD2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:67:LEU:HD23	5:S:220:CYS:SG	2.58	0.44
5:S:91:TYR:CD1	5:S:91:TYR:C	2.95	0.44
7:G:235:GLU:OE1	7:G:235:GLU:C	2.61	0.43
9:I:187:ARG:HB3	9:I:188:PRO:CD	2.48	0.43
10:J:216:ARG:NH2	12:Z:192:ASP:OD1	2.46	0.43
1:O:67:LEU:HD23	1:O:68:ASP:N	2.33	0.43
7:U:157:ASN:OD1	7:U:158:GLY:N	2.51	0.43
7:U:175:PHE:O	7:U:179:ILE:HG12	2.17	0.43
13:b:55:SER:OG	13:b:178:THR:OG1	2.33	0.43
3:Q:85:ILE:HD11	3:Q:130:TYR:CE1	2.53	0.43
4:R:153:TYR:CD2	4:R:153:TYR:C	2.96	0.43
7:U:60:MET:HB2	6:T:155:TYR:HD1	1.83	0.43
4:D:78:ALA:O	4:D:82:VAL:HG13	2.18	0.43
4:R:136:PHE:CE1	4:R:142:ILE:HD13	2.53	0.43
8:V:40:ASN:ND2	8:V:156:TYR:O	2.52	0.43
1:O:19:ASP:OD1	1:O:21:ASN:ND2	2.51	0.43
2:B:95:ILE:HG23	9:I:61:HIS:HB3	2.01	0.43
2:B:160:ALA:O	3:C:55:LEU:HD13	2.19	0.43
7:G:87:ALA:O	7:G:91:ILE:HG12	2.18	0.43
2:P:36:LEU:HD13	2:P:38:ILE:HD11	2.00	0.43
3:Q:44:ILE:O	3:Q:45:LEU:HD22	2.18	0.43
3:Q:186:GLU:OE2	3:Q:186:GLU:C	2.62	0.43
6:T:161:GLY:O	6:T:164:SER:OG	2.20	0.43
10:X:26:ASP:OD2	10:X:26:ASP:C	2.61	0.43
11:Y:65:VAL:HG13	11:Y:76:MET:HE3	2.00	0.43
13:N:49:LYS:C	13:N:50:THR:HG1	2.18	0.43
3:C:193:LEU:HD21	3:C:232:ILE:HD11	2.01	0.43
9:I:31:CYS:SG	9:I:32:SER:N	2.91	0.43
3:Q:38:ILE:HD11	3:Q:145:TYR:CB	2.48	0.43
3:C:35:ILE:HG22	3:C:36:GLY:N	2.34	0.43
4:D:80:ALA:O	4:D:84:VAL:HG23	2.19	0.43
4:D:131:THR:HG1	4:D:147:THR:HG1	1.67	0.43
6:F:80:ASP:OD1	6:F:80:ASP:N	2.50	0.43
12:L:125:LEU:HD23	12:L:125:LEU:C	2.44	0.43
13:N:128:ASP:OD1	13:N:129:ASN:N	2.51	0.43
14:M:173:ILE:HD11	14:M:205:ALA:O	2.18	0.43
3:Q:193:LEU:C	3:Q:193:LEU:HD23	2.43	0.43
11:Y:22:ILE:HD13	11:Y:22:ILE:N	2.33	0.43
11:Y:121:LEU:C	11:Y:122:SER:HG	2.18	0.43
1:A:79:THR:HG22	1:A:80:ASP:N	2.33	0.43
5:S:68:LEU:HD12	5:S:68:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:60:THR:HG23	10:X:61:ASP:N	2.34	0.43
1:A:117:ALA:HB3	1:A:156:GLU:OE2	2.19	0.43
7:G:69:ILE:HG21	7:G:219:SER:OG	2.18	0.43
7:G:94:ALA:HB2	7:G:118:ILE:HD11	2.01	0.43
4:D:230:ASP:O	4:D:234:THR:HG22	2.18	0.42
2:P:19:LEU:HB3	2:P:22:ILE:HD12	2.01	0.42
5:S:237:ILE:O	5:S:241:ILE:HG22	2.19	0.42
7:U:56:ASP:O	7:U:59:LYS:NZ	2.46	0.42
7:U:87:ALA:O	7:U:91:ILE:HG12	2.19	0.42
10:X:139:LEU:HD12	10:X:140:ILE:CD1	2.49	0.42
1:A:94:LEU:HG	7:G:120:LEU:HD21	2.00	0.42
3:C:46:GLY:HA2	3:C:212:LEU:HD23	2.01	0.42
8:H:119:GLU:OE1	8:H:119:GLU:C	2.62	0.42
8:H:189:ILE:O	8:H:190:GLN:C	2.63	0.42
8:V:18:SER:OG	8:V:227:LEU:HD23	2.19	0.42
1:A:132:THR:HG22	1:A:139:LEU:HD21	2.01	0.42
1:A:223:ASP:OD1	1:A:223:ASP:C	2.62	0.42
6:F:102:ASN:OD1	6:F:102:ASN:N	2.52	0.42
2:P:208:ILE:HG22	2:P:209:GLU:N	2.33	0.42
9:W:7:VAL:O	9:W:7:VAL:HG13	2.19	0.42
10:X:21:VAL:HG12	10:X:22:ALA:N	2.34	0.42
3:Q:76:VAL:HG21	3:Q:83:ALA:HB1	2.01	0.42
5:S:119:LEU:HD12	5:S:119:LEU:O	2.19	0.42
1:O:16:PHE:O	1:O:17:SER:OG	2.24	0.42
7:U:179:ILE:N	7:U:179:ILE:HD13	2.34	0.42
11:Y:152:THR:N	11:Y:155:GLU:OE2	2.51	0.42
1:A:145:MET:CG	1:A:174:ILE:HD12	2.50	0.42
2:B:82:ASP:HB2	2:B:132:LEU:HD23	2.02	0.42
5:E:72:ASP:O	5:E:229:PHE:N	2.39	0.42
8:H:40:ASN:ND2	8:H:156:TYR:O	2.52	0.42
10:J:44:ILE:HD11	10:J:199:GLU:OE2	2.19	0.42
12:L:50:ALA:N	14:M:157:SER:OG	2.53	0.42
4:R:34:ALA:O	4:R:35:ILE:HD13	2.19	0.42
5:S:68:LEU:HD12	5:S:68:LEU:N	2.34	0.42
9:I:8:CYS:SG	9:I:9:GLN:N	2.93	0.42
2:P:39:ARG:NH2	3:Q:57:ASP:OD2	2.52	0.42
2:P:56:LEU:HD13	1:O:171:ALA:O	2.20	0.42
3:Q:68:ILE:HD12	3:Q:68:ILE:N	2.34	0.42
7:U:23:GLN:O	7:U:27:ILE:HG13	2.19	0.42
6:F:133:MET:O	6:F:133:MET:HG2	2.19	0.42
2:P:102:GLY:O	2:P:103:SER:OG	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:51:ASP:OD1	14:a:128:ARG:NE	2.51	0.42
4:D:83:LEU:CD2	4:D:129:ILE:HD11	2.50	0.42
7:G:81:SER:O	7:G:81:SER:OG	2.37	0.42
4:R:227:GLU:CD	4:R:227:GLU:C	2.88	0.42
2:B:199:TYR:CB	2:B:203:LEU:HD11	2.51	0.41
6:F:11:ILE:HG21	6:F:123:SER:HB2	2.01	0.41
9:I:78:MET:O	9:I:82:ARG:HG2	2.20	0.41
10:J:201:LEU:HD12	10:J:208:ILE:HD11	2.01	0.41
12:L:4:LEU:HD11	12:L:139:LEU:HD11	1.96	0.41
14:M:59:LEU:O	14:M:60:SER:C	2.63	0.41
3:Q:35:ILE:HG22	3:Q:36:GLY:N	2.35	0.41
9:W:78:MET:O	9:W:82:ARG:HG2	2.20	0.41
10:X:112:VAL:HG22	10:X:134:LEU:HD22	2.02	0.41
5:E:243:VAL:O	5:E:243:VAL:CG1	2.68	0.41
10:J:36:THR:HG22	12:Z:166:ARG:HA	2.01	0.41
9:W:174:ASP:OD1	9:W:187:ARG:O	2.39	0.41
14:a:49:VAL:HG22	14:a:225:ILE:HB	2.01	0.41
1:O:147:ILE:HD11	1:O:241:PHE:HE1	1.85	0.41
7:G:218:PHE:HB3	7:G:232:ILE:HD12	2.00	0.41
3:Q:86:LEU:HD22	3:Q:117:ILE:HD11	2.02	0.41
3:Q:111:VAL:HG11	3:Q:148:TYR:CD1	2.56	0.41
12:Z:144:ASP:OD1	12:Z:145:TYR:N	2.54	0.41
2:B:149:ILE:HG22	2:B:150:ASP:N	2.35	0.41
2:B:189:HIS:O	2:B:193:LEU:HD23	2.20	0.41
6:F:91:GLU:OE2	6:F:91:GLU:HA	2.21	0.41
10:J:26:ASP:OD2	10:J:26:ASP:C	2.63	0.41
9:W:80:VAL:O	9:W:84:THR:HG23	2.21	0.41
10:X:13:LEU:HD13	10:X:151:VAL:HG12	2.02	0.41
1:O:67:LEU:HD23	1:O:67:LEU:C	2.45	0.41
1:A:50:ILE:HD11	1:A:85:SER:CB	2.50	0.41
1:A:181:SER:HB2	1:A:219:ILE:HD12	2.02	0.41
7:G:12:VAL:O	7:G:12:VAL:HG22	2.20	0.41
8:H:17:ASP:OD1	8:H:17:ASP:C	2.63	0.41
10:J:59:ALA:HB3	11:K:123:ASN:HD22	1.86	0.41
2:P:44:VAL:HG11	2:P:137:CYS:HB2	2.02	0.41
7:U:218:PHE:HB3	7:U:232:ILE:HD12	2.01	0.41
10:X:162:MET:HE3	10:X:166:LEU:HD22	2.01	0.41
1:A:94:LEU:O	1:A:97:VAL:HG22	2.20	0.41
5:E:82:MET:O	5:E:86:ARG:HG2	2.20	0.41
3:Q:68:ILE:HD12	3:Q:68:ILE:H	1.84	0.41
8:V:16:CYS:SG	8:V:34:ILE:HD12	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:201:LEU:C	7:U:201:LEU:HD23	2.46	0.41
9:I:7:VAL:HG23	9:I:7:VAL:O	2.20	0.41
9:I:147:THR:HG22	9:I:148:ILE:N	2.36	0.41
10:J:146:THR:O	10:J:147:ARG:HB3	2.21	0.41
9:W:79:CYS:O	9:W:83:LEU:CD2	2.68	0.41
10:X:136:ALA:HB2	10:X:150:VAL:HG23	2.01	0.41
1:A:231:VAL:HG22	1:A:249:ILE:HD11	2.03	0.41
3:C:68:ILE:HG21	3:C:110:LEU:HD11	2.02	0.41
5:E:66:LYS:O	5:E:67:LEU:HD12	2.21	0.41
6:F:13:TYR:OH	7:G:132:ARG:NH1	2.54	0.41
14:M:38:GLY:HA2	14:M:54:ASP:OD2	2.20	0.41
2:P:199:TYR:HB3	2:P:203:LEU:HD11	2.02	0.41
3:Q:17:ARG:O	3:Q:18:LEU:HB2	2.19	0.41
4:R:80:ALA:O	4:R:84:VAL:HG23	2.21	0.41
9:W:9:GLN:O	9:W:10:ASN:OD1	2.39	0.41
9:W:42:TRP:HB2	9:W:178:ILE:HD11	2.03	0.41
14:a:44:THR:CG2	14:a:149:LEU:HD13	2.47	0.41
14:a:59:LEU:O	14:a:60:SER:C	2.63	0.41
7:U:173:GLU:C	7:U:173:GLU:CD	2.89	0.41
6:T:185:GLU:OE1	6:T:185:GLU:N	2.47	0.41
11:Y:12:PHE:CD1	11:Y:12:PHE:C	2.98	0.41
5:E:42:VAL:HG11	5:E:196:ALA:HB2	2.02	0.41
12:L:63:ILE:HD12	12:L:74:ILE:HD13	2.03	0.41
5:S:72:ASP:O	5:S:229:PHE:N	2.39	0.41
6:T:167:SER:OG	6:T:197:SER:HB2	2.21	0.41
1:A:96:MET:HE2	1:A:96:MET:HB2	1.98	0.40
4:D:8:THR:O	4:D:8:THR:HG23	2.20	0.40
4:D:44:ALA:HB2	4:D:206:VAL:HG23	2.03	0.40
4:D:63:ILE:HD11	4:D:84:VAL:HG21	2.03	0.40
6:F:68:ASP:O	6:F:69:TYR:HB2	2.21	0.40
8:H:16:CYS:SG	8:H:34:ILE:HD12	2.61	0.40
9:I:41:ILE:HG22	9:I:100:LEU:HD11	2.03	0.40
3:Q:38:ILE:HG22	3:Q:160:PHE:O	2.21	0.40
5:S:91:TYR:CD2	5:S:119:LEU:HD22	2.56	0.40
8:V:172:SER:OG	13:b:58:LEU:HD23	2.21	0.40
1:A:115:VAL:HG22	1:A:116:ASN:N	2.36	0.40
3:C:114:ILE:O	3:C:117:ILE:HG22	2.21	0.40
5:E:71:ASP:OD2	5:E:72:ASP:N	2.49	0.40
5:E:85:ALA:O	5:E:89:ILE:HG12	2.20	0.40
10:J:21:VAL:HG12	10:J:22:ALA:N	2.37	0.40
10:J:47:MET:HE2	10:J:69:LEU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:164:PHE:HB3	11:K:195:VAL:HG21	2.02	0.40
1:O:220:LEU:HD23	1:O:220:LEU:HA	1.96	0.40
7:U:88:ARG:O	7:U:92:ASP:OD1	2.38	0.40
4:D:80:ALA:HA	4:D:129:ILE:HD13	2.03	0.40
5:E:111:SER:O	5:E:115:LEU:HG	2.21	0.40
6:F:138:HIS:O	6:F:139:ASN:CG	2.65	0.40
7:G:220:TRP:CD1	7:G:220:TRP:C	2.99	0.40
9:I:7:VAL:HG22	9:I:123:PRO:O	2.20	0.40
9:I:80:VAL:O	9:I:81:SER:C	2.65	0.40
9:I:138:LEU:O	9:I:142:TYR:N	2.51	0.40
10:J:203:LEU:HD23	10:J:203:LEU:H	1.86	0.40
12:L:65:ILE:HD13	12:L:65:ILE:HA	1.95	0.40
13:N:46:ILE:HG21	13:N:68:LEU:HB3	2.04	0.40
14:M:101:GLN:O	14:M:104:VAL:HG12	2.21	0.40
14:M:203:LYS:O	14:M:206:ILE:HG22	2.21	0.40
3:Q:117:ILE:HG13	3:Q:118:LYS:N	2.35	0.40
4:R:31:CYS:SG	4:R:32:ALA:N	2.94	0.40
4:R:178:GLU:N	4:R:178:GLU:CD	2.80	0.40
8:V:111:VAL:O	8:V:112:THR:C	2.65	0.40
9:W:45:GLY:C	9:W:52:LEU:HD21	2.46	0.40
7:U:216:VAL:O	7:U:216:VAL:HG13	2.21	0.40
11:Y:120:TYR:CZ	11:Y:121:LEU:HD11	2.57	0.40
10:J:60:THR:HG23	10:J:61:ASP:N	2.36	0.40
12:Z:4:LEU:HD13	12:Z:139:LEU:HD11	1.97	0.40
13:b:12:VAL:HG12	13:b:25:ALA:HB2	2.03	0.40
11:Y:188:VAL:O	11:Y:188:VAL:HG23	2.21	0.40
4:D:119:THR:O	4:D:119:THR:CG2	2.69	0.40
4:D:178:GLU:N	4:D:178:GLU:CD	2.80	0.40
6:F:121:GLN:NE2	7:G:132:ARG:O	2.54	0.40
9:I:9:GLN:O	9:I:10:ASN:OD1	2.40	0.40
2:P:160:ALA:O	3:Q:55:LEU:HD13	2.22	0.40
14:a:73:LYS:O	14:a:97:GLN:NE2	2.55	0.40
7:U:81:SER:O	7:U:81:SER:OG	2.33	0.40
7:U:220:TRP:CD1	7:U:220:TRP:C	2.99	0.40
6:T:187:ILE:HG23	6:T:211:LEU:HD21	2.03	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	A	242/260 (93%)	234 (97%)	8 (3%)	0	100	100
1	O	242/260 (93%)	234 (97%)	8 (3%)	0	100	100
2	B	225/235 (96%)	218 (97%)	7 (3%)	0	100	100
2	P	225/235 (96%)	214 (95%)	11 (5%)	0	100	100
3	C	238/246 (97%)	231 (97%)	7 (3%)	0	100	100
3	Q	238/246 (97%)	231 (97%)	7 (3%)	0	100	100
4	D	231/241 (96%)	228 (99%)	3 (1%)	0	100	100
4	R	231/241 (96%)	226 (98%)	5 (2%)	0	100	100
5	E	227/256 (89%)	220 (97%)	7 (3%)	0	100	100
5	S	227/256 (89%)	218 (96%)	9 (4%)	0	100	100
6	F	228/254 (90%)	215 (94%)	13 (6%)	0	100	100
6	T	228/254 (90%)	215 (94%)	13 (6%)	0	100	100
7	G	243/252 (96%)	238 (98%)	5 (2%)	0	100	100
7	U	243/252 (96%)	237 (98%)	6 (2%)	0	100	100
8	H	198/252 (79%)	191 (96%)	7 (4%)	0	100	100
8	V	198/252 (79%)	190 (96%)	8 (4%)	0	100	100
9	I	207/229 (90%)	191 (92%)	16 (8%)	0	100	100
9	W	207/229 (90%)	194 (94%)	13 (6%)	0	100	100
10	J	204/218 (94%)	192 (94%)	12 (6%)	0	100	100
10	X	204/218 (94%)	193 (95%)	11 (5%)	0	100	100
11	K	193/195 (99%)	186 (96%)	7 (4%)	0	100	100
11	Y	193/195 (99%)	186 (96%)	7 (4%)	0	100	100
12	L	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
12	Z	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
13	N	226/302 (75%)	216 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	b	226/302 (75%)	218 (96%)	8 (4%)	0	100	100
14	M	210/240 (88%)	203 (97%)	6 (3%)	1 (0%)	25	58
14	a	210/240 (88%)	203 (97%)	6 (3%)	1 (0%)	25	58
All	All	6162/6782 (91%)	5925 (96%)	235 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	M	189	LYS
14	a	189	LYS

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	192/231 (83%)	192 (100%)	0	100	100
1	O	192/231 (83%)	192 (100%)	0	100	100
2	B	167/205 (82%)	166 (99%)	1 (1%)	84	91
2	P	167/205 (82%)	167 (100%)	0	100	100
3	C	171/213 (80%)	170 (99%)	1 (1%)	84	91
3	Q	171/213 (80%)	170 (99%)	1 (1%)	84	91
4	D	175/207 (84%)	173 (99%)	2 (1%)	70	84
4	R	175/207 (84%)	174 (99%)	1 (1%)	84	91
5	E	178/223 (80%)	178 (100%)	0	100	100
5	S	178/223 (80%)	178 (100%)	0	100	100
6	F	181/227 (80%)	181 (100%)	0	100	100
6	T	181/227 (80%)	180 (99%)	1 (1%)	84	91
7	G	211/229 (92%)	211 (100%)	0	100	100
7	U	211/229 (92%)	211 (100%)	0	100	100
8	H	175/231 (76%)	174 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	175/231 (76%)	174 (99%)	1 (1%)	84	91
9	I	160/194 (82%)	160 (100%)	0	100	100
9	W	160/194 (82%)	160 (100%)	0	100	100
10	J	174/191 (91%)	173 (99%)	1 (1%)	84	91
10	X	174/191 (91%)	174 (100%)	0	100	100
11	K	165/174 (95%)	165 (100%)	0	100	100
11	Y	165/174 (95%)	165 (100%)	0	100	100
12	L	170/176 (97%)	170 (100%)	0	100	100
12	Z	170/176 (97%)	170 (100%)	0	100	100
13	N	194/266 (73%)	192 (99%)	2 (1%)	73	86
13	b	194/266 (73%)	194 (100%)	0	100	100
14	M	184/216 (85%)	184 (100%)	0	100	100
14	a	184/216 (85%)	184 (100%)	0	100	100
All	All	4994/5966 (84%)	4982 (100%)	12 (0%)	91	96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	70	GLU
3	C	92	LEU
4	D	96	LEU
4	D	148	GLU
8	H	146	PHE
10	J	139	LEU
13	N	72	ASN
13	N	208	GLU
3	Q	121	TYR
4	R	63	ILE
8	V	241	PHE
6	T	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	140	HIS

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Mol	Chain	Res	Type
1	A	243	GLN
2	B	148	GLN
4	D	39	ASN
5	E	106	ASN
5	E	227	GLN
6	F	31	GLN
6	F	174	ASN
7	G	123	HIS
8	H	10	ASN
8	H	51	HIS
8	H	61	HIS
8	H	143	ASN
8	H	168	ASN
9	I	73	GLN
9	I	85	GLN
10	J	8	ASN
10	J	63	GLN
10	J	118	HIS
11	K	123	ASN
12	L	106	HIS
13	N	38	GLN
13	N	65	HIS
14	M	101	GLN
2	P	71	HIS
3	Q	100	ASN
4	R	39	ASN
4	R	164	ASN
5	S	23	GLN
5	S	97	ASN
8	V	61	HIS
8	V	219	HIS
9	W	114	HIS
12	Z	106	HIS
13	b	65	HIS
1	O	53	GLN
7	U	54	ASN
7	U	112	HIS
6	T	117	GLN
6	T	174	ASN
6	T	176	HIS
10	X	63	GLN
11	Y	56	GLN

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Mol	Chain	Res	Type
11	Y	177	ASN
11	Y	186	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

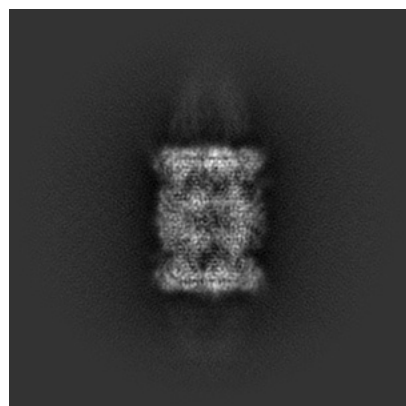
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72400. These allow visual inspection of the internal detail of the map and identification of artifacts.

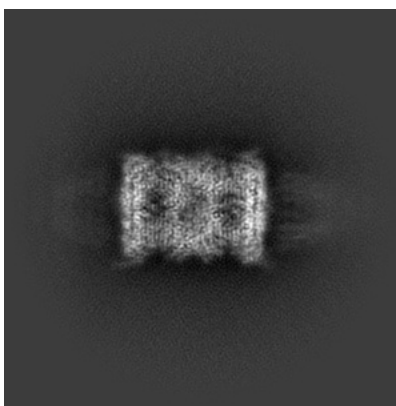
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

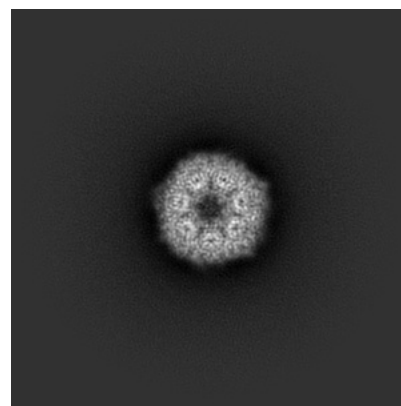
6.1.1 Primary map



X

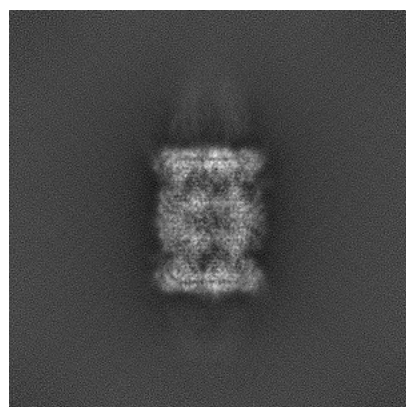


Y

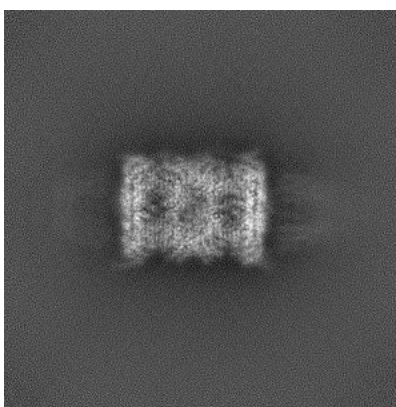


Z

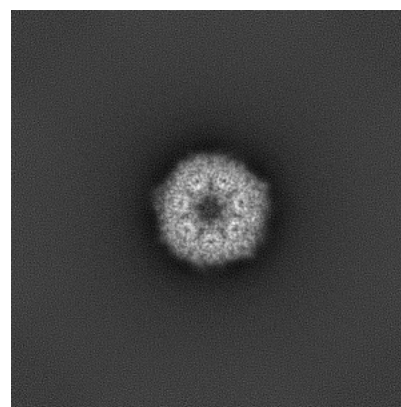
6.1.2 Raw map



X



Y

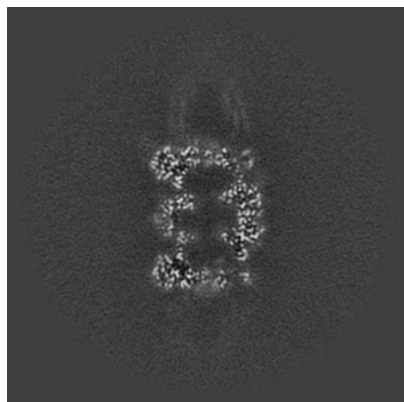


Z

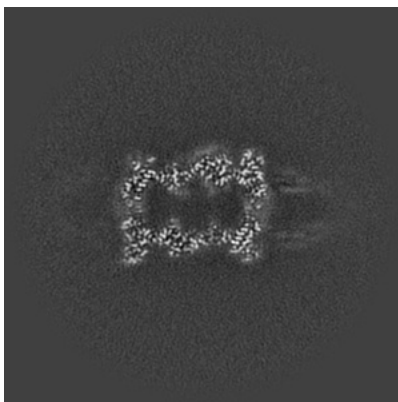
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

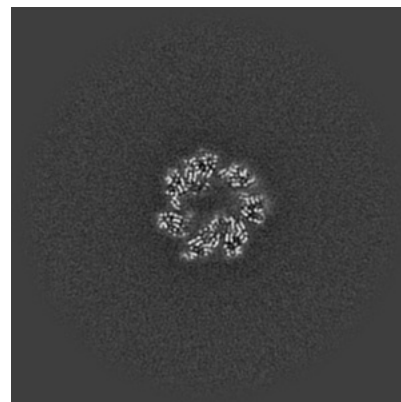
6.2.1 Primary map



X Index: 200

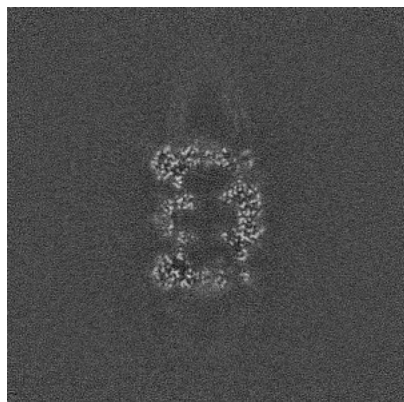


Y Index: 200

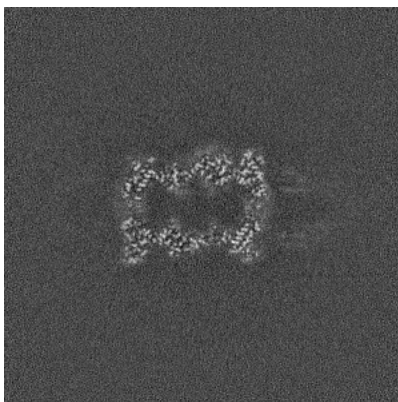


Z Index: 200

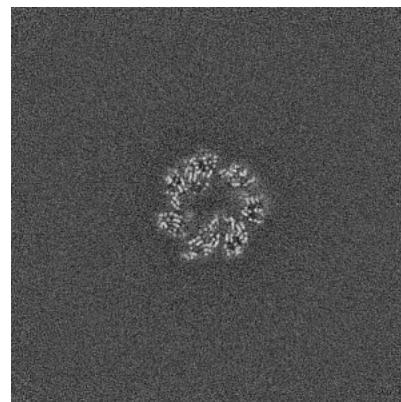
6.2.2 Raw map



X Index: 200



Y Index: 200

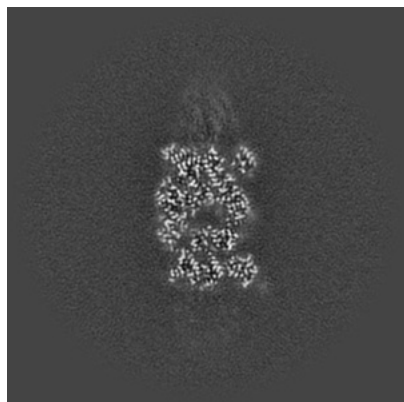


Z Index: 200

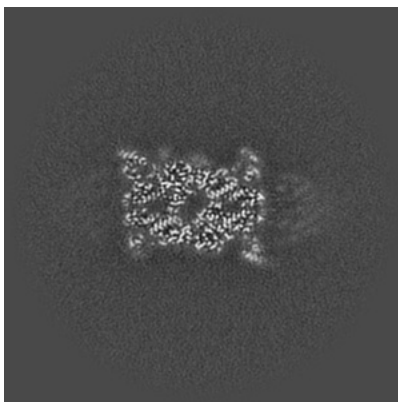
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

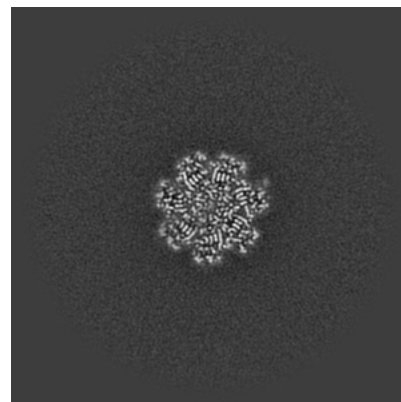
6.3.1 Primary map



X Index: 223

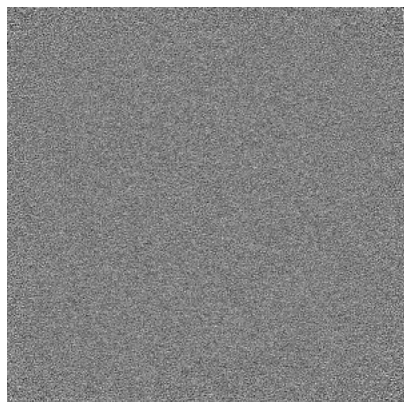


Y Index: 222

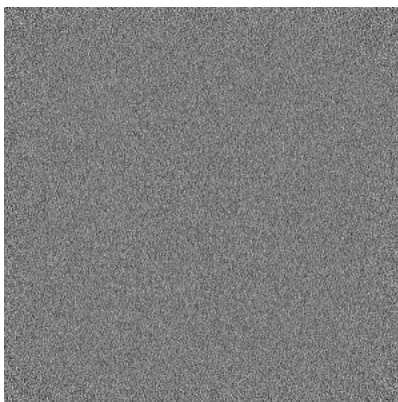


Z Index: 244

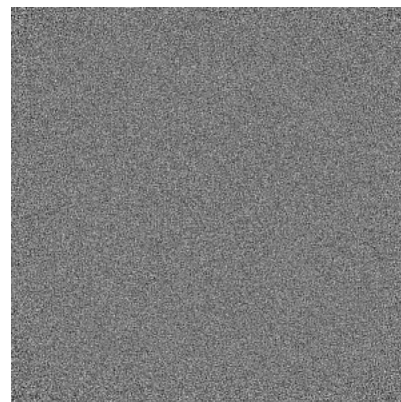
6.3.2 Raw map



X Index: 0



Y Index: 0

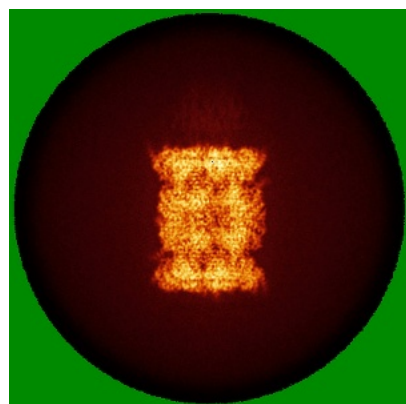


Z Index: 0

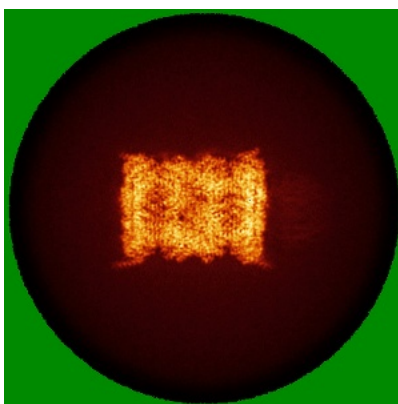
The images above show the largest variance slices of the map in three orthogonal directions.

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

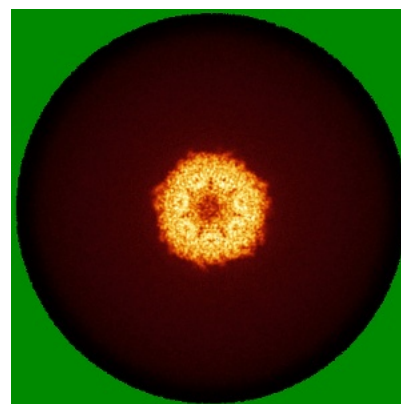
6.4.1 Primary map



X

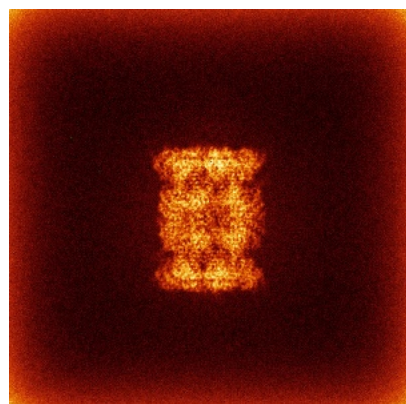


Y

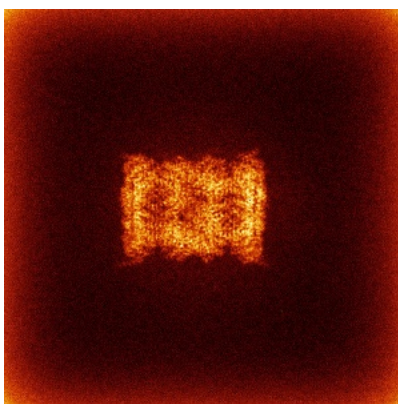


Z

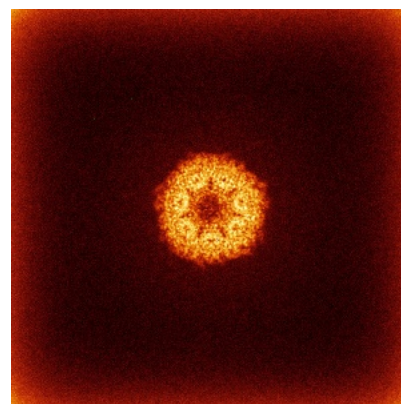
6.4.2 Raw map



X



Y

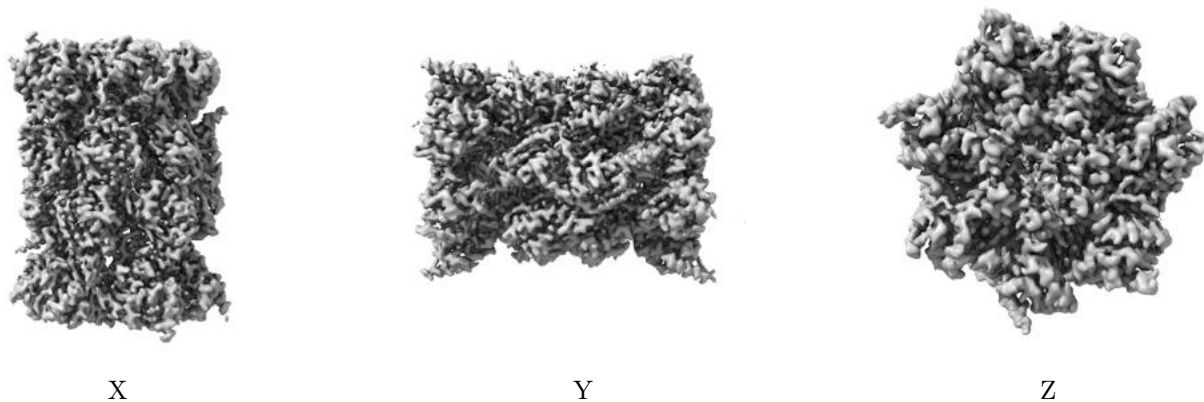


Z

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.

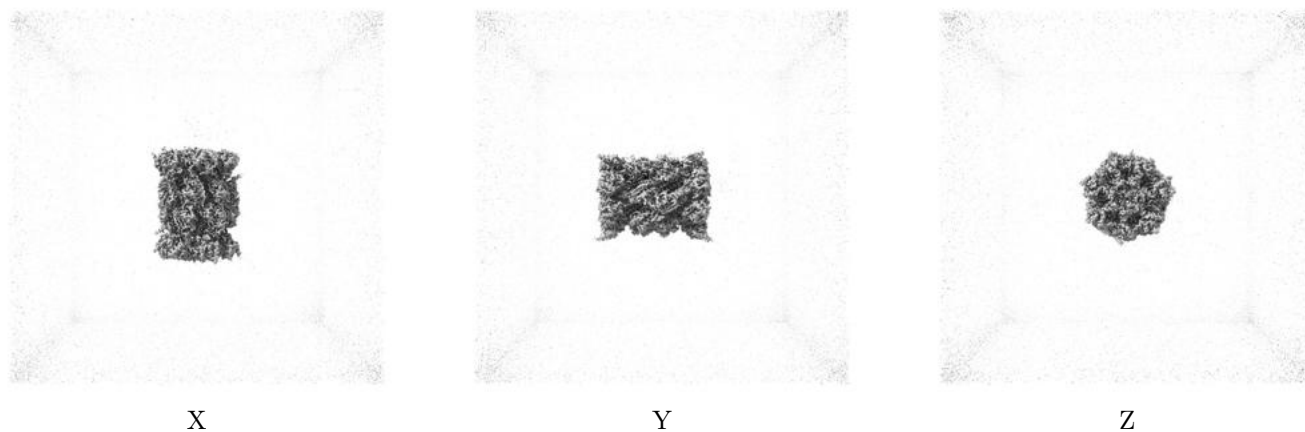
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

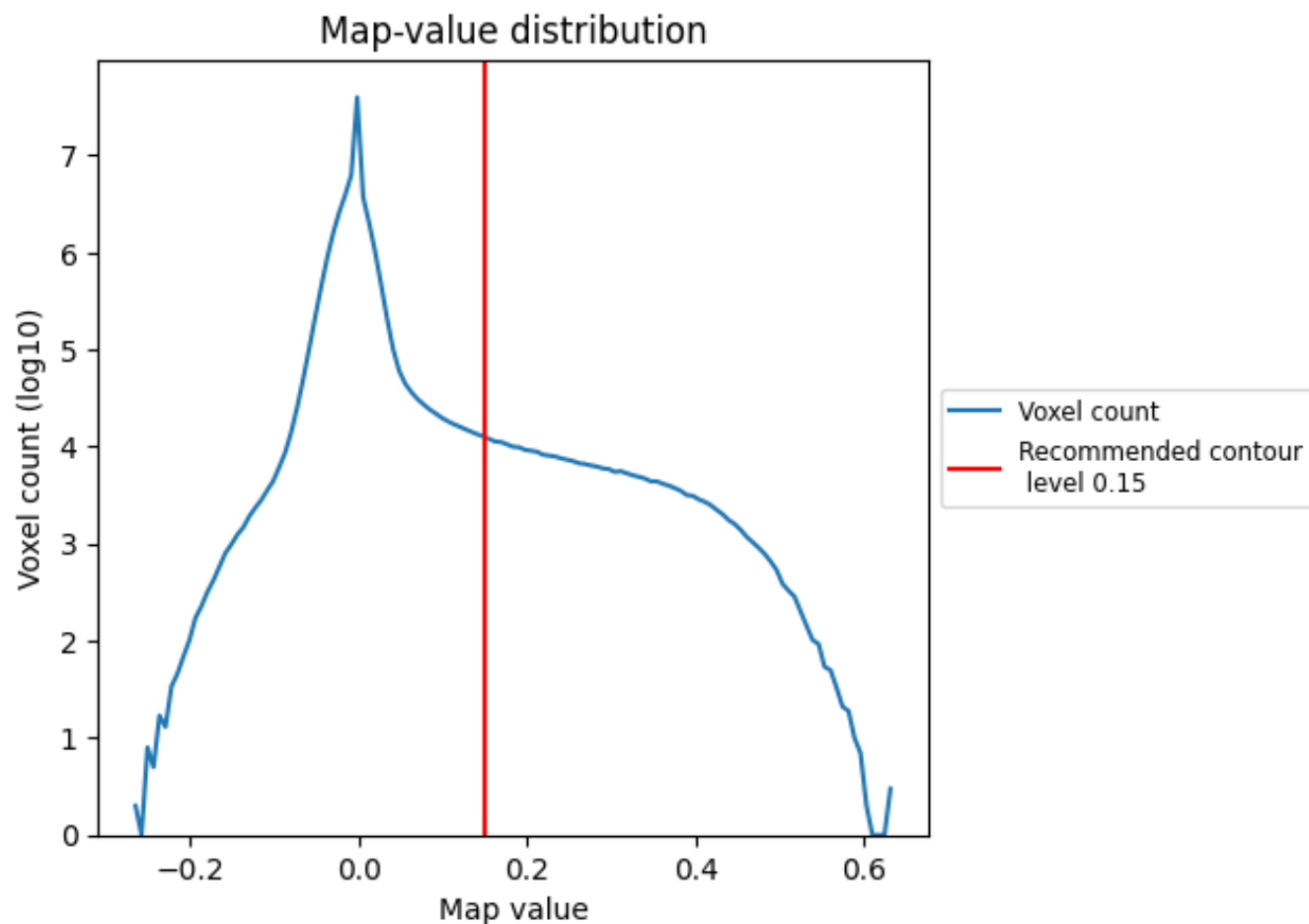
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

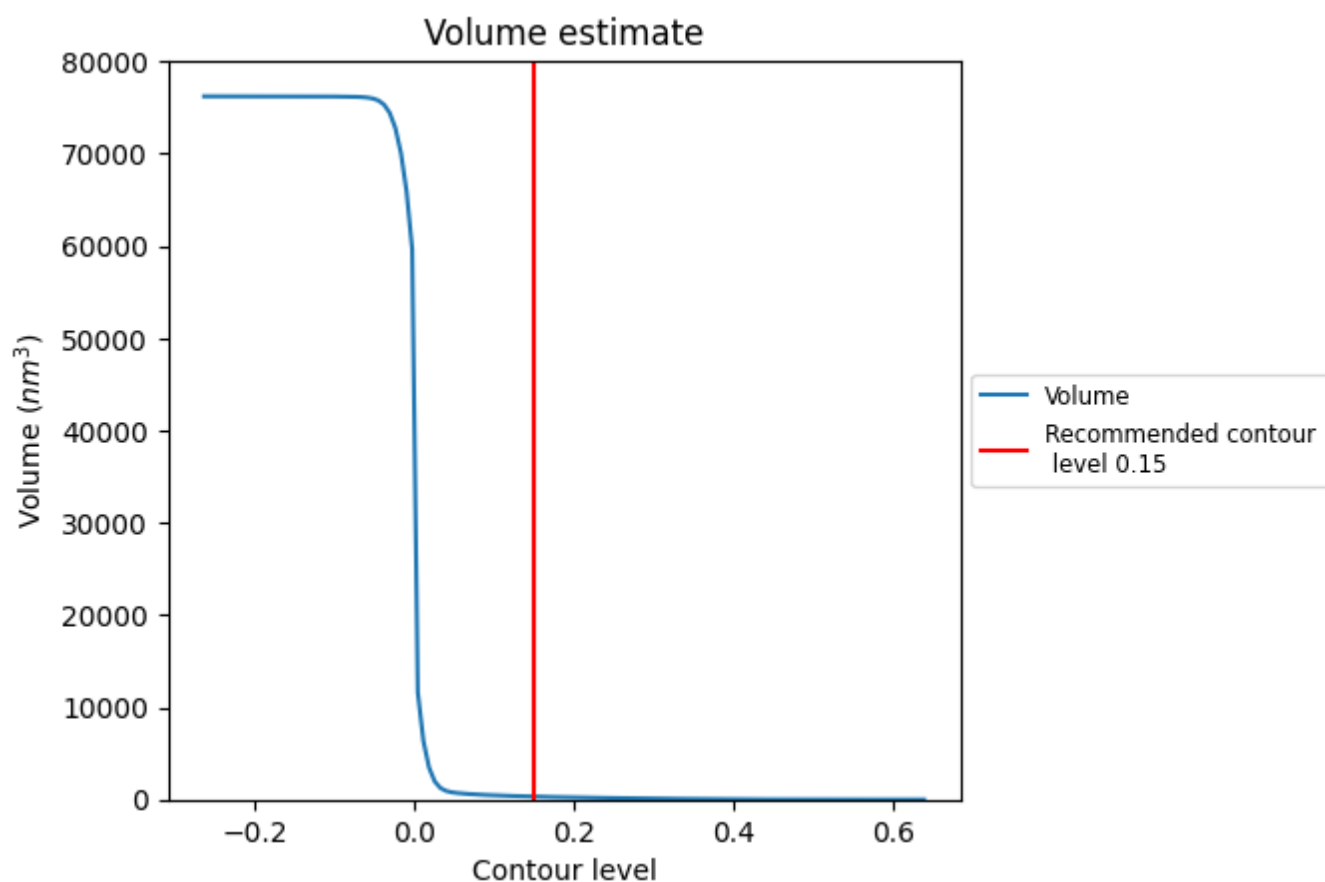
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

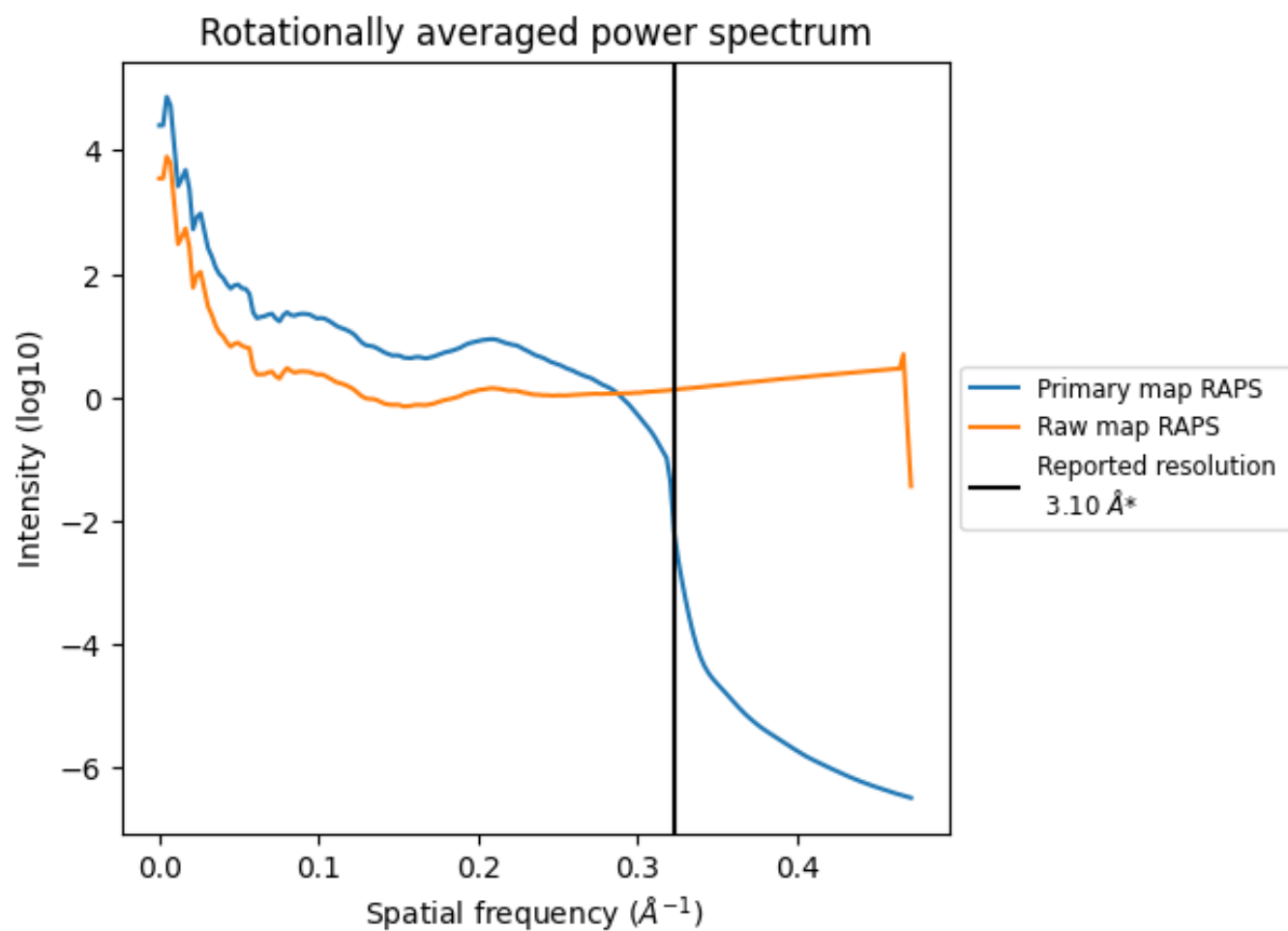
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 323 nm³; this corresponds to an approximate mass of 292 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 ⓘ

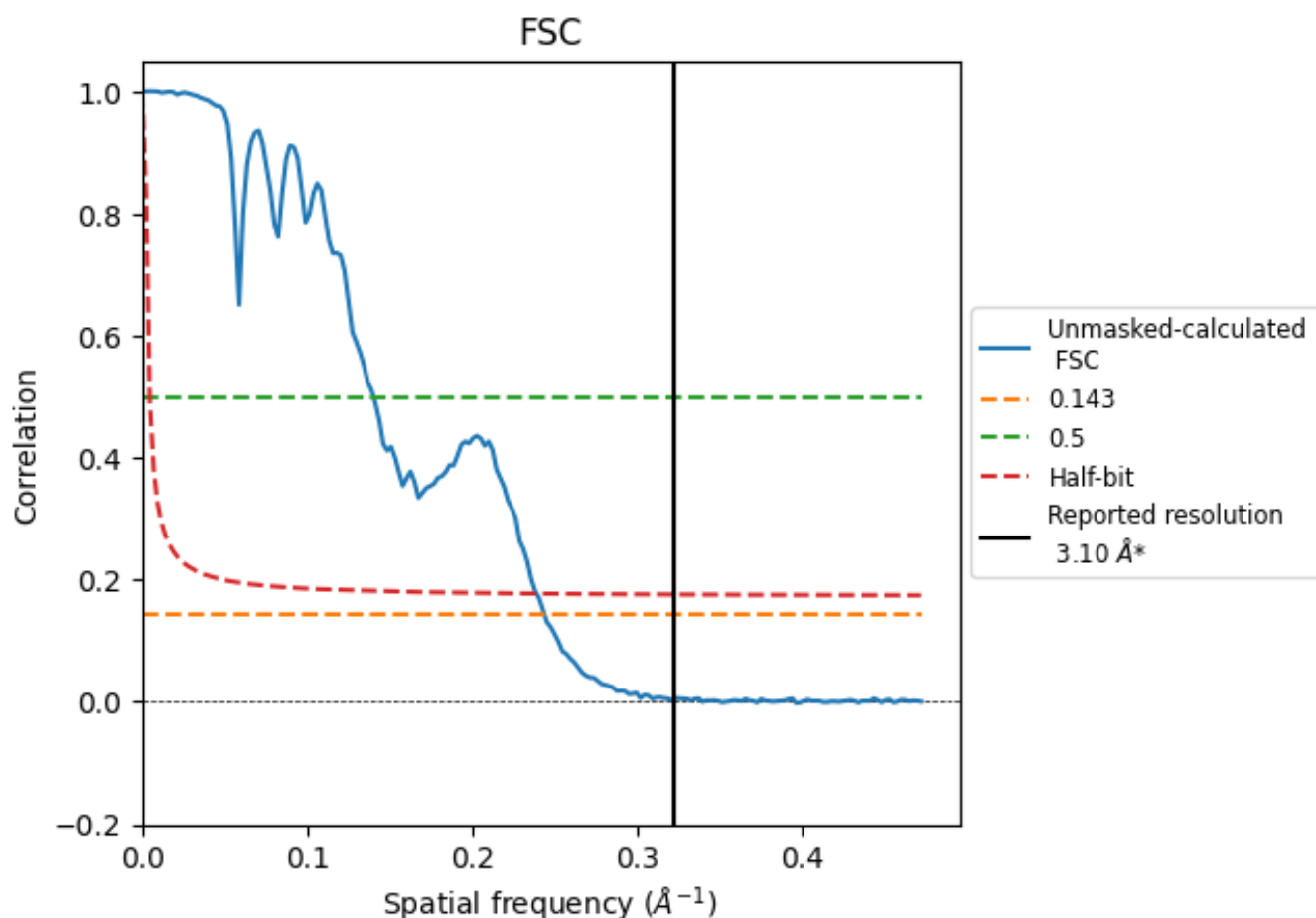


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

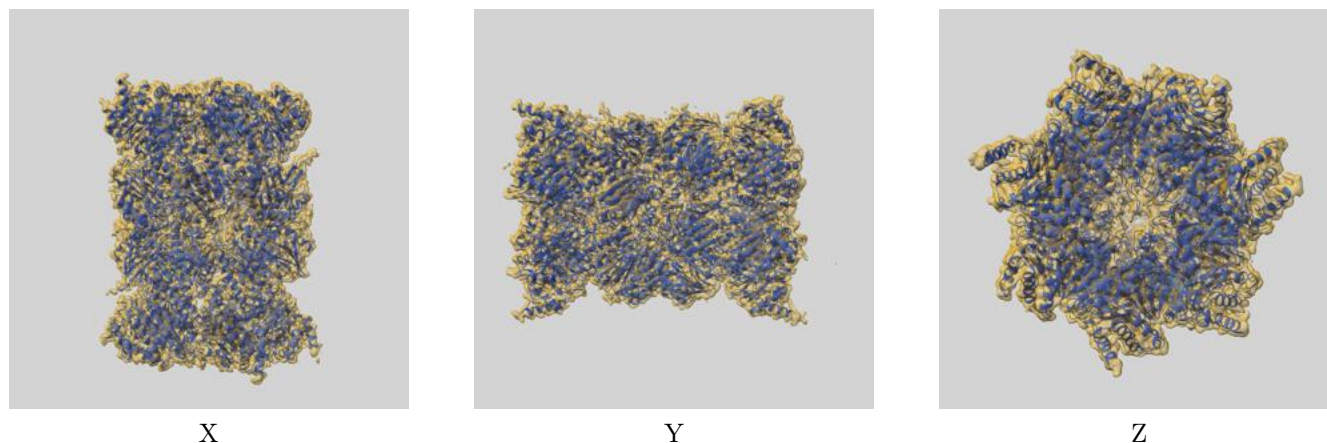
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.10	7.13	4.18

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

9 Map-model fit [i](#)

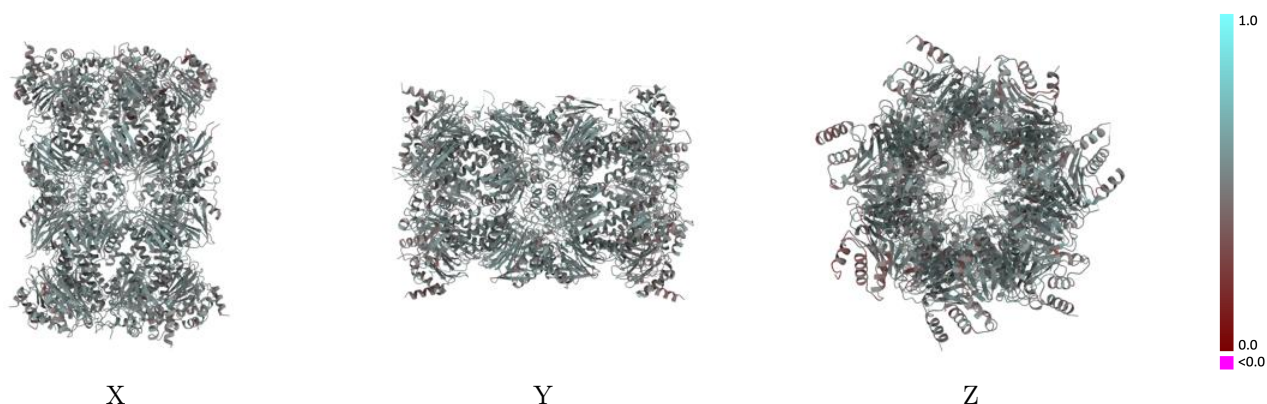
This section contains information regarding the fit between EMDB map EMD-72400 and PDB model 9Y1O. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



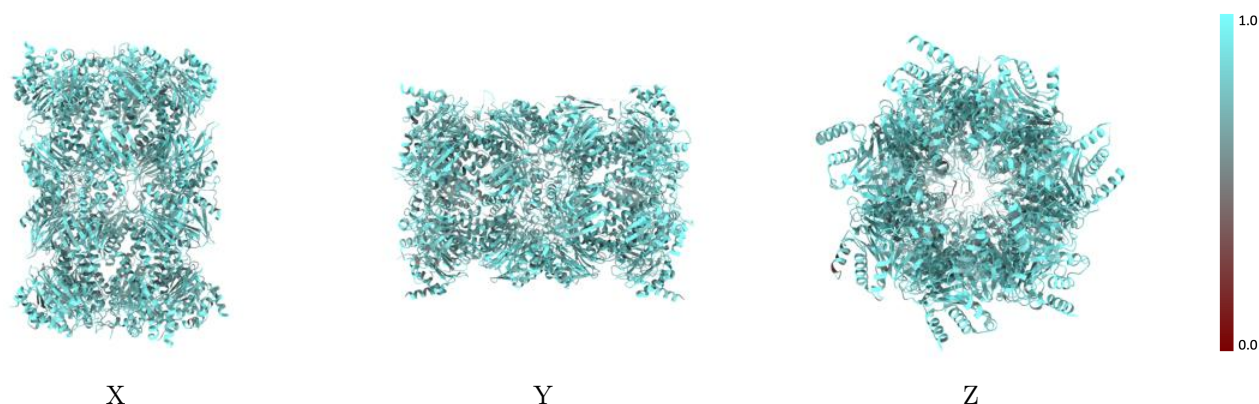
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



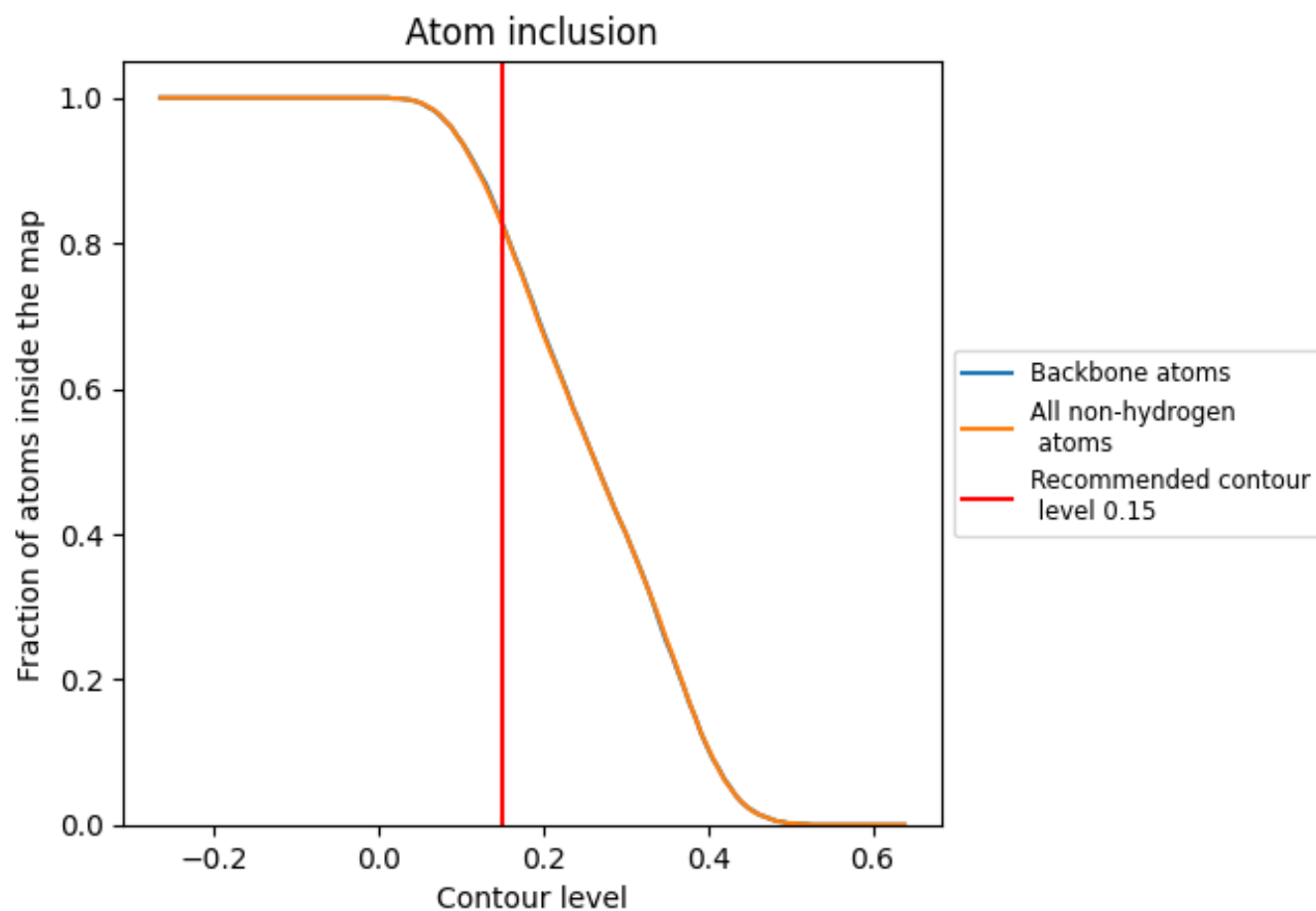
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.5150
A	 0.8080	 0.5130
B	 0.8070	 0.5050
C	 0.8190	 0.5150
D	 0.7940	 0.5050
E	 0.7640	 0.4890
F	 0.8050	 0.5130
G	 0.8350	 0.5240
H	 0.8190	 0.5300
I	 0.8170	 0.5250
J	 0.8270	 0.5280
K	 0.8300	 0.5330
L	 0.8380	 0.5310
M	 0.8160	 0.5280
N	 0.8500	 0.5400
O	 0.8480	 0.5020
P	 0.8590	 0.4980
Q	 0.8590	 0.4970
R	 0.8310	 0.4950
S	 0.8040	 0.4540
T	 0.8410	 0.4980
U	 0.8770	 0.5140
V	 0.8430	 0.5260
W	 0.8500	 0.5210
X	 0.8460	 0.5250
Y	 0.8480	 0.5290
Z	 0.8570	 0.5280
a	 0.8460	 0.5210
b	 0.8680	 0.5350

