



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:02 PM UTC

PDB ID : 8QYS / pdb_00008qys
EMDB ID : EMD-18761
Title : Human preholo proteasome 20S core particle
Authors : Schulman, B.A.; Hanna, J.W.; Harper, J.W.; Adolf, F.; Du, J.; Rawson, S.D.;
Walsh Jr, R.M.; Goodall, E.A.
Deposited on : 2023-10-26
Resolution : 3.89 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:

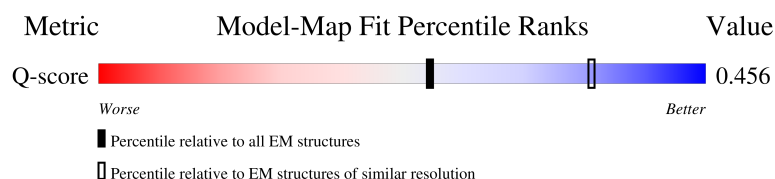
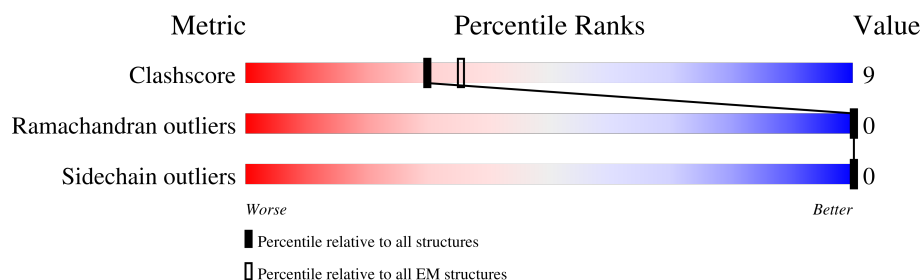
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.89 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	8712 (3.39 - 4.39)

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

Mol	Chain	Length	Quality of chain
1	A	234	 79% 19% .
1	R	234	 78% 20% .
2	B	248	 81% 19%
2	S	248	 82% 18%

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Mol	Chain	Length	Quality of chain
3	C	234	 85% 15%
3	T	234	 86% 14%
4	D	240	 77% 20% ..
4	U	240	 77% 20% ..
5	E	241	 82% 18%
5	V	241	 81% 19%
6	F	241	 80% 20%
6	W	241	 78% 22%
7	G	244	 78% 22%
7	X	244	 78% 22%
8	H	141	 60% 23% 16%
8	Y	141	 61% 23% 16%
9	I	288	 80% 14% 7%
9	Z	288	 79% 14% 7%
10	J	264	 75% 19% 6%
10	a	264	 77% 17% 6%
11	K	262	 72% 28%
11	b	262	 72% 28%
12	L	203	 74% 26%
12	c	203	 73% 27%
13	M	197	 72% 28%
13	d	197	 72% 28%
14	N	208	 80% 20%
14	e	208	 81% 19%
15	O	212	 80% 20%

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Mol	Chain	Length	Quality of chain	
15	f	212		
16	P	208		
16	g	208		
17	Q	197		
17	h	197		

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 57862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1720	1106	293	315	6		
1	R	229	Total	C	N	O	S	0	0
			1720	1106	293	315	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	248	Total	C	N	O	S	0	0
			1808	1149	311	338	10		
2	S	248	Total	C	N	O	S	0	0
			1808	1149	311	338	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	234	Total	C	N	O	S	0	0
			1744	1095	315	329	5		
3	T	234	Total	C	N	O	S	0	0
			1744	1095	315	329	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	236	Total	C	N	O	S	0	0
			1760	1110	294	344	12		
4	U	236	Total	C	N	O	S	0	0
			1760	1110	294	344	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	241	Total	C	N	O	S	0	0
			1863	1170	337	345	11		
5	V	241	Total	C	N	O	S	0	0
			1863	1170	337	345	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	241	Total	C	N	O	S	0	0
			1847	1172	315	349	11		
6	W	241	Total	C	N	O	S	0	0
			1847	1172	315	349	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1846	1172	314	348	12		
7	X	244	Total	C	N	O	S	0	0
			1846	1172	314	348	12		

- Molecule 8 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	118	Total	C	N	O	S	0	0
			937	595	157	180	5		
8	Y	118	Total	C	N	O	S	0	0
			937	595	157	180	5		

- Molecule 9 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	268	Total	C	N	O	S	0	0
			2040	1312	335	378	15		
9	Z	268	Total	C	N	O	S	0	0
			2040	1312	335	378	15		

- Molecule 10 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	248	Total	C	N	O	S	0	0
			1885	1216	307	348	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	248	Total	C	N	O	S	0	0
			1885	1216	307	348	14		

- Molecule 11 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	262	Total	C	N	O	S	0	0
			1980	1249	343	375	13		
11	b	262	Total	C	N	O	S	0	0
			1980	1249	343	375	13		

- Molecule 12 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	203	Total	C	N	O	S	0	0
			1585	1010	264	292	19		
12	c	203	Total	C	N	O	S	0	0
			1585	1010	264	292	19		

- Molecule 13 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	197	Total	C	N	O	S	0	0
			1568	1006	265	288	9		
13	d	197	Total	C	N	O	S	0	0
			1568	1006	265	288	9		

- Molecule 14 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	208	Total	C	N	O	S	0	0
			1607	1014	280	303	10		
14	e	208	Total	C	N	O	S	0	0
			1607	1014	280	303	10		

- Molecule 15 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
15	f	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

- Molecule 16 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	208	Total	C	N	O	S	0	0
			1623	1024	279	309	11		
16	g	208	Total	C	N	O	S	0	0
			1623	1024	279	309	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	234	THR	ILE	variant	UNP P28070
g	234	THR	ILE	variant	UNP P28070

- Molecule 17 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	197	Total	C	N	O	S	0	0
			1475	923	253	287	12		
17	h	197	Total	C	N	O	S	0	0
			1475	923	253	287	12		

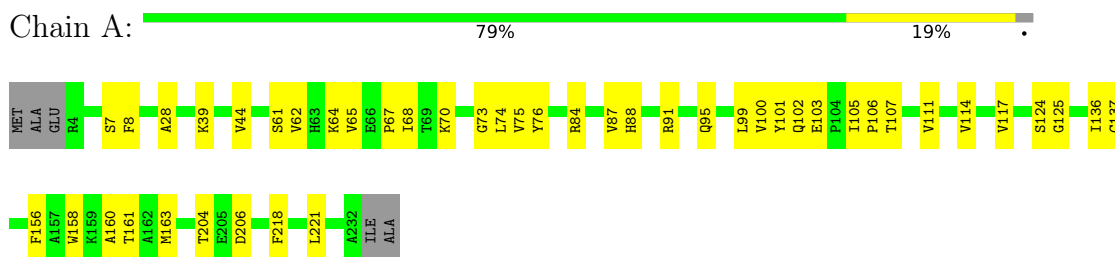
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	145	GLY	VAL	variant	UNP P28072
h	145	GLY	VAL	variant	UNP P28072

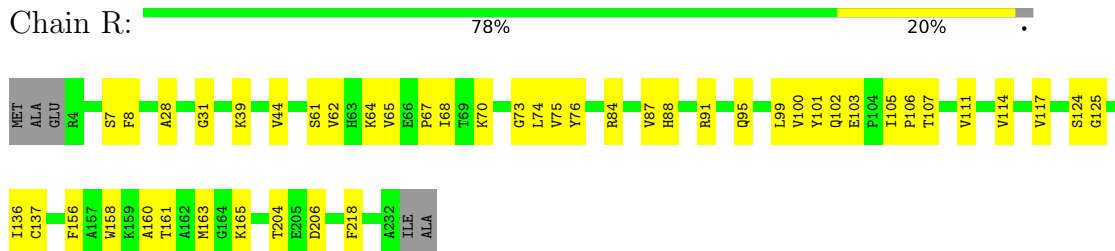
3 Residue-property plots

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.

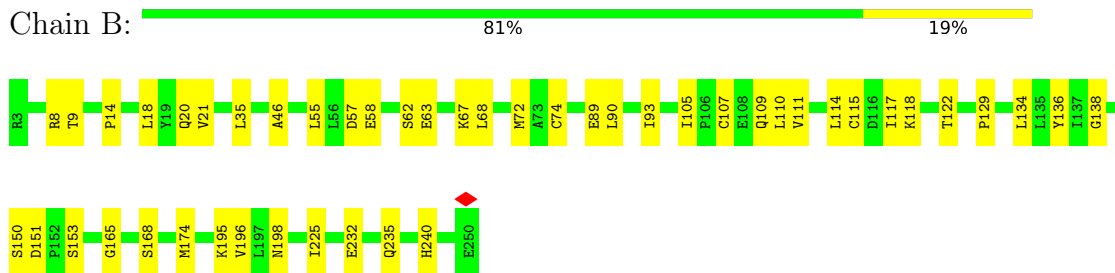
• Molecule 1: Proteasome subunit alpha type-2



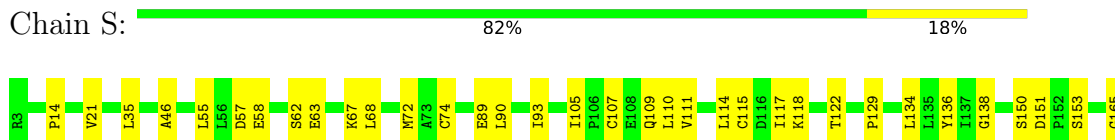
• Molecule 1: Proteasome subunit alpha type-2



• Molecule 2: Proteasome subunit alpha type-4

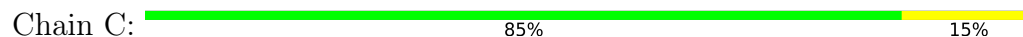


• Molecule 2: Proteasome subunit alpha type-4

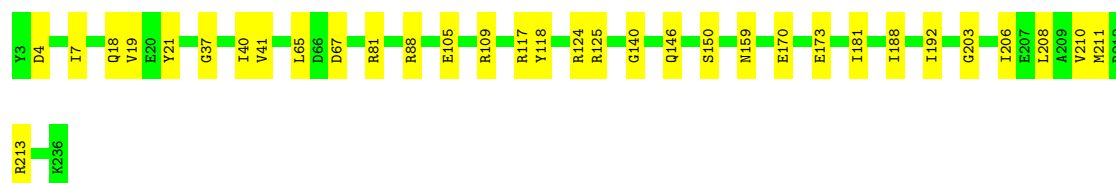




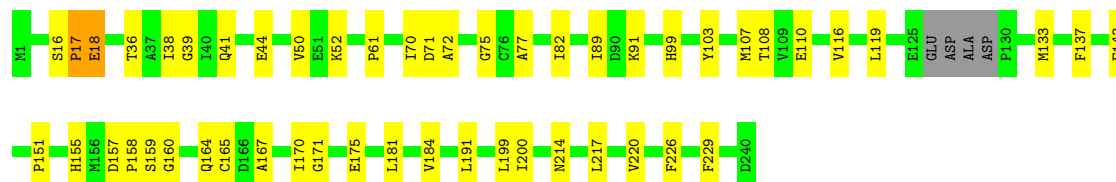
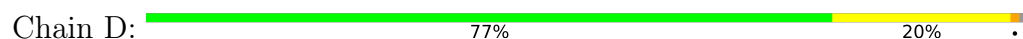
• Molecule 3: Proteasome subunit alpha type-7



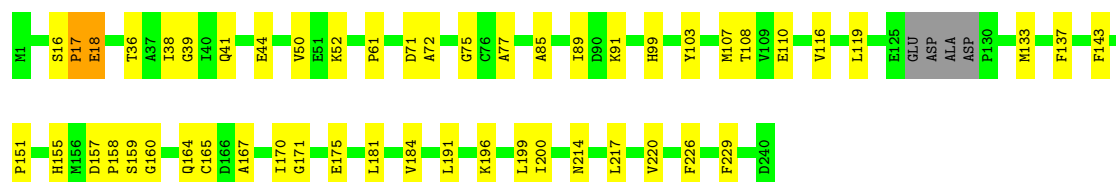
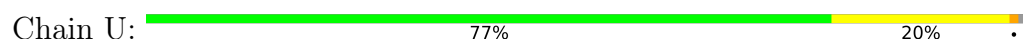
• Molecule 3: Proteasome subunit alpha type-7



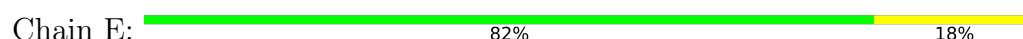
• Molecule 4: Proteasome subunit alpha type-5

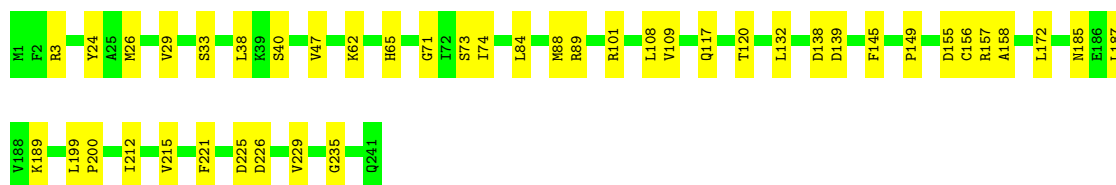


• Molecule 4: Proteasome subunit alpha type-5



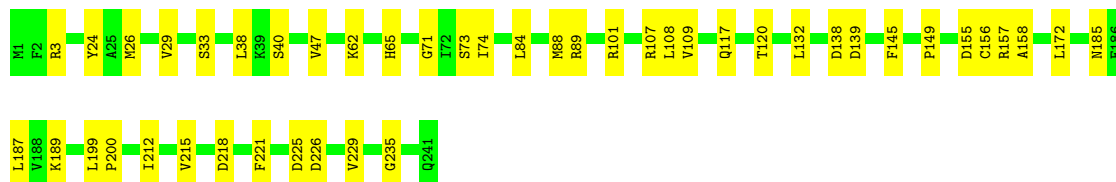
• Molecule 5: Proteasome subunit alpha type-1





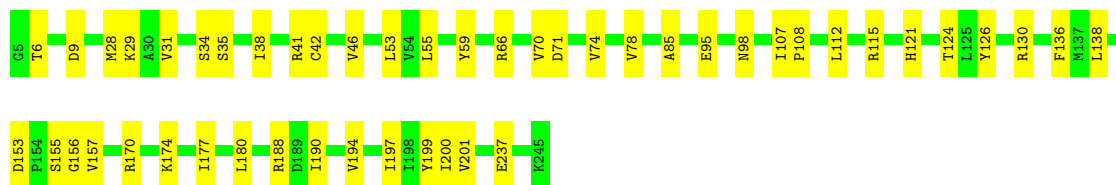
- Molecule 5: Proteasome subunit alpha type-1

Chain V: 81% 19%



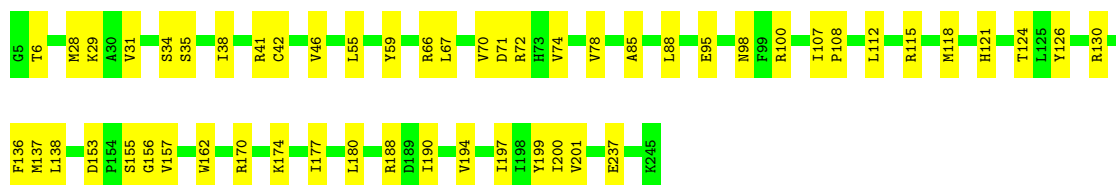
- Molecule 6: Proteasome subunit alpha type-3

Chain F: 80% 20%



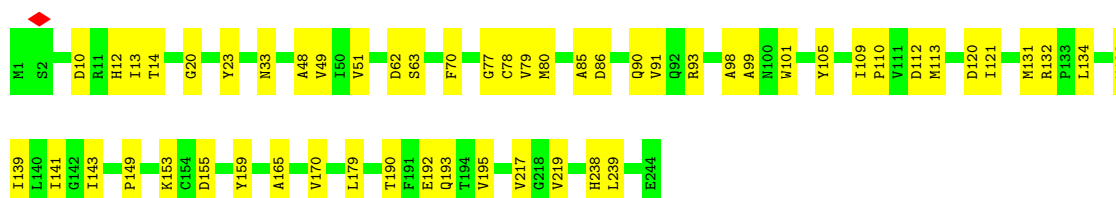
- Molecule 6: Proteasome subunit alpha type-3

Chain W: 78% 22%



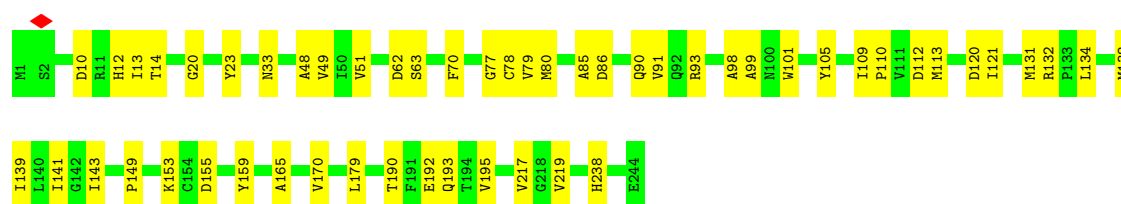
- Molecule 7: Proteasome subunit alpha type-6

Chain G: 78% 22%



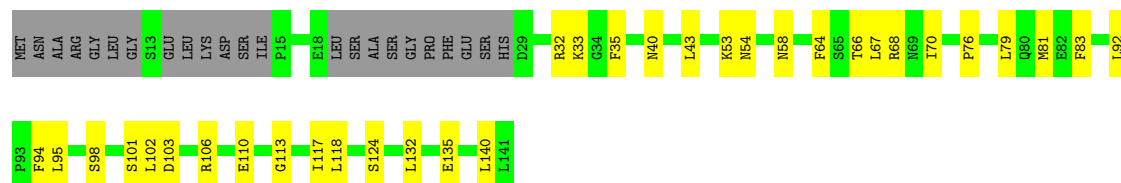
- Molecule 7: Proteasome subunit alpha type-6

Chain X:  78% 22%



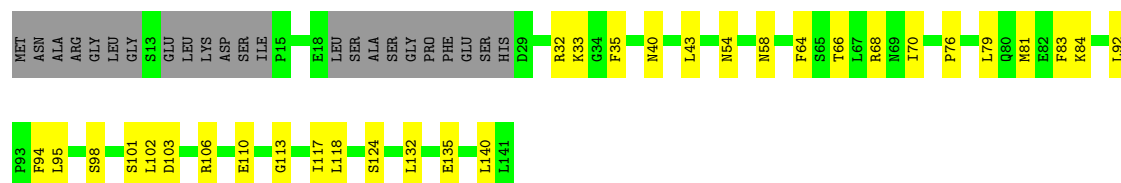
- Molecule 8: Proteasome maturation protein

Chain H:  60% 23% 16%



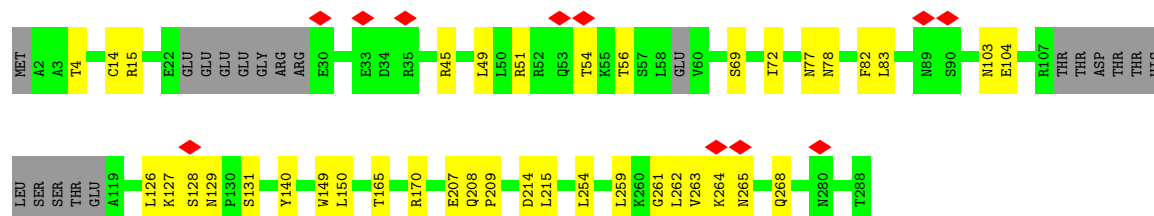
- Molecule 8: Proteasome maturation protein

Chain Y:  61% 23% 16%



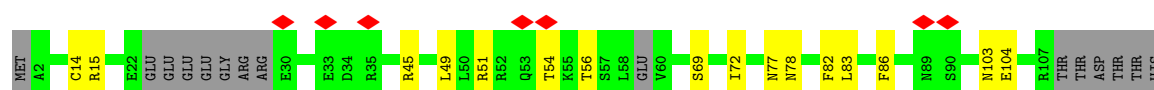
- Molecule 9: Proteasome assembly chaperone 1

Chain I:  80% 14% 7%



- Molecule 9: Proteasome assembly chaperone 1

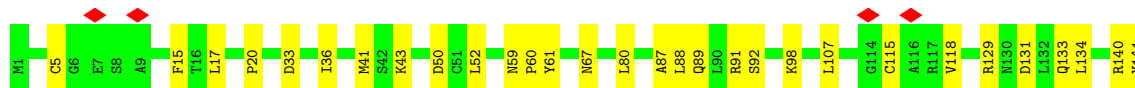
Chain Z:  79% 14% 7%





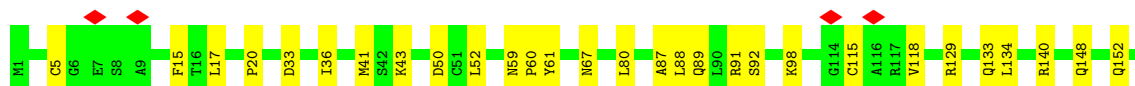
- Molecule 10: Proteasome assembly chaperone 2

Chain J: 75% 19% 6%



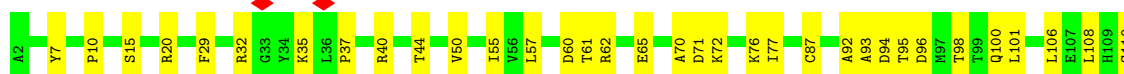
- Molecule 10: Proteasome assembly chaperone 2

Chain a: 77% 17% 6%



- Molecule 11: Proteasome subunit beta type-7

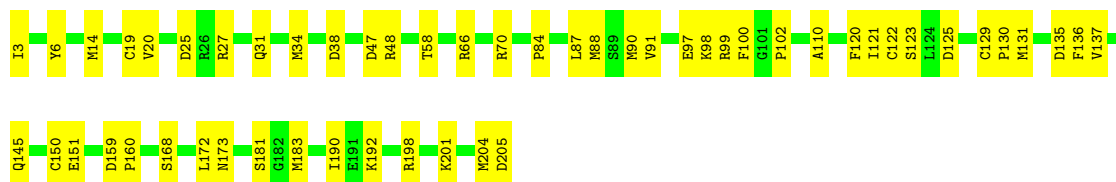
Chain K: 72% 28%





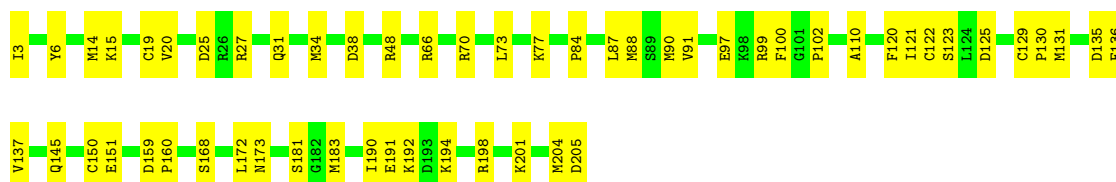
- Molecule 12: Proteasome subunit beta type-3

Chain L: 74% 26%



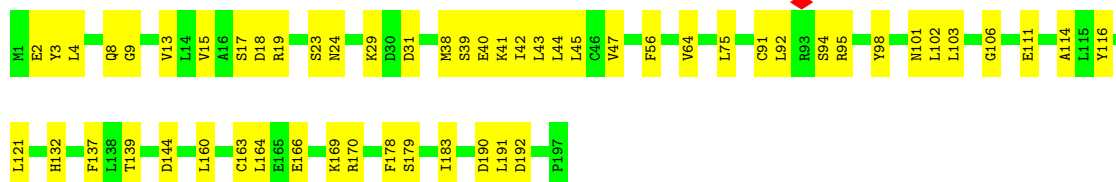
- Molecule 12: Proteasome subunit beta type-3

Chain c: 73% 27%



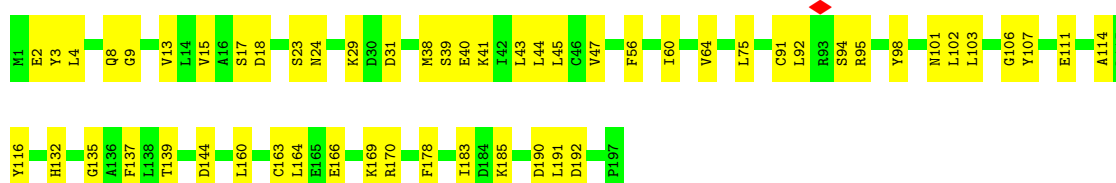
- Molecule 13: Proteasome subunit beta type-2

Chain M: 72% 28%



- Molecule 13: Proteasome subunit beta type-2

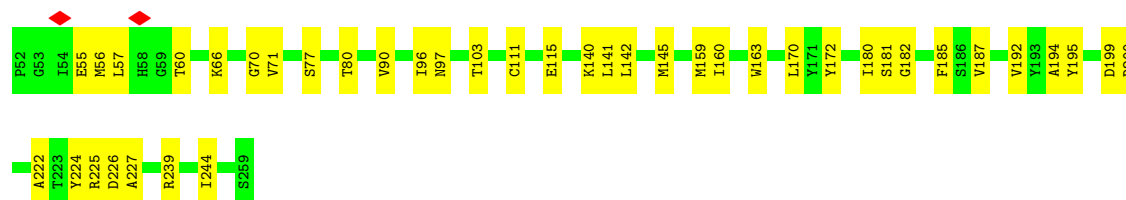
Chain d: 72% 28%



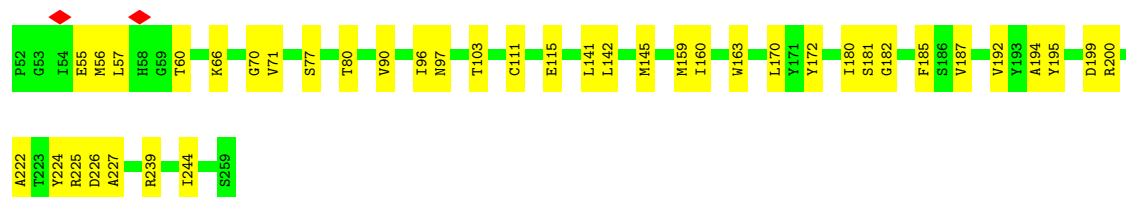
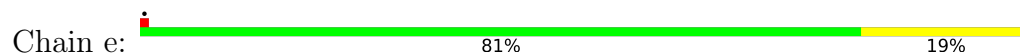
- Molecule 14: Proteasome subunit beta type-5

Chain N: 80% 20%

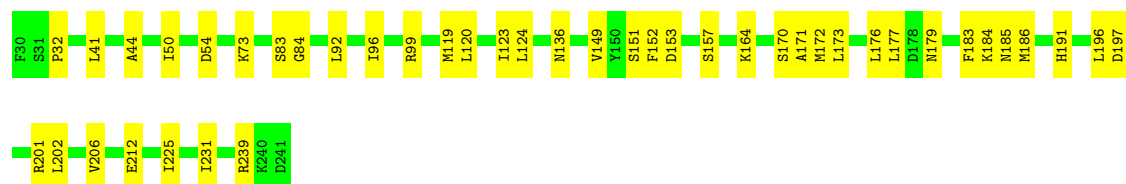
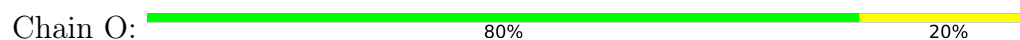




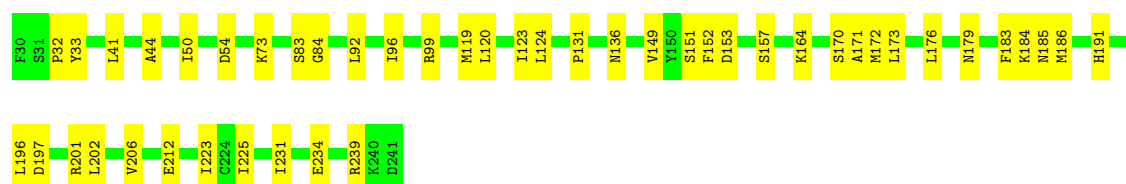
• Molecule 14: Proteasome subunit beta type-5



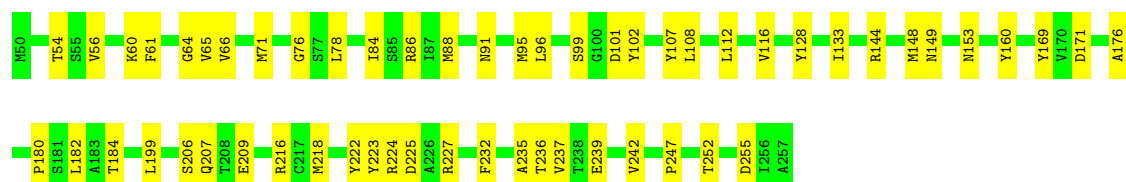
• Molecule 15: Proteasome subunit beta type-1



• Molecule 15: Proteasome subunit beta type-1

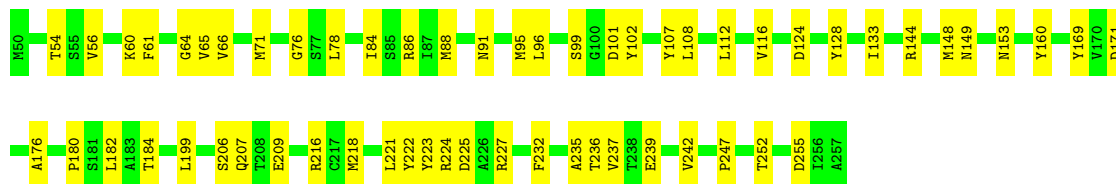


• Molecule 16: Proteasome subunit beta type-4



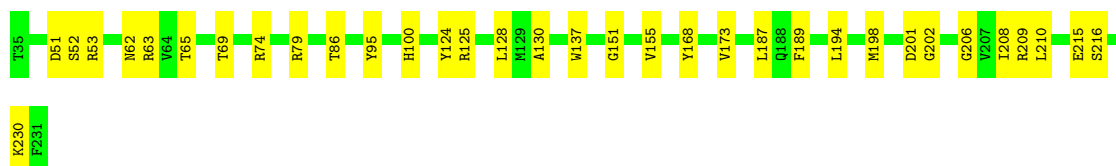
• Molecule 16: Proteasome subunit beta type-4

Chain g:  72% 28%



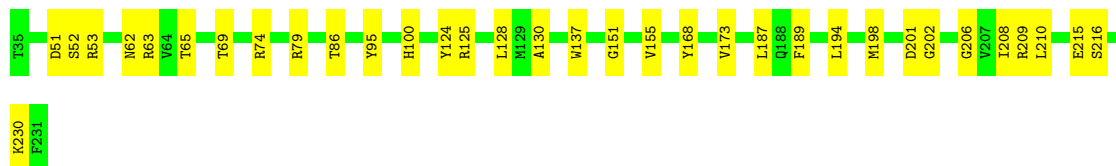
• Molecule 17: Proteasome subunit beta type-6

Chain Q:  83% 17%



• Molecule 17: Proteasome subunit beta type-6

Chain h:  83% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.688	Depositor
Minimum map value	-1.302	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.37	Depositor
Map size ($\text{\AA}$)	316.68, 316.68, 316.68	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.885, 1.885, 1.885	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/1759	0.32	0/2394
1	R	0.12	0/1759	0.32	0/2394
2	B	0.11	0/1837	0.31	0/2499
2	S	0.11	0/1837	0.31	0/2499
3	C	0.11	0/1767	0.27	0/2399
3	T	0.11	0/1767	0.27	0/2399
4	D	0.15	0/1788	0.38	3/2422 (0.1%)
4	U	0.15	0/1788	0.37	3/2422 (0.1%)
5	E	0.12	0/1899	0.32	0/2572
5	V	0.12	0/1899	0.32	0/2572
6	F	0.11	0/1882	0.30	0/2542
6	W	0.11	0/1882	0.30	0/2542
7	G	0.12	0/1879	0.29	0/2547
7	X	0.12	0/1879	0.29	0/2547
8	H	0.13	0/951	0.38	0/1277
8	Y	0.13	0/951	0.38	0/1277
9	I	0.09	0/2083	0.28	0/2839
9	Z	0.09	0/2083	0.28	0/2839
10	J	0.09	0/1925	0.26	0/2615
10	a	0.09	0/1925	0.26	0/2615
11	K	0.12	0/2015	0.28	0/2726
11	b	0.12	0/2015	0.28	0/2726
12	L	0.15	0/1614	0.35	0/2176
12	c	0.15	0/1614	0.35	0/2176
13	M	0.30	1/1601 (0.1%)	0.42	0/2168
13	d	0.30	1/1601 (0.1%)	0.42	0/2168
14	N	0.13	0/1640	0.33	0/2215
14	e	0.13	0/1640	0.34	0/2215
15	O	0.13	0/1673	0.32	0/2254
15	f	0.12	0/1673	0.30	0/2254
16	P	0.13	0/1654	0.32	0/2238
16	g	0.13	0/1654	0.32	0/2238
17	Q	0.13	0/1501	0.30	0/2030
17	h	0.13	0/1501	0.30	0/2030

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.14	2/58936 (0.0%)	0.32	6/79826 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	17	SER	CA-CB	-7.10	1.45	1.54
13	M	17	SER	CA-CB	-6.97	1.45	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	18	GLU	N-CA-C	6.62	120.67	112.59
4	D	17	PRO	CB-CA-C	6.29	121.94	111.56
4	U	18	GLU	N-CA-C	6.05	119.97	112.59
4	U	17	PRO	CB-CA-C	5.74	121.03	111.56
4	D	18	GLU	N-CA-CB	-5.54	102.06	110.92
4	U	18	GLU	N-CA-CB	-5.16	102.67	110.92

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	1720	0	1676	34	0
1	R	1720	0	1676	33	0
2	B	1808	0	1729	39	0
2	S	1808	0	1729	37	0
3	C	1744	0	1704	23	0
3	T	1744	0	1704	23	0
4	D	1760	0	1714	30	0
4	U	1760	0	1714	31	0
5	E	1863	0	1830	29	0
5	V	1863	0	1830	32	0
6	F	1847	0	1800	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	W	1847	0	1800	41	0
7	G	1846	0	1825	47	0
7	X	1846	0	1825	43	0
8	H	937	0	942	32	0
8	Y	937	0	942	32	0
9	I	2040	0	1967	26	0
9	Z	2040	0	1967	26	0
10	J	1885	0	1883	33	0
10	a	1885	0	1883	30	0
11	K	1980	0	2005	60	0
11	b	1980	0	2005	60	0
12	L	1585	0	1604	45	0
12	c	1585	0	1604	47	0
13	M	1568	0	1565	40	0
13	d	1568	0	1565	41	0
14	N	1607	0	1564	29	0
14	e	1607	0	1564	28	0
15	O	1643	0	1640	32	0
15	f	1643	0	1640	31	0
16	P	1623	0	1599	38	0
16	g	1623	0	1599	41	0
17	Q	1475	0	1437	25	0
17	h	1475	0	1437	25	0
All	All	57862	0	56968	1045	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 9.

All (1045) 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)
5:E:88:MET:HE1	5:E:108:LEU:HD21	1.54	0.88
5:V:88:MET:HE1	5:V:108:LEU:HD21	1.54	0.88
1:R:111:VAL:HG22	1:R:136:ILE:HD11	1.55	0.86
1:A:111:VAL:HG22	1:A:136:ILE:HD11	1.55	0.86
2:S:174:MET:HE1	2:S:196:VAL:HG22	1.62	0.82
2:B:174:MET:HE1	2:B:196:VAL:HG22	1.62	0.81
7:G:80:MET:HE1	7:G:138:MET:HA	1.64	0.79
15:f:196:LEU:HD11	15:f:225:ILE:HD11	1.64	0.79
7:G:78:CYS:HB2	7:G:80:MET:HE3	1.65	0.79
7:X:78:CYS:HB2	7:X:80:MET:HE3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:80:MET:HE1	7:X:138:MET:HA	1.64	0.77
15:O:196:LEU:HD11	15:O:225:ILE:HD11	1.65	0.77
14:e:194:ALA:HB2	14:e:222:ALA:HB2	1.68	0.74
11:K:113:THR:HG23	11:K:115:ARG:H	1.53	0.73
14:N:194:ALA:HB2	14:N:222:ALA:HB2	1.68	0.73
11:b:113:THR:HG23	11:b:115:ARG:H	1.53	0.72
17:Q:187:LEU:HD22	17:Q:210:LEU:HD23	1.72	0.72
8:H:68:ARG:HB2	8:H:76:PRO:HG2	1.72	0.72
11:K:55:ILE:HD11	11:K:151:PRO:HB3	1.72	0.71
17:h:187:LEU:HD22	17:h:210:LEU:HD23	1.72	0.71
17:h:52:SER:HB2	17:h:65:THR:H	1.55	0.71
12:L:34:MET:HG3	12:L:183:MET:HE1	1.71	0.71
8:Y:68:ARG:HB2	8:Y:76:PRO:HG2	1.72	0.70
17:Q:52:SER:HB2	17:Q:65:THR:H	1.55	0.70
11:K:62:ARG:HH21	11:K:213:GLY:HA3	1.56	0.70
11:b:62:ARG:HH21	11:b:213:GLY:HA3	1.56	0.70
12:c:34:MET:HG3	12:c:183:MET:HE1	1.71	0.70
6:F:42:CYS:HB3	6:F:190:ILE:HD13	1.74	0.69
6:W:42:CYS:HB3	6:W:190:ILE:HD13	1.74	0.69
16:P:60:LYS:HD3	16:P:180:PRO:HA	1.74	0.69
11:b:55:ILE:HD11	11:b:151:PRO:HB3	1.72	0.69
8:H:54:ASN:O	8:H:58:ASN:ND2	2.26	0.69
4:U:36:THR:HA	4:U:171:GLY:HA3	1.76	0.68
8:Y:54:ASN:O	8:Y:58:ASN:ND2	2.26	0.68
4:D:36:THR:HA	4:D:171:GLY:HA3	1.76	0.68
16:g:60:LYS:HD3	16:g:180:PRO:HA	1.74	0.68
17:Q:69:THR:OG1	17:Q:79:ARG:NH1	2.27	0.68
2:B:90:LEU:HD11	2:B:110:LEU:HG	1.76	0.68
13:M:44:LEU:HD11	13:M:102:LEU:HD23	1.74	0.68
17:h:69:THR:OG1	17:h:79:ARG:NH1	2.27	0.67
17:h:65:THR:O	17:h:209:ARG:NH1	2.28	0.67
1:A:68:ILE:HG23	1:A:91:ARG:HG2	1.76	0.67
2:S:90:LEU:HD11	2:S:110:LEU:HG	1.75	0.67
2:B:35:LEU:HB2	2:B:46:ALA:HB3	1.76	0.66
12:L:135:ASP:OD1	12:L:136:PHE:N	2.29	0.66
2:S:35:LEU:HB2	2:S:46:ALA:HB3	1.76	0.66
1:A:74:LEU:HB3	1:A:136:ILE:HG22	1.77	0.66
17:Q:65:THR:O	17:Q:209:ARG:NH1	2.28	0.66
1:R:68:ILE:HG23	1:R:91:ARG:HG2	1.76	0.66
6:F:6:THR:HG21	10:J:212:ASP:H	1.59	0.66
6:W:6:THR:HG21	10:a:212:ASP:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:68:ILE:HD11	1:R:74:LEU:HD23	1.78	0.65
1:A:68:ILE:HD11	1:A:74:LEU:HD23	1.78	0.65
13:d:44:LEU:HD11	13:d:102:LEU:HD23	1.78	0.65
4:D:52:LYS:HD3	4:D:214:ASN:HA	1.78	0.65
12:c:135:ASP:OD1	12:c:136:PHE:N	2.29	0.65
13:d:164:LEU:HD13	13:d:178:PHE:HD2	1.60	0.65
11:K:65:GLU:HG2	11:K:70:ALA:HB2	1.79	0.65
2:B:118:LYS:NZ	2:B:150:SER:OG	2.30	0.65
11:K:257:GLU:OE1	12:L:198:ARG:NH1	2.30	0.65
13:M:164:LEU:HD13	13:M:178:PHE:HD2	1.61	0.65
4:U:52:LYS:HD3	4:U:214:ASN:HA	1.78	0.65
11:b:65:GLU:HG2	11:b:70:ALA:HB2	1.79	0.65
7:G:131:MET:HE3	7:G:131:MET:HA	1.78	0.65
1:R:74:LEU:HB3	1:R:136:ILE:HG22	1.77	0.65
12:c:48:ARG:NH1	12:c:192:LYS:O	2.29	0.65
13:M:8:GLN:HG2	13:M:9:GLY:H	1.62	0.64
14:N:57:LEU:HD11	14:N:60:THR:HB	1.79	0.64
13:d:8:GLN:HG2	13:d:9:GLY:H	1.62	0.64
5:E:33:SER:OG	5:E:62:LYS:NZ	2.30	0.64
14:e:57:LEU:HD11	14:e:60:THR:HB	1.79	0.64
1:R:61:SER:OG	1:R:62:VAL:N	2.31	0.64
2:B:122:THR:O	3:C:125:ARG:NH1	2.31	0.64
1:A:117:VAL:HG23	8:H:98:SER:HB2	1.80	0.64
16:P:144:ARG:NH2	16:P:149:ASN:OD1	2.30	0.64
11:b:257:GLU:OE1	12:c:198:ARG:NH1	2.30	0.64
13:d:64:VAL:HG13	13:d:75:LEU:HD12	1.80	0.64
1:R:88:HIS:ND1	8:Y:110:GLU:OE2	2.31	0.64
2:S:118:LYS:NZ	2:S:150:SER:OG	2.30	0.64
16:g:144:ARG:NH2	16:g:149:ASN:OD1	2.30	0.64
13:M:29:LYS:NZ	13:M:31:ASP:O	2.31	0.64
14:N:141:LEU:O	14:N:145:MET:HG3	1.99	0.64
1:R:117:VAL:HG23	8:Y:98:SER:HB2	1.80	0.64
7:X:131:MET:HE3	7:X:131:MET:HA	1.78	0.64
13:d:29:LYS:NZ	13:d:31:ASP:O	2.31	0.64
3:C:140:GLY:O	3:C:213:ARG:NH2	2.31	0.63
12:L:48:ARG:NH1	12:L:192:LYS:O	2.31	0.63
3:T:140:GLY:O	3:T:213:ARG:NH2	2.31	0.63
2:S:122:THR:O	3:T:125:ARG:NH1	2.31	0.63
1:A:88:HIS:ND1	8:H:110:GLU:OE2	2.31	0.63
1:A:39:LYS:HA	1:A:44:VAL:HG12	1.80	0.63
4:D:70:ILE:HD11	4:D:89:ILE:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:ASN:ND2	13:M:95:ARG:O	2.31	0.63
11:b:60:ASP:OD1	11:b:61:THR:N	2.30	0.63
1:A:84:ARG:NH2	7:G:120:ASP:OD1	2.28	0.63
1:A:204:THR:HG23	1:A:206:ASP:H	1.63	0.62
16:P:99:SER:O	16:P:153:ASN:ND2	2.32	0.62
1:A:61:SER:OG	1:A:62:VAL:N	2.31	0.62
15:O:197:ASP:OD2	15:O:201:ARG:NH1	2.32	0.62
14:e:141:LEU:O	14:e:145:MET:HG3	1.99	0.62
7:G:93:ARG:HD3	7:G:121:ILE:HD13	1.81	0.62
15:f:197:ASP:OD2	15:f:201:ARG:NH1	2.32	0.62
2:B:115:CYS:SG	3:C:81:ARG:NH2	2.73	0.62
5:V:33:SER:OG	5:V:62:LYS:NZ	2.30	0.62
9:I:208:GLN:NE2	10:J:59:ASN:O	2.33	0.62
11:K:55:ILE:HB	11:K:221:ILE:HD11	1.82	0.62
16:g:99:SER:O	16:g:153:ASN:ND2	2.32	0.62
1:A:74:LEU:HD21	1:A:87:VAL:HG22	1.82	0.62
7:G:70:PHE:HD2	7:G:91:VAL:HG21	1.65	0.62
16:P:71:MET:HE1	16:P:247:PRO:HB3	1.82	0.62
7:X:70:PHE:HD2	7:X:91:VAL:HG21	1.65	0.62
1:R:39:LYS:HA	1:R:44:VAL:HG12	1.80	0.61
9:Z:208:GLN:NE2	10:a:59:ASN:O	2.33	0.61
11:b:55:ILE:HB	11:b:221:ILE:HD11	1.82	0.61
8:H:83:PHE:HE2	8:H:106:ARG:HE	1.49	0.61
1:R:204:THR:HG23	1:R:206:ASP:H	1.63	0.61
2:S:115:CYS:SG	3:T:81:ARG:NH2	2.73	0.61
8:Y:83:PHE:HE2	8:Y:106:ARG:HE	1.49	0.61
4:D:220:VAL:HG12	4:D:226:PHE:HA	1.83	0.61
16:P:76:GLY:O	16:P:227:ARG:NH2	2.31	0.61
1:R:74:LEU:HD21	1:R:87:VAL:HG22	1.82	0.60
4:U:18:GLU:OE1	4:U:18:GLU:N	2.32	0.60
14:N:55:GLU:HG3	14:N:56:MET:H	1.67	0.60
7:X:86:ASP:HB3	7:X:134:LEU:HD12	1.83	0.60
7:X:93:ARG:HD3	7:X:121:ILE:HD13	1.81	0.60
5:E:3:ARG:NH2	5:E:24:TYR:OH	2.35	0.60
7:G:86:ASP:HB3	7:G:134:LEU:HD12	1.83	0.60
14:e:55:GLU:HG3	14:e:56:MET:H	1.67	0.60
13:M:3:TYR:N	13:M:18:ASP:OD2	2.35	0.60
4:D:75:GLY:HA3	4:D:226:PHE:HE2	1.67	0.60
14:N:195:TYR:OH	13:d:170:ARG:NH1	2.35	0.60
16:P:112:LEU:HD11	16:P:133:ILE:HD12	1.84	0.60
5:E:120:THR:O	6:F:130:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:103:THR:OG1	14:N:159:MET:N	2.34	0.60
8:Y:40:ASN:ND2	13:d:95:ARG:O	2.32	0.60
2:B:72:MET:HE1	2:B:107:CYS:HA	1.84	0.59
16:g:71:MET:HE1	16:g:247:PRO:HB3	1.82	0.59
6:F:95:GLU:OE2	6:F:115:ARG:NH1	2.34	0.59
4:U:220:VAL:HG12	4:U:226:PHE:HA	1.83	0.59
11:K:60:ASP:OD1	11:K:61:THR:N	2.30	0.59
5:V:3:ARG:NH2	5:V:24:TYR:OH	2.35	0.59
13:M:64:VAL:HG13	13:M:75:LEU:HD12	1.83	0.59
5:V:101:ARG:HH21	16:g:128:TYR:HE1	1.50	0.59
6:W:95:GLU:OE2	6:W:115:ARG:NH1	2.34	0.59
3:C:192:ILE:HD11	3:C:208:LEU:HD11	1.85	0.59
13:d:3:TYR:N	13:d:18:ASP:OD2	2.35	0.59
2:B:89:GLU:HG3	8:H:95:LEU:HD21	1.85	0.59
14:N:172:TYR:CE1	14:N:187:VAL:HG11	2.37	0.59
1:R:101:TYR:O	1:R:103:GLU:N	2.35	0.59
5:V:120:THR:O	6:W:130:ARG:NH1	2.35	0.59
1:A:101:TYR:O	1:A:103:GLU:N	2.35	0.59
14:e:172:TYR:CE1	14:e:187:VAL:HG11	2.38	0.59
13:M:170:ARG:NH1	14:e:195:TYR:OH	2.35	0.59
2:S:111:VAL:HG22	2:S:136:TYR:HD2	1.68	0.59
14:e:103:THR:OG1	14:e:159:MET:N	2.34	0.59
16:g:88:MET:HB2	16:g:96:LEU:HB3	1.85	0.59
16:g:112:LEU:HD11	16:g:133:ILE:HD12	1.84	0.58
1:R:84:ARG:NH2	7:X:120:ASP:OD1	2.28	0.58
10:a:50:ASP:O	10:a:98:LYS:NZ	2.37	0.58
2:S:72:MET:HE1	2:S:107:CYS:HA	1.84	0.58
4:U:41:GLN:NE2	4:U:151:PRO:O	2.35	0.58
4:U:75:GLY:HA3	4:U:226:PHE:HE2	1.67	0.58
3:C:7:ILE:HG13	3:C:18:GLN:HG3	1.85	0.58
9:I:214:ASP:CG	9:I:215:LEU:H	2.12	0.58
11:K:35:LYS:O	12:L:3:ILE:N	2.37	0.58
13:d:2:GLU:HB2	13:d:47:VAL:HG11	1.85	0.58
4:D:18:GLU:OE1	4:D:18:GLU:N	2.31	0.58
2:S:89:GLU:HG3	8:Y:95:LEU:HD21	1.85	0.58
3:T:192:ILE:HD11	3:T:208:LEU:HD11	1.85	0.58
4:U:38:ILE:HD11	4:U:181:LEU:HD21	1.86	0.58
10:J:50:ASP:O	10:J:98:LYS:NZ	2.37	0.58
4:D:38:ILE:HD11	4:D:181:LEU:HD21	1.86	0.58
11:b:35:LYS:O	12:c:3:ILE:N	2.37	0.58
11:b:50:VAL:HG22	11:b:55:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:TRP:CD1	7:G:109:ILE:HG12	2.39	0.58
11:K:95:THR:HA	11:K:98:THR:HG22	1.86	0.58
5:E:101:ARG:HH21	16:P:128:TYR:HE1	1.50	0.57
10:J:59:ASN:ND2	10:J:67:ASN:O	2.37	0.57
14:e:57:LEU:N	14:e:80:THR:O	2.37	0.57
9:I:261:GLY:O	9:I:264:LYS:NZ	2.35	0.57
11:K:118:ARG:O	11:K:121:THR:OG1	2.22	0.57
4:D:41:GLN:NE2	4:D:151:PRO:O	2.35	0.57
7:X:12:HIS:CD2	7:X:14:THR:HG22	2.39	0.57
4:D:44:GLU:HG3	4:D:191:LEU:HB2	1.87	0.57
9:Z:214:ASP:CG	9:Z:215:LEU:H	2.12	0.57
7:X:101:TRP:CD1	7:X:109:ILE:HG12	2.39	0.57
11:b:118:ARG:O	11:b:121:THR:OG1	2.22	0.57
11:K:50:VAL:HG22	11:K:55:ILE:HD12	1.86	0.57
10:a:59:ASN:ND2	10:a:67:ASN:O	2.37	0.57
7:G:12:HIS:CD2	7:G:14:THR:HG22	2.39	0.57
11:b:95:THR:HA	11:b:98:THR:HG22	1.86	0.57
2:B:111:VAL:HG22	2:B:136:TYR:HD2	1.69	0.57
6:F:70:VAL:HB	6:F:74:VAL:HG23	1.87	0.57
13:M:2:GLU:HB2	13:M:47:VAL:HG11	1.85	0.57
13:M:39:SER:OG	13:M:40:GLU:N	2.38	0.57
15:O:179:ASN:HD22	12:c:173:ASN:HD21	1.53	0.57
1:R:99:LEU:HD22	8:Y:117:ILE:HG21	1.87	0.57
3:T:7:ILE:HG13	3:T:18:GLN:HG3	1.85	0.57
5:E:156:CYS:SG	5:E:157:ARG:N	2.78	0.56
3:T:117:ARG:NH1	8:Y:135:GLU:OE2	2.38	0.56
9:Z:149:TRP:HE3	9:Z:150:LEU:HD22	1.71	0.56
16:P:88:MET:HB2	16:P:96:LEU:HB3	1.85	0.56
7:G:10:ASP:HB3	7:G:23:TYR:HD2	1.71	0.56
1:R:44:VAL:HG21	1:R:137:CYS:HB2	1.88	0.56
5:V:156:CYS:SG	5:V:157:ARG:N	2.78	0.56
14:e:160:ILE:H	14:e:160:ILE:HD12	1.71	0.56
14:e:226:ASP:OD1	14:e:227:ALA:N	2.34	0.56
16:g:61:PHE:HB3	16:g:64:GLY:O	2.05	0.56
16:P:61:PHE:HB3	16:P:64:GLY:O	2.05	0.56
4:U:44:GLU:HG3	4:U:191:LEU:HB2	1.86	0.56
15:O:99:ARG:HD3	15:O:123:ILE:HD11	1.88	0.56
10:a:17:LEU:HB2	10:a:118:VAL:HA	1.88	0.56
2:B:67:LYS:HE3	2:B:225:ILE:HD12	1.88	0.56
1:A:44:VAL:HG21	1:A:137:CYS:HB2	1.88	0.56
9:I:265:ASN:ND2	9:I:268:GLN:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:70:VAL:HB	6:W:74:VAL:HG23	1.87	0.56
10:a:89:GLN:HE21	10:a:91:ARG:HH21	1.53	0.56
15:f:99:ARG:HD3	15:f:123:ILE:HD11	1.88	0.56
9:I:149:TRP:HE3	9:I:150:LEU:HD22	1.70	0.56
5:E:155:ASP:OD1	5:E:156:CYS:N	2.39	0.55
5:V:155:ASP:OD1	5:V:156:CYS:N	2.39	0.55
9:Z:261:GLY:O	9:Z:264:LYS:NZ	2.35	0.55
15:O:73:LYS:HE3	15:O:231:ILE:HD12	1.88	0.55
9:Z:265:ASN:ND2	9:Z:268:GLN:OE1	2.39	0.55
9:I:69:SER:HB3	9:I:131:SER:HB2	1.89	0.55
14:N:160:ILE:HD12	14:N:160:ILE:H	1.71	0.55
15:f:73:LYS:HE3	15:f:231:ILE:HD12	1.88	0.55
7:G:109:ILE:HG22	7:G:110:PRO:O	2.07	0.55
10:J:17:LEU:HB2	10:J:118:VAL:HA	1.88	0.55
16:g:76:GLY:O	16:g:227:ARG:NH2	2.31	0.55
1:A:99:LEU:HD22	8:H:117:ILE:HG21	1.87	0.55
10:J:89:GLN:HE21	10:J:91:ARG:HH21	1.53	0.55
9:Z:69:SER:HB3	9:Z:131:SER:HB2	1.89	0.55
16:g:206:SER:N	16:g:209:GLU:OE2	2.40	0.55
3:C:117:ARG:NH1	8:H:135:GLU:OE2	2.38	0.55
3:C:124:ARG:HH12	8:H:140:LEU:HD22	1.72	0.55
2:S:67:LYS:HE3	2:S:225:ILE:HD12	1.88	0.55
3:T:124:ARG:HH12	8:Y:140:LEU:HD22	1.72	0.55
1:A:64:LYS:HG2	1:A:76:TYR:HE1	1.72	0.54
3:C:105:GLU:OE2	3:C:109:ARG:NH2	2.40	0.54
11:K:37:PRO:HD3	12:L:3:ILE:HG13	1.89	0.54
12:L:173:ASN:HD21	15:f:179:ASN:HD22	1.53	0.54
3:T:146:GLN:OE1	3:T:159:ASN:ND2	2.40	0.54
9:I:54:THR:H	9:I:56:THR:HG23	1.72	0.54
5:V:40:SER:HB3	5:V:187:LEU:HD22	1.89	0.54
7:X:10:ASP:HB3	7:X:23:TYR:HD2	1.71	0.54
9:Z:82:PHE:HD2	9:Z:83:LEU:HD12	1.72	0.54
13:d:39:SER:OG	13:d:40:GLU:N	2.38	0.54
16:g:56:VAL:N	16:g:184:THR:OG1	2.37	0.54
13:M:4:LEU:HB2	13:M:132:HIS:HB2	1.90	0.54
3:T:105:GLU:OE2	3:T:109:ARG:NH2	2.40	0.54
7:G:48:ALA:HB1	7:G:141:ILE:HD11	1.90	0.54
9:I:72:ILE:HG12	9:I:165:THR:HB	1.90	0.54
9:I:82:PHE:HD2	9:I:83:LEU:HD12	1.72	0.54
7:X:48:ALA:HB1	7:X:141:ILE:HD11	1.90	0.54
7:X:109:ILE:HG22	7:X:110:PRO:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PRO:HB3	1:A:218:PHE:HD2	1.72	0.54
3:C:146:GLN:OE1	3:C:159:ASN:ND2	2.40	0.54
16:P:56:VAL:N	16:P:184:THR:OG1	2.37	0.54
1:R:64:LYS:HG2	1:R:76:TYR:HE1	1.72	0.54
9:Z:72:ILE:HG12	9:Z:165:THR:HB	1.90	0.54
1:A:107:THR:O	1:A:111:VAL:HG23	2.07	0.54
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.90	0.54
16:P:101:ASP:OD1	16:P:102:TYR:N	2.41	0.54
13:d:4:LEU:HB2	13:d:132:HIS:HB2	1.89	0.54
11:K:169:THR:HG22	11:K:174:SER:HB3	1.89	0.54
13:M:92:LEU:HD12	13:M:98:TYR:HB2	1.90	0.54
16:P:95:MET:HE1	16:P:235:ALA:HB3	1.90	0.54
16:g:169:TYR:CE2	16:g:171:ASP:HB2	2.43	0.54
7:X:165:ALA:HB1	7:X:179:LEU:HD13	1.90	0.54
9:Z:54:THR:H	9:Z:56:THR:HG23	1.72	0.54
16:P:169:TYR:CE2	16:P:171:ASP:HB2	2.43	0.54
13:d:92:LEU:HD12	13:d:98:TYR:HB2	1.90	0.54
14:N:239:ARG:HH22	14:N:244:ILE:HD13	1.72	0.54
16:g:101:ASP:OD1	16:g:102:TYR:N	2.41	0.54
9:I:77:ASN:OD1	9:I:78:ASN:N	2.40	0.53
14:N:57:LEU:N	14:N:80:THR:O	2.37	0.53
14:e:239:ARG:HH22	14:e:244:ILE:HD13	1.72	0.53
16:g:95:MET:HE1	16:g:235:ALA:HB3	1.90	0.53
16:P:206:SER:N	16:P:209:GLU:OE2	2.40	0.53
1:R:67:PRO:HB3	1:R:218:PHE:HD2	1.72	0.53
12:L:123:SER:HB2	12:L:137:VAL:HG21	1.90	0.53
11:b:169:THR:HG22	11:b:174:SER:HB3	1.88	0.53
12:c:123:SER:HB2	12:c:137:VAL:HG21	1.90	0.53
11:K:238:LYS:NZ	12:L:151:GLU:OE2	2.41	0.53
11:b:37:PRO:HD3	12:c:3:ILE:HG13	1.89	0.53
5:E:40:SER:HB3	5:E:187:LEU:HD22	1.89	0.53
1:R:107:THR:O	1:R:111:VAL:HG23	2.07	0.53
11:b:238:LYS:NZ	12:c:151:GLU:OE2	2.41	0.53
9:Z:77:ASN:OD1	9:Z:78:ASN:N	2.40	0.53
11:b:40:ARG:HD2	12:c:125:ASP:HB3	1.91	0.53
11:K:92:ALA:HA	11:K:95:THR:HG22	1.91	0.53
6:F:35:SER:OG	6:F:66:ARG:NH2	2.43	0.52
10:J:52:LEU:HD12	10:J:92:SER:HB3	1.92	0.52
12:L:88:MET:HE2	12:L:130:PRO:HB3	1.91	0.52
6:W:35:SER:OG	6:W:66:ARG:NH2	2.43	0.52
7:G:49:VAL:HA	7:G:219:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:ARG:HD2	12:L:125:ASP:HB3	1.91	0.52
11:K:71:ASP:OD1	11:K:72:LYS:N	2.42	0.52
5:V:73:SER:OG	5:V:74:ILE:N	2.42	0.52
7:X:101:TRP:HB3	7:X:109:ILE:HD11	1.91	0.52
11:b:71:ASP:OD1	11:b:72:LYS:N	2.42	0.52
5:E:84:LEU:HD23	5:E:132:LEU:HD11	1.91	0.52
9:I:103:ASN:ND2	9:I:140:TYR:O	2.42	0.52
9:Z:103:ASN:ND2	9:Z:140:TYR:O	2.42	0.52
6:W:153:ASP:HB2	6:W:157:VAL:HB	1.91	0.52
6:F:153:ASP:HB2	6:F:157:VAL:HB	1.90	0.52
11:b:92:ALA:HA	11:b:95:THR:HG22	1.92	0.52
4:U:103:TYR:OH	15:f:99:ARG:NH2	2.43	0.52
5:V:26:MET:HA	5:V:149:PRO:HG2	1.91	0.52
12:c:88:MET:HE2	12:c:130:PRO:HB3	1.92	0.52
15:f:223:ILE:HB	15:f:234:GLU:HB3	1.91	0.52
5:E:73:SER:OG	5:E:74:ILE:N	2.42	0.52
6:F:55:LEU:HD12	6:F:59:TYR:HE2	1.75	0.52
7:G:101:TRP:HB3	7:G:109:ILE:HD11	1.91	0.52
5:V:84:LEU:HD23	5:V:132:LEU:HD11	1.91	0.52
10:a:52:LEU:HD12	10:a:92:SER:HB3	1.92	0.52
2:B:122:THR:HG22	2:B:129:PRO:HB3	1.92	0.51
2:S:150:SER:OG	2:S:151:ASP:N	2.43	0.51
6:F:38:ILE:HD11	6:F:194:VAL:HG13	1.93	0.51
7:G:77:GLY:H	7:G:141:ILE:HG22	1.76	0.51
8:Y:43:LEU:O	11:b:20:ARG:NH2	2.43	0.51
11:K:32:ARG:NH1	12:L:31:GLN:OE1	2.43	0.51
14:N:226:ASP:OD1	14:N:227:ALA:N	2.34	0.51
15:O:183:PHE:HE2	15:O:191:HIS:HA	1.75	0.51
13:d:13:VAL:HG12	13:d:183:ILE:HB	1.92	0.51
5:E:26:MET:HA	5:E:149:PRO:HG2	1.91	0.51
9:I:51:ARG:O	9:I:56:THR:OG1	2.23	0.51
12:L:159:ASP:OD1	12:L:159:ASP:N	2.41	0.51
4:D:103:TYR:OH	15:O:99:ARG:NH2	2.43	0.51
4:D:159:SER:OG	4:D:160:GLY:N	2.44	0.51
11:b:32:ARG:NH1	12:c:31:GLN:OE1	2.43	0.51
16:g:84:ILE:HG22	17:h:155:VAL:HG21	1.93	0.51
2:B:150:SER:OG	2:B:151:ASP:N	2.43	0.51
1:R:7:SER:OG	1:R:8:PHE:N	2.44	0.51
7:X:77:GLY:H	7:X:141:ILE:HG22	1.75	0.51
7:G:139:ILE:HG12	7:G:153:LYS:HG3	1.93	0.51
11:K:110:SER:HA	11:K:113:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:13:VAL:HG12	13:M:183:ILE:HB	1.92	0.51
13:M:169:LYS:NZ	14:e:199:ASP:OD2	2.41	0.51
2:S:122:THR:HG22	2:S:129:PRO:HB3	1.92	0.51
7:X:139:ILE:HG12	7:X:153:LYS:HG3	1.93	0.51
1:A:105:ILE:HG13	1:A:106:PRO:O	2.11	0.51
6:W:55:LEU:HD12	6:W:59:TYR:HE2	1.76	0.51
7:X:49:VAL:HA	7:X:219:VAL:HG12	1.91	0.51
8:H:43:LEU:O	11:K:20:ARG:NH2	2.43	0.51
12:L:70:ARG:HG2	12:L:90:MET:HE1	1.93	0.51
12:c:70:ARG:HG2	12:c:90:MET:HE1	1.93	0.51
5:E:65:HIS:O	5:E:89:ARG:NH2	2.36	0.51
8:H:33:LYS:HB2	11:K:7:TYR:HE2	1.76	0.51
16:P:84:ILE:HG22	17:Q:155:VAL:HG21	1.93	0.51
4:U:85:ALA:O	4:U:89:ILE:HG12	2.10	0.50
6:W:38:ILE:HD11	6:W:194:VAL:HG13	1.93	0.50
3:C:37:GLY:HA2	3:C:181:ILE:HB	1.94	0.50
11:K:167:TYR:OH	17:Q:63:ARG:NH2	2.44	0.50
17:h:74:ARG:NH2	17:h:216:SER:O	2.45	0.50
9:Z:254:LEU:HD13	9:Z:263:VAL:HG11	1.93	0.50
11:b:167:TYR:OH	17:h:63:ARG:NH2	2.44	0.50
15:f:183:PHE:HE2	15:f:191:HIS:HA	1.75	0.50
16:g:56:VAL:HG12	16:g:56:VAL:O	2.11	0.50
2:B:198:ASN:HD22	2:B:240:HIS:CE1	2.30	0.50
7:X:33:ASN:HB3	7:X:170:VAL:HG23	1.94	0.50
4:D:116:VAL:HG11	4:D:143:PHE:HE2	1.76	0.50
9:I:45:ARG:NH1	9:I:104:GLU:OE1	2.45	0.50
4:U:159:SER:OG	4:U:160:GLY:N	2.44	0.50
10:a:231:LEU:HG	10:a:232:LYS:H	1.76	0.50
1:A:7:SER:OG	1:A:8:PHE:N	2.44	0.50
15:O:153:ASP:OD1	15:O:157:SER:N	2.44	0.50
8:Y:33:LYS:HB2	11:b:7:TYR:HE2	1.76	0.50
11:K:62:ARG:NH2	11:K:213:GLY:HA3	2.24	0.50
16:P:66:VAL:HG12	16:P:236:THR:HG22	1.93	0.50
17:Q:74:ARG:NH2	17:Q:216:SER:O	2.45	0.50
2:S:57:ASP:OD1	2:S:58:GLU:N	2.45	0.50
3:T:37:GLY:HA2	3:T:181:ILE:HB	1.94	0.50
10:a:194:SER:OG	10:a:199:ILE:O	2.30	0.50
11:b:252:THR:HG21	12:c:168:SER:HB3	1.94	0.50
2:B:57:ASP:OD1	2:B:58:GLU:N	2.45	0.50
16:P:237:VAL:HG23	16:P:242:VAL:HG22	1.94	0.50
11:b:110:SER:HA	11:b:113:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:66:VAL:HG12	16:g:236:THR:HG22	1.93	0.50
4:D:157:ASP:HB2	4:D:158:PRO:HD2	1.94	0.50
17:Q:137:TRP:CZ2	17:Q:215:GLU:HG2	2.47	0.50
4:U:116:VAL:HG11	4:U:143:PHE:HE2	1.76	0.50
16:P:56:VAL:HG12	16:P:56:VAL:O	2.11	0.49
4:U:91:LYS:HG3	4:U:119:LEU:HD22	1.94	0.49
6:F:78:VAL:HG11	6:F:85:ALA:HB1	1.93	0.49
10:J:60:PRO:HG3	10:J:91:ARG:HH22	1.77	0.49
15:O:96:ILE:HD12	15:O:119:MET:HE1	1.95	0.49
8:Y:35:PHE:HZ	13:d:56:PHE:HA	1.77	0.49
13:M:192:ASP:N	13:M:192:ASP:OD1	2.45	0.49
16:P:54:THR:H	16:P:86:ARG:HH22	1.60	0.49
4:U:50:VAL:HG21	4:U:77:ALA:HB1	1.93	0.49
13:d:135:GLY:O	13:d:139:THR:OG1	2.24	0.49
4:D:91:LYS:HG3	4:D:119:LEU:HD22	1.94	0.49
10:J:231:LEU:HG	10:J:232:LYS:H	1.76	0.49
2:S:198:ASN:HD22	2:S:240:HIS:CE1	2.30	0.49
9:Z:45:ARG:NH1	9:Z:104:GLU:OE1	2.45	0.49
10:a:60:PRO:HG3	10:a:91:ARG:HH22	1.77	0.49
12:c:159:ASP:OD1	12:c:159:ASP:N	2.41	0.49
13:d:94:SER:OG	13:d:95:ARG:N	2.45	0.49
16:g:237:VAL:HG23	16:g:242:VAL:HG22	1.94	0.49
17:h:125:ARG:HD2	17:h:151:GLY:HA2	1.94	0.49
1:A:73:GLY:HA3	1:A:218:PHE:CZ	2.48	0.49
7:G:33:ASN:HB3	7:G:170:VAL:HG23	1.94	0.49
11:K:252:THR:HG21	12:L:168:SER:HB3	1.94	0.49
1:R:95:GLN:HG3	11:b:108:LEU:HG	1.95	0.49
1:R:105:ILE:HG13	1:R:106:PRO:O	2.11	0.49
15:f:153:ASP:OD1	15:f:157:SER:N	2.45	0.49
1:A:95:GLN:HG3	11:K:108:LEU:HG	1.95	0.49
9:I:254:LEU:HD13	9:I:263:VAL:HG11	1.93	0.49
10:J:194:SER:OG	10:J:199:ILE:O	2.30	0.49
15:f:96:ILE:HD12	15:f:119:MET:HE1	1.95	0.49
16:P:225:ASP:O	17:h:53:ARG:NH2	2.46	0.49
1:R:73:GLY:HA3	1:R:218:PHE:CZ	2.47	0.49
1:R:100:VAL:HG12	1:R:101:TYR:CD1	2.48	0.49
5:V:109:VAL:HG21	5:V:145:PHE:HD2	1.76	0.49
6:W:78:VAL:HG11	6:W:85:ALA:HB1	1.93	0.49
12:c:27:ARG:HD3	12:c:181:SER:H	1.78	0.49
17:h:137:TRP:CZ2	17:h:215:GLU:HG2	2.47	0.49
10:J:41:MET:HG2	10:J:80:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:199:ASP:OD2	13:d:169:LYS:NZ	2.41	0.49
10:a:41:MET:HG2	10:a:80:LEU:HB2	1.95	0.49
13:M:111:GLU:O	13:M:111:GLU:HG2	2.13	0.49
15:O:179:ASN:ND2	12:c:173:ASN:HD21	2.11	0.49
7:X:190:THR:HG22	7:X:193:GLN:HB2	1.95	0.49
8:H:113:GLY:HA2	11:K:101:LEU:HD21	1.94	0.48
12:L:145:GLN:HG3	15:f:171:ALA:HB1	1.95	0.48
9:Z:14:CYS:SG	9:Z:15:ARG:N	2.86	0.48
16:g:65:VAL:H	16:g:237:VAL:HG12	1.78	0.48
1:A:100:VAL:HG12	1:A:101:TYR:CD1	2.48	0.48
7:G:190:THR:HG22	7:G:193:GLN:HB2	1.95	0.48
13:M:94:SER:OG	13:M:95:ARG:N	2.45	0.48
16:P:65:VAL:H	16:P:237:VAL:HG12	1.78	0.48
17:Q:125:ARG:HD2	17:Q:151:GLY:HA2	1.94	0.48
3:T:4:ASP:OD2	3:T:21:TYR:OH	2.28	0.48
3:T:188:ILE:HD11	3:T:210:VAL:HG22	1.95	0.48
16:g:54:THR:H	16:g:86:ARG:HH22	1.60	0.48
12:L:173:ASN:HD21	15:f:179:ASN:ND2	2.11	0.48
11:b:203:ALA:HA	11:b:206:ILE:HG22	1.95	0.48
9:I:259:LEU:HG	9:I:262:LEU:HD12	1.95	0.48
16:P:255:ASP:N	16:P:255:ASP:OD1	2.46	0.48
2:S:90:LEU:HD13	2:S:114:LEU:HD22	1.94	0.48
11:b:62:ARG:NH2	11:b:213:GLY:HA3	2.24	0.48
13:d:38:MET:HE1	13:d:60:ILE:HG23	1.94	0.48
5:E:109:VAL:HG21	5:E:145:PHE:HD2	1.76	0.48
9:I:14:CYS:SG	9:I:15:ARG:N	2.86	0.48
11:K:155:SER:HB2	11:K:168:VAL:HG21	1.95	0.48
1:R:161:THR:HG22	1:R:163:MET:H	1.78	0.48
1:A:161:THR:HG22	1:A:163:MET:H	1.78	0.48
3:C:65:LEU:HD23	3:C:88:ARG:HG3	1.96	0.48
17:Q:53:ARG:NH2	16:g:225:ASP:O	2.46	0.48
13:d:23:SER:OG	13:d:24:ASN:N	2.46	0.48
3:C:188:ILE:HD11	3:C:210:VAL:HG22	1.95	0.48
4:D:50:VAL:HG21	4:D:77:ALA:HB1	1.94	0.48
12:L:87:LEU:HA	12:L:90:MET:HB2	1.95	0.48
13:M:23:SER:OG	13:M:24:ASN:N	2.46	0.48
2:S:114:LEU:HD23	2:S:136:TYR:OH	2.14	0.48
9:Z:259:LEU:HG	9:Z:262:LEU:HD12	1.95	0.48
10:a:181:ILE:HD12	10:a:182:PRO:HD2	1.96	0.48
2:B:105:ILE:HD13	2:B:110:LEU:HD13	1.96	0.48
12:L:27:ARG:HD3	12:L:181:SER:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:171:ALA:HB1	12:c:145:GLN:HG3	1.95	0.48
16:P:223:TYR:HE1	16:P:252:THR:HB	1.79	0.48
12:c:87:LEU:HA	12:c:90:MET:HB2	1.95	0.48
13:d:111:GLU:O	13:d:111:GLU:HG2	2.13	0.48
2:B:90:LEU:HD13	2:B:114:LEU:HD22	1.94	0.48
2:B:114:LEU:HD23	2:B:136:TYR:OH	2.14	0.48
6:F:29:LYS:HE3	6:F:29:LYS:HB2	1.62	0.48
7:G:105:TYR:HB3	11:K:121:THR:HG22	1.95	0.48
11:K:183:ASP:OD2	16:g:216:ARG:NH1	2.47	0.48
8:Y:113:GLY:HA2	11:b:101:LEU:HD21	1.95	0.48
8:Y:117:ILE:HG13	8:Y:118:LEU:HG	1.96	0.48
11:b:155:SER:HB2	11:b:168:VAL:HG21	1.95	0.48
2:B:21:VAL:HG21	2:B:153:SER:HB2	1.96	0.47
5:E:225:ASP:OD1	5:E:226:ASP:N	2.45	0.47
6:F:136:PHE:CZ	6:F:138:LEU:HD13	2.49	0.47
11:K:203:ALA:HA	11:K:206:ILE:HG22	1.96	0.47
15:O:32:PRO:HG2	16:P:148:MET:HE1	1.96	0.47
2:S:21:VAL:HG21	2:S:153:SER:HB2	1.96	0.47
4:U:157:ASP:HB2	4:U:158:PRO:HD2	1.94	0.47
7:X:99:ALA:HB1	17:h:95:TYR:HE1	1.79	0.47
16:g:255:ASP:OD1	16:g:255:ASP:N	2.46	0.47
17:h:51:ASP:HB2	17:h:198:MET:HE1	1.96	0.47
4:D:133:MET:HE3	4:D:137:PHE:CZ	2.50	0.47
8:H:117:ILE:HG13	8:H:118:LEU:HG	1.96	0.47
10:J:181:ILE:HD12	10:J:182:PRO:HD2	1.96	0.47
13:M:166:GLU:HB2	14:e:200:ARG:HH21	1.79	0.47
17:Q:173:VAL:HG23	17:Q:189:PHE:HZ	1.79	0.47
1:R:102:GLN:HE22	11:b:100:GLN:CD	2.21	0.47
6:W:136:PHE:CZ	6:W:138:LEU:HD13	2.49	0.47
17:h:173:VAL:HG23	17:h:189:PHE:HZ	1.79	0.47
7:G:99:ALA:HB1	17:Q:95:TYR:HE1	1.79	0.47
3:T:65:LEU:HD23	3:T:88:ARG:HG3	1.96	0.47
17:h:79:ARG:HD2	17:h:86:THR:OG1	2.15	0.47
7:G:49:VAL:HG21	7:G:195:VAL:HG22	1.96	0.47
10:J:36:ILE:HD13	10:J:41:MET:HE3	1.97	0.47
13:M:101:ASN:HB3	13:M:132:HIS:CE1	2.50	0.47
13:M:144:ASP:OD2	14:e:225:ARG:NH2	2.48	0.47
4:U:133:MET:HE3	4:U:137:PHE:CZ	2.49	0.47
7:X:12:HIS:HD2	7:X:14:THR:H	1.63	0.47
7:X:105:TYR:HB3	11:b:121:THR:HG22	1.95	0.47
10:a:36:ILE:HD13	10:a:41:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:c:38:ASP:OD1	12:c:38:ASP:N	2.44	0.47
16:g:54:THR:H	16:g:86:ARG:NH2	2.13	0.47
11:K:170:MET:HE3	11:K:170:MET:HB3	1.80	0.47
17:Q:51:ASP:HB2	17:Q:198:MET:HE1	1.96	0.47
13:d:192:ASP:OD1	13:d:192:ASP:N	2.46	0.47
15:f:202:LEU:O	15:f:206:VAL:HG23	2.15	0.47
16:g:160:TYR:HE2	16:g:239:GLU:HB3	1.80	0.47
2:B:118:LYS:HB2	2:B:118:LYS:HE3	1.77	0.47
3:C:4:ASP:OD1	3:C:4:ASP:N	2.46	0.47
4:D:199:LEU:HD21	4:D:217:LEU:HD21	1.96	0.47
5:E:47:VAL:HG22	5:E:212:ILE:HG13	1.97	0.47
8:H:35:PHE:HZ	13:M:56:PHE:HA	1.78	0.47
11:K:147:ASP:OD1	11:K:149:THR:OG1	2.28	0.47
14:N:200:ARG:HH21	13:d:166:GLU:HB2	1.79	0.47
14:N:225:ARG:NH2	13:d:144:ASP:OD2	2.48	0.47
15:O:185:ASN:HB3	12:c:172:LEU:HD23	1.96	0.47
15:O:202:LEU:O	15:O:206:VAL:HG23	2.15	0.47
2:S:107:CYS:O	2:S:111:VAL:HG23	2.15	0.47
4:U:99:HIS:CG	4:U:107:MET:HE1	2.49	0.47
5:V:225:ASP:OD1	5:V:226:ASP:N	2.45	0.47
6:W:112:LEU:HD23	6:W:138:LEU:HD21	1.96	0.47
16:g:223:TYR:HE1	16:g:252:THR:HB	1.79	0.47
4:D:155:HIS:NE2	4:D:170:ILE:HD13	2.30	0.47
17:Q:194:LEU:HD23	17:Q:208:ILE:HG23	1.97	0.47
1:R:101:TYR:HE1	12:c:90:MET:SD	2.38	0.47
12:c:19:CYS:SG	12:c:160:PRO:HG3	2.55	0.47
1:A:101:TYR:HE1	12:L:90:MET:SD	2.38	0.47
7:X:192:GLU:OE1	7:X:238:HIS:NE2	2.48	0.47
14:e:170:LEU:HD23	14:e:170:LEU:O	2.15	0.47
8:H:53:LYS:HE2	8:H:53:LYS:HB2	1.83	0.47
12:L:172:LEU:HD23	15:f:185:ASN:HB3	1.96	0.47
15:O:212:GLU:HG2	15:O:239:ARG:HH11	1.80	0.47
6:W:121:HIS:O	6:W:124:THR:HG22	2.15	0.47
9:Z:49:LEU:HD23	9:Z:51:ARG:H	1.79	0.47
16:g:88:MET:HE2	16:g:88:MET:HB3	1.78	0.47
4:D:175:GLU:OE1	4:D:175:GLU:N	2.44	0.46
10:J:129:ARG:HH21	10:J:134:LEU:HD13	1.80	0.46
16:P:160:TYR:HE2	16:P:239:GLU:HB3	1.80	0.46
12:c:205:ASP:N	12:c:205:ASP:OD1	2.48	0.46
2:B:235:GLN:OE1	2:B:235:GLN:N	2.44	0.46
4:D:99:HIS:CG	4:D:107:MET:HE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:79:ARG:HD2	17:Q:86:THR:OG1	2.15	0.46
5:V:47:VAL:HG22	5:V:212:ILE:HG13	1.97	0.46
9:I:49:LEU:HD23	9:I:51:ARG:H	1.79	0.46
9:I:209:PRO:HD3	10:J:252:ARG:HH12	1.80	0.46
12:L:19:CYS:SG	12:L:160:PRO:HG3	2.55	0.46
12:L:58:THR:OG1	13:M:121:LEU:O	2.30	0.46
3:T:4:ASP:OD1	3:T:4:ASP:N	2.46	0.46
4:U:155:HIS:NE2	4:U:170:ILE:HD13	2.30	0.46
5:V:117:GLN:O	5:V:120:THR:HG22	2.15	0.46
7:X:51:VAL:HG12	7:X:217:VAL:HG22	1.97	0.46
7:X:70:PHE:CD2	7:X:91:VAL:HG21	2.48	0.46
14:e:181:SER:OG	14:e:182:GLY:N	2.48	0.46
16:g:218:MET:HG3	16:g:232:PHE:CE2	2.51	0.46
7:G:12:HIS:HD2	7:G:14:THR:H	1.62	0.46
10:a:181:ILE:HG22	10:a:188:LYS:HD3	1.97	0.46
13:d:45:LEU:HD12	13:d:103:LEU:HD23	1.97	0.46
15:f:44:ALA:HB2	15:f:149:VAL:HG23	1.98	0.46
1:A:102:GLN:HE22	11:K:100:GLN:CD	2.21	0.46
5:E:215:VAL:HB	5:E:221:PHE:HD1	1.81	0.46
10:J:33:ASP:OD1	10:J:61:TYR:OH	2.27	0.46
12:L:38:ASP:OD1	12:L:38:ASP:N	2.44	0.46
15:O:44:ALA:HB2	15:O:149:VAL:HG23	1.97	0.46
7:X:49:VAL:HG21	7:X:195:VAL:HG22	1.96	0.46
9:Z:126:LEU:HG	9:Z:128:SER:H	1.81	0.46
11:b:60:ASP:OD2	11:b:212:SER:HB2	2.16	0.46
12:c:120:PHE:CZ	12:c:122:CYS:HB3	2.51	0.46
6:F:112:LEU:HD23	6:F:138:LEU:HD21	1.96	0.46
10:J:181:ILE:HG22	10:J:188:LYS:HD3	1.97	0.46
10:J:231:LEU:HD21	10:J:244:ARG:HB3	1.97	0.46
11:K:60:ASP:OD2	11:K:212:SER:HB2	2.16	0.46
12:L:47:ASP:OD1	12:L:48:ARG:N	2.47	0.46
14:N:170:LEU:O	14:N:170:LEU:HD23	2.15	0.46
16:P:218:MET:HG3	16:P:232:PHE:CE2	2.51	0.46
2:S:117:ILE:HG23	8:Y:94:PHE:HE1	1.81	0.46
8:Y:124:SER:HB3	11:b:10:PRO:HG2	1.98	0.46
9:Z:209:PRO:HD3	10:a:252:ARG:HH12	1.80	0.46
14:e:103:THR:HG1	14:e:159:MET:H	1.61	0.46
15:f:32:PRO:HG2	16:g:148:MET:HE1	1.97	0.46
15:f:136:ASN:HB2	15:f:152:PHE:HD2	1.80	0.46
6:F:121:HIS:CD2	7:G:85:ALA:HB1	2.51	0.46
6:F:121:HIS:O	6:F:124:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:38:MET:HB2	13:M:42:ILE:HB	1.97	0.46
16:P:54:THR:H	16:P:86:ARG:NH2	2.13	0.46
16:P:169:TYR:O	16:P:176:ALA:HA	2.16	0.46
5:V:215:VAL:HB	5:V:221:PHE:HD1	1.81	0.46
9:Z:51:ARG:O	9:Z:56:THR:OG1	2.23	0.46
10:a:5:CYS:SG	10:a:43:LYS:NZ	2.88	0.46
10:a:129:ARG:HH21	10:a:134:LEU:HD13	1.80	0.46
4:U:175:GLU:OE1	4:U:175:GLU:N	2.44	0.46
5:V:199:LEU:HD12	5:V:200:PRO:HD2	1.98	0.46
2:B:107:CYS:O	2:B:111:VAL:HG23	2.15	0.46
2:B:117:ILE:HG23	8:H:94:PHE:HE1	1.81	0.46
7:G:192:GLU:OE1	7:G:238:HIS:NE2	2.48	0.46
16:P:78:LEU:HD12	17:h:168:TYR:CZ	2.51	0.46
17:Q:86:THR:HG22	17:Q:130:ALA:HB1	1.98	0.46
2:S:105:ILE:HD13	2:S:110:LEU:HD13	1.96	0.46
2:S:235:GLN:OE1	2:S:235:GLN:N	2.44	0.46
13:d:101:ASN:HB3	13:d:132:HIS:CE1	2.50	0.46
7:G:51:VAL:HG12	7:G:217:VAL:HG22	1.97	0.46
12:c:25:ASP:N	12:c:25:ASP:OD1	2.49	0.46
5:E:138:ASP:OD1	5:E:139:ASP:N	2.47	0.45
12:L:205:ASP:OD1	12:L:205:ASP:N	2.48	0.45
13:M:45:LEU:HD12	13:M:103:LEU:HD23	1.96	0.45
1:R:70:LYS:HB3	1:R:70:LYS:HE3	1.81	0.45
7:X:98:ALA:HA	7:X:109:ILE:HD11	1.98	0.45
16:g:169:TYR:O	16:g:176:ALA:HA	2.16	0.45
6:F:126:TYR:CG	8:H:81:MET:HE1	2.51	0.45
9:I:126:LEU:HG	9:I:128:SER:H	1.81	0.45
14:N:181:SER:OG	14:N:182:GLY:N	2.48	0.45
16:P:216:ARG:NH1	11:b:183:ASP:OD2	2.47	0.45
5:V:158:ALA:HB1	5:V:172:LEU:HD21	1.99	0.45
6:W:67:LEU:HD23	6:W:67:LEU:HA	1.85	0.45
10:a:160:TRP:CG	10:a:223:TYR:HH	2.34	0.45
11:b:106:LEU:HD23	11:b:106:LEU:HA	1.86	0.45
11:b:190:GLU:HG2	11:b:191:GLU:H	1.81	0.45
2:B:62:SER:OG	2:B:63:GLU:N	2.48	0.45
8:H:124:SER:HB3	11:K:10:PRO:HG2	1.98	0.45
10:J:5:CYS:SG	10:J:43:LYS:NZ	2.89	0.45
2:S:62:SER:OG	2:S:63:GLU:N	2.48	0.45
2:S:68:LEU:HD21	2:S:74:CYS:SG	2.57	0.45
13:M:160:LEU:O	13:M:164:LEU:HG	2.17	0.45
6:W:121:HIS:CD2	7:X:85:ALA:HB1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:231:LEU:HD21	10:a:244:ARG:HB3	1.97	0.45
15:f:212:GLU:HG2	15:f:239:ARG:HH11	1.81	0.45
17:h:86:THR:HG22	17:h:130:ALA:HB1	1.98	0.45
2:B:68:LEU:HD21	2:B:74:CYS:SG	2.57	0.45
5:E:117:GLN:O	5:E:120:THR:HG22	2.15	0.45
14:N:192:VAL:HG11	13:d:137:PHE:HB3	1.98	0.45
15:O:136:ASN:HB2	15:O:152:PHE:HD2	1.82	0.45
9:Z:128:SER:OG	9:Z:129:ASN:N	2.49	0.45
10:a:33:ASP:OD1	10:a:61:TYR:OH	2.27	0.45
12:c:183:MET:HB3	12:c:204:MET:HE1	1.98	0.45
13:d:190:ASP:OD1	13:d:191:LEU:N	2.49	0.45
16:g:206:SER:OG	16:g:207:GLN:N	2.50	0.45
17:h:194:LEU:HD23	17:h:208:ILE:HG23	1.97	0.45
8:H:67:LEU:HD23	8:H:67:LEU:HA	1.82	0.45
2:S:174:MET:HE3	2:S:174:MET:HB3	1.75	0.45
2:S:174:MET:SD	2:S:195:LYS:NZ	2.87	0.45
13:d:160:LEU:O	13:d:164:LEU:HG	2.17	0.45
6:F:197:ILE:HA	6:F:200:ILE:HG22	1.97	0.45
7:G:143:ILE:HA	7:G:149:PRO:HA	1.99	0.45
5:V:65:HIS:O	5:V:89:ARG:NH2	2.36	0.45
12:c:84:PRO:HB2	12:c:120:PHE:CD2	2.52	0.45
7:G:70:PHE:CD2	7:G:91:VAL:HG21	2.48	0.45
12:L:120:PHE:CZ	12:L:122:CYS:HB3	2.51	0.45
6:W:124:THR:O	7:X:132:ARG:NH2	2.34	0.45
6:W:126:TYR:CG	8:Y:81:MET:HE1	2.51	0.45
6:W:155:SER:OG	6:W:156:GLY:N	2.50	0.45
11:b:29:PHE:CZ	12:c:6:TYR:HB2	2.51	0.45
11:b:154:TYR:OH	11:b:164:LYS:NZ	2.49	0.45
5:E:199:LEU:HD12	5:E:200:PRO:HD2	1.98	0.45
7:G:98:ALA:HA	7:G:109:ILE:HD11	1.98	0.45
13:M:190:ASP:OD1	13:M:191:LEU:N	2.49	0.45
16:P:206:SER:OG	16:P:207:GLN:N	2.50	0.45
16:P:224:ARG:NE	11:b:182:GLU:OE1	2.50	0.45
11:b:94:ASP:OD2	12:c:99:ARG:NH2	2.50	0.45
11:b:106:LEU:HD11	11:b:122:ALA:HB2	1.99	0.45
6:F:107:ILE:HD12	6:F:108:PRO:HD2	1.99	0.45
6:F:199:TYR:OH	6:F:237:GLU:OE2	2.31	0.45
11:K:29:PHE:CZ	12:L:6:TYR:HB2	2.52	0.45
11:K:154:TYR:OH	11:K:164:LYS:NZ	2.49	0.45
11:K:219:CYS:O	11:K:221:ILE:HG23	2.17	0.45
7:X:12:HIS:CD2	7:X:13:ILE:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:139:THR:HB	13:d:163:CYS:SG	2.57	0.45
10:J:129:ARG:HD2	10:J:207:PHE:CD2	2.52	0.44
17:Q:168:TYR:CZ	16:g:78:LEU:HD12	2.51	0.44
6:W:34:SER:OG	6:W:35:SER:N	2.50	0.44
10:a:148:GLN:O	10:a:152:GLN:CB	2.65	0.44
11:b:209:ASP:OD1	11:b:210:LEU:N	2.50	0.44
12:c:73:LEU:HD23	12:c:73:LEU:HA	1.88	0.44
14:e:142:LEU:HD23	14:e:160:ILE:HD11	1.99	0.44
6:F:177:ILE:HA	6:F:180:LEU:HD13	1.98	0.44
6:F:188:ARG:HD3	6:F:188:ARG:HA	1.77	0.44
10:J:148:GLN:O	10:J:152:GLN:CB	2.65	0.44
6:W:107:ILE:HD12	6:W:108:PRO:HD2	1.99	0.44
6:W:197:ILE:HA	6:W:200:ILE:HG22	1.97	0.44
7:X:143:ILE:HA	7:X:149:PRO:HA	1.99	0.44
10:a:129:ARG:HD2	10:a:207:PHE:CD2	2.52	0.44
13:d:41:LYS:O	13:d:106:GLY:HA2	2.17	0.44
5:E:158:ALA:HB1	5:E:172:LEU:HD21	1.99	0.44
7:G:12:HIS:CD2	7:G:13:ILE:H	2.35	0.44
10:J:133:GLN:OE1	10:J:140:ARG:NH2	2.50	0.44
13:M:43:LEU:HG	13:M:183:ILE:HD11	1.99	0.44
7:X:112:ASP:OD1	7:X:113:MET:N	2.51	0.44
10:a:133:GLN:OE1	10:a:140:ARG:NH2	2.50	0.44
11:b:203:ALA:O	11:b:206:ILE:HG22	2.17	0.44
16:g:107:TYR:HD2	16:g:108:LEU:HD12	1.83	0.44
16:g:221:LEU:HD12	16:g:221:LEU:HA	1.88	0.44
2:B:232:GLU:HA	2:B:235:GLN:HE22	1.82	0.44
6:F:34:SER:OG	6:F:35:SER:N	2.50	0.44
9:I:170:ARG:HA	9:I:170:ARG:HD3	1.68	0.44
14:N:224:TYR:CE2	12:c:204:MET:HE2	2.53	0.44
15:O:153:ASP:OD1	15:O:153:ASP:N	2.50	0.44
6:W:118:MET:HE2	6:W:118:MET:HB2	1.84	0.44
12:c:100:PHE:O	12:c:102:PRO:HD3	2.17	0.44
13:d:29:LYS:HB3	14:e:180:ILE:HD11	1.98	0.44
13:d:164:LEU:HD22	13:d:178:PHE:CE2	2.53	0.44
11:K:190:GLU:HG2	11:K:191:GLU:H	1.81	0.44
13:M:137:PHE:HB3	14:e:192:VAL:HG11	1.98	0.44
15:O:92:LEU:HD21	15:O:124:LEU:HD21	2.00	0.44
5:V:26:MET:O	5:V:29:VAL:HG12	2.18	0.44
11:b:111:LEU:HD23	11:b:111:LEU:HA	1.86	0.44
12:L:84:PRO:HB2	12:L:120:PHE:CD2	2.52	0.44
13:M:29:LYS:HB3	14:N:180:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:142:LEU:HD23	14:N:160:ILE:HD11	1.99	0.44
2:S:232:GLU:HA	2:S:235:GLN:HE22	1.82	0.44
5:V:189:LYS:NZ	5:V:235:GLY:H	2.16	0.44
1:A:65:VAL:HG12	1:A:75:VAL:HB	2.00	0.44
2:B:111:VAL:HG22	2:B:136:TYR:CD2	2.52	0.44
3:C:99:GLU:OE2	14:N:140:LYS:NZ	2.37	0.44
5:E:189:LYS:NZ	5:E:235:GLY:H	2.16	0.44
12:L:183:MET:HB3	12:L:204:MET:HE1	1.98	0.44
1:R:28:ALA:HB2	7:X:20:GLY:HA3	2.00	0.44
12:c:87:LEU:O	12:c:91:VAL:HG23	2.18	0.44
16:g:222:TYR:HE2	16:g:252:THR:HG21	1.83	0.44
3:C:117:ARG:HD3	8:H:140:LEU:HD21	2.00	0.44
13:M:139:THR:HB	13:M:163:CYS:SG	2.57	0.44
3:T:118:TYR:HE1	3:T:124:ARG:HD2	1.83	0.44
10:a:180:ARG:HA	10:a:188:LYS:NZ	2.33	0.44
5:E:26:MET:O	5:E:29:VAL:HG12	2.18	0.44
10:J:60:PRO:O	10:J:250:SER:OG	2.36	0.44
11:K:195:LYS:HG2	11:K:218:LEU:HD13	1.99	0.44
11:K:203:ALA:O	11:K:206:ILE:HG22	2.17	0.44
11:K:230:ARG:HA	11:K:231:PRO:HA	1.84	0.44
12:L:204:MET:HE2	14:e:224:TYR:CE2	2.53	0.44
14:N:103:THR:HG1	14:N:159:MET:H	1.61	0.44
11:b:219:CYS:O	11:b:221:ILE:HG23	2.18	0.44
16:g:160:TYR:CE2	16:g:239:GLU:HB3	2.52	0.44
2:B:90:LEU:O	2:B:93:ILE:HG22	2.18	0.43
7:G:90:GLN:HG3	7:G:134:LEU:HD11	2.00	0.43
11:K:209:ASP:OD1	11:K:210:LEU:N	2.50	0.43
12:L:20:VAL:HG21	12:L:110:ALA:HB1	2.00	0.43
13:M:114:ALA:HB1	13:M:116:TYR:HE1	1.83	0.43
16:P:107:TYR:HD2	16:P:108:LEU:HD12	1.83	0.43
4:U:196:LYS:O	4:U:200:ILE:HG12	2.17	0.43
5:V:3:ARG:HH11	10:a:256:GLY:HA3	1.83	0.43
7:X:155:ASP:OD1	7:X:159:TYR:N	2.51	0.43
11:b:195:LYS:HG2	11:b:218:LEU:HD13	1.99	0.43
14:e:182:GLY:HA3	14:e:185:PHE:HE1	1.83	0.43
15:f:92:LEU:HD21	15:f:124:LEU:HD21	2.00	0.43
15:f:176:LEU:HD22	15:f:206:VAL:HG22	2.00	0.43
17:h:69:THR:HG1	17:h:79:ARG:NH1	2.14	0.43
1:A:70:LYS:HB3	1:A:70:LYS:HE3	1.81	0.43
3:C:118:TYR:HE1	3:C:124:ARG:HD2	1.83	0.43
11:K:44:THR:OG1	11:K:76:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:25:ASP:OD1	12:L:25:ASP:N	2.49	0.43
13:M:164:LEU:HD22	13:M:178:PHE:CE2	2.53	0.43
2:S:134:LEU:HB3	2:S:136:TYR:CE1	2.53	0.43
6:W:126:TYR:CE2	7:X:131:MET:HE1	2.53	0.43
6:W:177:ILE:HA	6:W:180:LEU:HD13	1.98	0.43
2:B:174:MET:SD	2:B:195:LYS:NZ	2.87	0.43
16:P:160:TYR:CE2	16:P:239:GLU:HB3	2.52	0.43
4:U:217:LEU:HB3	4:U:229:PHE:HD2	1.84	0.43
6:F:71:ASP:HB3	6:F:74:VAL:HG22	2.01	0.43
7:G:112:ASP:OD1	7:G:113:MET:N	2.51	0.43
11:K:94:ASP:OD2	12:L:99:ARG:NH2	2.50	0.43
14:N:182:GLY:HA3	14:N:185:PHE:HE1	1.83	0.43
15:O:170:SER:C	15:O:172:MET:H	2.26	0.43
3:T:203:GLY:H	3:T:206:ILE:HD13	1.83	0.43
7:X:90:GLN:HG3	7:X:134:LEU:HD11	2.00	0.43
17:h:198:MET:HE3	17:h:206:GLY:N	2.34	0.43
3:C:41:VAL:HG23	3:C:211:MET:HB3	2.00	0.43
7:G:155:ASP:OD1	7:G:159:TYR:N	2.51	0.43
12:L:100:PHE:O	12:L:102:PRO:HD3	2.17	0.43
15:O:54:ASP:OD1	15:O:54:ASP:N	2.51	0.43
17:Q:230:LYS:HA	17:Q:230:LYS:HD2	1.82	0.43
3:T:41:VAL:HG23	3:T:211:MET:HB3	2.00	0.43
4:U:199:LEU:HD21	4:U:217:LEU:HD21	2.00	0.43
10:a:36:ILE:HD11	10:a:87:ALA:HB3	2.01	0.43
3:C:203:GLY:H	3:C:206:ILE:HD13	1.83	0.43
10:J:180:ARG:HA	10:J:188:LYS:NZ	2.33	0.43
11:K:57:LEU:HD23	11:K:87:CYS:SG	2.59	0.43
15:O:176:LEU:HD22	15:O:206:VAL:HG22	2.00	0.43
1:A:28:ALA:HB2	7:G:20:GLY:HA3	2.00	0.43
4:D:16:SER:O	4:D:17:PRO:C	2.61	0.43
6:F:126:TYR:CE2	7:G:131:MET:HE1	2.53	0.43
6:F:155:SER:OG	6:F:156:GLY:N	2.50	0.43
8:H:66:THR:O	8:H:70:ILE:HG22	2.19	0.43
11:K:106:LEU:HD11	11:K:122:ALA:HB2	1.99	0.43
11:K:165:LEU:HD11	17:Q:62:ASN:OD1	2.19	0.43
16:P:180:PRO:HB2	16:P:199:LEU:HD13	2.01	0.43
16:P:222:TYR:HE2	16:P:252:THR:HG21	1.83	0.43
17:Q:201:ASP:OD1	17:Q:202:GLY:N	2.52	0.43
2:S:90:LEU:O	2:S:93:ILE:HG22	2.18	0.43
5:V:71:GLY:HA3	5:V:221:PHE:CZ	2.53	0.43
5:V:218:ASP:OD1	5:V:218:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:84:LYS:HB2	8:Y:84:LYS:HE3	1.84	0.43
5:E:3:ARG:HH11	10:J:256:GLY:HA3	1.83	0.43
7:G:62:ASP:OD1	7:G:63:SER:N	2.52	0.43
11:K:182:GLU:OE1	16:g:224:ARG:NE	2.50	0.43
12:L:87:LEU:O	12:L:91:VAL:HG23	2.18	0.43
11:b:169:THR:HB	11:b:178:MET:HB2	2.01	0.43
12:c:20:VAL:HG21	12:c:110:ALA:HB1	2.00	0.43
13:d:4:LEU:HD22	13:d:45:LEU:HD13	2.00	0.43
14:e:111:CYS:O	14:e:115:GLU:HG2	2.19	0.43
15:f:54:ASP:OD1	15:f:54:ASP:N	2.51	0.43
10:J:36:ILE:HD11	10:J:87:ALA:HB3	2.01	0.43
8:Y:101:SER:C	8:Y:103:ASP:H	2.27	0.43
4:D:108:THR:HG22	4:D:110:GLU:HG2	2.01	0.43
5:E:185:ASN:O	5:E:189:LYS:HG2	2.19	0.43
8:H:95:LEU:HD23	8:H:95:LEU:HA	1.77	0.43
9:I:214:ASP:CG	9:I:215:LEU:N	2.77	0.43
13:M:4:LEU:HD22	13:M:45:LEU:HD13	1.99	0.43
17:Q:198:MET:HE3	17:Q:206:GLY:N	2.34	0.43
7:X:62:ASP:OD1	7:X:63:SER:N	2.52	0.43
8:Y:40:ASN:HD21	13:d:95:ARG:C	2.25	0.43
13:d:114:ALA:HB1	13:d:116:TYR:HE1	1.83	0.43
15:f:33:TYR:OH	15:f:131:PRO:O	2.31	0.43
1:A:160:ALA:HB3	2:B:55:LEU:HD13	2.01	0.42
4:D:52:LYS:NZ	4:D:61:PRO:O	2.38	0.42
5:E:71:GLY:HA3	5:E:221:PHE:CZ	2.53	0.42
13:M:19:ARG:HD2	13:M:179:SER:HB2	2.01	0.42
5:V:38:LEU:HB3	5:V:187:LEU:HD11	2.01	0.42
6:W:137:MET:HE2	6:W:137:MET:HB3	1.89	0.42
8:Y:66:THR:O	8:Y:70:ILE:HG22	2.19	0.42
9:Z:207:GLU:HB3	9:Z:209:PRO:HD2	2.01	0.42
11:b:44:THR:OG1	11:b:76:LYS:NZ	2.51	0.42
11:b:57:LEU:HD23	11:b:87:CYS:SG	2.59	0.42
2:B:134:LEU:HB3	2:B:136:TYR:CE1	2.53	0.42
5:E:226:ASP:O	5:E:229:VAL:HG22	2.19	0.42
6:F:201:VAL:HG13	6:F:201:VAL:O	2.19	0.42
11:K:93:ALA:HB2	12:L:129:CYS:HB2	2.00	0.42
13:M:18:ASP:N	13:M:18:ASP:OD1	2.51	0.42
2:S:109:GLN:N	2:S:109:GLN:OE1	2.52	0.42
6:W:71:ASP:OD1	6:W:72:ARG:N	2.48	0.42
6:W:201:VAL:HG13	6:W:201:VAL:O	2.19	0.42
8:Y:101:SER:O	8:Y:102:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:8:GLN:HG2	13:d:9:GLY:N	2.31	0.42
16:g:180:PRO:HB2	16:g:199:LEU:HD13	2.01	0.42
4:D:181:LEU:HA	4:D:184:VAL:HG12	2.02	0.42
6:W:41:ARG:HA	6:W:46:VAL:HA	2.01	0.42
9:Z:170:ARG:HA	9:Z:170:ARG:HD3	1.68	0.42
13:d:18:ASP:N	13:d:18:ASP:OD1	2.51	0.42
14:N:77:SER:OG	14:N:90:VAL:N	2.52	0.42
1:R:65:VAL:HG12	1:R:75:VAL:HB	2.00	0.42
7:X:70:PHE:HB2	7:X:78:CYS:SG	2.59	0.42
7:X:79:VAL:HG12	7:X:139:ILE:HB	2.01	0.42
12:c:172:LEU:HD11	12:c:201:LYS:O	2.19	0.42
13:d:43:LEU:HG	13:d:183:ILE:HD11	1.99	0.42
2:B:117:ILE:HG23	8:H:94:PHE:CE1	2.55	0.42
12:L:204:MET:HE3	12:L:204:MET:HA	2.01	0.42
14:N:111:CYS:O	14:N:115:GLU:HG2	2.19	0.42
3:T:117:ARG:HD3	8:Y:140:LEU:HD21	2.00	0.42
4:U:39:GLY:O	4:U:167:ALA:HA	2.19	0.42
11:b:93:ALA:HB2	12:c:129:CYS:HB2	2.00	0.42
11:b:96:ASP:OD2	11:b:100:GLN:NE2	2.52	0.42
17:h:201:ASP:OD1	17:h:202:GLY:N	2.52	0.42
5:E:156:CYS:SG	5:E:158:ALA:N	2.93	0.42
11:K:169:THR:HB	11:K:178:MET:HB2	2.01	0.42
11:K:251:THR:HG23	15:f:186:MET:HG2	2.02	0.42
14:N:66:LYS:HB3	14:N:71:VAL:HG22	2.02	0.42
1:R:160:ALA:HB3	2:S:55:LEU:HD13	2.00	0.42
2:S:117:ILE:HG23	8:Y:94:PHE:CE1	2.54	0.42
4:U:108:THR:HG22	4:U:110:GLU:HG2	2.01	0.42
5:V:156:CYS:SG	5:V:158:ALA:N	2.93	0.42
5:V:185:ASN:O	5:V:189:LYS:HG2	2.19	0.42
6:W:29:LYS:HE3	6:W:29:LYS:HB2	1.62	0.42
6:W:98:ASN:C	6:W:98:ASN:HD22	2.27	0.42
6:W:188:ARG:HA	6:W:188:ARG:HD3	1.77	0.42
2:B:109:GLN:N	2:B:109:GLN:OE1	2.52	0.42
3:C:170:GLU:O	3:C:173:GLU:HG3	2.20	0.42
4:D:39:GLY:O	4:D:167:ALA:HA	2.19	0.42
4:D:71:ASP:OD1	4:D:72:ALA:N	2.48	0.42
6:F:126:TYR:CD1	8:H:81:MET:HE1	2.55	0.42
8:H:32:ARG:NH2	8:H:132:LEU:HD22	2.35	0.42
8:H:101:SER:C	8:H:103:ASP:H	2.27	0.42
4:D:217:LEU:HB3	4:D:229:PHE:HD2	1.83	0.42
5:E:38:LEU:HB3	5:E:187:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:15:PHE:O	10:J:115:CYS:HB2	2.20	0.42
11:K:96:ASP:OD2	11:K:100:GLN:NE2	2.52	0.42
12:L:172:LEU:HD11	12:L:201:LYS:O	2.19	0.42
5:V:226:ASP:O	5:V:229:VAL:HG22	2.19	0.42
6:W:71:ASP:HB3	6:W:74:VAL:HG22	2.01	0.42
10:a:162:GLU:HG3	10:a:163:MET:N	2.35	0.42
2:B:14:PRO:HA	3:C:21:TYR:CE1	2.55	0.42
6:F:98:ASN:C	6:F:98:ASN:HD22	2.27	0.42
9:I:128:SER:OG	9:I:129:ASN:N	2.49	0.42
10:J:162:GLU:HG3	10:J:163:MET:N	2.35	0.42
17:Q:69:THR:HG1	17:Q:79:ARG:NH1	2.13	0.42
12:c:191:GLU:OE2	12:c:194:LYS:NZ	2.34	0.42
12:c:204:MET:HE3	12:c:204:MET:HA	2.01	0.42
13:d:13:VAL:O	13:d:15:VAL:HG13	2.20	0.42
15:f:151:SER:HB2	15:f:164:LYS:HG2	2.02	0.42
7:G:179:LEU:HD23	7:G:179:LEU:HA	1.86	0.42
9:I:207:GLU:HB3	9:I:209:PRO:HD2	2.01	0.42
11:K:110:SER:HB2	11:K:117:PRO:HG3	2.02	0.42
13:M:41:LYS:O	13:M:106:GLY:HA2	2.20	0.42
3:T:40:ILE:HD12	3:T:40:ILE:HA	1.96	0.42
4:U:52:LYS:NZ	4:U:61:PRO:O	2.38	0.42
6:W:126:TYR:CD1	8:Y:81:MET:HE1	2.55	0.42
8:Y:32:ARG:NH2	8:Y:132:LEU:HD22	2.35	0.42
9:Z:265:ASN:ND2	9:Z:268:GLN:HB2	2.35	0.42
14:e:77:SER:OG	14:e:90:VAL:N	2.52	0.42
15:f:170:SER:C	15:f:172:MET:H	2.26	0.42
2:B:90:LEU:HB2	2:B:114:LEU:HD22	2.02	0.41
6:F:156:GLY:HA3	7:G:85:ALA:HB2	2.01	0.41
7:G:70:PHE:HB2	7:G:78:CYS:SG	2.59	0.41
8:Y:95:LEU:HD23	8:Y:95:LEU:HA	1.77	0.41
9:I:127:LYS:HA	9:I:127:LYS:HD3	1.78	0.41
14:N:96:ILE:HG13	14:N:97:ASN:OD1	2.20	0.41
1:R:156:PHE:HB2	1:R:158:TRP:CD1	2.55	0.41
2:S:14:PRO:HA	3:T:21:TYR:CE1	2.55	0.41
15:f:50:ILE:HG12	15:f:225:ILE:HG13	2.02	0.41
2:B:165:GLY:O	2:B:168:SER:HB3	2.20	0.41
6:F:53:LEU:HD23	6:F:53:LEU:HA	1.87	0.41
7:G:12:HIS:HD2	7:G:14:THR:HG22	1.84	0.41
7:G:239:LEU:HD12	7:G:239:LEU:HA	1.89	0.41
9:I:265:ASN:ND2	9:I:268:GLN:HB2	2.35	0.41
10:J:20:PRO:HD2	10:J:88:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:77:ILE:HG21	11:K:219:CYS:SG	2.60	0.41
2:S:72:MET:HG2	2:S:138:GLY:HA3	2.02	0.41
9:Z:214:ASP:CG	9:Z:215:LEU:N	2.77	0.41
14:e:96:ILE:HG13	14:e:97:ASN:OD1	2.19	0.41
1:A:156:PHE:HB2	1:A:158:TRP:CD1	2.55	0.41
8:H:101:SER:O	8:H:102:LEU:HB3	2.19	0.41
11:K:165:LEU:HD21	17:Q:62:ASN:CG	2.46	0.41
14:N:70:GLY:HA2	14:N:163:TRP:HZ3	1.85	0.41
15:O:183:PHE:CE2	15:O:191:HIS:HA	2.56	0.41
2:S:90:LEU:HB2	2:S:114:LEU:HD22	2.02	0.41
5:V:138:ASP:OD1	5:V:139:ASP:N	2.47	0.41
12:c:15:LYS:HB2	12:c:15:LYS:HE3	1.89	0.41
15:f:153:ASP:OD1	15:f:153:ASP:N	2.50	0.41
17:h:230:LYS:HA	17:h:230:LYS:HD2	1.82	0.41
8:H:64:PHE:HE1	8:H:79:LEU:HD23	1.86	0.41
12:L:14:MET:HE2	12:L:150:CYS:SG	2.61	0.41
13:M:13:VAL:O	13:M:15:VAL:HG13	2.20	0.41
4:U:71:ASP:OD1	4:U:72:ALA:N	2.49	0.41
4:U:181:LEU:HA	4:U:184:VAL:HG12	2.02	0.41
7:X:98:ALA:HA	7:X:109:ILE:CD1	2.50	0.41
8:Y:35:PHE:HD2	13:d:91:CYS:HB3	1.86	0.41
11:b:110:SER:HB2	11:b:117:PRO:HG3	2.02	0.41
15:f:120:LEU:HD21	15:f:136:ASN:HD22	1.86	0.41
7:G:23:TYR:OH	10:J:131:ASP:OD1	2.32	0.41
7:G:98:ALA:HA	7:G:109:ILE:CD1	2.50	0.41
15:O:83:SER:OG	15:O:84:GLY:N	2.54	0.41
15:O:151:SER:HB2	15:O:164:LYS:HG2	2.02	0.41
1:R:114:VAL:HA	1:R:117:VAL:HG12	2.03	0.41
8:Y:64:PHE:HE1	8:Y:79:LEU:HD23	1.86	0.41
12:c:20:VAL:HG13	12:c:190:ILE:HD12	2.03	0.41
14:e:70:GLY:HA2	14:e:163:TRP:HZ3	1.84	0.41
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.92	0.41
3:C:157:LYS:HB2	3:C:157:LYS:HE3	1.81	0.41
4:D:164:GLN:NE2	4:D:165:CYS:O	2.53	0.41
12:L:66:ARG:NH2	12:L:97:GLU:OE2	2.52	0.41
15:O:50:ILE:HG12	15:O:225:ILE:HG13	2.02	0.41
15:O:196:LEU:HD12	15:O:196:LEU:HA	1.88	0.41
2:S:197:LEU:HD12	2:S:197:LEU:HA	1.89	0.41
5:V:212:ILE:HD12	5:V:212:ILE:H	1.86	0.41
9:Z:86:PHE:HA	9:Z:269:SER:OG	2.21	0.41
12:c:66:ARG:NH2	12:c:97:GLU:OE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:83:SER:OG	15:f:84:GLY:N	2.53	0.41
15:f:184:LYS:HE3	15:f:184:LYS:HB3	1.87	0.41
2:B:18:LEU:HD23	2:B:18:LEU:HA	1.81	0.41
5:E:212:ILE:H	5:E:212:ILE:HD12	1.86	0.41
4:U:164:GLN:NE2	4:U:165:CYS:O	2.53	0.41
6:W:88:LEU:HD23	6:W:88:LEU:HA	1.86	0.41
7:X:112:ASP:OD1	7:X:113:MET:HG2	2.21	0.41
9:Z:127:LYS:HA	9:Z:127:LYS:HD3	1.78	0.41
10:a:20:PRO:HD2	10:a:88:LEU:HB3	2.03	0.41
11:b:77:ILE:HG21	11:b:219:CYS:SG	2.60	0.41
11:b:165:LEU:HD11	17:h:62:ASN:OD1	2.19	0.41
12:c:20:VAL:HG23	12:c:121:ILE:HD11	2.03	0.41
13:d:107:TYR:CE2	13:d:185:LYS:HB3	2.56	0.41
16:g:169:TYR:HB2	16:g:182:LEU:HD21	2.01	0.41
2:B:9:THR:HB	2:B:20:GLN:HG2	2.03	0.41
3:C:148:ASP:OD1	3:C:149:PRO:HD2	2.21	0.41
6:F:9:ASP:OD1	6:F:9:ASP:N	2.45	0.41
6:F:41:ARG:HA	6:F:46:VAL:HA	2.01	0.41
6:F:170:ARG:O	6:F:174:LYS:HG2	2.21	0.41
7:G:112:ASP:OD1	7:G:113:MET:HG2	2.21	0.41
8:H:70:ILE:HD11	17:Q:100:HIS:HB2	2.03	0.41
8:H:92:LEU:HD23	8:H:92:LEU:HA	1.85	0.41
11:K:40:ARG:NH2	12:L:131:MET:HG2	2.36	0.41
11:K:77:ILE:HG13	11:K:219:CYS:SG	2.61	0.41
15:O:41:LEU:HD12	15:O:173:LEU:HD12	2.03	0.41
15:O:186:MET:HG2	11:b:251:THR:HG23	2.02	0.41
16:P:169:TYR:HB2	16:P:182:LEU:HD21	2.01	0.41
1:R:31:GLY:HA2	1:R:165:LYS:NZ	2.36	0.41
1:R:124:SER:OG	1:R:125:GLY:N	2.54	0.41
2:S:111:VAL:HG22	2:S:136:TYR:CD2	2.52	0.41
2:S:165:GLY:O	2:S:168:SER:HB3	2.20	0.41
3:T:170:GLU:O	3:T:173:GLU:HG3	2.20	0.41
6:W:156:GLY:HA3	7:X:85:ALA:HB2	2.01	0.41
11:b:135:GLY:C	11:b:137:ILE:H	2.29	0.41
14:e:55:GLU:O	14:e:56:MET:HG2	2.21	0.41
15:f:41:LEU:HD12	15:f:173:LEU:HD12	2.02	0.41
16:g:91:ASN:HB3	16:g:116:VAL:HG21	2.03	0.41
1:A:124:SER:OG	1:A:125:GLY:N	2.54	0.41
10:J:107:LEU:HD12	10:J:199:ILE:HD12	2.03	0.41
12:L:20:VAL:HG23	12:L:121:ILE:HD11	2.03	0.41
17:Q:124:TYR:HB3	17:Q:128:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:28:MET:O	6:W:31:VAL:HG12	2.20	0.41
6:W:71:ASP:CG	6:W:100:ARG:HH12	2.29	0.41
6:W:170:ARG:O	6:W:174:LYS:HG2	2.21	0.41
10:a:17:LEU:HB2	10:a:118:VAL:HG22	2.03	0.41
17:h:124:TYR:HB3	17:h:128:LEU:HD23	2.03	0.41
6:F:28:MET:O	6:F:31:VAL:HG12	2.20	0.40
8:H:35:PHE:HD2	13:M:91:CYS:HB3	1.86	0.40
13:M:38:MET:HE3	13:M:44:LEU:HB3	2.03	0.40
4:U:133:MET:HE3	4:U:137:PHE:HZ	1.85	0.40
5:V:107:ARG:NE	16:g:124:ASP:OD2	2.53	0.40
8:Y:70:ILE:HD11	17:h:100:HIS:HB2	2.03	0.40
11:b:170:MET:HE3	11:b:170:MET:HB3	1.80	0.40
1:A:158:TRP:CG	1:A:161:THR:HG1	2.39	0.40
2:B:72:MET:HG2	2:B:138:GLY:HA3	2.02	0.40
11:K:111:LEU:HD23	11:K:111:LEU:HA	1.86	0.40
14:N:55:GLU:O	14:N:56:MET:HG2	2.21	0.40
15:O:41:LEU:HD11	15:O:177:LEU:HD11	2.02	0.40
15:O:184:LYS:HE3	15:O:184:LYS:HB3	1.87	0.40
5:V:189:LYS:HZ1	5:V:235:GLY:H	1.67	0.40
10:a:15:PHE:O	10:a:115:CYS:HB2	2.20	0.40
11:b:77:ILE:HG13	11:b:219:CYS:SG	2.61	0.40
11:b:230:ARG:HA	11:b:231:PRO:HA	1.84	0.40
12:c:14:MET:HE2	12:c:150:CYS:SG	2.61	0.40
12:c:77:LYS:HE3	12:c:77:LYS:HB3	1.89	0.40
14:e:66:LYS:HB3	14:e:71:VAL:HG22	2.04	0.40
1:A:114:VAL:HA	1:A:117:VAL:HG12	2.03	0.40
4:D:200:ILE:HD13	4:D:200:ILE:HA	1.90	0.40
16:P:91:ASN:HB3	16:P:116:VAL:HG21	2.03	0.40
4:U:16:SER:O	4:U:17:PRO:C	2.64	0.40
6:W:197:ILE:O	6:W:200:ILE:HG22	2.21	0.40
7:X:10:ASP:OD1	7:X:10:ASP:N	2.54	0.40
11:b:40:ARG:NH2	12:c:131:MET:HG2	2.36	0.40
12:c:123:SER:HB3	12:c:131:MET:SD	2.61	0.40
3:C:19:VAL:CG1	3:C:150:SER:HB2	2.52	0.40
6:F:124:THR:O	7:G:132:ARG:NH2	2.34	0.40
7:G:10:ASP:N	7:G:10:ASP:OD1	2.54	0.40
7:G:79:VAL:HG12	7:G:139:ILE:HB	2.01	0.40
11:K:15:SER:HB3	12:L:98:LYS:HG2	2.02	0.40
15:O:120:LEU:HD21	15:O:136:ASN:HD22	1.87	0.40
3:T:67:ASP:OD1	3:T:67:ASP:N	2.53	0.40
6:W:41:ARG:HG2	6:W:162:TRP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:ARG:NH2	9:I:4:THR:HG21	2.37	0.40
4:D:82:ILE:HD13	4:D:82:ILE:HA	1.94	0.40
10:J:141:TYR:OH	10:J:162:GLU:OE1	2.36	0.40
10:J:214:ILE:H	10:J:214:ILE:HG13	1.74	0.40
12:L:20:VAL:HG13	12:L:190:ILE:HD12	2.03	0.40
3:T:19:VAL:CG1	3:T:150:SER:HB2	2.52	0.40
4:U:107:MET:HA	4:U:107:MET:HE2	2.03	0.40
6:W:199:TYR:OH	6:W:237:GLU:OE2	2.31	0.40
8:Y:92:LEU:HD23	8:Y:92:LEU:HA	1.85	0.40
11:b:165:LEU:HD21	17:h:62:ASN:CG	2.46	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	227/234 (97%)	199 (88%)	28 (12%)	0	100	100
1	R	227/234 (97%)	199 (88%)	28 (12%)	0	100	100
2	B	246/248 (99%)	211 (86%)	35 (14%)	0	100	100
2	S	246/248 (99%)	210 (85%)	36 (15%)	0	100	100
3	C	232/234 (99%)	206 (89%)	26 (11%)	0	100	100
3	T	232/234 (99%)	206 (89%)	26 (11%)	0	100	100
4	D	232/240 (97%)	215 (93%)	17 (7%)	0	100	100
4	U	232/240 (97%)	215 (93%)	17 (7%)	0	100	100
5	E	239/241 (99%)	210 (88%)	29 (12%)	0	100	100
5	V	239/241 (99%)	211 (88%)	28 (12%)	0	100	100
6	F	239/241 (99%)	215 (90%)	24 (10%)	0	100	100
6	W	239/241 (99%)	215 (90%)	24 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	242/244 (99%)	226 (93%)	16 (7%)	0	100	100
7	X	242/244 (99%)	227 (94%)	15 (6%)	0	100	100
8	H	113/141 (80%)	100 (88%)	13 (12%)	0	100	100
8	Y	113/141 (80%)	100 (88%)	13 (12%)	0	100	100
9	I	260/288 (90%)	234 (90%)	26 (10%)	0	100	100
9	Z	260/288 (90%)	234 (90%)	26 (10%)	0	100	100
10	J	242/264 (92%)	229 (95%)	13 (5%)	0	100	100
10	a	242/264 (92%)	229 (95%)	13 (5%)	0	100	100
11	K	260/262 (99%)	240 (92%)	20 (8%)	0	100	100
11	b	260/262 (99%)	240 (92%)	20 (8%)	0	100	100
12	L	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
12	c	201/203 (99%)	183 (91%)	18 (9%)	0	100	100
13	M	195/197 (99%)	167 (86%)	28 (14%)	0	100	100
13	d	195/197 (99%)	167 (86%)	28 (14%)	0	100	100
14	N	206/208 (99%)	184 (89%)	22 (11%)	0	100	100
14	e	206/208 (99%)	184 (89%)	22 (11%)	0	100	100
15	O	210/212 (99%)	186 (89%)	24 (11%)	0	100	100
15	f	210/212 (99%)	185 (88%)	25 (12%)	0	100	100
16	P	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
16	g	206/208 (99%)	188 (91%)	18 (9%)	0	100	100
17	Q	195/197 (99%)	175 (90%)	20 (10%)	0	100	100
17	h	195/197 (99%)	175 (90%)	20 (10%)	0	100	100
All	All	7490/7724 (97%)	6737 (90%)	753 (10%)	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	A	171/191 (90%)	171 (100%)	0	100	100
1	R	171/191 (90%)	171 (100%)	0	100	100
2	B	173/208 (83%)	173 (100%)	0	100	100
2	S	173/208 (83%)	173 (100%)	0	100	100
3	C	173/198 (87%)	173 (100%)	0	100	100
3	T	173/198 (87%)	173 (100%)	0	100	100
4	D	186/202 (92%)	186 (100%)	0	100	100
4	U	186/202 (92%)	186 (100%)	0	100	100
5	E	197/207 (95%)	197 (100%)	0	100	100
5	V	197/207 (95%)	197 (100%)	0	100	100
6	F	189/198 (96%)	189 (100%)	0	100	100
6	W	189/198 (96%)	189 (100%)	0	100	100
7	G	193/208 (93%)	193 (100%)	0	100	100
7	X	193/208 (93%)	193 (100%)	0	100	100
8	H	109/128 (85%)	109 (100%)	0	100	100
8	Y	109/128 (85%)	109 (100%)	0	100	100
9	I	217/262 (83%)	217 (100%)	0	100	100
9	Z	217/262 (83%)	217 (100%)	0	100	100
10	J	208/237 (88%)	208 (100%)	0	100	100
10	a	208/237 (88%)	208 (100%)	0	100	100
11	K	213/213 (100%)	213 (100%)	0	100	100
11	b	213/213 (100%)	213 (100%)	0	100	100
12	L	172/172 (100%)	172 (100%)	0	100	100
12	c	172/172 (100%)	172 (100%)	0	100	100
13	M	166/168 (99%)	166 (100%)	0	100	100
13	d	166/168 (99%)	166 (100%)	0	100	100
14	N	161/162 (99%)	161 (100%)	0	100	100
14	e	161/162 (99%)	161 (100%)	0	100	100
15	O	177/177 (100%)	177 (100%)	0	100	100
15	f	177/177 (100%)	177 (100%)	0	100	100
16	P	171/171 (100%)	171 (100%)	0	100	100
16	g	171/171 (100%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	152/153 (99%)	152 (100%)	0	100	100
17	h	152/153 (99%)	152 (100%)	0	100	100
All	All	6056/6510 (93%)	6056 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	100	GLN
2	B	155	ASN
2	B	198	ASN
3	C	18	GLN
3	C	94	HIS
4	D	152	GLN
4	D	182	GLN
5	E	65	HIS
6	F	181	GLN
7	G	12	HIS
7	G	33	ASN
9	I	40	GLN
9	I	208	GLN
10	J	58	ASN
12	L	173	ASN
15	O	86	HIS
2	S	100	GLN
2	S	155	ASN
2	S	198	ASN
3	T	18	GLN
4	U	152	GLN
4	U	182	GLN
4	U	204	GLN
6	W	181	GLN
7	X	12	HIS
7	X	33	ASN
9	Z	40	GLN
12	c	157	ASN
12	c	173	ASN
15	f	86	HIS
16	g	153	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.

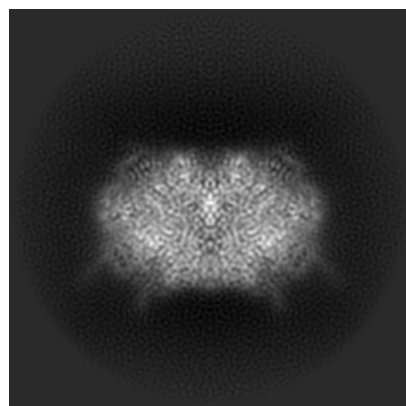
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18761. These allow visual inspection of the internal detail of the map and identification of artifacts.

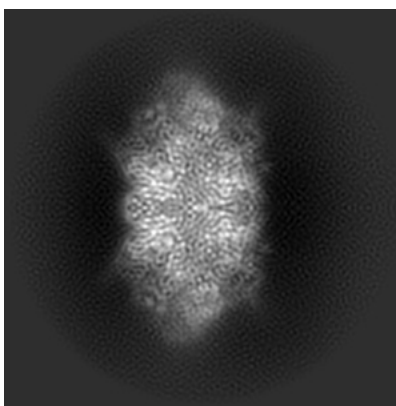
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

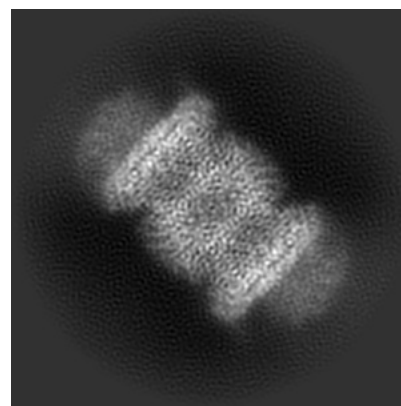
6.1.1 Primary map



X

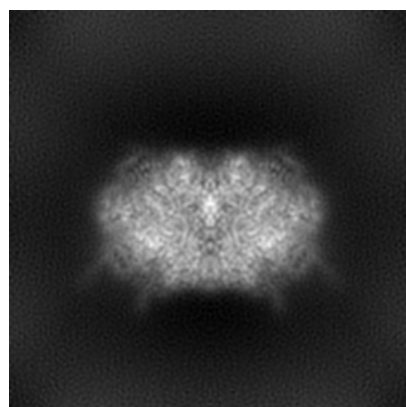


Y

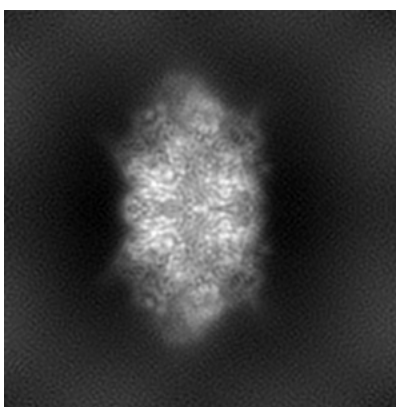


Z

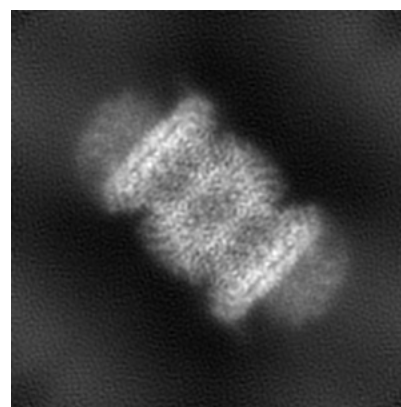
6.1.2 Raw map



X



Y

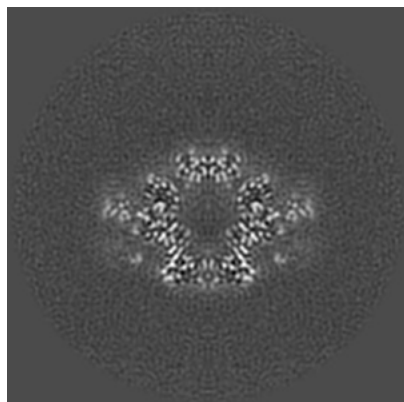


Z

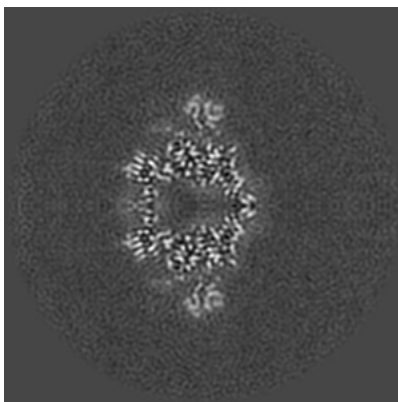
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

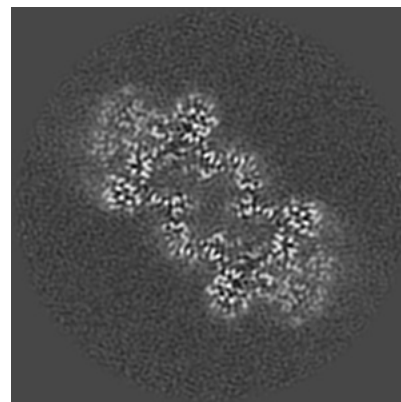
6.2.1 Primary map



X Index: 84

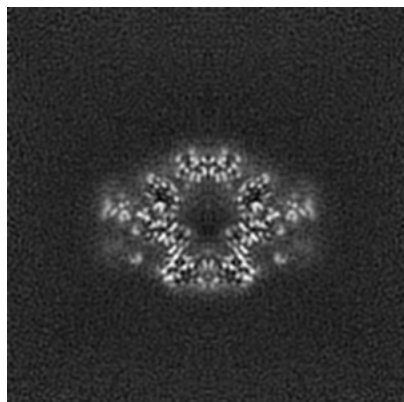


Y Index: 84

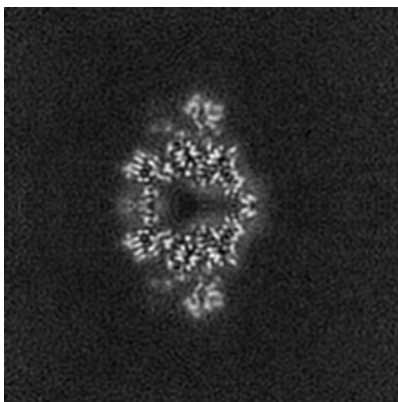


Z Index: 84

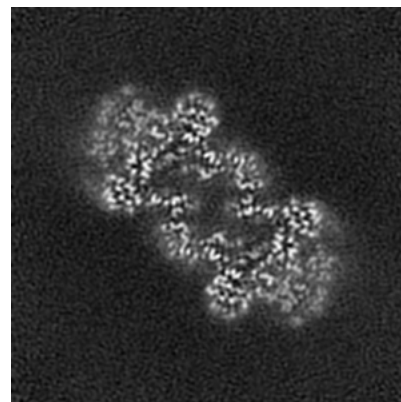
6.2.2 Raw map



X Index: 84



Y Index: 84

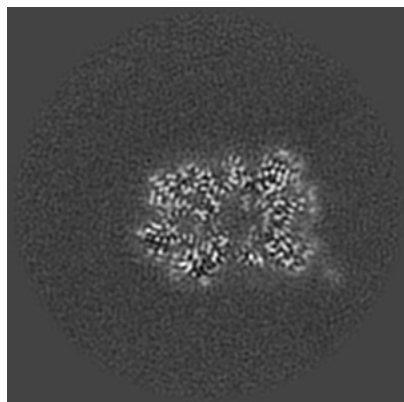


Z Index: 84

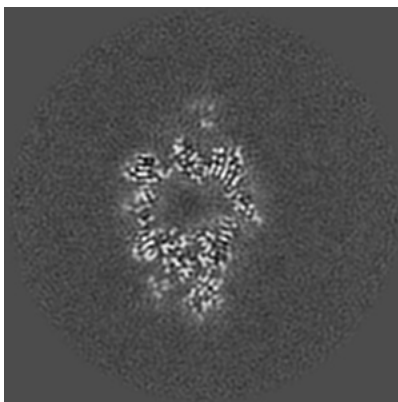
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

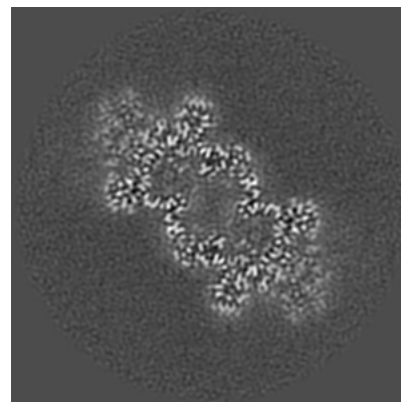
6.3.1 Primary map



X Index: 72

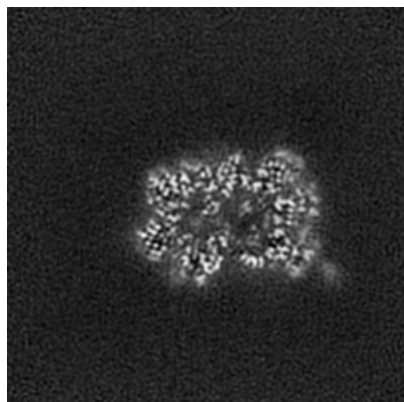


Y Index: 86

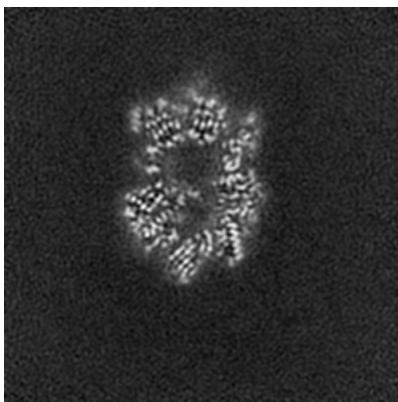


Z Index: 86

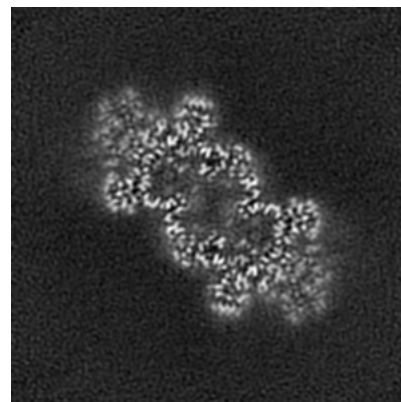
6.3.2 Raw map



X Index: 73



Y Index: 74

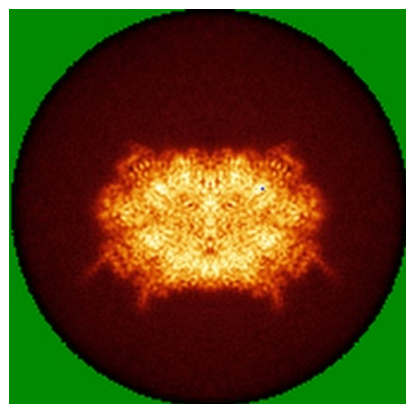


Z Index: 86

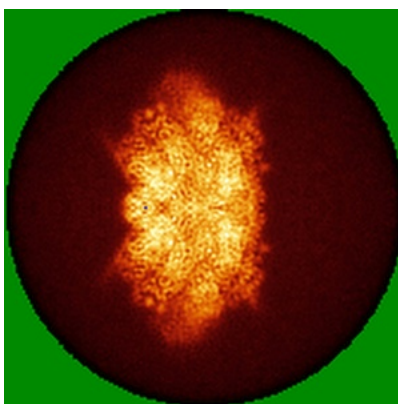
The images above show the largest variance slices of the map in three orthogonal directions.

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

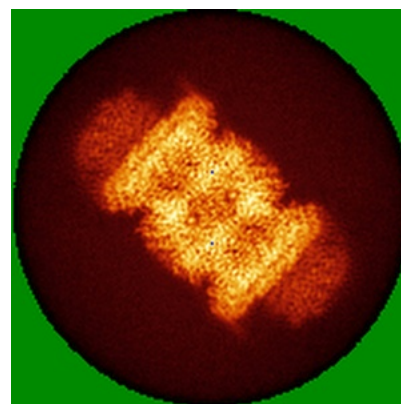
6.4.1 Primary map



X

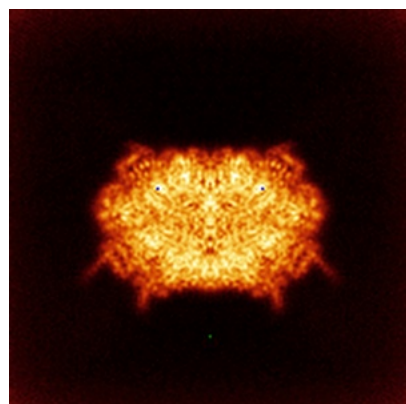


Y

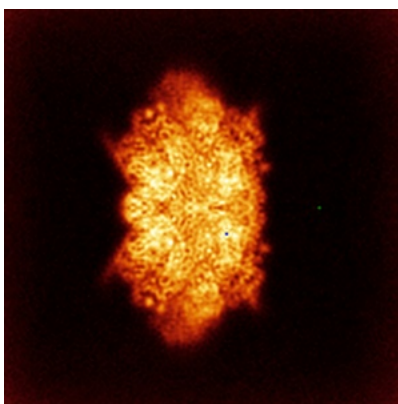


Z

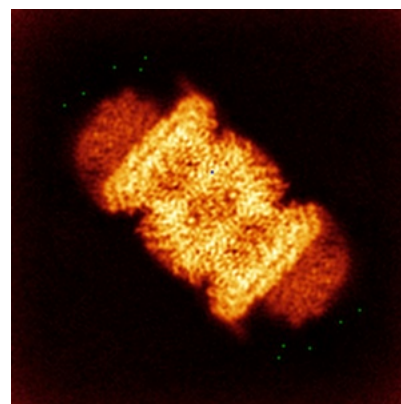
6.4.2 Raw map



X



Y

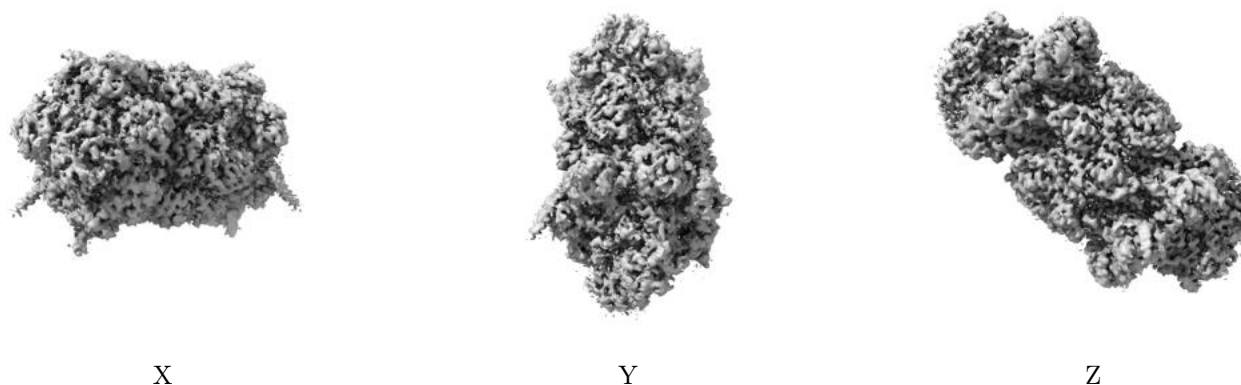


Z

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.

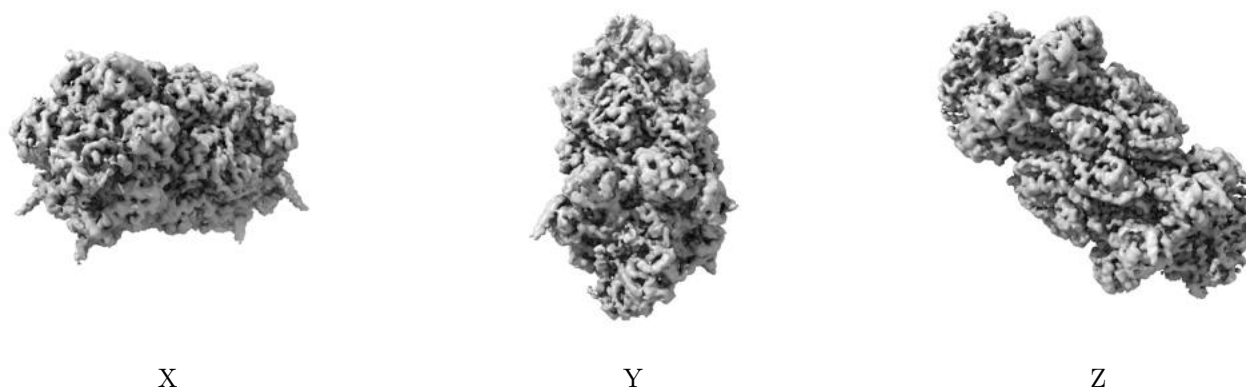
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.37. 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.

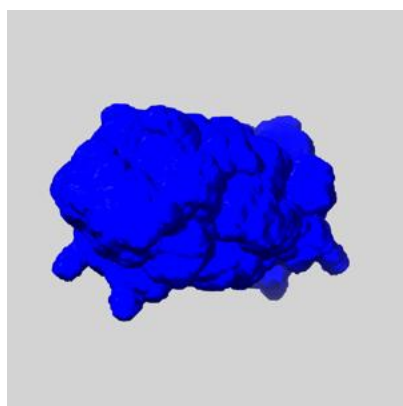
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

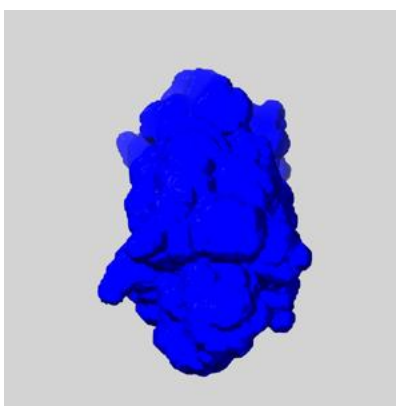
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

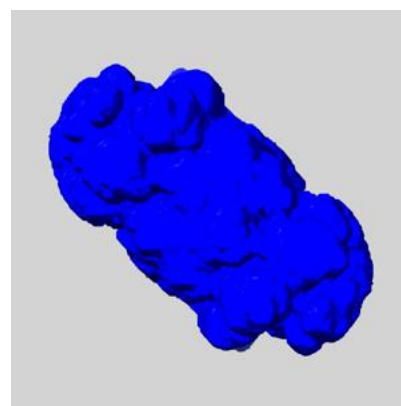
6.6.1 emd_18761_msk_1.map [i](#)



X



Y

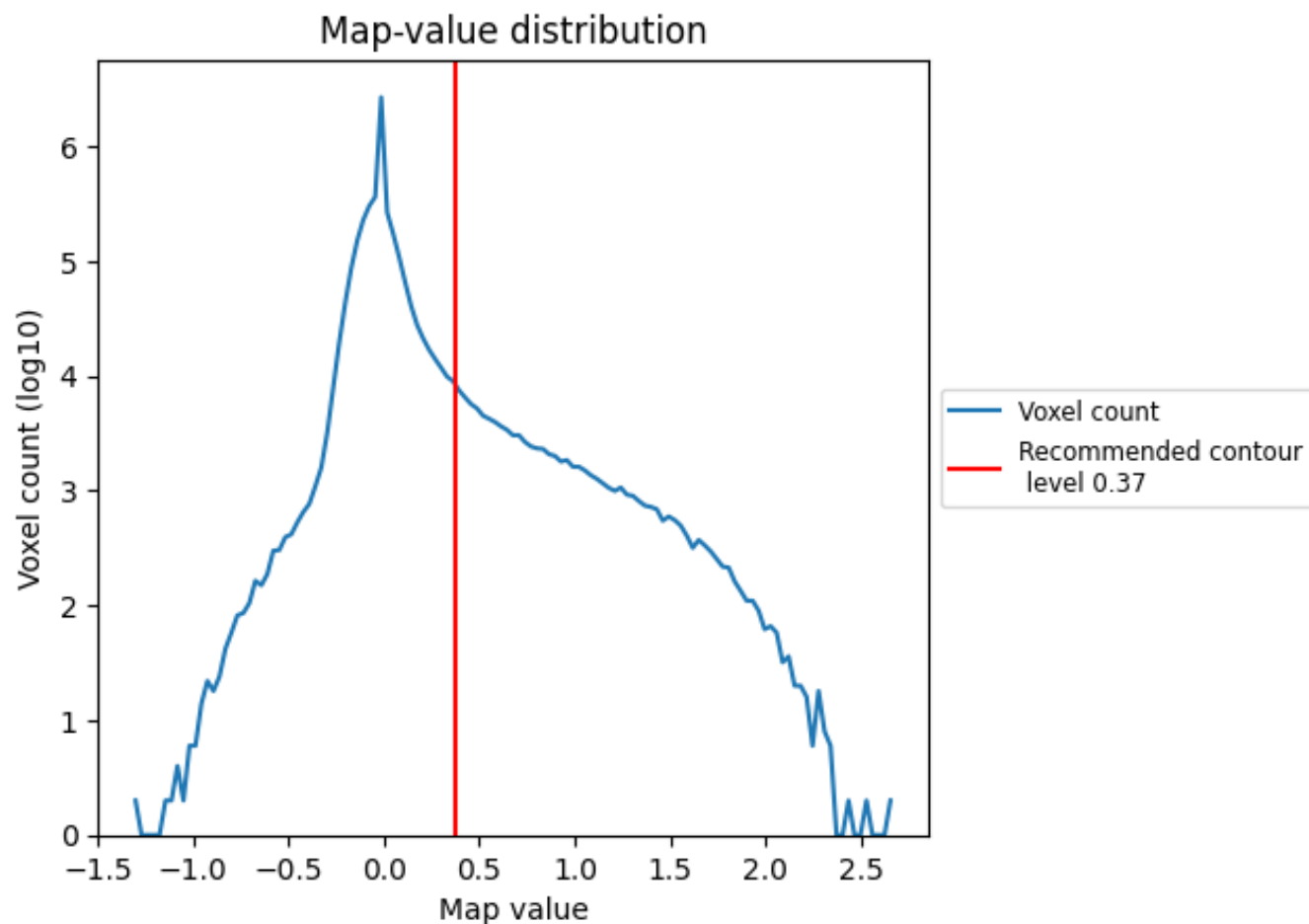


Z

7 Map analysis [i](#)

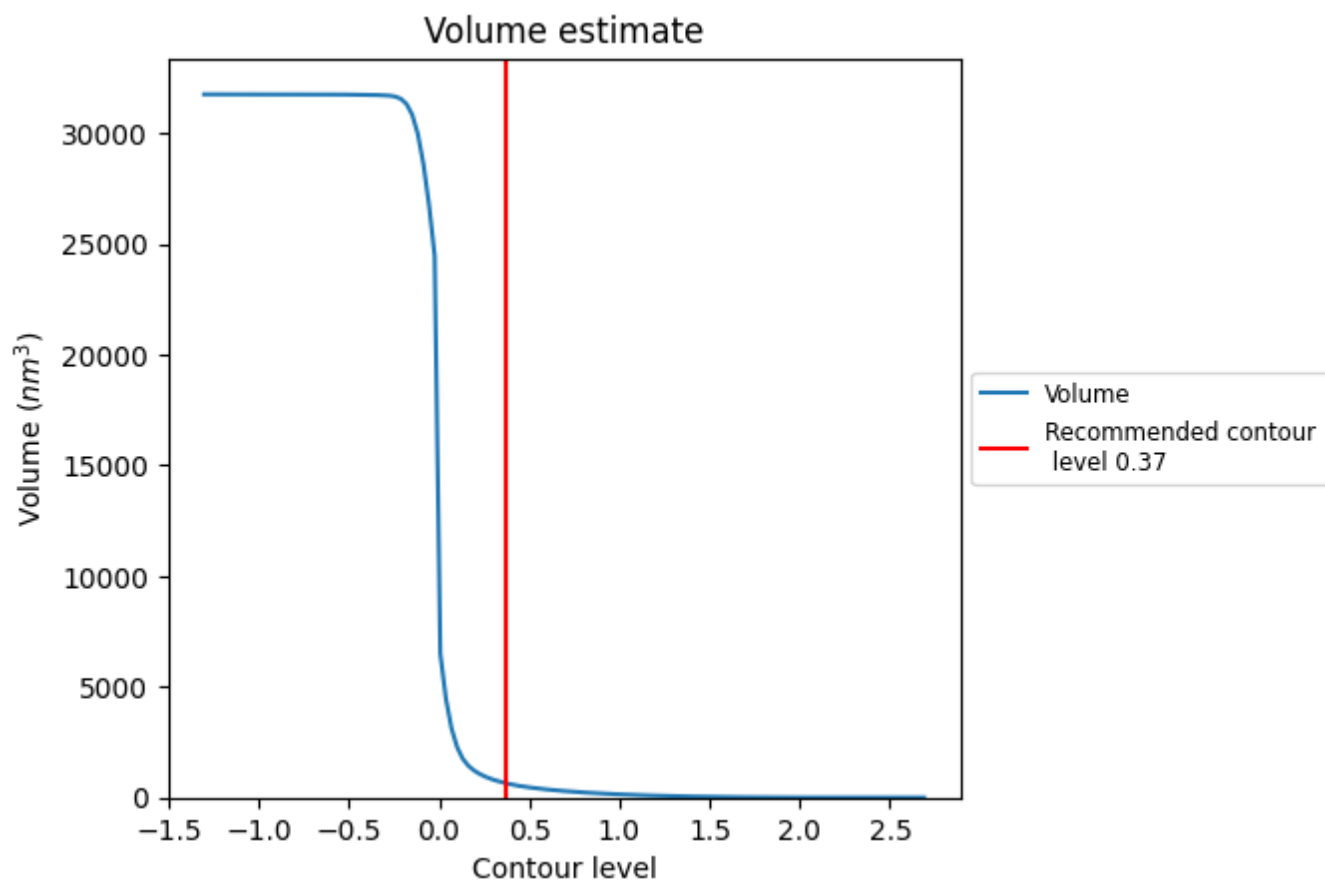
This section contains the results of statistical analysis of the map.

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.

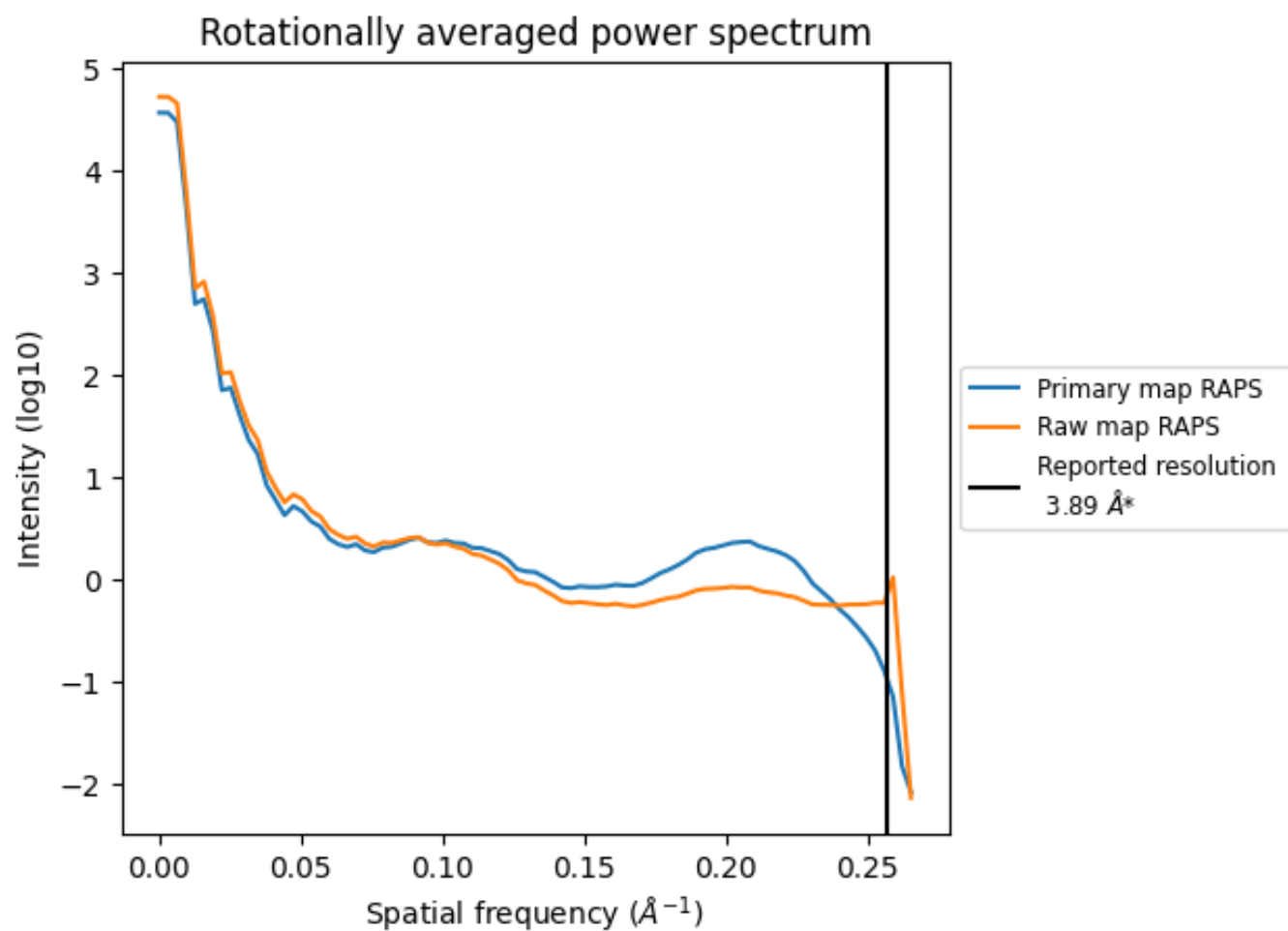
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 649 nm³; this corresponds to an approximate mass of 587 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 [i](#)

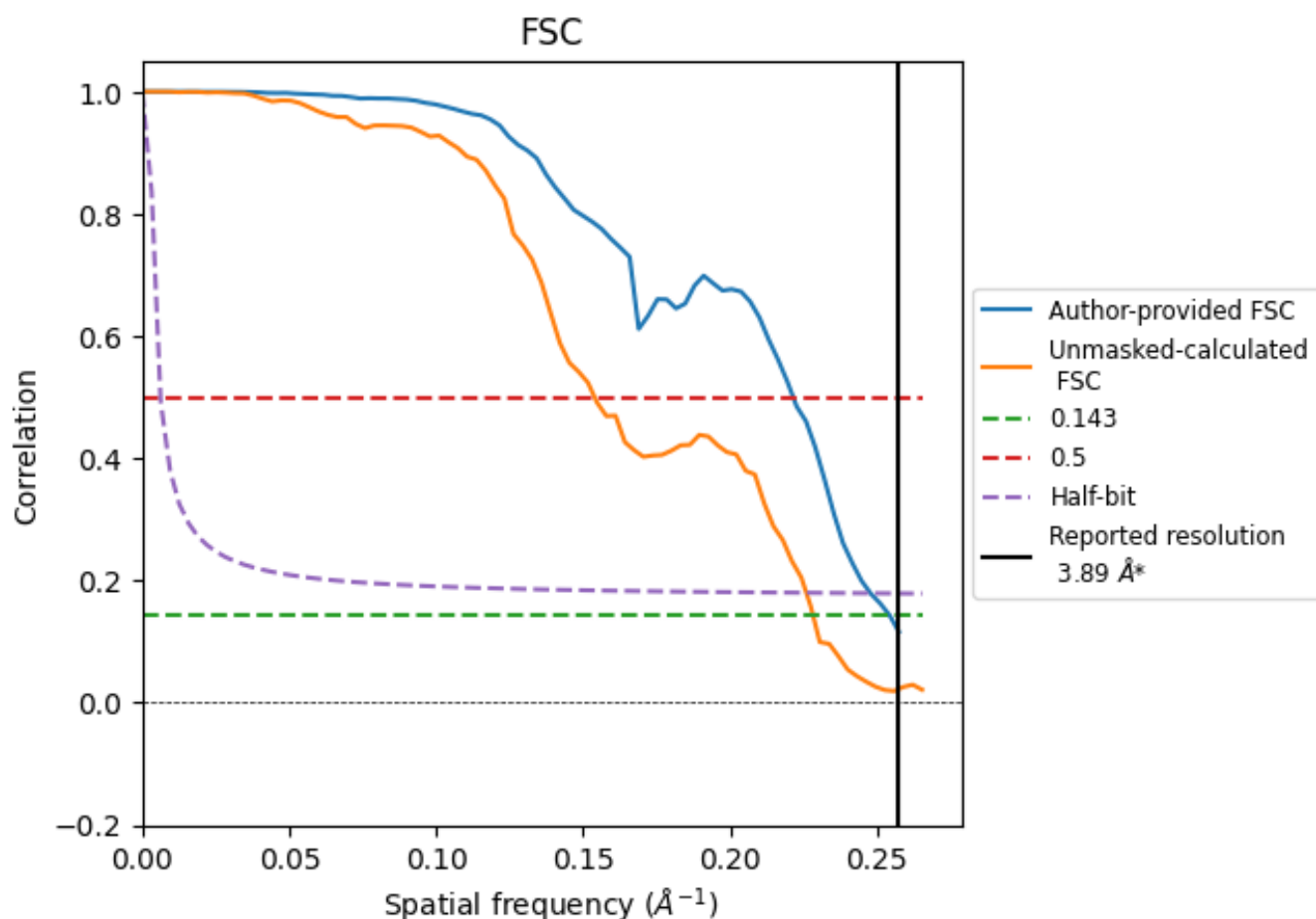


*Reported resolution corresponds to spatial frequency of 0.257 Å⁻¹

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 0.257 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.93	4.52	4.04
Unmasked-calculated*	4.38	6.50	4.43

*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 4.38 differs from the reported value 3.89 by more than 10 %

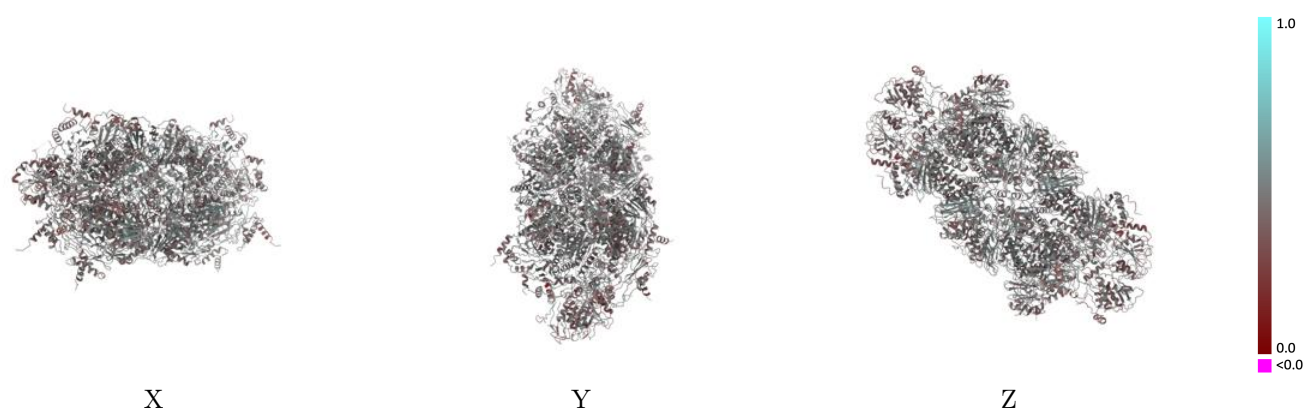
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18761 and PDB model 8QYS. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

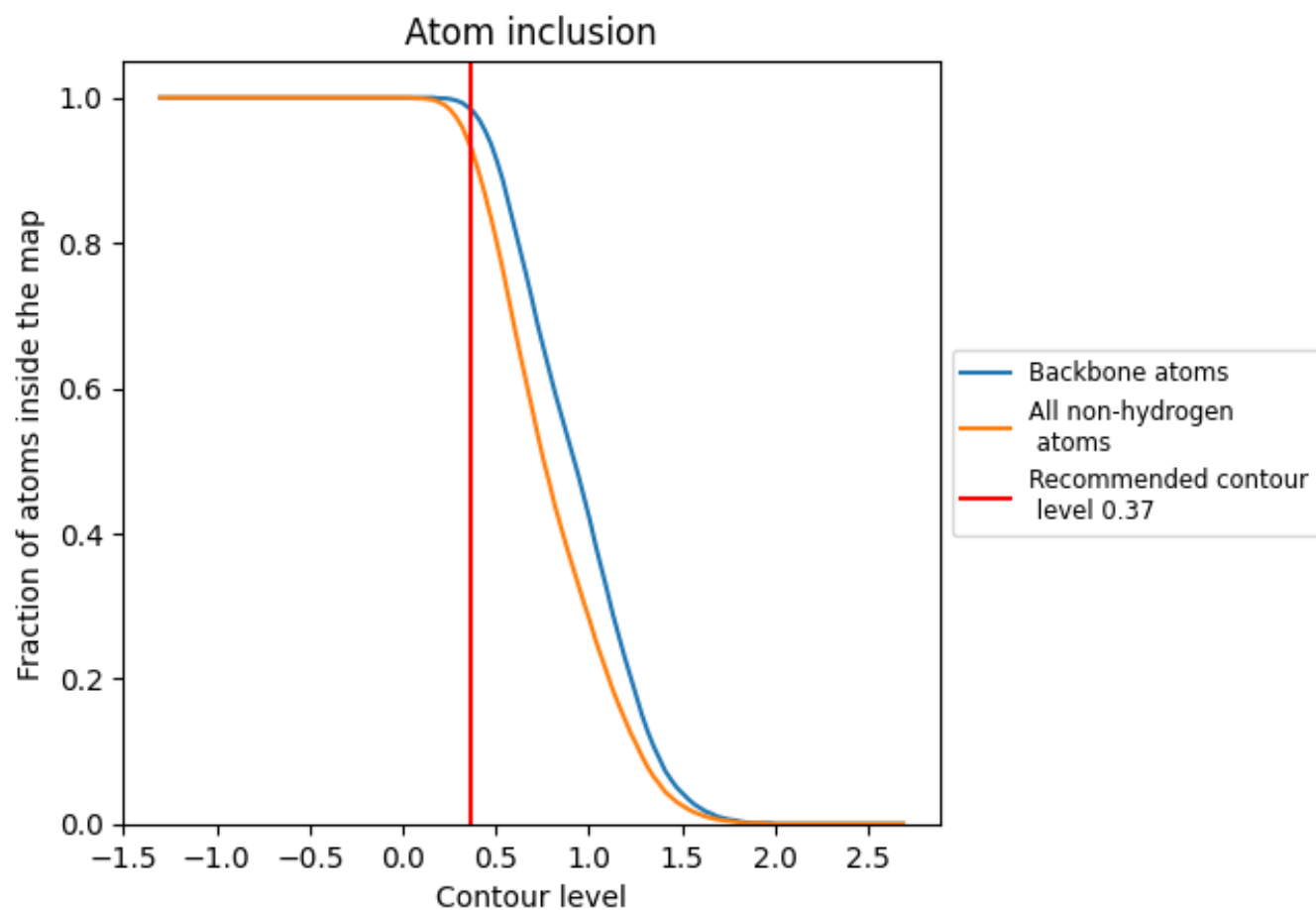


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.37) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.4560
A	 0.9590	 0.4560
B	 0.9630	 0.4660
C	 0.9560	 0.4600
D	 0.9400	 0.4510
E	 0.9500	 0.4670
F	 0.9540	 0.4530
G	 0.9430	 0.4530
H	 0.8120	 0.4430
I	 0.8260	 0.4180
J	 0.8730	 0.4270
K	 0.9190	 0.4620
L	 0.9450	 0.4760
M	 0.9450	 0.4690
N	 0.9440	 0.4610
O	 0.9390	 0.4720
P	 0.9540	 0.4650
Q	 0.9480	 0.4630
R	 0.9590	 0.4560
S	 0.9630	 0.4690
T	 0.9570	 0.4620
U	 0.9400	 0.4520
V	 0.9500	 0.4670
W	 0.9540	 0.4530
X	 0.9430	 0.4500
Y	 0.8110	 0.4420
Z	 0.8260	 0.4160
a	 0.8730	 0.4260
b	 0.9190	 0.4640
c	 0.9450	 0.4740
d	 0.9440	 0.4660
e	 0.9440	 0.4610
f	 0.9400	 0.4720
g	 0.9540	 0.4660
h	 0.9480	 0.4650

