



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:20 AM UTC

PDB ID : 6TU3 / pdb_00006tu3
EMDB ID : EMD-10586
Title : Rat 20S proteasome
Authors : Deshmukh, F.K.; Polkinghorn, C.R.; Elad, N.; Sharon, M.
Deposited on : 2020-01-02
Resolution : 2.70 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

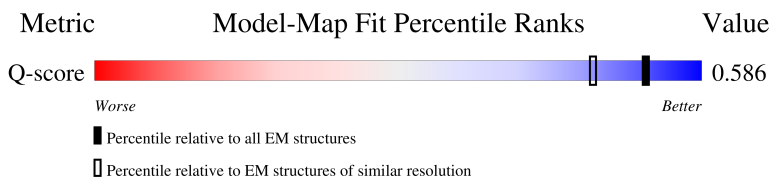
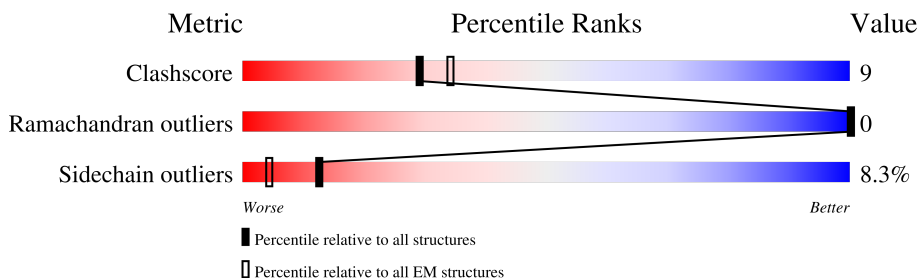
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	246	
1	O	246	
2	B	234	
2	P	234	

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Mol	Chain	Length	Quality of chain
3	C	261	
3	Q	261	
4	D	254	
4	R	254	
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	238	
8	V	238	
9	I	277	
9	W	277	
10	J	205	
10	X	205	
11	K	201	
11	Y	201	
12	L	263	
12	Z	263	
13	M	240	
13	a	240	
14	N	263	
14	b	263	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 47002 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total	C	N	O	S	0	0
			1789	1131	305	340	13		
1	O	240	Total	C	N	O	S	0	0
			1789	1131	305	340	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1765	1131	299	329	6		
2	P	229	Total	C	N	O	S	0	0
			1765	1131	299	329	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1902	1201	330	361	10		
3	Q	247	Total	C	N	O	S	0	0
			1902	1201	330	361	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1778	1125	318	330	5		
4	R	232	Total	C	N	O	S	0	0
			1778	1125	318	330	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1743	1095	295	343	10		
5	S	233	Total	C	N	O	S	0	0
			1743	1095	295	343	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	234	Total	C	N	O	S	0	0
			1787	1127	325	324	11		
6	T	234	Total	C	N	O	S	0	0
			1787	1127	325	324	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1853	1179	319	344	11		
7	U	239	Total	C	N	O	S	0	0
			1853	1179	319	344	11		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1507	942	259	295	11		
8	V	202	Total	C	N	O	S	0	0
			1507	942	259	295	11		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	197	Total	C	N	O	S	0	0
			1453	920	247	277	9		
9	W	197	Total	C	N	O	S	0	0
			1453	920	247	277	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1592	1013	265	295	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1592	1013	265	295	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	197	Total	C	N	O	S	0	0
			1552	997	260	286	9		
11	Y	197	Total	C	N	O	S	0	0
			1552	997	260	286	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total	C	N	O	S	0	0
			1534	972	265	288	9		
12	Z	201	Total	C	N	O	S	0	0
			1534	972	265	288	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1626	1033	277	306	10		
13	a	212	Total	C	N	O	S	0	0
			1626	1033	277	306	10		

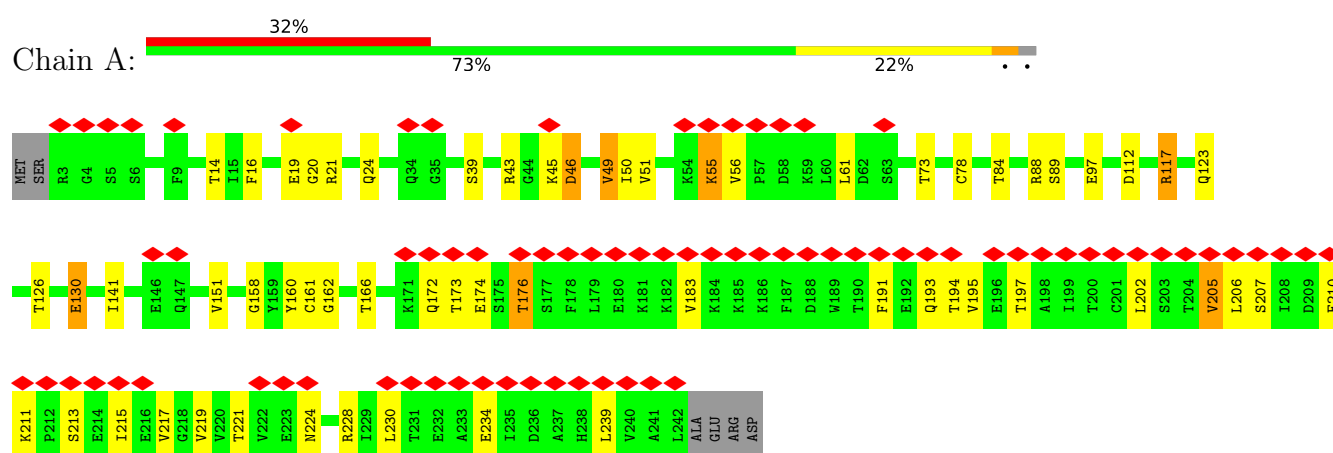
- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1620	1023	283	303	11		
14	b	212	Total	C	N	O	S	0	0
			1620	1023	283	303	11		

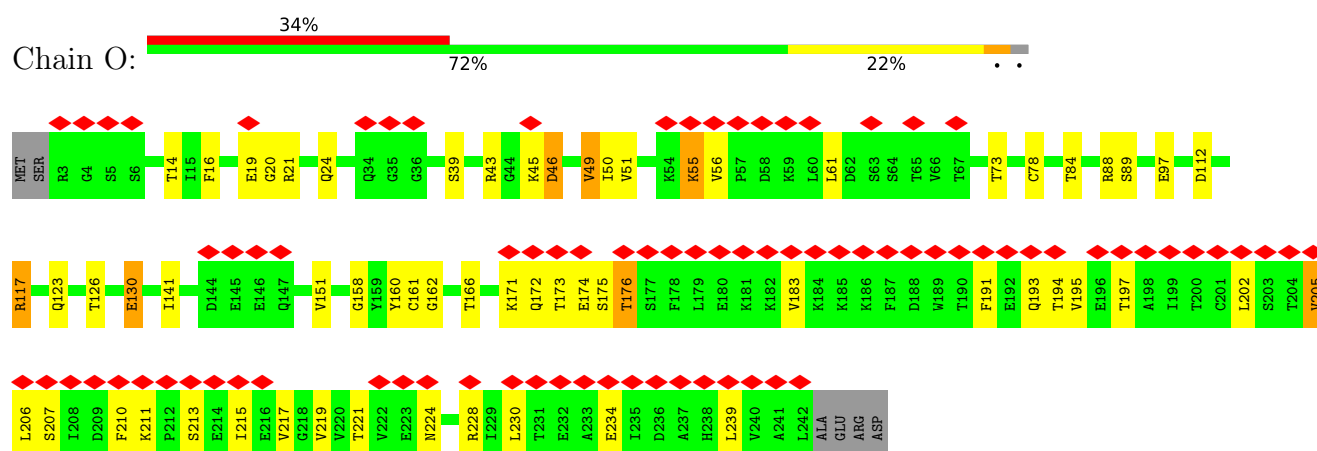
3 Residue-property plots

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.

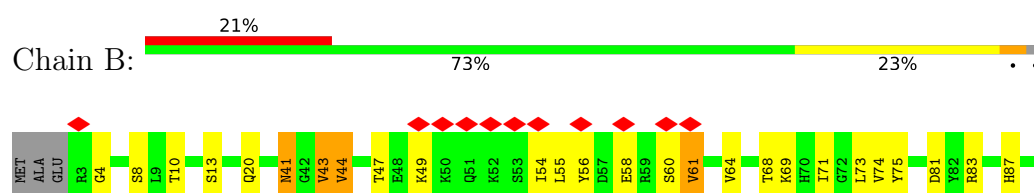
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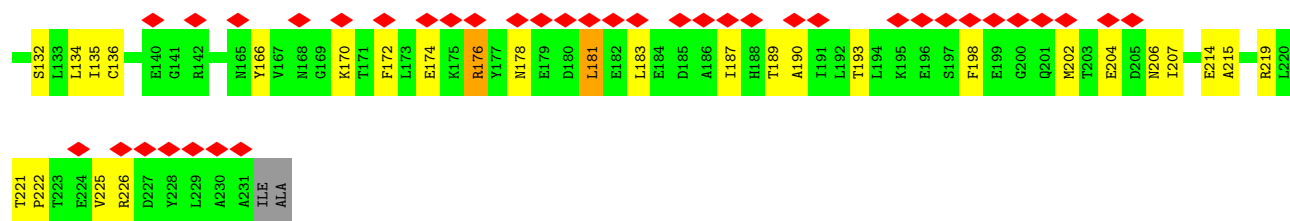


• Molecule 1: Proteasome subunit alpha type-6

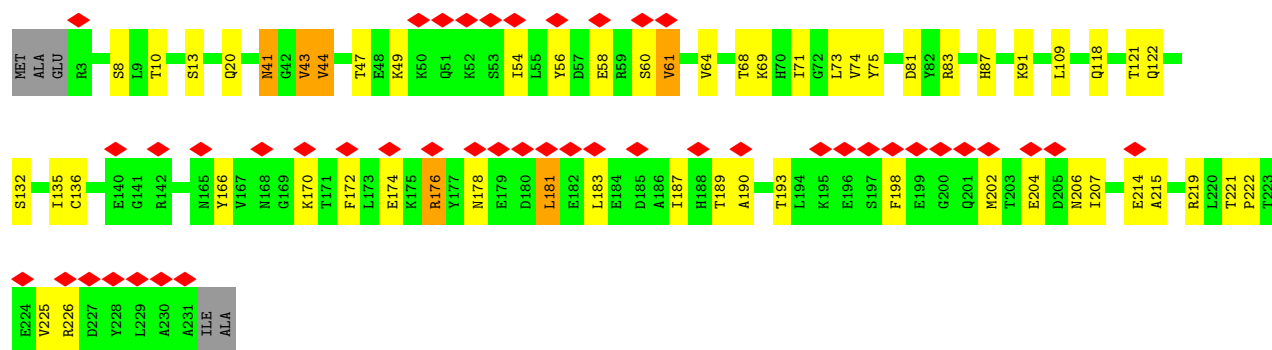
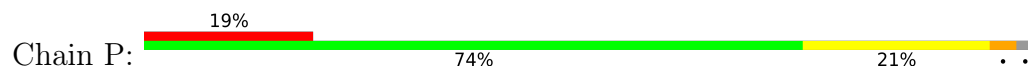


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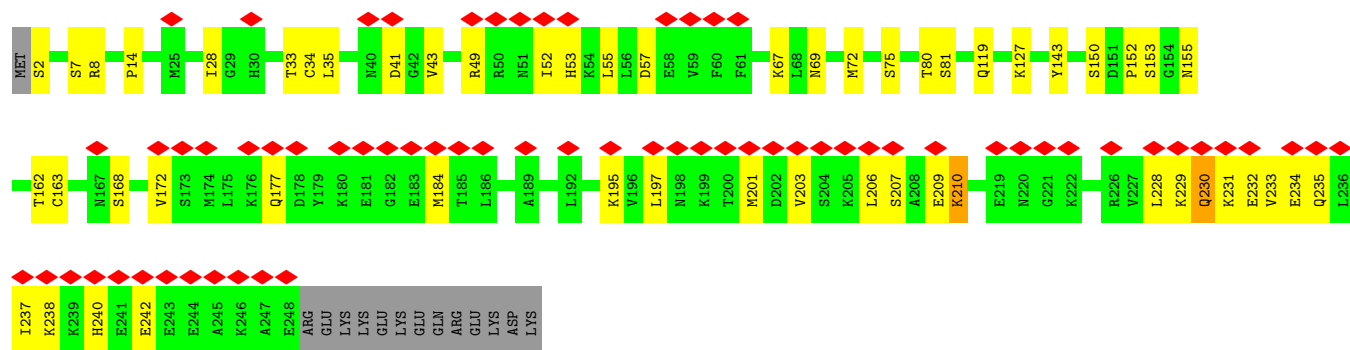
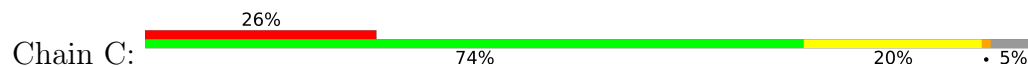




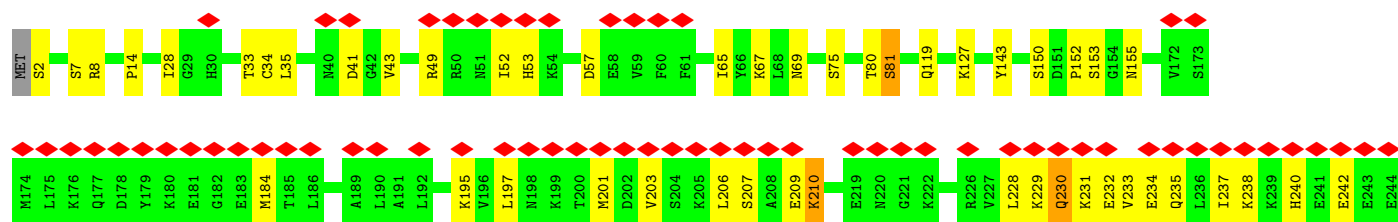
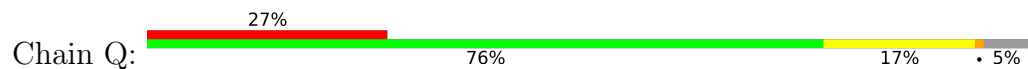
• Molecule 2: Proteasome subunit alpha type-2

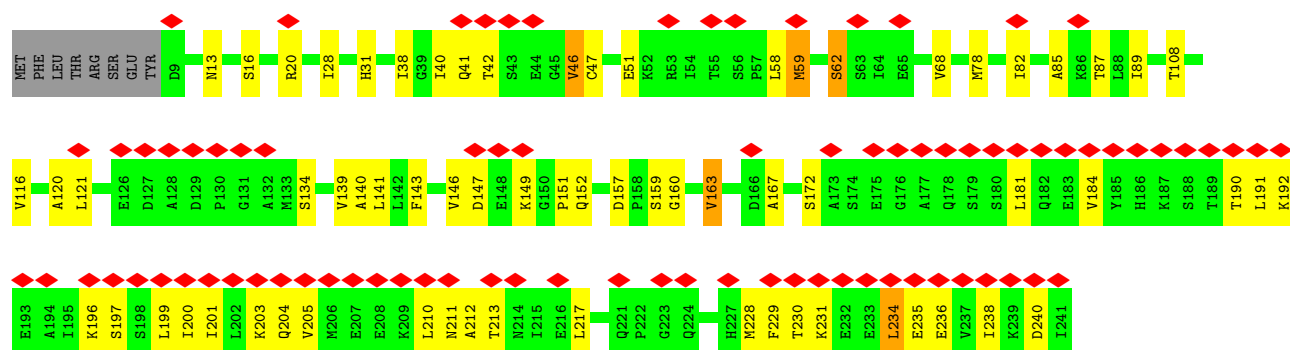


• Molecule 3: Proteasome subunit alpha type-4

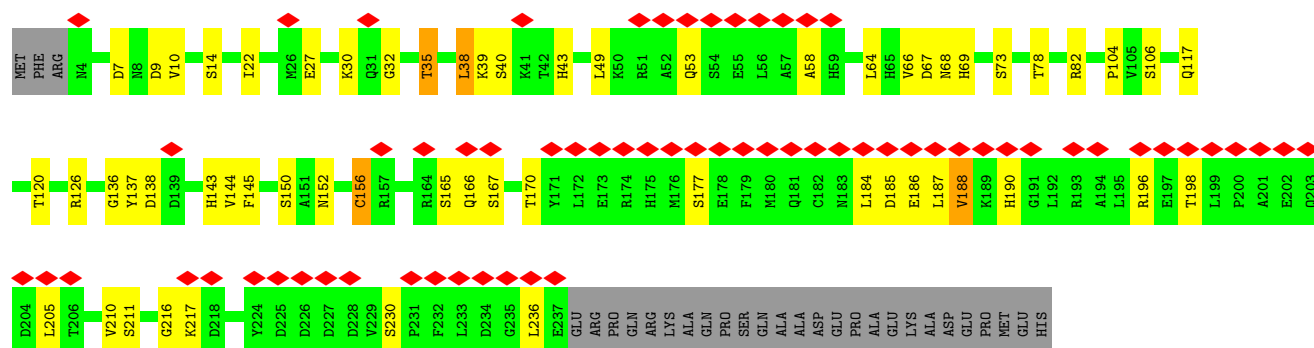


• Molecule 3: Proteasome subunit alpha type-4

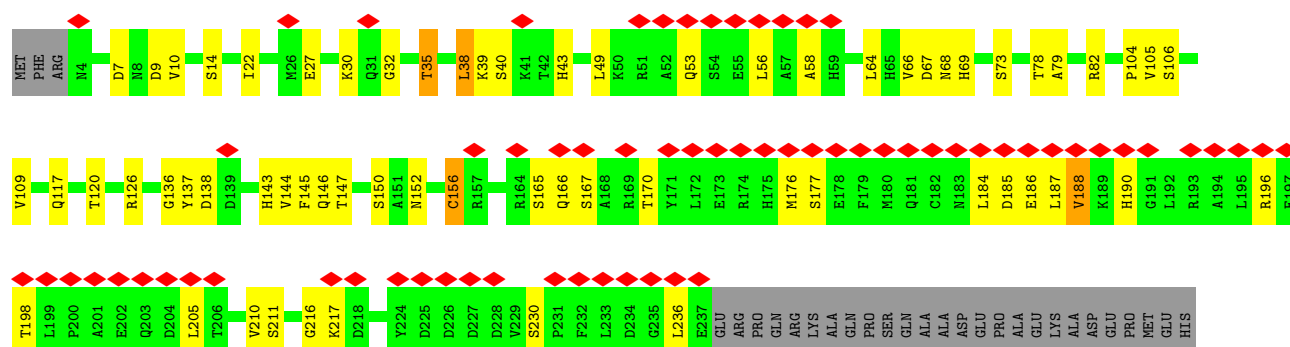




• Molecule 6: Proteasome subunit alpha type-1

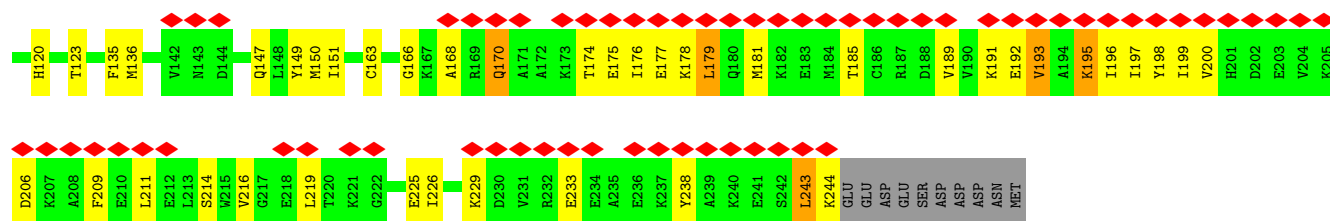


• Molecule 6: Proteasome subunit alpha type-1

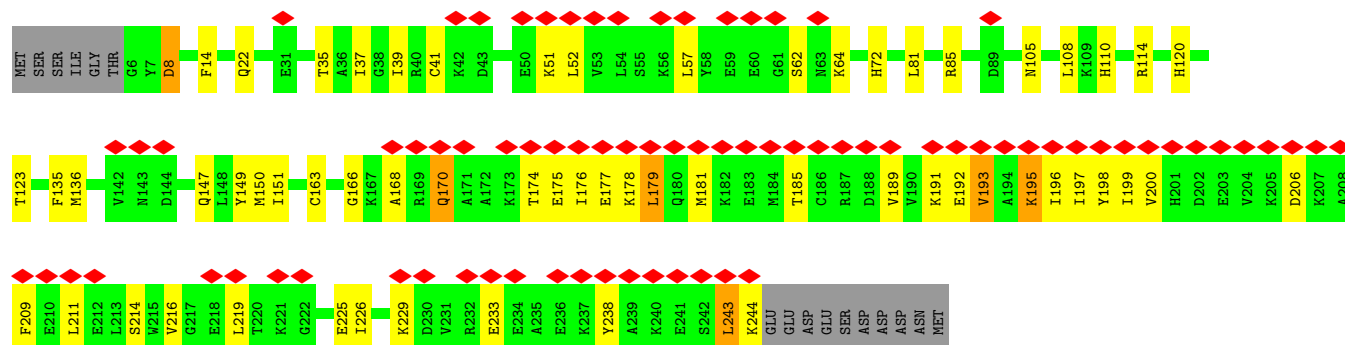


• Molecule 7: Proteasome subunit alpha type-3

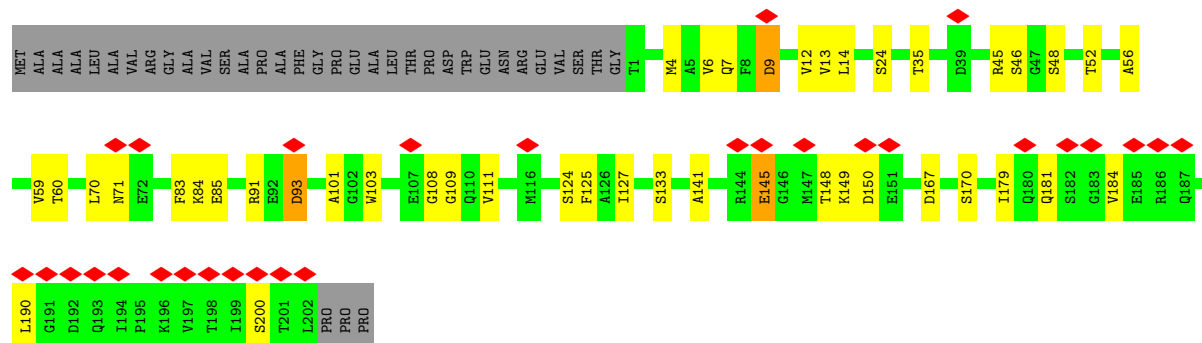




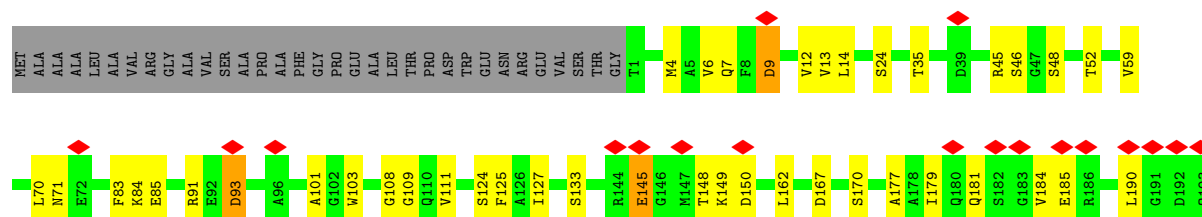
• Molecule 7: Proteasome subunit alpha type-3

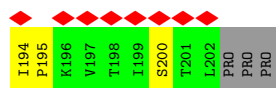


• Molecule 8: Proteasome subunit beta type-6

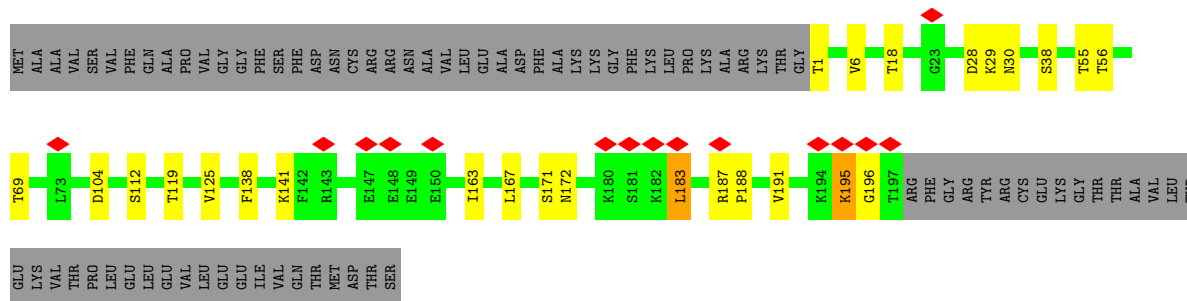


• Molecule 8: Proteasome subunit beta type-6

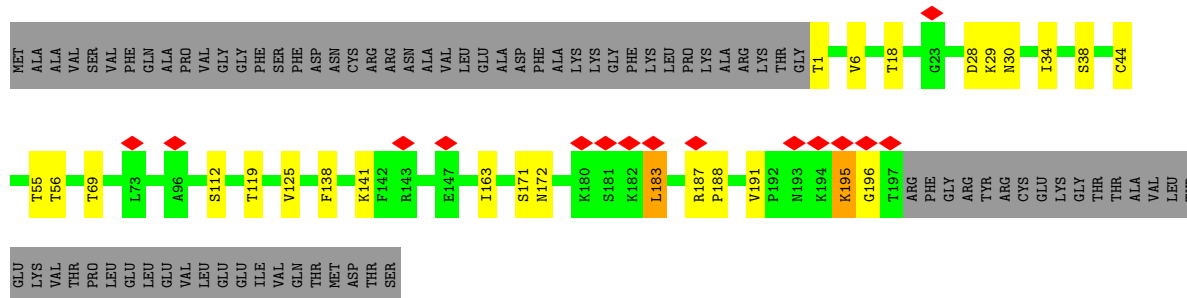




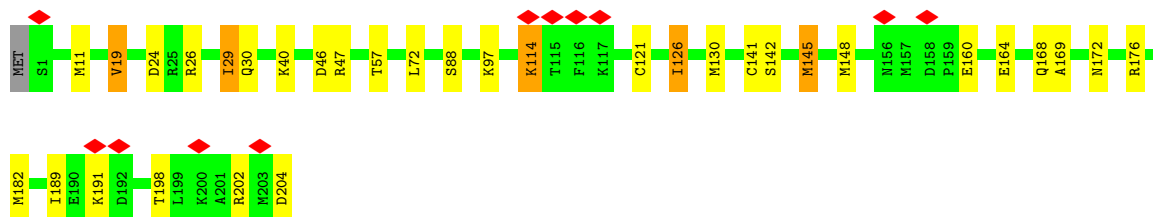
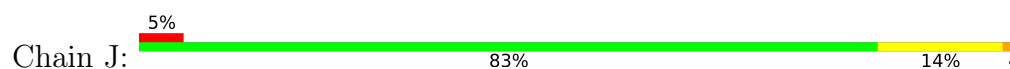
• Molecule 9: Proteasome subunit beta type-7



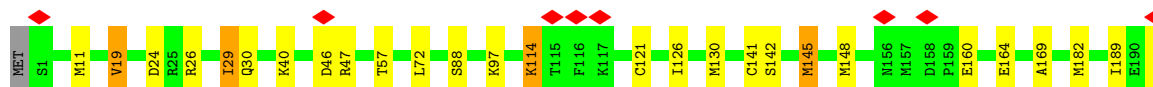
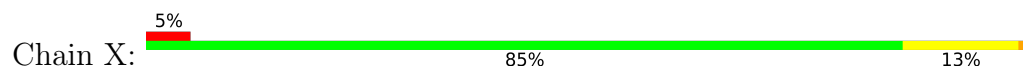
• Molecule 9: Proteasome subunit beta type-7

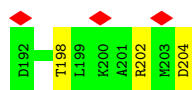


• Molecule 10: Proteasome subunit beta type-3

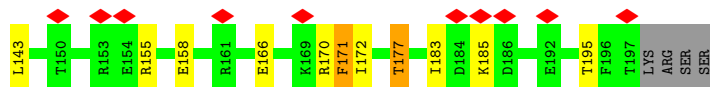
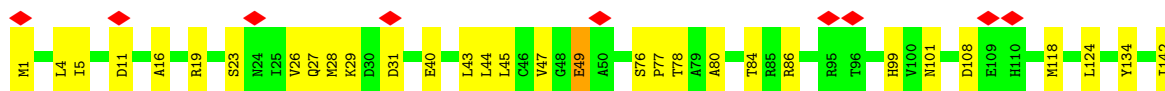
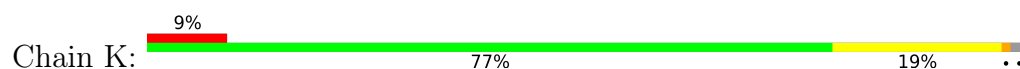


• Molecule 10: Proteasome subunit beta type-3

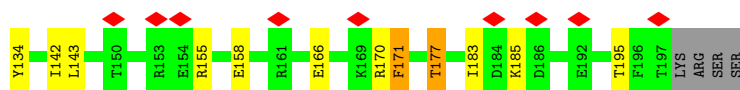
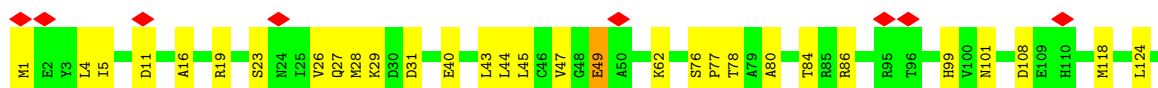
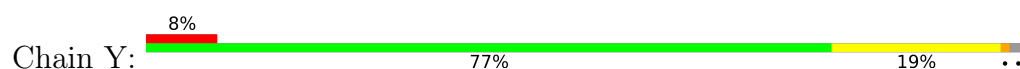




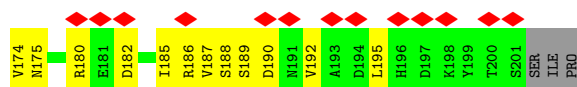
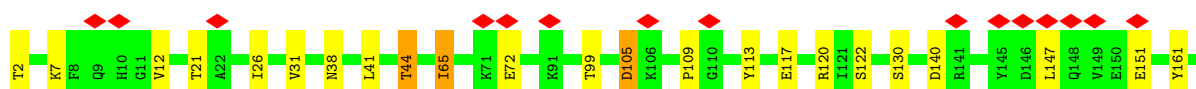
• Molecule 11: Proteasome subunit beta type-2



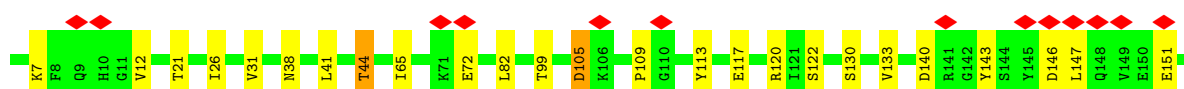
• Molecule 11: Proteasome subunit beta type-2

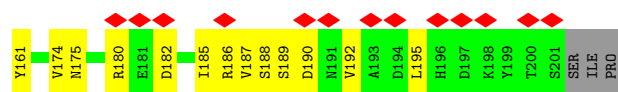


• Molecule 12: Proteasome subunit beta type-5

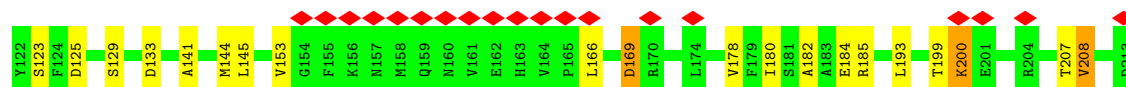


• Molecule 12: Proteasome subunit beta type-5

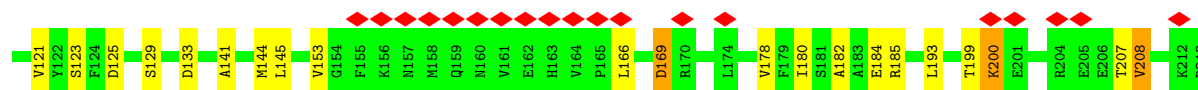
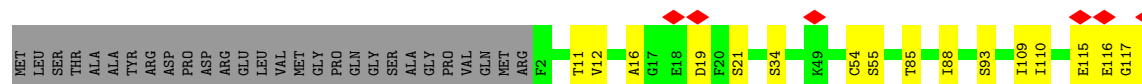




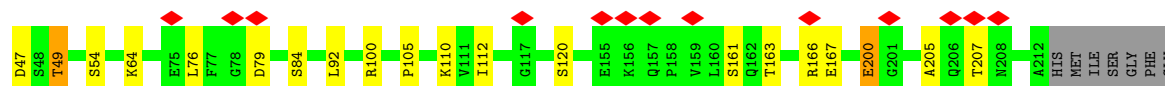
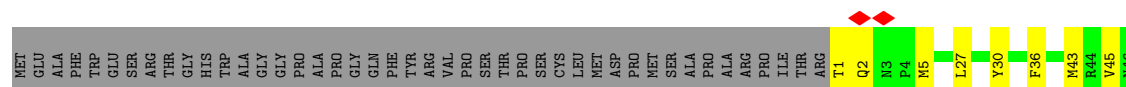
- Molecule 13: Proteasome subunit beta type-1



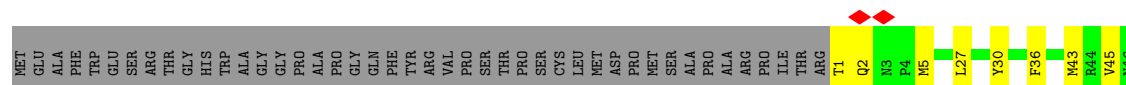
- Molecule 13: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	245800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.247	Depositor
Minimum map value	-0.161	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.043	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	0.25	0/1818	0.50	0/2464
1	O	0.26	0/1818	0.50	0/2464
2	B	0.28	0/1804	0.62	6/2447 (0.2%)
2	P	0.28	0/1804	0.62	6/2447 (0.2%)
3	C	0.26	0/1930	0.55	1/2606 (0.0%)
3	Q	0.26	0/1930	0.55	1/2606 (0.0%)
4	D	0.26	0/1805	0.59	2/2442 (0.1%)
4	R	0.26	0/1805	0.59	2/2442 (0.1%)
5	E	0.23	0/1770	0.45	0/2394
5	S	0.23	0/1770	0.45	0/2394
6	F	0.30	0/1821	0.64	3/2467 (0.1%)
6	T	0.30	0/1821	0.64	3/2467 (0.1%)
7	G	0.27	0/1888	0.55	1/2543 (0.0%)
7	U	0.27	0/1888	0.55	1/2543 (0.0%)
8	H	0.25	0/1533	0.42	0/2078
8	V	0.25	0/1533	0.42	0/2078
9	I	0.28	0/1478	0.53	1/2004 (0.0%)
9	W	0.28	0/1478	0.53	1/2004 (0.0%)
10	J	0.29	0/1621	0.49	0/2185
10	X	0.29	0/1621	0.49	0/2185
11	K	0.27	0/1583	0.49	0/2145
11	Y	0.28	0/1583	0.49	0/2145
12	L	0.23	0/1565	0.48	1/2118 (0.0%)
12	Z	0.24	0/1565	0.48	1/2118 (0.0%)
13	M	0.28	0/1656	0.51	1/2235 (0.0%)
13	a	0.28	0/1656	0.51	1/2235 (0.0%)
14	N	0.29	0/1651	0.52	0/2236
14	b	0.29	0/1651	0.52	0/2236
All	All	0.27	0/47846	0.53	32/64728 (0.0%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	215	GLN	CA-C-N	8.30	128.37	119.90
4	D	215	GLN	C-N-CA	8.30	128.37	119.90
4	R	215	GLN	CA-C-N	8.26	128.32	119.90
4	R	215	GLN	C-N-CA	8.26	128.32	119.90
6	F	66	VAL	N-CA-C	-7.56	105.78	111.90
6	T	66	VAL	N-CA-C	-7.52	105.81	111.90
12	L	187	VAL	N-CA-C	7.08	118.03	111.45
12	Z	187	VAL	N-CA-C	7.06	118.02	111.45
2	B	60	SER	N-CA-C	6.55	118.42	111.28
2	P	60	SER	N-CA-C	6.54	118.41	111.28
2	P	176	ARG	N-CA-C	6.26	118.11	111.28
2	B	176	ARG	N-CA-C	6.24	118.08	111.28
6	T	32	GLY	N-CA-C	5.74	119.94	112.25
6	F	32	GLY	N-CA-C	5.73	119.93	112.25
13	M	117	GLY	N-CA-C	5.68	123.64	114.90
13	a	117	GLY	N-CA-C	5.66	123.61	114.90
9	W	141	LYS	N-CA-C	5.61	122.02	113.61
9	I	141	LYS	N-CA-C	5.59	121.99	113.61
7	G	243	LEU	N-CA-C	5.43	117.20	111.28
7	U	243	LEU	N-CA-C	5.41	117.18	111.28
3	Q	52	ILE	N-CA-C	5.39	117.36	112.29
3	C	52	ILE	N-CA-C	5.38	117.35	112.29
2	P	58	GLU	N-CA-C	5.28	117.04	111.28
2	B	58	GLU	N-CA-C	5.26	117.02	111.28
2	P	61	VAL	N-CA-C	5.26	115.47	108.11
2	B	61	VAL	N-CA-C	5.25	115.47	108.11
6	F	156	CYS	N-CA-C	5.18	117.12	108.99
6	T	156	CYS	N-CA-C	5.18	117.12	108.99
2	P	215	ALA	N-CA-C	5.13	119.40	113.20
2	B	215	ALA	N-CA-C	5.12	119.39	113.20
2	P	181	LEU	N-CA-C	5.05	117.66	110.24
2	B	181	LEU	N-CA-C	5.02	117.61	110.24

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	1789	0	1745	31	0
1	O	1789	0	1745	32	0
2	B	1765	0	1746	49	0
2	P	1765	0	1746	48	0
3	C	1902	0	1903	34	0
3	Q	1902	0	1903	34	0
4	D	1778	0	1795	54	0
4	R	1778	0	1795	58	0
5	E	1743	0	1708	46	0
5	S	1743	0	1708	48	0
6	F	1787	0	1762	36	0
6	T	1787	0	1762	40	0
7	G	1853	0	1842	55	0
7	U	1853	0	1842	55	0
8	H	1507	0	1464	27	0
8	V	1507	0	1464	29	0
9	I	1453	0	1458	32	0
9	W	1453	0	1458	30	0
10	J	1592	0	1612	18	0
10	X	1592	0	1612	15	0
11	K	1552	0	1542	31	0
11	Y	1552	0	1542	32	0
12	L	1534	0	1487	20	0
12	Z	1534	0	1487	23	0
13	M	1626	0	1615	34	0
13	a	1626	0	1615	34	0
14	N	1620	0	1581	16	0
14	b	1620	0	1581	18	0
All	All	47002	0	46520	873	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 (873) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:41:CYS:SG	7:G:189:VAL:HG21	1.56	1.45
7:U:41:CYS:SG	7:U:189:VAL:HG21	1.56	1.44
9:I:195:LYS:HD3	13:a:184:GLU:CG	1.48	1.40
4:R:5:ARG:NH2	3:Q:8:ARG:HH21	0.95	1.40
2:B:172:PHE:HZ	2:B:176:ARG:NH1	1.23	1.35
2:P:172:PHE:HZ	2:P:176:ARG:NH1	1.23	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:195:LYS:HD3	13:a:184:GLU:CD	1.51	1.34
13:M:184:GLU:CG	9:W:195:LYS:HD3	1.56	1.32
4:D:218:LYS:NZ	4:D:220:LEU:HD12	1.47	1.29
4:R:218:LYS:NZ	4:R:220:LEU:HD12	1.47	1.29
11:K:77:PRO:CD	11:K:108:ASP:OD2	1.80	1.29
11:Y:77:PRO:CD	11:Y:108:ASP:OD2	1.80	1.28
4:R:5:ARG:NH2	3:Q:8:ARG:NH2	1.80	1.28
6:F:38:LEU:CD1	6:F:187:LEU:HD11	1.65	1.26
6:T:38:LEU:CD1	6:T:187:LEU:HD11	1.65	1.25
3:C:8:ARG:HH21	4:D:5:ARG:NH2	1.35	1.23
5:E:203:LYS:HG2	5:E:210:LEU:CD1	1.70	1.21
5:S:203:LYS:HG2	5:S:210:LEU:CD1	1.70	1.20
4:D:139:ASP:OD2	4:D:141:THR:OG1	1.61	1.17
4:R:139:ASP:OD2	4:R:141:THR:OG1	1.61	1.16
9:I:195:LYS:HG2	13:a:184:GLU:OE2	1.44	1.16
2:B:172:PHE:CZ	2:B:176:ARG:NH1	2.13	1.14
2:P:172:PHE:CZ	2:P:176:ARG:NH1	2.13	1.14
11:Y:77:PRO:HD2	11:Y:108:ASP:OD2	1.00	1.14
11:K:77:PRO:HD2	11:K:108:ASP:OD2	0.99	1.13
7:G:195:LYS:HD3	7:G:199:ILE:HD11	1.28	1.12
6:T:38:LEU:CD1	6:T:187:LEU:CD1	2.29	1.11
6:F:38:LEU:CD1	6:F:187:LEU:CD1	2.29	1.10
9:I:195:LYS:CD	13:a:184:GLU:CD	2.24	1.09
4:R:139:ASP:CG	4:R:141:THR:OG1	1.96	1.09
5:S:203:LYS:CG	5:S:210:LEU:HD13	1.82	1.09
7:U:195:LYS:HD3	7:U:199:ILE:HD11	1.28	1.09
5:E:203:LYS:CG	5:E:210:LEU:HD13	1.82	1.08
5:S:203:LYS:HG2	5:S:210:LEU:HD13	1.31	1.08
4:D:139:ASP:CG	4:D:141:THR:OG1	1.96	1.08
9:I:195:LYS:CD	13:a:184:GLU:CG	2.32	1.07
6:F:38:LEU:HD12	6:F:187:LEU:HD11	1.11	1.07
6:T:38:LEU:HD12	6:T:187:LEU:HD11	1.11	1.07
13:M:184:GLU:CD	9:W:195:LYS:HD3	1.79	1.06
13:M:184:GLU:OE2	9:W:195:LYS:HG2	1.55	1.06
4:R:218:LYS:HZ2	4:R:220:LEU:CD1	1.69	1.06
4:R:218:LYS:NZ	4:R:220:LEU:CD1	2.19	1.05
5:E:203:LYS:HG2	5:E:210:LEU:HD13	1.31	1.05
4:D:218:LYS:HZ2	4:D:220:LEU:CD1	1.69	1.05
12:Z:186:ARG:NH1	12:Z:189:SER:HB2	1.71	1.05
12:L:186:ARG:NH1	12:L:189:SER:HB2	1.71	1.04
4:D:218:LYS:NZ	4:D:220:LEU:CD1	2.19	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:77:PRO:CD	11:K:108:ASP:CG	2.33	1.02
11:Y:77:PRO:CD	11:Y:108:ASP:CG	2.33	1.00
7:U:41:CYS:SG	7:U:189:VAL:CG2	2.51	0.98
7:G:41:CYS:SG	7:G:189:VAL:CG2	2.51	0.98
3:Q:49:ARG:HD2	3:Q:209:GLU:O	1.62	0.98
7:G:52:LEU:HD21	7:G:206:ASP:OD2	1.64	0.98
11:K:77:PRO:HD3	11:K:108:ASP:OD1	1.64	0.97
3:C:8:ARG:HH21	4:D:5:ARG:HH22	1.06	0.97
3:C:49:ARG:HD2	3:C:209:GLU:O	1.62	0.97
9:I:195:LYS:HD3	13:a:184:GLU:HG2	1.44	0.96
7:U:52:LEU:HD21	7:U:206:ASP:OD2	1.64	0.96
11:Y:77:PRO:HD3	11:Y:108:ASP:OD1	1.64	0.95
4:R:64:ALA:HB2	4:R:217:LEU:HD22	1.47	0.94
9:I:195:LYS:HG2	13:a:184:GLU:CD	1.91	0.94
4:D:64:ALA:HB2	4:D:217:LEU:HD22	1.47	0.93
5:S:203:LYS:HG2	5:S:210:LEU:HD12	1.51	0.93
1:A:210:PHE:O	1:A:239:LEU:HD21	1.69	0.93
11:Y:77:PRO:HD2	11:Y:108:ASP:CG	1.94	0.92
11:K:77:PRO:HD2	11:K:108:ASP:CG	1.94	0.92
5:E:203:LYS:HG2	5:E:210:LEU:HD12	1.51	0.92
13:M:184:GLU:CG	9:W:195:LYS:CD	2.46	0.92
9:I:195:LYS:CE	13:a:184:GLU:HG3	1.98	0.91
4:D:64:ALA:HB2	4:D:217:LEU:CD2	2.01	0.91
2:P:56:TYR:HD1	1:O:161:CYS:HG	1.07	0.91
9:I:195:LYS:CG	13:a:184:GLU:CD	2.44	0.91
13:M:184:GLU:HG2	9:W:195:LYS:HD3	1.49	0.91
1:O:210:PHE:O	1:O:239:LEU:HD21	1.69	0.91
7:G:229:LYS:O	7:G:233:GLU:HG3	1.71	0.90
7:U:191:LYS:HE2	7:U:238:TYR:CE2	2.07	0.90
2:B:204:GLU:HG2	2:B:222:PRO:HB3	1.53	0.90
2:P:204:GLU:HG2	2:P:222:PRO:HB3	1.53	0.89
4:R:64:ALA:HB2	4:R:217:LEU:CD2	2.01	0.89
7:G:191:LYS:HE2	7:G:238:TYR:CE2	2.07	0.89
3:C:8:ARG:NH2	4:D:5:ARG:NH2	2.19	0.89
7:U:229:LYS:O	7:U:233:GLU:HG3	1.71	0.89
7:U:195:LYS:CD	7:U:199:ILE:HD11	2.03	0.87
7:G:195:LYS:CD	7:G:199:ILE:HD11	2.03	0.86
13:M:184:GLU:HG3	9:W:195:LYS:HD3	1.53	0.86
3:C:206:LEU:HD12	3:C:237:ILE:HD11	1.56	0.85
3:Q:206:LEU:HD12	3:Q:237:ILE:HD11	1.56	0.85
4:D:218:LYS:HZ2	4:D:220:LEU:HD12	0.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:218:LYS:HZ2	4:R:220:LEU:HD12	0.76	0.85
6:F:137:TYR:OH	6:F:217:LYS:HD3	1.77	0.84
6:T:137:TYR:OH	6:T:217:LYS:HD3	1.77	0.84
13:M:184:GLU:CD	9:W:195:LYS:HG2	2.01	0.84
2:P:204:GLU:OE1	2:P:226:ARG:HG3	1.78	0.84
2:B:204:GLU:OE1	2:B:226:ARG:HG3	1.78	0.84
1:A:158:GLY:O	2:B:83:ARG:NH2	2.11	0.83
13:M:184:GLU:CD	9:W:195:LYS:CD	2.51	0.83
4:R:5:ARG:HH22	3:Q:8:ARG:NH2	1.55	0.83
8:H:91:ARG:NH1	14:N:1:THR:HG23	1.93	0.83
3:Q:238:LYS:O	3:Q:242:GLU:HG3	1.79	0.83
4:R:5:ARG:HH22	3:Q:8:ARG:HH21	0.83	0.82
3:C:238:LYS:O	3:C:242:GLU:HG3	1.79	0.82
4:R:40:ILE:HG22	4:R:212:ARG:HG2	1.61	0.82
4:D:40:ILE:HG22	4:D:212:ARG:HG2	1.61	0.82
11:K:77:PRO:HD3	11:K:108:ASP:CG	2.02	0.81
6:F:205:LEU:HD22	6:F:210:VAL:HG11	1.62	0.81
6:F:38:LEU:HD11	6:F:187:LEU:CD1	2.10	0.81
7:U:170:GLN:HE21	7:U:170:GLN:HA	1.44	0.80
2:P:204:GLU:CG	2:P:222:PRO:HB3	2.12	0.80
11:Y:77:PRO:HD3	11:Y:108:ASP:CG	2.03	0.80
5:S:108:THR:HA	5:S:147:ASP:OD2	1.82	0.80
5:E:108:THR:HA	5:E:147:ASP:OD2	1.82	0.80
7:G:170:GLN:HE21	7:G:170:GLN:HA	1.44	0.80
2:B:204:GLU:CG	2:B:222:PRO:HB3	2.12	0.79
7:G:108:LEU:CD2	7:G:149:TYR:CD1	2.66	0.79
6:T:38:LEU:HD11	6:T:187:LEU:CD1	2.10	0.79
6:T:205:LEU:HD22	6:T:210:VAL:HG11	1.63	0.79
4:R:5:ARG:HH21	3:Q:8:ARG:HH21	1.24	0.79
4:D:139:ASP:OD1	4:D:140:GLY:N	2.16	0.79
13:M:180:ILE:HG23	9:W:195:LYS:CE	2.12	0.79
2:B:204:GLU:OE1	2:B:226:ARG:NH1	2.15	0.78
9:I:195:LYS:CG	13:a:184:GLU:OE2	2.27	0.78
2:P:204:GLU:OE1	2:P:226:ARG:NH1	2.15	0.78
7:U:108:LEU:CD2	7:U:149:TYR:CD1	2.66	0.78
4:R:139:ASP:OD1	4:R:140:GLY:N	2.16	0.78
7:G:195:LYS:HD3	7:G:199:ILE:CD1	2.12	0.78
8:V:7:GLN:NE2	8:V:109:GLY:O	2.17	0.77
7:U:52:LEU:CD2	7:U:206:ASP:OD2	2.32	0.77
5:S:230:THR:O	5:S:234:LEU:HB2	1.85	0.77
7:G:52:LEU:CD2	7:G:206:ASP:OD2	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:7:GLN:NE2	8:H:109:GLY:O	2.17	0.76
5:E:230:THR:O	5:E:234:LEU:HB2	1.85	0.76
13:M:184:GLU:HG3	9:W:195:LYS:CD	2.13	0.76
6:F:205:LEU:HD22	6:F:210:VAL:CG1	2.16	0.76
8:H:93:ASP:OD1	8:H:93:ASP:N	2.19	0.76
4:R:226:GLU:O	4:R:229:VAL:CG1	2.34	0.76
8:H:91:ARG:NH1	14:N:1:THR:CG2	2.48	0.76
4:D:226:GLU:O	4:D:229:VAL:CG1	2.34	0.75
6:T:38:LEU:CD1	6:T:187:LEU:HD12	2.17	0.75
5:E:203:LYS:CG	5:E:210:LEU:CD1	2.50	0.75
9:I:195:LYS:CD	13:a:184:GLU:HG3	2.11	0.75
11:K:77:PRO:CD	11:K:108:ASP:OD1	2.32	0.75
2:B:204:GLU:CD	2:B:222:PRO:HB3	2.12	0.74
2:P:204:GLU:CD	2:P:222:PRO:HB3	2.12	0.74
6:T:205:LEU:HD22	6:T:210:VAL:CG1	2.16	0.74
7:U:195:LYS:HD3	7:U:199:ILE:CD1	2.12	0.74
4:D:218:LYS:HZ1	4:D:220:LEU:CD1	1.98	0.74
7:G:175:GLU:OE2	7:G:196:ILE:HD12	1.88	0.74
13:M:184:GLU:CD	9:W:195:LYS:CG	2.61	0.74
6:T:184:LEU:O	6:T:188:VAL:HG22	1.88	0.74
11:K:171:PHE:O	11:Y:27:GLN:NE2	2.20	0.74
6:F:184:LEU:O	6:F:188:VAL:HG22	1.88	0.73
8:V:93:ASP:OD1	8:V:93:ASP:N	2.19	0.73
7:U:175:GLU:OE2	7:U:196:ILE:HD12	1.88	0.73
6:T:38:LEU:HD11	6:T:187:LEU:HD12	1.71	0.73
9:I:195:LYS:HE2	13:a:184:GLU:HG3	1.71	0.72
3:C:206:LEU:HD12	3:C:237:ILE:CD1	2.19	0.72
7:G:195:LYS:CD	7:G:199:ILE:CD1	2.67	0.72
7:U:195:LYS:CD	7:U:199:ILE:CD1	2.67	0.72
3:Q:206:LEU:HD12	3:Q:237:ILE:CD1	2.19	0.72
2:B:172:PHE:HZ	2:B:176:ARG:HH12	1.35	0.72
4:R:184:ASP:OD1	4:R:184:ASP:N	2.23	0.72
5:E:40:ILE:HD11	5:E:181:LEU:HD11	1.73	0.71
6:F:196:ARG:HH12	6:F:236:LEU:HB3	1.55	0.71
7:U:191:LYS:HE2	7:U:238:TYR:HE2	1.56	0.71
2:B:204:GLU:CD	2:B:222:PRO:CB	2.49	0.71
7:U:198:TYR:HB3	7:U:243:LEU:HD11	1.72	0.71
14:b:1:THR:CG2	8:V:91:ARG:NH1	2.54	0.71
4:R:218:LYS:HZ1	4:R:220:LEU:CD1	1.98	0.71
4:R:139:ASP:OD1	4:R:141:THR:OG1	2.09	0.71
6:F:38:LEU:CD1	6:F:187:LEU:HD12	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:83:ARG:NH2	1:O:158:GLY:O	2.24	0.70
14:b:1:THR:HG23	8:V:91:ARG:NH1	2.06	0.70
3:C:228:LEU:HD22	3:C:232:GLU:OE2	1.92	0.70
11:Y:77:PRO:CD	11:Y:108:ASP:OD1	2.32	0.70
5:S:40:ILE:HD11	5:S:181:LEU:HD11	1.73	0.70
4:D:139:ASP:OD1	4:D:141:THR:OG1	2.09	0.70
2:P:172:PHE:HZ	2:P:176:ARG:HH12	1.36	0.70
3:Q:228:LEU:HD22	3:Q:232:GLU:OE2	1.92	0.70
6:F:38:LEU:HD11	6:F:187:LEU:HD12	1.71	0.70
1:O:174:GLU:HG3	1:O:205:VAL:HG11	1.74	0.70
4:D:226:GLU:O	4:D:229:VAL:HG12	1.92	0.69
7:G:198:TYR:HB3	7:G:243:LEU:HD11	1.72	0.69
7:U:185:THR:O	7:U:189:VAL:HG23	1.92	0.69
2:P:204:GLU:CD	2:P:222:PRO:CB	2.49	0.69
4:R:226:GLU:O	4:R:229:VAL:HG12	1.92	0.69
6:T:196:ARG:HH12	6:T:236:LEU:HB3	1.55	0.69
7:G:185:THR:O	7:G:189:VAL:HG23	1.92	0.69
2:B:64:VAL:O	2:B:219:ARG:NH1	2.25	0.69
12:L:147:LEU:HG	12:L:151:GLU:HB2	1.74	0.69
13:M:184:GLU:HG3	9:W:195:LYS:CE	2.21	0.69
7:G:191:LYS:HE2	7:G:238:TYR:CD2	2.28	0.68
2:P:64:VAL:O	2:P:219:ARG:NH1	2.25	0.68
11:Y:40:GLU:O	11:Y:40:GLU:HG2	1.93	0.68
7:U:191:LYS:HE2	7:U:238:TYR:CD2	2.28	0.68
12:Z:147:LEU:HG	12:Z:151:GLU:HB2	1.74	0.68
1:A:174:GLU:HG3	1:A:205:VAL:HG11	1.74	0.68
2:B:178:ASN:HB3	2:B:181:LEU:HG	1.76	0.68
12:Z:186:ARG:NH1	12:Z:189:SER:CB	2.55	0.67
1:A:123:GLN:NE2	2:B:81:ASP:OD1	2.27	0.67
11:K:40:GLU:O	11:K:40:GLU:HG2	1.93	0.67
7:G:108:LEU:HD21	7:G:149:TYR:CD1	2.30	0.67
5:E:160:GLY:O	6:F:82:ARG:NH2	2.27	0.67
7:G:191:LYS:HE2	7:G:238:TYR:HE2	1.56	0.67
10:J:202:ARG:NH2	10:J:204:ASP:OD2	2.28	0.67
12:L:186:ARG:HH11	12:L:189:SER:HB2	1.60	0.67
5:S:203:LYS:CG	5:S:210:LEU:CD1	2.50	0.67
5:E:212:ALA:CB	5:E:235:GLU:HG2	2.25	0.66
13:M:180:ILE:HG23	9:W:195:LYS:HE3	1.77	0.66
6:F:40:SER:HB3	6:F:187:LEU:HD22	1.76	0.66
11:K:27:GLN:NE2	11:Y:171:PHE:O	2.29	0.66
6:T:40:SER:HB3	6:T:187:LEU:HD22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:202:ARG:NH2	10:X:204:ASP:OD2	2.28	0.66
2:B:190:ALA:O	2:B:193:THR:CG2	2.44	0.66
13:M:180:ILE:HG23	9:W:195:LYS:HE2	1.76	0.66
7:U:108:LEU:HD21	7:U:149:TYR:CD1	2.30	0.66
2:P:190:ALA:O	2:P:193:THR:CG2	2.44	0.66
7:U:214:SER:OG	7:U:225:GLU:O	2.14	0.66
5:S:212:ALA:CB	5:S:235:GLU:HG2	2.25	0.66
2:B:172:PHE:CZ	2:B:176:ARG:CZ	2.79	0.66
1:A:46:ASP:N	1:A:46:ASP:OD1	2.28	0.65
1:O:46:ASP:OD1	1:O:46:ASP:N	2.28	0.65
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.78	0.65
2:P:178:ASN:HB3	2:P:181:LEU:HG	1.76	0.65
7:G:179:LEU:HD21	7:G:192:GLU:HG2	1.77	0.65
11:K:118:MET:HE2	11:K:124:LEU:HD13	1.78	0.65
2:P:172:PHE:CZ	2:P:176:ARG:CZ	2.79	0.65
14:N:1:THR:N	14:N:105:PRO:O	2.29	0.65
14:b:1:THR:N	14:b:105:PRO:O	2.29	0.65
4:D:189:LYS:O	4:D:193:LYS:HG2	1.96	0.65
4:R:189:LYS:O	4:R:193:LYS:HG2	1.96	0.65
11:Y:118:MET:HE2	11:Y:124:LEU:HD13	1.78	0.65
4:R:5:ARG:HH21	3:Q:8:ARG:NH2	1.87	0.65
5:S:210:LEU:C	5:S:210:LEU:HD23	2.22	0.65
1:O:172:GLN:O	1:O:176:THR:OG1	2.16	0.64
5:S:85:ALA:HB2	5:S:139:VAL:HG11	1.80	0.64
6:F:67:ASP:OD1	6:F:68:ASN:N	2.28	0.64
11:K:26:VAL:HG12	11:K:27:GLN:N	2.12	0.64
11:Y:26:VAL:HG12	11:Y:27:GLN:N	2.12	0.64
7:U:179:LEU:HD21	7:U:192:GLU:HG2	1.77	0.64
1:A:172:GLN:O	1:A:176:THR:OG1	2.16	0.64
3:C:8:ARG:NH2	4:D:5:ARG:HH22	1.87	0.64
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.78	0.64
5:E:210:LEU:HD23	5:E:210:LEU:C	2.22	0.64
10:J:29:ILE:HG22	10:J:30:GLN:H	1.63	0.64
12:Z:186:ARG:HH11	12:Z:189:SER:HB2	1.60	0.64
2:P:81:ASP:OD1	1:O:123:GLN:NE2	2.31	0.63
6:T:67:ASP:OD1	6:T:68:ASN:N	2.28	0.63
10:X:29:ILE:HG22	10:X:30:GLN:H	1.63	0.63
13:a:16:ALA:HB2	13:a:121:VAL:HG23	1.81	0.63
5:E:85:ALA:HB2	5:E:139:VAL:HG11	1.80	0.63
5:E:203:LYS:CD	5:E:210:LEU:HD13	2.29	0.63
13:M:16:ALA:HB2	13:M:121:VAL:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:199:THR:HG22	13:a:200:LYS:H	1.64	0.62
3:C:119:GLN:HG3	4:D:78:ALA:HB1	1.80	0.62
10:X:19:VAL:HG23	10:X:189:ILE:HB	1.82	0.62
5:S:203:LYS:CD	5:S:210:LEU:HD13	2.29	0.62
3:C:34:CYS:HG	3:C:75:SER:HG	1.46	0.62
11:Y:177:THR:HG23	11:Y:195:THR:HG22	1.81	0.62
9:I:183:LEU:C	9:I:183:LEU:HD13	2.25	0.61
9:W:183:LEU:HD13	9:W:183:LEU:C	2.25	0.61
13:M:199:THR:HG22	13:M:200:LYS:H	1.64	0.61
4:D:208:LEU:HD22	4:D:220:LEU:HD22	1.83	0.61
4:D:218:LYS:HZ1	4:D:220:LEU:HD11	1.65	0.61
12:L:186:ARG:NH1	12:L:189:SER:CB	2.55	0.61
4:D:139:ASP:OD1	4:D:141:THR:N	2.33	0.61
11:K:177:THR:HG23	11:K:195:THR:HG22	1.81	0.61
13:a:109:ILE:HG22	13:a:109:ILE:O	2.00	0.61
4:D:184:ASP:OD1	4:D:184:ASP:N	2.23	0.60
2:P:190:ALA:O	2:P:193:THR:HG23	2.01	0.60
2:P:214:GLU:N	2:P:214:GLU:OE1	2.34	0.60
2:B:189:THR:O	2:B:193:THR:HG22	2.00	0.60
4:R:139:ASP:OD1	4:R:141:THR:N	2.33	0.60
10:J:19:VAL:HG23	10:J:189:ILE:HB	1.82	0.60
13:M:145:LEU:HD21	13:M:182:ALA:HB2	1.83	0.60
13:M:109:ILE:O	13:M:109:ILE:HG22	2.00	0.60
13:a:145:LEU:HD21	13:a:182:ALA:HB2	1.83	0.60
3:Q:231:LYS:O	3:Q:235:GLN:HG3	2.02	0.60
2:B:214:GLU:OE1	2:B:214:GLU:N	2.34	0.60
2:P:49:LYS:NZ	2:P:61:VAL:O	2.32	0.60
8:V:145:GLU:N	8:V:145:GLU:OE2	2.34	0.60
8:H:145:GLU:OE2	8:H:145:GLU:N	2.34	0.60
10:J:148:MET:HG2	10:J:169:ALA:HA	1.83	0.60
2:P:189:THR:O	2:P:193:THR:HG22	2.00	0.60
4:R:208:LEU:HD22	4:R:220:LEU:HD22	1.83	0.60
12:Z:7:LYS:HD2	12:Z:109:PRO:HB2	1.84	0.60
3:C:231:LYS:O	3:C:235:GLN:HG3	2.01	0.59
4:R:116:GLN:O	4:R:119:THR:OG1	2.20	0.59
2:B:44:VAL:HG23	2:B:183:LEU:HD11	1.84	0.59
2:P:44:VAL:HG23	2:P:183:LEU:HD11	1.84	0.59
10:X:148:MET:HG2	10:X:169:ALA:HA	1.83	0.59
3:C:229:LYS:O	3:C:233:VAL:HG23	2.03	0.59
6:T:82:ARG:NH2	5:S:160:GLY:O	2.27	0.59
2:B:190:ALA:O	2:B:193:THR:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:229:LYS:O	3:Q:233:VAL:HG23	2.03	0.59
3:C:41:ASP:OD1	3:C:41:ASP:N	2.34	0.59
2:B:174:GLU:OE2	3:C:53:HIS:HE1	1.85	0.58
8:H:6:VAL:HG23	8:H:125:PHE:HB3	1.85	0.58
11:K:4:LEU:HD22	11:K:45:LEU:HD23	1.85	0.58
11:Y:49:GLU:HG3	11:Y:99:HIS:HB3	1.85	0.58
2:P:174:GLU:OE2	3:Q:53:HIS:HE1	1.86	0.58
4:R:31:THR:OG1	4:R:163:ARG:O	2.21	0.58
5:E:236:GLU:O	5:E:240:ASP:CG	2.46	0.58
4:R:218:LYS:HZ1	4:R:220:LEU:HD11	1.65	0.58
5:S:236:GLU:O	5:S:240:ASP:CG	2.46	0.58
4:R:226:GLU:O	4:R:229:VAL:HG13	2.03	0.58
12:L:7:LYS:HD2	12:L:109:PRO:HB2	1.84	0.58
3:Q:41:ASP:OD1	3:Q:41:ASP:N	2.34	0.58
8:V:6:VAL:HG23	8:V:125:PHE:HB3	1.85	0.58
1:A:112:ASP:OD1	1:A:112:ASP:N	2.36	0.58
4:D:226:GLU:O	4:D:229:VAL:HG13	2.03	0.58
4:R:221:SER:HB2	4:R:222:PRO:HD2	1.85	0.58
5:E:234:LEU:O	5:E:238:ILE:HG13	2.04	0.58
4:D:31:THR:OG1	4:D:163:ARG:O	2.21	0.57
4:R:158:ALA:HB1	4:R:172:LEU:HD21	1.86	0.57
5:S:234:LEU:O	5:S:238:ILE:HG13	2.04	0.57
11:K:49:GLU:HG3	11:K:99:HIS:HB3	1.85	0.57
4:D:116:GLN:O	4:D:119:THR:OG1	2.20	0.57
7:G:39:ILE:HG12	7:G:176:ILE:HD11	1.86	0.57
2:B:204:GLU:CG	2:B:222:PRO:CB	2.82	0.57
1:O:112:ASP:OD1	1:O:112:ASP:N	2.36	0.57
11:Y:4:LEU:HD22	11:Y:45:LEU:HD23	1.85	0.57
9:I:195:LYS:CE	13:a:180:ILE:HG23	2.34	0.56
14:b:5:MET:HE3	14:b:30:TYR:HE1	1.70	0.56
7:U:39:ILE:HG12	7:U:176:ILE:HD11	1.86	0.56
7:U:174:THR:O	7:U:177:GLU:HG2	2.05	0.56
4:D:221:SER:HB2	4:D:222:PRO:HD2	1.85	0.56
5:E:146:VAL:O	5:E:147:ASP:OD1	2.23	0.56
6:T:186:GLU:O	6:T:190:HIS:CD2	2.58	0.56
14:b:1:THR:HG21	8:V:91:ARG:NH1	2.20	0.56
3:C:153:SER:OG	3:C:155:ASN:OD1	2.23	0.56
3:C:207:SER:HB2	3:C:210:LYS:HG3	1.86	0.56
7:G:174:THR:O	7:G:177:GLU:HG2	2.06	0.56
7:G:214:SER:OG	7:G:225:GLU:O	2.14	0.56
13:M:180:ILE:CG2	9:W:195:LYS:HE2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:74:VAL:HG22	2:P:75:TYR:H	1.71	0.56
10:X:47:ARG:NH1	10:X:191:LYS:O	2.38	0.56
3:Q:207:SER:HB2	3:Q:210:LYS:HG3	1.86	0.56
4:D:158:ALA:HB1	4:D:172:LEU:HD21	1.86	0.56
6:F:186:GLU:O	6:F:190:HIS:CD2	2.58	0.56
7:U:191:LYS:CE	7:U:238:TYR:CE2	2.87	0.56
9:I:195:LYS:HD3	13:a:184:GLU:OE1	2.01	0.56
12:Z:117:GLU:N	12:Z:117:GLU:OE2	2.39	0.56
14:N:5:MET:HE3	14:N:30:TYR:HE1	1.70	0.56
7:U:52:LEU:HD11	7:U:206:ASP:OD2	2.06	0.56
2:B:74:VAL:HG22	2:B:75:TYR:H	1.71	0.56
10:J:47:ARG:NH1	10:J:191:LYS:O	2.38	0.56
1:A:19:GLU:HB2	1:A:21:ARG:HG3	1.88	0.56
2:B:49:LYS:NZ	2:B:61:VAL:O	2.32	0.56
3:C:143:TYR:OH	4:D:57:ARG:NH2	2.39	0.56
12:L:182:ASP:OD1	12:L:182:ASP:N	2.34	0.56
2:P:41:ASN:OD1	2:P:41:ASN:N	2.39	0.55
1:O:171:LYS:O	1:O:175:SER:OG	2.14	0.55
7:G:108:LEU:HD21	7:G:149:TYR:HD1	1.70	0.55
9:I:28:ASP:HB2	10:J:130:MET:CE	2.36	0.55
1:A:123:GLN:O	1:A:126:THR:OG1	2.22	0.55
9:I:30:ASN:OD1	9:I:187:ARG:NH1	2.36	0.55
10:X:141:CYS:O	10:X:145:MET:HG2	2.06	0.55
1:O:221:THR:OG1	1:O:224:ASN:OD1	2.23	0.55
5:S:31:HIS:HE1	5:S:139:VAL:C	2.15	0.55
5:S:146:VAL:O	5:S:147:ASP:OD1	2.23	0.55
9:W:28:ASP:OD1	9:W:29:LYS:N	2.40	0.55
10:X:130:MET:CE	9:W:28:ASP:HB2	2.37	0.55
4:D:146:GLN:OE1	4:D:159:ASN:ND2	2.40	0.55
4:R:208:LEU:CD2	4:R:220:LEU:HD22	2.37	0.55
5:E:31:HIS:HE1	5:E:139:VAL:C	2.14	0.55
2:B:41:ASN:N	2:B:41:ASN:OD1	2.39	0.55
13:M:145:LEU:HD22	13:M:178:VAL:HG13	1.88	0.55
11:Y:80:ALA:O	11:Y:84:THR:OG1	2.25	0.55
1:O:19:GLU:HB2	1:O:21:ARG:HG3	1.88	0.55
7:G:52:LEU:HD11	7:G:206:ASP:OD2	2.06	0.54
6:T:137:TYR:CZ	6:T:217:LYS:HD3	2.42	0.54
9:I:28:ASP:OD1	9:I:29:LYS:N	2.40	0.54
12:L:117:GLU:OE2	12:L:117:GLU:N	2.39	0.54
5:E:236:GLU:O	5:E:240:ASP:OD2	2.25	0.54
7:G:191:LYS:CE	7:G:238:TYR:CE2	2.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:26:VAL:CG1	11:Y:27:GLN:N	2.71	0.54
7:U:108:LEU:HD21	7:U:149:TYR:HD1	1.70	0.54
13:a:145:LEU:HD22	13:a:178:VAL:HG13	1.88	0.54
4:R:146:GLN:OE1	4:R:159:ASN:ND2	2.40	0.54
1:O:123:GLN:O	1:O:126:THR:OG1	2.22	0.54
11:K:26:VAL:CG1	11:K:27:GLN:N	2.71	0.54
4:R:78:ALA:HB1	3:Q:119:GLN:HG3	1.89	0.54
4:D:208:LEU:CD2	4:D:220:LEU:HD22	2.37	0.54
8:H:12:VAL:HG21	8:H:101:ALA:HB1	1.89	0.54
10:J:141:CYS:O	10:J:145:MET:HG2	2.07	0.54
13:M:169:ASP:OD1	13:M:169:ASP:N	2.41	0.54
9:I:28:ASP:HB2	10:J:130:MET:HE3	1.88	0.54
2:P:204:GLU:CG	2:P:222:PRO:CB	2.82	0.53
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.90	0.53
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.89	0.53
5:E:31:HIS:HE1	5:E:140:ALA:N	2.07	0.53
8:H:12:VAL:HG11	8:H:111:VAL:HG23	1.90	0.53
6:F:117:GLN:O	6:F:120:THR:OG1	2.26	0.53
6:F:137:TYR:CZ	6:F:217:LYS:HD3	2.42	0.53
13:a:153:VAL:HG22	13:a:166:LEU:HD11	1.90	0.53
2:B:174:GLU:OE2	3:C:53:HIS:CE1	2.60	0.53
6:T:117:GLN:O	6:T:120:THR:OG1	2.27	0.53
6:T:126:ARG:HG2	5:S:13:ASN:HB3	1.90	0.53
3:Q:153:SER:OG	3:Q:155:ASN:OD1	2.23	0.53
9:I:195:LYS:CE	13:a:184:GLU:CG	2.72	0.53
1:A:161:CYS:SG	2:B:56:TYR:HD1	2.30	0.53
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.89	0.53
1:O:50:ILE:HD11	1:O:141:ILE:HG12	1.91	0.53
5:S:236:GLU:O	5:S:240:ASP:OD2	2.25	0.53
8:V:12:VAL:HG11	8:V:111:VAL:HG23	1.90	0.53
13:a:115:GLU:CD	13:a:115:GLU:H	2.17	0.53
1:A:50:ILE:HD11	1:A:141:ILE:HG12	1.91	0.53
11:Y:19:ARG:HB3	11:Y:31:ASP:HA	1.90	0.53
12:Z:105:ASP:OD1	12:Z:105:ASP:N	2.39	0.53
4:R:204:LYS:O	4:R:204:LYS:HG3	2.09	0.53
13:M:123:SER:OG	13:M:133:ASP:OD1	2.21	0.53
1:A:221:THR:OG1	1:A:224:ASN:OD1	2.23	0.52
6:F:53:GLN:OE1	6:F:58:ALA:O	2.27	0.52
13:M:153:VAL:HG22	13:M:166:LEU:HD11	1.90	0.52
8:V:12:VAL:HG21	8:V:101:ALA:HB1	1.90	0.52
1:A:176:THR:HG22	2:B:55:LEU:CD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:204:LYS:HG3	4:D:204:LYS:O	2.09	0.52
8:V:167:ASP:OD2	8:V:170:SER:OG	2.27	0.52
8:H:141:ALA:HB2	8:V:162:LEU:HD11	1.91	0.52
9:I:187:ARG:HB3	9:I:188:PRO:HD3	1.90	0.52
12:L:105:ASP:N	12:L:105:ASP:OD1	2.39	0.52
10:J:160:GLU:O	10:J:164:GLU:HG2	2.10	0.52
8:H:7:GLN:HA	8:H:12:VAL:HG12	1.91	0.52
11:K:19:ARG:HB3	11:K:31:ASP:HA	1.90	0.52
11:Y:5:ILE:HD11	11:Y:143:LEU:HD11	1.91	0.52
11:Y:47:VAL:HG23	11:Y:101:ASN:HB2	1.91	0.52
9:W:30:ASN:OD1	9:W:187:ARG:NH1	2.36	0.52
3:Q:201:MET:HG2	3:Q:203:VAL:HG22	1.92	0.52
4:D:217:LEU:HG	4:D:217:LEU:O	2.09	0.52
6:T:186:GLU:O	6:T:190:HIS:HD2	1.93	0.52
10:X:160:GLU:O	10:X:164:GLU:HG2	2.10	0.52
11:K:5:ILE:HD11	11:K:143:LEU:HD11	1.91	0.52
5:E:199:LEU:O	5:E:203:LYS:HG3	2.10	0.52
6:F:186:GLU:O	6:F:190:HIS:HD2	1.93	0.52
5:S:41:GLN:NE2	5:S:151:PRO:O	2.43	0.52
11:K:47:VAL:HG23	11:K:101:ASN:HB2	1.91	0.52
14:b:205:ALA:C	14:b:207:THR:H	2.17	0.52
4:R:217:LEU:HG	4:R:217:LEU:O	2.09	0.52
5:S:199:LEU:O	5:S:203:LYS:HG3	2.10	0.52
2:B:190:ALA:O	2:B:193:THR:HG22	2.10	0.52
3:C:201:MET:HG2	3:C:203:VAL:HG22	1.92	0.52
2:B:118:GLN:O	2:B:121:THR:OG1	2.28	0.51
6:T:53:GLN:OE1	6:T:58:ALA:O	2.27	0.51
14:N:205:ALA:C	14:N:207:THR:H	2.17	0.51
13:M:115:GLU:CD	13:M:115:GLU:H	2.17	0.51
5:S:197:SER:O	5:S:201:ILE:HG13	2.11	0.51
2:B:87:HIS:NE2	2:B:91:LYS:HE3	2.25	0.51
7:G:120:HIS:O	7:G:123:THR:OG1	2.27	0.51
8:H:91:ARG:NH1	14:N:1:THR:HG21	2.24	0.51
2:P:87:HIS:NE2	2:P:91:LYS:HE3	2.25	0.51
6:T:56:LEU:CD2	5:S:167:ALA:HB3	2.40	0.51
9:W:195:LYS:HE3	9:W:196:GLY:H	1.75	0.51
1:O:51:VAL:HG12	1:O:217:VAL:HG12	1.93	0.51
5:S:31:HIS:HE1	5:S:140:ALA:N	2.07	0.51
5:E:197:SER:O	5:E:201:ILE:HG13	2.11	0.51
2:P:174:GLU:OE2	3:Q:53:HIS:CE1	2.63	0.51
2:P:190:ALA:O	2:P:193:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:7:GLN:HA	8:V:12:VAL:HG12	1.91	0.51
14:N:45:VAL:HB	14:N:49:THR:HB	1.93	0.51
13:a:169:ASP:N	13:a:169:ASP:OD1	2.41	0.51
14:b:45:VAL:HB	14:b:49:THR:HB	1.93	0.51
7:U:108:LEU:CD2	7:U:149:TYR:CE1	2.94	0.51
1:A:51:VAL:HG12	1:A:217:VAL:HG12	1.93	0.51
7:G:108:LEU:CD2	7:G:149:TYR:CE1	2.94	0.51
3:Q:28:ILE:HD11	3:Q:152:PRO:HG3	1.92	0.51
1:A:24:GLN:NE2	7:G:14:PHE:H	2.09	0.51
6:T:39:LYS:HD3	6:T:144:VAL:HG23	1.93	0.51
7:U:120:HIS:O	7:U:123:THR:OG1	2.28	0.51
9:I:195:LYS:HE3	9:I:196:GLY:H	1.75	0.50
1:A:224:ASN:HD21	1:A:228:ARG:HE	1.60	0.50
4:D:23:GLN:HA	4:D:26:VAL:HG12	1.94	0.50
13:M:184:GLU:OE2	9:W:195:LYS:CG	2.44	0.50
3:C:28:ILE:HD11	3:C:152:PRO:HG3	1.92	0.50
5:E:41:GLN:NE2	5:E:151:PRO:O	2.43	0.50
8:H:45:ARG:HD2	8:H:52:THR:HB	1.94	0.50
2:P:118:GLN:O	2:P:121:THR:OG1	2.28	0.50
1:O:97:GLU:OE1	1:O:117:ARG:NH1	2.38	0.50
1:O:202:LEU:HD22	1:O:210:PHE:CE2	2.46	0.50
4:D:156:TRP:CE2	5:E:59:MET:HG3	2.47	0.50
6:T:53:GLN:HE22	5:S:163:VAL:HG11	1.76	0.50
12:Z:175:ASN:OD1	12:Z:189:SER:OG	2.24	0.50
1:O:84:THR:O	1:O:88:ARG:HG2	2.11	0.50
6:F:39:LYS:HD3	6:F:144:VAL:HG23	1.93	0.50
1:O:224:ASN:HD21	1:O:228:ARG:HE	1.60	0.50
6:F:196:ARG:NH1	6:F:236:LEU:HB3	2.26	0.50
4:R:23:GLN:HA	4:R:26:VAL:HG12	1.94	0.50
4:R:47:LYS:HE3	4:R:207:GLU:HB2	1.93	0.50
3:Q:230:GLN:O	3:Q:234:GLU:HG3	2.12	0.50
1:A:84:THR:O	1:A:88:ARG:HG2	2.11	0.50
2:B:202:MET:HE1	2:B:207:ILE:HG21	1.94	0.50
2:P:166:TYR:O	2:P:170:LYS:HG2	2.12	0.50
7:U:8:ASP:O	7:U:22:GLN:NE2	2.44	0.50
1:A:202:LEU:HD22	1:A:210:PHE:CE2	2.46	0.50
4:D:47:LYS:HE3	4:D:207:GLU:HB2	1.93	0.50
11:K:170:ARG:HH21	12:Z:140:ASP:CG	2.19	0.50
11:Y:19:ARG:HH21	11:Y:31:ASP:HB2	1.77	0.50
2:B:122:GLN:O	3:C:127:LYS:HG3	2.12	0.50
8:H:167:ASP:OD2	8:H:170:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:80:ALA:O	11:K:84:THR:OG1	2.25	0.50
7:U:37:ILE:HD11	7:U:193:VAL:HG22	1.94	0.50
8:V:148:THR:OG1	8:V:149:LYS:N	2.45	0.50
7:G:108:LEU:CD2	7:G:149:TYR:HD1	2.24	0.49
2:P:202:MET:HE1	2:P:207:ILE:HG21	1.94	0.49
4:D:76:LEU:H	4:D:129:ILE:HG22	1.77	0.49
14:N:92:LEU:HD21	14:N:110:LYS:HD2	1.94	0.49
2:B:44:VAL:HG21	2:B:187:ILE:HG12	1.93	0.49
5:E:97:GLN:HG3	12:L:65:ILE:HG13	1.95	0.49
13:a:123:SER:OG	13:a:133:ASP:OD1	2.21	0.49
14:b:92:LEU:HD21	14:b:110:LYS:HD2	1.94	0.49
7:G:37:ILE:HD11	7:G:193:VAL:HG22	1.94	0.49
5:S:62:SER:O	5:S:62:SER:OG	2.30	0.49
9:I:195:LYS:HE3	13:a:180:ILE:HG23	1.94	0.49
10:J:24:ASP:OD1	10:J:40:LYS:NZ	2.43	0.49
8:H:145:GLU:N	8:H:145:GLU:CD	2.71	0.49
9:I:183:LEU:C	9:I:183:LEU:CD1	2.86	0.49
12:Z:186:ARG:HH12	12:Z:189:SER:HB2	1.69	0.49
7:U:81:LEU:O	7:U:85:ARG:HG3	2.13	0.49
8:V:45:ARG:HD2	8:V:52:THR:HB	1.94	0.49
7:G:195:LYS:HD2	7:G:199:ILE:HD12	1.95	0.49
8:H:103:TRP:CH2	8:H:181:GLN:HG3	2.48	0.49
2:P:44:VAL:HG21	2:P:187:ILE:HG12	1.93	0.49
2:P:204:GLU:CG	2:P:222:PRO:CA	2.91	0.49
8:V:145:GLU:N	8:V:145:GLU:CD	2.71	0.49
10:X:24:ASP:OD1	10:X:40:LYS:NZ	2.42	0.49
12:Z:7:LYS:O	12:Z:143:TYR:OH	2.28	0.49
3:C:230:GLN:O	3:C:234:GLU:HG3	2.12	0.48
8:V:103:TRP:CH2	8:V:181:GLN:HG3	2.48	0.48
7:G:81:LEU:O	7:G:85:ARG:HG3	2.13	0.48
11:K:19:ARG:HH21	11:K:31:ASP:HB2	1.77	0.48
13:M:144:MET:HE1	13:M:185:ARG:HB2	1.95	0.48
7:U:195:LYS:HD2	7:U:199:ILE:HD12	1.95	0.48
1:A:16:PHE:HD1	1:A:20:GLY:HA2	1.78	0.48
4:D:204:LYS:NZ	4:D:222:PRO:O	2.40	0.48
4:R:76:LEU:H	4:R:129:ILE:HG22	1.77	0.48
7:U:195:LYS:HD2	7:U:199:ILE:CD1	2.42	0.48
11:K:5:ILE:HG22	11:K:16:ALA:HB3	1.96	0.48
12:L:175:ASN:OD1	12:L:189:SER:OG	2.24	0.48
10:X:11:MET:HE1	10:X:169:ALA:HB3	1.95	0.48
2:B:166:TYR:O	2:B:170:LYS:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:212:ALA:O	5:E:231:LYS:NZ	2.46	0.48
9:W:183:LEU:C	9:W:183:LEU:CD1	2.86	0.48
7:G:110:HIS:O	7:G:114:ARG:HG2	2.14	0.48
12:L:44:THR:O	12:L:99:THR:HG22	2.13	0.48
1:A:160:TYR:CG	1:A:160:TYR:O	2.67	0.48
6:F:117:GLN:HG3	7:G:82:ALA:HB1	1.95	0.48
7:G:195:LYS:HD2	7:G:199:ILE:CD1	2.42	0.48
4:R:156:TRP:CE2	5:S:59:MET:HG3	2.48	0.48
1:O:16:PHE:HD1	1:O:20:GLY:HA2	1.78	0.48
7:U:110:HIS:O	7:U:114:ARG:HG2	2.14	0.48
6:T:7:ASP:OD1	6:T:7:ASP:N	2.40	0.48
13:a:144:MET:HE1	13:a:185:ARG:HB2	1.95	0.48
12:L:140:ASP:CG	11:Y:170:ARG:HH21	2.22	0.48
7:G:51:LYS:NZ	7:G:62:SER:O	2.47	0.47
12:L:38:ASN:HD21	12:L:41:LEU:HD12	1.79	0.47
6:T:43:HIS:CD2	6:T:216:GLY:HA3	2.49	0.47
14:b:5:MET:HE3	14:b:30:TYR:CE1	2.49	0.47
4:R:215:GLN:N	4:R:216:PRO:CD	2.77	0.47
2:P:10:THR:HG23	2:P:20:GLN:HB2	1.96	0.47
12:Z:38:ASN:HD21	12:Z:41:LEU:HD12	1.79	0.47
10:J:168:GLN:O	10:J:172:ASN:ND2	2.44	0.47
13:M:184:GLU:HG3	9:W:195:LYS:HE2	1.95	0.47
1:O:160:TYR:CG	1:O:160:TYR:O	2.67	0.47
1:A:97:GLU:OE1	1:A:117:ARG:NH1	2.38	0.47
4:D:215:GLN:N	4:D:216:PRO:CD	2.77	0.47
12:Z:44:THR:O	12:Z:99:THR:HG22	2.14	0.47
1:A:130:GLU:HG2	2:B:4:GLY:HA2	1.96	0.47
6:F:35:THR:HG21	6:F:73:SER:OG	2.15	0.47
6:T:79:ALA:HB3	5:S:121:LEU:HD12	1.96	0.47
11:Y:5:ILE:HG22	11:Y:16:ALA:HB3	1.96	0.47
10:J:11:MET:HE1	10:J:169:ALA:HB3	1.95	0.47
7:U:135:PHE:CZ	7:U:151:ILE:HD12	2.49	0.47
2:P:54:ILE:HG12	2:P:54:ILE:O	2.15	0.47
10:X:114:LYS:HB3	10:X:114:LYS:HE3	1.46	0.47
12:Z:190:ASP:OD1	12:Z:195:LEU:HG	2.15	0.47
5:S:212:ALA:O	5:S:231:LYS:NZ	2.46	0.47
6:F:27:GLU:HA	6:F:30:LYS:HE2	1.97	0.47
7:G:135:PHE:CZ	7:G:151:ILE:HD12	2.50	0.47
8:V:71:ASN:C	8:V:71:ASN:HD22	2.23	0.47
4:R:29:GLY:O	4:R:163:ARG:HG2	2.15	0.47
2:B:204:GLU:CG	2:B:222:PRO:CA	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:9:ASP:OD1	8:V:9:ASP:N	2.47	0.47
4:D:29:GLY:O	4:D:163:ARG:HG2	2.15	0.46
6:F:43:HIS:CD2	6:F:216:GLY:HA3	2.49	0.46
8:H:71:ASN:C	8:H:71:ASN:HD22	2.23	0.46
12:L:190:ASP:OD1	12:L:195:LEU:HG	2.15	0.46
14:N:5:MET:HE3	14:N:30:TYR:CE1	2.49	0.46
4:R:57:ARG:NH2	3:Q:143:TYR:OH	2.48	0.46
7:U:51:LYS:NZ	7:U:62:SER:O	2.47	0.46
2:B:10:THR:HG23	2:B:20:GLN:HB2	1.96	0.46
6:F:104:PRO:HA	6:F:138:ASP:OD2	2.16	0.46
11:Y:62:LYS:HD2	4:R:96:LEU:HD22	1.97	0.46
7:G:8:ASP:O	7:G:22:GLN:NE2	2.44	0.46
7:U:72:HIS:CE1	7:U:105:ASN:HB3	2.50	0.46
2:B:54:ILE:O	2:B:54:ILE:HG12	2.15	0.46
8:H:148:THR:OG1	8:H:149:LYS:N	2.45	0.46
9:I:195:LYS:NZ	13:a:184:GLU:HG3	2.29	0.46
6:T:196:ARG:NH1	6:T:236:LEU:HB3	2.26	0.46
4:R:21:TYR:CE1	3:Q:14:PRO:HA	2.51	0.46
7:U:168:ALA:HB1	7:U:200:VAL:CG1	2.46	0.46
5:S:210:LEU:C	5:S:210:LEU:CD2	2.88	0.46
2:B:204:GLU:HG2	2:B:204:GLU:O	2.16	0.46
2:P:204:GLU:HG2	2:P:204:GLU:O	2.16	0.46
5:S:181:LEU:HD12	5:S:181:LEU:HA	1.78	0.46
1:A:230:LEU:HD22	1:A:234:GLU:OE1	2.16	0.46
7:G:52:LEU:CD1	7:G:206:ASP:OD2	2.64	0.46
7:G:72:HIS:CE1	7:G:105:ASN:HB3	2.50	0.46
8:H:56:ALA:O	8:H:60:THR:OG1	2.31	0.46
6:T:104:PRO:HA	6:T:138:ASP:OD2	2.16	0.46
10:J:29:ILE:O	10:J:30:GLN:C	2.59	0.46
6:T:27:GLU:HA	6:T:30:LYS:HE2	1.97	0.46
10:X:202:ARG:HE	10:X:202:ARG:HB3	1.50	0.46
2:P:43:VAL:HB	2:P:136:CYS:SG	2.56	0.46
8:V:59:VAL:HG11	8:V:83:PHE:CE2	2.51	0.46
1:A:161:CYS:SG	1:A:162:GLY:N	2.89	0.46
4:D:67:ASP:OD1	4:D:67:ASP:N	2.49	0.46
7:G:168:ALA:HB1	7:G:200:VAL:CG1	2.46	0.46
4:R:185:ASP:O	4:R:189:LYS:HD3	2.16	0.46
9:W:191:VAL:O	9:W:191:VAL:HG12	2.16	0.45
3:C:67:LYS:HE2	3:C:69:ASN:O	2.16	0.45
5:E:210:LEU:C	5:E:210:LEU:CD2	2.88	0.45
8:H:9:ASP:OD1	8:H:9:ASP:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:VAL:HB	2:B:136:CYS:SG	2.56	0.45
8:H:59:VAL:HG11	8:H:83:PHE:CE2	2.51	0.45
6:T:35:THR:HG21	6:T:73:SER:OG	2.15	0.45
1:O:230:LEU:HD22	1:O:234:GLU:OE1	2.16	0.45
7:U:52:LEU:CD1	7:U:206:ASP:OD2	2.64	0.45
13:M:193:LEU:HB3	13:M:208:VAL:HG23	1.99	0.45
13:a:125:ASP:OD1	13:a:129:SER:N	2.50	0.45
13:a:193:LEU:HB3	13:a:208:VAL:HG23	1.99	0.45
4:R:189:LYS:HB3	4:R:189:LYS:HE3	1.85	0.45
7:U:219:LEU:H	7:U:219:LEU:HD23	1.81	0.45
2:B:221:THR:O	2:B:225:VAL:HG23	2.17	0.45
4:D:173:GLU:HA	5:E:58:LEU:HD11	1.99	0.45
7:G:219:LEU:HD23	7:G:219:LEU:H	1.81	0.45
13:M:199:THR:HG22	13:M:200:LYS:N	2.31	0.45
11:Y:11:ASP:OD1	11:Y:11:ASP:N	2.49	0.45
9:I:195:LYS:HD2	9:I:195:LYS:HA	1.58	0.45
10:J:114:LYS:HB3	10:J:114:LYS:HE3	1.46	0.45
3:Q:67:LYS:HE2	3:Q:69:ASN:O	2.16	0.45
2:B:174:GLU:HG2	3:C:55:LEU:HD11	1.98	0.45
11:Y:1:MET:HG3	11:Y:134:TYR:CG	2.52	0.45
4:D:26:VAL:HG21	4:D:130:SER:HB2	1.99	0.45
11:K:11:ASP:OD1	11:K:11:ASP:N	2.49	0.45
10:X:130:MET:HE3	9:W:28:ASP:HB2	1.98	0.45
4:R:40:ILE:CG2	4:R:212:ARG:HG2	2.42	0.45
1:O:161:CYS:SG	1:O:162:GLY:N	2.89	0.45
7:G:39:ILE:HG21	7:G:189:VAL:CG1	2.48	0.44
9:I:191:VAL:HG12	9:I:191:VAL:O	2.16	0.44
2:P:221:THR:O	2:P:225:VAL:HG23	2.17	0.44
10:X:29:ILE:O	10:X:30:GLN:C	2.59	0.44
12:Z:82:LEU:HD23	12:Z:82:LEU:HA	1.87	0.44
12:Z:182:ASP:OD1	12:Z:182:ASP:N	2.34	0.44
4:R:26:VAL:HG21	4:R:130:SER:HB2	1.99	0.44
1:A:55:LYS:HE3	1:A:55:LYS:HB3	1.61	0.44
4:D:185:ASP:O	4:D:189:LYS:HD3	2.16	0.44
11:K:170:ARG:HA	11:K:170:ARG:HD3	1.83	0.44
13:M:125:ASP:OD1	13:M:129:SER:N	2.50	0.44
4:R:204:LYS:NZ	4:R:222:PRO:O	2.40	0.44
5:S:141:LEU:HD23	5:S:143:PHE:CZ	2.53	0.44
3:Q:28:ILE:O	3:Q:28:ILE:HG22	2.17	0.44
5:E:16:SER:OG	5:E:20:ARG:HB2	2.18	0.44
12:Z:161:TYR:HD1	12:Z:192:VAL:HG13	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:67:ASP:N	4:R:67:ASP:OD1	2.49	0.44
8:V:179:ILE:HD13	8:V:184:VAL:HG22	2.00	0.44
2:P:118:GLN:HG3	3:Q:81:SER:HB3	2.00	0.44
1:A:202:LEU:HD22	1:A:210:PHE:HE2	1.82	0.44
14:b:79:ASP:OD1	14:b:79:ASP:N	2.35	0.44
7:U:35:THR:HA	7:U:166:GLY:HA3	1.99	0.44
12:L:161:TYR:HD1	12:L:192:VAL:HG13	1.81	0.44
3:Q:195:LYS:HG3	3:Q:240:HIS:HE1	1.82	0.44
2:B:198:PHE:HZ	2:B:206:ASN:HB3	1.83	0.44
8:H:4:MET:HG3	8:H:127:ILE:HG22	2.00	0.44
11:K:1:MET:HG3	11:K:134:TYR:CG	2.52	0.44
14:b:1:THR:HG23	8:V:91:ARG:HH11	1.78	0.44
3:C:14:PRO:HA	4:D:21:TYR:CE1	2.53	0.44
6:F:38:LEU:HD13	6:F:187:LEU:CD1	2.39	0.44
7:G:175:GLU:O	7:G:178:LYS:HG2	2.18	0.44
8:H:179:ILE:HD13	8:H:184:VAL:HG22	2.00	0.44
13:M:200:LYS:HE3	13:M:200:LYS:HB3	1.73	0.44
14:N:79:ASP:OD1	14:N:79:ASP:N	2.35	0.44
14:b:166:ARG:NH1	14:b:200:GLU:OE1	2.51	0.44
5:S:16:SER:OG	5:S:20:ARG:HB2	2.18	0.44
1:O:55:LYS:HB3	1:O:55:LYS:HE3	1.61	0.43
8:V:4:MET:HG3	8:V:127:ILE:HG22	2.00	0.43
4:D:46:GLU:HG2	4:D:47:LYS:N	2.33	0.43
11:K:43:LEU:HD12	11:K:183:ILE:HD11	2.00	0.43
4:R:46:GLU:HG2	4:R:47:LYS:N	2.33	0.43
2:B:190:ALA:C	2:B:193:THR:HG22	2.44	0.43
3:C:28:ILE:O	3:C:28:ILE:HG22	2.17	0.43
4:D:40:ILE:CG2	4:D:212:ARG:HG2	2.42	0.43
7:G:28:LYS:HE2	7:G:28:LYS:HB3	1.80	0.43
14:N:166:ARG:NH1	14:N:200:GLU:OE1	2.51	0.43
14:N:205:ALA:O	14:N:207:THR:N	2.51	0.43
11:Y:43:LEU:HD12	11:Y:183:ILE:HD11	2.00	0.43
5:S:228:MET:HE2	5:S:228:MET:HB3	1.89	0.43
1:A:191:PHE:O	1:A:193:GLN:N	2.52	0.43
2:B:134:LEU:HD23	2:B:134:LEU:HA	1.87	0.43
3:C:195:LYS:HG3	3:C:240:HIS:HE1	1.82	0.43
2:P:198:PHE:HZ	2:P:206:ASN:HB3	1.83	0.43
1:O:191:PHE:O	1:O:193:GLN:N	2.52	0.43
1:O:202:LEU:HD22	1:O:210:PHE:HE2	1.82	0.43
5:S:85:ALA:O	5:S:89:ILE:HG12	2.18	0.43
5:E:85:ALA:O	5:E:89:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:120:ALA:O	5:E:121:LEU:HB2	2.18	0.43
5:E:211:ASN:ND2	5:E:213:THR:HG22	2.33	0.43
7:G:35:THR:HA	7:G:166:GLY:HA3	1.99	0.43
12:L:186:ARG:HH12	12:L:189:SER:HB2	1.69	0.43
13:M:116:GLU:CD	13:M:118:LYS:HE3	2.44	0.43
6:T:53:GLN:NE2	5:S:163:VAL:HG11	2.33	0.43
1:O:130:GLU:H	1:O:130:GLU:HG3	1.42	0.43
4:D:30:SER:HB3	4:D:48:LYS:HE3	2.00	0.43
5:E:141:LEU:HD23	5:E:143:PHE:CZ	2.53	0.43
6:F:185:ASP:O	6:F:188:VAL:HG23	2.19	0.43
2:P:190:ALA:C	2:P:193:THR:HG22	2.44	0.43
13:a:116:GLU:CD	13:a:118:LYS:HE3	2.44	0.43
14:b:205:ALA:O	14:b:207:THR:N	2.51	0.43
7:U:39:ILE:HG21	7:U:189:VAL:CG1	2.48	0.43
8:V:84:LYS:HE2	8:V:84:LYS:HB3	1.88	0.43
6:F:185:ASP:OD1	6:F:185:ASP:N	2.52	0.43
12:L:113:TYR:O	12:L:120:ARG:HA	2.19	0.43
2:P:183:LEU:O	2:P:187:ILE:HG13	2.19	0.43
6:T:185:ASP:OD1	6:T:185:ASP:N	2.52	0.43
4:R:41:VAL:HG11	4:R:134:VAL:HB	2.01	0.43
2:B:183:LEU:O	2:B:187:ILE:HG13	2.19	0.43
7:G:179:LEU:HD12	7:G:181:MET:HB3	2.01	0.43
1:O:202:LEU:HD23	1:O:206:LEU:HD12	2.00	0.43
7:U:179:LEU:HD12	7:U:181:MET:HB3	2.01	0.43
5:S:120:ALA:O	5:S:121:LEU:HB2	2.18	0.43
5:S:203:LYS:HD2	5:S:210:LEU:HB3	2.00	0.43
5:S:211:ASN:ND2	5:S:213:THR:HG22	2.33	0.43
8:H:103:TRP:CZ2	8:H:181:GLN:HG3	2.54	0.42
7:U:136:MET:SD	7:U:163:CYS:HB3	2.59	0.42
5:S:184:VAL:HG11	5:S:197:SER:HB3	2.01	0.42
5:E:13:ASN:HB3	6:F:126:ARG:HG2	2.00	0.42
5:E:196:LYS:O	5:E:200:ILE:HD12	2.20	0.42
6:T:185:ASP:O	6:T:188:VAL:HG23	2.19	0.42
11:Y:26:VAL:CG2	12:Z:133:VAL:HG12	2.49	0.42
3:C:72:MET:HE2	3:C:72:MET:HB3	1.89	0.42
4:D:41:VAL:HG11	4:D:134:VAL:HB	2.01	0.42
8:H:150:ASP:N	8:H:150:ASP:OD1	2.53	0.42
12:L:147:LEU:HD12	12:L:147:LEU:HA	1.87	0.42
11:Y:23:SER:HB3	11:Y:28:MET:HG3	2.01	0.42
12:Z:21:THR:HG22	12:Z:26:ILE:HA	2.01	0.42
7:U:175:GLU:O	7:U:178:LYS:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:78:MET:HG3	5:S:82:ILE:HD12	2.01	0.42
5:E:203:LYS:HD2	5:E:210:LEU:HB3	2.00	0.42
8:H:103:TRP:HA	8:H:108:GLY:O	2.20	0.42
6:T:176:MET:HE3	7:U:57:LEU:HD23	2.01	0.42
10:J:176:ARG:NH1	12:Z:26:ILE:O	2.52	0.42
11:K:23:SER:HB3	11:K:28:MET:HG3	2.00	0.42
13:a:199:THR:HG22	13:a:200:LYS:N	2.31	0.42
4:R:5:ARG:CZ	3:Q:8:ARG:HE	2.33	0.42
4:R:173:GLU:HA	5:S:58:LEU:HD11	2.02	0.42
1:A:202:LEU:HD23	1:A:206:LEU:HD12	2.00	0.42
5:E:163:VAL:HG11	6:F:53:GLN:HE22	1.85	0.42
5:E:184:VAL:HG11	5:E:197:SER:HB3	2.01	0.42
13:M:11:THR:HG21	13:M:141:ALA:HB3	2.02	0.42
10:X:26:ARG:HB2	10:X:182:MET:HG2	2.02	0.42
9:W:18:THR:OG1	9:W:172:ASN:HB2	2.19	0.42
9:W:195:LYS:HD2	9:W:195:LYS:HA	1.58	0.42
7:U:181:MET:HB3	7:U:181:MET:HE3	1.88	0.42
9:I:18:THR:OG1	9:I:172:ASN:HB2	2.19	0.42
6:T:69:HIS:O	6:T:136:GLY:HA2	2.20	0.42
14:b:205:ALA:C	14:b:207:THR:N	2.78	0.42
4:R:30:SER:HB3	4:R:48:LYS:HE3	2.00	0.42
7:U:168:ALA:CB	7:U:200:VAL:CG1	2.98	0.42
7:U:243:LEU:O	7:U:244:LYS:HB2	2.20	0.42
5:S:41:GLN:HA	5:S:46:VAL:HG12	2.01	0.42
4:D:13:ASP:N	4:D:13:ASP:OD1	2.53	0.42
6:F:69:HIS:O	6:F:136:GLY:HA2	2.20	0.42
12:Z:113:TYR:O	12:Z:120:ARG:HA	2.19	0.42
8:V:103:TRP:CZ2	8:V:181:GLN:HG3	2.54	0.42
5:E:41:GLN:HA	5:E:46:VAL:HG12	2.01	0.42
5:E:149:LYS:HD2	5:E:152:GLN:HE22	1.85	0.42
7:G:136:MET:SD	7:G:163:CYS:HB3	2.59	0.42
2:P:204:GLU:CG	2:P:222:PRO:HA	2.50	0.42
13:a:11:THR:HG21	13:a:141:ALA:HB3	2.02	0.42
13:a:88:ILE:HG22	13:a:110:ILE:HD13	2.02	0.42
6:F:7:ASP:OD1	6:F:7:ASP:N	2.40	0.41
7:G:181:MET:HB3	7:G:181:MET:HE3	1.88	0.41
9:W:112:SER:OG	9:W:125:VAL:HG21	2.20	0.41
5:S:196:LYS:O	5:S:200:ILE:HD12	2.20	0.41
3:C:162:THR:OG1	3:C:163:CYS:N	2.53	0.41
9:I:167:LEU:HD23	9:I:167:LEU:HA	1.91	0.41
14:N:205:ALA:C	14:N:207:THR:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:146:GLN:HG2	6:T:147:THR:N	2.35	0.41
11:Y:142:ILE:HD11	11:Y:166:GLU:HG2	2.02	0.41
4:R:13:ASP:OD1	4:R:13:ASP:N	2.53	0.41
5:S:229:PHE:HB3	5:S:234:LEU:HG	2.02	0.41
12:L:21:THR:HG22	12:L:26:ILE:HA	2.01	0.41
14:N:43:MET:SD	14:N:64:LYS:HG2	2.60	0.41
2:P:69:LYS:O	2:P:69:LYS:HG2	2.20	0.41
12:Z:146:ASP:OD1	12:Z:146:ASP:N	2.52	0.41
14:b:157:GLN:HA	14:b:158:PRO:HD3	1.87	0.41
3:Q:34:CYS:SG	3:Q:75:SER:OG	2.69	0.41
8:V:150:ASP:N	8:V:150:ASP:OD1	2.53	0.41
4:D:7:ILE:HD12	4:D:124:ARG:N	2.36	0.41
7:G:168:ALA:CB	7:G:200:VAL:CG1	2.98	0.41
4:R:7:ILE:HD12	4:R:124:ARG:N	2.36	0.41
1:O:224:ASN:ND2	1:O:228:ARG:HE	2.18	0.41
7:U:108:LEU:HD22	7:U:149:TYR:CE1	2.56	0.41
8:V:103:TRP:HA	8:V:108:GLY:O	2.20	0.41
3:C:168:SER:O	3:C:172:VAL:HG23	2.21	0.41
5:E:78:MET:HG3	5:E:82:ILE:HD12	2.01	0.41
5:E:229:PHE:HB3	5:E:234:LEU:HG	2.02	0.41
12:L:180:ARG:HH21	12:L:185:ILE:HG23	1.85	0.41
13:M:88:ILE:HG22	13:M:110:ILE:HD13	2.02	0.41
12:Z:180:ARG:HH21	12:Z:185:ILE:HG23	1.85	0.41
7:G:195:LYS:O	7:G:199:ILE:HG13	2.20	0.41
5:E:208:GLU:HB3	5:E:209:LYS:H	1.77	0.41
10:J:126:ILE:H	10:J:126:ILE:HG12	1.78	0.41
14:b:27:LEU:HD12	14:b:36:PHE:O	2.21	0.41
3:Q:195:LYS:HG3	3:Q:240:HIS:CE1	2.56	0.41
3:Q:197:LEU:HD23	3:Q:197:LEU:HA	1.93	0.41
1:A:224:ASN:ND2	1:A:228:ARG:HE	2.18	0.41
2:B:204:GLU:CG	2:B:222:PRO:HA	2.50	0.41
6:F:143:HIS:HB3	6:F:145:PHE:CE1	2.56	0.41
7:G:243:LEU:O	7:G:244:LYS:HB2	2.20	0.41
2:P:71:ILE:HG23	2:P:136:CYS:O	2.21	0.41
11:Y:155:ARG:O	11:Y:158:GLU:HB2	2.20	0.41
1:A:49:VAL:HG11	1:A:195:VAL:HG12	2.03	0.41
7:G:198:TYR:CZ	7:G:209:PHE:HZ	2.39	0.41
8:H:84:LYS:HE2	8:H:84:LYS:HB3	1.88	0.41
9:I:112:SER:OG	9:I:125:VAL:HG21	2.20	0.41
9:I:195:LYS:CD	13:a:184:GLU:HG2	2.28	0.41
10:J:26:ARG:HB2	10:J:182:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:142:ILE:HD11	11:K:166:GLU:HG2	2.02	0.41
14:N:76:LEU:HD23	14:N:76:LEU:HA	1.87	0.41
6:T:105:VAL:O	6:T:109:VAL:HG23	2.21	0.41
6:T:143:HIS:HB3	6:T:145:PHE:CE1	2.56	0.41
1:O:24:GLN:NE2	7:U:14:PHE:H	2.18	0.41
7:U:195:LYS:O	7:U:199:ILE:HG13	2.20	0.41
5:S:47:CYS:HB3	5:S:191:LEU:HD11	2.03	0.41
3:Q:65:ILE:HD13	3:Q:65:ILE:HA	1.90	0.41
3:C:195:LYS:HG3	3:C:240:HIS:CE1	2.56	0.41
6:F:144:VAL:HB	6:F:156:CYS:O	2.21	0.41
11:K:155:ARG:O	11:K:158:GLU:HB2	2.20	0.41
11:K:172:ILE:HG22	11:Y:27:GLN:HG3	2.03	0.41
2:P:170:LYS:HE3	2:P:170:LYS:HB3	1.82	0.41
14:b:64:LYS:HB3	14:b:64:LYS:HE2	1.75	0.41
4:D:23:GLN:O	4:D:26:VAL:HG12	2.21	0.40
9:I:104:ASP:OD1	9:I:104:ASP:N	2.54	0.40
6:T:144:VAL:HB	6:T:156:CYS:O	2.21	0.40
7:U:179:LEU:CD2	7:U:192:GLU:HG2	2.47	0.40
5:S:203:LYS:HG3	5:S:210:LEU:HD13	1.92	0.40
8:V:177:ALA:HA	8:V:185:GLU:O	2.21	0.40
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.93	0.40
5:E:47:CYS:HB3	5:E:191:LEU:HD11	2.03	0.40
5:E:181:LEU:HD12	5:E:181:LEU:HA	1.78	0.40
2:P:122:GLN:O	3:Q:127:LYS:HG3	2.22	0.40
14:b:43:MET:SD	14:b:64:LYS:HG2	2.60	0.40
4:R:23:GLN:O	4:R:26:VAL:HG12	2.21	0.40
1:O:50:ILE:O	1:O:217:VAL:HA	2.21	0.40
7:U:198:TYR:CZ	7:U:209:PHE:HZ	2.39	0.40
7:U:233:GLU:HG3	7:U:233:GLU:H	1.72	0.40
5:E:27:ALA:O	5:E:31:HIS:HD2	2.04	0.40
5:E:62:SER:O	5:E:62:SER:OG	2.30	0.40
14:N:27:LEU:HD12	14:N:36:PHE:O	2.21	0.40
2:P:204:GLU:OE1	2:P:226:ARG:CZ	2.70	0.40
9:W:34:ILE:HG12	9:W:44:CYS:SG	2.62	0.40
7:U:108:LEU:CD2	7:U:149:TYR:HD1	2.23	0.40
2:B:71:ILE:HG23	2:B:136:CYS:O	2.21	0.40
3:C:177:GLN:O	3:C:177:GLN:HG2	2.21	0.40
7:G:179:LEU:CD2	7:G:192:GLU:HG2	2.47	0.40
7:G:200:VAL:O	7:G:200:VAL:HG12	2.20	0.40
10:J:204:ASP:OD1	10:J:204:ASP:N	2.54	0.40
2:B:69:LYS:HG2	2:B:69:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:LYS:HD2	4:D:219:ILE:N	2.37	0.40
6:F:150:SER:O	6:F:152:ASN:N	2.55	0.40
6:T:150:SER:O	6:T:152:ASN:N	2.55	0.40
1:O:49:VAL:HG11	1:O:195:VAL:HG12	2.03	0.40
5:S:149:LYS:HD2	5:S:152:GLN:HE22	1.85	0.40
8:V:194:ILE:HA	8:V:195:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/246 (97%)	226 (95%)	12 (5%)	0	100	100
1	O	238/246 (97%)	226 (95%)	12 (5%)	0	100	100
2	B	227/234 (97%)	217 (96%)	10 (4%)	0	100	100
2	P	227/234 (97%)	217 (96%)	10 (4%)	0	100	100
3	C	245/261 (94%)	231 (94%)	14 (6%)	0	100	100
3	Q	245/261 (94%)	232 (95%)	13 (5%)	0	100	100
4	D	230/254 (91%)	219 (95%)	11 (5%)	0	100	100
4	R	230/254 (91%)	219 (95%)	11 (5%)	0	100	100
5	E	231/241 (96%)	210 (91%)	21 (9%)	0	100	100
5	S	231/241 (96%)	210 (91%)	21 (9%)	0	100	100
6	F	232/263 (88%)	217 (94%)	15 (6%)	0	100	100
6	T	232/263 (88%)	217 (94%)	15 (6%)	0	100	100
7	G	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
7	U	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
8	H	200/238 (84%)	195 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	200/238 (84%)	195 (98%)	5 (2%)	0	100	100
9	I	195/277 (70%)	183 (94%)	12 (6%)	0	100	100
9	W	195/277 (70%)	183 (94%)	12 (6%)	0	100	100
10	J	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	X	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
11	K	195/201 (97%)	178 (91%)	17 (9%)	0	100	100
11	Y	195/201 (97%)	178 (91%)	17 (9%)	0	100	100
12	L	199/263 (76%)	189 (95%)	10 (5%)	0	100	100
12	Z	199/263 (76%)	189 (95%)	10 (5%)	0	100	100
13	M	210/240 (88%)	201 (96%)	9 (4%)	0	100	100
13	a	210/240 (88%)	201 (96%)	9 (4%)	0	100	100
14	N	210/263 (80%)	187 (89%)	23 (11%)	0	100	100
14	b	210/263 (80%)	187 (89%)	23 (11%)	0	100	100
All	All	6102/6882 (89%)	5749 (94%)	353 (6%)	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	184/210 (88%)	158 (86%)	26 (14%)	3	9
1	O	184/210 (88%)	158 (86%)	26 (14%)	3	9
2	B	182/191 (95%)	171 (94%)	11 (6%)	17	41
2	P	182/191 (95%)	171 (94%)	11 (6%)	17	41
3	C	197/221 (89%)	185 (94%)	12 (6%)	17	40
3	Q	197/221 (89%)	185 (94%)	12 (6%)	17	40
4	D	184/215 (86%)	165 (90%)	19 (10%)	7	18
4	R	184/215 (86%)	165 (90%)	19 (10%)	7	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	185/203 (91%)	164 (89%)	21 (11%)	5	14
5	S	185/203 (91%)	164 (89%)	21 (11%)	5	14
6	F	186/224 (83%)	167 (90%)	19 (10%)	7	18
6	T	186/224 (83%)	167 (90%)	19 (10%)	7	18
7	G	192/212 (91%)	180 (94%)	12 (6%)	16	39
7	U	192/212 (91%)	180 (94%)	12 (6%)	16	39
8	H	156/185 (84%)	142 (91%)	14 (9%)	9	23
8	V	156/185 (84%)	142 (91%)	14 (9%)	9	23
9	I	154/227 (68%)	142 (92%)	12 (8%)	11	29
9	W	154/227 (68%)	142 (92%)	12 (8%)	11	29
10	J	174/175 (99%)	161 (92%)	13 (8%)	12	31
10	X	174/175 (99%)	161 (92%)	13 (8%)	12	31
11	K	162/172 (94%)	153 (94%)	9 (6%)	19	44
11	Y	162/172 (94%)	153 (94%)	9 (6%)	19	44
12	L	151/205 (74%)	140 (93%)	11 (7%)	13	32
12	Z	151/205 (74%)	141 (93%)	10 (7%)	15	36
13	M	172/200 (86%)	160 (93%)	12 (7%)	14	34
13	a	172/200 (86%)	160 (93%)	12 (7%)	14	34
14	N	165/215 (77%)	153 (93%)	12 (7%)	13	32
14	b	165/215 (77%)	153 (93%)	12 (7%)	13	32
All	All	4888/5710 (86%)	4483 (92%)	405 (8%)	12	26

All (405) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	39	SER
1	A	43	ARG
1	A	45	LYS
1	A	46	ASP
1	A	49	VAL
1	A	55	LYS
1	A	56	VAL
1	A	61	LEU
1	A	73	THR

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Mol	Chain	Res	Type
1	A	78	CYS
1	A	89	SER
1	A	117	ARG
1	A	130	GLU
1	A	166	THR
1	A	173	THR
1	A	176	THR
1	A	183	VAL
1	A	194	THR
1	A	197	THR
1	A	205	VAL
1	A	207	SER
1	A	211	LYS
1	A	213	SER
1	A	215	ILE
1	A	219	VAL
2	B	8	SER
2	B	13	SER
2	B	41	ASN
2	B	43	VAL
2	B	44	VAL
2	B	47	THR
2	B	68	THR
2	B	73	LEU
2	B	109	LEU
2	B	132	SER
2	B	135	ILE
3	C	2	SER
3	C	7	SER
3	C	33	THR
3	C	35	LEU
3	C	43	VAL
3	C	57	ASP
3	C	80	THR
3	C	81	SER
3	C	150	SER
3	C	184	MET
3	C	210	LYS
3	C	230	GLN
4	D	2	SER
4	D	8	THR
4	D	13	ASP

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Mol	Chain	Res	Type
4	D	35	VAL
4	D	41	VAL
4	D	50	VAL
4	D	52	LYS
4	D	67	ASP
4	D	69	VAL
4	D	141	THR
4	D	181	ILE
4	D	184	ASP
4	D	187	THR
4	D	195	LEU
4	D	198	VAL
4	D	206	ILE
4	D	208	LEU
4	D	210	VAL
4	D	229	VAL
5	E	28	ILE
5	E	38	ILE
5	E	42	THR
5	E	46	VAL
5	E	51	GLU
5	E	59	MET
5	E	62	SER
5	E	68	VAL
5	E	87	THR
5	E	116	VAL
5	E	134	SER
5	E	157	ASP
5	E	159	SER
5	E	163	VAL
5	E	172	SER
5	E	190	THR
5	E	192	LYS
5	E	204	GLN
5	E	205	VAL
5	E	217	LEU
5	E	234	LEU
6	F	9	ASP
6	F	10	VAL
6	F	14	SER
6	F	22	ILE
6	F	35	THR

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Mol	Chain	Res	Type
6	F	38	LEU
6	F	49	LEU
6	F	64	LEU
6	F	78	THR
6	F	106	SER
6	F	165	SER
6	F	166	GLN
6	F	167	SER
6	F	170	THR
6	F	177	SER
6	F	188	VAL
6	F	198	THR
6	F	211	SER
6	F	230	SER
7	G	8	ASP
7	G	64	LYS
7	G	147	GLN
7	G	150	MET
7	G	170	GLN
7	G	179	LEU
7	G	193	VAL
7	G	195	LYS
7	G	197	ILE
7	G	211	LEU
7	G	216	VAL
7	G	226	ILE
8	H	9	ASP
8	H	13	VAL
8	H	24	SER
8	H	35	THR
8	H	46	SER
8	H	48	SER
8	H	70	LEU
8	H	85	GLU
8	H	93	ASP
8	H	124	SER
8	H	133	SER
8	H	145	GLU
8	H	190	LEU
8	H	200	SER
9	I	1	THR
9	I	6	VAL

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Mol	Chain	Res	Type
9	I	38	SER
9	I	55	THR
9	I	56	THR
9	I	69	THR
9	I	119	THR
9	I	138	PHE
9	I	163	ILE
9	I	171	SER
9	I	183	LEU
9	I	195	LYS
10	J	19	VAL
10	J	29	ILE
10	J	46	ASP
10	J	57	THR
10	J	72	LEU
10	J	88	SER
10	J	97	LYS
10	J	114	LYS
10	J	121	CYS
10	J	126	ILE
10	J	142	SER
10	J	145	MET
10	J	198	THR
11	K	29	LYS
11	K	44	LEU
11	K	49	GLU
11	K	76	SER
11	K	78	THR
11	K	86	ARG
11	K	171	PHE
11	K	177	THR
11	K	185	LYS
12	L	2	THR
12	L	12	VAL
12	L	31	VAL
12	L	44	THR
12	L	65	ILE
12	L	72	GLU
12	L	105	ASP
12	L	122	SER
12	L	130	SER
12	L	174	VAL

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Mol	Chain	Res	Type
12	L	188	SER
13	M	12	VAL
13	M	19	ASP
13	M	21	SER
13	M	34	SER
13	M	54	CYS
13	M	55	SER
13	M	85	THR
13	M	93	SER
13	M	169	ASP
13	M	200	LYS
13	M	207	THR
13	M	208	VAL
14	N	2	GLN
14	N	47	ASP
14	N	49	THR
14	N	54	SER
14	N	84	SER
14	N	100	ARG
14	N	112	ILE
14	N	120	SER
14	N	161	SER
14	N	163	THR
14	N	167	GLU
14	N	200	GLU
2	P	8	SER
2	P	13	SER
2	P	41	ASN
2	P	43	VAL
2	P	44	VAL
2	P	47	THR
2	P	68	THR
2	P	73	LEU
2	P	109	LEU
2	P	132	SER
2	P	135	ILE
6	T	9	ASP
6	T	10	VAL
6	T	14	SER
6	T	22	ILE
6	T	35	THR
6	T	38	LEU

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Mol	Chain	Res	Type
6	T	49	LEU
6	T	64	LEU
6	T	78	THR
6	T	106	SER
6	T	165	SER
6	T	166	GLN
6	T	167	SER
6	T	170	THR
6	T	177	SER
6	T	188	VAL
6	T	198	THR
6	T	211	SER
6	T	230	SER
10	X	19	VAL
10	X	29	ILE
10	X	46	ASP
10	X	57	THR
10	X	72	LEU
10	X	88	SER
10	X	97	LYS
10	X	114	LYS
10	X	121	CYS
10	X	126	ILE
10	X	142	SER
10	X	145	MET
10	X	198	THR
11	Y	29	LYS
11	Y	44	LEU
11	Y	49	GLU
11	Y	76	SER
11	Y	78	THR
11	Y	86	ARG
11	Y	171	PHE
11	Y	177	THR
11	Y	185	LYS
12	Z	12	VAL
12	Z	31	VAL
12	Z	44	THR
12	Z	65	ILE
12	Z	72	GLU
12	Z	105	ASP
12	Z	122	SER

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Mol	Chain	Res	Type
12	Z	130	SER
12	Z	174	VAL
12	Z	188	SER
13	a	12	VAL
13	a	19	ASP
13	a	21	SER
13	a	34	SER
13	a	54	CYS
13	a	55	SER
13	a	85	THR
13	a	93	SER
13	a	169	ASP
13	a	200	LYS
13	a	207	THR
13	a	208	VAL
14	b	2	GLN
14	b	47	ASP
14	b	49	THR
14	b	54	SER
14	b	84	SER
14	b	100	ARG
14	b	112	ILE
14	b	120	SER
14	b	161	SER
14	b	163	THR
14	b	167	GLU
14	b	200	GLU
9	W	1	THR
9	W	6	VAL
9	W	38	SER
9	W	55	THR
9	W	56	THR
9	W	69	THR
9	W	119	THR
9	W	138	PHE
9	W	163	ILE
9	W	171	SER
9	W	183	LEU
9	W	195	LYS
4	R	2	SER
4	R	8	THR
4	R	13	ASP

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Mol	Chain	Res	Type
4	R	35	VAL
4	R	41	VAL
4	R	50	VAL
4	R	52	LYS
4	R	67	ASP
4	R	69	VAL
4	R	141	THR
4	R	181	ILE
4	R	184	ASP
4	R	187	THR
4	R	195	LEU
4	R	198	VAL
4	R	206	ILE
4	R	208	LEU
4	R	210	VAL
4	R	229	VAL
1	O	14	THR
1	O	39	SER
1	O	43	ARG
1	O	45	LYS
1	O	46	ASP
1	O	49	VAL
1	O	55	LYS
1	O	56	VAL
1	O	61	LEU
1	O	73	THR
1	O	78	CYS
1	O	89	SER
1	O	117	ARG
1	O	130	GLU
1	O	166	THR
1	O	173	THR
1	O	176	THR
1	O	183	VAL
1	O	194	THR
1	O	197	THR
1	O	205	VAL
1	O	207	SER
1	O	211	LYS
1	O	213	SER
1	O	215	ILE
1	O	219	VAL

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Mol	Chain	Res	Type
7	U	8	ASP
7	U	64	LYS
7	U	147	GLN
7	U	150	MET
7	U	170	GLN
7	U	179	LEU
7	U	193	VAL
7	U	195	LYS
7	U	197	ILE
7	U	211	LEU
7	U	216	VAL
7	U	226	ILE
5	S	28	ILE
5	S	38	ILE
5	S	42	THR
5	S	46	VAL
5	S	51	GLU
5	S	59	MET
5	S	62	SER
5	S	68	VAL
5	S	87	THR
5	S	116	VAL
5	S	134	SER
5	S	157	ASP
5	S	159	SER
5	S	163	VAL
5	S	172	SER
5	S	190	THR
5	S	192	LYS
5	S	204	GLN
5	S	205	VAL
5	S	217	LEU
5	S	234	LEU
3	Q	2	SER
3	Q	7	SER
3	Q	33	THR
3	Q	35	LEU
3	Q	43	VAL
3	Q	57	ASP
3	Q	80	THR
3	Q	81	SER
3	Q	150	SER

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Mol	Chain	Res	Type
3	Q	184	MET
3	Q	210	LYS
3	Q	230	GLN
8	V	9	ASP
8	V	13	VAL
8	V	24	SER
8	V	35	THR
8	V	46	SER
8	V	48	SER
8	V	70	LEU
8	V	85	GLU
8	V	93	ASP
8	V	124	SER
8	V	133	SER
8	V	145	GLU
8	V	190	LEU
8	V	200	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	24	GLN
1	A	100	ASN
2	B	62	HIS
3	C	53	HIS
3	C	95	GLN
3	C	109	GLN
3	C	142	HIS
3	C	167	ASN
3	C	230	GLN
4	D	54	GLN
4	D	92	GLN
5	E	31	HIS
5	E	41	GLN
5	E	73	HIS
5	E	152	GLN
5	E	211	ASN
6	F	4	ASN
6	F	43	HIS
6	F	53	GLN
6	F	166	GLN

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Mol	Chain	Res	Type
6	F	190	HIS
7	G	72	HIS
7	G	110	HIS
7	G	170	GLN
8	H	7	GLN
8	H	62	GLN
8	H	71	ASN
8	H	77	HIS
8	H	110	GLN
8	H	154	GLN
9	I	35	HIS
10	J	156	ASN
10	J	161	HIS
11	K	55	GLN
11	K	61	GLN
11	K	63	ASN
11	K	87	ASN
12	L	9	GLN
12	L	191	ASN
13	M	80	ASN
13	M	146	GLN
13	M	157	ASN
14	N	2	GLN
14	N	61	GLN
2	P	62	HIS
6	T	21	GLN
6	T	43	HIS
6	T	53	GLN
6	T	166	GLN
6	T	190	HIS
10	X	156	ASN
11	Y	55	GLN
11	Y	61	GLN
11	Y	63	ASN
11	Y	87	ASN
12	Z	9	GLN
12	Z	191	ASN
13	a	146	GLN
13	a	157	ASN
14	b	61	GLN
9	W	35	HIS
4	R	54	GLN

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Mol	Chain	Res	Type
4	R	92	GLN
1	O	12	HIS
1	O	24	GLN
7	U	72	HIS
7	U	110	HIS
7	U	170	GLN
5	S	31	HIS
5	S	41	GLN
5	S	73	HIS
5	S	152	GLN
5	S	211	ASN
3	Q	53	HIS
3	Q	95	GLN
3	Q	109	GLN
3	Q	167	ASN
3	Q	230	GLN
8	V	7	GLN
8	V	62	GLN
8	V	71	ASN
8	V	77	HIS
8	V	110	GLN
8	V	123	GLN
8	V	154	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

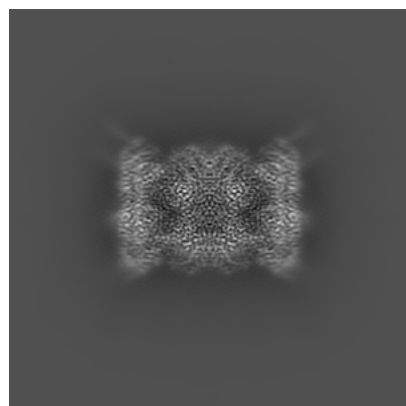
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10586. These allow visual inspection of the internal detail of the map and identification of artifacts.

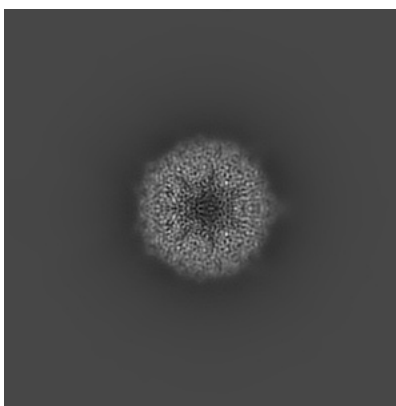
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

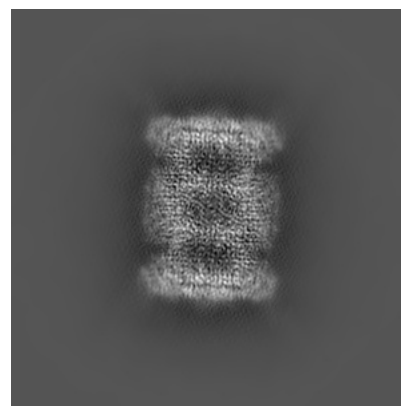
6.1.1 Primary map



X

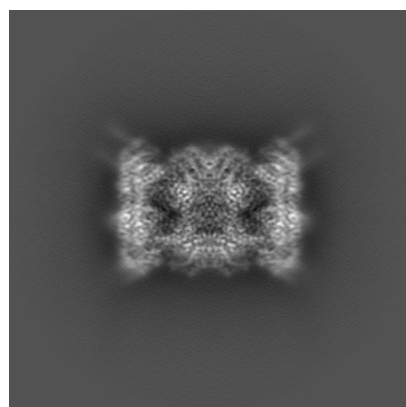


Y

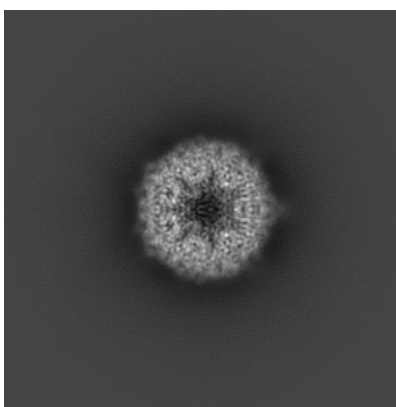


Z

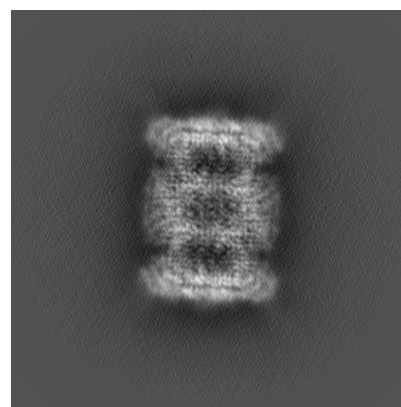
6.1.2 Raw map



X



Y

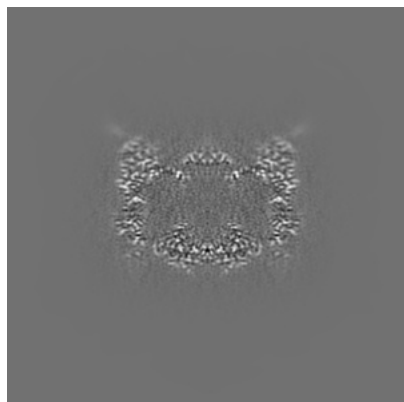


Z

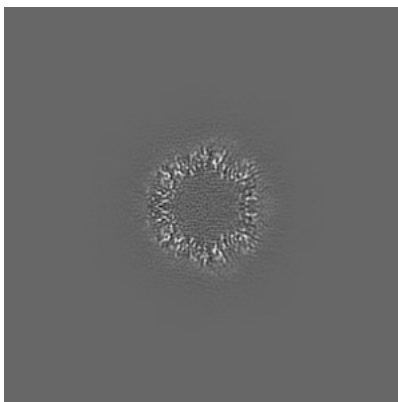
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

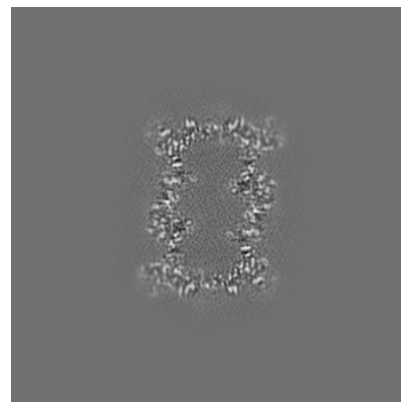
6.2.1 Primary map



X Index: 200

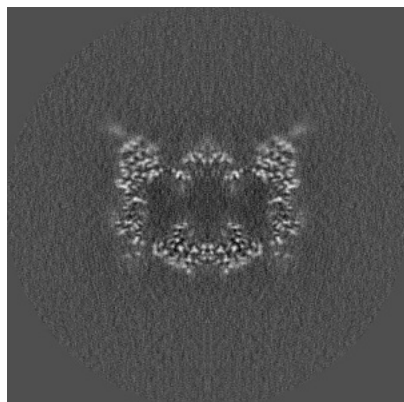


Y Index: 200

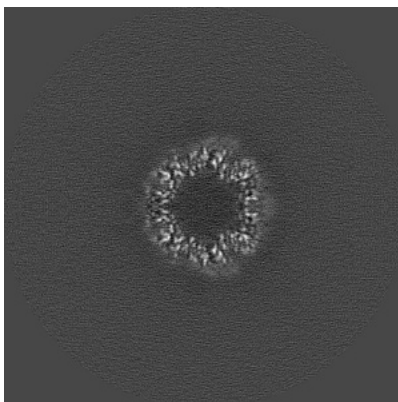


Z Index: 200

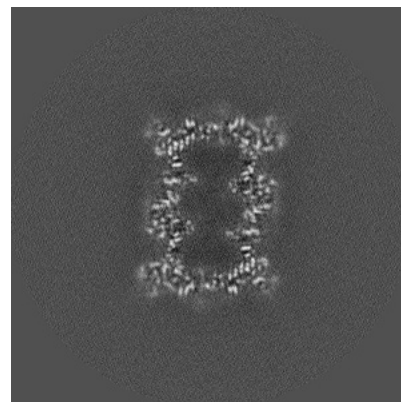
6.2.2 Raw map



X Index: 200



Y Index: 200

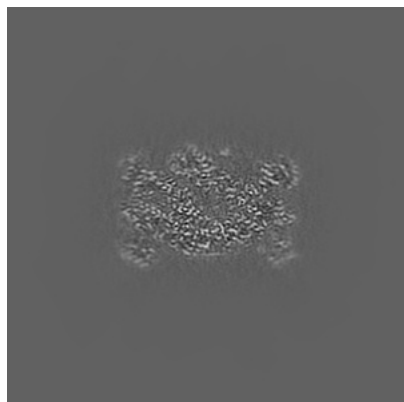


Z Index: 200

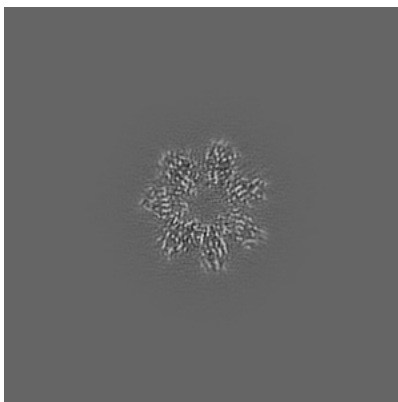
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

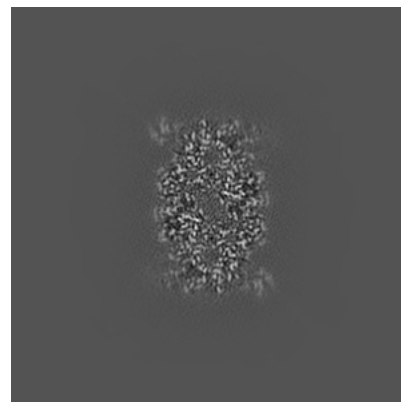
6.3.1 Primary map



X Index: 167

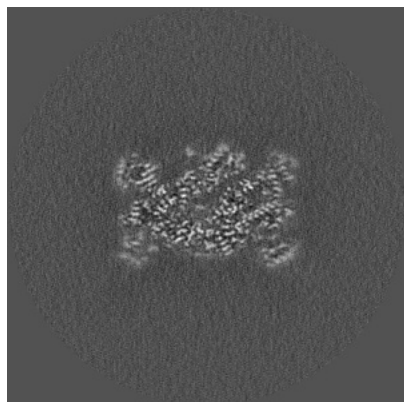


Y Index: 178

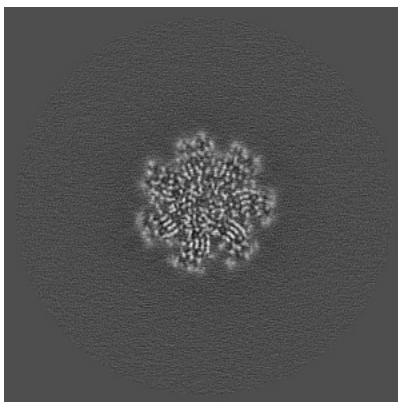


Z Index: 170

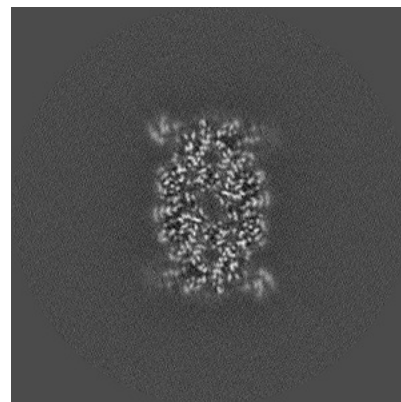
6.3.2 Raw map



X Index: 234



Y Index: 270

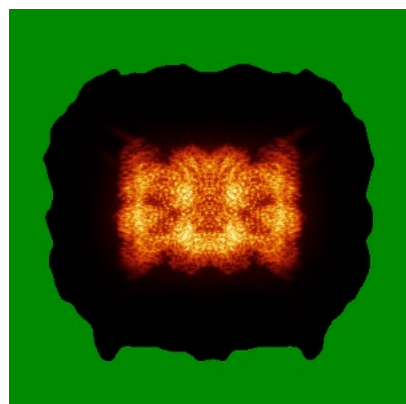


Z Index: 170

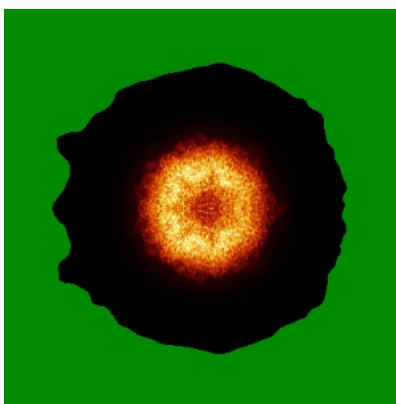
The images above show the largest variance slices of the map in three orthogonal directions.

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

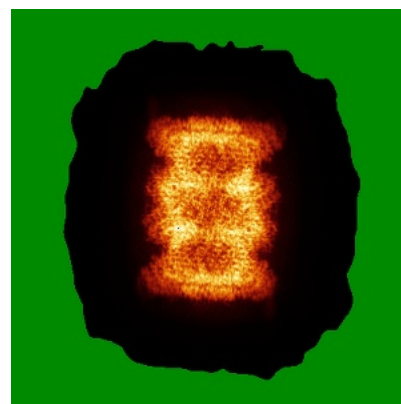
6.4.1 Primary map



X

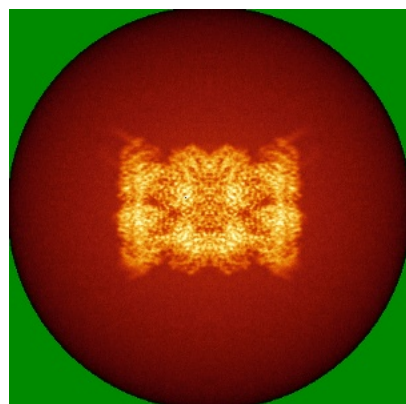


Y

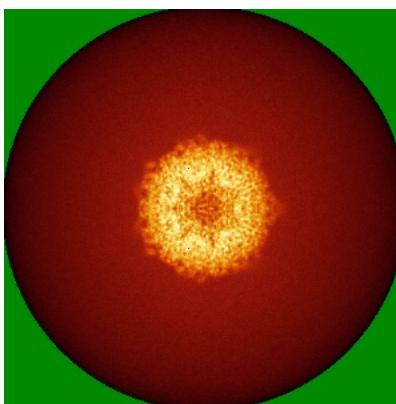


Z

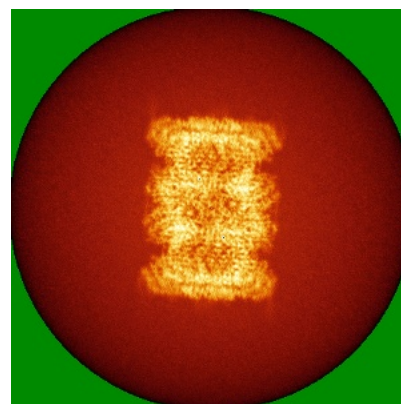
6.4.2 Raw map



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.

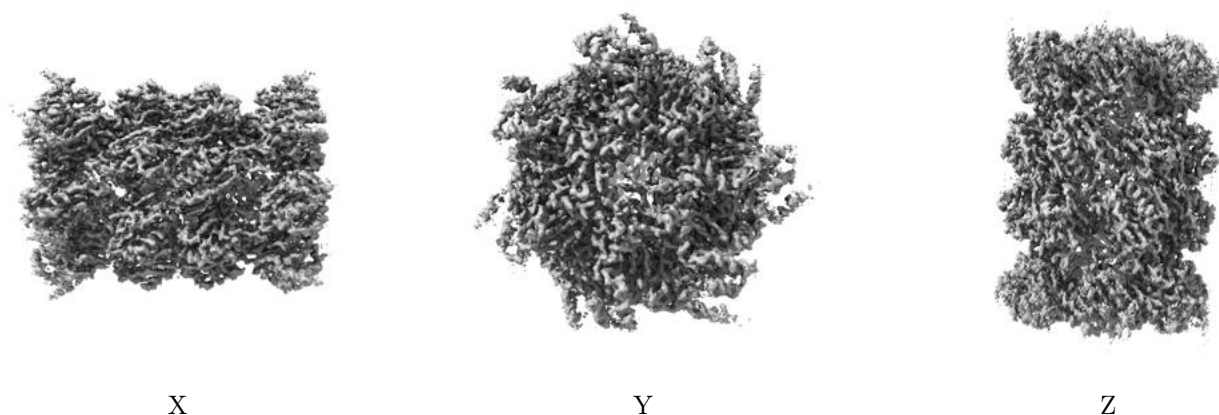
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.043. 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.

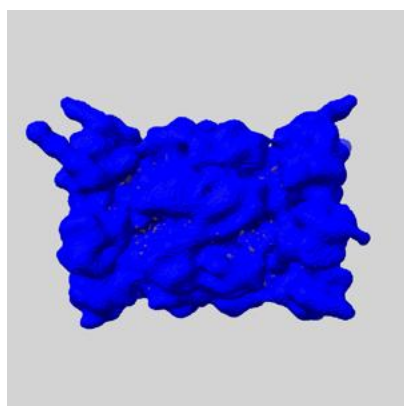
6.6 Mask visualisation [i](#)

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

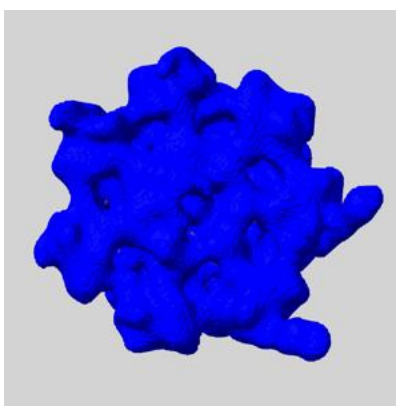
A mask typically either:

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

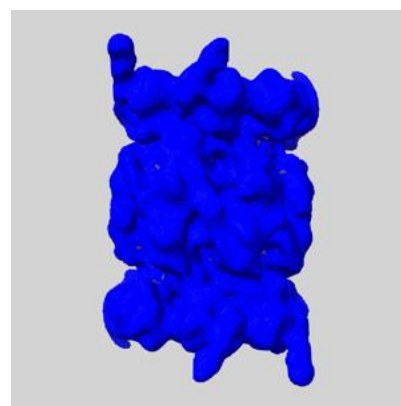
6.6.1 emd_10586_msk_1.map [i](#)



X



Y

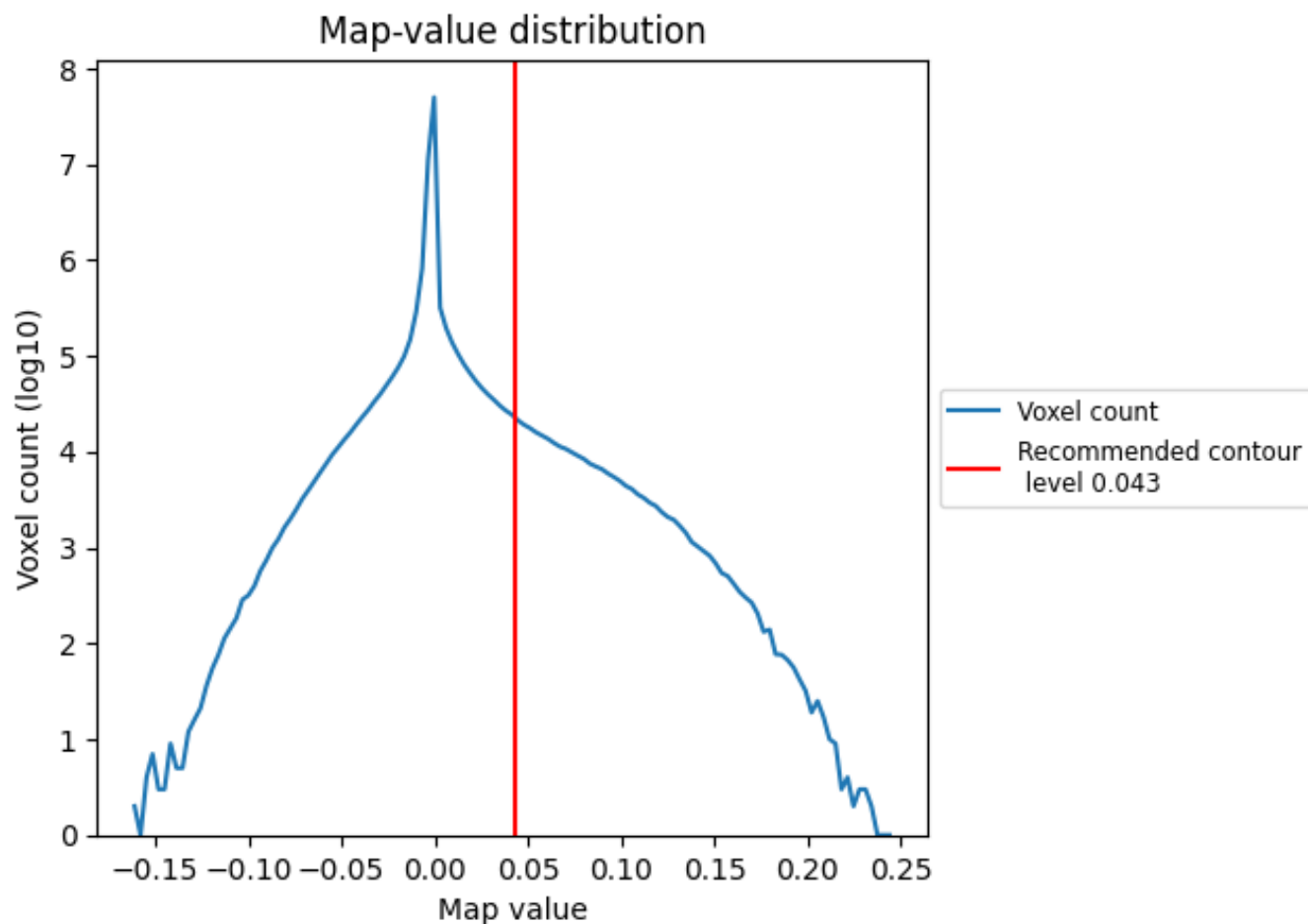


Z

7 Map analysis [i](#)

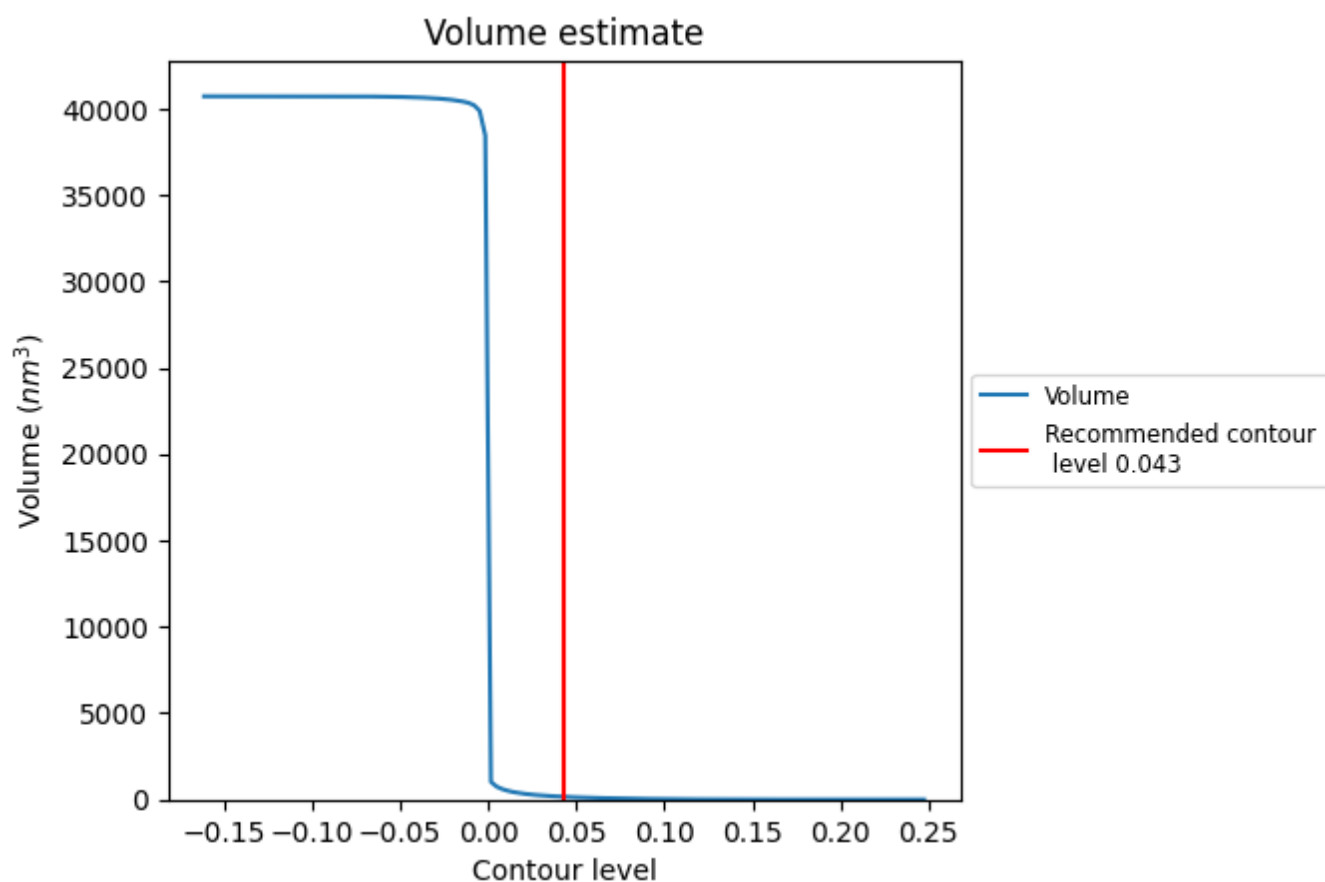
This section contains the results of statistical analysis of the map.

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.

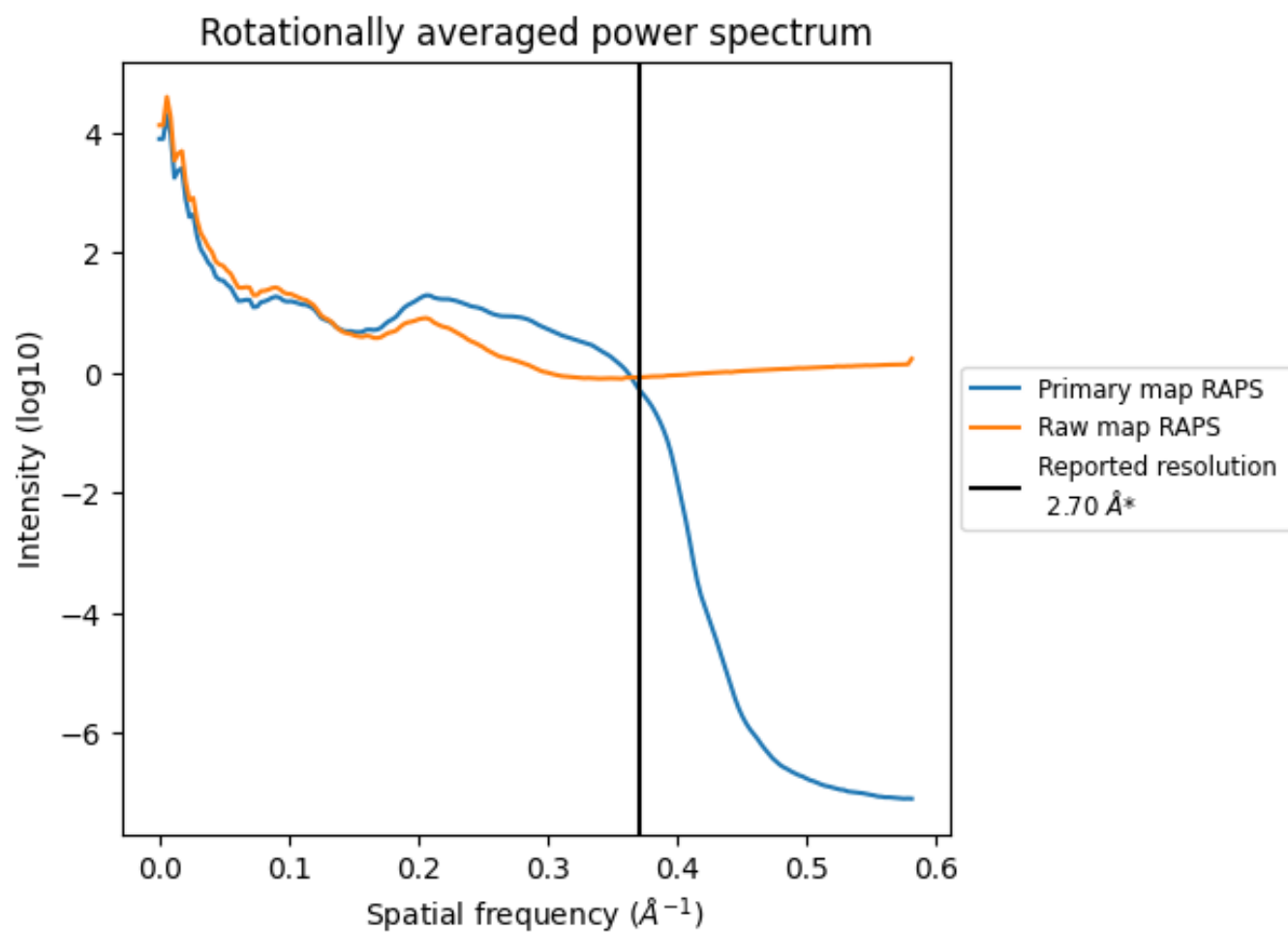
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160 nm^3 ; this corresponds to an approximate mass of 144 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 ⓘ

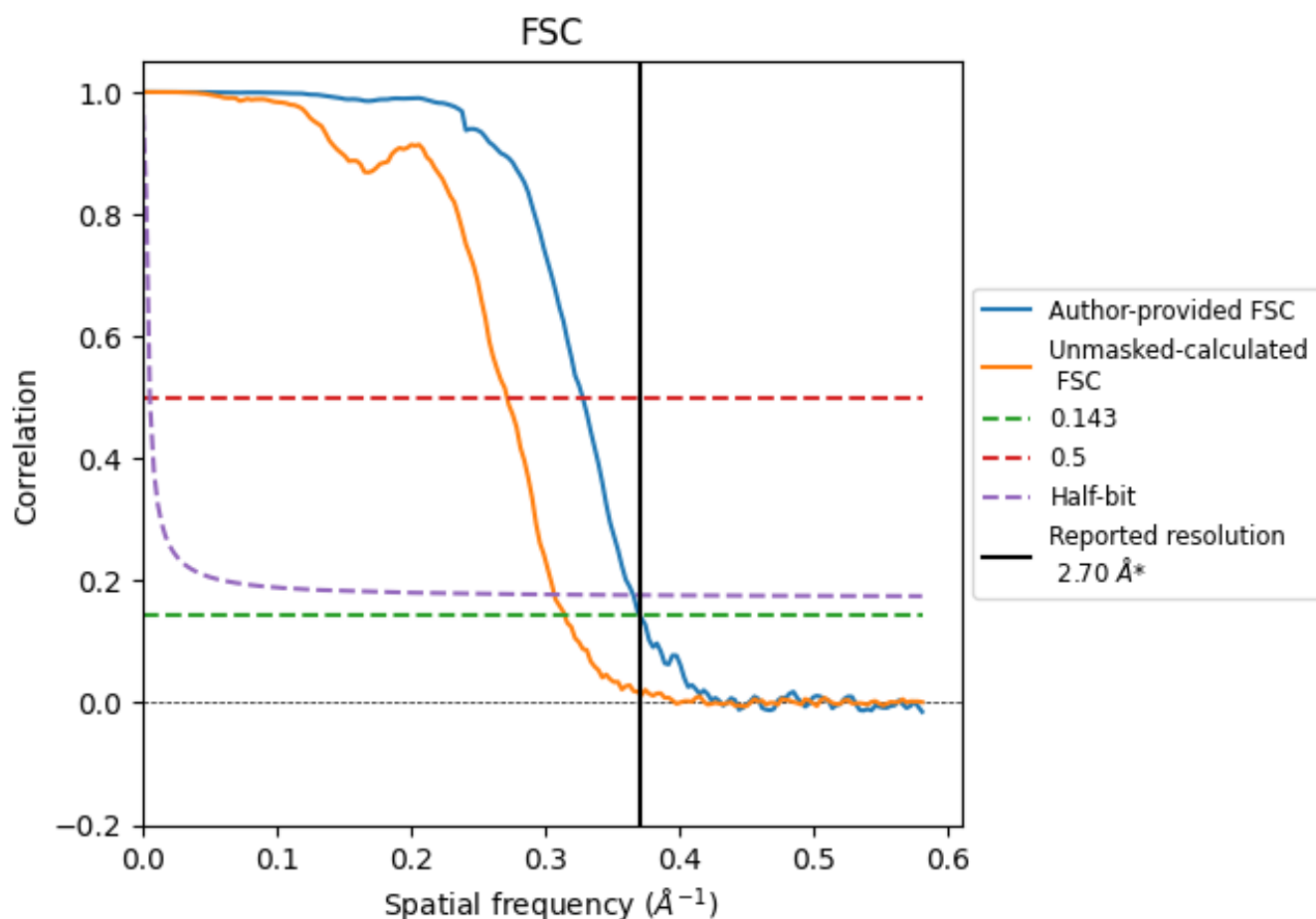


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

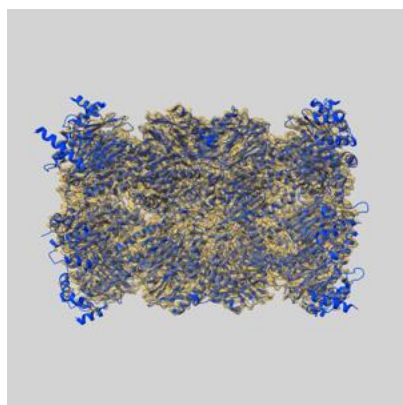
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.05	2.73
Unmasked-calculated*	3.18	3.68	3.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.7 by more than 10 %

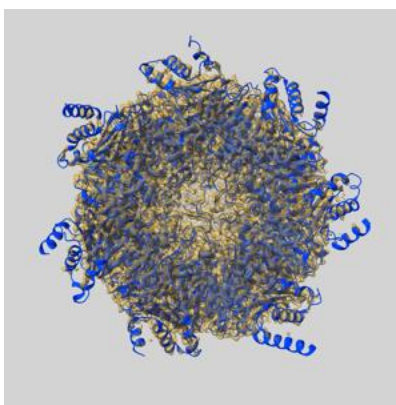
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10586 and PDB model 6TU3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

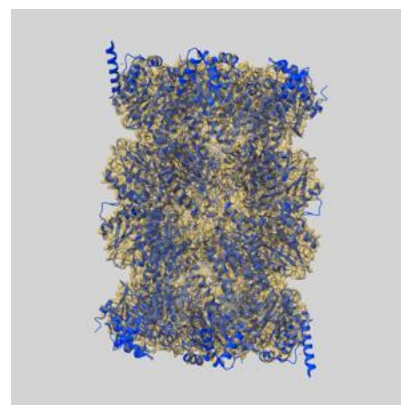
9.1 Map-model overlay [i](#)



X



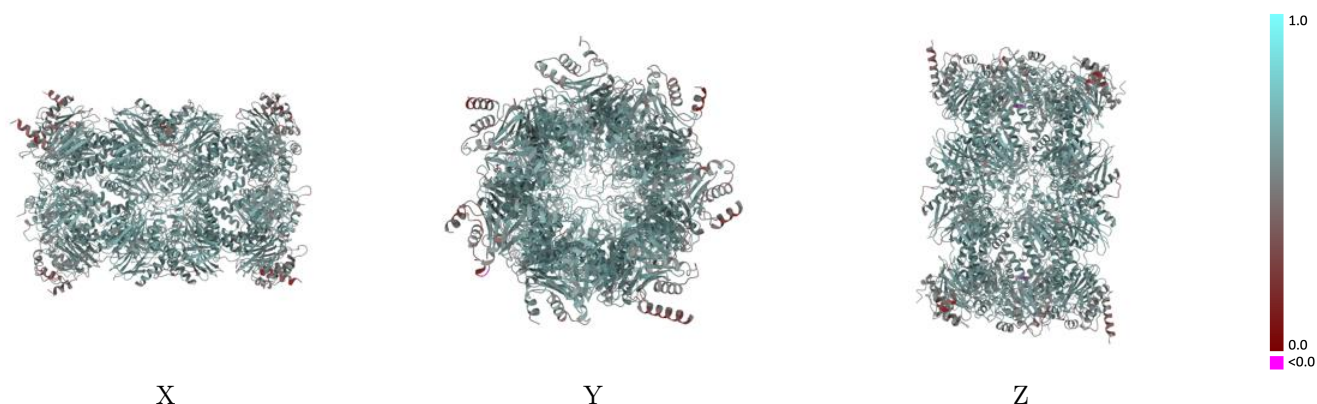
Y



Z

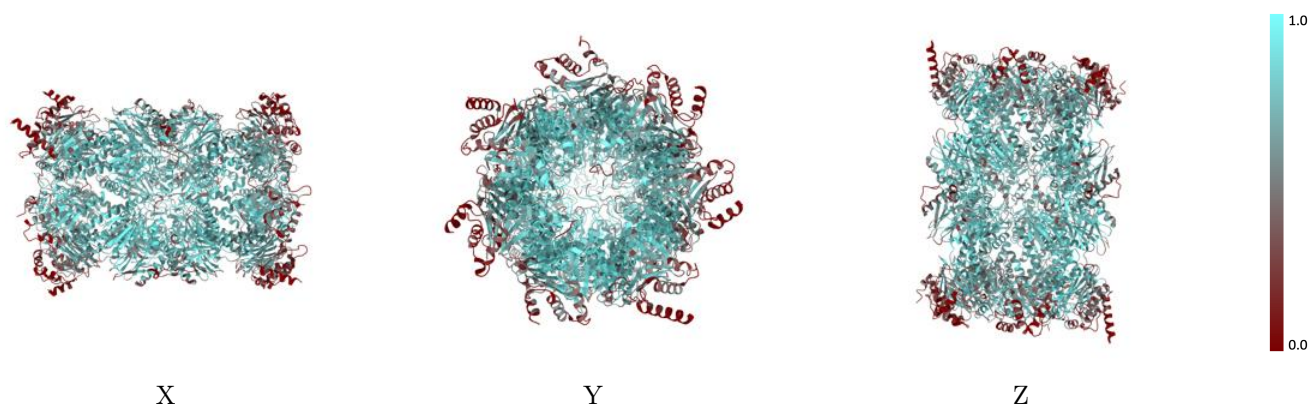
The images above show the 3D surface view of the map at the recommended contour level 0.043 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



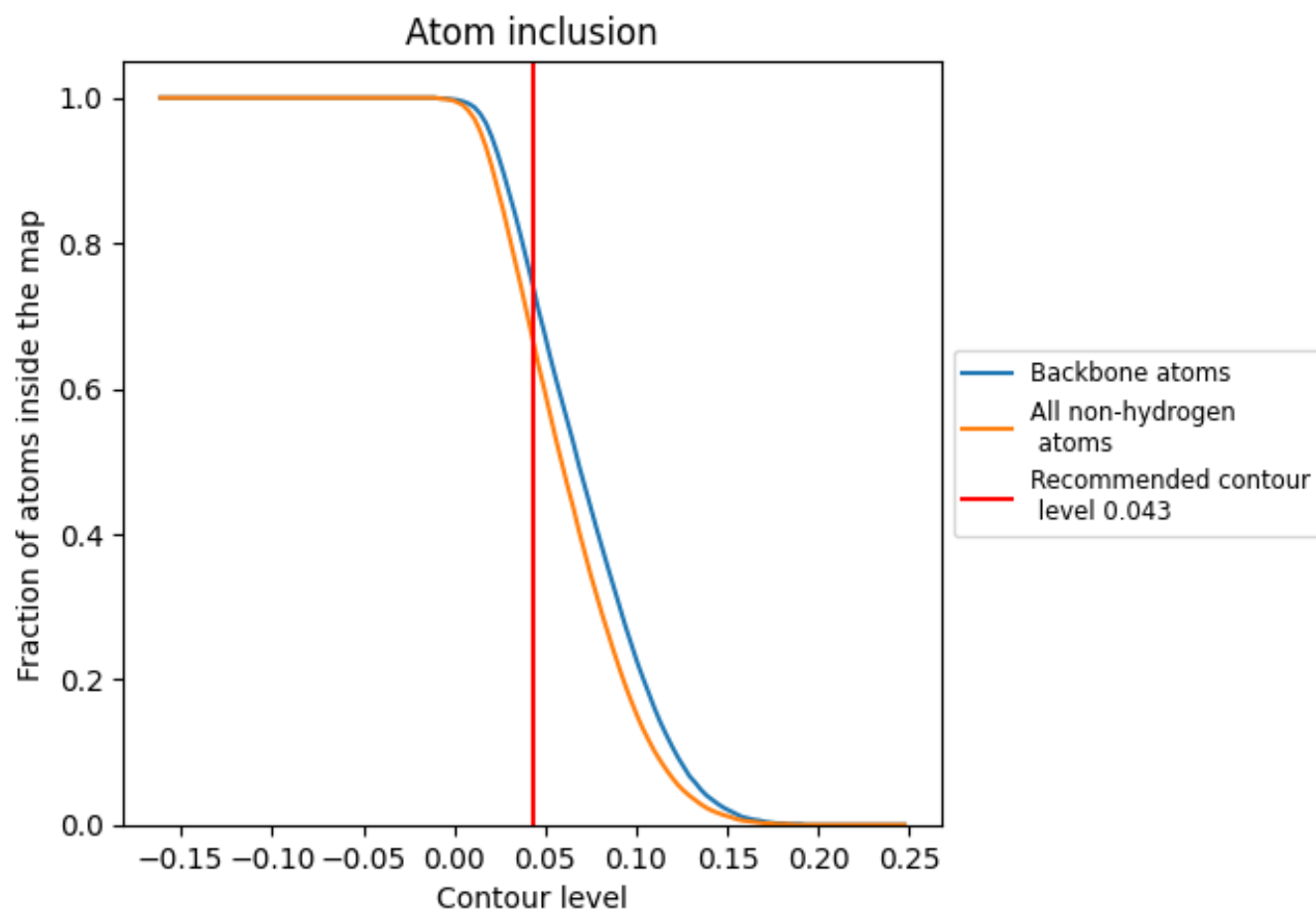
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.043).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 67% 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 (0.043) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6690	 0.5860
A	 0.5800	 0.5600
B	 0.6810	 0.5970
C	 0.6020	 0.5600
D	 0.5260	 0.5540
E	 0.5270	 0.5550
F	 0.5920	 0.5710
G	 0.5670	 0.5550
H	 0.7560	 0.6100
I	 0.7990	 0.6190
J	 0.8040	 0.6230
K	 0.7470	 0.6070
L	 0.7110	 0.5980
M	 0.7500	 0.6030
N	 0.8150	 0.6260
O	 0.5670	 0.5550
P	 0.6840	 0.5970
Q	 0.5970	 0.5560
R	 0.5290	 0.5530
S	 0.5260	 0.5540
T	 0.5940	 0.5690
U	 0.5660	 0.5540
V	 0.7680	 0.6120
W	 0.8020	 0.6200
X	 0.8030	 0.6210
Y	 0.7560	 0.6040
Z	 0.7130	 0.5960
a	 0.7500	 0.6050
b	 0.8200	 0.6240

