



Full wwPDB EM Validation Report ⓘ

Aug 18, 2025 – 08:53 PM EDT

PDB ID : 9C6G / pdb_00009c6g
EMDB ID : EMD-45246
Title : Mcm double hexamer from human
Authors : Liu, C.; Xu, N.; Lin, Q.
Deposited on : 2024-06-07
Resolution : 4.26 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

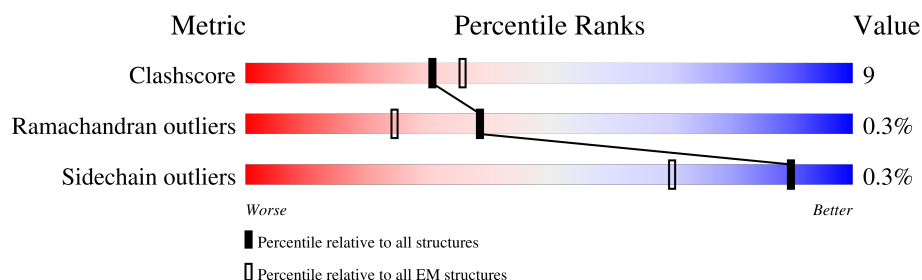
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.26 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	0	863	<div> <div>21%</div> <div>48%</div> <div>13%</div> <div>39%</div> </div>
1	4	863	<div> <div>22%</div> <div>49%</div> <div>13%</div> <div>39%</div> </div>
2	2	904	<div> <div>27%</div> <div>53%</div> <div>9%</div> <div>38%</div> </div>
2	8	904	<div> <div>27%</div> <div>51%</div> <div>11%</div> <div>38%</div> </div>
3	3	808	<div> <div>8%</div> <div>53%</div> <div>15%</div> <div>31%</div> </div>
3	9	808	<div> <div>7%</div> <div>53%</div> <div>15%</div> <div>31%</div> </div>
4	5	734	<div> <div>21%</div> <div>63%</div> <div>16%</div> <div>20%</div> </div>
4	A	734	<div> <div>21%</div> <div>63%</div> <div>16%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
5	6	821	<div><div></div><div>32%</div><div>63%</div><div>18%</div><div>19%</div></div>
5	B	821	<div><div></div><div>31%</div><div>61%</div><div>19%</div><div>19%</div></div>
6	7	719	<div><div></div><div>25%</div><div>70%</div><div>17%</div><div>13%</div></div>
6	C	719	<div><div></div><div>25%</div><div>70%</div><div>16%</div><div>13%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 55961 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 DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	529	Total	C	N	O	S	0	0
			4226	2669	745	788	24		
1	4	529	Total	C	N	O	S	0	0
			4227	2670	745	788	24		

- Molecule 2 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	560	Total	C	N	O	S	0	0
			4443	2800	797	823	23		
2	8	560	Total	C	N	O	S	0	0
			4443	2800	797	823	23		

- Molecule 3 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	557	Total	C	N	O	S	0	0
			4397	2756	778	839	24		
3	9	557	Total	C	N	O	S	0	0
			4397	2756	778	839	24		

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

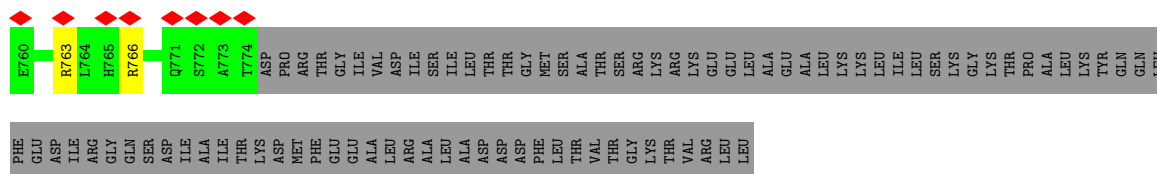
Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	585	Total	C	N	O	S	0	0
			4621	2918	815	855	33		
4	A	585	Total	C	N	O	S	0	0
			4621	2918	815	855	33		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

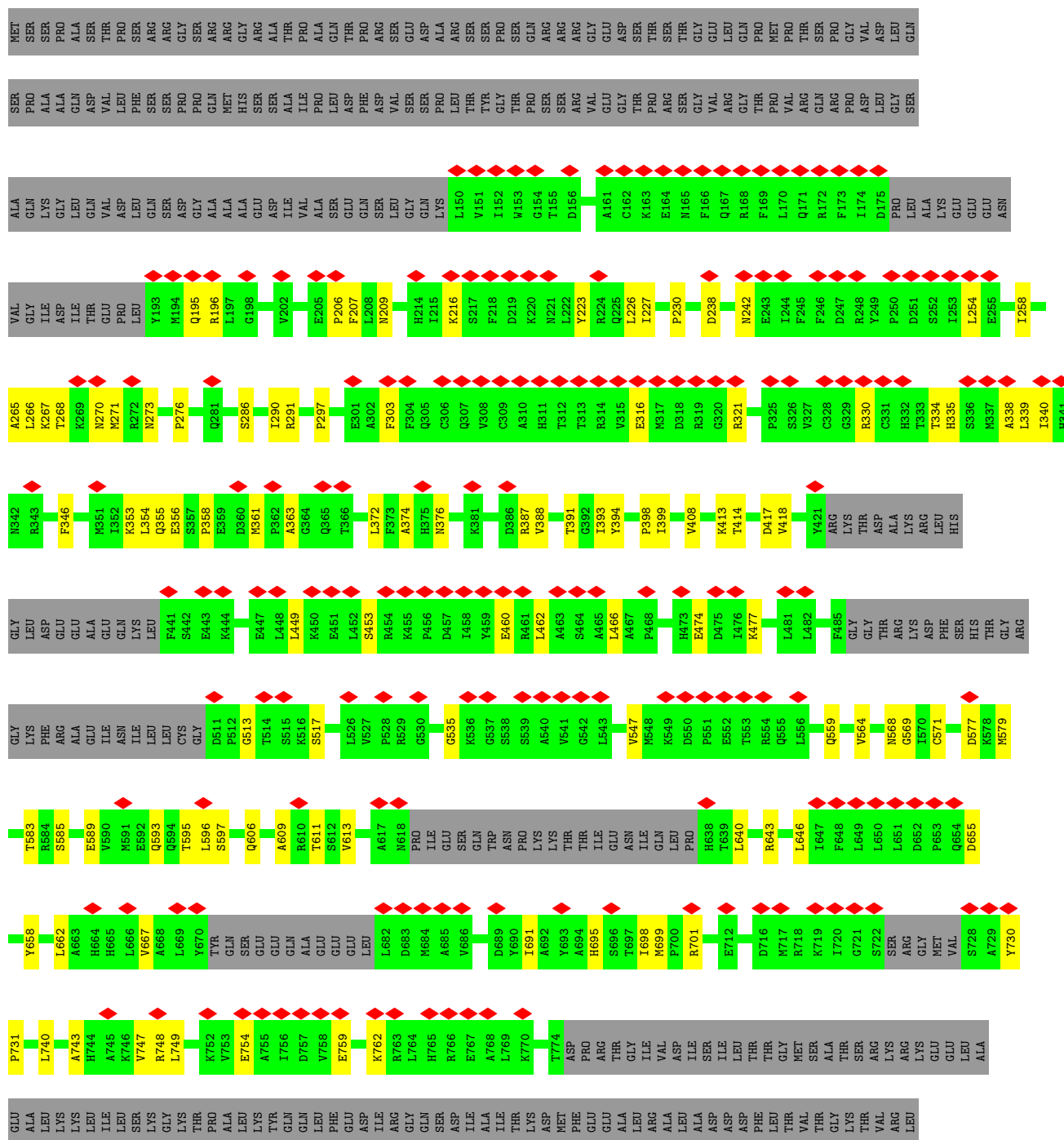
Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	661	Total	C	N	O	S	0	0
			5335	3355	946	1007	27		
5	B	661	Total	C	N	O	S	0	0
			5335	3355	946	1007	27		

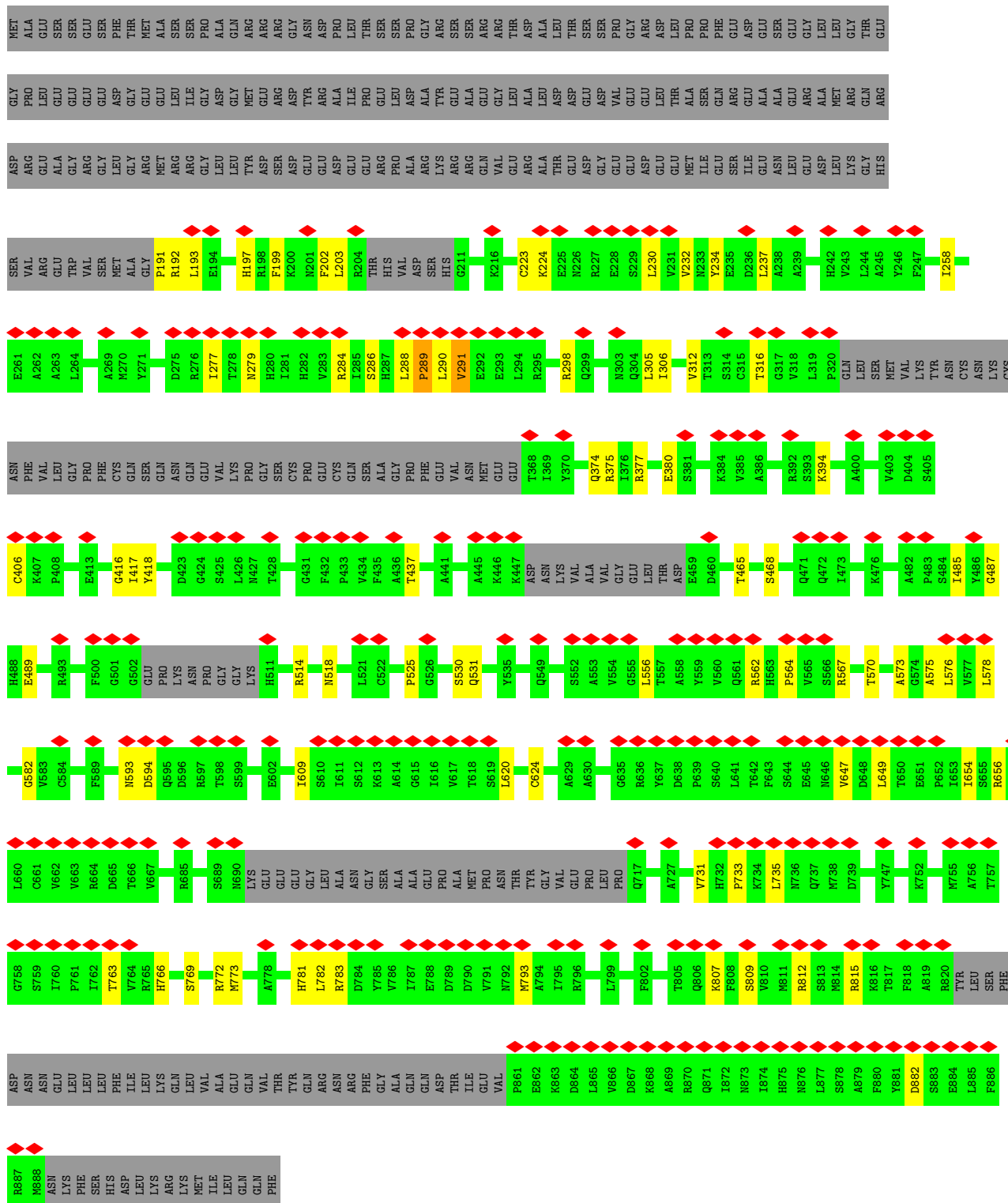
- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	623	Total	C	N	O	S	0	0
			4958	3101	886	940	31		
6	C	623	Total	C	N	O	S	0	0
			4958	3101	886	940	31		



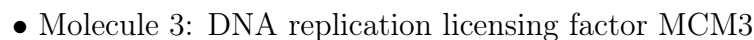
• Molecule 1: DNA replication licensing factor MCM4

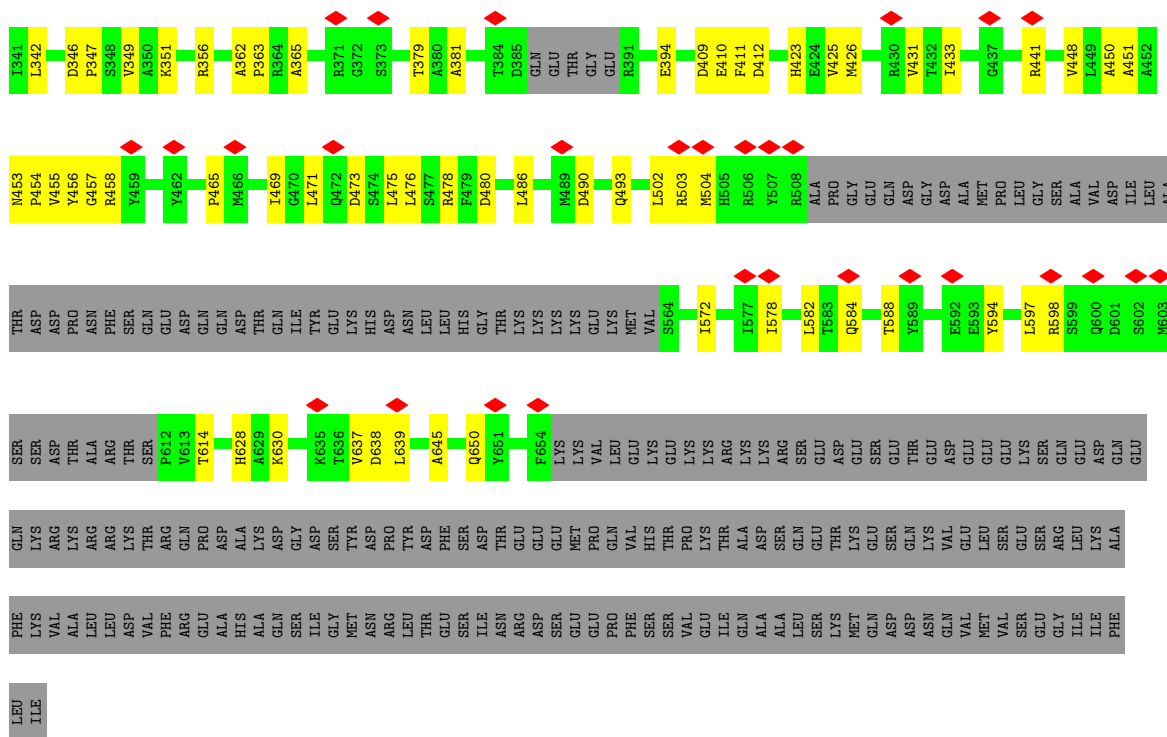




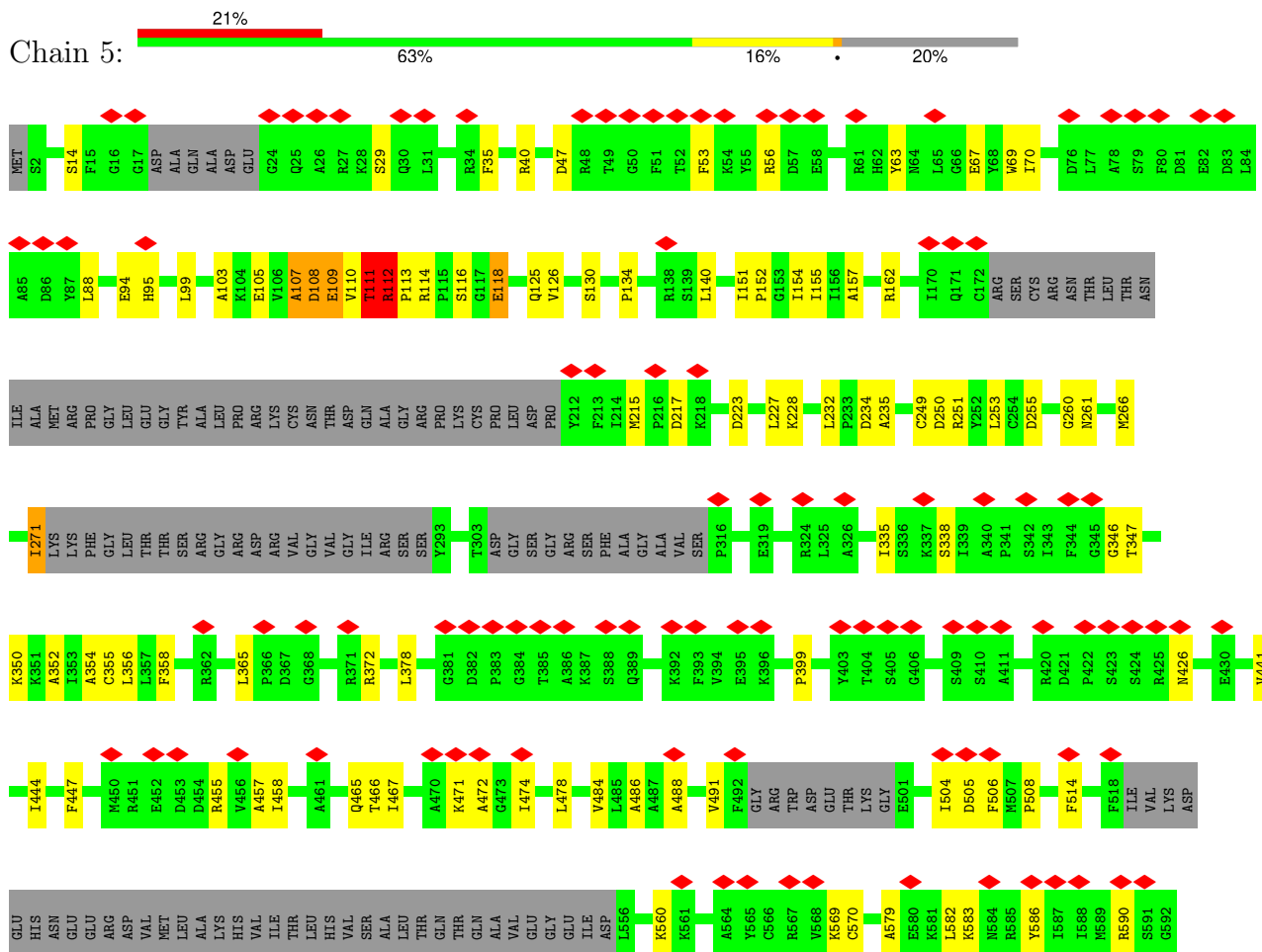
Chain 8:

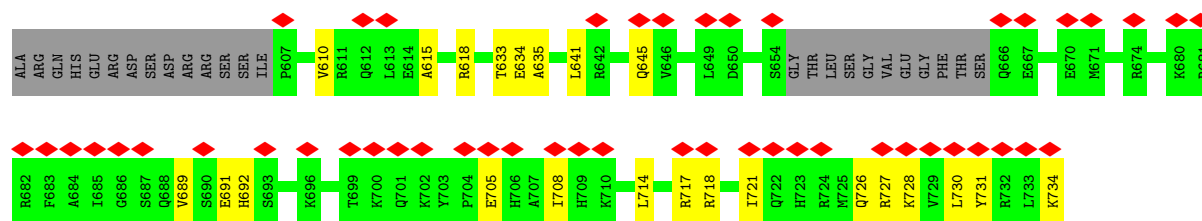




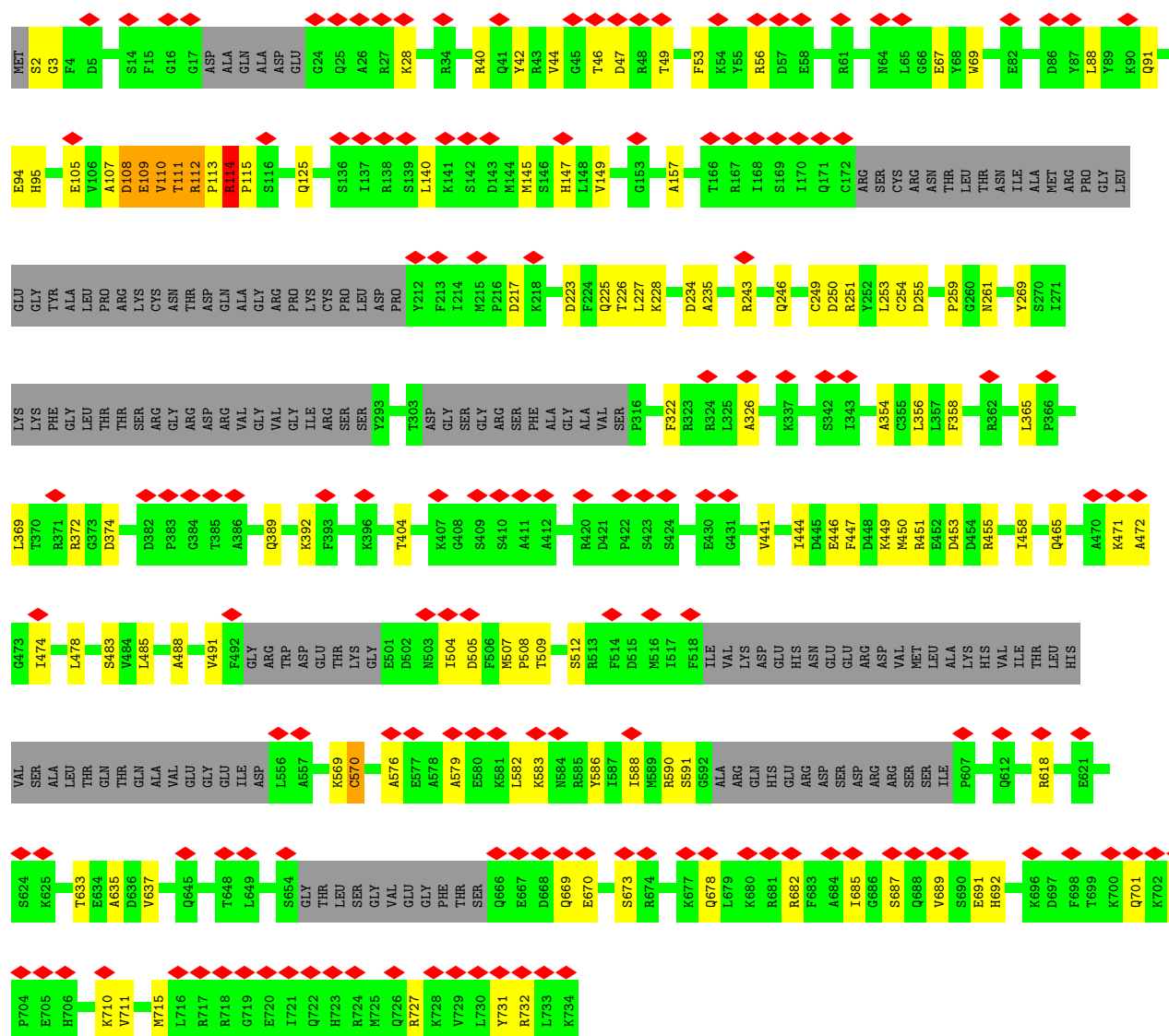


- Molecule 4: DNA replication licensing factor MCM5



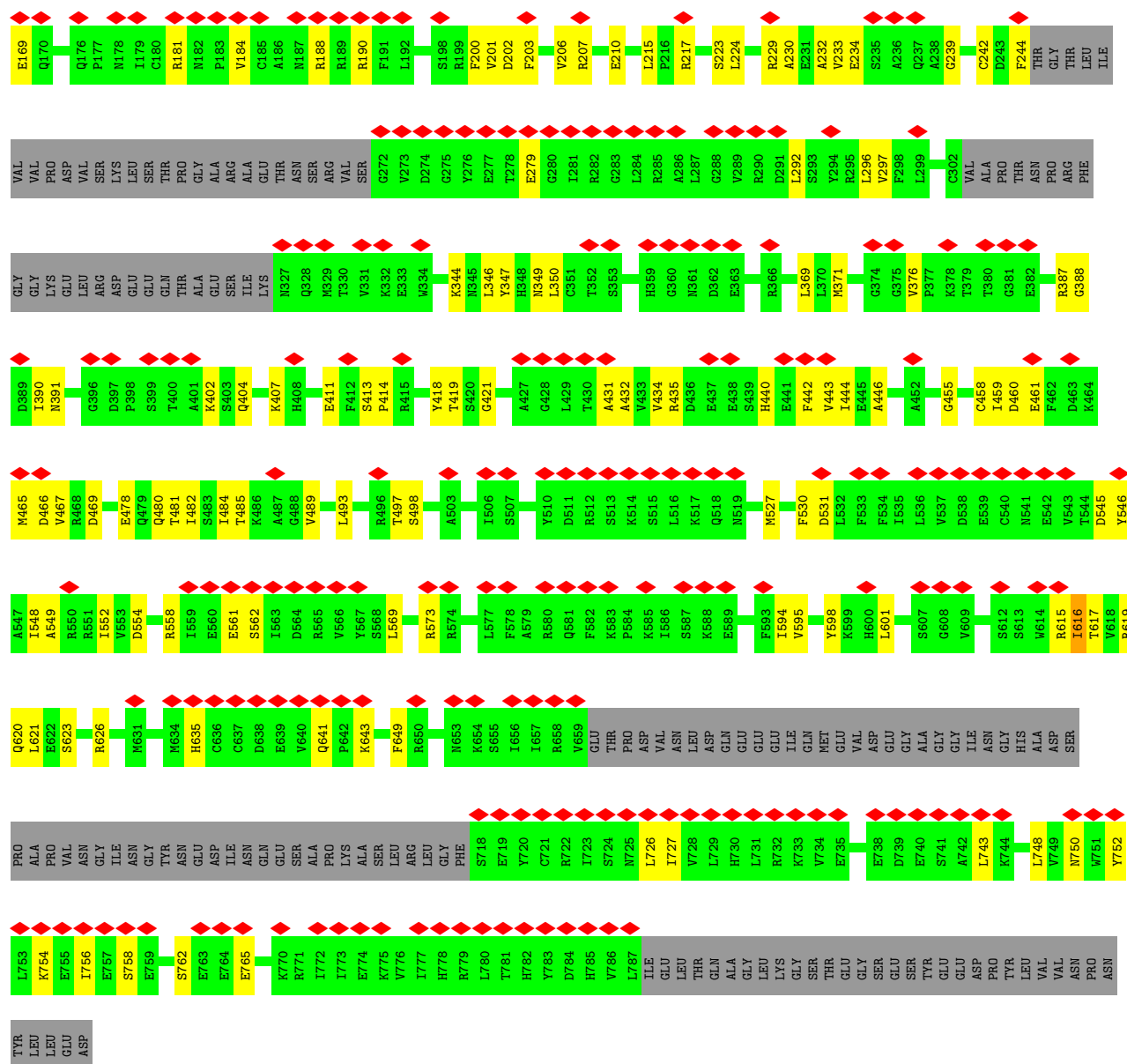


• Molecule 4: DNA replication licensing factor MCM5

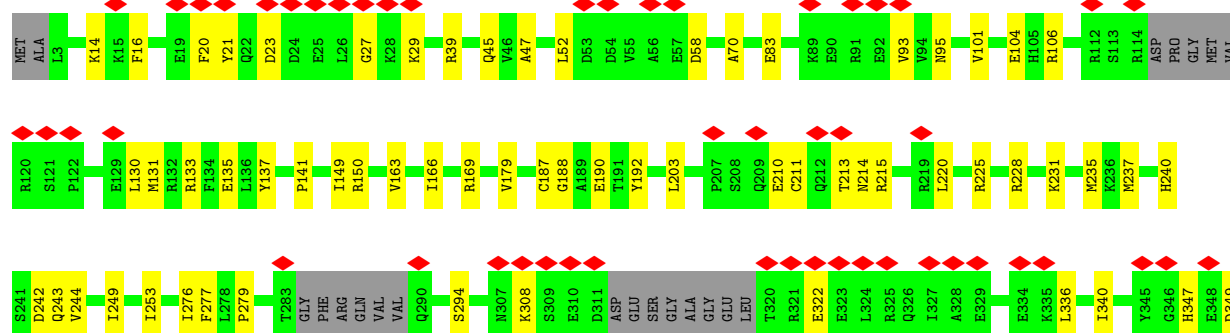


• Molecule 5: DNA replication licensing factor MCM6





• Molecule 6: DNA replication licensing factor MCM7





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.169	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

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	0	0.19	0/4296	0.46	2/5804 (0.0%)
1	4	0.19	0/4299	0.45	0/5809
2	2	0.15	0/4518	0.40	0/6093
2	8	0.15	0/4518	0.41	0/6093
3	3	0.47	11/4459 (0.2%)	0.50	7/6014 (0.1%)
3	9	0.44	6/4459 (0.1%)	0.54	10/6014 (0.2%)
4	5	0.30	2/4690 (0.0%)	0.50	6/6288 (0.1%)
4	A	0.27	2/4690 (0.0%)	0.61	9/6288 (0.1%)
5	6	0.17	0/5420	0.42	0/7302
5	B	0.18	0/5420	0.42	0/7302
6	7	0.18	0/5034	0.39	0/6792
6	C	0.18	0/5034	0.38	0/6792
All	All	0.26	21/56837 (0.0%)	0.46	34/76591 (0.0%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	137	VAL	CA-CB	-8.76	1.43	1.53
3	9	200	THR	CA-C	8.06	1.62	1.52
3	9	265	VAL	CA-CB	-8.02	1.44	1.54
3	3	132	THR	C-O	-7.85	1.14	1.24
4	5	110	VAL	CA-C	-6.84	1.44	1.52
3	9	201	ILE	CA-C	6.83	1.60	1.52
3	3	267	GLN	CA-C	-6.63	1.44	1.53
3	3	137	VAL	CA-C	-6.55	1.45	1.53
3	3	132	THR	N-CA	-6.29	1.38	1.46
3	9	265	VAL	CA-C	-5.91	1.45	1.52
3	9	266	LYS	CA-C	-5.74	1.45	1.52
3	3	132	THR	CA-C	-5.73	1.45	1.52
4	A	111	THR	CA-C	-5.73	1.45	1.52
3	3	137	VAL	C-O	-5.63	1.17	1.23
4	5	118	GLU	CA-C	-5.33	1.45	1.52
4	A	110	VAL	CA-C	-5.33	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	201	ILE	CA-CB	-5.17	1.46	1.55
3	3	136	LEU	CA-C	-5.16	1.45	1.53
3	3	134	CYS	CA-CB	-5.08	1.45	1.53
3	3	134	CYS	C-O	-5.05	1.17	1.23
3	9	265	VAL	C-O	-5.04	1.19	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	114	ARG	CA-C-N	21.48	141.80	119.89
4	A	114	ARG	C-N-CA	21.48	141.80	119.89
3	9	268	MET	N-CA-C	10.84	126.67	113.12
4	5	107	ALA	O-C-N	10.68	133.44	122.12
4	5	111	THR	N-CA-C	-9.90	100.04	111.03
4	5	118	GLU	N-CA-C	-8.80	92.05	110.80
3	9	201	ILE	N-CA-C	8.79	123.19	108.86
4	A	107	ALA	O-C-N	8.70	132.40	122.22
3	9	201	ILE	CA-C-N	8.28	135.36	122.94
3	9	201	ILE	C-N-CA	8.28	135.36	122.94
4	A	109	GLU	N-CA-C	8.27	119.98	110.97
3	3	201	ILE	CB-CA-C	-8.13	97.68	110.69
3	3	201	ILE	N-CA-C	7.65	121.33	108.86
4	5	109	GLU	N-CA-C	7.59	119.24	110.97
3	3	137	VAL	CB-CA-C	-7.29	103.36	111.23
3	9	136	LEU	CA-C-N	-7.27	112.92	123.10
3	9	136	LEU	C-N-CA	-7.27	112.92	123.10
4	A	108	ASP	N-CA-C	-7.02	102.69	111.11
4	5	111	THR	CB-CA-C	-6.60	100.72	110.95
4	A	111	THR	N-CA-C	-6.25	104.09	111.03
3	9	200	THR	N-CA-C	6.11	119.00	109.52
3	9	201	ILE	CB-CA-C	-6.08	100.96	110.69
4	5	108	ASP	N-CA-C	-5.69	101.98	111.37
3	9	268	MET	CB-CG-SD	-5.64	95.79	112.70
4	A	109	GLU	CA-C-N	-5.64	112.44	121.35
4	A	109	GLU	C-N-CA	-5.64	112.44	121.35
3	3	269	SER	N-CA-C	5.63	122.79	110.80
1	0	359	GLU	CA-C-N	5.59	130.07	122.19
1	0	359	GLU	C-N-CA	5.59	130.07	122.19
3	3	137	VAL	N-CA-C	5.52	116.32	107.98
3	3	270	LYS	N-CA-C	-5.50	105.18	111.07
4	A	111	THR	CB-CA-C	-5.50	102.43	110.95
3	3	268	MET	N-CA-C	5.44	122.39	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9	265	VAL	N-CA-CB	-5.38	102.86	111.58

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	0	4226	0	4252	80	0
1	4	4227	0	4255	74	0
2	2	4443	0	4481	57	0
2	8	4443	0	4481	63	0
3	3	4397	0	4434	99	0
3	9	4397	0	4434	102	0
4	5	4621	0	4703	100	0
4	A	4621	0	4703	93	0
5	6	5335	0	5358	93	0
5	B	5335	0	5358	106	0
6	7	4958	0	5002	74	0
6	C	4958	0	5002	77	0
All	All	55961	0	56463	977	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 (977) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:112:ARG:HB3	4:A:113:PRO:CD	1.27	1.50
4:5:112:ARG:HB3	4:5:113:PRO:CD	1.46	1.44
4:A:112:ARG:CB	4:A:113:PRO:CD	2.18	1.17
4:A:112:ARG:HB3	4:A:113:PRO:HD3	1.24	1.13
4:5:112:ARG:HB3	4:5:113:PRO:HD2	1.15	1.09
4:5:112:ARG:CB	4:5:113:PRO:CD	2.31	1.08
4:5:112:ARG:HB3	4:5:113:PRO:HD3	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:136:LEU:HD13	3:9:138:ARG:CD	1.86	1.02
1:0:690:TYR:CE1	1:0:690:TYR:CE2	2.39	1.00
4:5:105:GLU:O	4:5:108:ASP:HB2	1.61	0.99
4:A:112:ARG:HB3	4:A:113:PRO:HD2	1.01	0.98
4:A:105:GLU:O	4:A:108:ASP:HB3	1.65	0.96
4:5:105:GLU:O	4:5:108:ASP:CB	2.16	0.94
3:3:188:TYR:HH	4:A:2:SER:N	1.66	0.93
3:3:362:ALA:HB1	3:3:365:ALA:HB3	1.53	0.90
4:A:112:ARG:CB	4:A:113:PRO:HD2	1.89	0.90
4:5:271:ILE:HD12	4:5:271:ILE:H	1.39	0.87
4:A:114:ARG:O	4:A:114:ARG:NE	2.07	0.86
3:3:338:ASP:OD2	3:3:478:ARG:NH2	2.09	0.85
4:A:40:ARG:HD3	4:A:109:GLU:OE1	1.77	0.85
3:3:133:LYS:NZ	3:3:392:ARG:HD3	1.91	0.85
3:9:471:LEU:HB3	3:9:476:LEU:HD11	1.58	0.84
4:A:114:ARG:CB	4:A:115:PRO:HD2	2.07	0.83
1:0:162:CYS:HB2	1:0:166:PHE:HB3	1.61	0.83
3:9:136:LEU:HD13	3:9:138:ARG:HD3	1.59	0.82
4:5:112:ARG:CB	4:5:113:PRO:HD2	2.05	0.81
4:5:569:LYS:HD2	4:5:570:CYS:H	1.45	0.81
4:A:569:LYS:HD2	4:A:570:CYS:H	1.45	0.81
4:A:125:GLN:HE22	4:A:250:ASP:HB3	1.45	0.80
5:B:465:MET:HA	5:B:469:ASP:HB3	1.62	0.80
4:A:105:GLU:O	4:A:108:ASP:CB	2.30	0.79
4:5:111:THR:HG22	4:5:114:ARG:NH2	1.98	0.79
2:2:380:GLU:HB2	2:2:394:LYS:HE2	1.64	0.79
5:6:202:ASP:HB3	5:6:230:ALA:HB2	1.65	0.78
5:6:431:ALA:HB1	5:6:444:ILE:HA	1.66	0.78
5:B:387:ARG:NH2	5:B:478:GLU:O	2.15	0.78
3:3:324:GLY:HA3	3:3:327:ARG:HH22	1.48	0.77
4:A:112:ARG:CB	4:A:113:PRO:HD3	1.97	0.77
1:4:376:ASN:ND2	1:4:418:VAL:O	2.17	0.76
6:C:52:LEU:HD12	6:C:141:PRO:HD3	1.68	0.76
6:C:93:VAL:HG12	6:C:95:ASN:H	1.49	0.76
1:0:690:TYR:CE2	1:0:690:TYR:OH	2.38	0.76
2:2:230:LEU:HB3	2:2:284:ARG:HD3	1.66	0.76
3:9:136:LEU:HD21	3:9:138:ARG:CZ	2.16	0.76
3:3:339:ILE:HG21	3:3:623:ARG:HG3	1.68	0.76
1:0:690:TYR:CE1	1:0:690:TYR:OH	2.39	0.75
3:9:136:LEU:HD21	3:9:138:ARG:NH2	2.02	0.75
6:7:495:TYR:HE1	6:7:504:ASN:HB2	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:136:LEU:HD13	3:9:138:ARG:HD2	1.69	0.74
4:5:111:THR:HG22	4:5:114:ARG:HH21	1.52	0.74
3:3:334:HIS:O	3:3:336:ARG:NH1	2.21	0.73
1:4:597:SER:HA	1:4:606:GLN:HA	1.70	0.73
2:8:413:GLU:HG2	2:8:445:ALA:HB2	1.70	0.73
4:A:471:LYS:HD3	4:A:474:ILE:HD12	1.70	0.73
4:5:112:ARG:CB	4:5:113:PRO:HD3	2.09	0.73
3:3:340:ASN:ND2	3:3:426:MET:SD	2.62	0.72
3:3:234:ARG:O	3:3:268:MET:HB2	1.90	0.72
6:7:380:MET:HE1	6:7:518:LEU:HB3	1.72	0.72
3:9:136:LEU:CD1	3:9:138:ARG:CD	2.65	0.72
5:B:141:VAL:H	5:B:239:GLY:HA2	1.54	0.72
5:B:181:ARG:HH21	5:B:184:VAL:HG11	1.54	0.72
4:5:63:TYR:HE1	4:5:114:ARG:HH12	1.38	0.72
4:A:114:ARG:HB2	4:A:115:PRO:HD2	1.71	0.71
4:A:669:GLN:O	4:A:673:SER:OG	2.08	0.71
3:9:136:LEU:CD1	3:9:138:ARG:HD3	2.20	0.71
2:8:679:VAL:O	2:8:682:SER:OG	2.09	0.71
2:2:306:ILE:N	2:2:416:GLY:O	2.22	0.70
6:C:133:ARG:HD2	6:C:228:ARG:HH12	1.56	0.70
3:9:136:LEU:HD12	3:9:136:LEU:N	2.05	0.70
6:C:381:GLY:N	6:C:488:ALA:O	2.17	0.70
2:8:575:ALA:HA	2:8:578:LEU:HD12	1.74	0.69
1:0:640:LEU:O	1:0:643:ARG:NE	2.25	0.69
2:2:298:ARG:HH12	5:6:57:GLU:HB3	1.57	0.69
4:5:347:THR:HA	4:5:350:LYS:HD2	1.73	0.69
3:9:478:ARG:O	3:9:478:ARG:NH1	2.25	0.69
4:5:40:ARG:HG2	4:5:109:GLU:OE2	1.92	0.69
6:C:210:GLU:OE2	6:C:214:ASN:ND2	2.25	0.69
1:0:474:GLU:HB2	1:0:477:LYS:HD2	1.74	0.68
6:7:363:ASP:O	6:7:618:ARG:NH2	2.26	0.68
6:C:380:MET:HE1	6:C:518:LEU:HB3	1.75	0.68
3:3:146:HIS:CE1	3:3:175:PRO:HG2	2.28	0.68
6:C:469:ILE:HG22	6:C:471:LYS:H	1.57	0.68
1:0:379:VAL:O	1:0:381:LYS:NZ	2.26	0.68
5:B:371:MET:HE2	5:B:498:SER:HB3	1.74	0.68
6:7:52:LEU:HD12	6:7:141:PRO:HD3	1.75	0.68
1:0:597:SER:HA	1:0:606:GLN:HA	1.76	0.68
3:9:334:HIS:O	3:9:336:ARG:NH1	2.27	0.68
5:6:725:ASN:HA	5:6:729:LEU:HD12	1.76	0.68
3:9:134:CYS:SG	3:9:231:PRO:HG3	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:344:LYS:HG3	5:B:635:HIS:HE1	1.58	0.67
1:4:569:GLY:O	1:4:611:THR:OG1	2.12	0.67
1:0:270:ASN:HB3	1:0:273:ASN:HB2	1.77	0.67
2:2:564:PRO:HD2	2:2:567:ARG:HD2	1.76	0.67
6:7:93:VAL:HG12	6:7:95:ASN:H	1.58	0.67
4:A:389:GLN:HA	4:A:392:LYS:HD2	1.76	0.67
3:3:379:THR:OG1	3:3:435:LYS:NZ	2.28	0.67
1:4:358:PRO:HB2	1:4:361:MET:HB2	1.77	0.67
3:9:594:TYR:HA	3:9:597:LEU:HD12	1.77	0.67
4:5:727:ARG:NH1	4:5:727:ARG:O	2.28	0.67
5:B:376:VAL:HG13	5:B:388:GLY:HA3	1.77	0.67
3:3:478:ARG:O	3:3:478:ARG:NH1	2.28	0.66
4:5:105:GLU:O	4:5:108:ASP:HB3	1.93	0.66
2:8:576:LEU:HD11	2:8:604:MET:HG2	1.78	0.66
5:6:444:ILE:HG21	5:6:489:VAL:HG11	1.76	0.66
4:5:125:GLN:HE22	4:5:250:ASP:HB3	1.59	0.66
2:2:312:VAL:HG11	2:2:406:CYS:HB3	1.77	0.66
3:9:339:ILE:HG12	3:9:480:ASP:HB2	1.78	0.66
6:C:397:LEU:HA	6:C:560:ARG:HH21	1.60	0.66
4:5:579:ALA:HA	4:5:582:LEU:HB2	1.78	0.65
1:0:699:MET:O	1:0:701:ARG:NH1	2.29	0.65
4:A:374:ASP:OD1	4:A:483:SER:OG	2.13	0.65
4:A:223:ASP:HB2	4:A:251:ARG:HA	1.78	0.65
2:2:609:ILE:HD12	2:2:620:LEU:HD12	1.78	0.65
4:A:91:GLN:O	4:A:95:HIS:ND1	2.23	0.65
1:0:287:GLY:H	1:0:388:VAL:HB	1.62	0.65
1:0:747:VAL:HG12	1:0:748:ARG:HG3	1.79	0.65
1:4:354:LEU:HD22	1:4:388:VAL:HG21	1.77	0.65
2:2:575:ALA:HA	2:2:578:LEU:HD12	1.79	0.65
4:A:727:ARG:O	4:A:727:ARG:NH1	2.29	0.65
5:6:440:HIS:CE1	5:6:442:PHE:HB2	2.32	0.65
5:B:36:GLU:OE2	5:B:45:LYS:NZ	2.30	0.64
3:9:340:ASN:HB2	3:9:448:VAL:O	1.98	0.64
5:B:413:SER:O	5:B:418:TYR:OH	2.11	0.64
4:A:114:ARG:H	4:A:114:ARG:CZ	2.09	0.64
3:3:268:MET:HE3	3:3:268:MET:C	2.21	0.64
1:4:398:PRO:HB2	1:4:408:VAL:HG11	1.79	0.64
1:0:598:ILE:N	1:0:605:CYS:O	2.23	0.64
3:3:414:MET:O	3:3:419:ARG:NH2	2.30	0.64
5:6:84:TYR:OH	5:6:297:VAL:O	2.16	0.64
3:9:362:ALA:HB1	3:9:365:ALA:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:496:ASN:H	6:7:499:ARG:HH21	1.46	0.63
3:9:136:LEU:HD12	3:9:136:LEU:H	1.64	0.63
1:4:270:ASN:HB3	1:4:273:ASN:HB2	1.80	0.63
6:C:379:LEU:O	6:C:488:ALA:N	2.31	0.63
2:8:422:TYR:HB2	2:8:436:ALA:HB1	1.80	0.63
2:8:551:ALA:HB3	2:8:555:GLY:HA3	1.81	0.63
4:A:678:GLN:HG2	4:A:682:ARG:HD2	1.79	0.63
1:0:563:LEU:HB3	1:0:596:LEU:HD11	1.81	0.63
3:9:234:ARG:O	3:9:268:MET:HB2	1.99	0.63
5:B:181:ARG:HE	5:B:184:VAL:HG21	1.64	0.63
1:4:271:MET:HE1	1:4:286:SER:HB2	1.81	0.63
2:2:556:LEU:HD22	2:2:576:LEU:HG	1.81	0.62
3:9:356:ARG:HG2	4:A:369:LEU:HD22	1.81	0.62
3:9:503:ARG:HH21	4:A:576:ALA:HA	1.64	0.62
3:9:16:GLN:NE2	3:9:82:ASP:OD2	2.32	0.62
5:B:434:VAL:HA	5:B:440:HIS:HB2	1.81	0.62
6:C:516:ASP:OD1	6:C:517:LEU:N	2.33	0.62
6:C:622:VAL:HG12	6:C:624:VAL:H	1.65	0.62
5:B:466:ASP:OD1	5:B:467:VAL:N	2.29	0.62
6:7:376:ASN:ND2	6:7:462:MET:SD	2.73	0.62
4:5:271:ILE:HD12	4:5:271:ILE:N	2.02	0.62
3:3:133:LYS:HG3	3:3:394:GLU:HG2	1.81	0.62
1:4:453:SER:HB3	1:4:748:ARG:HE	1.65	0.62
5:6:82:GLU:HB3	5:6:85:ARG:HB2	1.81	0.61
2:8:528:ALA:O	2:8:532:PHE:N	2.32	0.61
4:A:112:ARG:CG	4:A:113:PRO:HD3	2.30	0.61
4:A:471:LYS:HG2	4:A:472:ALA:H	1.65	0.61
5:B:61:LEU:HD12	5:B:112:VAL:HG21	1.82	0.61
2:2:812:ARG:HA	2:2:815:ARG:HE	1.65	0.61
5:6:411:GLU:HB3	5:6:418:TYR:HE1	1.66	0.61
5:6:413:SER:OG	5:6:573:ARG:NH2	2.34	0.61
2:8:297:LEU:HB3	2:8:380:GLU:OE2	2.01	0.61
5:B:414:PRO:HG2	5:B:573:ARG:HH22	1.66	0.61
1:0:340:ILE:HB	5:B:85:ARG:HH12	1.66	0.60
1:4:754:GLU:N	1:4:754:GLU:OE1	2.34	0.60
5:6:417:VAL:HG23	5:6:452:ALA:HB2	1.82	0.60
2:8:430:ASN:ND2	2:8:566:SER:OG	2.34	0.60
4:A:588:ILE:O	4:A:591:SER:OG	2.18	0.60
3:3:113:PRO:HD2	3:3:203:GLU:HG3	1.82	0.60
6:7:374:ASN:O	6:7:611:ARG:NH1	2.34	0.60
5:B:431:ALA:HB1	5:B:444:ILE:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:418:TYR:HB3	2:2:437:THR:HG21	1.83	0.60
3:3:133:LYS:HZ2	3:3:392:ARG:HD3	1.66	0.60
4:5:726:GLN:HG2	4:5:730:LEU:HD12	1.83	0.60
2:8:647:VAL:HG12	2:8:649:LEU:H	1.67	0.60
2:8:867:ASP:OD1	2:8:871:GLN:NE2	2.35	0.60
3:9:136:LEU:HD22	3:9:138:ARG:NE	2.17	0.60
6:C:616:LEU:HD13	6:C:632:GLU:HG3	1.81	0.60
2:2:377:ARG:NH1	2:2:573:ALA:O	2.34	0.60
3:3:114:ARG:HH12	3:3:212:GLN:HG3	1.66	0.60
4:5:105:GLU:C	4:5:108:ASP:HB2	2.27	0.60
3:3:19:TYR:CG	3:3:76:PHE:HD1	2.20	0.60
5:6:726:LEU:HD12	5:6:727:ILE:HB	1.84	0.60
5:B:598:TYR:HA	5:B:601:LEU:HD13	1.83	0.60
2:2:659:ILE:HD11	2:2:773:MET:HE1	1.83	0.59
4:5:590:ARG:HH12	4:5:610:VAL:HG22	1.67	0.59
5:6:69:GLU:HG2	5:6:76:SER:HB2	1.84	0.59
1:4:374:ALA:HB2	1:4:417:ASP:HA	1.84	0.59
3:9:136:LEU:CD2	3:9:138:ARG:CZ	2.80	0.59
5:6:215:LEU:HD13	5:6:219:SER:HB2	1.83	0.59
6:7:406:GLY:HA3	6:7:445:ASP:H	1.67	0.59
6:C:471:LYS:HD3	6:C:473:GLY:H	1.66	0.59
4:5:70:ILE:HG13	4:5:126:VAL:HG22	1.83	0.59
1:0:385:GLY:HA3	1:0:565:LEU:HD21	1.85	0.59
3:9:215:ARG:NH2	4:A:255:ASP:OD2	2.36	0.59
3:9:340:ASN:ND2	3:9:426:MET:SD	2.75	0.59
3:9:578:ILE:O	3:9:630:LYS:NZ	2.36	0.59
3:9:441:ARG:HD3	6:C:248:ASN:HA	1.85	0.59
5:6:429:LEU:H	5:6:446:ALA:HA	1.67	0.59
2:2:377:ARG:HD3	2:2:573:ALA:HB3	1.85	0.58
2:2:489:GLU:N	2:2:489:GLU:OE1	2.36	0.58
5:B:554:ASP:O	5:B:558:ARG:NH2	2.32	0.58
1:0:714:TYR:OH	5:B:546:TYR:O	2.20	0.58
1:4:449:LEU:O	1:4:453:SER:OG	2.18	0.58
4:5:399:PRO:HG3	4:5:560:LYS:HG2	1.83	0.58
3:9:423:HIS:CE1	3:9:475:LEU:HD22	2.38	0.58
3:3:134:CYS:CB	3:3:231:PRO:HG3	2.34	0.58
2:8:579:ALA:HB3	2:8:584:CYS:HB3	1.85	0.58
4:A:583:LYS:HA	4:A:586:TYR:HD2	1.69	0.58
6:C:213:THR:O	6:C:215:ARG:NH1	2.36	0.58
6:C:616:LEU:HD11	6:C:636:LEU:HD12	1.86	0.58
3:3:327:ARG:HD2	6:7:541:HIS:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:186:ALA:HA	5:6:190:ARG:HH22	1.68	0.58
6:7:392:SER:OG	6:7:396:ARG:NH1	2.36	0.58
1:0:399:ILE:HD11	1:0:413:LYS:HB2	1.84	0.58
3:3:376:VAL:HA	3:3:396:GLY:HA3	1.86	0.58
5:6:466:ASP:OD1	5:6:467:VAL:N	2.37	0.58
6:7:516:ASP:OD1	6:7:517:LEU:N	2.36	0.58
3:9:340:ASN:HD22	3:9:448:VAL:HB	1.69	0.58
6:C:190:GLU:OE1	6:C:192:TYR:OH	2.22	0.58
4:5:504:ILE:HG21	4:5:508:PRO:HB3	1.84	0.58
1:0:763:ARG:HG2	1:0:766:ARG:HH21	1.68	0.58
3:9:136:LEU:CD2	3:9:138:ARG:NE	2.67	0.58
3:9:425:VAL:HG22	3:9:431:VAL:HG22	1.85	0.58
6:C:387:LYS:O	6:C:390:LEU:HG	2.03	0.58
2:2:525:PRO:HA	2:2:530:SER:HB3	1.85	0.57
1:4:374:ALA:HB3	1:4:418:VAL:H	1.69	0.57
3:9:185:GLU:HB2	6:C:72:ARG:HH22	1.68	0.57
5:B:391:ASN:O	5:B:531:ASP:N	2.36	0.57
2:2:203:LEU:HD11	2:2:258:ILE:HG23	1.86	0.57
4:5:67:GLU:OE1	4:5:69:TRP:NE1	2.33	0.57
3:9:326:GLU:O	3:9:327:ARG:NH1	2.36	0.57
5:B:233:VAL:HG12	5:B:234:GLU:HG2	1.86	0.57
3:3:326:GLU:O	3:3:327:ARG:NH1	2.38	0.57
1:0:663:ALA:HA	6:C:606:LEU:HD21	1.86	0.57
1:0:710:LEU:HD11	1:0:738:ILE:HB	1.87	0.57
5:6:207:ARG:NE	5:6:224:LEU:O	2.28	0.57
4:A:67:GLU:HB3	4:A:69:TRP:CD1	2.39	0.57
2:8:489:GLU:OE1	2:8:489:GLU:N	2.36	0.57
4:A:110:VAL:O	4:A:110:VAL:HG22	2.04	0.57
2:2:199:PHE:HE2	2:2:258:ILE:HD13	1.69	0.57
3:3:16:GLN:NE2	3:3:82:ASP:OD2	2.38	0.57
3:3:455:VAL:HG21	4:5:718:ARG:CZ	2.35	0.57
3:9:133:LYS:HG2	3:9:200:THR:HB	1.87	0.57
5:B:432:ALA:HB3	5:B:440:HIS:CE1	2.40	0.57
6:C:45:GLN:NE2	6:C:47:ALA:O	2.31	0.57
2:2:193:LEU:O	2:2:197:HIS:ND1	2.36	0.57
3:9:19:TYR:CG	3:9:76:PHE:HD1	2.23	0.57
4:5:471:LYS:HG2	4:5:472:ALA:H	1.70	0.56
5:6:777:ILE:HA	5:6:780:LEU:HD12	1.86	0.56
6:7:190:GLU:OE1	6:7:192:TYR:OH	2.23	0.56
1:0:596:LEU:O	1:0:607:LEU:N	2.33	0.56
1:4:474:GLU:HB2	1:4:477:LYS:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:460:ASP:OD1	5:6:461:GLU:N	2.38	0.56
1:0:291:ARG:NH1	1:0:550:ASP:OD2	2.38	0.56
2:2:518:ASN:ND2	2:2:656:ARG:O	2.38	0.56
3:9:63:ASN:O	3:9:67:ASN:ND2	2.37	0.56
5:B:411:GLU:HA	5:B:418:TYR:CE1	2.40	0.56
1:0:470:ILE:HB	1:0:477:LYS:HE2	1.87	0.56
5:6:527:MET:HA	5:6:530:PHE:HD2	1.70	0.56
1:0:334:THR:HG22	1:0:342:ASN:HD21	1.71	0.56
4:5:134:PRO:HB2	4:5:152:PRO:HD3	1.86	0.56
5:B:201:VAL:HG23	5:B:202:ASP:H	1.71	0.56
5:B:43:GLU:HB2	5:B:46:TYR:HD2	1.70	0.56
5:B:558:ARG:NH1	5:B:561:GLU:O	2.38	0.56
1:4:265:ALA:HB3	1:4:391:THR:HG21	1.87	0.56
5:6:62:VAL:HG23	5:6:114:PHE:HA	1.86	0.56
5:6:109:ASP:OD1	5:6:110:PHE:N	2.37	0.56
4:A:125:GLN:NE2	4:A:250:ASP:HB3	2.18	0.56
5:B:481:THR:HG1	5:B:493:LEU:H	1.51	0.56
5:B:292:LEU:HD21	5:B:297:VAL:HG21	1.87	0.56
4:5:157:ALA:HB3	4:5:228:LYS:HB2	1.87	0.56
1:0:373:PHE:CZ	1:0:415:HIS:HD2	2.24	0.56
6:7:210:GLU:OE2	6:7:214:ASN:ND2	2.39	0.56
4:A:678:GLN:OE1	4:A:701:GLN:NE2	2.38	0.56
2:8:465:THR:O	2:8:468:SER:OG	2.16	0.55
5:B:455:GLY:O	5:B:497:THR:OG1	2.24	0.55
3:3:268:MET:C	3:3:268:MET:SD	2.88	0.55
6:7:361:GLY:HA3	6:7:373:GLY:HA2	1.88	0.55
5:B:419:THR:OG1	5:B:458:CYS:N	2.27	0.55
1:0:341:HIS:H	5:B:85:ARG:HH22	1.53	0.55
4:A:509:THR:O	4:A:512:SER:OG	2.24	0.55
2:2:781:HIS:HB3	2:2:783:ARG:HG3	1.87	0.55
4:5:234:ASP:OD1	4:5:235:ALA:N	2.40	0.55
2:8:261:GLU:HA	2:8:264:LEU:HD12	1.87	0.55
2:2:223:CYS:SG	2:2:224:LYS:N	2.80	0.55
3:3:136:LEU:CD2	3:3:438:ILE:HG13	2.36	0.55
4:5:112:ARG:CG	4:5:113:PRO:HD3	2.36	0.55
5:6:394:ILE:HG23	5:6:534:PHE:HB2	1.89	0.55
5:6:397:ASP:O	5:6:504:ASN:ND2	2.40	0.55
6:7:135:GLU:OE1	6:7:137:TYR:OH	2.19	0.55
5:B:84:TYR:OH	5:B:297:VAL:O	2.24	0.55
6:C:39:ARG:NH1	6:C:45:GLN:HB2	2.22	0.55
2:2:232:VAL:O	2:2:286:SER:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:496:ALA:HA	2:8:499:LEU:HD12	1.88	0.55
3:9:203:GLU:HB3	3:9:208:ALA:HB2	1.89	0.55
3:3:43:ASN:OD1	3:3:95:TYR:OH	2.23	0.55
5:6:201:VAL:HG23	5:6:202:ASP:H	1.72	0.55
4:A:234:ASP:OD1	4:A:235:ALA:N	2.39	0.55
5:B:210:GLU:HB3	5:B:215:LEU:HD11	1.89	0.55
5:B:344:LYS:HG3	5:B:635:HIS:CE1	2.41	0.55
6:C:163:VAL:HG23	6:C:237:MET:HE1	1.89	0.55
5:6:397:ASP:OD2	5:6:403:SER:N	2.40	0.54
5:6:117:LEU:HB3	5:6:136:ARG:HH22	1.72	0.54
2:8:432:PHE:CD2	2:8:436:ALA:HA	2.41	0.54
3:3:114:ARG:NH1	3:3:212:GLN:HE21	2.05	0.54
4:A:372:ARG:HG3	4:A:465:GLN:HE22	1.72	0.54
6:C:275:GLY:HA2	6:C:301:HIS:HD2	1.73	0.54
3:3:234:ARG:HH21	3:3:364:ARG:NH1	2.06	0.54
5:6:434:VAL:HA	5:6:440:HIS:HB3	1.89	0.54
4:A:46:THR:HG1	4:A:49:THR:HG1	1.51	0.54
1:0:656:GLU:HG3	6:C:586:VAL:HG13	1.90	0.54
4:5:53:PHE:HD2	4:5:56:ARG:HH21	1.55	0.54
2:8:658:ASP:OD1	2:8:659:ILE:N	2.41	0.54
1:0:754:GLU:OE1	1:0:754:GLU:N	2.35	0.54
1:4:303:PHE:HE1	1:4:316:GLU:HB2	1.73	0.54
2:8:223:CYS:SG	2:8:224:LYS:N	2.75	0.54
3:9:502:LEU:HD13	4:A:579:ALA:HB1	1.90	0.54
5:B:726:LEU:HD12	5:B:727:ILE:HB	1.89	0.54
4:5:471:LYS:HD3	4:5:474:ILE:HD12	1.90	0.54
5:B:350:LEU:HD13	5:B:369:LEU:HD11	1.89	0.54
6:7:504:ASN:OD1	6:7:505:ILE:N	2.41	0.54
3:3:112:SER:H	3:3:115:THR:HB	1.74	0.53
5:6:181:ARG:HG2	5:6:184:VAL:HB	1.89	0.53
5:B:83:PHE:HA	5:B:86:VAL:HG22	1.90	0.53
1:4:640:LEU:O	1:4:643:ARG:NE	2.39	0.53
5:B:147:VAL:HG13	5:B:202:ASP:OD2	2.08	0.53
5:B:421:GLY:HA2	5:B:460:ASP:H	1.72	0.53
1:0:529:ARG:HH22	1:0:565:LEU:HB3	1.72	0.53
1:4:748:ARG:NH1	1:4:754:GLU:OE2	2.41	0.53
1:4:759:GLU:HA	1:4:762:LYS:HD3	1.91	0.53
5:6:444:ILE:HG13	5:6:489:VAL:HG21	1.91	0.53
3:9:146:HIS:NE2	3:9:175:PRO:HG2	2.24	0.53
4:A:508:PRO:HG3	4:A:710:LYS:HE3	1.90	0.53
5:B:143:ARG:HE	5:B:443:VAL:HG12	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:655:ASP:HB3	1:4:658:TYR:HD2	1.73	0.53
5:6:120:ARG:HB2	5:6:136:ARG:HE	1.73	0.53
5:B:82:GLU:HB3	5:B:85:ARG:HB2	1.91	0.53
5:B:411:GLU:O	5:B:418:TYR:OH	2.25	0.53
6:C:516:ASP:OD2	6:C:611:ARG:NH1	2.31	0.53
1:0:270:ASN:OD1	1:0:273:ASN:ND2	2.41	0.53
4:5:140:LEU:HD11	4:5:151:ILE:HD13	1.91	0.53
3:9:340:ASN:HB3	3:9:448:VAL:H	1.73	0.53
6:C:150:ARG:NH2	6:C:249:ILE:O	2.33	0.53
6:7:469:ILE:HG22	6:7:471:LYS:H	1.73	0.53
6:7:495:TYR:CE1	6:7:504:ASN:HB2	2.41	0.53
5:6:83:PHE:HA	5:6:86:VAL:HG22	1.91	0.52
5:6:459:ILE:HD12	5:6:499:ILE:HG23	1.91	0.52
3:9:454:PRO:O	3:9:457:GLY:N	2.41	0.52
1:0:388:VAL:HG13	1:0:390:VAL:HG23	1.90	0.52
2:2:316:THR:OG1	2:2:374:GLN:OE1	2.20	0.52
2:2:658:ASP:OD1	2:2:659:ILE:N	2.42	0.52
6:7:354:LEU:O	6:7:358:LEU:N	2.35	0.52
6:C:516:ASP:HB2	6:C:611:ARG:HH22	1.73	0.52
2:2:647:VAL:HG12	2:2:649:LEU:H	1.74	0.52
5:B:151:LEU:HA	5:B:200:PHE:CE1	2.44	0.52
3:3:340:ASN:HB2	3:3:448:VAL:O	2.10	0.52
6:C:182:TYR:HB2	6:C:191:THR:HB	1.90	0.52
3:3:471:LEU:HB3	3:3:476:LEU:HD11	1.92	0.52
5:B:558:ARG:O	5:B:562:SER:OG	2.26	0.52
6:7:211:CYS:O	6:7:215:ARG:N	2.42	0.52
3:9:136:LEU:HD11	3:9:138:ARG:NH1	2.24	0.52
3:3:327:ARG:HD2	6:7:541:HIS:CE1	2.45	0.52
4:5:731:TYR:O	4:5:734:LYS:NZ	2.34	0.52
6:7:213:THR:O	6:7:215:ARG:NH1	2.43	0.52
3:9:363:PRO:HG2	3:9:572:ILE:HD13	1.90	0.52
5:B:77:THR:O	5:B:81:GLU:HG2	2.10	0.52
6:7:627:LYS:O	6:7:631:ASN:ND2	2.43	0.52
5:B:56:PRO:HB2	5:B:58:ARG:HG3	1.92	0.52
1:0:390:VAL:HG13	1:0:418:VAL:HG13	1.92	0.52
2:2:375:ARG:HH12	2:2:570:THR:HG23	1.74	0.52
5:6:440:HIS:HE1	5:6:442:PHE:HB2	1.74	0.52
5:B:446:ALA:HB2	5:B:484:ILE:HD11	1.91	0.52
3:3:63:ASN:O	3:3:67:ASN:ND2	2.40	0.51
4:5:457:ALA:HB1	4:5:467:ILE:HD11	1.92	0.51
1:4:589:GLU:O	1:4:593:GLN:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:407:LYS:HE2	5:B:458:CYS:HB3	1.93	0.51
1:4:335:HIS:O	1:4:339:LEU:HB2	2.10	0.51
3:9:351:LYS:HD3	3:9:451:ALA:HB1	1.91	0.51
5:B:151:LEU:HA	5:B:200:PHE:HE1	1.76	0.51
3:3:146:HIS:NE2	3:3:175:PRO:HG2	2.25	0.51
4:5:223:ASP:HB2	4:5:251:ARG:HA	1.91	0.51
3:9:136:LEU:HD12	3:9:136:LEU:O	2.11	0.51
1:0:378:LEU:O	1:0:381:LYS:HG2	2.10	0.51
2:2:234:TYR:HA	2:2:237:LEU:HD12	1.93	0.51
4:5:356:LEU:HD21	4:5:441:VAL:HG21	1.92	0.51
6:C:70:ALA:HB3	6:C:276:ILE:HG23	1.92	0.51
3:3:349:VAL:HG12	3:3:349:VAL:O	2.11	0.51
5:B:482:ILE:HG22	5:B:484:ILE:HG13	1.92	0.51
1:0:314:ARG:HD2	1:0:317:MET:HG2	1.93	0.51
5:6:77:THR:O	5:6:81:GLU:HG2	2.10	0.51
6:7:279:PRO:O	4:A:2:SER:OG	2.29	0.51
1:0:460:GLU:N	1:0:460:GLU:OE1	2.44	0.51
3:3:134:CYS:SG	3:3:135:SER:N	2.83	0.51
1:4:399:ILE:HD11	1:4:413:LYS:HB2	1.92	0.51
4:5:615:ALA:HA	4:5:618:ARG:HH11	1.76	0.51
4:A:157:ALA:HB3	4:A:228:LYS:HB2	1.93	0.51
5:B:460:ASP:OD1	5:B:461:GLU:N	2.40	0.51
3:3:290:THR:HG21	3:3:632:ARG:HH21	1.75	0.50
5:6:146:PRO:HG2	5:6:148:HIS:CE1	2.46	0.50
6:7:471:LYS:HD3	6:7:473:GLY:H	1.76	0.50
2:8:432:PHE:HD2	2:8:436:ALA:HA	1.76	0.50
6:C:337:ALA:HB1	6:C:351:LYS:HE3	1.92	0.50
1:4:699:MET:O	1:4:701:ARG:NH1	2.43	0.50
6:7:163:VAL:HG23	6:7:237:MET:HE1	1.92	0.50
3:9:76:PHE:CE2	3:9:100:VAL:HG11	2.46	0.50
3:3:456:TYR:O	3:3:458:ARG:NH1	2.45	0.50
1:4:393:ILE:HB	1:4:417:ASP:HB2	1.93	0.50
4:5:506:PHE:HB3	4:5:717:ARG:HH22	1.75	0.50
6:7:336:LEU:O	6:7:340:ILE:HG13	2.11	0.50
5:B:569:LEU:HD23	5:B:569:LEU:H	1.76	0.50
5:6:181:ARG:HA	5:6:184:VAL:HB	1.94	0.50
5:6:482:ILE:HG22	5:6:484:ILE:HG13	1.92	0.50
5:6:598:TYR:HA	5:6:601:LEU:HD13	1.94	0.50
3:3:200:THR:OG1	3:3:392:ARG:NH2	2.45	0.50
1:4:568:ASN:H	1:4:611:THR:HB	1.77	0.50
6:7:407:ARG:NH2	6:7:409:SER:O	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:691:GLU:HG2	4:A:692:HIS:HD2	1.77	0.50
6:7:187:CYS:SG	6:7:188:GLY:N	2.84	0.50
2:8:199:PHE:CE2	2:8:203:LEU:HD11	2.47	0.50
5:B:347:TYR:HA	5:B:350:LEU:HD12	1.93	0.50
1:0:397:VAL:HG22	1:0:415:HIS:CE1	2.47	0.50
1:4:286:SER:HB3	1:4:387:ARG:HH21	1.76	0.50
5:6:544:THR:O	5:6:548:ILE:HG13	2.11	0.50
4:A:491:VAL:HG21	4:A:505:ASP:HB3	1.94	0.50
3:9:598:ARG:HB2	3:9:614:THR:HG21	1.93	0.50
2:2:649:LEU:HB3	2:2:654:ILE:HD11	1.94	0.49
3:3:454:PRO:O	3:3:456:TYR:N	2.45	0.49
6:7:347:HIS:CE1	6:7:385:VAL:HG21	2.47	0.49
5:B:743:LEU:HD12	5:B:748:LEU:HD21	1.93	0.49
6:C:620:ARG:NH1	6:C:629:ASP:OD1	2.42	0.49
5:6:780:LEU:HD22	5:6:786:VAL:HG23	1.94	0.49
3:9:490:ASP:OD2	3:9:493:GLN:NE2	2.44	0.49
4:A:633:THR:HG23	4:A:635:ALA:H	1.77	0.49
1:0:265:ALA:HB3	1:0:391:THR:HG21	1.93	0.49
4:5:130:SER:H	4:5:266:MET:HE1	1.77	0.49
4:5:271:ILE:CD1	4:5:271:ILE:C	2.86	0.49
5:6:402:LYS:HD2	5:6:404:GLN:NE2	2.26	0.49
2:8:586:ILE:HD13	2:8:626:VAL:HG13	1.94	0.49
3:3:76:PHE:CD2	3:3:100:VAL:HG11	2.48	0.49
3:3:454:PRO:O	3:3:457:GLY:N	2.44	0.49
3:3:465:PRO:O	3:3:469:ILE:HG12	2.13	0.49
5:6:114:PHE:CE2	5:6:117:LEU:HD22	2.47	0.49
6:7:610:LEU:O	6:7:614:THR:OG1	2.27	0.49
5:B:141:VAL:HG13	5:B:206:VAL:HG13	1.95	0.49
3:3:477:SER:O	3:3:616:ARG:NH1	2.45	0.49
6:7:149:ILE:HD11	6:7:237:MET:HE3	1.93	0.49
2:8:774:ALA:HB1	2:8:786:VAL:HG21	1.95	0.49
5:B:527:MET:HA	5:B:530:PHE:HD2	1.77	0.49
6:C:232:PHE:CE1	6:C:256:LEU:HD13	2.47	0.49
2:2:199:PHE:CE2	2:2:258:ILE:HD13	2.46	0.49
5:B:150:GLU:HB2	5:B:203:PHE:CZ	2.48	0.49
5:B:545:ASP:HA	5:B:548:ILE:HD12	1.94	0.49
5:B:750:ASN:OD1	5:B:754:LYS:NZ	2.45	0.49
6:C:406:GLY:HA3	6:C:445:ASP:O	2.13	0.49
2:2:518:ASN:HB2	2:2:658:ASP:OD1	2.12	0.49
4:A:670:GLU:O	4:A:703:TYR:OH	2.30	0.49
5:B:31:LEU:O	5:B:34:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:698:ILE:HG13	1:4:749:LEU:HG	1.94	0.49
3:9:136:LEU:CD1	3:9:136:LEU:C	2.85	0.49
3:9:582:LEU:HD23	3:9:637:VAL:HG21	1.94	0.49
3:3:76:PHE:CE2	3:3:100:VAL:HG11	2.47	0.49
3:3:430:ARG:NH2	3:3:441:ARG:O	2.46	0.49
1:4:513:GLY:HA2	1:4:517:SER:H	1.77	0.49
4:5:125:GLN:HB2	4:5:251:ARG:CZ	2.42	0.49
3:9:454:PRO:O	3:9:456:TYR:N	2.46	0.49
6:C:149:ILE:HD11	6:C:237:MET:HE3	1.95	0.49
3:3:325:VAL:HA	3:3:337:GLY:HA3	1.95	0.49
5:6:142:VAL:HA	5:6:445:GLU:OE2	2.11	0.49
3:9:136:LEU:HD11	3:9:138:ARG:CZ	2.42	0.49
3:9:279:GLU:N	3:9:279:GLU:OE1	2.46	0.49
3:9:638:ASP:OD1	3:9:639:LEU:N	2.46	0.49
3:3:355:LEU:HD11	3:3:451:ALA:HB3	1.95	0.48
4:5:455:ARG:HA	4:5:458:ILE:HG22	1.95	0.48
3:9:111:VAL:HG21	3:9:116:LEU:HD13	1.95	0.48
6:C:187:CYS:SG	6:C:188:GLY:N	2.87	0.48
1:4:691:ILE:O	1:4:695:HIS:HB2	2.13	0.48
5:6:363:GLU:OE1	5:6:363:GLU:N	2.42	0.48
3:9:409:ASP:OD1	3:9:410:GLU:N	2.45	0.48
6:C:49:TYR:HB3	6:C:139:GLN:HE21	1.78	0.48
6:C:169:ARG:NH2	6:C:428:THR:OG1	2.47	0.48
1:4:303:PHE:CE1	1:4:316:GLU:HB2	2.48	0.48
1:4:535:GLY:HA3	1:4:579:MET:SD	2.53	0.48
5:6:75:LEU:O	5:6:79:ILE:HG12	2.13	0.48
6:7:322:GLU:OE1	6:7:322:GLU:N	2.41	0.48
2:8:485:ILE:HG13	2:8:487:GLY:H	1.78	0.48
3:9:245:PRO:HA	3:9:256:PHE:CE1	2.47	0.48
3:9:584:GLN:O	3:9:588:THR:OG1	2.30	0.48
4:A:586:TYR:O	4:A:590:ARG:N	2.41	0.48
5:B:619:ARG:O	5:B:623:SER:N	2.44	0.48
2:2:731:VAL:HG12	2:2:733:PRO:HD3	1.95	0.48
1:4:595:THR:HA	1:4:609:ALA:HB3	1.96	0.48
2:8:796:ARG:O	2:8:800:GLU:HG3	2.14	0.48
3:9:76:PHE:CD2	3:9:100:VAL:HG11	2.48	0.48
4:A:217:ASP:OD1	4:A:217:ASP:N	2.47	0.48
3:3:206:GLU:HG2	3:3:207:LYS:HG3	1.95	0.48
4:5:721:ILE:H	4:5:721:ILE:HD12	1.79	0.48
5:6:407:LYS:HE2	5:6:458:CYS:HB3	1.94	0.48
4:A:67:GLU:HB3	4:A:69:TRP:NE1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:226:THR:HG23	4:A:246:GLN:HE21	1.79	0.48
4:A:356:LEU:HD21	4:A:441:VAL:HG21	1.96	0.48
3:3:130:ILE:HG13	3:3:233:ASP:O	2.14	0.48
5:6:584:PRO:HB2	5:6:586:ILE:HG13	1.96	0.48
6:7:387:LYS:O	6:7:390:LEU:HG	2.14	0.48
4:A:685:ILE:HG22	4:A:687:SER:H	1.79	0.48
3:3:136:LEU:HA	3:3:136:LEU:HD12	1.46	0.47
3:3:279:GLU:N	3:3:279:GLU:OE1	2.47	0.47
1:4:361:MET:C	1:4:363:ALA:H	2.22	0.47
6:7:381:GLY:HA2	6:7:490:PRO:HG3	1.96	0.47
3:9:136:LEU:HD22	3:9:138:ARG:HE	1.79	0.47
6:C:157:VAL:HA	6:C:277:PHE:HD2	1.79	0.47
6:C:380:MET:HA	6:C:488:ALA:HB3	1.95	0.47
2:2:191:PRO:HB2	2:2:192:ARG:HD2	1.95	0.47
5:6:291:ASP:O	5:6:295:ARG:NH1	2.47	0.47
4:A:259:PRO:HB2	4:A:478:LEU:HD21	1.96	0.47
3:3:304:ALA:HB3	3:3:314:LYS:HE2	1.96	0.47
4:5:14:SER:HA	6:C:189:ALA:HB2	1.96	0.47
4:5:378:LEU:HD22	4:5:514:PHE:HD2	1.79	0.47
4:5:447:PHE:H	4:5:488:ALA:HB2	1.80	0.47
4:A:322:PHE:O	4:A:326:ALA:N	2.38	0.47
1:0:169:PHE:O	1:0:173:PHE:N	2.37	0.47
1:0:730:TYR:N	1:0:731:PRO:HD2	2.29	0.47
3:3:215:ARG:NH2	4:5:255:ASP:OD2	2.39	0.47
5:6:724:SER:HA	5:6:728:VAL:HB	1.97	0.47
2:8:534:LYS:O	2:8:537:GLU:HG2	2.14	0.47
1:0:366:THR:HG22	6:C:476:THR:HA	1.96	0.47
1:0:754:GLU:HG2	1:0:756:ILE:H	1.78	0.47
4:5:130:SER:N	4:5:266:MET:HE1	2.29	0.47
2:8:215:PHE:CE1	2:8:266:VAL:HG21	2.49	0.47
3:9:266:LYS:HE2	3:9:266:LYS:HB3	1.45	0.47
5:B:65:PHE:HZ	5:B:114:PHE:HD2	1.62	0.47
2:2:793:MET:SD	2:2:793:MET:N	2.87	0.47
5:6:20:ASP:OD1	5:6:21:GLU:N	2.48	0.47
5:B:20:ASP:OD1	5:B:21:GLU:N	2.47	0.47
6:C:327:ILE:HG23	6:C:335:LYS:HE2	1.95	0.47
3:3:188:TYR:OH	4:A:2:SER:N	2.39	0.47
1:4:238:ASP:O	1:4:242:ASN:ND2	2.43	0.47
4:5:444:ILE:HB	4:5:486:ALA:HA	1.95	0.47
4:5:714:LEU:O	4:5:718:ARG:HG2	2.15	0.47
2:8:793:MET:SD	2:8:793:MET:N	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:421:GLY:HA2	5:B:459:ILE:HA	1.96	0.47
5:B:549:ALA:HA	5:B:552:ILE:HD12	1.96	0.47
5:B:762:SER:HB2	5:B:765:GLU:HB2	1.96	0.47
2:2:576:LEU:HD23	2:2:624:CYS:SG	2.55	0.47
3:3:268:MET:C	3:3:268:MET:CE	2.85	0.47
1:4:564:VAL:HG22	1:4:596:LEU:HD22	1.96	0.47
3:9:36:VAL:O	3:9:39:LEU:HG	2.15	0.47
3:9:68:ASN:ND2	3:9:71:GLU:OE2	2.48	0.47
3:3:133:LYS:HZ3	3:3:392:ARG:HD3	1.75	0.47
2:8:304:GLN:O	2:8:417:ILE:HA	2.15	0.47
3:3:624:LEU:HD22	3:3:648:LEU:HD23	1.97	0.46
1:4:195:GLN:HE22	1:4:196:ARG:HH21	1.62	0.46
4:5:641:LEU:O	4:5:645:GLN:N	2.49	0.46
2:8:297:LEU:HD13	2:8:380:GLU:HG2	1.97	0.46
3:3:234:ARG:HH12	3:3:402:ASP:HB3	1.78	0.46
2:8:298:ARG:HH12	5:B:57:GLU:HB2	1.78	0.46
1:4:646:LEU:HD11	1:4:740:LEU:HD11	1.97	0.46
4:5:634:GLU:OE1	4:5:634:GLU:N	2.44	0.46
6:7:101:VAL:O	6:7:104:GLU:HG3	2.15	0.46
6:7:203:LEU:O	6:7:220:LEU:HD11	2.15	0.46
2:8:511:HIS:HB2	2:8:513:VAL:HG13	1.97	0.46
4:A:249:CYS:HB3	4:A:253:LEU:HB2	1.97	0.46
5:B:72:ASN:HB3	5:B:75:LEU:HG	1.98	0.46
6:C:101:VAL:O	6:C:104:GLU:HG3	2.15	0.46
6:C:240:HIS:O	6:C:244:VAL:HG23	2.15	0.46
6:7:253:ILE:HD11	6:7:277:PHE:HE1	1.80	0.46
2:8:215:PHE:HE1	2:8:266:VAL:HG21	1.80	0.46
3:9:281:ILE:HA	3:9:284:ILE:HD12	1.98	0.46
4:A:455:ARG:HA	4:A:458:ILE:HG22	1.97	0.46
5:B:402:LYS:C	5:B:404:GLN:H	2.24	0.46
1:0:606:GLN:OE1	5:B:217:ARG:NH2	2.48	0.46
1:4:206:PRO:HA	1:4:258:ILE:HG12	1.97	0.46
1:4:547:VAL:HA	1:4:559:GLN:HB2	1.97	0.46
4:5:113:PRO:O	4:5:113:PRO:HG2	2.15	0.46
3:3:133:LYS:HG3	3:3:394:GLU:CG	2.45	0.46
4:5:94:GLU:HG2	4:5:95:HIS:N	2.31	0.46
3:9:349:VAL:HG12	3:9:349:VAL:O	2.15	0.46
4:A:689:VAL:HG12	4:A:689:VAL:O	2.16	0.46
5:B:65:PHE:HZ	5:B:114:PHE:CD2	2.34	0.46
5:B:371:MET:HG3	5:B:390:ILE:HG21	1.96	0.46
2:2:289:PRO:O	2:2:291:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:600:GLN:NE2	3:3:650:GLN:OE1	2.49	0.46
4:5:491:VAL:HG11	4:5:505:ASP:HB3	1.96	0.46
3:9:306:SER:HA	3:9:504:MET:HE3	1.97	0.46
4:A:451:ARG:HD2	4:A:453:ASP:HB2	1.97	0.46
6:C:451:ALA:O	6:C:455:ARG:HG3	2.16	0.46
3:3:470:GLY:HA3	4:5:718:ARG:NH2	2.30	0.46
5:6:143:ARG:HD2	5:6:207:ARG:HG3	1.98	0.46
5:6:429:LEU:N	5:6:446:ALA:HA	2.30	0.46
3:9:379:THR:HA	3:9:394:GLU:O	2.16	0.46
5:B:620:GLN:OE1	5:B:620:GLN:N	2.44	0.46
1:0:207:PHE:O	1:0:209:ASN:ND2	2.49	0.46
3:3:195:ASP:OD1	3:3:223:ASP:HA	2.16	0.46
3:9:293:LYS:HE3	3:9:294:ASP:H	1.81	0.46
4:A:404:THR:HG22	4:A:444:ILE:HA	1.97	0.46
2:8:248:LEU:HB2	2:8:249:PRO:HD3	1.98	0.46
3:9:57:LYS:HB2	3:9:57:LYS:HE2	1.72	0.46
3:9:136:LEU:CD1	3:9:138:ARG:NE	2.78	0.46
4:A:53:PHE:HB2	4:A:56:ARG:HB2	1.97	0.46
4:A:225:GLN:HB2	4:A:254:CYS:SG	2.56	0.46
5:B:229:ARG:HG3	5:B:232:ALA:H	1.81	0.46
1:0:289:VAL:HB	1:0:384:PRO:HA	1.97	0.45
4:5:466:THR:OG1	4:5:478:LEU:O	2.25	0.45
5:6:143:ARG:HG3	5:6:443:VAL:HG11	1.96	0.45
6:7:369:MET:SD	6:7:372:ARG:NH2	2.86	0.45
5:B:188:ARG:HD3	5:B:190:ARG:HH21	1.81	0.45
5:B:758:SER:O	5:B:758:SER:OG	2.32	0.45
1:4:334:THR:HG23	1:4:338:ALA:HB3	1.98	0.45
4:5:111:THR:HB	4:5:114:ARG:HD2	1.97	0.45
4:5:125:GLN:NE2	4:5:250:ASP:OD2	2.49	0.45
5:6:652:LEU:HD22	5:6:656:ILE:HD11	1.98	0.45
2:8:461:VAL:HA	2:8:464:ILE:HB	1.97	0.45
1:0:577:ASP:HA	1:0:584:ARG:HH22	1.81	0.45
2:2:525:PRO:HA	2:2:530:SER:CB	2.47	0.45
1:4:571:CYS:H	1:4:613:VAL:HG22	1.80	0.45
1:4:730:TYR:N	1:4:731:PRO:HD2	2.31	0.45
5:6:419:THR:HG21	5:6:459:ILE:HA	1.98	0.45
2:8:412:ILE:HA	2:8:445:ALA:HB3	1.98	0.45
2:2:199:PHE:O	2:2:202:PHE:HB2	2.17	0.45
5:6:417:VAL:HG22	5:6:451:LEU:HD23	1.98	0.45
6:7:150:ARG:NH2	6:7:249:ILE:O	2.37	0.45
2:8:601:HIS:HA	2:8:604:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:235:VAL:HG12	3:9:267:GLN:HG3	1.98	0.45
3:9:628:HIS:HD2	3:9:645:ALA:HB2	1.82	0.45
5:B:201:VAL:HG23	5:B:202:ASP:N	2.30	0.45
1:4:290:ILE:HD11	1:4:355:GLN:HB2	1.99	0.45
1:4:354:LEU:HD11	1:4:372:LEU:HD22	1.98	0.45
1:4:374:ALA:HB3	1:4:418:VAL:HG23	1.98	0.45
2:8:749:ASP:O	2:8:752:LYS:HG2	2.17	0.45
5:B:346:LEU:HD12	5:B:349:ASN:HD22	1.81	0.45
5:B:387:ARG:HH12	5:B:480:GLN:HG3	1.82	0.45
6:C:528:ASP:HA	6:C:531:LEU:HD12	1.99	0.45
2:2:203:LEU:HD21	2:2:258:ILE:HG23	1.99	0.45
4:5:447:PHE:HB3	4:5:488:ALA:HB2	1.98	0.45
5:6:431:ALA:HB1	5:6:444:ILE:HD13	1.98	0.45
3:9:473:ASP:O	3:9:476:LEU:HD13	2.16	0.45
4:A:114:ARG:CG	4:A:115:PRO:HD2	2.46	0.45
1:0:547:VAL:HG13	1:0:600:LYS:HZ3	1.81	0.45
4:5:372:ARG:HG3	4:5:465:GLN:HE22	1.82	0.45
6:7:16:PHE:HA	6:7:20:PHE:HB3	1.98	0.45
6:7:130:LEU:HD13	6:7:179:VAL:HG11	1.97	0.45
4:A:582:LEU:HD22	4:A:637:VAL:HG21	1.98	0.45
6:C:232:PHE:HE1	6:C:256:LEU:HD13	1.82	0.45
1:0:276:PRO:HB3	6:C:175:PRO:HB3	1.98	0.45
5:6:392:VAL:HG23	5:6:532:LEU:HB2	1.99	0.45
6:7:358:LEU:HD22	6:7:398:ALA:HB2	1.99	0.45
4:A:243:ARG:HA	4:A:243:ARG:HD3	1.83	0.45
5:B:617:THR:HG23	5:B:619:ARG:H	1.82	0.45
1:0:283:ILE:HD11	1:0:416:ILE:HD12	1.99	0.45
6:7:242:ASP:OD1	6:7:243:GLN:N	2.50	0.45
2:8:733:PRO:HD3	2:8:779:ARG:HH22	1.81	0.45
3:9:650:GLN:O	3:9:650:GLN:NE2	2.46	0.45
4:5:47:ASP:OD1	4:5:47:ASP:N	2.50	0.44
3:9:130:ILE:HG13	3:9:233:ASP:O	2.18	0.44
6:C:628:GLU:OE1	6:C:628:GLU:N	2.49	0.44
3:3:178:ASP:HB2	3:3:184:LEU:HD21	1.98	0.44
1:4:462:LEU:O	1:4:466:LEU:HB2	2.17	0.44
4:5:691:GLU:HG2	4:5:692:HIS:HD2	1.83	0.44
5:6:422:LYS:O	5:6:424:SER:N	2.51	0.44
5:6:620:GLN:OE1	5:6:620:GLN:N	2.42	0.44
2:8:306:ILE:HB	2:8:418:TYR:HE1	1.82	0.44
2:8:522:CYS:HB3	2:8:662:VAL:HG23	2.00	0.44
1:0:321:ARG:NH2	6:C:185:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:226:LEU:HD12	1:4:227:ILE:HG23	1.97	0.44
4:5:217:ASP:N	4:5:217:ASP:OD1	2.48	0.44
4:5:583:LYS:HA	4:5:586:TYR:HD2	1.83	0.44
6:C:424:SER:OG	6:C:425:GLY:N	2.50	0.44
3:3:412:ASP:OD1	3:3:412:ASP:N	2.50	0.44
1:4:354:LEU:HD13	1:4:388:VAL:HG11	2.00	0.44
5:6:148:HIS:O	5:6:203:PHE:HE1	2.00	0.44
5:B:485:THR:HA	5:B:489:VAL:O	2.16	0.44
2:2:514:ARG:O	2:2:772:ARG:NE	2.50	0.44
3:3:223:ASP:N	3:3:223:ASP:OD1	2.49	0.44
6:7:21:TYR:HB2	6:7:29:LYS:HB2	2.00	0.44
5:B:207:ARG:HH21	5:B:223:SER:HB2	1.82	0.44
1:0:283:ILE:HD12	1:0:285:ILE:HD11	2.00	0.44
3:3:206:GLU:OE2	3:3:364:ARG:NE	2.51	0.44
1:4:316:GLU:OE2	1:4:321:ARG:NH1	2.50	0.44
4:5:107:ALA:C	4:5:109:GLU:N	2.71	0.44
3:9:271:ASP:OD1	3:9:271:ASP:N	2.49	0.44
4:A:47:ASP:OD1	4:A:47:ASP:N	2.50	0.44
4:A:88:LEU:HD23	4:A:88:LEU:HA	1.86	0.44
6:C:547:PRO:HB2	6:C:551:PHE:HD2	1.83	0.44
6:C:577:LEU:HD21	6:C:629:ASP:HB2	1.99	0.44
3:9:471:LEU:HD23	3:9:471:LEU:HA	1.80	0.44
6:C:366:PRO:O	6:C:367:ARG:NH1	2.50	0.44
6:C:375:ILE:HG22	6:C:377:ILE:HG13	2.00	0.44
1:0:577:ASP:OD1	1:0:577:ASP:N	2.51	0.44
3:3:57:LYS:HE2	3:3:57:LYS:HB2	1.74	0.44
3:3:153:LYS:HE2	3:3:153:LYS:HB3	1.73	0.44
4:5:705:GLU:O	4:5:708:ILE:HG12	2.18	0.44
2:8:292:GLU:HG2	2:8:295:ARG:HB2	2.00	0.44
3:9:40:ILE:HG23	3:9:91:TYR:CD2	2.53	0.44
3:9:139:PRO:HD2	6:C:294:SER:O	2.18	0.44
4:5:335:ILE:O	4:5:338:SER:OG	2.27	0.44
4:5:444:ILE:HD12	4:5:484:VAL:HG13	1.98	0.44
5:6:152:VAL:H	5:6:200:PHE:HZ	1.66	0.44
3:9:153:LYS:HB3	3:9:153:LYS:HE2	1.77	0.44
4:A:354:ALA:O	4:A:358:PHE:HD1	2.00	0.44
6:C:504:ASN:OD1	6:C:505:ILE:N	2.51	0.44
1:4:667:VAL:HG11	6:7:610:LEU:HD13	1.99	0.43
6:C:58:ASP:OD1	6:C:58:ASP:N	2.50	0.43
1:0:575:GLU:HB3	1:0:578:LYS:HB2	2.00	0.43
3:3:36:VAL:O	3:3:39:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:460:ASP:HA	3:3:468:ASN:HD22	1.82	0.43
4:5:689:VAL:O	4:5:689:VAL:HG12	2.18	0.43
5:6:371:MET:SD	5:6:500:LEU:HD12	2.58	0.43
3:9:43:ASN:OD1	3:9:95:TYR:OH	2.32	0.43
4:A:114:ARG:NE	4:A:114:ARG:C	2.72	0.43
4:A:507:MET:C	4:A:509:THR:H	2.26	0.43
3:3:40:ILE:HG23	3:3:91:TYR:CD2	2.54	0.43
4:5:140:LEU:HD23	4:5:140:LEU:HA	1.88	0.43
3:9:60:LYS:HE3	3:9:61:ARG:HH21	1.82	0.43
5:B:230:ALA:HA	5:B:233:VAL:HG23	2.01	0.43
5:B:595:VAL:HG22	5:B:621:LEU:HD11	2.00	0.43
3:3:628:HIS:HB3	3:3:641:ASP:HB3	1.99	0.43
4:5:365:LEU:HD23	4:5:365:LEU:HA	1.85	0.43
5:6:139:GLY:O	5:6:241:LYS:HA	2.19	0.43
5:6:509:HIS:NE2	5:6:512:ARG:HB2	2.33	0.43
2:8:586:ILE:HB	2:8:628:ALA:HB2	2.01	0.43
5:B:421:GLY:CA	5:B:460:ASP:H	2.31	0.43
1:0:296:ILE:HB	1:0:349:LYS:HG2	2.00	0.43
1:0:352:ILE:HB	1:0:372:LEU:HB3	2.00	0.43
1:0:559:GLN:O	1:0:600:LYS:NZ	2.51	0.43
1:4:330:ARG:HH22	5:6:273:VAL:HG11	1.83	0.43
4:5:155:ILE:HD13	4:5:227:LEU:HD13	2.01	0.43
5:6:198:SER:HB2	5:6:200:PHE:CD2	2.53	0.43
5:6:398:PRO:CB	5:6:508:GLY:HA2	2.48	0.43
6:7:14:LYS:NZ	6:7:83:GLU:OE1	2.44	0.43
4:A:447:PHE:O	4:A:450:MET:HG2	2.17	0.43
4:A:485:LEU:HD23	4:A:485:LEU:HA	1.88	0.43
4:A:731:TYR:CD2	4:A:732:ARG:HG2	2.52	0.43
2:2:562:ARG:NH1	4:5:691:GLU:O	2.52	0.43
3:3:494:ASP:HB3	4:5:590:ARG:HH21	1.83	0.43
1:4:207:PHE:N	1:4:258:ILE:HG23	2.33	0.43
1:4:355:GLN:HE21	1:4:356:GLU:N	2.17	0.43
6:7:131:MET:HE3	6:7:131:MET:HB3	1.91	0.43
2:8:736:ASN:ND2	2:8:739:ASP:OD2	2.50	0.43
1:0:733:GLN:O	1:0:737:LEU:N	2.44	0.43
2:2:769:SER:HB3	2:2:773:MET:HE3	2.00	0.43
1:4:577:ASP:OD1	1:4:577:ASP:N	2.50	0.43
3:9:221:LEU:HD13	3:9:225:LEU:O	2.19	0.43
4:A:372:ARG:HB3	4:A:618:ARG:HE	1.84	0.43
1:0:159:VAL:C	1:0:161:ALA:H	2.27	0.43
1:0:234:ILE:N	1:0:235:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:590:ARG:NH1	4:5:610:VAL:HG22	2.33	0.43
6:7:58:ASP:OD1	6:7:58:ASP:N	2.49	0.43
3:9:268:MET:O	3:9:268:MET:SD	2.77	0.43
1:0:254:LEU:HD23	1:0:254:LEU:H	1.84	0.43
1:0:291:ARG:HB3	1:0:559:GLN:HE22	1.83	0.43
1:0:589:GLU:HG3	1:0:593:GLN:HG3	1.99	0.43
2:2:763:THR:OG1	2:2:766:HIS:ND1	2.50	0.43
4:5:232:LEU:HD23	4:5:232:LEU:HA	1.83	0.43
4:5:261:ASN:HD22	4:5:261:ASN:HA	1.68	0.43
5:6:416:ALA:HA	5:6:456:VAL:O	2.18	0.43
6:7:451:ALA:O	6:7:455:ARG:HG3	2.19	0.43
1:4:216:LYS:NZ	1:4:266:LEU:HD13	2.34	0.43
6:7:39:ARG:NH1	6:7:45:GLN:HB2	2.33	0.43
2:8:398:LEU:HD22	2:8:402:LEU:HB2	1.99	0.43
3:9:379:THR:C	3:9:381:ALA:H	2.27	0.43
3:9:453:ASN:HD21	3:9:458:ARG:HH22	1.65	0.43
4:A:149:VAL:HG11	4:A:269:TYR:HB2	2.00	0.43
1:4:394:TYR:OH	1:4:414:THR:OG1	2.22	0.42
4:5:111:THR:O	4:5:113:PRO:HD2	2.19	0.42
5:6:153:SER:HB3	5:6:199:ARG:HG3	2.01	0.42
3:9:223:ASP:OD1	3:9:223:ASP:N	2.50	0.42
4:A:113:PRO:O	4:A:113:PRO:HG2	2.19	0.42
4:A:261:ASN:HD22	4:A:261:ASN:HA	1.68	0.42
3:3:145:VAL:O	3:3:186:THR:OG1	2.28	0.42
5:6:201:VAL:HG23	5:6:202:ASP:N	2.34	0.42
6:7:133:ARG:HD2	6:7:228:ARG:HH12	1.83	0.42
2:8:389:ARG:NH1	2:8:390:LEU:O	2.52	0.42
5:B:75:LEU:O	5:B:79:ILE:HG12	2.19	0.42
5:B:388:GLY:HA2	5:B:626:ARG:NH1	2.33	0.42
6:C:131:MET:HE3	6:C:131:MET:HB3	1.94	0.42
2:2:530:SER:OG	2:2:531:GLN:NE2	2.39	0.42
3:3:135:SER:OG	3:3:136:LEU:N	2.52	0.42
3:3:650:GLN:O	3:3:650:GLN:NE2	2.47	0.42
1:4:474:GLU:OE1	1:4:474:GLU:N	2.38	0.42
1:4:743:ALA:O	1:4:747:VAL:HG23	2.19	0.42
2:8:581:ARG:H	2:8:623:ARG:HB2	1.83	0.42
3:9:628:HIS:CD2	3:9:645:ALA:HB2	2.54	0.42
3:3:134:CYS:HB3	3:3:231:PRO:HG3	2.00	0.42
1:4:579:MET:HE3	1:4:583:THR:HG21	2.00	0.42
6:C:461:VAL:HG12	6:C:462:MET:HE2	2.01	0.42
6:C:609:ILE:HA	6:C:612:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:359:GLU:O	1:0:360:ASP:OD1	2.38	0.42
2:2:485:ILE:C	2:2:487:GLY:H	2.28	0.42
2:2:593:ASN:OD1	2:2:594:ASP:N	2.53	0.42
1:4:747:VAL:HG12	1:4:748:ARG:HG3	2.02	0.42
4:5:29:SER:OG	6:C:210:GLU:OE2	2.36	0.42
5:6:229:ARG:HG3	5:6:231:GLU:H	1.85	0.42
4:A:42:TYR:CE2	4:A:44:VAL:HB	2.54	0.42
4:A:225:GLN:OE1	4:A:254:CYS:HA	2.18	0.42
5:B:434:VAL:HA	5:B:440:HIS:CB	2.49	0.42
3:3:114:ARG:HH22	3:3:212:GLN:HG2	1.83	0.42
1:4:466:LEU:HD23	1:4:466:LEU:HA	1.90	0.42
4:5:67:GLU:HB3	4:5:69:TRP:CD1	2.55	0.42
4:5:354:ALA:O	4:5:358:PHE:HD1	2.03	0.42
5:6:333:GLU:HA	5:6:336:LYS:NZ	2.34	0.42
4:A:145:MET:O	4:A:147:HIS:ND1	2.52	0.42
6:C:164:ARG:HB3	6:C:240:HIS:HE1	1.85	0.42
1:0:238:ASP:O	1:0:242:ASN:ND2	2.47	0.42
2:8:411:GLU:O	2:8:445:ALA:HB3	2.20	0.42
2:8:485:ILE:C	2:8:487:GLY:H	2.28	0.42
2:8:584:CYS:H	2:8:624:CYS:HB2	1.85	0.42
3:9:342:LEU:HD12	3:9:450:ALA:O	2.19	0.42
3:9:412:ASP:OD1	3:9:412:ASP:N	2.51	0.42
5:B:146:PRO:HG2	5:B:148:HIS:NE2	2.34	0.42
6:C:97:ASP:O	6:C:101:VAL:HG23	2.18	0.42
6:C:274:THR:O	6:C:301:HIS:N	2.51	0.42
3:3:143:ARG:HD2	3:3:158:ARG:HE	1.84	0.42
3:3:341:ILE:HG12	3:3:481:LEU:HD12	2.02	0.42
1:4:276:PRO:HG2	6:7:231:LYS:HG2	2.02	0.42
4:5:249:CYS:HB3	4:5:253:LEU:HB2	2.01	0.42
5:6:141:VAL:HG23	5:6:240:ASP:O	2.20	0.42
5:6:182:ASN:HB2	5:6:183:PRO:HD3	2.02	0.42
6:7:308:LYS:HE3	6:7:400:ARG:HH21	1.84	0.42
3:9:346:ASP:HB2	3:9:349:VAL:HG21	2.02	0.42
3:9:465:PRO:O	3:9:469:ILE:HG12	2.20	0.42
6:C:130:LEU:HD13	6:C:179:VAL:HG11	2.01	0.42
3:3:444:ALA:O	3:3:446:CYS:N	2.53	0.42
4:5:35:PHE:CD1	4:5:99:LEU:HD13	2.55	0.42
5:B:224:LEU:HD22	5:B:296:LEU:HD23	2.02	0.42
5:B:620:GLN:HA	5:B:623:SER:HB3	2.01	0.42
1:0:474:GLU:OE1	1:0:474:GLU:N	2.40	0.42
2:2:288:LEU:O	2:2:289:PRO:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:305:LEU:HA	2:2:417:ILE:HG12	2.01	0.42
3:3:8:ASP:HB3	6:C:3:LEU:HD11	2.01	0.42
3:3:112:SER:O	3:3:116:LEU:N	2.49	0.42
3:3:139:PRO:HD2	6:7:294:SER:O	2.20	0.42
5:6:217:ARG:HA	5:6:217:ARG:NH1	2.35	0.42
5:6:435:ARG:HA	5:6:435:ARG:HD2	1.90	0.42
2:8:512:LYS:HA	2:8:514:ARG:HH11	1.85	0.42
3:9:136:LEU:HD13	3:9:138:ARG:NE	2.32	0.42
3:9:311:ASP:OD1	3:9:312:TYR:N	2.53	0.42
3:9:347:PRO:O	3:9:349:VAL:HG23	2.20	0.42
3:9:486:LEU:HD23	3:9:486:LEU:H	1.84	0.42
6:C:184:CYS:SG	6:C:185:ASP:N	2.93	0.42
1:0:267:LYS:NZ	1:0:268:THR:O	2.53	0.41
1:0:478:LYS:O	1:0:482:LEU:HG	2.19	0.41
2:2:199:PHE:CE2	2:2:258:ILE:HG21	2.55	0.41
3:3:23:LEU:HB3	3:3:83:PHE:CD2	2.55	0.41
3:3:268:MET:HE3	3:3:269:SER:N	2.35	0.41
1:4:223:TYR:O	1:4:226:LEU:HG	2.20	0.41
6:7:379:LEU:HB3	6:7:387:LYS:NZ	2.34	0.41
3:9:379:THR:H	3:9:433:ILE:HD13	1.85	0.41
4:A:731:TYR:O	4:A:732:ARG:NE	2.52	0.41
5:B:125:GLU:O	5:B:127:THR:HG23	2.20	0.41
1:0:452:LEU:HB3	1:0:458:ILE:HG21	2.02	0.41
2:2:731:VAL:HG11	2:2:782:LEU:HD11	2.00	0.41
1:4:254:LEU:HD23	1:4:254:LEU:H	1.85	0.41
4:5:579:ALA:O	4:5:583:LYS:N	2.49	0.41
6:7:169:ARG:O	6:7:235:MET:HA	2.20	0.41
2:8:288:LEU:O	2:8:289:PRO:C	2.63	0.41
3:9:195:ASP:OD1	3:9:223:ASP:HA	2.20	0.41
5:B:279:GLU:OE1	5:B:279:GLU:N	2.50	0.41
6:C:30:GLN:O	6:C:35:ASN:ND2	2.52	0.41
6:C:534:ALA:O	6:C:537:ILE:HG22	2.20	0.41
1:0:368:HIS:NE2	6:C:172:GLU:OE1	2.53	0.41
1:0:590:VAL:HG22	1:0:596:LEU:HA	2.01	0.41
1:4:267:LYS:NZ	1:4:268:THR:O	2.53	0.41
5:6:147:VAL:HG13	5:6:203:PHE:O	2.20	0.41
5:6:334:TRP:HB2	5:6:575:TYR:CZ	2.55	0.41
6:7:501:LEU:HD12	6:7:504:ASN:HD21	1.85	0.41
4:A:711:VAL:O	4:A:715:MET:HG2	2.20	0.41
5:B:123:ILE:HA	5:B:126:LEU:HD12	2.02	0.41
3:3:9:ASP:HB3	3:3:12:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:207:PHE:O	1:4:209:ASN:ND2	2.53	0.41
1:4:291:ARG:HH21	1:4:353:LYS:HD2	1.84	0.41
2:8:546:THR:OG1	2:8:547:THR:N	2.54	0.41
5:B:98:VAL:HG11	5:B:103:GLU:HB2	2.01	0.41
1:0:373:PHE:O	1:0:373:PHE:CG	2.73	0.41
3:3:460:ASP:HA	3:3:468:ASN:ND2	2.35	0.41
5:6:402:LYS:HB2	5:6:404:GLN:HG2	2.02	0.41
5:6:411:GLU:O	5:6:413:SER:N	2.52	0.41
5:6:520:ILE:HG12	5:6:522:LEU:HG	2.01	0.41
6:7:461:VAL:HG12	6:7:462:MET:HE2	2.01	0.41
2:8:533:LEU:HB3	2:8:585:LEU:HD11	2.03	0.41
6:C:322:GLU:OE1	6:C:322:GLU:N	2.43	0.41
2:2:582:GLY:O	2:2:624:CYS:HA	2.21	0.41
3:3:366:ILE:HD12	3:3:367:PRO:HD2	2.02	0.41
1:4:460:GLU:OE1	1:4:460:GLU:N	2.44	0.41
4:5:162:ARG:HD3	4:5:426:ASN:ND2	2.36	0.41
4:A:140:LEU:HD23	4:A:140:LEU:HA	1.84	0.41
4:A:365:LEU:HD23	4:A:365:LEU:HA	1.87	0.41
2:2:277:ILE:C	2:2:279:ASN:H	2.29	0.41
6:7:23:ASP:HA	6:7:27:GLY:HA2	2.02	0.41
6:7:106:ARG:NE	6:7:192:TYR:OH	2.53	0.41
4:A:114:ARG:HA	4:A:115:PRO:HD3	1.84	0.41
6:C:56:ALA:HB2	6:C:63:VAL:HG21	2.03	0.41
2:2:518:ASN:HD22	2:2:658:ASP:H	1.69	0.41
2:2:735:LEU:H	2:2:735:LEU:HD23	1.85	0.41
3:3:115:THR:O	3:3:117:THR:N	2.54	0.41
3:3:471:LEU:HA	3:3:471:LEU:HD23	1.70	0.41
4:5:727:ARG:HG3	4:5:728:LYS:HE3	2.02	0.41
5:6:787:LEU:H	5:6:787:LEU:HD23	1.86	0.41
6:7:45:GLN:NE2	6:7:47:ALA:O	2.47	0.41
6:7:70:ALA:HB3	6:7:276:ILE:HG23	2.01	0.41
6:7:366:PRO:O	6:7:367:ARG:NH1	2.54	0.41
6:7:382:ASP:OD2	6:7:489:ASN:ND2	2.54	0.41
6:7:546:GLN:O	6:7:548:PRO:HD3	2.21	0.41
2:8:882:ASP:N	2:8:882:ASP:OD1	2.52	0.41
4:A:28:LYS:NZ	4:A:94:GLU:OE2	2.47	0.41
4:A:446:GLU:HB3	4:A:449:LYS:HB2	2.02	0.41
4:A:569:LYS:CD	4:A:570:CYS:H	2.25	0.41
1:0:335:HIS:O	1:0:339:LEU:HB2	2.21	0.41
3:3:486:LEU:HD23	3:3:486:LEU:H	1.85	0.41
3:3:583:THR:O	3:3:587:ALA:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:70:ILE:HD11	4:5:103:ALA:HB1	2.03	0.41
4:5:215:MET:HB3	4:5:217:ASP:OD1	2.21	0.41
5:6:31:LEU:HD23	5:6:34:LEU:HD12	2.03	0.41
6:7:349:ASP:OD1	6:7:349:ASP:N	2.54	0.41
6:7:535:GLN:O	6:7:538:THR:OG1	2.39	0.41
2:8:512:LYS:HA	2:8:514:ARG:NH1	2.36	0.41
2:8:768:GLU:O	2:8:771:ILE:HG22	2.20	0.41
3:9:453:ASN:HD21	3:9:458:ARG:NH2	2.19	0.41
4:A:226:THR:O	4:A:227:LEU:HD23	2.21	0.41
4:A:504:ILE:HG21	4:A:507:MET:O	2.21	0.41
5:B:435:ARG:HD2	5:B:435:ARG:HA	1.90	0.41
5:B:641:GLN:HB2	5:B:643:LYS:HG2	2.02	0.41
6:C:35:ASN:O	6:C:39:ARG:HG3	2.21	0.41
1:0:169:PHE:CE1	1:0:173:PHE:HB2	2.56	0.41
1:0:222:LEU:HD23	1:0:222:LEU:HA	1.89	0.41
1:0:535:GLY:C	1:0:537:GLY:H	2.29	0.41
1:0:575:GLU:HB3	1:0:578:LYS:HG3	2.03	0.41
3:3:494:ASP:HB3	4:5:590:ARG:NH2	2.36	0.41
1:4:662:LEU:HD23	6:7:606:LEU:HD23	2.03	0.41
5:6:408:HIS:HA	5:6:411:GLU:HG3	2.02	0.41
2:8:304:GLN:N	2:8:417:ILE:HG23	2.36	0.41
2:8:412:ILE:HG22	2:8:444:VAL:HG13	2.03	0.41
2:8:576:LEU:HD23	2:8:624:CYS:SG	2.61	0.41
3:9:321:LEU:HD23	3:9:321:LEU:HA	1.88	0.41
4:A:447:PHE:HB3	4:A:488:ALA:HB2	2.02	0.41
6:C:349:ASP:OD1	6:C:349:ASP:N	2.54	0.41
1:0:338:ALA:HA	5:B:85:ARG:HH21	1.85	0.40
3:3:268:MET:CE	3:3:268:MET:O	2.69	0.40
4:5:154:ILE:HD11	4:5:260:GLY:HA2	2.04	0.40
5:6:555:LEU:O	5:6:558:ARG:HG2	2.21	0.40
6:7:166:ILE:HD11	6:7:240:HIS:CD2	2.57	0.40
6:7:240:HIS:O	6:7:244:VAL:HG23	2.20	0.40
3:9:128:GLU:HG2	3:9:236:GLN:HG2	2.03	0.40
4:A:2:SER:OG	4:A:3:GLY:N	2.54	0.40
5:B:594:ILE:HG23	5:B:649:PHE:HE1	1.86	0.40
5:B:615:ARG:O	5:B:616:ILE:C	2.64	0.40
6:C:546:GLN:O	6:C:548:PRO:HD3	2.20	0.40
1:0:226:LEU:HD12	1:0:227:ILE:HG23	2.03	0.40
4:5:352:ALA:O	4:5:355:CYS:HB2	2.21	0.40
2:8:288:LEU:HA	2:8:289:PRO:HD2	1.94	0.40
3:9:411:PHE:HD2	3:9:450:ALA:HB1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:440:HIS:CE1	5:B:442:PHE:HB2	2.57	0.40
2:2:882:ASP:OD1	2:2:882:ASP:N	2.53	0.40
4:5:88:LEU:HD23	4:5:88:LEU:HA	1.90	0.40
4:5:346:GLY:O	4:5:350:LYS:HG3	2.22	0.40
4:5:372:ARG:HG3	4:5:465:GLN:NE2	2.37	0.40
4:5:633:THR:HG23	4:5:635:ALA:H	1.86	0.40
5:6:228:LEU:HB3	5:6:232:ALA:HB2	2.03	0.40
5:6:431:ALA:CB	5:6:444:ILE:HA	2.43	0.40
5:B:69:GLU:HA	5:B:73:GLN:HA	2.02	0.40
1:0:158:ASN:HB3	1:0:161:ALA:HA	2.04	0.40
1:0:291:ARG:NH2	1:0:353:LYS:HD2	2.36	0.40
2:2:465:THR:O	2:2:468:SER:OG	2.28	0.40
2:2:807:LYS:HG2	2:2:809:SER:H	1.86	0.40
3:3:135:SER:HB2	3:3:392:ARG:HG2	2.02	0.40
1:4:230:PRO:HD2	6:7:225:ARG:HH22	1.87	0.40
1:4:297:PRO:HB2	1:4:346:PHE:HB3	2.03	0.40
1:4:339:LEU:HB3	1:4:340:ILE:HD12	2.03	0.40
5:6:764:GLU:O	5:6:767:ILE:HG22	2.22	0.40
6:7:374:ASN:O	6:7:375:ILE:HD13	2.22	0.40
2:8:533:LEU:H	2:8:533:LEU:HG	1.73	0.40
5:B:97:PHE:O	5:B:99:LYS:NZ	2.50	0.40
5:B:242:CYS:HB3	5:B:244:PHE:HE1	1.86	0.40
1:4:585:SER:HB2	5:6:423:ALA:O	2.22	0.40
5:6:80:GLN:HA	5:6:83:PHE:CE2	2.57	0.40
2:8:308:THR:O	2:8:414:LEU:N	2.49	0.40
5:B:36:GLU:CD	5:B:45:LYS:HD3	2.46	0.40
5:B:752:TYR:O	5:B:756:ILE:HG12	2.22	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	0	515/863 (60%)	477 (93%)	38 (7%)	0	100	100
1	4	515/863 (60%)	477 (93%)	38 (7%)	0	100	100
2	2	546/904 (60%)	506 (93%)	37 (7%)	3 (0%)	25	63
2	8	546/904 (60%)	512 (94%)	31 (6%)	3 (0%)	25	63
3	3	543/808 (67%)	506 (93%)	35 (6%)	2 (0%)	30	67
3	9	543/808 (67%)	504 (93%)	37 (7%)	2 (0%)	30	67
4	5	567/734 (77%)	526 (93%)	38 (7%)	3 (0%)	25	63
4	A	567/734 (77%)	536 (94%)	29 (5%)	2 (0%)	30	67
5	6	653/821 (80%)	602 (92%)	49 (8%)	2 (0%)	37	72
5	B	653/821 (80%)	605 (93%)	46 (7%)	2 (0%)	37	72
6	7	615/719 (86%)	585 (95%)	30 (5%)	0	100	100
6	C	615/719 (86%)	591 (96%)	23 (4%)	1 (0%)	44	78
All	All	6878/9698 (71%)	6427 (93%)	431 (6%)	20 (0%)	38	72

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	289	PRO
3	3	269	SER
3	3	455	VAL
4	5	112	ARG
4	5	116	SER
5	6	616	ILE
2	8	289	PRO
3	9	455	VAL
4	A	112	ARG
5	B	616	ILE
4	5	118	GLU
2	2	290	LEU
5	6	169	GLU
2	8	290	LEU
3	9	270	LYS
4	A	570	CYS
2	2	291	VAL
2	8	291	VAL
5	B	169	GLU
6	C	385	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	470/753 (62%)	470 (100%)	0	100	100
1	4	470/753 (62%)	470 (100%)	0	100	100
2	2	488/781 (62%)	488 (100%)	0	100	100
2	8	488/781 (62%)	488 (100%)	0	100	100
3	3	482/707 (68%)	476 (99%)	6 (1%)	67	79
3	9	482/707 (68%)	477 (99%)	5 (1%)	73	82
4	5	501/625 (80%)	498 (99%)	3 (1%)	84	88
4	A	501/625 (80%)	499 (100%)	2 (0%)	89	91
5	6	595/724 (82%)	595 (100%)	0	100	100
5	B	595/724 (82%)	595 (100%)	0	100	100
6	7	542/619 (88%)	542 (100%)	0	100	100
6	C	542/619 (88%)	542 (100%)	0	100	100
All	All	6156/8418 (73%)	6140 (100%)	16 (0%)	90	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	133	LYS
3	3	136	LEU
3	3	200	THR
3	3	201	ILE
3	3	268	MET
3	3	271	ASP
4	5	111	THR
4	5	112	ARG
4	5	271	ILE
3	9	136	LEU
3	9	201	ILE
3	9	265	VAL
3	9	266	LYS
3	9	267	GLN

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Mol	Chain	Res	Type
4	A	111	THR
4	A	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	231	GLN
1	0	264	ASN
1	0	332	HIS
1	0	335	HIS
1	0	342	ASN
1	0	355	GLN
1	0	375	HIS
1	0	415	HIS
1	0	483	GLN
1	0	555	GLN
1	0	559	GLN
2	2	518	ASN
2	2	621	GLN
3	3	52	ASN
3	3	439	HIS
3	3	500	HIS
3	3	600	GLN
3	3	650	GLN
1	4	195	GLN
1	4	209	ASN
1	4	225	GLN
1	4	231	GLN
1	4	264	ASN
1	4	273	ASN
1	4	305	GLN
1	4	335	HIS
1	4	355	GLN
1	4	559	GLN
1	4	568	ASN
1	4	593	GLN
4	5	122	GLN
4	5	125	GLN
4	5	261	ASN
4	5	300	GLN
4	5	459	HIS
4	5	489	ASN

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Mol	Chain	Res	Type
4	5	612	GLN
4	5	678	GLN
4	5	692	HIS
5	6	140	GLN
5	6	171	GLN
5	6	178	ASN
5	6	196	ASN
5	6	237	GLN
5	6	361	ASN
5	6	404	GLN
5	6	635	HIS
6	7	82	GLN
6	7	212	GLN
6	7	214	ASN
6	7	223	GLN
6	7	347	HIS
6	7	364	GLN
6	7	376	ASN
6	7	402	GLN
6	7	464	GLN
6	7	479	ASN
6	7	522	GLN
6	7	542	GLN
6	7	543	HIS
6	7	631	ASN
2	8	280	HIS
2	8	419	HIS
2	8	443	HIS
2	8	518	ASN
2	8	561	GLN
2	8	607	GLN
2	8	621	GLN
2	8	687	HIS
3	9	52	ASN
3	9	267	GLN
3	9	439	HIS
3	9	453	ASN
4	A	30	GLN
4	A	246	GLN
4	A	261	ASN
4	A	300	GLN
4	A	459	HIS

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Mol	Chain	Res	Type
4	A	489	ASN
4	A	692	HIS
4	A	701	GLN
5	B	187	ASN
5	B	196	ASN
5	B	345	ASN
5	B	349	ASN
5	B	509	HIS
5	B	635	HIS
6	C	139	GLN
6	C	209	GLN
6	C	212	GLN
6	C	347	HIS
6	C	541	HIS

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.

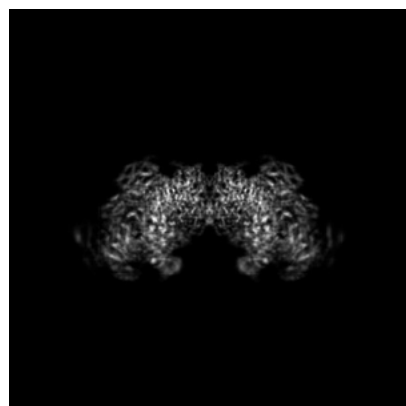
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45246. These allow visual inspection of the internal detail of the map and identification of artifacts.

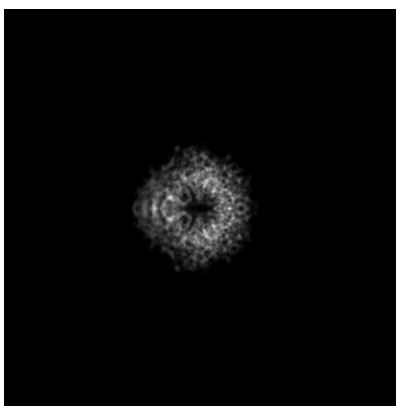
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

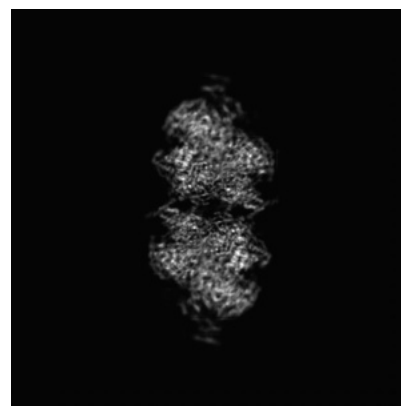
6.1.1 Primary map



X

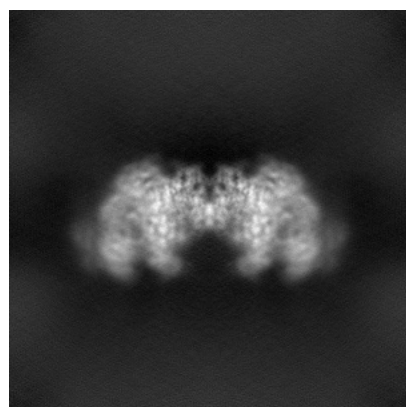


Y

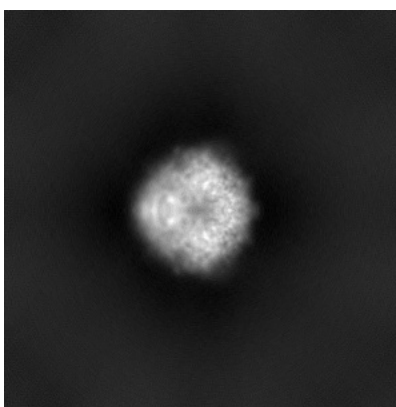


Z

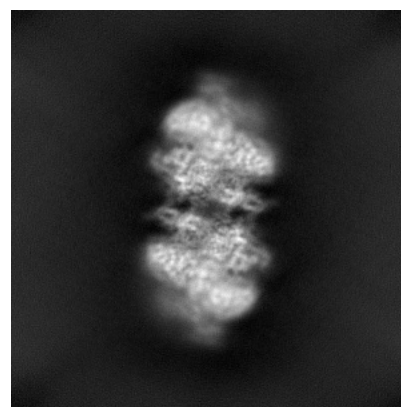
6.1.2 Raw map



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

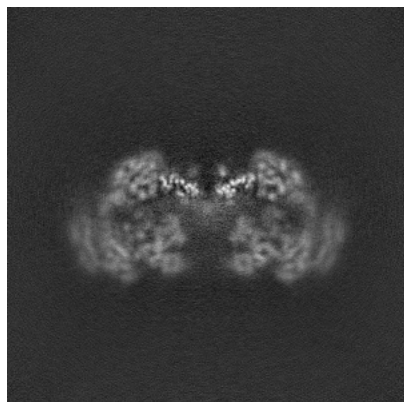


Y Index: 200

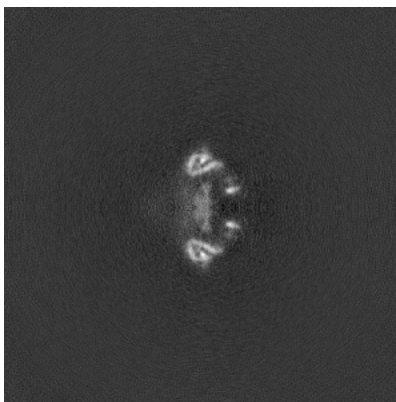


Z Index: 200

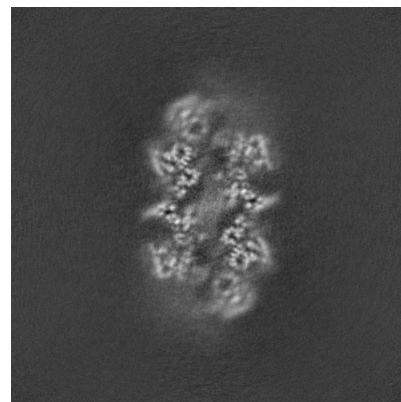
6.2.2 Raw map



X Index: 200



Y Index: 200

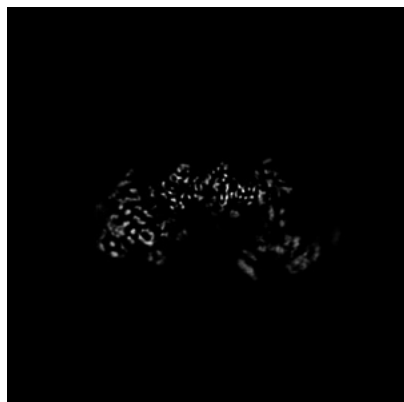


Z Index: 200

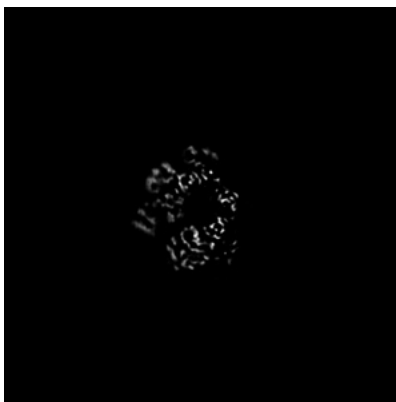
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

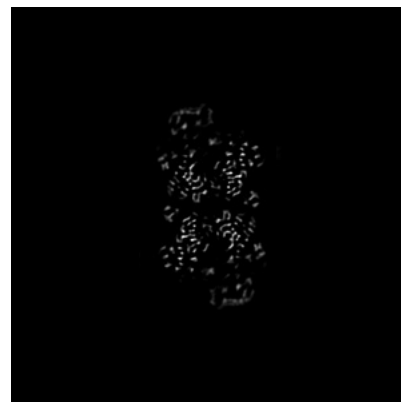
6.3.1 Primary map



X Index: 217

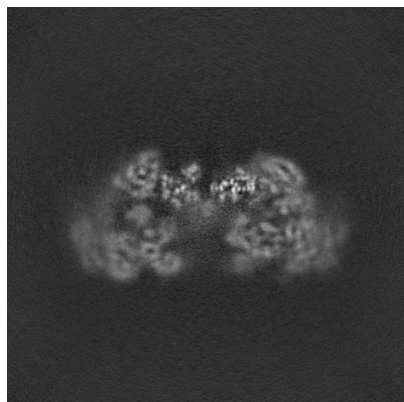


Y Index: 154

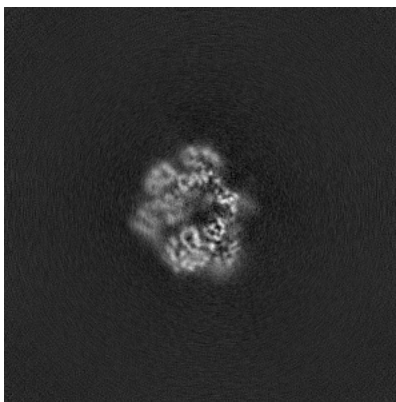


Z Index: 210

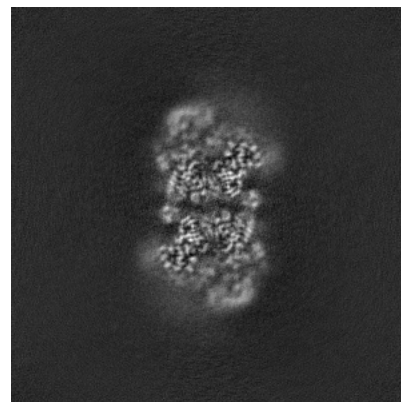
6.3.2 Raw map



X Index: 193



Y Index: 154

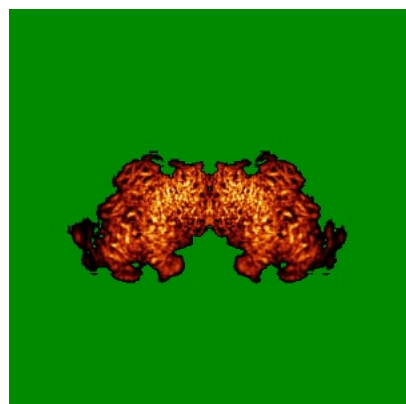


Z Index: 211

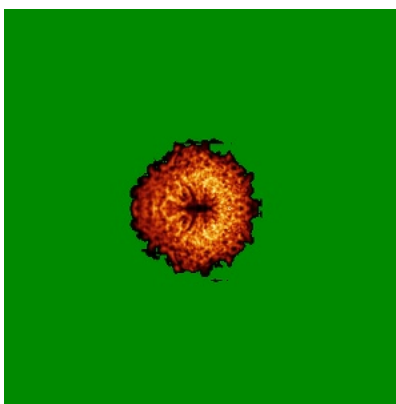
The images above show the largest variance slices of the map in three orthogonal directions.

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

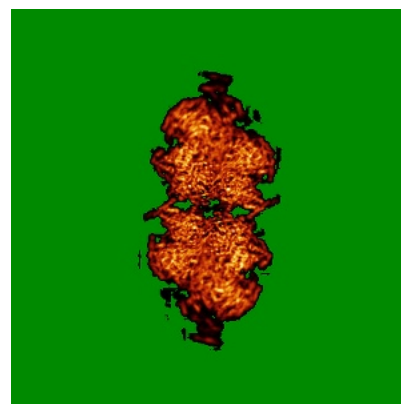
6.4.1 Primary map



X

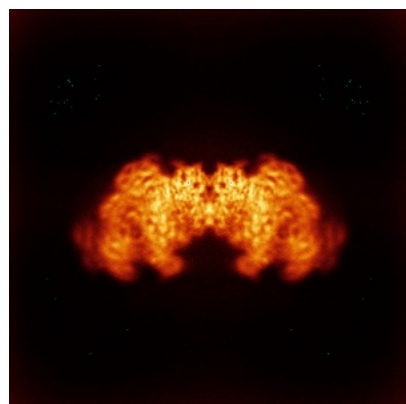


Y

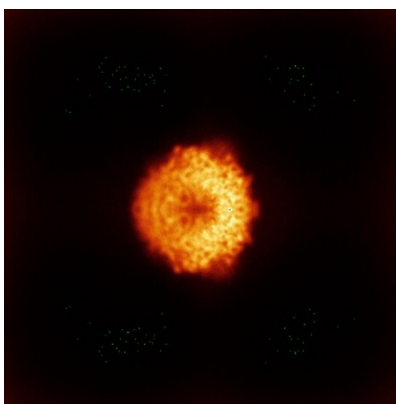


Z

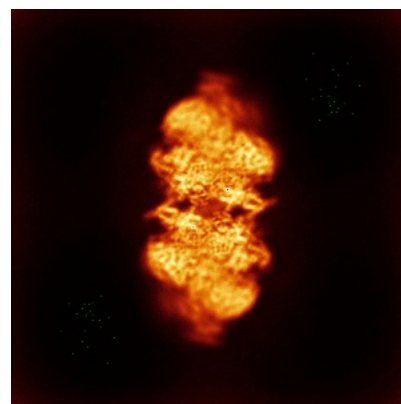
6.4.2 Raw map



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.

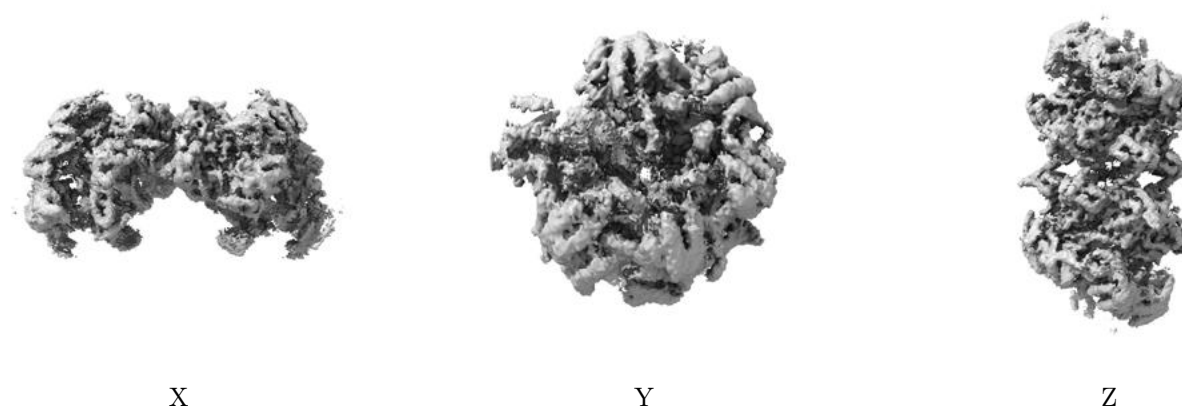
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

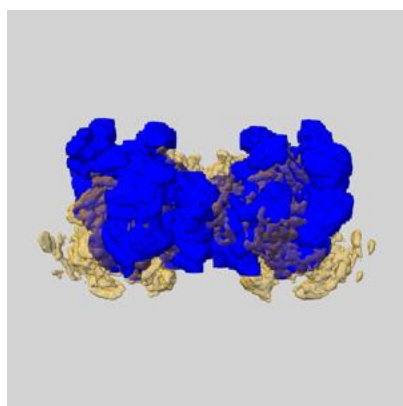
6.6 Mask visualisation [i](#)

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

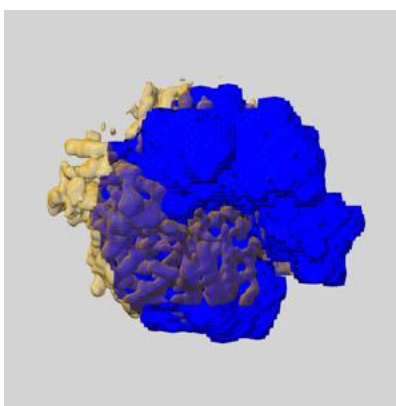
A mask typically either:

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

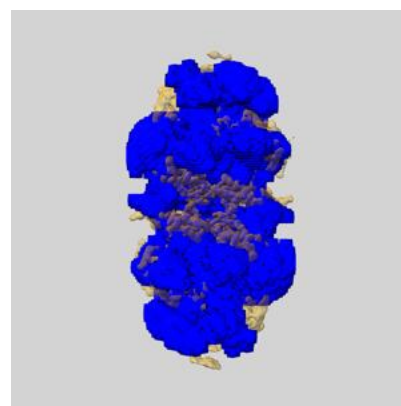
6.6.1 emd_45246_msk_1.map [i](#)



X



Y

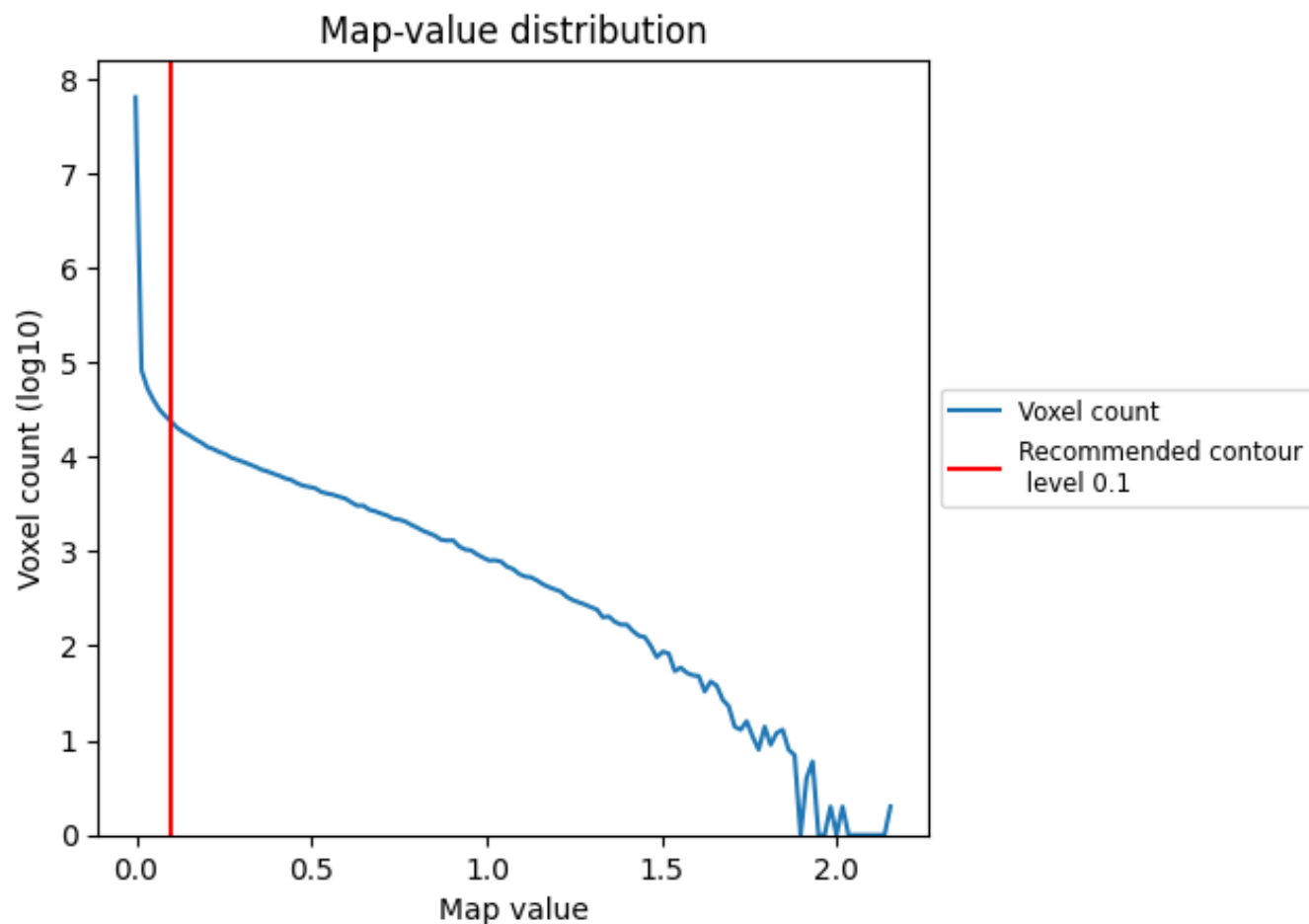


Z

7 Map analysis [i](#)

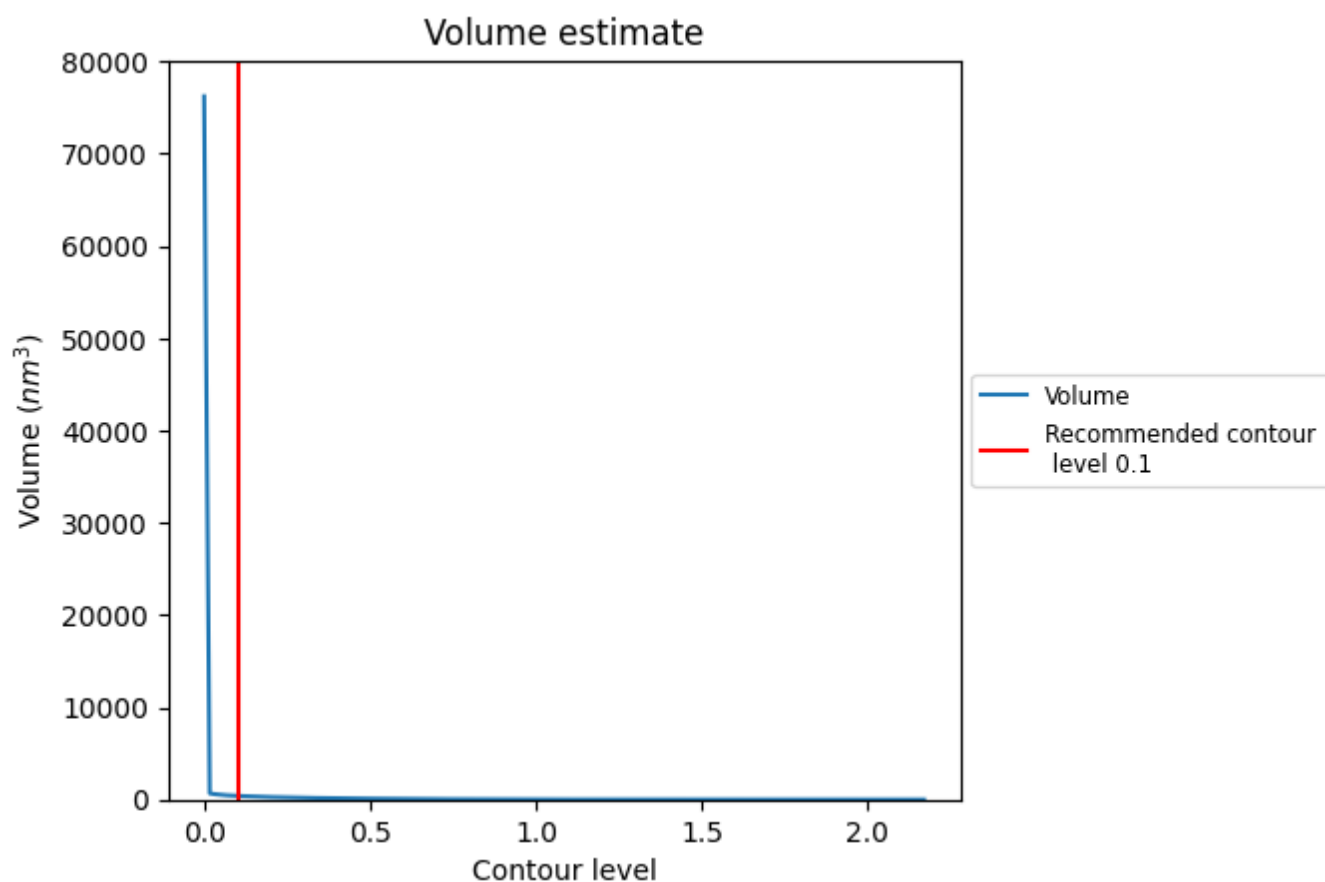
This section contains the results of statistical analysis of the map.

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.

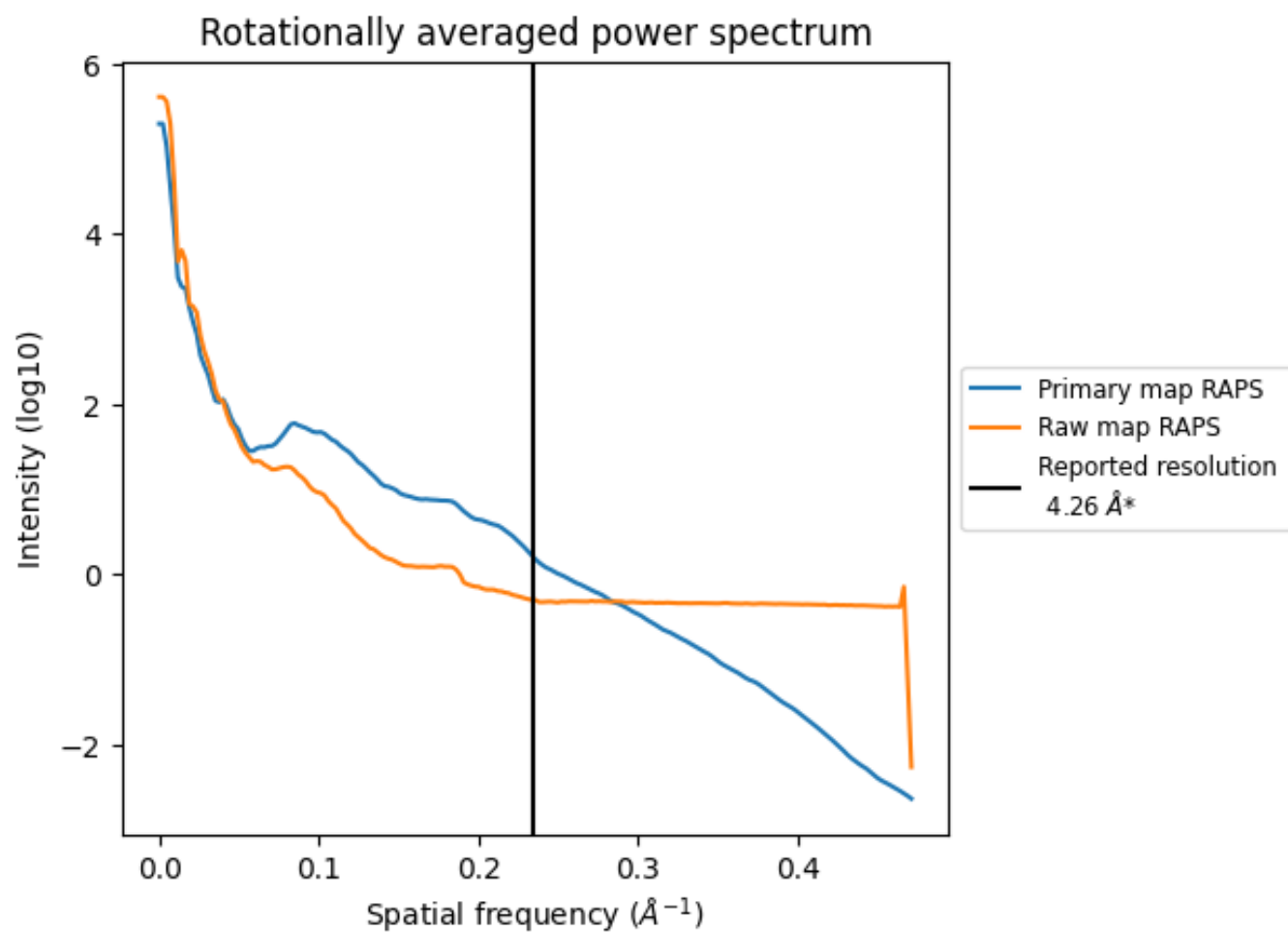
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 397 nm^3 ; this corresponds to an approximate mass of 358 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 ⓘ

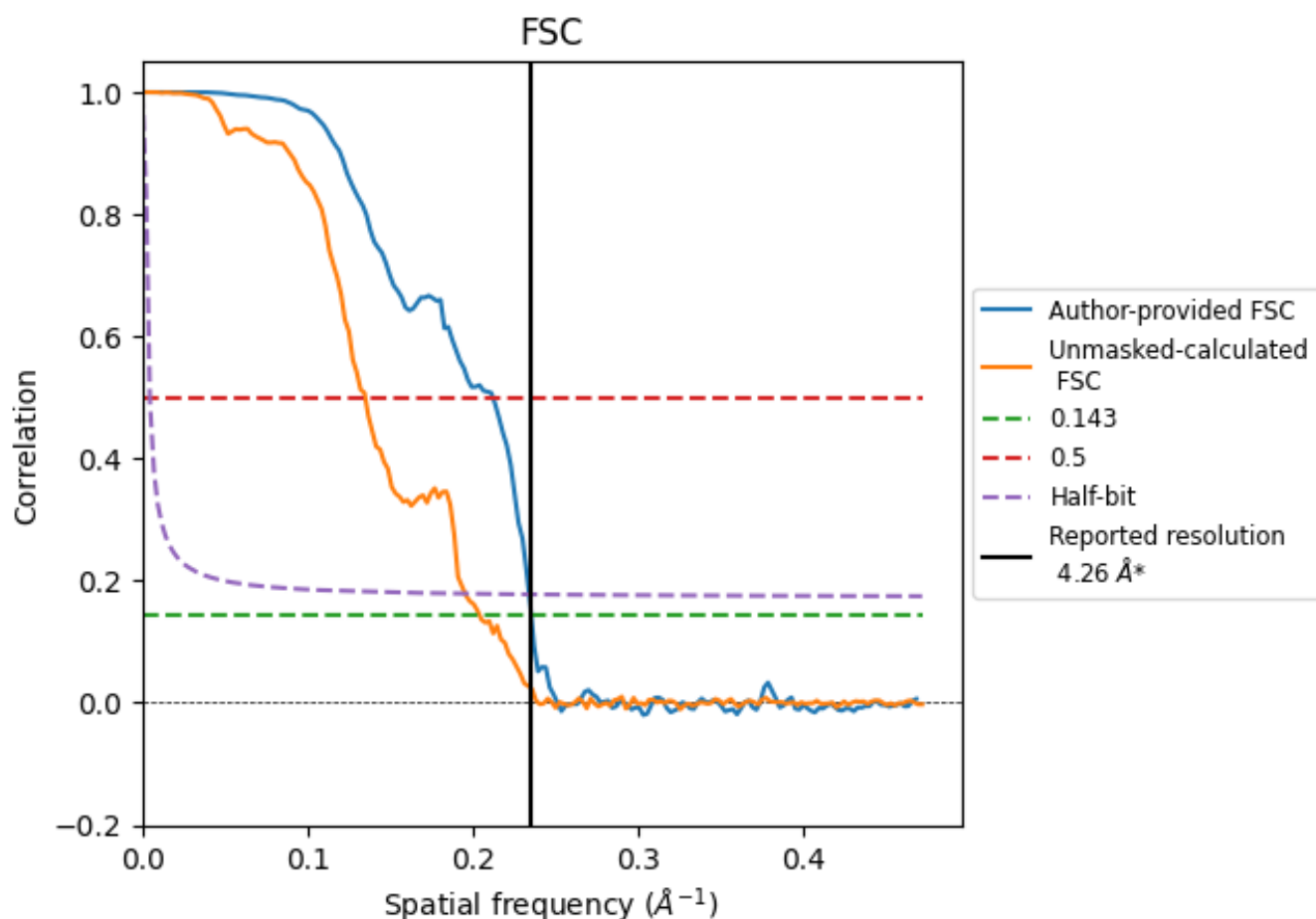


*Reported resolution corresponds to spatial frequency of 0.235 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.235 \AA^{-1}

8.2 Resolution estimates [i](#)

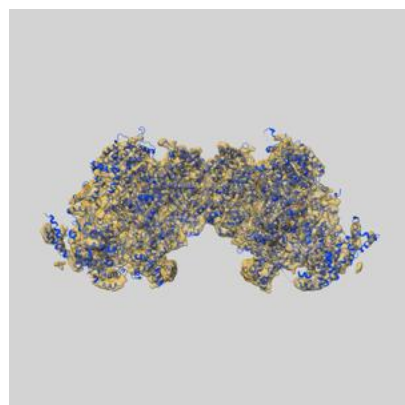
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.26	-	-
Author-provided FSC curve	4.25	4.71	4.27
Unmasked-calculated*	4.90	7.41	5.12

*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 4.90 differs from the reported value 4.26 by more than 10 %

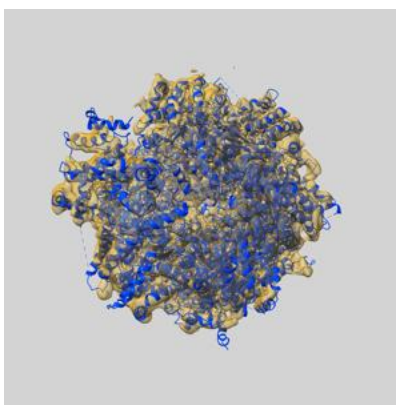
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45246 and PDB model 9C6G. Per-residue inclusion information can be found in section [3](#) on page [6](#).

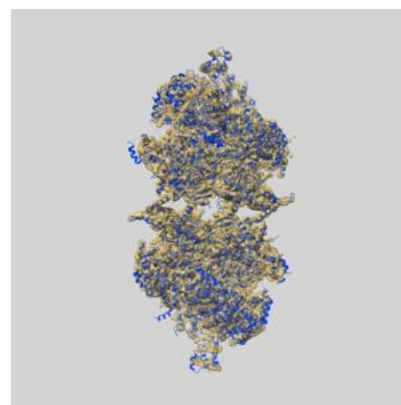
9.1 Map-model overlay [i](#)



X



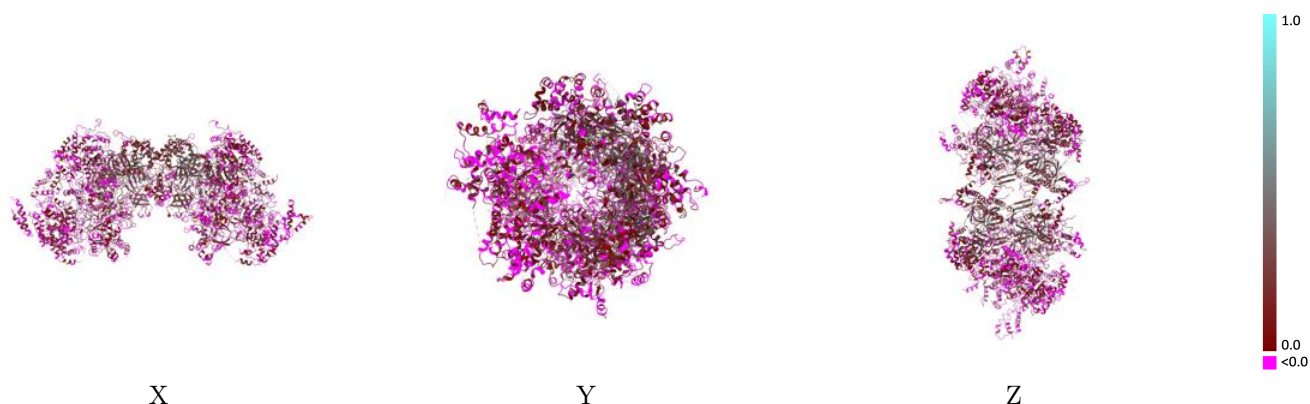
Y



Z

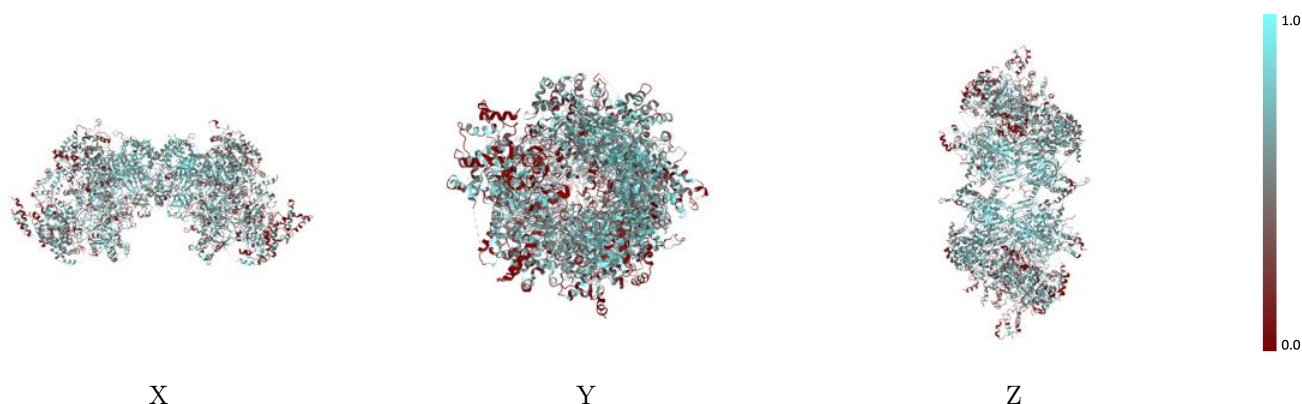
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



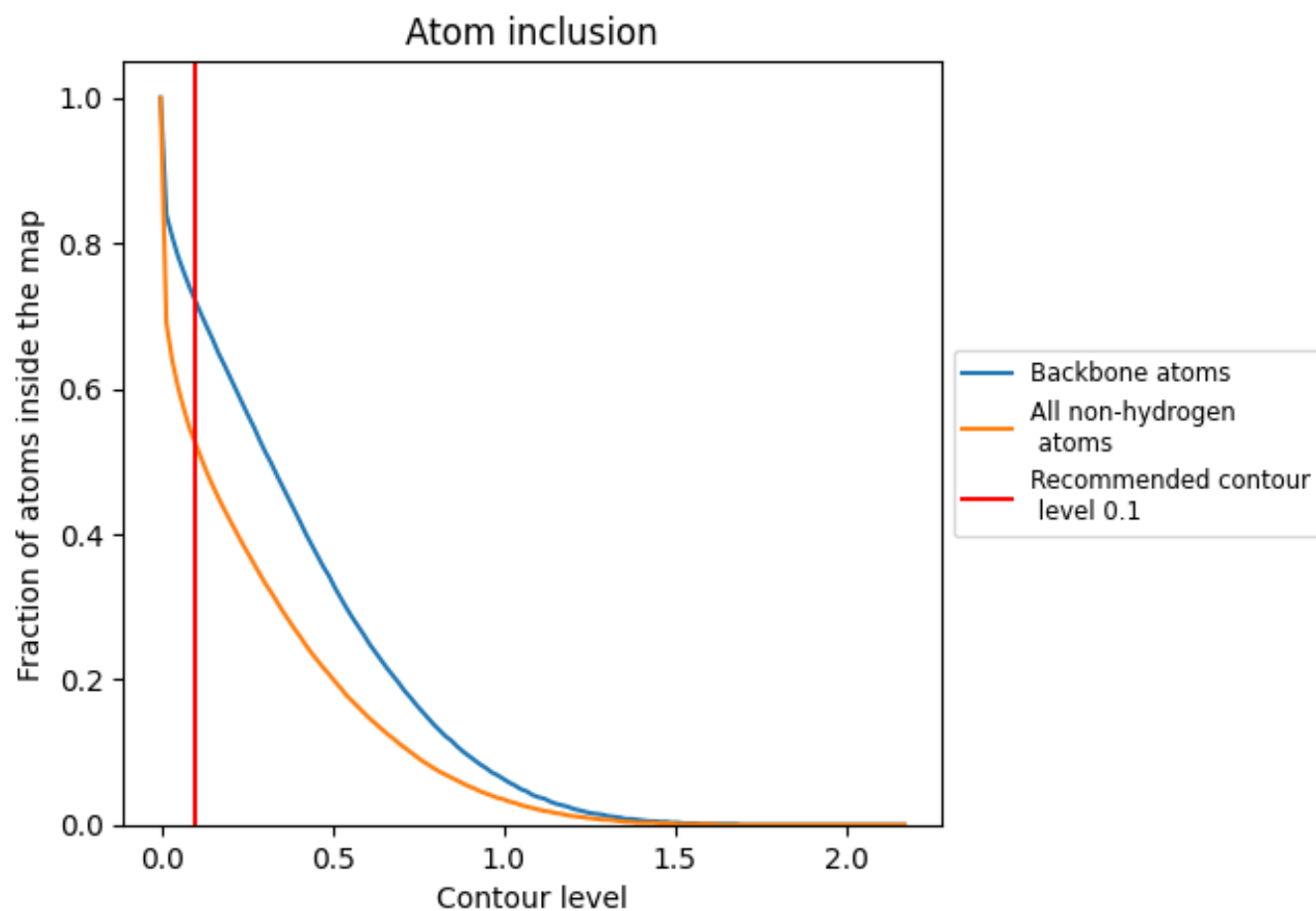
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 52% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5240	<div></div> 0.1120
0	<div></div> 0.4950	<div></div> 0.0960
2	<div></div> 0.4500	<div></div> 0.0400
3	<div></div> 0.6610	<div></div> 0.2190
4	<div></div> 0.4730	<div></div> 0.0870
5	<div></div> 0.5400	<div></div> 0.1260
6	<div></div> 0.4570	<div></div> 0.0520
7	<div></div> 0.5460	<div></div> 0.1520
8	<div></div> 0.4580	<div></div> 0.0440
9	<div></div> 0.6660	<div></div> 0.2180
A	<div></div> 0.5420	<div></div> 0.1220
B	<div></div> 0.4710	<div></div> 0.0530
C	<div></div> 0.5480	<div></div> 0.1490

1.0

0.0

<0.0