



## Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 12:22 PM EDT

PDB ID : 10DQ / pdb\_000010dq  
EMDB ID : EMD-75095  
Title : Cbf1-CCAN-CEN complex  
Authors : Mengqiu, J.; Sue, B.  
Deposited on : 2026-01-14  
Resolution : 3.90 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](mailto: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>.

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

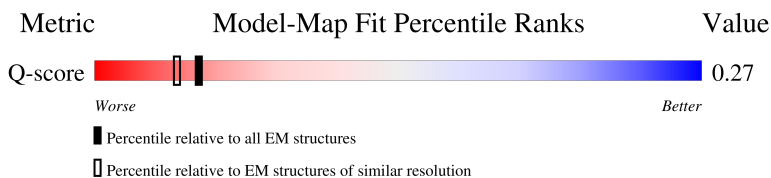
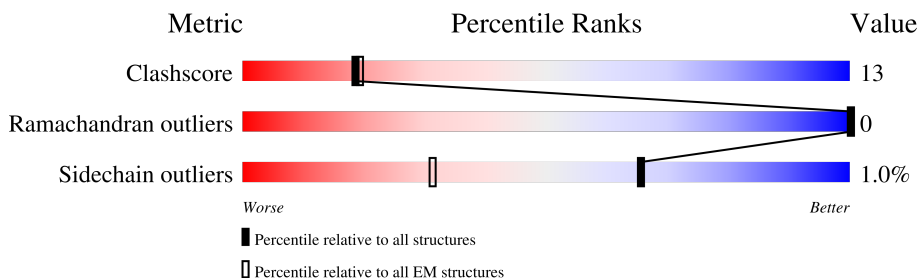
EMDB validation analysis : 0.0.1.dev133  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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.




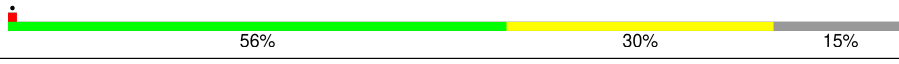

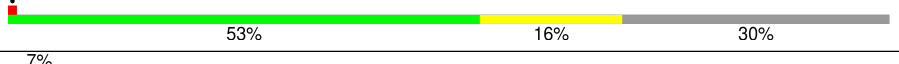
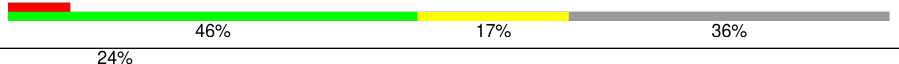

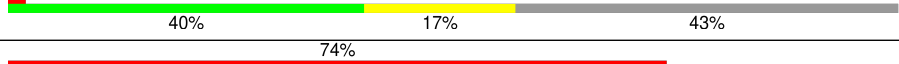
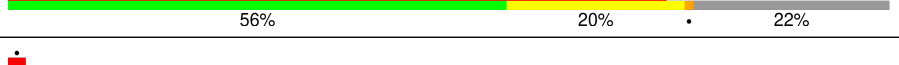

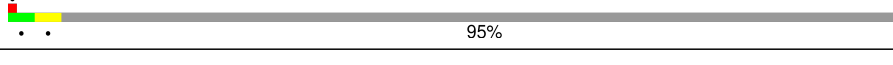
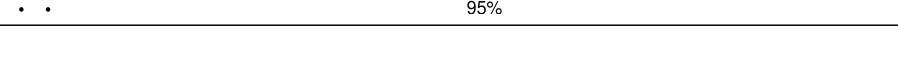
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 ( 3.40 - 4.40 )

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  $\geq 3$ , 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	351	 20% 9% 71%
1	B	351	 23% 7% 70%
2	D	508	 17% 95%
3	H	181	 17% 57% 36% 6%

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Mol	Chain	Length	Quality of chain
4	I	733	
5	K	239	
6	L	245	
7	N	458	
8	O	368	
9	P	369	
10	Q	406	
11	T	361	
12	U	324	
13	W	89	
14	Y	238	
15	Z	153	
16	E	508	

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 28461 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 Centromere-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	101	Total	C	N	O	S	0	0
			822	507	152	161	2		
1	B	107	Total	C	N	O	S	0	0
			876	542	161	171	2		

- Molecule 2 is a DNA chain called DNA (508-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	D	27	Total	C	N	O	P	0	0
			552	266	100	159	27		

- Molecule 3 is a protein called Inner kinetochore subunit MCM16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	171	Total	C	N	O	S	0	0
			1412	890	247	273	2		

- Molecule 4 is a protein called Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	679	Total	C	N	O	S	0	0
			5496	3559	917	990	30		

- Molecule 5 is a protein called Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	219	Total	C	N	O	S	0	0
			1762	1113	304	340	5		

- Molecule 6 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	241	1941	1244	320	366	11	0	0

- Molecule 7 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	391	3166	2053	537	563	13	0	0

- Molecule 8 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	241	1979	1277	328	369	5	0	0

- Molecule 9 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	P	257	2116	1358	366	378	14	0	0

- Molecule 10 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Q	258	2144	1355	375	405	9	0	0

- Molecule 11 is a protein called Inner kinetochore subunit CNN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	T	92	761	488	125	144	4	0	0

- Molecule 12 is a protein called K7\_Ame1p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	184	1485	928	255	299	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	269	GLU	GLY	conflict	UNP G2W9L4

- Molecule 13 is a protein called Inner kinetochore subunit WIP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	W	69	551	348	96	105	2	0	0

- Molecule 14 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Y	223	1663	1027	281	349	6	0	0

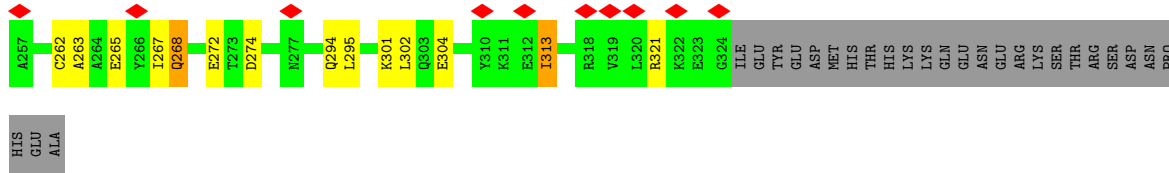
- Molecule 15 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Z	151	1180	740	204	235	1	0	0

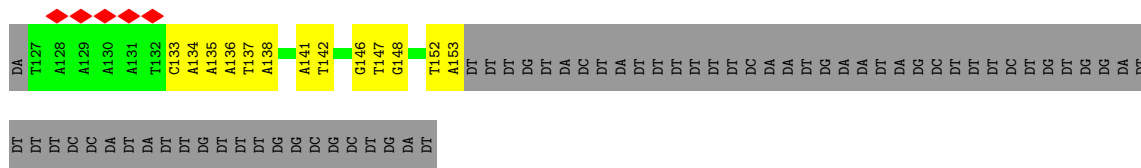
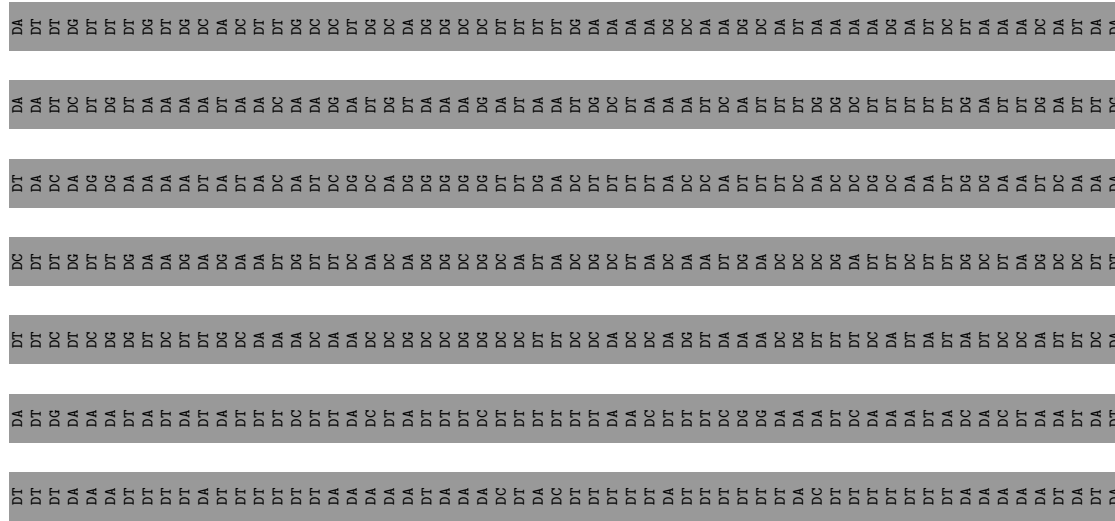
- Molecule 16 is a DNA chain called DNA (508-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	E	27	555	268	95	165	27	0	0

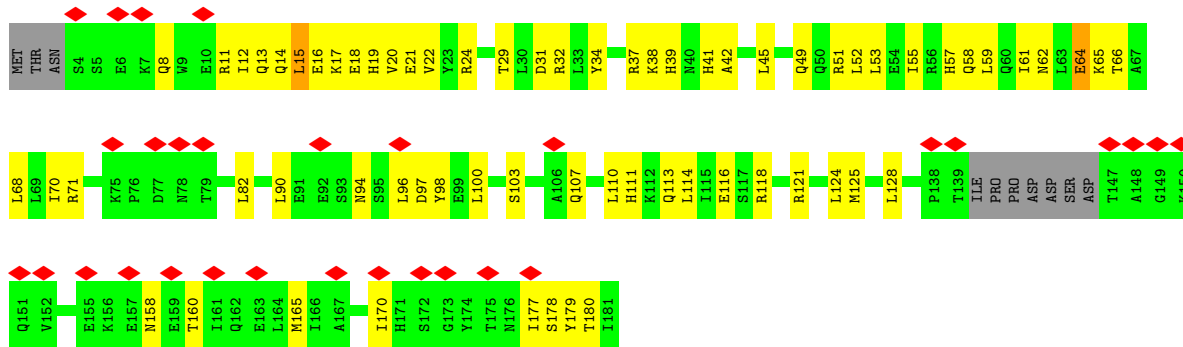




• Molecule 2: DNA (508-MER)



• Molecule 3: Inner kinetochore subunit MCM16



• Molecule 4: Inner kinetochore subunit CTF3













## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11639	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.739	Depositor
Minimum map value	-0.298	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.14	Depositor
Map size ( $\text{\AA}$ )	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.07, 1.07, 1.07	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.13	0/828	0.34	0/1108
1	B	0.13	0/884	0.35	0/1182
2	D	0.16	0/619	0.36	0/952
3	H	0.13	0/1429	0.37	0/1923
4	I	0.13	0/5620	0.38	0/7623
5	K	0.13	0/1784	0.37	0/2404
6	L	0.13	0/1981	0.36	0/2684
7	N	0.13	0/3239	0.33	0/4372
8	O	0.13	0/2017	0.34	0/2713
9	P	0.11	0/2149	0.31	0/2888
10	Q	0.14	0/2175	0.38	0/2913
11	T	0.13	0/772	0.41	0/1040
12	U	0.14	0/1499	0.35	0/2018
13	W	0.15	0/557	0.37	0/748
14	Y	0.13	0/1672	0.37	0/2252
15	Z	0.12	0/1195	0.33	0/1616
16	E	0.18	0/621	0.39	0/957
All	All	0.13	0/29041	0.36	0/39393

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
14	Y	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	Y	187	ASP	Peptide

## 5.2 Too-close contacts [i](#)

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	822	0	845	24	0
1	B	876	0	896	21	0
2	D	552	0	307	15	0
3	H	1412	0	1451	76	0
4	I	5496	0	5615	179	0
5	K	1762	0	1796	67	0
6	L	1941	0	1946	52	0
7	N	3166	0	3220	103	0
8	O	1979	0	1995	47	0
9	P	2116	0	2189	48	0
10	Q	2144	0	2195	62	0
11	T	761	0	781	38	0
12	U	1485	0	1465	50	0
13	W	551	0	559	24	0
14	Y	1663	0	1588	53	0
15	Z	1180	0	1108	36	0
16	E	555	0	310	13	0
All	All	28461	0	28266	736	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 13.

All (736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:370:LEU:HG	10:Q:374:MET:HE1	1.44	0.98
10:Q:357:LEU:HD11	15:Z:105:LEU:HD22	1.65	0.78
14:Y:12:ILE:O	14:Y:16:LEU:HB2	1.85	0.77
10:Q:207:LEU:HD11	12:U:177:LEU:HD21	1.67	0.76
1:A:228:LYS:HD3	16:E:10:DA:H3'	1.67	0.75
10:Q:356:LEU:HD21	14:Y:153:LYS:HD3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:121:ARG:HH22	5:K:110:ILE:HG23	1.52	0.75
1:A:247:ASP:HA	1:A:252:ARG:HH21	1.50	0.74
9:P:304:MET:HE3	9:P:305:PRO:HD2	1.67	0.74
14:Y:39:CYS:SG	14:Y:40:ARG:NH2	2.60	0.74
4:I:294:THR:HB	4:I:331:MET:HB3	1.70	0.73
9:P:194:MET:HE3	9:P:194:MET:HA	1.71	0.73
3:H:17:LYS:HD2	5:K:77:ASN:HD21	1.54	0.73
14:Y:190:ILE:HB	15:Z:125:MET:HE3	1.71	0.73
3:H:107:GLN:OE1	4:I:467:GLN:NE2	2.22	0.73
8:O:321:GLN:N	8:O:321:GLN:OE1	2.22	0.71
4:I:150:THR:HG21	4:I:186:SER:HB2	1.72	0.71
1:A:295:LEU:HD22	1:B:295:LEU:HB3	1.71	0.71
4:I:383:ILE:HD11	4:I:416:VAL:HA	1.72	0.71
3:H:8:GLN:HG3	5:K:5:LYS:HD2	1.72	0.71
7:N:283:LEU:HB3	9:P:210:SER:HB3	1.73	0.70
4:I:494:THR:HG21	4:I:541:ILE:HG23	1.73	0.70
6:L:56:TYR:HB2	6:L:75:PHE:HB2	1.72	0.70
14:Y:74:ARG:HH21	15:Z:72:LEU:HB3	1.56	0.70
5:K:97:SER:HA	5:K:100:GLN:HE21	1.55	0.70
5:K:86:SER:O	5:K:90:LEU:HD22	1.91	0.70
13:W:51:GLN:O	13:W:55:ARG:HG2	1.92	0.70
4:I:379:ILE:HG12	4:I:380:PRO:HD3	1.74	0.69
10:Q:269:LEU:HD21	10:Q:273:ARG:HH21	1.57	0.69
8:O:329:ILE:O	14:Y:106:GLN:NE2	2.26	0.69
3:H:170:ILE:HD11	4:I:135:ILE:HD13	1.74	0.69
9:P:217:ILE:HG12	9:P:232:LEU:HD23	1.75	0.69
14:Y:43:LYS:O	14:Y:47:ILE:HG12	1.93	0.69
3:H:103:SER:HB2	5:K:93:MET:HE2	1.73	0.69
4:I:291:TRP:HB3	4:I:333:ARG:HE	1.57	0.69
7:N:102:GLU:HG2	7:N:103:LYS:HD2	1.74	0.68
15:Z:53:VAL:O	15:Z:57:LEU:HD22	1.92	0.68
3:H:53:LEU:O	3:H:57:HIS:ND1	2.18	0.68
4:I:603:LEU:HB3	4:I:611:PHE:HE2	1.58	0.68
10:Q:253:GLN:HE22	14:Y:4:THR:HG22	1.60	0.67
14:Y:47:ILE:HA	14:Y:50:ARG:HG2	1.75	0.67
4:I:202:SER:HA	6:L:94:ASN:HB2	1.76	0.67
12:U:179:GLN:NE2	14:Y:36:ASN:OD1	2.28	0.67
4:I:191:LEU:HD22	4:I:204:ILE:HD12	1.77	0.66
11:T:277:ASP:HA	13:W:1:MET:HE1	1.78	0.66
4:I:255:ILE:O	4:I:259:LEU:HD23	1.95	0.65
14:Y:10:ASN:O	14:Y:14:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:68:LEU:HD11	5:K:72:PHE:H	1.62	0.65
6:L:127:ALA:HB1	6:L:231:ARG:HB3	1.76	0.65
10:Q:203:LYS:HE3	12:U:173:LEU:HD11	1.79	0.65
11:T:272:PRO:HG3	11:T:306:LEU:HD21	1.79	0.64
15:Z:5:GLN:O	15:Z:9:ASN:ND2	2.31	0.64
4:I:102:THR:HB	4:I:107:GLN:HE21	1.63	0.64
4:I:590:ASN:HA	4:I:594:ARG:HB2	1.80	0.64
2:D:137:DT:N3	16:E:18:DA:N1	2.44	0.64
4:I:198:VAL:HG13	4:I:200:ALA:H	1.62	0.64
11:T:285:PHE:HE1	13:W:55:ARG:HB3	1.63	0.64
16:E:7:DC:H2'	16:E:8:DA:C8	2.31	0.64
3:H:18:GLU:O	3:H:22:VAL:HG12	1.98	0.64
8:O:318:PHE:HB3	8:O:326:SER:HB3	1.79	0.63
4:I:345:LEU:HD12	4:I:350:ARG:HG2	1.81	0.63
12:U:198:SER:HA	12:U:201:GLU:HG3	1.80	0.63
4:I:193:ARG:HD3	4:I:265:LEU:HD21	1.80	0.62
4:I:359:TRP:O	4:I:363:GLN:HG2	2.00	0.62
4:I:33:GLU:OE2	4:I:34:LYS:NZ	2.32	0.62
9:P:276:ASN:ND2	12:U:297:ASP:OD2	2.33	0.62
10:Q:340:ILE:HA	14:Y:158:GLN:HE22	1.64	0.62
4:I:469:ILE:HD11	4:I:485:LEU:HD23	1.82	0.62
7:N:100:LYS:HB3	7:N:103:LYS:HD3	1.81	0.62
2:D:133:DC:H3'	7:N:22:LYS:HZ1	1.65	0.61
4:I:52:LEU:HD11	4:I:63:LYS:HG2	1.82	0.61
7:N:39:TRP:CE2	7:N:88:GLN:HG3	2.35	0.61
15:Z:57:LEU:HD13	15:Z:60:ARG:HH12	1.64	0.61
2:D:138:DA:OP1	11:T:283:ARG:NH2	2.31	0.61
8:O:356:GLU:O	8:O:360:ASN:ND2	2.34	0.61
4:I:5:LEU:HD13	4:I:40:LEU:HG	1.80	0.61
7:N:244:GLN:NE2	7:N:437:SER:O	2.33	0.61
8:O:206:LEU:HD21	8:O:271:VAL:HG23	1.82	0.61
1:B:229:GLU:OE2	1:B:233:ARG:NH2	2.33	0.61
15:Z:70:SER:O	15:Z:74:ARG:HG2	2.00	0.61
7:N:237:THR:HG21	12:U:231:LYS:HB3	1.82	0.61
12:U:238:ASP:O	12:U:242:GLU:HG3	2.01	0.61
4:I:698:VAL:HG13	4:I:702:MET:HE3	1.83	0.61
4:I:215:ARG:HD2	4:I:215:ARG:O	2.01	0.60
4:I:443:ILE:HD13	4:I:461:THR:HG21	1.83	0.60
14:Y:99:ASN:HB3	14:Y:105:PRO:HD3	1.82	0.60
15:Z:50:ASP:HA	15:Z:53:VAL:HG22	1.83	0.60
7:N:152:LEU:HD13	7:N:153:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:195:ILE:HD12	7:N:195:ILE:H	1.66	0.60
10:Q:250:GLN:O	10:Q:254:ASN:ND2	2.34	0.60
14:Y:194:PHE:CE2	15:Z:126:VAL:HA	2.37	0.60
8:O:348:LEU:HA	8:O:358:LYS:HD2	1.84	0.60
7:N:121:VAL:HG11	7:N:211:ILE:HD11	1.83	0.60
16:E:6:DT:H2'	16:E:7:DC:C6	2.37	0.59
5:K:226:LYS:NZ	11:T:342:GLU:OE1	2.34	0.59
9:P:316:LEU:HD22	9:P:317:PRO:HD2	1.84	0.59
10:Q:358:PRO:HA	10:Q:361:LYS:HZ1	1.67	0.59
4:I:50:ARG:NH1	4:I:84:GLU:OE2	2.35	0.59
5:K:27:LYS:HE2	5:K:28:GLN:HE22	1.66	0.59
10:Q:255:ASN:HD21	12:U:212:ARG:HG3	1.67	0.59
6:L:195:GLU:OE1	7:N:391:ASN:ND2	2.34	0.59
2:D:136:DA:OP1	4:I:219:LYS:NZ	2.36	0.58
1:A:315:TYR:HD1	1:A:318:ARG:HH22	1.51	0.58
3:H:100:LEU:HD12	5:K:90:LEU:HD11	1.84	0.58
1:B:232:ARG:HD3	6:L:212:GLY:HA3	1.84	0.58
3:H:57:HIS:O	3:H:61:ILE:HG12	2.03	0.58
4:I:388:MET:HE3	4:I:388:MET:HA	1.85	0.58
7:N:164:SER:OG	10:Q:247:ARG:NH2	2.37	0.58
11:T:285:PHE:HD1	13:W:55:ARG:HD2	1.69	0.58
12:U:296:VAL:HG22	14:Y:177:LEU:HD22	1.86	0.58
5:K:103:MET:HE3	5:K:103:MET:O	2.04	0.58
4:I:569:MET:HE3	4:I:569:MET:HA	1.86	0.57
10:Q:244:ILE:HG23	12:U:202:LEU:HD23	1.85	0.57
12:U:302:TYR:OH	14:Y:183:GLU:OE2	2.22	0.57
6:L:208:VAL:HG22	6:L:216:ILE:HG12	1.87	0.57
5:K:174:LEU:O	5:K:178:VAL:HG23	2.04	0.57
6:L:23:LEU:HG	6:L:27:LEU:HD23	1.86	0.57
6:L:124:LEU:HD22	6:L:232:VAL:HG13	1.86	0.57
6:L:198:MET:HE2	7:N:431:LEU:HD21	1.85	0.57
7:N:190:GLN:HB3	7:N:192:LYS:HZ2	1.70	0.57
1:A:274:ASP:O	1:A:278:ILE:HG22	2.05	0.57
10:Q:277:MET:HE2	10:Q:277:MET:HA	1.85	0.57
8:O:188:ILE:HG22	8:O:195:ILE:HG12	1.85	0.57
10:Q:163:LEU:HD11	10:Q:215:LYS:HD2	1.86	0.57
4:I:350:ARG:HB3	4:I:391:LYS:HZ1	1.70	0.57
5:K:193:THR:HG23	5:K:195:ASN:H	1.69	0.57
15:Z:93:ALA:O	15:Z:97:ILE:HG12	2.05	0.57
1:A:224:LYS:HB3	1:A:229:GLU:HG3	1.86	0.56
16:E:5:DG:H2'	16:E:6:DT:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:297:THR:O	11:T:301:ILE:HG12	2.04	0.56
2:D:152:DT:H1'	2:D:153:DA:H5'	1.87	0.56
4:I:709:ASN:O	4:I:712:ARG:NE	2.37	0.56
8:O:357:LEU:HA	8:O:360:ASN:HD21	1.71	0.56
4:I:314:TYR:HA	4:I:317:LYS:HE3	1.86	0.56
5:K:93:MET:SD	5:K:97:SER:OG	2.62	0.56
6:L:58:MET:HE3	6:L:73:PHE:HB2	1.88	0.56
7:N:85:ASN:OD1	7:N:86:VAL:N	2.38	0.56
4:I:313:ASP:O	4:I:317:LYS:HG3	2.06	0.56
8:O:310:VAL:HG23	8:O:311:LYS:H	1.69	0.56
4:I:550:ASP:HB3	4:I:553:LEU:HB3	1.87	0.56
7:N:59:ASP:O	7:N:63:GLU:HG2	2.05	0.56
7:N:40:PHE:HD1	7:N:44:GLY:HA2	1.70	0.56
13:W:2:ASP:HB2	13:W:4:GLU:HG3	1.87	0.56
3:H:158:ASN:HD21	5:K:145:ASN:HB2	1.71	0.56
5:K:22:LYS:HZ1	5:K:70:ILE:HG12	1.71	0.56
14:Y:38:VAL:HG22	15:Z:29:LEU:HD22	1.88	0.55
6:L:85:MET:HA	6:L:85:MET:HE2	1.88	0.55
9:P:166:GLN:NE2	9:P:190:CYS:SG	2.79	0.55
10:Q:353:VAL:HG12	14:Y:156:ALA:HB2	1.87	0.55
13:W:6:LEU:HD23	13:W:47:ALA:HB1	1.88	0.55
1:B:249:LEU:O	1:B:252:ARG:NH1	2.38	0.55
3:H:20:VAL:HG21	5:K:77:ASN:HD22	1.71	0.55
6:L:114:ILE:HD12	6:L:240:ILE:HD13	1.89	0.55
10:Q:258:LEU:HB3	12:U:216:LEU:HD23	1.89	0.55
6:L:81:MET:SD	6:L:241:GLN:NE2	2.80	0.55
8:O:169:VAL:HA	8:O:172:MET:SD	2.46	0.55
3:H:125:MET:SD	4:I:350:ARG:NH1	2.79	0.55
10:Q:337:ASN:OD1	12:U:284:ARG:NH2	2.35	0.55
12:U:176:ARG:HH12	14:Y:40:ARG:HH22	1.55	0.55
14:Y:41:LEU:HD23	15:Z:29:LEU:HD23	1.89	0.55
4:I:235:LYS:HE2	4:I:248:ALA:HB1	1.88	0.55
4:I:168:LEU:HD23	4:I:204:ILE:HG21	1.88	0.55
5:K:218:GLU:HG2	5:K:226:LYS:HG2	1.88	0.55
10:Q:251:GLU:HA	10:Q:254:ASN:HD22	1.71	0.55
10:Q:269:LEU:HD12	12:U:223:VAL:HG23	1.88	0.55
5:K:96:GLN:O	5:K:100:GLN:HG3	2.07	0.54
3:H:90:LEU:O	3:H:94:ASN:ND2	2.41	0.54
5:K:6:ASP:OD2	5:K:6:ASP:N	2.35	0.54
11:T:348:LEU:HD11	13:W:44:LEU:HD11	1.90	0.54
1:B:294:GLN:O	9:P:369:ARG:NE	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:24:ARG:HH12	4:I:501:ASN:HB3	1.72	0.54
4:I:359:TRP:CD1	4:I:363:GLN:HE21	2.24	0.54
4:I:644:ILE:O	4:I:648:ARG:HG2	2.07	0.54
10:Q:363:TYR:OH	12:U:288:ASN:ND2	2.40	0.54
15:Z:73:LEU:O	15:Z:77:GLU:HG2	2.07	0.54
7:N:210:ILE:HG21	7:N:258:LEU:HB3	1.88	0.54
12:U:275:SER:OG	12:U:276:GLN:N	2.37	0.54
7:N:427:VAL:HG23	7:N:431:LEU:HD23	1.90	0.54
4:I:568:LEU:HD22	4:I:578:VAL:HG22	1.90	0.54
8:O:351:SER:OG	8:O:353:ASP:OD1	2.26	0.54
12:U:176:ARG:HH12	14:Y:40:ARG:NH2	2.06	0.54
4:I:10:LEU:O	4:I:13:THR:OG1	2.22	0.53
14:Y:110:ILE:O	14:Y:114:ILE:HD12	2.08	0.53
12:U:300:ASP:HB3	12:U:304:GLY:H	1.73	0.53
3:H:51:ARG:HG2	4:I:540:ASP:HB2	1.90	0.53
4:I:383:ILE:HD12	4:I:419:GLY:HA3	1.89	0.53
7:N:203:ALA:HB3	7:N:212:PHE:HB2	1.90	0.53
7:N:340:VAL:C	7:N:341:MET:HE2	2.34	0.53
10:Q:233:ASP:N	10:Q:233:ASP:OD1	2.41	0.53
15:Z:7:LEU:O	15:Z:11:VAL:HG12	2.08	0.53
3:H:11:ARG:HH22	7:N:320:GLU:HB2	1.73	0.53
5:K:137:HIS:HB3	5:K:139:ARG:HD3	1.90	0.53
10:Q:386:ILE:HD11	12:U:305:LEU:HD21	1.91	0.53
11:T:345:HIS:ND1	11:T:353:GLN:OE1	2.35	0.53
3:H:42:ALA:HB1	5:K:48:VAL:HG22	1.89	0.53
3:H:58:GLN:HG3	4:I:501:ASN:HB2	1.90	0.53
3:H:125:MET:HE1	4:I:388:MET:HB3	1.90	0.53
4:I:632:THR:OG1	4:I:633:ILE:N	2.41	0.53
7:N:160:GLN:NE2	7:N:196:SER:OG	2.42	0.53
9:P:173:ASP:N	9:P:173:ASP:OD1	2.39	0.53
10:Q:203:LYS:O	10:Q:207:LEU:HD23	2.09	0.53
3:H:179:TYR:HE2	4:I:79:LYS:HB3	1.73	0.53
4:I:439:PHE:O	4:I:443:ILE:HG22	2.09	0.53
4:I:565:LYS:HG2	4:I:721:TYR:HE1	1.74	0.53
5:K:103:MET:HE3	5:K:107:GLN:HB2	1.90	0.53
6:L:7:PHE:HE1	6:L:221:ILE:HG22	1.72	0.53
11:T:333:ILE:HD11	13:W:53:ILE:HD11	1.91	0.53
1:A:310:TYR:HD1	9:P:285:VAL:HG23	1.73	0.53
1:B:226:SER:O	1:B:230:VAL:HG23	2.09	0.53
4:I:568:LEU:HA	4:I:571:TYR:HD2	1.74	0.53
10:Q:141:ARG:O	10:Q:141:ARG:NH1	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:383:GLU:HG3	12:U:298:LEU:HD13	1.91	0.53
15:Z:25:PHE:CE1	15:Z:29:LEU:HD12	2.44	0.53
3:H:71:ARG:HG3	4:I:621:PRO:HD3	1.90	0.53
15:Z:56:GLU:O	15:Z:60:ARG:HG3	2.08	0.53
1:A:242:ILE:HG21	1:A:256:LYS:HE3	1.90	0.52
5:K:54:THR:O	5:K:58:ARG:HG2	2.09	0.52
3:H:118:ARG:NH2	4:I:390:ASN:OD1	2.43	0.52
4:I:492:LEU:HD21	9:P:105:LEU:HD22	1.90	0.52
5:K:157:LYS:HD2	5:K:175:THR:HG21	1.91	0.52
6:L:214:THR:HB	6:L:223:THR:HG23	1.90	0.52
12:U:217:ASN:O	12:U:221:ILE:HG22	2.09	0.52
2:D:134:DA:H2''	2:D:135:DA:N7	2.25	0.52
4:I:141:GLN:O	4:I:180:TYR:OH	2.24	0.52
4:I:253:ASN:OD1	4:I:257:MET:HE2	2.09	0.52
5:K:138:ILE:HA	5:K:141:ARG:HD3	1.90	0.52
8:O:347:ALA:O	8:O:358:LYS:NZ	2.36	0.52
14:Y:24:ASP:HA	15:Z:49:ARG:HH12	1.74	0.52
15:Z:48:ALA:O	15:Z:52:ARG:HG2	2.09	0.52
3:H:37:ARG:NH2	8:O:130:ASP:OD2	2.43	0.52
5:K:177:GLU:O	5:K:181:LEU:HG	2.09	0.52
6:L:77:GLY:HA3	6:L:85:MET:HE2	1.92	0.52
7:N:384:LYS:NZ	16:E:16:DA:OP1	2.32	0.52
12:U:170:LEU:HD23	12:U:173:LEU:HD21	1.91	0.52
4:I:235:LYS:HE3	4:I:252:GLN:HB2	1.92	0.52
6:L:43:ASP:N	6:L:43:ASP:OD1	2.43	0.52
6:L:225:THR:HG22	6:L:227:SER:H	1.74	0.52
8:O:207:GLU:O	9:P:238:GLN:NE2	2.37	0.52
8:O:295:HIS:HD2	8:O:309:PHE:HB2	1.74	0.52
2:D:133:DC:H2''	2:D:134:DA:C8	2.45	0.52
3:H:13:GLN:O	3:H:16:GLU:HG2	2.09	0.52
3:H:111:HIS:HA	3:H:114:LEU:HD12	1.91	0.52
3:H:121:ARG:O	3:H:125:MET:HG3	2.09	0.52
4:I:140:TRP:CZ3	4:I:171:ILE:HD12	2.44	0.52
15:Z:108:LEU:O	15:Z:112:ILE:HG12	2.10	0.52
1:B:252:ARG:HE	7:N:443:MET:HE1	1.74	0.52
4:I:64:VAL:HA	4:I:67:VAL:HG22	1.92	0.52
2:D:137:DT:H2''	2:D:138:DA:C8	2.44	0.52
4:I:334:ASP:OD1	4:I:334:ASP:N	2.42	0.52
7:N:75:ILE:HA	7:N:79:TYR:HB2	1.91	0.52
8:O:313:ILE:HA	8:O:331:ASP:HB3	1.92	0.52
4:I:94:VAL:O	4:I:97:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:200:TYR:O	10:Q:204:GLU:HG2	2.10	0.52
4:I:168:LEU:O	4:I:171:ILE:HG22	2.11	0.51
10:Q:323:VAL:O	10:Q:327:ASN:ND2	2.43	0.51
3:H:18:GLU:O	3:H:21:GLU:HG3	2.10	0.51
11:T:285:PHE:CE1	13:W:55:ARG:HB3	2.44	0.51
4:I:514:SER:O	4:I:518:ILE:HG22	2.09	0.51
4:I:542:MET:HA	4:I:545:VAL:HG22	1.92	0.51
6:L:10:ILE:HD11	6:L:87:LEU:HD23	1.92	0.51
10:Q:170:THR:HA	12:U:181:ILE:HD11	1.92	0.51
4:I:165:PRO:HG2	5:K:235:GLU:HB3	1.92	0.51
7:N:303:ASP:OD1	7:N:305:SER:OG	2.29	0.51
7:N:333:PHE:CE1	7:N:432:ALA:HA	2.45	0.51
9:P:269:THR:HG22	9:P:284:ARG:HB2	1.93	0.51
7:N:161:LEU:HB2	7:N:197:ARG:HD2	1.93	0.51
3:H:59:LEU:HD11	4:I:610:PHE:HE2	1.75	0.51
8:O:291:LYS:O	8:O:292:LYS:HG2	2.11	0.51
11:T:276:MET:SD	11:T:280:HIS:ND1	2.84	0.51
11:T:337:VAL:HA	11:T:340:MET:HB3	1.93	0.51
11:T:285:PHE:CD1	13:W:55:ARG:HD2	2.46	0.50
12:U:220:ILE:HA	12:U:223:VAL:HG12	1.92	0.50
1:B:301:LYS:O	1:B:304:GLU:HG3	2.11	0.50
4:I:94:VAL:HG11	11:T:357:GLU:HG3	1.92	0.50
7:N:227:SER:O	7:N:231:THR:OG1	2.24	0.50
9:P:285:VAL:HA	9:P:293:THR:HA	1.92	0.50
13:W:74:TYR:HD1	13:W:76:TYR:HE1	1.57	0.50
1:B:294:GLN:HB3	9:P:369:ARG:NH1	2.26	0.50
4:I:67:VAL:HA	4:I:71:PHE:HD2	1.75	0.50
4:I:203:GLN:NE2	6:L:92:THR:O	2.44	0.50
4:I:483:LEU:HD13	4:I:534:TYR:HB3	1.93	0.50
4:I:543:ASN:OD1	4:I:544:LYS:N	2.44	0.50
9:P:262:ILE:O	9:P:266:LYS:HB2	2.11	0.50
3:H:121:ARG:HG3	3:H:125:MET:HE3	1.94	0.50
5:K:194:LEU:HG	5:K:228:ILE:HD11	1.93	0.50
13:W:9:TYR:O	13:W:12:ARG:HG3	2.11	0.50
14:Y:203:VAL:O	14:Y:206:GLU:HG3	2.10	0.50
4:I:575:ASN:O	4:I:579:ARG:NE	2.44	0.50
7:N:82:ASP:OD1	7:N:82:ASP:N	2.43	0.50
7:N:92:ILE:HG13	7:N:93:ASP:N	2.25	0.50
3:H:17:LYS:HD2	5:K:77:ASN:ND2	2.24	0.50
3:H:34:TYR:O	3:H:38:LYS:HG2	2.12	0.50
4:I:582:ASN:HA	4:I:585:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:35:LEU:HD12	7:N:39:TRP:CZ2	2.47	0.50
7:N:88:GLN:N	7:N:88:GLN:OE1	2.45	0.50
4:I:259:LEU:HD12	4:I:263:HIS:NE2	2.26	0.50
4:I:512:PHE:CE2	4:I:545:VAL:HG11	2.47	0.50
5:K:36:ILE:HA	5:K:39:ARG:HG2	1.94	0.50
9:P:300:PHE:HZ	10:Q:332:LEU:HD13	1.76	0.50
14:Y:136:ASP:N	14:Y:136:ASP:OD1	2.44	0.50
7:N:374:SER:OG	7:N:375:ARG:N	2.45	0.50
1:B:218:GLU:HB2	1:B:221:LYS:HB2	1.93	0.50
5:K:206:ARG:NH2	11:T:353:GLN:OE1	2.45	0.50
9:P:345:ILE:HD12	10:Q:336:LEU:HD11	1.94	0.50
12:U:212:ARG:O	12:U:212:ARG:HD3	2.12	0.50
12:U:251:LYS:HE3	12:U:255:ARG:HH21	1.77	0.50
2:D:147:DT:H2'	2:D:148:DG:C8	2.47	0.49
12:U:194:ASP:OD2	14:Y:56:ARG:N	2.33	0.49
3:H:107:GLN:HG2	5:K:100:GLN:HE22	1.76	0.49
4:I:61:VAL:HA	4:I:64:VAL:HG22	1.92	0.49
8:O:296:ASP:OD1	8:O:296:ASP:N	2.44	0.49
10:Q:340:ILE:HA	14:Y:158:GLN:NE2	2.27	0.49
14:Y:94:GLY:HA3	14:Y:116:ASP:CG	2.37	0.49
15:Z:122:PHE:O	15:Z:126:VAL:HG12	2.12	0.49
4:I:261:GLU:HA	4:I:264:GLN:HE21	1.75	0.49
4:I:583:GLN:HA	4:I:586:MET:SD	2.52	0.49
7:N:223:LEU:HA	12:U:221:ILE:HD13	1.93	0.49
9:P:366:MET:N	9:P:366:MET:HE2	2.28	0.49
6:L:9:GLY:N	6:L:114:ILE:HD11	2.27	0.49
5:K:167:ASN:H	5:K:200:LYS:HZ2	1.61	0.49
6:L:11:SER:HB3	6:L:110:ILE:HB	1.93	0.49
14:Y:198:ASN:O	14:Y:201:LEU:HD12	2.11	0.49
7:N:40:PHE:CD1	7:N:44:GLY:HA2	2.47	0.49
7:N:245:LYS:HG3	7:N:246:ILE:HD12	1.94	0.49
9:P:364:PRO:HG3	12:U:263:LEU:HD21	1.93	0.49
11:T:336:ASN:ND2	11:T:338:ASP:OD1	2.45	0.49
12:U:135:ILE:HG23	12:U:189:LEU:HD22	1.94	0.49
3:H:62:ASN:HB2	4:I:637:PRO:HG2	1.95	0.49
6:L:14:LEU:HD23	6:L:109:VAL:HG11	1.94	0.49
9:P:359:ASN:HA	9:P:363:PHE:CD2	2.47	0.49
10:Q:376:GLN:NE2	10:Q:377:MET:HG2	2.28	0.49
11:T:272:PRO:HB3	11:T:306:LEU:HD11	1.94	0.49
11:T:285:PHE:HB2	13:W:55:ARG:NH1	2.27	0.49
14:Y:182:LYS:HD2	14:Y:188:ASP:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:293:VAL:HG13	4:I:298:GLN:HB2	1.93	0.49
11:T:286:LEU:HD22	11:T:291:ILE:HB	1.94	0.49
11:T:350:LEU:HA	11:T:353:GLN:HE21	1.77	0.49
1:A:308:ASN:O	1:A:311:LYS:HG2	2.13	0.49
4:I:59:ASP:O	4:I:62:THR:OG1	2.26	0.49
4:I:67:VAL:HA	4:I:71:PHE:CD2	2.48	0.49
4:I:140:TRP:HZ3	4:I:174:CYS:HB3	1.78	0.49
7:N:444:ASN:OD1	8:O:229:LYS:NZ	2.45	0.49
8:O:316:GLU:HG3	8:O:328:SER:HB2	1.94	0.49
6:L:112:TRP:HE1	6:L:240:ILE:HD11	1.77	0.49
7:N:43:PHE:HD2	7:N:88:GLN:HE22	1.59	0.49
2:D:141:DA:C8	2:D:142:DT:H72	2.47	0.48
7:N:93:ASP:OD1	7:N:201:TYR:OH	2.21	0.48
9:P:280:LEU:HD23	9:P:298:ILE:HD11	1.96	0.48
16:E:11:DT:H2''	16:E:12:DG:H8	1.78	0.48
4:I:625:PHE:O	4:I:629:LYS:HB2	2.13	0.48
14:Y:98:ARG:O	14:Y:102:GLU:HG2	2.12	0.48
15:Z:116:THR:HA	15:Z:119:LEU:HG	1.94	0.48
4:I:194:PHE:O	4:I:198:VAL:HG12	2.13	0.48
7:N:126:ALA:O	7:N:129:ILE:HG12	2.14	0.48
8:O:320:LYS:HB3	8:O:321:GLN:OE1	2.14	0.48
14:Y:164:LEU:HB2	15:Z:112:ILE:HD11	1.96	0.48
4:I:208:ILE:O	4:I:211:ILE:HG22	2.12	0.48
4:I:260:SER:O	4:I:264:GLN:HG3	2.12	0.48
5:K:206:ARG:HH22	11:T:353:GLN:HB2	1.79	0.48
3:H:160:THR:HG22	5:K:233:PHE:HB2	1.95	0.48
4:I:198:VAL:HG22	4:I:200:ALA:HB3	1.95	0.48
4:I:489:MET:HE2	4:I:489:MET:N	2.28	0.48
11:T:305:SER:O	11:T:308:ILE:HG22	2.13	0.48
16:E:9:DC:H2''	16:E:10:DA:C8	2.49	0.48
7:N:322:ARG:O	7:N:325:ARG:HG3	2.13	0.48
10:Q:349:ASP:O	10:Q:353:VAL:HG22	2.14	0.48
1:A:278:ILE:O	1:A:282:THR:HG23	2.13	0.48
12:U:217:ASN:HA	12:U:220:ILE:HG22	1.96	0.48
1:B:294:GLN:HB3	9:P:369:ARG:CZ	2.44	0.48
4:I:509:THR:O	4:I:513:ILE:HG23	2.14	0.48
5:K:103:MET:O	5:K:106:LEU:HD12	2.14	0.48
12:U:280:ASP:OD1	12:U:280:ASP:N	2.46	0.48
14:Y:188:ASP:OD1	14:Y:188:ASP:N	2.46	0.47
3:H:70:ILE:HD13	4:I:664:ILE:HD13	1.96	0.47
4:I:143:SER:OG	11:T:351:GLU:OE2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:465:VAL:O	4:I:468:MET:HE3	2.13	0.47
5:K:199:SER:HA	5:K:202:ILE:HG12	1.96	0.47
9:P:170:GLN:NE2	9:P:186:ASN:OD1	2.41	0.47
6:L:168:GLU:HA	6:L:171:GLU:HG2	1.95	0.47
6:L:227:SER:OG	6:L:228:LEU:N	2.47	0.47
1:B:228:LYS:HD2	2:D:146:DG:O5'	2.13	0.47
4:I:436:PHE:O	4:I:440:MET:HG2	2.14	0.47
5:K:164:LEU:HG	5:K:166:ASP:HB2	1.96	0.47
6:L:191:TYR:CE1	6:L:195:GLU:HG3	2.49	0.47
10:Q:211:LEU:HA	10:Q:214:ILE:HG12	1.96	0.47
10:Q:255:ASN:O	10:Q:259:GLU:HG3	2.14	0.47
11:T:352:LEU:O	11:T:356:ILE:HG12	2.15	0.47
12:U:184:GLN:HB3	12:U:185:MET:HE2	1.96	0.47
3:H:121:ARG:NH2	5:K:110:ILE:HG23	2.26	0.47
10:Q:161:SER:O	10:Q:164:ARG:HG2	2.14	0.47
14:Y:42:LEU:HD12	14:Y:43:LYS:HD3	1.97	0.47
4:I:66:ILE:HG23	4:I:70:CYS:SG	2.55	0.47
7:N:124:GLN:NE2	8:O:305:MET:HE3	2.29	0.47
7:N:375:ARG:NH2	7:N:418:ASP:OD2	2.47	0.47
8:O:130:ASP:OD1	8:O:130:ASP:N	2.48	0.47
4:I:195:GLN:NE2	4:I:203:GLN:OE1	2.48	0.47
6:L:150:GLU:HB2	6:L:206:THR:HG21	1.96	0.47
7:N:7:LEU:O	7:N:133:GLN:NE2	2.48	0.47
9:P:187:TYR:HB2	9:P:199:ILE:HG22	1.97	0.47
4:I:397:ILE:O	4:I:401:CYS:HB2	2.15	0.47
14:Y:36:ASN:O	14:Y:40:ARG:HG2	2.15	0.47
3:H:34:TYR:HD1	8:O:128:VAL:HG13	1.79	0.47
4:I:253:ASN:O	4:I:257:MET:HG3	2.15	0.47
4:I:704:LEU:O	4:I:709:ASN:ND2	2.47	0.47
8:O:123:MET:HE2	8:O:123:MET:HA	1.96	0.47
12:U:147:GLU:N	12:U:147:GLU:OE1	2.48	0.47
1:A:276:ALA:O	1:A:279:GLU:HG3	2.15	0.46
4:I:200:ALA:O	6:L:94:ASN:ND2	2.48	0.46
14:Y:82:MET:HA	14:Y:82:MET:HE2	1.97	0.46
4:I:4:ILE:HD13	4:I:34:LYS:HE2	1.97	0.46
4:I:462:CYS:HA	4:I:465:VAL:HG22	1.97	0.46
7:N:115:ASP:HB3	12:U:237:HIS:NE2	2.30	0.46
4:I:6:ASP:HB3	4:I:44:GLN:HG2	1.96	0.46
4:I:254:THR:HA	4:I:257:MET:HE3	1.97	0.46
9:P:358:CYS:O	9:P:362:LEU:HB2	2.15	0.46
11:T:289:ASN:CG	13:W:62:ARG:HH21	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:276:VAL:HG11	9:P:315:PHE:HE1	1.81	0.46
10:Q:335:MET:HB2	10:Q:335:MET:HE3	1.85	0.46
14:Y:114:ILE:HD11	14:Y:157:LEU:HD23	1.97	0.46
3:H:34:TYR:HA	3:H:37:ARG:HG2	1.97	0.46
3:H:64:GLU:O	3:H:68:LEU:HD23	2.16	0.46
11:T:319:LEU:HD13	13:W:42:LYS:HB3	1.96	0.46
1:A:302:LEU:HD23	1:B:302:LEU:HD22	1.97	0.46
1:A:312:GLU:HB3	1:B:313:ILE:HD11	1.98	0.46
7:N:285:ASP:OD1	7:N:286:TYR:N	2.49	0.46
9:P:363:PHE:HB3	9:P:366:MET:HG2	1.98	0.46
1:A:315:TYR:O	1:A:319:VAL:HG23	2.16	0.46
12:U:185:MET:HE2	12:U:185:MET:N	2.29	0.46
1:A:283:LEU:O	1:A:286:LEU:HG	2.15	0.46
3:H:97:ASP:HB3	4:I:552:LEU:HD21	1.98	0.46
6:L:22:LYS:HG3	6:L:102:TRP:HE1	1.81	0.46
1:A:224:LYS:HG2	13:W:74:TYR:CE1	2.50	0.46
4:I:476:ASP:OD1	4:I:477:LYS:N	2.49	0.46
4:I:701:LEU:HD21	4:I:718:LEU:HD12	1.97	0.46
5:K:5:LYS:HD3	5:K:8:LEU:HD12	1.97	0.46
6:L:202:ARG:NH2	7:N:306:PHE:O	2.49	0.46
7:N:23:GLN:CD	7:N:92:ILE:HD12	2.41	0.46
8:O:276:VAL:HG11	9:P:315:PHE:CE1	2.51	0.46
8:O:295:HIS:CD2	8:O:309:PHE:HB2	2.51	0.46
10:Q:249:SER:O	10:Q:253:GLN:HG2	2.16	0.46
12:U:155:LEU:N	12:U:175:LEU:HD21	2.31	0.46
4:I:607:SER:H	5:K:58:ARG:NH2	2.14	0.46
7:N:77:TYR:O	7:N:81:PRO:HB3	2.15	0.46
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.80	0.45
5:K:171:ILE:O	5:K:175:THR:OG1	2.28	0.45
7:N:253:ASN:HB3	7:N:380:VAL:HG13	1.98	0.45
14:Y:25:TYR:HA	14:Y:43:LYS:HE3	1.98	0.45
1:A:221:LYS:HD3	13:W:76:TYR:CD2	2.51	0.45
2:D:136:DA:H2"	2:D:137:DT:C4	2.51	0.45
10:Q:205:ARG:HH21	10:Q:208:GLU:CD	2.25	0.45
3:H:39:HIS:CE1	5:K:49:ASN:H	2.34	0.45
6:L:13:GLN:HB2	6:L:84:PRO:HB2	1.98	0.45
6:L:110:ILE:C	6:L:111:MET:HE2	2.41	0.45
3:H:31:ASP:OD1	3:H:57:HIS:NE2	2.49	0.45
7:N:46:SER:OG	7:N:79:TYR:O	2.33	0.45
3:H:124:LEU:HD13	5:K:114:LEU:HG	1.98	0.45
4:I:312:VAL:HG13	4:I:316:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:228:ILE:O	7:N:232:ILE:HG22	2.16	0.45
15:Z:4:GLU:OE2	15:Z:69:ARG:NH1	2.38	0.45
4:I:355:SER:OG	4:I:356:PRO:HD3	2.16	0.45
7:N:139:ILE:HG21	7:N:223:LEU:HD21	1.98	0.45
9:P:365:ASP:HB2	9:P:366:MET:HE2	1.97	0.45
3:H:118:ARG:HB2	4:I:423:LEU:HD21	1.99	0.45
7:N:273:TYR:OH	9:P:144:THR:O	2.32	0.45
12:U:176:ARG:HH22	14:Y:40:ARG:CZ	2.30	0.45
12:U:310:ASN:O	12:U:314:GLU:HG2	2.16	0.45
15:Z:50:ASP:OD1	15:Z:51:ALA:N	2.50	0.45
3:H:68:LEU:HD11	5:K:72:PHE:N	2.32	0.45
3:H:170:ILE:HD11	4:I:135:ILE:HA	1.99	0.45
5:K:161:VAL:HG12	5:K:171:ILE:HG22	1.98	0.45
8:O:199:ARG:CZ	8:O:225:LYS:HD3	2.47	0.45
1:B:265:GLU:HA	1:B:268:GLN:OE1	2.17	0.45
11:T:291:ILE:HD13	13:W:62:ARG:HD3	1.98	0.45
4:I:636:ILE:HG22	4:I:639:LEU:H	1.82	0.44
5:K:27:LYS:HE2	5:K:28:GLN:NE2	2.31	0.44
7:N:28:PRO:O	7:N:32:LEU:HD23	2.17	0.44
7:N:318:GLU:HB2	7:N:321:ILE:HG22	1.98	0.44
7:N:404:PHE:HB3	7:N:409:ILE:HD12	1.98	0.44
8:O:160:LEU:HB2	9:P:131:LEU:HD21	2.00	0.44
14:Y:45:GLN:O	14:Y:49:LYS:HG2	2.18	0.44
16:E:2:DT:H2''	16:E:3:DA:C4	2.53	0.44
10:Q:130:PHE:CE2	10:Q:217:LYS:HB3	2.52	0.44
10:Q:280:LYS:O	10:Q:284:LYS:HE3	2.18	0.44
4:I:509:THR:OG1	4:I:510:MET:SD	2.74	0.44
2:D:134:DA:H2''	2:D:135:DA:C8	2.52	0.44
7:N:9:ASP:O	7:N:85:ASN:ND2	2.33	0.44
7:N:24:LEU:HD12	7:N:32:LEU:HD11	1.98	0.44
7:N:250:SER:O	7:N:253:ASN:N	2.50	0.44
1:A:242:ILE:HD12	1:A:242:ILE:HA	1.88	0.44
9:P:299:ASN:ND2	9:P:322:SER:OG	2.37	0.44
10:Q:169:ASN:ND2	12:U:188:ASP:OD2	2.50	0.44
16:E:13:DA:H2''	16:E:14:DT:H71	1.99	0.44
11:T:349:PRO:O	11:T:353:GLN:HG2	2.17	0.44
3:H:49:GLN:HB3	5:K:53:PHE:CE2	2.53	0.44
3:H:52:LEU:HA	3:H:55:ILE:HD12	1.99	0.44
3:H:128:LEU:HD23	3:H:128:LEU:HA	1.79	0.44
6:L:22:LYS:HA	6:L:22:LYS:HD2	1.74	0.44
10:Q:142:LEU:HD22	10:Q:146:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:184:GLU:O	10:Q:187:GLN:HG3	2.17	0.44
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.86	0.44
3:H:29:THR:HA	3:H:32:ARG:HG2	2.00	0.44
7:N:85:ASN:HB3	7:N:88:GLN:OE1	2.17	0.44
14:Y:200:LYS:HA	14:Y:203:VAL:HG12	1.99	0.44
4:I:540:ASP:OD1	4:I:540:ASP:N	2.51	0.44
6:L:10:ILE:HG12	6:L:111:MET:HE1	2.00	0.44
6:L:182:HIS:O	6:L:186:ASP:HB2	2.18	0.44
7:N:28:PRO:O	7:N:31:VAL:HG22	2.17	0.44
10:Q:234:ILE:HA	12:U:192:ILE:HD11	2.00	0.44
11:T:340:MET:HE2	11:T:340:MET:HB2	1.88	0.44
1:B:321:ARG:HD2	1:B:321:ARG:HA	1.86	0.43
4:I:186:SER:O	4:I:190:ILE:HG12	2.17	0.43
4:I:315:MET:HE2	4:I:315:MET:O	2.18	0.43
5:K:24:TYR:OH	8:O:147:LEU:HG	2.18	0.43
6:L:39:ARG:NH1	6:L:51:ASP:HB2	2.33	0.43
6:L:168:GLU:HG2	6:L:169:SER:N	2.32	0.43
7:N:25:MET:HE1	7:N:69:ASN:HA	1.99	0.43
7:N:324:LEU:HD23	7:N:324:LEU:HA	1.85	0.43
8:O:277:GLU:OE2	8:O:277:GLU:HA	2.18	0.43
1:B:268:GLN:O	1:B:272:GLU:HG2	2.18	0.43
2:D:133:DC:H3'	7:N:22:LYS:NZ	2.32	0.43
3:H:118:ARG:HA	4:I:388:MET:HE1	1.99	0.43
3:H:165:MET:HE1	3:H:180:THR:OG1	2.18	0.43
4:I:647:LEU:HD13	4:I:696:LEU:HD11	1.99	0.43
9:P:333:ASN:HB3	9:P:336:ASP:OD1	2.18	0.43
11:T:338:ASP:HA	11:T:341:PHE:CE2	2.53	0.43
1:A:266:TYR:HE2	1:B:267:ILE:HD11	1.83	0.43
3:H:14:GLN:HG3	7:N:319:PRO:HG2	1.99	0.43
4:I:425:LYS:HB2	4:I:425:LYS:HE2	1.86	0.43
5:K:71:GLY:HA2	5:K:74:LEU:HD12	2.00	0.43
8:O:353:ASP:OD1	8:O:353:ASP:N	2.49	0.43
9:P:304:MET:HE3	9:P:304:MET:HA	1.99	0.43
10:Q:130:PHE:HB3	12:U:141:LEU:HD11	2.00	0.43
10:Q:364:THR:OG1	12:U:282:SER:OG	2.25	0.43
14:Y:36:ASN:OD1	14:Y:40:ARG:NH1	2.52	0.43
3:H:110:LEU:O	3:H:114:LEU:HG	2.18	0.43
4:I:443:ILE:HG23	4:I:458:PHE:HD1	1.84	0.43
4:I:704:LEU:HD12	4:I:711:TYR:HB2	2.00	0.43
7:N:163:ASP:OD2	7:N:197:ARG:NH2	2.45	0.43
9:P:101:THR:O	9:P:105:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:142:PHE:HB3	12:U:146:PHE:CE1	2.53	0.43
4:I:9:ILE:O	4:I:13:THR:HG23	2.18	0.43
1:A:309:ALA:O	1:A:313:ILE:HG12	2.19	0.43
2:D:135:DA:H2"	2:D:136:DA:C8	2.54	0.43
9:P:128:ILE:HG13	9:P:132:THR:HG21	1.99	0.43
9:P:257:ILE:HG12	9:P:351:LYS:HG2	2.01	0.43
10:Q:247:ARG:O	10:Q:251:GLU:HG2	2.18	0.43
10:Q:269:LEU:HA	12:U:227:ILE:HD11	2.01	0.43
3:H:45:LEU:HB3	5:K:48:VAL:HG21	2.01	0.43
3:H:121:ARG:NH2	5:K:111:ASN:OD1	2.52	0.43
4:I:9:ILE:HG12	4:I:48:LEU:HD13	1.99	0.43
9:P:231:LEU:HB3	9:P:232:LEU:HD12	2.00	0.43
11:T:271:LYS:HB3	11:T:272:PRO:HD3	2.01	0.43
12:U:155:LEU:HA	12:U:175:LEU:HD11	2.00	0.43
4:I:510:MET:SD	4:I:510:MET:N	2.92	0.43
7:N:23:GLN:OE1	7:N:92:ILE:HD12	2.19	0.43
8:O:309:PHE:HD1	8:O:314:LYS:HA	1.83	0.43
13:W:70:LEU:HD21	13:W:74:TYR:OH	2.19	0.43
15:Z:71:ARG:HG3	15:Z:72:LEU:N	2.34	0.43
15:Z:100:LEU:O	15:Z:103:GLN:HG2	2.18	0.43
4:I:312:VAL:HG12	4:I:359:TRP:CD1	2.54	0.43
4:I:546:PHE:HE1	4:I:557:ALA:HB1	1.84	0.43
5:K:101:LYS:O	5:K:105:LEU:HD23	2.19	0.43
5:K:156:LEU:HD12	5:K:179:MET:SD	2.59	0.43
10:Q:207:LEU:HD21	12:U:177:LEU:HD11	2.00	0.43
3:H:70:ILE:HA	4:I:664:ILE:CD1	2.49	0.43
3:H:98:TYR:HD2	4:I:710:PRO:HD3	1.84	0.43
4:I:518:ILE:HG13	4:I:521:GLN:HE21	1.84	0.43
6:L:164:GLU:HB2	7:N:401:LYS:HB2	2.00	0.43
10:Q:252:LEU:HD22	14:Y:67:TYR:HE2	1.84	0.43
11:T:279:LYS:O	11:T:283:ARG:HB2	2.19	0.43
4:I:116:HIS:HD1	4:I:226:LEU:HG	1.84	0.42
4:I:565:LYS:HG2	4:I:721:TYR:CE1	2.53	0.42
4:I:727:LYS:HE3	4:I:728:TYR:CZ	2.54	0.42
6:L:196:THR:O	6:L:196:THR:OG1	2.31	0.42
7:N:89:LEU:HA	7:N:92:ILE:HG12	2.00	0.42
7:N:255:MET:HB3	7:N:255:MET:HE3	1.82	0.42
8:O:337:SER:OG	8:O:340:ASN:OD1	2.24	0.42
10:Q:185:MET:HE1	10:Q:199:ILE:HD12	2.00	0.42
10:Q:323:VAL:HG12	10:Q:327:ASN:HD21	1.83	0.42
14:Y:49:LYS:HD3	15:Z:19:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:5:DG:H2'	16:E:6:DT:H6	1.81	0.42
3:H:16:GLU:O	3:H:20:VAL:HG13	2.19	0.42
3:H:19:HIS:HD2	5:K:19:ILE:HG13	1.84	0.42
4:I:178:PRO:HG2	11:T:347:LEU:HD13	2.01	0.42
4:I:407:LYS:HG2	4:I:446:TRP:CH2	2.53	0.42
4:I:506:ARG:HH11	5:K:82:ARG:HG3	1.84	0.42
7:N:8:GLU:N	7:N:8:GLU:OE1	2.53	0.42
7:N:125:PRO:HA	7:N:146:MET:HE1	2.01	0.42
8:O:285:PHE:CE2	8:O:306:VAL:HG11	2.54	0.42
10:Q:185:MET:HE3	10:Q:196:VAL:HA	2.01	0.42
14:Y:74:ARG:HE	15:Z:72:LEU:HG	1.83	0.42
14:Y:100:ARG:HA	14:Y:100:ARG:HH11	1.84	0.42
4:I:429:ILE:HG23	4:I:481:LEU:HD22	2.01	0.42
4:I:506:ARG:HA	4:I:506:ARG:HD2	1.82	0.42
8:O:167:GLU:OE2	9:P:153:ARG:NH1	2.52	0.42
8:O:273:LEU:O	8:O:277:GLU:HG2	2.19	0.42
12:U:157:ASP:HB3	12:U:171:TYR:CZ	2.55	0.42
4:I:215:ARG:HA	4:I:218:LEU:HD21	2.00	0.42
4:I:219:LYS:HA	4:I:222:ARG:HE	1.84	0.42
7:N:149:HIS:HB3	7:N:152:LEU:O	2.19	0.42
8:O:146:LYS:O	8:O:146:LYS:NZ	2.43	0.42
9:P:189:PHE:CE2	9:P:244:LEU:HD23	2.53	0.42
1:A:291:ASN:O	1:A:294:GLN:HG2	2.20	0.42
1:B:252:ARG:HA	1:B:252:ARG:HD3	1.83	0.42
3:H:68:LEU:HD21	5:K:71:GLY:HA3	2.01	0.42
4:I:505:ASN:OD1	4:I:507:PHE:HD2	2.03	0.42
5:K:139:ARG:HG2	5:K:140:THR:N	2.35	0.42
7:N:233:SER:O	7:N:234:GLU:HG2	2.20	0.42
9:P:105:LEU:HA	9:P:108:ILE:HD12	2.01	0.42
15:Z:115:LYS:HA	15:Z:115:LYS:HD3	1.82	0.42
4:I:178:PRO:HG3	13:W:55:ARG:HH22	1.85	0.42
6:L:102:TRP:CE3	6:L:103:LEU:HD23	2.54	0.42
7:N:84:LEU:HA	7:N:84:LEU:HD23	1.81	0.42
7:N:165:ASN:ND2	7:N:193:PRO:HD2	2.35	0.42
10:Q:185:MET:SD	10:Q:196:VAL:HG22	2.60	0.42
4:I:210:THR:O	11:T:287:ASN:HB3	2.19	0.42
7:N:253:ASN:ND2	7:N:381:PRO:HD2	2.34	0.42
15:Z:114:GLU:O	15:Z:118:GLU:HG2	2.19	0.42
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.86	0.42
4:I:42:SER:HB3	4:I:43:PRO:HD3	2.02	0.42
4:I:242:HIS:HA	4:I:243:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:504:SER:HB2	5:K:78:PHE:CE1	2.55	0.42
6:L:72:LYS:HB3	6:L:72:LYS:HE3	1.77	0.42
7:N:155:LEU:N	7:N:204:PHE:O	2.51	0.42
7:N:208:SER:HB3	7:N:260:PRO:HB3	2.01	0.42
7:N:386:GLY:H	7:N:439:SER:HB3	1.85	0.42
3:H:96:LEU:O	3:H:100:LEU:HD13	2.19	0.42
3:H:177:ILE:HD13	4:I:86:ILE:HG22	2.02	0.42
4:I:539:PRO:HB3	4:I:584:TYR:HE1	1.85	0.42
4:I:542:MET:H	4:I:542:MET:HG3	1.68	0.42
5:K:103:MET:CE	5:K:107:GLN:HB2	2.50	0.42
6:L:10:ILE:HD13	6:L:85:MET:HG3	2.02	0.42
9:P:253:LYS:HD3	9:P:253:LYS:HA	1.89	0.42
9:P:284:ARG:HB3	9:P:362:LEU:HD12	2.02	0.42
14:Y:80:GLN:O	14:Y:83:GLU:HG2	2.20	0.42
3:H:128:LEU:HD12	4:I:346:ILE:HD13	2.02	0.41
4:I:291:TRP:HZ2	4:I:311:ASP:HB2	1.85	0.41
4:I:504:SER:N	5:K:81:LEU:HD11	2.35	0.41
7:N:298:MET:SD	7:N:324:LEU:HB3	2.60	0.41
3:H:178:SER:HA	4:I:83:LEU:HD13	2.01	0.41
4:I:686:TRP:CG	4:I:687:ILE:H	2.37	0.41
7:N:27:LEU:HD22	7:N:31:VAL:HG21	2.01	0.41
7:N:85:ASN:O	7:N:89:LEU:HG	2.20	0.41
7:N:113:ARG:HD3	7:N:119:TYR:CD1	2.54	0.41
8:O:298:ASP:OD1	8:O:298:ASP:N	2.53	0.41
14:Y:24:ASP:HA	15:Z:49:ARG:NH1	2.36	0.41
16:E:2:DT:H2''	16:E:3:DA:C5	2.55	0.41
4:I:364:LEU:HD23	4:I:396:ILE:HD12	2.02	0.41
4:I:581:GLN:HA	4:I:584:TYR:CD2	2.55	0.41
5:K:78:PHE:O	5:K:82:ARG:HB3	2.20	0.41
6:L:177:TYR:CE2	6:L:186:ASP:HB3	2.56	0.41
7:N:97:MET:HE1	7:N:201:TYR:CD1	2.55	0.41
8:O:225:LYS:HB3	8:O:234:PHE:CE1	2.55	0.41
9:P:239:LYS:H	9:P:239:LYS:HG2	1.74	0.41
10:Q:324:THR:HA	10:Q:327:ASN:HD22	1.84	0.41
13:W:36:SER:OG	13:W:37:SER:N	2.51	0.41
14:Y:42:LEU:O	14:Y:45:GLN:NE2	2.53	0.41
15:Z:62:LYS:O	15:Z:66:ILE:HG12	2.20	0.41
4:I:158:THR:HB	4:I:328:ARG:HH12	1.85	0.41
4:I:505:ASN:O	4:I:509:THR:HG23	2.21	0.41
11:T:305:SER:HA	11:T:308:ILE:HG22	2.03	0.41
11:T:355:ARG:HD2	13:W:41:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HD13	1:B:262:CYS:SG	2.60	0.41
3:H:62:ASN:HB3	4:I:501:ASN:HD21	1.85	0.41
4:I:84:GLU:HA	4:I:87:ASN:HD22	1.84	0.41
4:I:565:LYS:HB2	4:I:581:GLN:NE2	2.36	0.41
6:L:17:GLU:OE2	6:L:17:GLU:N	2.49	0.41
6:L:45:ASP:OD1	6:L:45:ASP:N	2.53	0.41
6:L:147:LEU:HD13	6:L:208:VAL:HG12	2.02	0.41
7:N:270:TRP:CD1	8:O:237:LYS:HE2	2.56	0.41
8:O:269:LYS:NZ	10:Q:330:HIS:O	2.48	0.41
10:Q:349:ASP:HB3	10:Q:352:GLU:HB3	2.02	0.41
15:Z:62:LYS:HA	15:Z:62:LYS:HD3	1.87	0.41
4:I:465:VAL:O	4:I:469:ILE:HG12	2.20	0.41
4:I:518:ILE:HA	4:I:521:GLN:HG3	2.02	0.41
4:I:543:ASN:HB2	4:I:604:PHE:HB3	2.02	0.41
4:I:711:TYR:HB3	4:I:714:ILE:HD11	2.02	0.41
5:K:231:ILE:HG13	5:K:233:PHE:CE2	2.56	0.41
8:O:341:LYS:HD2	14:Y:106:GLN:HE22	1.86	0.41
10:Q:342:SER:HB3	14:Y:155:GLN:HE21	1.85	0.41
15:Z:46:LEU:O	15:Z:49:ARG:HG3	2.20	0.41
4:I:586:MET:HA	4:I:589:THR:OG1	2.21	0.41
6:L:4:THR:HG22	6:L:222:VAL:HB	2.01	0.41
6:L:209:ILE:HG23	6:L:215:LYS:HB3	2.02	0.41
7:N:27:LEU:HD23	7:N:27:LEU:HA	1.88	0.41
3:H:41:HIS:NE2	5:K:46:LYS:HB2	2.35	0.41
3:H:61:ILE:HA	3:H:64:GLU:OE2	2.21	0.41
3:H:65:LYS:HD2	5:K:75:THR:HB	2.03	0.41
4:I:148:TRP:O	4:I:151:PRO:HD2	2.21	0.41
4:I:660:PHE:CE1	4:I:662:SER:HB3	2.55	0.41
4:I:712:ARG:H	4:I:712:ARG:HG2	1.70	0.41
6:L:121:MET:HE1	6:L:218:ARG:HA	2.02	0.41
7:N:59:ASP:HA	7:N:62:ILE:HG12	2.03	0.41
7:N:72:VAL:HA	7:N:75:ILE:HG12	2.02	0.41
7:N:228:ILE:HG22	7:N:240:PHE:HE2	1.85	0.41
7:N:401:LYS:HB3	7:N:403:LYS:HE3	2.02	0.41
9:P:197:PHE:CZ	9:P:248:ASP:HB2	2.55	0.41
10:Q:364:THR:O	10:Q:368:LYS:HG2	2.21	0.41
11:T:355:ARG:O	11:T:355:ARG:HD3	2.21	0.41
13:W:6:LEU:HD22	13:W:51:GLN:HE21	1.86	0.41
13:W:70:LEU:HD11	13:W:74:TYR:OH	2.20	0.41
14:Y:43:LYS:O	14:Y:46:VAL:HG12	2.21	0.41
16:E:11:DT:H2"	16:E:12:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:12:ILE:HD12	3:H:15:LEU:HD22	2.03	0.41
4:I:444:PHE:HB2	4:I:458:PHE:CE1	2.56	0.41
7:N:74:ARG:HB3	7:N:79:TYR:HE1	1.86	0.41
7:N:162:PHE:CE2	7:N:196:SER:HB2	2.56	0.41
8:O:166:LEU:HD12	8:O:166:LEU:HA	1.90	0.41
12:U:300:ASP:HB3	12:U:304:GLY:N	2.35	0.41
14:Y:81:ILE:HD12	14:Y:81:ILE:HA	1.96	0.41
3:H:66:THR:O	3:H:70:ILE:HG12	2.20	0.40
3:H:113:GLN:O	3:H:116:GLU:HG3	2.22	0.40
4:I:329:LYS:HA	4:I:329:LYS:HD3	1.92	0.40
4:I:362:TRP:HZ2	6:L:83:VAL:HG12	1.86	0.40
8:O:309:PHE:HA	8:O:313:ILE:O	2.20	0.40
10:Q:158:MET:H	10:Q:158:MET:HG3	1.58	0.40
15:Z:114:GLU:O	15:Z:117:SER:OG	2.30	0.40
1:B:249:LEU:HD21	1:B:263:ALA:HA	2.03	0.40
7:N:115:ASP:OD1	7:N:115:ASP:N	2.54	0.40
4:I:332:SER:OG	4:I:334:ASP:OD1	2.39	0.40
4:I:510:MET:HA	4:I:513:ILE:HG12	2.02	0.40
4:I:718:LEU:HD23	4:I:718:LEU:HA	1.89	0.40
7:N:129:ILE:CG2	7:N:146:MET:HE2	2.50	0.40
9:P:235:ARG:HA	9:P:235:ARG:HD2	1.90	0.40
15:Z:73:LEU:HD23	15:Z:74:ARG:HH12	1.86	0.40
3:H:82:LEU:HB3	5:K:72:PHE:HZ	1.86	0.40
3:H:121:ARG:HG2	4:I:388:MET:HG3	2.03	0.40
4:I:371:GLN:HG3	6:L:242:PHE:HE1	1.87	0.40
7:N:23:GLN:NE2	7:N:96:LEU:HD13	2.37	0.40
7:N:88:GLN:O	7:N:92:ILE:HG23	2.22	0.40
8:O:218:LYS:HA	8:O:219:PRO:HD3	1.93	0.40
4:I:48:LEU:HD12	4:I:48:LEU:HA	1.87	0.40
4:I:171:ILE:HD12	4:I:171:ILE:HA	1.92	0.40
7:N:98:ILE:HD11	7:N:147:PHE:HE2	1.86	0.40
7:N:136:LEU:HD23	7:N:136:LEU:HA	1.84	0.40
7:N:291:GLY:HA3	9:P:150:MET:HE1	2.02	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	99/351 (28%)	96 (97%)	3 (3%)	0	100	100
1	B	105/351 (30%)	104 (99%)	1 (1%)	0	100	100
3	H	167/181 (92%)	164 (98%)	3 (2%)	0	100	100
4	I	669/733 (91%)	646 (97%)	23 (3%)	0	100	100
5	K	213/239 (89%)	210 (99%)	3 (1%)	0	100	100
6	L	239/245 (98%)	236 (99%)	3 (1%)	0	100	100
7	N	383/458 (84%)	364 (95%)	19 (5%)	0	100	100
8	O	237/368 (64%)	224 (94%)	13 (6%)	0	100	100
9	P	251/369 (68%)	240 (96%)	11 (4%)	0	100	100
10	Q	254/406 (63%)	251 (99%)	3 (1%)	0	100	100
11	T	90/361 (25%)	88 (98%)	2 (2%)	0	100	100
12	U	180/324 (56%)	173 (96%)	7 (4%)	0	100	100
13	W	65/89 (73%)	65 (100%)	0	0	100	100
14	Y	217/238 (91%)	209 (96%)	8 (4%)	0	100	100
15	Z	149/153 (97%)	146 (98%)	3 (2%)	0	100	100
All	All	3318/4866 (68%)	3216 (97%)	102 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	89/305 (29%)	89 (100%)	0	100	100
1	B	94/305 (31%)	90 (96%)	4 (4%)	26	49
3	H	162/172 (94%)	160 (99%)	2 (1%)	63	72
4	I	631/683 (92%)	625 (99%)	6 (1%)	68	75
5	K	202/223 (91%)	202 (100%)	0	100	100
6	L	217/221 (98%)	214 (99%)	3 (1%)	59	71
7	N	353/416 (85%)	350 (99%)	3 (1%)	73	77
8	O	226/347 (65%)	222 (98%)	4 (2%)	51	67
9	P	241/344 (70%)	238 (99%)	3 (1%)	63	72
10	Q	242/378 (64%)	241 (100%)	1 (0%)	84	83
11	T	89/339 (26%)	89 (100%)	0	100	100
12	U	168/309 (54%)	166 (99%)	2 (1%)	63	72
13	W	57/76 (75%)	56 (98%)	1 (2%)	51	67
14	Y	175/219 (80%)	175 (100%)	0	100	100
15	Z	121/143 (85%)	119 (98%)	2 (2%)	53	68
All	All	3067/4480 (68%)	3036 (99%)	31 (1%)	65	75

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	238	ILE
1	B	268	GLN
1	B	274	ASP
1	B	313	ILE
3	H	15	LEU
3	H	64	GLU
4	I	59	ASP
4	I	253	ASN
4	I	389	ASP
4	I	411	LEU
4	I	503	THR
4	I	518	ILE
6	L	83	VAL
6	L	145	SER
6	L	222	VAL
7	N	142	CYS
7	N	225	LEU
7	N	299	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	O	208	VAL
8	O	266	LEU
8	O	353	ASP
8	O	361	HIS
9	P	128	ILE
9	P	209	ASP
9	P	282	VAL
10	Q	268	LEU
12	U	167	ARG
12	U	299	MET
13	W	62	ARG
15	Z	25	PHE
15	Z	81	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	308	ASN
3	H	8	GLN
3	H	19	HIS
3	H	50	GLN
3	H	88	ASN
3	H	102	GLN
3	H	107	GLN
3	H	176	ASN
4	I	46	GLN
4	I	141	GLN
4	I	212	ASN
4	I	242	HIS
4	I	264	GLN
4	I	363	GLN
4	I	467	GLN
4	I	505	ASN
5	K	28	GLN
5	K	77	ASN
5	K	100	GLN
5	K	163	ASN
5	K	212	ASN
5	K	234	ASN
6	L	13	GLN
6	L	241	GLN
7	N	165	ASN

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Mol	Chain	Res	Type
7	N	435	ASN
8	O	122	GLN
8	O	360	ASN
9	P	259	GLN
9	P	359	ASN
10	Q	246	ASN
10	Q	250	GLN
10	Q	253	GLN
10	Q	254	ASN
10	Q	255	ASN
10	Q	327	ASN
10	Q	330	HIS
10	Q	382	HIS
13	W	51	GLN
14	Y	77	GLN
14	Y	145	ASN
15	Z	9	ASN
15	Z	41	HIS
15	Z	102	GLN
15	Z	106	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.

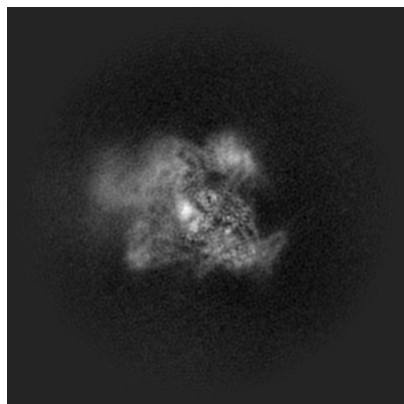
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75095. These allow visual inspection of the internal detail of the map and identification of artifacts.

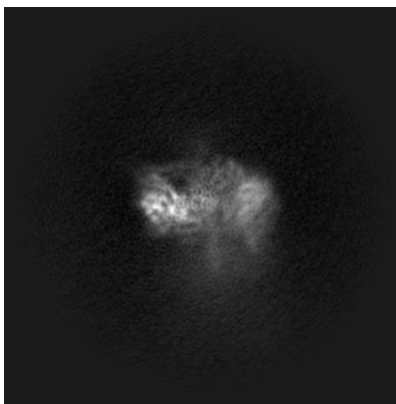
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

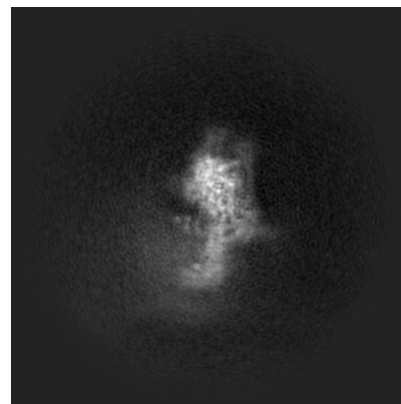
#### 6.1.1 Primary map



X

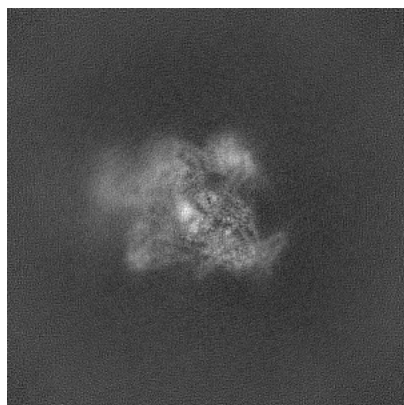


Y

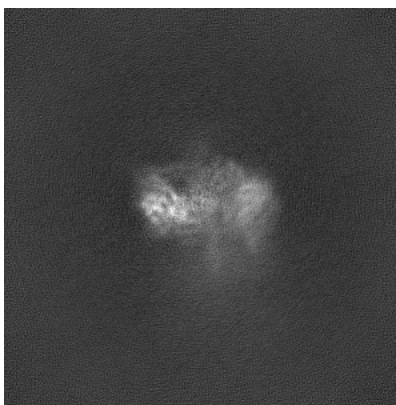


Z

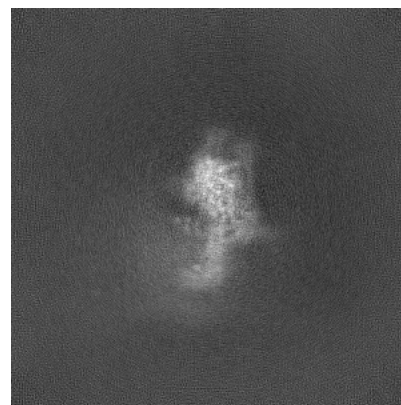
#### 6.1.2 Raw map



X



Y

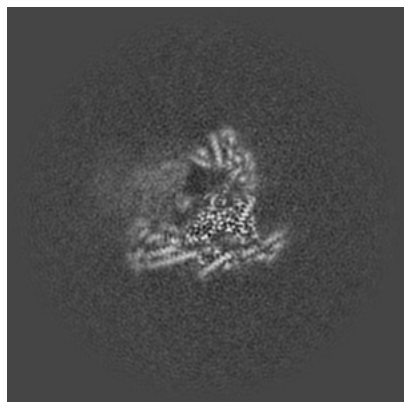


Z

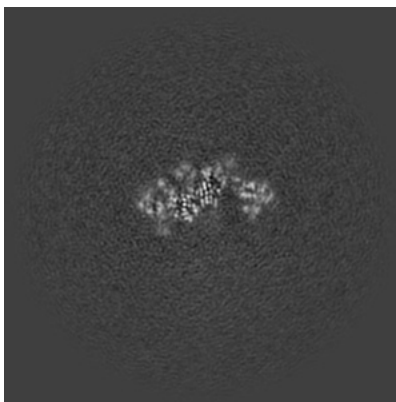
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

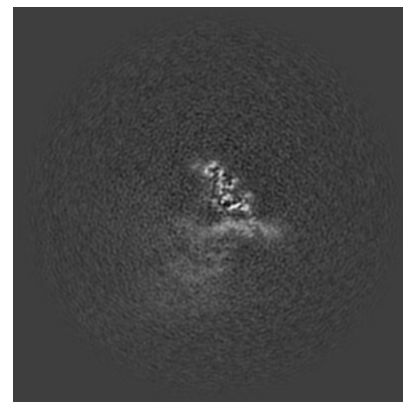
### 6.2.1 Primary map



X Index: 200

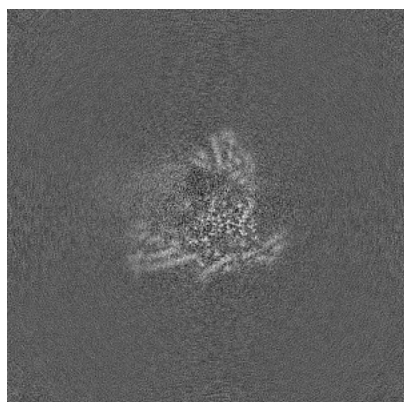


Y Index: 200

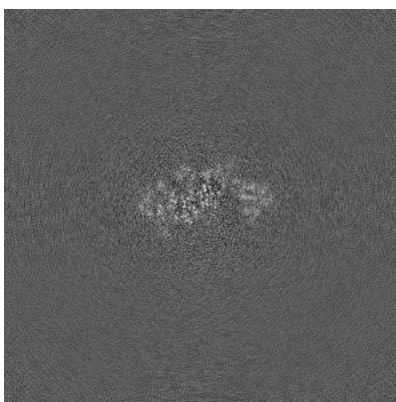


Z Index: 200

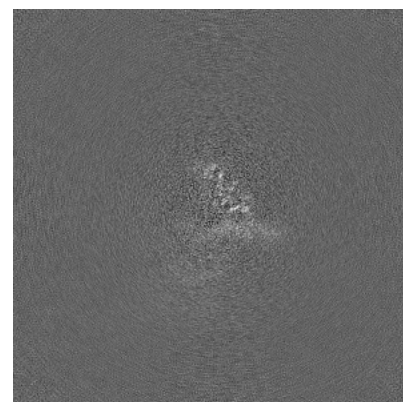
### 6.2.2 Raw map



X Index: 200



Y Index: 200

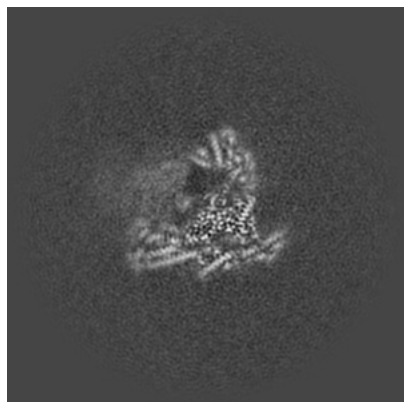


Z Index: 200

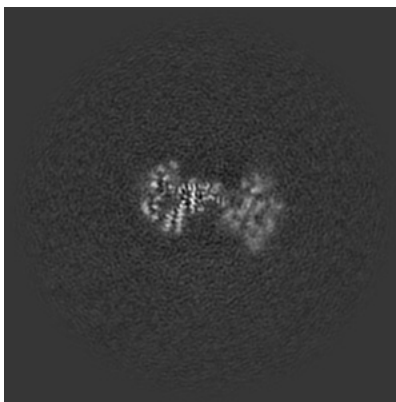
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

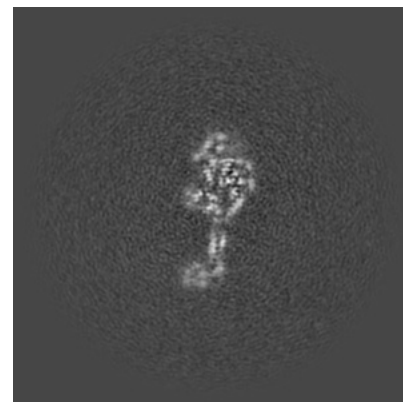
### 6.3.1 Primary map



X Index: 200

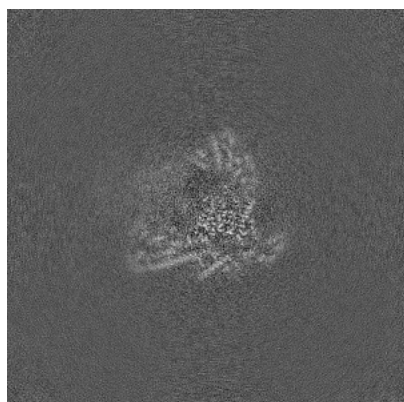


Y Index: 221

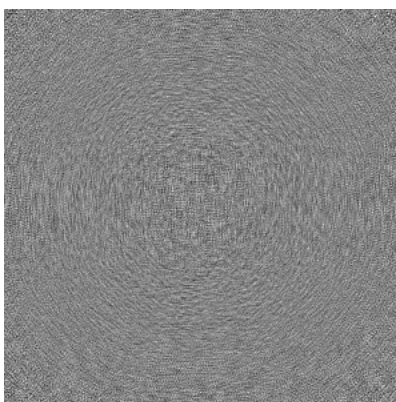


Z Index: 156

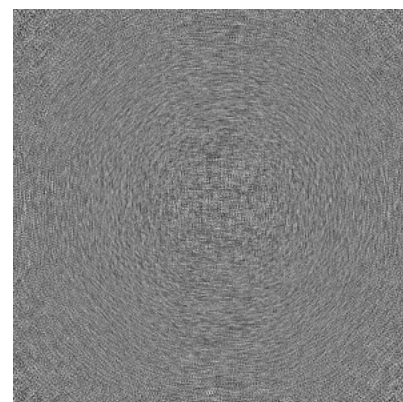
### 6.3.2 Raw map



X Index: 201



Y Index: 0

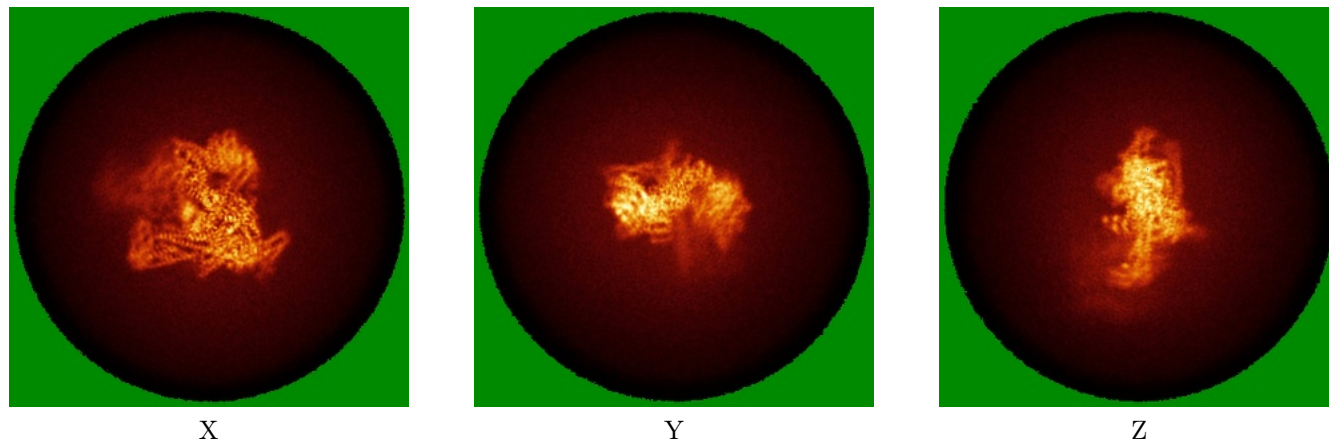


Z Index: 0

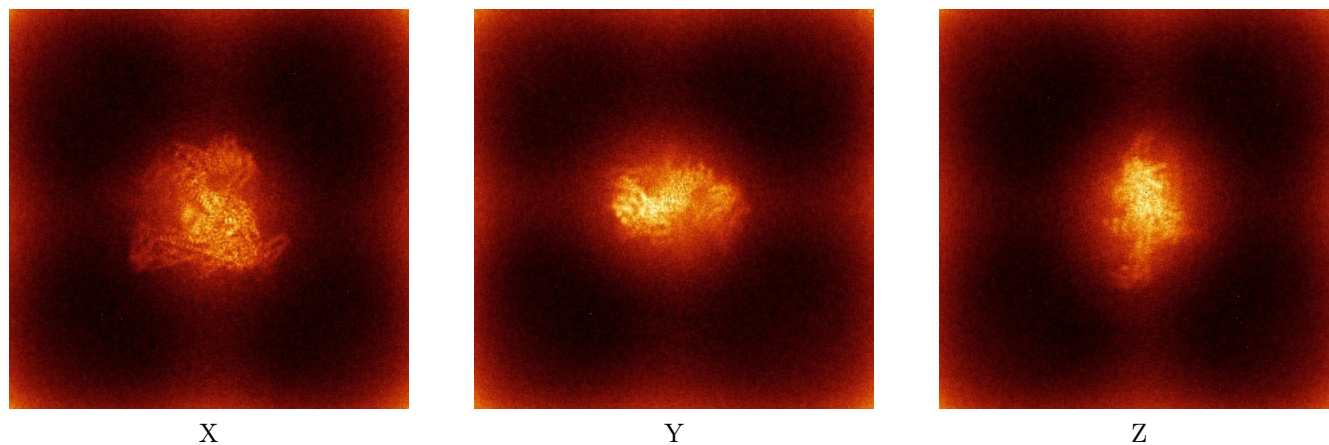
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



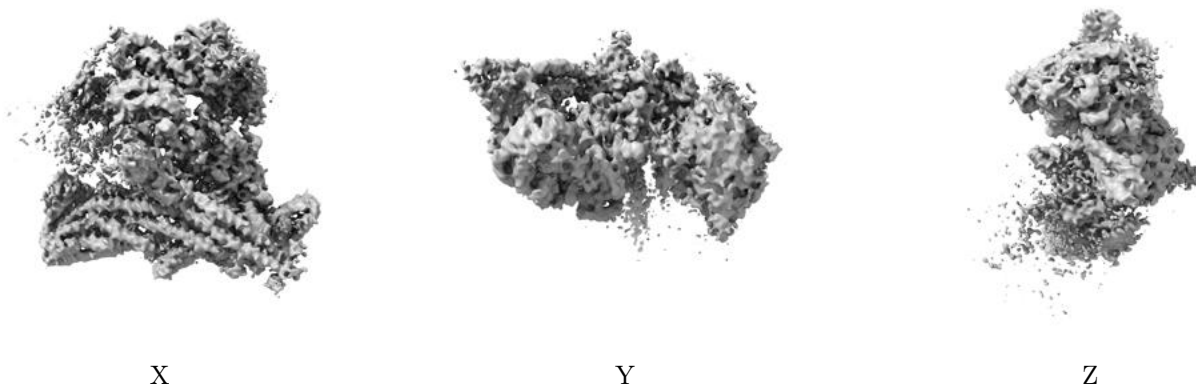
### 6.4.2 Raw map



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.

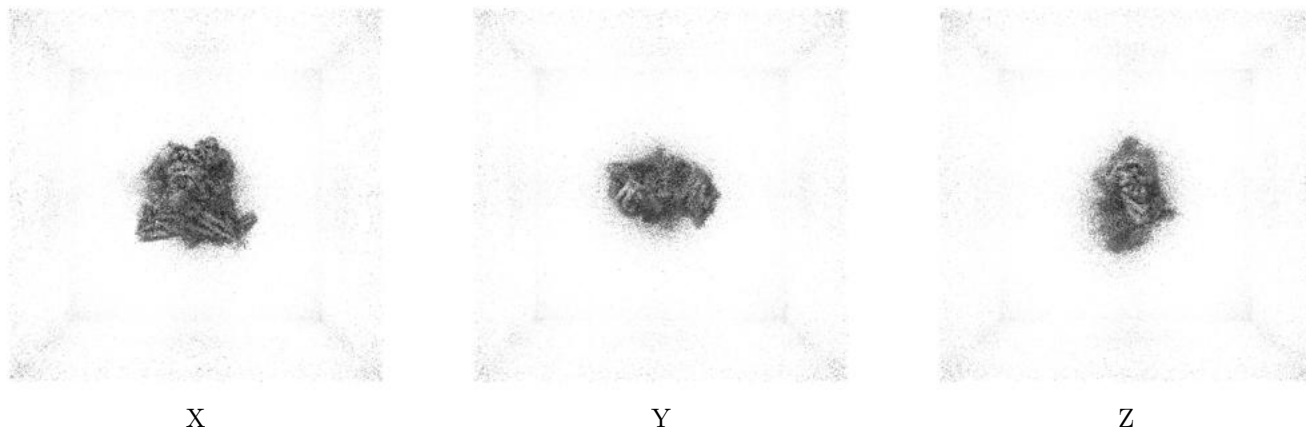
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

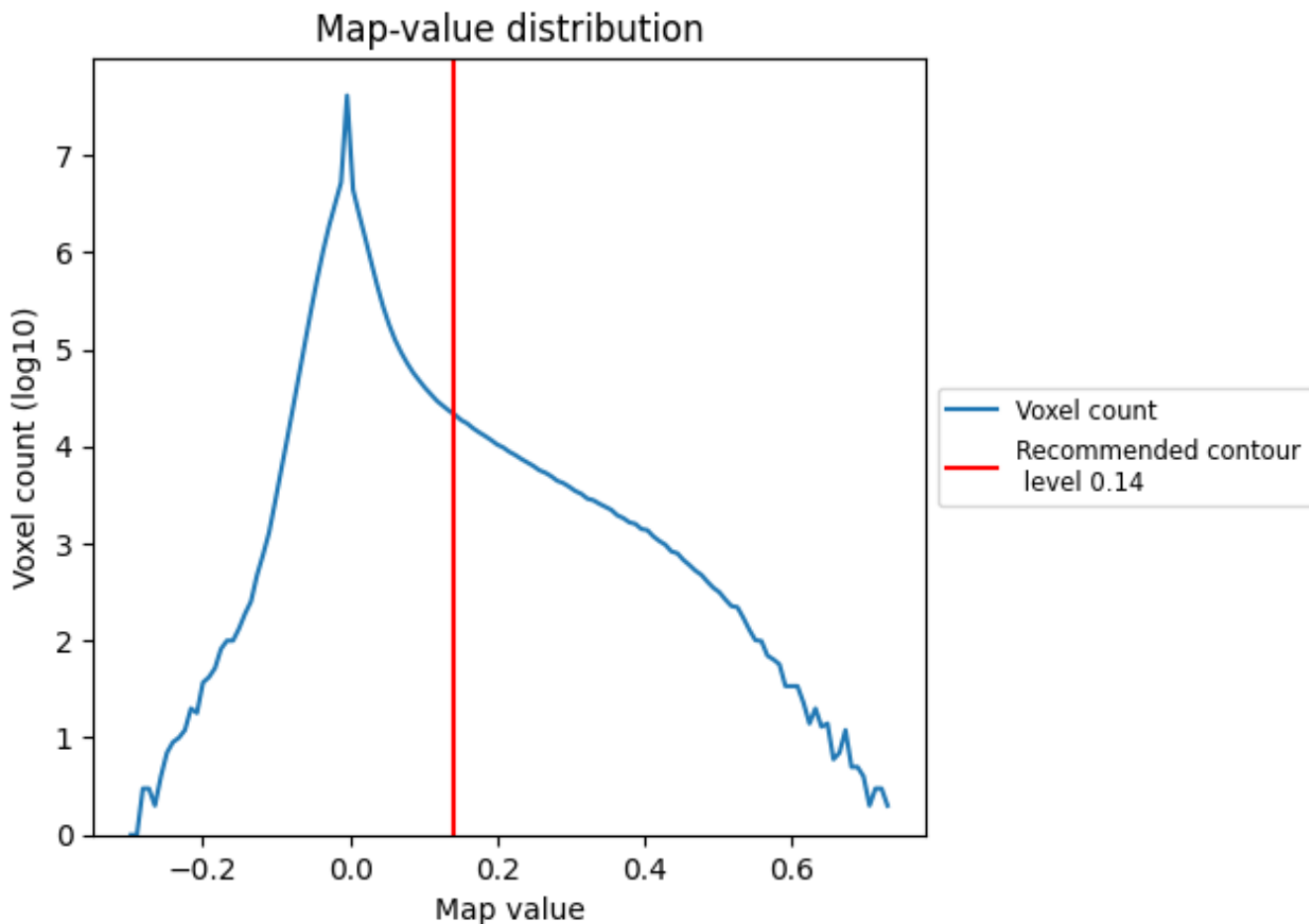
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

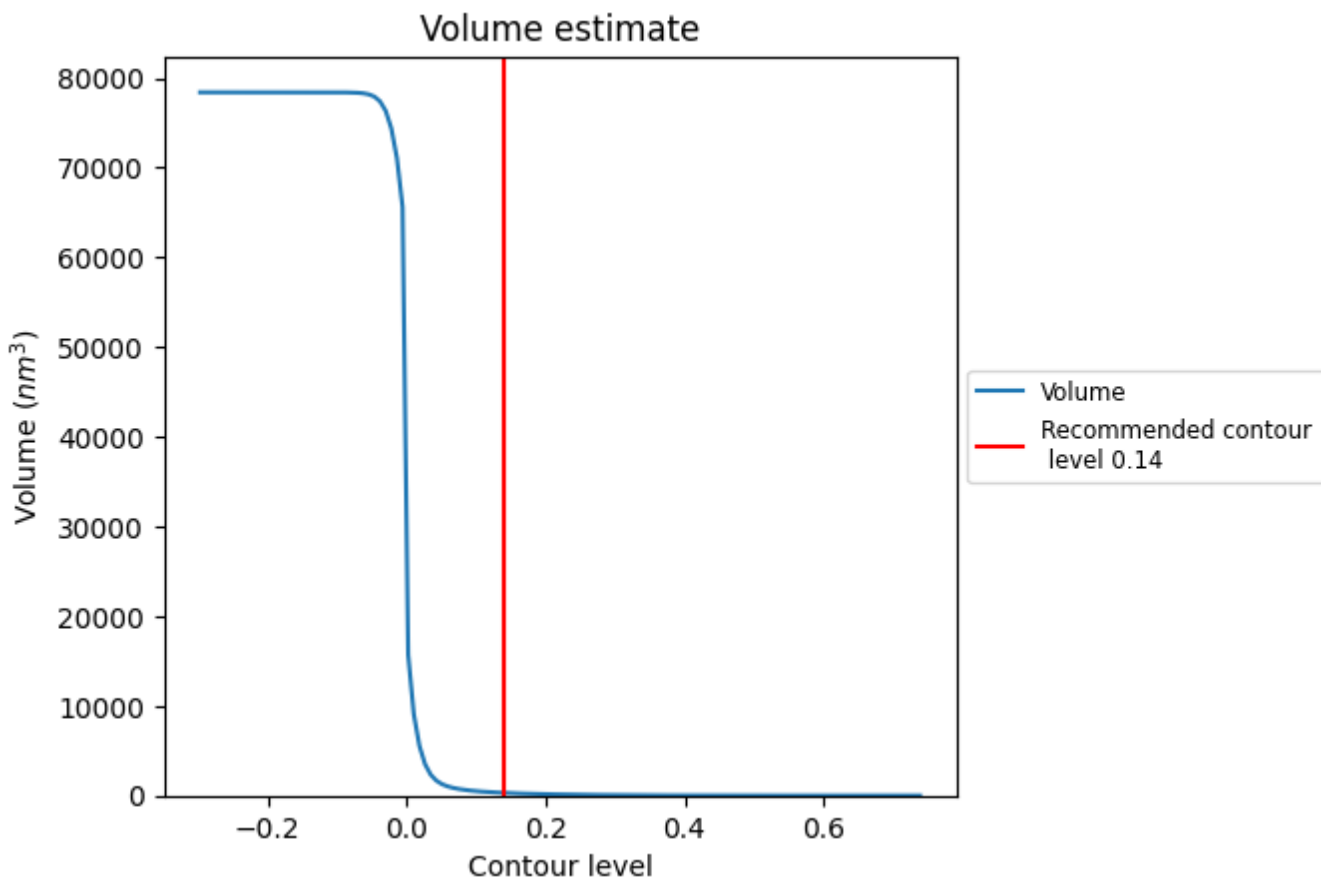
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

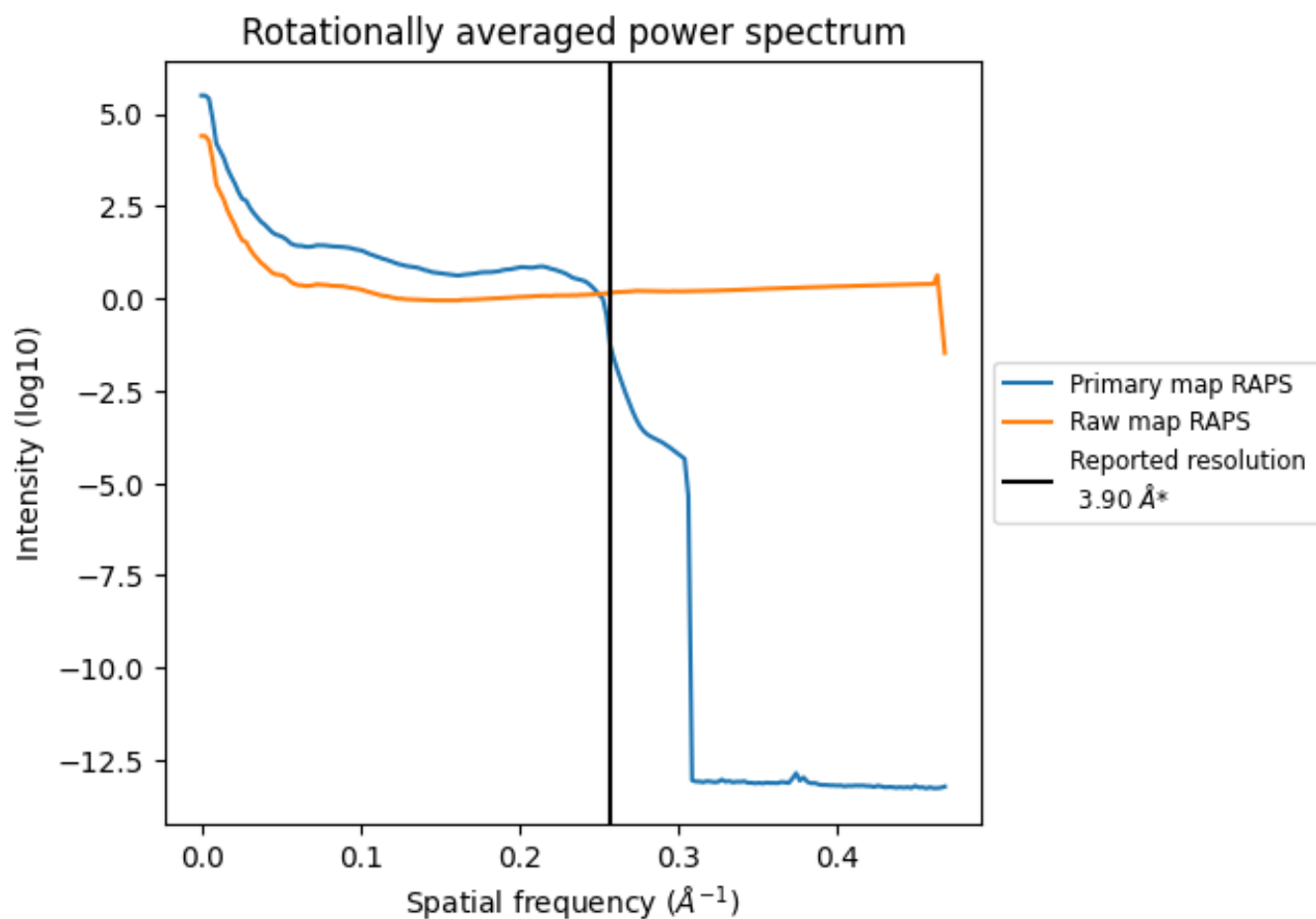
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300  $\text{nm}^3$ ; this corresponds to an approximate mass of 271 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

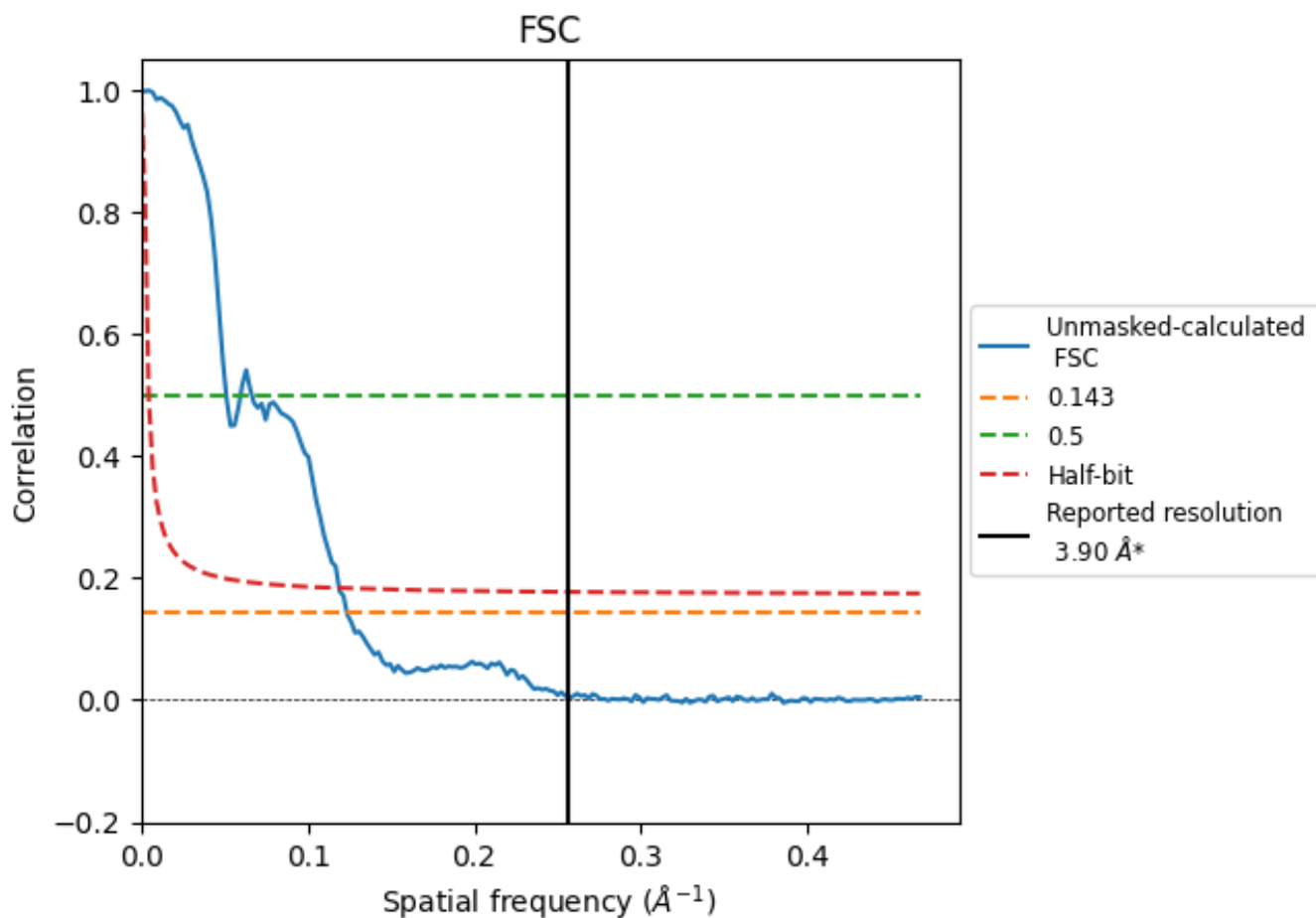


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

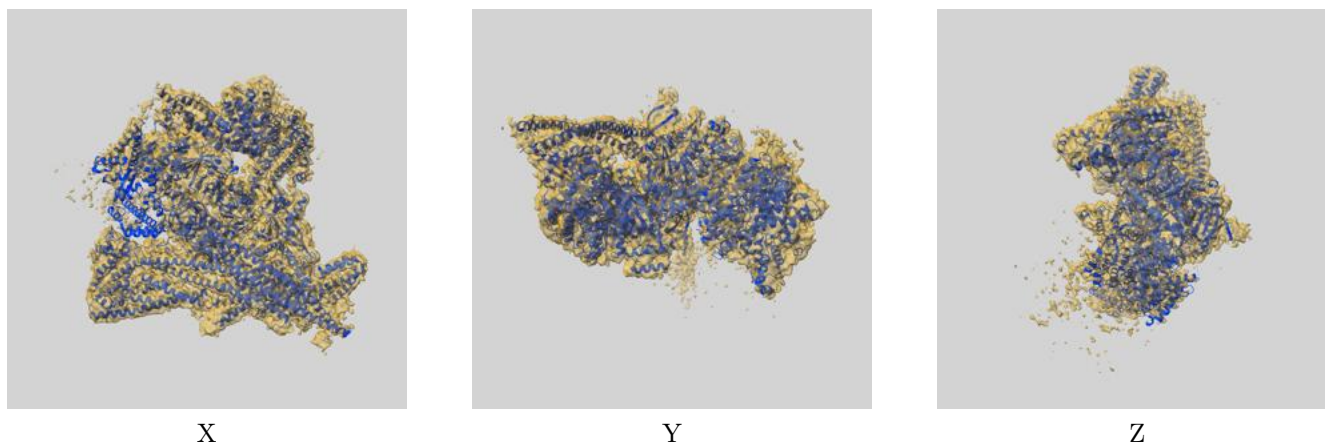
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.09	19.57	8.41

\*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 8.09 differs from the reported value 3.9 by more than 10 %

## 9 Map-model fit [i](#)

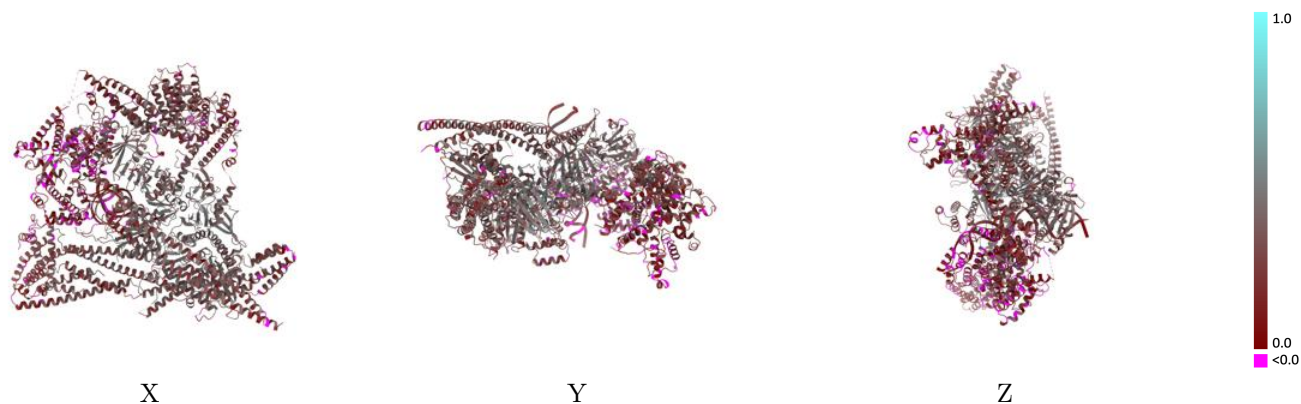
This section contains information regarding the fit between EMDB map EMD-75095 and PDB model 10DQ. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



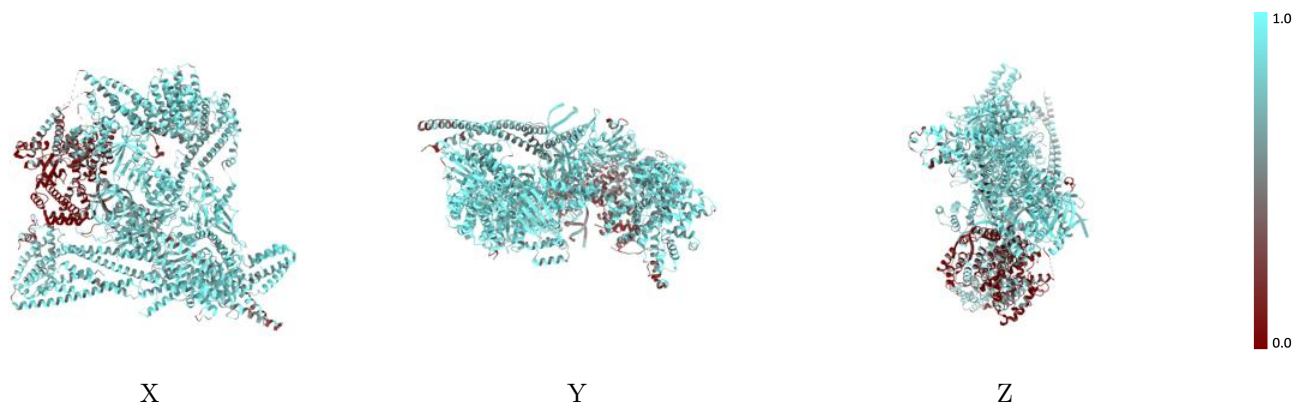
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



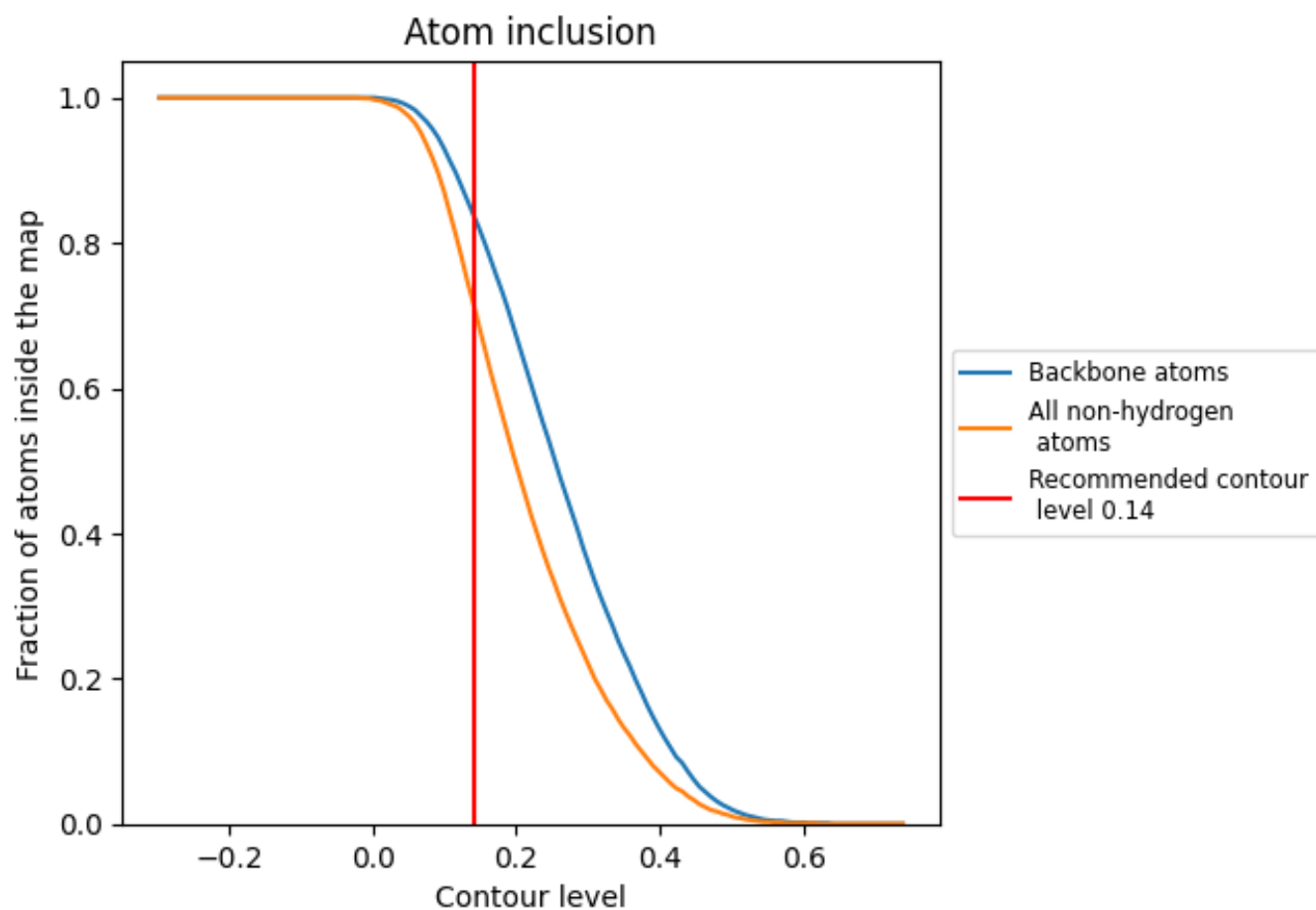
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).





































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 72% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7170	 0.2700
A	 0.6580	 0.2810
B	 0.6530	 0.2980
D	 0.7450	 0.1970
E	 0.6580	 0.1720
H	 0.6790	 0.1720
I	 0.6100	 0.1880
K	 0.5220	 0.1700
L	 0.8650	 0.3750
N	 0.8660	 0.3740
O	 0.8640	 0.3720
P	 0.8620	 0.3740
Q	 0.7380	 0.2540
T	 0.1020	 0.1470
U	 0.8230	 0.2960
W	 0.0780	 0.1330
Y	 0.8540	 0.2920
Z	 0.8400	 0.2650

