



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:36 AM UTC

PDB ID : 8XX5 / pdb_00008xx5
EMDB ID : EMD-38746
Title : ASFV RNAP M1249L C-tail occupied complex1 (MCOC1)
Authors : Zhu, G.L.; Zhu, Y.; Zhu, Z.X.; Sun, F.; Zheng, H.X.
Deposited on : 2024-01-17
Resolution : 2.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

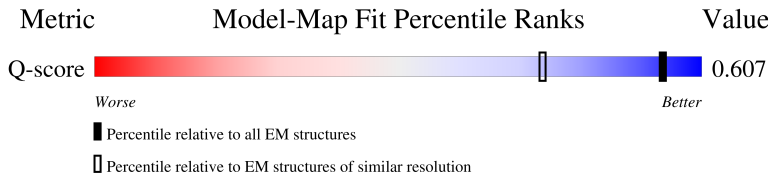
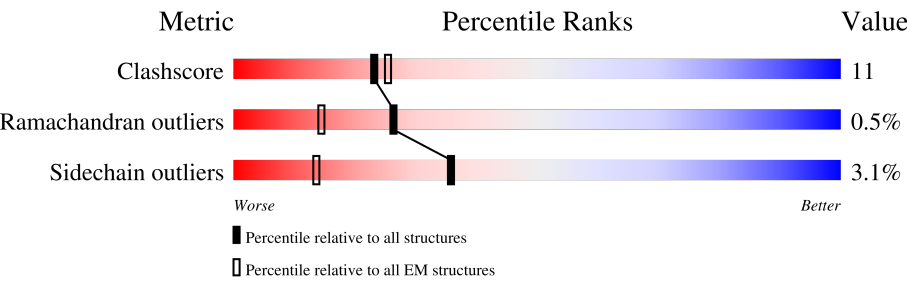
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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	5628 (1.90 - 2.90)

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	B	1235	70% 28% ..
2	C	359	77% 22% .
3	D	205	6% 72% 27%
4	F	334	22% 63% 34% .

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Mol	Chain	Length	Quality of chain
5	G	105	10% 67% 31%
6	H	80	71% 29%
7	I	1183	10% 54% 25% 20%
8	E	139	8% 60% 31% 7%
9	A	1440	73% 24%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 38337 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-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1222	Total	C	N	O	S	0	0
			9672	6107	1701	1813	51		

- Molecule 2 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	359	Total	C	N	O	S	0	0
			2915	1890	482	530	13		

- Molecule 3 is a protein called DNA-directed RNA polymerase RPB5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	205	Total	C	N	O	S	0	0
			1669	1088	278	295	8		

- Molecule 4 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	334	Total	C	N	O	S	0	0
			2686	1726	444	502	14		

- Molecule 5 is a protein called C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	105	Total	C	N	O	S	0	0
			816	507	141	153	15		

- Molecule 6 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	80	Total	C	N	O	S	0	0
			631	411	102	111	7		

- Molecule 7 is a protein called M1249L.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	952	Total	C	N	O	S	0	0
			7761	4991	1279	1453	38		

- Molecule 8 is a protein called C147L.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	129	Total	C	N	O	S	0	0
			1021	648	167	200	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1404	Total	C	N	O	S	0	0
			11158	7082	1937	2078	61		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	Zn	0
			1	1	
10	G	2	Total	Zn	0
			2	2	
10	H	1	Total	Zn	0
			1	1	
10	I	1	Total	Zn	0
			1	1	
10	A	2	Total	Zn	0
			2	2	

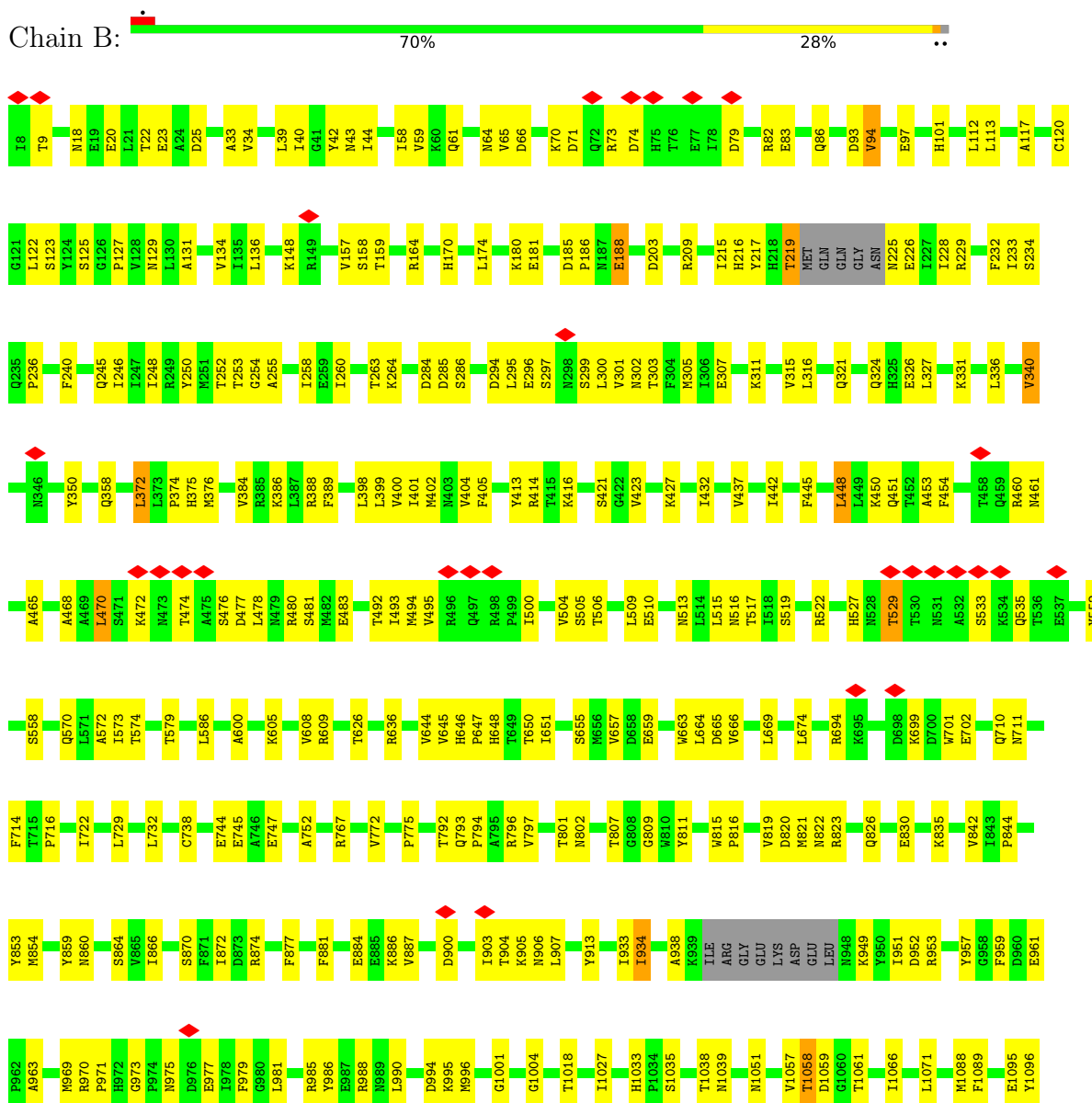
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

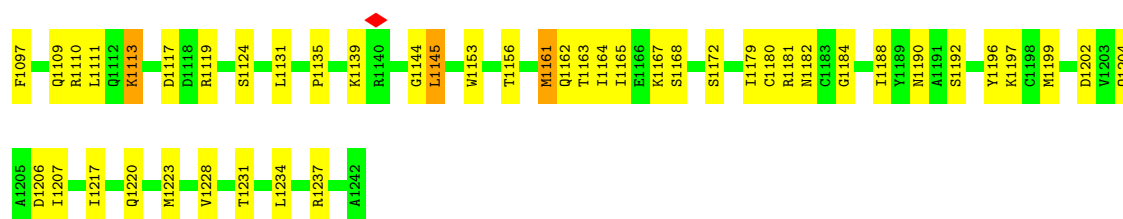
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

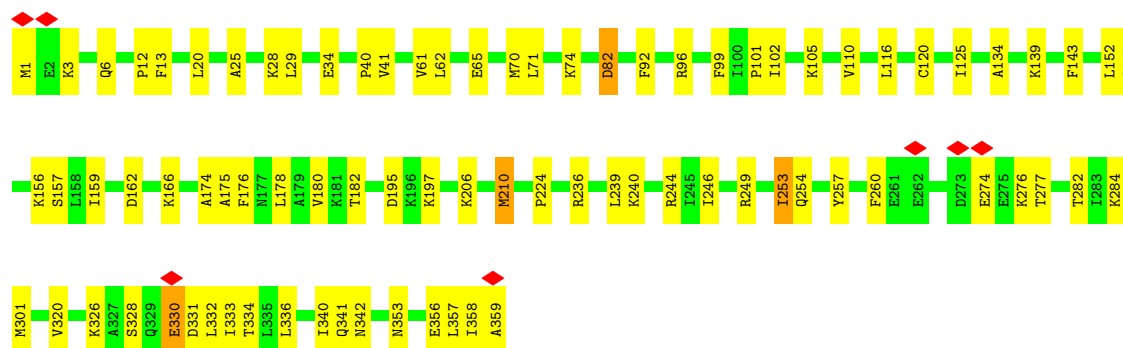
- Molecule 1: DNA-directed RNA polymerase subunit beta





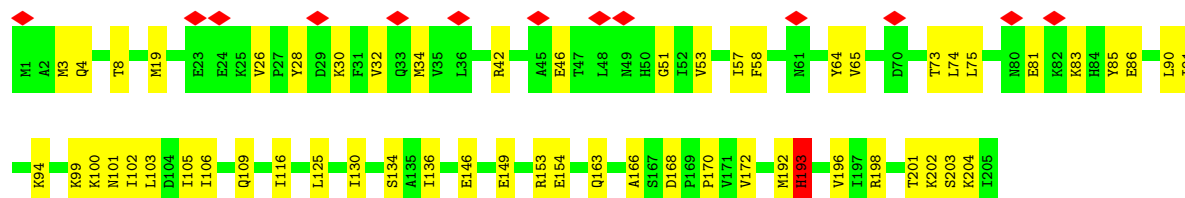
- Molecule 2: DNA-directed RNA polymerase RPB3-11 homolog

Chain C: 77% 22% .



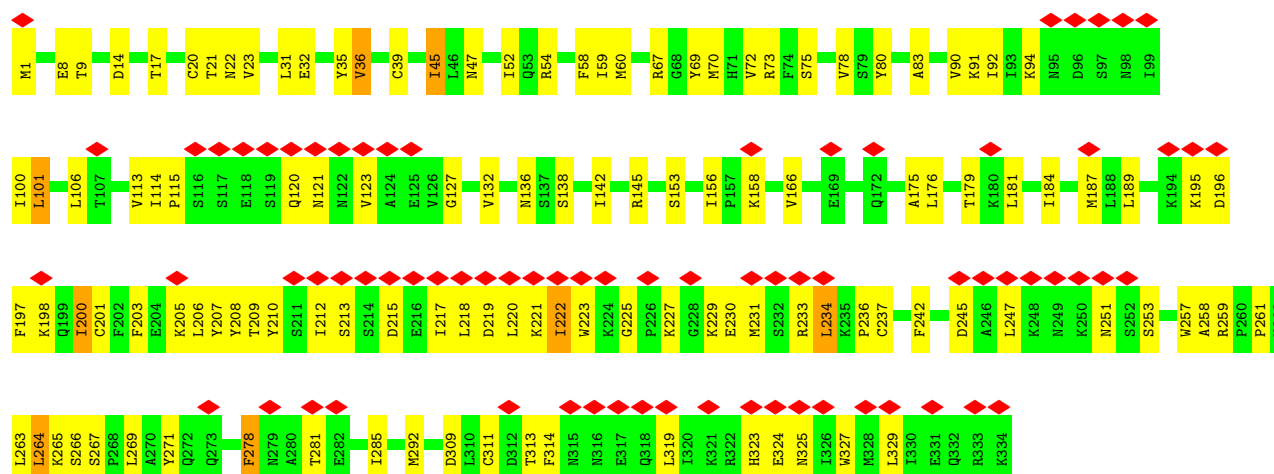
- Molecule 3: DNA-directed RNA polymerase RPB5 homolog

Chain D: 6% 72% 27% .

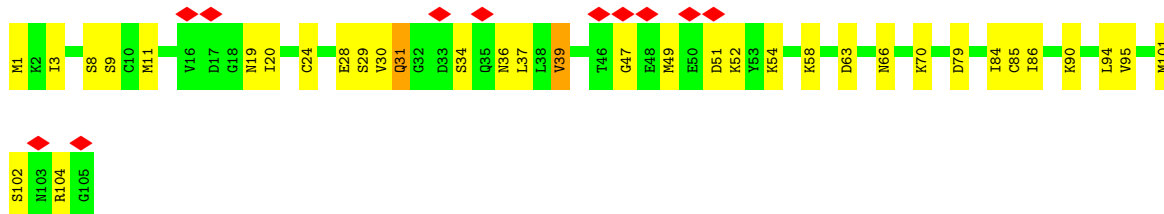


- Molecule 4: D339L

Chain F: 22% 63% 34% .



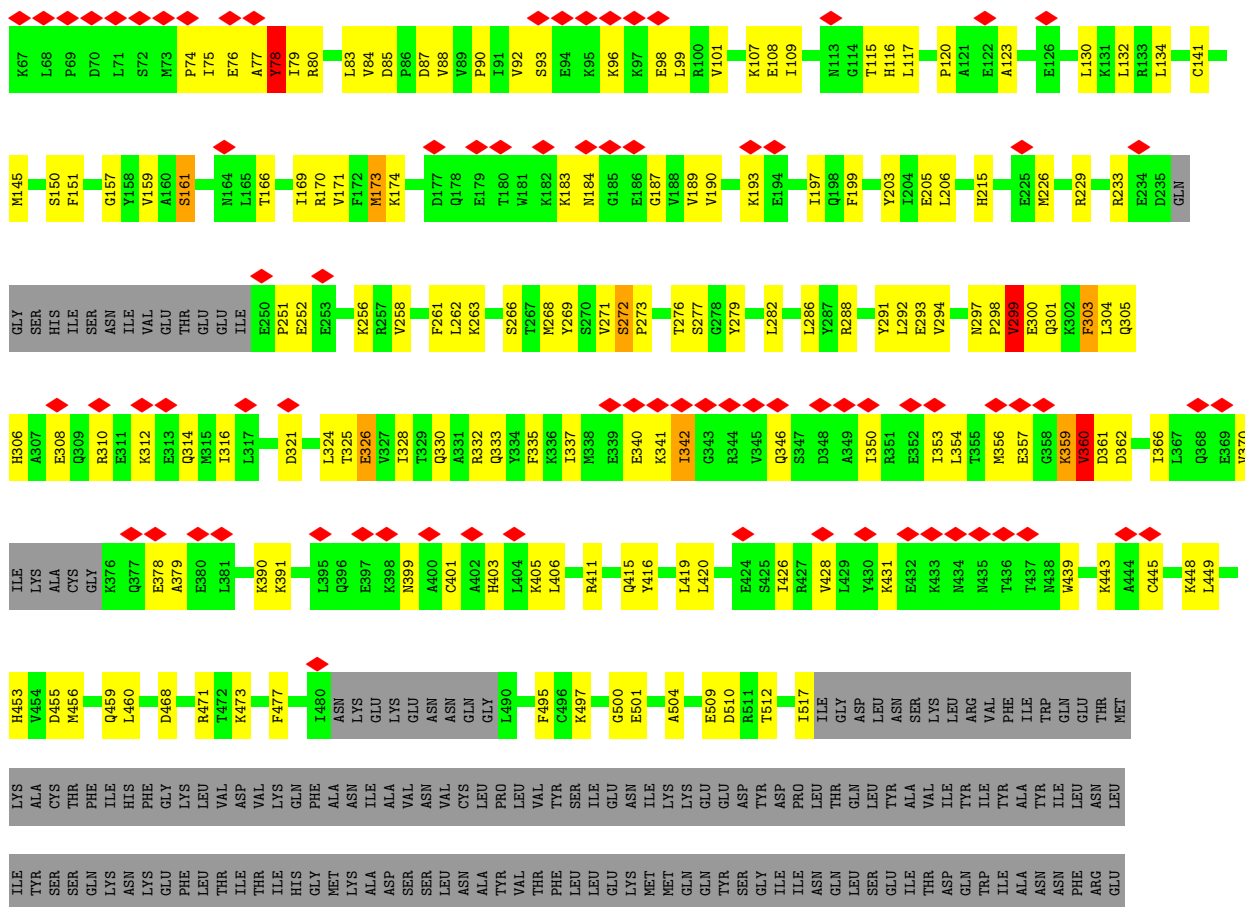
- Molecule 5: C122R

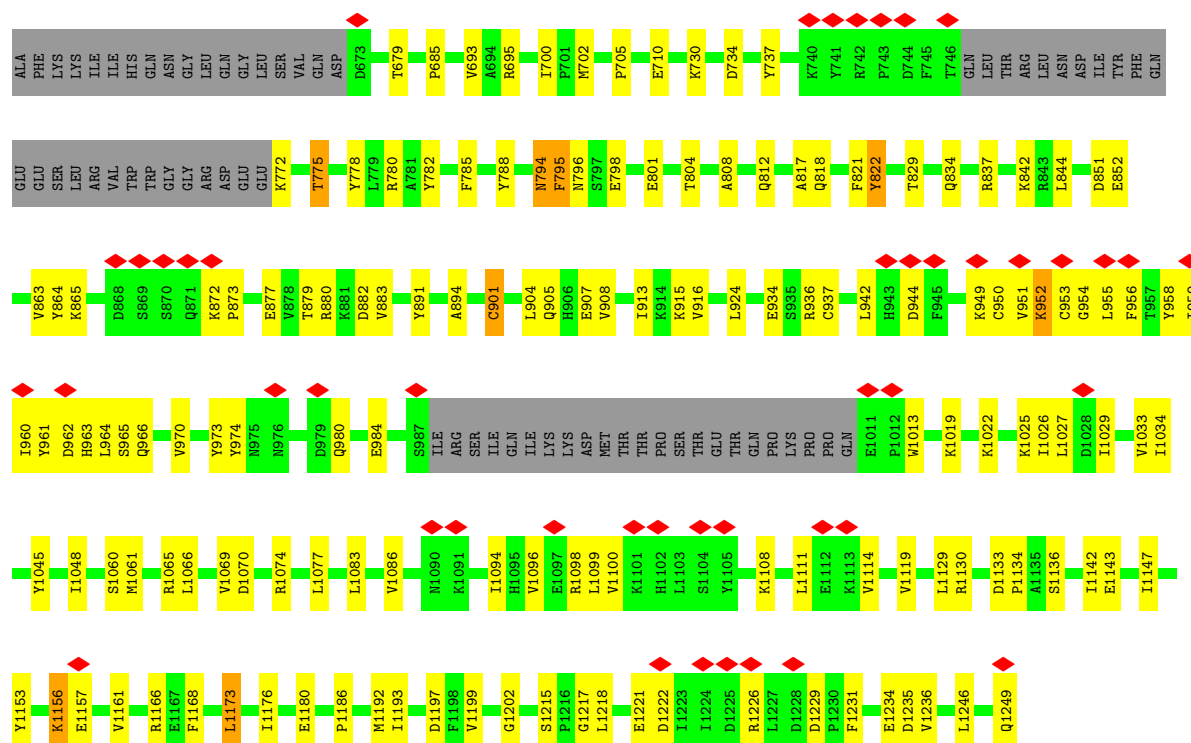


- Molecule 6: DNA-directed RNA polymerase RPB10 homolog

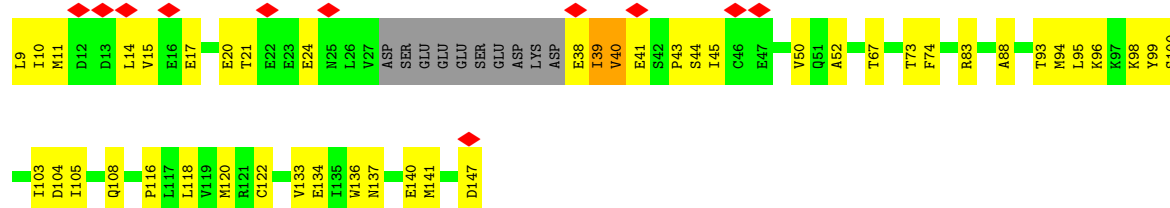


- Molecule 7: M1249L

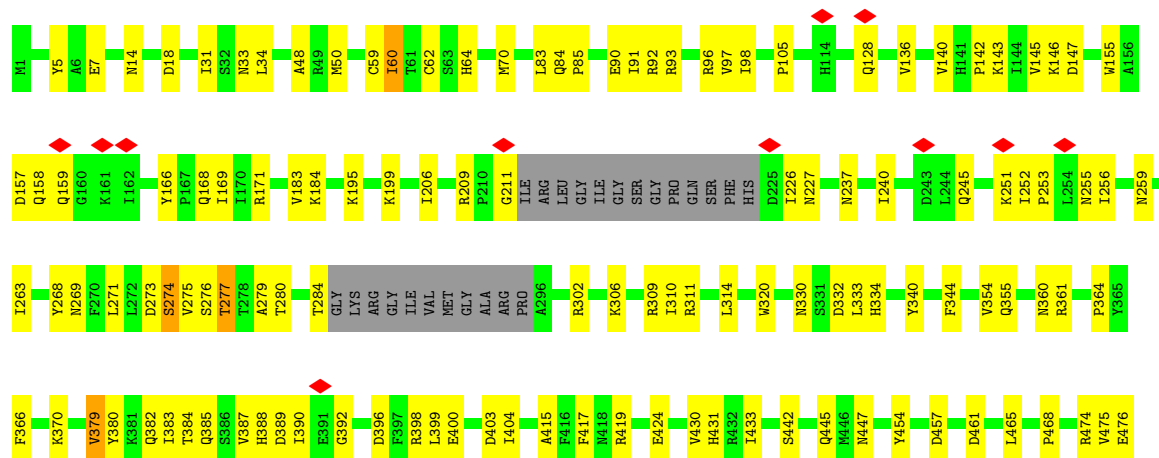




• Molecule 8: C147L



• Molecule 9: DNA-directed RNA polymerase subunit





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372305	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.327	Depositor
Minimum map value	-1.740	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	B	0.14	0/9866	0.31	0/13352
2	C	0.12	0/2977	0.28	0/4022
3	D	0.14	0/1708	0.35	0/2311
4	F	0.14	0/2739	0.35	0/3709
5	G	0.12	0/828	0.31	0/1109
6	H	0.14	0/644	0.26	0/872
7	I	0.14	0/7930	0.37	2/10718 (0.0%)
8	E	0.14	0/1033	0.31	0/1398
9	A	0.13	0/11374	0.31	1/15409 (0.0%)
All	All	0.13	0/39099	0.32	3/52900 (0.0%)

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
7	I	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	78	TYR	N-CA-C	-6.28	106.58	114.56
9	A	226	ILE	N-CA-C	-5.89	108.11	113.71
7	I	78	TYR	CA-CB-CG	5.10	123.08	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	I	952	LYS	Peptide

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	B	9672	0	9630	242	0
2	C	2915	0	2994	50	0
3	D	1669	0	1713	37	0
4	F	2686	0	2721	85	0
5	G	816	0	813	26	0
6	H	631	0	659	17	0
7	I	7761	0	7748	223	0
8	E	1021	0	1054	35	0
9	A	11158	0	11260	249	0
10	A	2	0	0	0	0
10	B	1	0	0	0	0
10	G	2	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
11	A	1	0	0	0	0
All	All	38337	0	38592	850	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 11.

All (850) 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)
9:A:1125:LEU:HD12	9:A:1195:ILE:HD11	1.59	0.82
7:I:936:ARG:HG2	9:A:1189:SER:HB2	1.61	0.82
9:A:582:MET:HG3	9:A:725:PRO:HG2	1.61	0.82
2:C:61:VAL:HA	2:C:65:GLU:HB2	1.63	0.80
7:I:173:MET:HE1	7:I:203:TYR:HB2	1.64	0.80
1:B:316:LEU:HA	1:B:324:GLN:HE22	1.51	0.76
9:A:240:ILE:HD11	9:A:259:ASN:HB3	1.68	0.75
9:A:142:PRO:HB3	9:A:158:GLN:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:168:GLN:NE2	9:A:245:GLN:OE1	2.21	0.73
4:F:267:SER:HB2	4:F:269:LEU:HD13	1.70	0.73
1:B:605:LYS:HE3	1:B:609:ARG:HH11	1.56	0.71
7:I:960:ILE:HG13	7:I:962:ASP:H	1.56	0.71
7:I:354:LEU:HD23	7:I:360:VAL:HA	1.72	0.71
7:I:460:LEU:HD21	7:I:473:LYS:HD2	1.73	0.71
7:I:772:LYS:HA	7:I:772:LYS:HE2	1.72	0.71
7:I:353:ILE:HG13	7:I:356:MET:HE2	1.72	0.71
1:B:657:VAL:HG23	1:B:659:GLU:HG3	1.73	0.71
1:B:294:ASP:HB2	1:B:608:VAL:HG11	1.73	0.70
3:D:101:ASN:O	3:D:105:ILE:HD12	1.91	0.70
9:A:1015:THR:H	9:A:1018:GLN:HE21	1.37	0.70
1:B:494:MET:HG3	8:E:14:LEU:HD21	1.73	0.70
9:A:1158:PHE:HZ	9:A:1200:ARG:HH22	1.40	0.70
7:I:951:VAL:HG22	7:I:952:LYS:HG3	1.74	0.69
8:E:137:ASN:ND2	8:E:140:GLU:OE1	2.25	0.69
7:I:328:ILE:HD13	7:I:361:ASP:HB3	1.73	0.69
4:F:14:ASP:HA	4:F:67:ARG:HG2	1.74	0.69
1:B:1051:ASN:HD21	1:B:1058:THR:HB	1.57	0.69
1:B:579:THR:HA	1:B:666:VAL:HG23	1.74	0.69
1:B:284:ASP:HB2	5:G:9:SER:HA	1.75	0.68
9:A:672:GLU:OE1	9:A:714:ARG:NH2	2.25	0.68
1:B:900:ASP:H	1:B:903:ILE:HB	1.59	0.68
4:F:245:ASP:OD1	4:F:251:ASN:ND2	2.25	0.68
9:A:1057:MET:HG2	9:A:1074:ILE:HD11	1.75	0.68
1:B:264:LYS:NZ	7:I:1202:GLY:O	2.24	0.68
7:I:268:MET:HE1	7:I:308:GLU:HG2	1.75	0.68
1:B:792:THR:HG23	1:B:1038:THR:HA	1.76	0.68
1:B:70:LYS:HG3	7:I:1192:MET:HG3	1.76	0.68
9:A:380:TYR:HB3	9:A:404:ILE:HB	1.75	0.67
7:I:370:VAL:HG11	7:I:379:ALA:HB2	1.76	0.67
7:I:904:LEU:HB2	7:I:907:GLU:HG3	1.77	0.67
9:A:876:SER:HB2	9:A:1283:LYS:HB2	1.76	0.67
7:I:399:ASN:ND2	7:I:445:CYS:SG	2.67	0.67
1:B:835:LYS:HE2	6:H:42:PRO:HB3	1.76	0.67
1:B:877:PHE:O	1:B:1110:ARG:NH1	2.27	0.67
7:I:145:MET:HE1	7:I:159:VAL:HG21	1.76	0.67
4:F:205:LYS:HZ3	4:F:212:ILE:HD13	1.60	0.67
1:B:650:THR:HB	1:B:663:TRP:HB2	1.76	0.66
1:B:1033:HIS:CE1	1:B:1039:ASN:HD22	2.13	0.66
7:I:924:LEU:HD21	9:A:683:ARG:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:400:GLU:N	9:A:400:GLU:OE1	2.28	0.66
1:B:295:LEU:HD11	5:G:1:MET:HE1	1.76	0.66
1:B:236:PRO:HA	1:B:375:HIS:HA	1.77	0.66
4:F:259:ARG:NH2	4:F:267:SER:O	2.28	0.66
7:I:293:GLU:HG2	7:I:297:ASN:HB2	1.78	0.66
1:B:1206:ASP:OD2	1:B:1237:ARG:NH2	2.27	0.66
9:A:1125:LEU:HD13	9:A:1190:ILE:HG21	1.78	0.65
5:G:63:ASP:OD2	9:A:777:ARG:NH1	2.29	0.65
9:A:415:ALA:HB2	9:A:433:ILE:HD11	1.78	0.65
2:C:28:LYS:HD2	6:H:23:LYS:HE2	1.76	0.65
1:B:995:LYS:HG2	1:B:1111:LEU:HD12	1.77	0.65
1:B:180:LYS:HD3	1:B:186:PRO:HG3	1.79	0.65
1:B:510:GLU:O	1:B:516:ASN:ND2	2.30	0.65
1:B:650:THR:HG21	1:B:744:GLU:HG3	1.77	0.65
1:B:881:PHE:HB2	1:B:988:ARG:HG3	1.78	0.64
7:I:477:PHE:O	7:I:497:LYS:N	2.29	0.64
1:B:988:ARG:NH2	1:B:1117:ASP:OD1	2.29	0.64
9:A:90:GLU:OE1	9:A:93:ARG:NH1	2.31	0.64
1:B:217:TYR:HA	1:B:228:ILE:HG13	1.79	0.64
5:G:19:ASN:ND2	5:G:31:GLN:OE1	2.30	0.64
1:B:74:ASP:HA	1:B:79:ASP:HB3	1.80	0.64
4:F:189:LEU:HB3	4:F:223:TRP:HB2	1.80	0.64
4:F:324:GLU:OE2	4:F:325:ASN:ND2	2.30	0.64
7:I:96:LYS:HD3	7:I:98:GLU:HB3	1.79	0.64
3:D:65:VAL:O	3:D:99:LYS:NZ	2.31	0.64
9:A:928:ARG:HD3	9:A:997:LEU:HD21	1.78	0.64
1:B:303:THR:O	1:B:307:GLU:HG3	1.98	0.64
1:B:1167:LYS:NZ	9:A:320:TRP:O	2.31	0.63
8:E:93:THR:HG22	8:E:95:LEU:H	1.64	0.63
7:I:251:PRO:HB2	7:I:256:LYS:HG2	1.80	0.63
6:H:48:GLN:HA	7:I:822:TYR:HA	1.81	0.63
1:B:830:GLU:OE2	6:H:72:THR:OG1	2.17	0.62
9:A:1002:ILE:HG23	9:A:1006:LEU:HD12	1.81	0.62
2:C:330:GLU:O	2:C:334:THR:HG23	1.99	0.62
1:B:844:PRO:HG2	6:H:74:LEU:HD11	1.80	0.62
1:B:994:ASP:OD2	1:B:1110:ARG:NH2	2.33	0.62
4:F:209:THR:HG21	4:F:261:PRO:HB3	1.81	0.62
8:E:96:LYS:O	8:E:98:LYS:NZ	2.33	0.62
7:I:1070:ASP:OD2	7:I:1074:ARG:NH2	2.32	0.62
7:I:794:ASN:O	7:I:796:ASN:N	2.31	0.62
2:C:110:VAL:HB	2:C:134:ALA:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:8:GLU:OE2	4:F:73:ARG:NH1	2.32	0.61
9:A:559:LEU:HD22	9:A:639:LEU:HD22	1.82	0.61
1:B:1066:ILE:HD11	1:B:1071:LEU:HD11	1.82	0.61
1:B:1161:MET:C	1:B:1163:THR:H	2.08	0.61
4:F:52:ILE:HD11	4:F:75:SER:HB2	1.82	0.61
3:D:26:VAL:HB	3:D:30:LYS:HD3	1.82	0.61
1:B:881:PHE:HB3	1:B:986:TYR:HB2	1.81	0.61
7:I:117:LEU:HD21	9:A:136:VAL:HG11	1.82	0.61
1:B:250:TYR:HD2	1:B:401:ILE:HD13	1.66	0.61
1:B:900:ASP:HB2	1:B:903:ILE:HG13	1.83	0.61
9:A:7:GLU:OE1	9:A:1421:ARG:NH2	2.33	0.61
2:C:254:GLN:NE2	2:C:341:GLN:OE1	2.34	0.60
7:I:401:CYS:HB3	7:I:403:HIS:HD2	1.65	0.60
1:B:73:ARG:HH21	1:B:453:ALA:HB2	1.66	0.60
1:B:83:GLU:OE1	1:B:83:GLU:N	2.32	0.60
7:I:401:CYS:HB3	7:I:403:HIS:CD2	2.36	0.60
1:B:1033:HIS:NE2	9:A:656:MET:SD	2.75	0.60
8:E:88:ALA:O	9:A:355:GLN:NE2	2.35	0.60
1:B:1059:ASP:HB2	7:I:821:PHE:CE1	2.37	0.60
1:B:752:ALA:HB3	1:B:772:VAL:HG23	1.84	0.60
3:D:42:ARG:NH2	3:D:85:TYR:OH	2.22	0.60
4:F:242:PHE:HE1	4:F:251:ASN:HB2	1.67	0.60
7:I:312:LYS:O	7:I:316:ILE:HG12	2.02	0.60
1:B:522:ARG:NH2	1:B:572:ALA:O	2.34	0.60
6:H:28:TYR:HE2	6:H:49:ILE:HG23	1.67	0.60
7:I:1022:LYS:O	7:I:1026:ILE:HG12	2.01	0.60
7:I:695:ARG:HG2	7:I:702:MET:HA	1.83	0.59
1:B:1124:SER:HA	9:A:320:TRP:HB3	1.85	0.59
7:I:500:GLY:HA3	9:A:392:GLY:HA3	1.83	0.59
1:B:203:ASP:N	1:B:505:SER:O	2.35	0.59
1:B:913:TYR:OH	1:B:952:ASP:OD2	2.20	0.59
7:I:1133:ASP:HB3	7:I:1136:SER:HB2	1.84	0.59
9:A:1100:ASN:HB3	9:A:1103:VAL:HG12	1.84	0.59
1:B:65:VAL:HG11	1:B:442:ILE:HD11	1.83	0.59
1:B:513:ASN:HA	1:B:811:TYR:HA	1.84	0.59
1:B:1164:ILE:O	1:B:1168:SER:HB2	2.02	0.59
4:F:233:ARG:HB3	4:F:234:LEU:HD12	1.85	0.59
7:I:944:ASP:HA	7:I:950:CYS:HB2	1.84	0.59
9:A:84:GLN:NE2	9:A:195:LYS:O	2.35	0.59
1:B:835:LYS:NZ	1:B:1059:ASP:OD2	2.36	0.59
2:C:276:LYS:HG3	2:C:326:LYS:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:863:VAL:HG22	7:I:877:GLU:HG2	1.83	0.59
9:A:833:LEU:HG	9:A:1359:LEU:HD22	1.84	0.59
4:F:197:PHE:CZ	4:F:221:LYS:HB3	2.37	0.59
7:I:85:ASP:OD2	7:I:203:TYR:OH	2.21	0.59
1:B:859:TYR:OH	9:A:332:ASP:OD2	2.21	0.59
8:E:103:ILE:HG23	9:A:475:VAL:HG22	1.84	0.59
7:I:1197:ASP:OD1	7:I:1197:ASP:N	2.34	0.58
8:E:24:GLU:HG2	9:A:1385:ARG:HH21	1.68	0.58
9:A:277:THR:HG23	9:A:1393:GLN:HG2	1.85	0.58
1:B:970:ARG:O	7:I:679:THR:OG1	2.17	0.58
2:C:236:ARG:NH1	2:C:359:ALA:OXT	2.36	0.58
1:B:297:SER:OG	1:B:302:ASN:ND2	2.36	0.58
9:A:14:ASN:OD1	9:A:1402:SER:OG	2.19	0.58
1:B:887:VAL:HG11	1:B:934:ILE:HG21	1.86	0.58
7:I:190:VAL:HG11	7:I:199:PHE:HB2	1.86	0.58
7:I:303:PHE:HA	7:I:306:HIS:HB3	1.85	0.58
9:A:1076:ARG:NH2	9:A:1317:SER:O	2.36	0.58
1:B:509:LEU:HD11	1:B:517:THR:HG23	1.86	0.58
2:C:70:MET:HG2	2:C:166:LYS:HB3	1.85	0.58
1:B:34:VAL:HG13	1:B:39:LEU:HG	1.86	0.58
7:I:183:LYS:NZ	8:E:38:GLU:OE1	2.37	0.58
8:E:99:TYR:CZ	8:E:108:GLN:HG3	2.39	0.58
4:F:9:THR:OG1	4:F:35:TYR:OH	2.21	0.58
7:I:1019:LYS:HE2	7:I:1147:ILE:HG12	1.85	0.58
1:B:123:SER:OG	1:B:483:GLU:OE2	2.17	0.57
4:F:1:MET:N	4:F:80:TYR:O	2.36	0.57
2:C:101:PRO:HG2	6:H:13:PRO:HB3	1.85	0.57
4:F:200:ILE:HG13	4:F:201:CYS:N	2.17	0.57
9:A:18:ASP:OD1	9:A:18:ASP:N	2.37	0.57
2:C:328:SER:OG	2:C:331:ASP:OD2	2.17	0.57
4:F:217:ILE:HG12	4:F:218:LEU:HD12	1.87	0.57
6:H:17:TYR:HB3	6:H:58:LEU:HD22	1.87	0.57
7:I:512:THR:HG23	9:A:211:GLY:HA3	1.87	0.57
9:A:1177:ARG:NH1	9:A:1179:GLU:OE2	2.37	0.57
1:B:66:ASP:OD1	1:B:86:GLN:NE2	2.37	0.57
4:F:197:PHE:HZ	4:F:221:LYS:HB3	1.68	0.57
1:B:23:GLU:HG3	7:I:834:GLN:HE22	1.70	0.56
1:B:872:ILE:HG12	1:B:990:LEU:HB3	1.87	0.56
7:I:134:LEU:HG	7:I:187:GLY:HA2	1.86	0.56
7:I:1176:ILE:O	7:I:1180:GLU:HG2	2.05	0.56
8:E:147:ASP:N	8:E:147:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:94:LYS:HB3	4:F:101:LEU:HB2	1.86	0.56
7:I:294:VAL:HG13	7:I:303:PHE:HZ	1.69	0.56
1:B:284:ASP:N	5:G:8:SER:O	2.37	0.56
3:D:30:LYS:HZ2	3:D:34:MET:HE2	1.70	0.56
1:B:113:LEU:HD12	7:I:685:PRO:HG2	1.86	0.56
1:B:938:ALA:HB3	1:B:951:ILE:HG23	1.88	0.56
6:H:41:ILE:HD12	7:I:818:GLN:HG3	1.86	0.56
7:I:266:SER:HB3	7:I:273:PRO:HD3	1.86	0.56
7:I:359:LYS:C	7:I:361:ASP:H	2.14	0.56
9:A:206:ILE:HA	9:A:209:ARG:HG3	1.87	0.56
4:F:23:VAL:HG21	9:A:1433:GLU:HG2	1.88	0.56
1:B:495:VAL:HG22	8:E:10:ILE:HG12	1.88	0.56
1:B:996:MET:O	1:B:1004:GLY:N	2.37	0.56
4:F:309:ASP:O	4:F:313:THR:HG22	2.06	0.56
9:A:330:ASN:ND2	9:A:445:GLN:OE1	2.39	0.56
9:A:857:GLU:OE2	9:A:1332:ARG:NH2	2.38	0.56
4:F:205:LYS:HG3	4:F:215:ASP:HB3	1.88	0.56
8:E:20:GLU:OE1	9:A:1393:GLN:HG3	2.06	0.56
8:E:74:PHE:HE2	9:A:1039:GLU:HG2	1.70	0.56
7:I:705:PRO:HB3	7:I:710:GLU:HG3	1.88	0.55
7:I:780:ARG:HH22	7:I:798:GLU:HB3	1.72	0.55
9:A:1087:GLU:CD	9:A:1087:GLU:H	2.14	0.55
7:I:321:ASP:O	7:I:325:THR:HG23	2.06	0.55
9:A:431:HIS:NE2	9:A:454:TYR:OH	2.31	0.55
4:F:181:LEU:HA	4:F:184:ILE:HD12	1.88	0.55
7:I:1249:GLN:NE2	9:A:457:ASP:OD2	2.39	0.55
1:B:18:ASN:ND2	1:B:714:PHE:O	2.37	0.55
4:F:285:ILE:HG12	7:I:205:GLU:HG3	1.88	0.55
1:B:209:ARG:NH1	1:B:744:GLU:OE1	2.37	0.55
1:B:535:GLN:HG2	7:I:1229:ASP:HA	1.89	0.55
1:B:860:ASN:HA	1:B:864:SER:HB2	1.89	0.55
7:I:251:PRO:HD2	7:I:256:LYS:HE3	1.87	0.55
9:A:1306:ASP:OD1	9:A:1307:ASP:N	2.40	0.55
1:B:226:GLU:OE2	1:B:229:ARG:HB2	2.06	0.55
1:B:904:THR:C	1:B:906:ASN:H	2.12	0.55
7:I:356:MET:HE3	7:I:357:GLU:HG2	1.88	0.55
7:I:801:GLU:O	7:I:804:THR:OG1	2.24	0.55
6:H:23:LYS:O	6:H:27:GLU:HG3	2.07	0.54
8:E:73:THR:OG1	9:A:1036:ASN:OD1	2.23	0.54
9:A:862:ALA:HB2	9:A:1351:ARG:HD2	1.89	0.54
9:A:932:VAL:HG22	9:A:1029:GLN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:MET:HE3	2:C:176:PHE:CZ	2.43	0.54
5:G:20:ILE:HD12	5:G:20:ILE:H	1.71	0.54
8:E:40:VAL:HG12	8:E:41:GLU:H	1.73	0.54
1:B:1199:MET:HE3	1:B:1199:MET:HA	1.90	0.54
7:I:88:VAL:O	7:I:107:LYS:NZ	2.37	0.54
1:B:1220:GLN:HA	1:B:1223:MET:HE3	1.88	0.54
1:B:1162:GLN:NE2	9:A:476:GLU:OE2	2.41	0.54
9:A:50:MET:HB3	9:A:206:ILE:HG13	1.90	0.54
1:B:400:VAL:HG22	1:B:405:PHE:HB2	1.90	0.54
7:I:145:MET:HG3	7:I:151:PHE:CD1	2.42	0.54
7:I:1129:LEU:O	7:I:1133:ASP:N	2.37	0.54
9:A:158:GLN:OE1	9:A:159:GLN:NE2	2.41	0.54
9:A:1152:VAL:HA	9:A:1155:MET:HB2	1.89	0.54
9:A:904:ASP:HB3	9:A:1000:MET:HG3	1.89	0.54
9:A:1274:MET:O	9:A:1275:ARG:NH1	2.40	0.54
7:I:340:GLU:OE1	7:I:340:GLU:N	2.37	0.54
1:B:215:ILE:HD12	1:B:400:VAL:HG21	1.88	0.54
1:B:971:PRO:HG2	1:B:979:PHE:CZ	2.43	0.54
2:C:125:ILE:HD11	2:C:152:LEU:HG	1.90	0.54
2:C:282:THR:HG23	2:C:320:VAL:HG22	1.89	0.54
2:C:25:ALA:O	2:C:29:LEU:HB2	2.08	0.53
3:D:166:ALA:HB3	3:D:203:SER:HB2	1.90	0.53
7:I:77:ALA:HA	7:I:80:ARG:HB3	1.90	0.53
9:A:1371:LYS:HD3	9:A:1388:LEU:HD23	1.90	0.53
7:I:1153:TYR:O	7:I:1166:ARG:NH1	2.41	0.53
9:A:499:GLN:NE2	9:A:617:TYR:OH	2.35	0.53
1:B:586:LEU:HD23	1:B:664:LEU:HD11	1.91	0.53
9:A:1342:VAL:HG12	9:A:1343:MET:HE2	1.89	0.53
7:I:406:LEU:HB3	7:I:426:ILE:HD11	1.88	0.53
1:B:299:SER:HB3	1:B:302:ASN:HB2	1.91	0.53
1:B:20:GLU:HG2	1:B:716:PRO:HG2	1.90	0.53
9:A:209:ARG:HB2	9:A:227:ASN:HD21	1.73	0.53
3:D:58:PHE:HE2	3:D:90:LEU:HB3	1.74	0.53
5:G:102:SER:O	5:G:104:ARG:N	2.42	0.53
7:I:880:ARG:NH1	9:A:713:ASP:OD2	2.42	0.53
7:I:905:GLN:HE22	9:A:714:ARG:CZ	2.21	0.53
7:I:949:LYS:HG2	7:I:974:TYR:CD2	2.44	0.53
4:F:220:LEU:HD22	4:F:229:LYS:HE3	1.91	0.53
6:H:4:PRO:HG2	6:H:14:ILE:HD11	1.91	0.53
1:B:793:GLN:HB3	1:B:796:ARG:HG2	1.90	0.53
1:B:821:MET:HB2	1:B:884:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:ARG:NE	7:I:509:GLU:OE2	2.35	0.53
3:D:4:GLN:HG2	3:D:28:TYR:CE2	2.43	0.53
3:D:64:TYR:CE1	3:D:74:LEU:HB2	2.42	0.53
5:G:1:MET:HE2	5:G:3:ILE:HD11	1.91	0.53
7:I:346:GLN:O	7:I:350:ILE:HG12	2.09	0.53
7:I:1086:VAL:HG11	7:I:1100:VAL:HG21	1.91	0.53
9:A:396:ASP:O	9:A:398:ARG:N	2.40	0.53
9:A:491:LYS:O	9:A:1349:ASN:N	2.41	0.53
9:A:734:VAL:HG21	9:A:745:MET:HG3	1.91	0.53
7:I:1013:TRP:NE1	7:I:1143:GLU:OE1	2.41	0.52
9:A:1196:ILE:O	9:A:1200:ARG:HB2	2.09	0.52
4:F:115:PRO:O	4:F:121:ASN:ND2	2.43	0.52
7:I:915:LYS:HD2	7:I:915:LYS:O	2.09	0.52
1:B:644:VAL:HG23	1:B:645:VAL:HG23	1.90	0.52
4:F:101:LEU:HD23	4:F:113:VAL:HG23	1.91	0.52
9:A:591:THR:HA	9:A:601:GLY:HA3	1.91	0.52
9:A:382:GLN:O	9:A:385:GLN:NE2	2.35	0.52
1:B:957:TYR:OH	1:B:961:GLU:O	2.27	0.52
2:C:116:LEU:HG	2:C:157:SER:HB3	1.90	0.52
4:F:114:ILE:HG23	4:F:153:SER:HA	1.92	0.52
4:F:319:LEU:O	4:F:323:HIS:ND1	2.43	0.52
4:F:9:THR:HG1	4:F:35:TYR:HH	1.52	0.52
9:A:59:CYS:O	9:A:60:ILE:HB	2.10	0.52
9:A:973:TYR:OH	9:A:985:THR:O	2.27	0.52
9:A:1185:MET:HE1	9:A:1221:ILE:HD12	1.91	0.52
1:B:1059:ASP:HB2	7:I:821:PHE:HE1	1.73	0.52
9:A:83:LEU:HD22	9:A:91:ILE:HD13	1.91	0.52
1:B:233:ILE:HG12	1:B:245:GLN:HG3	1.91	0.52
3:D:85:TYR:O	3:D:116:ILE:HD12	2.10	0.52
9:A:419:ARG:NH1	9:A:461:ASP:OD2	2.41	0.52
1:B:413:TYR:HA	1:B:416:LYS:HB2	1.91	0.52
2:C:3:LYS:O	2:C:6:GLN:NE2	2.43	0.52
1:B:117:ALA:HA	1:B:122:LEU:HB2	1.91	0.51
1:B:255:ALA:HB2	1:B:315:VAL:HG11	1.92	0.51
1:B:973:GLY:N	1:B:977:GLU:O	2.38	0.51
7:I:258:VAL:HG12	7:I:282:LEU:HD11	1.91	0.51
9:A:569:ARG:NH2	9:A:606:LYS:O	2.42	0.51
9:A:875:LEU:HD21	9:A:883:LYS:HD3	1.92	0.51
2:C:178:LEU:O	2:C:224:PRO:HD3	2.10	0.51
8:E:43:PRO:HB2	8:E:45:ILE:HG12	1.91	0.51
1:B:904:THR:O	1:B:906:ASN:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1095:GLU:OE1	9:A:526:HIS:NE2	2.44	0.51
2:C:153:GLN:HB2	2:C:156:LYS:HG3	1.90	0.51
4:F:213:SER:O	4:F:213:SER:OG	2.29	0.51
4:F:222:ILE:HG21	4:F:267:SER:HA	1.92	0.51
5:G:11:MET:HE1	5:G:30:VAL:HG23	1.91	0.51
9:A:310:ILE:HA	9:A:314:LEU:HD12	1.91	0.51
1:B:101:HIS:HB2	1:B:112:LEU:HB2	1.92	0.51
1:B:157:VAL:HG23	1:B:470:LEU:HD11	1.91	0.51
2:C:102:ILE:HG22	2:C:143:PHE:HB3	1.92	0.51
8:E:122:CYS:HA	8:E:133:VAL:HG12	1.91	0.51
1:B:515:LEU:HD13	1:B:842:VAL:HG21	1.91	0.51
7:I:354:LEU:HD21	7:I:366:ILE:HG12	1.93	0.51
7:I:455:ASP:OD1	7:I:459:GLN:NE2	2.44	0.51
7:I:952:LYS:HD2	7:I:954:GLY:O	2.10	0.51
9:A:277:THR:HG22	9:A:279:ALA:H	1.75	0.51
7:I:261:PHE:HB2	7:I:300:GLU:HG2	1.92	0.51
1:B:285:ASP:OD1	1:B:286:SER:N	2.43	0.51
5:G:95:VAL:HG12	5:G:101:MET:HG2	1.91	0.51
7:I:193:LYS:O	7:I:197:ILE:HD12	2.11	0.51
9:A:468:PRO:HB2	9:A:474:ARG:HG3	1.92	0.51
3:D:83:LYS:HE2	3:D:85:TYR:CZ	2.45	0.51
8:E:95:LEU:HD12	8:E:105:ILE:HG23	1.91	0.51
1:B:170:HIS:ND1	7:I:788:TYR:OH	2.38	0.51
3:D:81:GLU:OE1	3:D:85:TYR:OH	2.19	0.51
4:F:23:VAL:HG11	4:F:54:ARG:CZ	2.41	0.51
4:F:31:LEU:HD11	4:F:72:VAL:HG11	1.92	0.51
2:C:13:PHE:HD2	2:C:40:PRO:HB2	1.75	0.50
7:I:808:ALA:O	7:I:812:GLN:HG2	2.10	0.50
9:A:1159:LEU:HD11	9:A:1167:PRO:HD3	1.93	0.50
1:B:450:LYS:HD3	1:B:451:GLN:OE1	2.09	0.50
5:G:47:GLY:H	5:G:49:MET:HE2	1.77	0.50
7:I:326:GLU:OE2	9:A:360:ASN:ND2	2.43	0.50
7:I:495:PHE:CG	9:A:389:ASP:HB2	2.46	0.50
9:A:1339:ILE:O	9:A:1343:MET:HG2	2.12	0.50
1:B:79:ASP:OD1	1:B:82:ARG:NH2	2.41	0.50
1:B:181:GLU:OE1	7:I:778:TYR:OH	2.22	0.50
3:D:146:GLU:O	3:D:149:GLU:HG3	2.11	0.50
9:A:1070:ASN:ND2	9:A:1090:GLN:OE1	2.41	0.50
1:B:423:VAL:HG12	1:B:427:LYS:HE3	1.91	0.50
1:B:907:LEU:HD22	1:B:913:TYR:CZ	2.47	0.50
2:C:260:PHE:CG	2:C:333:ILE:HG13	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:904:THR:HG23	1:B:907:LEU:HG	1.93	0.50
9:A:166:TYR:HB2	9:A:169:ILE:HD12	1.94	0.50
9:A:553:LYS:HG2	9:A:598:LEU:HG	1.93	0.50
9:A:1155:MET:HE3	9:A:1209:MET:HE1	1.93	0.50
9:A:1371:LYS:NZ	9:A:1389:SER:O	2.44	0.50
2:C:332:LEU:O	2:C:336:LEU:HG	2.11	0.50
9:A:959:GLN:O	9:A:963:MET:HG3	2.11	0.50
9:A:1205:ASN:HB3	9:A:1230:SER:HB2	1.93	0.50
1:B:1162:GLN:HG3	9:A:1425:MET:HE2	1.93	0.50
2:C:92:PHE:O	2:C:96:ARG:HG2	2.12	0.50
7:I:879:THR:OG1	7:I:882:ASP:OD1	2.30	0.50
9:A:876:SER:OG	9:A:877:ASP:N	2.44	0.50
1:B:148:LYS:HG3	1:B:454:PHE:CZ	2.47	0.50
3:D:19:MET:HE1	3:D:53:VAL:HG11	1.94	0.50
7:I:75:ILE:HG12	7:I:99:LEU:HD21	1.93	0.50
7:I:78:TYR:CD1	7:I:78:TYR:C	2.89	0.50
8:E:67:THR:OG1	8:E:134:GLU:OE1	2.20	0.50
9:A:1374:LEU:HD21	9:A:1384:LEU:HG	1.92	0.50
4:F:1:MET:HE1	4:F:184:ILE:HD13	1.93	0.49
2:C:65:GLU:OE1	2:C:249:ARG:NH2	2.45	0.49
7:I:340:GLU:H	7:I:340:GLU:CD	2.19	0.49
9:A:97:VAL:HG23	9:A:98:ILE:HG23	1.93	0.49
9:A:1162:HIS:HB3	9:A:1165:LEU:HD12	1.94	0.49
1:B:819:VAL:HG21	1:B:969:MET:HE1	1.94	0.49
1:B:1192:SER:O	7:I:415:GLN:HA	2.12	0.49
7:I:510:ASP:OD1	7:I:510:ASP:N	2.39	0.49
9:A:1172:ALA:HB2	9:A:1229:GLU:HG3	1.94	0.49
1:B:372:LEU:O	1:B:386:LYS:HD3	2.13	0.49
1:B:376:MET:HE2	1:B:389:PHE:HB2	1.94	0.49
1:B:1018:THR:HG22	1:B:1088:MET:HG2	1.95	0.49
1:B:1089:PHE:HA	1:B:1096:TYR:HA	1.94	0.49
7:I:960:ILE:HG23	7:I:961:TYR:H	1.77	0.49
8:E:120:MET:HE2	9:A:1428:ASP:OD2	2.12	0.49
1:B:294:ASP:OD2	1:B:609:ARG:NE	2.45	0.49
1:B:1119:ARG:O	1:B:1139:LYS:NZ	2.36	0.49
2:C:254:GLN:HB2	2:C:340:ILE:HG21	1.94	0.49
7:I:937:CYS:HA	7:I:950:CYS:HA	1.95	0.49
9:A:302:ARG:O	9:A:309:ARG:N	2.41	0.49
9:A:424:GLU:CD	9:A:1051:GLU:HG3	2.38	0.49
7:I:229:ARG:HE	7:I:233:ARG:HD3	1.77	0.49
7:I:305:GLN:HA	7:I:308:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:132:LEU:HD22	7:I:173:MET:HG2	1.94	0.49
7:I:340:GLU:HG2	7:I:341:LYS:H	1.77	0.49
7:I:78:TYR:C	7:I:78:TYR:HD1	2.20	0.49
7:I:517:ILE:O	9:A:34:LEU:N	2.39	0.49
9:A:1074:ILE:O	9:A:1078:GLN:HG3	2.13	0.49
1:B:158:SER:HB3	1:B:478:LEU:HB3	1.95	0.48
1:B:299:SER:OG	1:B:300:LEU:N	2.46	0.48
4:F:229:LYS:O	4:F:231:MET:N	2.45	0.48
7:I:74:PRO:O	7:I:76:GLU:N	2.46	0.48
7:I:269:TYR:HD2	7:I:271:VAL:HG13	1.77	0.48
9:A:653:THR:HA	9:A:656:MET:HE2	1.95	0.48
7:I:183:LYS:NZ	7:I:184:ASN:HB2	2.28	0.48
9:A:48:ALA:HB3	9:A:60:ILE:HD12	1.95	0.48
9:A:370:LYS:HE3	9:A:390:ILE:HG22	1.95	0.48
9:A:725:PRO:HB3	9:A:731:PHE:CE2	2.48	0.48
1:B:870:SER:O	1:B:874:ARG:HG3	2.13	0.48
2:C:61:VAL:HG21	2:C:246:ILE:HG13	1.95	0.48
5:G:11:MET:HE3	5:G:24:CYS:HB2	1.95	0.48
9:A:619:LEU:O	9:A:623:ARG:HG2	2.13	0.48
1:B:646:HIS:CE1	1:B:648:HIS:HB2	2.49	0.48
7:I:262:LEU:HD12	7:I:282:LEU:HD12	1.94	0.48
7:I:403:HIS:ND1	7:I:449:LEU:HD12	2.29	0.48
1:B:448:LEU:HD11	1:B:461:ASN:HB3	1.95	0.48
1:B:1144:GLY:O	1:B:1145:LEU:HB2	2.14	0.48
4:F:220:LEU:HD23	4:F:220:LEU:H	1.79	0.48
1:B:22:THR:OG1	1:B:25:ASP:OD1	2.32	0.48
1:B:853:TYR:O	9:A:650:THR:OG1	2.25	0.48
7:I:1029:ILE:HD12	7:I:1033:VAL:HB	1.96	0.48
9:A:366:PHE:HB2	9:A:399:LEU:HD11	1.96	0.48
9:A:1273:LEU:HD13	9:A:1292:ALA:HB3	1.95	0.48
2:C:74:LYS:HB2	2:C:162:ASP:HB3	1.96	0.48
3:D:75:LEU:HB3	3:D:109:GLN:HG2	1.95	0.48
3:D:192:MET:O	3:D:193:HIS:CD2	2.66	0.48
4:F:120:GLN:HE21	4:F:156:ILE:HD11	1.79	0.48
4:F:258:ALA:HB3	4:F:278:PHE:CE2	2.49	0.48
9:A:269:ASN:O	9:A:273:ASP:HB2	2.13	0.48
1:B:350:TYR:HA	7:I:1193:ILE:HG12	1.96	0.48
1:B:874:ARG:HG2	2:C:99:PHE:CE1	2.48	0.48
1:B:1188:ILE:HB	1:B:1197:LYS:HG2	1.96	0.48
1:B:448:LEU:HD13	1:B:465:ALA:HB2	1.96	0.48
1:B:1059:ASP:OD1	1:B:1061:THR:OG1	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:95:LEU:HD11	8:E:108:GLN:HB2	1.94	0.48
1:B:573:ILE:HG23	1:B:574:THR:HG23	1.95	0.47
1:B:1184:GLY:HA3	1:B:1231:THR:HG23	1.96	0.47
3:D:100:LYS:HA	3:D:103:LEU:HD12	1.96	0.47
4:F:20:CYS:C	4:F:22:ASN:H	2.21	0.47
7:I:183:LYS:HZ3	7:I:184:ASN:HB2	1.78	0.47
9:A:354:VAL:N	9:A:403:ASP:O	2.34	0.47
9:A:1175:CYS:HB2	9:A:1226:TYR:HA	1.96	0.47
9:A:1200:ARG:NH2	9:A:1208:ILE:O	2.46	0.47
1:B:404:VAL:O	5:G:52:LYS:HE3	2.15	0.47
1:B:665:ASP:OD1	1:B:665:ASP:N	2.47	0.47
7:I:737:TYR:O	7:I:782:TYR:OH	2.25	0.47
1:B:866:ILE:HB	1:B:1027:ILE:HB	1.96	0.47
4:F:198:LYS:H	4:F:198:LYS:HD2	1.79	0.47
7:I:96:LYS:HD2	7:I:96:LYS:C	2.39	0.47
7:I:108:GLU:HB3	7:I:116:HIS:CE1	2.50	0.47
1:B:608:VAL:HG13	1:B:609:ARG:HD2	1.96	0.47
9:A:684:LEU:HB2	9:A:689:ILE:HD12	1.96	0.47
9:A:1196:ILE:HG13	9:A:1210:HIS:CD2	2.49	0.47
9:A:1213:GLU:CD	9:A:1213:GLU:H	2.23	0.47
1:B:820:ASP:HB3	1:B:823:ARG:HG3	1.96	0.47
3:D:153:ARG:NH1	3:D:154:GLU:OE2	2.47	0.47
4:F:21:THR:HB	9:A:1440:TYR:CE1	2.50	0.47
7:I:90:PRO:HD3	7:I:107:LYS:HZ3	1.79	0.47
2:C:82:ASP:HB3	2:C:159:ILE:HG13	1.96	0.47
9:A:310:ILE:HG21	9:A:1387:ALA:HA	1.96	0.47
9:A:754:GLN:HA	9:A:787:PHE:HA	1.96	0.47
1:B:33:ALA:HA	1:B:729:LEU:HD22	1.96	0.47
1:B:185:ASP:HB3	1:B:188:GLU:HB3	1.96	0.47
2:C:353:ASN:ND2	2:C:356:GLU:OE2	2.44	0.47
3:D:163:GLN:HG2	3:D:201:THR:HG21	1.95	0.47
6:H:69:HIS:O	6:H:73:THR:OG1	2.25	0.47
7:I:90:PRO:HA	7:I:130:LEU:HD23	1.97	0.47
7:I:391:LYS:HD2	7:I:391:LYS:N	2.29	0.47
8:E:136:TRP:CE3	8:E:141:MET:HE3	2.50	0.47
9:A:62:CYS:SG	9:A:64:HIS:HB2	2.55	0.47
9:A:171:ARG:NH2	9:A:199:LYS:HB2	2.30	0.47
9:A:1262:ILE:HB	9:A:1265:ILE:HD12	1.96	0.47
3:D:101:ASN:OD1	3:D:102:ILE:N	2.47	0.47
4:F:83:ALA:HB1	4:F:136:ASN:HA	1.96	0.47
4:F:200:ILE:HG22	4:F:311:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:140:VAL:O	9:A:158:GLN:NE2	2.48	0.47
9:A:145:VAL:HB	9:A:155:TRP:HB2	1.96	0.47
9:A:921:SER:O	9:A:921:SER:OG	2.32	0.47
9:A:1220:PRO:HG2	9:A:1222:ILE:HD11	1.96	0.47
4:F:233:ARG:CZ	4:F:234:LEU:H	2.29	0.47
9:A:1438:GLU:HG3	9:A:1439:ASN:OD1	2.15	0.46
1:B:835:LYS:HG2	1:B:1057:VAL:HG12	1.98	0.46
1:B:747:GLU:HG2	9:A:767:SER:OG	2.16	0.46
1:B:1204:GLN:HA	7:I:150:SER:OG	2.15	0.46
5:G:54:LYS:HB3	5:G:54:LYS:HE3	1.76	0.46
6:H:78:LYS:HD3	7:I:817:ALA:HA	1.97	0.46
4:F:206:LEU:HD23	4:F:207:TYR:CZ	2.50	0.46
5:G:37:LEU:HD12	9:A:1133:TYR:HB3	1.97	0.46
6:H:21:PHE:HB2	6:H:58:LEU:HD11	1.96	0.46
7:I:299:VAL:O	7:I:301:GLN:N	2.48	0.46
7:I:1061:MET:O	7:I:1130:ARG:NH1	2.49	0.46
7:I:1100:VAL:O	7:I:1108:LYS:NZ	2.37	0.46
3:D:57:ILE:HG12	3:D:91:ILE:HD12	1.96	0.46
7:I:92:VAL:HG21	7:I:109:ILE:HD12	1.98	0.46
9:A:252:ILE:HG23	9:A:256:ILE:HB	1.96	0.46
9:A:340:TYR:CE1	9:A:465:LEU:HD22	2.51	0.46
1:B:432:ILE:HG12	1:B:481:SER:HB3	1.96	0.46
1:B:1153:TRP:CE2	9:A:830:ILE:HG21	2.51	0.46
4:F:259:ARG:HA	4:F:263:LEU:HD12	1.97	0.46
5:G:58:LYS:HE3	5:G:58:LYS:HB3	1.57	0.46
1:B:529:THR:HG21	7:I:1221:GLU:HA	1.97	0.46
4:F:60:MET:HG2	9:A:5:TYR:CD1	2.51	0.46
5:G:39:VAL:HG11	9:A:1174:TRP:HZ3	1.80	0.46
7:I:161:SER:HA	7:I:166:THR:O	2.16	0.46
1:B:767:ARG:HE	9:A:776:PRO:HG3	1.80	0.46
2:C:353:ASN:O	2:C:357:LEU:HB2	2.16	0.46
3:D:102:ILE:O	3:D:106:ILE:HG12	2.16	0.46
7:I:324:LEU:O	7:I:328:ILE:HG12	2.15	0.46
7:I:439:TRP:CD2	7:I:448:LYS:HG2	2.51	0.46
9:A:1087:GLU:OE2	9:A:1087:GLU:N	2.45	0.46
1:B:474:THR:C	1:B:476:SER:H	2.23	0.46
7:I:252:GLU:O	7:I:256:LYS:N	2.36	0.46
9:A:860:LEU:HD21	9:A:1030:TYR:HE1	1.80	0.46
1:B:527:HIS:CE1	7:I:1217:GLY:HA3	2.51	0.46
9:A:146:LYS:NZ	9:A:147:ASP:O	2.49	0.46
1:B:97:GLU:HB2	1:B:127:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ARG:HG3	1:B:701:TRP:CD2	2.51	0.45
1:B:797:VAL:O	1:B:801:THR:HG23	2.16	0.45
2:C:62:LEU:HD11	2:C:239:LEU:HD23	1.98	0.45
4:F:21:THR:HA	9:A:1437:THR:HG22	1.98	0.45
4:F:166:VAL:HG21	4:F:292:MET:HE2	1.98	0.45
4:F:196:ASP:O	4:F:200:ILE:HG23	2.16	0.45
4:F:220:LEU:HB3	4:F:229:LYS:NZ	2.31	0.45
7:I:955:LEU:HB3	7:I:956:PHE:H	1.48	0.45
9:A:1345:ASP:N	9:A:1345:ASP:OD1	2.49	0.45
1:B:468:ALA:HB1	1:B:472:LYS:HE3	1.97	0.45
1:B:492:THR:HG23	8:E:14:LEU:HD12	1.98	0.45
1:B:1179:ILE:HG21	1:B:1234:LEU:HD13	1.98	0.45
4:F:225:GLY:O	4:F:227:LYS:HD2	2.16	0.45
5:G:20:ILE:HD11	5:G:37:LEU:HD13	1.98	0.45
7:I:293:GLU:OE2	7:I:297:ASN:ND2	2.48	0.45
7:I:949:LYS:HD2	7:I:970:VAL:HG13	1.98	0.45
9:A:85:PRO:HD2	9:A:271:LEU:HD12	1.98	0.45
1:B:97:GLU:OE2	1:B:129:ASN:ND2	2.37	0.45
4:F:145:ARG:HD2	4:F:145:ARG:HA	1.82	0.45
6:H:60:ILE:HD13	6:H:70:LEU:HD22	1.97	0.45
7:I:332:ARG:NH1	9:A:364:PRO:O	2.50	0.45
7:I:865:LYS:HB2	7:I:894:ALA:HB2	1.98	0.45
9:A:1124:ARG:HG3	9:A:1124:ARG:HH11	1.81	0.45
1:B:93:ASP:HB3	1:B:131:ALA:HB3	1.99	0.45
1:B:234:SER:HB3	1:B:374:PRO:HD2	1.98	0.45
7:I:288:ARG:HB2	8:E:147:ASP:OD1	2.17	0.45
7:I:1077:LEU:HD13	7:I:1119:VAL:HG13	1.98	0.45
9:A:340:TYR:CZ	9:A:344:PHE:HB3	2.52	0.45
1:B:815:TRP:CG	1:B:816:PRO:HD3	2.52	0.45
1:B:877:PHE:HB3	1:B:1110:ARG:HD2	1.97	0.45
7:I:141:CYS:HB3	8:E:45:ILE:HG21	1.99	0.45
7:I:844:LEU:HG	9:A:671:ASN:HB3	1.99	0.45
7:I:864:TYR:HB3	7:I:891:TYR:HB3	1.98	0.45
7:I:1065:ARG:O	7:I:1069:VAL:HG23	2.17	0.45
9:A:255:ASN:OD1	9:A:256:ILE:N	2.49	0.45
1:B:1119:ARG:HD3	9:A:442:SER:HB3	1.98	0.45
1:B:1135:PRO:HG3	9:A:320:TRP:CE2	2.51	0.45
9:A:665:GLU:HB3	9:A:718:PRO:HG3	1.97	0.45
1:B:216:HIS:NE2	1:B:219:THR:HG23	2.32	0.45
7:I:310:ARG:O	7:I:314:GLN:HG3	2.17	0.45
7:I:695:ARG:HG3	7:I:700:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:TYR:HE1	1:B:254:GLY:HA2	1.82	0.45
1:B:906:ASN:HD22	1:B:951:ILE:HD11	1.82	0.45
3:D:202:LYS:HA	3:D:202:LYS:HD3	1.63	0.45
7:I:1157:GLU:N	7:I:1157:GLU:OE1	2.50	0.45
1:B:468:ALA:O	1:B:472:LYS:HB2	2.17	0.45
1:B:600:ALA:HB1	7:I:1060:SER:HB2	1.99	0.45
4:F:59:ILE:HD11	9:A:1431:MET:SD	2.56	0.45
7:I:949:LYS:HD3	7:I:949:LYS:HA	1.50	0.45
8:E:118:LEU:HB2	9:A:1430:ILE:HG12	1.99	0.45
4:F:175:ALA:HB1	4:F:247:LEU:HD23	1.99	0.44
6:H:28:TYR:O	6:H:32:LYS:HG2	2.17	0.44
7:I:359:LYS:C	7:I:361:ASP:N	2.75	0.44
9:A:184:LYS:HA	9:A:184:LYS:HD3	1.71	0.44
1:B:120:CYS:HB2	1:B:122:LEU:HG	1.98	0.44
2:C:240:LYS:O	2:C:244:ARG:HD3	2.17	0.44
7:I:145:MET:HE2	7:I:145:MET:HB2	1.62	0.44
9:A:379:VAL:HG12	9:A:403:ASP:OD1	2.17	0.44
9:A:383:ILE:HG13	9:A:384:THR:HG23	1.98	0.44
7:I:1094:ILE:HD13	7:I:1094:ILE:HA	1.85	0.44
9:A:536:THR:HG22	9:A:631:LYS:HE3	1.99	0.44
1:B:699:LYS:HE3	1:B:699:LYS:HB2	1.74	0.44
4:F:324:GLU:HG2	4:F:325:ASN:OD1	2.18	0.44
7:I:734:ASP:OD1	7:I:734:ASP:N	2.48	0.44
7:I:1098:ARG:HG2	7:I:1099:LEU:HD12	1.99	0.44
9:A:1122:PHE:CE1	9:A:1126:ILE:HD11	2.53	0.44
2:C:236:ARG:HG3	2:C:358:ILE:HB	1.99	0.44
4:F:45:ILE:HA	4:F:78:VAL:HG12	1.99	0.44
7:I:120:PRO:HG2	7:I:123:ALA:HB2	2.00	0.44
7:I:411:ARG:HG3	9:A:384:THR:HA	1.98	0.44
9:A:430:VAL:HB	9:A:482:SER:HA	1.99	0.44
9:A:1074:ILE:HG22	9:A:1078:GLN:HG3	2.00	0.44
1:B:61:GLN:O	1:B:64:ASN:ND2	2.51	0.44
1:B:305:MET:HG2	1:B:398:LEU:HD12	2.00	0.44
1:B:694:ARG:HG3	1:B:701:TRP:CE2	2.53	0.44
7:I:963:HIS:ND1	7:I:964:LEU:O	2.51	0.44
1:B:1161:MET:O	1:B:1163:THR:N	2.50	0.44
4:F:233:ARG:HD2	4:F:233:ARG:HA	1.89	0.44
9:A:1179:GLU:HG3	9:A:1222:ILE:HD12	1.99	0.44
1:B:870:SER:HA	2:C:174:ALA:HB2	1.99	0.44
7:I:980:GLN:O	7:I:984:GLU:HG3	2.17	0.44
7:I:1022:LYS:HA	7:I:1025:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:SER:HA	1:B:570:GLN:HE22	1.83	0.44
1:B:796:ARG:NH2	1:B:1001:GLY:O	2.51	0.44
2:C:105:LYS:HD2	2:C:105:LYS:HA	1.81	0.44
4:F:265:LYS:HA	4:F:265:LYS:HD3	1.63	0.44
7:I:471:ARG:HG3	7:I:504:ALA:HB3	1.99	0.44
7:I:420:LEU:HD12	7:I:420:LEU:HA	1.84	0.43
9:A:512:ARG:HA	9:A:602:VAL:HG12	2.00	0.43
9:A:1057:MET:CG	9:A:1074:ILE:HD11	2.47	0.43
1:B:232:PHE:HB3	1:B:246:ILE:HG12	1.99	0.43
7:I:170:ARG:O	7:I:174:LYS:HB2	2.18	0.43
7:I:883:VAL:HG11	9:A:580:PRO:HA	2.00	0.43
9:A:92:ARG:O	9:A:96:ARG:HG3	2.17	0.43
9:A:334:HIS:HE1	9:A:535:GLN:HG2	1.83	0.43
9:A:599:ILE:HG22	9:A:600:GLU:HG2	2.00	0.43
9:A:955:LYS:HB3	9:A:955:LYS:HE3	1.72	0.43
1:B:794:PRO:HB3	9:A:805:GLU:HG2	2.01	0.43
1:B:18:ASN:HB2	1:B:711:ASN:HD21	1.82	0.43
7:I:468:ASP:OD2	7:I:471:ARG:NH2	2.51	0.43
8:E:17:GLU:HG2	9:A:274:SER:HA	2.00	0.43
9:A:900:ARG:NH1	9:A:903:LYS:HD3	2.34	0.43
1:B:674:LEU:HD23	1:B:738:CYS:HB3	1.99	0.43
1:B:701:TRP:CE2	1:B:702:GLU:HG3	2.54	0.43
4:F:58:PHE:HB2	4:F:69:TYR:CZ	2.53	0.43
4:F:91:LYS:HE3	4:F:127:GLY:HA2	2.00	0.43
4:F:219:ASP:OD1	4:F:219:ASP:N	2.52	0.43
7:I:333:GLN:O	7:I:337:ILE:HD12	2.19	0.43
7:I:1045:TYR:HA	7:I:1048:ILE:HD12	2.00	0.43
9:A:361:ARG:O	9:A:364:PRO:HD2	2.18	0.43
9:A:1179:GLU:OE1	9:A:1179:GLU:N	2.51	0.43
1:B:246:ILE:HG22	1:B:260:ILE:HG23	1.99	0.43
4:F:218:LEU:HD13	4:F:229:LYS:HD3	1.99	0.43
4:F:242:PHE:HE2	4:F:257:TRP:HZ2	1.65	0.43
7:I:788:TYR:HB2	7:I:795:PHE:CE1	2.54	0.43
1:B:229:ARG:HH12	7:I:1222:ASP:CG	2.26	0.43
1:B:710:GLN:NE2	1:B:767:ARG:O	2.45	0.43
2:C:257:TYR:OH	2:C:336:LEU:HD13	2.18	0.43
4:F:236:PRO:HD3	4:F:271:TYR:CE1	2.53	0.43
7:I:1234:GLU:HA	9:A:306:LYS:HE2	1.99	0.43
7:I:1236:VAL:HG22	9:A:823:GLY:HA3	1.99	0.43
7:I:1246:LEU:HD13	9:A:819:THR:HG21	2.01	0.43
9:A:945:SER:HB2	9:A:1018:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1382:VAL:O	9:A:1386:MET:HG3	2.19	0.43
1:B:125:SER:HB3	1:B:159:THR:HB	2.00	0.43
1:B:963:ALA:HB2	1:B:986:TYR:CZ	2.54	0.43
9:A:594:ARG:HB2	9:A:599:ILE:HD11	2.01	0.43
9:A:1203:HIS:HA	9:A:1204:PRO:HD3	1.91	0.43
7:I:294:VAL:HG13	7:I:303:PHE:CZ	2.51	0.43
7:I:730:LYS:HD3	7:I:730:LYS:HA	1.74	0.43
9:A:873:ILE:HD11	9:A:1000:MET:HE1	2.01	0.43
1:B:904:THR:C	1:B:906:ASN:N	2.77	0.43
2:C:12:PRO:HA	2:C:41:VAL:HA	2.00	0.43
4:F:156:ILE:HG22	4:F:158:LYS:H	1.84	0.43
4:F:195:LYS:HG2	4:F:311:CYS:HB2	2.00	0.43
7:I:693:VAL:HG21	7:I:782:TYR:CG	2.54	0.43
7:I:1083:LEU:HD22	7:I:1168:PHE:CG	2.54	0.43
9:A:728:ASN:HB3	9:A:731:PHE:HB3	2.01	0.43
1:B:136:LEU:HB3	1:B:454:PHE:HE1	1.84	0.42
7:I:76:GLU:HG2	7:I:77:ALA:N	2.32	0.42
7:I:272:SER:HA	7:I:273:PRO:HD3	1.84	0.42
7:I:279:TYR:HB2	7:I:282:LEU:HB3	2.00	0.42
7:I:949:LYS:NZ	7:I:953:CYS:SG	2.92	0.42
7:I:949:LYS:NZ	7:I:970:VAL:HG22	2.34	0.42
9:A:1124:ARG:HG3	9:A:1124:ARG:NH1	2.34	0.42
1:B:58:ILE:HD11	1:B:240:PHE:HB3	2.01	0.42
1:B:646:HIS:CD2	1:B:647:PRO:HD2	2.54	0.42
4:F:123:VAL:HG11	4:F:329:LEU:HD11	2.01	0.42
6:H:75:ASP:HB3	6:H:78:LYS:HD2	2.01	0.42
7:I:780:ARG:NH2	7:I:798:GLU:HB3	2.33	0.42
9:A:884:PHE:HA	9:A:1009:VAL:HG21	2.01	0.42
1:B:552:TYR:HB3	1:B:669:LEU:HD13	2.01	0.42
7:I:291:TYR:HB3	7:I:303:PHE:CZ	2.54	0.42
7:I:780:ARG:NH2	7:I:798:GLU:OE1	2.52	0.42
9:A:1433:GLU:O	9:A:1437:THR:HG23	2.18	0.42
1:B:43:ASN:OD1	1:B:44:ILE:N	2.52	0.42
1:B:399:LEU:HD22	1:B:404:VAL:HG11	2.01	0.42
1:B:527:HIS:HB3	7:I:1218:LEU:HG	2.02	0.42
1:B:1196:TYR:OH	1:B:1207:ILE:N	2.49	0.42
2:C:70:MET:HE2	2:C:175:ALA:HB3	2.01	0.42
2:C:120:CYS:HB2	7:I:775:THR:HA	2.00	0.42
3:D:4:GLN:O	3:D:8:THR:HG22	2.20	0.42
5:G:49:MET:HG3	5:G:51:ASP:OD1	2.18	0.42
7:I:405:LYS:HB2	7:I:405:LYS:HE3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:1066:LEU:HD11	7:I:1134:PRO:HB3	2.01	0.42
9:A:692:PRO:HG2	9:A:695:LEU:HD12	2.02	0.42
1:B:398:LEU:HD23	1:B:401:ILE:HD12	2.01	0.42
1:B:1190:ASN:ND2	9:A:62:CYS:O	2.49	0.42
1:B:1228:VAL:HG11	9:A:1395:LEU:HD11	2.01	0.42
3:D:198:ARG:NH2	9:A:1361:THR:O	2.40	0.42
5:G:70:LYS:HD2	5:G:70:LYS:HA	1.69	0.42
9:A:143:LYS:HB3	9:A:157:ASP:HB2	2.02	0.42
9:A:893:LEU:HD12	9:A:958:LEU:HD22	2.01	0.42
9:A:1322:THR:HG23	9:A:1326:TYR:HD2	1.85	0.42
1:B:636:ARG:NH2	1:B:651:ILE:O	2.53	0.42
1:B:722:ILE:HD11	1:B:732:LEU:HD11	2.00	0.42
4:F:36:VAL:HG22	4:F:47:ASN:HA	2.01	0.42
4:F:203:PHE:HZ	4:F:314:PHE:HB2	1.84	0.42
7:I:229:ARG:NE	7:I:233:ARG:HD3	2.35	0.42
7:I:353:ILE:O	7:I:353:ILE:HG12	2.19	0.42
7:I:431:LYS:HG2	7:I:443:LYS:HG3	2.02	0.42
7:I:495:PHE:CD1	9:A:389:ASP:HB2	2.54	0.42
7:I:937:CYS:HB2	7:I:942:LEU:O	2.19	0.42
8:E:83:ARG:HD3	8:E:116:PRO:HD2	2.01	0.42
8:E:104:ASP:O	8:E:108:GLN:HG2	2.19	0.42
4:F:196:ASP:OD1	4:F:196:ASP:N	2.46	0.42
7:I:958:TYR:HD1	7:I:959:ILE:HG13	1.85	0.42
9:A:720:MET:HB3	9:A:720:MET:HE3	1.84	0.42
9:A:1178:LEU:HD11	9:A:1225:ILE:HD12	2.02	0.42
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.89	0.42
1:B:807:THR:CG2	1:B:1109:GLN:HB3	2.49	0.42
1:B:809:GLY:HA2	1:B:826:GLN:HB3	2.02	0.42
2:C:139:LYS:HA	2:C:139:LYS:HD3	1.86	0.42
3:D:168:ASP:OD2	3:D:170:PRO:HD2	2.20	0.42
4:F:54:ARG:HH12	9:A:1433:GLU:CD	2.27	0.42
9:A:1076:ARG:HB3	9:A:1077:PRO:HD3	2.02	0.42
9:A:1107:LYS:HB2	9:A:1291:TYR:CZ	2.55	0.42
1:B:854:MET:HE1	1:B:1097:PHE:CZ	2.55	0.42
1:B:1165:ILE:HD11	9:A:1419:VAL:HG21	2.02	0.42
2:C:206:LYS:C	9:A:517:MET:HE2	2.44	0.42
3:D:125:LEU:HD21	3:D:172:VAL:HG11	2.02	0.42
4:F:220:LEU:HD13	4:F:264:LEU:HD21	2.01	0.42
7:I:258:VAL:HG11	7:I:286:LEU:HD11	2.02	0.42
8:E:74:PHE:CE2	9:A:1039:GLU:HG2	2.53	0.42
8:E:94:MET:HE1	9:A:1435:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:491:LYS:HG3	9:A:1348:PRO:HB3	2.02	0.42
9:A:923:LEU:HD12	9:A:923:LEU:HA	1.78	0.42
9:A:1202:LYS:O	9:A:1202:LYS:HD3	2.19	0.42
2:C:71:LEU:HG	2:C:102:ILE:HG21	2.02	0.42
2:C:277:THR:HG23	2:C:332:LEU:HD22	2.01	0.42
2:C:301:MET:SD	2:C:342:ASN:ND2	2.93	0.42
4:F:32:GLU:O	4:F:36:VAL:HB	2.20	0.42
4:F:90:VAL:HG21	4:F:132:VAL:HB	2.02	0.42
4:F:323:HIS:HB2	4:F:327:TRP:NE1	2.35	0.42
7:I:362:ASP:O	7:I:366:ILE:HG13	2.20	0.42
7:I:1226:ARG:HE	8:E:21:THR:HG21	1.84	0.42
9:A:1195:ILE:HD13	9:A:1259:ILE:HG13	2.02	0.42
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.91	0.41
3:D:193:HIS:CD2	3:D:193:HIS:C	2.97	0.41
9:A:631:LYS:HA	9:A:631:LYS:HD2	1.80	0.41
1:B:414:ARG:HD2	1:B:747:GLU:OE2	2.20	0.41
1:B:669:LEU:HD23	1:B:669:LEU:HA	1.89	0.41
1:B:874:ARG:HA	2:C:99:PHE:CZ	2.55	0.41
7:I:79:ILE:O	7:I:83:LEU:HG	2.19	0.41
7:I:269:TYR:CD2	7:I:271:VAL:HG13	2.54	0.41
7:I:403:HIS:HA	7:I:406:LEU:HD12	2.02	0.41
9:A:98:ILE:HA	9:A:105:PRO:HA	2.02	0.41
9:A:128:GLN:CD	9:A:128:GLN:H	2.28	0.41
9:A:844:VAL:HG11	9:A:1355:MET:HE1	2.01	0.41
1:B:71:ASP:OD2	1:B:82:ARG:NE	2.41	0.41
1:B:134:VAL:HG11	1:B:445:PHE:CZ	2.56	0.41
1:B:296:GLU:OE1	1:B:296:GLU:HA	2.20	0.41
1:B:336:LEU:O	1:B:340:VAL:HB	2.21	0.41
1:B:650:THR:HG23	1:B:745:GLU:HB2	2.02	0.41
1:B:1113:LYS:HB2	1:B:1113:LYS:HE2	1.71	0.41
4:F:208:TYR:HE2	4:F:210:TYR:HB2	1.86	0.41
7:I:403:HIS:HA	7:I:406:LEU:HB2	2.02	0.41
7:I:851:ASP:HB3	7:I:901:CYS:SG	2.60	0.41
9:A:1190:ILE:HD13	9:A:1190:ILE:HA	1.85	0.41
1:B:775:PRO:HB3	9:A:798:SER:OG	2.20	0.41
1:B:1217:ILE:HG21	9:A:70:MET:HB3	2.02	0.41
3:D:46:GLU:HG2	3:D:51:GLY:O	2.19	0.41
4:F:142:ILE:HB	4:F:145:ARG:HG2	2.02	0.41
7:I:107:LYS:HA	7:I:107:LYS:HD2	1.86	0.41
7:I:842:LYS:HD3	7:I:842:LYS:C	2.45	0.41
9:A:510:LEU:O	9:A:552:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:616:ILE:HG13	9:A:617:TYR:N	2.34	0.41
9:A:1155:MET:HE2	9:A:1155:MET:HB3	1.80	0.41
1:B:326:GLU:HG2	1:B:331:LYS:HB2	2.03	0.41
2:C:210:MET:HE2	2:C:210:MET:HB2	1.82	0.41
2:C:253:ILE:HD11	2:C:340:ILE:HD11	2.02	0.41
3:D:51:GLY:HA3	3:D:86:GLU:HG2	2.01	0.41
3:D:94:LYS:HE2	3:D:94:LYS:HB3	1.88	0.41
4:F:106:LEU:HD11	4:F:309:ASP:CG	2.45	0.41
7:I:286:LEU:O	7:I:292:LEU:HG	2.21	0.41
7:I:390:LYS:HB2	7:I:390:LYS:HE3	1.81	0.41
7:I:456:MET:HE3	7:I:456:MET:HB2	1.78	0.41
7:I:1027:LEU:HD11	7:I:1173:LEU:HD13	2.02	0.41
1:B:316:LEU:HD13	1:B:324:GLN:HE22	1.86	0.41
4:F:233:ARG:C	4:F:234:LEU:HD12	2.46	0.41
7:I:1156:LYS:HB3	7:I:1156:LYS:HE2	1.35	0.41
9:A:475:VAL:O	9:A:479:LEU:HB2	2.21	0.41
1:B:957:TYR:CZ	1:B:959:PHE:HB2	2.56	0.41
1:B:1181:ARG:O	1:B:1181:ARG:HG2	2.21	0.41
1:B:1192:SER:HB3	7:I:416:TYR:CE1	2.56	0.41
7:I:157:GLY:HA3	7:I:215:HIS:NE2	2.36	0.41
7:I:1069:VAL:HG11	7:I:1142:ILE:HG13	2.02	0.41
7:I:1111:LEU:HD23	7:I:1111:LEU:HA	1.86	0.41
1:B:301:VAL:HG12	1:B:402:MET:SD	2.61	0.41
1:B:358:GLN:HB2	7:I:1186:PRO:HB3	2.03	0.41
1:B:767:ARG:HH22	9:A:781:GLU:CD	2.29	0.41
2:C:274:GLU:C	2:C:276:LYS:H	2.29	0.41
2:C:333:ILE:HD13	2:C:333:ILE:HA	1.94	0.41
3:D:64:TYR:HE1	3:D:74:LEU:HB2	1.84	0.41
4:F:8:GLU:HG2	4:F:73:ARG:HD3	2.01	0.41
5:G:49:MET:HE3	5:G:52:LYS:HB2	2.03	0.41
5:G:84:ILE:HG22	5:G:86:ILE:HG23	2.03	0.41
7:I:169:ILE:HG12	7:I:206:LEU:HD21	2.02	0.41
7:I:913:ILE:HD13	7:I:913:ILE:HA	1.87	0.41
7:I:964:LEU:O	7:I:966:GLN:N	2.53	0.41
7:I:1231:PHE:CE2	9:A:817:LEU:HB3	2.55	0.41
9:A:483:VAL:HA	9:A:486:TRP:CD1	2.56	0.41
9:A:519:LYS:HB3	9:A:519:LYS:HE3	1.82	0.41
9:A:915:VAL:HA	9:A:918:PHE:CZ	2.56	0.41
9:A:1074:ILE:C	9:A:1077:PRO:HD2	2.46	0.41
9:A:1144:MET:HE2	9:A:1144:MET:HB2	1.83	0.41
9:A:1162:HIS:HB3	9:A:1165:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:VAL:O	1:B:388:ARG:HG3	2.20	0.41
1:B:437:VAL:HG13	1:B:470:LEU:HD13	2.03	0.41
1:B:822:ASN:HA	1:B:881:PHE:CZ	2.56	0.41
3:D:28:TYR:O	3:D:32:VAL:HG22	2.21	0.41
7:I:263:LYS:O	7:I:266:SER:OG	2.38	0.41
7:I:852:GLU:HA	7:I:916:VAL:HG22	2.03	0.41
7:I:872:LYS:HB3	7:I:873:PRO:HD3	2.02	0.41
9:A:750:ALA:C	9:A:791:SER:HB3	2.46	0.41
9:A:876:SER:HB3	9:A:879:GLU:OE2	2.21	0.41
1:B:248:ILE:HG12	1:B:258:ILE:HG12	2.03	0.40
1:B:474:THR:O	1:B:476:SER:N	2.54	0.40
1:B:605:LYS:HG2	1:B:609:ARG:HD3	2.03	0.40
3:D:3:MET:HA	3:D:3:MET:HE3	2.04	0.40
3:D:130:ILE:HG23	3:D:136:ILE:HD13	2.04	0.40
4:F:39:CYS:HB2	4:F:142:ILE:O	2.22	0.40
5:G:85:CYS:SG	5:G:90:LYS:HE2	2.61	0.40
5:G:94:LEU:H	5:G:102:SER:HB3	1.86	0.40
7:I:1235:ASP:HA	9:A:311:ARG:HH22	1.85	0.40
9:A:251:LYS:HA	9:A:251:LYS:HD2	1.87	0.40
1:B:18:ASN:HD22	1:B:18:ASN:HA	1.64	0.40
1:B:42:TYR:OH	1:B:522:ARG:HA	2.21	0.40
1:B:59:VAL:HB	1:B:94:VAL:HG21	2.03	0.40
1:B:311:LYS:O	1:B:315:VAL:HG23	2.21	0.40
1:B:1156:THR:OG1	9:A:1422:ILE:HD11	2.20	0.40
4:F:176:LEU:O	4:F:179:THR:HB	2.21	0.40
8:E:39:ILE:HD12	9:A:183:VAL:HG11	2.03	0.40
9:A:276:SER:O	9:A:280:THR:OG1	2.22	0.40
9:A:1015:THR:OG1	9:A:1017:GLU:HG3	2.21	0.40
1:B:225:ASN:C	1:B:252:THR:HG1	2.28	0.40
1:B:460:ARG:HD2	1:B:460:ARG:O	2.21	0.40
1:B:476:SER:O	1:B:480:ARG:HB3	2.21	0.40
1:B:900:ASP:H	1:B:903:ILE:CB	2.32	0.40
1:B:957:TYR:CE2	1:B:959:PHE:HB2	2.56	0.40
7:I:298:PRO:O	7:I:299:VAL:C	2.63	0.40
9:A:31:ILE:HD12	9:A:33:ASN:ND2	2.37	0.40
9:A:85:PRO:HB3	9:A:268:TYR:CD2	2.57	0.40
9:A:237:ASN:HA	9:A:263:ILE:HD11	2.04	0.40
9:A:904:ASP:C	9:A:1000:MET:HE3	2.46	0.40
9:A:1247:ALA:O	9:A:1251:VAL:HG23	2.21	0.40
1:B:558:SER:O	1:B:802:ASN:ND2	2.54	0.40
1:B:674:LEU:HB2	1:B:772:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1180:CYS:C	1:B:1182:ASN:H	2.29	0.40
3:D:192:MET:O	3:D:193:HIS:CG	2.74	0.40
3:D:204:LYS:H	3:D:204:LYS:HG2	1.56	0.40
4:F:158:LYS:HA	4:F:158:LYS:HD2	1.73	0.40
7:I:226:MET:HE2	7:I:226:MET:HB3	2.00	0.40
7:I:301:GLN:HA	7:I:304:LEU:HB2	2.03	0.40
7:I:378:GLU:H	7:I:378:GLU:HG2	1.74	0.40
8:E:14:LEU:HD23	8:E:14:LEU:HA	1.89	0.40
9:A:938:VAL:HG13	9:A:1014:ILE:HD11	2.03	0.40
9:A:1182:LYS:HD2	9:A:1182:LYS:O	2.22	0.40
1:B:174:LEU:HD22	7:I:785:PHE:HD1	1.87	0.40
1:B:886:LYS:HA	1:B:981:LEU:H	1.86	0.40
5:G:20:ILE:HD12	5:G:20:ILE:N	2.36	0.40
5:G:28:GLU:HG3	5:G:29:SER:N	2.35	0.40
7:I:79:ILE:HG23	7:I:130:LEU:HD11	2.04	0.40
7:I:501:GLU:HB2	9:A:388:HIS:CE1	2.57	0.40
7:I:837:ARG:HD3	9:A:663:HIS:CG	2.56	0.40
8:E:100:SER:OG	9:A:361:ARG:NE	2.41	0.40
9:A:333:LEU:O	9:A:447:ASN:ND2	2.41	0.40
9:A:514:ASN:HD22	9:A:519:LYS:HA	1.85	0.40
9:A:934:VAL:HG13	9:A:1026:ILE:HD11	2.04	0.40
9:A:1077:PRO:HG3	9:A:1342:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1216/1235 (98%)	1157 (95%)	54 (4%)	5 (0%)	30	43
2	C	357/359 (99%)	343 (96%)	14 (4%)	0	100	100
3	D	203/205 (99%)	197 (97%)	5 (2%)	1 (0%)	24	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	332/334 (99%)	304 (92%)	21 (6%)	7 (2%)	5	7
5	G	103/105 (98%)	92 (89%)	10 (10%)	1 (1%)	12	20
6	H	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
7	I	938/1183 (79%)	869 (93%)	62 (7%)	7 (1%)	18	28
8	E	125/139 (90%)	113 (90%)	10 (8%)	2 (2%)	7	11
9	A	1394/1440 (97%)	1349 (97%)	42 (3%)	3 (0%)	43	58
All	All	4746/5080 (93%)	4501 (95%)	219 (5%)	26 (0%)	26	37

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	266	SER
7	I	299	VAL
7	I	359	LYS
7	I	360	VAL
7	I	795	PHE
9	A	60	ILE
1	B	905	LYS
4	F	222	ILE
7	I	342	ILE
4	F	70	MET
4	F	100	ILE
4	F	230	GLU
5	G	31	GLN
7	I	822	TYR
1	B	477	ASP
4	F	138	SER
8	E	52	ALA
9	A	253	PRO
9	A	277	THR
1	B	934	ILE
1	B	1161	MET
4	F	45	ILE
8	E	39	ILE
1	B	421	SER
3	D	193	HIS
7	I	965	SER

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	B	1063/1074 (99%)	1031 (97%)	32 (3%)	36	58
2	C	328/328 (100%)	316 (96%)	12 (4%)	30	51
3	D	185/185 (100%)	181 (98%)	4 (2%)	45	67
4	F	308/308 (100%)	296 (96%)	12 (4%)	28	48
5	G	96/96 (100%)	91 (95%)	5 (5%)	21	36
6	H	70/70 (100%)	69 (99%)	1 (1%)	59	79
7	I	859/1069 (80%)	821 (96%)	38 (4%)	25	43
8	E	119/129 (92%)	113 (95%)	6 (5%)	22	38
9	A	1240/1269 (98%)	1218 (98%)	22 (2%)	51	73
All	All	4268/4528 (94%)	4136 (97%)	132 (3%)	36	57

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	THR
1	B	40	ILE
1	B	94	VAL
1	B	164	ARG
1	B	188	GLU
1	B	219	THR
1	B	253	THR
1	B	263	THR
1	B	321	GLN
1	B	340	VAL
1	B	372	LEU
1	B	448	LEU
1	B	470	LEU
1	B	493	ILE
1	B	500	ILE
1	B	504	VAL
1	B	506	THR
1	B	529	THR

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Mol	Chain	Res	Type
1	B	533	SER
1	B	626	THR
1	B	655	SER
1	B	933	ILE
1	B	949	LYS
1	B	975	ASN
1	B	985	ARG
1	B	1035	SER
1	B	1058	THR
1	B	1113	LYS
1	B	1131	LEU
1	B	1145	LEU
1	B	1172	SER
1	B	1202	ASP
2	C	1	MET
2	C	20	LEU
2	C	34	GLU
2	C	82	ASP
2	C	180	VAL
2	C	182	THR
2	C	195	ASP
2	C	197	LYS
2	C	210	MET
2	C	253	ILE
2	C	284	LYS
2	C	330	GLU
3	D	73	THR
3	D	134	SER
3	D	193	HIS
3	D	196	VAL
4	F	17	THR
4	F	36	VAL
4	F	92	ILE
4	F	101	LEU
4	F	187	MET
4	F	200	ILE
4	F	234	LEU
4	F	237	CYS
4	F	253	SER
4	F	264	LEU
4	F	278	PHE
4	F	281	THR

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Mol	Chain	Res	Type
5	G	34	SER
5	G	36	ASN
5	G	39	VAL
5	G	66	ASN
5	G	79	ASP
6	H	16	THR
7	I	78	TYR
7	I	84	VAL
7	I	87	ASP
7	I	93	SER
7	I	101	VAL
7	I	115	THR
7	I	161	SER
7	I	171	VAL
7	I	173	MET
7	I	189	VAL
7	I	272	SER
7	I	276	THR
7	I	277	SER
7	I	299	VAL
7	I	303	PHE
7	I	326	GLU
7	I	330	GLN
7	I	335	PHE
7	I	342	ILE
7	I	360	VAL
7	I	419	LEU
7	I	428	VAL
7	I	453	HIS
7	I	775	THR
7	I	794	ASN
7	I	829	THR
7	I	901	CYS
7	I	908	VAL
7	I	934	GLU
7	I	973	TYR
7	I	1034	ILE
7	I	1096	VAL
7	I	1114	VAL
7	I	1156	LYS
7	I	1161	VAL
7	I	1173	LEU

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Mol	Chain	Res	Type
7	I	1199	VAL
7	I	1215	SER
8	E	9	LEU
8	E	11	MET
8	E	15	VAL
8	E	40	VAL
8	E	44	SER
8	E	50	VAL
9	A	274	SER
9	A	275	VAL
9	A	284	THR
9	A	379	VAL
9	A	387	VAL
9	A	417	PHE
9	A	500	VAL
9	A	535	GLN
9	A	577	VAL
9	A	613	SER
9	A	703	LYS
9	A	727	THR
9	A	817	LEU
9	A	830	ILE
9	A	923	LEU
9	A	1206	THR
9	A	1212	VAL
9	A	1230	SER
9	A	1242	THR
9	A	1295	THR
9	A	1402	SER
9	A	1419	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	61	GLN
1	B	108	ASN
1	B	139	HIS
1	B	145	GLN
1	B	173	HIS
1	B	207	ASN
1	B	242	ASN

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Mol	Chain	Res	Type
1	B	302	ASN
1	B	314	HIS
1	B	324	GLN
1	B	325	HIS
1	B	461	ASN
1	B	507	GLN
1	B	525	ASN
1	B	531	ASN
1	B	570	GLN
1	B	704	HIS
1	B	717	GLN
1	B	826	GLN
1	B	861	GLN
1	B	869	GLN
1	B	975	ASN
1	B	1002	ASN
1	B	1039	ASN
1	B	1090	ASN
2	C	7	ASN
2	C	19	ASN
2	C	153	GLN
2	C	292	ASN
2	C	311	GLN
3	D	67	HIS
3	D	144	GLN
3	D	148	GLN
3	D	157	GLN
3	D	193	HIS
4	F	42	ASN
4	F	121	ASN
4	F	128	GLN
4	F	146	GLN
4	F	174	GLN
4	F	183	ASN
4	F	238	ASN
7	I	309	GLN
7	I	319	GLN
7	I	399	ASN
7	I	403	HIS
7	I	435	ASN
7	I	818	GLN
7	I	828	ASN

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Mol	Chain	Res	Type
7	I	905	GLN
7	I	1174	ASN
9	A	33	ASN
9	A	55	HIS
9	A	68	GLN
9	A	158	GLN
9	A	159	GLN
9	A	190	ASN
9	A	334	HIS
9	A	388	HIS
9	A	535	GLN
9	A	568	GLN
9	A	587	GLN
9	A	638	GLN
9	A	707	ASN
9	A	765	GLN
9	A	852	GLN
9	A	1018	GLN
9	A	1128	GLN
9	A	1197	ASN
9	A	1365	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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

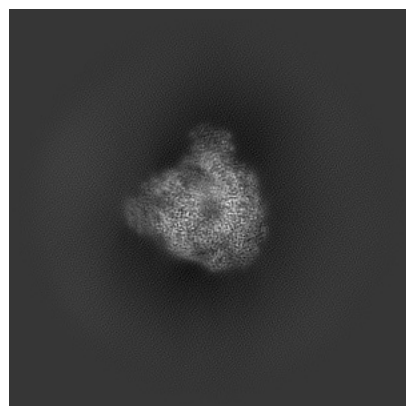
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38746. These allow visual inspection of the internal detail of the map and identification of artifacts.

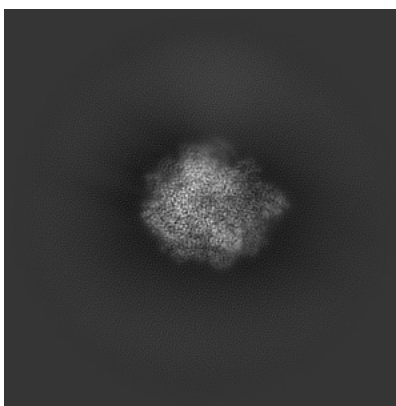
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

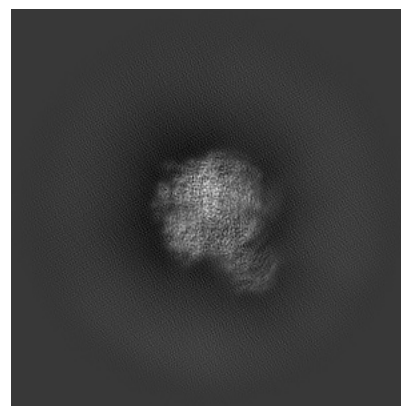
6.1.1 Primary map



X

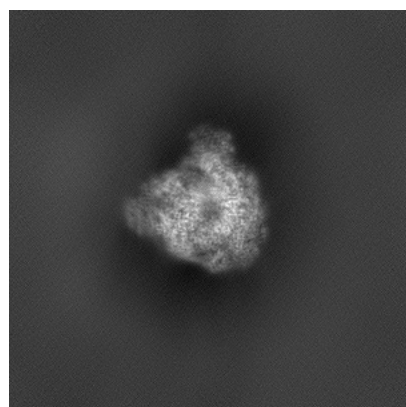


Y

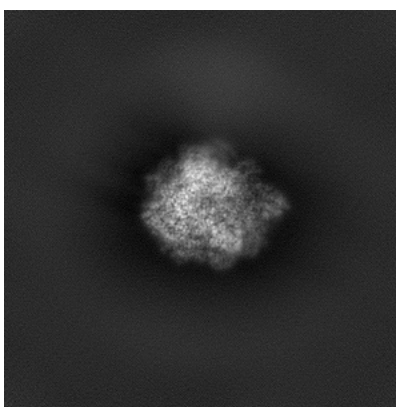


Z

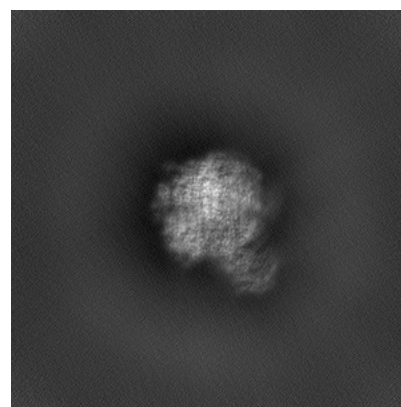
6.1.2 Raw map



X



Y

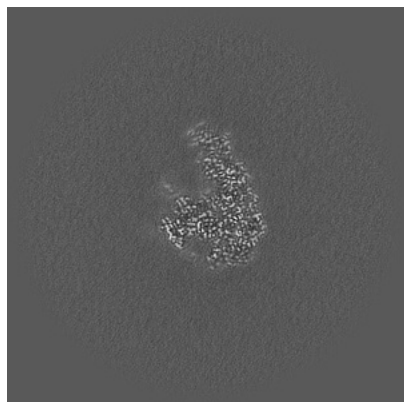


Z

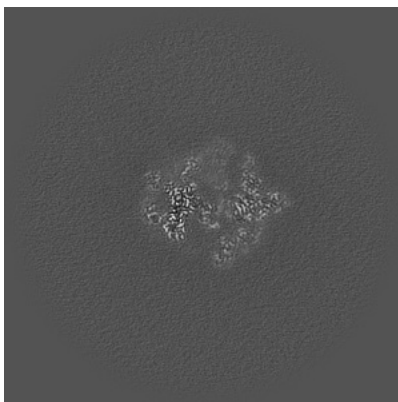
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

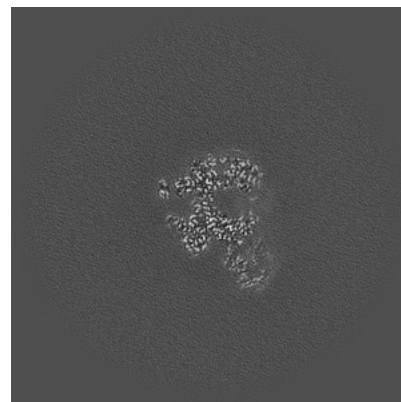
6.2.1 Primary map



X Index: 256

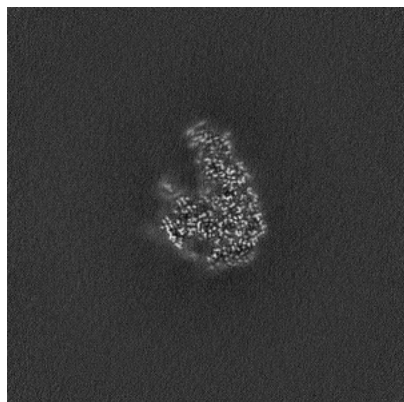


Y Index: 256

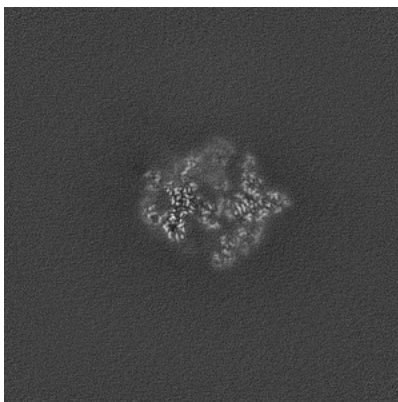


Z Index: 256

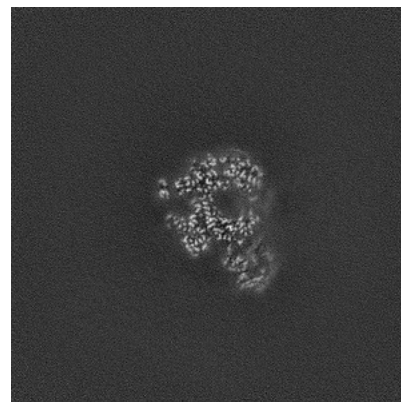
6.2.2 Raw map



X Index: 256



Y Index: 256

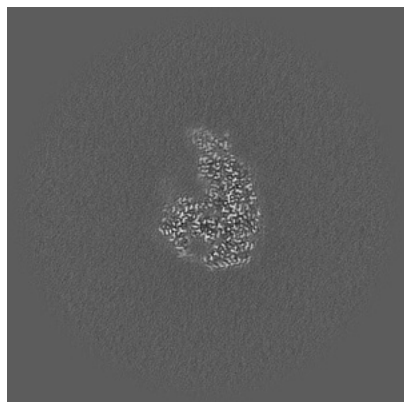


Z Index: 256

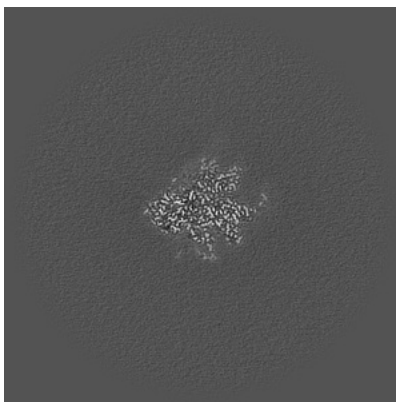
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

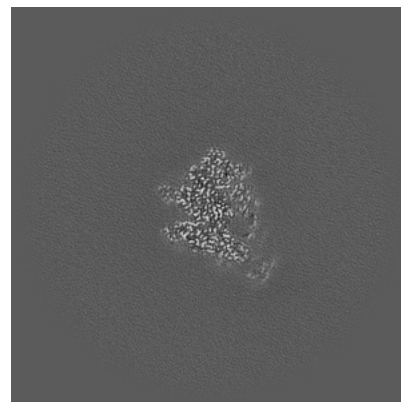
6.3.1 Primary map



X Index: 251

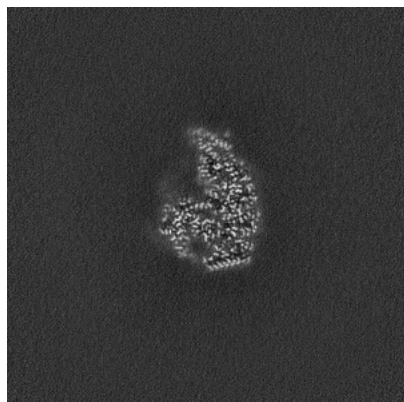


Y Index: 288

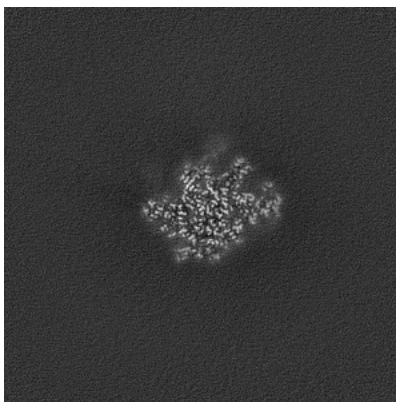


Z Index: 230

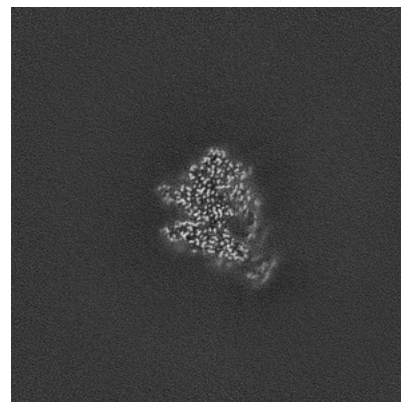
6.3.2 Raw map



X Index: 250



Y Index: 280

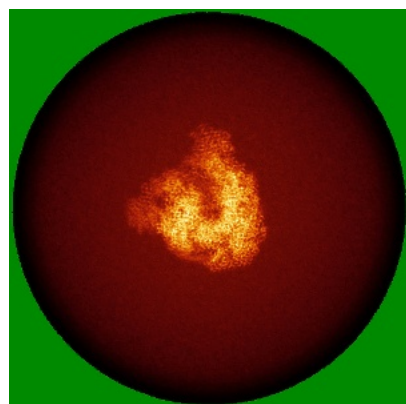


Z Index: 230

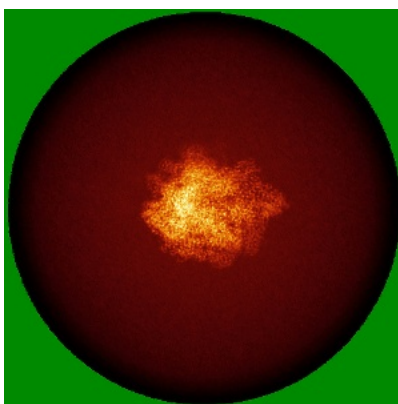
The images above show the largest variance slices of the map in three orthogonal directions.

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

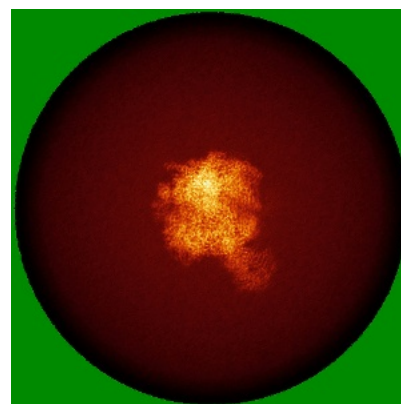
6.4.1 Primary map



X

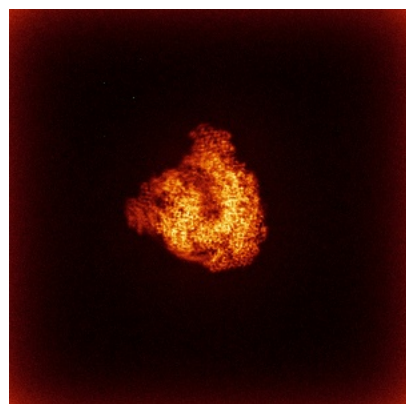


Y

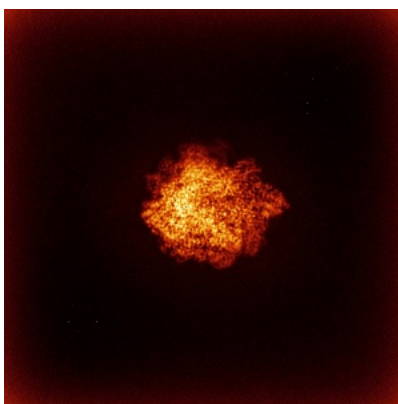


Z

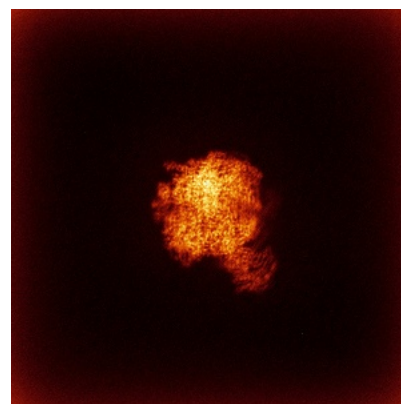
6.4.2 Raw map



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](#)

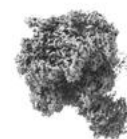
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. 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



X



Y



Z

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.

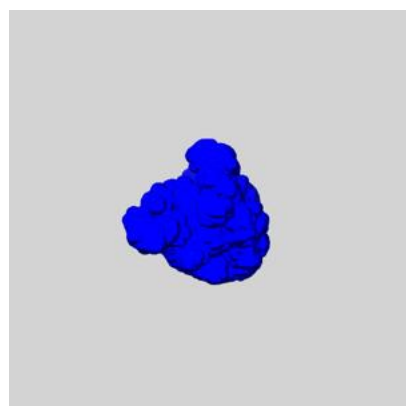
6.6 Mask visualisation [i](#)

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

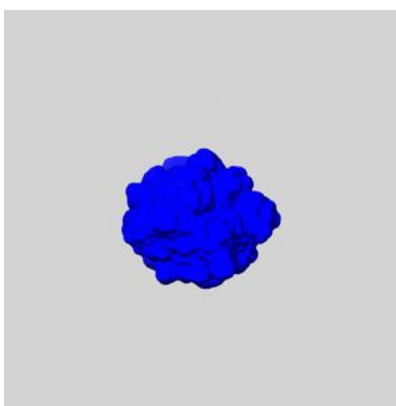
A mask typically either:

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

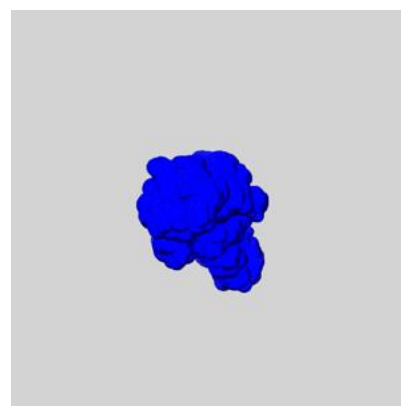
6.6.1 emd_38746_msk_1.map [i](#)



X



Y

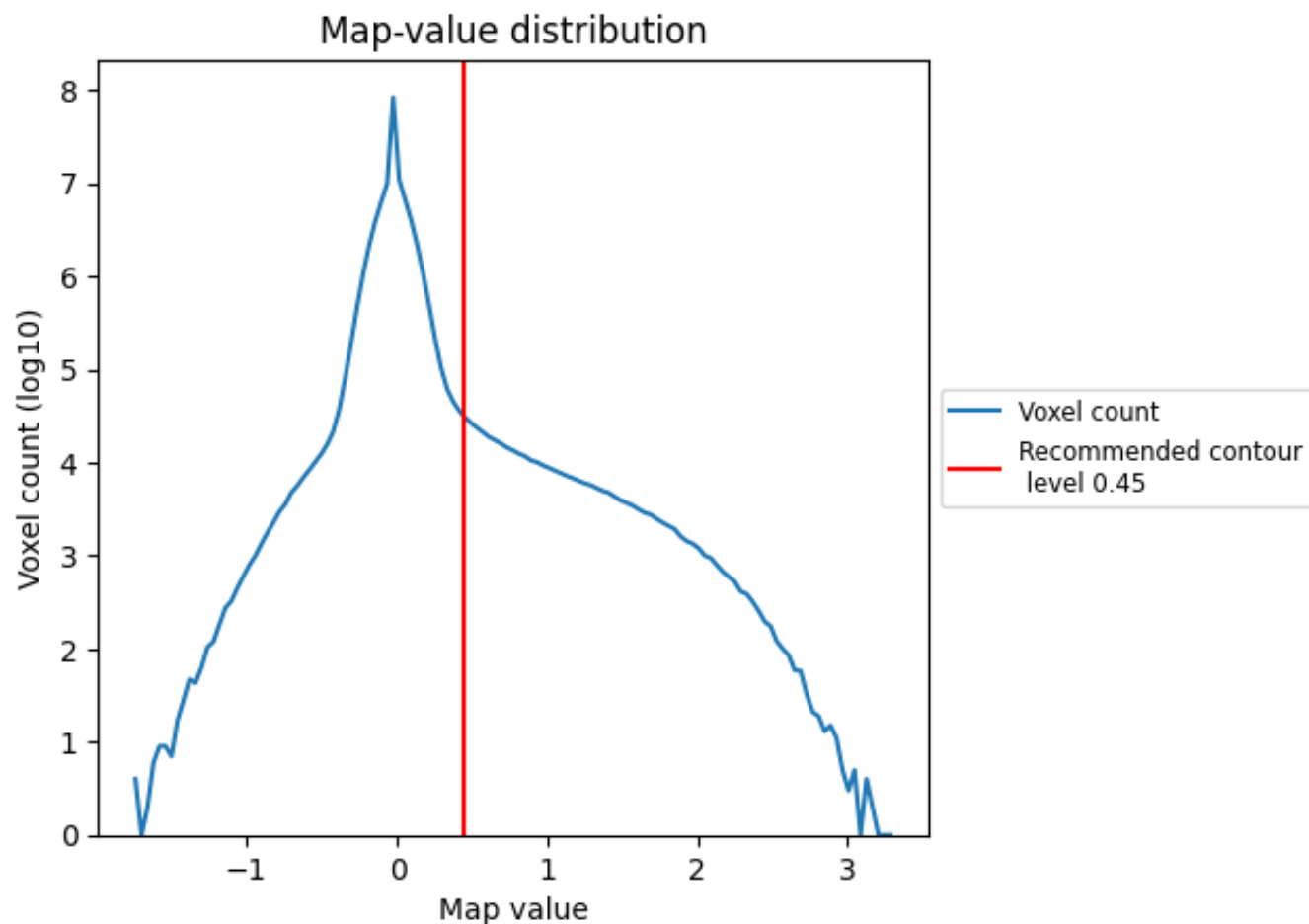


Z

7 Map analysis [i](#)

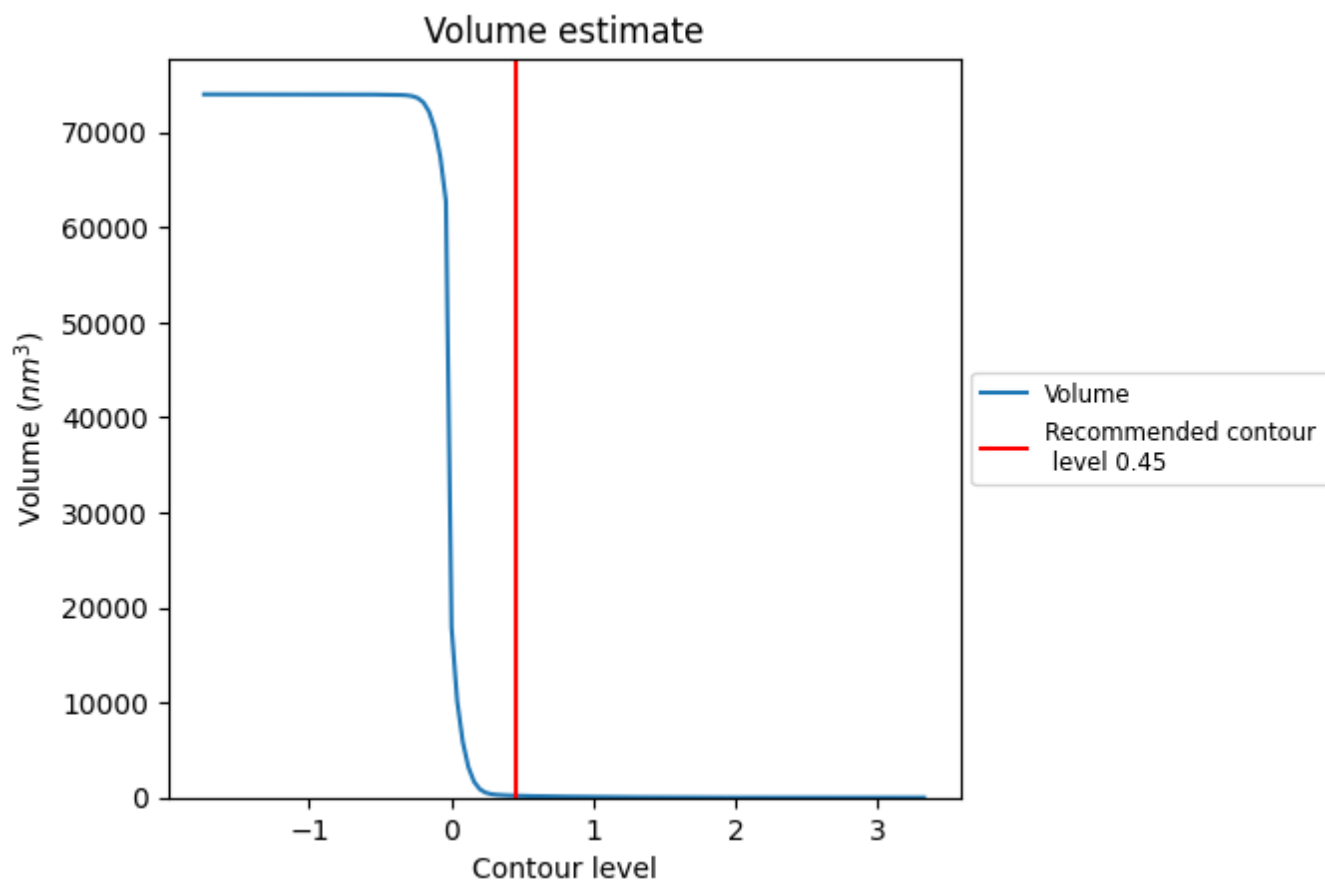
This section contains the results of statistical analysis of the map.

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.

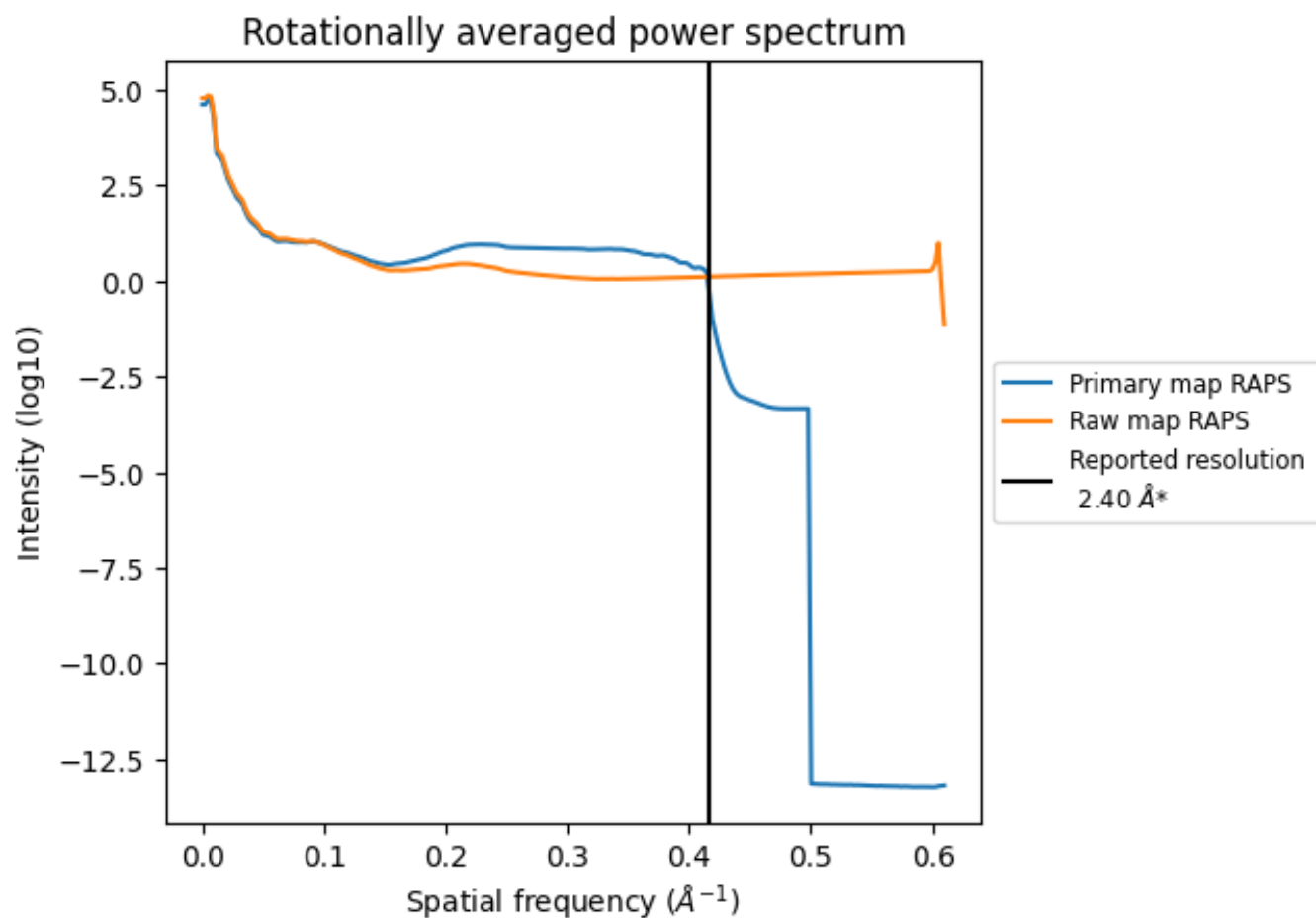
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm³; this corresponds to an approximate mass of 178 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 ⓘ

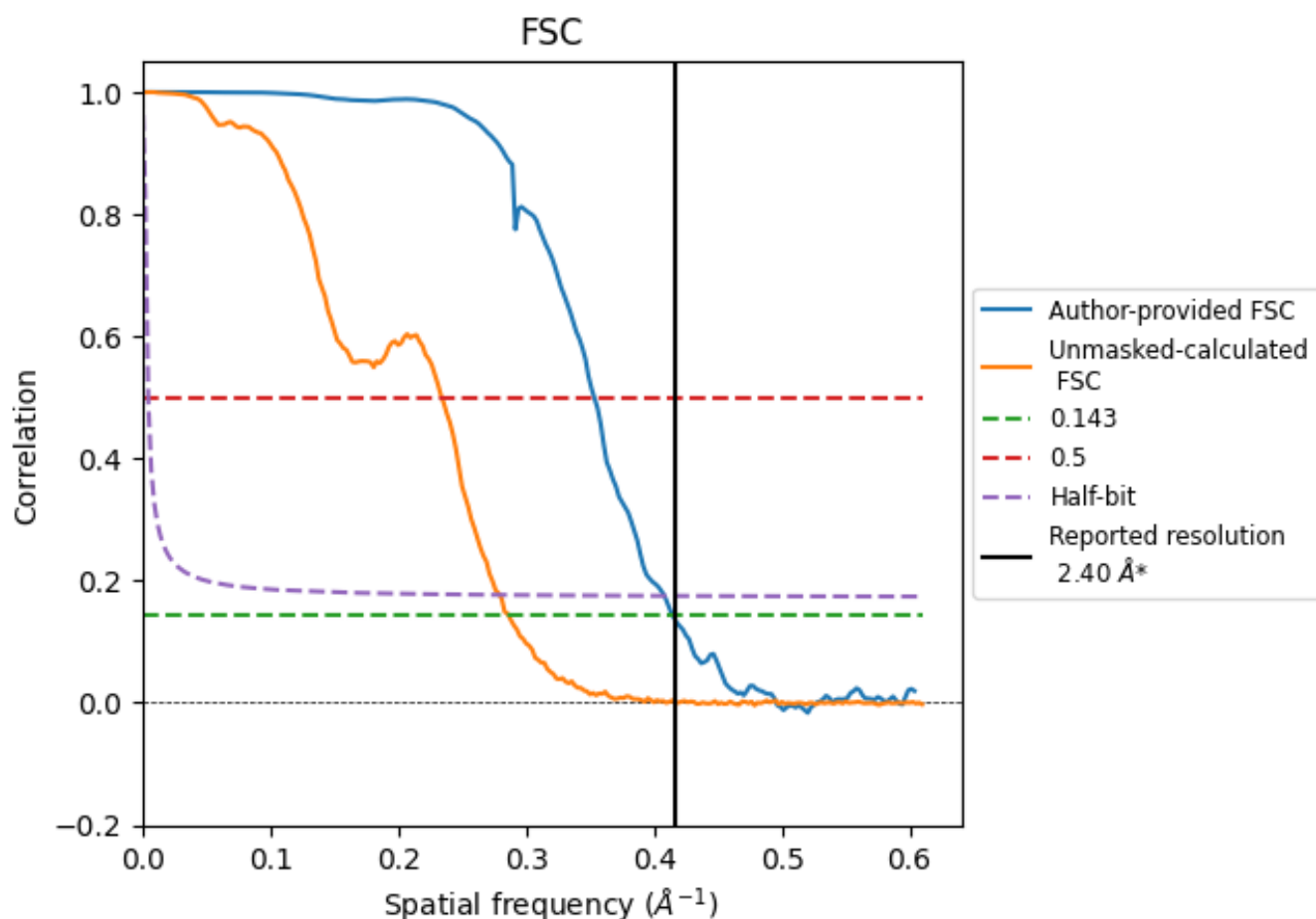


*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

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 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

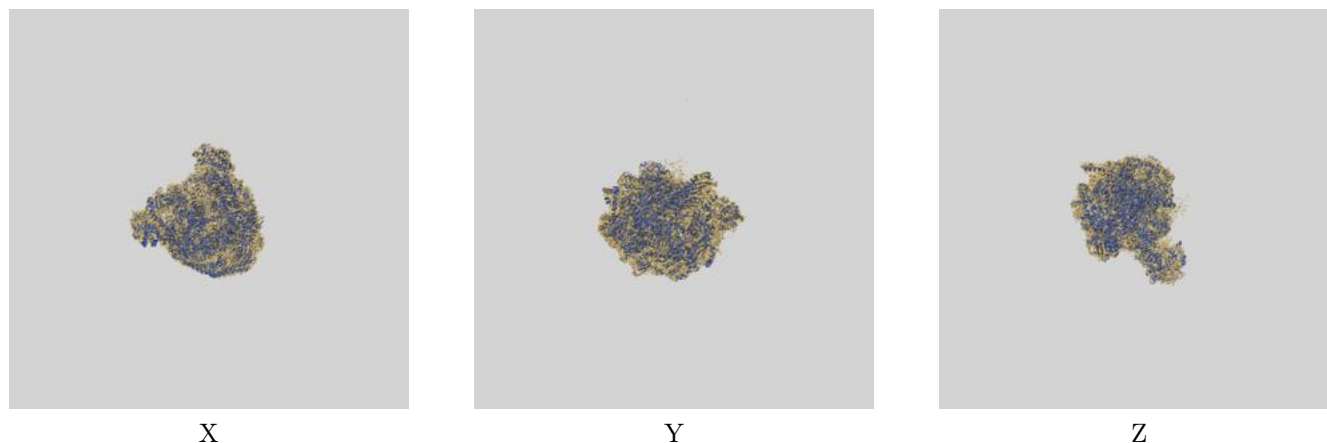
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.41	2.83	2.45
Unmasked-calculated*	3.49	4.27	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

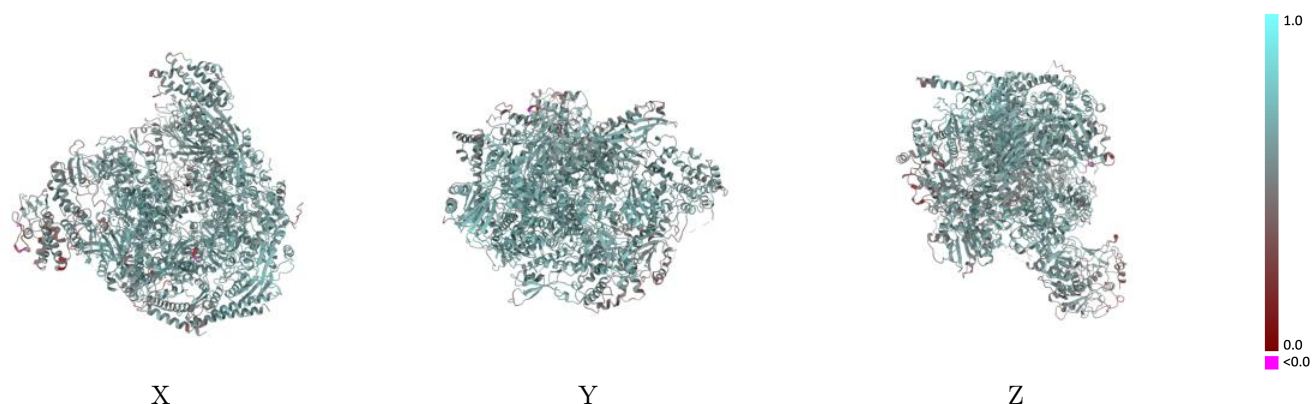
This section contains information regarding the fit between EMDB map EMD-38746 and PDB model 8XX5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



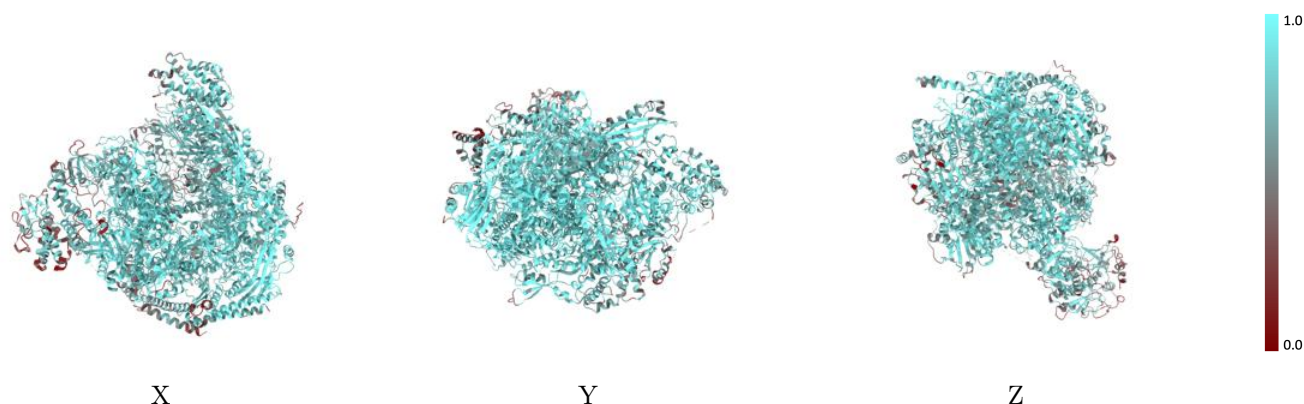
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



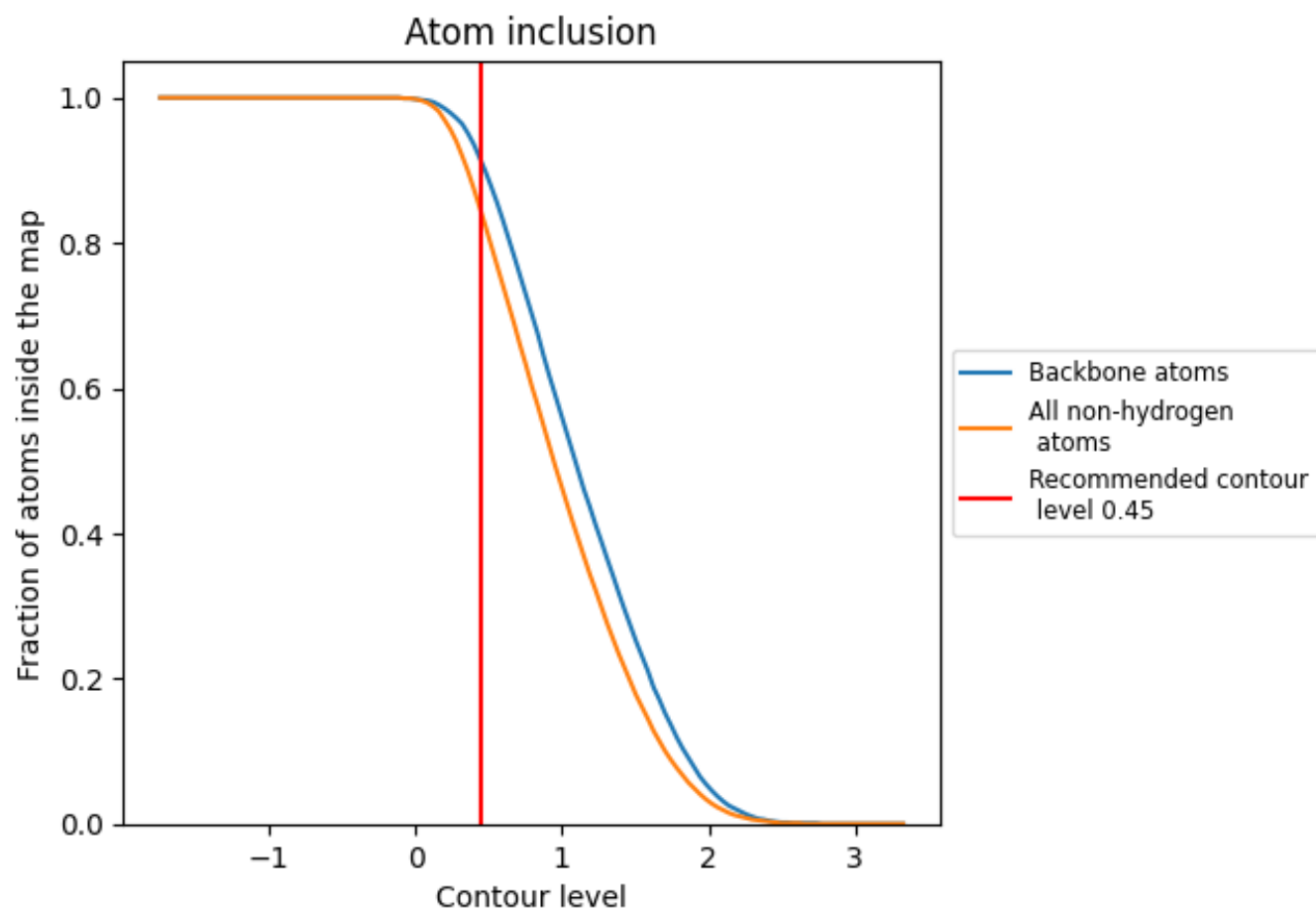
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.6070
A	0.8950	0.6330
B	0.9050	0.6350
C	0.9100	0.6440
D	0.8120	0.5830
E	0.8320	0.6230
F	0.6620	0.5120
G	0.8200	0.5720
H	0.9680	0.6630
I	0.7240	0.5570

1.0

0.0

<0.0