Full wwPDB EM Validation Report ⓘ

Jan 20, 2025 – 02:41 PM JST

PDB ID	:	8Y0E
EMDB ID	:	EMD-38802
Title	:	ASFV RNAP M1249L C-tail occupied complex4 (MCOC4)
Authors	:	Zhu, G.L.; Zhu, Y.; Zhu, Z.X.; Sun, F.; Zheng, H.X.
Deposited on	:	2024-01-22
Resolution	:	3.00 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:

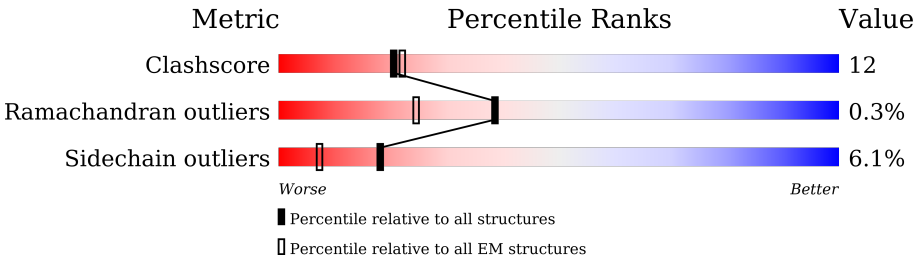
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1450	5% 68% 26%
2	B	1242	10% 62% 32%
3	C	359	74% 25%
4	D	205	8% 75% 22%
5	E	147	7% 52% 18% 27%
6	F	339	47% 45% 22% 30%
7	G	105	11% 61% 36%
8	H	80	5% 51% 32% 14%

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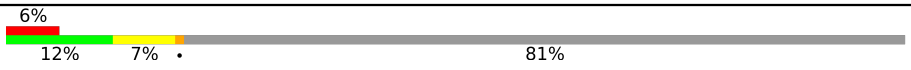
Mol	Chain	Length	Quality of chain
9	I	1249	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31248 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1400	11157	7085	1939	2071	62	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1200	9493	5994	1666	1782	51	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	358	2907	1885	481	529	12	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase RPB5 homolog.

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

- Molecule 5 is a protein called C147L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	107	839	533	144	157	5	0	0

- Molecule 6 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	237	1906	1226	315	354	11	0	0

- Molecule 7 is a protein called C122R.

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

- Molecule 8 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	69	Total	C	N	O	S	0	0
			553	362	89	95	7		

- Molecule 9 is a protein called M1249L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	239	Total	C	N	O	S	0	0
			1901	1221	301	371	8		

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

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

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

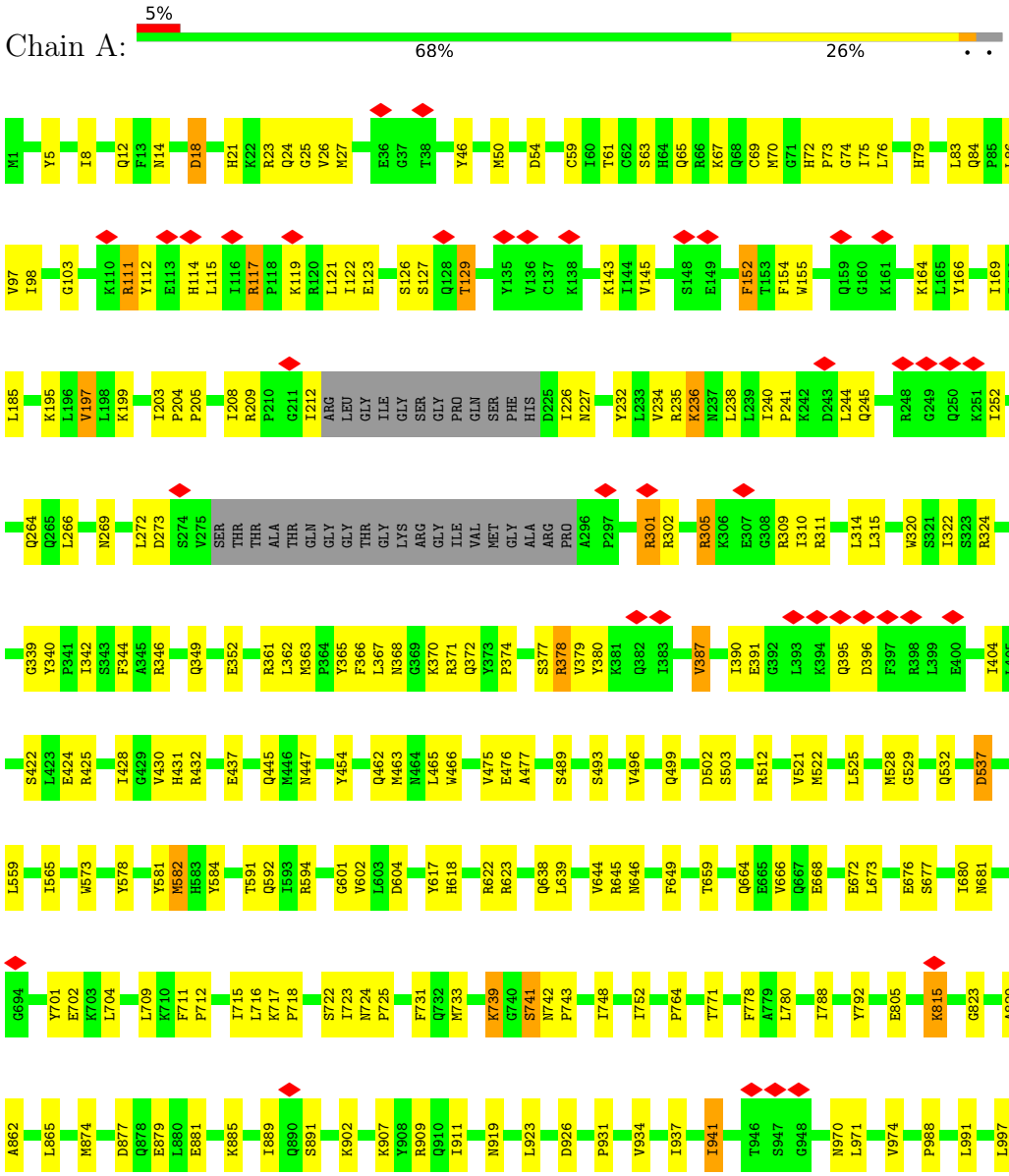
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	

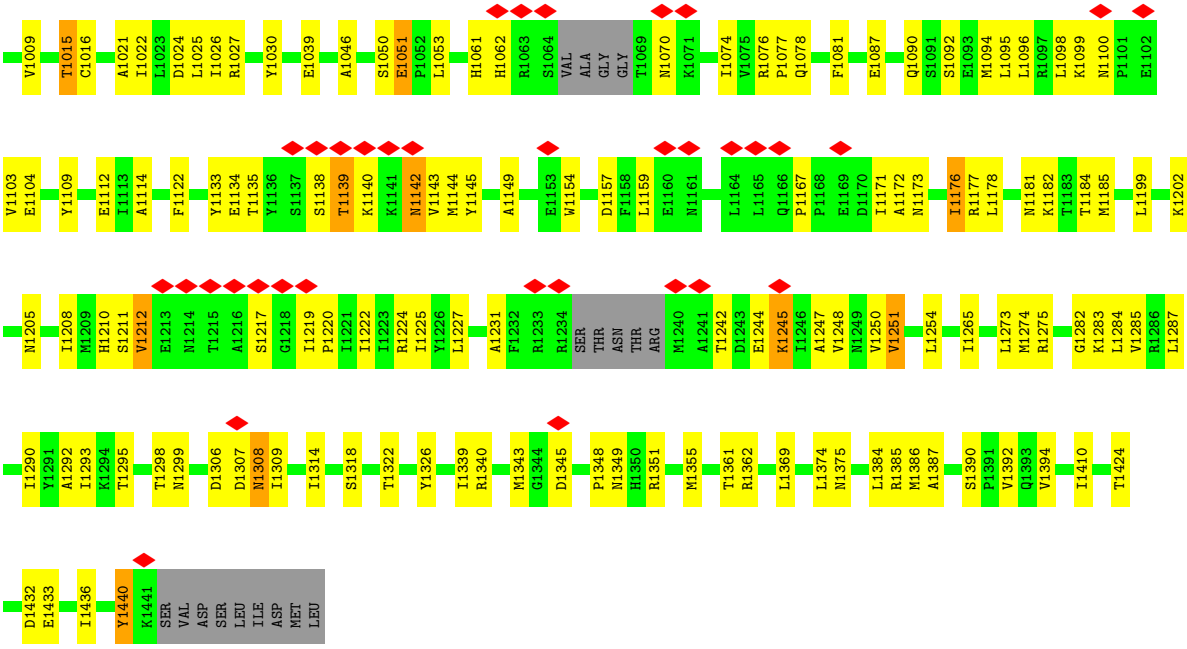
3 Residue-property plots (i)

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

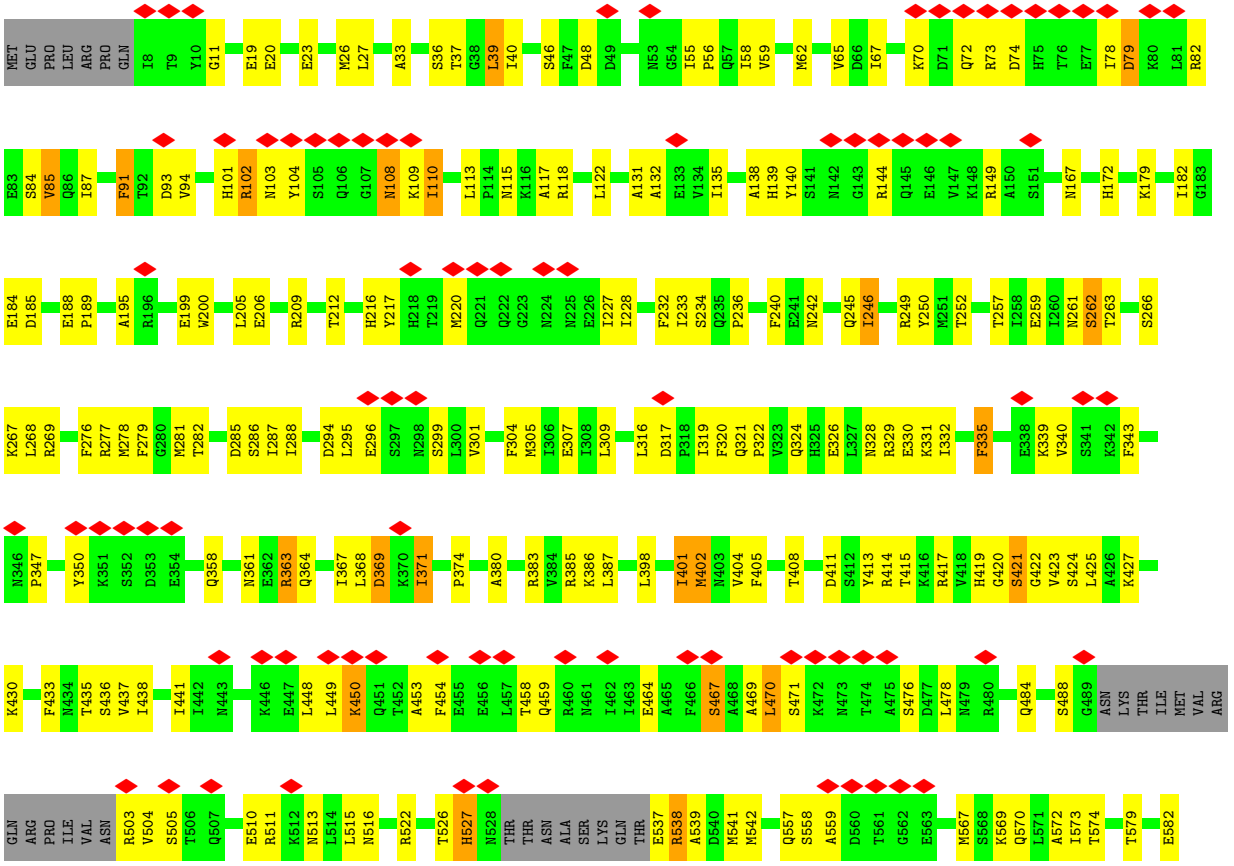
Chain A:

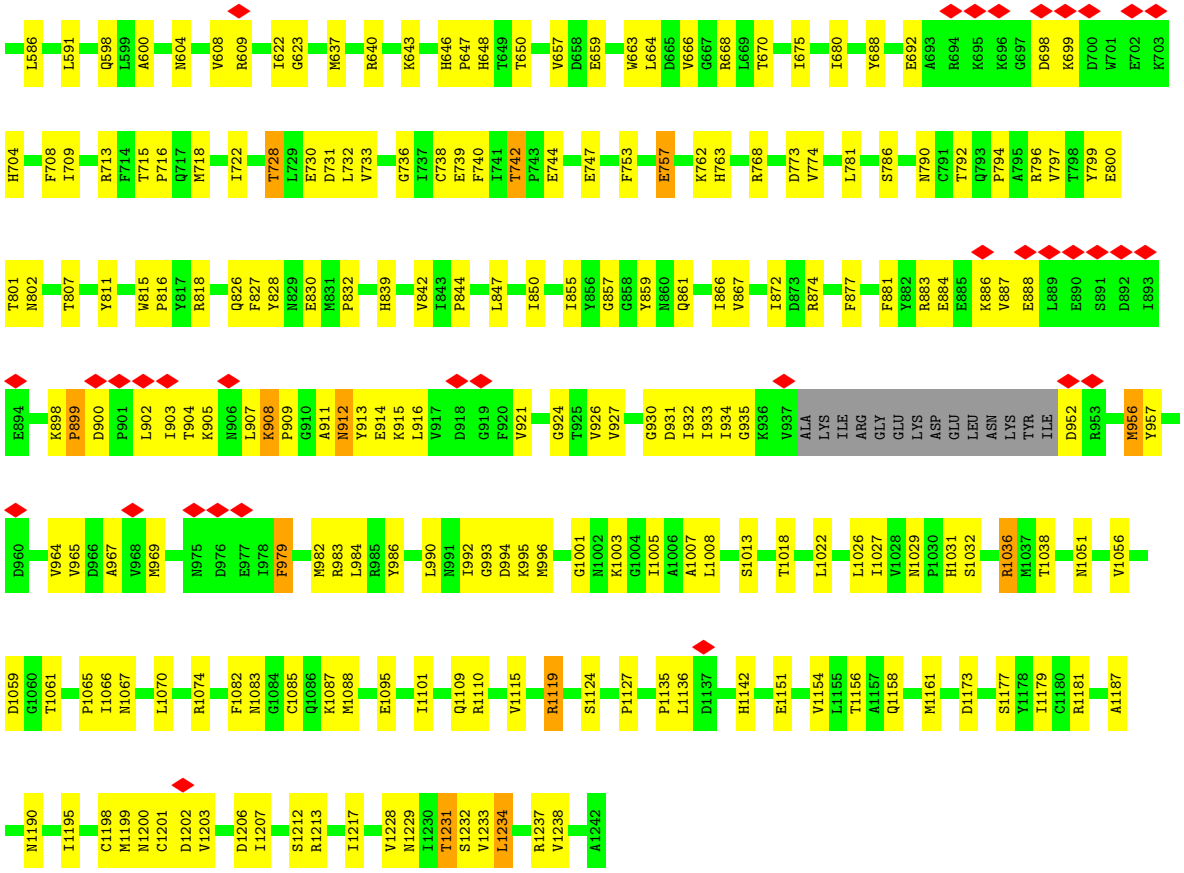




• Molecule 2: DNA-directed RNA polymerase subunit beta

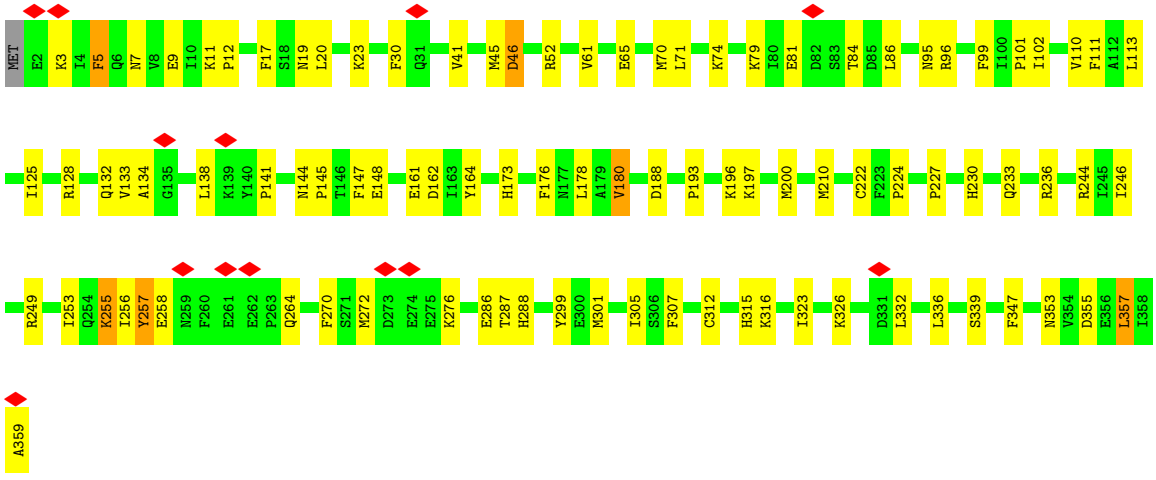
Chain B:





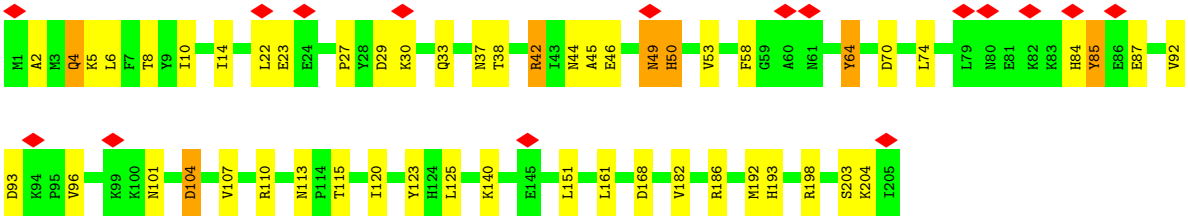
• Molecule 3: DNA-directed RNA polymerase RPB3-11 homolog

Chain C:



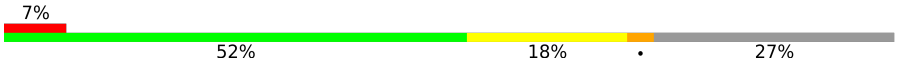
• Molecule 4: DNA-directed RNA polymerase RPB5 homolog

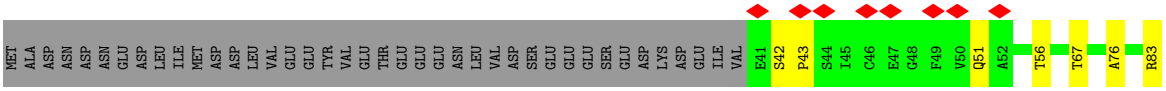
Chain D:

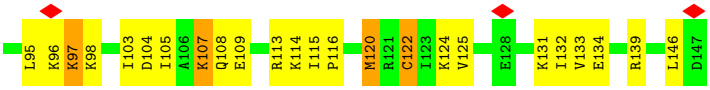


• Molecule 5: C147L

Chain E:

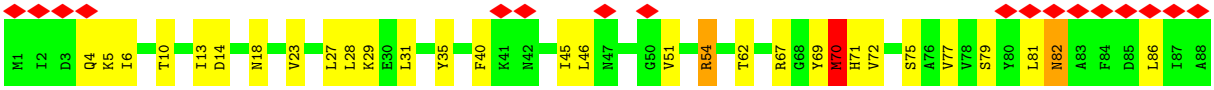


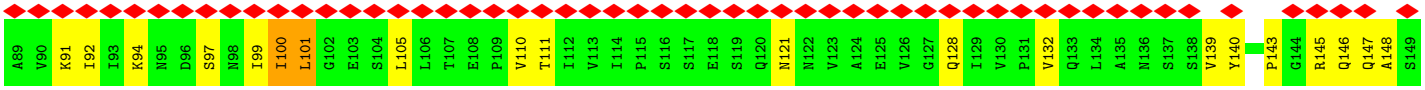


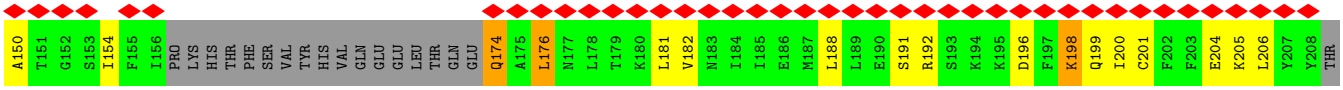


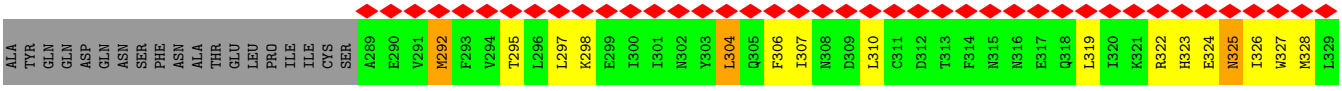
• Molecule 6: D339L

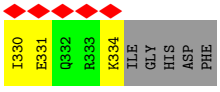
Chain F:





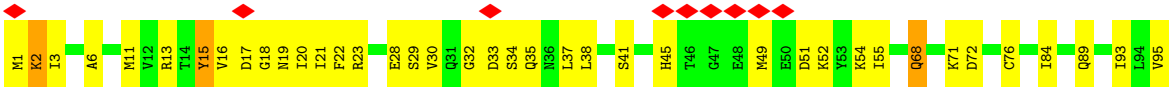


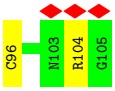




• Molecule 7: C122R

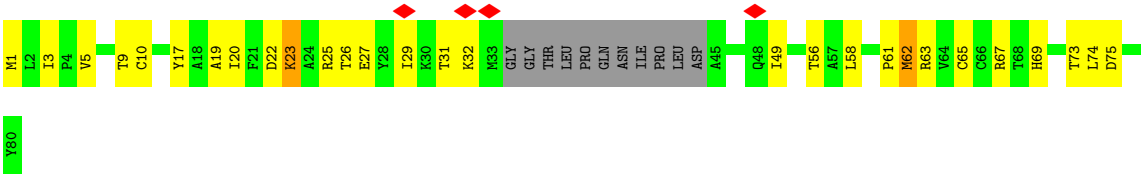
Chain G:





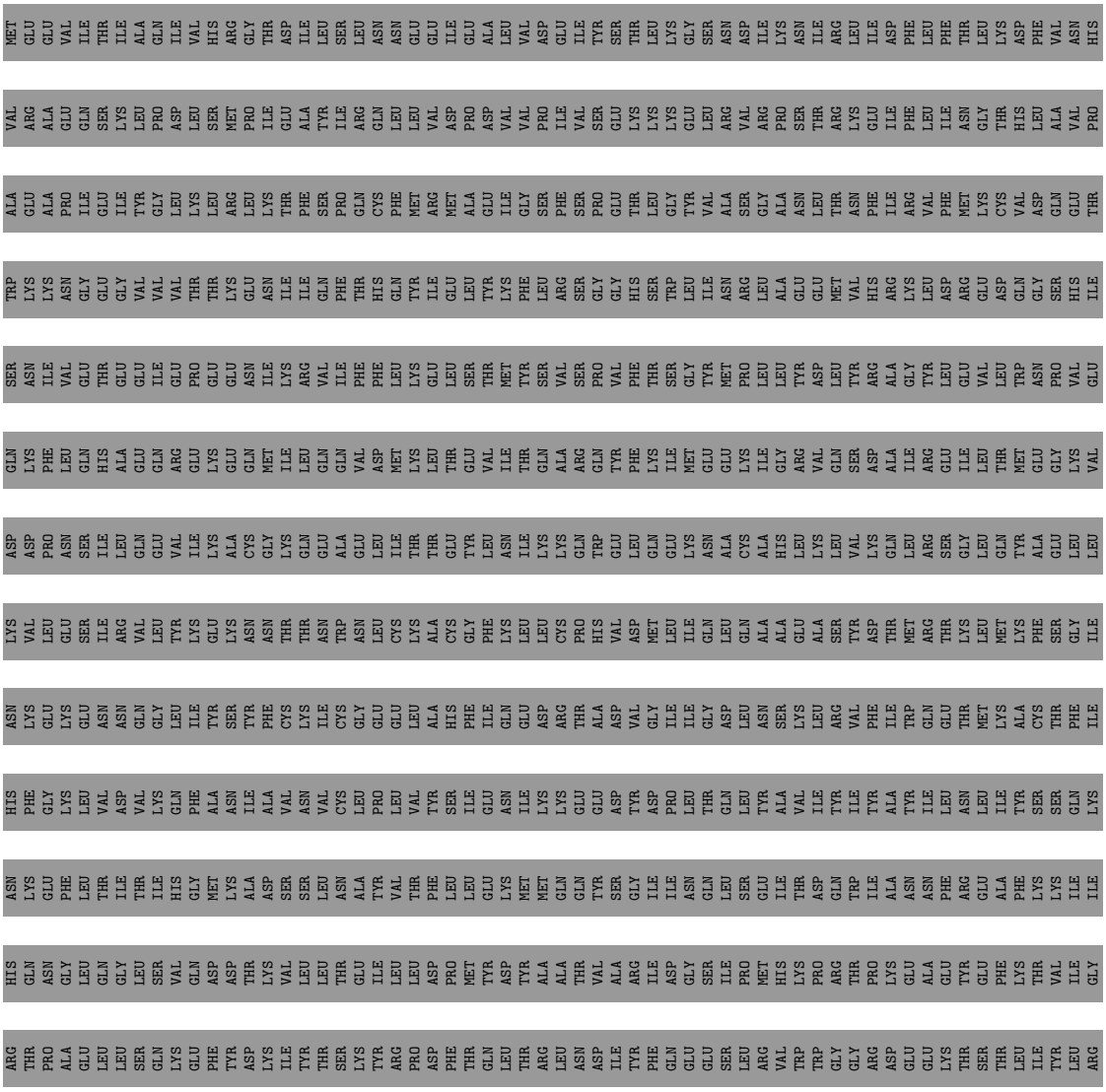
• Molecule 8: DNA-directed RNA polymerase RPB10 homolog

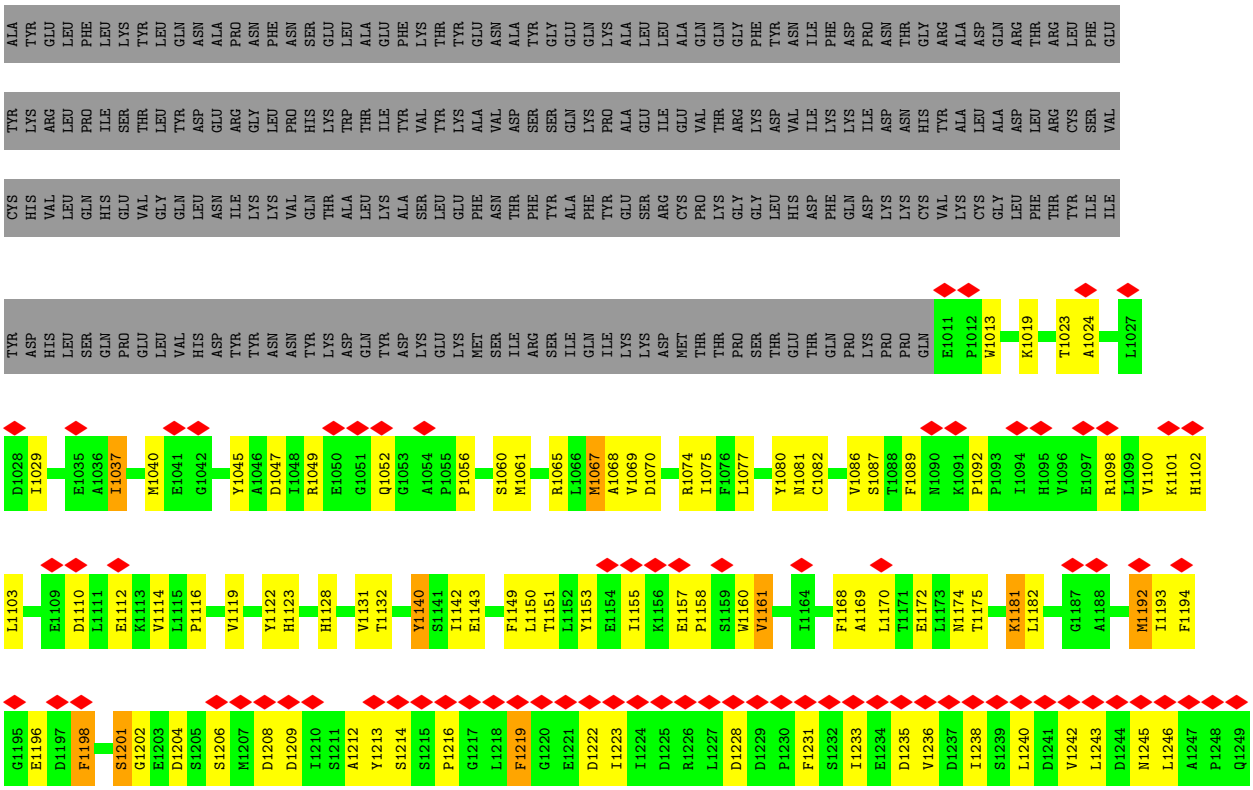
Chain H:



• Molecule 9: M1249L

Chain I:




ALA TYR GLU LEU PHE LEU LYS TYR LEU GLN ASN ALA PRO ASN PHE ASN SER GLU LEU ALA GLU PHE LYS THR TYR GLU ASN ALA TYR GLY GLU GLN LYS ALA LEU LEU ALA GLN GLN GLY PHE TYR ASN ILE PHE ASP PRO ASN THR GLY ARG ALA ASP GLN ARG THR ARG LEU PHE GLU
TYR LYS ARG LEU PRO ILE SER THR LEU TYR ASP GLU ARG GLY LEU PRO HIS LYS TRP THR ILE TYR VAL TYR LYS ALA VAL ASP SER SER GLN LYS PRO ALA GLU ILE GLU VAL THR ARG LYS ASP VAL LEU HIS ASP PHE GLN ASP LYS LYS VAL LYS ILE ASP ASN HIS TYR ALA LEU ALA ASP LEU ARG CYS SER VAL
CYS HIS VAL LEU GLN HIS GLU VAL GLY GLN LEU ASN ILE LYS LYS VAL GLN THR ALA LEU LYS ALA SER LEU GLU PHE ASN THR PHE TYR ALA PHE TYR GLN ILE GLN LYS PRO ALA GLU SER ARG CYS PRO LYS GLY GLY LEU HIS ASP PHE GLN ASP LYS CYS VAL LYS CYS GLY LEU PHE THR TYR ILE ILE
TYR ASP HIS LEU SER GLN PRO GLU LEU VAL HIS ASP TYR TYR ASN ASN TYR LYS ASP GLN TYR ASP LYS GLU LYS MET SER ILE ARG SER ILE GLN ILE LYS LYS ASP MET THR THR PRO SER THR GLU THR GLN PRO LYS PRO PRO GLN E1011 P1012 W1013 K1019 T1023 A1024 L1027
D1028 I1029 E1035 A1036 I1037 M1040 E1041 G1042 Y1045 A1046 D1047 I1048 R1049 E1050 G1051 Q1052 G1053 A1054 P1055 P1056 S1060 M1061 R1065 L1066 M1067 A1068 V1069 D1070 R1074 I1075 F1076 L1077 Y1080 N1081 C1082 V1086 S1087 T1088 F1089 N1090 K1091 P1092 P1093 I1094 H1095 V1096 E1097 R1098 L1099 V1100 K1101 H1102
L1103 E1109 D1110 L1111 E1112 K1113 V1114 L1115 P1116 V1119 Y1122 H1123 H1128 V1131 T1132 Y1140 S1141 I1142 E1143 F1149 L1150 T1151 L1152 Y1153 E1154 I1155 K1156 E1157 P1158 S1159 W1160 V1161 I1164 F1168 A1169 L1170 T1171 E1172 L1173 N1174 T1175 K1181 L1182 G1187 A1188 M1192 I1193 F1194
G1195 E1196 D1197 F1198 S1201 G1202 E1203 D1204 S1205 S1206 M1207 D1208 D1209 I1210 S1211 A1212 Y1213 S1214 S1215 P1216 G1217 L1218 F1219 G1220 E1221 D1222 I1223 I1224 D1225 R1226 L1227 D1228 D1229 P1230 F1231 S1232 I1233 E1234 D1235 V1236 D1237 I1238 S1239 L1240 D1241 V1242 L1243 D1244 N1245 L1246 A1247 P1248 Q1249

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65385	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 ($e^-/Å^2$)	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	2.077	Depositor
Minimum map value	-0.969	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.4	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: MG, ZN

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	0.33	0/11373	0.51	0/15402
2	B	0.33	0/9684	0.53	2/13104 (0.0%)
3	C	0.34	0/2969	0.51	0/4012
4	D	0.32	0/1708	0.49	0/2311
5	E	0.32	0/851	0.51	0/1151
6	F	0.28	0/1936	0.50	1/2616 (0.0%)
7	G	0.34	0/828	0.57	0/1109
8	H	0.35	0/563	0.54	0/758
9	I	0.28	0/1947	0.46	0/2648
All	All	0.33	0/31859	0.51	3/43111 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	899	PRO	CA-N-CD	-12.09	94.58	111.50
2	B	899	PRO	N-CD-CG	-6.37	93.64	103.20
6	F	143	PRO	CA-N-CD	-5.15	104.30	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11157	0	11278	255	0
2	B	9493	0	9426	295	0
3	C	2907	0	2982	62	0
4	D	1669	0	1713	25	0
5	E	839	0	883	22	0
6	F	1906	0	1943	55	0
7	G	816	0	813	31	0
8	H	553	0	580	22	0
9	I	1901	0	1860	63	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
11	A	1	0	0	0	0
All	All	31248	0	31478	749	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 12.

All (749) 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)
1:A:431:HIS:HE2	1:A:454:TYR:HH	1.12	0.91
3:C:353:ASN:O	3:C:357:LEU:HB2	1.79	0.82
8:H:17:TYR:HB3	8:H:58:LEU:HD22	1.61	0.81
1:A:1074:ILE:HG22	1:A:1078:GLN:HG3	1.63	0.81
2:B:205:LEU:HG	2:B:505:SER:HB2	1.65	0.79
4:D:49:ASN:O	4:D:49:ASN:ND2	2.17	0.77
2:B:281:MET:HB3	9:I:1067:MET:HG3	1.69	0.75
3:C:65:GLU:OE1	3:C:249:ARG:NH2	2.18	0.75
4:D:42:ARG:NH2	4:D:85:TYR:OH	2.19	0.74
1:A:1092:SER:HG	1:A:1298:THR:HG1	1.34	0.74
2:B:294:ASP:OD2	2:B:609:ARG:NH1	2.20	0.74
2:B:1051:ASN:OD1	2:B:1074:ARG:NH2	2.20	0.73
2:B:227:ILE:HG22	2:B:228:ILE:H	1.50	0.73
1:A:92:ARG:HH11	1:A:96:ARG:HH21	1.37	0.72
2:B:115:ASN:ND2	2:B:182:ILE:O	2.22	0.72
4:D:37:ASN:OD1	4:D:38:THR:N	2.23	0.72
1:A:301:ARG:HH22	1:A:305:ARG:HB2	1.55	0.71
2:B:411:ASP:OD1	2:B:538:ARG:NH2	2.23	0.71
2:B:967:ALA:HB3	2:B:983:ARG:H	1.54	0.71
2:B:367:ILE:O	2:B:371:ILE:HB	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:SER:OG	1:A:1349:ASN:ND2	2.23	0.70
1:A:311:ARG:HH22	9:I:1235:ASP:HA	1.56	0.70
1:A:301:ARG:O	1:A:301:ARG:NE	2.18	0.70
1:A:646:ASN:ND2	2:B:1095:GLU:OE1	2.20	0.69
2:B:924:GLY:N	2:B:965:VAL:O	2.24	0.69
2:B:899:PRO:O	2:B:899:PRO:HD2	1.92	0.69
2:B:558:SER:O	2:B:802:ASN:ND2	2.25	0.68
2:B:329:ARG:HA	2:B:332:ILE:HD12	1.75	0.68
4:D:29:ASP:O	4:D:33:GLN:HG2	1.93	0.68
1:A:502:ASP:OD2	2:B:1029:ASN:ND2	2.22	0.68
2:B:70:LYS:HE3	9:I:1192:MET:HA	1.73	0.68
1:A:1114:ALA:HB2	1:A:1293:ILE:HG21	1.74	0.68
4:D:192:MET:O	4:D:193:HIS:ND1	2.26	0.68
4:D:22:LEU:HD23	4:D:44:ASN:HB3	1.75	0.68
1:A:395:GLN:NE2	1:A:396:ASP:OD1	2.26	0.68
2:B:19:GLU:OE2	2:B:19:GLU:N	2.24	0.68
3:C:253:ILE:HA	3:C:256:ILE:HD12	1.75	0.67
1:A:1087:GLU:N	1:A:1087:GLU:OE2	2.27	0.67
1:A:1205:ASN:HB2	1:A:1231:ALA:HB2	1.77	0.67
8:H:10:CYS:SG	8:H:63:ARG:NH1	2.68	0.67
2:B:586:LEU:HD23	2:B:664:LEU:HD11	1.76	0.67
2:B:70:LYS:NZ	9:I:1194:PHE:O	2.28	0.67
2:B:916:LEU:HD22	2:B:935:GLY:H	1.59	0.67
1:A:1208:ILE:HD12	1:A:1225:ILE:HG22	1.77	0.66
9:I:1037:ILE:HG22	9:I:1069:VAL:HG22	1.77	0.66
2:B:1018:THR:HG22	2:B:1088:MET:HG2	1.77	0.66
1:A:93:ARG:HD2	1:A:121:LEU:HG	1.77	0.66
6:F:324:GLU:HG2	6:F:327:TRP:HD1	1.60	0.66
1:A:1245:LYS:HE3	1:A:1245:LYS:HA	1.77	0.66
5:E:83:ARG:HD3	5:E:116:PRO:HD2	1.78	0.66
2:B:277:ARG:HB2	2:B:282:THR:HG22	1.78	0.66
1:A:1432:ASP:OD2	5:E:139:ARG:NH2	2.28	0.66
1:A:232:TYR:HB3	1:A:266:LEU:HD21	1.77	0.66
9:I:1170:LEU:O	9:I:1174:ASN:ND2	2.29	0.66
7:G:2:LYS:HD3	7:G:30:VAL:HG21	1.79	0.65
1:A:1138:SER:O	1:A:1140:LYS:N	2.29	0.65
2:B:830:GLU:HG3	2:B:847:LEU:HA	1.78	0.65
2:B:228:ILE:HG21	2:B:401:ILE:HG12	1.78	0.65
3:C:257:TYR:HE1	3:C:336:LEU:HB2	1.61	0.65
4:D:42:ARG:NE	4:D:44:ASN:OD1	2.30	0.65
9:I:1114:VAL:HG11	9:I:1161:VAL:HG11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:H	1:A:169:ILE:HD12	1.62	0.65
2:B:994:ASP:OD2	2:B:1110:ARG:NH2	2.30	0.65
2:B:321:GLN:OE1	2:B:324:GLN:NE2	2.30	0.64
1:A:578:TYR:HE1	1:A:742:ASN:HD21	1.46	0.64
2:B:216:HIS:ND1	2:B:217:TYR:O	2.30	0.64
1:A:889:ILE:HG22	1:A:891:SER:H	1.62	0.64
2:B:404:VAL:HG13	7:G:52:LYS:HG3	1.80	0.64
6:F:46:LEU:HD11	6:F:79:SER:HB3	1.79	0.64
9:I:1086:VAL:HG11	9:I:1100:VAL:HG11	1.79	0.63
1:A:1182:LYS:HA	1:A:1185:MET:HB2	1.79	0.63
2:B:728:THR:OG1	2:B:730:GLU:OE1	2.15	0.63
9:I:1047:ASP:HB3	9:I:1052:GLN:HE22	1.63	0.63
2:B:113:LEU:HD22	2:B:182:ILE:HD11	1.80	0.63
2:B:522:ARG:NH2	2:B:572:ALA:O	2.31	0.63
6:F:31:LEU:HD11	6:F:72:VAL:HG11	1.79	0.63
9:I:1056:PRO:O	9:I:1065:ARG:NH2	2.31	0.63
3:C:96:ARG:NH2	3:C:148:GLU:O	2.22	0.63
2:B:877:PHE:O	2:B:1110:ARG:NH1	2.30	0.63
2:B:73:ARG:HH22	2:B:453:ALA:HA	1.64	0.62
2:B:722:ILE:HD11	2:B:732:LEU:HD11	1.81	0.62
2:B:510:GLU:O	2:B:516:ASN:ND2	2.32	0.62
2:B:902:LEU:HD23	2:B:902:LEU:H	1.63	0.62
2:B:1212:SER:OG	2:B:1213:ARG:N	2.29	0.62
1:A:430:VAL:HG21	1:A:477:ALA:HB1	1.80	0.62
1:A:377:SER:HA	1:A:390:ILE:HB	1.81	0.62
1:A:1098:LEU:HB2	1:A:1104:GLU:HB3	1.82	0.62
3:C:276:LYS:HG2	3:C:326:LYS:HD2	1.80	0.62
2:B:650:THR:HB	2:B:663:TRP:HB2	1.82	0.61
2:B:622:ILE:HD12	2:B:622:ILE:O	2.01	0.61
1:A:1386:MET:HG2	1:A:1394:VAL:HG23	1.81	0.61
1:A:1440:TYR:OH	5:E:83:ARG:NH2	2.33	0.61
2:B:467:SER:O	2:B:471:SER:OG	2.18	0.61
2:B:600:ALA:HB1	9:I:1060:SER:HB2	1.83	0.61
7:G:19:ASN:OD1	7:G:20:ILE:N	2.33	0.61
1:A:23:ARG:HH11	5:E:43:PRO:HG3	1.65	0.61
1:A:74:GLY:O	1:A:203:ILE:N	2.33	0.61
2:B:437:VAL:HG22	2:B:470:LEU:HD11	1.83	0.61
3:C:230:HIS:HB3	3:C:233:GLN:HE21	1.66	0.61
2:B:206:GLU:OE1	2:B:569:LYS:NZ	2.30	0.61
9:I:1077:LEU:HD13	9:I:1119:VAL:HG13	1.83	0.60
1:A:489:SER:HB2	1:A:496:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:NE2	1:A:195:LYS:O	2.34	0.60
1:A:98:ILE:HD13	1:A:177:VAL:HG22	1.83	0.60
3:C:326:LYS:HE2	3:C:326:LYS:HA	1.83	0.60
7:G:17:ASP:OD1	7:G:18:GLY:N	2.34	0.60
1:A:551:ASP:OD1	1:A:552:GLY:N	2.34	0.60
1:A:1159:LEU:HD11	1:A:1167:PRO:HD3	1.83	0.60
9:I:1193:ILE:HD12	9:I:1193:ILE:H	1.67	0.60
3:C:180:VAL:HG22	3:C:222:CYS:HB3	1.83	0.60
1:A:380:TYR:HB3	1:A:404:ILE:HB	1.83	0.60
2:B:140:TYR:HB2	2:B:144:ARG:HB2	1.84	0.60
1:A:1227:LEU:HD11	1:A:1250:VAL:HG11	1.84	0.60
2:B:85:VAL:HG11	2:B:449:LEU:HD11	1.84	0.60
3:C:96:ARG:NH1	8:H:3:ILE:O	2.28	0.60
1:A:693:ILE:HD12	1:A:693:ILE:H	1.67	0.59
1:A:367:LEU:O	1:A:371:ARG:NH2	2.35	0.59
2:B:792:THR:HG23	2:B:1038:THR:HA	1.84	0.59
2:B:797:VAL:O	2:B:801:THR:HG23	2.03	0.59
2:B:902:LEU:HG	2:B:903:ILE:HG12	1.85	0.59
2:B:904:THR:HG23	2:B:907:LEU:HD22	1.85	0.59
2:B:915:LYS:NZ	2:B:931:ASP:OD2	2.28	0.59
1:A:97:VAL:HG11	1:A:185:LEU:HD21	1.85	0.59
1:A:324:ARG:NH1	1:A:462:GLN:OE1	2.36	0.59
2:B:233:ILE:HD13	2:B:245:GLN:HB2	1.85	0.59
2:B:934:ILE:HD12	2:B:934:ILE:O	2.03	0.59
1:A:1096:LEU:HD22	1:A:1314:ILE:HD12	1.84	0.59
1:A:592:GLN:HE21	1:A:594:ARG:HG3	1.67	0.58
1:A:1275:ARG:HB2	1:A:1290:ILE:HD12	1.84	0.58
9:I:1204:ASP:OD1	9:I:1206:SER:OG	2.20	0.58
1:A:322:ILE:HG13	1:A:466:TRP:HB3	1.85	0.58
2:B:881:PHE:HB3	2:B:986:TYR:HB2	1.86	0.58
8:H:69:HIS:O	8:H:73:THR:OG1	2.20	0.58
1:A:1176:ILE:HG23	1:A:1225:ILE:HG13	1.85	0.58
2:B:167:ASN:HA	2:B:172:HIS:CG	2.39	0.58
2:B:844:PRO:HD2	8:H:74:LEU:HD11	1.84	0.58
3:C:305:ILE:HD11	3:C:323:ILE:HG23	1.85	0.58
4:D:107:VAL:HG12	4:D:110:ARG:HH21	1.69	0.58
4:D:58:PHE:O	4:D:123:TYR:OH	2.22	0.58
3:C:148:GLU:HG3	8:H:19:ALA:HB2	1.86	0.58
2:B:1083:ASN:ND2	2:B:1085:CYS:SG	2.77	0.58
1:A:681:ASN:ND2	1:A:780:LEU:O	2.35	0.58
1:A:681:ASN:OD1	1:A:701:TYR:OH	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:113:ARG:NH1	5:E:139:ARG:O	2.36	0.58
1:A:209:ARG:NH1	1:A:227:ASN:OD1	2.35	0.57
1:A:1138:SER:OG	1:A:1139:THR:N	2.37	0.57
1:A:1225:ILE:HD12	1:A:1254:LEU:HD13	1.85	0.57
2:B:72:GLN:HG2	2:B:82:ARG:HG2	1.86	0.57
2:B:866:ILE:HG23	2:B:1008:LEU:HB3	1.85	0.57
3:C:110:VAL:H	3:C:134:ALA:HB3	1.69	0.57
3:C:256:ILE:O	3:C:264:GLN:NE2	2.38	0.57
7:G:6:ALA:O	9:I:1123:HIS:NE2	2.33	0.57
1:A:352:GLU:OE1	1:A:361:ARG:NH2	2.29	0.57
1:A:1210:HIS:ND1	1:A:1211:SER:O	2.35	0.57
2:B:753:PHE:CE2	2:B:757:GLU:HG3	2.39	0.57
2:B:827:PHE:O	8:H:1:MET:N	2.35	0.57
3:C:227:PRO:HG2	3:C:230:HIS:HB2	1.86	0.57
2:B:55:ILE:O	2:B:59:VAL:HG23	2.05	0.57
1:A:418:ASN:HB2	1:A:428:ILE:HG12	1.86	0.57
2:B:1059:ASP:OD1	2:B:1061:THR:OG1	2.22	0.57
2:B:11:GLY:O	2:B:713:ARG:NH1	2.38	0.57
2:B:276:PHE:HB3	2:B:287:ILE:HD12	1.87	0.57
1:A:241:PRO:HG2	1:A:244:LEU:HG	1.87	0.56
6:F:145:ARG:NH1	6:F:146:GLN:OE1	2.37	0.56
1:A:342:ILE:HD12	1:A:437:GLU:HG2	1.86	0.56
1:A:970:ASN:O	1:A:1027:ARG:NH2	2.37	0.56
2:B:135:ILE:HG13	2:B:149:ARG:HG2	1.87	0.56
2:B:688:TYR:O	2:B:692:GLU:HG2	2.05	0.56
6:F:91:LYS:HZ3	6:F:105:LEU:H	1.52	0.56
1:A:333:LEU:O	1:A:447:ASN:ND2	2.38	0.56
2:B:317:ASP:N	2:B:324:GLN:OE1	2.38	0.56
1:A:1144:MET:HG2	1:A:1149:ALA:HA	1.88	0.56
1:A:310:ILE:HA	1:A:314:LEU:HD12	1.85	0.56
2:B:268:LEU:HD23	2:B:340:VAL:HG12	1.88	0.56
2:B:363:ARG:NH2	9:I:1201:SER:O	2.39	0.56
1:A:1361:THR:O	4:D:198:ARG:NH2	2.37	0.56
1:A:1133:TYR:OH	7:G:17:ASP:O	2.11	0.56
2:B:199:GLU:OE2	2:B:818:ARG:NH1	2.37	0.56
2:B:1201:CYS:O	2:B:1203:VAL:N	2.39	0.56
5:E:97:LYS:HD2	5:E:98:LYS:N	2.21	0.56
6:F:14:ASP:HA	6:F:67:ARG:HG2	1.87	0.56
6:F:139:VAL:HG13	6:F:150:ALA:HB2	1.88	0.56
9:I:1019:LYS:HG2	9:I:1150:LEU:HD21	1.88	0.56
2:B:424:SER:HB3	2:B:504:VAL:HA	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:648:HIS:O	2:B:668:ARG:NH1	2.34	0.55
9:I:1089:PHE:HB2	9:I:1092:PRO:HG3	1.88	0.55
5:E:122:CYS:HB2	5:E:133:VAL:HG12	1.89	0.55
2:B:768:ARG:NH1	7:G:68:GLN:OE1	2.32	0.55
6:F:174:GLN:N	6:F:174:GLN:HE21	2.04	0.55
1:A:422:SER:HB3	2:B:1154:VAL:HG21	1.89	0.55
1:A:21:HIS:HB3	1:A:75:ILE:HD12	1.88	0.55
1:A:92:ARG:HH11	1:A:96:ARG:NH2	2.03	0.55
1:A:352:GLU:HG3	1:A:407:ARG:HE	1.71	0.55
3:C:193:PRO:HG2	3:C:196:LYS:HD3	1.88	0.55
1:A:877:ASP:OD2	1:A:902:LYS:NZ	2.35	0.55
5:E:115:ILE:O	5:E:139:ARG:NH1	2.40	0.55
1:A:475:VAL:HG22	5:E:103:ILE:HG23	1.89	0.55
2:B:420:GLY:O	2:B:422:GLY:N	2.38	0.55
2:B:319:ILE:HD11	2:B:339:LYS:HD3	1.88	0.55
2:B:579:THR:HA	2:B:666:VAL:HG23	1.89	0.54
6:F:4:GLN:HA	6:F:77:VAL:HA	1.89	0.54
1:A:1142:ASN:HD21	1:A:1144:MET:HB2	1.72	0.54
2:B:866:ILE:HB	2:B:1027:ILE:HB	1.87	0.54
1:A:377:SER:O	1:A:378:ARG:NH1	2.41	0.54
1:A:805:GLU:HG2	2:B:794:PRO:HB3	1.88	0.54
2:B:227:ILE:HD11	2:B:252:THR:HA	1.90	0.54
6:F:192:ARG:HG3	6:F:200:ILE:HD13	1.89	0.54
1:A:419:ARG:HG3	1:A:463:MET:HG2	1.90	0.54
1:A:522:MET:HB3	3:C:210:MET:HB3	1.90	0.54
2:B:898:LYS:HG2	2:B:899:PRO:HD3	1.89	0.54
1:A:164:LYS:HD2	1:A:166:TYR:CE1	2.43	0.54
2:B:84:SER:O	2:B:139:HIS:N	2.35	0.54
2:B:262:SER:O	2:B:266:SER:OG	2.25	0.54
3:C:101:PRO:HD2	3:C:147:PHE:CZ	2.43	0.54
3:C:138:LEU:HD13	3:C:141:PRO:HA	1.90	0.54
8:H:62:MET:HE2	8:H:62:MET:HA	1.90	0.54
1:A:926:ASP:OD1	1:A:926:ASP:N	2.38	0.54
2:B:78:ILE:HG22	2:B:82:ARG:HH21	1.73	0.54
2:B:108:ASN:N	2:B:108:ASN:OD1	2.40	0.54
2:B:921:VAL:HG21	2:B:933:ILE:HG22	1.90	0.54
6:F:91:LYS:N	6:F:91:LYS:HD2	2.23	0.54
1:A:1134:GLU:HB3	7:G:37:LEU:HD23	1.90	0.53
2:B:826:GLN:NE2	2:B:828:TYR:O	2.38	0.53
2:B:786:SER:HB2	2:B:800:GLU:HG2	1.90	0.53
3:C:12:PRO:HA	3:C:41:VAL:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:TYR:CE2	7:G:38:LEU:HB2	2.43	0.53
2:B:993:GLY:HA2	2:B:1005:ILE:HG23	1.90	0.53
6:F:111:THR:OG1	6:F:147:GLN:NE2	2.37	0.53
2:B:926:VAL:HG22	2:B:964:VAL:HG22	1.90	0.53
2:B:288:ILE:HG22	2:B:295:LEU:HD21	1.91	0.53
3:C:20:LEU:HD22	3:C:20:LEU:H	1.73	0.53
1:A:18:ASP:OD2	1:A:199:LYS:N	2.33	0.53
1:A:346:ARG:NH2	1:A:372:GLN:O	2.42	0.53
1:A:499:GLN:HB3	1:A:503:SER:HB2	1.91	0.53
1:A:1273:LEU:HD11	1:A:1292:ALA:HB3	1.91	0.53
1:A:673:LEU:HD21	1:A:712:PRO:HD3	1.91	0.53
4:D:6:LEU:O	4:D:10:ILE:HG22	2.07	0.53
2:B:573:ILE:HG23	2:B:574:THR:HG23	1.90	0.53
9:I:1080:TYR:OH	9:I:1116:PRO:O	2.12	0.53
2:B:216:HIS:HB3	9:I:1219:PHE:CE2	2.44	0.53
2:B:417:ARG:NH1	2:B:744:GLU:OE2	2.41	0.53
4:D:64:TYR:CZ	4:D:74:LEU:HD12	2.44	0.53
1:A:752:ILE:HB	1:A:788:ILE:HB	1.90	0.53
2:B:46:SER:OG	2:B:421:SER:OG	2.25	0.53
7:G:54:LYS:HA	7:G:54:LYS:HE2	1.91	0.53
1:A:332:ASP:OD2	2:B:859:TYR:OH	2.23	0.52
8:H:61:PRO:HG2	8:H:63:ARG:HD2	1.91	0.52
3:C:236:ARG:NE	3:C:359:ALA:OXT	2.42	0.52
6:F:319:LEU:HA	6:F:322:ARG:HB3	1.90	0.52
1:A:823:GLY:HA3	9:I:1236:VAL:HG22	1.90	0.52
1:A:1154:TRP:HA	1:A:1157:ASP:HB2	1.91	0.52
2:B:82:ARG:HD3	2:B:138:ALA:HB1	1.91	0.52
5:E:122:CYS:SG	5:E:131:LYS:NZ	2.63	0.52
6:F:206:LEU:HD21	6:F:330:ILE:HG21	1.91	0.52
9:I:1061:MET:HE2	9:I:1131:VAL:HA	1.90	0.52
1:A:63:SER:O	2:B:1190:ASN:ND2	2.42	0.52
3:C:249:ARG:NH1	3:C:286:GLU:OE2	2.43	0.52
6:F:110:VAL:HG22	6:F:148:ALA:HB3	1.92	0.52
2:B:330:GLU:OE2	2:B:361:ASN:ND2	2.30	0.52
2:B:582:GLU:O	2:B:582:GLU:HG2	2.09	0.52
3:C:113:LEU:HD21	3:C:125:ILE:HG21	1.90	0.52
3:C:128:ARG:HB3	3:C:145:PRO:HB2	1.92	0.52
4:D:53:VAL:HG22	4:D:87:GLU:HB3	1.91	0.52
1:A:330:ASN:ND2	1:A:445:GLN:OE1	2.43	0.52
1:A:919:ASN:OD1	1:A:1340:ARG:NH2	2.42	0.52
2:B:688:TYR:HE1	7:G:76:CYS:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:CYS:O	1:A:61:THR:N	2.40	0.52
1:A:988:PRO:HD2	1:A:991:LEU:HD12	1.92	0.52
1:A:14:ASN:O	2:B:1229:ASN:N	2.41	0.51
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.91	0.51
2:B:305:MET:HG2	2:B:398:LEU:HD23	1.92	0.51
1:A:119:LYS:HD2	1:A:122:ILE:HD11	1.92	0.51
2:B:296:GLU:N	2:B:296:GLU:OE1	2.42	0.51
9:I:1013:TRP:NE1	9:I:1143:GLU:OE1	2.35	0.51
1:A:252:ILE:HD13	1:A:256:ILE:HG22	1.92	0.51
1:A:512:ARG:HA	1:A:602:VAL:HG12	1.93	0.51
1:A:573:TRP:N	1:A:604:ASP:OD2	2.44	0.51
1:A:1220:PRO:HG2	1:A:1222:ILE:HD11	1.92	0.51
2:B:526:THR:O	2:B:527:HIS:ND1	2.43	0.51
7:G:45:HIS:NE2	7:G:89:GLN:OE1	2.44	0.51
1:A:24:GLN:OE1	2:B:1200:ASN:ND2	2.37	0.51
1:A:1375:ASN:OD1	1:A:1385:ARG:NE	2.44	0.51
6:F:325:ASN:OD1	6:F:325:ASN:N	2.39	0.51
9:I:1158:PRO:HG2	9:I:1161:VAL:HG13	1.93	0.51
1:A:1275:ARG:O	1:A:1287:LEU:N	2.40	0.51
2:B:992:ILE:HG23	2:B:1007:ALA:HA	1.92	0.51
1:A:1070:ASN:ND2	1:A:1090:GLN:OE1	2.36	0.51
1:A:70:MET:HB3	2:B:1217:ILE:HG21	1.91	0.51
1:A:909:ARG:NH1	1:A:1282:GLY:O	2.42	0.51
1:A:76:LEU:HD22	1:A:234:VAL:HG22	1.93	0.50
2:B:513:ASN:HA	2:B:811:TYR:HA	1.93	0.50
2:B:1177:SER:OG	2:B:1217:ILE:HD11	2.11	0.50
1:A:1247:ALA:O	1:A:1251:VAL:HG12	2.11	0.50
1:A:370:LYS:HE3	1:A:391:GLU:HG3	1.92	0.50
2:B:285:ASP:HB2	7:G:3:ILE:HG21	1.92	0.50
6:F:35:TYR:HE2	6:F:40:PHE:CD1	2.28	0.50
2:B:414:ARG:HG2	2:B:415:THR:HG23	1.93	0.50
1:A:46:TYR:CZ	1:A:212:ILE:HG12	2.47	0.50
1:A:171:ARG:HA	1:A:197:VAL:HG21	1.94	0.50
1:A:1051:GLU:OE1	1:A:1051:GLU:N	2.44	0.50
2:B:206:GLU:HG2	2:B:526:THR:HA	1.93	0.50
3:C:272:MET:N	3:C:276:LYS:O	2.42	0.50
1:A:537:ASP:OD1	1:A:537:ASP:N	2.33	0.50
1:A:907:LYS:HE3	1:A:911:ILE:HD11	1.94	0.50
2:B:874:ARG:HG2	3:C:99:PHE:CE1	2.47	0.50
2:B:903:ILE:O	2:B:905:LYS:N	2.43	0.50
6:F:176:LEU:HD23	6:F:176:LEU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:188:LEU:O	6:F:191:SER:OG	2.24	0.50
8:H:26:THR:O	8:H:29:ILE:HG12	2.11	0.50
3:C:5:PHE:CZ	3:C:45:MET:HG2	2.47	0.50
1:A:25:GLY:HA3	1:A:75:ILE:HG12	1.92	0.50
1:A:565:ILE:HG22	1:A:623:ARG:HD3	1.93	0.50
2:B:56:PRO:HA	2:B:94:VAL:HG11	1.94	0.50
2:B:236:PRO:HG3	2:B:374:PRO:HB2	1.94	0.49
2:B:263:THR:HG22	9:I:1212:ALA:HB3	1.94	0.49
2:B:304:PHE:O	2:B:307:GLU:HG3	2.12	0.49
2:B:316:LEU:HD21	2:B:321:GLN:HE22	1.77	0.49
1:A:1374:LEU:HD21	1:A:1384:LEU:HG	1.92	0.49
2:B:93:ASP:HB3	2:B:131:ALA:HB3	1.94	0.49
3:C:79:LYS:HE2	3:C:161:GLU:HB2	1.93	0.49
8:H:25:ARG:O	8:H:29:ILE:HG23	2.11	0.49
1:A:1345:ASP:OD1	1:A:1345:ASP:N	2.45	0.49
2:B:404:VAL:O	7:G:52:LYS:NZ	2.46	0.49
2:B:1161:MET:SD	2:B:1161:MET:N	2.86	0.49
1:A:340:TYR:CE1	1:A:465:LEU:HD22	2.47	0.49
1:A:680:ILE:HD13	1:A:704:LEU:HB3	1.94	0.49
2:B:1032:SER:O	2:B:1036:ARG:HB2	2.11	0.49
1:A:1181:ASN:ND2	1:A:1184:THR:OG1	2.45	0.49
2:B:675:ILE:HD11	2:B:739:GLU:HB3	1.94	0.49
1:A:865:LEU:HD12	1:A:1349:ASN:HD21	1.78	0.49
6:F:94:LYS:O	6:F:97:SER:OG	2.22	0.49
1:A:172:GLU:OE2	1:A:172:GLU:HA	2.13	0.49
2:B:73:ARG:NH2	2:B:79:ASP:OD2	2.38	0.49
7:G:51:ASP:OD2	7:G:52:LYS:N	2.46	0.49
1:A:419:ARG:HB2	1:A:463:MET:SD	2.52	0.49
2:B:261:ASN:HA	2:B:266:SER:HA	1.95	0.49
2:B:877:PHE:HB3	2:B:1110:ARG:HD2	1.95	0.49
2:B:908:LYS:NZ	2:B:909:PRO:O	2.46	0.49
1:A:5:TYR:HB3	6:F:69:TYR:HB3	1.94	0.49
1:A:79:HIS:ND1	1:A:240:ILE:O	2.32	0.49
2:B:227:ILE:HG22	2:B:228:ILE:HG22	1.94	0.49
2:B:1206:ASP:OD2	2:B:1237:ARG:NH2	2.46	0.49
7:G:22:PHE:HE1	7:G:32:GLY:HA3	1.78	0.49
8:H:22:ASP:OD1	8:H:22:ASP:N	2.46	0.49
1:A:559:LEU:HD22	1:A:639:LEU:HD22	1.95	0.48
1:A:672:GLU:O	1:A:676:GLU:HG3	2.13	0.48
5:E:95:LEU:HD22	5:E:105:ILE:HG23	1.96	0.48
2:B:82:ARG:HB2	2:B:140:TYR:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:331:GLU:HA	6:F:334:LYS:HE3	1.95	0.48
1:A:1211:SER:OG	1:A:1212:VAL:N	2.46	0.48
2:B:101:HIS:N	2:B:110:ILE:O	2.39	0.48
3:C:178:LEU:O	3:C:224:PRO:HD3	2.13	0.48
3:C:332:LEU:O	3:C:336:LEU:HG	2.13	0.48
5:E:67:THR:OG1	5:E:134:GLU:OE2	2.30	0.48
1:A:934:VAL:HG13	1:A:1026:ILE:HD11	1.96	0.48
2:B:515:LEU:HD23	2:B:842:VAL:HG11	1.95	0.48
2:B:279:PHE:CE1	2:B:368:LEU:HD23	2.48	0.48
2:B:1179:ILE:HG21	2:B:1232:SER:HB2	1.94	0.48
2:B:1187:ALA:HB1	2:B:1207:ILE:HD12	1.95	0.48
8:H:32:LYS:HD3	8:H:49:ILE:HG22	1.96	0.48
9:I:1070:ASP:OD2	9:I:1074:ARG:NH2	2.45	0.48
2:B:934:ILE:HG23	2:B:982:MET:HE3	1.96	0.48
7:G:6:ALA:HA	9:I:1119:VAL:HG11	1.95	0.48
9:I:1238:ILE:HD13	9:I:1246:LEU:HD21	1.95	0.48
1:A:529:GLY:HA2	1:A:532:GLN:HG3	1.96	0.48
2:B:242:ASN:HD21	9:I:1213:TYR:HE1	1.62	0.48
2:B:657:VAL:HB	2:B:659:GLU:HG3	1.95	0.48
1:A:269:ASN:O	1:A:273:ASP:HB2	2.14	0.48
1:A:1173:ASN:ND2	7:G:18:GLY:HA2	2.28	0.48
2:B:484:GLN:O	2:B:488:SER:OG	2.31	0.48
4:D:27:PRO:HD2	4:D:30:LYS:HB3	1.95	0.48
1:A:8:ILE:HD12	2:B:1232:SER:HB3	1.96	0.48
1:A:428:ILE:O	2:B:1158:GLN:NE2	2.38	0.48
2:B:320:PHE:O	2:B:324:GLN:HG3	2.13	0.48
2:B:1179:ILE:HB	2:B:1234:LEU:HD11	1.95	0.48
1:A:127:SER:HG	1:A:129:THR:HG1	1.60	0.47
2:B:328:ASN:HA	9:I:1075:ILE:HD11	1.95	0.47
7:G:11:MET:HB3	7:G:22:PHE:HB3	1.96	0.47
6:F:304:LEU:O	6:F:307:ILE:HG12	2.13	0.47
1:A:378:ARG:HB3	1:A:406:TYR:HB2	1.97	0.47
1:A:235:ARG:HA	1:A:238:LEU:HD12	1.97	0.47
1:A:741:SER:HB3	1:A:743:PRO:HD2	1.97	0.47
2:B:65:VAL:HG13	9:I:1206:SER:HB3	1.96	0.47
2:B:91:PHE:HA	2:B:132:ALA:HA	1.95	0.47
3:C:272:MET:HB2	3:C:276:LYS:HB2	1.95	0.47
1:A:83:LEU:HD23	1:A:197:VAL:HG12	1.95	0.47
1:A:103:GLY:HA3	1:A:176:ARG:HB3	1.96	0.47
1:A:664:GLN:O	1:A:668:GLU:HG2	2.14	0.47
1:A:1390:SER:O	1:A:1394:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ARG:HG3	2:B:109:LYS:HA	1.96	0.47
2:B:1127:PRO:HB2	2:B:1136:LEU:HD23	1.95	0.47
1:A:349:GLN:NE2	1:A:408:ASP:OD1	2.38	0.47
1:A:1002:ILE:HG23	1:A:1006:LEU:HD12	1.96	0.47
2:B:20:GLU:HG2	2:B:716:PRO:HG2	1.96	0.47
2:B:85:VAL:HA	2:B:138:ALA:HA	1.97	0.47
2:B:304:PHE:HD2	2:B:402:MET:HE2	1.80	0.47
2:B:421:SER:O	2:B:425:LEU:HB2	2.14	0.47
3:C:257:TYR:CE1	3:C:336:LEU:HB2	2.44	0.47
4:D:151:LEU:HD21	4:D:161:LEU:HD11	1.95	0.47
6:F:292:MET:HA	6:F:295:THR:HG22	1.96	0.47
2:B:118:ARG:NH2	2:B:184:GLU:OE2	2.47	0.47
1:A:1244:GLU:OE2	7:G:15:TYR:OH	2.26	0.47
2:B:796:ARG:HG3	2:B:1038:THR:HG22	1.96	0.47
2:B:709:ILE:HD11	2:B:762:LYS:HE3	1.95	0.47
3:C:288:HIS:CE1	3:C:312:CYS:HB2	2.51	0.47
9:I:1045:TYR:CE1	9:I:1181:LYS:HE3	2.50	0.47
1:A:860:LEU:O	1:A:1351:ARG:NH1	2.48	0.46
2:B:414:ARG:HE	2:B:747:GLU:CD	2.18	0.46
2:B:796:ARG:NH2	2:B:1001:GLY:O	2.47	0.46
6:F:92:ILE:HG23	6:F:101:LEU:O	2.16	0.46
1:A:422:SER:OG	2:B:1151:GLU:OE2	2.23	0.46
1:A:1171:ILE:HG22	1:A:1172:ALA:O	2.15	0.46
2:B:305:MET:O	2:B:309:LEU:HG	2.15	0.46
5:E:124:LYS:HD2	5:E:124:LYS:HA	1.62	0.46
1:A:1322:THR:HG23	1:A:1326:TYR:HD2	1.80	0.46
2:B:234:SER:OG	2:B:374:PRO:HD2	2.15	0.46
2:B:850:ILE:HG21	2:B:1022:LEU:HD11	1.97	0.46
1:A:320:TRP:CE2	2:B:1135:PRO:HG3	2.50	0.46
7:G:33:ASP:O	7:G:35:GLN:N	2.49	0.46
1:A:145:VAL:HG23	1:A:155:TRP:HB2	1.97	0.46
1:A:330:ASN:HB2	1:A:445:GLN:HB3	1.97	0.46
2:B:39:LEU:HD11	2:B:781:LEU:HD22	1.97	0.46
2:B:956:MET:HG2	2:B:957:TYR:H	1.81	0.46
8:H:32:LYS:HE2	8:H:32:LYS:HB3	1.73	0.46
1:A:261:GLN:OE1	1:A:261:GLN:HA	2.15	0.46
1:A:1177:ARG:HD2	1:A:1224:ARG:NH1	2.31	0.46
2:B:591:LEU:HD22	2:B:598:GLN:HG2	1.98	0.46
2:B:1187:ALA:CB	2:B:1207:ILE:HD12	2.45	0.46
1:A:331:SER:O	1:A:638:GLN:NE2	2.47	0.46
1:A:1432:ASP:O	1:A:1436:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:715:THR:HG23	2:B:718:MET:HE3	1.98	0.46
2:B:796:ARG:HA	2:B:799:TYR:HD2	1.81	0.46
2:B:1088:MET:HG3	2:B:1101:ILE:HB	1.97	0.46
2:B:604:ASN:O	2:B:608:VAL:HG23	2.16	0.46
3:C:17:PHE:O	3:C:23:LYS:HE3	2.16	0.46
1:A:881:GLU:O	1:A:885:LYS:HB3	2.15	0.46
1:A:974:VAL:HG12	1:A:1027:ARG:HE	1.81	0.45
2:B:296:GLU:HB2	2:B:609:ARG:HH22	1.81	0.45
4:D:203:SER:OG	4:D:204:LYS:N	2.49	0.45
7:G:21:ILE:HD12	7:G:21:ILE:O	2.16	0.45
1:A:1306:ASP:OD1	1:A:1308:ASN:N	2.47	0.45
2:B:343:PHE:HA	9:I:1196:GLU:HG3	1.97	0.45
2:B:358:GLN:HG2	9:I:1182:LEU:HA	1.98	0.45
3:C:9:GLU:OE1	3:C:11:LYS:HG2	2.17	0.45
4:D:92:VAL:HG11	4:D:96:VAL:HG11	1.97	0.45
6:F:81:LEU:HB2	6:F:139:VAL:HG21	1.97	0.45
9:I:1049:ARG:HB3	9:I:1049:ARG:NH1	2.31	0.45
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.70	0.45
3:C:3:LYS:HB3	3:C:3:LYS:HE3	1.63	0.45
3:C:30:PHE:HA	3:C:128:ARG:HH12	1.81	0.45
1:A:723:ILE:HD13	1:A:731:PHE:HB2	1.97	0.45
1:A:941:ILE:HG21	1:A:1022:ILE:HD11	1.99	0.45
2:B:1173:ASP:OD1	2:B:1173:ASP:N	2.49	0.45
6:F:298:LYS:HA	6:F:298:LYS:HD3	1.73	0.45
7:G:71:LYS:HE3	7:G:71:LYS:HB2	1.88	0.45
2:B:527:HIS:CG	2:B:527:HIS:O	2.69	0.45
1:A:72:HIS:N	1:A:205:PRO:HB3	2.32	0.45
1:A:521:VAL:HB	1:A:549:LEU:HB3	1.97	0.45
4:D:101:ASN:OD1	4:D:101:ASN:N	2.48	0.45
1:A:86:LEU:HD23	1:A:272:LEU:HD21	1.97	0.45
1:A:92:ARG:HB2	1:A:154:PHE:CE1	2.52	0.45
1:A:860:LEU:HD22	1:A:931:PRO:HB3	1.99	0.45
1:A:1181:ASN:OD1	1:A:1181:ASN:N	2.46	0.45
2:B:140:TYR:HD1	2:B:144:ARG:HE	1.64	0.45
2:B:216:HIS:HB3	9:I:1219:PHE:CZ	2.52	0.45
2:B:458:THR:HG22	2:B:459:GLN:H	1.82	0.45
2:B:1036:ARG:HB3	2:B:1038:THR:HG23	1.99	0.45
1:A:368:ASN:ND2	1:A:374:PRO:O	2.50	0.45
1:A:829:ALA:HA	1:A:1369:LEU:HD13	1.99	0.45
1:A:1135:THR:HB	1:A:1173:ASN:HA	1.98	0.45
2:B:884:GLU:HA	2:B:983:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:MET:HB3	3:C:301:MET:HE2	1.76	0.45
1:A:26:VAL:HG22	1:A:73:PRO:O	2.17	0.45
2:B:58:ILE:HA	2:B:62:MET:HG3	1.98	0.45
2:B:887:VAL:O	2:B:979:PHE:HB2	2.17	0.45
9:I:1128:HIS:O	9:I:1132:THR:OG1	2.28	0.45
1:A:115:LEU:HG	1:A:119:LYS:HB3	1.99	0.45
1:A:234:VAL:O	1:A:238:LEU:HG	2.17	0.45
1:A:717:LYS:HB3	1:A:718:PRO:HD3	1.99	0.45
9:I:1087:SER:OG	9:I:1112:GLU:OE2	2.26	0.45
1:A:937:ILE:HG23	1:A:1025:LEU:HD23	1.99	0.44
2:B:205:LEU:HD23	2:B:205:LEU:HA	1.80	0.44
6:F:100:ILE:HG13	6:F:121:ASN:OD1	2.17	0.44
9:I:1160:TRP:CE3	9:I:1161:VAL:HG12	2.52	0.44
9:I:1233:ILE:HG23	9:I:1236:VAL:HB	1.99	0.44
1:A:344:PHE:HE1	2:B:1119:ARG:HE	1.65	0.44
1:A:431:HIS:NE2	1:A:454:TYR:OH	2.23	0.44
2:B:380:ALA:HB1	2:B:383:ARG:NH1	2.31	0.44
2:B:670:THR:HG23	2:B:742:THR:HG23	2.00	0.44
7:G:23:ARG:NH2	7:G:29:SER:OG	2.50	0.44
1:A:417:PHE:CD2	1:A:465:LEU:HD12	2.52	0.44
1:A:1053:LEU:HD11	1:A:1081:PHE:HE2	1.83	0.44
1:A:1122:PHE:CZ	1:A:1199:LEU:HD11	2.52	0.44
2:B:262:SER:OG	2:B:263:THR:N	2.50	0.44
2:B:404:VAL:HG12	2:B:405:PHE:CD2	2.51	0.44
2:B:1233:VAL:O	2:B:1234:LEU:HB2	2.16	0.44
4:D:2:ALA:O	4:D:6:LEU:HB2	2.17	0.44
1:A:117:ARG:H	1:A:117:ARG:HG2	1.35	0.44
1:A:778:PHE:CE2	7:G:84:ILE:HG23	2.52	0.44
2:B:23:GLU:HG3	2:B:1065:PRO:HD3	1.99	0.44
2:B:27:LEU:HD23	2:B:27:LEU:HA	1.87	0.44
2:B:680:ILE:HD12	2:B:680:ILE:HA	1.81	0.44
6:F:188:LEU:HB3	6:F:304:LEU:HD11	2.00	0.44
2:B:1082:PHE:HB3	3:C:200:MET:SD	2.58	0.44
2:B:1095:GLU:HG2	3:C:52:ARG:CZ	2.48	0.44
4:D:104:ASP:OD2	4:D:104:ASP:N	2.51	0.44
2:B:209:ARG:NE	2:B:212:THR:OG1	2.47	0.44
2:B:329:ARG:NH2	9:I:1068:ALA:O	2.51	0.44
2:B:427:LYS:HD2	2:B:503:ARG:HB2	2.00	0.44
1:A:123:GLU:O	1:A:126:SER:OG	2.33	0.44
2:B:322:PRO:HD2	2:B:335:PHE:HE2	1.82	0.44
2:B:933:ILE:O	2:B:934:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:VAL:HA	3:C:65:GLU:HB2	1.99	0.44
6:F:13:ILE:HD11	6:F:70:MET:HE3	1.99	0.44
6:F:27:LEU:HD23	6:F:51:VAL:HG11	1.99	0.44
1:A:525:LEU:HB2	3:C:299:TYR:CE2	2.53	0.44
2:B:419:HIS:HB3	2:B:423:VAL:HB	2.00	0.44
2:B:449:LEU:HG	2:B:454:PHE:CE1	2.53	0.44
2:B:913:TYR:O	2:B:916:LEU:HD12	2.18	0.44
6:F:46:LEU:N	6:F:77:VAL:O	2.50	0.44
1:A:666:VAL:HG23	1:A:718:PRO:HB2	1.99	0.44
1:A:844:VAL:HG11	1:A:1355:MET:HE1	1.98	0.44
2:B:438:ILE:HG21	9:I:1206:SER:HA	2.00	0.44
2:B:957:TYR:HE1	2:B:984:LEU:HD22	1.83	0.44
3:C:12:PRO:HB3	3:C:41:VAL:HG12	2.00	0.44
4:D:92:VAL:HG12	4:D:93:ASP:H	1.83	0.44
6:F:91:LYS:HE2	6:F:105:LEU:HB2	2.00	0.44
8:H:9:THR:HB	8:H:65:CYS:HB2	2.00	0.44
1:A:649:PHE:HB3	2:B:855:ILE:HD12	2.00	0.43
2:B:185:ASP:HB3	2:B:188:GLU:HG2	2.00	0.43
2:B:347:PRO:HA	2:B:350:TYR:CE1	2.53	0.43
2:B:1237:ARG:NH1	6:F:10:THR:OG1	2.45	0.43
9:I:1024:ALA:HB1	9:I:1029:ILE:O	2.18	0.43
2:B:109:LYS:HB2	2:B:109:LYS:HE2	1.68	0.43
2:B:301:VAL:HA	2:B:402:MET:HE1	2.00	0.43
2:B:369:ASP:O	2:B:386:LYS:NZ	2.51	0.43
2:B:371:ILE:HD12	2:B:371:ILE:HA	1.83	0.43
2:B:558:SER:OG	2:B:559:ALA:N	2.51	0.43
2:B:1067:ASN:HB3	2:B:1070:LEU:HB2	1.99	0.43
3:C:71:LEU:HG	3:C:102:ILE:HG21	2.00	0.43
5:E:104:ASP:O	5:E:108:GLN:HG2	2.18	0.43
1:A:1015:THR:OG1	1:A:1016:CYS:N	2.50	0.43
2:B:249:ARG:NH1	2:B:259:GLU:OE1	2.47	0.43
3:C:244:ARG:HD3	3:C:244:ARG:HA	1.77	0.43
3:C:315:HIS:CD2	3:C:316:LYS:HG3	2.53	0.43
5:E:124:LYS:HB2	5:E:132:ILE:HB	2.01	0.43
1:A:1386:MET:HG2	1:A:1394:VAL:CG2	2.47	0.43
2:B:281:MET:HE2	2:B:286:SER:HB3	2.00	0.43
3:C:188:ASP:OD1	3:C:188:ASP:N	2.39	0.43
3:C:255:LYS:O	3:C:258:GLU:HG3	2.18	0.43
1:A:65:GLN:O	1:A:67:LYS:N	2.51	0.43
2:B:816:PRO:CB	3:C:86:LEU:HB3	2.48	0.43
2:B:1008:LEU:HD12	2:B:1008:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:GLU:HB2	3:C:84:THR:HG23	2.00	0.43
5:E:95:LEU:HD21	5:E:108:GLN:HB2	2.01	0.43
1:A:152:PHE:CD1	1:A:264:GLN:HG2	2.53	0.43
1:A:1154:TRP:HH2	1:A:1224:ARG:HG3	1.82	0.43
2:B:886:LYS:HD2	2:B:979:PHE:HE1	1.84	0.43
4:D:4:GLN:O	4:D:8:THR:HG22	2.19	0.43
6:F:198:LYS:HD3	6:F:199:GLN:H	1.83	0.43
1:A:315:LEU:HD11	1:A:1387:ALA:HB1	2.00	0.43
1:A:1265:ILE:HG23	1:A:1295:THR:HB	2.00	0.43
2:B:279:PHE:HB2	2:B:387:LEU:HD11	2.01	0.43
2:B:557:GLN:CD	2:B:570:GLN:HG3	2.39	0.43
3:C:70:MET:HG2	3:C:176:PHE:CE1	2.53	0.43
3:C:246:ILE:HG21	3:C:347:PHE:CZ	2.53	0.43
1:A:112:TYR:HE1	1:A:123:GLU:HG2	1.84	0.43
2:B:364:GLN:O	2:B:367:ILE:HG13	2.19	0.43
6:F:132:VAL:HG22	6:F:154:ILE:HD13	2.01	0.43
1:A:26:VAL:HG11	1:A:61:THR:HG21	2.01	0.43
1:A:499:GLN:NE2	1:A:617:TYR:OH	2.51	0.43
5:E:120:MET:O	5:E:120:MET:HG3	2.18	0.43
6:F:6:ILE:HA	6:F:75:SER:HA	2.00	0.43
6:F:28:LEU:HD23	6:F:28:LEU:HA	1.76	0.43
6:F:82:ASN:OD1	6:F:82:ASN:N	2.51	0.43
1:A:419:ARG:NH1	9:I:1245:ASN:HB3	2.34	0.43
1:A:815:LYS:HE3	1:A:815:LYS:HB3	1.74	0.43
2:B:40:ILE:HG13	2:B:189:PRO:HG3	2.00	0.43
2:B:815:TRP:CG	2:B:816:PRO:HD3	2.54	0.43
9:I:1037:ILE:HB	9:I:1142:ILE:HD11	2.01	0.43
9:I:1240:LEU:C	9:I:1242:VAL:H	2.22	0.43
1:A:344:PHE:HZ	2:B:1119:ARG:HG3	1.83	0.42
1:A:1021:ALA:HA	1:A:1024:ASP:OD2	2.19	0.42
2:B:363:ARG:HG3	2:B:364:GLN:N	2.34	0.42
2:B:559:ALA:HA	2:B:802:ASN:HD21	1.83	0.42
2:B:796:ARG:HA	2:B:799:TYR:CD2	2.53	0.42
2:B:1238:VAL:H	6:F:71:HIS:CD2	2.37	0.42
5:E:114:LYS:HE2	5:E:114:LYS:HB2	1.79	0.42
9:I:1243:LEU:HA	9:I:1246:LEU:HD23	2.01	0.42
1:A:425:ARG:NH2	1:A:1039:GLU:OE1	2.52	0.42
1:A:997:LEU:HD13	4:D:192:MET:HB2	2.00	0.42
2:B:72:GLN:HE21	2:B:454:PHE:HE2	1.67	0.42
2:B:205:LEU:HD21	2:B:527:HIS:HB3	2.01	0.42
2:B:646:HIS:CG	2:B:647:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:THR:CG2	2:B:1109:GLN:HB3	2.50	0.42
2:B:883:ARG:HB2	2:B:986:TYR:HE1	1.85	0.42
2:B:911:ALA:HB1	2:B:932:ILE:HD11	2.00	0.42
4:D:14:ILE:HD12	4:D:45:ALA:HB2	2.01	0.42
1:A:502:ASP:OD2	2:B:861:GLN:HG2	2.19	0.42
1:A:1076:ARG:HB3	1:A:1077:PRO:HD3	2.00	0.42
1:A:1283:LYS:HE2	1:A:1285:VAL:HG12	2.01	0.42
2:B:404:VAL:C	2:B:405:PHE:HD2	2.23	0.42
3:C:46:ASP:N	3:C:46:ASP:OD1	2.52	0.42
3:C:74:LYS:HB2	3:C:162:ASP:HB3	2.01	0.42
5:E:96:LYS:HA	5:E:96:LYS:HD3	1.82	0.42
6:F:86:LEU:HB3	6:F:306:PHE:HB2	2.01	0.42
9:I:1122:TYR:HA	9:I:1140:TYR:OH	2.18	0.42
1:A:244:LEU:HD11	1:A:256:ILE:HD12	2.01	0.42
1:A:362:LEU:HA	1:A:365:TYR:HD2	1.83	0.42
1:A:377:SER:O	1:A:378:ARG:HB2	2.19	0.42
2:B:995:LYS:HD2	2:B:1003:LYS:HD2	2.02	0.42
2:B:1087:LYS:HB3	2:B:1087:LYS:HE2	1.85	0.42
6:F:196:ASP:OD2	6:F:198:LYS:NZ	2.43	0.42
9:I:1223:ILE:H	9:I:1223:ILE:HG13	1.61	0.42
1:A:92:ARG:HB2	1:A:154:PHE:HE1	1.84	0.42
1:A:739:LYS:HA	1:A:739:LYS:HD3	1.88	0.42
2:B:102:ARG:HG2	2:B:109:LYS:HD3	2.01	0.42
2:B:427:LYS:O	2:B:430:LYS:HG2	2.20	0.42
2:B:435:THR:OG1	2:B:436:SER:N	2.52	0.42
2:B:733:VAL:HG11	2:B:740:PHE:CE2	2.54	0.42
6:F:5:LYS:HD3	6:F:5:LYS:HA	1.81	0.42
6:F:128:GLN:NE2	6:F:326:ILE:HD11	2.35	0.42
9:I:1019:LYS:O	9:I:1023:THR:OG1	2.38	0.42
1:A:204:PRO:HB3	1:A:208:ILE:HD11	2.02	0.42
1:A:1410:ILE:HG12	2:B:1156:THR:HG21	2.02	0.42
2:B:640:ARG:NH2	2:B:736:GLY:O	2.44	0.42
2:B:1198:CYS:SG	2:B:1199:MET:N	2.92	0.42
8:H:23:LYS:O	8:H:27:GLU:HG2	2.19	0.42
9:I:1155:ILE:HD12	9:I:1155:ILE:HA	1.87	0.42
2:B:773:ASP:OD1	2:B:774:VAL:N	2.52	0.42
5:E:76:ALA:HB1	5:E:146:LEU:HD11	2.01	0.42
9:I:1201:SER:OG	9:I:1202:GLY:N	2.53	0.42
1:A:50:MET:SD	1:A:74:GLY:HA3	2.60	0.42
1:A:185:LEU:HD12	1:A:185:LEU:HA	1.78	0.42
1:A:748:ILE:HA	1:A:792:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:ALA:O	1:A:1050:SER:OG	2.38	0.42
6:F:91:LYS:NZ	6:F:105:LEU:H	2.14	0.42
6:F:310:LEU:HD23	6:F:310:LEU:HA	1.91	0.42
9:I:1192:MET:SD	9:I:1193:ILE:HG13	2.59	0.42
1:A:112:TYR:CE1	1:A:123:GLU:HG2	2.55	0.42
1:A:971:LEU:HD23	1:A:999:ARG:HG3	2.01	0.42
1:A:1094:MET:HE1	1:A:1299:ASN:H	1.85	0.42
1:A:1176:ILE:HD11	1:A:1178:LEU:HD21	2.02	0.42
2:B:79:ASP:CG	2:B:82:ARG:HH12	2.23	0.42
2:B:598:GLN:HA	2:B:623:GLY:HA2	2.01	0.42
1:A:336:ASP:OD1	1:A:432:ARG:NH2	2.49	0.42
1:A:1100:ASN:HB3	1:A:1103:VAL:HG22	2.02	0.42
2:B:33:ALA:O	2:B:37:THR:HG23	2.20	0.42
2:B:539:ALA:HB1	9:I:1231:PHE:HD2	1.85	0.42
9:I:1089:PHE:N	9:I:1089:PHE:CD1	2.87	0.42
9:I:1149:PHE:CD1	9:I:1169:ALA:HB1	2.54	0.42
1:A:370:LYS:HG2	1:A:377:SER:HB3	2.02	0.41
2:B:326:GLU:HG2	2:B:331:LYS:HB2	2.01	0.41
2:B:911:ALA:HA	2:B:930:GLY:O	2.20	0.41
3:C:5:PHE:HB3	3:C:353:ASN:HB3	2.03	0.41
6:F:201:CYS:O	6:F:204:GLU:HG2	2.19	0.41
6:F:319:LEU:HB3	6:F:323:HIS:CE1	2.54	0.41
1:A:226:ILE:HD12	1:A:226:ILE:HA	1.92	0.41
1:A:618:HIS:O	1:A:622:ARG:HG2	2.20	0.41
1:A:716:LEU:HD13	1:A:716:LEU:HA	1.88	0.41
1:A:764:PRO:HA	1:A:771:THR:HA	2.02	0.41
1:A:1343:MET:HG3	1:A:1348:PRO:HD2	2.02	0.41
1:A:1433:GLU:OE2	6:F:54:ARG:NH2	2.53	0.41
2:B:708:PHE:O	2:B:763:HIS:HA	2.20	0.41
9:I:1082:CYS:HB3	9:I:1089:PHE:HE2	1.85	0.41
2:B:267:LYS:HE3	2:B:267:LYS:HB3	1.91	0.41
2:B:539:ALA:HB1	9:I:1231:PHE:CD2	2.56	0.41
2:B:1056:VAL:HG12	8:H:49:ILE:O	2.21	0.41
1:A:659:THR:HG1	1:A:722:SER:HG	1.65	0.41
2:B:67:ILE:HD11	9:I:1198:PHE:HD1	1.86	0.41
2:B:179:LYS:O	2:B:182:ILE:HG22	2.20	0.41
2:B:790:ASN:OD1	2:B:790:ASN:N	2.53	0.41
3:C:111:PHE:CD2	3:C:132:GLN:HB2	2.55	0.41
6:F:97:SER:O	6:F:99:ILE:N	2.53	0.41
7:G:93:ILE:HG23	7:G:104:ARG:HB2	2.01	0.41
1:A:181:THR:O	1:A:185:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:O	1:A:309:ARG:N	2.45	0.41
1:A:733:MET:SD	2:B:1031:HIS:HA	2.61	0.41
2:B:646:HIS:CD2	2:B:647:PRO:HD2	2.55	0.41
2:B:872:ILE:HG12	2:B:990:LEU:HB3	2.03	0.41
6:F:86:LEU:HD13	6:F:86:LEU:HA	1.90	0.41
7:G:28:GLU:HB2	9:I:1081:ASN:HD21	1.85	0.41
8:H:29:ILE:HG22	8:H:49:ILE:CD1	2.51	0.41
9:I:1172:GLU:O	9:I:1175:THR:HG22	2.21	0.41
1:A:715:ILE:O	1:A:718:PRO:HD2	2.19	0.41
2:B:441:ILE:HD13	2:B:469:ALA:HB3	2.02	0.41
2:B:464:GLU:HA	2:B:467:SER:OG	2.21	0.41
2:B:913:TYR:OH	2:B:952:ASP:OD2	2.31	0.41
2:B:1115:VAL:O	2:B:1119:ARG:HB3	2.20	0.41
6:F:29:LYS:HB3	6:F:29:LYS:HE3	1.84	0.41
8:H:56:THR:HB	8:H:67:ARG:HH22	1.85	0.41
9:I:1100:VAL:HG23	9:I:1103:LEU:HD12	2.01	0.41
1:A:111:ARG:O	1:A:114:HIS:NE2	2.54	0.41
1:A:862:ALA:HB2	1:A:1351:ARG:HD2	2.02	0.41
2:B:268:LEU:HD12	2:B:268:LEU:HA	1.75	0.41
2:B:433:PHE:HA	2:B:478:LEU:HD11	2.01	0.41
2:B:450:LYS:HA	2:B:450:LYS:HD3	1.88	0.41
2:B:643:LYS:HB3	2:B:643:LYS:HE3	1.83	0.41
2:B:867:VAL:HG12	2:B:1026:LEU:HD22	2.02	0.41
3:C:110:VAL:HB	3:C:134:ALA:HB2	2.03	0.41
4:D:46:GLU:OE2	4:D:50:HIS:HA	2.20	0.41
7:G:13:ARG:HD3	7:G:15:TYR:OH	2.21	0.41
1:A:645:ARG:HH22	2:B:857:GLY:HA2	1.85	0.41
1:A:923:LEU:HD21	1:A:1274:MET:O	2.19	0.41
1:A:1339:ILE:O	1:A:1343:MET:HG2	2.21	0.41
2:B:26:MET:HB3	2:B:774:VAL:HG13	2.03	0.41
2:B:470:LEU:HD23	2:B:470:LEU:HA	1.80	0.41
2:B:511:ARG:HB3	2:B:811:TYR:HD2	1.86	0.41
2:B:567:MET:CE	2:B:567:MET:HA	2.51	0.41
3:C:30:PHE:HE2	8:H:20:ILE:HG13	1.86	0.41
5:E:107:LYS:HB2	5:E:107:LYS:HE3	1.89	0.41
7:G:16:VAL:HA	7:G:17:ASP:HA	1.67	0.41
7:G:55:ILE:HD12	7:G:55:ILE:H	1.85	0.41
1:A:320:TRP:HB3	2:B:1124:SER:HA	2.03	0.41
1:A:379:VAL:O	1:A:387:VAL:HA	2.20	0.41
1:A:528:MET:SD	3:C:307:PHE:HA	2.61	0.41
1:A:582:MET:HB2	1:A:725:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:THR:HA	1:A:601:GLY:HA3	2.02	0.41
1:A:874:MET:SD	1:A:1284:LEU:HD23	2.61	0.41
1:A:1099:LYS:HE3	1:A:1307:ASP:O	2.21	0.41
2:B:195:ALA:HB3	2:B:200:TRP:CD1	2.56	0.41
2:B:832:PRO:HG2	2:B:839:HIS:CE1	2.56	0.41
5:E:95:LEU:CD1	5:E:109:GLU:HG3	2.51	0.41
1:A:339:GLY:N	1:A:445:GLN:O	2.38	0.40
2:B:58:ILE:HD11	2:B:240:PHE:HB3	2.03	0.40
2:B:912:ASN:OD1	2:B:914:GLU:N	2.43	0.40
3:C:301:MET:CE	3:C:339:SER:HB3	2.51	0.40
9:I:1065:ARG:O	9:I:1069:VAL:HG23	2.21	0.40
1:A:236:LYS:HA	1:A:236:LYS:HD3	1.87	0.40
1:A:1142:ASN:ND2	1:A:1144:MET:HB2	2.35	0.40
2:B:1181:ARG:HB2	2:B:1234:LEU:HD22	2.03	0.40
6:F:206:LEU:HD22	6:F:327:TRP:HZ3	1.86	0.40
6:F:206:LEU:HD22	6:F:327:TRP:CZ3	2.56	0.40
8:H:27:GLU:O	8:H:31:THR:HG23	2.21	0.40
2:B:78:ILE:HG22	2:B:82:ARG:NH2	2.36	0.40
7:G:95:VAL:HG12	7:G:96:CYS:H	1.87	0.40
1:A:1109:TYR:O	1:A:1112:GLU:HG2	2.22	0.40
2:B:257:THR:OG1	2:B:269:ARG:HB3	2.21	0.40
2:B:927:VAL:HG13	2:B:931:ASP:HB2	2.03	0.40
3:C:96:ARG:O	8:H:5:VAL:HG21	2.21	0.40
1:A:12:GLN:HB2	2:B:1231:THR:HG23	2.03	0.40
1:A:166:TYR:OH	1:A:252:ILE:HD11	2.22	0.40
1:A:363:MET:HE3	1:A:366:PHE:HB3	2.03	0.40
1:A:677:SER:HB2	1:A:709:LEU:HD21	2.03	0.40
2:B:232:PHE:HB3	2:B:246:ILE:HG12	2.04	0.40
2:B:449:LEU:HG	2:B:454:PHE:CZ	2.57	0.40
2:B:637:MET:HA	2:B:637:MET:CE	2.51	0.40
2:B:1013:SER:H	2:B:1013:SER:HG	1.64	0.40
6:F:181:LEU:HB3	6:F:297:LEU:HD13	2.03	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	1390/1450 (96%)	1326 (95%)	60 (4%)	4 (0%)	37	70
2	B	1192/1242 (96%)	1107 (93%)	81 (7%)	4 (0%)	37	70
3	C	356/359 (99%)	341 (96%)	15 (4%)	0	100	100
4	D	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
5	E	105/147 (71%)	91 (87%)	13 (12%)	1 (1%)	13	46
6	F	231/339 (68%)	211 (91%)	17 (7%)	3 (1%)	10	39
7	G	103/105 (98%)	94 (91%)	8 (8%)	1 (1%)	13	46
8	H	65/80 (81%)	64 (98%)	1 (2%)	0	100	100
9	I	237/1249 (19%)	222 (94%)	15 (6%)	0	100	100
All	All	3882/5176 (75%)	3653 (94%)	216 (6%)	13 (0%)	38	70

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1139	THR
1	A	1142	ASN
2	B	1202	ASP
7	G	34	SER
6	F	70	MET
2	B	421	SER
1	A	1143	VAL
6	F	100	ILE
1	A	582	MET
2	B	103	ASN
2	B	1234	LEU
5	E	42	SER
6	F	45	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1242/1279 (97%)	1185 (95%)	57 (5%)	23 56
2	B	1042/1081 (96%)	982 (94%)	60 (6%)	17 48
3	C	327/328 (100%)	310 (95%)	17 (5%)	19 52
4	D	185/185 (100%)	166 (90%)	19 (10%)	6 24
5	E	97/136 (71%)	90 (93%)	7 (7%)	12 39
6	F	218/312 (70%)	201 (92%)	17 (8%)	10 36
7	G	96/96 (100%)	89 (93%)	7 (7%)	11 39
8	H	61/70 (87%)	58 (95%)	3 (5%)	21 54
9	I	215/1130 (19%)	191 (89%)	24 (11%)	5 21
All	All	3483/4617 (75%)	3272 (94%)	211 (6%)	18 46

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	27	MET
1	A	54	ASP
1	A	69	CYS
1	A	111	ARG
1	A	117	ARG
1	A	129	THR
1	A	143	LYS
1	A	152	PHE
1	A	197	VAL
1	A	236	LYS
1	A	245	GLN
1	A	255	ASN
1	A	301	ARG
1	A	305	ARG
1	A	378	ARG
1	A	387	VAL
1	A	417	PHE
1	A	424	GLU
1	A	476	GLU
1	A	537	ASP
1	A	581	TYR
1	A	584	TYR
1	A	644	VAL
1	A	685	LEU
1	A	689	ILE

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Mol	Chain	Res	Type
1	A	702	GLU
1	A	711	PHE
1	A	724	ASN
1	A	739	LYS
1	A	741	SER
1	A	815	LYS
1	A	879	GLU
1	A	941	ILE
1	A	1009	VAL
1	A	1015	THR
1	A	1030	TYR
1	A	1051	GLU
1	A	1061	HIS
1	A	1062	HIS
1	A	1095	LEU
1	A	1176	ILE
1	A	1202	LYS
1	A	1212	VAL
1	A	1217	SER
1	A	1219	ILE
1	A	1242	THR
1	A	1245	LYS
1	A	1248	VAL
1	A	1251	VAL
1	A	1308	ASN
1	A	1309	ILE
1	A	1318	SER
1	A	1362	ARG
1	A	1392	VAL
1	A	1424	THR
1	A	1440	TYR
2	B	36	SER
2	B	39	LEU
2	B	48	ASP
2	B	74	ASP
2	B	79	ASP
2	B	85	VAL
2	B	87	ILE
2	B	91	PHE
2	B	102	ARG
2	B	104	TYR
2	B	108	ASN

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Mol	Chain	Res	Type
2	B	110	ILE
2	B	220	MET
2	B	246	ILE
2	B	250	TYR
2	B	262	SER
2	B	278	MET
2	B	299	SER
2	B	335	PHE
2	B	363	ARG
2	B	369	ASP
2	B	371	ILE
2	B	385	ARG
2	B	401	ILE
2	B	402	MET
2	B	408	THR
2	B	413	TYR
2	B	448	LEU
2	B	450	LYS
2	B	467	SER
2	B	470	LEU
2	B	476	SER
2	B	527	HIS
2	B	537	GLU
2	B	538	ARG
2	B	541	MET
2	B	542	MET
2	B	698	ASP
2	B	699	LYS
2	B	704	HIS
2	B	728	THR
2	B	731	ASP
2	B	738	CYS
2	B	742	THR
2	B	757	GLU
2	B	888	GLU
2	B	900	ASP
2	B	908	LYS
2	B	912	ASN
2	B	956	MET
2	B	969	MET
2	B	979	PHE
2	B	996	MET

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Mol	Chain	Res	Type
2	B	1036	ARG
2	B	1066	ILE
2	B	1119	ARG
2	B	1142	HIS
2	B	1195	ILE
2	B	1228	VAL
2	B	1231	THR
3	C	5	PHE
3	C	7	ASN
3	C	19	ASN
3	C	46	ASP
3	C	95	ASN
3	C	133	VAL
3	C	144	ASN
3	C	164	TYR
3	C	173	HIS
3	C	180	VAL
3	C	197	LYS
3	C	255	LYS
3	C	257	TYR
3	C	270	PHE
3	C	287	THR
3	C	355	ASP
3	C	357	LEU
4	D	4	GLN
4	D	5	LYS
4	D	23	GLU
4	D	42	ARG
4	D	49	ASN
4	D	50	HIS
4	D	64	TYR
4	D	70	ASP
4	D	84	HIS
4	D	85	TYR
4	D	104	ASP
4	D	113	ASN
4	D	115	THR
4	D	120	ILE
4	D	125	LEU
4	D	140	LYS
4	D	168	ASP
4	D	182	VAL

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Mol	Chain	Res	Type
4	D	186	ARG
5	E	51	GLN
5	E	56	THR
5	E	97	LYS
5	E	107	LYS
5	E	120	MET
5	E	122	CYS
5	E	125	VAL
6	F	18	ASN
6	F	23	VAL
6	F	54	ARG
6	F	62	THR
6	F	70	MET
6	F	82	ASN
6	F	101	LEU
6	F	140	TYR
6	F	174	GLN
6	F	176	LEU
6	F	182	VAL
6	F	198	LYS
6	F	205	LYS
6	F	292	MET
6	F	304	LEU
6	F	325	ASN
6	F	328	MET
7	G	1	MET
7	G	2	LYS
7	G	15	TYR
7	G	41	SER
7	G	49	MET
7	G	68	GLN
7	G	72	ASP
8	H	23	LYS
8	H	62	MET
8	H	75	ASP
9	I	1037	ILE
9	I	1040	MET
9	I	1067	MET
9	I	1098	ARG
9	I	1101	LYS
9	I	1102	HIS
9	I	1110	ASP

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Mol	Chain	Res	Type
9	I	1140	TYR
9	I	1151	THR
9	I	1153	TYR
9	I	1157	GLU
9	I	1161	VAL
9	I	1168	PHE
9	I	1181	LYS
9	I	1192	MET
9	I	1198	PHE
9	I	1201	SER
9	I	1208	ASP
9	I	1209	ASP
9	I	1214	SER
9	I	1216	PRO
9	I	1219	PHE
9	I	1222	ASP
9	I	1228	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	ASN
1	A	445	GLN
1	A	592	GLN
2	B	1083	ASN
3	C	233	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

Of 7 ligands modelled in this entry, 7 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.

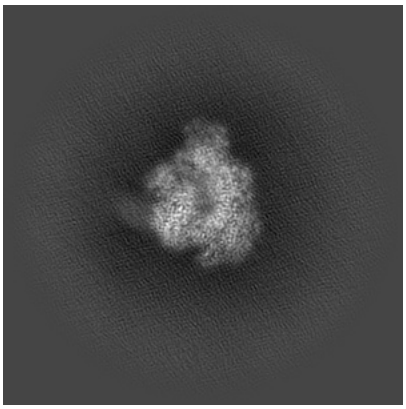
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38802. These allow visual inspection of the internal detail of the map and identification of artifacts.

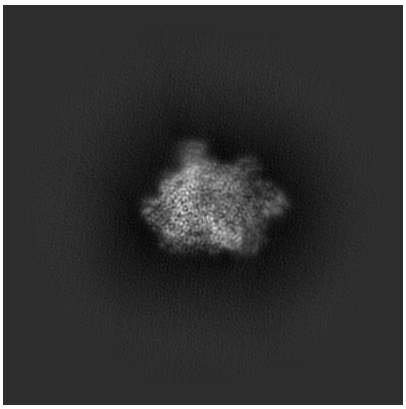
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

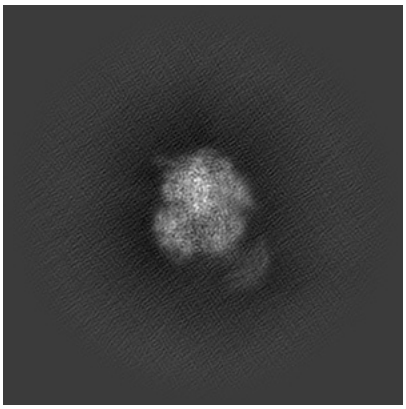
6.1.1 Primary map



X

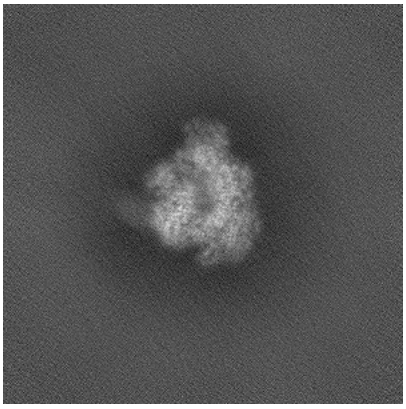


Y

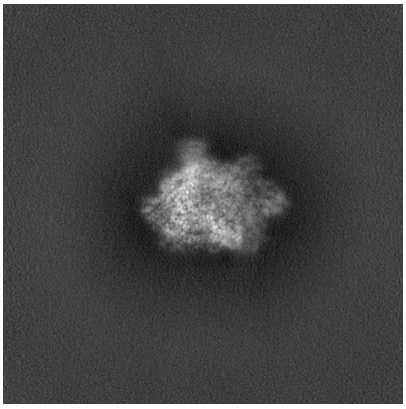


Z

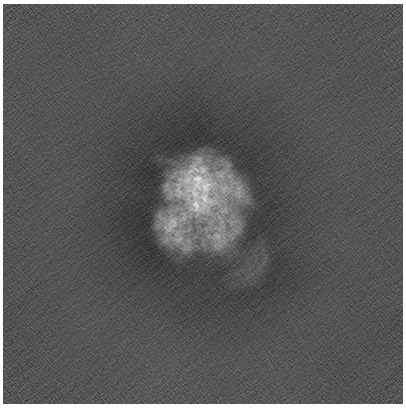
6.1.2 Raw map



X



Y

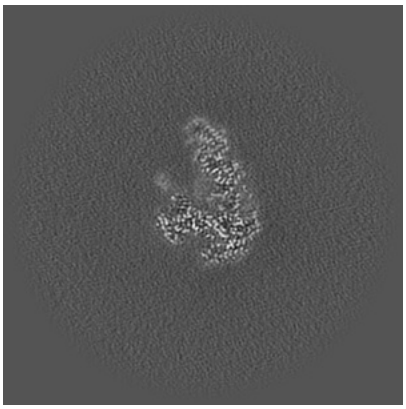


Z

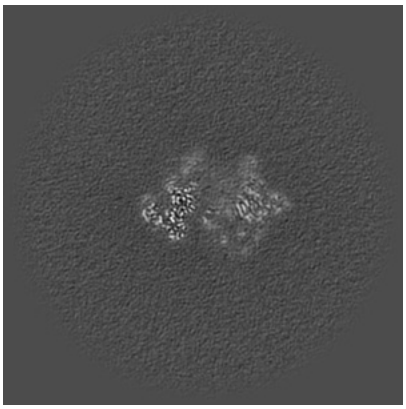
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

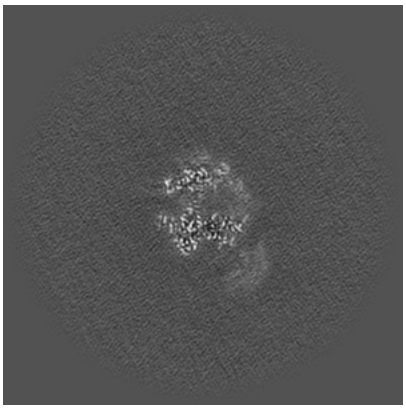
6.2.1 Primary map



X Index: 256

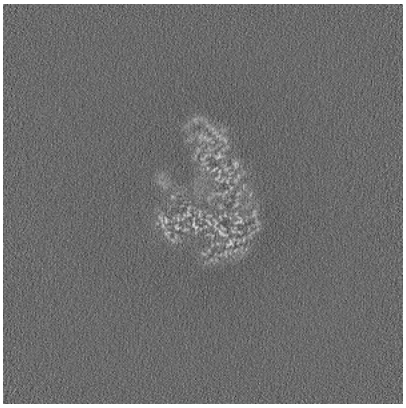


Y Index: 256

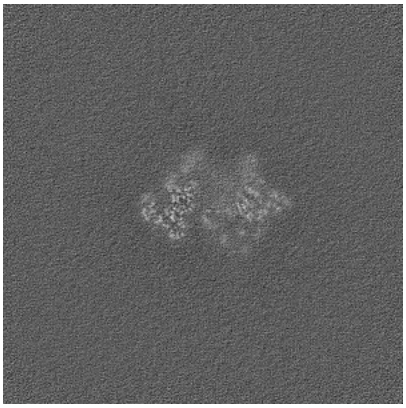


Z Index: 256

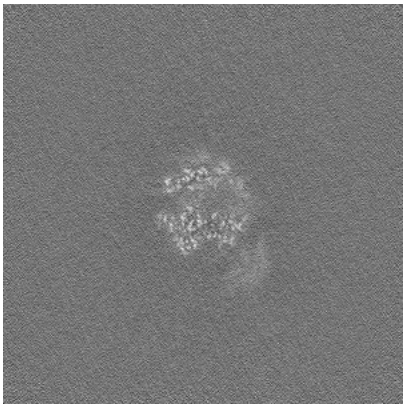
6.2.2 Raw map



X Index: 256



Y Index: 256

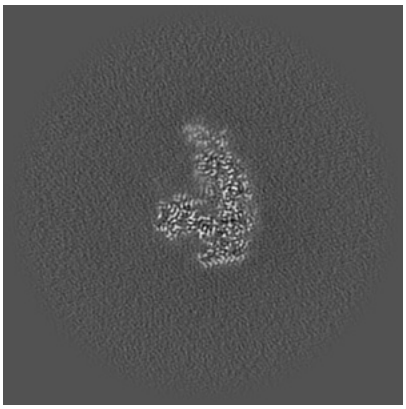


Z Index: 256

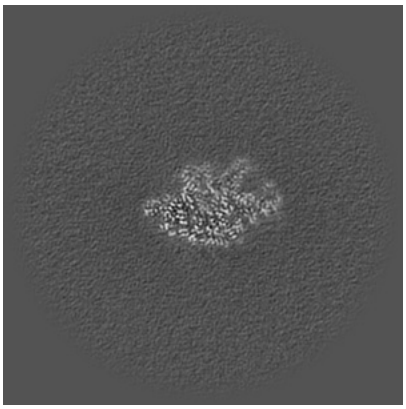
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

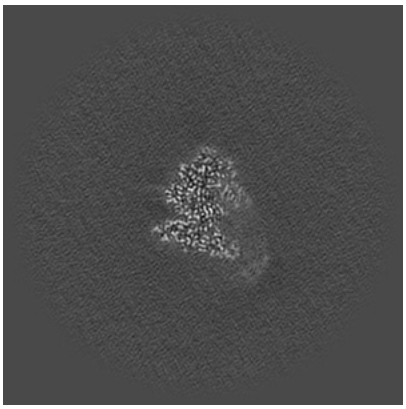
6.3.1 Primary map



X Index: 249

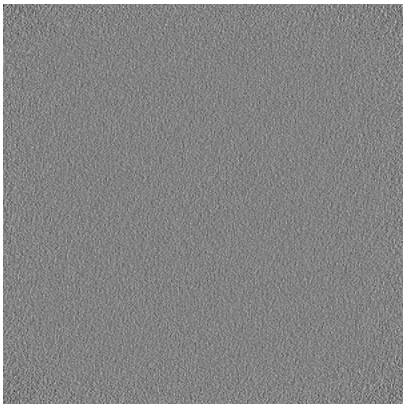


Y Index: 280

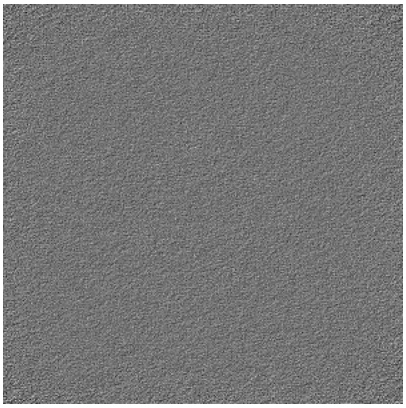


Z Index: 232

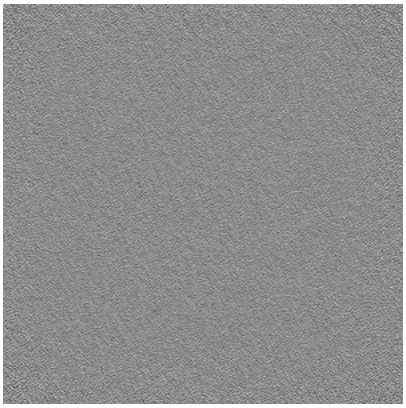
6.3.2 Raw map



X Index: 0



Y Index: 0

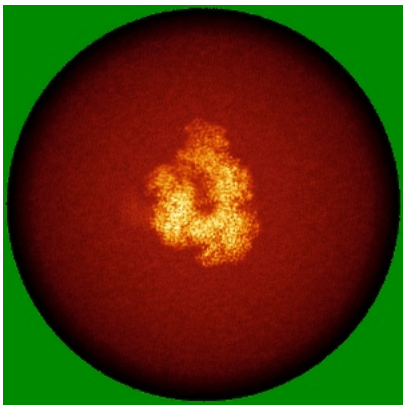


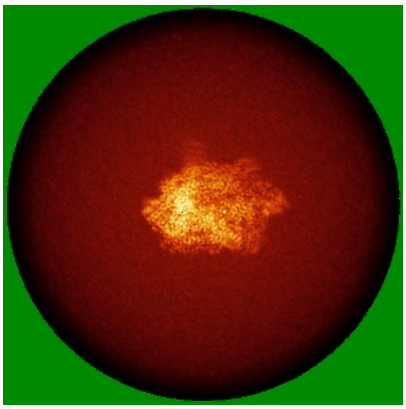
Z Index: 0

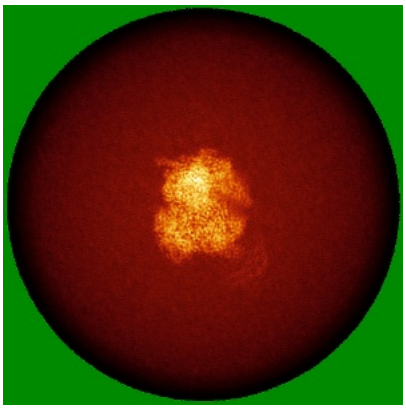
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

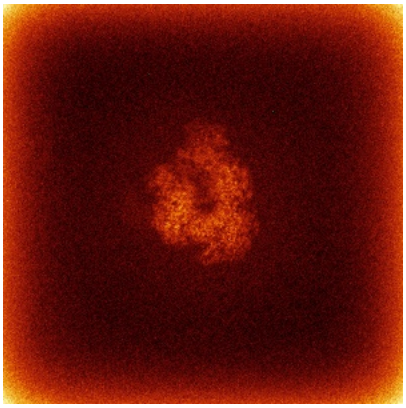
6.4.1 Primary map

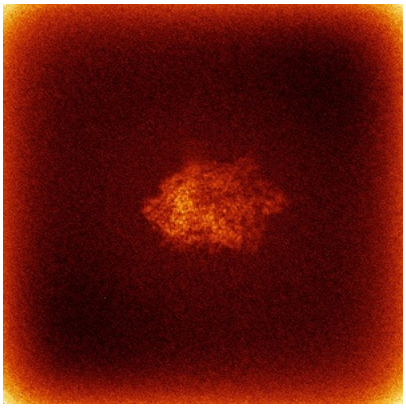

X

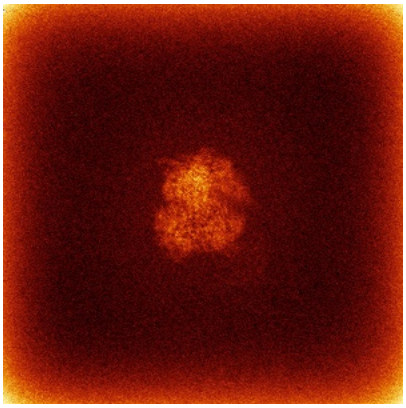

Y


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 0.4. 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.

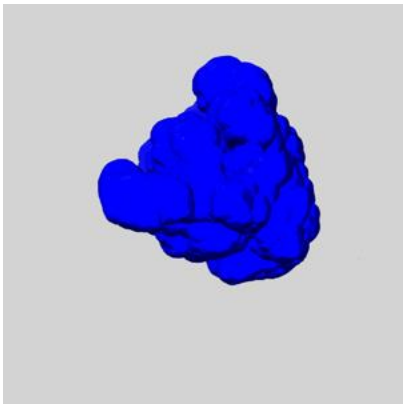
6.6 Mask visualisation (i)

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

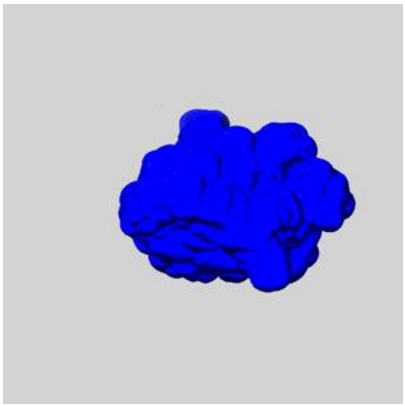
A mask typically either:

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

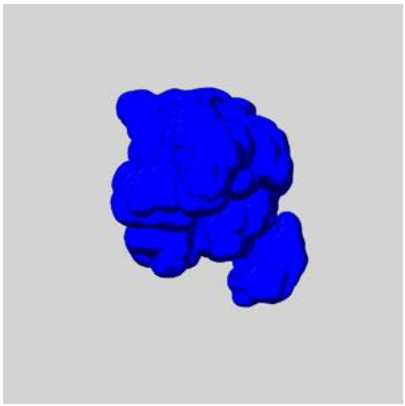
6.6.1 emd_38802_msk_1.map (i)



X



Y

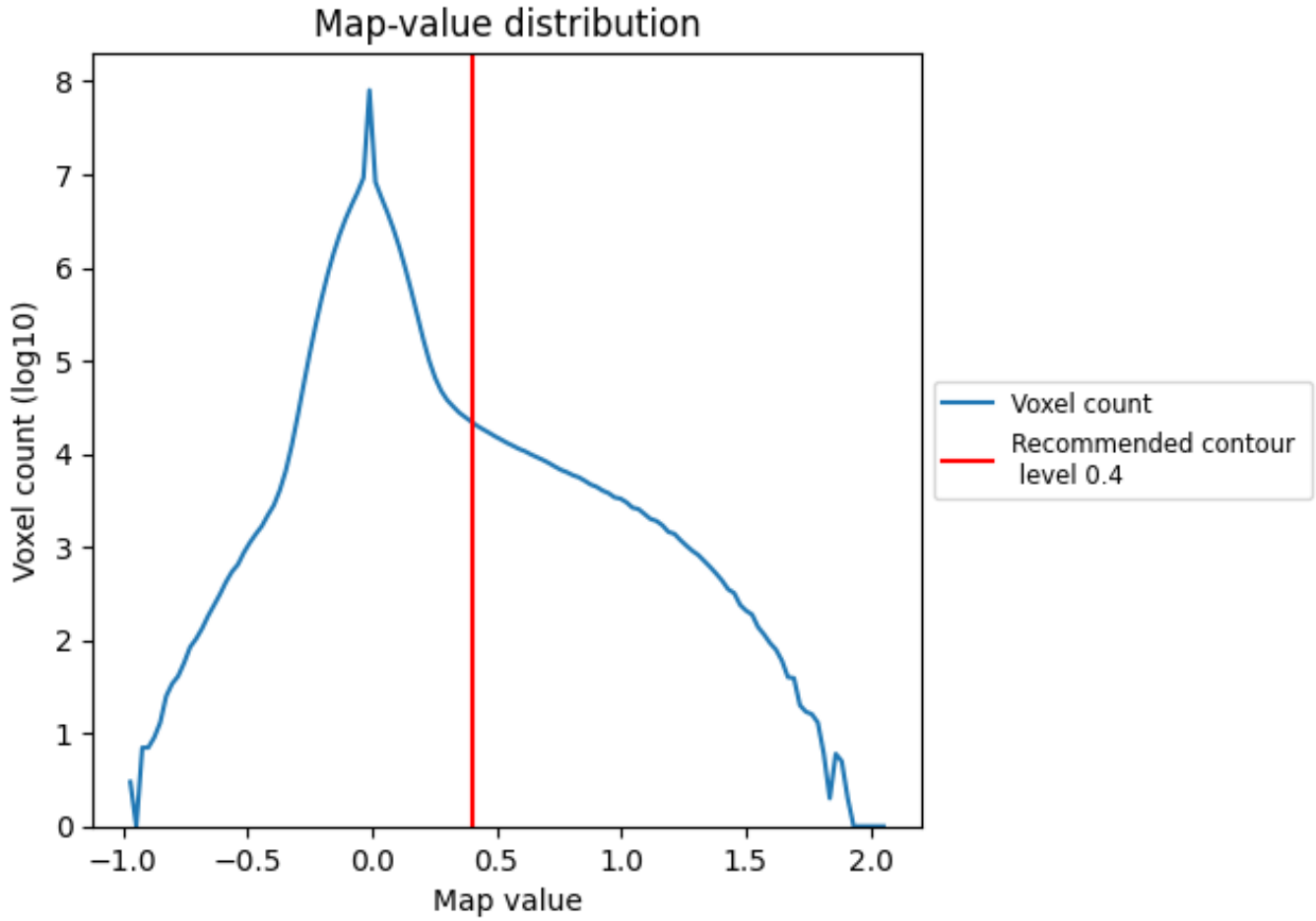


Z

7 Map analysis

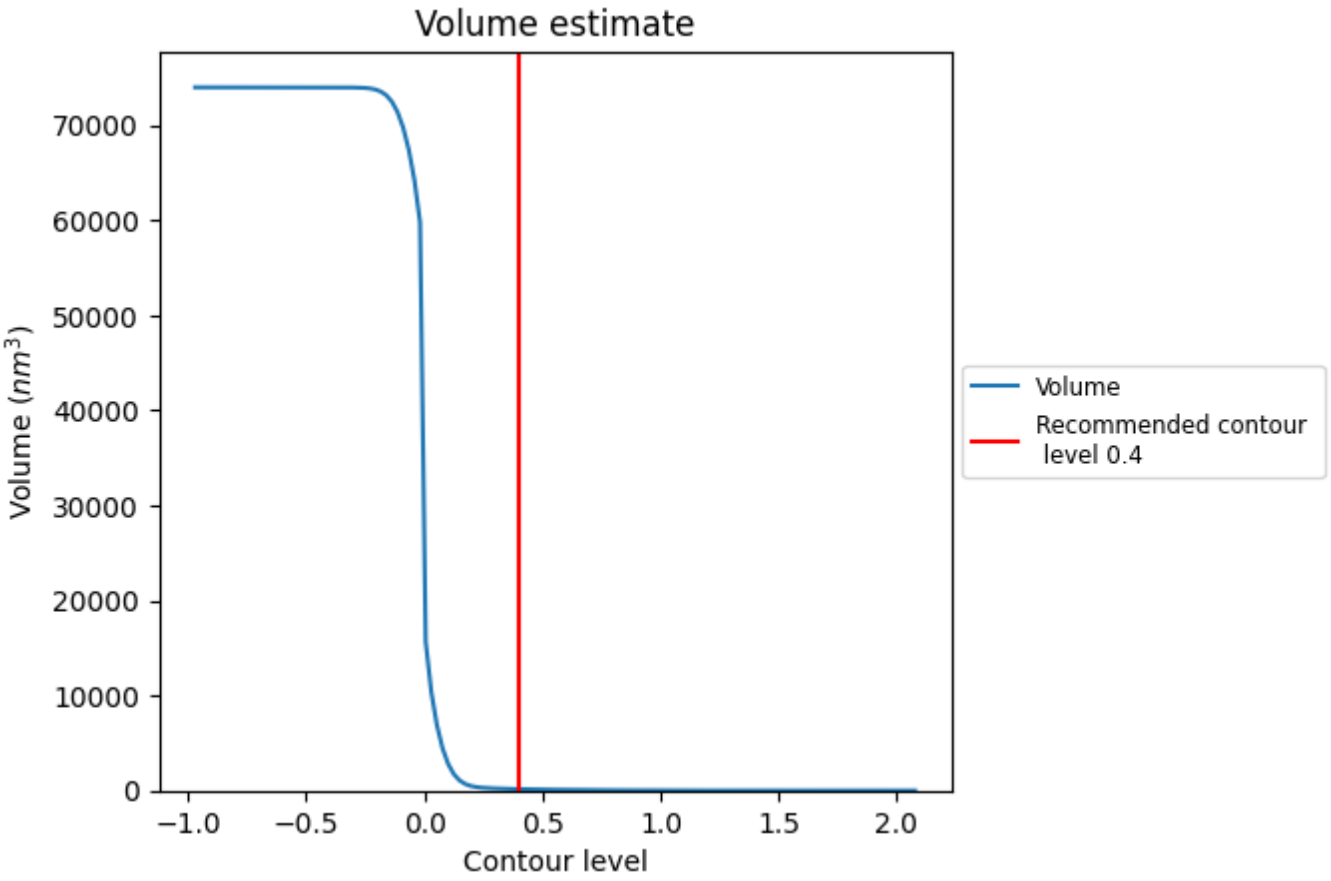
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

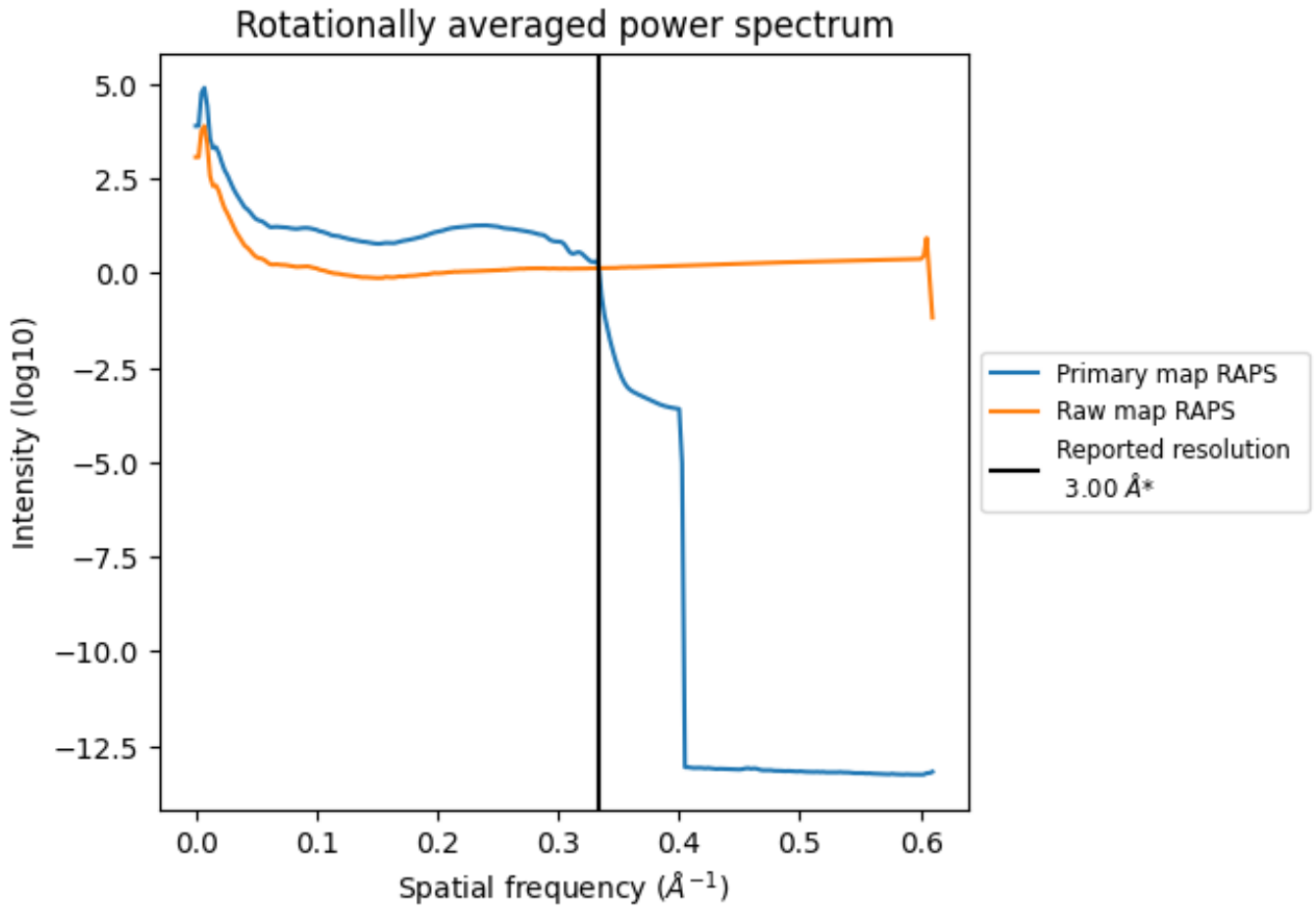
7.2 Volume estimate (i)



The volume at the recommended contour level is 152 nm^3; this corresponds to an approximate mass of 138 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)

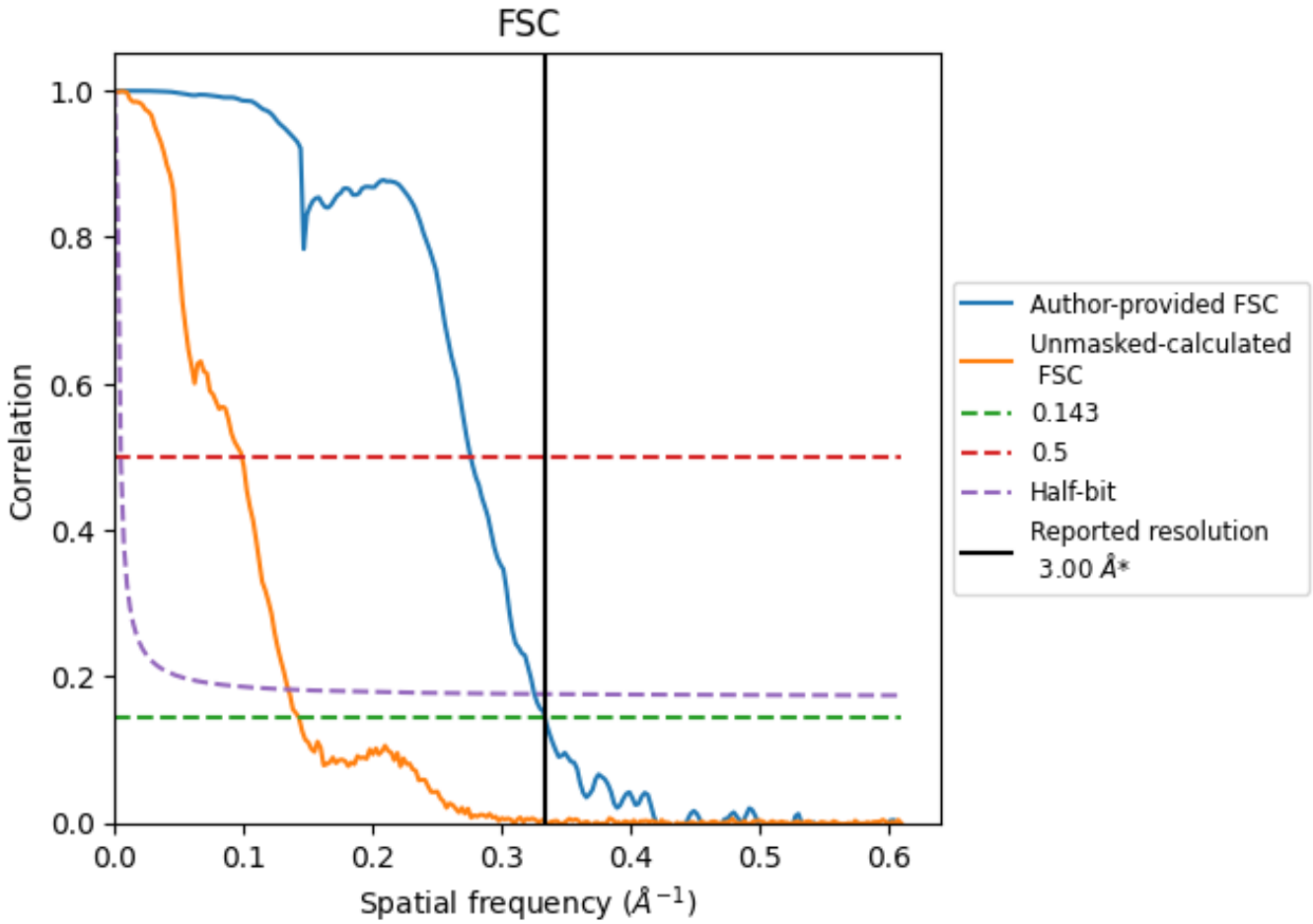


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

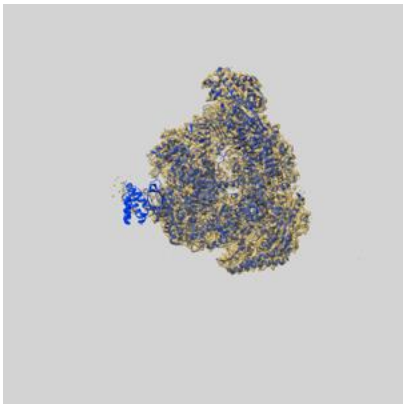
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.62	3.07
Unmasked-calculated*	7.00	10.16	7.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 3.0 by more than 10 %

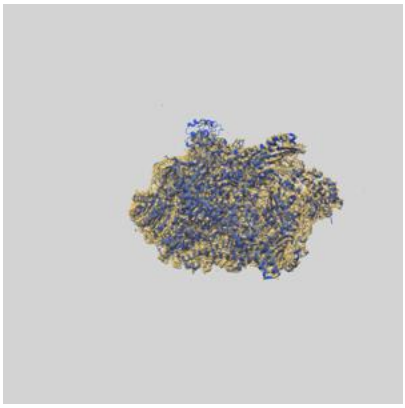
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38802 and PDB model 8Y0E. Per-residue inclusion information can be found in section 3 on page 6.

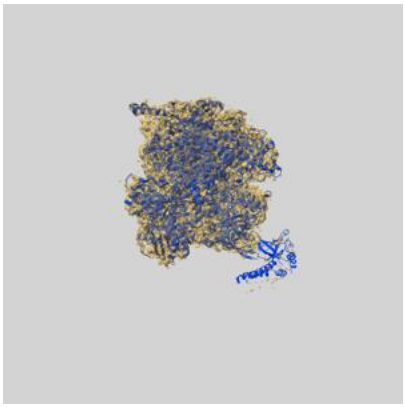
9.1 Map-model overlay



X



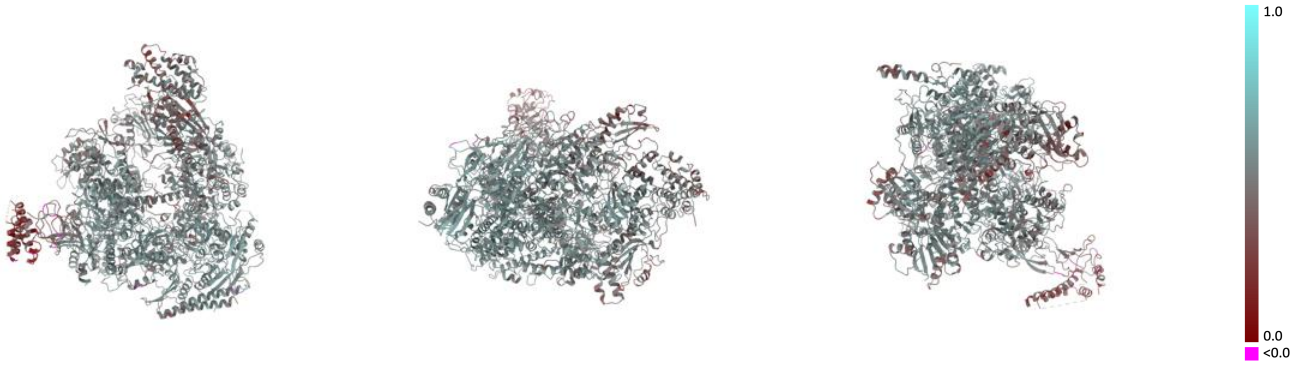
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

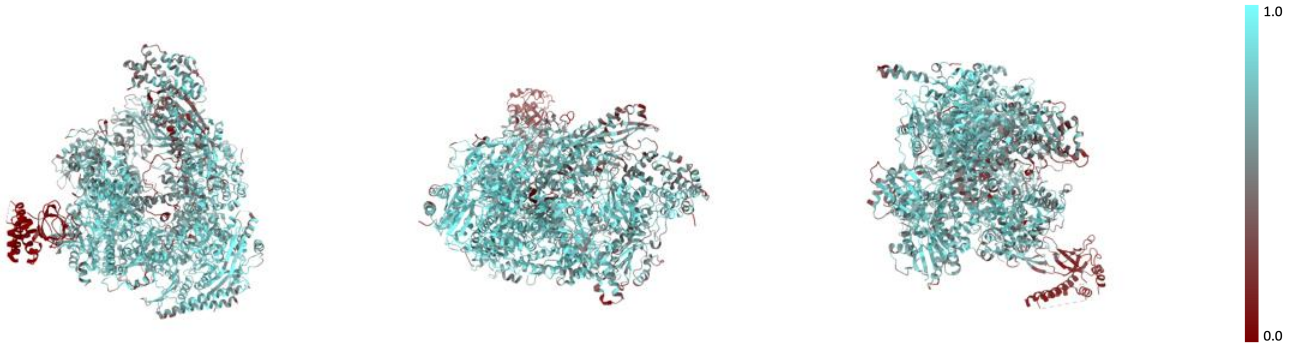
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

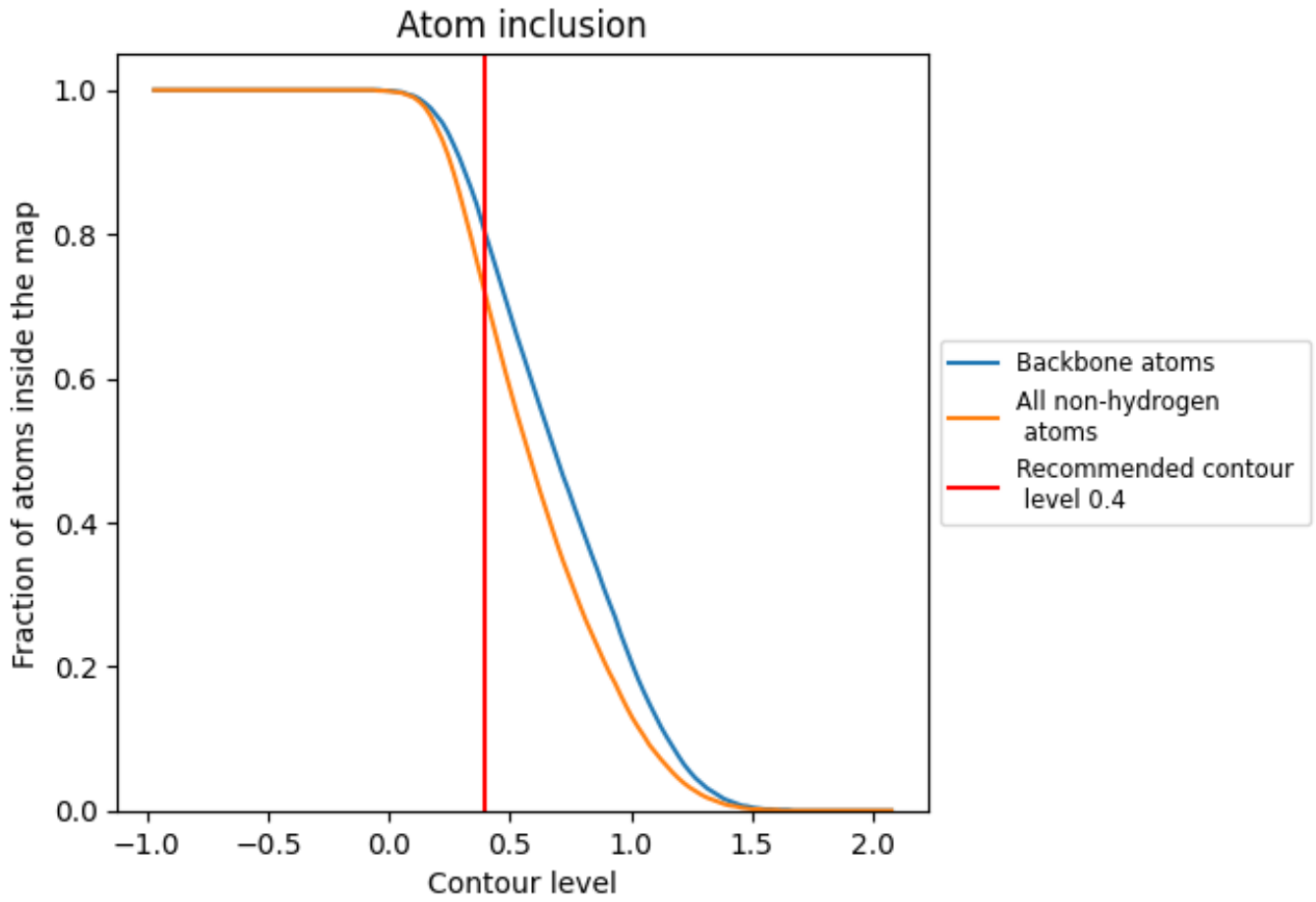
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.5130
A	0.7760	0.5350
B	0.7350	0.5150
C	0.7880	0.5440
D	0.7360	0.5160
E	0.7470	0.5410
F	0.2690	0.3700
G	0.7110	0.5080
H	0.8150	0.5450
I	0.5170	0.4480