Full wwPDB EM Validation Report

Feb 27, 2022 – 06:13 am GMT

PDB ID	:	7PD4
EMDB ID	:	EMD-13330
Title	:	structure of Adenylyl cyclase 9 in complex with MANT-GTP
Authors	:	Qi, C.; Korkhov, V.M.
Deposited on	:	2021-08-04
Resolution	:	4.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

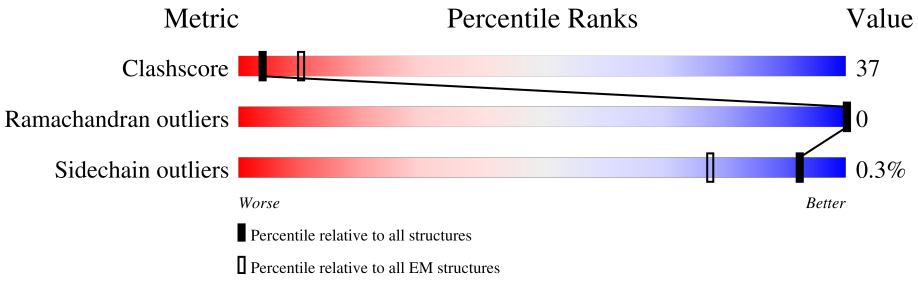
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance

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

The reported resolution of this entry is 4.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1354	24% 38% 38%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6676 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 Adenylate cyclase 9.

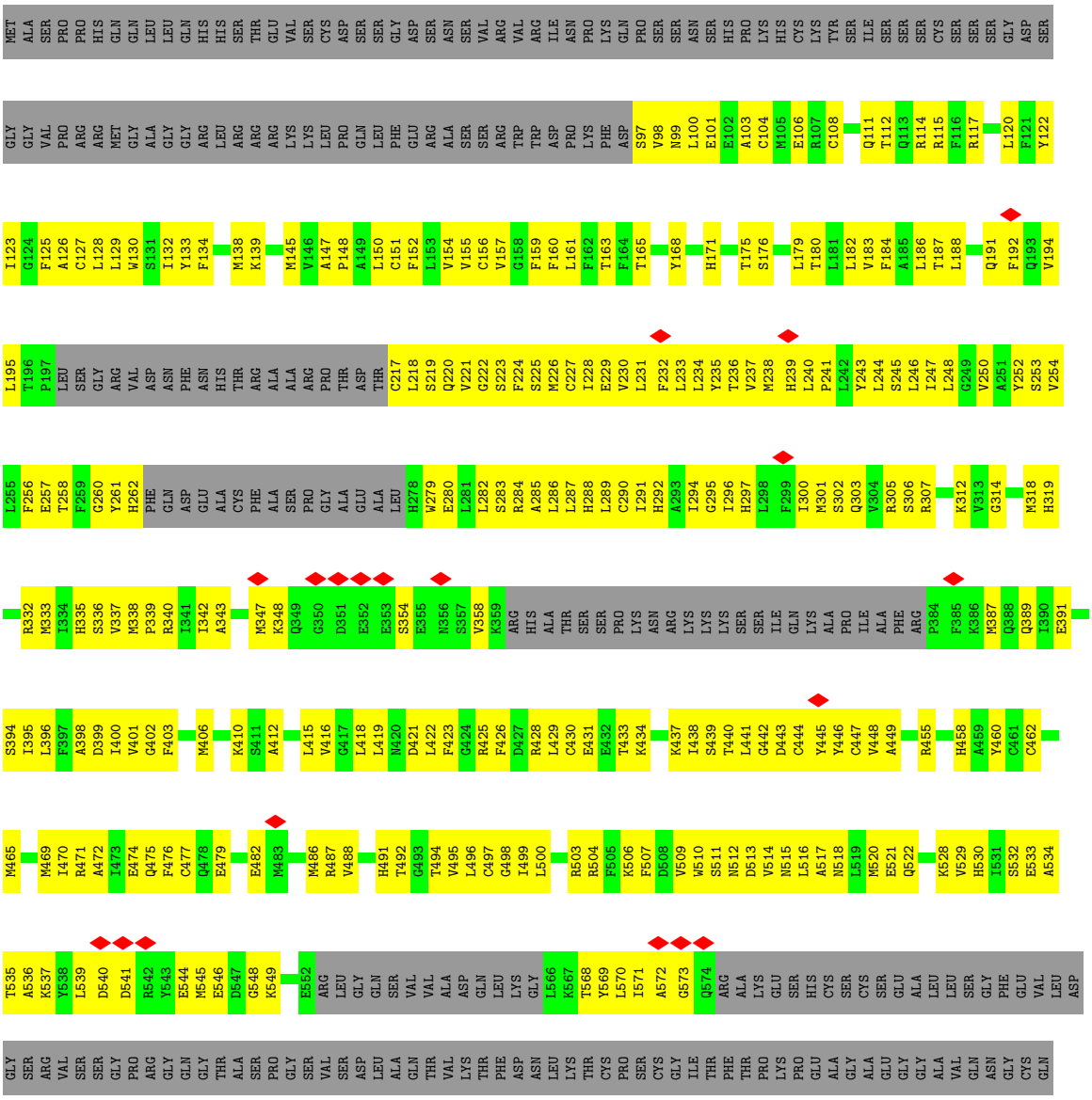
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	842	6676	4329	1098	1194	55	0	0

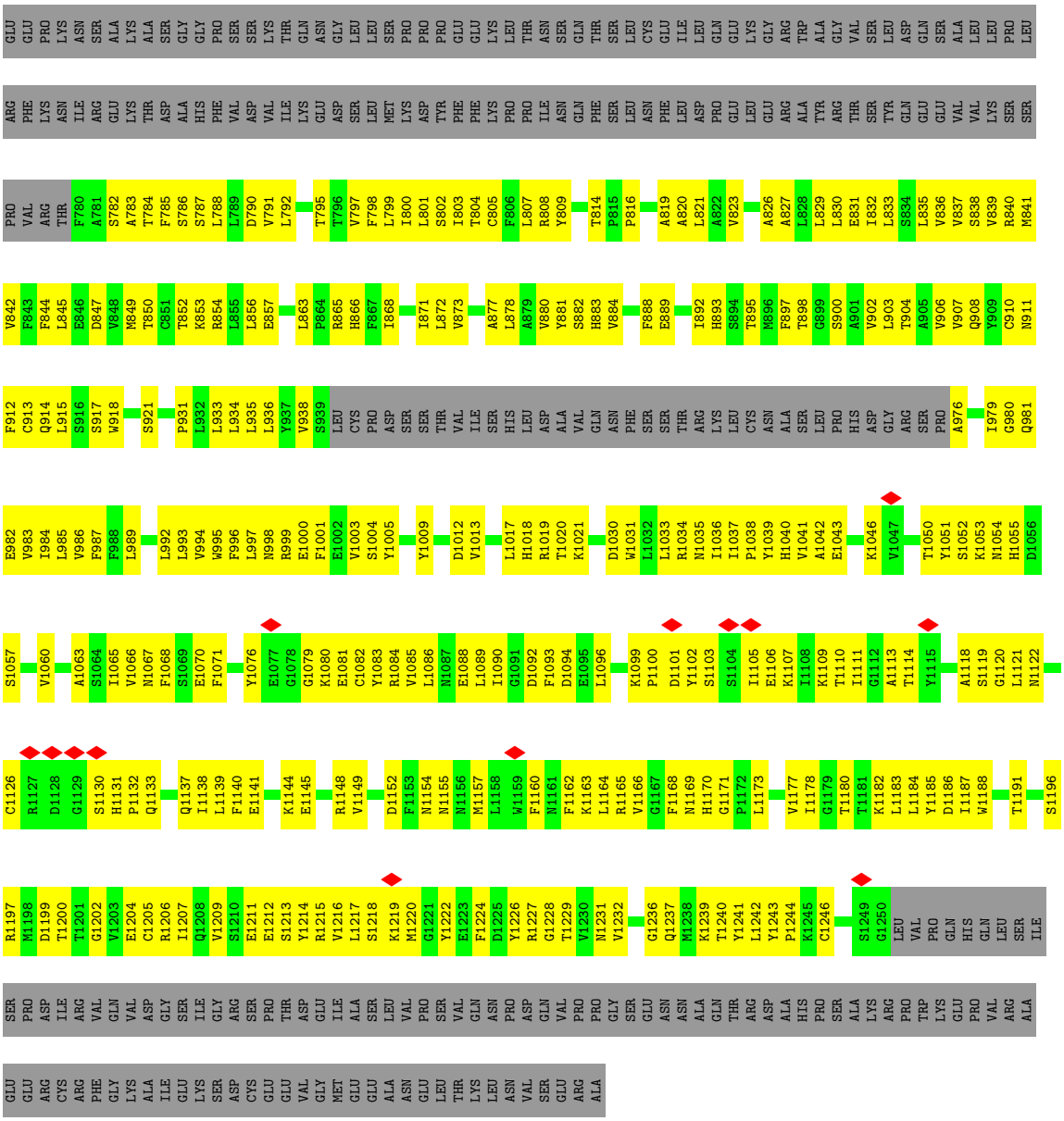
3 Residue-property plots (i)

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: Adenylate cyclase 9

Chain A:




GLU GLU PRO LYS ASN SER ALA LYS ALA SER GLY GLY PRO SER SER LYS THR GLN ASN GLY LEU LEU SER PRO PRO PRO GLU GLU LYS LEU THR ASN SER GLN THR SER LEU CYS GLU ILE LEU GLN GLU LYS GLY ARG TRP ALA GLY VAL SER LEU ASP GLN SER ALA LEU LEU PRO LEU
ARG PHE LYS ASN ILE ARG GLU LYS THR ASP ALA HIS PHE VAL ASP VAL ILE LYS GLU ASP SER LEU VAL PRO PRO LYS ASP TYR PHE PHE LYS PRO PRO ILE ASN GLN PHE SER LEU ASN PHE LEU ASP PRO GLU LEU GLU ARG ALA TYR ARG THR SER TYR GLN GLU GLU VAL VAL LYS SER SER
PRO VAL ARG THR F780 A781 S782 A783 T784 F785 S786 S787 L788 L789 D790 V791 L792 T795 T796 V797 F798 L799 I800 L801 S802 I803 T804 C805 F806 L807 R808 Y809 T814 P815 P816 A819 A820 L821 A822 V823 A826 A827 L828 L829 L830 E831 I832 L833 S834 L835 V836 V837 S838 V839 R840 M841
V842 F843 F844 L845 E846 D847 V848 M849 T850 C851 T852 K853 R854 L855 L856 E857 L863 P864 R865 H866 F867 I868 I871 L872 V873 A877 L878 A879 V880 Y881 S882 H883 V884 F888 E889 I892 H893 S894 T895 M896 F897 T898 G899 S900 A901 V902 L903 T904 A905 V906 V907 Q908 Y909 C910 N911
F912 C913 Q914 L915 S916 S917 W918 S921 P931 L932 L933 L934 L935 L936 Y937 V938 S939 LEU CYS PRO ASP SER SER THR VAL ILE SER HIS LEU ASP ALA VAL GLN ASN PHE SER SER THR ARG LYS LEU CYS ASN ALA SER LEU PRO HIS ASP GLY ARG SER PRO A976 I979 G980 Q981
E982 V983 I984 L985 V986 F987 F988 L989 L992 L993 V994 W995 F996 L997 N998 R999 E1000 F1001 E1002 V1003 S1004 Y1005 Y1009 D1012 V1013 L1017 H1018 R1019 T1020 K1021 D1030 W1031 L1032 L1033 R1034 N1035 I1036 I1037 P1038 Y1039 H1040 V1041 A1042 E1043 K1046 V1047 T1050 Y1051 S1052 K1053 N1054 H1055 D1056
S1057 V1060 A1063 S1064 I1065 V1066 N1067 F1068 S1069 E1070 F1071 Y1076 E1077 G1078 G1079 K1080 E1081 C1082 Y1083 R1084 V1085 L1086 N1087 E1088 L1089 I1090 G1091 D1092 F1093 D1094 E1095 L1096 K1099 P1100 D1101 Y1102 S1103 S1104 I1105 E1106 K1107 I1108 K1109 T1110 I1111 G1112 A1113 T1114 Y1115 A1118 S1119 G1120 L1121 N1122
C1126 R1127 D1128 G1129 S1130 H1131 P1132 Q1133 Q1137 I1138 L1139 F1140 E1141 K1144 E1145 R1148 V1149 D1152 F1153 N1154 N1155 N1156 M1157 L1158 W1159 F1160 N1161 F1162 K1163 L1164 R1165 V1166 G1167 F1168 N1169 H1170 G1171 P1172 L1173 V1177 I1178 G1179 T1180 T1181 K1182 L1183 L1184 Y1185 D1186 I1187 W1188 T1191 S1196
R1197 M1198 D1199 T1200 T1201 G1202 V1203 E1204 C1205 R1206 I1207 Q1208 V1209 S1210 E1211 E1212 S1213 Y1214 R1215 V1216 L1217 S1218 K1219 M1220 G1221 Y1222 E1223 F1224 D1225 Y1226 R1227 G1228 T1229 V1230 N1231 V1232 G1236 Q1237 M1238 K1239 T1240 Y1241 L1242 Y1243 P1244 K1245 C1246 S1249 G1250 LEU VAL PRO GLN HIS GLN LEU SER ILE
SER PRO ASP ILE ARG VAL GLN VAL ASP GLY SER ILE GLY ARG SER PRO THR ASP GLU ILE ALA SER LEU VAL PRO SER VAL GLN ASN PRO ASP GLN VAL PRO PRO GLY SER GLU ASN ASN ALA GLN THR ARG ASP ALA HIS PRO SER ALA LYS ARG PRO TRP LYS GLU PRO VAL ARG ALA
GLU GLU ARG CYS ARG PHE GLY LYS ALA ILE GLU GLU LYS SER ASP CYS GLU GLU GLU VAL GLY MET GLU GLU ALA ASN GLU LEU THR LYS LEU ASN VAL SER GLU ARG ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141446	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	243.0, 243.0, 243.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.34	0/6822	0.49	0/9226

There are no bond length outliers.

There are no bond angle outliers.

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	6676	0	6696	497	0
All	All	6676	0	6696	497	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 37.

All (497) 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:1111:ILE:H	1:A:1114:THR:HB	1.34	0.89
1:A:1106:GLU:HB2	1:A:1118:ALA:O	1.70	0.89
1:A:528:LYS:HA	1:A:571:ILE:O	1.73	0.88
1:A:800:ILE:HA	1:A:803:ILE:HD12	1.56	0.87
1:A:240:LEU:HB2	1:A:245:SER:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:MET:HG2	1:A:498:GLY:HA3	1.56	0.84
1:A:108:CYS:O	1:A:111:GLN:NE2	2.12	0.82
1:A:1165:ARG:HH21	1:A:1200:THR:HA	1.45	0.82
1:A:120:LEU:HA	1:A:123:ILE:HD12	1.62	0.81
1:A:1227:ARG:HB2	1:A:1242:LEU:HG	1.65	0.78
1:A:1110:THR:OG1	1:A:1114:THR:O	2.03	0.76
1:A:1206:ARG:NH1	1:A:1244:PRO:O	2.21	0.73
1:A:808:ARG:O	1:A:808:ARG:NH1	2.22	0.73
1:A:284:ARG:O	1:A:288:HIS:ND1	2.19	0.73
1:A:335:HIS:O	1:A:340:ARG:NH1	2.22	0.72
1:A:111:GLN:OE1	1:A:115:ARG:NH1	2.24	0.71
1:A:234:LEU:HD12	1:A:238:MET:HG3	1.73	0.71
1:A:1178:ILE:HB	1:A:1184:LEU:HB2	1.72	0.70
1:A:455:ARG:HB3	1:A:458:HIS:HB3	1.73	0.70
1:A:857:GLU:OE2	1:A:865:ARG:NH2	2.19	0.70
1:A:1042:ALA:O	1:A:1046:LYS:HB2	1.91	0.70
1:A:416:VAL:HA	1:A:419:LEU:HD12	1.74	0.70
1:A:138:MET:SD	1:A:139:LYS:NZ	2.64	0.70
1:A:220:GLN:O	1:A:223:SER:OG	2.10	0.69
1:A:394:SER:HA	1:A:492:THR:HG22	1.75	0.68
1:A:1170:HIS:CE1	1:A:1212:GLU:HG2	2.29	0.68
1:A:312:LYS:HD3	1:A:1012:ASP:HA	1.76	0.67
1:A:827:ALA:HA	1:A:830:LEU:HD12	1.75	0.67
1:A:783:ALA:O	1:A:786:SER:OG	2.12	0.67
1:A:908:GLN:OE1	1:A:911:ASN:ND2	2.28	0.66
1:A:976:ALA:HA	1:A:979:ILE:HD11	1.77	0.66
1:A:1036:ILE:HG23	1:A:1037:ILE:HG23	1.77	0.66
1:A:792:LEU:O	1:A:795:THR:OG1	2.11	0.66
1:A:993:LEU:O	1:A:997:LEU:HG	1.95	0.66
1:A:495:VAL:HG11	1:A:509:VAL:HB	1.77	0.66
1:A:139:LYS:NZ	1:A:217:CYS:O	2.27	0.65
1:A:241:PRO:HB2	1:A:244:LEU:HB2	1.78	0.65
1:A:931:PRO:O	1:A:935:LEU:HG	1.96	0.65
1:A:127:CYS:HA	1:A:130:TRP:HD1	1.61	0.65
1:A:279:TRP:HA	1:A:282:LEU:HD13	1.78	0.65
1:A:429:LEU:HB3	1:A:465:MET:HG3	1.76	0.65
1:A:114:ARG:HA	1:A:117:ARG:HE	1.61	0.65
1:A:1226:TYR:HE1	1:A:1239:LYS:HG3	1.61	0.65
1:A:1232:VAL:O	1:A:1236:GLY:N	2.29	0.65
1:A:401:VAL:HG22	1:A:487:ARG:HH11	1.62	0.65
1:A:234:LEU:HD11	1:A:240:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:SER:OG	1:A:458:HIS:ND1	2.24	0.65
1:A:115:ARG:NH2	1:A:1000:GLU:OE2	2.29	0.65
1:A:227:CYS:HG	1:A:252:TYR:HE2	1.45	0.65
1:A:986:VAL:O	1:A:989:LEU:HG	1.96	0.65
1:A:799:LEU:O	1:A:802:SER:OG	2.15	0.64
1:A:836:VAL:HA	1:A:839:VAL:HG12	1.78	0.64
1:A:1053:LYS:NZ	1:A:1054:ASN:O	2.25	0.64
1:A:244:LEU:HD23	1:A:247:ILE:HD11	1.78	0.64
1:A:333:MET:HG3	1:A:1033:LEU:HD21	1.79	0.64
1:A:850:THR:OG1	1:A:854:ARG:NH1	2.31	0.64
1:A:391:GLU:HA	1:A:494:THR:HA	1.80	0.64
1:A:788:LEU:HD11	1:A:842:VAL:HG21	1.80	0.64
1:A:820:ALA:HA	1:A:882:SER:HB2	1.80	0.64
1:A:1137:GLN:O	1:A:1222:TYR:OH	2.14	0.64
1:A:897:PHE:O	1:A:900:SER:OG	2.15	0.63
1:A:844:PHE:HE1	1:A:854:ARG:HH22	1.47	0.63
1:A:1083:TYR:HA	1:A:1086:LEU:HD12	1.81	0.63
1:A:425:ARG:NH1	1:A:472:ALA:O	2.31	0.62
1:A:528:LYS:HG2	1:A:572:ALA:HB2	1.81	0.62
1:A:460:TYR:OH	1:A:540:ASP:OD1	2.18	0.62
1:A:868:ILE:HA	1:A:871:ILE:HD12	1.81	0.62
1:A:1165:ARG:NE	1:A:1199:ASP:O	2.33	0.62
1:A:912:PHE:HB3	1:A:915:LEU:HG	1.81	0.62
1:A:426:PHE:HA	1:A:429:LEU:HD12	1.80	0.62
1:A:1111:ILE:N	1:A:1114:THR:HB	2.12	0.61
1:A:458:HIS:O	1:A:462:CYS:HB2	2.00	0.61
1:A:512:ASN:O	1:A:516:LEU:N	2.33	0.61
1:A:429:LEU:HD13	1:A:469:MET:HG2	1.83	0.61
1:A:433:THR:HG21	1:A:465:MET:HB2	1.82	0.61
1:A:497:CYS:HB3	1:A:509:VAL:HG12	1.83	0.61
1:A:1232:VAL:N	1:A:1236:GLY:O	2.28	0.60
1:A:412:ALA:O	1:A:1052:SER:OG	2.15	0.60
1:A:290:CYS:O	1:A:294:ILE:HG22	2.02	0.60
1:A:335:HIS:CE1	1:A:340:ARG:HA	2.36	0.60
1:A:288:HIS:O	1:A:292:HIS:ND1	2.35	0.60
1:A:790:ASP:OD1	1:A:791:VAL:N	2.34	0.60
1:A:236:THR:HG23	1:A:237:VAL:HG23	1.82	0.60
1:A:1040:HIS:CE1	1:A:1122:ASN:HD21	2.19	0.60
1:A:396:LEU:HD21	1:A:447:CYS:HB2	1.84	0.60
1:A:1178:ILE:N	1:A:1184:LEU:O	2.24	0.60
1:A:548:GLY:HA3	1:A:570:LEU:HG	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HA	1:A:132:ILE:HG12	1.84	0.59
1:A:819:ALA:O	1:A:823:VAL:HG22	2.03	0.59
1:A:297:HIS:O	1:A:300:ILE:HG12	2.03	0.59
1:A:790:ASP:OD2	1:A:914:GLN:NE2	2.35	0.59
1:A:184:PHE:HZ	1:A:234:LEU:HD22	1.67	0.59
1:A:504:ARG:N	1:A:1035:ASN:OD1	2.34	0.59
1:A:863:LEU:O	1:A:866:HIS:HB2	2.03	0.59
1:A:935:LEU:HA	1:A:938:VAL:HB	1.85	0.59
1:A:127:CYS:HA	1:A:130:TRP:CD1	2.38	0.58
1:A:415:LEU:HD12	1:A:418:LEU:HD11	1.85	0.58
1:A:1186:ASP:OD1	1:A:1187:ILE:N	2.33	0.58
1:A:410:LYS:HG3	1:A:415:LEU:HD13	1.86	0.58
1:A:287:LEU:HG	1:A:904:THR:HG21	1.84	0.58
1:A:98:VAL:HG13	1:A:99:ASN:H	1.68	0.58
1:A:401:VAL:HG23	1:A:487:ARG:H	1.67	0.58
1:A:1033:LEU:HA	1:A:1036:ILE:HG22	1.85	0.58
1:A:1206:ARG:HH12	1:A:1246:CYS:H	1.50	0.58
1:A:229:GLU:O	1:A:233:LEU:HG	2.03	0.58
1:A:1068:PHE:HA	1:A:1162:PHE:CE1	2.39	0.57
1:A:97:SER:HB2	1:A:100:LEU:HD12	1.85	0.57
1:A:126:ALA:O	1:A:129:LEU:HG	2.04	0.57
1:A:471:ARG:O	1:A:474:GLU:HG2	2.04	0.57
1:A:387:MET:HB2	1:A:1080:LYS:HE2	1.87	0.57
1:A:910:CYS:HA	1:A:998:ASN:HD22	1.70	0.57
1:A:438:ILE:HB	1:A:446:TYR:CD2	2.40	0.57
1:A:1099:LYS:HB2	1:A:1102:TYR:HB2	1.87	0.57
1:A:220:GLN:OE1	1:A:220:GLN:N	2.38	0.57
1:A:1018:HIS:HA	1:A:1021:LYS:HD2	1.85	0.57
1:A:305:ARG:NH1	1:A:1004:SER:OG	2.37	0.57
1:A:910:CYS:HB2	1:A:994:VAL:HG23	1.85	0.57
1:A:224:PHE:O	1:A:228:ILE:HG12	2.05	0.56
1:A:833:LEU:O	1:A:837:VAL:HG23	2.05	0.56
1:A:1082:CYS:O	1:A:1086:LEU:HG	2.04	0.56
1:A:179:LEU:O	1:A:183:VAL:HG23	2.05	0.56
1:A:795:THR:HG22	1:A:831:GLU:HB3	1.87	0.56
1:A:491:HIS:HD2	1:A:513:ASP:HA	1.71	0.56
1:A:849:MET:O	1:A:852:THR:OG1	2.23	0.56
1:A:893:HIS:O	1:A:897:PHE:HB2	2.06	0.56
1:A:1106:GLU:HG3	1:A:1121:LEU:HD12	1.87	0.56
1:A:1065:ILE:H	1:A:1113:ALA:HB1	1.71	0.56
1:A:536:ALA:HA	1:A:539:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:ILE:HA	1:A:982:GLU:HG3	1.88	0.55
1:A:1068:PHE:HA	1:A:1162:PHE:HE1	1.71	0.55
1:A:1066:VAL:H	1:A:1164:LEU:HA	1.72	0.55
1:A:288:HIS:O	1:A:291:ILE:HG22	2.07	0.55
1:A:336:SER:OG	1:A:1183:LEU:N	2.40	0.55
1:A:785:PHE:HA	1:A:788:LEU:HD12	1.88	0.55
1:A:801:LEU:O	1:A:804:THR:OG1	2.21	0.55
1:A:403:PHE:CD1	1:A:443:ASP:HB3	2.41	0.55
1:A:826:ALA:O	1:A:829:LEU:HG	2.06	0.55
1:A:868:ILE:O	1:A:872:LEU:HG	2.07	0.55
1:A:895:THR:O	1:A:898:THR:OG1	2.24	0.55
1:A:1101:ASP:OD1	1:A:1101:ASP:N	2.40	0.55
1:A:981:GLN:O	1:A:985:LEU:HG	2.06	0.55
1:A:1063:ALA:HB1	1:A:1164:LEU:HD12	1.89	0.55
1:A:1145:GLU:O	1:A:1149:VAL:HG23	2.06	0.54
1:A:228:ILE:HG23	1:A:291:ILE:HG12	1.89	0.54
1:A:305:ARG:NH2	1:A:1005:TYR:HD1	2.06	0.54
1:A:791:VAL:O	1:A:795:THR:HG23	2.07	0.54
1:A:981:GLN:O	1:A:984:ILE:HG12	2.07	0.54
1:A:319:HIS:CE1	1:A:1019:ARG:HG2	2.42	0.54
1:A:280:GLU:O	1:A:283:SER:OG	2.14	0.54
1:A:532:SER:O	1:A:535:THR:OG1	2.25	0.54
1:A:235:TYR:CE1	1:A:295:GLY:HA3	2.43	0.54
1:A:241:PRO:HG2	1:A:244:LEU:HD12	1.90	0.54
1:A:247:ILE:HG13	1:A:248:LEU:HD22	1.90	0.54
1:A:337:VAL:O	1:A:338:MET:HE2	2.08	0.54
1:A:878:LEU:HD12	1:A:881:TYR:HB2	1.90	0.54
1:A:881:TYR:CZ	1:A:931:PRO:HG2	2.43	0.54
1:A:986:VAL:HG23	1:A:989:LEU:HD21	1.90	0.54
1:A:496:LEU:HD11	1:A:1083:TYR:CZ	2.44	0.53
1:A:1226:TYR:CE1	1:A:1239:LYS:HG3	2.43	0.53
1:A:826:ALA:O	1:A:830:LEU:HG	2.09	0.53
1:A:438:ILE:HB	1:A:446:TYR:HD2	1.71	0.53
1:A:1009:TYR:O	1:A:1013:VAL:HG23	2.09	0.53
1:A:546:GLU:O	1:A:570:LEU:N	2.25	0.53
1:A:788:LEU:HD23	1:A:838:SER:HB2	1.90	0.53
1:A:863:LEU:HA	1:A:866:HIS:ND1	2.24	0.53
1:A:1086:LEU:O	1:A:1090:ILE:HG12	2.08	0.53
1:A:873:VAL:HG22	1:A:908:GLN:HE22	1.74	0.53
1:A:998:ASN:HA	1:A:1001:PHE:CD2	2.44	0.53
1:A:903:LEU:O	1:A:907:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:THR:O	1:A:1237:GLN:NE2	2.41	0.53
1:A:821:LEU:HD12	1:A:821:LEU:H	1.74	0.53
1:A:1180:THR:C	1:A:1182:LYS:H	2.10	0.53
1:A:442:GLY:HA2	1:A:1188:TRP:HD1	1.73	0.52
1:A:1196:SER:O	1:A:1200:THR:OG1	2.20	0.52
1:A:403:PHE:CG	1:A:443:ASP:HB3	2.44	0.52
1:A:1040:HIS:CE1	1:A:1041:VAL:HG13	2.45	0.52
1:A:804:THR:O	1:A:807:LEU:HG	2.09	0.52
1:A:1057:SER:HA	1:A:1171:GLY:O	2.10	0.52
1:A:1131:HIS:CE1	1:A:1133:GLN:HB2	2.44	0.52
1:A:533:GLU:HA	1:A:569:TYR:HE2	1.74	0.52
1:A:1067:ASN:HB2	1:A:1070:GLU:OE2	2.10	0.52
1:A:1216:VAL:HG23	1:A:1217:LEU:HD22	1.91	0.52
1:A:429:LEU:O	1:A:433:THR:OG1	2.23	0.52
1:A:448:VAL:HG22	1:A:449:ALA:H	1.74	0.52
1:A:159:PHE:O	1:A:163:THR:OG1	2.27	0.52
1:A:881:TYR:OH	1:A:931:PRO:HG2	2.09	0.52
1:A:254:VAL:O	1:A:258:THR:HG23	2.10	0.52
1:A:477:CYS:HB2	1:A:482:GLU:O	2.10	0.52
1:A:222:GLY:O	1:A:225:SER:OG	2.23	0.52
1:A:1060:VAL:HG11	1:A:1191:THR:HG22	1.92	0.52
1:A:221:VAL:HA	1:A:224:PHE:HB3	1.91	0.51
1:A:888:PHE:HE2	1:A:895:THR:HG23	1.75	0.51
1:A:250:VAL:HG12	1:A:292:HIS:CD2	2.46	0.51
1:A:314:GLY:O	1:A:318:MET:HG2	2.10	0.51
1:A:983:VAL:HB	1:A:987:PHE:CZ	2.46	0.51
1:A:401:VAL:H	1:A:486:MET:HA	1.74	0.51
1:A:933:LEU:O	1:A:936:LEU:HB3	2.10	0.51
1:A:798:PHE:O	1:A:801:LEU:HB3	2.11	0.51
1:A:986:VAL:HA	1:A:989:LEU:HD23	1.93	0.51
1:A:881:TYR:HA	1:A:884:VAL:HG23	1.93	0.51
1:A:129:LEU:HD21	1:A:989:LEU:HD22	1.93	0.51
1:A:261:TYR:HB3	1:A:262:HIS:CE1	2.46	0.51
1:A:476:PHE:HA	1:A:479:GLU:HB3	1.92	0.51
1:A:303:GLN:O	1:A:306:SER:OG	2.25	0.51
1:A:303:GLN:O	1:A:307:ARG:HG2	2.11	0.51
1:A:419:LEU:HB3	1:A:423:PHE:CE2	2.46	0.51
1:A:165:THR:HG22	1:A:168:TYR:HB2	1.92	0.51
1:A:257:GLU:HB3	1:A:288:HIS:NE2	2.26	0.51
1:A:833:LEU:HA	1:A:836:VAL:HG22	1.93	0.51
1:A:1085:VAL:O	1:A:1088:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLN:NE2	1:A:496:LEU:HB3	2.26	0.50
1:A:491:HIS:CG	1:A:516:LEU:HD22	2.44	0.50
1:A:1131:HIS:CD2	1:A:1132:PRO:HD2	2.46	0.50
1:A:1213:SER:HA	1:A:1216:VAL:HG22	1.93	0.50
1:A:829:LEU:HA	1:A:832:ILE:HG22	1.93	0.50
1:A:910:CYS:SG	1:A:998:ASN:HB3	2.52	0.50
1:A:1001:PHE:O	1:A:1004:SER:OG	2.21	0.50
1:A:290:CYS:HB3	1:A:800:ILE:HD11	1.94	0.50
1:A:150:LEU:O	1:A:154:VAL:HG13	2.12	0.50
1:A:354:SER:O	1:A:358:VAL:HG23	2.12	0.50
1:A:296:ILE:O	1:A:300:ILE:HG23	2.13	0.49
1:A:504:ARG:HB2	1:A:1107:LYS:NZ	2.27	0.49
1:A:188:LEU:HD11	1:A:256:PHE:HA	1.95	0.49
1:A:227:CYS:SG	1:A:252:TYR:HE2	2.35	0.49
1:A:285:ALA:O	1:A:289:LEU:HG	2.13	0.49
1:A:224:PHE:CZ	1:A:287:LEU:HD23	2.47	0.49
1:A:343:ALA:O	1:A:347:MET:HG2	2.12	0.49
1:A:904:THR:O	1:A:907:VAL:HG22	2.13	0.49
1:A:97:SER:OG	1:A:101:GLU:HG3	2.12	0.49
1:A:1017:LEU:HB3	1:A:1021:LYS:HE3	1.93	0.49
1:A:518:ASN:OD1	1:A:522:GLN:NE2	2.46	0.49
1:A:1119:SER:HB3	1:A:1139:LEU:HD11	1.93	0.49
1:A:301:MET:SD	1:A:302:SER:N	2.85	0.49
1:A:399:ASP:O	1:A:487:ARG:HG2	2.13	0.49
1:A:332:ARG:HE	1:A:333:MET:HE2	1.76	0.49
1:A:335:HIS:CE1	1:A:343:ALA:HB3	2.48	0.49
1:A:335:HIS:HE1	1:A:340:ARG:HA	1.78	0.49
1:A:548:GLY:H	1:A:569:TYR:HA	1.75	0.49
1:A:1038:PRO:HD2	1:A:1041:VAL:HG21	1.93	0.49
1:A:830:LEU:O	1:A:833:LEU:HG	2.12	0.49
1:A:395:ILE:HG21	1:A:514:VAL:HA	1.93	0.49
1:A:1186:ASP:HB3	1:A:1188:TRP:CZ2	2.48	0.49
1:A:1043:GLU:OE2	1:A:1046:LYS:NZ	2.45	0.48
1:A:120:LEU:HD22	1:A:156:CYS:HB3	1.94	0.48
1:A:128:LEU:O	1:A:132:ILE:HG23	2.13	0.48
1:A:797:VAL:HA	1:A:800:ILE:HG12	1.95	0.48
1:A:881:TYR:HA	1:A:884:VAL:CG2	2.42	0.48
1:A:243:TYR:O	1:A:247:ILE:HG12	2.14	0.48
1:A:241:PRO:O	1:A:245:SER:N	2.34	0.48
1:A:475:GLN:O	1:A:479:GLU:HB2	2.13	0.48
1:A:809:TYR:CZ	1:A:816:PRO:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PRO:HD3	1:A:506:LYS:HZ1	1.79	0.48
1:A:898:THR:O	1:A:902:VAL:HG13	2.13	0.48
1:A:97:SER:HB2	1:A:100:LEU:HB2	1.95	0.48
1:A:888:PHE:CZ	1:A:935:LEU:HD22	2.49	0.48
1:A:288:HIS:H	1:A:288:HIS:HD1	1.61	0.48
1:A:530:HIS:NE2	1:A:568:THR:HB	2.28	0.48
1:A:130:TRP:O	1:A:134:PHE:HD2	1.95	0.48
1:A:103:ALA:HA	1:A:106:GLU:CD	2.34	0.48
1:A:253:SER:HB2	1:A:288:HIS:HD2	1.79	0.48
1:A:280:GLU:O	1:A:284:ARG:HG2	2.13	0.48
1:A:503:ARG:HH11	1:A:1094:ASP:HB3	1.79	0.48
1:A:533:GLU:O	1:A:537:LYS:N	2.46	0.48
1:A:814:THR:O	1:A:816:PRO:HD3	2.14	0.48
1:A:1126:CYS:SG	1:A:1130:SER:OG	2.66	0.48
1:A:423:PHE:HA	1:A:426:PHE:CD2	2.49	0.48
1:A:921:SER:HB2	1:A:995:TRP:CE3	2.48	0.48
1:A:159:PHE:CE2	1:A:179:LEU:HD13	2.50	0.47
1:A:223:SER:HA	1:A:226:MET:SD	2.53	0.47
1:A:400:ILE:O	1:A:487:ARG:NH1	2.47	0.47
1:A:495:VAL:CG1	1:A:509:VAL:HB	2.42	0.47
1:A:284:ARG:O	1:A:287:LEU:HB2	2.13	0.47
1:A:1060:VAL:CG1	1:A:1191:THR:HG22	2.44	0.47
1:A:496:LEU:HD23	1:A:510:TRP:O	2.14	0.47
1:A:784:THR:HA	1:A:787:SER:OG	2.14	0.47
1:A:983:VAL:HA	1:A:986:VAL:HG12	1.97	0.47
1:A:192:PHE:O	1:A:194:VAL:N	2.46	0.47
1:A:227:CYS:O	1:A:231:LEU:HD23	2.14	0.47
1:A:250:VAL:HA	1:A:292:HIS:HE2	1.78	0.47
1:A:465:MET:O	1:A:469:MET:HG3	2.14	0.47
1:A:782:SER:OG	1:A:785:PHE:HB2	2.13	0.47
1:A:1033:LEU:O	1:A:1037:ILE:N	2.42	0.47
1:A:1137:GLN:HB2	1:A:1220:MET:SD	2.53	0.47
1:A:1141:GLU:OE2	1:A:1222:TYR:OH	2.33	0.47
1:A:1197:ARG:HD3	1:A:1232:VAL:HA	1.97	0.47
1:A:133:TYR:HD2	1:A:134:PHE:CD2	2.33	0.47
1:A:179:LEU:O	1:A:182:LEU:HB3	2.14	0.47
1:A:913:CYS:SG	1:A:1001:PHE:HB2	2.55	0.47
1:A:992:LEU:O	1:A:995:TRP:HB3	2.15	0.47
1:A:1119:SER:OG	1:A:1120:GLY:N	2.45	0.47
1:A:221:VAL:HG11	1:A:900:SER:HB3	1.97	0.47
1:A:226:MET:O	1:A:229:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:LEU:HA	1:A:906:VAL:HG12	1.96	0.47
1:A:1177:VAL:HA	1:A:1185:TYR:HA	1.97	0.47
1:A:224:PHE:HZ	1:A:287:LEU:HB3	1.80	0.46
1:A:802:SER:HA	1:A:805:CYS:SG	2.54	0.46
1:A:1140:PHE:HB3	1:A:1222:TYR:CZ	2.50	0.46
1:A:1076:TYR:HB2	1:A:1079:GLY:HA2	1.97	0.46
1:A:101:GLU:HA	1:A:104:CYS:SG	2.56	0.46
1:A:492:THR:HG23	1:A:535:THR:HG22	1.98	0.46
1:A:125:PHE:O	1:A:128:LEU:HB3	2.16	0.46
1:A:148:PRO:HA	1:A:151:CYS:SG	2.56	0.46
1:A:226:MET:O	1:A:230:VAL:HG23	2.15	0.46
1:A:430:CYS:SG	1:A:437:LYS:HB3	2.56	0.46
1:A:520:MET:O	1:A:530:HIS:ND1	2.45	0.46
1:A:931:PRO:O	1:A:934:LEU:HB3	2.15	0.46
1:A:152:PHE:HZ	1:A:183:VAL:HG22	1.80	0.46
1:A:152:PHE:CD1	1:A:186:LEU:HD22	2.51	0.46
1:A:171:HIS:O	1:A:175:THR:OG1	2.32	0.46
1:A:221:VAL:O	1:A:225:SER:N	2.28	0.46
1:A:283:SER:O	1:A:287:LEU:HD13	2.16	0.46
1:A:853:LYS:H	1:A:853:LYS:HD2	1.81	0.46
1:A:1207:ILE:HB	1:A:1243:TYR:HB3	1.98	0.46
1:A:1227:ARG:H	1:A:1241:TYR:HA	1.80	0.46
1:A:888:PHE:CE2	1:A:895:THR:HG23	2.51	0.46
1:A:1081:GLU:HA	1:A:1084:ARG:NH1	2.31	0.46
1:A:402:GLY:O	1:A:406:MET:HG3	2.15	0.46
1:A:422:LEU:HB3	1:A:426:PHE:CZ	2.51	0.46
1:A:1034:ARG:HH22	1:A:1039:TYR:N	2.13	0.46
1:A:853:LYS:HA	1:A:856:LEU:HB2	1.98	0.46
1:A:1152:ASP:HA	1:A:1155:ASN:ND2	2.31	0.45
1:A:1239:LYS:HG2	1:A:1241:TYR:CE2	2.51	0.45
1:A:120:LEU:HD11	1:A:159:PHE:HB3	1.98	0.45
1:A:418:LEU:HB2	1:A:476:PHE:CZ	2.50	0.45
1:A:539:LEU:HG	1:A:541:ASP:H	1.81	0.45
1:A:1071:PHE:HB3	1:A:1162:PHE:CZ	2.51	0.45
1:A:1090:ILE:HA	1:A:1093:PHE:CD2	2.51	0.45
1:A:506:LYS:HG3	1:A:507:PHE:N	2.30	0.45
1:A:993:LEU:HD23	1:A:994:VAL:N	2.32	0.45
1:A:1211:GLU:O	1:A:1215:ARG:HG3	2.16	0.45
1:A:286:LEU:HD11	1:A:800:ILE:HB	1.98	0.45
1:A:1066:VAL:HG21	1:A:1204:GLU:HB3	1.98	0.45
1:A:903:LEU:HD12	1:A:904:THR:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ILE:HG13	1:A:443:ASP:O	2.17	0.45
1:A:415:LEU:O	1:A:418:LEU:HG	2.16	0.45
1:A:438:ILE:HG12	1:A:447:CYS:HA	1.99	0.45
1:A:999:ARG:O	1:A:1003:VAL:HG23	2.17	0.45
1:A:1218:SER:HA	1:A:1222:TYR:O	2.17	0.45
1:A:286:LEU:HD21	1:A:800:ILE:HB	1.99	0.45
1:A:441:LEU:N	1:A:446:TYR:HE1	2.15	0.45
1:A:1197:ARG:HE	1:A:1232:VAL:HA	1.81	0.45
1:A:233:LEU:HA	1:A:236:THR:HG22	1.98	0.45
1:A:389:GLN:HA	1:A:496:LEU:HA	1.98	0.45
1:A:1205:CYS:O	1:A:1244:PRO:HG2	2.17	0.45
1:A:111:GLN:NE2	1:A:112:THR:OG1	2.50	0.45
1:A:243:TYR:CE2	1:A:244:LEU:HG	2.51	0.45
1:A:422:LEU:O	1:A:425:ARG:HB2	2.17	0.45
1:A:1168:PHE:CE2	1:A:1213:SER:HB2	2.52	0.45
1:A:303:GLN:HB2	1:A:307:ARG:HH22	1.82	0.44
1:A:431:GLU:O	1:A:434:LYS:NZ	2.37	0.44
1:A:499:ILE:HG12	1:A:507:PHE:HA	1.97	0.44
1:A:98:VAL:HG13	1:A:99:ASN:N	2.32	0.44
1:A:342:ILE:H	1:A:342:ILE:HD12	1.83	0.44
1:A:358:VAL:HA	1:A:1031:TRP:CH2	2.52	0.44
1:A:495:VAL:HA	1:A:511:SER:HB3	1.99	0.44
1:A:784:THR:O	1:A:788:LEU:HG	2.17	0.44
1:A:1089:LEU:HA	1:A:1092:ASP:OD2	2.16	0.44
1:A:1231:ASN:HA	1:A:1237:GLN:HA	1.99	0.44
1:A:797:VAL:O	1:A:800:ILE:HG12	2.18	0.44
1:A:983:VAL:O	1:A:986:VAL:HG12	2.17	0.44
1:A:399:ASP:HA	1:A:443:ASP:O	2.18	0.44
1:A:400:ILE:HD12	1:A:443:ASP:HA	1.99	0.44
1:A:418:LEU:HB2	1:A:476:PHE:HZ	1.83	0.44
1:A:1105:ILE:HD11	1:A:1138:ILE:HG13	1.99	0.44
1:A:1207:ILE:O	1:A:1209:VAL:HG23	2.18	0.44
1:A:1212:GLU:HA	1:A:1215:ARG:HD2	1.99	0.44
1:A:103:ALA:O	1:A:106:GLU:HB2	2.18	0.44
1:A:184:PHE:O	1:A:187:THR:OG1	2.31	0.44
1:A:280:GLU:HG2	1:A:897:PHE:CE1	2.53	0.44
1:A:439:SER:OG	1:A:440:THR:N	2.50	0.44
1:A:1013:VAL:O	1:A:1017:LEU:HG	2.18	0.44
1:A:832:ILE:HD12	1:A:835:LEU:HD13	1.99	0.44
1:A:157:VAL:HA	1:A:160:PHE:HB3	1.99	0.44
1:A:297:HIS:O	1:A:301:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:THR:OG1	1:A:445:TYR:HD1	2.00	0.44
1:A:442:GLY:HA2	1:A:1188:TRP:CD1	2.53	0.44
1:A:1160:PHE:HE2	1:A:1162:PHE:CD1	2.36	0.44
1:A:286:LEU:HA	1:A:289:LEU:HG	1.99	0.43
1:A:339:PRO:HD3	1:A:506:LYS:NZ	2.33	0.43
1:A:877:ALA:O	1:A:880:VAL:HG12	2.18	0.43
1:A:1140:PHE:O	1:A:1144:LYS:HG3	2.18	0.43
1:A:332:ARG:HH21	1:A:333:MET:HE1	1.83	0.43
1:A:437:LYS:HA	1:A:447:CYS:SG	2.58	0.43
1:A:840:ARG:NH1	1:A:847:ASP:HB2	2.33	0.43
1:A:147:ALA:HB3	1:A:148:PRO:HD3	1.99	0.43
1:A:358:VAL:HG13	1:A:1031:TRP:CZ3	2.52	0.43
1:A:236:THR:HG23	1:A:237:VAL:H	1.83	0.43
1:A:499:ILE:O	1:A:500:LEU:HD23	2.18	0.43
1:A:530:HIS:HA	1:A:570:LEU:HD23	2.00	0.43
1:A:549:LYS:HA	1:A:568:THR:OG1	2.19	0.43
1:A:1173:LEU:HA	1:A:1188:TRP:O	2.19	0.43
1:A:218:LEU:HD23	1:A:219:SER:O	2.18	0.43
1:A:233:LEU:HD21	1:A:993:LEU:HD11	2.00	0.43
1:A:399:ASP:N	1:A:521:GLU:OE2	2.48	0.43
1:A:418:LEU:HA	1:A:421:ASP:OD1	2.18	0.43
1:A:1214:TYR:CE1	1:A:1224:PHE:HB2	2.54	0.43
1:A:226:MET:O	1:A:227:CYS:C	2.56	0.43
1:A:496:LEU:HD11	1:A:1083:TYR:CE2	2.54	0.43
1:A:980:GLY:O	1:A:984:ILE:HG23	2.18	0.43
1:A:1197:ARG:NE	1:A:1232:VAL:HA	2.33	0.43
1:A:232:PHE:O	1:A:235:TYR:HB2	2.19	0.43
1:A:443:ASP:N	1:A:443:ASP:OD1	2.48	0.43
1:A:503:ARG:NH1	1:A:1094:ASP:O	2.51	0.43
1:A:1017:LEU:O	1:A:1020:THR:OG1	2.27	0.43
1:A:176:SER:O	1:A:180:THR:HG22	2.18	0.43
1:A:191:GLN:NE2	1:A:260:GLY:HA2	2.34	0.43
1:A:1228:GLY:O	1:A:1240:THR:N	2.39	0.43
1:A:401:VAL:HG23	1:A:487:ARG:N	2.33	0.43
1:A:441:LEU:N	1:A:444:CYS:O	2.50	0.43
1:A:246:LEU:O	1:A:250:VAL:HG13	2.18	0.42
1:A:512:ASN:HA	1:A:515:ASN:ND2	2.34	0.42
1:A:1169:ASN:ND2	1:A:1212:GLU:OE2	2.52	0.42
1:A:1050:THR:OG1	1:A:1051:TYR:N	2.52	0.42
1:A:1209:VAL:HG21	1:A:1224:PHE:CE1	2.54	0.42
1:A:195:LEU:HD23	1:A:195:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:THR:HG1	1:A:445:TYR:HD1	1.66	0.42
1:A:784:THR:OG1	1:A:841:MET:HE3	2.20	0.42
1:A:805:CYS:HB2	1:A:883:HIS:CD2	2.53	0.42
1:A:528:LYS:HB3	1:A:570:LEU:HB3	2.00	0.42
1:A:1102:TYR:HD1	1:A:1105:ILE:HG13	1.84	0.42
1:A:145:MET:O	1:A:148:PRO:HD2	2.20	0.42
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.71	0.42
1:A:389:GLN:OE1	1:A:494:THR:OG1	2.37	0.42
1:A:475:GLN:O	1:A:479:GLU:CB	2.68	0.42
1:A:534:ALA:O	1:A:537:LYS:HG2	2.19	0.42
1:A:840:ARG:NH1	1:A:845:LEU:HB3	2.34	0.42
1:A:1030:ASP:O	1:A:1034:ARG:HG2	2.19	0.42
1:A:1207:ILE:O	1:A:1242:LEU:HA	2.19	0.42
1:A:491:HIS:HB3	1:A:517:ALA:HB2	2.02	0.42
1:A:1055:HIS:HB2	1:A:1173:LEU:HD12	2.02	0.42
1:A:154:VAL:HA	1:A:157:VAL:HG12	2.01	0.42
1:A:280:GLU:OE2	1:A:284:ARG:HD3	2.19	0.42
1:A:873:VAL:CG2	1:A:908:GLN:HE22	2.33	0.42
1:A:232:PHE:HD1	1:A:235:TYR:HD1	1.68	0.42
1:A:338:MET:HB3	1:A:343:ALA:HB2	2.01	0.42
1:A:168:TYR:HA	1:A:171:HIS:HB2	2.02	0.41
1:A:474:GLU:HA	1:A:477:CYS:SG	2.60	0.41
1:A:921:SER:HB2	1:A:995:TRP:CZ3	2.54	0.41
1:A:1166:VAL:HG23	1:A:1207:ILE:HG23	2.02	0.41
1:A:151:CYS:O	1:A:154:VAL:HG22	2.19	0.41
1:A:250:VAL:O	1:A:253:SER:OG	2.27	0.41
1:A:1157:MET:HB3	1:A:1160:PHE:O	2.20	0.41
1:A:151:CYS:O	1:A:155:VAL:HG22	2.20	0.41
1:A:152:PHE:CE1	1:A:182:LEU:HG	2.54	0.41
1:A:398:ALA:O	1:A:444:CYS:HA	2.20	0.41
1:A:491:HIS:CE1	1:A:534:ALA:HB3	2.56	0.41
1:A:545:MET:HA	1:A:571:ILE:HD13	2.02	0.41
1:A:1093:PHE:O	1:A:1096:LEU:HB2	2.20	0.41
1:A:1107:LYS:HG3	1:A:1107:LYS:O	2.20	0.41
1:A:111:GLN:HA	1:A:114:ARG:CZ	2.50	0.41
1:A:449:ALA:HB3	1:A:458:HIS:HB2	2.02	0.41
1:A:992:LEU:HD12	1:A:996:PHE:HE2	1.85	0.41
1:A:1109:LYS:HE3	1:A:1109:LYS:HB2	1.96	0.41
1:A:1165:ARG:HD2	1:A:1202:GLY:C	2.41	0.41
1:A:159:PHE:CZ	1:A:179:LEU:HB2	2.56	0.41
1:A:232:PHE:HA	1:A:235:TYR:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:LEU:HB3	1:A:1001:PHE:CZ	2.55	0.41
1:A:195:LEU:HD13	1:A:262:HIS:HA	2.03	0.41
1:A:900:SER:O	1:A:903:LEU:HG	2.20	0.41
1:A:1001:PHE:CD1	1:A:1001:PHE:N	2.85	0.41
1:A:1100:PRO:O	1:A:1103:SER:OG	2.24	0.41
1:A:1102:TYR:CD1	1:A:1105:ILE:HG13	2.56	0.41
1:A:224:PHE:CZ	1:A:228:ILE:HD11	2.55	0.41
1:A:1066:VAL:HG23	1:A:1164:LEU:HA	2.03	0.41
1:A:239:HIS:O	1:A:239:HIS:ND1	2.54	0.41
1:A:399:ASP:O	1:A:486:MET:HB2	2.21	0.41
1:A:497:CYS:HB2	1:A:507:PHE:CZ	2.55	0.41
1:A:544:GLU:N	1:A:573:GLY:O	2.37	0.41
1:A:888:PHE:CG	1:A:889:GLU:N	2.89	0.41
1:A:1067:ASN:CG	1:A:1163:LYS:H	2.21	0.41
1:A:1160:PHE:HE2	1:A:1162:PHE:CG	2.39	0.41
1:A:491:HIS:NE2	1:A:516:LEU:HD13	2.36	0.41
1:A:787:SER:O	1:A:791:VAL:HG23	2.21	0.41
1:A:1066:VAL:N	1:A:1163:LYS:O	2.54	0.41
1:A:1148:ARG:CZ	1:A:1148:ARG:HB2	2.51	0.41
1:A:336:SER:HA	1:A:1182:LYS:NZ	2.36	0.40
1:A:403:PHE:CE1	1:A:443:ASP:HB3	2.56	0.40
1:A:428:ARG:O	1:A:431:GLU:HG2	2.21	0.40
1:A:892:ILE:HA	1:A:895:THR:HB	2.03	0.40
1:A:917:SER:OG	1:A:918:TRP:N	2.54	0.40
1:A:935:LEU:HG	1:A:935:LEU:H	1.73	0.40
1:A:1067:ASN:HD21	1:A:1162:PHE:HA	1.85	0.40
1:A:1154:ASN:ND2	1:A:1162:PHE:H	2.19	0.40
1:A:133:TYR:HE2	1:A:134:PHE:CE1	2.40	0.40
1:A:152:PHE:CZ	1:A:183:VAL:HA	2.57	0.40
1:A:294:ILE:CD1	1:A:908:GLN:HA	2.51	0.40
1:A:122:TYR:CD2	1:A:233:LEU:HD11	2.56	0.40
1:A:232:PHE:HD1	1:A:232:PHE:HA	1.70	0.40
1:A:400:ILE:HB	1:A:403:PHE:HB2	2.03	0.40
1:A:232:PHE:HD1	1:A:235:TYR:CD1	2.39	0.40
1:A:286:LEU:O	1:A:286:LEU:HD23	2.21	0.40
1:A:511:SER:HG	1:A:513:ASP:HB2	1.87	0.40
1:A:1034:ARG:HH12	1:A:1038:PRO:C	2.25	0.40
1:A:470:ILE:HD13	1:A:470:ILE:HA	1.92	0.40
1:A:488:VAL:HG12	1:A:529:VAL:HG23	2.03	0.40
1:A:1137:GLN:O	1:A:1141:GLU:HG2	2.21	0.40
1:A:1217:LEU:HD12	1:A:1222:TYR:CE2	2.56	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	828/1354 (61%)	731 (88%)	97 (12%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	729/1176 (62%)	727 (100%)	2 (0%)	92 95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	LYS
1	A	1219	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	HIS
1	A	356	ASN
1	A	512	ASN

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Mol	Chain	Res	Type
1	A	515	ASN
1	A	1044	GLN
1	A	1122	ASN
1	A	1135	HIS
1	A	1154	ASN
1	A	1155	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

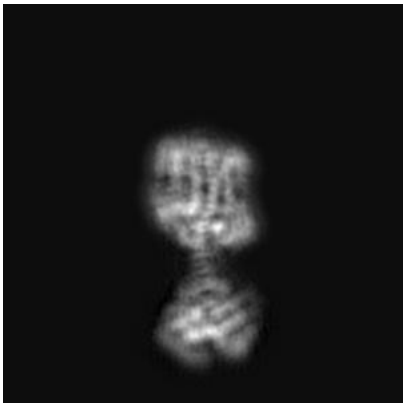
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13330. These allow visual inspection of the internal detail of the map and identification of artifacts.

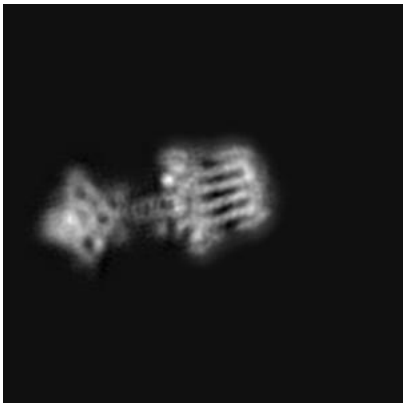
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

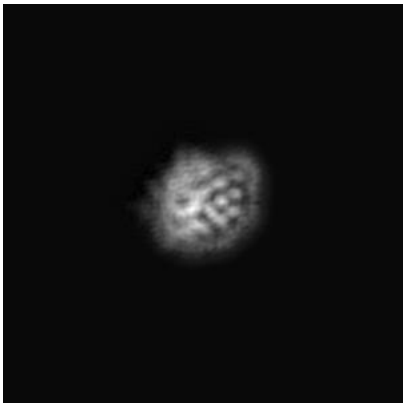
6.1.1 Primary map



X



Y

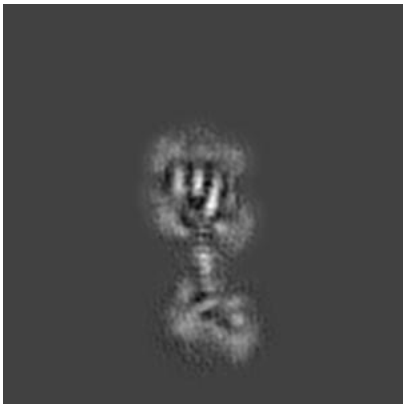


Z

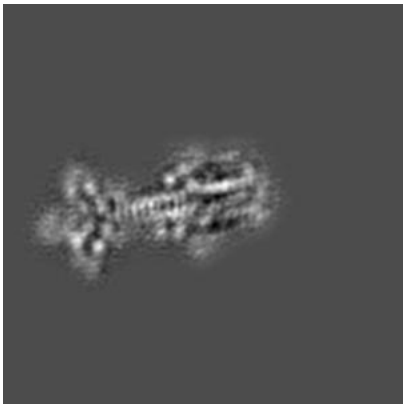
The images above show the map projected in three orthogonal directions.

6.2 Central slices

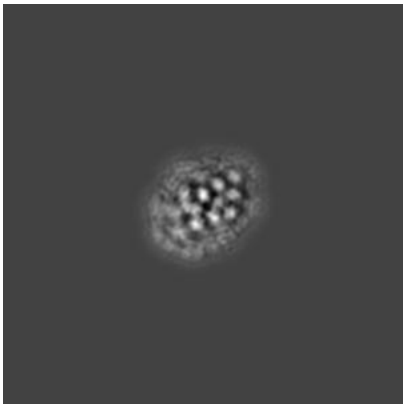
6.2.1 Primary map



X Index: 150



Y Index: 150

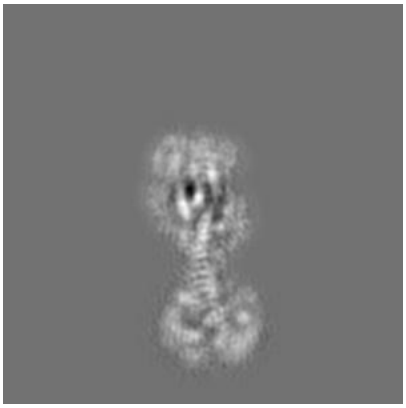


Z Index: 150

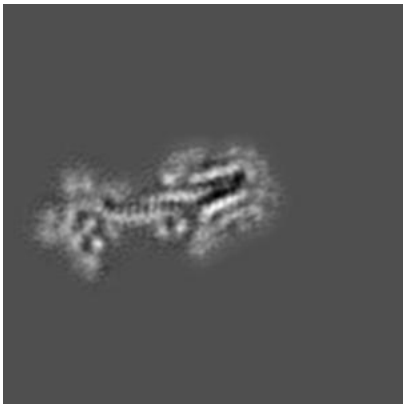
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

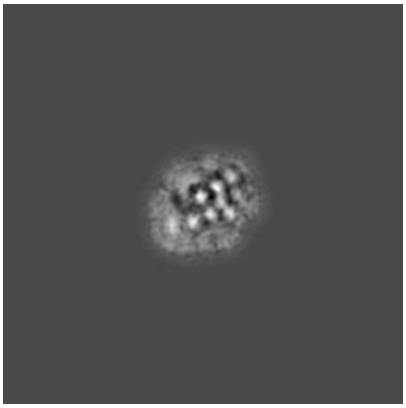
6.3.1 Primary map



X Index: 143



Y Index: 145



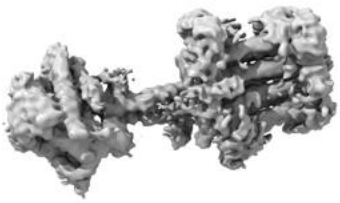
Z Index: 144

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

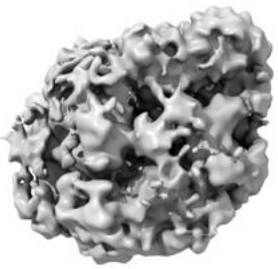
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

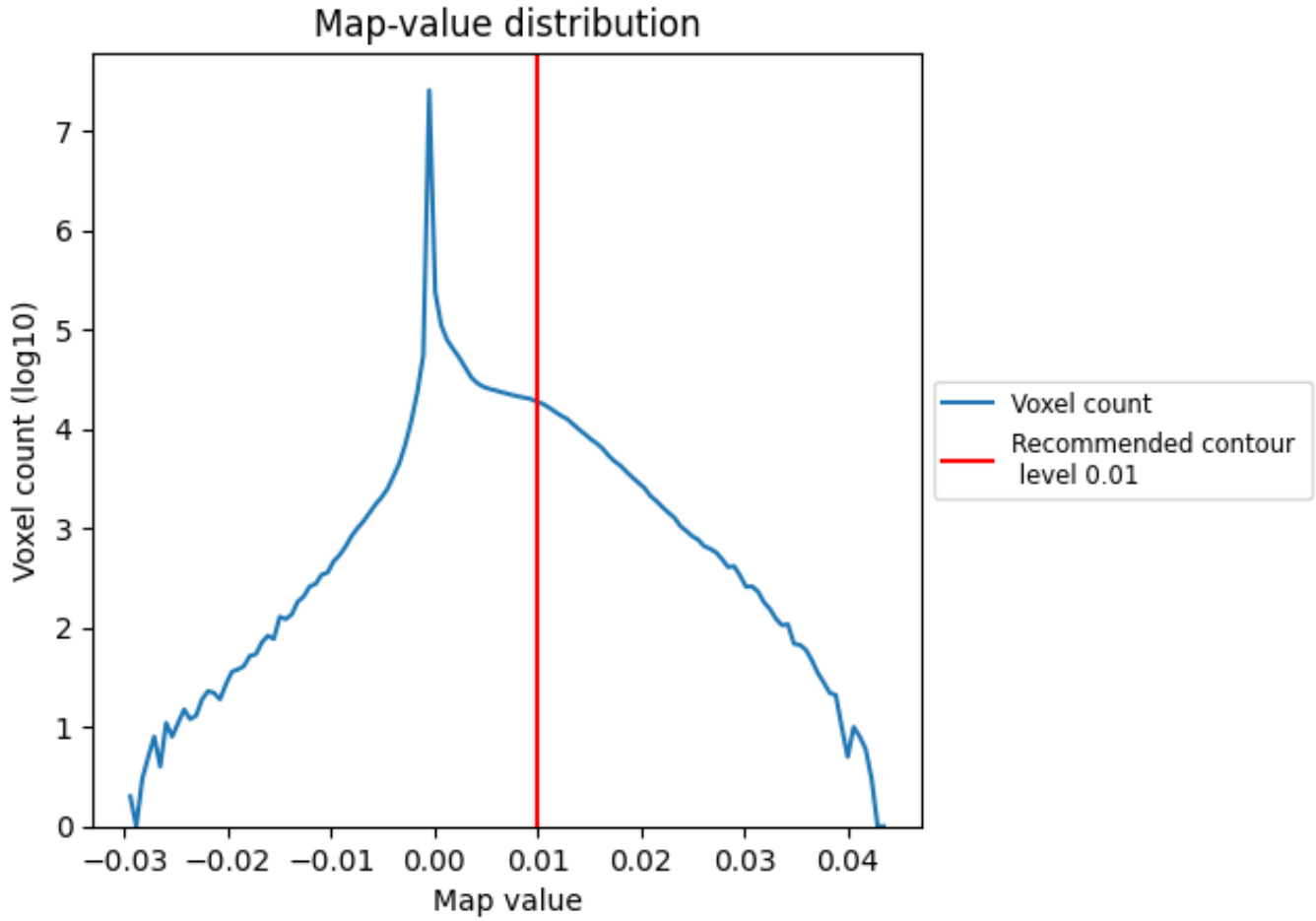
6.5 Mask visualisation (i)

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

7 Map analysis

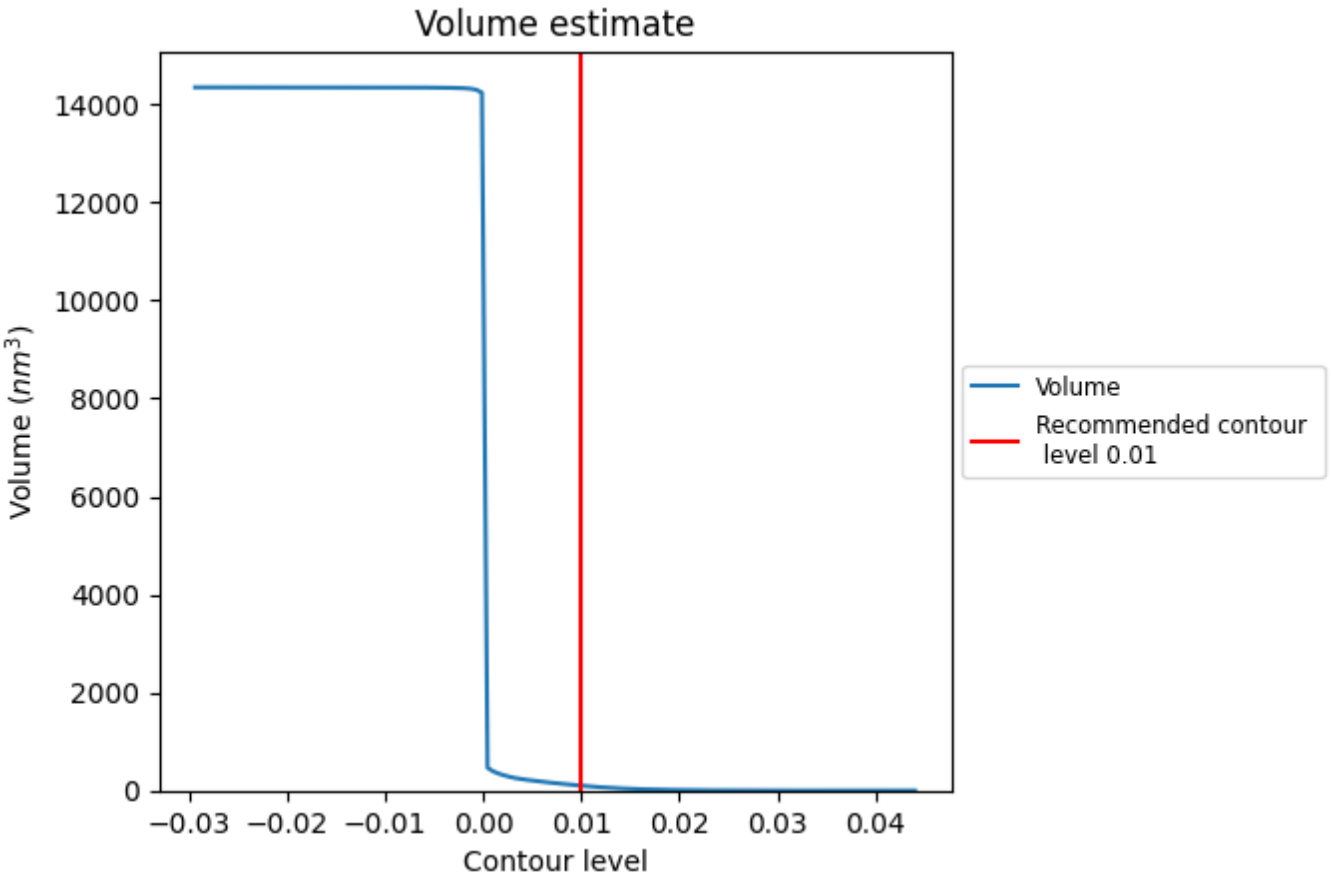
This section contains the results of statistical analysis of the map.

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.

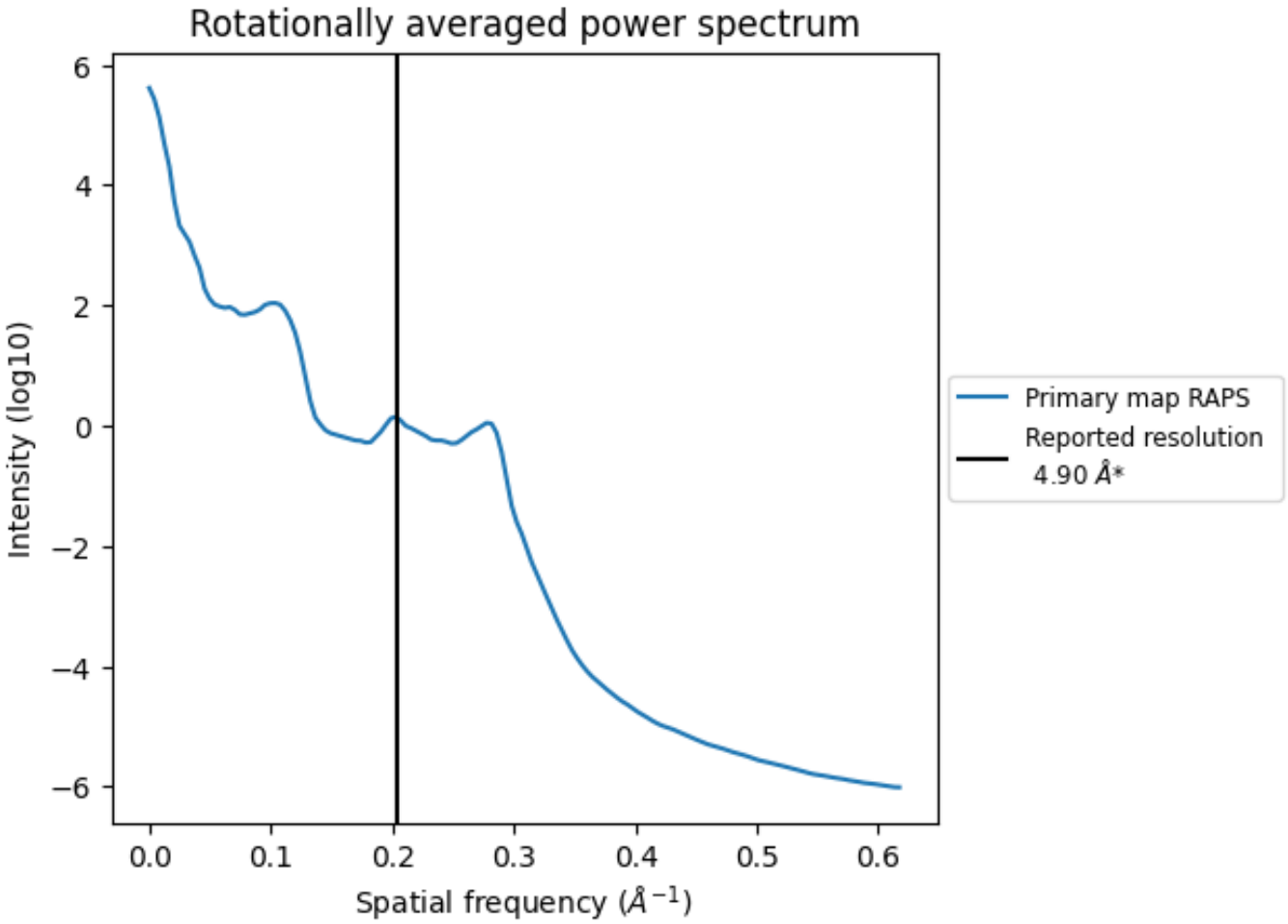
7.2 Volume estimate



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 90 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)

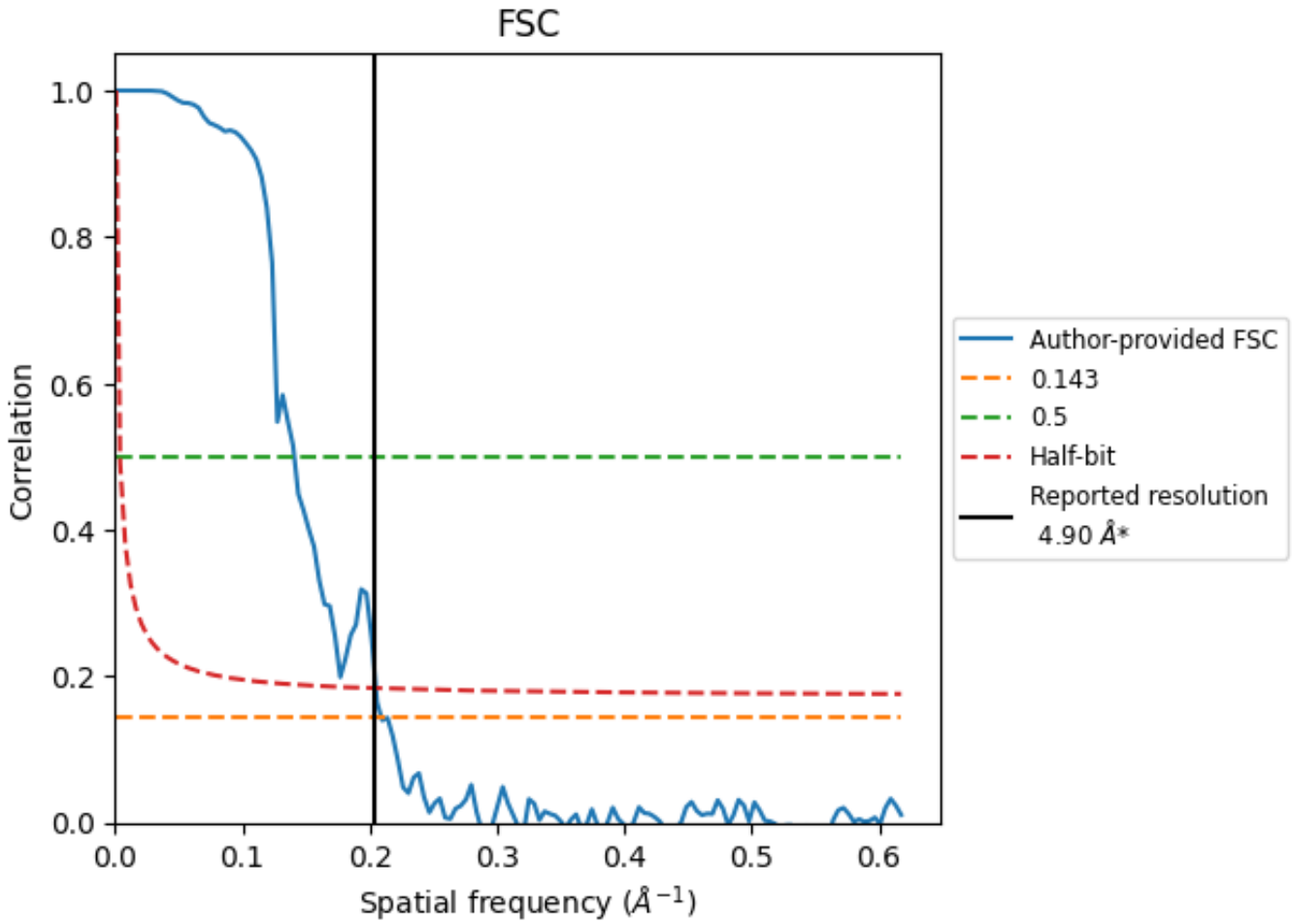


*Reported resolution corresponds to spatial frequency of 0.204 Å^{-1}

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 0.204 Å^{-1}

8.2 Resolution estimates (i)

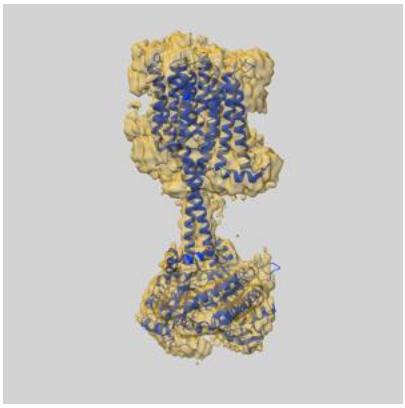
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.78	7.10	4.88
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

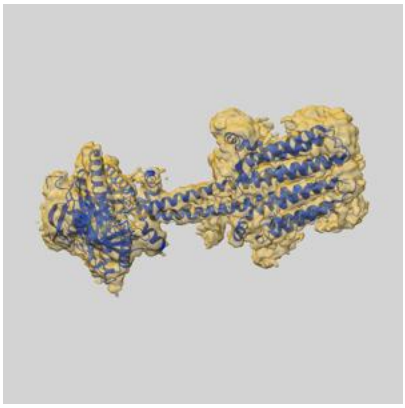
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13330 and PDB model 7PD4. Per-residue inclusion information can be found in section 3 on page 4.

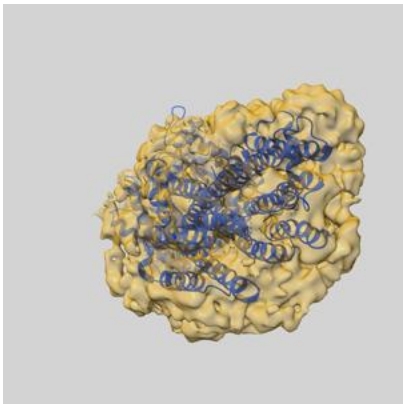
9.1 Map-model overlay



X



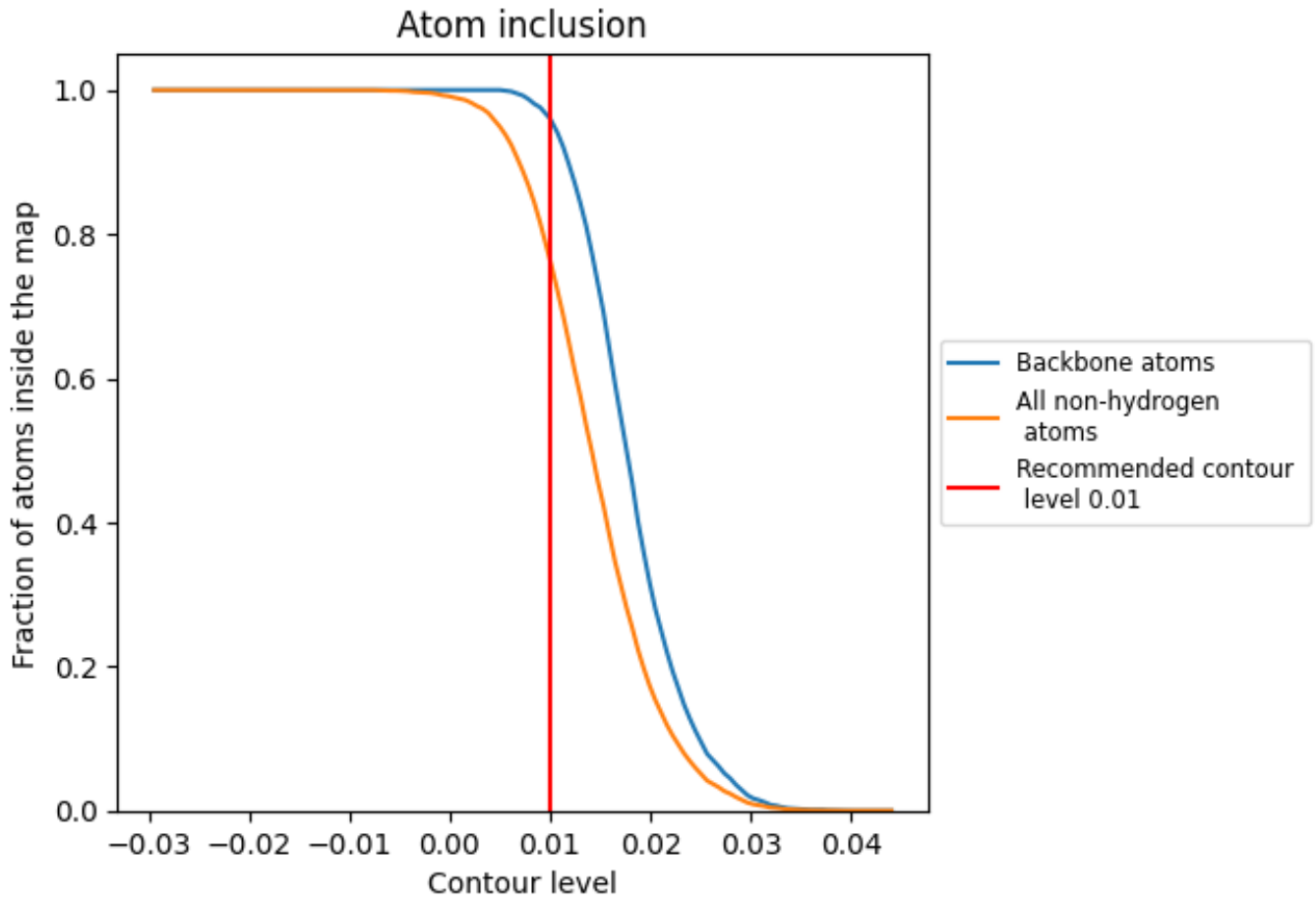
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.