Full wwPDB EM Validation Report

Jun 2, 2025 – 04:39 PM JST

PDB ID	:	8YQZ / pdb_00008yqz
EMDB ID	:	EMD-39511
Title	:	African swine fever virus RNA Polymerase–DNA complex
Authors	:	Feng, X.Y.
Deposited on	:	2024-03-20
Resolution	:	2.78 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

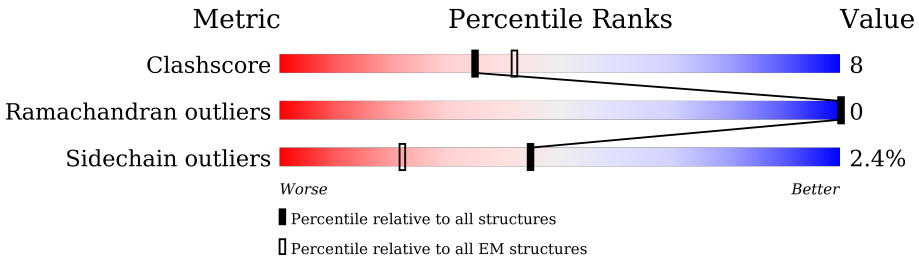
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.78 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	82% 75% 19% • 5%
2	B	1242	88% 75% 21% •
3	C	359	82% 86% 13% ••
4	D	205	81% 83% 17%
5	E	147	56% 60% 12% 28%
6	F	339	96% 73% 27% •
7	G	105	41% 44% 12% 44%
8	H	80	86% 76% 22% •

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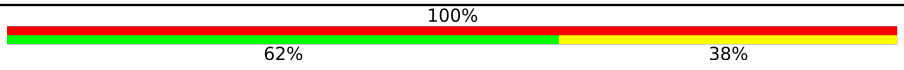
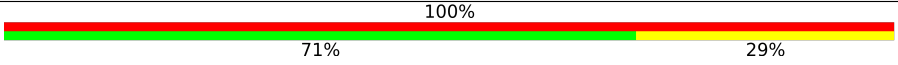
Mol	Chain	Length	Quality of chain
9	X	8	
10	Y	7	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29943 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	1375	10954	6958	1906	2030	60	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	1196	9459	5983	1653	1773	50	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	357	2897	1880	480	525	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	1668	1088	278	294	8	0	0

- Molecule 5 is a protein called C147L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	106	829	528	143	153	5	0	0

- Molecule 6 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	339	2727	1753	451	509	14	0	0

- Molecule 7 is a protein called C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	59	Total	C	N	O	S	0	0
			468	295	80	85	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	80	Total	C	N	O	S	0	0
			630	411	102	110	7		

- Molecule 9 is a DNA chain called DNA (5'-D(P*GP*CP*CP*GP*AP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	8	Total	C	N	O	P	0	0
			165	77	34	46	8		

- Molecule 10 is a DNA chain called DNA (5'-D(P*TP*CP*GP*GP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	7	Total	C	N	O	P	0	0
			141	67	23	44	7		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

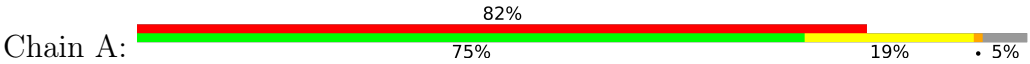
Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Zn	0
			1	1	
12	B	1	Total	Zn	0
			1	1	
12	G	1	Total	Zn	0
			1	1	
12	H	1	Total	Zn	0
			1	1	

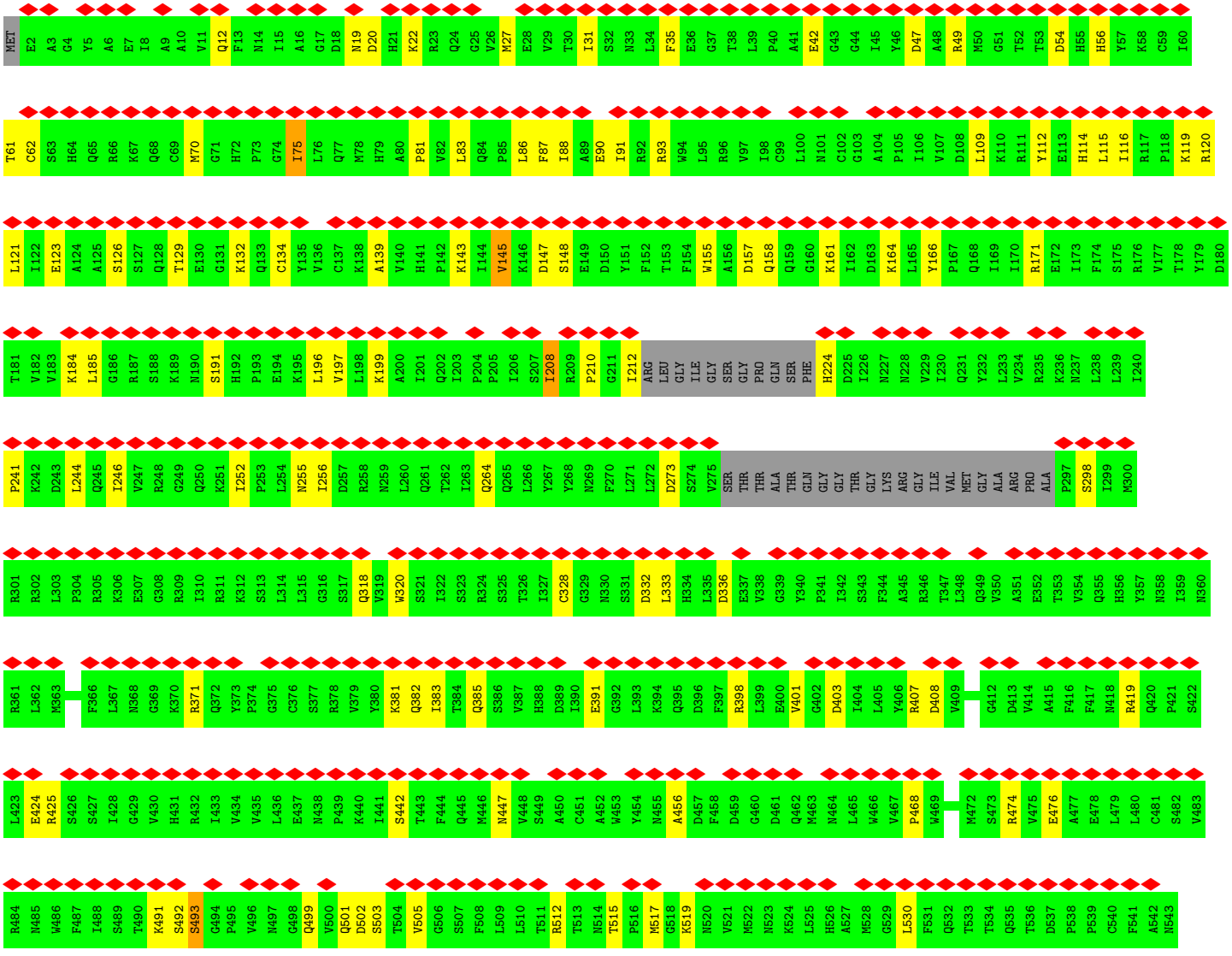
3 Residue-property plots (i)

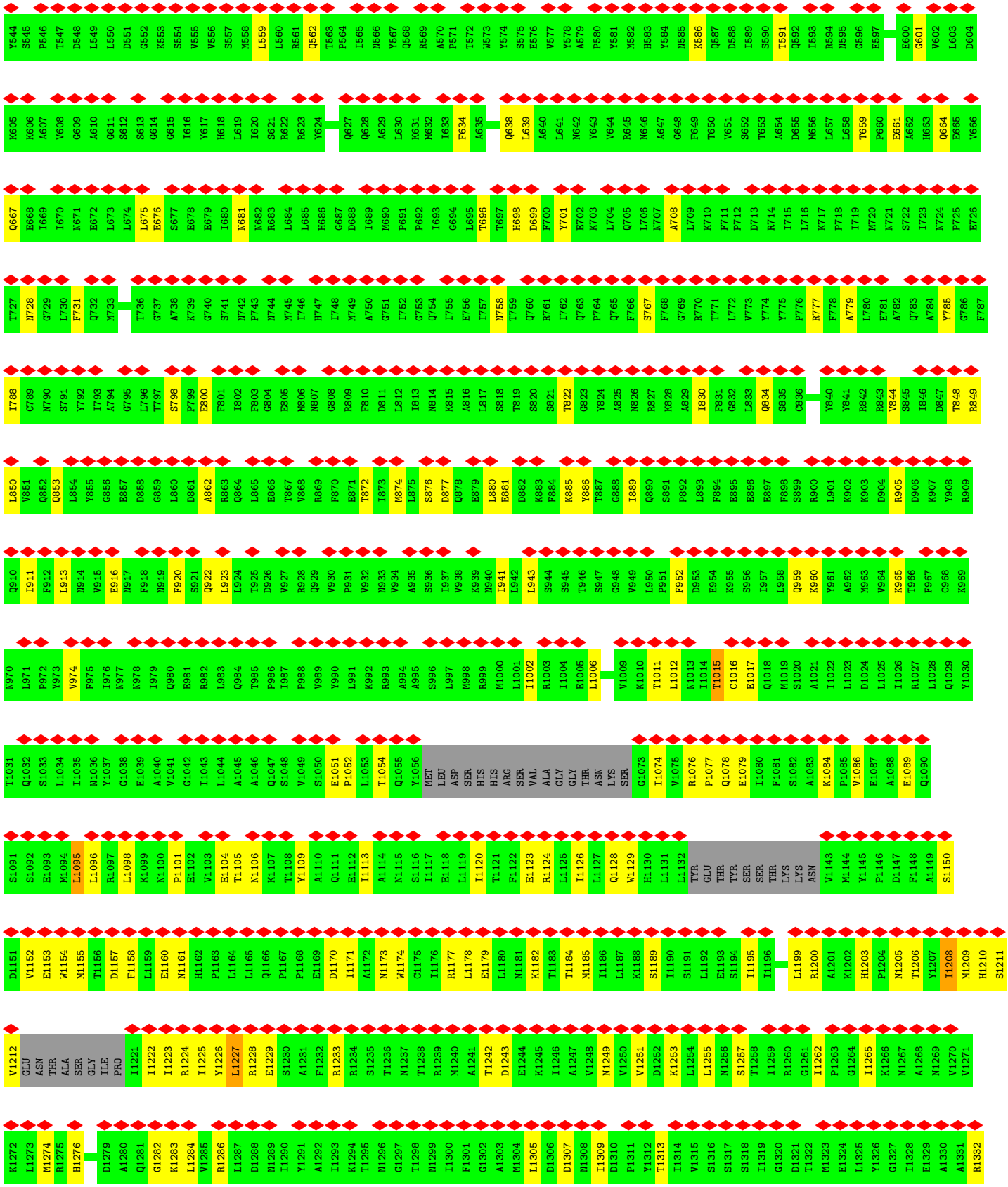
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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:



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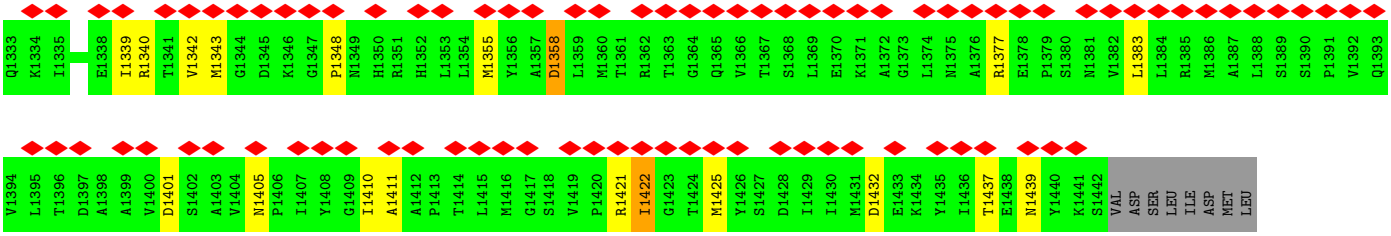
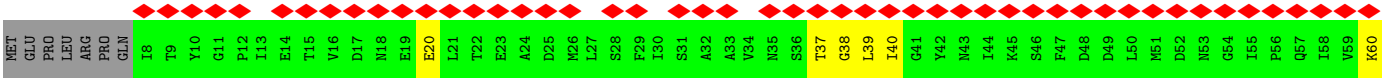
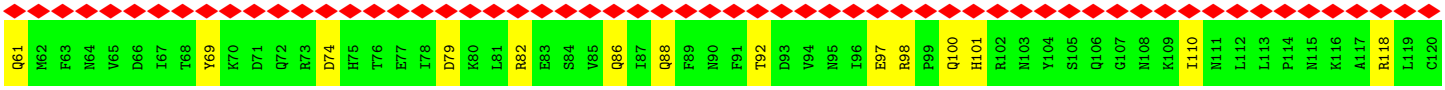
K605 K606 A607 V608 G609 A610 G611 S612 S613 G614 G615 I616 Y617 H618 L619 I620 S621 R622 R623 Y624 Q627 Q628 A629 L630 K631 M632 I633 F634 A635 Q638 L639 A640 L641 N642 Y643 V644 R645 N646 A647 G648 F649 T650 V651 S652 T653 A654 D655 M656 L657 L658 T659 P660 E661 A662 H663 Q664 E665 V666
Q667 E668 I669 I670 N671 E672 L673 L674 L675 E676 S677 E678 E679 I680 N681 N682 R683 L684 L685 H686 G687 D688 I689 M690 P691 P692 I693 G694 L695 T696 T697 H698 D699 F700 Y701 E702 K703 L704 Q705 L706 N707 A708 L709 K710 F711 P712 D713 R714 I715 L716 K717 P718 I719 M720 N721 S722 I723 N724 P725 E726
T727 N728 G729 L730 F731 Q732 M733 T736 G737 A738 K739 G740 S741 N742 P743 N744 M745 I746 H747 I748 M749 A750 G751 I752 G753 Q754 I755 E756 I757 N758 T759 Q760 R761 I762 Q763 P764 Q765 F766 S767 F768 G769 R770 T771 L772 V773 Y774 Y775 P776 R777 F778 A779 L780 E781 A782 Q783 A784 Y785 G786 F787
I788 C789 N790 S791 Y792 I793 A794 G795 L796 T797 S798 P799 E800 F801 I802 F803 G804 E805 M806 N807 G808 R809 F810 D811 L812 I813 N814 K815 A816 L817 S818 T819 S820 S821 T822 G823 Y824 A825 N826 R827 K828 A829 I830 F831 G832 L833 Q834 S835 C836 Y840 Y841 R842 R843 V844 S845 I846 D847 T848 R849
L850 V851 Q852 Q853 L854 Y855 G856 E857 D858 G859 L860 D861 A862 R863 Q864 L865 E866 T867 V868 R869 F870 E871 T872 I873 M874 L875 S876 D877 Q878 E879 L880 E881 D882 K883 F884 K885 Y886 T887 G888 I889 Q890 S891 P892 L893 F894 E895 E896 E897 F898 S899 R900 L901 K902 K903 D904 R905 D906 K907 Y908 R909
Q910 I911 F912 L913 N914 V915 E916 N917 F918 N919 F920 S921 Q922 L923 L924 T925 D926 V927 R928 Q929 V930 P931 V932 N933 V934 A935 S936 I937 V938 K939 N940 I941 L942 L943 S944 S945 T946 S947 G948 V949 L950 P951 F952 D953 E954 K955 S956 I957 L958 Q959 K960 Y961 A962 M963 V964 K965 T966 F967 C968 K969
N970 L971 P972 Y973 V974 F975 I976 N977 N978 I979 Q980 E981 R982 L983 Q984 T985 P986 I987 P988 V989 Y990 L991 K992 R993 A994 A995 S996 L997 M998 R999 M1000 L1001 I1002 R1003 I1004 E1005 L1006 V1009 K1010 T1011 L1012 N1013 I1014 T1015 C1016 E1017 Q1018 M1019 S1020 A1021 I1022 L1023 D1024 L1025 I1026 R1027 L1028 Q1029 Y1030
T1031 Q1032 S1033 L1034 I1035 N1036 Y1037 G1038 E1039 A1040 V1041 G1042 I1043 L1044 A1045 A1046 Q1047 S1048 V1049 S1050 E1051 P1052 L1053 T1054 Q1055 Y1056 MET LEU ASP SER HIS HIS ARG SER VAL ALA GLY GLY THR ASN LYS SER G1073 I1074 V1075 R1076 P1077 Q1078 E1079 I1080 F1081 S1082 A1083 K1084 P1085 V1086 E1087 A1088 E1089 Q1090
S1091 S1092 E1093 M1094 L1095 L1096 R1097 L1098 K1099 N1100 P1101 E1102 V1103 E1104 T1105 N1106 K1107 T1108 Y1109 A1110 Q1111 E1112 I1113 A1114 N1115 S1116 I1117 E1118 L1119 I1120 T1121 F1122 E1123 R1124 L1125 I1126 L1127 Q1128 W1129 H1130 L1131 L1132 TYR GLU THR TYR SER SER THR LYS LYS ASN V1143 M1144 Y1145 P1146 D1147 F1148 A1149 S1150
D1151 V1152 E1153 W1154 M1155 T1156 D1157 F1158 L1159 E1160 N1161 H1162 P1163 L1164 L1165 Q1166 P1167 P1168 E1169 D1170 I1171 A1172 N1173 W1174 C1175 I1176 R1177 L1178 E1179 L1180 N1181 K1182 T1183 T1184 M1185 I1186 L1187 K1188 S1189 I1190 S1191 L1192 E1193 S1194 I1195 I1196 L1199 R1200 A1201 K1202 H1203 P1204 N1205 T1206 Y1207 I1208 M1209 H1210 S1211
V1212 GLU ASN THR ALA SER GLY ILE PRO I1221 I1222 I1223 R1224 I1225 Y1226 L1227 R1228 E1229 S1230 A1231 F1232 R1233 R1234 S1235 T1236 N1237 T1238 R1239 M1240 A1241 T1242 D1243 E1244 K1245 I1246 A1247 V1248 N1249 V1250 V1251 D1252 K1253 L1254 L1255 N1256 S1257 T1258 I1259 R1260 G1261 I1262 P1263 G1264 I1265 K1266 N1267 A1268 N1269 V1270 V1271
K1272 L1273 M1274 R1275 H1276 D1279 A1280 Q1281 G1282 K1283 L1284 V1285 R1286 L1287 D1288 N1289 I1290 Y1291 A1292 I1293 K1294 T1295 N1296 G1297 T1298 N1299 I1300 F1301 G1302 A1303 M1304 L1305 D1306 D1307 N1308 I1309 D1310 P1311 Y1312 T1313 I1314 V1315 S1316 S1317 S1318 I1319 G1320 D1321 T1322 M1323 E1324 L1325 Y1326 G1327 I1328 E1329 A1330 A1331 R1332

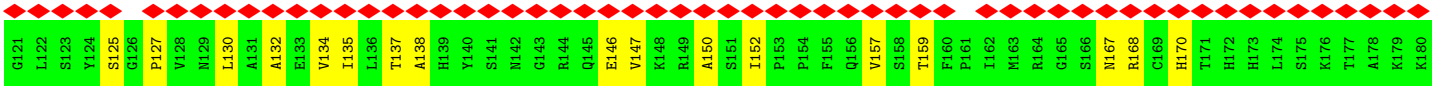


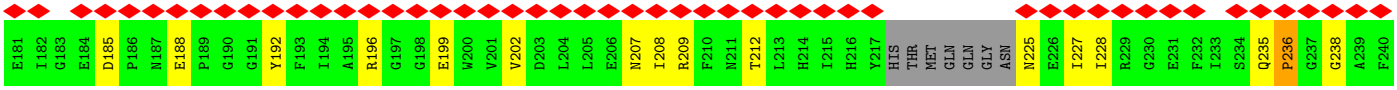
• Molecule 2: DNA-directed RNA polymerase subunit beta

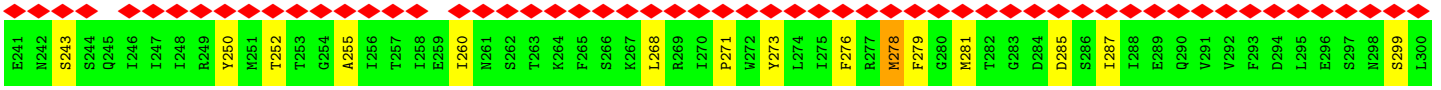
Chain B:

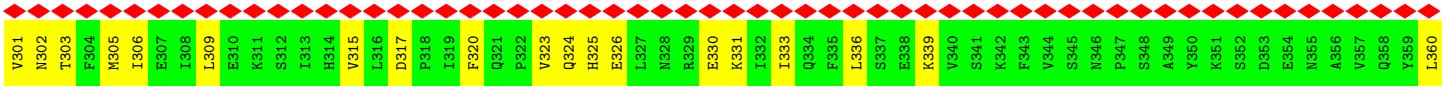


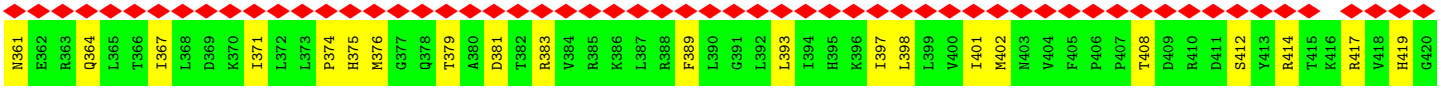


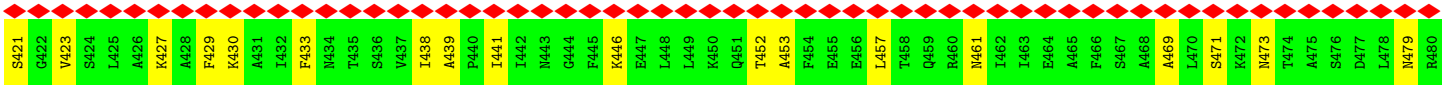


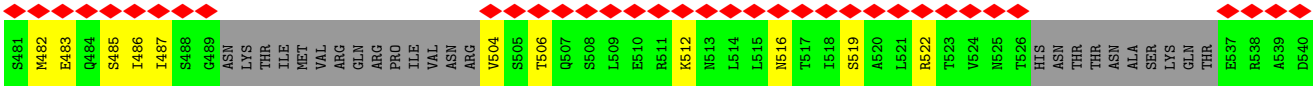


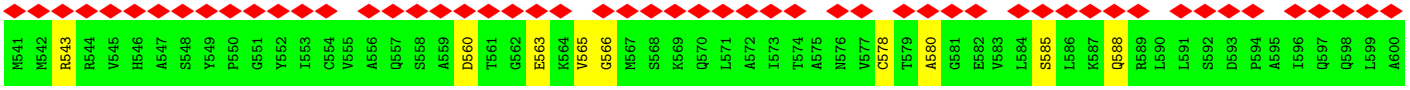


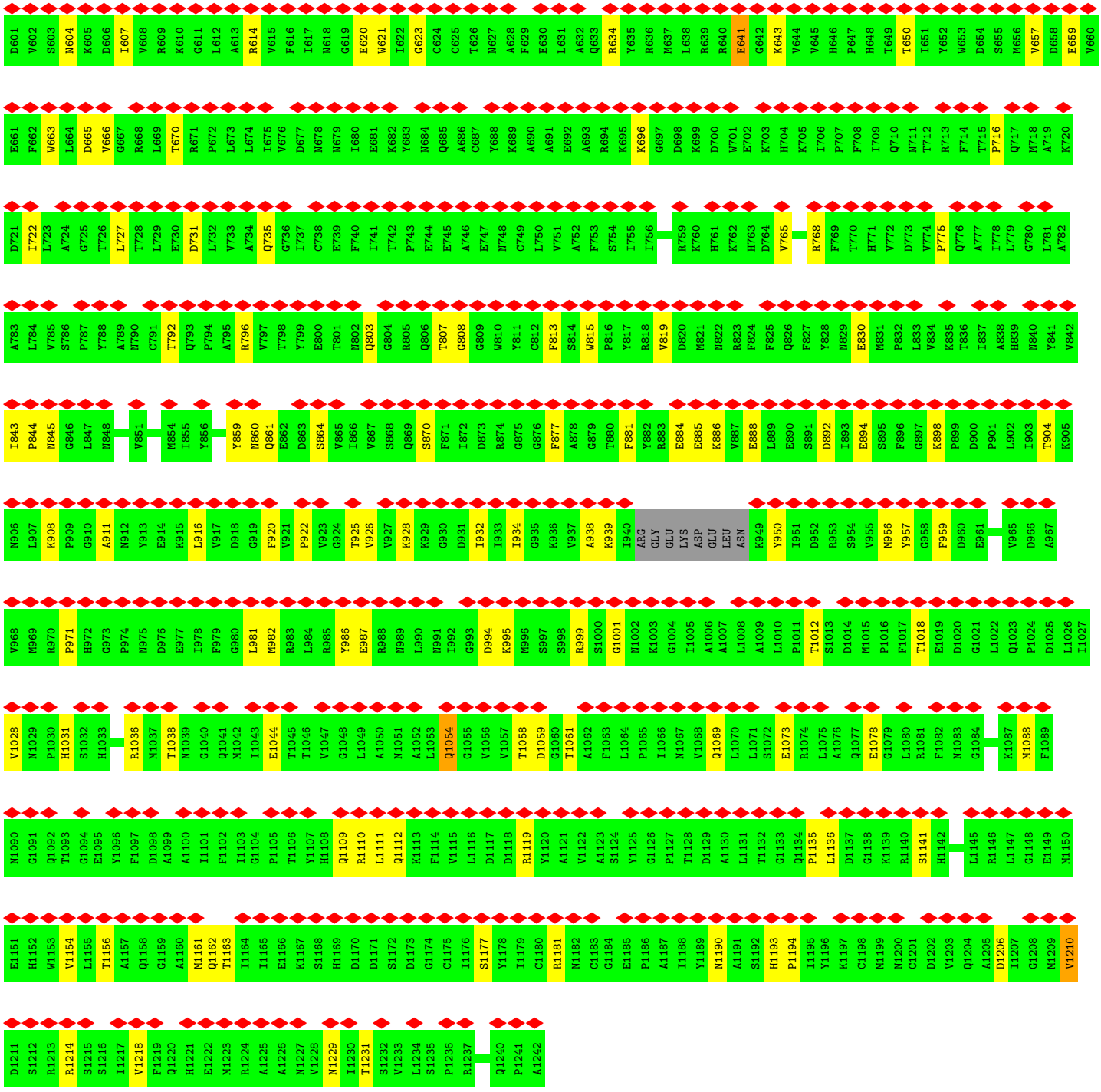






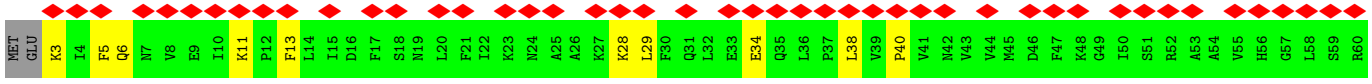


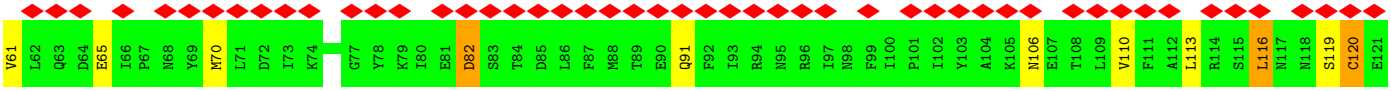


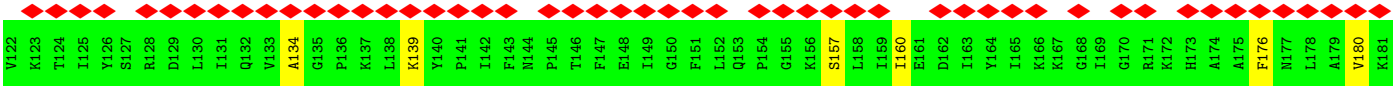


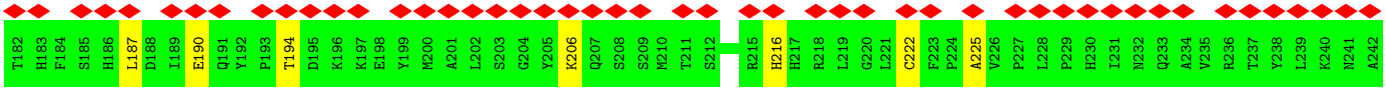
• Molecule 3: DNA-directed RNA polymerase RPB3-11 homolog

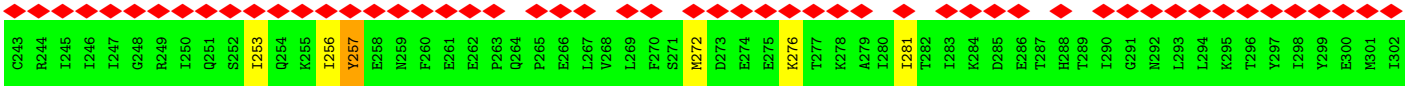
Chain C:

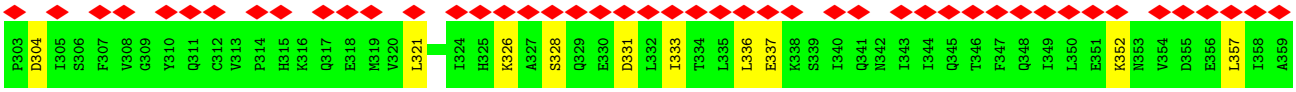






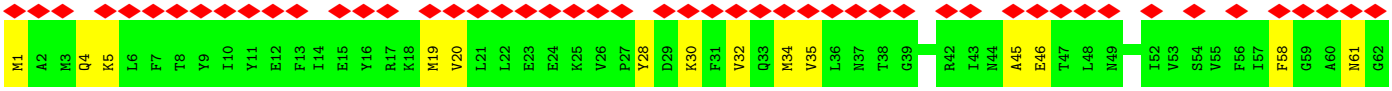


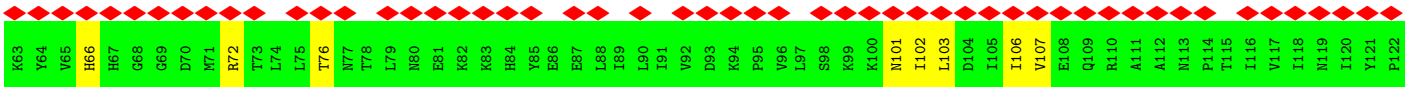


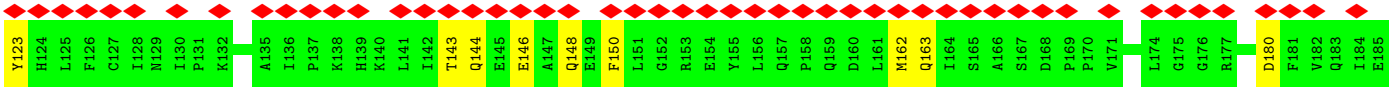


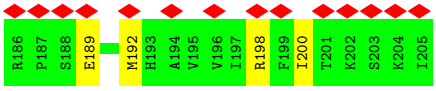
• Molecule 4: DNA-directed RNA polymerase RPB5 homolog

Chain D:



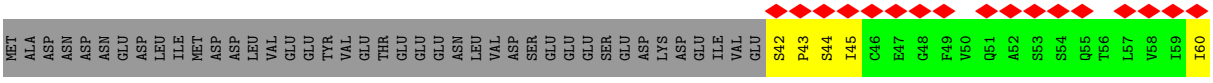


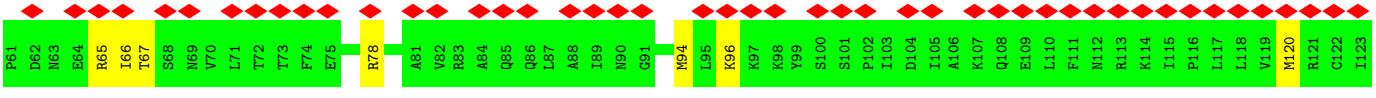


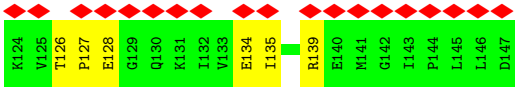


• Molecule 5: C147L

Chain E:

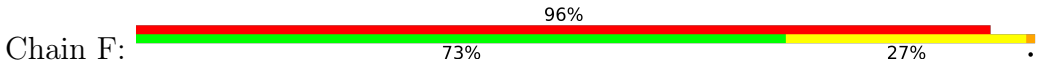


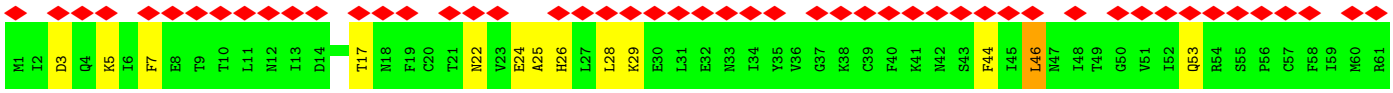


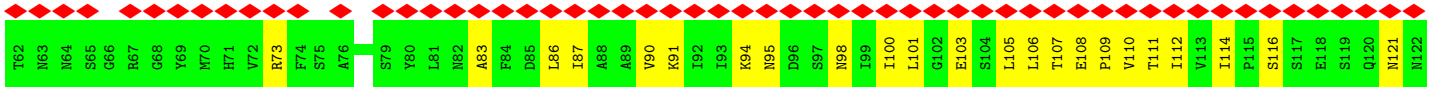


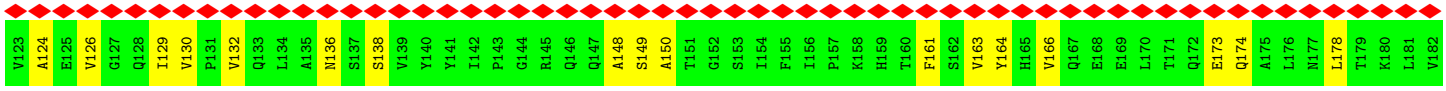
• Molecule 6: D339L

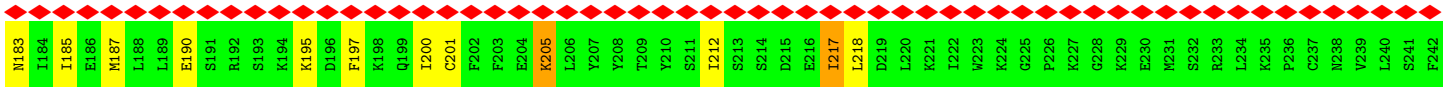
Chain F:

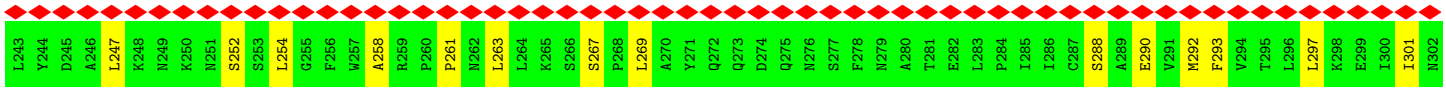


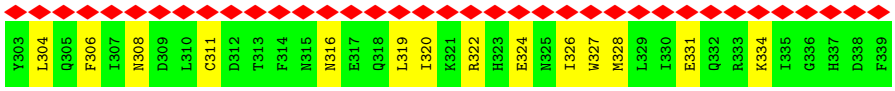






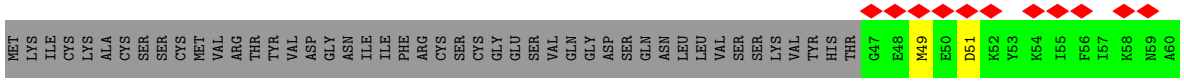


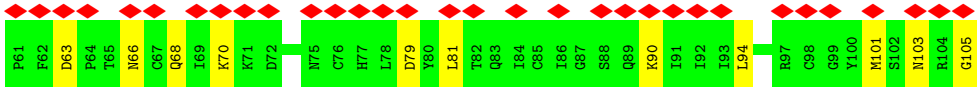




• Molecule 7: C122R

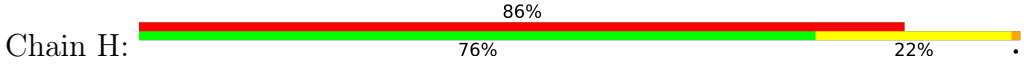
Chain G:

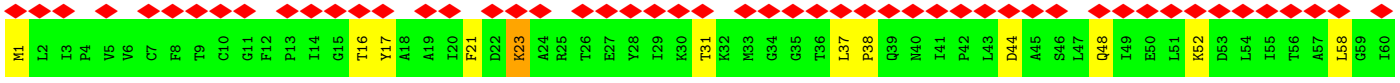




• Molecule 8: DNA-directed RNA polymerase RPB10 homolog

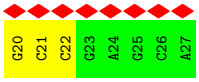
Chain H:





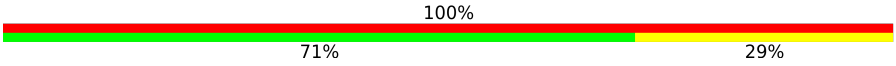
• Molecule 9: DNA (5'-D(P*GP*CP*CP*GP*AP*GP*CP*A)-3')

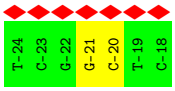
Chain X:



• Molecule 10: DNA (5'-D(P*TP*CP*GP*GP*CP*TP*C)-3')

Chain Y:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266388	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 ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.090	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0129	Depositor
Map size (Å)	258.56, 258.56, 258.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.80799997, 0.80799997, 0.80799997	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	0.35	0/11163	0.45	2/15116 (0.0%)
2	B	0.30	0/9648	0.44	3/13055 (0.0%)
3	C	0.36	0/2959	0.41	0/4000
4	D	0.30	0/1707	0.44	0/2311
5	E	0.36	0/841	0.45	0/1139
6	F	0.20	0/2782	0.39	0/3767
7	G	0.26	0/476	0.41	0/638
8	H	0.37	0/643	0.46	0/872
9	X	0.19	0/185	0.40	0/283
10	Y	0.22	0/156	0.38	0/238
All	All	0.32	0/30560	0.44	5/41419 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1101	PRO	N-CD-CG	-8.09	91.07	103.20
2	B	323	VAL	N-CA-C	-6.03	107.25	113.10
1	A	1101	PRO	CA-N-CD	-5.49	104.31	112.00
2	B	971	PRO	N-CD-CG	-5.39	95.11	103.20
2	B	236	PRO	CA-N-CD	-5.29	104.59	112.00

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	10954	0	11085	175	0
2	B	9459	0	9413	177	0
3	C	2897	0	2976	31	0
4	D	1668	0	1713	21	0
5	E	829	0	877	17	0
6	F	2727	0	2755	56	0
7	G	468	0	467	10	0
8	H	630	0	659	12	0
9	X	165	0	89	4	0
10	Y	141	0	80	3	0
11	A	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
All	All	29943	0	30114	466	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 8.

All (466) 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)
2:B:807:THR:OG1	2:B:845:ASN:ND2	1.99	0.95
6:F:91:LYS:HG3	6:F:105:LEU:HD11	1.56	0.87
5:E:42:SER:OG	5:E:43:PRO:HD3	1.74	0.86
1:A:121:LEU:HD23	1:A:185:LEU:HG	1.58	0.84
1:A:83:LEU:H	1:A:264:GLN:HE22	1.28	0.81
1:A:515:THR:HG22	1:A:517:MET:H	1.48	0.79
1:A:1078:GLN:OE1	1:A:1084:LYS:NZ	2.14	0.76
1:A:109:LEU:HD13	1:A:184:LYS:HD3	1.65	0.76
2:B:892:ASP:O	2:B:939:LYS:NZ	2.20	0.75
6:F:22:ASN:O	6:F:26:HIS:ND1	2.19	0.75
6:F:164:TYR:HB2	6:F:292:MET:HE1	1.68	0.75
2:B:138:ALA:HB3	2:B:146:GLU:HB3	1.70	0.73
1:A:1128:GLN:N	1:A:1179:GLU:OE1	2.22	0.73
2:B:886:LYS:NZ	2:B:888:GLU:OE2	2.22	0.72
9:X:21:DC:N3	10:Y:-21:DG:N1	2.31	0.72
5:E:96:LYS:HE3	5:E:96:LYS:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:THR:HG22	1:A:905:ARG:HG3	1.73	0.70
6:F:95:ASN:ND2	6:F:124:ALA:O	2.24	0.70
1:A:1123:GLU:HG3	1:A:1255:LEU:HD12	1.72	0.70
1:A:1200:ARG:NE	1:A:1206:THR:O	2.23	0.70
2:B:543:ARG:NH1	2:B:563:GLU:O	2.24	0.70
6:F:173:GLU:OE2	6:F:174:GLN:NE2	2.25	0.70
8:H:17:TYR:HB3	8:H:58:LEU:HD22	1.74	0.69
2:B:911:ALA:HB2	2:B:956:MET:HE2	1.73	0.69
1:A:1126:ILE:HG21	1:A:1178:LEU:HD23	1.75	0.69
1:A:1432:ASP:OD2	5:E:139:ARG:NH2	2.23	0.69
1:A:381:LYS:NZ	1:A:403:ASP:OD2	2.25	0.69
2:B:130:LEU:HD22	2:B:157:VAL:HG21	1.76	0.68
1:A:1203:HIS:NE2	1:A:1257:SER:OG	2.25	0.68
1:A:1425:MET:HE2	2:B:1161:MET:HB3	1.74	0.67
1:A:91:ILE:HG12	1:A:196:LEU:HD23	1.77	0.67
1:A:501:GLN:O	2:B:1031:HIS:NE2	2.26	0.67
2:B:1229:ASN:HD22	5:E:45:ILE:HG13	1.60	0.67
1:A:145:VAL:HG13	1:A:155:TRP:HB2	1.76	0.67
6:F:46:LEU:HD21	6:F:108:GLU:HG2	1.76	0.66
5:E:67:THR:OG1	5:E:134:GLU:OE1	2.14	0.66
2:B:236:PRO:HD3	2:B:374:PRO:HB2	1.78	0.66
3:C:82:ASP:OD1	3:C:82:ASP:N	2.25	0.66
1:A:49:ARG:O	1:A:61:THR:OG1	2.14	0.66
6:F:293:PHE:O	6:F:297:LEU:HG	1.96	0.66
6:F:94:LYS:HB3	6:F:101:LEU:HB3	1.78	0.65
6:F:267:SER:HB2	6:F:269:LEU:HD22	1.79	0.65
2:B:792:THR:HG23	2:B:1038:THR:HA	1.76	0.65
2:B:1162:GLN:HE21	5:E:78:ARG:HH11	1.45	0.65
4:D:163:GLN:O	4:D:198:ARG:NH1	2.30	0.64
4:D:102:ILE:O	4:D:106:ILE:HG12	1.97	0.64
2:B:330:GLU:HA	2:B:333:ILE:HD12	1.80	0.64
2:B:486:ILE:HG13	2:B:487:ILE:HG13	1.80	0.64
2:B:330:GLU:OE2	2:B:361:ASN:ND2	2.31	0.64
2:B:486:ILE:O	2:B:506:THR:OG1	2.14	0.64
2:B:393:LEU:O	2:B:397:ILE:HD12	1.98	0.64
2:B:1059:ASP:OD2	2:B:1061:THR:OG1	2.15	0.64
1:A:886:TYR:HE2	1:A:889:ILE:HD12	1.64	0.63
3:C:110:VAL:HB	3:C:134:ALA:HB3	1.80	0.63
1:A:728:ASN:HD22	1:A:731:PHE:H	1.45	0.63
1:A:877:ASP:OD1	1:A:1282:GLY:HA3	1.99	0.62
1:A:1182:LYS:HA	1:A:1185:MET:HE1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:ARG:NH1	1:A:1226:TYR:OH	2.32	0.62
2:B:657:VAL:HG23	2:B:659:GLU:HG3	1.82	0.62
3:C:190:GLU:HB2	3:C:206:LYS:HD2	1.82	0.62
4:D:58:PHE:O	4:D:123:TYR:OH	2.17	0.61
2:B:621:TRP:NE1	2:B:623:GLY:O	2.33	0.61
2:B:908:LYS:HB3	2:B:956:MET:HE3	1.83	0.61
7:G:101:MET:HG2	7:G:105:GLY:HA3	1.82	0.61
1:A:1332:ARG:NH1	1:A:1358:ASP:OD1	2.34	0.60
2:B:278:MET:HE1	2:B:336:LEU:HD22	1.83	0.60
1:A:241:PRO:HG2	1:A:244:LEU:HB2	1.84	0.60
6:F:304:LEU:O	6:F:308:ASN:ND2	2.33	0.60
1:A:916:GLU:OE2	1:A:923:LEU:HD13	2.02	0.60
1:A:116:ILE:HG13	1:A:119:LYS:HG3	1.83	0.60
2:B:885:GLU:HB2	2:B:982:MET:HB3	1.83	0.60
1:A:676:GLU:HG2	1:A:708:ALA:HB1	1.83	0.59
1:A:681:ASN:OD1	1:A:701:TYR:OH	2.19	0.59
2:B:360:LEU:O	2:B:364:GLN:NE2	2.34	0.59
9:X:20:DG:H1	10:Y:-20:DC:H42	1.51	0.59
2:B:844:PRO:HG2	8:H:74:LEU:HD11	1.85	0.59
2:B:208:ILE:HD12	2:B:208:ILE:H	1.68	0.59
6:F:164:TYR:HB2	6:F:292:MET:CE	2.32	0.59
6:F:328:MET:HA	6:F:331:GLU:HB2	1.84	0.58
2:B:920:PHE:HE1	2:B:934:ILE:HG23	1.67	0.58
1:A:1274:MET:SD	1:A:1286:ARG:NH1	2.77	0.58
2:B:650:THR:HB	2:B:663:TRP:HB2	1.84	0.58
2:B:807:THR:HG1	2:B:845:ASN:HD21	1.46	0.58
6:F:163:VAL:HG22	6:F:258:ALA:HB2	1.86	0.58
6:F:166:VAL:HG23	6:F:292:MET:HE3	1.86	0.58
1:A:90:GLU:OE1	1:A:93:ARG:NH1	2.36	0.58
1:A:333:LEU:O	1:A:447:ASN:ND2	2.29	0.58
1:A:332:ASP:OD2	2:B:859:TYR:OH	2.21	0.58
1:A:696:THR:HG23	1:A:699:ASP:H	1.69	0.58
1:A:143:LYS:HB3	1:A:157:ASP:HB3	1.86	0.57
5:E:120:MET:HG3	5:E:135:ILE:HD13	1.85	0.57
1:A:491:LYS:HZ2	1:A:492:SER:HB3	1.70	0.57
1:A:1152:VAL:HG23	1:A:1155:MET:HE2	1.86	0.57
1:A:1184:THR:OG1	1:A:1185:MET:SD	2.62	0.57
2:B:485:SER:HG	2:B:504:VAL:N	2.02	0.57
1:A:1177:ARG:HH11	1:A:1222:ILE:HD11	1.70	0.57
7:G:81:LEU:HD23	7:G:94:LEU:HB3	1.86	0.57
6:F:319:LEU:HD23	6:F:322:ARG:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:324:GLU:HA	6:F:327:TRP:CD1	2.39	0.57
1:A:468:PRO:HB2	1:A:474:ARG:HG3	1.86	0.57
2:B:260:ILE:HG21	2:B:371:ILE:HD12	1.86	0.57
1:A:844:VAL:HG11	1:A:1355:MET:HE1	1.87	0.57
2:B:86:GLN:HB3	2:B:137:THR:HB	1.87	0.56
1:A:1410:ILE:HD12	2:B:1156:THR:HG21	1.88	0.56
2:B:202:VAL:HA	2:B:506:THR:HG22	1.86	0.56
1:A:273:ASP:N	1:A:298:SER:OG	2.35	0.56
5:E:42:SER:OG	5:E:43:PRO:CD	2.52	0.56
5:E:65:ARG:HG2	5:E:134:GLU:HG2	1.86	0.56
1:A:1150:SER:O	1:A:1154:TRP:N	2.33	0.56
2:B:999:ARG:NH2	2:B:1044:GLU:OE2	2.35	0.56
3:C:190:GLU:CD	3:C:190:GLU:H	2.13	0.56
3:C:328:SER:OG	3:C:331:ASP:OD1	2.24	0.56
1:A:1126:ILE:HD13	1:A:1129:TRP:HB3	1.86	0.56
2:B:1069:GLN:NE2	2:B:1073:GLU:OE2	2.35	0.56
6:F:116:SER:OG	6:F:121:ASN:ND2	2.39	0.56
2:B:302:ASN:O	2:B:306:ILE:HD12	2.05	0.56
1:A:1305:LEU:HB3	4:D:1:MET:HB3	1.86	0.56
1:A:872:THR:HG23	1:A:880:LEU:HD13	1.88	0.56
1:A:1096:LEU:HD22	1:A:1309:ILE:HG21	1.87	0.56
2:B:580:ALA:HB2	2:B:666:VAL:HG13	1.88	0.56
2:B:134:VAL:HB	2:B:150:ALA:HB3	1.88	0.56
2:B:118:ARG:NH2	2:B:192:TYR:OH	2.38	0.55
3:C:113:LEU:HD23	3:C:160:ILE:HD12	1.88	0.55
4:D:1:MET:HE3	4:D:5:LYS:HE2	1.88	0.55
2:B:235:GLN:NE2	2:B:238:GLY:O	2.35	0.55
1:A:54:ASP:OD2	1:A:56:HIS:ND1	2.38	0.55
1:A:134:CYS:HB3	1:A:139:ALA:H	1.71	0.55
6:F:53:GLN:OE1	6:F:73:ARG:NH1	2.39	0.55
3:C:6:GLN:HA	3:C:357:LEU:HD11	1.89	0.55
1:A:1209:MET:HE3	1:A:1209:MET:HA	1.89	0.54
1:A:1109:TYR:CZ	1:A:1113:ILE:HD11	2.43	0.54
1:A:1052:PRO:HG2	1:A:1348:PRO:HD3	1.90	0.54
6:F:183:ASN:O	6:F:187:MET:HG2	2.07	0.54
2:B:255:ALA:HB2	2:B:315:VAL:HG11	1.90	0.54
1:A:35:PHE:HE2	1:A:212:ILE:HG21	1.72	0.54
1:A:1340:ARG:NH2	4:D:189:GLU:OE2	2.41	0.54
2:B:429:PHE:O	2:B:433:PHE:HB2	2.08	0.54
1:A:255:ASN:OD1	1:A:256:ILE:N	2.41	0.53
1:A:147:ASP:OD1	1:A:148:SER:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:THR:O	1:A:1313:THR:HG22	2.08	0.53
1:A:158:GLN:HB3	1:A:161:LYS:HB3	1.90	0.53
1:A:1051:GLU:HB3	1:A:1052:PRO:HD3	1.91	0.53
1:A:336:ASP:OD1	1:A:336:ASP:N	2.42	0.53
2:B:20:GLU:HG2	2:B:716:PRO:HG2	1.90	0.53
4:D:30:LYS:O	4:D:34:MET:HG3	2.08	0.53
3:C:38:LEU:HD23	3:C:225:ALA:HB1	1.91	0.53
3:C:272:MET:HE2	3:C:276:LYS:HD2	1.91	0.53
1:A:442:SER:HB3	2:B:1119:ARG:HD3	1.91	0.52
1:A:850:LEU:HB3	4:D:162:MET:HE2	1.91	0.52
2:B:315:VAL:O	2:B:324:GLN:NE2	2.43	0.52
1:A:1208:ILE:HG13	1:A:1223:ILE:HD11	1.91	0.52
1:A:1195:ILE:O	1:A:1199:LEU:HD12	2.10	0.52
2:B:987:GLU:HG3	3:C:91:GLN:CD	2.34	0.52
1:A:1249:ASN:O	1:A:1253:LYS:N	2.36	0.52
2:B:417:ARG:NH1	2:B:665:ASP:OD2	2.43	0.52
2:B:60:LYS:HB2	2:B:61:GLN:OE1	2.10	0.52
2:B:74:ASP:N	2:B:74:ASP:OD1	2.41	0.52
3:C:61:VAL:HA	3:C:65:GLU:HB2	1.90	0.52
6:F:320:ILE:HG23	6:F:327:TRP:HE1	1.75	0.52
1:A:81:PRO:HD3	1:A:199:LYS:HE2	1.92	0.52
1:A:1174:TRP:HZ2	1:A:1243:ASP:HB3	1.75	0.52
2:B:320:PHE:CZ	2:B:339:LYS:HE3	2.45	0.52
2:B:722:ILE:HG13	2:B:727:LEU:HD23	1.92	0.51
1:A:22:LYS:HA	1:A:75:ILE:HD13	1.92	0.51
1:A:1185:MET:SD	1:A:1185:MET:N	2.83	0.51
2:B:881:PHE:HB3	2:B:986:TYR:HB2	1.91	0.51
7:G:49:MET:HE1	7:G:103:ASN:HB2	1.91	0.51
1:A:499:GLN:HB3	1:A:503:SER:HB2	1.93	0.51
2:B:101:HIS:N	2:B:110:ILE:O	2.35	0.51
6:F:24:GLU:CD	6:F:24:GLU:H	2.18	0.51
6:F:25:ALA:O	6:F:29:LYS:HG3	2.11	0.51
2:B:235:GLN:OE1	2:B:243:SER:OG	2.29	0.51
1:A:62:CYS:O	2:B:1190:ASN:ND2	2.41	0.51
2:B:299:SER:O	2:B:303:THR:HG23	2.11	0.51
2:B:482:MET:HG3	2:B:483:GLU:N	2.26	0.51
1:A:371:ARG:NH1	1:A:391:GLU:OE2	2.44	0.51
2:B:97:GLU:HG3	2:B:127:PRO:HD2	1.93	0.51
6:F:200:ILE:HG22	6:F:311:CYS:SG	2.51	0.51
2:B:375:HIS:HD2	2:B:620:GLU:HB3	1.75	0.51
2:B:132:ALA:HB3	2:B:152:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:ASN:HB3	5:E:94:MET:SD	2.51	0.50
2:B:877:PHE:O	2:B:1110:ARG:NH1	2.43	0.50
2:B:482:MET:O	2:B:486:ILE:HG23	2.11	0.50
4:D:1:MET:SD	4:D:4:GLN:HB3	2.50	0.50
2:B:79:ASP:HA	2:B:82:ARG:HH12	1.77	0.50
2:B:957:TYR:CZ	2:B:959:PHE:HB2	2.46	0.50
6:F:138:SER:O	6:F:150:ALA:HA	2.12	0.50
1:A:70:MET:HE1	2:B:1214:ARG:HG3	1.93	0.50
2:B:1177:SER:HB3	2:B:1210:VAL:HG22	1.93	0.50
1:A:493:SER:OG	1:A:862:ALA:O	2.17	0.50
1:A:407:ARG:NH1	1:A:408:ASP:O	2.45	0.49
2:B:486:ILE:HG13	2:B:487:ILE:N	2.27	0.49
8:H:21:PHE:HB2	8:H:58:LEU:HD11	1.94	0.49
9:X:21:DC:N4	10:Y:-21:DG:O6	2.20	0.49
2:B:209:ARG:NE	2:B:212:THR:HG21	2.26	0.49
2:B:604:ASN:HA	2:B:607:ILE:HG12	1.94	0.49
2:B:227:ILE:HG13	2:B:228:ILE:HG23	1.94	0.49
2:B:285:ASP:OD1	2:B:285:ASP:N	2.45	0.49
2:B:324:GLN:HG3	2:B:325:HIS:CD2	2.47	0.49
2:B:1190:ASN:O	2:B:1194:PRO:HA	2.13	0.49
4:D:103:LEU:O	4:D:107:VAL:HG12	2.12	0.49
1:A:1098:LEU:HD12	1:A:1104:GLU:HA	1.94	0.49
2:B:543:ARG:HD3	2:B:565:VAL:O	2.13	0.49
8:H:37:LEU:HD12	8:H:38:PRO:HD2	1.94	0.49
2:B:486:ILE:HG22	2:B:504:VAL:HB	1.95	0.49
2:B:389:PHE:O	2:B:393:LEU:HG	2.13	0.49
3:C:333:ILE:O	3:C:337:GLU:HG2	2.12	0.49
2:B:185:ASP:OD1	2:B:813:PHE:HB2	2.11	0.49
2:B:922:PRO:HG2	2:B:925:THR:HG21	1.95	0.49
6:F:263:LEU:HD11	6:F:269:LEU:HG	1.95	0.49
2:B:202:VAL:HG11	2:B:421:SER:HA	1.95	0.49
4:D:143:THR:OG1	4:D:146:GLU:HG3	2.13	0.49
1:A:1307:ASP:N	1:A:1307:ASP:OD1	2.45	0.48
1:A:586:LYS:HA	1:A:586:LYS:HD3	1.64	0.48
1:A:20:ASP:OD1	5:E:44:SER:OG	2.26	0.48
2:B:271:PRO:HB2	2:B:273:TYR:CE1	2.48	0.48
2:B:281:MET:HG2	2:B:287:ILE:HD13	1.96	0.48
3:C:3:LYS:NZ	3:C:357:LEU:HG	2.28	0.48
2:B:870:SER:HG	2:B:1012:THR:HG1	1.61	0.48
1:A:1174:TRP:HD1	1:A:1227:LEU:HD11	1.79	0.48
1:A:208:ILE:HD11	2:B:1218:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:TYR:CD2	2:B:199:GLU:HG2	2.49	0.47
2:B:1058:THR:HG22	8:H:48:GLN:HE22	1.79	0.47
6:F:3:ASP:N	6:F:3:ASP:OD1	2.46	0.47
2:B:1181:ARG:HB2	2:B:1206:ASP:HB3	1.96	0.47
1:A:1129:TRP:HB2	1:A:1178:LEU:HG	1.96	0.47
2:B:916:LEU:HD21	2:B:932:ILE:HG22	1.96	0.47
2:B:1162:GLN:NE2	5:E:78:ARG:HH11	2.10	0.47
2:B:457:LEU:HD22	2:B:461:ASN:HB3	1.96	0.47
2:B:894:GLU:HG2	2:B:938:ALA:HB2	1.96	0.47
5:E:127:PRO:HD2	5:E:128:GLU:OE2	2.14	0.47
2:B:995:LYS:HD2	2:B:1111:LEU:HD12	1.97	0.47
3:C:281:ILE:HD13	3:C:321:LEU:HD23	1.95	0.47
1:A:320:TRP:CE2	2:B:1135:PRO:HG3	2.50	0.47
1:A:501:GLN:O	2:B:1031:HIS:CE1	2.67	0.47
1:A:1185:MET:O	1:A:1189:SER:N	2.48	0.47
2:B:512:LYS:HD3	2:B:516:ASN:ND2	2.30	0.47
2:B:423:VAL:O	2:B:427:LYS:HG2	2.14	0.47
3:C:139:LYS:HA	3:C:139:LYS:HD3	1.66	0.47
2:B:727:LEU:HD12	2:B:731:ASP:OD1	2.15	0.46
5:E:120:MET:HG3	5:E:135:ILE:CD1	2.45	0.46
1:A:210:PRO:HD2	1:A:224:HIS:CE1	2.51	0.46
1:A:519:LYS:HE3	1:A:519:LYS:HB3	1.64	0.46
2:B:69:TYR:CZ	2:B:446:LYS:HG2	2.50	0.46
2:B:438:ILE:HG13	2:B:439:ALA:N	2.31	0.46
6:F:288:SER:OG	6:F:290:GLU:OE2	2.30	0.46
1:A:87:PHE:O	1:A:91:ILE:HG13	2.16	0.46
3:C:352:LYS:HE3	3:C:352:LYS:HB3	1.53	0.46
1:A:171:ARG:HB2	1:A:197:VAL:HG11	1.97	0.46
2:B:479:ASN:HA	2:B:482:MET:HG2	1.97	0.46
4:D:19:MET:HB3	4:D:45:ALA:HB1	1.96	0.46
2:B:39:LEU:O	2:B:522:ARG:NH1	2.42	0.46
6:F:98:ASN:O	6:F:116:SER:HB3	2.16	0.46
7:G:90:LYS:HB3	7:G:90:LYS:HE3	1.65	0.46
2:B:441:ILE:HA	2:B:469:ALA:HB1	1.98	0.46
2:B:796:ARG:HH22	2:B:1036:ARG:HH21	1.63	0.46
6:F:212:ILE:HG12	6:F:217:ILE:HG12	1.98	0.46
1:A:1233:ARG:HA	1:A:1233:ARG:HD2	1.74	0.46
2:B:379:THR:OG1	2:B:381:ASP:OD1	2.17	0.46
3:C:34:GLU:N	3:C:34:GLU:OE1	2.49	0.46
6:F:212:ILE:HG21	6:F:217:ILE:HD11	1.97	0.46
1:A:166:TYR:CD2	1:A:246:ILE:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:GLN:HA	2:B:367:ILE:HG22	1.98	0.46
2:B:870:SER:OG	2:B:1012:THR:OG1	2.33	0.46
3:C:70:MET:HG2	3:C:176:PHE:CE1	2.51	0.46
2:B:1054:GLN:NE2	2:B:1078:GLU:OE1	2.49	0.45
6:F:83:ALA:HB1	6:F:136:ASN:HA	1.98	0.45
1:A:1211:SER:OG	1:A:1212:VAL:N	2.48	0.45
2:B:803:GLN:OE1	2:B:1001:GLY:HA2	2.16	0.45
1:A:19:ASN:OD1	1:A:19:ASN:N	2.48	0.45
2:B:167:ASN:OD1	2:B:168:ARG:NH1	2.49	0.45
2:B:807:THR:HB	2:B:1109:GLN:HB3	1.99	0.45
1:A:559:LEU:HD22	1:A:639:LEU:HD22	1.99	0.45
1:A:1173:ASN:N	1:A:1173:ASN:OD1	2.50	0.45
2:B:904:THR:HA	2:B:950:TYR:HB2	1.99	0.45
5:E:60:ILE:HD12	5:E:134:GLU:HG3	1.98	0.45
1:A:112:TYR:HB3	1:A:120:ARG:HB2	1.98	0.45
1:A:252:ILE:HD12	1:A:256:ILE:HG22	1.99	0.45
1:A:952:PHE:C	1:A:952:PHE:CD2	2.95	0.45
2:B:196:ARG:NH2	2:B:487:ILE:HD13	2.32	0.45
2:B:830:GLU:HG2	8:H:73:THR:HA	1.99	0.45
6:F:87:ILE:HD12	6:F:112:ILE:HD11	1.99	0.45
6:F:108:GLU:O	6:F:110:VAL:HG23	2.17	0.45
1:A:798:SER:OG	2:B:775:PRO:HB3	2.17	0.45
1:A:1079:GLU:OE1	1:A:1089:GLU:HA	2.17	0.45
2:B:1018:THR:HG22	2:B:1088:MET:HG2	1.99	0.45
1:A:591:THR:HA	1:A:601:GLY:HA3	1.99	0.44
9:X:21:DC:H2”	9:X:22:DC:C6	2.52	0.44
1:A:1177:ARG:C	1:A:1178:LEU:HD12	2.42	0.44
2:B:430:LYS:HD2	2:B:430:LYS:HA	1.70	0.44
2:B:614:ARG:HD3	2:B:621:TRP:CZ2	2.52	0.44
6:F:110:VAL:HG13	6:F:148:ALA:HB3	1.98	0.44
1:A:31:ILE:HD11	1:A:42:GLU:O	2.17	0.44
1:A:114:HIS:CE1	1:A:115:LEU:HG	2.52	0.44
1:A:382:GLN:NE2	1:A:401:VAL:O	2.50	0.44
6:F:5:LYS:HD3	6:F:7:PHE:CZ	2.53	0.44
1:A:923:LEU:HD12	1:A:1276:HIS:HE1	1.83	0.44
3:C:180:VAL:HG22	3:C:222:CYS:HB3	1.99	0.44
6:F:106:LEU:HD12	6:F:107:THR:N	2.32	0.44
1:A:1251:VAL:HG13	1:A:1255:LEU:HD23	2.00	0.44
1:A:1401:ASP:OD2	1:A:1401:ASP:N	2.50	0.44
2:B:479:ASN:O	2:B:483:GLU:HG2	2.17	0.44
4:D:20:VAL:HG22	4:D:46:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ARG:HD2	1:A:456:ALA:HB2	2.00	0.44
1:A:923:LEU:HD12	1:A:1276:HIS:CE1	2.52	0.44
3:C:119:SER:OG	3:C:120:CYS:N	2.49	0.44
3:C:257:TYR:HB3	3:C:337:GLU:OE2	2.18	0.44
1:A:876:SER:HB3	1:A:1283:LYS:HG3	2.00	0.44
1:A:1015:THR:HG22	1:A:1016:CYS:H	1.83	0.44
2:B:60:LYS:HE2	2:B:92:THR:O	2.18	0.44
2:B:118:ARG:NE	2:B:199:GLU:OE1	2.40	0.44
1:A:960:LYS:NZ	1:A:1011:THR:O	2.45	0.44
2:B:543:ARG:HB3	2:B:566:GLY:HA3	2.00	0.44
6:F:44:PHE:CZ	6:F:109:PRO:HG2	2.53	0.44
2:B:305:MET:O	2:B:309:LEU:HD12	2.17	0.43
2:B:381:ASP:OD1	2:B:381:ASP:N	2.44	0.43
2:B:843:ILE:HD11	8:H:79:TYR:CD2	2.53	0.43
6:F:103:GLU:OE2	6:F:111:THR:OG1	2.34	0.43
1:A:208:ILE:HG13	2:B:1218:VAL:HG13	1.98	0.43
1:A:123:GLU:O	1:A:126:SER:OG	2.32	0.43
1:A:849:ARG:NH1	1:A:1377:ARG:O	2.49	0.43
1:A:1158:PHE:HA	1:A:1161:ASN:HD22	1.83	0.43
1:A:1208:ILE:HD12	1:A:1225:ILE:HG23	2.00	0.43
2:B:125:SER:HB3	2:B:159:THR:HB	2.00	0.43
2:B:994:ASP:OD2	2:B:1110:ARG:NH2	2.52	0.43
6:F:22:ASN:HB3	6:F:26:HIS:CE1	2.53	0.43
6:F:316:ASN:HD21	6:F:319:LEU:HG	1.82	0.43
1:A:318:GLN:NE2	2:B:1136:LEU:O	2.52	0.43
1:A:822:THR:HG21	1:A:1054:THR:HA	2.00	0.43
2:B:39:LEU:O	2:B:40:ILE:HD13	2.18	0.43
2:B:100:GLN:HG3	2:B:110:ILE:O	2.19	0.43
2:B:279:PHE:CG	2:B:383:ARG:HD2	2.53	0.43
1:A:834:GLN:HE22	1:A:1411:ALA:HB2	1.84	0.43
1:A:911:ILE:HD13	4:D:192:MET:O	2.19	0.43
2:B:185:ASP:HB3	2:B:188:GLU:HB3	2.01	0.43
2:B:225:ASN:O	2:B:252:THR:HG23	2.19	0.43
2:B:305:MET:HG3	2:B:398:LEU:HD23	2.00	0.43
2:B:471:SER:OG	2:B:473:ASN:OD1	2.32	0.43
2:B:860:ASN:OD1	2:B:860:ASN:N	2.51	0.43
1:A:920:PHE:CE2	1:A:1095:LEU:HB2	2.53	0.43
2:B:815:TRP:CD1	2:B:815:TRP:H	2.35	0.43
6:F:174:GLN:O	6:F:178:LEU:HG	2.19	0.43
6:F:205:LYS:HE2	6:F:205:LYS:N	2.34	0.43
1:A:164:LYS:HE3	1:A:164:LYS:HB2	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:ILE:O	1:A:1077:PRO:HD2	2.18	0.43
2:B:88:GLN:HB3	2:B:135:ILE:O	2.18	0.43
2:B:808:GLY:HA2	2:B:1112:GLN:OE1	2.19	0.43
6:F:324:GLU:HG3	6:F:327:TRP:HD1	1.84	0.43
8:H:1:MET:HB3	8:H:76:TYR:HB2	2.01	0.43
8:H:69:HIS:O	8:H:73:THR:OG1	2.29	0.43
1:A:425:ARG:HA	2:B:1154:VAL:HG13	2.00	0.43
1:A:1157:ASP:O	1:A:1160:GLU:HG3	2.19	0.43
1:A:1205:ASN:HA	1:A:1228:ARG:HD3	2.00	0.43
2:B:299:SER:OG	7:G:51:ASP:OD2	2.33	0.43
3:C:116:LEU:HD13	3:C:157:SER:HB3	2.00	0.43
1:A:35:PHE:CE2	1:A:212:ILE:HG21	2.51	0.43
1:A:698:HIS:HA	7:G:90:LYS:HD2	2.01	0.43
2:B:130:LEU:HB2	2:B:157:VAL:HG23	2.01	0.43
2:B:453:ALA:O	2:B:457:LEU:HG	2.19	0.43
2:B:885:GLU:O	2:B:981:LEU:HD12	2.18	0.43
3:C:187:LEU:HB2	3:C:216:HIS:CD2	2.54	0.43
1:A:1383:LEU:H	1:A:1405:ASN:ND2	2.17	0.42
7:G:49:MET:HE1	7:G:103:ASN:HD22	1.84	0.42
2:B:957:TYR:CE2	2:B:959:PHE:HB2	2.53	0.42
3:C:28:LYS:HD3	8:H:23:LYS:NZ	2.33	0.42
3:C:257:TYR:CZ	3:C:336:LEU:HD13	2.54	0.42
1:A:27:MET:HE3	1:A:47:ASP:OD2	2.19	0.42
1:A:512:ARG:HE	1:A:512:ARG:HB3	1.61	0.42
1:A:1120:ILE:HD12	1:A:1124:ARG:HD3	2.01	0.42
2:B:696:LYS:HE3	2:B:696:LYS:HB3	1.92	0.42
1:A:1174:TRP:CD1	1:A:1227:LEU:HD11	2.55	0.42
2:B:376:MET:HE1	2:B:389:PHE:HB2	2.01	0.42
2:B:665:ASP:OD1	2:B:665:ASP:N	2.52	0.42
3:C:11:LYS:HE2	3:C:11:LYS:HB2	1.56	0.42
3:C:276:LYS:NZ	3:C:326:LYS:HE2	2.35	0.42
5:E:126:THR:HG22	5:E:127:PRO:HD2	2.01	0.42
6:F:331:GLU:HA	6:F:334:LYS:HE3	2.01	0.42
1:A:767:SER:O	1:A:777:ARG:NH1	2.53	0.42
1:A:853:GLN:HE22	4:D:150:PHE:HZ	1.68	0.42
1:A:1017:GLU:H	1:A:1017:GLU:CD	2.27	0.42
1:A:1106:ASN:ND2	1:A:1109:TYR:HB2	2.34	0.42
2:B:235:GLN:HA	2:B:236:PRO:HD2	1.90	0.42
4:D:72:ARG:O	4:D:76:THR:HG23	2.19	0.42
7:G:70:LYS:HD2	7:G:70:LYS:HA	1.77	0.42
1:A:12:GLN:HB2	2:B:1231:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ILE:HG23	1:A:800:GLU:HG2	2.02	0.42
1:A:1177:ARG:HD2	1:A:1222:ILE:HD11	2.01	0.42
4:D:28:TYR:O	4:D:32:VAL:HG12	2.20	0.42
1:A:661:GLU:OE2	1:A:661:GLU:N	2.51	0.42
2:B:98:ARG:HB3	2:B:170:HIS:CE1	2.55	0.42
6:F:252:SER:OG	6:F:254:LEU:HG	2.19	0.42
8:H:44:ASP:O	8:H:48:GLN:HG2	2.20	0.42
1:A:1274:MET:HE3	1:A:1274:MET:HB2	1.89	0.42
1:A:476:GLU:OE2	2:B:1163:THR:OG1	2.30	0.42
1:A:874:MET:SD	1:A:1284:LEU:HD23	2.60	0.42
2:B:137:THR:HG23	2:B:147:VAL:HG22	2.01	0.42
3:C:13:PHE:HD2	3:C:40:PRO:HB2	1.84	0.42
6:F:185:ILE:HG13	6:F:301:ILE:HG12	2.01	0.42
1:A:1123:GLU:OE2	1:A:1255:LEU:HB3	2.19	0.42
1:A:1177:ARG:HG3	1:A:1224:ARG:HG2	2.02	0.42
2:B:207:ASN:HB3	2:B:419:HIS:CE1	2.55	0.42
1:A:1182:LYS:HA	1:A:1185:MET:CE	2.49	0.41
3:C:106:ASN:OD1	3:C:106:ASN:N	2.51	0.41
6:F:86:LEU:HD21	6:F:306:PHE:CD2	2.55	0.41
1:A:634:PHE:O	1:A:638:GLN:HG2	2.19	0.41
2:B:326:GLU:OE2	2:B:331:LYS:HB2	2.19	0.41
6:F:161:PHE:CD1	6:F:261:PRO:HD3	2.55	0.41
6:F:263:LEU:HD21	6:F:269:LEU:O	2.20	0.41
1:A:1262:ILE:HB	1:A:1265:ILE:HD12	2.00	0.41
1:A:1421:ARG:O	1:A:1422:ILE:HG13	2.20	0.41
3:C:256:ILE:HD13	3:C:256:ILE:HA	1.90	0.41
1:A:383:ILE:HD12	1:A:383:ILE:HA	1.97	0.41
1:A:385:GLN:N	1:A:385:GLN:OE1	2.53	0.41
1:A:661:GLU:CD	1:A:661:GLU:H	2.27	0.41
1:A:1002:ILE:O	1:A:1006:LEU:HB2	2.21	0.41
1:A:1177:ARG:HA	1:A:1224:ARG:HA	2.02	0.41
2:B:37:THR:HG22	2:B:38:GLY:O	2.20	0.41
2:B:641:GLU:OE1	2:B:643:LYS:N	2.52	0.41
2:B:641:GLU:CD	2:B:643:LYS:H	2.28	0.41
4:D:34:MET:HE2	4:D:34:MET:HB3	1.74	0.41
5:E:45:ILE:H	5:E:45:ILE:HG12	1.74	0.41
6:F:100:ILE:HB	6:F:114:ILE:HB	2.02	0.41
6:F:195:LYS:HE3	6:F:308:ASN:HA	2.01	0.41
1:A:70:MET:HE3	1:A:70:MET:HA	2.01	0.41
1:A:1178:LEU:HB2	1:A:1223:ILE:HG23	2.03	0.41
2:B:928:LYS:HE2	2:B:928:LYS:HB2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:ASP:OD1	2:B:560:ASP:N	2.51	0.41
1:A:913:LEU:HD23	1:A:913:LEU:HA	1.88	0.41
2:B:207:ASN:ND2	2:B:208:ILE:HD12	2.36	0.41
6:F:187:MET:HA	6:F:190:GLU:HG2	2.02	0.41
6:F:200:ILE:HG13	6:F:201:CYS:N	2.34	0.41
1:A:381:LYS:NZ	1:A:398:ARG:O	2.50	0.41
1:A:965:LYS:HB3	1:A:965:LYS:HE3	1.71	0.41
2:B:412:SER:OG	2:B:414:ARG:HG2	2.21	0.41
1:A:881:GLU:O	1:A:885:LYS:HB3	2.21	0.41
1:A:1076:ARG:HB3	1:A:1077:PRO:HD3	2.03	0.41
1:A:1339:ILE:O	1:A:1343:MET:HG2	2.20	0.41
2:B:276:PHE:HD2	2:B:287:ILE:HG23	1.85	0.41
2:B:898:LYS:HG3	2:B:916:LEU:HB2	2.02	0.41
4:D:180:ASP:HB2	4:D:200:ILE:HD12	2.03	0.41
6:F:130:VAL:HG12	6:F:326:ILE:HG13	2.02	0.41
1:A:1170:ASP:OD1	1:A:1229:GLU:HB2	2.21	0.41
2:B:138:ALA:N	2:B:146:GLU:O	2.45	0.41
7:G:63:ASP:HB3	7:G:66:ASN:ND2	2.35	0.41
1:A:1150:SER:HA	1:A:1153:GLU:HB3	2.03	0.40
1:A:1210:HIS:HA	1:A:1223:ILE:HD13	2.03	0.40
1:A:1242:THR:OG1	1:A:1243:ASP:N	2.54	0.40
8:H:52:LYS:HE3	8:H:62:MET:HE3	2.03	0.40
1:A:779:ALA:O	1:A:785:TYR:OH	2.30	0.40
2:B:317:ASP:OD2	2:B:320:PHE:HD2	2.03	0.40
2:B:483:GLU:HA	2:B:486:ILE:HG12	2.03	0.40
2:B:585:SER:O	2:B:588:GLN:HG3	2.21	0.40
2:B:1193:HIS:O	2:B:1193:HIS:ND1	2.53	0.40
1:A:758:ASN:N	1:A:758:ASN:HD22	2.18	0.40
4:D:144:GLN:O	4:D:148:GLN:HB2	2.21	0.40
6:F:90:VAL:O	6:F:129:ILE:HA	2.20	0.40
6:F:197:PHE:CE1	6:F:218:LEU:HD22	2.56	0.40
1:A:129:THR:HG22	1:A:132:LYS:NZ	2.36	0.40
1:A:502:ASP:HB2	2:B:861:GLN:NE2	2.37	0.40
2:B:207:ASN:HD22	2:B:207:ASN:HA	1.72	0.40
2:B:768:ARG:NH2	7:G:68:GLN:OE1	2.54	0.40
3:C:304:ASP:OD2	3:C:304:ASP:N	2.54	0.40
2:B:228:ILE:HG12	2:B:250:TYR:HB3	2.02	0.40
2:B:543:ARG:HH12	2:B:563:GLU:HG2	1.86	0.40
2:B:819:VAL:HG12	2:B:884:GLU:HB2	2.03	0.40
4:D:61:ASN:HA	4:D:66:HIS:HE1	1.86	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	1363/1450 (94%)	1314 (96%)	49 (4%)	0	100	100
2	B	1186/1242 (96%)	1143 (96%)	43 (4%)	0	100	100
3	C	355/359 (99%)	344 (97%)	11 (3%)	0	100	100
4	D	203/205 (99%)	196 (97%)	7 (3%)	0	100	100
5	E	104/147 (71%)	102 (98%)	2 (2%)	0	100	100
6	F	337/339 (99%)	321 (95%)	16 (5%)	0	100	100
7	G	57/105 (54%)	53 (93%)	4 (7%)	0	100	100
8	H	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
All	All	3683/3927 (94%)	3549 (96%)	134 (4%)	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	1219/1279 (95%)	1184 (97%)	35 (3%)	37	68
2	B	1038/1081 (96%)	1018 (98%)	20 (2%)	52	79
3	C	326/328 (99%)	318 (98%)	8 (2%)	42	73
4	D	185/185 (100%)	183 (99%)	2 (1%)	70	88
5	E	96/136 (71%)	95 (99%)	1 (1%)	73	89
6	F	312/312 (100%)	303 (97%)	9 (3%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	54/96 (56%)	53 (98%)	1 (2%)	52 79
8	H	70/70 (100%)	66 (94%)	4 (6%)	17 43
All	All	3300/3487 (95%)	3220 (98%)	80 (2%)	45 74

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
1	A	86	LEU
1	A	88	ILE
1	A	145	VAL
1	A	191	SER
1	A	208	ILE
1	A	328	CYS
1	A	424	GLU
1	A	493	SER
1	A	505	VAL
1	A	530	LEU
1	A	562	GLN
1	A	659	THR
1	A	664	GLN
1	A	667	GLN
1	A	675	LEU
1	A	830	ILE
1	A	848	THR
1	A	922	GLN
1	A	941	ILE
1	A	943	LEU
1	A	959	GLN
1	A	974	VAL
1	A	1012	LEU
1	A	1015	THR
1	A	1086	VAL
1	A	1095	LEU
1	A	1105	THR
1	A	1171	ILE
1	A	1208	ILE
1	A	1227	LEU
1	A	1342	VAL
1	A	1358	ASP
1	A	1422	ILE

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Mol	Chain	Res	Type
1	A	1437	THR
2	B	268	LEU
2	B	278	MET
2	B	301	VAL
2	B	401	ILE
2	B	402	MET
2	B	408	THR
2	B	452	THR
2	B	519	SER
2	B	578	CYS
2	B	634	ARG
2	B	641	GLU
2	B	670	THR
2	B	735	GLN
2	B	765	VAL
2	B	864	SER
2	B	926	VAL
2	B	1028	VAL
2	B	1054	GLN
2	B	1141	SER
2	B	1210	VAL
3	C	5	PHE
3	C	29	LEU
3	C	82	ASP
3	C	116	LEU
3	C	120	CYS
3	C	194	THR
3	C	253	ILE
3	C	257	TYR
4	D	35	VAL
4	D	101	ASN
5	E	66	ILE
6	F	17	THR
6	F	28	LEU
6	F	46	LEU
6	F	126	VAL
6	F	132	VAL
6	F	149	SER
6	F	205	LYS
6	F	217	ILE
6	F	247	LEU
7	G	79	ASP

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Mol	Chain	Res	Type
8	H	16	THR
8	H	23	LYS
8	H	31	THR
8	H	71	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	21	HIS
1	A	64	HIS
1	A	68	GLN
1	A	114	HIS
1	A	224	HIS
1	A	228	ASN
1	A	264	GLN
1	A	265	GLN
1	A	269	ASN
1	A	418	ASN
1	A	420	GLN
1	A	455	ASN
1	A	464	ASN
1	A	501	GLN
1	A	566	ASN
1	A	592	GLN
1	A	646	ASN
1	A	663	HIS
1	A	698	HIS
1	A	728	ASN
1	A	758	ASN
1	A	763	GLN
1	A	834	GLN
1	A	853	GLN
1	A	878	GLN
1	A	1013	ASN
1	A	1106	ASN
1	A	1115	ASN
1	A	1161	ASN
1	A	1197	ASN
1	A	1276	HIS
1	A	1349	ASN
1	A	1439	ASN

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Mol	Chain	Res	Type
2	B	64	ASN
2	B	207	ASN
2	B	216	HIS
2	B	325	HIS
2	B	364	GLN
2	B	419	HIS
2	B	557	GLN
2	B	598	GLN
2	B	761	HIS
2	B	829	ASN
2	B	845	ASN
2	B	861	GLN
2	B	906	ASN
2	B	912	ASN
2	B	972	HIS
2	B	991	ASN
2	B	1039	ASN
2	B	1108	HIS
2	B	1112	GLN
2	B	1142	HIS
2	B	1162	GLN
2	B	1182	ASN
2	B	1227	ASN
2	B	1229	ASN
3	C	19	ASN
3	C	207	GLN
3	C	216	HIS
3	C	259	ASN
3	C	345	GLN
4	D	77	ASN
4	D	119	ASN
4	D	144	GLN
6	F	4	GLN
6	F	121	ASN
6	F	146	GLN
7	G	89	GLN
7	G	103	ASN
8	H	48	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

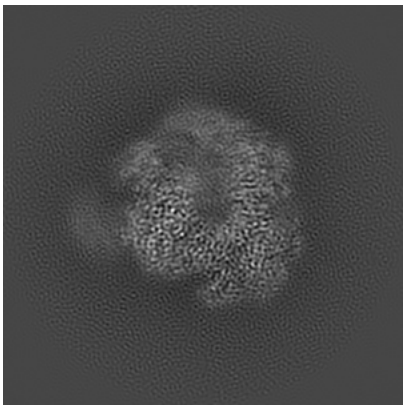
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39511. These allow visual inspection of the internal detail of the map and identification of artifacts.

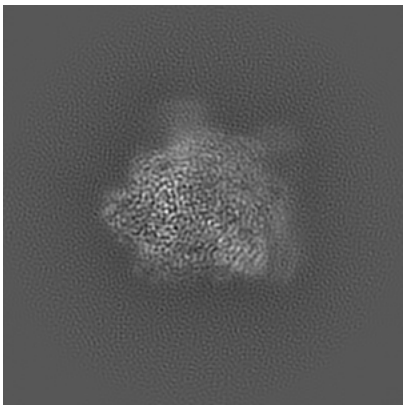
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

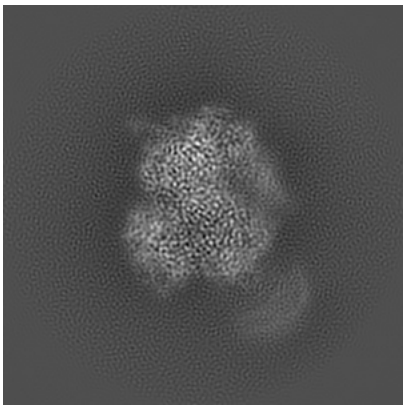
6.1.1 Primary map



X

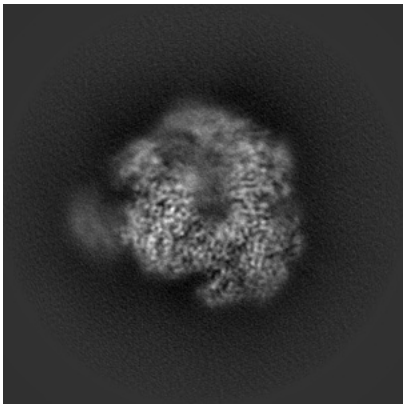


Y

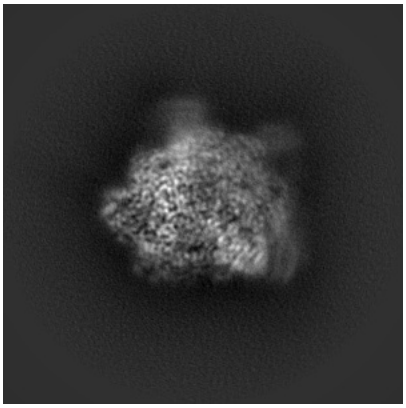


Z

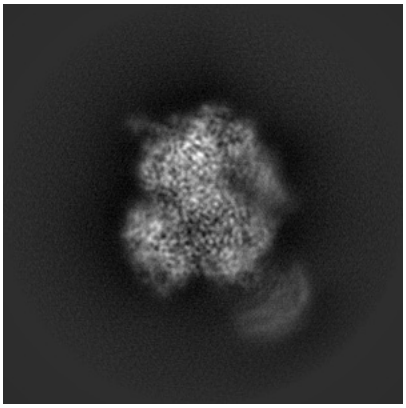
6.1.2 Raw map



X



Y

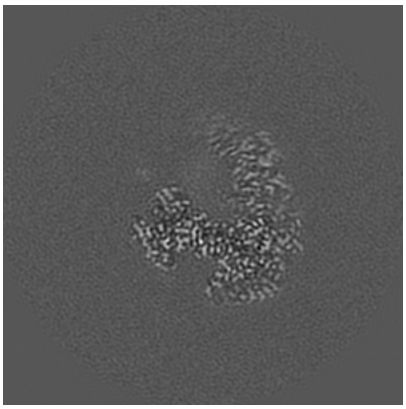


Z

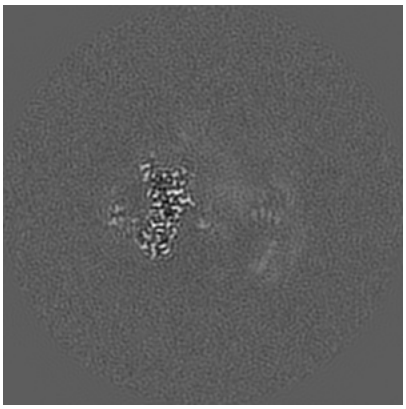
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

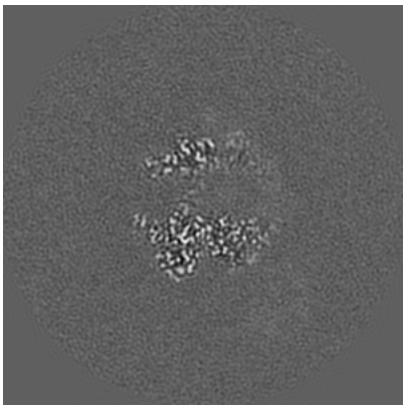
6.2.1 Primary map



X Index: 160

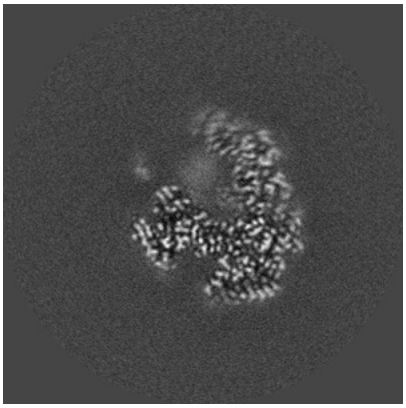


Y Index: 160

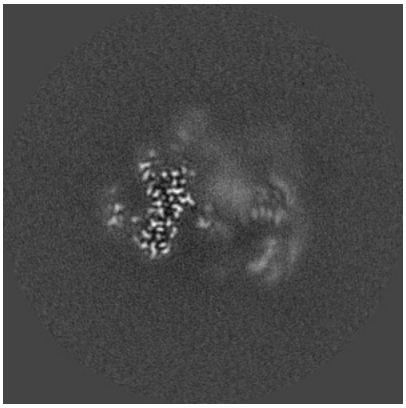


Z Index: 160

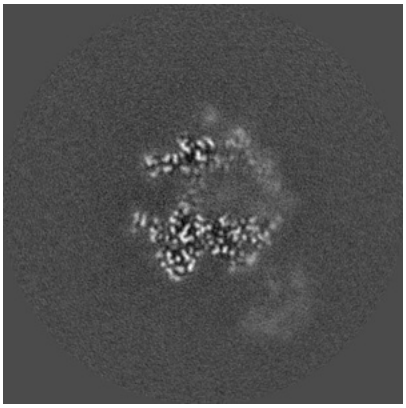
6.2.2 Raw map



X Index: 160



Y Index: 160

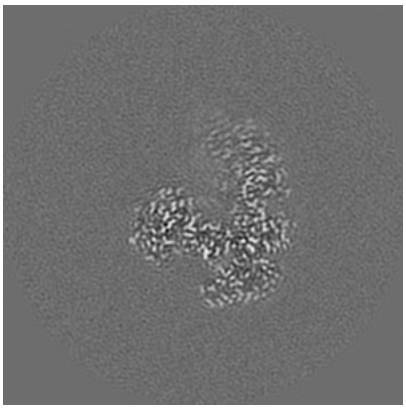


Z Index: 160

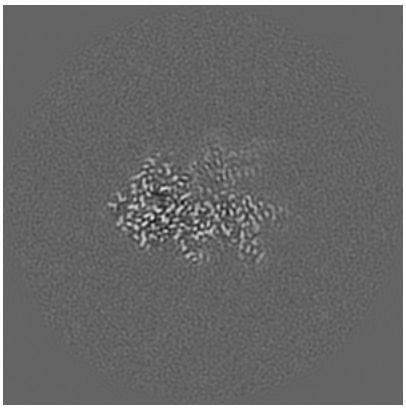
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

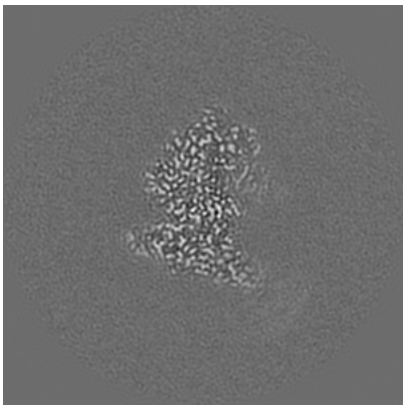
6.3.1 Primary map



X Index: 155

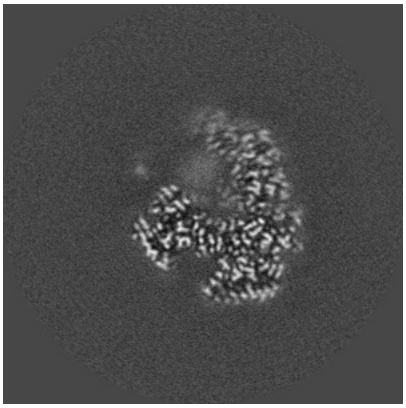


Y Index: 199

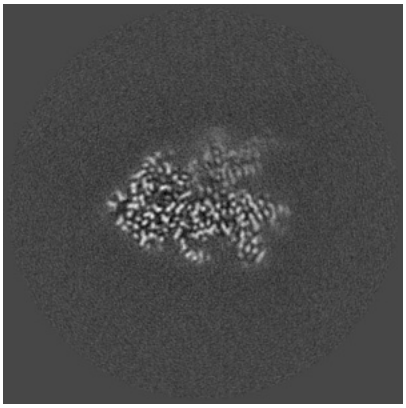


Z Index: 135

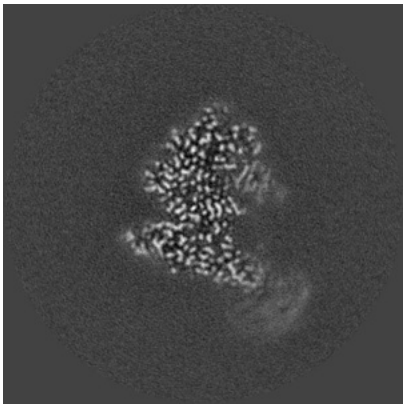
6.3.2 Raw map



X Index: 159



Y Index: 199

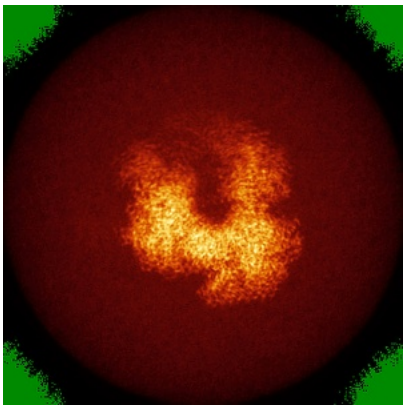


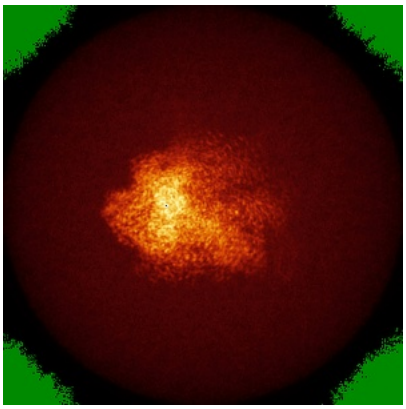
Z Index: 135

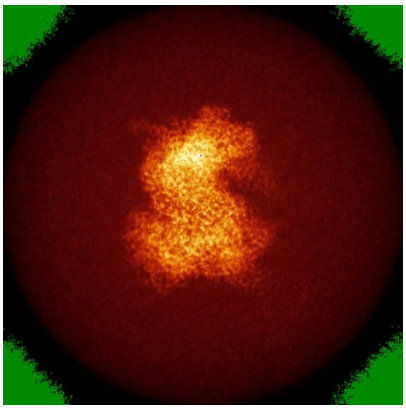
The images above show the largest variance slices of the map in three orthogonal directions.

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

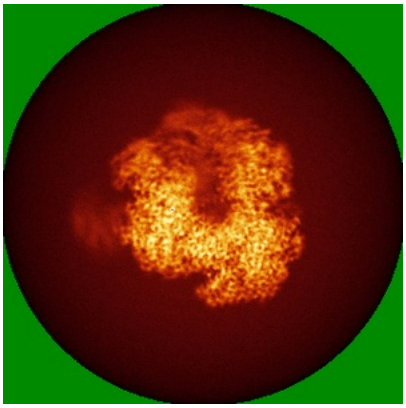
6.4.1 Primary map

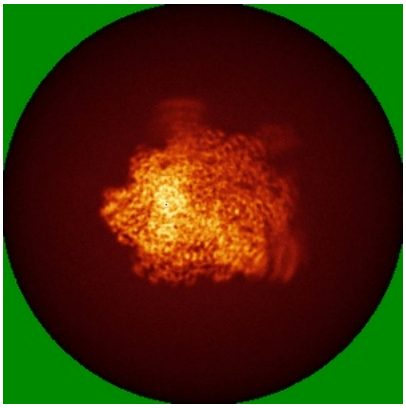

X

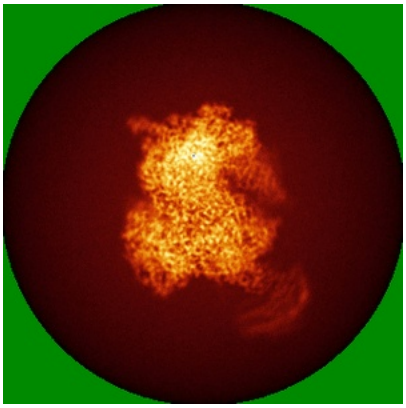

Y


Z

6.4.2 Raw map


X

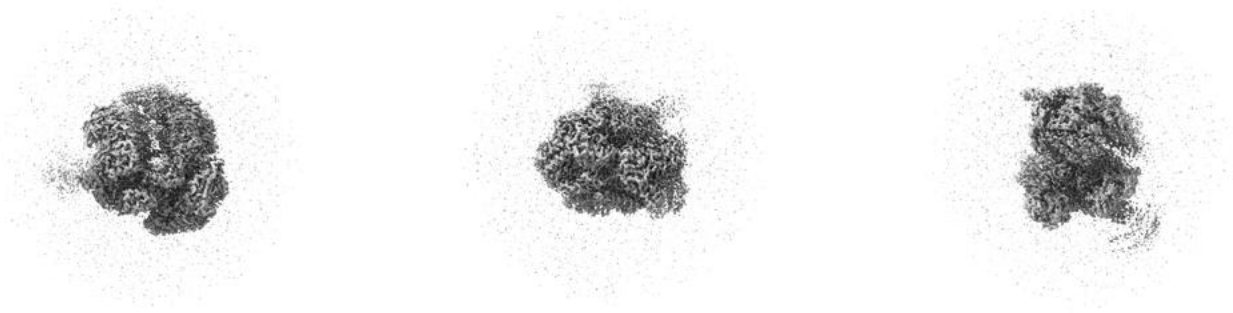

Y


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)

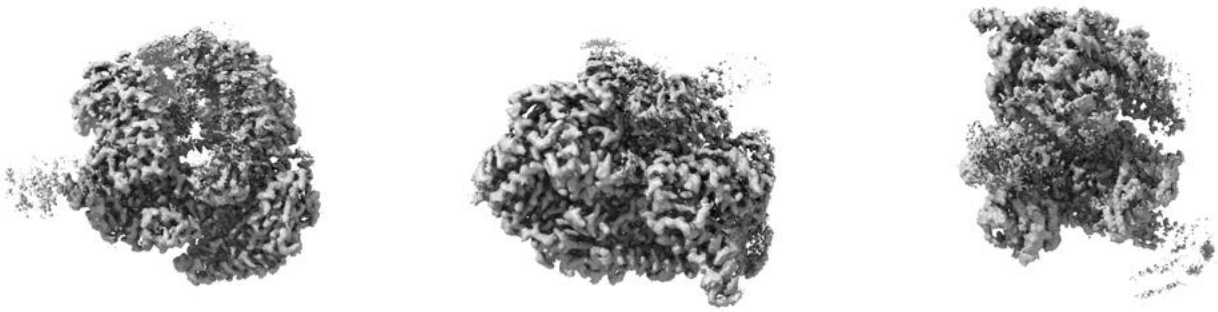
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0129. 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.

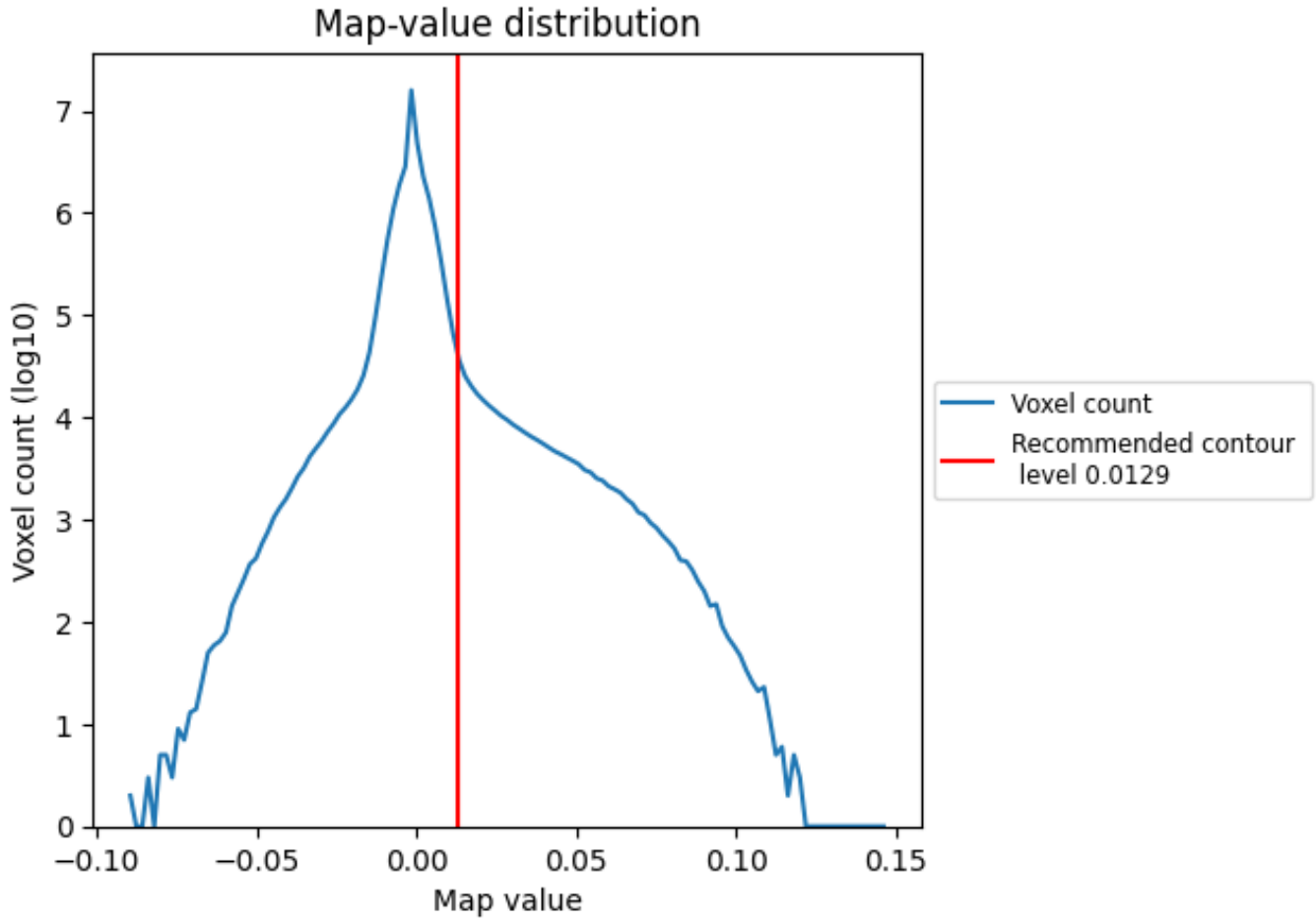
6.6 Mask visualisation (i)

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

7 Map analysis

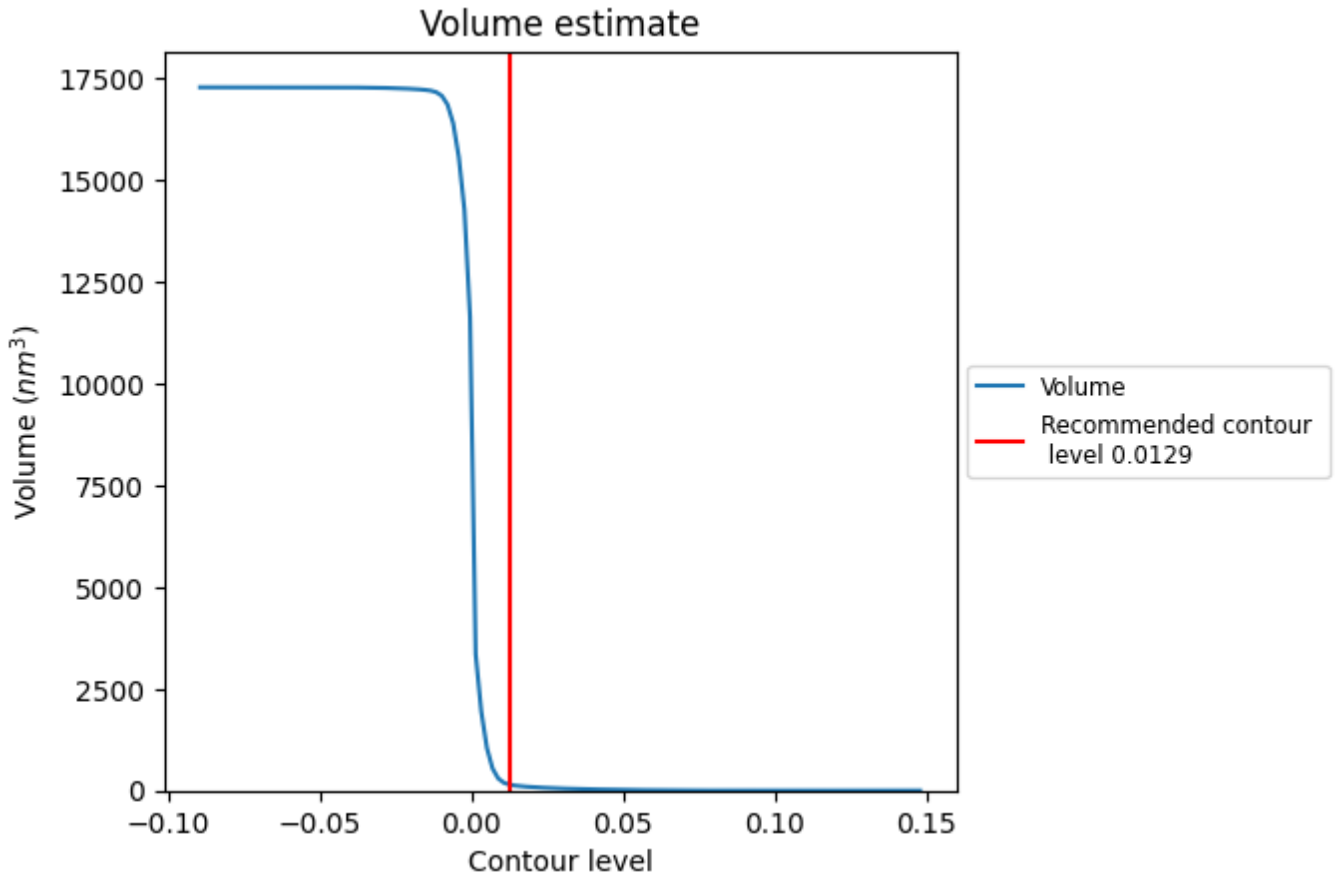
This section contains the results of statistical analysis of the map.

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.

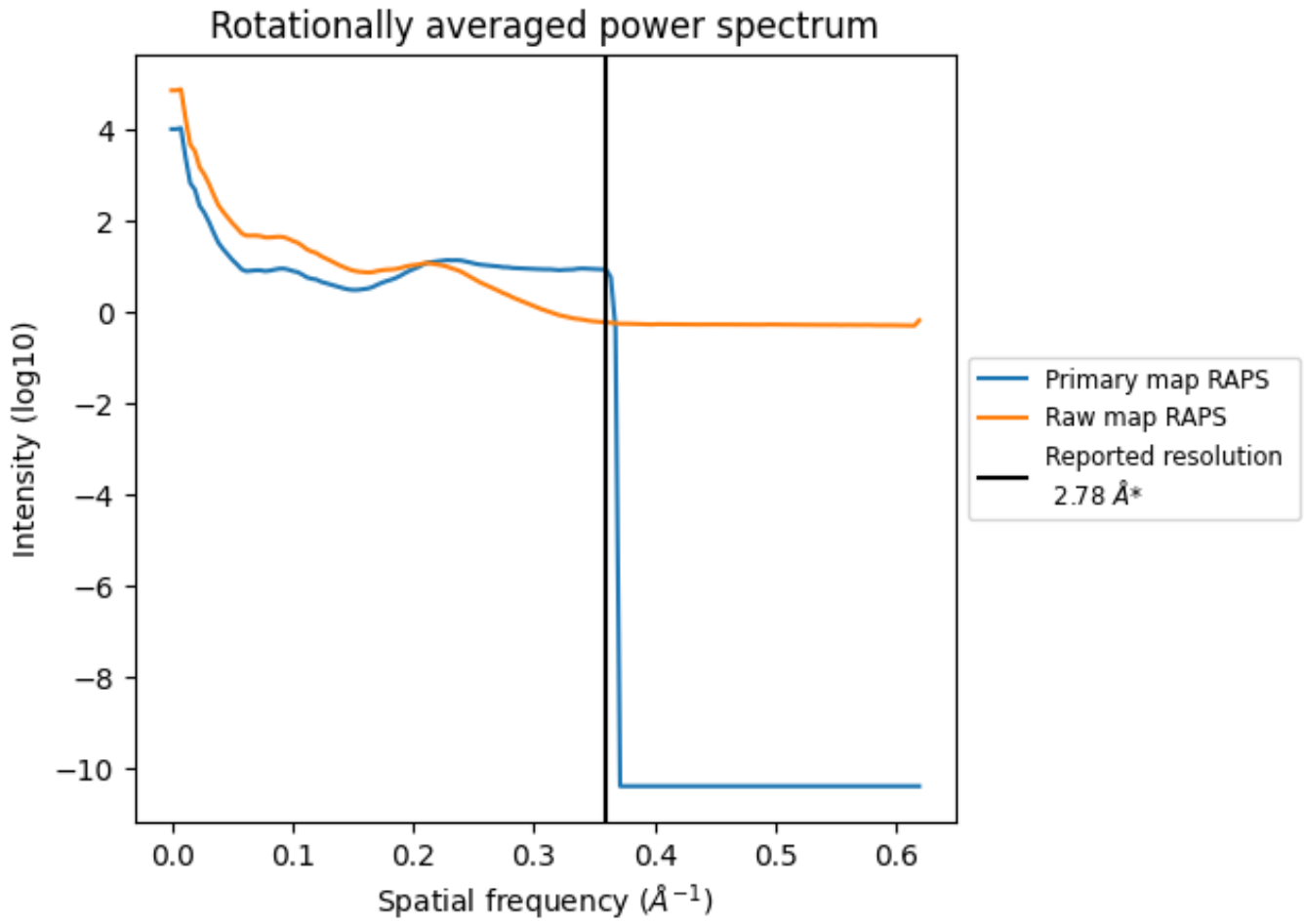
7.2 Volume estimate



The volume at the recommended contour level is 141 nm^3; this corresponds to an approximate mass of 127 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)

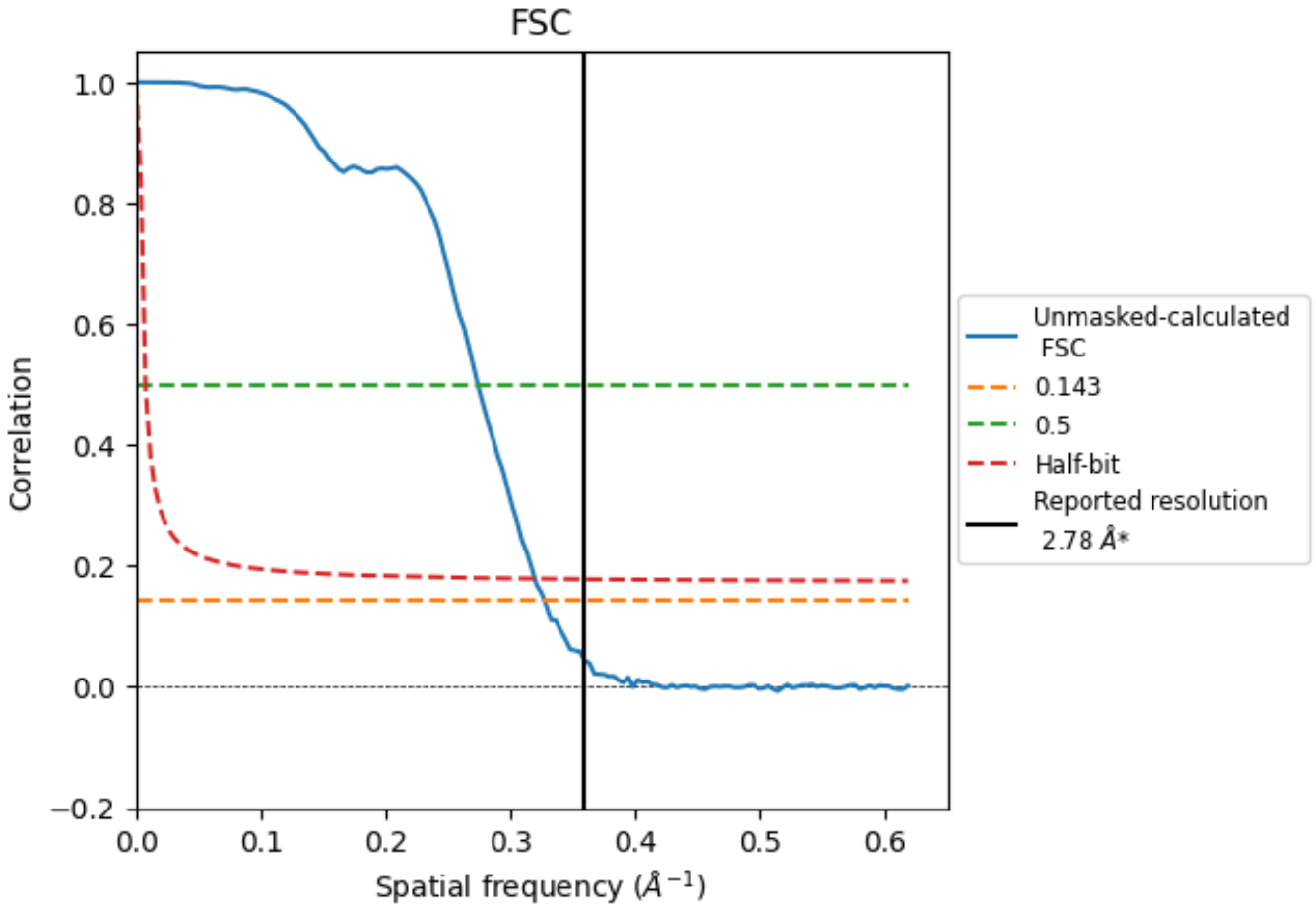


*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

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 0.360 Å^{-1}

8.2 Resolution estimates (i)

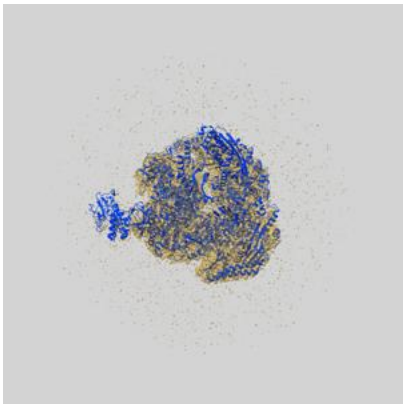
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.06	3.65	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.78 by more than 10 %

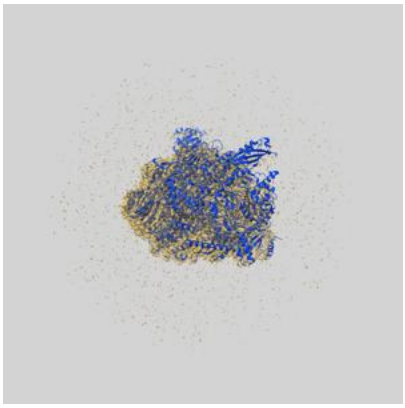
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39511 and PDB model 8YQZ. Per-residue inclusion information can be found in section 3 on page 6.

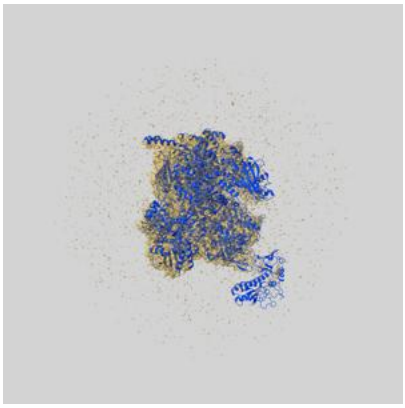
9.1 Map-model overlay



X



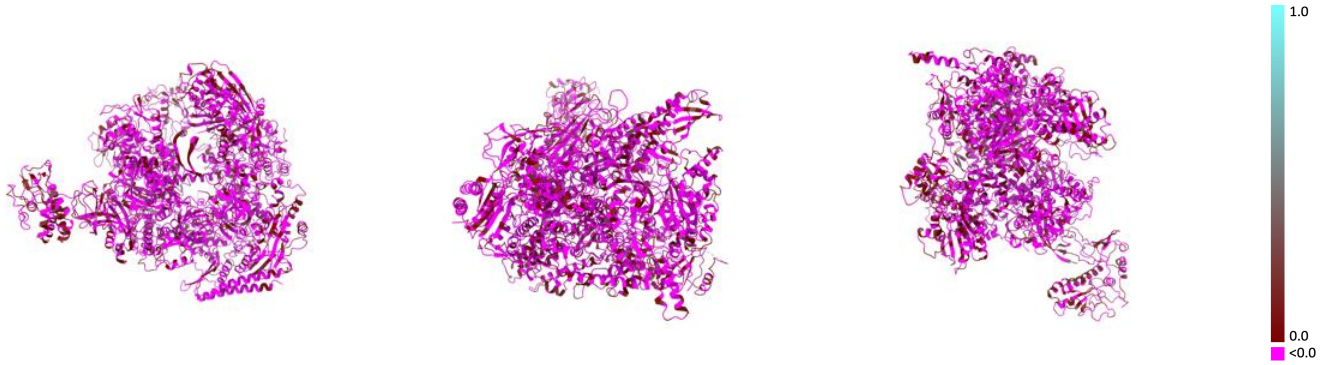
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0129 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.

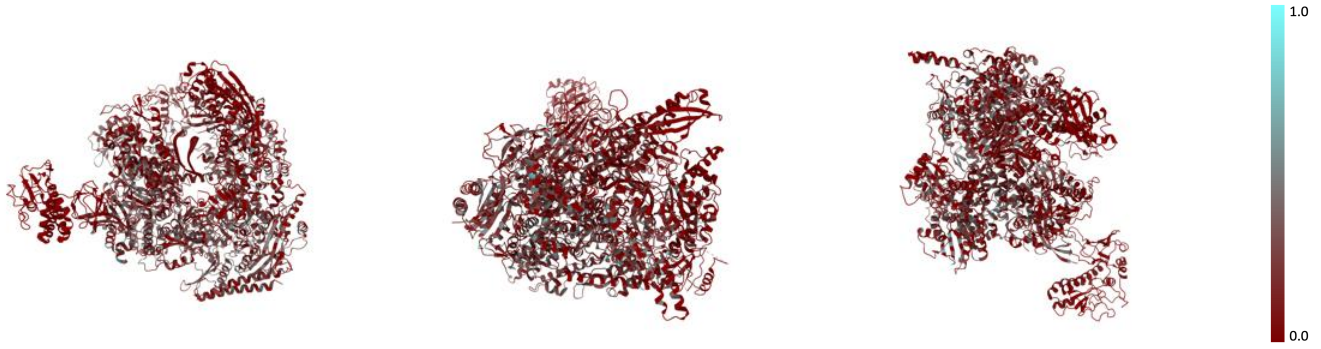
9.2 Q-score mapped to coordinate model



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.

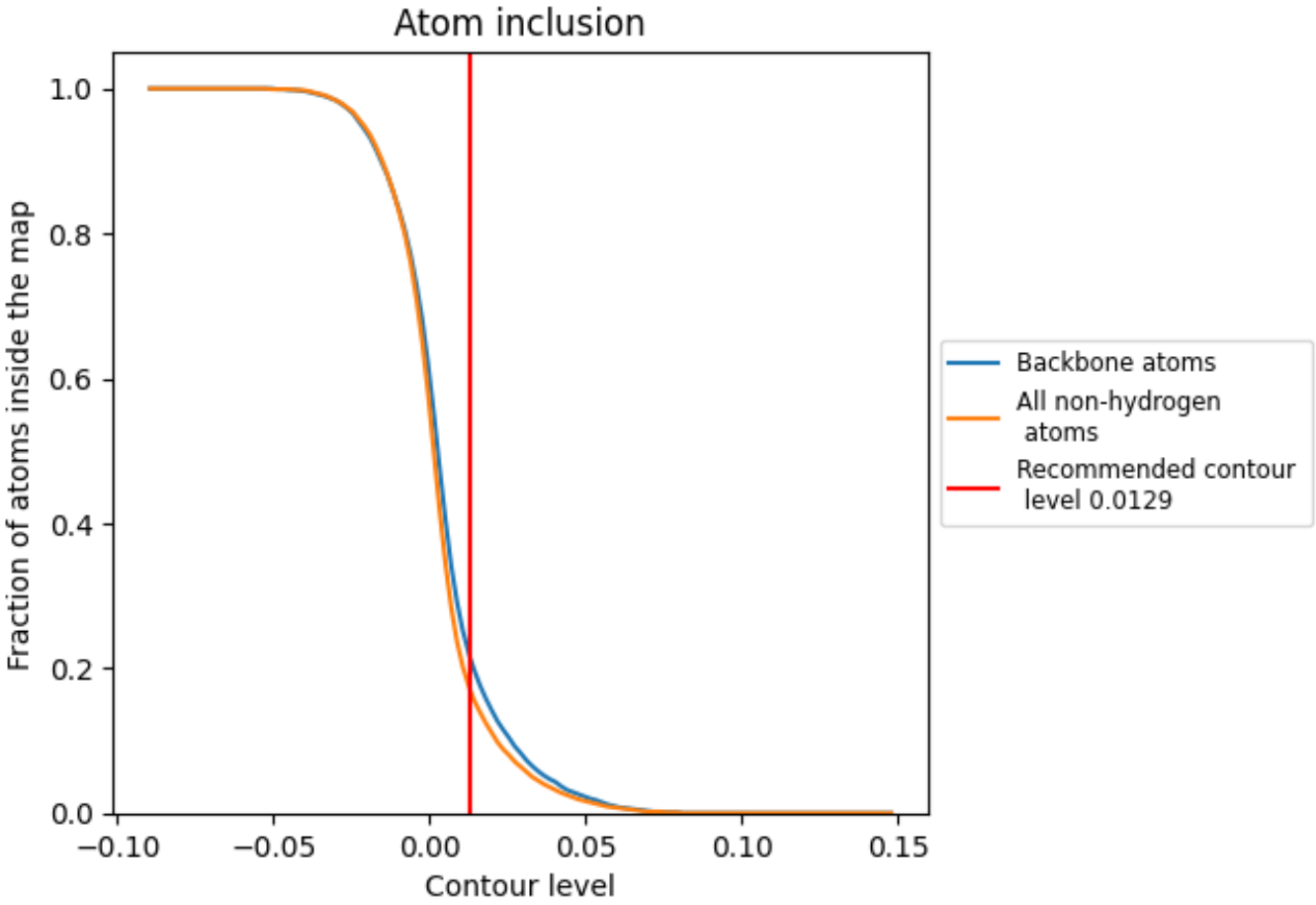
9.3 Atom inclusion mapped to coordinate model



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 (0.0129).

9.4 Atom inclusion (i)



At the recommended contour level, 22% of all backbone atoms, 17% 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 (0.0129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1710	-0.0810
A	0.2010	-0.0910
B	0.1300	-0.0990
C	0.2320	-0.0920
D	0.2530	-0.0250
E	0.2540	-0.0690
F	0.0530	-0.0120
G	0.2230	-0.0700
H	0.1880	-0.0890
X	0.0360	0.0190
Y	0.0140	-0.0090