Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 09:27 pm GMT

PDB ID	:	6EU3
EMDB ID	:	EMD-3958
Title	:	Apo RNA Polymerase III - closed conformation (cPOL3)
Authors	:	Abascal-Palacios, G.; Ramsay, E.P.; Beuron, F.; Morris, E.; Vannini, A.
Deposited on	:	2017-10-27
Resolution	:	3.30 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:

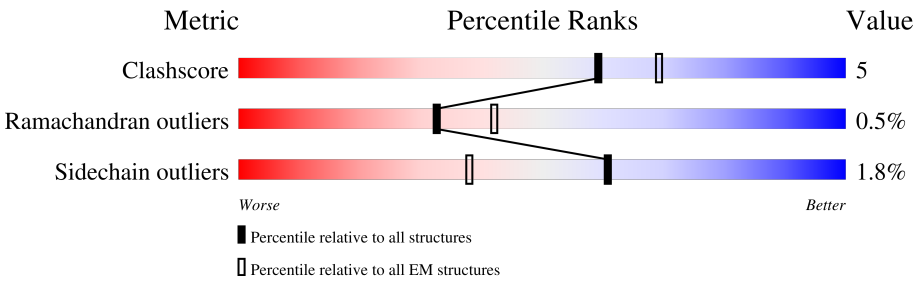
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1460	74%, 81%, 14%, •
2	B	1149	74%, 81%, 15%, • •
3	C	335	73%, 85%, 14%, •
4	D	161	51%, 62%, 11%, •, 26%
5	E	215	78%, 81%, 19%
6	F	155	40%, 45%, 9%, 46%
7	G	212	67%, 74%, 16%, 10%
8	H	146	82%, 77%, 18%, • •

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Mol	Chain	Length	Quality of chain
9	I	110	29% 33% 5% 62%
10	J	70	64% 86% 10%
11	K	142	51% 61% 10% 29%
12	L	70	44% 54% 10% 36%
13	M	282	44% 47% 11% 41%
14	N	422	21% 20% 5% 75%
15	O	654	56% 69% 12% 18%
16	P	317	25% 32% 5% 61%
17	Q	251	9% 15% 84%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 38330 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1402	10980	6924	1930	2068	58	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1114	8788	5558	1516	1654	60	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	335	2655	1681	454	511	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	119	977	628	156	187	6	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1759	1116	310	321	12	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	671	429	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	191	1544	1007	250	281	6	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	140	1120	703	188	224	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	42	321	204	47	64	6	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	68	558	356	97	99	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	792	496	130	161	5	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	45	358	221	71	62	4	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	165	1347	862	229	255	1	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	105	802	508	144	147	3	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	537	4316	2748	739	810	19	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	123	1024	667	161	192	4	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	40	311	204	50	57	0	0

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
18	A	2	2	2	0
18	B	1	1	1	0
18	I	1	1	1	0
18	J	1	1	1	0
18	L	1	1	1	0

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

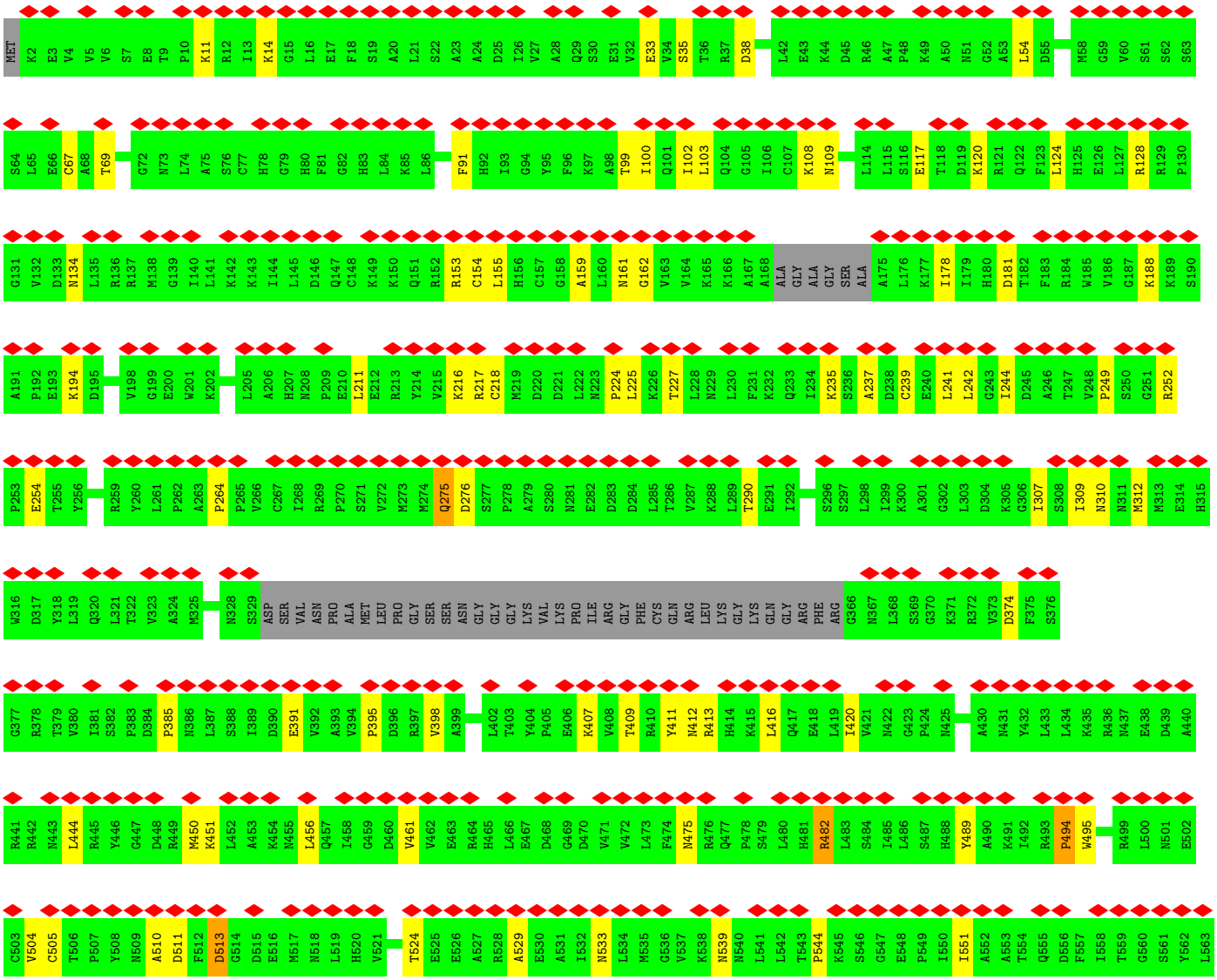
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
19	A	1	1	1	0

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: DNA-directed RNA polymerase III subunit RPC1

Chain A:



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N625 L626 D627 A628 K629 N630 K631 V632 F633 V634 P635 P636 K637 S638 K639 S640 L641 P642 N643 E644 M645 S646 Q647 N648 D649 G650 F651 V652 T653 I654 R655 G656 S657 Q658 I659 L660 S661 G662 V663 M664 D665 K666 S667 V668 L669 G670 D671 G672 K673 K674 H675 S676 V677 F678 Y679 T680 I681 L682 R683 D684

E689 A690 A691 N692 A693 M694 N695 R696 M697 A698 K699 L700 C701 A702 R703 F704 L705 G706 N707 R708 G709 F710 S711 I712 G713 I714 N715 D716 V717 T718 P719 A720 D721 D722 L723 K724 Q725 K726 K727 E728 E729 L730 V731 E732 I733 A734 Y735 H736 K737 C738 D739 E740 L741 I742 T743 L744 F745 N746 K747

G748 E749 L750 E751 T752 Q753 P754 G755 C756 N757 E758 E759 Q760 T761 L762 E763 A764 K765 I766 G767 G768 L769 L770 S771 K772 V773 R774 E775 E776 V777 G778 D779 V780 C781 I782 N783 E784 L785 D786 N787 W788 L792 I793 M794 A795 T796 S799 K800 G801 S802 T803 L804 N805 V806 S807 Q808 M809 V810

A811 V812 V813 G814 Q815 Q816 I817 I818 S819 G820 N821 R822 V823 P824 D825 G826 F827 Q828 D829 R830 S831 L832 P833 H834 F835 P836 K837 N838 S839 K840 T841 P842 Q843 S844 K845 G846 F847 V848 R849 N850 S851 F852 F853 S854 G855 L856 S857 P858 P859 E860 F861 L862 F863 H864 A865 I866 S867 G868 R869 E870

G871 L872 V873 D874 T875 A876 V877 K878 T879 A880 E881 T882 G883 Y884 M885 S886 R887 R888 L889 M890 K891 S892 L893 E894 D895 L896 S897 C898 Q899 Y900 D901 N902 T903 V904 R905 T906 S907 A908 N909 G910 I911 V912 Q913 F914 T915 Y916 G917 G918 D919 G920 L921 D922 P923 L924 E925 G928 N929 A930 Q931

P932 V933 N934 F935 N936 R937 S938 W939 D940 H941 A942 Y943 N944 I945 T946 F947 N948 N949 Q950 D951 K952 G953 L954 L955 P956 Y957 A958 I959 M960 E961 T962 A963 N964 E965 I966 L967 G968 P969 L970 E971 E972 R973 L974 V975 R976 Y977 D978 N979 S980 G981 C982 L983 V984 K985 R986 E987 D988 L989 N990 K991

A992 E993 Y994 V995 D996 Q997 Y998 D999 A1000 E1001 R1002 D1003 F1004 Y1005 H1006 S1007 L1008 R1009 E1010 Y1011 I1012 N1013 G1014 K1015 A1016 T1017 A1018 L1019 A1020 N1021 L1022 R1023 K1024 S1025 R1026 G1027 M1028 L1029 G1030 L1031 L1032 E1033 P1034 P1035 A1036 K1037 E1038 L1039 Q1040 G1041 I1042 D1043 P1044 D1045 E1046 T1047 V1048 P1049 D1050 N1051

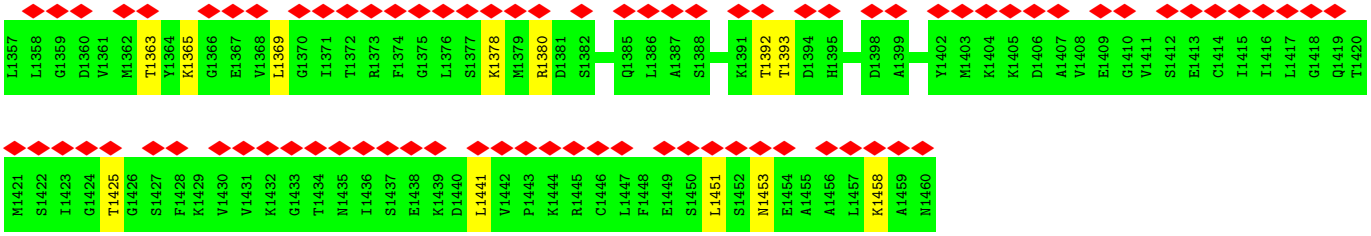
V1052 K1053 T1054 S1055 V1056 S1057 Q1058 L1059 Y1060 R1061 I1062 S1063 E1064 K1065 S1066 V1067 R1068 K1069 F1070 Y1071 L1072 E1073 I1074 A1075 L1076 K1077 Y1078 R1079 K1080 A1081 R1082 L1083 E1084 P1085 G1086 T1087 A1088 I1089 G1090 A1091 I1092 G1093 A1094 Q1095 S1096 I1097 G1098 E1099 P1100 G1101 T1102 Q1103 M1104 T1105 L1106 K1107 T1108 F1109 H1110 F1111

A1112 G1113 V1114 A1115 S1116 M1117 N1118 V1119 T1120 L1121 G1122 V1123 P1124 R1125 E1128 I1129 I1130 N1131 A1132 S1133 K1134 V1135 I1136 S1137 T1138 P1139 I1140 I1141 N1142 A1143 V1144 L1145 V1146 N1147 D1148 N1149 D1150 E1151 R1152 A1153 A1154 R1155 V1156 V1157 K1158 G1159 R1160 V1161 E1162 K1163 T1164 L1165 D1168 V1169 A1170 F1171 Y1172 V1173

Q1174 D1175 V1176 Y1177 K1178 D1179 N1180 L1181 S1182 F1183 I1184 Q1185 V1186 R1187 I1188 D1189 L1190 G1191 T1192 I1193 D1194 K1195 L1196 Q1197 L1198 E1199 L1200 T1201 I1202 E1203 D1204 I1205 A1206 I1209 A1212 S1213 K1214 L1215 K1216 I1217 Q1218 D1221 V1222 N1223 I1224 I1225 G1226 K1227 D1228 R1229 I1230 A1231 I1232 N1233 V1234 F1235 P1236

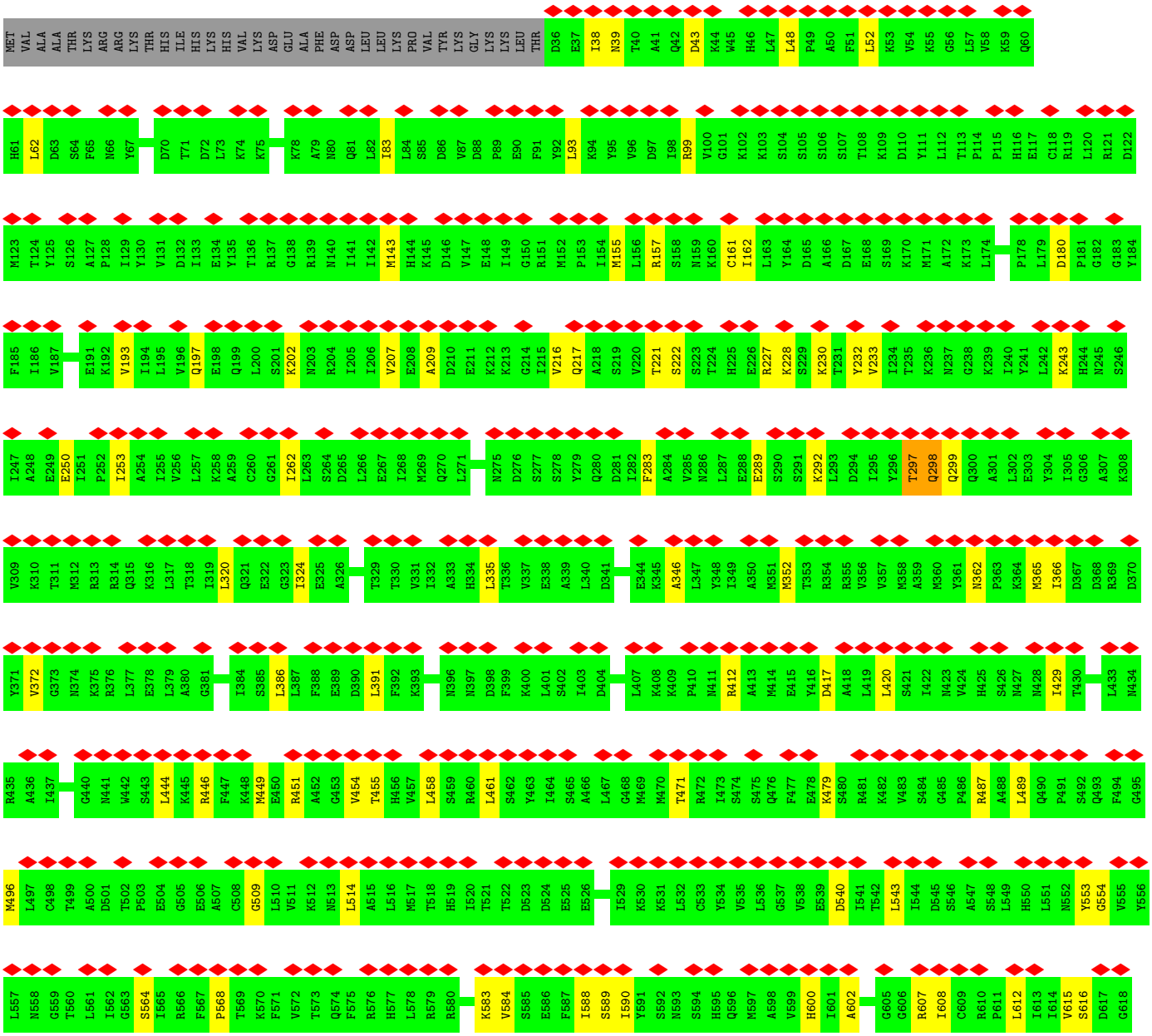
GLU GLY TYR LYS ALA LYS SER ILE SER THR SER ALA LYS GLU PRO S1252 E1253 N1254 D1255 V1256 F1257 Y1258 R1259 M1260 Q1261 Q1262 L1263 R1264 R1265 A1266 L1267 P1268 D1269 V1270 V1271 V1272 K1273 G1274 L1275 P1276 D1277 I1278 S1279 R1280 A1281 V1282 I1283 N1284 I1285 R1286 D1287 D1288 G1289 K1290 R1291 E1292 L1293 L1294 V1295 E1296

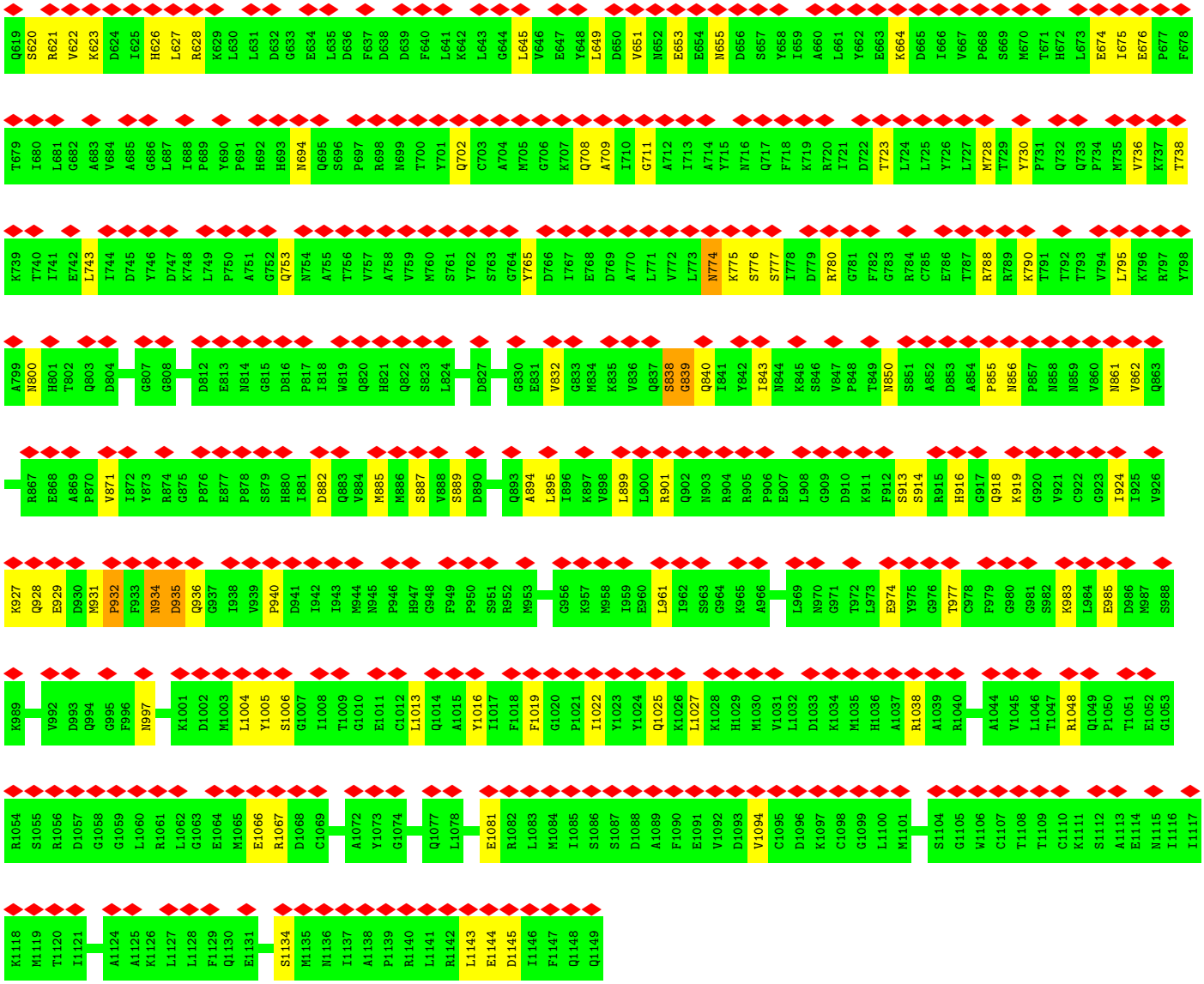
G1297 Y1298 G1299 L1300 R1301 D1302 V1303 M1304 C1305 T1306 D1307 G1308 V1309 I1310 G1311 S1312 R1313 T1314 T1315 T1316 N1317 H1318 V1319 L1320 E1321 V1322 F1323 S1324 V1325 L1326 G1327 I1328 E1329 A1330 A1331 R1332 Y1333 S1334 I1335 I1336 R1337 E1338 I1339 N1340 Y1341 T1342 M1343 S1344 N1345 H1346 G1347 M1348 S1349 V1350 D1351 P1352 R1353 H1354 I1355 Q1356



• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

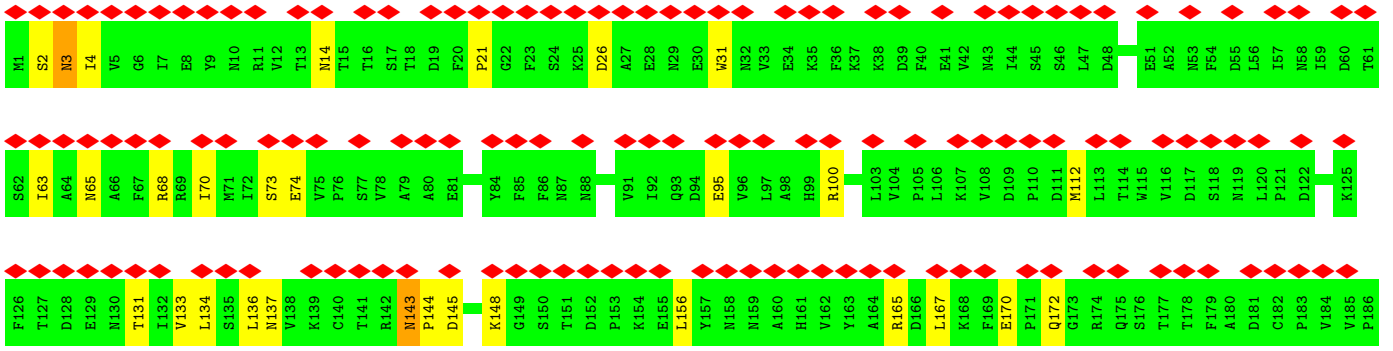
Chain B:

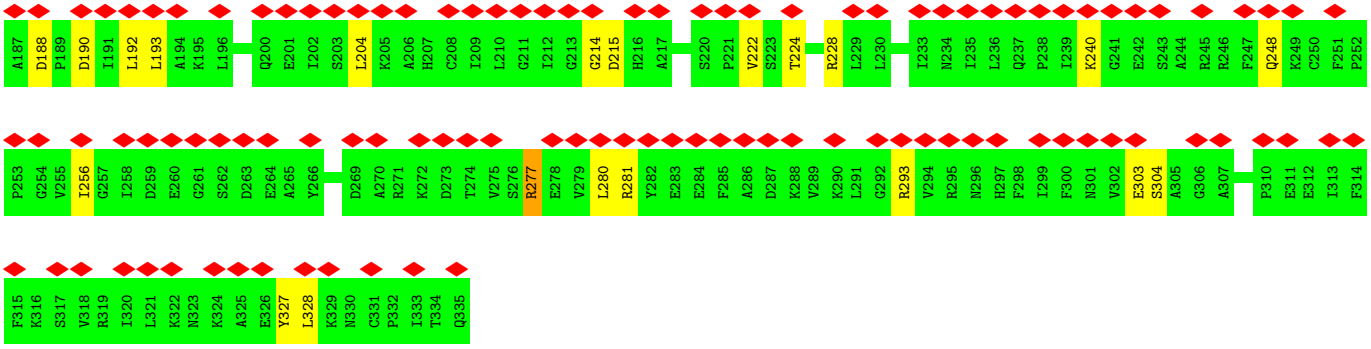




- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

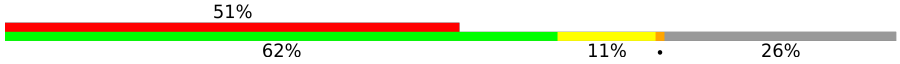
Chain C:

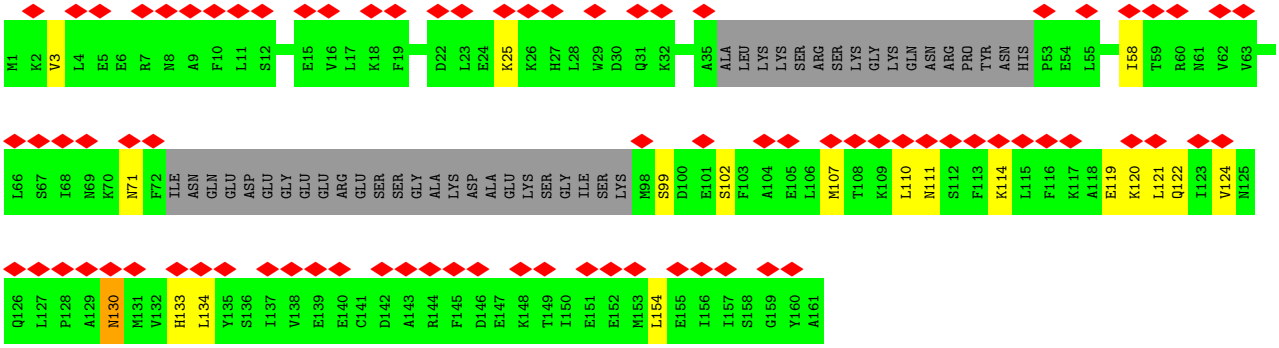




• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D:



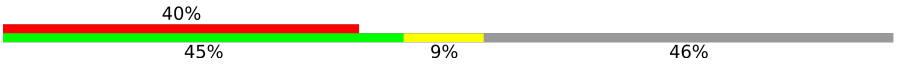


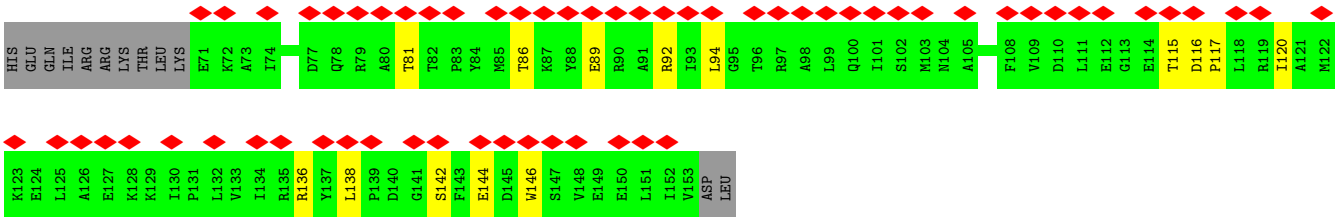
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

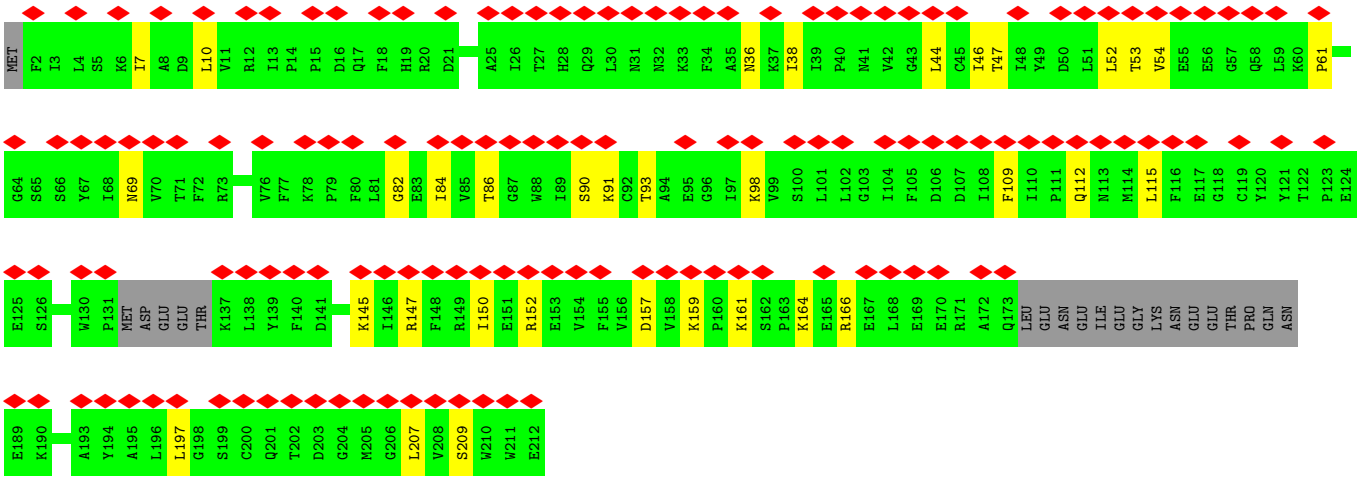
Chain F:





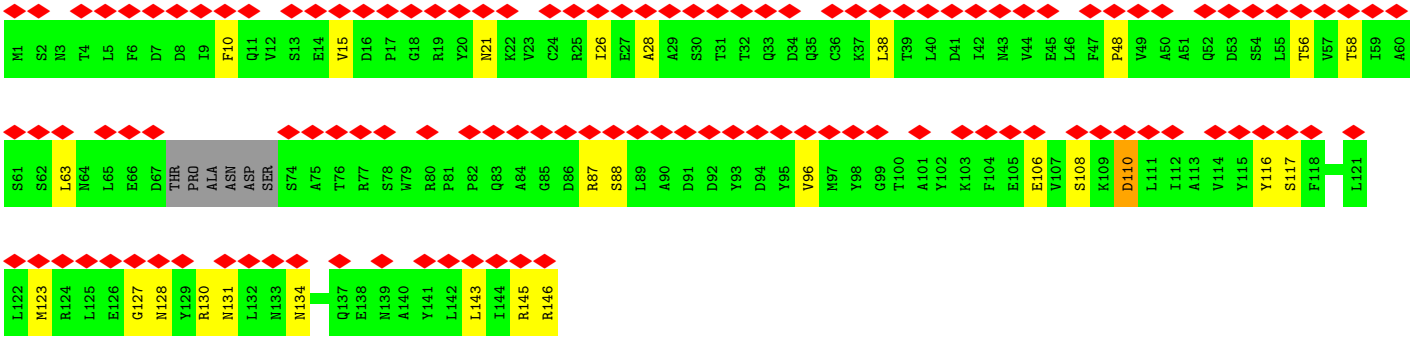
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:



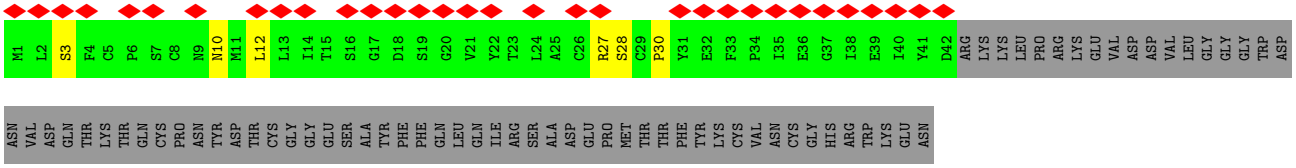
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



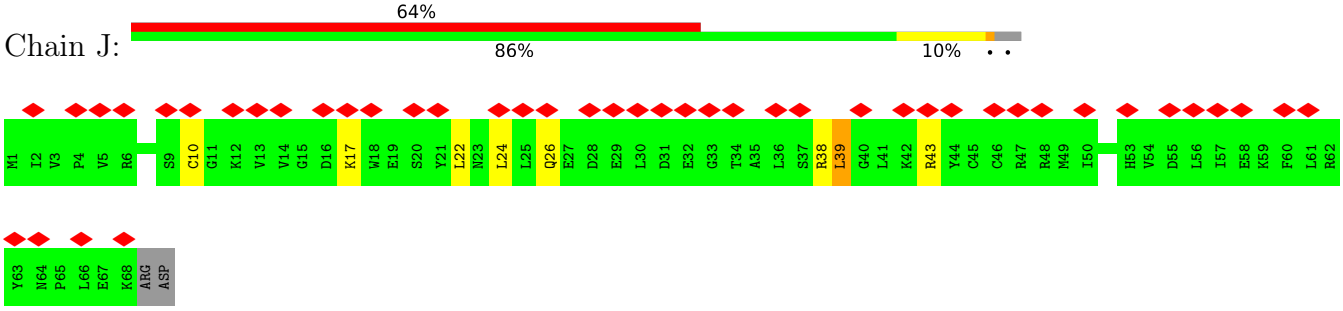
• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

Chain I:



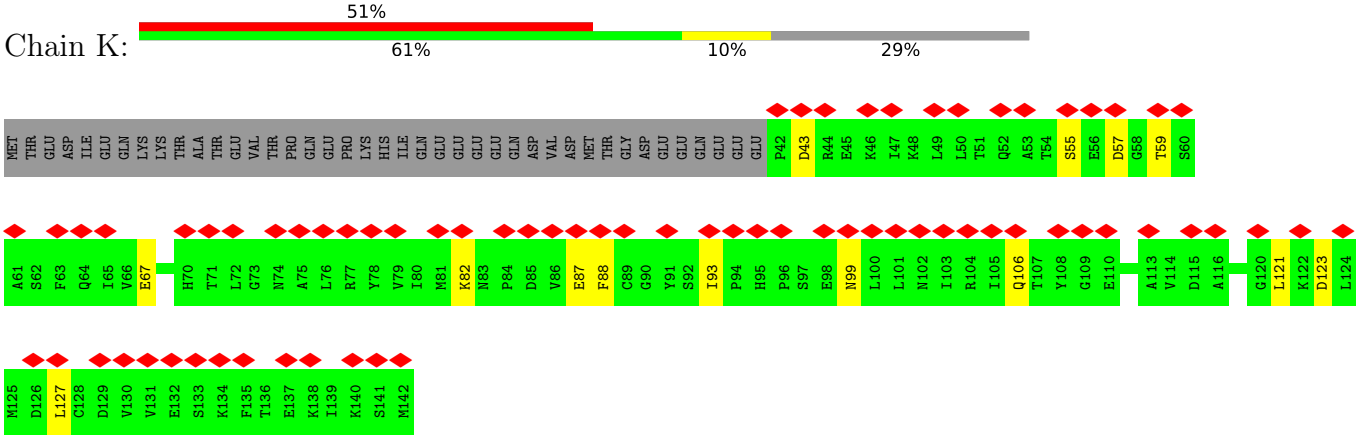
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



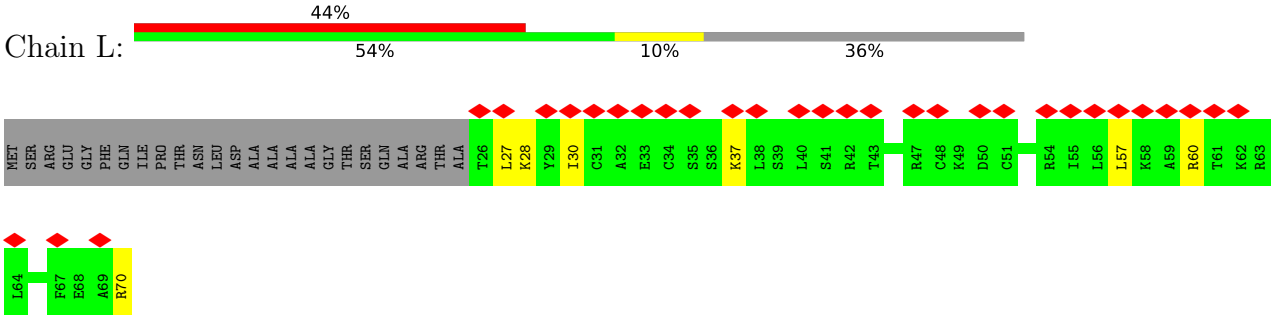
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



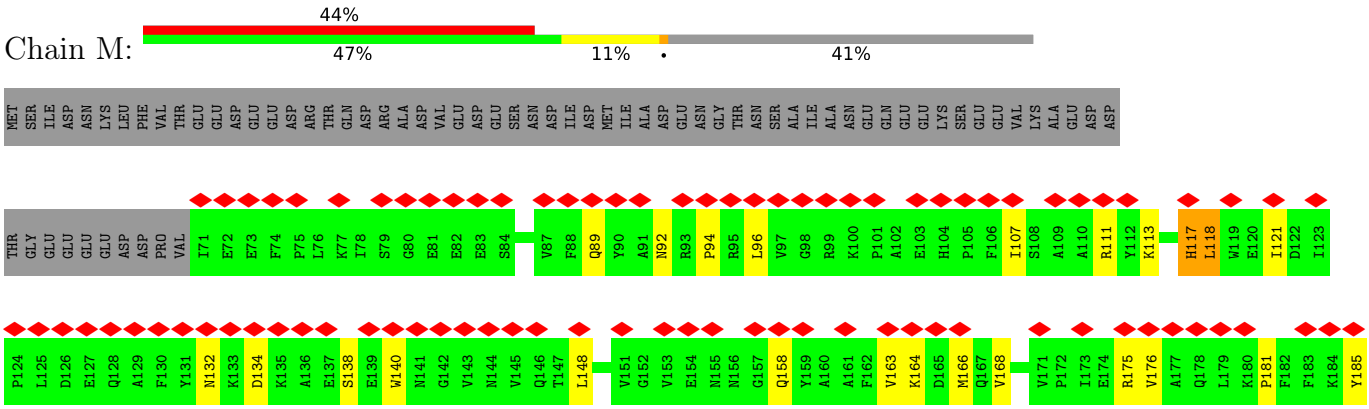
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

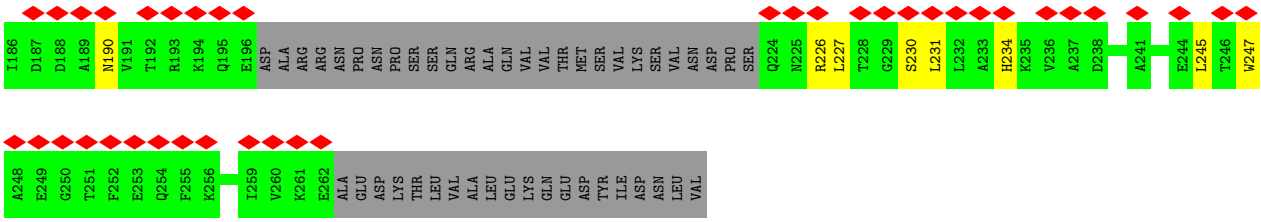
Chain L:



• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

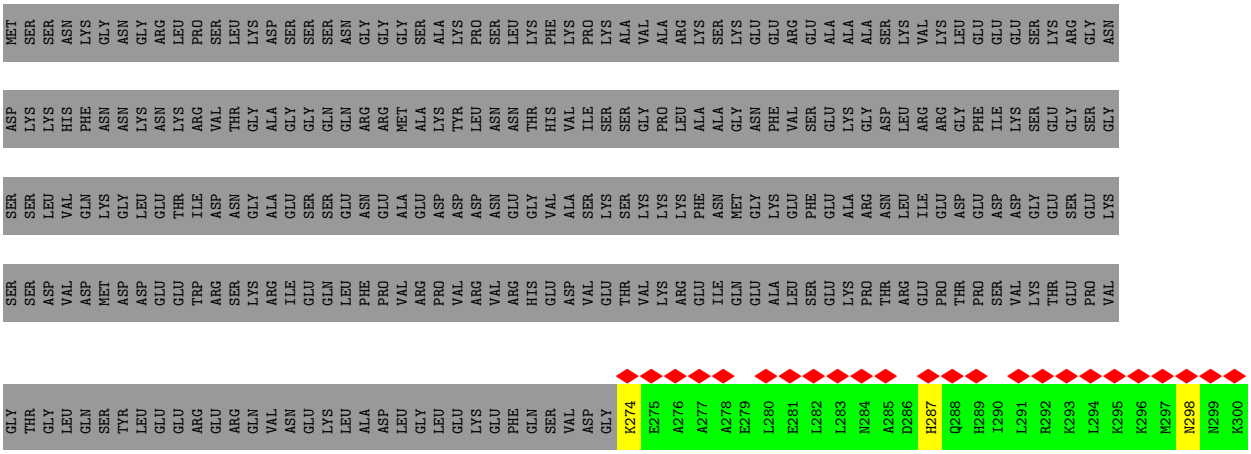
Chain M:

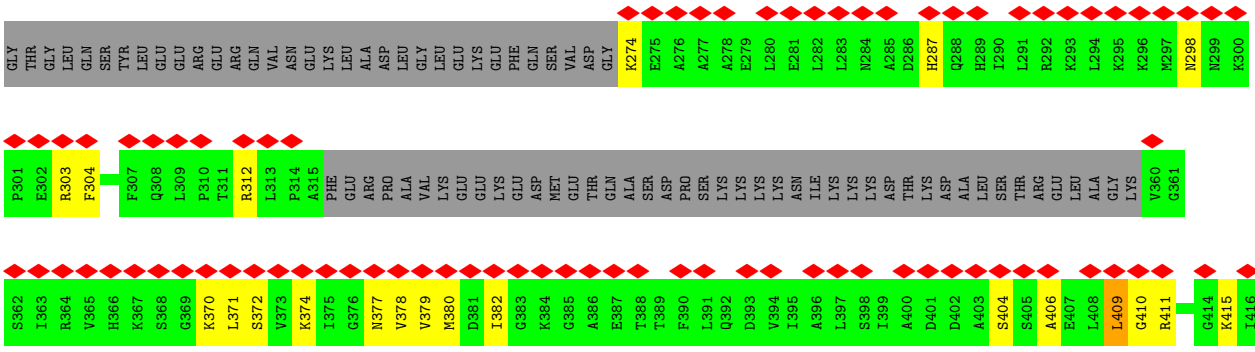


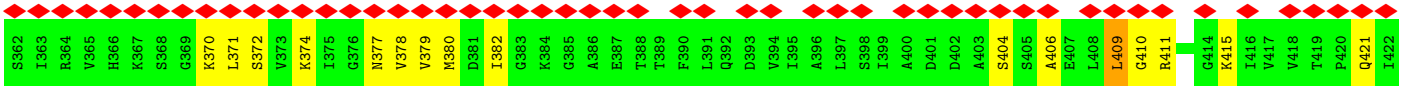


- Molecule 14: DNA-directed RNA polymerase III subunit RPC4

Chain N:

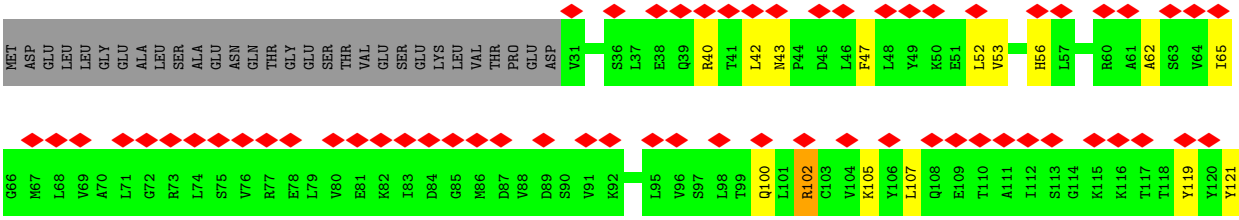


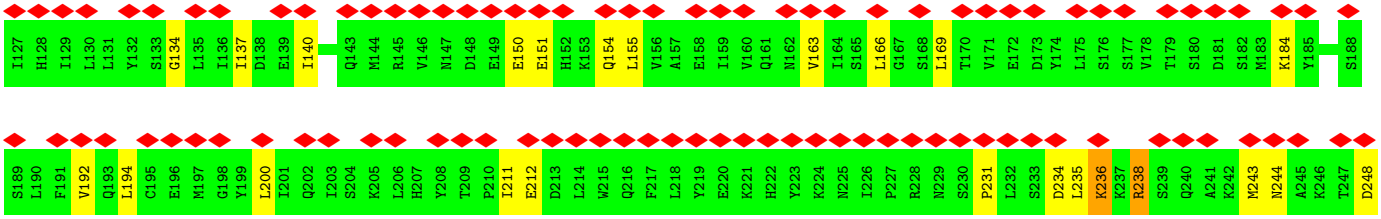


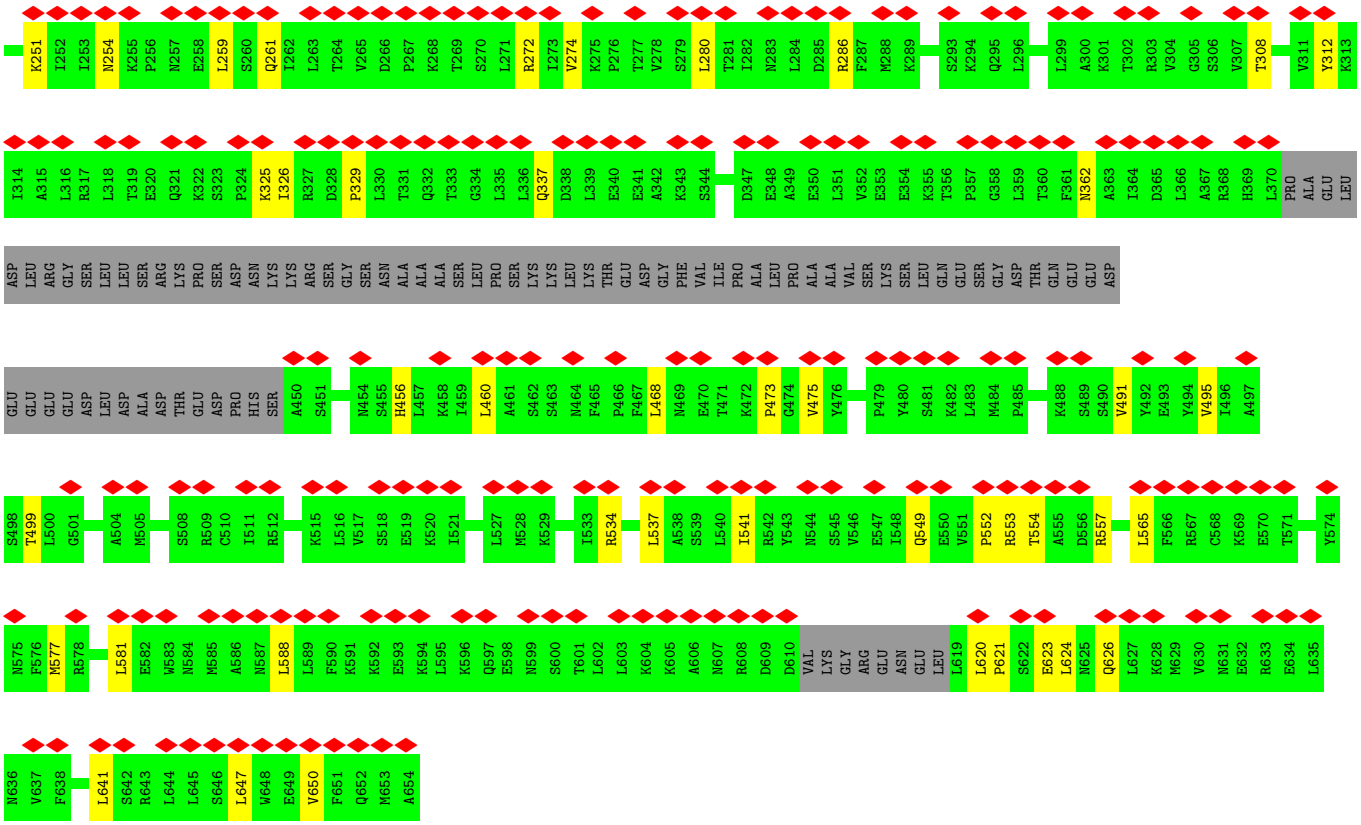


- Molecule 15: DNA-directed RNA polymerase III subunit RPC3

Chain O:

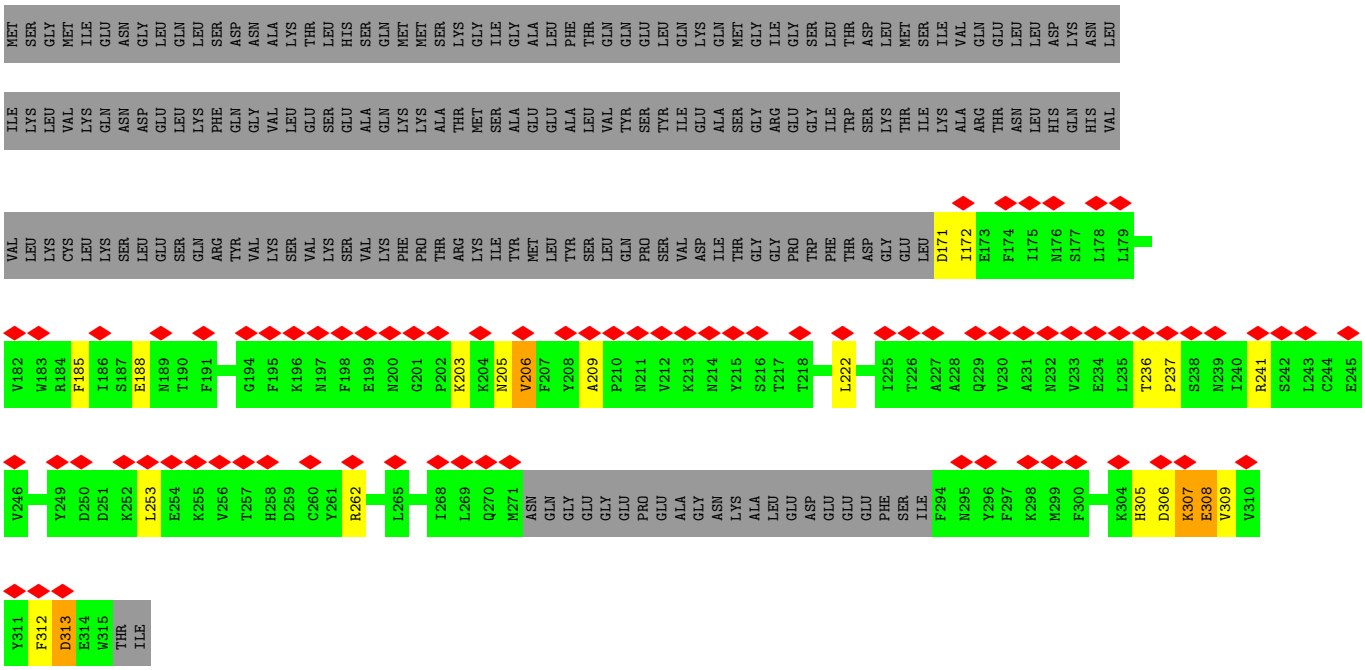






• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

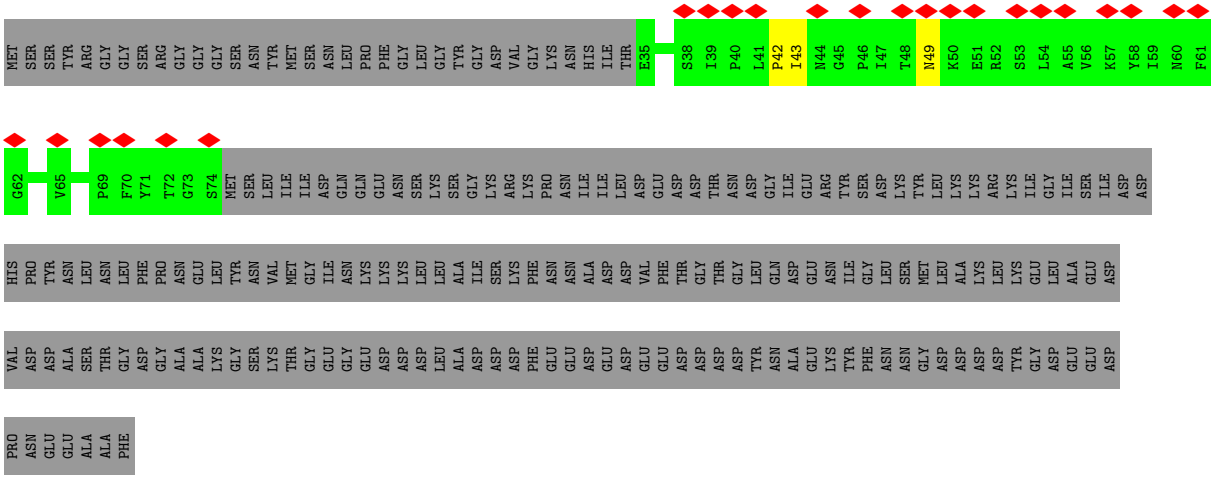
Chain P:



• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

Chain Q:

9%
15%
84%


MET SER SER TYR ARG GLY GLY SER ARG GLY GLY GLY SER ASN TYR MET SER ASN LEU PRO PHE GLY LEU GLY TYR GLY ASP VAL GLY LYS ASN HIS ILE THR E35 S38 I39 P40 L41 P42 I43 N44 G45 P46 I47 T48 N49 K50 E51 R52 S53 L54 A55 V56 K57 Y58 I59 N60 F61
G62 V65 P69 F70 Y71 T72 G73 S74 MET SER LEU ILE ILE ASP GLN GLN GLU GLU ASN SER LYS SER GLY LYS ARG LYS PRO ASN ILE ILE LEU ASP GLU ASP ASP THR ASN ASP GLY ILE GLU ARG TYR SER ASP LYS TYR LEU LYS LYS ARG LYS ILE GLY ILE SER ILE ASP ASP
HIS PRO TYR ASN LEU ASN LEU PHE PRO ASN GLU LEU TYR ASN VAL MET GLY ILE ASN LYS LYS LYS LEU LEU LEU ALA ILE SER LYS PHE ASN ASN ALA ASP ASP VAL PHE THR GLY THR GLY LEU GLN ASP GLU ASN ILE GLY LEU SER MET LEU ALA LYS LEU LYS GLU LEU ALA GLU ASP
VAL ASP ASP ALA SER THR GLY ASP GLY ALA ALA LYS GLY SER LYS THR GLY GLU GLY GLU ASP ASP ASP LEU ALA ASP ASP ASP PHE GLU GLU ASP GLU ASP GLU GLU ASP ASP ASP ASP TYR ASN ALA GLU LYS TYR PHE ASN ASN GLY ASP ASP ASP ASP TYR GLY ASP GLU GLU ASP
PRO ASN GLU GLU ALA ALA PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62306	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 ($e^-/Å^2$)	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	0.385	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	323.4, 323.4, 323.4	wwPDB
Map dimensions	308, 308, 308	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/11176	0.61	6/15104 (0.0%)
2	B	0.28	0/8943	0.60	2/12068 (0.0%)
3	C	0.28	0/2711	0.57	1/3676 (0.0%)
4	D	0.27	0/991	0.58	0/1328
5	E	0.30	0/1795	0.52	0/2416
6	F	0.28	0/683	0.58	0/923
7	G	0.28	0/1583	0.57	0/2146
8	H	0.29	0/1138	0.61	1/1540 (0.1%)
9	I	0.29	0/328	0.62	0/445
10	J	0.30	0/567	0.66	1/761 (0.1%)
11	K	0.27	0/803	0.62	1/1083 (0.1%)
12	L	0.30	0/360	0.67	0/478
13	M	0.29	0/1378	0.64	0/1863
14	N	0.29	0/810	0.73	1/1088 (0.1%)
15	O	0.27	0/4380	0.61	0/5908
16	P	0.33	0/1050	0.74	0/1424
17	Q	0.42	0/320	0.73	0/434
All	All	0.29	0/39016	0.61	13/52685 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	8
3	C	0	1
8	H	0	1
12	L	0	1
13	M	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	3
15	O	0	3
16	P	0	8
17	Q	0	1
All	All	0	36

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	409	LEU	N-CA-C	-6.86	92.49	111.00
1	A	54	LEU	CA-CB-CG	6.78	130.89	115.30
3	C	156	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	276	ASP	CB-CG-OD1	6.42	124.08	118.30
10	J	39	LEU	CA-CB-CG	6.10	129.33	115.30
2	B	335	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	1351	ASP	CB-CG-OD1	5.75	123.47	118.30
8	H	110	ASP	CB-CG-OD1	5.74	123.46	118.30
11	K	57	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	513	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	275	GLN	C-N-CA	5.19	134.69	121.70
1	A	585	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	839	GLY	N-CA-C	5.01	125.64	113.10

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1351	ASP	Peptide
1	A	218	CYS	Peptide
1	A	275	GLN	Peptide
1	A	494	PRO	Peptide
1	A	511	ASP	Peptide
1	A	631	LYS	Peptide
2	B	297	THR	Peptide
2	B	298	GLN	Peptide
2	B	583	LYS	Peptide
2	B	838	SER	Peptide
2	B	856	ASN	Peptide
2	B	889	SER	Peptide
2	B	932	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	B	934	ASN	Peptide
3	C	3	ASN	Peptide
8	H	108	SER	Peptide
12	L	28	LYS	Peptide
13	M	107	ILE	Peptide
13	M	117	HIS	Peptide
13	M	166	MET	Peptide
13	M	96	LEU	Peptide
14	N	377	ASN	Peptide
14	N	379	VAL	Peptide
14	N	410	GLY	Peptide
15	O	238	ARG	Peptide
15	O	248	ASP	Peptide
15	O	326	ILE	Peptide
16	P	205	ASN	Peptide
16	P	209	ALA	Peptide
16	P	236	THR	Peptide
16	P	306	ASP	Peptide
16	P	307	LYS	Peptide
16	P	308	GLU	Peptide
16	P	312	PHE	Peptide
16	P	313	ASP	Peptide
17	Q	43	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10980	0	11096	118	0
2	B	8788	0	8903	104	0
3	C	2655	0	2628	29	0
4	D	977	0	983	10	0
5	E	1759	0	1788	23	0
6	F	671	0	692	10	0
7	G	1544	0	1540	19	0
8	H	1120	0	1089	16	0
9	I	321	0	306	4	0
10	J	558	0	573	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	792	0	790	11	0
12	L	358	0	382	4	0
13	M	1347	0	1315	17	0
14	N	802	0	851	16	0
15	O	4316	0	4485	44	0
16	P	1024	0	992	6	0
17	Q	311	0	315	1	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
All	All	38330	0	38728	373	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 5.

All (373) 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:162:GLY:HA3	1:A:181:ASP:O	1.86	0.75
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.73	0.70
15:O:107:LEU:O	15:O:119:TYR:HB2	1.92	0.69
1:A:475:ASN:HD21	2:B:1066:GLU:HG2	1.60	0.65
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.79	0.65
7:G:90:SER:HB2	7:G:98:LYS:HG3	1.80	0.64
2:B:589:SER:HB3	2:B:653:GLU:HG3	1.81	0.63
2:B:607:ARG:HH11	2:B:651:VAL:HB	1.64	0.63
4:D:58:ILE:HD12	7:G:36:ASN:HD21	1.64	0.63
6:F:138:LEU:HB2	6:F:142:SER:HB2	1.81	0.63
2:B:887:SER:HB2	2:B:895:LEU:HB3	1.81	0.62
1:A:869:ARG:HH21	2:B:509:GLY:HA2	1.62	0.62
15:O:552:PRO:HG3	15:O:557:ARG:HA	1.80	0.62
1:A:1328:ILE:HD13	5:E:178:ILE:HG13	1.83	0.61
1:A:235:LYS:HG3	1:A:237:ALA:H	1.64	0.61
1:A:216:LYS:HD3	1:A:217:ARG:HG3	1.83	0.61
3:C:277:ARG:HB2	3:C:280:LEU:HD12	1.83	0.60
15:O:40:ARG:NH2	16:P:313:ASP:OD1	2.34	0.60
1:A:482:ARG:HH11	1:A:544:PRO:HG3	1.66	0.60
2:B:694:ASN:HD21	2:B:916:HIS:HD2	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.84	0.59
2:B:52:LEU:HD22	2:B:743:LEU:HD23	1.84	0.59
1:A:38:ASP:HB2	1:A:290:THR:HG23	1.83	0.59
1:A:1369:LEU:HD11	1:A:1378:LYS:HB3	1.85	0.59
1:A:1152:ARG:NH1	1:A:1197:GLN:OE1	2.36	0.59
1:A:573:ARG:HH22	11:K:87:GLU:HB3	1.67	0.58
3:C:63:ILE:HD13	11:K:127:LEU:HD21	1.85	0.58
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.36	0.58
2:B:675:ILE:HG22	2:B:676:GLU:HG3	1.83	0.58
2:B:776:SER:O	2:B:780:ARG:NH1	2.37	0.58
3:C:2:SER:O	3:C:14:ASN:ND2	2.37	0.58
1:A:252:ARG:NH2	1:A:254:GLU:OE2	2.36	0.58
1:A:652:VAL:HG22	1:A:662:GLY:HA3	1.87	0.57
1:A:154:CYS:SG	1:A:155:LEU:N	2.77	0.57
1:A:1184:ILE:HD12	1:A:1232:ILE:HB	1.86	0.57
10:J:24:LEU:HD12	10:J:39:LEU:HD12	1.86	0.57
1:A:103:LEU:O	1:A:108:LYS:NZ	2.37	0.57
2:B:612:LEU:HD12	2:B:649:LEU:HD12	1.84	0.57
10:J:22:LEU:O	10:J:26:GLN:NE2	2.38	0.57
2:B:788:ARG:NH1	2:B:882:ASP:OD2	2.38	0.56
2:B:588:ILE:HA	2:B:602:ALA:O	2.05	0.56
1:A:869:ARG:HD3	2:B:489:LEU:HB2	1.88	0.56
1:A:1206:ALA:HB2	1:A:1224:ILE:HD11	1.87	0.56
2:B:496:MET:HB3	2:B:608:ILE:HD12	1.87	0.56
15:O:620:LEU:HD22	15:O:623:GLU:HG2	1.87	0.56
6:F:92:ARG:HH21	7:G:61:PRO:HG3	1.69	0.56
1:A:505:CYS:HB2	1:A:510:ALA:HB3	1.88	0.56
8:H:58:THR:HB	8:H:143:LEU:HB2	1.88	0.56
1:A:407:LYS:HG2	1:A:461:VAL:HG22	1.86	0.56
1:A:1185:GLN:OE1	1:A:1229:ARG:NH1	2.39	0.56
16:P:203:LYS:HB2	16:P:206:VAL:HG22	1.87	0.55
2:B:299:GLN:HG3	13:M:190:ASN:HD22	1.71	0.55
1:A:533:ASN:O	1:A:539:ASN:ND2	2.40	0.55
2:B:622:VAL:HG22	2:B:645:LEU:HD23	1.88	0.55
15:O:137:ILE:HA	15:O:140:ILE:HG22	1.89	0.55
4:D:110:LEU:HD21	4:D:120:LYS:HB2	1.87	0.55
9:I:28:SER:O	13:M:185:TYR:OH	2.25	0.55
2:B:202:LYS:HB3	2:B:222:SER:HB2	1.89	0.55
2:B:882:ASP:HB3	2:B:901:ARG:HE	1.72	0.54
14:N:304:PHE:CE1	14:N:409:LEU:HB3	2.41	0.54
7:G:84:ILE:HD11	7:G:147:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:THR:HG22	7:G:145:LYS:HD2	1.89	0.54
13:M:163:VAL:HG22	13:M:168:VAL:HG22	1.90	0.54
1:A:654:ILE:HG12	1:A:659:ILE:HG13	1.90	0.54
1:A:1059:LEU:HD11	8:H:106:GLU:HB2	1.89	0.54
1:A:1441:LEU:HD21	7:G:54:VAL:HG22	1.89	0.54
2:B:838:SER:O	2:B:840:GLN:N	2.39	0.54
14:N:409:LEU:N	14:N:409:LEU:HD12	2.23	0.54
1:A:1055:SER:HB2	8:H:131:ASN:HD22	1.73	0.53
6:F:89:GLU:OE2	6:F:136:ARG:NH2	2.41	0.53
1:A:1023:ARG:NH2	1:A:1045:ASP:OD1	2.41	0.53
15:O:43:ASN:HB2	15:O:47:PHE:HB2	1.90	0.53
15:O:312:TYR:HB2	15:O:460:LEU:HD21	1.89	0.53
3:C:143:ASN:HD22	3:C:144:PRO:HD2	1.73	0.53
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.40	0.53
1:A:391:GLU:HG2	1:A:489:TYR:HB2	1.91	0.53
2:B:62:LEU:HA	2:B:155:MET:HE1	1.90	0.53
2:B:207:VAL:HG22	2:B:217:GLN:HG3	1.90	0.53
1:A:504:VAL:HG12	1:A:551:ILE:HD11	1.91	0.53
2:B:774:ASN:ND2	2:B:775:LYS:O	2.42	0.53
1:A:1278:ILE:HG13	1:A:1297:GLY:HA3	1.89	0.53
5:E:4:GLU:O	5:E:8:ASN:ND2	2.38	0.53
6:F:117:PRO:HA	6:F:120:ILE:HG12	1.91	0.52
2:B:209:ALA:HB2	2:B:366:ILE:HG21	1.90	0.52
7:G:91:LYS:NZ	7:G:93:THR:OG1	2.42	0.52
7:G:98:LYS:HB3	7:G:109:PHE:HD1	1.74	0.52
14:N:303:ARG:HG3	14:N:411:ARG:HB2	1.91	0.52
15:O:194:LEU:HD22	15:O:200:LEU:HG	1.91	0.52
1:A:1332:ARG:HB3	1:A:1363:THR:HG21	1.92	0.52
2:B:543:LEU:HG	13:M:176:VAL:HG11	1.91	0.52
5:E:185:ALA:HA	5:E:190:LEU:HD13	1.92	0.52
8:H:48:PRO:O	8:H:146:ARG:NH2	2.42	0.52
14:N:409:LEU:N	14:N:409:LEU:CD1	2.73	0.52
1:A:1304:MET:HG2	5:E:142:VAL:HG11	1.90	0.52
2:B:927:LYS:NZ	3:C:214:GLY:O	2.43	0.52
13:M:230:SER:O	13:M:234:HIS:ND1	2.41	0.52
2:B:612:LEU:HD22	2:B:674:GLU:HA	1.90	0.51
15:O:150:GLU:HG2	15:O:151:GLU:HG3	1.92	0.51
1:A:652:VAL:HG21	1:A:668:VAL:HG21	1.91	0.51
1:A:224:PRO:HA	1:A:227:THR:HG22	1.91	0.51
1:A:1253:GLU:OE2	9:I:27:ARG:NH1	2.44	0.51
1:A:1425:THR:HG22	6:F:92:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:736:VAL:HG12	2:B:974:GLU:HB2	1.92	0.51
14:N:380:MET:SD	14:N:421:GLN:NE2	2.83	0.51
1:A:873:VAL:HG21	2:B:487:ARG:HB3	1.92	0.51
1:A:1329:GLU:OE2	5:E:200:ARG:NE	2.44	0.51
7:G:161:LYS:HZ2	7:G:166:ARG:HA	1.76	0.51
2:B:553:TYR:HD2	2:B:568:PRO:HG2	1.76	0.51
14:N:372:SER:HB2	14:N:382:ILE:HG22	1.91	0.51
15:O:102:ARG:O	15:O:123:ASN:ND2	2.43	0.51
1:A:1351:ASP:O	1:A:1353:ARG:N	2.44	0.51
1:A:894:GLU:OE2	2:B:1067:ARG:NH1	2.44	0.51
2:B:623:LYS:H	2:B:626:HIS:HD2	1.58	0.51
1:A:307:ILE:HD11	1:A:312:MET:HG2	1.91	0.50
1:A:808:GLN:HE21	1:A:813:VAL:HG13	1.77	0.50
7:G:52:LEU:HD12	7:G:53:THR:HG22	1.93	0.50
2:B:197:GLN:HE22	2:B:454:VAL:HG22	1.75	0.50
1:A:813:VAL:HG23	1:A:851:SER:HA	1.92	0.50
2:B:616:SER:HG	2:B:621:ARG:HH21	1.57	0.50
1:A:413:ARG:NH1	1:A:456:LEU:O	2.41	0.50
2:B:372:VAL:HB	2:B:651:VAL:HG11	1.93	0.50
2:B:554:GLY:HA2	2:B:564:SER:HA	1.93	0.50
3:C:100:ARG:NH1	3:C:193:LEU:O	2.45	0.50
1:A:1323:PHE:HE1	1:A:1328:ILE:HG13	1.77	0.50
3:C:143:ASN:ND2	3:C:145:ASP:OD1	2.44	0.50
15:O:308:THR:HG23	15:O:456:HIS:HB3	1.94	0.50
11:K:67:GLU:HA	11:K:99:ASN:HB3	1.93	0.50
15:O:163:VAL:HA	15:O:169:LEU:HD13	1.93	0.50
1:A:124:LEU:HD23	1:A:128:ARG:HH12	1.77	0.50
8:H:127:GLY:HA3	8:H:130:ARG:HH21	1.77	0.49
1:A:1160:ARG:NH1	1:A:1307:ASP:O	2.45	0.49
2:B:738:THR:HG23	2:B:977:THR:HA	1.95	0.49
1:A:124:LEU:HD12	1:A:241:LEU:HD21	1.94	0.49
1:A:788:TRP:NE1	8:H:21:ASN:OD1	2.45	0.49
2:B:543:LEU:O	13:M:89:GLN:NE2	2.43	0.49
14:N:304:PHE:CE1	14:N:409:LEU:CB	2.96	0.49
9:I:3:SER:HB2	9:I:12:LEU:HD11	1.95	0.49
1:A:1258:TYR:O	1:A:1262:GLN:NE2	2.45	0.49
5:E:50:MET:SD	5:E:52:ARG:NH1	2.79	0.49
13:M:113:LYS:HE3	13:M:118:LEU:HB3	1.93	0.49
1:A:623:VAL:HG13	1:A:656:GLY:HA2	1.95	0.48
1:A:1223:ASN:HD21	1:A:1231:ALA:HB3	1.78	0.48
1:A:1365:LYS:NZ	1:A:1378:LYS:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:VAL:HG22	2:B:233:VAL:HG23	1.94	0.48
1:A:1121:LEU:O	1:A:1342:THR:OG1	2.32	0.48
2:B:800:ASN:HD22	2:B:855:PRO:HG2	1.78	0.48
2:B:1005:TYR:OH	3:C:293:ARG:NH1	2.47	0.48
5:E:109:ILE:HG22	5:E:133:GLU:HB2	1.94	0.48
12:L:27:LEU:HD11	12:L:37:LYS:HD2	1.95	0.48
1:A:14:LYS:HD3	2:B:1144:GLU:HB3	1.96	0.48
1:A:1120:THR:HG22	1:A:1125:ARG:HB2	1.96	0.48
1:A:1194:ASP:O	1:A:1197:GLN:NE2	2.46	0.48
2:B:901:ARG:NH1	3:C:95:GLU:OE1	2.38	0.48
5:E:47:CYS:HA	5:E:53:PRO:HA	1.94	0.48
5:E:32:GLN:HE21	5:E:36:GLU:HG3	1.79	0.48
5:E:171:LYS:H	5:E:174:GLN:HE21	1.61	0.48
1:A:109:ASN:HD22	1:A:159:ALA:HB2	1.79	0.48
1:A:249:PRO:HB2	15:O:42:LEU:HD22	1.94	0.48
2:B:243:LYS:HA	2:B:250:GLU:HG2	1.96	0.48
3:C:224:THR:OG1	3:C:303:GLU:OE1	2.30	0.48
3:C:327:TYR:OH	11:K:43:ASP:OD2	2.32	0.48
1:A:409:THR:HG23	1:A:411:TYR:H	1.78	0.48
1:A:1136:ILE:HD11	1:A:1139:PRO:HB3	1.96	0.48
1:A:1451:LEU:HD13	4:D:107:MET:HG3	1.95	0.48
2:B:711:GLY:HA2	2:B:728:MET:HB2	1.96	0.48
2:B:929:GLU:OE2	3:C:73:SER:OG	2.25	0.47
2:B:940:PRO:HG3	2:B:1019:PHE:HE1	1.78	0.47
7:G:152:ARG:HB3	7:G:197:LEU:HD12	1.96	0.47
1:A:211:LEU:O	15:O:553:ARG:NH2	2.48	0.47
16:P:222:LEU:HB2	16:P:241:ARG:NH1	2.28	0.47
2:B:38:ILE:HG13	2:B:628:ARG:HG2	1.96	0.47
4:D:130:ASN:H	4:D:133:HIS:CE1	2.33	0.47
2:B:161:CYS:SG	2:B:162:ILE:N	2.87	0.47
1:A:117:GLU:HG3	15:O:212:GLU:HG3	1.96	0.47
5:E:119:SER:O	5:E:122:LYS:NZ	2.47	0.47
13:M:134:ASP:O	13:M:138:SER:CB	2.63	0.47
1:A:832:LEU:HD21	1:A:862:LEU:HD23	1.97	0.47
2:B:43:ASP:HB3	2:B:627:LEU:HD13	1.97	0.47
2:B:217:GLN:HB3	2:B:232:TYR:HB3	1.96	0.47
3:C:188:ASP:OD1	3:C:188:ASP:N	2.46	0.47
5:E:91:LYS:HE3	15:O:231:PRO:HG2	1.96	0.47
15:O:499:THR:HG23	17:Q:42:PRO:HA	1.97	0.47
15:O:581:LEU:HD11	15:O:647:LEU:HD12	1.97	0.47
2:B:227:ARG:NH2	2:B:449:MET:SD	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:287:HIS:HB3	14:N:371:LEU:HD13	1.96	0.47
15:O:140:ILE:HD11	15:O:194:LEU:HD21	1.96	0.47
1:A:1058:GLN:NE2	8:H:134:ASN:O	2.48	0.47
14:N:374:LYS:HA	14:N:380:MET:HG2	1.97	0.47
1:A:385:PRO:HD2	2:B:765:TYR:CD1	2.50	0.46
2:B:931:MET:HB3	2:B:940:PRO:HD2	1.97	0.46
2:B:193:VAL:HG21	2:B:458:LEU:HD23	1.96	0.46
2:B:702:GLN:HE22	2:B:1025:GLN:HE22	1.63	0.46
2:B:850:ASN:ND2	2:B:862:VAL:O	2.45	0.46
15:O:552:PRO:HB2	15:O:554:THR:HG22	1.96	0.46
1:A:33:GLU:HG2	1:A:35:SER:H	1.80	0.46
2:B:788:ARG:HB3	2:B:899:LEU:HD11	1.98	0.46
13:M:245:LEU:HD21	14:N:404:SER:HA	1.96	0.46
5:E:97:VAL:HG13	5:E:127:ILE:HD11	1.97	0.46
4:D:119:GLU:HA	4:D:122:GLN:HB2	1.97	0.46
13:M:117:HIS:CE1	13:M:175:ARG:HH12	2.34	0.46
15:O:549:GLN:O	15:O:565:LEU:HB2	2.15	0.46
2:B:776:SER:HB2	2:B:928:GLN:HB2	1.98	0.46
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.98	0.46
1:A:264:PRO:HG3	2:B:1134:SER:HB2	1.98	0.46
1:A:529:ALA:O	1:A:533:ASN:ND2	2.49	0.46
3:C:21:PRO:HD2	11:K:82:LYS:HA	1.98	0.46
7:G:10:LEU:HA	7:G:69:ASN:HA	1.97	0.46
13:M:158:GLN:HE22	14:N:415:LYS:HE3	1.81	0.46
1:A:967:LEU:HD22	1:A:1009:ARG:HH21	1.81	0.46
2:B:262:ILE:HG12	2:B:346:ALA:HB1	1.98	0.46
2:B:540:ASP:HB3	2:B:543:LEU:HD13	1.96	0.46
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.84	0.46
15:O:52:LEU:O	15:O:56:HIS:ND1	2.47	0.46
2:B:832:VAL:HB	12:L:60:ARG:HA	1.98	0.45
7:G:112:GLN:HG2	7:G:115:LEU:HD22	1.98	0.45
7:G:157:ASP:HB3	7:G:159:LYS:HG3	1.97	0.45
15:O:621:PRO:HA	15:O:624:LEU:HD23	1.97	0.45
1:A:374:ASP:OD1	2:B:1038:ARG:NH1	2.36	0.45
2:B:934:ASN:O	2:B:936:GLN:N	2.48	0.45
8:H:63:LEU:HB3	8:H:88:SER:HB2	1.99	0.45
1:A:597:ILE:HB	1:A:603:LEU:HB2	1.98	0.45
1:A:1332:ARG:HA	1:A:1335:ILE:HG22	1.98	0.45
2:B:1094:VAL:HG23	2:B:1143:LEU:HD11	1.97	0.45
13:M:121:ILE:HG22	13:M:148:LEU:HB2	1.98	0.45
1:A:1112:ALA:HB1	1:A:1116:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ASP:HB3	1:A:984:VAL:HG12	1.98	0.45
1:A:1458:LYS:NZ	4:D:111:ASN:O	2.45	0.45
5:E:124:VAL:HG23	5:E:132:ILE:HG13	1.99	0.45
14:N:304:PHE:N	14:N:304:PHE:CD1	2.85	0.45
14:N:382:ILE:HG12	14:N:421:GLN:HB3	1.99	0.45
15:O:100:GLN:NE2	15:O:166:LEU:O	2.48	0.45
15:O:588:LEU:HD23	15:O:641:LEU:HD23	1.97	0.45
3:C:215:ASP:OD1	12:L:70:ARG:NH2	2.50	0.45
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.99	0.45
1:A:225:LEU:HD23	15:O:541:ILE:HG22	1.99	0.45
1:A:895:ASP:OD2	1:A:1380:ARG:NH1	2.50	0.45
1:A:955:LEU:HB3	1:A:958:ALA:HB3	1.98	0.45
1:A:980:SER:HB3	5:E:160:GLU:HG2	1.98	0.45
2:B:157:ARG:NH2	2:B:180:ASP:OD1	2.50	0.45
2:B:461:LEU:HD23	2:B:708:GLN:HA	1.99	0.45
4:D:99:SER:HA	4:D:102:SER:HB2	1.98	0.45
5:E:101:GLN:HE21	5:E:127:ILE:HG13	1.82	0.45
1:A:239:CYS:HB3	1:A:244:ILE:HB	1.98	0.44
2:B:253:ILE:HD11	2:B:283:PHE:HE1	1.81	0.44
7:G:38:ILE:HG12	7:G:44:LEU:HD13	1.99	0.44
16:P:171:ASP:HA	16:P:172:ILE:HA	1.65	0.44
1:A:420:ILE:HG23	1:A:444:LEU:HD21	1.99	0.44
1:A:1209:ILE:HA	1:A:1212:ALA:HB2	2.00	0.44
15:O:235:LEU:HD13	15:O:238:ARG:HB2	1.99	0.44
1:A:703:ARG:NH2	11:K:93:ILE:O	2.50	0.44
1:A:1084:GLU:HB3	6:F:86:THR:HG23	1.98	0.44
12:L:30:ILE:N	12:L:57:LEU:O	2.51	0.44
15:O:200:LEU:HB3	15:O:280:LEU:HD12	1.99	0.44
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.99	0.44
1:A:533:ASN:HD21	6:F:94:LEU:HD23	1.82	0.44
1:A:1198:LEU:HD23	1:A:1273:LYS:HD3	1.99	0.44
2:B:765:TYR:HD2	2:B:924:ILE:HB	1.82	0.44
11:K:67:GLU:N	11:K:99:ASN:O	2.50	0.44
13:M:247:TRP:HD1	14:N:406:ALA:HB1	1.82	0.44
15:O:53:VAL:HG11	15:O:65:ILE:HG21	1.99	0.44
2:B:709:ALA:HA	2:B:1027:LEU:HA	1.98	0.44
5:E:66:GLU:HA	5:E:69:ILE:HD12	2.00	0.44
2:B:935:ASP:HB2	3:C:228:ARG:HB3	1.99	0.44
3:C:100:ARG:NH2	3:C:192:LEU:O	2.50	0.44
14:N:304:PHE:N	14:N:304:PHE:HD1	2.15	0.44
15:O:192:VAL:HG23	15:O:274:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:ASN:HB3	1:A:951:ASP:HB2	1.99	0.44
2:B:289:GLU:HA	2:B:292:LYS:HD3	1.99	0.44
2:B:386:LEU:HB3	2:B:444:LEU:HD21	2.00	0.44
2:B:1004:LEU:HB2	2:B:1013:LEU:HD12	1.98	0.44
8:H:96:VAL:HG12	8:H:143:LEU:HD23	1.99	0.44
1:A:1161:VAL:HG11	1:A:1295:VAL:HG11	1.98	0.44
1:A:1175:ASP:HA	1:A:1183:PHE:O	2.18	0.44
4:D:121:LEU:HA	4:D:124:VAL:HG12	2.00	0.44
16:P:222:LEU:HD21	16:P:237:PRO:HG3	1.99	0.44
1:A:153:ARG:HB3	15:O:337:GLN:HB3	1.99	0.43
1:A:1026:ARG:HH22	8:H:110:ASP:H	1.66	0.43
2:B:417:ASP:HA	2:B:420:LEU:HB2	2.00	0.43
3:C:136:LEU:HB3	3:C:204:LEU:HG	2.00	0.43
4:D:134:LEU:HD13	4:D:154:LEU:HD11	2.00	0.43
8:H:10:PHE:HD2	8:H:38:LEU:HD22	1.83	0.43
2:B:197:GLN:OE1	2:B:451:ARG:NH1	2.51	0.43
2:B:391:LEU:HD23	2:B:429:ILE:HA	1.99	0.43
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.99	0.43
1:A:719:PRO:HB3	1:A:723:LEU:HD23	2.00	0.43
1:A:966:ILE:HA	1:A:970:LEU:HD12	2.01	0.43
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.99	0.43
1:A:91:PHE:HE1	1:A:99:THR:HG21	1.83	0.43
1:A:309:ILE:HG13	1:A:310:ASN:H	1.83	0.43
3:C:70:ILE:HB	3:C:74:GLU:HB2	2.01	0.43
3:C:131:THR:O	3:C:172:GLN:NE2	2.51	0.43
5:E:113:GLN:NE2	5:E:137:GLU:OE2	2.51	0.43
6:F:81:THR:HG1	6:F:146:TRP:HE1	1.66	0.43
6:F:115:THR:HG22	6:F:116:ASP:H	1.84	0.43
13:M:134:ASP:O	13:M:138:SER:HB3	2.18	0.43
15:O:259:LEU:HG	15:O:261:GLN:H	1.83	0.43
1:A:67:CYS:SG	1:A:69:THR:OG1	2.72	0.43
1:A:612:LEU:HD23	1:A:616:PRO:HA	2.00	0.43
2:B:961:LEU:HD11	2:B:1022:ILE:HD11	2.00	0.43
3:C:133:VAL:HG23	3:C:170:GLU:HB2	2.01	0.43
5:E:34:GLU:HA	5:E:37:LEU:HD23	2.01	0.43
1:A:1213:SER:OG	1:A:1218:GLN:NE2	2.52	0.43
2:B:843:ILE:HB	2:B:871:VAL:HG12	2.01	0.43
15:O:134:GLY:HA2	15:O:137:ILE:HG12	2.01	0.43
2:B:935:ASP:HB3	2:B:1005:TYR:HE2	1.84	0.43
11:K:55:SER:OG	11:K:59:THR:O	2.36	0.43
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:723:THR:HA	2:B:790:LYS:HB3	2.01	0.42
7:G:46:ILE:HG22	7:G:47:THR:HG23	2.00	0.42
1:A:524:THR:HG22	2:B:1081:GLU:HG3	2.01	0.42
15:O:495:VAL:HG21	15:O:577:MET:HE1	2.00	0.42
2:B:730:TYR:O	2:B:753:GLN:NE2	2.40	0.42
15:O:211:ILE:HG23	15:O:329:PRO:HB3	2.01	0.42
2:B:885:MET:SD	2:B:887:SER:OG	2.76	0.42
15:O:154:GLN:HG2	15:O:155:LEU:HD22	2.02	0.42
3:C:65:ASN:OD1	3:C:68:ARG:NH2	2.52	0.42
3:C:328:LEU:HB3	11:K:121:LEU:HD21	2.01	0.42
15:O:623:GLU:HA	15:O:626:GLN:HB3	2.01	0.42
4:D:3:VAL:HA	7:G:7:ILE:HG22	2.01	0.42
5:E:35:VAL:HG13	5:E:36:GLU:HG2	2.01	0.42
8:H:28:ALA:HB3	8:H:38:LEU:HB3	2.02	0.42
2:B:320:LEU:HA	2:B:324:ILE:HB	2.02	0.42
2:B:471:THR:HG22	2:B:514:LEU:HB2	2.02	0.42
2:B:615:VAL:HG12	2:B:620:SER:HA	2.01	0.42
9:I:30:PRO:HG3	13:M:140:TRP:HZ2	1.84	0.42
16:P:185:PHE:HA	16:P:188:GLU:HG2	2.02	0.42
1:A:102:ILE:HG13	1:A:242:LEU:HD22	2.01	0.41
1:A:828:GLN:HB3	2:B:655:ASN:HD21	1.84	0.41
2:B:983:LYS:HG3	2:B:985:GLU:H	1.84	0.41
8:H:15:VAL:HG22	8:H:26:ILE:HG22	2.02	0.41
2:B:774:ASN:HB3	2:B:777:SER:HB3	2.02	0.41
1:A:1392:THR:HG22	1:A:1393:THR:H	1.85	0.41
2:B:913:SER:HB2	2:B:1027:LEU:HD11	2.01	0.41
3:C:26:ASP:OD1	3:C:26:ASP:N	2.52	0.41
5:E:78:LEU:HB3	5:E:107:THR:HG23	2.03	0.41
5:E:86:PRO:HA	5:E:113:GLN:HG2	2.02	0.41
1:A:953:GLY:HA2	1:A:1063:SER:HA	2.02	0.41
2:B:934:ASN:HB3	2:B:1004:LEU:HD23	2.01	0.41
13:M:227:LEU:HB3	13:M:231:LEU:HB2	2.03	0.41
15:O:62:ALA:HA	15:O:65:ILE:HG22	2.03	0.41
2:B:932:PRO:HB2	2:B:1004:LEU:HD13	2.01	0.41
1:A:100:ILE:HD11	1:A:178:ILE:HD12	2.01	0.41
1:A:1234:VAL:HG11	1:A:1260:MET:HE1	2.02	0.41
3:C:248:GLN:HA	3:C:256:ILE:HD11	2.01	0.41
7:G:207:LEU:HD23	7:G:209:SER:H	1.85	0.41
1:A:11:LYS:HA	2:B:1145:ASP:HA	2.02	0.41
2:B:590:ILE:HA	2:B:600:HIS:O	2.20	0.41
3:C:134:LEU:HD12	3:C:167:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:VAL:HA	3:C:304:SER:HA	2.03	0.41
6:F:144:GLU:HG2	6:F:146:TRP:CD1	2.56	0.41
13:M:92:ASN:HD21	13:M:181:PRO:HD3	1.86	0.41
2:B:193:VAL:O	2:B:455:THR:HA	2.21	0.41
2:B:230:LYS:NZ	2:B:352:MET:SD	2.89	0.41
3:C:31:TRP:CE2	11:K:123:ASP:HB3	2.56	0.41
15:O:491:VAL:HG11	15:O:650:VAL:HG11	2.03	0.41
1:A:1150:ASP:O	1:A:1155:ARG:NH1	2.54	0.40
14:N:303:ARG:C	14:N:304:PHE:HD1	2.25	0.40
15:O:235:LEU:HD12	15:O:236:LYS:H	1.86	0.40
1:A:939:TRP:HZ2	1:A:1062:ILE:HD12	1.85	0.40
2:B:83:ILE:HD11	2:B:93:LEU:HD13	2.02	0.40
1:A:412:ASN:HB2	1:A:416:LEU:HD13	2.03	0.40
1:A:660:LEU:HD12	8:H:117:SER:HB3	2.03	0.40
1:A:816:GLN:NE2	1:A:867:SER:OG	2.51	0.40
2:B:935:ASP:HB3	2:B:1005:TYR:CE2	2.57	0.40
7:G:82:GLY:H	7:G:150:ILE:HB	1.86	0.40
15:O:473:PRO:HG2	15:O:475:VAL:HG12	2.02	0.40
15:O:534:ARG:HD3	15:O:537:LEU:HD12	2.03	0.40
1:A:711:SER:OG	2:B:1016:TYR:O	2.39	0.40
1:A:826:GLY:H	1:A:831:SER:HA	1.86	0.40
2:B:221:THR:HB	2:B:228:LYS:HB2	2.03	0.40
2:B:932:PRO:HG3	2:B:1006:SER:HA	2.04	0.40
8:H:56:THR:HB	8:H:145:ARG:HB3	2.04	0.40
15:O:231:PRO:HB3	15:O:234:ASP:HA	2.04	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	1394/1460 (96%)	1213 (87%)	174 (12%)	7 (0%)	29 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1112/1149 (97%)	979 (88%)	128 (12%)	5 (0%)	34	66
3	C	333/335 (99%)	299 (90%)	32 (10%)	2 (1%)	25	57
4	D	113/161 (70%)	96 (85%)	17 (15%)	0	100	100
5	E	213/215 (99%)	195 (92%)	18 (8%)	0	100	100
6	F	81/155 (52%)	68 (84%)	13 (16%)	0	100	100
7	G	185/212 (87%)	162 (88%)	23 (12%)	0	100	100
8	H	136/146 (93%)	115 (85%)	21 (15%)	0	100	100
9	I	40/110 (36%)	35 (88%)	5 (12%)	0	100	100
10	J	66/70 (94%)	56 (85%)	10 (15%)	0	100	100
11	K	99/142 (70%)	88 (89%)	11 (11%)	0	100	100
12	L	43/70 (61%)	36 (84%)	7 (16%)	0	100	100
13	M	161/282 (57%)	123 (76%)	36 (22%)	2 (1%)	13	42
14	N	101/422 (24%)	82 (81%)	18 (18%)	1 (1%)	15	46
15	O	531/654 (81%)	470 (88%)	60 (11%)	1 (0%)	47	77
16	P	119/317 (38%)	82 (69%)	31 (26%)	6 (5%)	2	14
17	Q	38/251 (15%)	28 (74%)	10 (26%)	0	100	100
All	All	4765/6151 (78%)	4127 (87%)	614 (13%)	24 (0%)	32	61

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	839	GLY
2	B	935	ASP
1	A	495	TRP
2	B	297	THR
16	P	309	VAL
1	A	513	ASP
2	B	298	GLN
3	C	4	ILE
13	M	118	LEU
16	P	206	VAL
1	A	494	PRO
1	A	1179	ASP
15	O	236	LYS
16	P	307	LYS
1	A	1352	PRO

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Mol	Chain	Res	Type
13	M	94	PRO
16	P	253	LEU
16	P	305	HIS
16	P	308	GLU
1	A	599	LYS
1	A	636	PRO
3	C	3	ASN
2	B	584	VAL
14	N	378	VAL

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	1215/1257 (97%)	1196 (98%)	19 (2%)	62	79
2	B	975/1006 (97%)	960 (98%)	15 (2%)	65	81
3	C	296/296 (100%)	289 (98%)	7 (2%)	49	73
4	D	110/145 (76%)	106 (96%)	4 (4%)	35	63
5	E	197/197 (100%)	193 (98%)	4 (2%)	55	76
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	170/190 (90%)	169 (99%)	1 (1%)	86	91
8	H	123/128 (96%)	121 (98%)	2 (2%)	62	79
9	I	38/98 (39%)	37 (97%)	1 (3%)	46	71
10	J	63/65 (97%)	62 (98%)	1 (2%)	62	79
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	143/249 (57%)	139 (97%)	4 (3%)	43	70
14	N	88/360 (24%)	84 (96%)	4 (4%)	27	58
15	O	493/593 (83%)	482 (98%)	11 (2%)	52	74
16	P	116/285 (41%)	115 (99%)	1 (1%)	78	87
17	Q	35/212 (16%)	34 (97%)	1 (3%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4266/5405 (79%)	4191 (98%)	75 (2%)	61 78

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	161	ASN
1	A	188	LYS
1	A	194	LYS
1	A	450	MET
1	A	451	LYS
1	A	482	ARG
1	A	643	ASN
1	A	774	ARG
1	A	948	ASN
1	A	973	ARG
1	A	990	ASN
1	A	1032	LEU
1	A	1104	MET
1	A	1163	LYS
1	A	1313	ARG
1	A	1332	ARG
1	A	1337	ARG
1	A	1453	ASN
2	B	39	ASN
2	B	48	LEU
2	B	99	ARG
2	B	143	MET
2	B	362	ASN
2	B	365	MET
2	B	412	ARG
2	B	446	ARG
2	B	479	LYS
2	B	664	LYS
2	B	774	ASN
2	B	861	ASN
2	B	919	LYS
2	B	997	ASN
2	B	1048	ARG
3	C	112	MET
3	C	137	ASN
3	C	143	ASN

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Mol	Chain	Res	Type
3	C	148	LYS
3	C	240	LYS
3	C	277	ARG
3	C	281	ARG
4	D	25	LYS
4	D	71	ASN
4	D	114	LYS
4	D	130	ASN
5	E	5	ASN
5	E	7	ARG
5	E	122	LYS
5	E	136	ASN
7	G	164	LYS
8	H	87	ARG
8	H	128	ASN
9	I	10	ASN
10	J	38	ARG
13	M	111	ARG
13	M	132	ASN
13	M	164	LYS
13	M	226	ARG
14	N	274	LYS
14	N	298	ASN
14	N	312	ARG
14	N	370	LYS
15	O	102	ARG
15	O	184	LYS
15	O	243	MET
15	O	244	ASN
15	O	251	LYS
15	O	254	ASN
15	O	272	ARG
15	O	286	ARG
15	O	325	LYS
15	O	362	ASN
15	O	468	LEU
16	P	262	ARG
17	Q	49	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	109	ASN
1	A	161	ASN
1	A	229	ASN
1	A	386	ASN
1	A	533	ASN
1	A	566	HIS
1	A	643	ASN
1	A	808	GLN
1	A	816	GLN
1	A	899	GLN
1	A	948	ASN
1	A	990	ASN
1	A	1218	GLN
1	A	1233	ASN
1	A	1254	ASN
1	A	1262	GLN
1	A	1354	HIS
1	A	1419	GLN
1	A	1453	ASN
2	B	39	ASN
2	B	334	HIS
2	B	362	ASN
2	B	456	HIS
2	B	593	ASN
2	B	596	GLN
2	B	626	HIS
2	B	774	ASN
2	B	861	ASN
2	B	893	GLN
2	B	916	HIS
2	B	997	ASN
2	B	1025	GLN
3	C	137	ASN
3	C	143	ASN
3	C	207	HIS
4	D	71	ASN
4	D	130	ASN
5	E	5	ASN
5	E	32	GLN
5	E	54	GLN
5	E	101	GLN
5	E	113	GLN

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Mol	Chain	Res	Type
5	E	136	ASN
5	E	174	GLN
7	G	36	ASN
8	H	128	ASN
10	J	26	GLN
13	M	92	ASN
13	M	117	HIS
13	M	132	ASN
13	M	155	ASN
13	M	158	GLN
13	M	190	ASN
14	N	298	ASN
14	N	421	GLN
15	O	244	ASN
15	O	254	ASN
15	O	362	ASN
15	O	464	ASN
15	O	544	ASN
15	O	579	GLN
15	O	584	ASN
15	O	631	ASN
17	Q	49	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)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

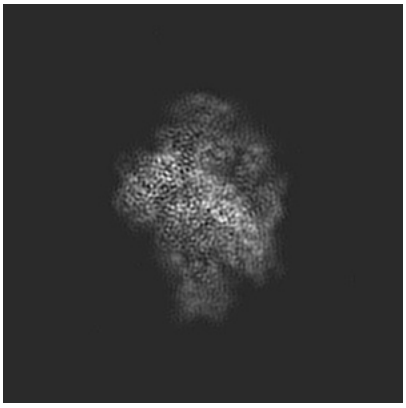
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3958. These allow visual inspection of the internal detail of the map and identification of artifacts.

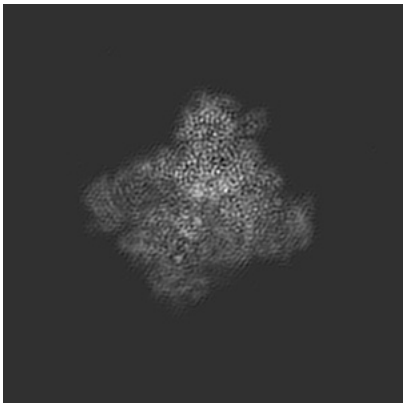
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

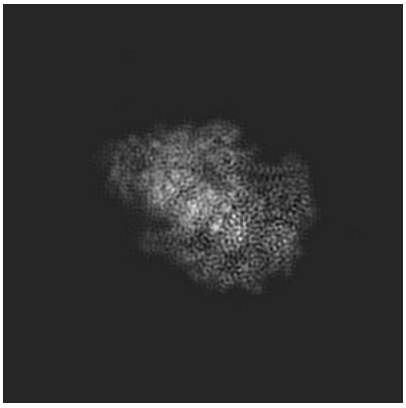
6.1.1 Primary map



X



Y

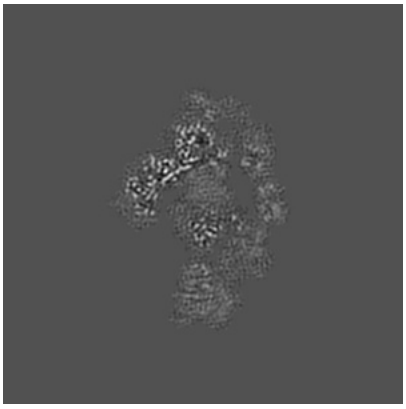


Z

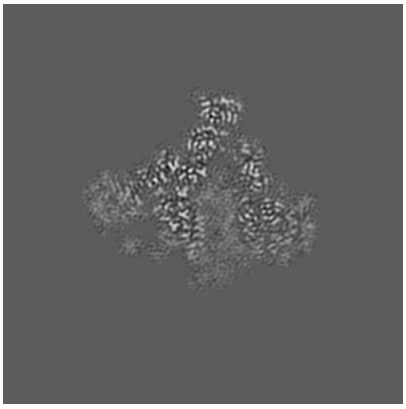
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

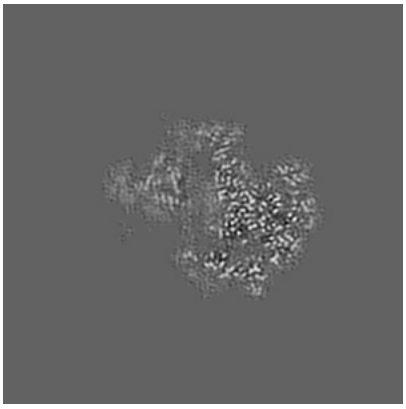
6.2.1 Primary map



X Index: 154



Y Index: 154

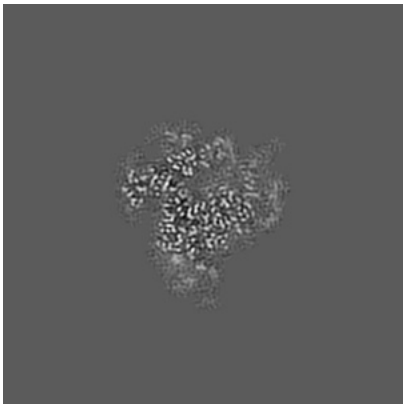


Z Index: 154

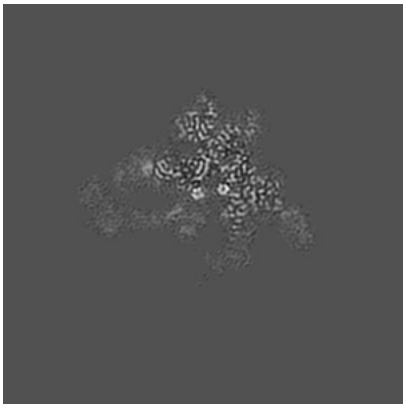
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

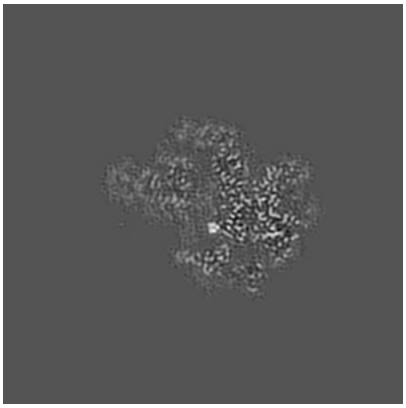
6.3.1 Primary map



X Index: 178



Y Index: 135



Z Index: 151

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

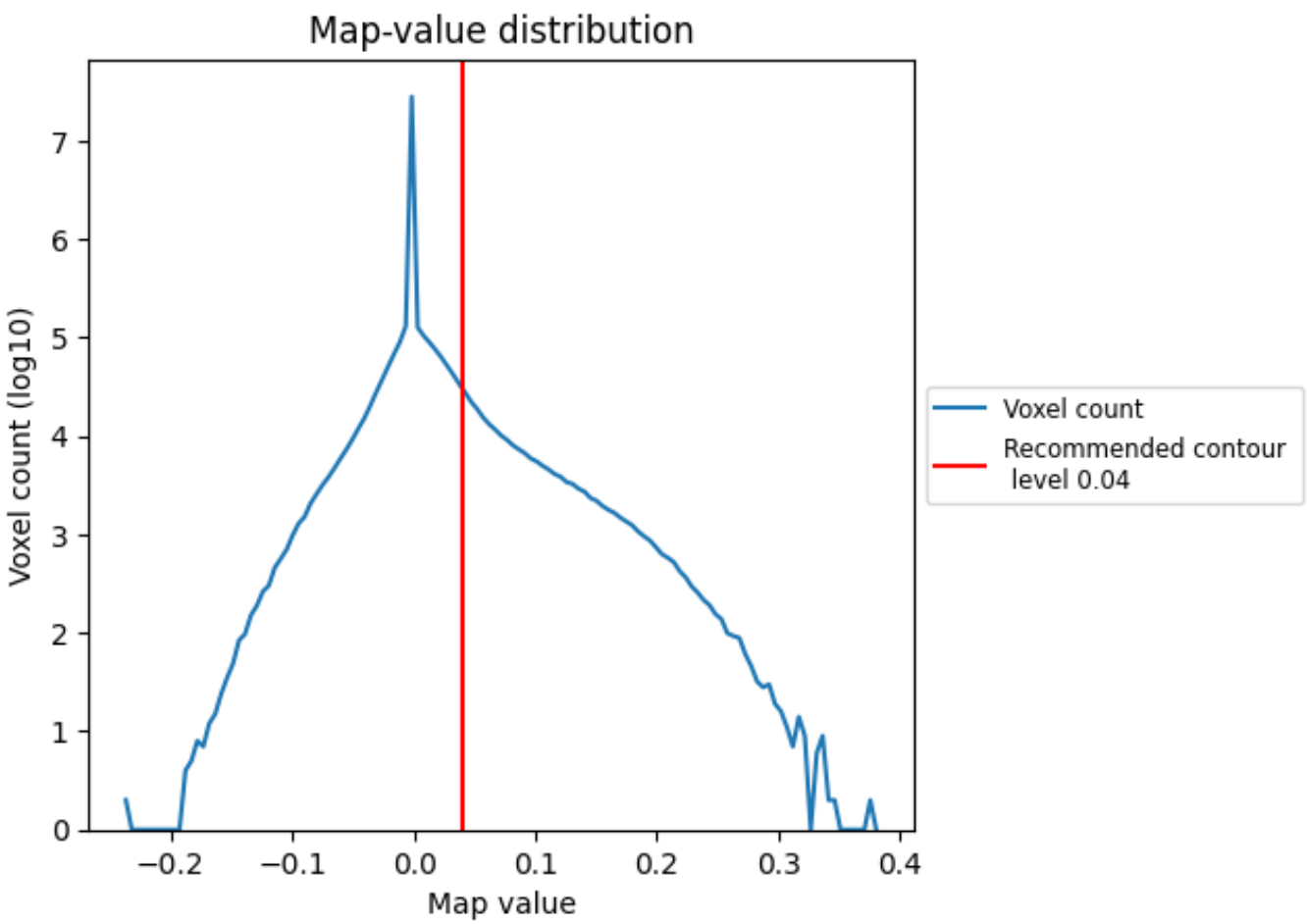
6.5 Mask visualisation (i)

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

7 Map analysis (i)

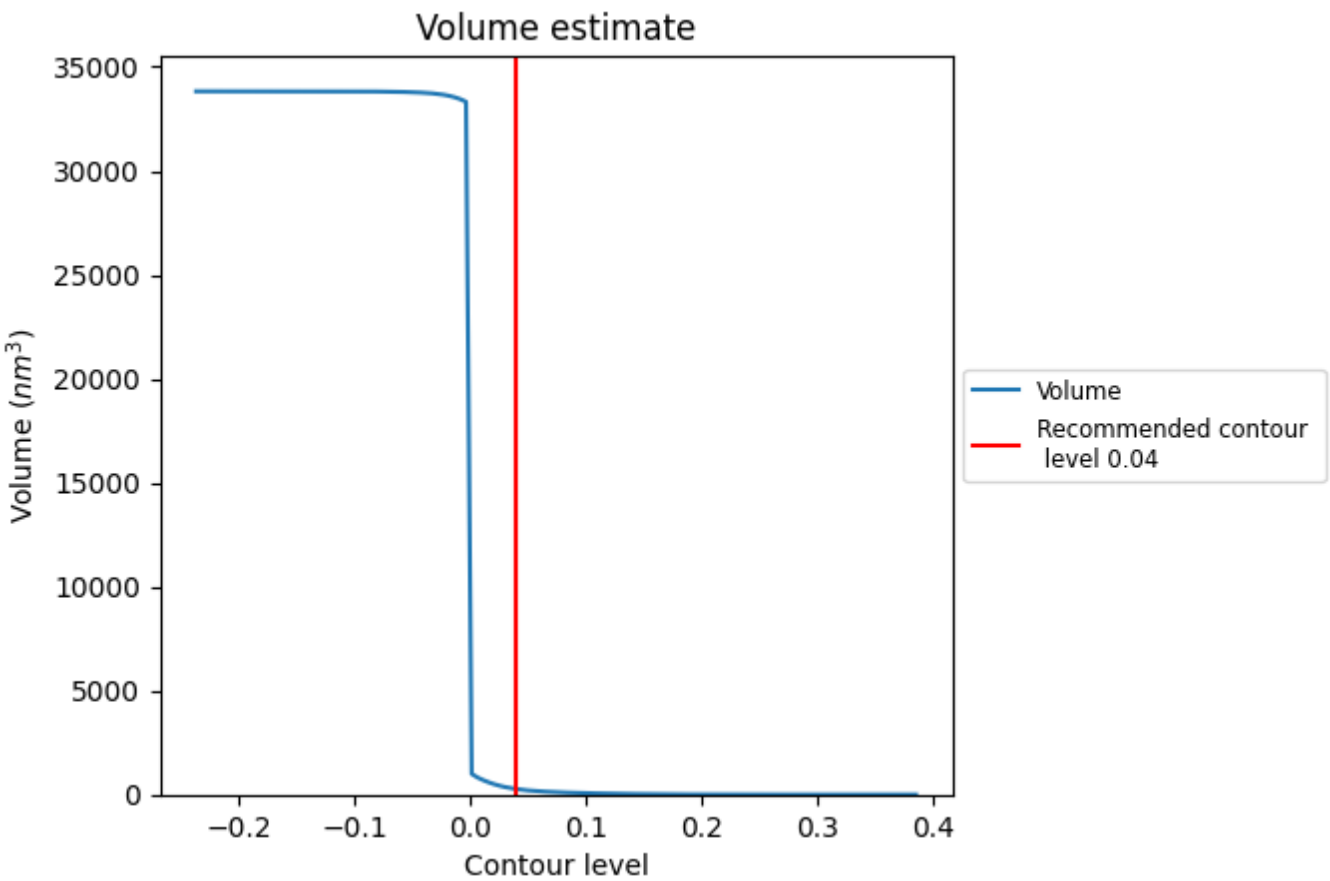
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

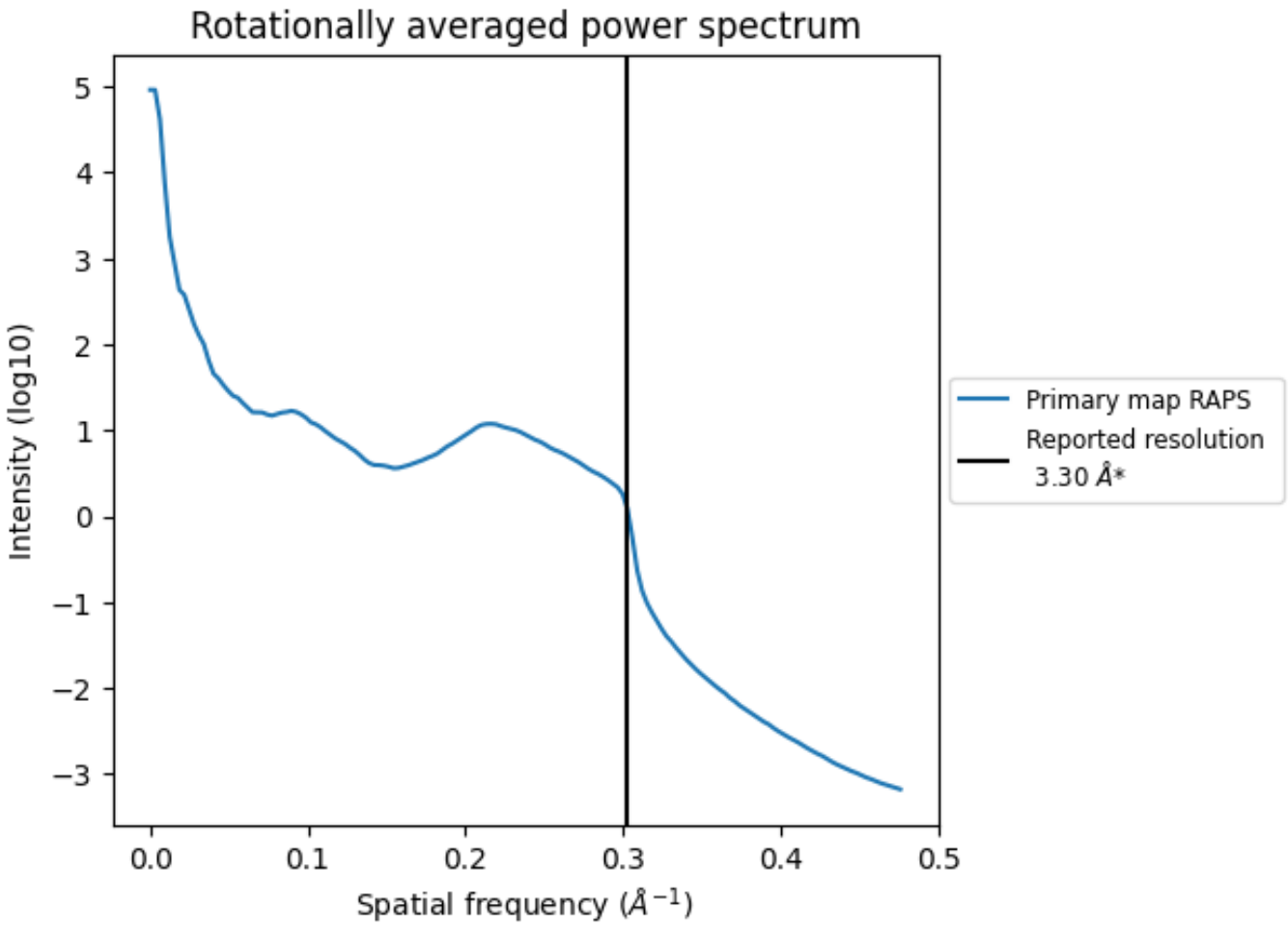
7.2 Volume estimate (i)



The volume at the recommended contour level is 265 nm^3; this corresponds to an approximate mass of 239 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)

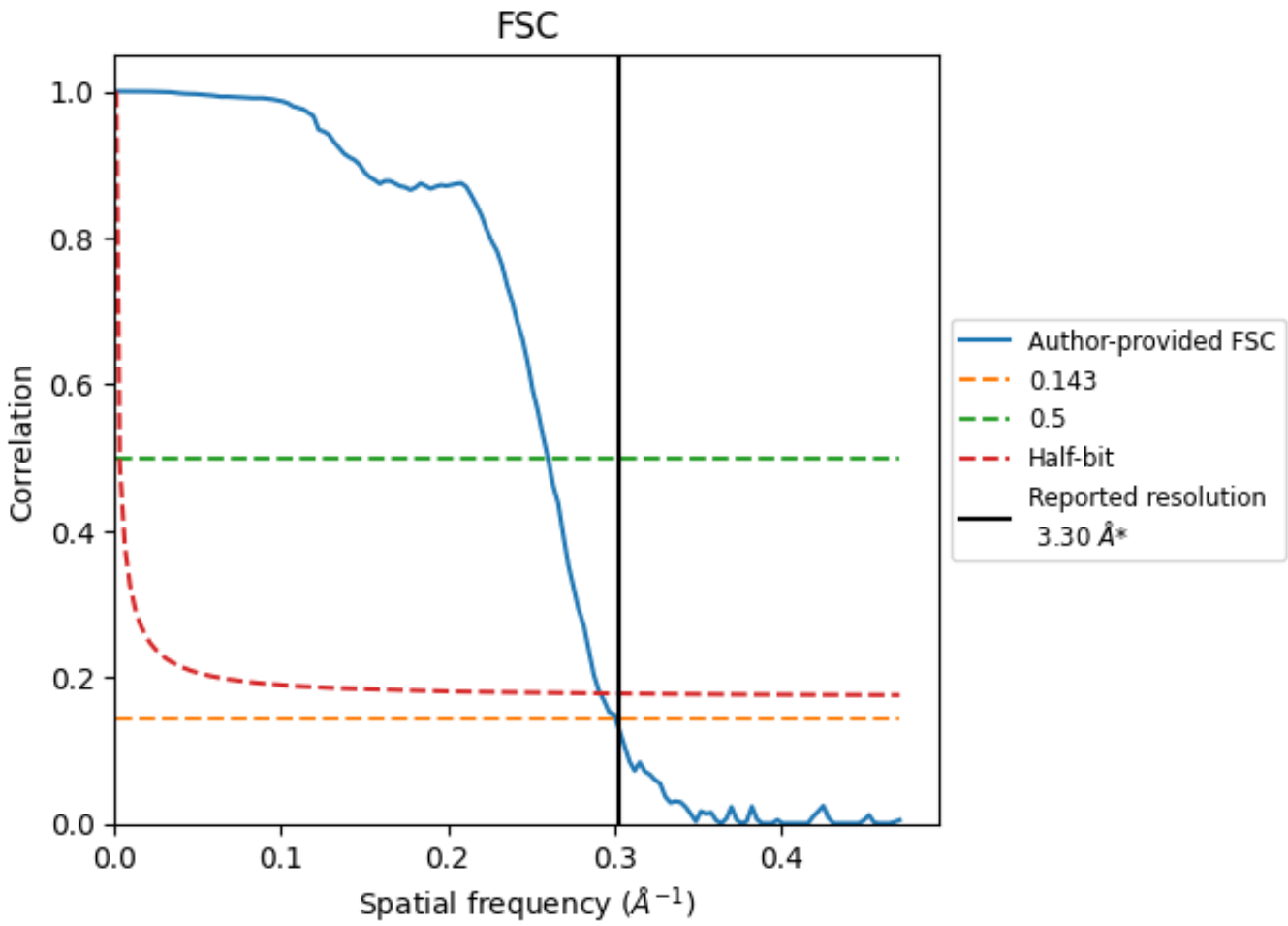


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

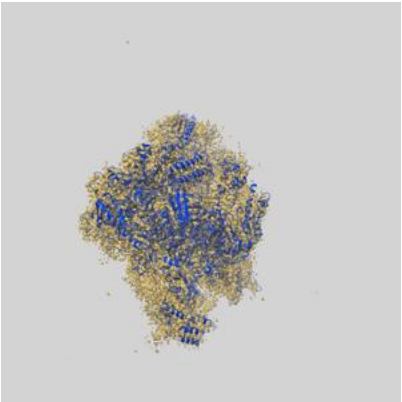
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.84	3.43
Unmasked-calculated*	-	-	-

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

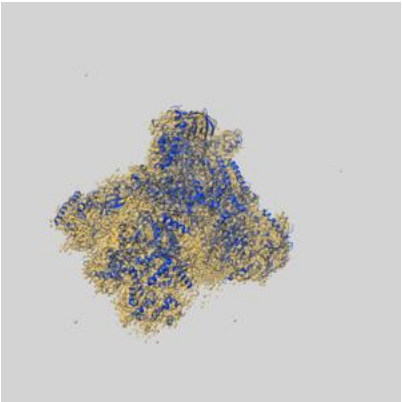
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3958 and PDB model 6EU3. Per-residue inclusion information can be found in section 3 on page 7.

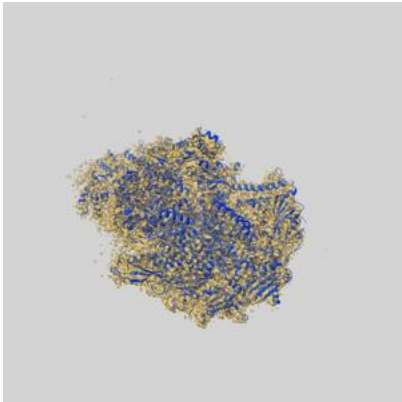
9.1 Map-model overlay (i)



X



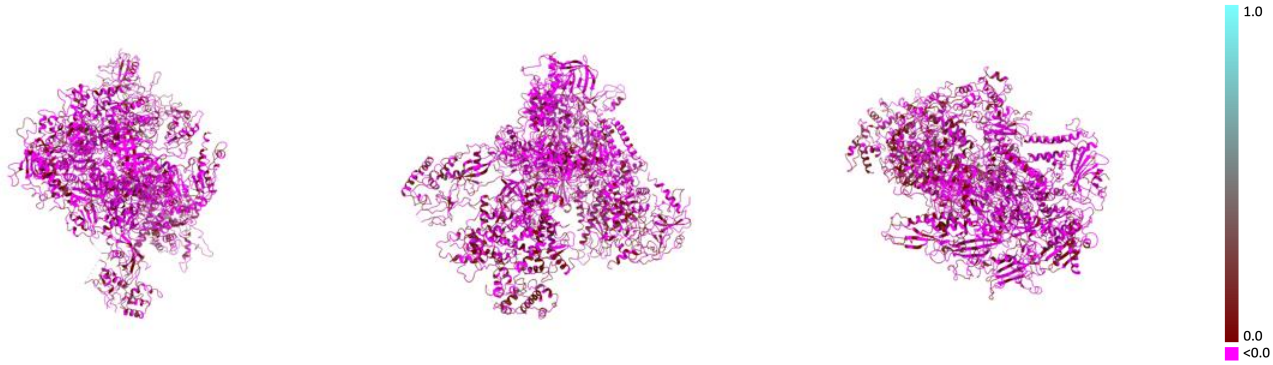
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

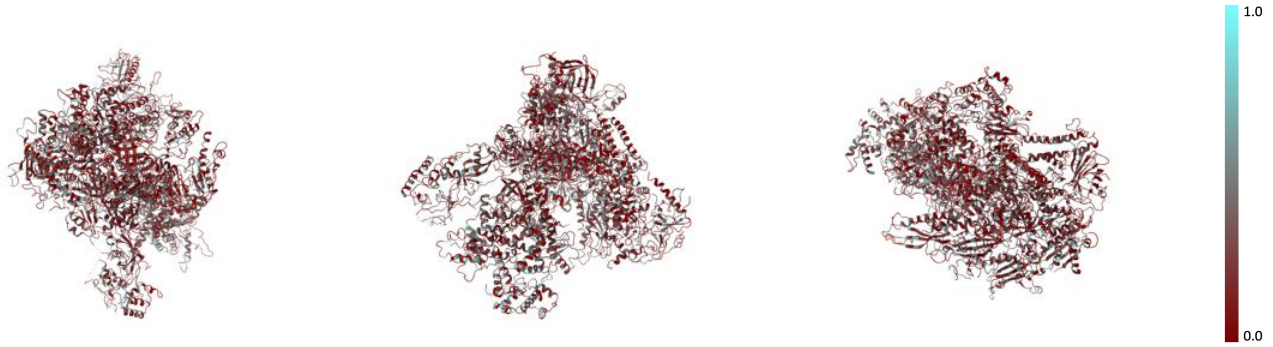
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

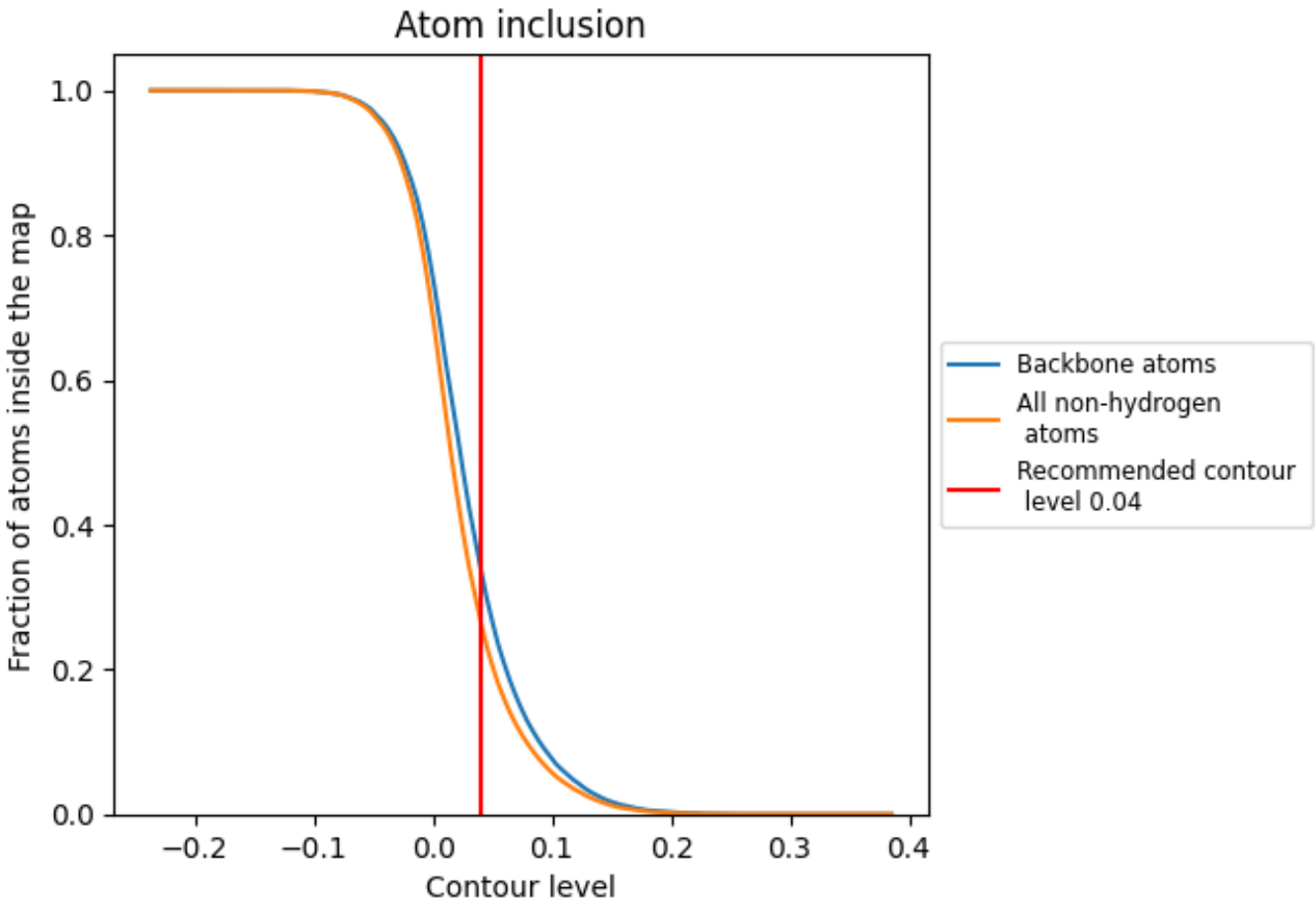
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 34% of all backbone atoms, 27% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2670	-0.0440
A	0.2539	-0.0610
B	0.2601	-0.0660
C	0.2795	-0.0740
D	0.3033	0.0660
E	0.2483	-0.0450
F	0.2802	-0.0660
G	0.2683	-0.0140
H	0.2143	-0.0990
I	0.2019	0.0320
J	0.2928	-0.0740
K	0.2580	-0.0830
L	0.3295	-0.0170
M	0.2500	0.0190
N	0.2121	-0.0360
O	0.3067	0.0000
P	0.3248	0.0430
Q	0.4104	0.0330