Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:20 am GMT

PDB ID	:	6GYL
EMDB ID	:	EMD-0091
Title	:	Structure of a yeast closed complex with distorted DNA (core CCdist)
Authors	:	Dienemann, C.; Schwalb, B.; Schilbach, S.; Cramer, P.
Deposited on	:	2018-06-30
Resolution	:	4.80 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

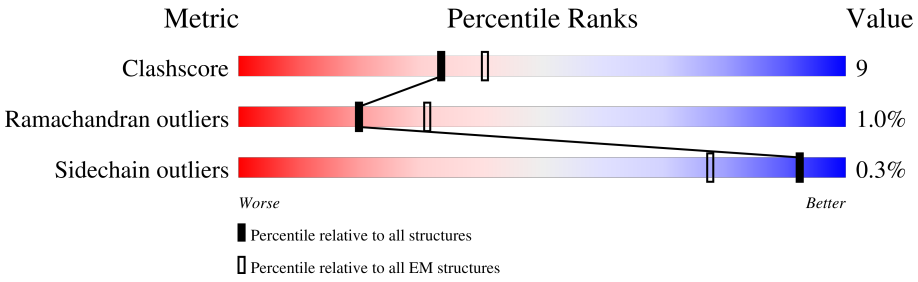
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.80 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	1733	44% 67% 14% 19%
2	B	1224	53% 73% 21% 6%
3	C	318	42% 68% 14% 18%
4	D	221	56% 61% 10% 29%
5	E	215	57% 88% 11%
6	F	155	26% 43% 10% 46%
7	G	171	57% 65% 35%
8	H	146	50% 71% 23% 7%

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Mol	Chain	Length	Quality of chain
9	I	122	53% 74% 20% 5%
10	J	70	46% 80% 13% 7%
11	K	120	53% 77% 17% 7%
12	L	70	36% 50% 14% 36%
13	M	345	50% 63% 18% 19%
14	N	56	48% 89% 11%
15	O	240	33% 57% 18% 25%
16	Q	735	11% 15% 5% 80%
17	R	400	27% 38% 10% 52%
18	T	56	39% 84% 16%
19	U	171	46% 40% 13% 46%
20	V	129	63% 67% 11% 22%
21	W	586	22% 24% 8% 67%
22	X	328	39% 42% 6% 51%

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 43409 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1398	10997	6931	1927	2078	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1152	9178	5807	1608	1708	55	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	262	2061	1299	343	406	13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1253	779	220	252	2	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	213	1744	1107	308	318	11	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	670	428	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

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

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

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 14 is a DNA chain called GAT1 promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	56	Total	C	N	O	P	0	0
			1129	540	204	329	56		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 16 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 17 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 18 is a DNA chain called GAT1 promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	56	Total	C	N	O	P	0	0
			1149	546	222	325	56		

- Molecule 19 is a protein called Transcription initiation factor IIA large subunit,Transcriptio n initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	123	LYS	-	expression tag	UNP P32774
V	124	HIS	-	expression tag	UNP P32774
V	125	HIS	-	expression tag	UNP P32774
V	126	HIS	-	expression tag	UNP P32774
V	127	HIS	-	expression tag	UNP P32774
V	128	HIS	-	expression tag	UNP P32774
V	129	HIS	-	expression tag	UNP P32774

- Molecule 21 is a protein called Transcription initiation factor IIE subunit alpha,Tfa1,Tfa1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	160	Total	C	N	O	S	0	0
			1004	620	184	196	4		

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	C	1	Total	Zn	0
			1	1	
23	I	2	Total	Zn	0
			2	2	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	
23	M	1	Total	Zn	0
			1	1	
23	W	1	Total	Zn	0
			1	1	

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

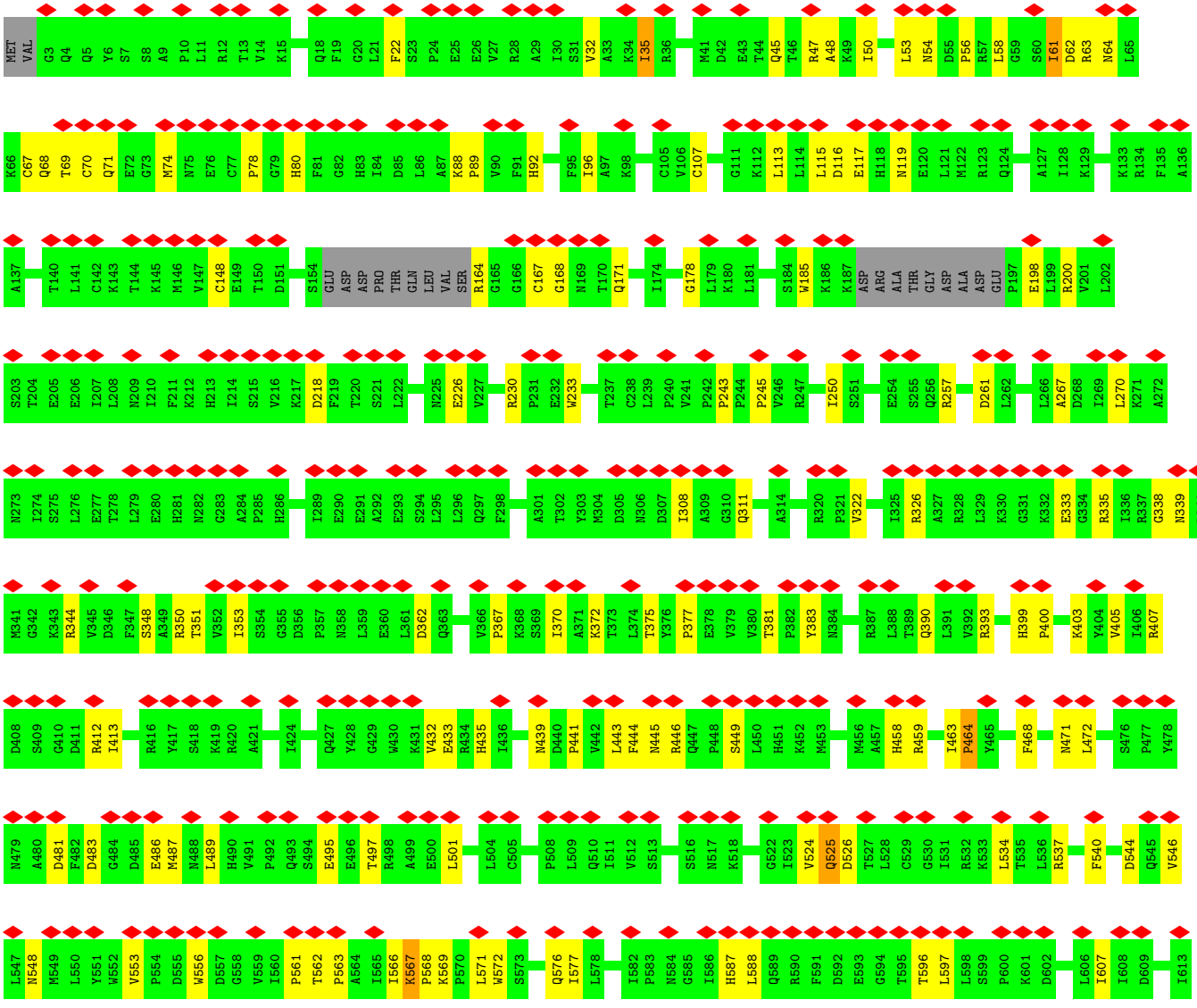
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
24	A	1	1	1	0

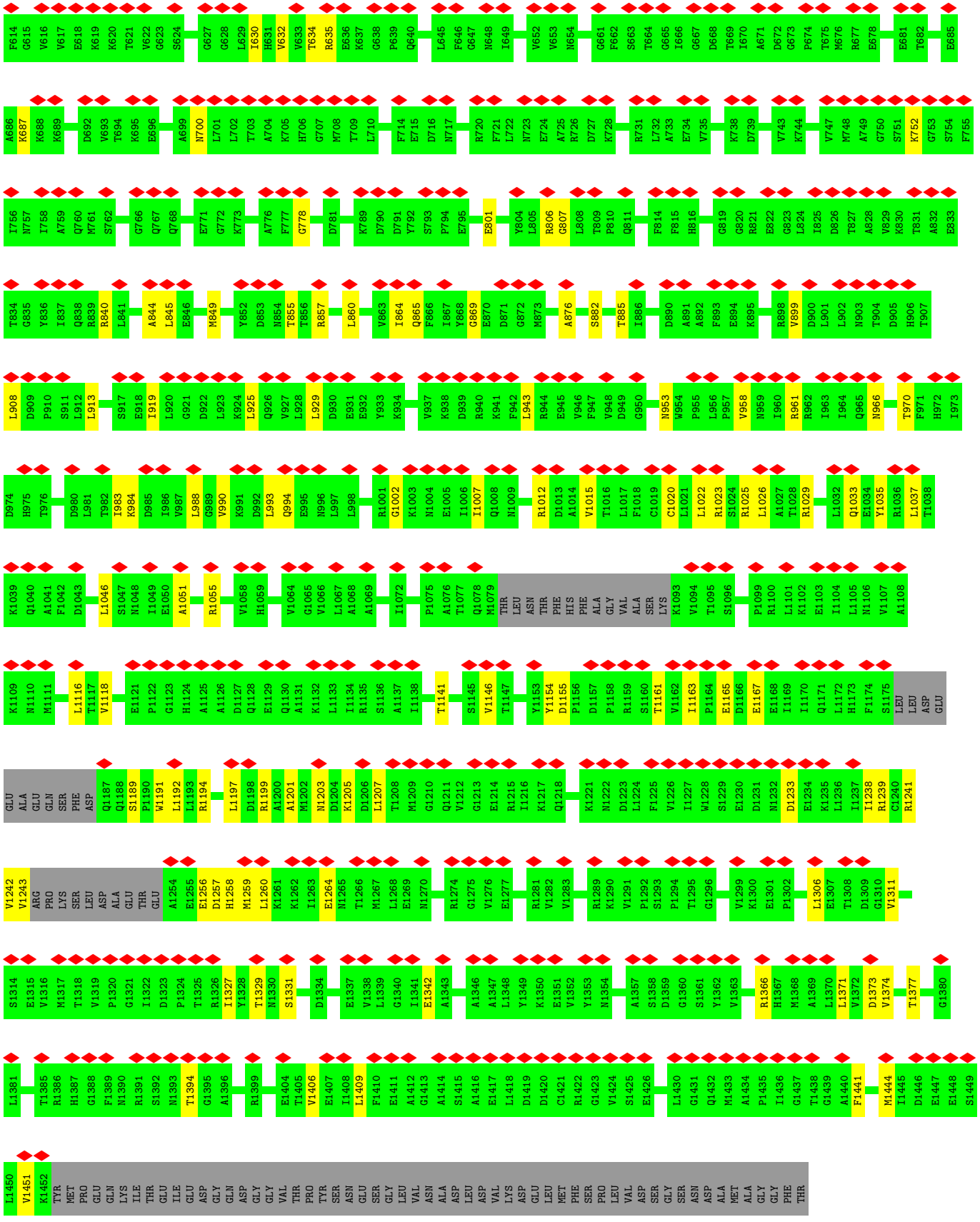
3 Residue-property plots (i)

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 II subunit RPB1

Chain A:

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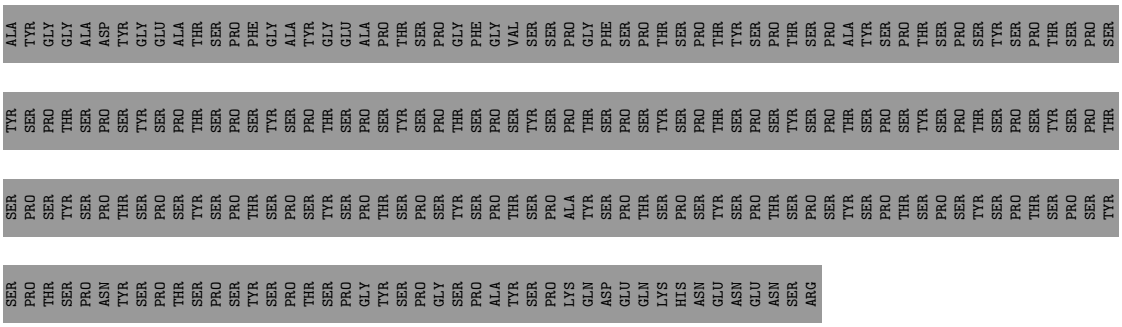
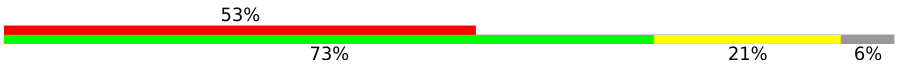
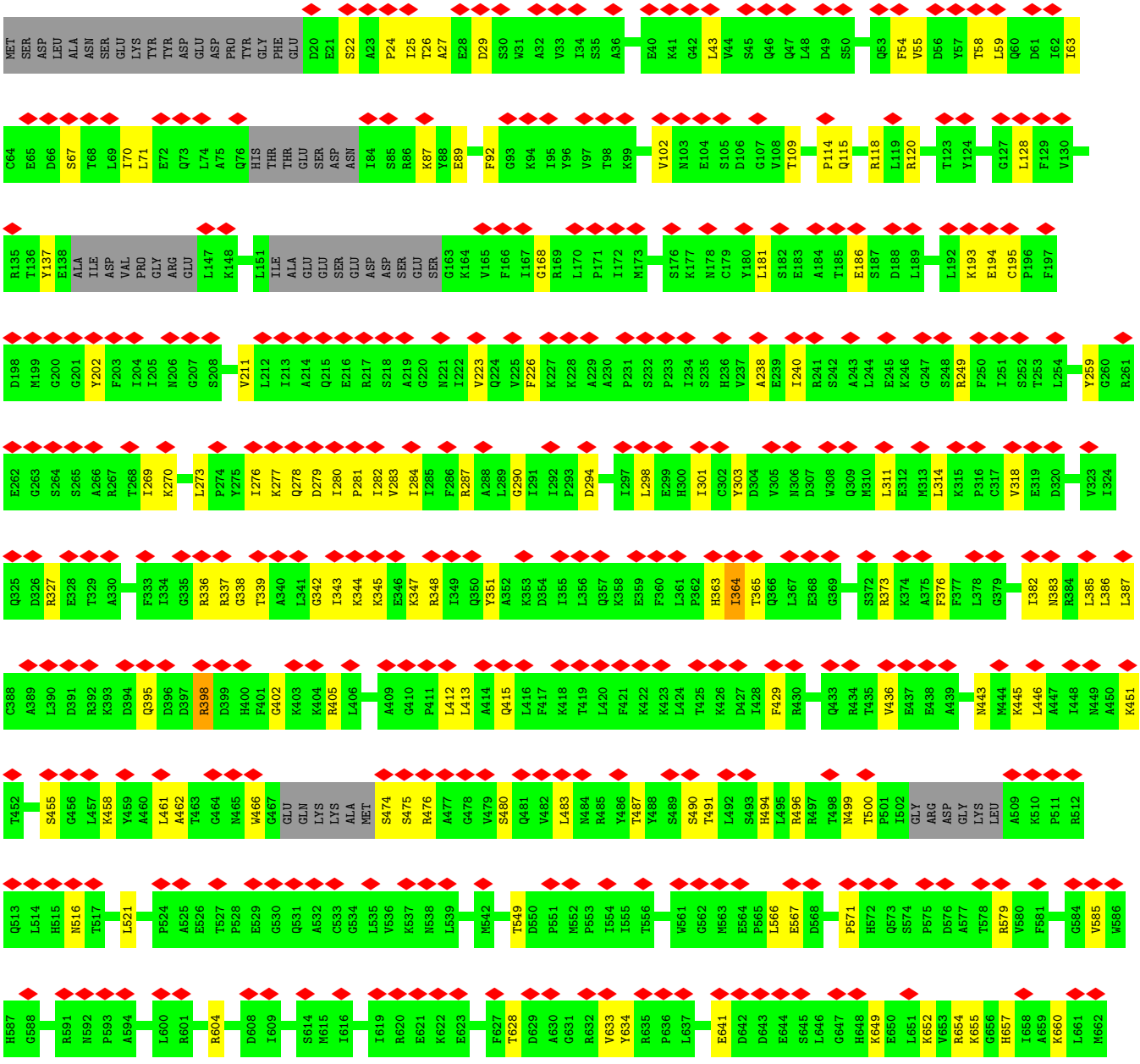
A686 K687 K688 K689 D692 V693 T694 K695 E696 A699 N700 L701 L702 T703 A704 K705 H706 G707 M708 T709 L710 F714 E715 D716 N717 R720 F721 L722 N723 E724 A725 R726 D727 K728 R731 L732 A733 E734 V735 K738 D739 V743 K744 V747 M748 A749 G750 S751 K752 G753 S754 F755
I756 N757 I758 A759 Q760 M761 S762 G766 Q767 Q768 E771 G772 K773 A776 F777 G778 D781 K789 D790 D791 Y792 S793 P794 E795 E801 Y804 L805 R806 G807 L808 T809 P810 Q811 F814 F815 H816 G819 G820 R821 E822 G823 L824 I825 D826 T827 A828 V829 K830 T831 A832 E833
T834 G835 Y836 I837 Q838 R839 R840 L841 A844 L845 E846 M849 Y852 D853 N854 T855 T856 R857 L860 V863 I864 Q865 F866 I867 Y868 G869 E870 D871 G872 M873 A876 S882 T885 I886 D890 A891 A892 F893 E894 K895 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907
L908 D909 P910 S911 L912 L913 S917 E918 I919 L920 G921 D922 L923 K924 L925 Q926 V927 L928 D930 E931 E932 Y933 K934 V937 K938 D939 R940 K941 F942 L943 R944 E945 V946 F947 V948 D949 G950 N953 W954 P955 L956 P957 V958 N959 I960 R961 R962 I963 I964 Q965 N966 T970 F971 H972 I973
D974 H975 T976 D980 L981 T982 I983 K984 D985 I986 V987 L988 G989 V990 K991 D992 L993 Q994 E995 N996 L997 L998 R1001 G1002 K1003 N1004 E1005 I1006 I1007 Q1008 N1009 R1012 D1013 A1014 V1015 T1016 L1017 F1018 C1019 C1020 L1021 L1022 R1023 S1024 R1025 L1026 A1027 T1028 R1029 L1032 Q1033 E1034 Y1035 R1036 L1037 T1038
K1039 Q1040 A1041 F1042 D1043 L1046 S1047 N1048 I1049 E1050 A1051 R1055 V1058 H1059 V1064 G1065 V1066 L1067 A1068 A1069 I1072 P1075 A1076 T1077 Q1078 M1079 THR LEU ASN THR PHE HIS PHE ALA GLY VAL ALA SER LYS K1093 V1094 T1095 S1096 P1099 R1100 L1101 K1102 E1103 I1104 L1105 N1106 V1107 A1108
K1109 N1110 M1111 L1116 T1117 V1118 E1121 P1122 G1123 H1124 A1125 A1126 D1127 Q1128 E1129 Q1130 A1131 K1132 L1133 I1134 R1135 S1136 A1137 I1138 T1141 S1145 V1146 T1147 Y1153 Y1154 D1155 P1156 D1157 P1158 R1159 S1160 T1161 V1162 I1163 P1164 E1165 D1166 E1167 E1168 I1169 I1170 Q1171 L1172 H1173 F1174 S1175 LEU LEU ASP GLU
GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189 P1190 W1191 L1192 L1193 R1194 L1197 D1198 R1199 A1200 A1201 M1202 N1203 D1204 K1205 D1206 L1207 T1208 M1209 G1210 Q1211 V1212 G1213 E1214 R1215 I1216 K1217 Q1218 K1221 N1222 D1223 L1224 F1225 V1226 I1227 W1228 S1229 E1230 D1231 N1232 D1233 E1234 K1235 L1236 I1237 I1238 R1239 C1240 R1241
V1242 V1243 ARG PRO LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 D1257 H1258 M1259 L1260 K1261 K1262 I1263 E1264 N1265 T1266 M1267 L1268 E1269 N1270 R1274 G1275 V1276 E1277 R1281 V1282 V1283 R1289 K1290 V1291 P1292 S1293 P1294 T1295 G1296 V1299 K1300 E1301 P1302 L1306 E1307 T1308 D1309 G1310 V1311
S1314 E1315 V1316 M1317 T1318 V1319 P1320 G1321 I1322 D1323 P1324 T1325 R1326 I1327 Y1328 T1329 N1330 S1331 D1334 E1337 V1338 L1339 G1340 I1341 E1342 A1343 A1346 A1347 L1348 Y1349 K1350 E1351 V1352 Y1353 N1354 A1357 S1358 D1359 G1360 S1361 Y1362 V1363 R1366 H1367 M1368 A1369 L1370 L1371 V1372 D1373 V1374 T1377 G1380
L1381 T1385 R1386 H1387 G1388 F1389 N1390 R1391 S1392 N1393 T1394 G1395 A1396 R1399 E1404 T1405 V1406 E1407 I1408 L1409 F1410 E1411 A1412 G1413 A1414 S1415 A1416 E1417 L1418 D1419 D1420 C1421 R1422 G1423 V1424 S1425 E1426 L1430 G1431 Q1432 M1433 A1434 P1435 I1436 G1437 T1438 G1439 A1440 F1441 M1444 I1445 D1446 E1447 E1448 S1449
L1450 V1451 K1452 TYR MET PRO GLU GLN LYS ILE THR GLU ILE GLU ASP GLY GLN ASP GLY GLY VAL THR PRO TYR SER ASN GLU SER GLY LEU VAL ASN ALA ASP LEU ASP VAL LYS ASP GLU LEU MET PHE SER PRO LEU VAL ASP SER GLY SER ASN ASP ALA MET ALA GLY GLY PHE THR

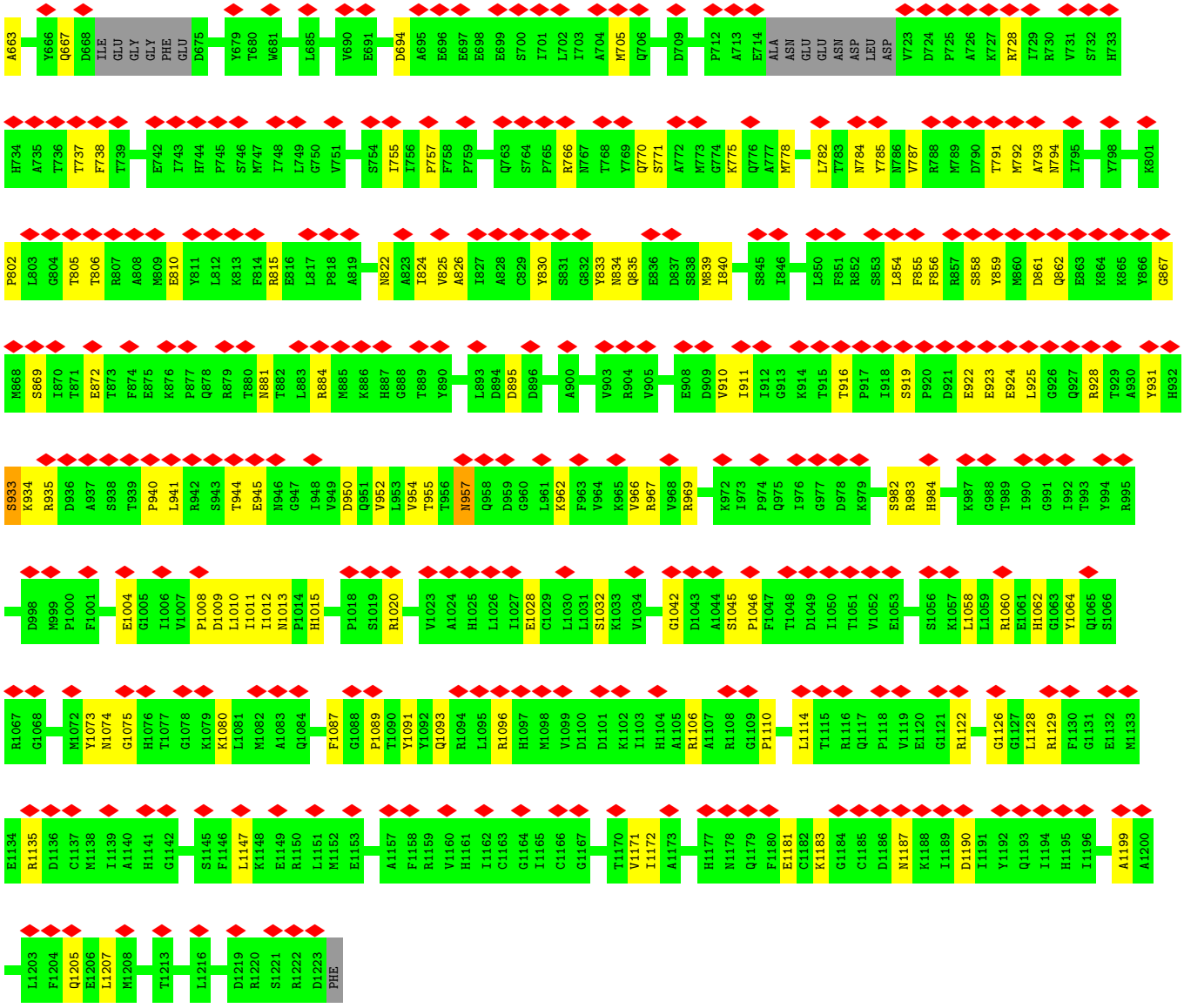


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

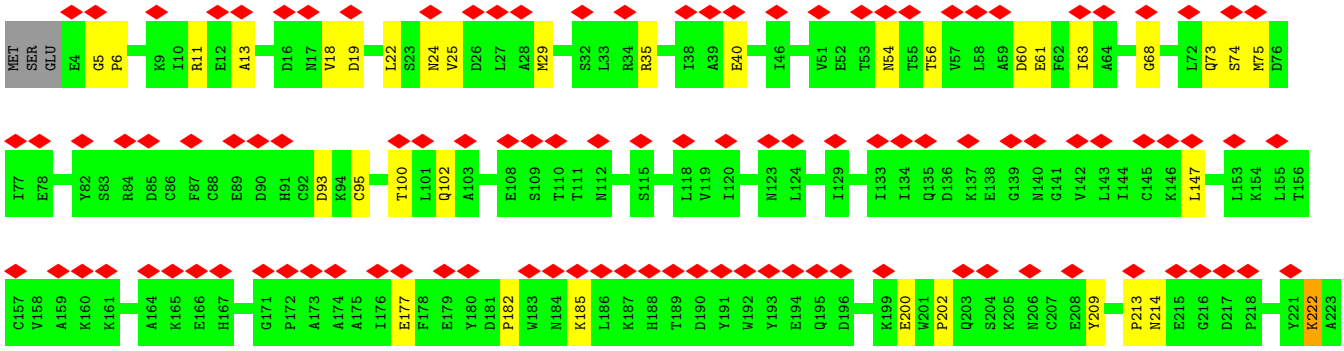


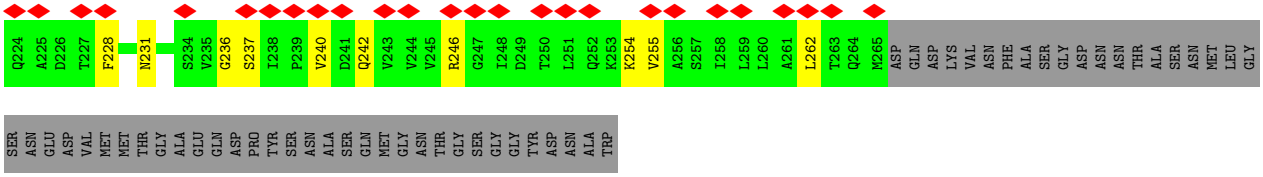




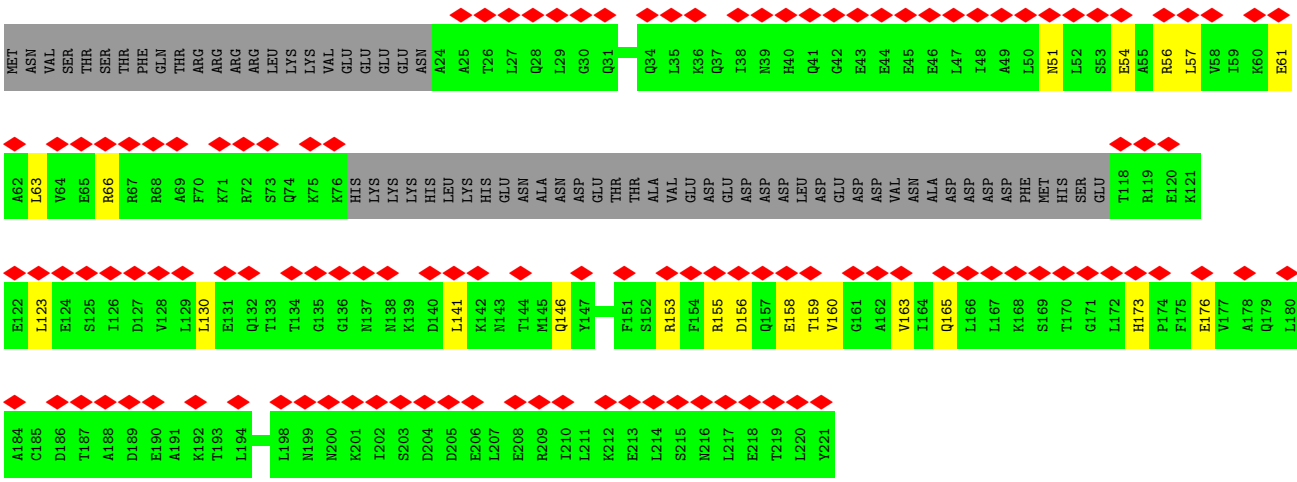
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

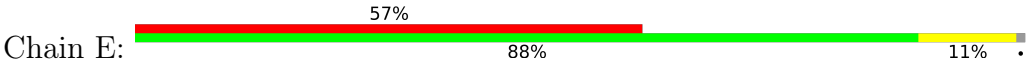


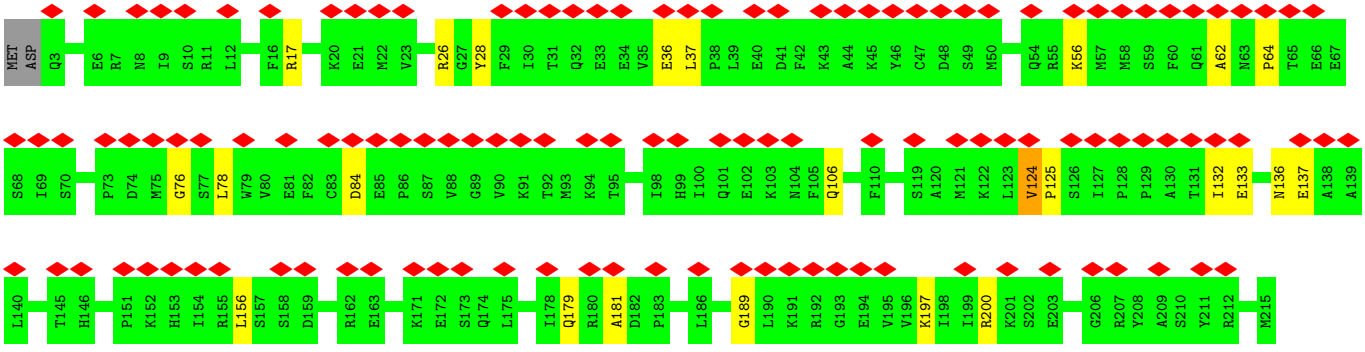


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

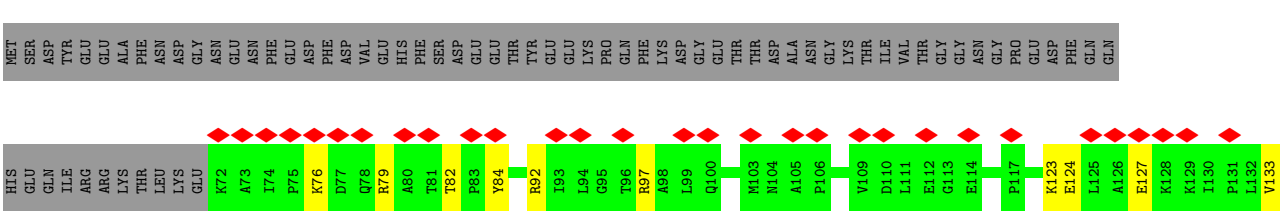


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



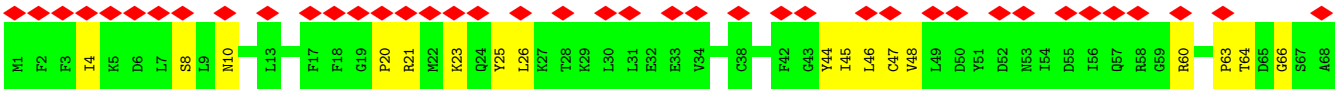


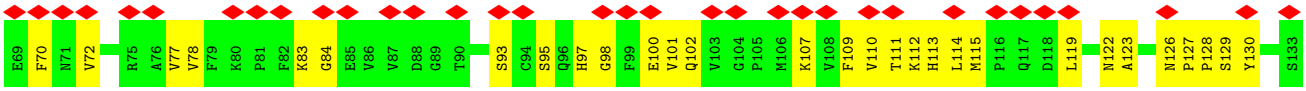
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

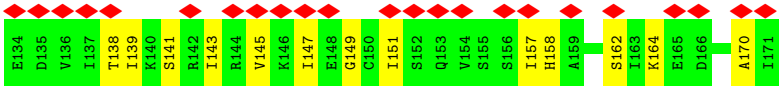


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

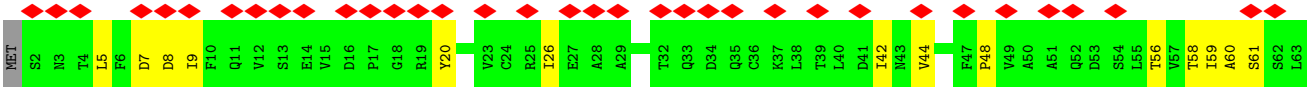


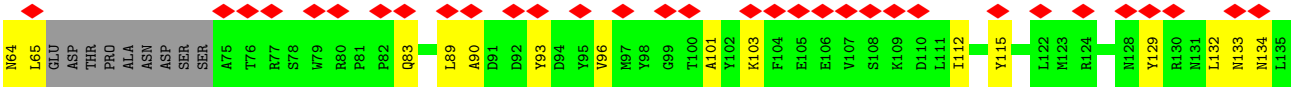


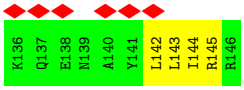


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

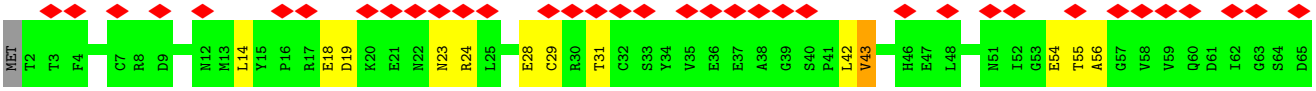


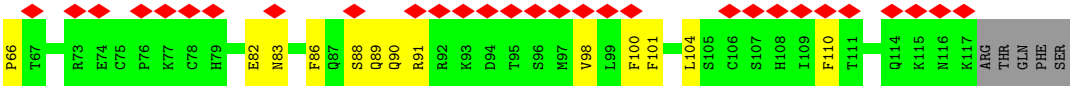




• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

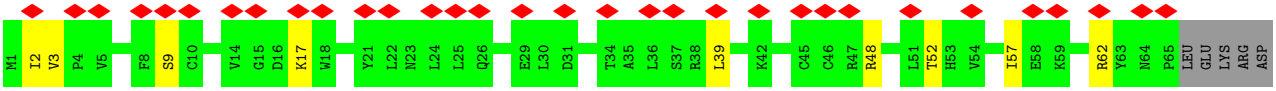
Chain I:



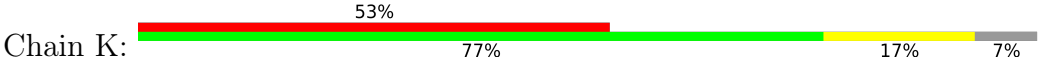


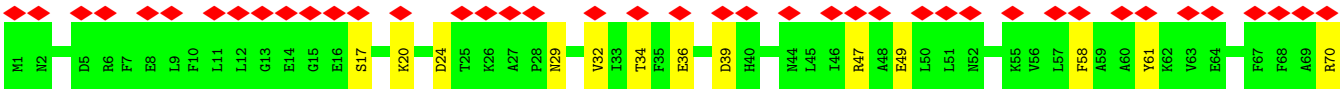
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

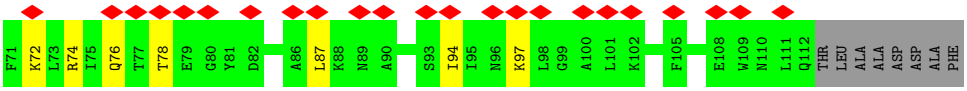
Chain J:



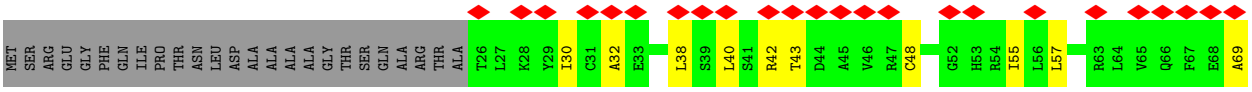
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11



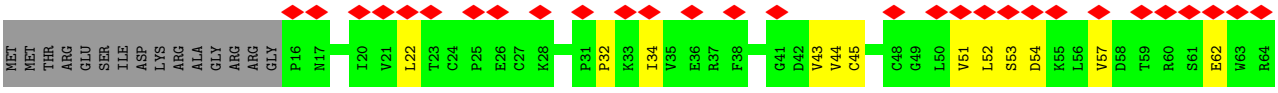


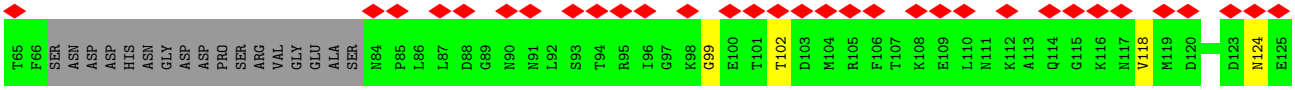


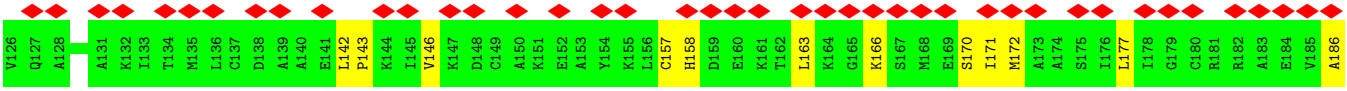
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

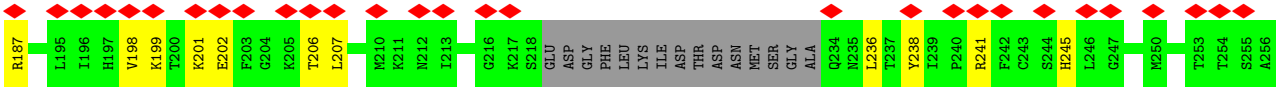


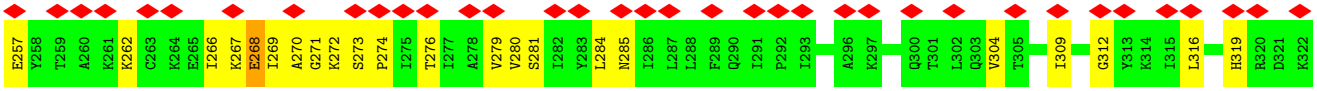
• Molecule 13: Transcription initiation factor IIB

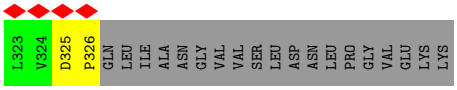




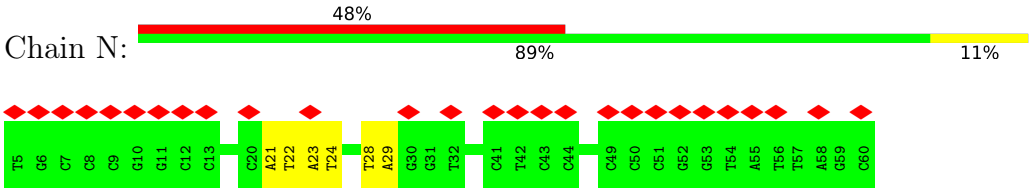




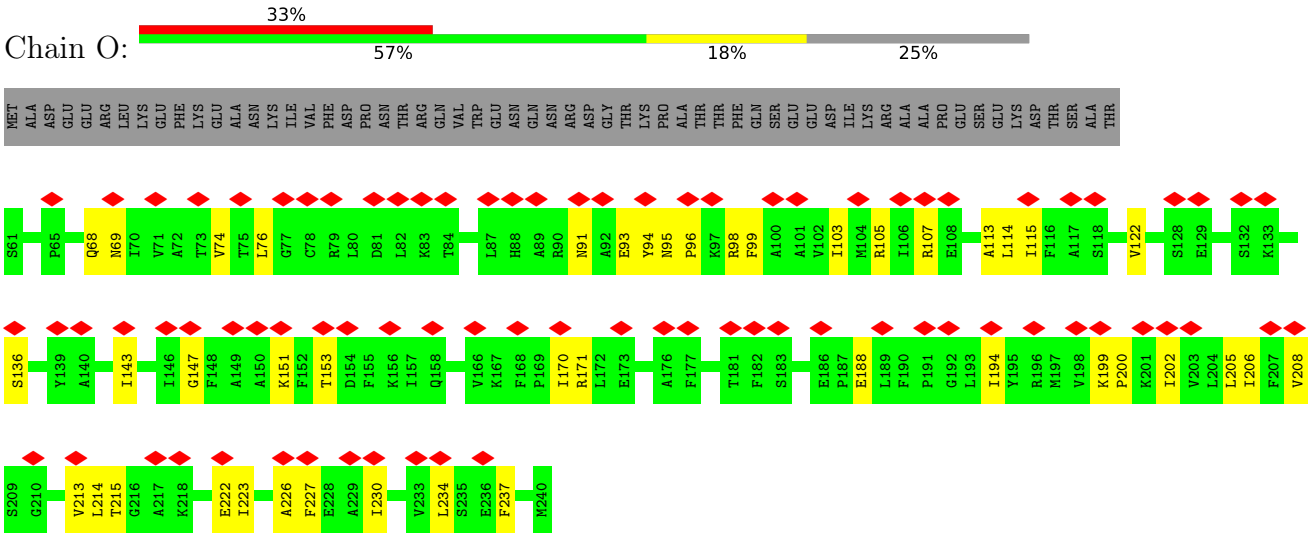




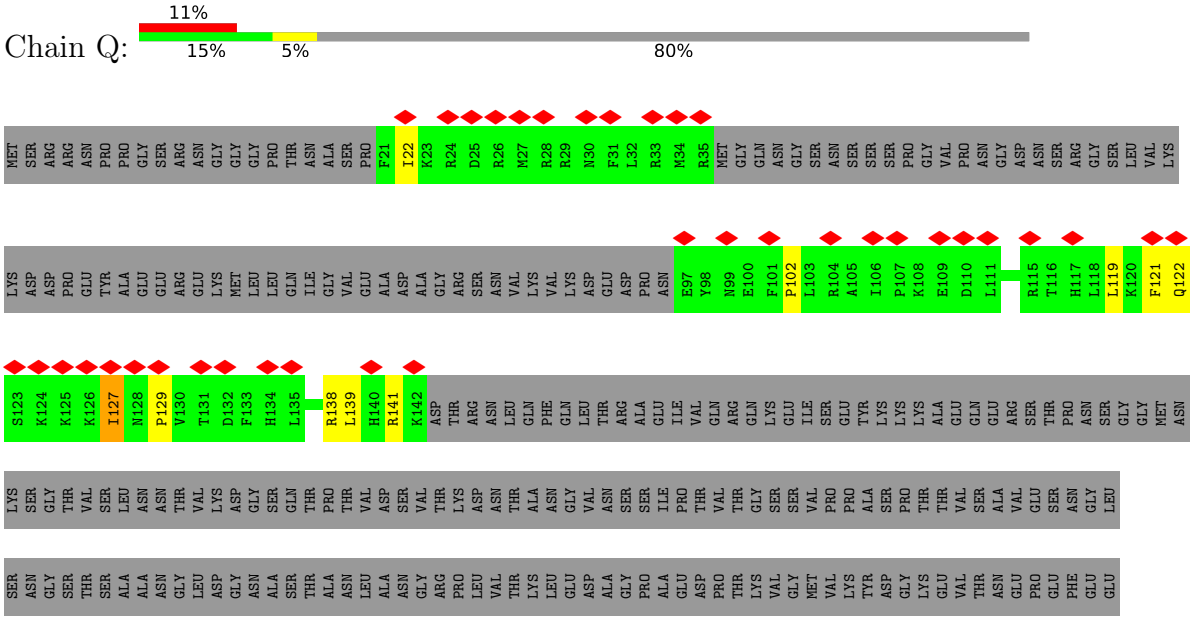
• Molecule 14: GAT1 promoter DNA

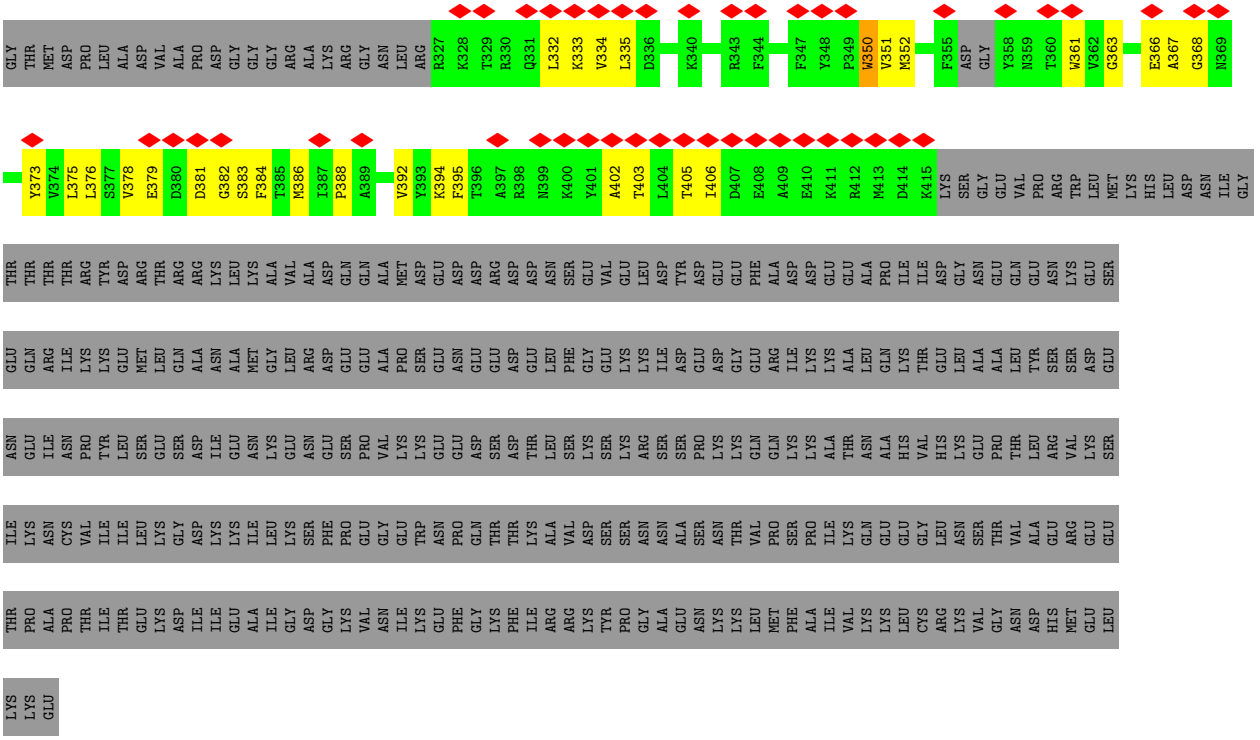


• Molecule 15: TATA-box-binding protein



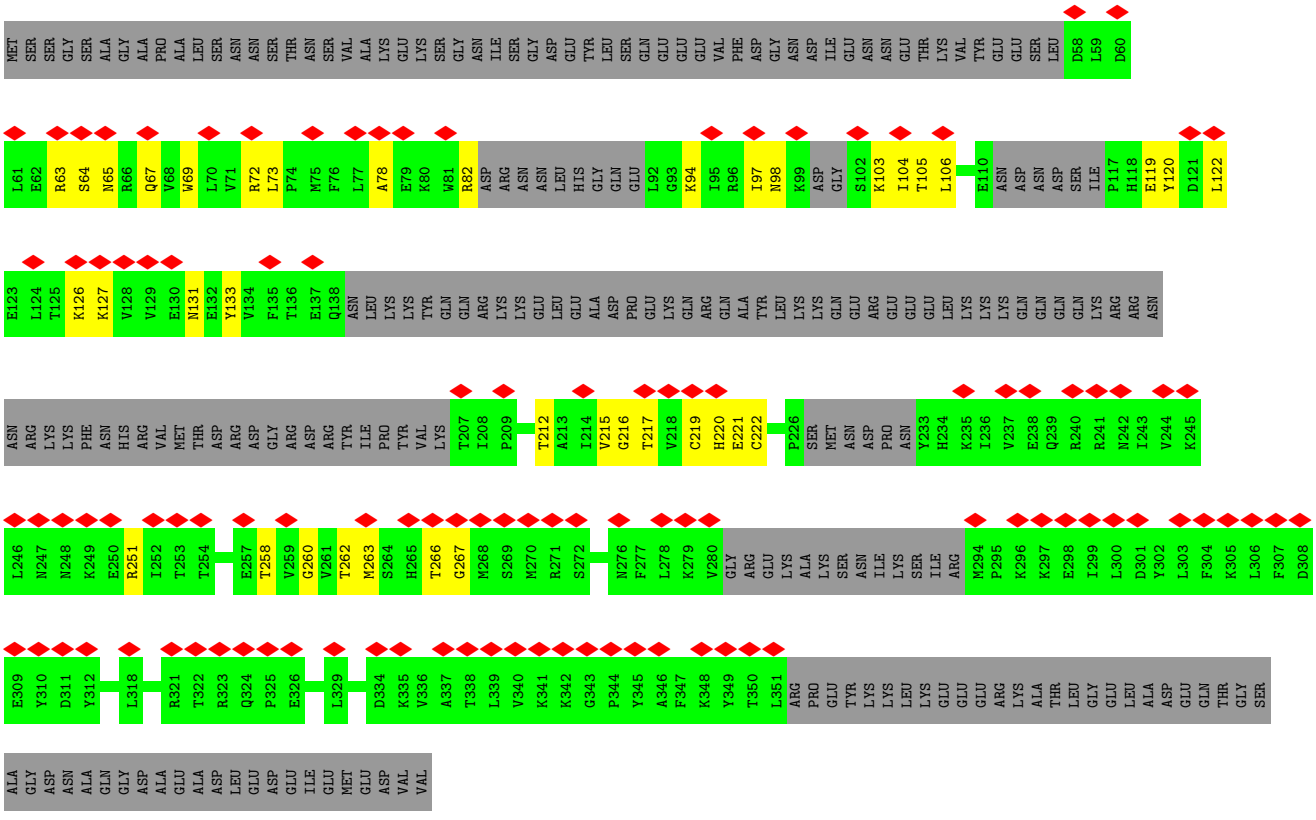
• Molecule 16: Transcription initiation factor IIF subunit alpha





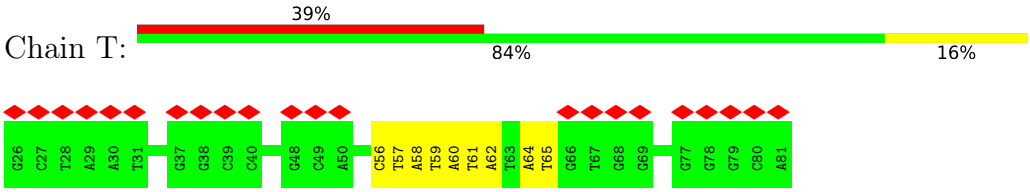
• Molecule 17: Transcription initiation factor IIF subunit beta

Chain R:



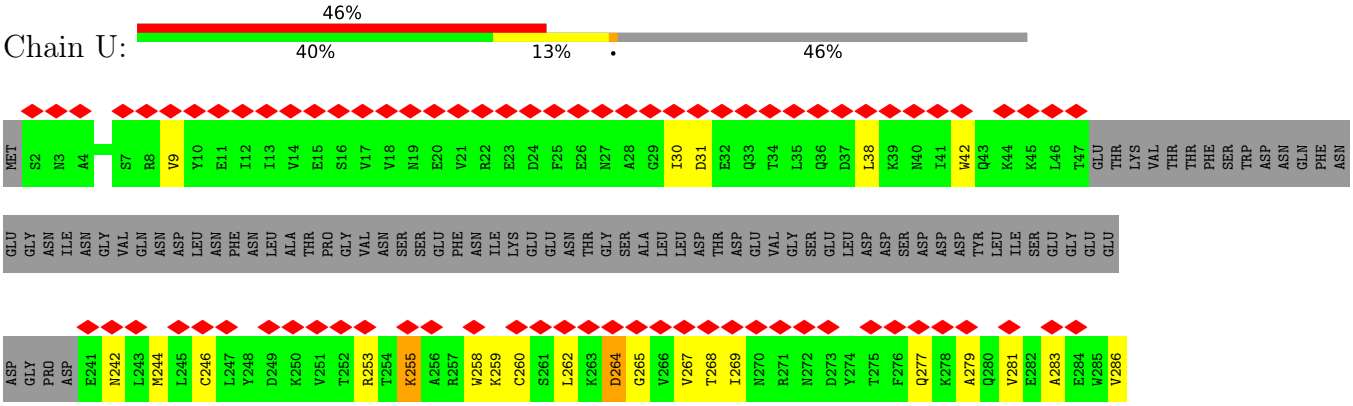
• Molecule 18: GAT1 promoter DNA

Chain T:



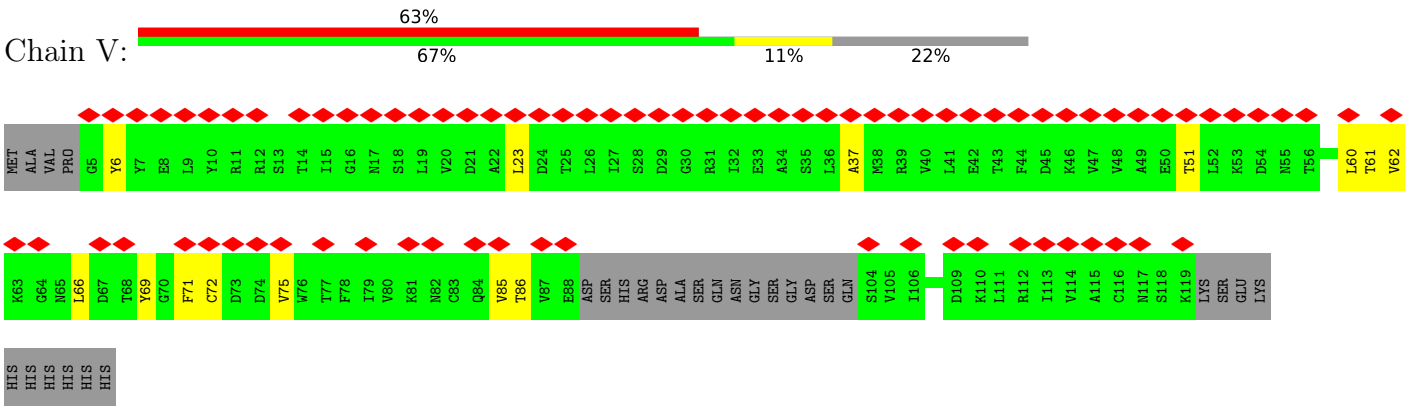
• Molecule 19: Transcription initiation factor IIA large subunit,Transcription initiation factor IIA large subunit

Chain U:



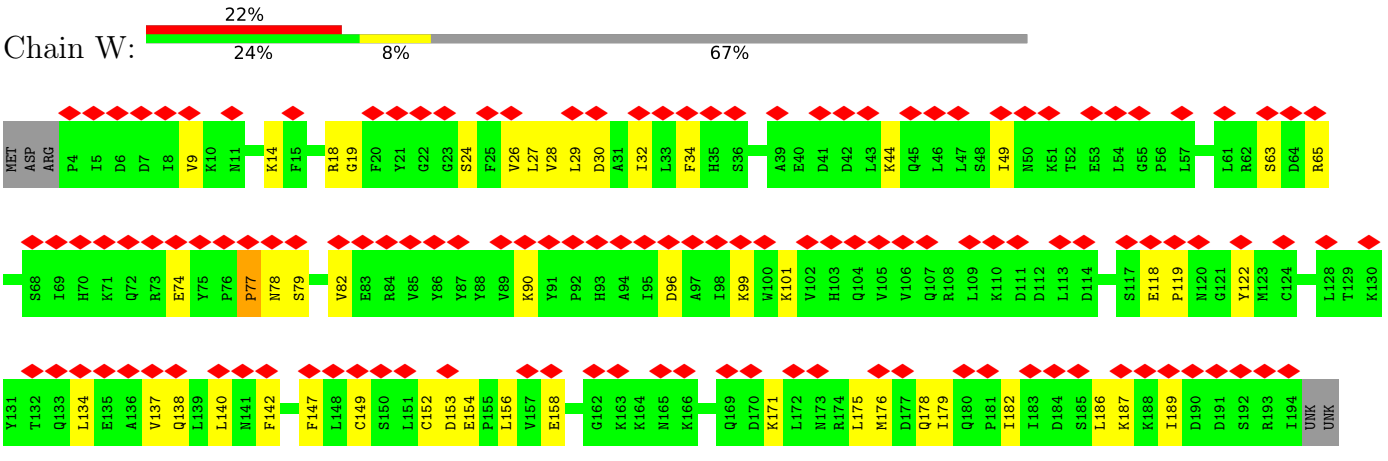
• Molecule 20: Transcription initiation factor IIA subunit 2

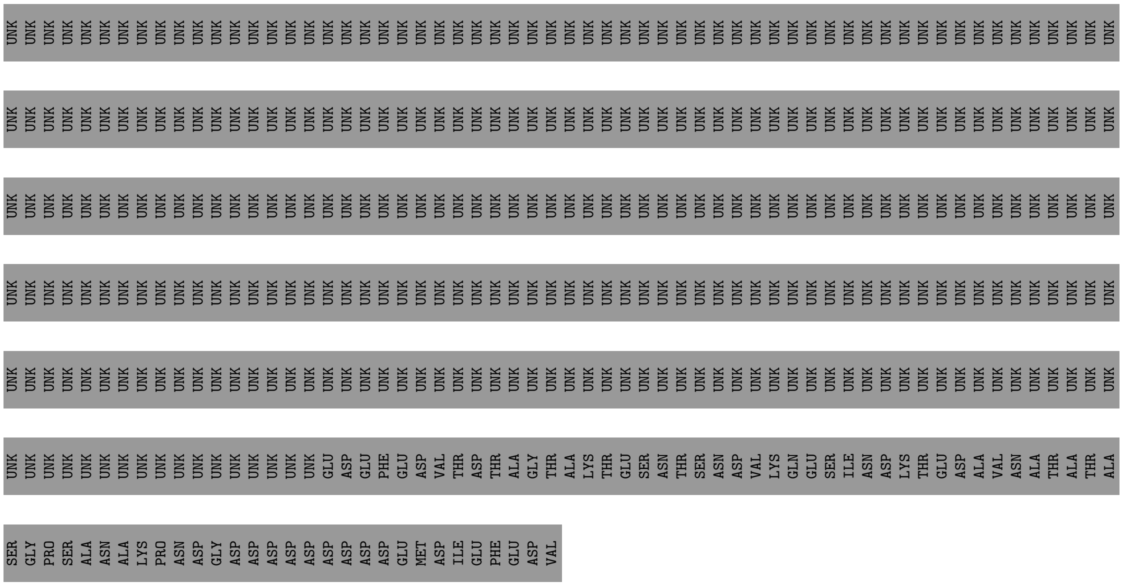
Chain V:



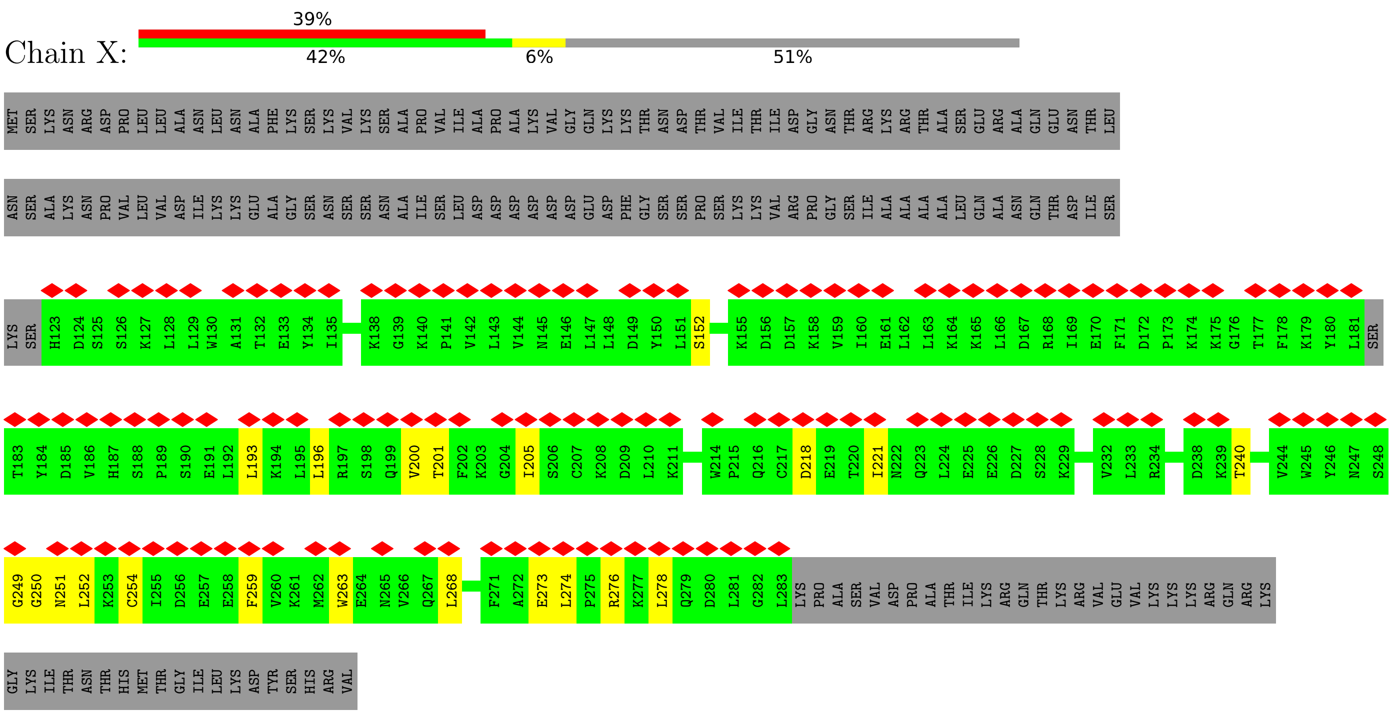
• Molecule 21: Transcription initiation factor IIE subunit alpha,Tfa1,Tfa1

Chain W:





• Molecule 22: Transcription initiation factor IIE subunit beta



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38000	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 ($e^-/Å^2$)	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.011	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0028	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/11192	0.41	0/15128
2	B	0.24	0/9357	0.40	0/12618
3	C	0.24	0/2099	0.40	0/2845
4	D	0.23	0/1262	0.37	0/1693
5	E	0.24	0/1780	0.38	0/2395
6	F	0.24	0/682	0.38	0/922
7	G	0.25	0/1368	0.42	0/1844
8	H	0.25	0/1107	0.42	0/1499
9	I	0.24	0/962	0.43	0/1295
10	J	0.28	0/541	0.41	0/727
11	K	0.24	0/922	0.39	0/1244
12	L	0.23	0/360	0.45	0/478
13	M	0.24	0/2204	0.40	0/2963
14	N	0.50	0/1264	0.85	0/1933
15	O	0.25	0/1443	0.43	0/1942
16	Q	0.26	0/1168	0.45	0/1579
17	R	0.24	0/1312	0.42	0/1777
18	T	0.49	0/1292	0.81	0/1981
19	U	0.22	0/766	0.38	0/1032
20	V	0.23	0/789	0.39	0/1066
21	W	0.24	0/1490	0.38	0/2014
22	X	0.24	0/1013	0.40	0/1385
All	All	0.27	0/44373	0.44	0/60360

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	10997	0	11081	159	0
2	B	9178	0	9195	163	0
3	C	2061	0	2029	29	0
4	D	1253	0	1275	12	0
5	E	1744	0	1772	13	0
6	F	670	0	690	10	0
7	G	1340	0	1357	76	0
8	H	1089	0	1062	20	0
9	I	944	0	899	28	0
10	J	532	0	542	6	0
11	K	904	0	911	13	0
12	L	358	0	381	7	0
13	M	2175	0	2283	50	0
14	N	1129	0	629	8	0
15	O	1416	0	1493	77	0
16	Q	1144	0	1034	29	0
17	R	1303	0	1110	29	0
18	T	1149	0	627	51	0
19	U	757	0	747	23	0
20	V	782	0	790	14	0
21	W	1469	0	1431	97	0
22	X	1004	0	730	38	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	43409	0	42068	748	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 9.

All (748) 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)
15:O:99:PHE:CD2	18:T:58:DA:H1'	1.23	1.65
15:O:98:ARG:HG2	18:T:58:DA:C5'	1.46	1.43
15:O:99:PHE:CG	18:T:58:DA:H1'	1.57	1.37
15:O:99:PHE:CZ	18:T:58:DA:N3	1.95	1.35
7:G:158:HIS:HB2	21:W:138:GLN:NE2	1.40	1.32
15:O:98:ARG:CD	18:T:58:DA:H5"	1.55	1.30
15:O:99:PHE:CB	18:T:58:DA:O4'	1.80	1.27
15:O:99:PHE:HB2	18:T:58:DA:O4'	1.10	1.26
15:O:99:PHE:CD2	18:T:58:DA:C1'	2.16	1.26
13:M:272:LYS:HE2	18:T:65:DT:O5'	1.36	1.25
7:G:97:HIS:CE1	21:W:122:TYR:HE2	1.54	1.24
7:G:158:HIS:CG	21:W:138:GLN:HE22	1.55	1.23
15:O:99:PHE:CG	18:T:58:DA:C1'	2.20	1.23
15:O:98:ARG:CG	18:T:58:DA:C5'	2.16	1.21
21:W:178:GLN:NE2	22:X:254:CYS:SG	2.12	1.21
7:G:113:HIS:HB3	21:W:118:GLU:OE2	1.06	1.20
15:O:98:ARG:CG	18:T:58:DA:H5'	1.73	1.19
7:G:113:HIS:CB	21:W:118:GLU:OE2	1.91	1.18
7:G:158:HIS:CB	21:W:138:GLN:HE22	1.55	1.16
15:O:103:ILE:HD13	18:T:59:DT:H5'	1.29	1.11
7:G:158:HIS:CB	21:W:138:GLN:NE2	2.09	1.10
21:W:65:ARG:NH2	22:X:274:LEU:HD23	1.67	1.09
15:O:98:ARG:O	18:T:57:DT:H2"	1.50	1.09
21:W:65:ARG:HH22	22:X:274:LEU:HB3	1.18	1.07
7:G:97:HIS:CE1	21:W:122:TYR:CE2	2.42	1.06
7:G:158:HIS:CD2	21:W:138:GLN:HE22	1.76	1.04
15:O:98:ARG:CD	18:T:58:DA:C5'	2.35	1.04
9:I:54:GLU:O	9:I:89:GLN:N	1.93	1.02
7:G:158:HIS:CG	21:W:138:GLN:NE2	2.28	1.00
19:U:242:ASN:HA	19:U:268:THR:O	1.62	0.99
21:W:65:ARG:NH2	22:X:274:LEU:CD2	2.25	0.99
15:O:99:PHE:CE1	18:T:58:DA:N3	2.31	0.99
14:N:24:DT:OP1	15:O:194:ILE:HD13	1.63	0.98
21:W:18:ARG:NE	22:X:250:GLY:H	1.60	0.97
15:O:103:ILE:CD1	18:T:59:DT:H5'	1.95	0.96
15:O:98:ARG:HD3	18:T:58:DA:H5"	1.47	0.95
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.40	0.93
15:O:99:PHE:CZ	18:T:58:DA:C2	2.58	0.91
17:R:106:LEU:O	17:R:119:GLU:HA	1.72	0.90
9:I:54:GLU:HB3	9:I:88:SER:OG	1.71	0.90
1:A:1444:MET:SD	7:G:60:ARG:HG3	2.12	0.90
15:O:98:ARG:CG	18:T:58:DA:H5"	1.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:138:ARG:O	16:Q:352:MET:HA	1.72	0.89
17:R:98:ASN:HB3	17:R:103:LYS:O	1.71	0.89
7:G:158:HIS:HB2	21:W:138:GLN:HE21	1.30	0.88
15:O:103:ILE:HD13	18:T:59:DT:C5’	2.05	0.87
13:M:274:PRO:HD2	15:O:188:GLU:HG2	1.57	0.87
7:G:158:HIS:CD2	21:W:138:GLN:NE2	2.40	0.87
15:O:99:PHE:CE2	18:T:58:DA:H1’	2.07	0.86
15:O:99:PHE:CE2	18:T:58:DA:N3	2.44	0.85
7:G:109:PHE:CZ	21:W:147:PHE:HZ	1.93	0.84
21:W:18:ARG:NH1	22:X:249:GLY:HA3	1.93	0.84
2:B:70:ILE:HD11	16:Q:333:LYS:HB2	1.59	0.83
21:W:65:ARG:HH22	22:X:274:LEU:CB	1.91	0.83
9:I:54:GLU:CB	9:I:88:SER:OG	2.27	0.83
3:C:11:ARG:NH1	3:C:209:TYR:OH	2.12	0.82
21:W:34:PHE:HB3	22:X:201:THR:HG22	1.58	0.82
21:W:14:LYS:O	21:W:18:ARG:HB2	1.79	0.82
9:I:54:GLU:HA	9:I:90:GLN:H	1.43	0.82
21:W:18:ARG:CZ	22:X:250:GLY:H	1.93	0.81
13:M:272:LYS:HE2	18:T:65:DT:C5’	2.10	0.80
18:T:60:DA:OP1	19:U:253:ARG:NH1	2.11	0.80
21:W:65:ARG:NH2	22:X:274:LEU:HB3	1.96	0.79
21:W:149:CYS:O	21:W:153:ASP:N	2.16	0.79
15:O:103:ILE:HD11	18:T:58:DA:H2”	1.65	0.79
7:G:158:HIS:CD2	21:W:138:GLN:OE1	2.37	0.78
21:W:101:LYS:HD3	22:X:263:TRP:CE2	2.18	0.78
2:B:835:GLN:HA	2:B:1013:ASN:ND2	1.99	0.78
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.18	0.77
4:D:57:LEU:O	4:D:61:GLU:HB2	1.84	0.77
13:M:272:LYS:CE	18:T:65:DT:O5’	2.28	0.77
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.67	0.76
15:O:98:ARG:HG3	18:T:57:DT:O3’	1.85	0.76
21:W:96:ASP:HB3	22:X:278:LEU:CD1	2.16	0.76
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.65	0.76
15:O:99:PHE:HB2	18:T:58:DA:C4’	2.16	0.76
2:B:839:MET:HG2	2:B:1012:ILE:HG22	1.66	0.76
16:Q:376:LEU:HD21	16:Q:386:MET:HE3	1.66	0.75
21:W:65:ARG:NH2	22:X:274:LEU:CB	2.49	0.75
11:K:20:LYS:HB2	11:K:34:THR:HB	1.67	0.75
8:H:56:THR:O	8:H:144:ILE:HA	1.86	0.75
7:G:113:HIS:CE1	21:W:119:PRO:HG2	2.22	0.75
15:O:98:ARG:HG2	18:T:58:DA:H5’	0.78	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:65:ARG:CZ	22:X:274:LEU:HD23	2.17	0.75
3:C:75:MET:O	3:C:246:ARG:NH2	2.21	0.74
3:C:56:THR:HG22	3:C:147:LEU:HD21	1.70	0.74
21:W:149:CYS:HB2	21:W:156:LEU:HD21	1.70	0.74
15:O:91:ASN:OD1	20:V:69:TYR:CE2	2.40	0.73
21:W:18:ARG:HB3	22:X:252:LEU:HD12	1.70	0.73
1:A:1055:ARG:NH1	6:F:154:ASP:O	2.20	0.73
13:M:279:VAL:HG11	13:M:304:VAL:HG11	1.70	0.73
1:A:441:PRO:HA	1:A:458:HIS:O	1.88	0.73
9:I:101:PHE:HB2	9:I:110:PHE:O	1.89	0.73
16:Q:127:ILE:HG22	16:Q:129:PRO:HD3	1.70	0.72
21:W:65:ARG:HH21	22:X:274:LEU:CD2	2.02	0.72
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.55	0.72
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.72	0.71
12:L:32:ALA:HB2	12:L:55:ILE:HB	1.70	0.71
7:G:101:VAL:HG21	7:G:145:VAL:HG21	1.73	0.70
16:Q:375:LEU:O	16:Q:386:MET:HA	1.91	0.70
9:I:19:ASP:HB3	9:I:24:ARG:O	1.92	0.70
7:G:10:ASN:HA	7:G:70:PHE:O	1.92	0.69
15:O:91:ASN:OD1	20:V:69:TYR:CZ	2.44	0.69
13:M:34:ILE:HG22	13:M:45:CYS:HA	1.75	0.69
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.73	0.69
13:M:236:LEU:HD11	13:M:257:GLU:HG3	1.74	0.69
13:M:274:PRO:HD2	15:O:188:GLU:CG	2.23	0.69
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.75	0.69
8:H:96:VAL:HA	8:H:142:LEU:O	1.93	0.69
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.74	0.68
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.75	0.68
2:B:373:ARG:HG3	2:B:566:LEU:HD23	1.75	0.68
2:B:825:VAL:HA	2:B:1010:LEU:O	1.93	0.68
21:W:18:ARG:CB	22:X:252:LEU:HD12	2.23	0.68
7:G:97:HIS:ND1	21:W:122:TYR:HE2	1.90	0.68
13:M:99:GLY:H	13:M:102:THR:HG21	1.58	0.68
7:G:113:HIS:CE1	21:W:119:PRO:HB2	2.30	0.67
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.23	0.67
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.77	0.67
13:M:157:CYS:SG	13:M:158:HIS:N	2.68	0.67
3:C:18:VAL:HG21	3:C:240:VAL:HG21	1.77	0.67
2:B:383:ASN:O	2:B:387:LEU:HB2	1.96	0.66
17:R:64:SER:HA	17:R:216:GLY:HA2	1.77	0.66
21:W:18:ARG:HG2	22:X:250:GLY:HA2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.77	0.66
2:B:67:SER:HB2	2:B:92:PHE:H	1.61	0.66
15:O:98:ARG:O	18:T:57:DT:C2'	2.36	0.66
15:O:107:ARG:HG2	19:U:286:VAL:O	1.95	0.66
1:A:807:GLY:HA3	2:B:728:ARG:HH21	1.60	0.66
2:B:770:GLN:NE2	2:B:982:SER:O	2.29	0.65
1:A:61:ILE:HG22	1:A:62:ASP:H	1.59	0.65
7:G:158:HIS:CD2	21:W:138:GLN:CD	2.70	0.65
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.78	0.65
3:C:11:ARG:NH2	3:C:19:ASP:OD2	2.30	0.65
2:B:1171:VAL:HA	2:B:1181:GLU:O	1.97	0.65
1:A:69:THR:HG23	1:A:80:HIS:CD2	2.32	0.65
7:G:109:PHE:CZ	21:W:147:PHE:CZ	2.81	0.65
7:G:97:HIS:ND1	21:W:122:TYR:CE2	2.63	0.64
13:M:267:LYS:HE2	13:M:270:ALA:HB2	1.78	0.64
2:B:826:ALA:HB3	2:B:1011:ILE:HG12	1.79	0.64
2:B:822:ASN:O	10:J:48:ARG:NH1	2.30	0.64
16:Q:121:PHE:HB2	17:R:131:ASN:HB3	1.78	0.64
1:A:178:GLY:HA2	1:A:311:GLN:HE22	1.63	0.64
4:D:173:HIS:HB3	4:D:176:GLU:HG3	1.80	0.64
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.70	0.64
1:A:860:LEU:HD11	1:A:1394:THR:HA	1.80	0.64
7:G:113:HIS:ND1	21:W:119:PRO:HD2	2.13	0.64
2:B:115:GLN:NE2	2:B:787:VAL:O	2.31	0.64
13:M:272:LYS:CE	18:T:65:DT:C5'	2.76	0.63
7:G:113:HIS:CA	21:W:118:GLU:OE2	2.46	0.63
13:M:267:LYS:HE2	15:O:208:VAL:HG11	1.79	0.63
1:A:32:VAL:HG12	2:B:1183:LYS:HE2	1.81	0.63
1:A:1329:THR:HG22	1:A:1331:SER:H	1.62	0.63
1:A:70:CYS:SG	1:A:80:HIS:CE1	2.91	0.63
17:R:126:LYS:HB3	17:R:221:GLU:HB2	1.79	0.63
3:C:13:ALA:HA	3:C:18:VAL:HG22	1.80	0.62
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.80	0.62
2:B:25:ILE:HA	2:B:655:LYS:HE3	1.82	0.62
2:B:249:ARG:HG2	2:B:415:GLN:HE22	1.64	0.62
1:A:68:GLN:O	1:A:71:GLN:NE2	2.33	0.62
2:B:944:THR:HG21	2:B:1122:ARG:HH12	1.63	0.62
2:B:490:SER:O	2:B:494:HIS:HB2	2.00	0.62
13:M:163:LEU:O	13:M:166:LYS:NZ	2.33	0.62
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.81	0.61
1:A:1451:VAL:HG12	7:G:20:PRO:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:785:TYR:O	2:B:967:ARG:NH1	2.32	0.61
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.81	0.61
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.33	0.61
15:O:99:PHE:CE1	18:T:58:DA:C2	2.87	0.61
21:W:101:LYS:HD2	22:X:263:TRP:CZ2	2.36	0.61
13:M:118:VAL:HG22	13:M:124:ASN:HD21	1.65	0.61
7:G:113:HIS:CE1	21:W:119:PRO:CG	2.82	0.61
3:C:25:VAL:HG13	3:C:29:MET:HB3	1.83	0.60
15:O:91:ASN:ND2	20:V:69:TYR:OH	2.32	0.60
13:M:22:LEU:HB3	13:M:52:LEU:HD23	1.83	0.60
7:G:113:HIS:O	21:W:118:GLU:OE2	2.20	0.60
16:Q:373:TYR:OH	17:R:72:ARG:NH2	2.34	0.60
19:U:259:LYS:HA	19:U:281:VAL:O	2.00	0.60
1:A:562:THR:O	1:A:576:GLN:NE2	2.34	0.60
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.34	0.60
16:Q:139:LEU:HA	16:Q:351:VAL:O	2.02	0.60
1:A:481:ASP:O	1:A:483:ASP:OD1	2.20	0.60
1:A:483:ASP:OD1	1:A:483:ASP:N	2.35	0.60
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.65	0.60
1:A:185:TRP:HB2	1:A:198:GLU:O	2.02	0.60
1:A:1257:ASP:OD1	1:A:1258:HIS:N	2.35	0.60
2:B:298:LEU:HD23	2:B:311:LEU:HD22	1.84	0.60
8:H:101:ALA:HA	8:H:115:TYR:O	2.02	0.60
21:W:65:ARG:HH21	22:X:274:LEU:HD22	1.66	0.60
1:A:537:ARG:HD2	8:H:20:TYR:CZ	2.37	0.59
1:A:115:LEU:O	1:A:164:ARG:NH1	2.35	0.59
4:D:66:ARG:NH2	7:G:47:CYS:SG	2.75	0.59
4:D:57:LEU:O	4:D:61:GLU:CB	2.50	0.59
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.36	0.59
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.83	0.59
13:M:281:SER:O	13:M:285:ASN:ND2	2.31	0.59
15:O:105:ARG:NE	19:U:253:ARG:NH2	2.50	0.59
2:B:193:LYS:HB3	2:B:787:VAL:HG21	1.83	0.59
22:X:200:VAL:HG12	22:X:201:THR:HG23	1.85	0.59
3:C:5:GLY:O	3:C:24:ASN:ND2	2.36	0.59
7:G:109:PHE:CE1	21:W:147:PHE:HZ	2.20	0.59
21:W:96:ASP:HB3	22:X:278:LEU:HD11	1.85	0.59
9:I:82:GLU:HG2	9:I:104:LEU:HD12	1.85	0.58
3:C:73:GLN:HE21	3:C:74:SER:H	1.50	0.58
16:Q:141:ARG:HA	16:Q:350:TRP:HA	1.85	0.58
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:284:LEU:HD22	13:M:316:LEU:HG	1.86	0.58
19:U:244:MET:HG3	19:U:267:VAL:HG22	1.86	0.58
1:A:1189:SER:N	1:A:1242:VAL:O	2.31	0.58
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.84	0.58
2:B:919:SER:HB2	2:B:922:GLU:HB2	1.84	0.58
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	1.86	0.58
2:B:969:ARG:NH2	3:C:60:ASP:OD2	2.36	0.58
7:G:84:GLY:CA	7:G:147:ILE:O	2.52	0.58
8:H:129:TYR:O	8:H:133:ASN:ND2	2.35	0.58
15:O:99:PHE:CB	18:T:58:DA:C4'	2.77	0.58
8:H:65:LEU:HD21	8:H:89:LEU:HD13	1.86	0.58
1:A:250:ILE:HD13	13:M:62:GLU:HG3	1.85	0.58
3:C:22:LEU:O	3:C:228:PHE:HB2	2.03	0.58
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.85	0.58
14:N:24:DT:P	15:O:194:ILE:HD13	2.44	0.58
15:O:68:GLN:OE1	18:T:62:DA:H5'	2.04	0.58
1:A:335:ARG:HH22	2:B:1114:LEU:HD11	1.69	0.57
3:C:54:ASN:HD21	3:C:63:ILE:HD12	1.68	0.57
1:A:333:GLU:OE1	2:B:1129:ARG:NH2	2.37	0.57
1:A:390:GLN:OE1	1:A:393:ARG:NH2	2.37	0.57
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.85	0.57
7:G:97:HIS:CE1	21:W:158:GLU:HG2	2.38	0.57
7:G:113:HIS:C	21:W:118:GLU:OE2	2.43	0.57
9:I:19:ASP:O	9:I:23:ASN:HA	2.04	0.57
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.36	0.57
1:A:443:LEU:HG	1:A:501:LEU:HD21	1.87	0.57
7:G:8:SER:HA	7:G:72:VAL:O	2.05	0.57
7:G:113:HIS:HB3	21:W:118:GLU:CD	2.11	0.57
17:R:104:ILE:HD11	17:R:122:LEU:HD22	1.86	0.57
1:A:62:ASP:O	1:A:64:ASN:N	2.35	0.57
2:B:881:ASN:O	2:B:933:SER:OG	2.23	0.57
11:K:29:ASN:ND2	11:K:78:THR:O	2.37	0.57
16:Q:122:GLN:HB2	16:Q:394:LYS:HE3	1.87	0.57
17:R:104:ILE:HD11	17:R:122:LEU:HB3	1.86	0.56
19:U:262:LEU:HB2	19:U:279:ALA:HB3	1.87	0.56
5:E:28:TYR:HA	5:E:64:PRO:HA	1.86	0.56
21:W:175:LEU:HB2	22:X:259:PHE:CZ	2.39	0.56
1:A:348:SER:HA	1:A:489:LEU:O	2.04	0.56
2:B:118:ARG:NH2	2:B:202:TYR:OH	2.38	0.56
2:B:858:SER:HA	2:B:966:VAL:O	2.04	0.56
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1009:ASP:OD2	10:J:48:ARG:NH2	2.38	0.56
3:C:73:GLN:NE2	3:C:237:SER:O	2.38	0.56
7:G:138:THR:HG22	7:G:139:ILE:H	1.70	0.56
9:I:55:THR:HG22	9:I:100:PHE:CD2	2.40	0.56
13:M:34:ILE:HG21	13:M:52:LEU:HD22	1.87	0.56
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.05	0.56
17:R:67:GLN:HB3	17:R:219:CYS:HB2	1.87	0.56
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.86	0.56
5:E:17:ARG:HH12	5:E:36:GLU:HA	1.71	0.56
7:G:107:LYS:NZ	21:W:142:PHE:CE1	2.73	0.56
13:M:177:LEU:HD22	13:M:207:LEU:HD11	1.87	0.56
7:G:84:GLY:HA2	7:G:147:ILE:O	2.05	0.56
2:B:794:ASN:HA	2:B:854:LEU:O	2.06	0.56
5:E:76:GLY:N	5:E:106:GLN:OE1	2.39	0.56
2:B:71:LEU:HD21	2:B:436:VAL:HG11	1.88	0.56
7:G:84:GLY:N	7:G:147:ILE:O	2.39	0.55
15:O:99:PHE:CB	18:T:58:DA:C1'	2.56	0.55
1:A:544:ASP:O	1:A:548:ASN:ND2	2.38	0.55
2:B:278:GLN:HB2	2:B:337:ARG:HD2	1.88	0.55
2:B:549:THR:HG1	2:B:628:THR:HG1	1.49	0.55
4:D:141:LEU:HD13	7:G:46:LEU:HB3	1.88	0.55
19:U:30:ILE:HG23	19:U:31:ASP:H	1.71	0.55
1:A:687:LYS:NZ	1:A:801:GLU:OE1	2.38	0.55
7:G:97:HIS:HE1	21:W:158:GLU:HG2	1.72	0.55
10:J:48:ARG:O	10:J:52:THR:OG1	2.14	0.55
15:O:74:VAL:HG21	15:O:136:SER:HB3	1.88	0.55
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.72	0.55
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.32	0.55
3:C:242:GLN:O	3:C:246:ARG:HB2	2.06	0.55
11:K:36:GLU:OE1	11:K:70:ARG:NH1	2.39	0.55
19:U:246:CYS:HB3	19:U:265:GLY:HA3	1.89	0.55
21:W:101:LYS:HB3	22:X:263:TRP:CZ3	2.42	0.55
1:A:845:LEU:HD11	1:A:1371:LEU:HD23	1.89	0.55
12:L:30:ILE:HB	12:L:57:LEU:HB2	1.88	0.55
2:B:211:VAL:O	2:B:480:SER:HA	2.07	0.54
1:A:908:LEU:HA	1:A:1029:ARG:HH22	1.72	0.54
1:A:1342:GLU:OE1	5:E:200:ARG:NH2	2.36	0.54
2:B:347:LYS:O	2:B:351:TYR:HB2	2.07	0.54
21:W:19:GLY:HA2	22:X:252:LEU:HB3	1.88	0.54
1:A:1441:PHE:O	6:F:92:ARG:NH1	2.41	0.54
15:O:69:ASN:HB2	18:T:61:DT:H1'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TRP:HZ3	1:A:200:ARG:HB2	1.72	0.54
2:B:298:LEU:HG	2:B:314:LEU:HD13	1.89	0.54
13:M:43:VAL:HG12	13:M:53:SER:HB3	1.90	0.54
15:O:205:LEU:HB2	15:O:213:VAL:HB	1.90	0.54
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.88	0.54
2:B:429:PHE:CZ	16:Q:332:LEU:HB2	2.43	0.54
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.90	0.54
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.90	0.54
17:R:127:LYS:HA	17:R:220:HIS:CE1	2.43	0.54
21:W:101:LYS:CD	22:X:263:TRP:CE2	2.89	0.54
1:A:588:LEU:HD13	1:A:632:VAL:HG21	1.89	0.54
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.88	0.54
8:H:112:ILE:HG23	8:H:132:LEU:HD12	1.89	0.54
9:I:56:ALA:O	9:I:89:GLN:HG3	2.08	0.54
9:I:54:GLU:HG2	9:I:90:GLN:HB3	1.89	0.54
14:N:28:DT:H3	14:N:29:DA:H62	1.55	0.54
2:B:55:VAL:HA	2:B:59:LEU:HD13	1.90	0.53
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.73	0.53
15:O:91:ASN:ND2	20:V:69:TYR:CZ	2.76	0.53
21:W:18:ARG:NE	22:X:250:GLY:N	2.43	0.53
7:G:158:HIS:HD2	21:W:138:GLN:OE1	1.88	0.53
2:B:833:TYR:HB2	2:B:840:ILE:HD11	1.90	0.53
1:A:899:VAL:H	1:A:929:LEU:HD11	1.72	0.53
10:J:2:ILE:HD13	10:J:57:ILE:HG21	1.90	0.53
13:M:241:ARG:O	13:M:245:HIS:ND1	2.34	0.53
9:I:29:CYS:SG	9:I:31:THR:OG1	2.66	0.53
21:W:14:LYS:NZ	21:W:30:ASP:OD1	2.41	0.53
21:W:96:ASP:HB3	22:X:278:LEU:HD12	1.90	0.53
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.39	0.53
17:R:98:ASN:CB	17:R:103:LYS:O	2.50	0.53
2:B:128:LEU:HB2	2:B:168:GLY:O	2.09	0.53
2:B:1042:GLY:HA2	16:Q:22:ILE:HA	1.90	0.53
7:G:47:CYS:SG	7:G:48:VAL:N	2.81	0.53
15:O:99:PHE:CE1	18:T:58:DA:C4	2.97	0.53
2:B:43:LEU:O	2:B:496:ARG:NH1	2.41	0.53
3:C:6:PRO:HB3	3:C:25:VAL:HG23	1.90	0.53
1:A:226:GLU:HA	1:A:230:ARG:HE	1.74	0.53
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.52
1:A:700:ASN:HB2	9:I:98:VAL:HG22	1.90	0.52
2:B:458:LYS:O	2:B:462:ALA:HB2	2.09	0.52
2:B:806:THR:HG23	2:B:1045:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:923:GLU:HB3	2:B:925:LEU:HG	1.91	0.52
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.73	0.52
21:W:175:LEU:HD23	22:X:259:PHE:CG	2.44	0.52
20:V:72:CYS:O	20:V:75:VAL:HB	2.10	0.52
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.73	0.52
3:C:100:THR:OG1	3:C:102:GLN:NE2	2.43	0.52
13:M:276:THR:HA	13:M:279:VAL:HG12	1.91	0.52
20:V:71:PHE:HA	20:V:75:VAL:O	2.09	0.52
15:O:93:GLU:OE2	15:O:105:ARG:NH1	2.41	0.52
1:A:445:ASN:OD1	1:A:449:SER:OG	2.21	0.52
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.92	0.52
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.91	0.52
2:B:445:LYS:NZ	17:R:267:GLY:O	2.36	0.52
7:G:107:LYS:HZ2	21:W:142:PHE:HE1	1.56	0.52
1:A:48:ALA:HB3	1:A:56:PRO:HD3	1.90	0.52
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.75	0.52
16:Q:366:GLU:O	16:Q:368:GLY:N	2.43	0.52
1:A:63:ARG:HA	1:A:74:MET:HG2	1.92	0.52
1:A:553:VAL:HB	1:A:556:TRP:HB2	1.92	0.52
2:B:791:THR:HG22	2:B:792:MET:HG3	1.91	0.52
7:G:111:THR:HB	7:G:114:LEU:HD13	1.92	0.52
15:O:113:ALA:HA	15:O:122:VAL:O	2.09	0.52
21:W:101:LYS:CD	22:X:263:TRP:CZ2	2.91	0.52
2:B:826:ALA:O	2:B:1011:ILE:HA	2.10	0.52
8:H:142:LEU:HG	8:H:144:ILE:HD11	1.92	0.52
16:Q:366:GLU:HB3	16:Q:392:VAL:HG13	1.90	0.52
17:R:73:LEU:HD23	17:R:78:ALA:HA	1.92	0.52
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.42	0.52
2:B:1060:ARG:NH1	3:C:200:GLU:O	2.42	0.52
13:M:199:LYS:O	13:M:201:LYS:N	2.42	0.52
17:R:105:THR:HA	17:R:120:TYR:O	2.09	0.52
2:B:1060:ARG:HH12	3:C:202:PRO:HD3	1.75	0.51
4:D:51:ASN:HD22	4:D:181:GLY:HA3	1.74	0.51
20:V:62:VAL:HG22	20:V:85:VAL:HG22	1.92	0.51
2:B:641:GLU:HB2	2:B:652:LYS:HE2	1.93	0.51
13:M:202:GLU:OE2	13:M:206:THR:OG1	2.24	0.51
2:B:342:GLY:O	2:B:344:LYS:N	2.41	0.51
11:K:61:TYR:HA	11:K:72:LYS:O	2.11	0.51
13:M:280:VAL:HG12	13:M:309:ILE:HA	1.92	0.51
15:O:99:PHE:CG	18:T:58:DA:O4'	2.34	0.51
22:X:193:LEU:HA	22:X:196:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.93	0.51
1:A:1154:TYR:HE2	9:I:18:GLU:HB2	1.75	0.51
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.39	0.51
2:B:22:SER:O	2:B:654:ARG:NH2	2.44	0.51
7:G:97:HIS:HE1	21:W:122:TYR:HE2	1.37	0.51
15:O:115:ILE:HD13	15:O:143:ILE:HD11	1.92	0.51
3:C:185:LYS:HE2	3:C:213:PRO:HB3	1.93	0.51
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.74	0.51
8:H:8:ASP:OD1	8:H:9:ILE:N	2.44	0.51
16:Q:334:VAL:HG12	16:Q:335:LEU:H	1.75	0.51
1:A:88:LYS:HD3	1:A:89:PRO:HD2	1.92	0.51
3:C:222:LYS:H	3:C:222:LYS:HD3	1.76	0.51
6:F:82:THR:HG22	6:F:84:TYR:H	1.76	0.51
2:B:771:SER:O	2:B:775:LYS:NZ	2.43	0.51
3:C:35:ARG:NH2	11:K:39:ASP:OD2	2.41	0.51
13:M:187:ARG:HH11	13:M:241:ARG:HH21	1.59	0.51
1:A:840:ARG:O	1:A:844:ALA:HB2	2.11	0.50
2:B:413:LEU:HD21	2:B:461:LEU:HD11	1.93	0.50
7:G:113:HIS:NE2	21:W:119:PRO:HB2	2.24	0.50
13:M:267:LYS:HE2	15:O:208:VAL:CG1	2.41	0.50
1:A:869:GLY:HA3	1:A:1366:ARG:HD2	1.93	0.50
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.93	0.50
19:U:283:ALA:HB1	20:V:66:LEU:HB2	1.94	0.50
2:B:102:VAL:O	2:B:109:THR:HA	2.12	0.50
2:B:376:PHE:HD2	2:B:566:LEU:HG	1.75	0.50
9:I:55:THR:HG22	9:I:100:PHE:CE2	2.47	0.50
9:I:86:PHE:O	9:I:100:PHE:HB2	2.12	0.50
1:A:961:ARG:NH1	1:A:1035:TYR:OH	2.44	0.50
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.50
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.93	0.50
15:O:202:ILE:HD11	15:O:222:GLU:HB3	1.94	0.50
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.93	0.50
2:B:755:ILE:O	2:B:983:ARG:NE	2.45	0.50
1:A:882:SER:O	1:A:1025:ARG:NH2	2.43	0.49
2:B:766:ARG:HE	2:B:1020:ARG:HB3	1.77	0.49
2:B:1091:TYR:HE2	2:B:1093:GLN:HE21	1.58	0.49
7:G:107:LYS:NZ	21:W:142:PHE:HE1	2.08	0.49
15:O:206:ILE:HD13	15:O:234:LEU:HD21	1.93	0.49
19:U:38:LEU:O	19:U:42:TRP:HB2	2.12	0.49
21:W:99:LYS:HG2	21:W:186:LEU:HD13	1.93	0.49
22:X:273:GLU:HG2	22:X:276:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:ARG:O	1:A:1033:GLN:HB3	2.12	0.49
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.93	0.49
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.12	0.49
2:B:226:PHE:HD1	2:B:395:GLN:HE21	1.60	0.49
21:W:24:SER:HA	21:W:27:LEU:HD22	1.94	0.49
1:A:597:LEU:HD13	8:H:103:LYS:HD3	1.94	0.49
1:A:984:LYS:O	1:A:988:LEU:HB2	2.12	0.49
1:A:1020:CYS:SG	1:A:1023:ARG:NH2	2.85	0.49
2:B:87:LYS:HB2	2:B:137:TYR:HB2	1.93	0.49
16:Q:119:LEU:HD12	17:R:133:TYR:HB2	1.93	0.49
2:B:793:ALA:O	2:B:855:PHE:HA	2.13	0.49
9:I:54:GLU:HA	9:I:90:GLN:N	2.21	0.49
1:A:69:THR:HG23	1:A:80:HIS:NE2	2.28	0.49
21:W:175:LEU:HD23	22:X:259:PHE:CD2	2.47	0.49
1:A:63:ARG:HH11	13:M:57:VAL:HG22	1.76	0.49
3:C:19:ASP:HB2	3:C:231:ASN:HD22	1.76	0.49
4:D:54:GLU:HB2	4:D:160:VAL:HG11	1.95	0.49
7:G:95:SER:OG	7:G:98:GLY:O	2.23	0.49
7:G:113:HIS:CE1	21:W:119:PRO:CB	2.94	0.49
15:O:105:ARG:NE	19:U:253:ARG:CZ	2.76	0.49
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.48	0.49
16:Q:381:ASP:OD1	16:Q:382:GLY:N	2.42	0.49
1:A:446:ARG:O	1:A:449:SER:OG	2.31	0.49
6:F:133:VAL:HA	6:F:147:SER:HA	1.95	0.49
1:A:495:GLU:OE1	1:A:495:GLU:N	2.46	0.49
1:A:526:ASP:OD1	2:B:1015:HIS:ND1	2.46	0.49
1:A:1199:ARG:NH1	1:A:1233:ASP:O	2.45	0.49
2:B:402:GLY:O	2:B:405:ARG:NH1	2.41	0.49
8:H:26:ILE:HG13	8:H:42:ILE:HD12	1.95	0.49
9:I:14:LEU:HA	9:I:28:GLU:O	2.13	0.49
15:O:98:ARG:CG	18:T:57:DT:O3'	2.59	0.49
1:A:381:THR:HG23	1:A:383:TYR:H	1.78	0.48
17:R:263:MET:O	17:R:266:THR:OG1	2.28	0.48
18:T:56:DC:OP2	18:T:56:DC:H2'	2.12	0.48
1:A:1116:LEU:HD11	1:A:1311:VAL:HG23	1.94	0.48
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.96	0.48
2:B:810:GLU:HB2	2:B:815:ARG:HH12	1.79	0.48
13:M:267:LYS:HG3	13:M:268:GLU:H	1.78	0.48
16:Q:352:MET:HG3	16:Q:361:TRP:HB2	1.94	0.48
17:R:73:LEU:HD23	17:R:78:ALA:CA	2.43	0.48
5:E:179:GLN:HG2	5:E:181:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:118:VAL:HG22	13:M:124:ASN:ND2	2.28	0.48
15:O:68:GLN:HB3	18:T:61:DT:H2"	1.94	0.48
9:I:19:ASP:CB	9:I:24:ARG:O	2.60	0.48
15:O:105:ARG:HE	19:U:253:ARG:NH2	2.10	0.48
15:O:105:ARG:CZ	19:U:253:ARG:CZ	2.92	0.48
21:W:77:PRO:O	21:W:79:SER:N	2.46	0.48
2:B:364:ILE:HG22	2:B:365:THR:HG22	1.96	0.48
16:Q:363:GLY:HA2	16:Q:395:PHE:HA	1.95	0.48
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.79	0.48
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.94	0.48
1:A:1444:MET:HE3	7:G:60:ARG:HA	1.95	0.48
7:G:44:TYR:OH	7:G:157:ILE:O	2.28	0.48
2:B:63:ILE:O	2:B:67:SER:HB3	2.13	0.48
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.96	0.48
6:F:76:LYS:HA	6:F:79:ARG:HE	1.79	0.48
1:A:481:ASP:OD2	1:A:483:ASP:OD2	2.31	0.48
11:K:32:VAL:HG22	11:K:74:ARG:HG2	1.94	0.48
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.95	0.47
9:I:54:GLU:CG	9:I:88:SER:OG	2.62	0.47
2:B:363:HIS:CD2	2:B:364:ILE:HG13	2.49	0.47
17:R:69:TRP:CD1	17:R:219:CYS:HB3	2.49	0.47
2:B:249:ARG:HG2	2:B:415:GLN:NE2	2.29	0.47
2:B:1004:GLU:OE1	2:B:1064:TYR:OH	2.27	0.47
14:N:24:DT:H1'	15:O:215:THR:HG21	1.97	0.47
21:W:18:ARG:NH1	22:X:249:GLY:CA	2.70	0.47
1:A:308:ILE:HG23	1:A:311:GLN:HB2	1.97	0.47
2:B:398:ARG:H	2:B:398:ARG:HD2	1.80	0.47
2:B:737:THR:OG1	9:I:66:PRO:O	2.27	0.47
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.47
21:W:74:GLU:CB	21:W:82:VAL:O	2.63	0.47
1:A:630:ILE:O	1:A:634:THR:OG1	2.27	0.47
2:B:924:GLU:H	2:B:928:ARG:HD2	1.80	0.47
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.96	0.47
2:B:70:ILE:HG22	2:B:89:GLU:HG3	1.97	0.47
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.95	0.47
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.80	0.47
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.95	0.47
8:H:89:LEU:HG	8:H:90:ALA:H	1.78	0.47
13:M:272:LYS:CE	18:T:65:DT:H5"	2.44	0.47
21:W:179:ILE:HD12	21:W:182:ILE:HD12	1.97	0.47
21:W:187:LYS:HD3	21:W:187:LYS:HA	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:214:LEU:HD22	15:O:223:ILE:HG23	1.96	0.47
17:R:97:ILE:HA	17:R:104:ILE:HG22	1.97	0.47
17:R:122:LEU:HD21	17:R:222:CYS:HB3	1.97	0.47
11:K:24:ASP:HB2	11:K:32:VAL:HG23	1.95	0.47
13:M:312:GLY:O	13:M:316:LEU:HB2	2.14	0.47
15:O:171:ARG:HB2	15:O:237:PHE:HB3	1.96	0.47
16:Q:102:PRO:HA	17:R:94:LYS:HA	1.97	0.47
18:T:56:DC:H2"	18:T:57:DT:C5	2.50	0.47
2:B:458:LYS:O	2:B:462:ALA:CB	2.63	0.47
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.96	0.47
2:B:336:ARG:HD2	2:B:348:ARG:NH1	2.30	0.46
15:O:99:PHE:CD2	18:T:58:DA:C2'	2.93	0.46
21:W:176:MET:HA	21:W:179:ILE:HG22	1.96	0.46
22:X:218:ASP:HA	22:X:221:ILE:HD12	1.97	0.46
1:A:1012:ARG:HH21	1:A:1015:VAL:HG11	1.81	0.46
2:B:931:TYR:O	2:B:933:SER:N	2.43	0.46
10:J:17:LYS:HB3	10:J:39:LEU:HD13	1.96	0.46
1:A:806:ARG:HD2	2:B:728:ARG:HA	1.97	0.46
20:V:60:LEU:HA	20:V:86:THR:O	2.15	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.81	0.46
2:B:194:GLU:HA	2:B:784:ASN:HD22	1.80	0.46
7:G:97:HIS:HE1	21:W:158:GLU:CG	2.29	0.46
15:O:91:ASN:CG	20:V:69:TYR:CZ	2.89	0.46
15:O:95:ASN:N	15:O:95:ASN:OD1	2.47	0.46
17:R:63:ARG:C	17:R:65:ASN:H	2.19	0.46
1:A:471:ASN:OD1	1:A:472:LEU:N	2.48	0.46
1:A:561:PRO:HB2	1:A:576:GLN:HE21	1.80	0.46
1:A:855:THR:HG21	1:A:857:ARG:HH21	1.81	0.46
9:I:88:SER:O	9:I:91:ARG:NH1	2.47	0.46
4:D:123:LEU:HD21	4:D:146:GLN:HA	1.97	0.46
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	1.98	0.46
6:F:135:ARG:HA	6:F:144:GLU:O	2.16	0.46
15:O:202:ILE:HG13	15:O:226:ALA:HB2	1.98	0.46
1:A:116:ASP:OD1	1:A:117:GLU:N	2.43	0.45
1:A:993:LEU:HD13	1:A:1046:LEU:HD22	1.98	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.16	0.45
18:T:61:DT:H2'	18:T:62:DA:C8	2.51	0.45
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.98	0.45
2:B:663:ALA:O	2:B:667:GLN:HB2	2.17	0.45
13:M:262:LYS:O	13:M:266:ILE:HG13	2.17	0.45
20:V:61:THR:HB	20:V:86:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:PRO:HG2	1:A:566:ILE:HG13	1.98	0.45
1:A:990:VAL:HG12	1:A:994:GLN:HE21	1.80	0.45
2:B:737:THR:HB	9:I:66:PRO:CB	2.47	0.45
7:G:123:ALA:HA	7:G:128:PRO:HB3	1.97	0.45
8:H:5:LEU:HD22	8:H:134:ASN:HB3	1.99	0.45
15:O:227:PHE:HA	15:O:230:ILE:HG22	1.99	0.45
1:A:596:THR:HG22	1:A:597:LEU:H	1.80	0.45
1:A:864:ILE:HG12	1:A:1374:VAL:HG22	1.97	0.45
2:B:301:ILE:O	2:B:383:ASN:ND2	2.49	0.45
4:D:63:LEU:HD13	4:D:130:LEU:HD13	1.99	0.45
1:A:45:GLN:O	1:A:257:ARG:NH1	2.41	0.45
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.52	0.45
16:Q:379:GLU:OE2	16:Q:383:SER:OG	2.35	0.45
20:V:23:LEU:HD13	20:V:37:ALA:HB1	1.99	0.45
1:A:463:ILE:HD12	1:A:464:PRO:O	2.17	0.45
2:B:933:SER:OG	2:B:934:LYS:N	2.49	0.45
7:G:97:HIS:CE1	21:W:158:GLU:CG	2.99	0.45
2:B:276:ILE:HA	2:B:338:GLY:HA3	1.99	0.45
2:B:859:TYR:OH	2:B:945:GLU:OE1	2.35	0.45
13:M:268:GLU:OE1	13:M:319:HIS:NE2	2.38	0.45
15:O:199:LYS:HA	15:O:200:PRO:HA	1.84	0.45
16:Q:402:ALA:O	16:Q:403:THR:HG23	2.16	0.45
18:T:61:DT:P	19:U:255:LYS:HZ2	2.39	0.45
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.98	0.45
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.00	0.45
18:T:64:DA:H2"	18:T:65:DT:C5	2.52	0.45
21:W:152:CYS:O	21:W:154:GLU:HG3	2.17	0.45
1:A:92:HIS:O	1:A:96:ILE:HG13	2.17	0.44
2:B:954:VAL:HG11	2:B:962:LYS:HE3	1.98	0.44
7:G:23:LYS:O	7:G:26:LEU:HB2	2.16	0.44
12:L:43:THR:HG22	12:L:43:THR:O	2.16	0.44
2:B:634:TYR:HA	2:B:694:ASP:HA	1.98	0.44
21:W:18:ARG:CG	22:X:250:GLY:HA2	2.47	0.44
1:A:350:ARG:HA	1:A:487:MET:O	2.17	0.44
1:A:587:HIS:HA	1:A:607:ILE:O	2.16	0.44
2:B:1172:ILE:HD11	2:B:1183:LYS:HD2	1.98	0.44
21:W:171:LYS:O	21:W:175:LEU:HB2	2.16	0.44
15:O:76:LEU:HD13	15:O:143:ILE:HG21	2.00	0.44
1:A:567:LYS:HA	1:A:568:PRO:HA	1.82	0.44
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.99	0.44
2:B:238:ALA:HB2	2:B:385:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:21:ARG:HG3	7:G:25:TYR:HE2	1.81	0.44
16:Q:352:MET:CG	16:Q:361:TRP:HB2	2.47	0.44
1:A:53:LEU:HD21	1:A:267:ALA:HB2	1.99	0.44
9:I:83:ASN:HA	9:I:104:LEU:HG	1.98	0.44
13:M:198:VAL:HG12	13:M:198:VAL:O	2.18	0.44
21:W:24:SER:HA	21:W:27:LEU:HB2	1.98	0.44
1:A:443:LEU:HD21	1:A:501:LEU:HD11	2.00	0.44
2:B:499:ASN:OD1	2:B:500:THR:N	2.50	0.44
8:H:5:LEU:HD11	8:H:61:SER:HB3	2.00	0.44
13:M:44:VAL:HG22	13:M:51:VAL:HA	2.00	0.44
13:M:166:LYS:HB3	13:M:170:SER:HB3	2.00	0.44
1:A:1051:ALA:O	1:A:1055:ARG:HG2	2.18	0.44
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.99	0.44
2:B:281:PRO:HD2	2:B:284:ILE:HD12	2.00	0.44
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.99	0.44
19:U:260:CYS:HB2	19:U:281:VAL:HB	1.99	0.44
1:A:882:SER:OG	1:A:953:ASN:ND2	2.51	0.43
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.43
9:I:54:GLU:HB3	9:I:88:SER:CB	2.46	0.43
19:U:9:VAL:HG13	20:V:51:THR:HG21	2.00	0.43
1:A:351:THR:O	1:A:486:GLU:HA	2.18	0.43
1:A:481:ASP:C	1:A:483:ASP:OD1	2.56	0.43
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.53	0.43
7:G:102:GLN:HE22	7:G:107:LYS:HE2	1.83	0.43
13:M:325:ASP:HB3	13:M:326:PRO:HD3	2.00	0.43
1:A:439:ASN:HA	1:A:459:ARG:HG3	1.99	0.43
1:A:1146:VAL:HG11	1:A:1207:LEU:CD1	2.47	0.43
7:G:113:HIS:HE1	21:W:119:PRO:HG2	1.78	0.43
9:I:54:GLU:CA	9:I:88:SER:OG	2.66	0.43
1:A:362:ASP:OD2	1:A:459:ARG:NH1	2.52	0.43
3:C:19:ASP:HA	3:C:231:ASN:HA	2.00	0.43
7:G:97:HIS:O	7:G:112:LYS:N	2.51	0.43
1:A:339:ASN:HB3	2:B:1199:ALA:HB1	2.01	0.43
1:A:405:VAL:HG13	1:A:432:VAL:HG22	2.01	0.43
6:F:123:LYS:NZ	6:F:127:GLU:OE2	2.51	0.43
8:H:64:ASN:OD1	8:H:65:LEU:N	2.52	0.43
19:U:267:VAL:HG12	19:U:269:ILE:HG13	2.00	0.43
2:B:279:ASP:OD1	2:B:279:ASP:N	2.50	0.43
2:B:412:LEU:HB3	2:B:466:TRP:CE2	2.53	0.43
17:R:133:TYR:CD1	17:R:217:THR:HG22	2.52	0.43
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:VAL:HG21	1:A:572:TRP:HB2	1.99	0.43
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.43
12:L:38:LEU:HD23	12:L:40:LEU:HD23	2.01	0.43
16:Q:388:PRO:HB2	17:R:82:ARG:NH1	2.34	0.43
1:A:348:SER:HB2	2:B:1128:LEU:HD12	2.01	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.00	0.43
1:A:966:ASN:O	1:A:970:THR:OG1	2.25	0.43
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.84	0.43
16:Q:376:LEU:HB2	17:R:69:TRP:HB2	2.01	0.43
1:A:412:ARG:NH2	13:M:54:ASP:OD1	2.36	0.43
2:B:223:VAL:HG22	2:B:240:ILE:HD12	2.00	0.43
7:G:143:ILE:HG13	7:G:170:ALA:HA	2.01	0.43
1:A:148:CYS:O	1:A:168:GLY:HA2	2.19	0.43
1:A:375:THR:HB	1:A:403:LYS:HD3	2.01	0.43
1:A:377:PRO:HB3	1:A:433:GLU:HG2	2.00	0.43
1:A:1260:LEU:O	1:A:1264:GLU:HG3	2.19	0.43
2:B:376:PHE:HE2	2:B:567:GLU:HA	1.84	0.43
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.52	0.43
5:E:56:LYS:NZ	5:E:84:ASP:OD2	2.43	0.43
1:A:849:MET:SD	1:A:849:MET:N	2.92	0.42
16:Q:376:LEU:CD2	16:Q:386:MET:HE3	2.44	0.42
17:R:105:THR:OG1	17:R:106:LEU:N	2.52	0.42
1:A:362:ASP:O	1:A:458:HIS:ND1	2.51	0.42
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.01	0.42
17:R:258:THR:O	17:R:260:GLY:N	2.42	0.42
17:R:262:THR:O	17:R:266:THR:HG23	2.19	0.42
2:B:283:VAL:O	2:B:287:ARG:HG2	2.19	0.42
7:G:138:THR:O	7:G:141:SER:OG	2.37	0.42
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.37	0.42
14:N:22:DT:H2'	14:N:23:DA:C8	2.55	0.42
21:W:63:SER:O	22:X:268:LEU:HD12	2.19	0.42
1:A:113:LEU:HD11	1:A:218:ASP:HA	2.01	0.42
1:A:372:LYS:HA	1:A:435:HIS:HD2	1.84	0.42
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.84	0.42
13:M:201:LYS:HG3	14:N:23:DA:P	2.60	0.42
13:M:268:GLU:C	13:M:270:ALA:H	2.23	0.42
1:A:54:ASN:OD1	1:A:54:ASN:N	2.52	0.42
2:B:910:VAL:HA	2:B:940:PRO:HA	2.01	0.42
21:W:9:VAL:HG22	21:W:189:ILE:HD13	2.01	0.42
13:M:187:ARG:NH1	13:M:241:ARG:HH21	2.17	0.42
18:T:61:DT:P	19:U:255:LYS:NZ	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:26:VAL:HA	21:W:29:LEU:HB3	2.00	0.42
21:W:178:GLN:CD	22:X:254:CYS:SG	2.90	0.42
4:D:158:GLU:OE1	4:D:158:GLU:N	2.41	0.42
13:M:142:LEU:HD23	13:M:146:VAL:HG11	2.01	0.42
19:U:253:ARG:HD2	19:U:258:TRP:CZ2	2.54	0.42
1:A:481:ASP:N	1:A:481:ASP:OD1	2.52	0.42
1:A:1035:TYR:HB3	1:A:1037:LEU:HG	2.01	0.42
7:G:83:LYS:HG2	7:G:149:GLY:HA2	2.01	0.42
1:A:913:LEU:HD11	1:A:919:ILE:HG13	2.02	0.42
7:G:98:GLY:HA3	7:G:110:VAL:O	2.20	0.42
9:I:55:THR:CG2	9:I:100:PHE:CE2	3.03	0.42
11:K:17:SER:HB2	11:K:20:LYS:HZ3	1.84	0.42
1:A:925:LEU:HD22	1:A:983:ILE:HB	2.00	0.41
1:A:1191:TRP:CZ3	1:A:1257:ASP:HB3	2.55	0.41
2:B:487:THR:HG23	2:B:490:SER:H	1.85	0.41
3:C:68:GLY:HA3	12:L:69:ALA:HB1	2.01	0.41
3:C:262:LEU:HD22	11:K:87:LEU:HD23	2.01	0.41
13:M:267:LYS:CE	15:O:208:VAL:CG1	2.98	0.41
15:O:68:GLN:HG3	18:T:62:DA:H4'	2.01	0.41
1:A:1012:ARG:HA	1:A:1015:VAL:HG12	2.02	0.41
7:G:126:ASN:HA	7:G:127:PRO:HA	1.96	0.41
7:G:151:ILE:HD11	21:W:134:LEU:HD23	2.02	0.41
13:M:267:LYS:CG	13:M:268:GLU:H	2.31	0.41
1:A:230:ARG:HB2	1:A:233:TRP:CG	2.55	0.41
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.54	0.41
21:W:44:LYS:NZ	21:W:49:ILE:O	2.50	0.41
1:A:497:THR:O	1:A:501:LEU:HB2	2.20	0.41
1:A:1022:LEU:O	1:A:1026:LEU:HB2	2.20	0.41
2:B:778:MET:HA	2:B:1096:ARG:HH12	1.86	0.41
2:B:895:ASP:OD2	12:L:42:ARG:NH2	2.54	0.41
5:E:124:VAL:H	5:E:125:PRO:HD2	1.85	0.41
6:F:76:LYS:HB3	6:F:79:ARG:HH21	1.85	0.41
1:A:167:CYS:SG	1:A:168:GLY:N	2.92	0.41
2:B:451:LYS:O	2:B:455:SER:HB2	2.20	0.41
2:B:950:ASP:HB2	2:B:969:ARG:HG2	2.02	0.41
2:B:1058:LEU:O	2:B:1062:HIS:ND1	2.50	0.41
4:D:56:ARG:HH22	4:D:155:ARG:HE	1.68	0.41
7:G:109:PHE:CD2	21:W:137:VAL:HG12	2.56	0.41
15:O:114:LEU:HD11	18:T:59:DT:O2	2.20	0.41
21:W:90:LYS:HD2	21:W:90:LYS:HA	1.95	0.41
21:W:140:LEU:HD22	21:W:147:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ILE:HG21	16:Q:335:LEU:HD21	2.01	0.41
2:B:24:PRO:HA	2:B:654:ARG:HH12	1.86	0.41
2:B:474:SER:O	2:B:476:ARG:N	2.53	0.41
4:D:159:THR:O	4:D:163:VAL:HG23	2.21	0.41
14:N:21:DA:H2'	14:N:22:DT:C6	2.56	0.41
14:N:28:DT:H3	14:N:29:DA:N6	2.18	0.41
2:B:26:THR:OG1	2:B:27:ALA:N	2.54	0.41
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	2.03	0.41
7:G:115:MET:O	7:G:164:LYS:NZ	2.49	0.41
13:M:143:PRO:HG2	13:M:146:VAL:HG23	2.03	0.41
15:O:105:ARG:NH2	19:U:253:ARG:NH1	2.68	0.41
1:A:481:ASP:CG	1:A:483:ASP:OD1	2.59	0.41
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.36	0.41
5:E:136:ASN:OD1	5:E:137:GLU:N	2.54	0.41
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.38	0.41
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.56	0.41
13:M:186:ALA:HB1	13:M:238:TYR:CZ	2.56	0.41
16:Q:378:VAL:HG22	16:Q:384:PHE:CD1	2.56	0.41
19:U:264:ASP:OD1	19:U:277:GLN:NE2	2.54	0.41
1:A:635:ARG:NH2	1:A:876:ALA:O	2.54	0.41
1:A:1194:ARG:HA	1:A:1238:ILE:O	2.20	0.41
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.02	0.41
15:O:107:ARG:HD3	19:U:286:VAL:HB	2.03	0.41
2:B:443:ASN:HD22	2:B:446:LEU:HG	1.86	0.40
2:B:649:LYS:HZ1	2:B:738:PHE:HD2	1.68	0.40
7:G:64:THR:C	7:G:66:GLY:H	2.25	0.40
7:G:122:ASN:HB3	7:G:129:SER:O	2.21	0.40
21:W:77:PRO:C	21:W:79:SER:H	2.23	0.40
1:A:885:THR:HB	1:A:943:LEU:HD12	2.03	0.40
1:A:1165:GLU:O	1:A:1167:GLU:N	2.55	0.40
2:B:26:THR:HG23	2:B:29:ASP:H	1.86	0.40
2:B:54:PHE:O	2:B:58:THR:HB	2.21	0.40
2:B:1183:LYS:HB3	2:B:1183:LYS:HE3	1.83	0.40
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.04	0.40
7:G:93:SER:OG	7:G:100:GLU:OE1	2.39	0.40
7:G:97:HIS:ND1	21:W:122:TYR:OH	2.49	0.40
16:Q:139:LEU:HD23	17:R:212:THR:HG21	2.03	0.40
2:B:259:TYR:HE1	2:B:270:LYS:HB2	1.85	0.40
2:B:867:GLY:C	2:B:869:SER:H	2.25	0.40
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.54	0.40
8:H:56:THR:HB	8:H:145:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:HIS:HA	2:B:660:LYS:HZ3	1.86	0.40
6:F:146:TRP:HB3	6:F:151:LEU:HD21	2.03	0.40
13:M:171:ILE:HD12	13:M:172:MET:HG3	2.03	0.40
15:O:91:ASN:OD1	20:V:69:TYR:CD2	2.74	0.40
21:W:28:VAL:O	21:W:32:ILE:HG13	2.22	0.40
2:B:186:GLU:OE2	10:J:62:ARG:NH1	2.52	0.40
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.03	0.40
2:B:1028:GLU:O	2:B:1032:SER:OG	2.26	0.40
15:O:151:LYS:HG2	15:O:153:THR:HG23	2.02	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	1386/1733 (80%)	1298 (94%)	77 (6%)	11 (1%)	19 59
2	B	1136/1224 (93%)	1064 (94%)	62 (6%)	10 (1%)	17 56
3	C	260/318 (82%)	236 (91%)	20 (8%)	4 (2%)	10 46
4	D	153/221 (69%)	145 (95%)	7 (5%)	1 (1%)	22 62
5	E	211/215 (98%)	202 (96%)	8 (4%)	1 (0%)	29 68
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100 100
7	G	169/171 (99%)	156 (92%)	12 (7%)	1 (1%)	25 65
8	H	132/146 (90%)	117 (89%)	12 (9%)	3 (2%)	6 36
9	I	114/122 (93%)	99 (87%)	15 (13%)	0	100 100
10	J	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4 30
11	K	110/120 (92%)	109 (99%)	1 (1%)	0	100 100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100 100
13	M	273/345 (79%)	252 (92%)	16 (6%)	5 (2%)	8 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	O	178/240 (74%)	164 (92%)	13 (7%)	1 (1%)	25 65
16	Q	140/735 (19%)	119 (85%)	17 (12%)	4 (3%)	4 31
17	R	176/400 (44%)	160 (91%)	15 (8%)	1 (1%)	25 65
19	U	88/171 (52%)	82 (93%)	4 (4%)	2 (2%)	6 36
20	V	96/129 (74%)	92 (96%)	3 (3%)	1 (1%)	15 53
21	W	189/586 (32%)	183 (97%)	4 (2%)	2 (1%)	14 51
22	X	156/328 (48%)	129 (83%)	23 (15%)	4 (3%)	5 34
All	All	5154/7499 (69%)	4781 (93%)	320 (6%)	53 (1%)	20 53

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	127	ILE
21	W	77	PRO
2	B	830	TYR
2	B	933	SER
7	G	63	PRO
13	M	269	ILE
16	Q	405	THR
21	W	78	ASN
22	X	251	ASN
2	B	277	LYS
2	B	475	SER
3	C	214	ASN
8	H	60	ALA
8	H	83	GLN
13	M	268	GLU
16	Q	406	ILE
19	U	255	LYS
22	X	152	SER
1	A	47	ARG
1	A	67	CYS
1	A	567	LYS
1	A	958	VAL
2	B	364	ILE
2	B	957	ASN
3	C	93	ASP
4	D	156	ASP
10	J	9	SER
19	U	264	ASP

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Mol	Chain	Res	Type
20	V	6	TYR
1	A	35	ILE
1	A	50	ILE
1	A	525	GLN
1	A	569	LYS
2	B	339	THR
2	B	705	MET
3	C	236	GLY
5	E	124	VAL
10	J	3	VAL
13	M	271	GLY
22	X	240	THR
1	A	464	PRO
2	B	1046	PRO
13	M	273	SER
16	Q	367	ALA
15	O	147	GLY
22	X	205	ILE
2	B	343	ILE
1	A	61	ILE
3	C	182	PRO
8	H	59	ILE
17	R	215	VAL
1	A	1327	ILE
13	M	32	PRO

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	1221/1520 (80%)	1218 (100%)	3 (0%)	93 96
2	B	1000/1061 (94%)	997 (100%)	3 (0%)	92 95
3	C	230/274 (84%)	228 (99%)	2 (1%)	78 87
4	D	139/200 (70%)	137 (99%)	2 (1%)	67 81
5	E	195/197 (99%)	194 (100%)	1 (0%)	88 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	73/137 (53%)	73 (100%)	0	100 100
7	G	152/152 (100%)	152 (100%)	0	100 100
8	H	119/128 (93%)	119 (100%)	0	100 100
9	I	110/116 (95%)	108 (98%)	2 (2%)	59 77
10	J	60/65 (92%)	60 (100%)	0	100 100
11	K	97/102 (95%)	97 (100%)	0	100 100
12	L	40/57 (70%)	40 (100%)	0	100 100
13	M	245/299 (82%)	245 (100%)	0	100 100
15	O	152/205 (74%)	152 (100%)	0	100 100
16	Q	109/641 (17%)	108 (99%)	1 (1%)	78 87
17	R	107/363 (30%)	106 (99%)	1 (1%)	78 87
19	U	84/154 (54%)	84 (100%)	0	100 100
20	V	90/115 (78%)	90 (100%)	0	100 100
21	W	155/244 (64%)	155 (100%)	0	100 100
22	X	62/295 (21%)	62 (100%)	0	100 100
All	All	4440/6325 (70%)	4425 (100%)	15 (0%)	92 95

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	444	PHE
1	A	1259	MET
2	B	398	ARG
2	B	579	ARG
2	B	604	ARG
3	C	95	CYS
3	C	222	LYS
4	D	153	ARG
4	D	165	GLN
5	E	37	LEU
9	I	42	LEU
9	I	43	VAL
16	Q	350	TRP
17	R	251	ARG

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	18	GLN
1	A	64	ASN
1	A	68	GLN
1	A	256	GLN
1	A	311	GLN
1	A	313	GLN
1	A	339	ASN
1	A	363	GLN
1	A	517	ASN
1	A	525	GLN
1	A	589	GLN
1	A	611	GLN
1	A	640	GLN
1	A	698	GLN
1	A	745	GLN
1	A	760	GLN
1	A	881	GLN
1	A	953	ASN
1	A	965	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1040	GLN
1	A	1130	GLN
1	A	1140	HIS
2	B	60	GLN
2	B	115	GLN
2	B	215	GLN
2	B	395	GLN
2	B	415	GLN
2	B	433	GLN
2	B	573	GLN
2	B	657	HIS
2	B	667	GLN
2	B	763	GLN
2	B	1093	GLN
2	B	1161	HIS
2	B	1193	GLN
2	B	1195	HIS
3	C	73	GLN
3	C	102	GLN
3	C	224	GLN
3	C	231	ASN

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Mol	Chain	Res	Type
3	C	242	GLN
3	C	264	GLN
4	D	157	GLN
4	D	165	GLN
4	D	179	GLN
5	E	54	GLN
7	G	102	GLN
7	G	158	HIS
8	H	83	GLN
9	I	60	GLN
10	J	53	HIS
11	K	112	GLN
13	M	90	ASN
13	M	114	GLN
13	M	193	GLN
13	M	235	ASN
15	O	91	ASN
15	O	158	GLN
16	Q	117	HIS
19	U	33	GLN
19	U	280	GLN
20	V	55	ASN
20	V	84	GLN
21	W	107	GLN
21	W	138	GLN
21	W	178	GLN
22	X	216	GLN
22	X	223	GLN
22	X	267	GLN
22	X	279	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 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.

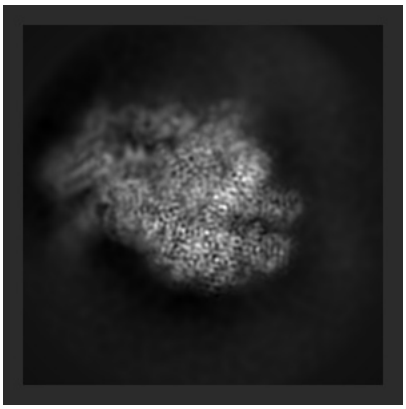
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0091. These allow visual inspection of the internal detail of the map and identification of artifacts.

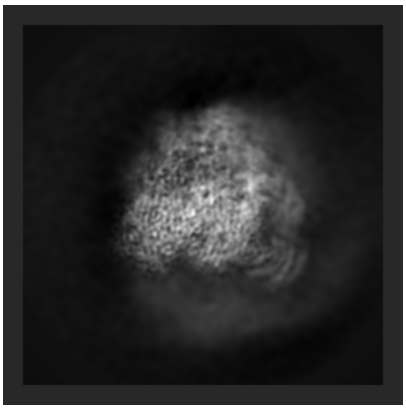
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

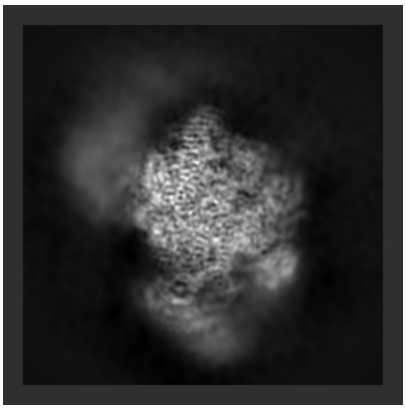
6.1.1 Primary map



X

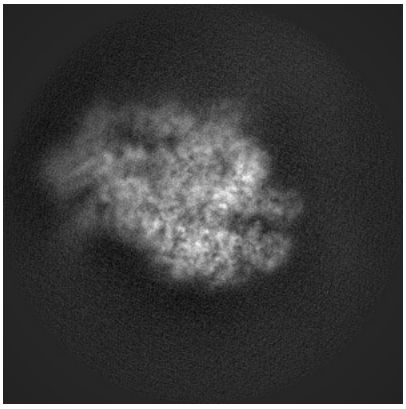


Y

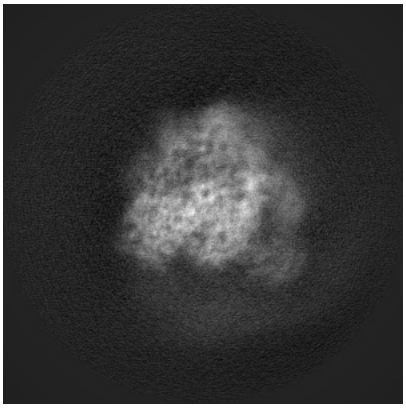


Z

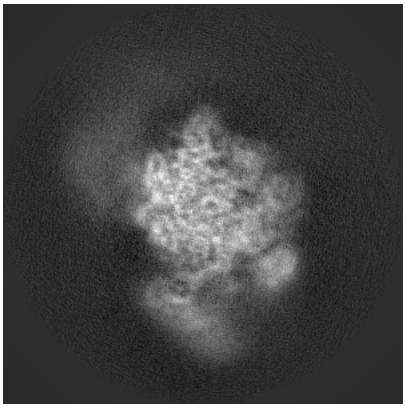
6.1.2 Raw map



X



Y

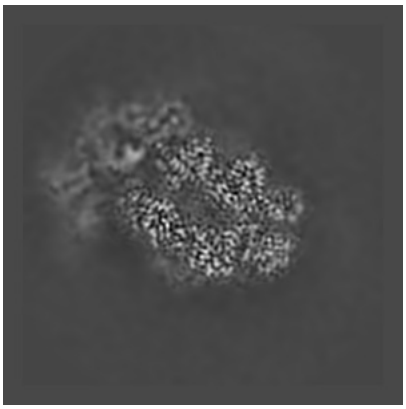


Z

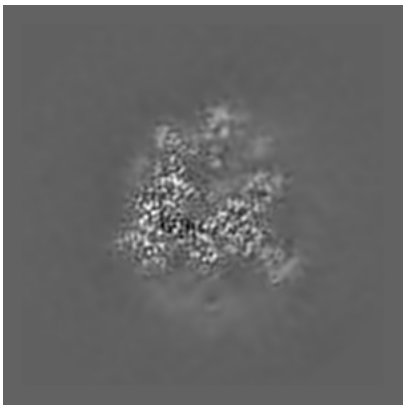
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

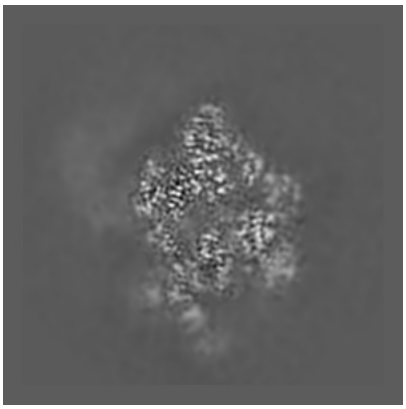
6.2.1 Primary map



X Index: 150

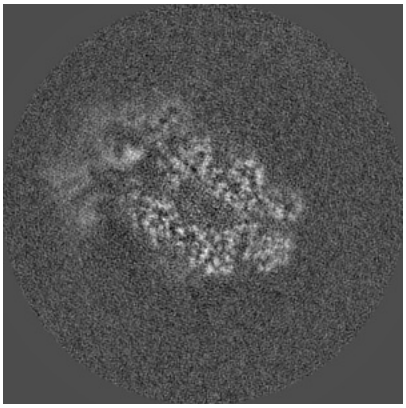


Y Index: 150

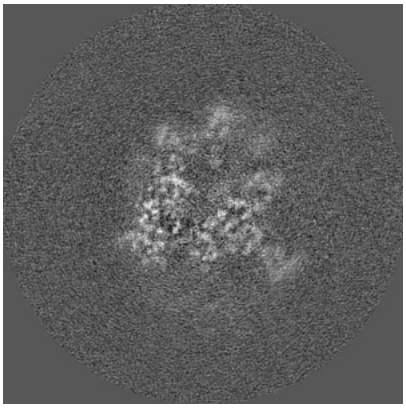


Z Index: 150

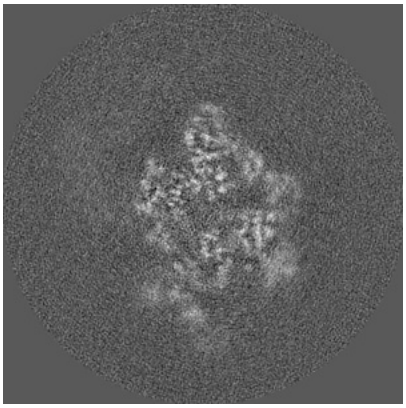
6.2.2 Raw map



X Index: 150



Y Index: 150

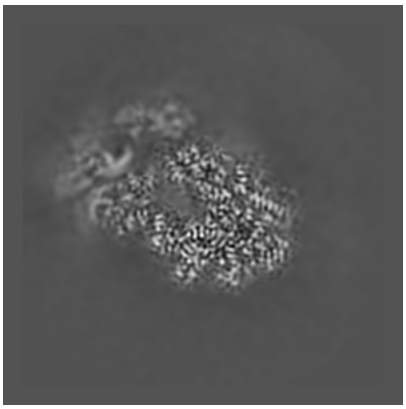


Z Index: 150

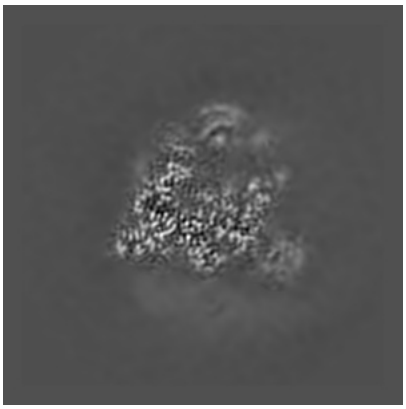
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

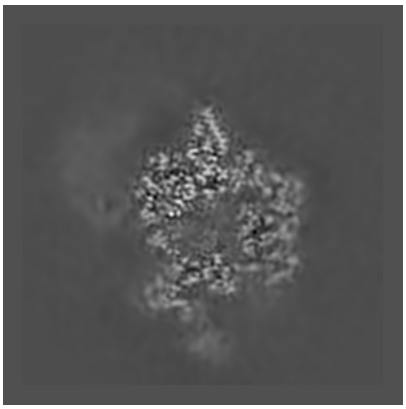
6.3.1 Primary map



X Index: 140

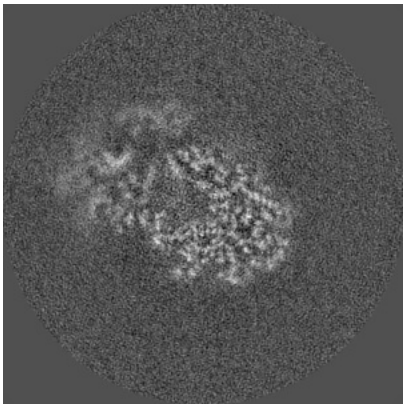


Y Index: 156

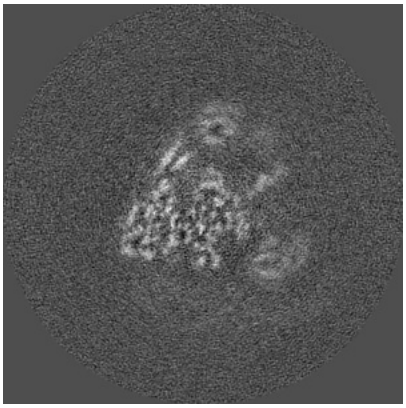


Z Index: 156

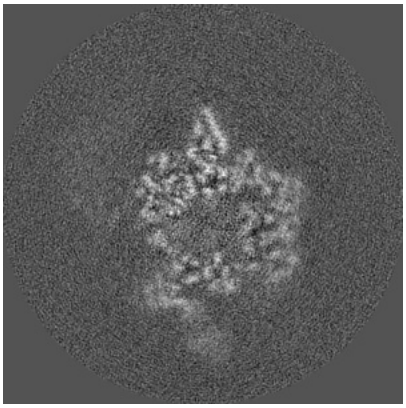
6.3.2 Raw map



X Index: 141



Y Index: 162

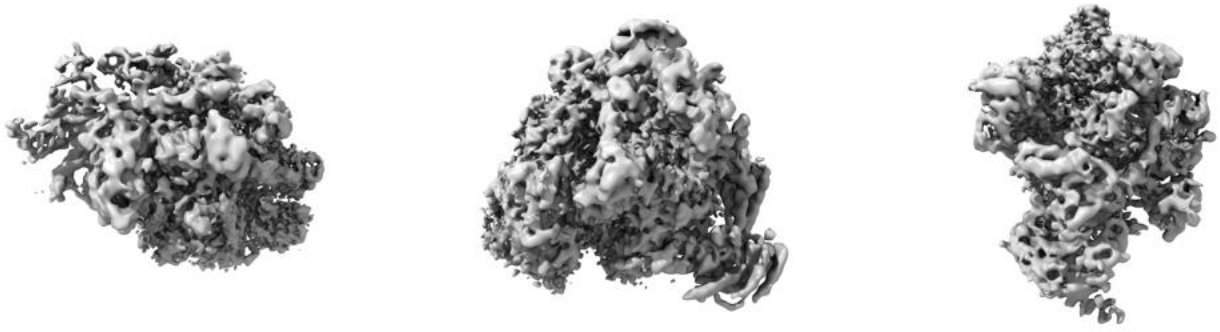


Z Index: 156

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 0.0028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

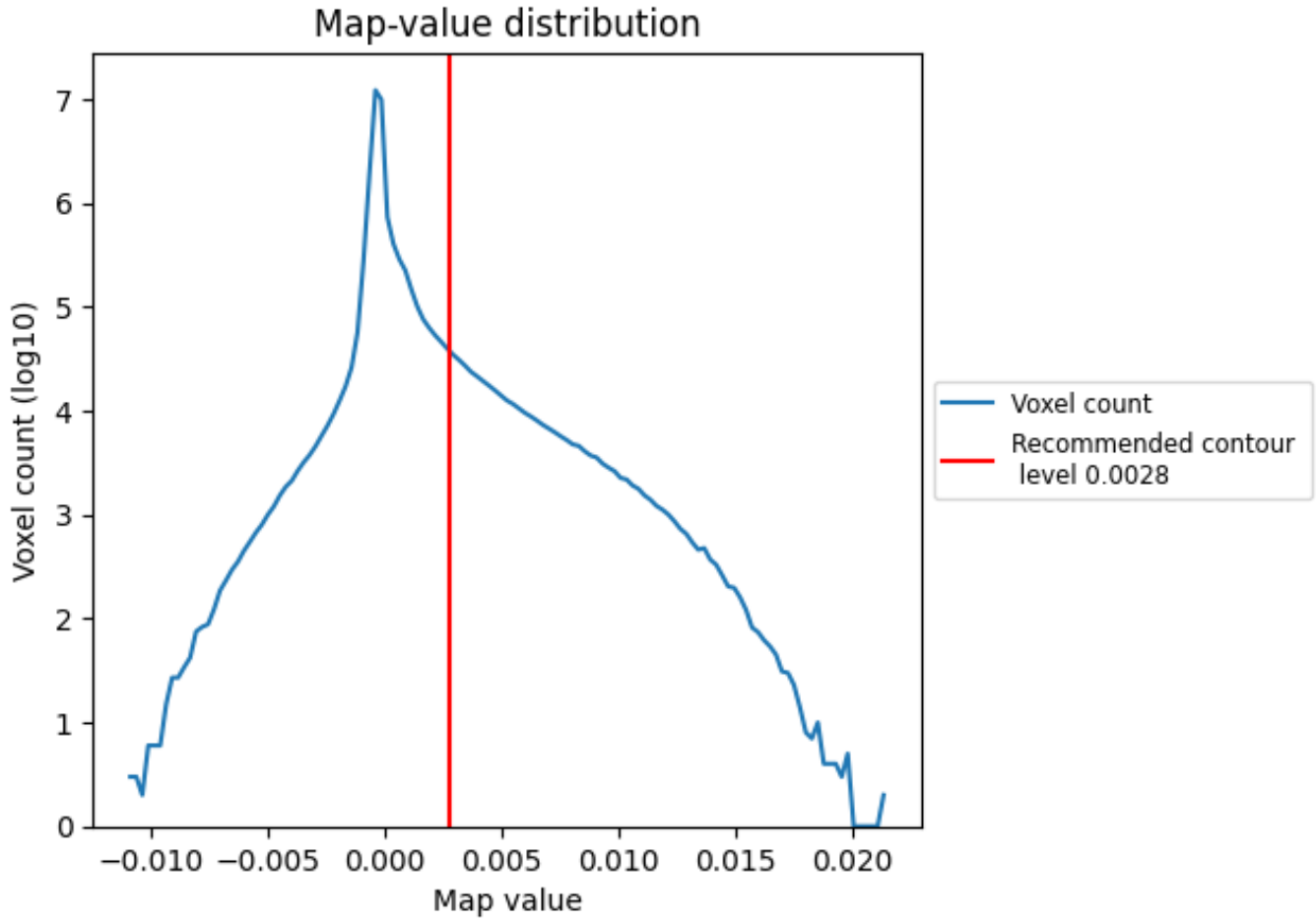
6.5 Mask visualisation (i)

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

7 Map analysis

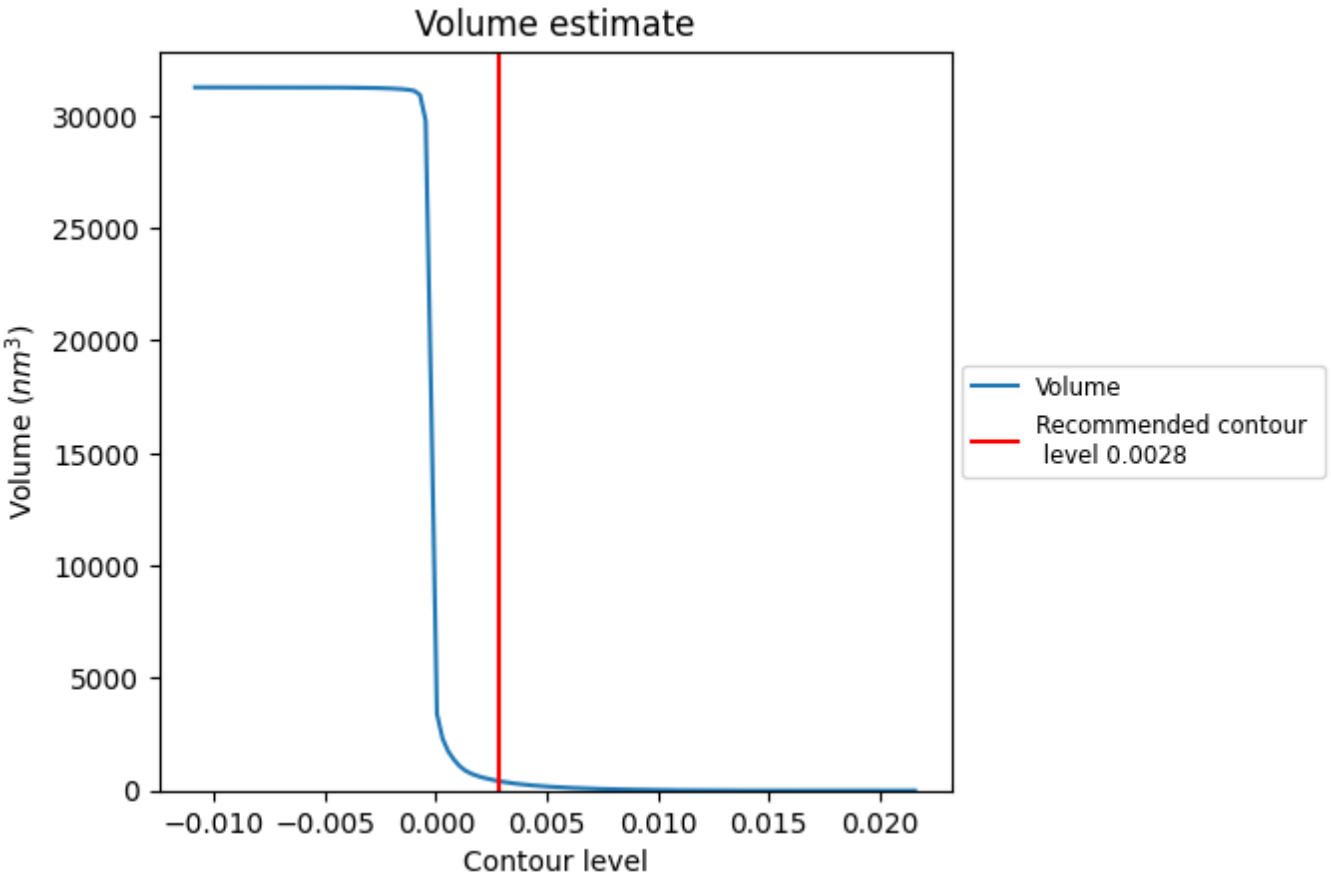
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

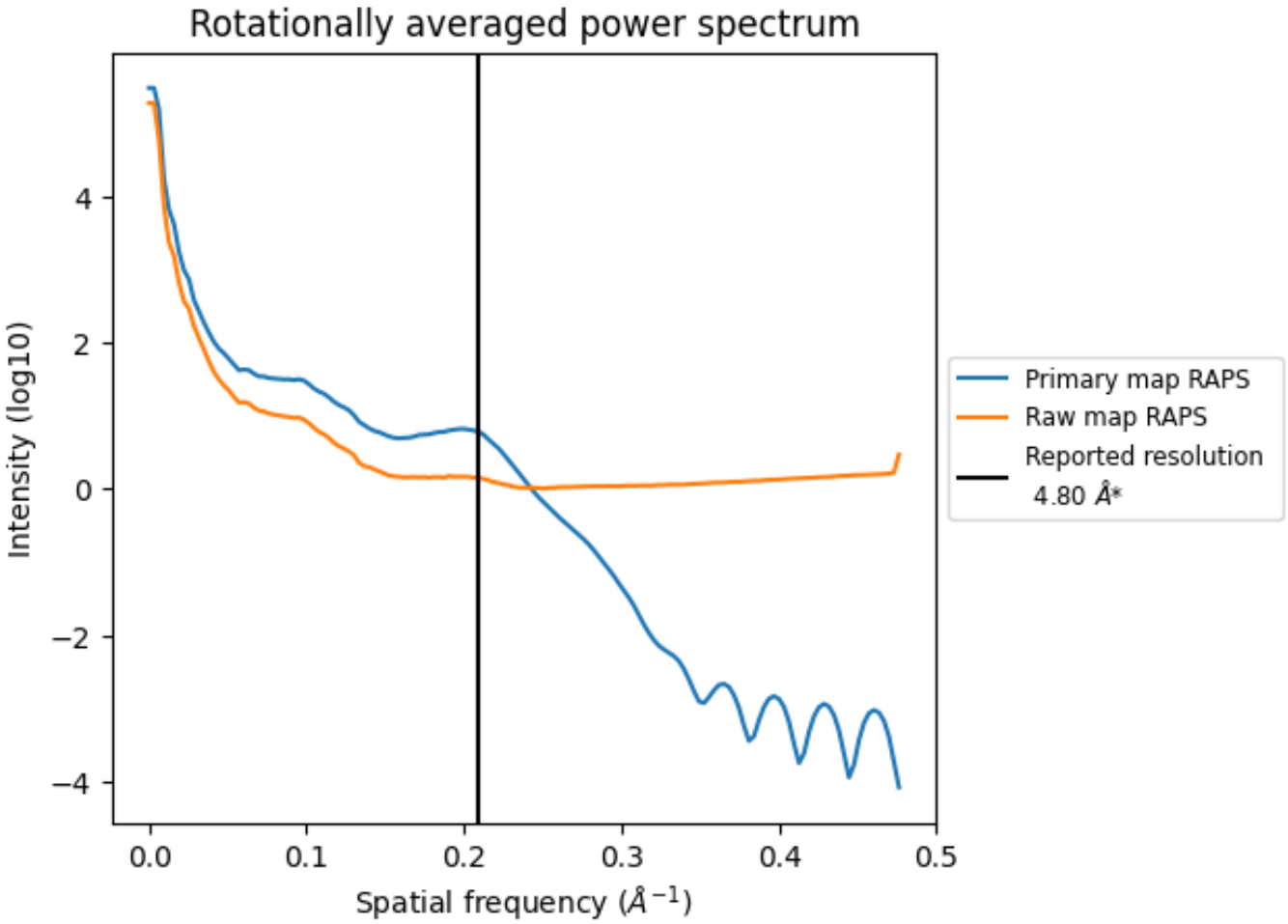
7.2 Volume estimate



The volume at the recommended contour level is 426 nm^3; this corresponds to an approximate mass of 385 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)

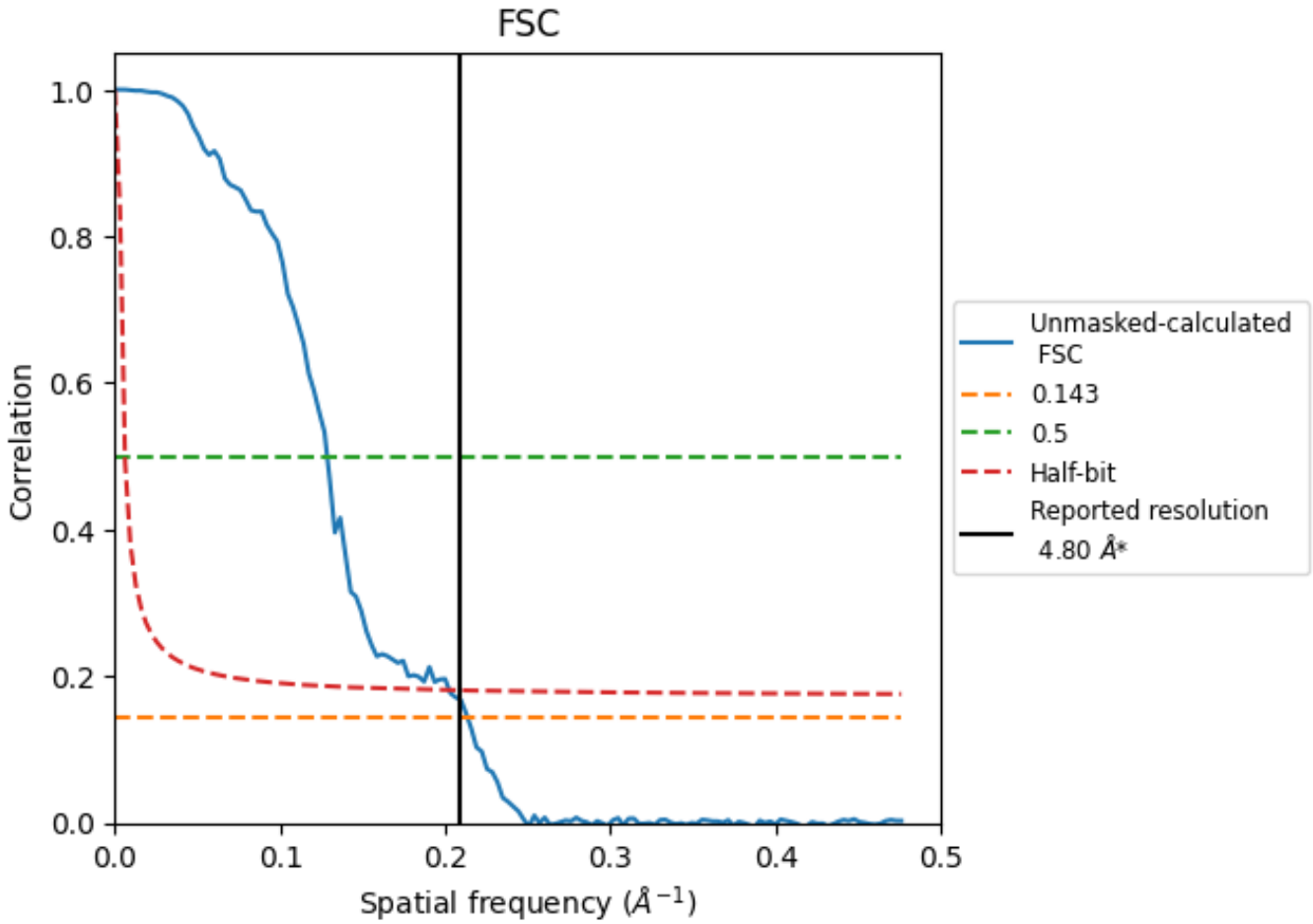


*Reported resolution corresponds to spatial frequency of 0.208 $Å^{-1}$

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 0.208 Å^{-1}

8.2 Resolution estimates (i)

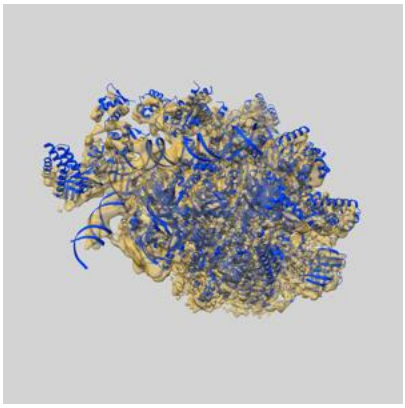
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	7.78	4.94

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

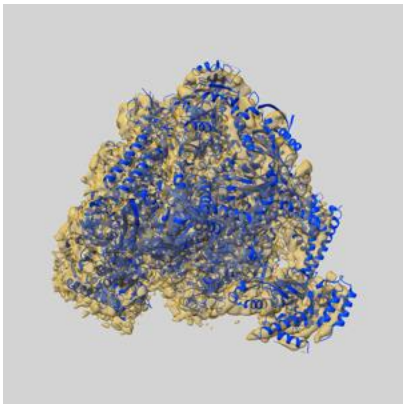
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0091 and PDB model 6GYL. Per-residue inclusion information can be found in section 3 on page 9.

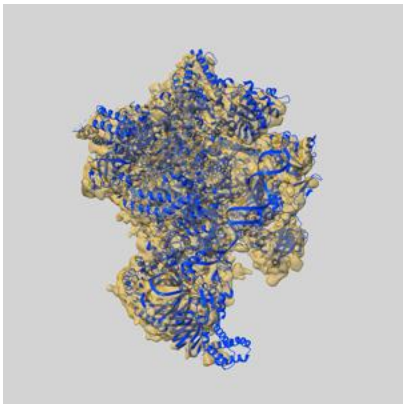
9.1 Map-model overlay



X



Y



Z

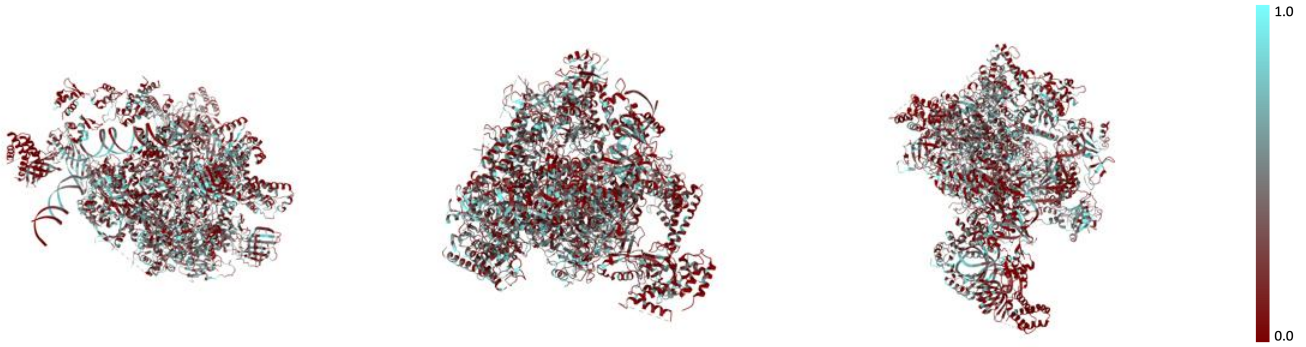
The images above show the 3D surface view of the map at the recommended contour level 0.0028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

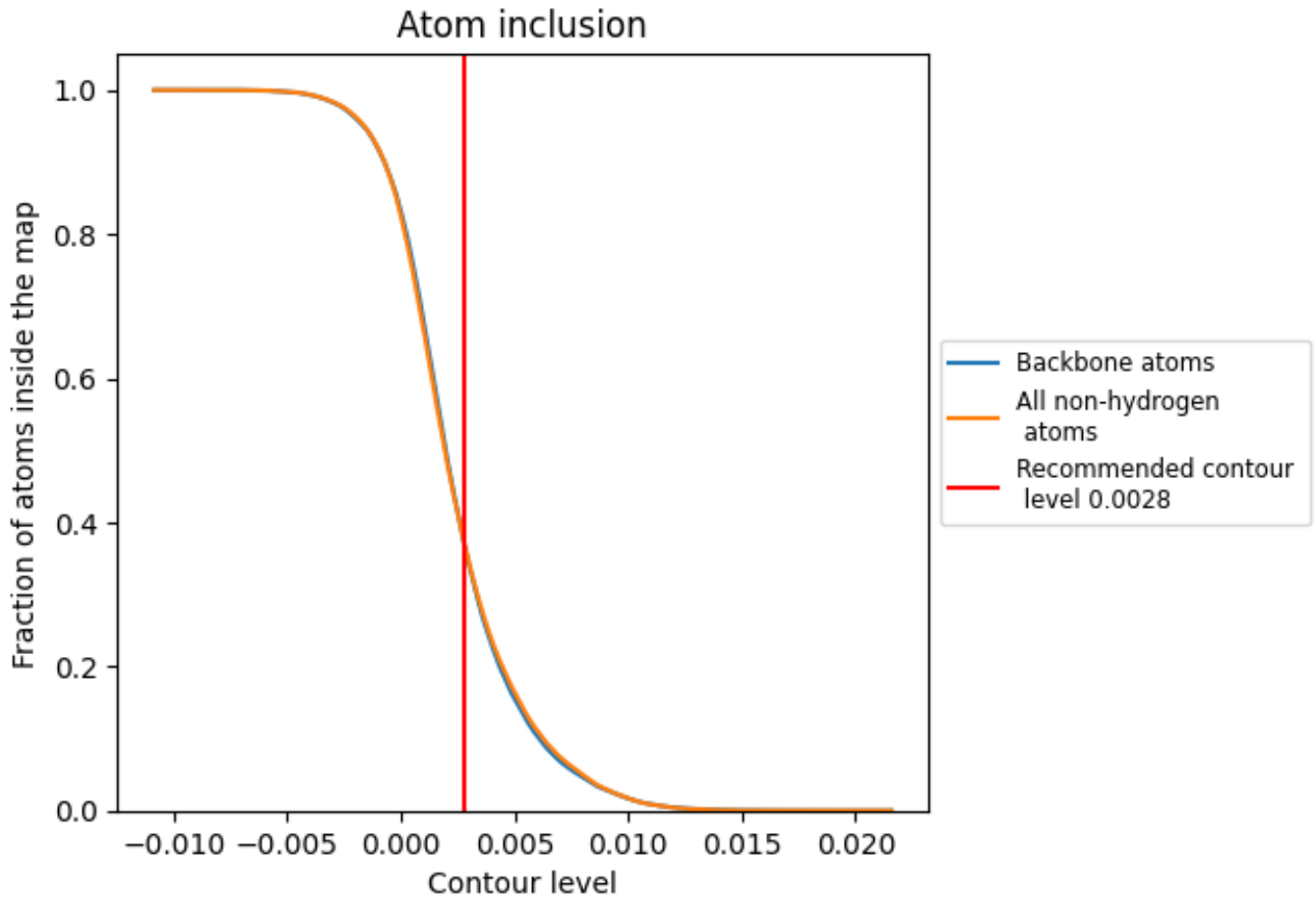
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0028).

9.4 Atom inclusion (i)



At the recommended contour level, 37% of all backbone atoms, 37% 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 (0.0028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3696	-0.0040
A	0.3840	-0.0110
B	0.3770	-0.0240
C	0.4248	-0.0310
D	0.1987	0.0040
E	0.3745	0.0120
F	0.4202	0.0230
G	0.3480	-0.0030
H	0.3779	-0.0040
I	0.3822	0.0160
J	0.4333	-0.0570
K	0.3850	-0.0410
L	0.3642	-0.0550
M	0.3360	-0.0170
N	0.4181	0.0710
O	0.4784	0.0280
Q	0.3802	0.0040
R	0.4093	-0.0100
T	0.4996	0.0660
U	0.1606	0.0330
V	0.1630	0.0540
W	0.3140	0.0240
X	0.2144	0.0330