Full wwPDB EM Validation Report (i)

Oct 12, 2022 – 04:37 PM EDT

PDB ID	:	7UNC
EMDB ID	:	EMD-26620
Title	:	Pol II-DSIF-SPT6-PAF1c-TFIIS complex with rewrapped nucleosome
Authors	:	Filipovski, M.; Vos, S.M.; Farnung, L.
Deposited on	:	2022-04-10
Resolution	:	3.00 Å(reported)
Based on initial models	:	3LZ0, 6TED

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:

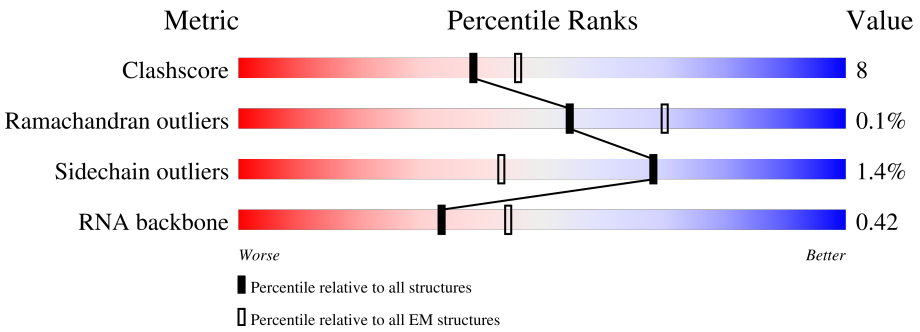
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1984	58% 13% • 28%
2	B	1251	75% 14% 11%
3	C	275	83% 11% 6%
4	D	184	66% • • 32%
5	E	210	79% 20%
6	F	127	54% 7% • 39%
7	G	172	86% 12% • •

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Mol	Chain	Length	Quality of chain
8	H	150	88% 11%
9	I	125	71% 22% 7%
10	J	67	79% 18%
11	K	117	79% 19%
12	L	58	71% 9% 19%
13	M	1729	31% 57% 42%
14	N	209	8% 48% 11% 33%
15	O	304	36% 51% 47%
16	P	16	56% 19% 19% 6%
17	Q	1179	24% 75% 25%
18	R	713	26% 34% 66%
19	T	215	19% 45% 9% 28%
20	U	666	15% 15% 84%
21	V	531	32% 45% 54%
22	W	305	98%
23	X	531	8% 92%
24	Z	1087	6% 23% 5% 72%
25	a	136	71% 29%
25	e	136	71% 29%
26	b	103	80% 19%
26	f	103	76% 24%
27	c	130	79% 21%
27	g	130	81% 19%
28	d	123	76% 23%
28	h	123	75% 24%

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 105742 atoms, of which 48112 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms							AltConf	Trace
			Total	C	H	N	O	P	S		
1	A	1426	22643	7074	11388	2014	2095	2	70	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	1117	17949	5665	9002	1571	1647	64	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	258	4096	1300	2024	356	410	6	0	0

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	126	1985	630	981	170	200	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	209	3458	1089	1738	300	323	8	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	H	N	O	S		
6	F	78	1284	401	658	106	114	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	171	2654	866	1321	214	245	8	0	0

- Molecule 8 is a protein called RPB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	149	2354	759	1157	195	238	5	0	0

- Molecule 9 is a protein called RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	116	1822	582	880	168	181	11	0	0

- Molecule 10 is a protein called RPB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	66	1068	339	544	88	91	6	0	0

- Molecule 11 is a protein called RPB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	115	1862	593	942	152	173	2	0	0

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	47	803	246	406	77	68	6	0	0

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
13	M	1002	5267	2004	1259	1002	1002	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
14	N	140	4480	1376	1594	490	880	140	0	0

- Molecule 15 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	161	645	322	161	162	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	SER	-	expression tag	UNP P23193
O	-1	ASN	-	expression tag	UNP P23193
O	0	ALA	-	expression tag	UNP P23193

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
16	P	16	502	148	170	49	119	16	0	0

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
17	Q	890	5356	1780	1796	890	890	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
18	R	244	1467	488	491	244	244	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
19	T	155	4885	1498	1719	629	884	155	0	0

- Molecule 20 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
20	U	104	626	208	210	104	104	0	0

- Molecule 21 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
21	V	244	1457	488	481	244	244	0	0

- Molecule 22 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
22	W	300	1817	600	617	300	300	0	0

- Molecule 23 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
23	X	43	259	86	87	43	43	0	0

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms							AltConf	Trace
			Total	C	H	N	O	P	S		
24	Z	307	4751	1495	2363	430	450	1	12	0	0

- Molecule 25 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	a	97	1643	506	841	155	138	3	0	0
			Total	C	H	N	O	S		
25	e	97	1640	504	839	155	139	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	102	ALA	GLY	engineered mutation	UNP P84233
e	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 26 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	b	83	1372	418	710	129	114	1	0	0
			Total	C	H	N	O	S		
26	f	78	1279	391	660	120	107	1	0	0

- Molecule 27 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
27	c	103	1642	501	847	155	139	0	0
			Total	C	H	N	O		
27	g	105	1674	510	865	158	141	0	0

- Molecule 28 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	d	95	1519	469	774	134	140	2	0	0
			Total	C	H	N	O	S		
28	h	93	1474	457	748	130	137	2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
29	A	2	2	2	0
			Total	Zn	
29	B	1	1	1	0
			Total	Zn	
29	C	1	1	1	0
			Total	Zn	
29	I	2	2	2	0
			Total	Zn	
29	J	1	1	1	0
			Total	Zn	
29	R	1	1	1	0

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

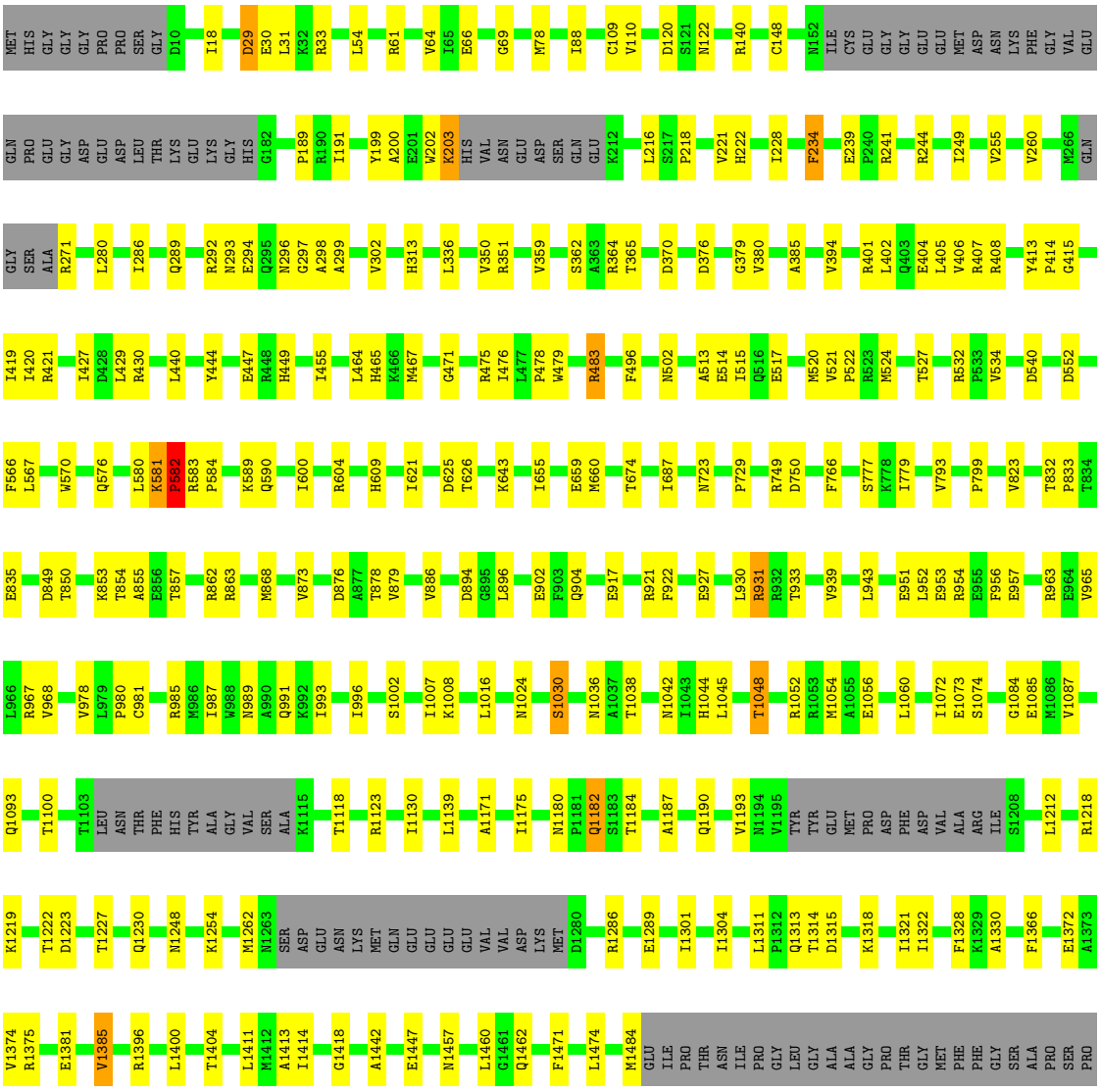
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
30	A	1	1	1	0

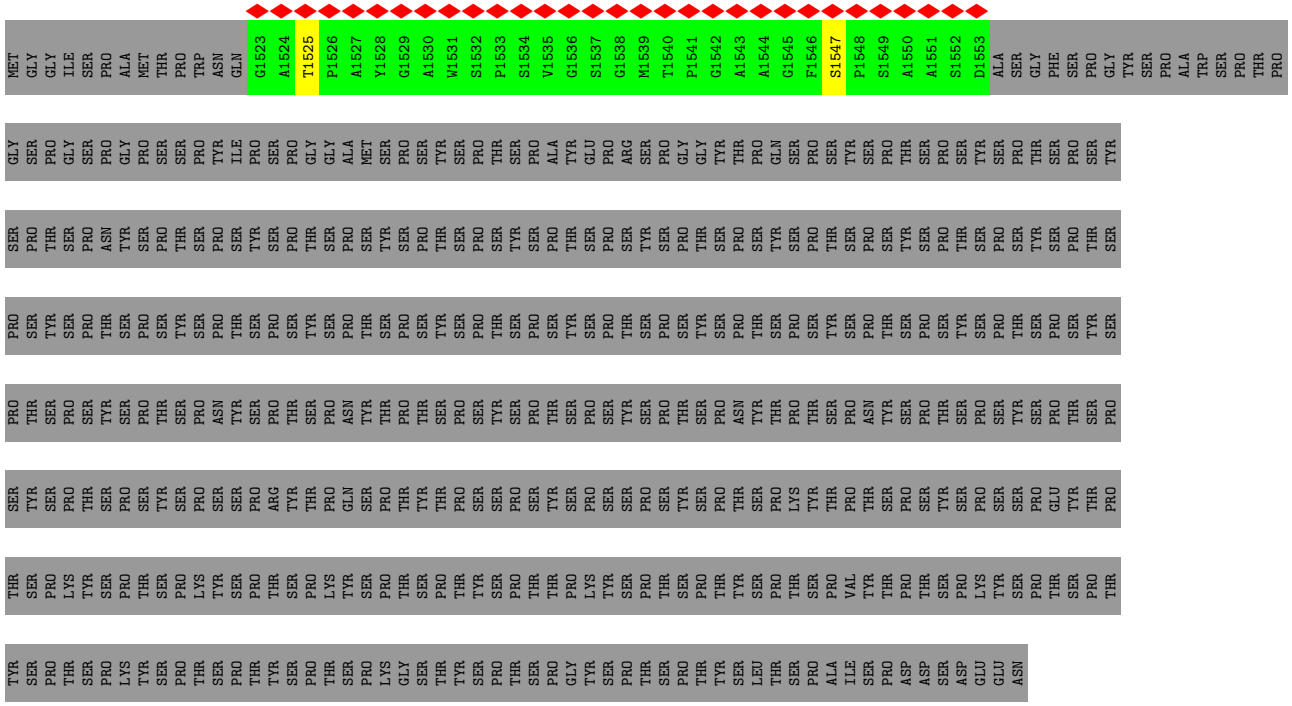
3 Residue-property plots (i)

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 subunit

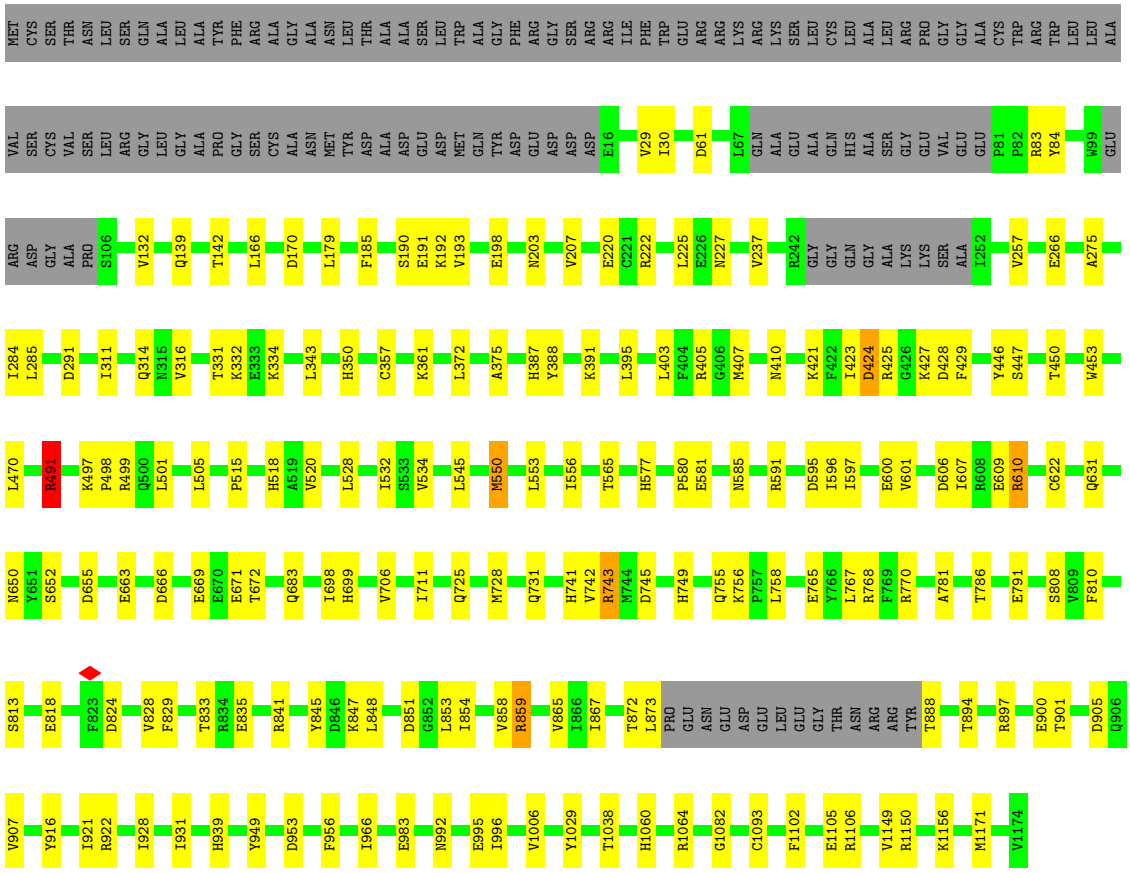
Chain A:





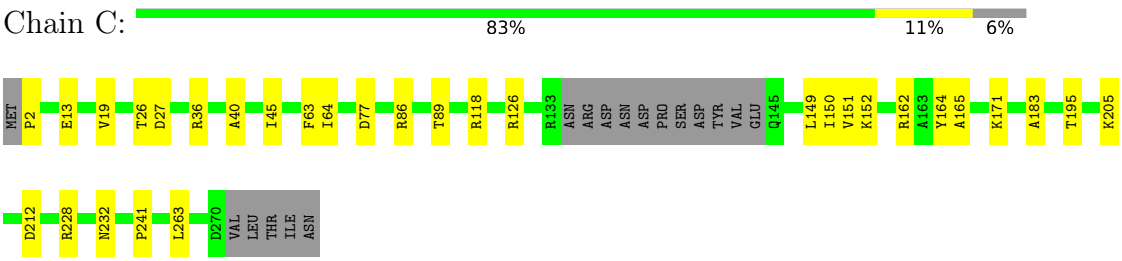
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B: 75% 14% 11%



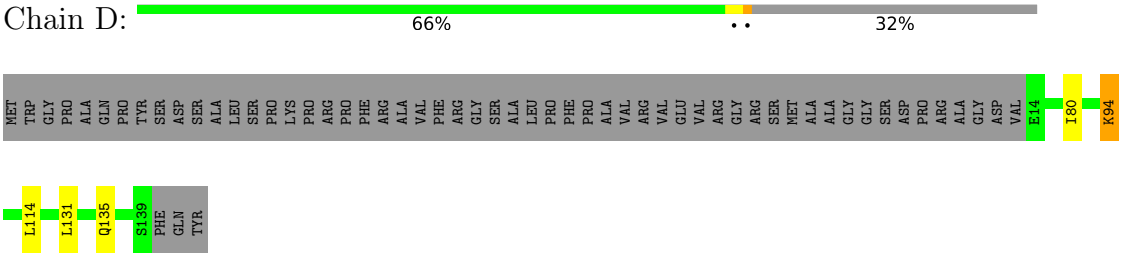
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



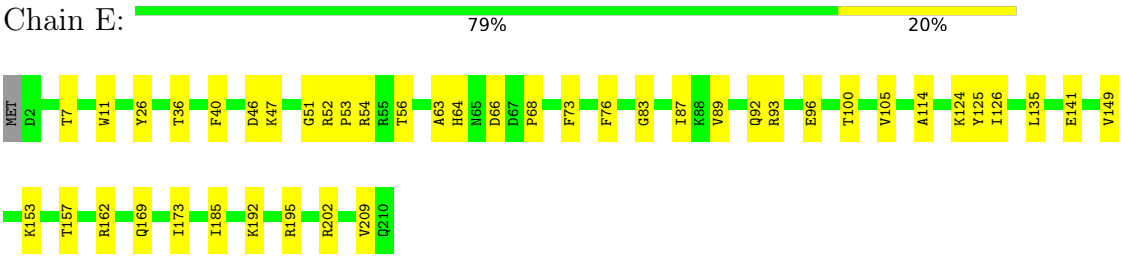
- Molecule 4: RPOL4c domain-containing protein

Chain D:



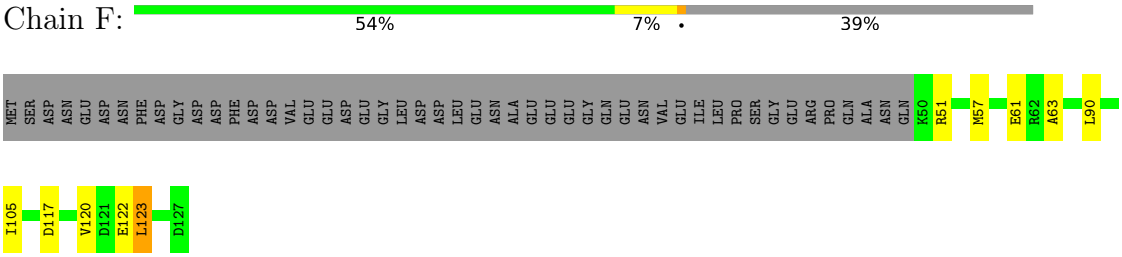
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:



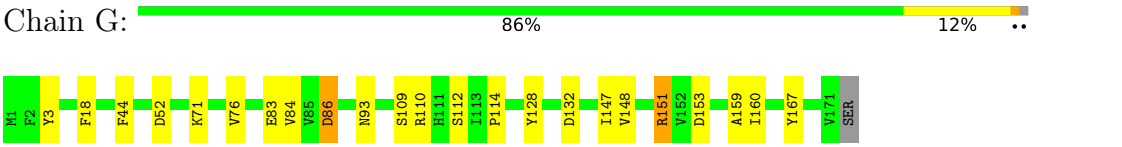
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



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

Chain G:



- Molecule 8: RPB8

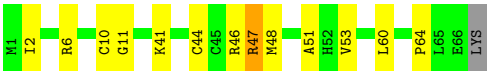
Chain H:

• Molecule 9: RPB9

Chain I:

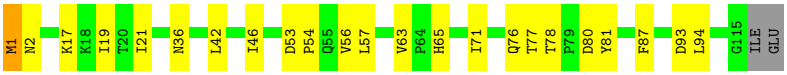
• Molecule 10: RPB10

Chain J:



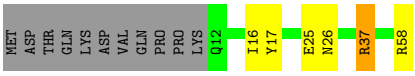
• Molecule 11: RPB11

Chain K:



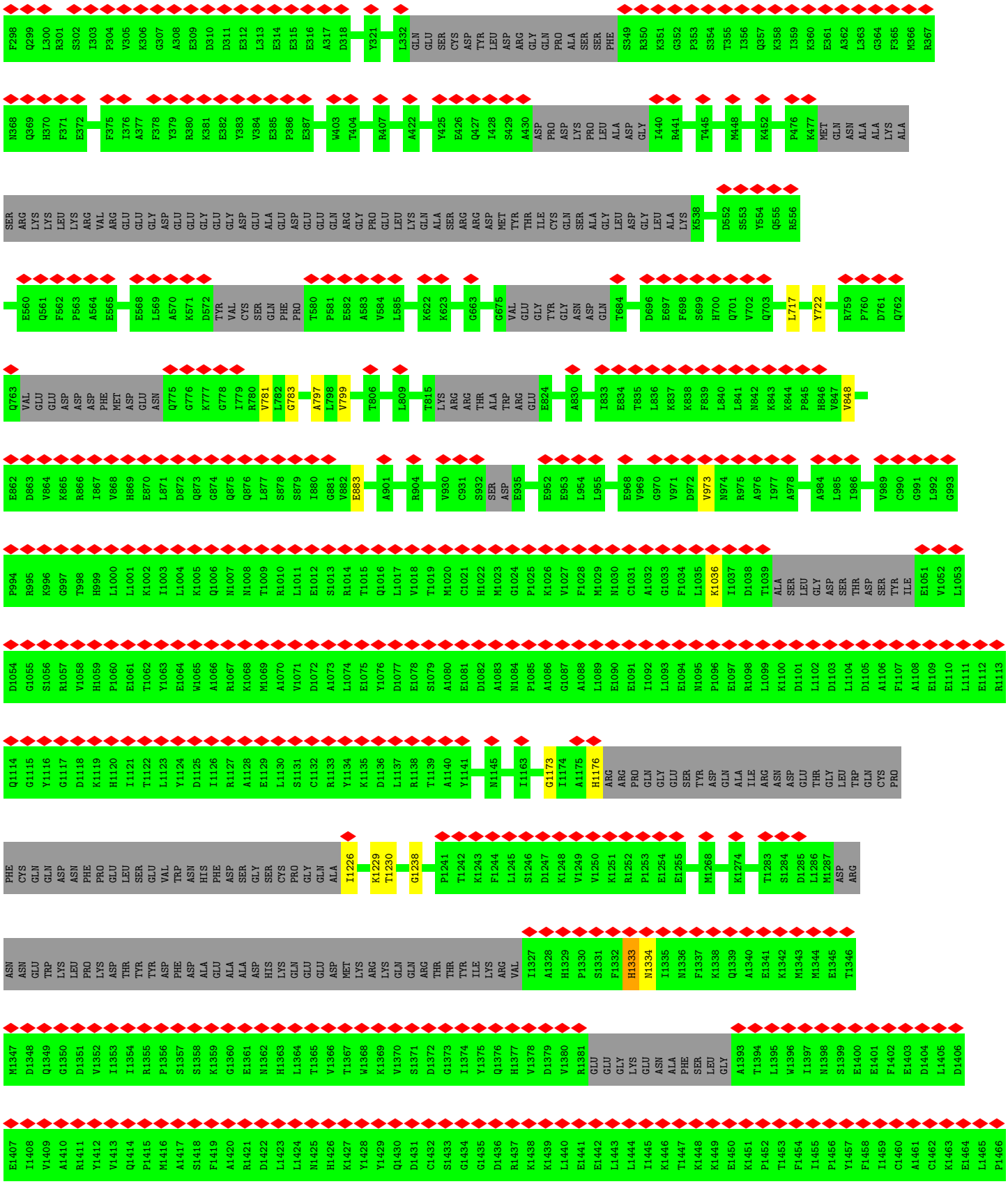
• Molecule 12: RNA polymerase II subunit K

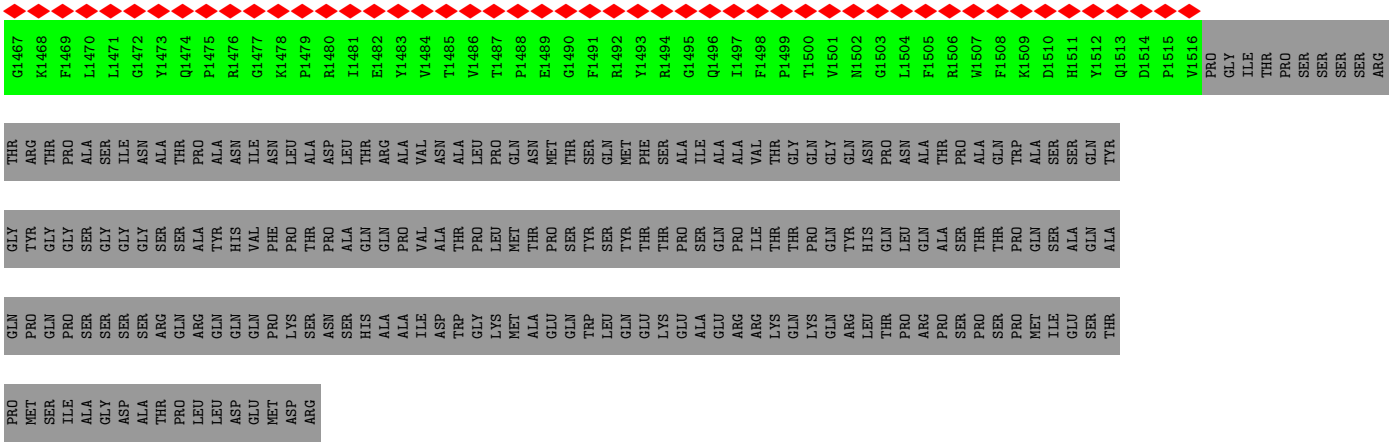
Chain L:



• Molecule 13: Transcription elongation factor SPT6

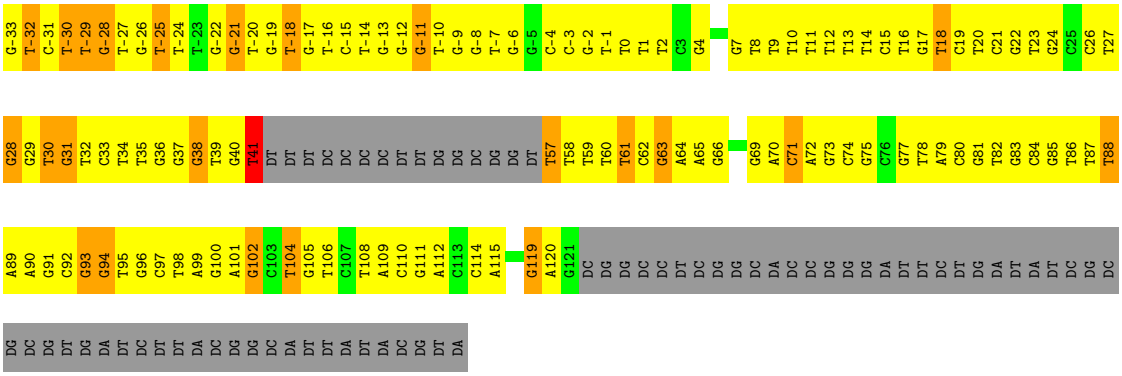
Chain M:


F298 Q299 L300 R301 S302 I303 P304 V305 K306 G307 A308 E309 D310 D311 E312 L313 E314 E315 E316 A317 D318 Y321 L332 GLN GLU SER CYS ASP TYR LEU ASP ARG GLY GLN PRO ALA SER SER PHE S349 R350 K351 G352 P353 S354 T355 I356 Q357 K358 I359 K360 E361 A362 L363 G364 F365 M366 R367
N368 Q369 H370 F371 E372 F375 I376 A377 F378 Y379 R380 K381 E382 Y383 Y384 E385 P386 E387 W403 T404 R407 A422 Y425 E426 Q427 I428 S429 A430 ASP PRO ASP LYS PRO LEU ALA ASP GLY I440 R441 T445 M448 K452 P476 K477 MET GLN ASN ALA ALA LYS ALA
SER ARG LYS LYS LEU LYS ARG VAL ARG GLU GLU GLY ASP GLU GLU GLY GLU GLY ASP GLU ALA GLU ASP GLU GLU GLN ARG GLY PRO GLU LEU LYS GLN ALA SER ARG ARG ASP MET TYR THR ILE CYS GLN SER ALA GLY LEU ASP GLY LEU ALA LYS K538 D552 S553 Y554 Q555 R556
E560 Q561 F562 P563 A564 E565 E568 L569 A570 K571 D572 TYR VAL CYS SER GLN PHE PRO T580 P581 E582 A583 V584 L585 K622 K623 G663 G675 VAL GLU GLY TYR GLY ASN ASP GLN T684 D696 E697 F698 S699 H700 Q701 V702 Q703 L717 Y722 R759 P760 D761 Q762
Q763 VAL GLU GLU ASP ASP ASP PHE MET ASP GLU ASN Q775 G776 K777 G778 I779 R780 V781 L782 G783 A797 L798 V799 T806 L809 T815 LYS ARG ARG THR ALA TRP ARG GLU E824 A830 I833 E834 T835 L836 K837 K838 F839 L840 L841 N842 K843 K844 P845 H846 V847 V848
E862 D863 V864 K865 R866 I867 V868 H869 E870 L871 D872 Q873 G874 Q875 Q876 L877 S878 S879 I880 G881 V882 E883 A901 R904 V930 C931 S932 SER ASP E935 E952 E953 L954 L955 E968 V969 G970 V971 D972 V973 N974 R975 A976 I977 A978 A984 L985 I986 V989 C990 G991 L992 G993
P994 R995 K996 G997 T998 H999 L1000 L1001 K1002 I1003 L1004 K1005 Q1006 N1007 N1008 T1009 R1010 L1011 E1012 S1013 R1014 T1015 Q1016 L1017 V1018 T1019 M1020 C1021 H1022 M1023 G1024 P1025 K1026 V1027 F1028 M1029 N1030 C1031 A1032 G1033 F1034 L1035 K1036 I1037 D1038 T1039 ALA SER LEU GLY ASP SER THR ASP SER TYR ILE E1051 V1052 L1053
D1054 G1055 S1056 R1057 V1058 H1059 P1060 E1061 T1062 Y1063 E1064 W1065 A1066 R1067 K1068 M1069 A1070 V1071 D1072 A1073 L1074 E1075 Y1076 D1077 E1078 S1079 A1080 E1081 D1082 A1083 N1084 P1085 A1086 G1087 A1088 L1089 E1090 E1091 I1092 L1093 E1094 N1095 P1096 E1097 R1098 L1099 K1100 D1101 L1102 D1103 L1104 D1105 A1106 F1107 A1108 E1109 E1110 L1111 E1112 R1113
Q1114 G1115 Y1116 G1117 D1118 K1119 H1120 I1121 T1122 L1123 Y1124 D1125 I1126 R1127 A1128 E1129 L1130 S1131 C1132 R1133 Y1134 K1135 D1136 L1137 R1138 T1139 A1140 Y1141 N1145 I1163 G1173 I1174 A1175 H1176 ARG ARG PRO GLN GLY GLU SER TYR ASP GLN ALA ILE ARG ASN ASP GLU THR GLY LEU TRP GLN CYS PRO
PHE CYS GLN GLN ASP ASN PHE PRO GLU LEU SER GLU VAL TRP ASN HIS PHE ASP SER GLY SER CYS PRO GLY GLN ALA I1226 K1229 T1230 G1238 P1241 T1242 K1243 F1244 L1245 S1246 D1247 K1248 V1249 V1250 K1251 R1252 P1253 E1254 E1255 M1268 K1274 T1283 S1284 D1285 L1286 M1287 ASP ARG
ASN ASN GLU TRP LYS LEU PRO LYS ASP THR TYR TYR ASP PHE ASP ALA GLU ALA ALA ASP HIS LYS GLN GLU GLU ASP MET LYS ARG LYS GLN GLN ARG THR THR TYR ILE LYS ARG VAL I1327 A1328 H1329 P1330 S1331 F1332 H1333 N1334 I1335 N1336 F1337 K1338 Q1339 A1340 E1341 K1342 M1343 M1344 E1345 T1346
M1347 D1348 Q1349 G1350 D1351 V1352 I1353 I1354 R1355 P1356 S1357 S1358 K1359 G1360 E1361 N1362 H1363 L1364 T1365 V1366 T1367 W1368 K1369 V1370 S1371 D1372 G1373 I1374 Y1375 Q1376 H1377 V1378 D1379 V1380 R1381 GLU GLU GLY LYS GLU ASN ALA PHE SER LEU GLY A1393 T1394 L1395 W1396 I1397 N1398 S1399 E1400 E1401 F1402 E1403 D1404 L1405 D1406
E1407 I1408 V1409 A1410 R1411 Y1412 V1413 Q1414 P1415 M1416 A1417 S1418 F1419 A1420 R1421 D1422 L1423 L1424 N1425 H1426 K1427 Y1428 Y1429 Q1430 D1431 C1432 S1433 G1434 G1435 D1436 R1437 K1438 K1439 L1440 E1441 E1442 L1443 L1444 L1445 K1446 T1447 K1448 K1449 E1450 K1451 P1452 T1453 F1454 I1455 P1456 Y1457 F1458 I1459 C1460 A1461 C1462 K1463 E1464 L1465 P1466



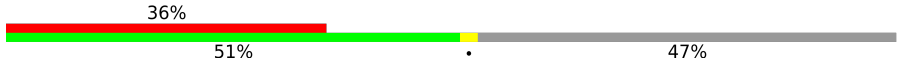
- Molecule 14: Non-template DNA

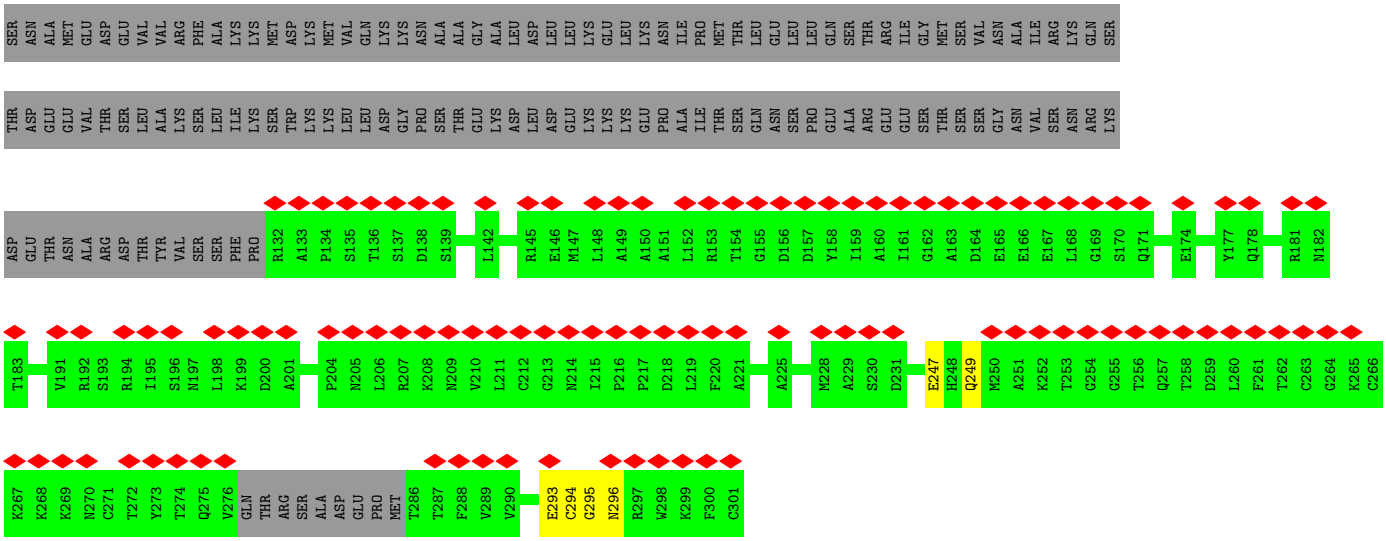
Chain N:



- Molecule 15: Transcription elongation factor A protein 1

Chain O:





- Molecule 16: RNA

Chain P: 56% 19% 19% 6%

G38 U41 U42 U43 U44 C45 C46 C47 C48 C53

• Molecule 17: RNA polymerase-associated protein CTR9 homolog

Chain Q: 24% 75% • 25%

MET SER R3 G4 S5 I6 E7 I8 P9 L10 R11 D12 T13 D14 E15 V16 I17 E18 L19 D20 F21 D22 Q23 L24 P25 E26 G27 D28 E29 V30 I31 S32 I33 L34 K35 Q36 E37 H38 T39 Q40 L41 H42 I43 W44 I45 A46 L47 A48 L49 E50 K53 Q54 G55 K56 T57 E58 E59 F60 V61

K62 L63 L64 E65 A66 A67 R68 I69 D70 G71 N72 L73 D74 Y75 R76 D77 H78 E79 K80 D81 Q82 M83 T84 C85 L86 D87 T88 L89 A90 A91 Y92 Y93 V94 Q95 Q96 A97 R98 K99 E100 K101 N102 K103 D104 N105 K106 K107 D108 L109 I110 T111 Q112 A113 T114 L115 L116 Y117 T118 M119 A120 D121

K122 I123 I124 M125 Q128 N129 L132 G133 R134 A135 C136 L139 L140 E141 G142 M145 D146 Q147 A148 D149 A150 N157 Q158 S159 P160 N161 N162 I163 P164 A165 L166 L167 G168 K169 K176 L183 A184 Y185 Y186 K187 K188 A189 L190 R191 T192 C196 P197 A198 E199 V200 R201 L202

G203 M204 G205 H206 C207 F208 V209 K210 L214 E215 R218 L219 E226 L227 K230 C231 V232 G233 A234 L235 V236 G237 L238 A239 V240 L241 E242 L243 N244 N245 K246 E247 A248 D249 S250 I251 K252 N253 G254 V255 Q256 L257 L258 S259 R260 A261 Y262 T263 I264 D265 P266 S267 N268 P269 M270 V271

L272 N273 H274 L275 A276 N277 H278 F279 F280 F281 K282 K283 D284 Y285 S286 K287 V288 Q289 H290 L291 A295 F296 H297 N298 T299 E300 V301 E302 E307 S308 C309 Y310 Q311 L312 Q334 F335 S338 S339 F340 V341 L342 K369 A370 Y371 P372 Y375 E389 G399 H400 L401 K402 K403

E406 Q407 Y408 P409 D410 D411 V412 E413 A414 W415 I416 E417 T425 D426 G429 S432 G435 E443 K444 L506 M510 V531 F663 R667 L723 A724 R725 D801 A808 T892 GLY GLU THR GLU ALA THR LYS GLU LYS LYS ARG GLY GLY GLY

GLY ARG ARG SER LYS LYS GLY GLY GLU PHE ASP GLU PHE VAL ASN ASP ASP THR ASP ASP ASP LEU PRO ILE SER LYS LYS LYS LYS ARG ARG LYS GLY SER GLY SER GLU GLN GLU GLY GLU ASP GLU GLU GLY GLY GLU ARG LYS LYS LYS ARG ARG ARG HIS PRO LYS GLY GLU

GLU GLY SER ASP ASP ASP GLU THR GLU ASN GLY PRO LYS PRO LYS LYS ARG ARG PRO PRO LYS ALA GLU LYS LYS LYS ALA PRO LYS PRO GLU ARG LEU PRO PRO SER MET LYS GLY LYS ILE LYS SER LYS ALA ILE ILE SER SER SER ASP ASP SER SER ASP GLU ASP LYS LEU LYS

ILE ALA ASP GLU GLY HIS PRO ARG ASN SER ASN SER ASN SER ASP SER ASP GLU ASP GLU GLN ARG LYS LYS CYS ALA SER SER GLU SER ASP SER ASP GLU ASN GLN ASN LYS SER GLY SER GLU ALA GLY SER PRO ARG ARG PRO ARG ARG GLN ARG SER ASP GLN ASP SER SER

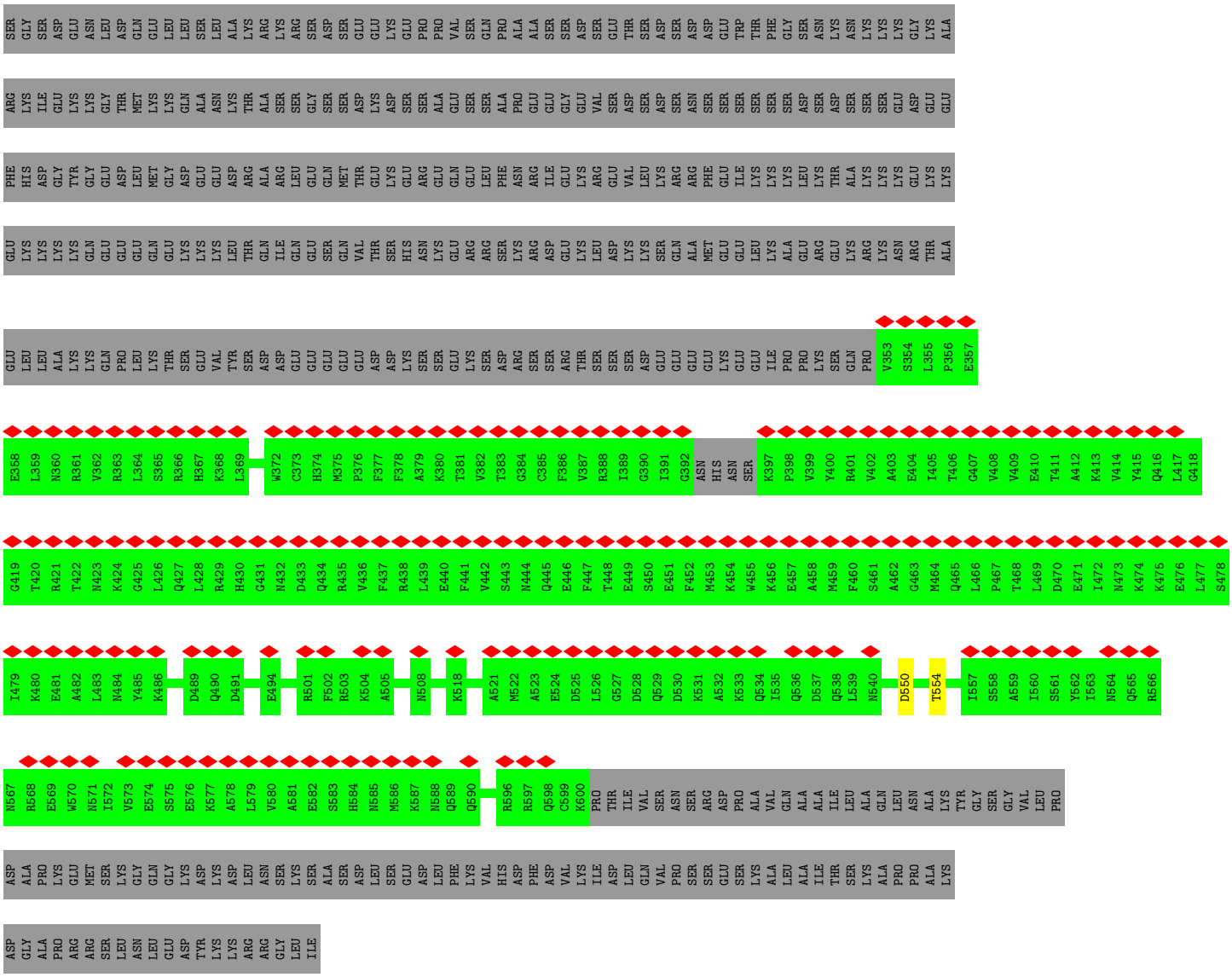
ASP GLN PRO SER ARG LYS ARG ARG PRO SER GLY SER GLU GLN SER ASP ASN GLU SER VAL GLN SER GLY ARG SER HIS SER GLY VAL SER GLU ASN ASP SER ARG PRO ALA SER PRO SER ALA GLU SER ASP HIS GLU SER GLU ARG GLY SER ASP ASN GLU GLY GLN GLY SER

GLY ASN GLU SER GLU PRO GLU GLY SER ASN ASN GLU ALA SER ASP ARG GLY SER GLU HIS GLY SER ASP ASP SER ASP GLU ASN LEU TYR PHE GLN

• Molecule 18: RNA polymerase-associated protein RTF1 homolog

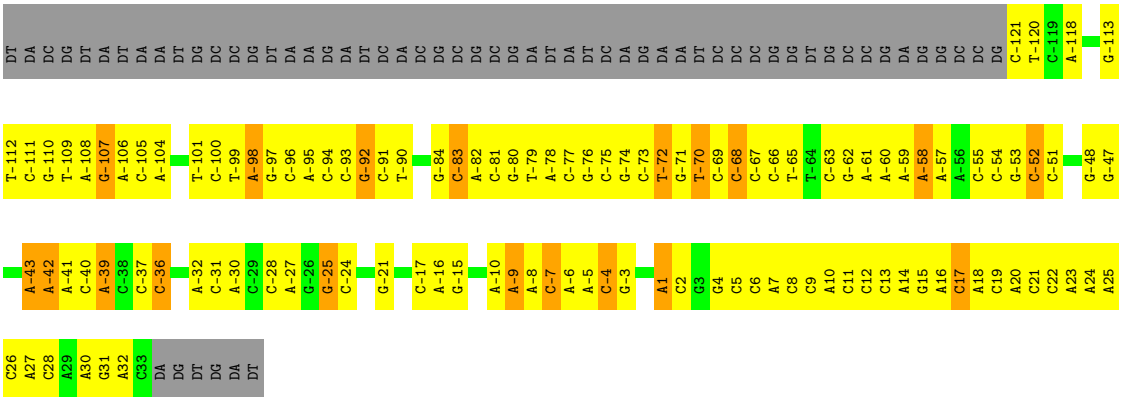
Chain R: 26% 34% 66%

SER ASN ALA MET ARG GLY ARG LEU CYS VAL GLY ARG ALA ALA ALA ALA ALA ALA ALA VAL ALA ALA VAL PRO LEU ALA GLY GLY GLN GLU GLY SER PRO GLY GLY GLY ARG ARG GLY SER ARG GLY THR THR MET VAL LYS LYS ARG LYS GLY ARG VAL VAL ILE ASP SER ASP THR GLU ASP



• Molecule 19: Template DNA

Chain T: 19% 45% 9% 28%



• Molecule 20: RNA polymerase-associated protein LEO1

Chain U: 15% 15% 84%

MET ALA ASP MET GLU ASP LEU PHE GLY SER ASP ALA ASP SER GLU ALA GLU ARG LYS ASP SER ASP SER GLY SER ASP SER ASP SER ASP GLN GLU ASN ALA ALA SER GLY SER ASN ALA SER GLY SER GLU SER ASP GLN ASP GLU ARG GLY ASP SER GLY GLN PRO SER ASN LYS GLU

LEU PHE GLY ASP ASP SER GLU ASP GLU GLY GLY ALA SER HIS HIS SER GLY SER ASP ASN HIS SER GLU ARG SER ASP ARG SER GLU ALA SER GLU ARG SER ASP HIS GLU ASP ASN ASP PRO SER ASP VAL ASP GLN HIS SER GLY SER GLU ALA PRO ASN ASP ASP GLU ASP GLU GLY

HIS ARG SER ASP GLY GLY SER HIS HIS SER SER GLU ALA GLU GLY SER GLU LYS ALA HIS SER ASP ASP GLU LYS TRP GLY ARG GLU ASP LYS SER ASP GLN SER ASP ASP GLU LYS ILE GLN ASN SER ASP ASP GLU GLU ARG ALA GLN GLY SER ASP GLU GLU LYS LEU GLN ASN ASP

ASP ASP GLU LYS MET GLN ASN THR ASP ASP GLU GLU ARG PRO GLN LEU SER ASP ASP GLU ARG GLN GLN LEU SER GLU GLU GLU ASP LYS ALA ASN SER ASP ASP GLU ARG PRO VAL ALA SER ASP ASN ASP ASP GLU LYS GLN SER ASP ASP GLU GLU GLN PRO GLN LEU SER ASP GLU

GLU LYS MET GLN ASN SER ASP ASP GLU ARG PRO GLN ALA SER ASP GLU GLU HIS ARG HIS SER ASP ASP GLU GLU GLU GLN ASP HIS LYS SER GLU SER ASP ALA ARG GLY SER ASP SER GLU ASP GLU VAL LEU ARG MET LYS ARG LYS ASN ALA ILE ALA SER ASP SER GLU ALA ASP SER

ASP THR GLU VAL PRO LYS ASP ASN SER GLY THR MET ASP LEU PHE GLY GLY ALA ASP ASP ILE SER SER GLY SER ASP GLY GLU ASP LYS PRO PRO THR PRO GLN GLY GLN PRO VAL ASP GLU ASN GLY LEU PRO GLN ASP GLN GLN GLU GLU GLU PRO ILE PRO GLU THR ARG ILE GLU VAL

GLU ILE PRO LYS VAL ASN THR ASP LEU G370 N371 D372 L373 Y374 F375 V376 K377 L378 P379 N380 F381 L382 S383 V384 E385 P386 R387 P388 F389 D390 P391 Q392 Y393 Y394 E395 D396 E397 F398 E399 ASP GLU GLU MET LEU ASP E406 E407 G408 R409 T410 R411 L412 K413 L414 K415 V416 E417 N418 THR ILE

ARG TRP ARG ILE ARG ARG ASP GLU GLU GLY ASN GLU ILE LYS GLU SER N437 A438 R439 I440 V441 K442 W443 S444 D445 G446 S447 M448 S449 L450 H451 L452 G453 N454 E455 V456 F457 D458 V459 Y460 K461 A462 P463 L464 Q465 G466 D467 H468 N469 H470 L471 F472 I473 R474 Q475 G476 T477 G478 L479 Q480

G481 Q482 A483 V484 F485 K486 T487 K488 L489 T490 F491 R492 P493 H494 S495 T496 D497 SER ALA THR HIS ARG LYS MET THR LEU SER LEU ALA ASP ARG CYS SER LYS THR GLN LYS ILE ARG ILE LEU PRO MET ALA GLY ARG ASP PRO GLU CYS GLN ARG THR GLU MET ILE LYS LYS GLU GLU

GLU ARG LEU ARG ALA SER ILE ARG ARG GLU SER GLN GLN ARG ARG MET ARG GLU LYS GLN HIS GLN ARG GLY LEU SER ALA SER TYR LEU GLU PRO ASP ARG TYR ASP GLU GLU GLU GLU GLU GLU SER ILE SER LEU ALA ALA ILE LYS ASN ARG TYR LYS GLY GLY ILE ARG GLU

GLU ARG ALA ARG ILE TYR SER SER ASP SER ASP GLU GLY SER GLU GLU ASP LYS ALA GLN ARG LEU LEU LYS ALA LYS LYS LEU THR SER ASP GLU GLU GLY GLY GLU PRO SER GLY LYS ARG LYS ALA GLU ASP ASP ASP LYS ALA ALA ASN LYS LYS HIS LYS LYS TYR VAL ILE SER ASP GLU

GLU GLU GLU ASP ASP ASP

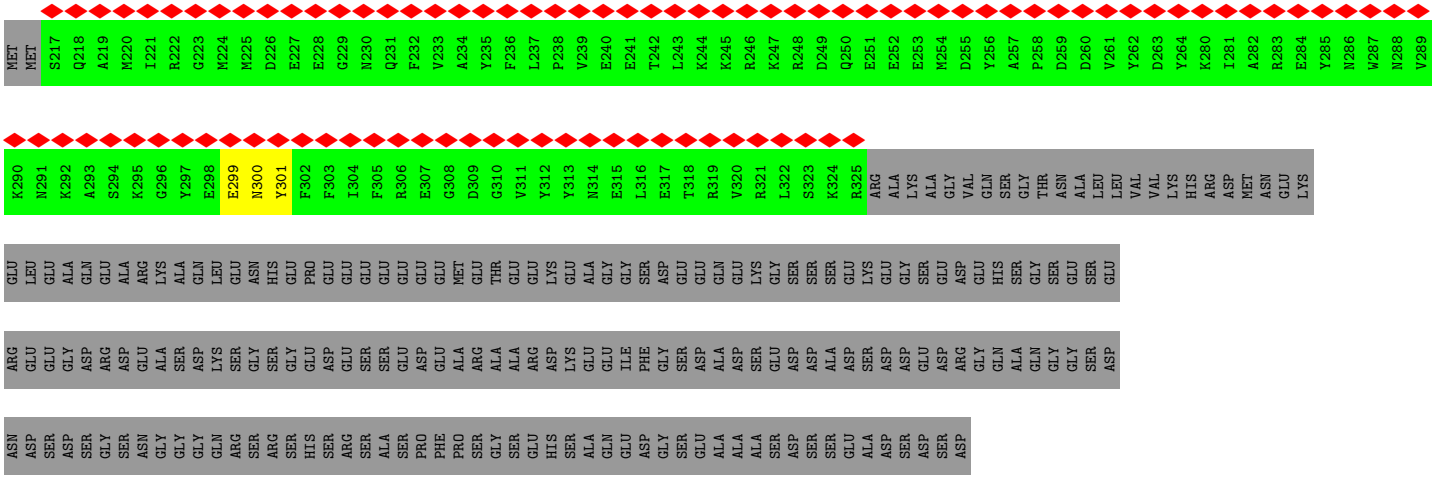
• Molecule 21: RNA polymerase II-associated factor 1 homolog

Chain V: 32% 45% 54%

MET ALA PRO THR ILE GLN THR GLN ALA GLN ARG GLU ASP GLY HIS ARG PRO ASN SER HIS ARG THR LEU PRO E25 N56 R57 F58 V59 Q60 Y61 K62 A63 T64 S65 L66 E67 K68 Q69 H70 K71 H72 D73 L74 L75 T76 E77 P78 D79 L80 G81 V82 T83 I84 D85 L86 I87 N88 P89

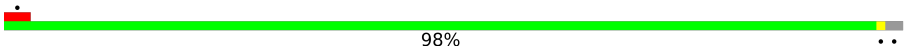
D90 P96 Q113 ALA PRO THR SER SER LYS R120 V127 V128 E135 Y136 I137 E140 F141 N142 ARG TYR GLY ILE SER ASN GLU LYS PRO GLU VAL LYS ILE GLY VAL SER VAL LYS GLN GLN PHE THR GLU GLU GLU ILE TYR K170 D171 R172 D173 S174 Q175 I176 T177 A178 I179

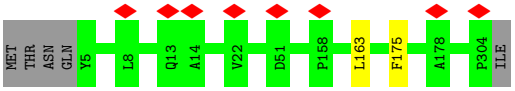
E180 K181 T182 F183 E184 D185 A186 Q187 K188 S189 I190 S191 Q192 H193 Y194 S195 K196 P197 R198 V199 T200 P201 V202 E203 V204 M205 P206 V207 PHE PRO ASP PHE LYS MET TRP ILE ASN PRO CYS ALA GLN VAL ILE PHE ASP SER ASP PRO ALA PRO LYS ASP THR SER GLY ALA ALA ALA LEU GLU



- Molecule 22: WDR61

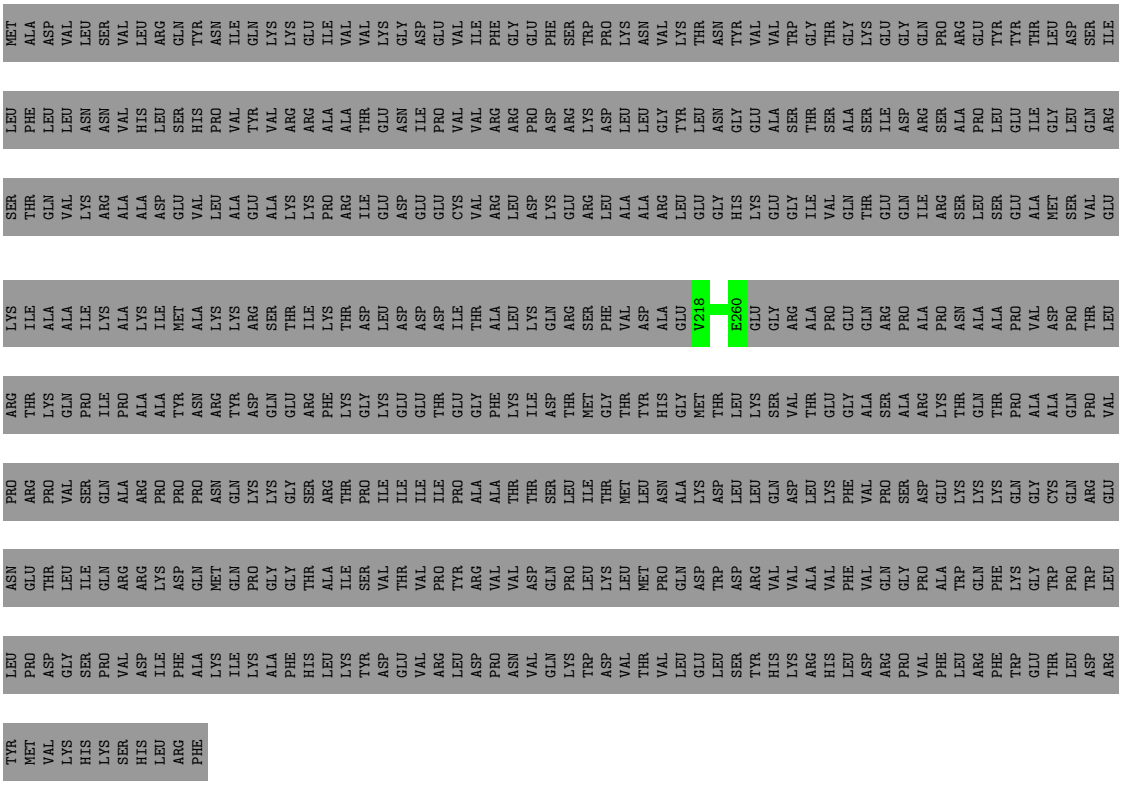
Chain W:





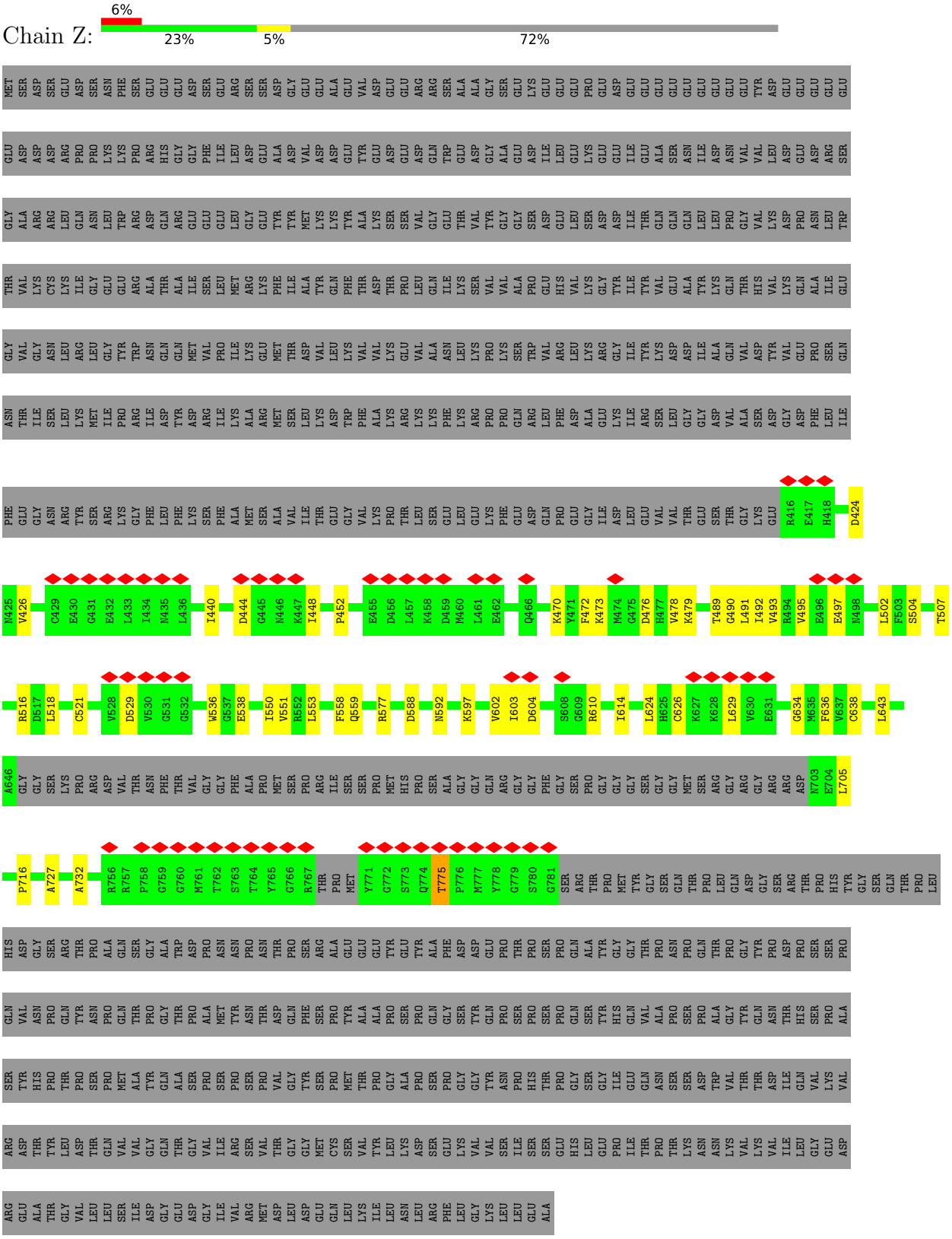
- Molecule 23: Parafibromin

Chain X:



- Molecule 24: Transcription elongation factor SPT5

Chain Z:

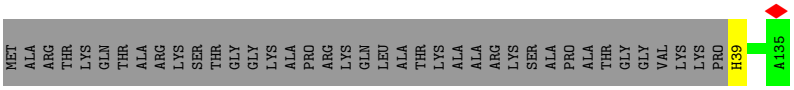


• Molecule 25: Histone H3.2

Chain a:

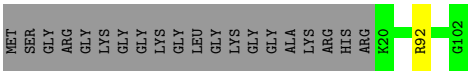
• Molecule 25: Histone H3.2

Chain e:



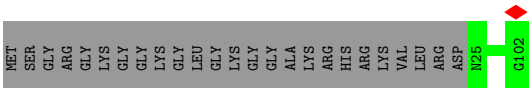
• Molecule 26: Histone H4

Chain b:



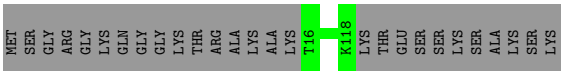
• Molecule 26: Histone H4

Chain f:



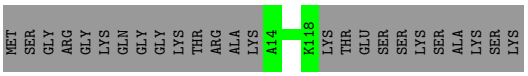
• Molecule 27: Histone H2A

Chain c:



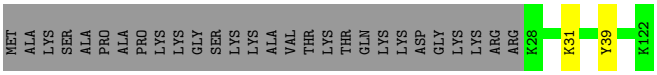
• Molecule 27: Histone H2A

Chain g:



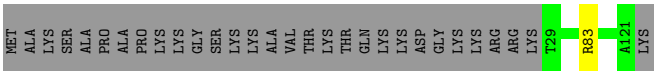
• Molecule 28: Histone H2B 1.1

Chain d:



• Molecule 28: Histone H2B 1.1

Chain h:


MET
ALA
LYS
SER
ALA
PRO
ALA
PRO
LYS
LYS
GLY
SER
LYS
LYS
ALA
VAL
THR
LYS
THR
GLN
LYS
LYS
ASP
GLY
LYS
LYS
ARG
ARG
LYS
T29
R83
A121
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105420	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.466	Depositor
Minimum map value	-0.485	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	373.5, 373.5, 373.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: TPO, ZN, MG, SEP

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	0.39	0/11437	0.61	2/15433 (0.0%)
2	B	0.42	0/9124	0.58	0/12313
3	C	0.42	0/2115	0.54	0/2873
4	D	0.26	0/1017	0.48	0/1368
5	E	0.33	0/1751	0.57	0/2366
6	F	0.45	0/636	0.57	0/859
7	G	0.29	0/1364	0.51	0/1853
8	H	0.38	0/1219	0.55	0/1644
9	I	0.33	0/964	0.54	0/1305
10	J	0.51	0/533	0.57	0/719
11	K	0.41	0/939	0.54	0/1271
12	L	0.41	0/403	0.66	0/536
13	M	0.26	0/3995	0.50	1/4971 (0.0%)
14	N	0.77	1/3226 (0.0%)	1.33	29/4986 (0.6%)
15	O	0.36	0/643	0.62	0/799
16	P	0.63	0/367	1.13	2/568 (0.4%)
17	Q	0.23	0/3559	0.47	0/4447
18	R	0.23	0/974	0.48	0/1214
19	T	0.80	1/3564 (0.0%)	1.19	22/5487 (0.4%)
20	U	0.25	0/413	0.48	0/511
21	V	0.27	0/972	0.53	0/1208
22	W	0.24	0/1199	0.55	0/1497
23	X	0.24	0/171	0.46	0/212
24	Z	0.26	0/2414	0.53	0/3250
25	a	0.30	0/814	0.62	0/1092
25	e	0.28	0/812	0.57	0/1088
26	b	0.33	0/669	0.60	0/894
26	f	0.32	0/626	0.59	0/837
27	c	0.28	0/805	0.56	0/1088
27	g	0.29	0/819	0.56	0/1106
28	d	0.29	0/756	0.50	0/1015
28	h	0.32	0/737	0.50	0/993

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.42	2/59037 (0.0%)	0.70	56/79803 (0.1%)

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	2
2	B	0	3
7	G	0	1
10	J	0	1
13	M	0	1
14	N	0	1
21	V	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	41	DT	C4'-O4'	5.26	1.50	1.45
19	T	-51	DC	C3'-O3'	-5.19	1.37	1.44

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	581	LYS	C-N-CD	-28.87	57.08	120.60
19	T	-42	DA	O4'-C1'-N9	10.77	115.54	108.00
14	N	28	DG	O4'-C1'-N9	10.03	115.02	108.00
14	N	38	DG	O4'-C1'-N9	9.74	114.82	108.00
19	T	1	DA	O4'-C1'-N9	9.66	114.76	108.00
14	N	93	DG	O4'-C1'-N9	9.51	114.66	108.00
14	N	24	DG	O4'-C1'-N9	8.59	114.01	108.00
14	N	-28	DG	O4'-C1'-N9	8.52	113.96	108.00
14	N	63	DG	O4'-C1'-N9	7.92	113.55	108.00
19	T	-43	DA	O4'-C4'-C3'	-7.88	101.27	106.00
14	N	18	DT	O4'-C1'-N1	7.69	113.38	108.00
14	N	95	DT	O4'-C1'-N1	7.49	113.24	108.00
1	A	582	PRO	CA-N-CD	-7.44	101.09	111.50
14	N	-32	DT	O4'-C1'-N1	7.42	113.19	108.00
13	M	1333	HIS	CA-C-N	-7.33	101.08	117.20
19	T	-107	DG	O4'-C1'-N9	7.31	113.12	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	74	DC	O4'-C1'-N1	7.19	113.03	108.00
19	T	-40	DC	O4'-C1'-N1	7.08	112.96	108.00
19	T	-7	DC	O4'-C1'-N1	6.88	112.81	108.00
19	T	-52	DC	O4'-C1'-N1	6.88	112.81	108.00
19	T	-70	DT	O4'-C1'-N1	6.54	112.58	108.00
19	T	-39	DA	OP1-P-OP2	-6.53	109.81	119.60
14	N	30	DT	OP1-P-OP2	-6.40	110.00	119.60
19	T	-72	DT	O4'-C1'-N1	6.33	112.43	108.00
14	N	-29	DT	O4'-C1'-N1	-6.32	103.58	108.00
14	N	57	DT	O4'-C1'-N1	6.19	112.33	108.00
19	T	-25	DG	O4'-C1'-N9	6.14	112.30	108.00
19	T	-40	DC	OP1-P-O3'	5.99	118.38	105.20
19	T	-58	DA	O4'-C1'-N9	5.99	112.19	108.00
14	N	88	DT	O4'-C1'-N1	-5.94	103.84	108.00
14	N	102	DG	O4'-C1'-N9	5.93	112.15	108.00
19	T	-92	DG	O4'-C1'-N9	5.91	112.14	108.00
19	T	-36	DC	O4'-C1'-N1	-5.90	103.87	108.00
14	N	31	DG	C1'-O4'-C4'	-5.64	104.46	110.10
14	N	71	DC	C1'-O4'-C4'	-5.59	104.51	110.10
14	N	24	DG	C1'-O4'-C4'	-5.58	104.52	110.10
14	N	94	DG	C1'-O4'-C4'	-5.51	104.59	110.10
19	T	-9	DA	O4'-C1'-N9	5.45	111.82	108.00
16	P	48	C	C5'-C4'-O4'	5.43	115.61	109.10
14	N	-21	DG	O4'-C1'-N9	-5.42	104.21	108.00
19	T	-98	DA	O4'-C1'-N9	5.32	111.72	108.00
14	N	-25	DT	O4'-C1'-N1	5.25	111.67	108.00
14	N	41	DT	O4'-C1'-N1	-5.23	104.34	108.00
14	N	-30	DT	O4'-C1'-N1	-5.19	104.36	108.00
14	N	104	DT	O4'-C1'-N1	5.19	111.64	108.00
19	T	-17	DC	O4'-C1'-N1	5.17	111.62	108.00
19	T	17	DC	C1'-O4'-C4'	-5.16	104.94	110.10
14	N	119	DG	O4'-C1'-N9	5.13	111.59	108.00
14	N	-18	DT	O4'-C1'-N1	5.12	111.59	108.00
14	N	28	DG	C1'-O4'-C4'	-5.10	105.00	110.10
14	N	61	DT	O4'-C1'-N1	5.09	111.56	108.00
19	T	-83	DC	C1'-O4'-C4'	-5.07	105.03	110.10
19	T	-68	DC	O4'-C1'-C2'	5.04	109.93	105.90
16	P	45	C	C5'-C4'-O4'	5.04	115.14	109.10
19	T	-4	DC	C1'-O4'-C4'	-5.02	105.08	110.10
14	N	-11	DG	O4'-C1'-N9	-5.02	104.49	108.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ARG	Sidechain
1	A	430	ARG	Sidechain
2	B	491	ARG	Sidechain
2	B	743	ARG	Sidechain
2	B	859	ARG	Sidechain
7	G	151	ARG	Sidechain
10	J	6	ARG	Sidechain
13	M	1333	HIS	Mainchain
14	N	41	DT	Sidechain
21	V	299	GLU	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	11255	11388	11374	221	0
2	B	8947	9002	8994	118	0
3	C	2072	2024	2019	21	0
4	D	1004	981	980	4	0
5	E	1720	1738	1737	29	0
6	F	626	658	657	8	0
7	G	1333	1321	1321	17	0
8	H	1197	1157	1156	9	0
9	I	942	880	872	17	0
10	J	524	544	540	11	0
11	K	920	942	942	17	0
12	L	397	406	405	4	0
13	M	4008	1259	1035	8	0
14	N	2886	1594	1596	160	0
15	O	645	0	171	30	0
16	P	332	170	169	3	0
17	Q	3560	1796	940	4	0
18	R	976	491	255	1	0
19	T	3166	1719	1720	133	0
20	U	416	210	111	2	0
21	V	976	481	240	2	0
22	W	1200	617	341	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	X	172	87	44	0	0
24	Z	2388	2363	2360	43	0
25	a	802	841	841	0	0
25	e	801	839	838	0	0
26	b	662	710	709	0	0
26	f	619	660	659	0	0
27	c	795	847	846	0	0
27	g	809	865	864	0	0
28	d	745	774	773	0	0
28	h	726	748	747	0	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	R	1	0	0	0	0
30	A	1	0	0	0	0
All	All	57630	48112	46256	753	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (753) 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:729:PRO:CG	15:O:249:GLN:O	1.79	1.27
1:A:1314:THR:C	15:O:295:GLY:HA3	1.56	1.23
1:A:729:PRO:HB3	15:O:247:GLU:O	1.38	1.21
1:A:203:LYS:NZ	19:T:-67:DC:OP1	1.75	1.20
1:A:729:PRO:CB	15:O:247:GLU:O	1.90	1.17
1:A:1314:THR:O	15:O:295:GLY:HA3	1.40	1.16
1:A:203:LYS:NZ	19:T:-67:DC:P	2.17	1.16
1:A:729:PRO:HG3	15:O:249:GLN:O	1.44	1.05
1:A:1315:ASP:CG	15:O:296:ASN:N	2.03	1.00
1:A:203:LYS:HZ3	19:T:-67:DC:P	1.84	0.97
1:A:729:PRO:CA	15:O:247:GLU:O	2.13	0.97
11:K:77:THR:OG1	11:K:81:TYR:O	1.83	0.96
1:A:1314:THR:C	15:O:295:GLY:CA	2.32	0.96
1:A:904:GLN:NE2	1:A:981:CYS:O	1.98	0.95
10:J:47:ARG:NH1	10:J:48:MET:SD	2.42	0.93
1:A:582:PRO:HG2	1:A:583:ARG:H	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.05	0.89
1:A:729:PRO:HG2	15:O:249:GLN:O	1.72	0.89
1:A:1313:GLN:O	15:O:295:GLY:HA2	1.74	0.86
1:A:729:PRO:HA	15:O:247:GLU:O	1.75	0.85
1:A:552:ASP:OD2	8:H:24:ARG:NH1	2.10	0.85
1:A:1130:ILE:O	1:A:1130:ILE:HD12	1.77	0.84
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.12	0.83
1:A:54:LEU:O	1:A:61:ARG:NH2	2.14	0.80
1:A:1330:ALA:HB3	15:O:294:CYS:CA	2.11	0.80
1:A:440:LEU:O	1:A:440:LEU:HD12	1.83	0.79
1:A:729:PRO:HB3	15:O:247:GLU:C	2.04	0.79
1:A:1024:ASN:O	5:E:162:ARG:NH2	2.17	0.78
1:A:296:ASN:OD1	1:A:297:GLY:N	2.17	0.77
1:A:1315:ASP:OD2	15:O:296:ASN:N	2.16	0.77
1:A:394:VAL:HG23	1:A:444:TYR:O	1.84	0.77
11:K:78:THR:OG1	11:K:80:ASP:OD1	2.02	0.77
1:A:66:GLU:OE1	1:A:271:ARG:NH2	2.18	0.76
1:A:1314:THR:HA	15:O:295:GLY:O	1.85	0.76
24:Z:602:VAL:HG21	24:Z:636:PHE:HE2	1.50	0.76
3:C:26:THR:HG22	3:C:27:ASP:H	1.49	0.76
1:A:1315:ASP:CG	15:O:296:ASN:H	1.88	0.75
14:N:-15:DC:H2'	14:N:-14:DT:H71	1.70	0.74
1:A:729:PRO:CB	15:O:249:GLN:O	2.36	0.73
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.21	0.73
1:A:239:GLU:OE2	1:A:241:ARG:NH1	2.21	0.73
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.71	0.73
1:A:203:LYS:HZ2	19:T:-67:DC:P	2.11	0.72
1:A:1218:ARG:O	1:A:1222:THR:HG23	1.88	0.72
5:E:153:LYS:O	5:E:157:THR:HG23	1.88	0.72
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.22	0.72
18:R:550:ASP:O	18:R:554:THR:N	2.23	0.71
14:N:57:DT:O2	19:T:-55:DC:N4	2.23	0.70
3:C:86:ARG:NH1	24:Z:716:PRO:O	2.24	0.70
11:K:93:ASP:OD1	11:K:94:LEU:N	2.25	0.70
1:A:447:GLU:OE2	2:B:1064:ARG:NH1	2.24	0.70
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.73	0.70
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.09	0.70
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.73	0.69
1:A:66:GLU:O	1:A:69:GLY:N	2.26	0.69
1:A:902:GLU:OE1	1:A:985:ARG:NH2	2.27	0.68
1:A:1315:ASP:N	15:O:295:GLY:HA3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:ILE:HD12	2:B:428:ASP:HA	1.76	0.68
9:I:109:ARG:HD3	9:I:124:THR:HG21	1.76	0.68
14:N:9:DT:H2"	14:N:10:DT:H71	1.75	0.68
14:N:-28:DG:H2"	14:N:-27:DT:H72	1.75	0.67
24:Z:602:VAL:HG21	24:Z:636:PHE:CE2	2.29	0.67
1:A:581:LYS:NZ	8:H:85:ALA:O	2.27	0.67
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.28	0.67
1:A:1314:THR:O	15:O:295:GLY:CA	2.31	0.67
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.25	0.67
14:N:98:DT:O2	19:T:-97:DG:N2	2.28	0.66
17:Q:506:LEU:O	17:Q:510:MET:N	2.28	0.66
24:Z:478:VAL:HG11	24:Z:492:ILE:HG23	1.77	0.66
14:N:86:DT:H2'	14:N:87:DT:H72	1.77	0.66
1:A:832:THR:HG22	1:A:833:PRO:HD2	1.78	0.65
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.78	0.65
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.78	0.65
24:Z:550:ILE:HD13	24:Z:558:PHE:HB3	1.78	0.64
1:A:1400:LEU:O	1:A:1404:THR:HG23	1.98	0.64
14:N:59:DT:H2'	14:N:60:DT:H72	1.79	0.64
7:G:110:ARG:NH1	7:G:114:PRO:O	2.30	0.64
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.25	0.63
9:I:81:THR:HG23	9:I:96:PHE:CD2	2.33	0.63
2:B:824:ASP:O	2:B:872:THR:HG23	1.98	0.63
14:N:41:DT:H5'	14:N:41:DT:C6	2.33	0.63
14:N:63:DG:H1'	14:N:64:DA:N7	2.14	0.63
1:A:582:PRO:HG2	1:A:583:ARG:N	2.09	0.63
19:T:11:DC:H2"	19:T:12:DC:C5	2.34	0.63
1:A:203:LYS:HZ1	19:T:-67:DC:P	2.20	0.63
14:N:32:DT:H2"	14:N:33:DC:C6	2.34	0.62
1:A:455:ILE:HG23	1:A:520:MET:HE1	1.80	0.62
1:A:1007:ILE:HD12	1:A:1008:LYS:N	2.14	0.62
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.14	0.62
2:B:266:GLU:OE1	2:B:266:GLU:O	2.18	0.62
24:Z:473:LYS:O	24:Z:492:ILE:HD11	1.99	0.62
1:A:933:THR:O	1:A:1002:SER:N	2.33	0.61
1:A:1318:LYS:HZ3	15:O:293:GLU:C	2.03	0.61
2:B:931:ILE:HD12	2:B:931:ILE:H	1.65	0.61
11:K:1:MET:SD	11:K:2:ASN:N	2.73	0.61
19:T:-72:DT:H1'	19:T:-71:DG:C8	2.35	0.61
1:A:886:VAL:HG12	5:E:169:GLN:O	2.00	0.61
2:B:845:TYR:HA	2:B:865:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:-107:DG:H1'	19:T:-106:DA:C8	2.36	0.61
1:A:582:PRO:CG	1:A:583:ARG:N	2.64	0.61
14:N:-8:DG:N2	19:T:9:DC:O2	2.33	0.61
19:T:-37:DC:H2'	19:T:-36:DC:C5	2.36	0.61
1:A:1314:THR:CA	15:O:295:GLY:O	2.49	0.61
5:E:96:GLU:OE1	5:E:96:GLU:N	2.27	0.60
14:N:87:DT:H2'	14:N:88:DT:H72	1.83	0.60
19:T:16:DA:H2"	19:T:17:DC:C6	2.36	0.60
1:A:873:VAL:HG22	1:A:879:VAL:HG22	1.83	0.60
1:A:1315:ASP:N	15:O:295:GLY:O	2.35	0.60
9:I:31:GLU:N	9:I:31:GLU:OE1	2.34	0.60
14:N:97:DC:H2"	14:N:98:DT:C6	2.37	0.60
6:F:120:VAL:HG12	6:F:120:VAL:O	2.02	0.60
6:F:105:ILE:HD12	6:F:117:ASP:HB3	1.83	0.60
1:A:965:VAL:O	1:A:968:VAL:HG22	2.01	0.60
2:B:423:ILE:HD13	2:B:429:PHE:CD1	2.37	0.60
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.83	0.60
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.84	0.59
13:M:1230:THR:O	13:M:1238:GLY:N	2.35	0.59
14:N:33:DC:H2"	14:N:34:DT:H71	1.84	0.59
14:N:61:DT:H2"	14:N:62:DC:C5	2.36	0.59
8:H:63:THR:O	8:H:84:ARG:NH1	2.35	0.59
14:N:99:DA:H2"	14:N:100:DG:C8	2.37	0.59
1:A:479:TRP:O	1:A:483:ARG:NH2	2.36	0.59
14:N:26:DC:O2	19:T:-25:DG:N2	2.35	0.59
14:N:69:DG:H2"	14:N:70:DA:C8	2.38	0.59
2:B:198:GLU:OE2	2:B:391:LYS:NZ	2.20	0.59
6:F:51:ARG:NH1	6:F:122:GLU:OE1	2.33	0.59
24:Z:626:CYS:HB3	24:Z:629:LEU:HD12	1.84	0.59
10:J:10:CYS:SG	10:J:11:GLY:N	2.76	0.59
24:Z:610:ARG:HD2	24:Z:629:LEU:HD21	1.85	0.58
14:N:57:DT:C6	14:N:57:DT:O5'	2.56	0.58
14:N:13:DT:H2'	14:N:14:DT:H71	1.84	0.58
14:N:58:DT:H2'	14:N:59:DT:H71	1.84	0.58
19:T:-61:DA:H2'	19:T:-60:DA:C8	2.39	0.58
24:Z:492:ILE:HG22	24:Z:502:LEU:HB3	1.85	0.58
1:A:413:TYR:O	1:A:415:GLY:N	2.37	0.58
1:A:1315:ASP:N	15:O:295:GLY:C	2.57	0.58
7:G:147:ILE:HG23	7:G:159:ALA:HB1	1.86	0.58
14:N:31:DG:C2	19:T:-30:DA:C2	2.91	0.58
2:B:631:GLN:O	2:B:683:GLN:NE2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:THR:O	1:A:854:THR:HG23	2.03	0.57
19:T:-67:DC:H2'	19:T:-66:DC:C6	2.38	0.57
2:B:275:ALA:O	2:B:314:GLN:NE2	2.36	0.57
14:N:9:DT:H2"	14:N:10:DT:C7	2.33	0.57
14:N:93:DG:H1'	14:N:94:DG:C8	2.39	0.57
1:A:189:PRO:CB	1:A:200:ALA:HB1	2.35	0.57
24:Z:492:ILE:HD12	24:Z:495:VAL:CG1	2.34	0.57
19:T:-92:DG:H1'	19:T:-91:DC:C6	2.40	0.57
19:T:21:DC:H2"	19:T:22:DC:C5	2.39	0.57
2:B:867:ILE:HD12	2:B:894:THR:HG21	1.87	0.57
1:A:1045:LEU:HD11	1:A:1072:ILE:HD13	1.86	0.56
1:A:1190:GLN:O	1:A:1193:VAL:HG12	2.04	0.56
1:A:404:GLU:OE2	1:A:407:ARG:NH1	2.38	0.56
19:T:8:DC:H2"	19:T:9:DC:C6	2.41	0.56
14:N:-25:DT:C6	14:N:-24:DT:H72	2.40	0.56
14:N:77:DG:H2"	14:N:78:DT:C5	2.41	0.56
1:A:1087:VAL:HG23	1:A:1400:LEU:HD21	1.87	0.56
8:H:32:SER:OG	8:H:37:MET:N	2.39	0.56
14:N:-28:DG:H1'	14:N:-27:DT:C6	2.40	0.56
19:T:-105:DC:H1'	19:T:-104:DA:C8	2.41	0.56
14:N:81:DG:H2'	14:N:82:DT:H72	1.87	0.56
19:T:-80:DG:H2"	19:T:-79:DT:C5	2.40	0.56
19:T:-78:DA:H2"	19:T:-77:DC:C5	2.41	0.56
19:T:1:DA:H2"	19:T:2:DC:C5	2.40	0.56
1:A:402:LEU:O	1:A:406:VAL:HG23	2.06	0.56
14:N:104:DT:H2"	14:N:105:DG:C8	2.41	0.56
1:A:1318:LYS:NZ	15:O:293:GLU:C	2.60	0.56
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.39	0.55
24:Z:478:VAL:HG21	24:Z:502:LEU:HD22	1.87	0.55
1:A:582:PRO:CG	1:A:583:ARG:H	2.12	0.55
14:N:22:DG:H2'	14:N:23:DT:H71	1.87	0.55
1:A:359:VAL:HG23	1:A:362:SER:OG	2.06	0.55
21:V:196:LYS:O	21:V:198:ARG:N	2.38	0.55
2:B:227:ASN:OD1	2:B:405:ARG:NH2	2.36	0.55
10:J:53:VAL:O	10:J:53:VAL:HG13	2.06	0.55
14:N:-2:DG:H2"	14:N:-1:DT:C5	2.41	0.55
22:W:163:LEU:O	22:W:175:PHE:N	2.33	0.55
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.88	0.55
7:G:147:ILE:HD12	7:G:147:ILE:H	1.72	0.55
14:N:81:DG:C2	19:T:-80:DG:N2	2.75	0.55
14:N:38:DG:H2"	14:N:39:DT:C5	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:18:DT:H1'	14:N:19:DC:C6	2.42	0.54
5:E:126:ILE:HG23	5:E:126:ILE:O	2.07	0.54
24:Z:492:ILE:HD12	24:Z:495:VAL:HG13	1.89	0.54
11:K:17:LYS:O	11:K:36:ASN:ND2	2.32	0.54
14:N:10:DT:H2'	14:N:11:DT:H72	1.89	0.54
14:N:15:DC:H2'	14:N:16:DT:H72	1.89	0.54
1:A:1227:THR:N	1:A:1230:GLN:OE1	2.38	0.54
14:N:11:DT:H2'	14:N:12:DT:H72	1.89	0.54
3:C:149:LEU:HG	10:J:2:ILE:HD11	1.90	0.54
13:M:1173:GLY:O	13:M:1229:LYS:N	2.41	0.54
24:Z:588:ASP:OD1	24:Z:592:ASN:N	2.35	0.54
9:I:81:THR:HG23	9:I:96:PHE:HD2	1.73	0.54
19:T:-91:DC:H2'	19:T:-90:DT:H71	1.90	0.54
19:T:-68:DC:H2'	19:T:-67:DC:C5	2.43	0.54
2:B:907:VAL:HG13	2:B:921:ILE:HG12	1.90	0.54
9:I:22:ASN:ND2	9:I:41:ASN:OD1	2.41	0.53
19:T:27:DA:H2"	19:T:28:DC:C6	2.44	0.53
24:Z:638:CYS:SG	24:Z:643:LEU:HD21	2.48	0.53
3:C:77:ASP:OD2	3:C:126:ARG:NH2	2.40	0.53
14:N:-1:DT:H2"	14:N:0:DT:C7	2.39	0.53
2:B:515:PRO:O	2:B:520:VAL:HA	2.09	0.53
2:B:534:VAL:N	2:B:600:GLU:OE1	2.40	0.53
1:A:413:TYR:O	1:A:449:HIS:ND1	2.42	0.53
1:A:200:ALA:HB2	1:A:216:LEU:HD21	1.91	0.53
2:B:343:LEU:O	2:B:361:LYS:NZ	2.30	0.53
14:N:-17:DG:C2	19:T:18:DA:C2	2.97	0.53
19:T:-113:DG:H2'	19:T:-112:DT:H72	1.91	0.53
14:N:32:DT:H2"	14:N:33:DC:C5	2.44	0.52
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.74	0.52
1:A:1322:ILE:HD12	1:A:1322:ILE:H	1.75	0.52
14:N:108:DT:O3'	14:N:109:DA:C8	2.62	0.52
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.91	0.52
9:I:42:CYS:SG	9:I:43:ASP:N	2.83	0.52
1:A:951:GLU:OE1	1:A:954:ARG:NH1	2.41	0.52
12:L:37:ARG:H	12:L:37:ARG:HD3	1.75	0.52
13:M:783:GLY:N	13:M:797:ALA:O	2.42	0.52
14:N:7:DG:C2	19:T:-6:DA:C2	2.98	0.52
1:A:406:VAL:HG21	1:A:440:LEU:HD23	1.92	0.52
1:A:514:GLU:HA	6:F:63:ALA:HB1	1.91	0.52
1:A:853:LYS:O	1:A:857:THR:HG23	2.10	0.52
2:B:848:LEU:HD23	2:B:865:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:2:ASN:OD1	11:K:2:ASN:O	2.26	0.52
1:A:1052:ARG:NE	1:A:1056:GLU:OE2	2.42	0.52
2:B:139:GLN:OE1	2:B:139:GLN:N	2.42	0.52
14:N:29:DG:N2	19:T:-28:DC:O2	2.43	0.52
24:Z:516:ARG:HG2	24:Z:516:ARG:HH11	1.75	0.52
1:A:621:ILE:HG23	1:A:621:ILE:O	2.10	0.52
1:A:1315:ASP:N	15:O:295:GLY:CA	2.72	0.52
2:B:897:ARG:HB2	2:B:900:GLU:HG3	1.92	0.52
14:N:39:DT:C4	14:N:40:DG:C6	2.98	0.52
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.42	0.52
14:N:-1:DT:H2"	14:N:0:DT:C5	2.45	0.51
14:N:78:DT:H1'	14:N:79:DA:C5	2.45	0.51
14:N:105:DG:C2	19:T:-104:DA:C2	2.98	0.51
19:T:-42:DA:H1'	19:T:-41:DA:C8	2.44	0.51
24:Z:424:ASP:HB2	24:Z:440:ILE:HD12	1.92	0.51
14:N:-20:DT:H2"	14:N:-19:DG:C8	2.46	0.51
1:A:989:ASN:O	1:A:993:ILE:HG13	2.11	0.51
14:N:-16:DT:H2"	14:N:-15:DC:C6	2.45	0.51
19:T:30:DA:H4'	19:T:31:DG:OP1	2.10	0.51
7:G:84:VAL:HG23	7:G:84:VAL:O	2.11	0.51
13:M:973:VAL:N	13:M:1036:LYS:O	2.44	0.51
1:A:567:LEU:HD23	1:A:570:TRP:HB2	1.91	0.51
2:B:595:ASP:OD1	2:B:596:ILE:N	2.38	0.51
16:P:48:C:O2	19:T:-47:DG:N2	2.43	0.51
13:M:717:LEU:O	13:M:722:TYR:N	2.36	0.51
1:A:1414:ILE:O	1:A:1414:ILE:HG22	2.10	0.51
19:T:-55:DC:C2'	19:T:-55:DC:O2	2.58	0.51
1:A:1044:HIS:O	1:A:1048:THR:HG23	2.12	0.50
2:B:257:VAL:HB	2:B:266:GLU:OE1	2.11	0.50
2:B:758:LEU:HD11	10:J:47:ARG:HB2	1.93	0.50
14:N:98:DT:H2"	14:N:99:DA:N7	2.26	0.50
19:T:20:DA:H2"	19:T:21:DC:C5	2.46	0.50
1:A:600:ILE:HG23	1:A:655:ILE:HG22	1.93	0.50
1:A:1311:LEU:O	1:A:1313:GLN:NE2	2.45	0.50
2:B:818:GLU:OE1	2:B:828:VAL:HA	2.11	0.50
14:N:84:DC:H2"	14:N:85:DG:C8	2.46	0.50
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.47	0.50
1:A:902:GLU:O	1:A:978:VAL:HA	2.12	0.50
1:A:930:LEU:HB3	1:A:939:VAL:HG12	1.93	0.50
3:C:45:ILE:HG22	3:C:165:ALA:HB1	1.93	0.50
3:C:162:ARG:NH1	3:C:164:TYR:OH	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:728:MET:HA	2:B:731:GLN:OE1	2.12	0.50
7:G:86:ASP:OD1	7:G:86:ASP:N	2.40	0.50
14:N:75:DG:C2	19:T:-74:DG:C2	3.00	0.50
14:N:79:DA:H2"	14:N:80:DC:C6	2.47	0.50
24:Z:629:LEU:HB2	24:Z:634:GLY:HA2	1.94	0.50
13:M:781:VAL:O	13:M:799:VAL:N	2.43	0.50
17:Q:291:LEU:O	17:Q:295:ALA:N	2.42	0.50
19:T:13:DC:H2"	19:T:14:DA:C8	2.47	0.50
1:A:1366:PHE:HA	1:A:1374:VAL:CG2	2.42	0.50
3:C:263:LEU:HD13	11:K:19:ILE:HD13	1.94	0.49
21:V:88:ASN:O	21:V:90:ASP:N	2.45	0.49
14:N:102:DG:N2	19:T:-101:DT:O2	2.45	0.49
19:T:-9:DA:H1'	19:T:-8:DA:C8	2.47	0.49
24:Z:626:CYS:CB	24:Z:629:LEU:HD12	2.41	0.49
2:B:786:THR:O	2:B:786:THR:HG22	2.13	0.49
1:A:401:ARG:O	1:A:405:LEU:HD13	2.12	0.49
5:E:54:ARG:NH1	5:E:56:THR:OG1	2.45	0.49
14:N:35:DT:H1'	14:N:36:DG:N7	2.26	0.49
24:Z:602:VAL:HG22	24:Z:643:LEU:CD2	2.42	0.49
1:A:406:VAL:HG13	1:A:429:LEU:HD11	1.95	0.49
1:A:576:GLN:O	1:A:590:GLN:NE2	2.45	0.49
1:A:1381:GLU:O	1:A:1385:VAL:HG13	2.12	0.49
2:B:854:ILE:HG22	2:B:921:ILE:HD13	1.93	0.49
7:G:52:ASP:N	7:G:71:LYS:O	2.44	0.49
19:T:-94:DC:H1'	19:T:-93:DC:C6	2.48	0.49
19:T:-53:DG:C6	19:T:-52:DC:N4	2.81	0.49
19:T:15:DG:H2"	19:T:16:DA:C8	2.47	0.49
1:A:30:GLU:HA	1:A:33:ARG:HE	1.77	0.49
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.43	0.49
2:B:395:LEU:HD11	2:B:532:ILE:HB	1.93	0.49
2:B:867:ILE:HB	2:B:894:THR:HG22	1.95	0.49
14:N:98:DT:H2"	14:N:99:DA:C8	2.48	0.49
2:B:553:LEU:HA	2:B:556:ILE:HD12	1.94	0.49
1:A:140:ARG:NH2	1:A:234:PHE:O	2.44	0.49
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.36	0.49
3:C:205:LYS:NZ	3:C:212:ASP:O	2.46	0.49
14:N:28:DG:C2	19:T:-27:DA:C2	3.01	0.49
24:Z:603:ILE:HG23	24:Z:604:ASP:N	2.27	0.49
1:A:868:MET:HG2	1:A:1404:THR:HG21	1.94	0.49
2:B:421:LYS:HD3	2:B:425:ARG:HE	1.78	0.49
3:C:150:ILE:O	3:C:151:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:89:DA:H1'	14:N:90:DA:N7	2.27	0.49
7:G:3:TYR:N	7:G:76:VAL:O	2.46	0.48
19:T:-84:DG:H2"	19:T:-83:DC:C6	2.48	0.48
2:B:607:ILE:HG21	9:I:72:VAL:HA	1.95	0.48
14:N:12:DT:C2'	14:N:13:DT:H71	2.42	0.48
19:T:22:DC:H2"	19:T:23:DA:C8	2.49	0.48
1:A:1318:LYS:HD2	15:O:294:CYS:C	2.33	0.48
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.95	0.48
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.53	0.48
14:N:-33:DG:H2'	14:N:-32:DT:H72	1.96	0.48
14:N:21:DC:H1'	14:N:22:DG:C8	2.48	0.48
19:T:-98:DA:H1'	19:T:-97:DG:C8	2.47	0.48
24:Z:479:LYS:NZ	24:Z:521:CYS:O	2.25	0.48
2:B:446:TYR:CE1	2:B:450:THR:HG21	2.48	0.48
1:A:18:ILE:HD11	2:B:1149:VAL:HG21	1.95	0.48
14:N:12:DT:H2"	14:N:13:DT:H71	1.96	0.48
20:U:450:LEU:N	20:U:457:PHE:O	2.47	0.48
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.36	0.48
2:B:565:THR:HG22	2:B:577:HIS:O	2.13	0.48
14:N:4:DG:C2	19:T:-3:DG:C2	3.02	0.48
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.95	0.48
1:A:286:ILE:HD12	1:A:313:HIS:CD2	2.48	0.48
1:A:1314:THR:C	15:O:295:GLY:C	2.72	0.48
1:A:1330:ALA:CB	15:O:294:CYS:CA	2.88	0.48
14:N:-8:DG:H2'	14:N:-7:DT:H71	1.96	0.48
24:Z:504:SER:OG	24:Z:507:THR:O	2.28	0.48
2:B:423:ILE:HD13	2:B:429:PHE:HD1	1.79	0.48
19:T:-68:DC:H2'	19:T:-67:DC:C6	2.49	0.48
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.78	0.47
8:H:128:ASP:N	8:H:128:ASP:OD1	2.44	0.47
19:T:-70:DT:H1'	19:T:-69:DC:C6	2.48	0.47
1:A:421:ARG:HE	1:A:427:ILE:HD11	1.79	0.47
1:A:1314:THR:C	15:O:295:GLY:O	2.53	0.47
2:B:491:ARG:H	2:B:491:ARG:HD2	1.79	0.47
2:B:992:ASN:O	10:J:46:ARG:NH1	2.47	0.47
11:K:80:ASP:OD1	11:K:80:ASP:N	2.47	0.47
14:N:38:DG:H2"	14:N:39:DT:C7	2.44	0.47
1:A:1322:ILE:HD12	1:A:1322:ILE:N	2.28	0.47
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.96	0.47
19:T:-121:DC:H2"	19:T:-120:DT:C6	2.49	0.47
1:A:793:VAL:HG23	1:A:793:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:17:TYR:O	12:L:26:ASN:N	2.40	0.47
13:M:1176:HIS:C	13:M:1226:ILE:N	2.68	0.47
14:N:-30:DT:C2'	14:N:-29:DT:H71	2.44	0.47
14:N:33:DC:H1'	14:N:34:DT:C5	2.49	0.47
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.96	0.47
1:A:364:ARG:NH1	1:A:502:ASN:OD1	2.47	0.47
2:B:818:GLU:HB2	2:B:916:TYR:HB3	1.97	0.47
14:N:-22:DG:O3'	14:N:-21:DG:C8	2.67	0.47
14:N:63:DG:N2	19:T:-62:DG:N2	2.62	0.47
1:A:1130:ILE:O	1:A:1130:ILE:CD1	2.57	0.47
14:N:15:DC:H2'	14:N:16:DT:C7	2.45	0.47
5:E:76:PHE:CE2	5:E:105:VAL:HG11	2.50	0.47
14:N:-26:DG:C5	14:N:-25:DT:C4	3.01	0.47
14:N:29:DG:C2'	14:N:30:DT:H71	2.45	0.47
19:T:-101:DT:H2"	19:T:-100:DC:C6	2.50	0.47
19:T:10:DA:H2"	19:T:11:DC:C5	2.49	0.47
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.97	0.47
3:C:212:ASP:OD1	3:C:212:ASP:N	2.46	0.47
19:T:-62:DG:C2	19:T:-61:DA:C2	3.02	0.47
4:D:114:LEU:HD21	7:G:167:TYR:HB2	1.97	0.47
14:N:72:DA:H1'	14:N:73:DG:C5	2.50	0.47
1:A:222:HIS:ND1	1:A:249:ILE:HD11	2.30	0.47
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.40	0.47
14:N:-4:DC:H2'	14:N:-3:DC:C6	2.49	0.47
1:A:31:LEU:O	1:A:31:LEU:HD23	2.15	0.46
2:B:220:GLU:OE2	2:B:222:ARG:NE	2.36	0.46
9:I:12:VAL:HG22	9:I:50:ASN:HD22	1.80	0.46
14:N:114:DC:H2'	14:N:115:DA:C8	2.49	0.46
1:A:527:THR:HG22	1:A:532:ARG:O	2.15	0.46
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.97	0.46
24:Z:478:VAL:HB	24:Z:518:LEU:HD21	1.97	0.46
24:Z:597:LYS:N	24:Z:614:ILE:O	2.47	0.46
17:Q:663:PHE:O	17:Q:667:ARG:N	2.42	0.46
14:N:-1:DT:H2"	14:N:0:DT:H71	1.96	0.46
14:N:78:DT:O3'	14:N:79:DA:C8	2.69	0.46
14:N:111:DG:C2	19:T:-110:DG:N2	2.84	0.46
24:Z:426:VAL:HG13	24:Z:440:ILE:HD11	1.97	0.46
1:A:540:ASP:C	1:A:540:ASP:OD1	2.54	0.46
1:A:749:ARG:NH1	1:A:750:ASP:OD1	2.48	0.46
1:A:963:ARG:O	1:A:967:ARG:HG3	2.16	0.46
2:B:706:VAL:HG13	2:B:767:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:755:GLN:HB3	10:J:51:ALA:HB1	1.97	0.46
14:N:36:DG:C6	14:N:37:DG:C6	3.03	0.46
19:T:-63:DC:H2"	19:T:-62:DG:N7	2.31	0.46
1:A:218:PRO:O	1:A:221:VAL:HG22	2.15	0.46
1:A:464:LEU:HD22	1:A:1100:THR:HG21	1.97	0.46
5:E:105:VAL:HG13	5:E:135:LEU:HD12	1.97	0.46
14:N:33:DC:H2"	14:N:34:DT:C7	2.46	0.46
14:N:65:DA:H2'	14:N:66:DG:C8	2.50	0.46
1:A:191:ILE:HA	1:A:199:TYR:O	2.15	0.46
1:A:471:GLY:O	1:A:521:VAL:HG23	2.16	0.46
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.51	0.46
2:B:606:ASP:O	2:B:609:GLU:O	2.34	0.46
4:D:80:ILE:HD12	4:D:80:ILE:N	2.31	0.46
14:N:-6:DG:C2	19:T:7:DA:C2	3.04	0.46
7:G:109:SER:HB3	24:Z:493:VAL:HG21	1.97	0.46
10:J:41:LYS:HA	10:J:41:LYS:HE2	1.97	0.46
14:N:-12:DG:H1'	14:N:-11:DG:N7	2.31	0.46
14:N:41:DT:C6	14:N:41:DT:C3'	2.99	0.46
1:A:1321:ILE:O	1:A:1321:ILE:HG23	2.15	0.46
14:N:77:DG:N2	19:T:-76:DG:C2	2.84	0.46
14:N:114:DC:C2	19:T:-113:DG:N2	2.84	0.46
1:A:687:ILE:HD11	1:A:766:PHE:CE1	2.51	0.45
2:B:61:ASP:OD1	2:B:61:ASP:C	2.54	0.45
5:E:149:VAL:O	5:E:192:LYS:N	2.47	0.45
7:G:93:ASN:O	7:G:128:TYR:OH	2.26	0.45
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.97	0.45
14:N:-28:DG:H2"	14:N:-27:DT:C7	2.43	0.45
14:N:104:DT:H2"	14:N:105:DG:H8	1.81	0.45
19:T:-58:DA:H1'	19:T:-57:DA:C8	2.51	0.45
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.51	0.45
1:A:793:VAL:CG2	1:A:799:PRO:HD3	2.46	0.45
1:A:854:THR:OG1	1:A:855:ALA:N	2.49	0.45
2:B:853:LEU:HD23	2:B:867:ILE:HG23	1.98	0.45
19:T:-79:DT:H2"	19:T:-78:DA:N7	2.31	0.45
19:T:-62:DG:H1'	19:T:-61:DA:C8	2.52	0.45
19:T:-53:DG:O6	19:T:-52:DC:N4	2.49	0.45
7:G:160:ILE:HB	24:Z:491:LEU:HD13	1.98	0.45
14:N:61:DT:O3'	14:N:62:DC:C6	2.69	0.45
19:T:-101:DT:H2"	19:T:-100:DC:C5	2.51	0.45
24:Z:478:VAL:HG23	24:Z:478:VAL:O	2.16	0.45
1:A:222:HIS:HB2	1:A:249:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:THR:O	2:B:142:THR:HG23	2.17	0.45
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.49	0.45
5:E:52:ARG:N	5:E:53:PRO:HD3	2.32	0.45
5:E:185:ILE:HD12	5:E:209:VAL:CG2	2.46	0.45
14:N:-30:DT:H2'	14:N:-29:DT:H71	1.99	0.45
14:N:1:DT:H2"	14:N:2:DT:C6	2.51	0.45
14:N:20:DT:H2"	14:N:21:DC:C5	2.50	0.45
14:N:26:DC:H2'	14:N:27:DT:H71	1.96	0.45
1:A:566:PHE:HB3	1:A:674:THR:HG22	1.99	0.45
1:A:1087:VAL:HG23	1:A:1400:LEU:CD2	2.47	0.45
14:N:-9:DG:H1'	14:N:-8:DG:C8	2.52	0.45
19:T:-96:DC:H2'	19:T:-95:DA:C8	2.51	0.45
19:T:-10:DA:H2"	19:T:-9:DA:C8	2.52	0.45
24:Z:536:TRP:NE1	24:Z:551:VAL:O	2.48	0.45
1:A:404:GLU:O	1:A:408:ARG:HG3	2.16	0.45
1:A:467:MET:HG2	1:A:534:VAL:HG21	1.99	0.45
19:T:18:DA:H2'	19:T:19:DC:C5	2.51	0.45
1:A:987:ILE:O	1:A:991:GLN:HG3	2.17	0.45
2:B:666:ASP:O	2:B:669:GLU:N	2.50	0.45
2:B:873:LEU:HD12	2:B:888:THR:N	2.32	0.45
14:N:72:DA:C2	19:T:-71:DG:C2	3.05	0.45
1:A:515:ILE:HD11	2:B:1102:PHE:CD1	2.52	0.45
2:B:1105:GLU:HG3	2:B:1106:ARG:N	2.32	0.45
14:N:100:DG:H1'	14:N:101:DA:N7	2.32	0.45
14:N:109:DA:H1'	14:N:110:DC:O4'	2.17	0.45
2:B:743:ARG:NH1	2:B:745:ASP:OD1	2.50	0.45
14:N:33:DC:C2'	14:N:34:DT:H71	2.46	0.45
14:N:93:DG:N1	19:T:-92:DG:N1	2.64	0.45
14:N:119:DG:O3'	14:N:120:DA:C8	2.70	0.45
1:A:293:ASN:O	1:A:298:ALA:N	2.44	0.44
1:A:419:ILE:CD1	1:A:440:LEU:HB3	2.47	0.44
5:E:93:ARG:HA	5:E:96:GLU:OE1	2.17	0.44
14:N:13:DT:H5'	14:N:13:DT:C6	2.52	0.44
14:N:83:DG:C2	19:T:-82:DA:C2	3.06	0.44
2:B:84:TYR:HA	2:B:132:VAL:HA	1.98	0.44
2:B:669:GLU:O	2:B:672:THR:HG22	2.18	0.44
2:B:905:ASP:OD2	2:B:922:ARG:NH2	2.47	0.44
2:B:928:ILE:HD12	2:B:928:ILE:H	1.83	0.44
19:T:23:DA:C2'	19:T:24:DA:C8	3.01	0.44
1:A:832:THR:HG22	1:A:833:PRO:CD	2.45	0.44
1:A:1052:ARG:HE	1:A:1056:GLU:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ASN:N	2:B:222:ARG:O	2.35	0.44
2:B:553:LEU:HD12	2:B:556:ILE:HD12	1.98	0.44
19:T:-112:DT:H2"	19:T:-111:DC:C6	2.53	0.44
14:N:105:DG:C8	14:N:106:DT:H72	2.52	0.44
1:A:64:VAL:HG11	1:A:78:MET:HA	1.99	0.44
1:A:583:ARG:HG3	1:A:584:PRO:HD2	1.99	0.44
1:A:921:ARG:HD2	1:A:956:PHE:CG	2.53	0.44
5:E:83:GLY:HA2	5:E:114:ALA:HB2	1.99	0.44
14:N:-33:DG:H2'	14:N:-32:DT:C7	2.48	0.44
14:N:29:DG:N2	19:T:-28:DC:C2	2.86	0.44
14:N:90:DA:C6	14:N:91:DG:C6	3.05	0.44
19:T:-100:DC:H1'	19:T:-99:DT:C4	2.53	0.44
1:A:203:LYS:NZ	19:T:-67:DC:OP2	2.32	0.44
5:E:11:TRP:HA	5:E:40:PHE:CE2	2.53	0.44
5:E:26:TYR:HA	5:E:64:HIS:HA	2.00	0.44
14:N:-32:DT:O2	19:T:32:DA:C2	2.71	0.44
19:T:-5:DA:H2"	19:T:-4:DC:C6	2.53	0.44
1:A:289:GLN:O	1:A:292:ARG:HG2	2.18	0.44
2:B:166:LEU:HG	2:B:170:ASP:HB2	2.00	0.44
2:B:818:GLU:OE2	2:B:829:PHE:CE1	2.70	0.44
6:F:120:VAL:O	6:F:120:VAL:CG1	2.64	0.44
14:N:-18:DT:H2"	14:N:-17:DG:H8	1.82	0.44
19:T:-80:DG:H2"	19:T:-79:DT:C6	2.53	0.44
19:T:-32:DA:H2"	19:T:-31:DC:C6	2.52	0.44
19:T:21:DC:H2"	19:T:22:DC:C6	2.53	0.44
1:A:385:ALA:HB2	1:A:476:ILE:HD12	2.00	0.44
14:N:35:DT:C2	14:N:36:DG:O6	2.70	0.44
1:A:1413:ALA:O	1:A:1418:GLY:HA3	2.18	0.44
9:I:69:ILE:HD13	9:I:71:ASP:HB2	1.99	0.44
14:N:-26:DG:C2	19:T:27:DA:C2	3.05	0.44
14:N:29:DG:H2"	14:N:30:DT:H71	2.00	0.44
19:T:-25:DG:H1'	19:T:-24:DC:C6	2.53	0.44
1:A:862:ARG:HG3	1:A:863:ARG:N	2.33	0.43
24:Z:476:ASP:O	24:Z:478:VAL:HG13	2.18	0.43
1:A:1474:LEU:HD12	6:F:105:ILE:HD11	2.00	0.43
5:E:173:ILE:O	5:E:209:VAL:HA	2.18	0.43
14:N:-13:DG:H2"	14:N:-12:DG:N7	2.33	0.43
1:A:927:GLU:HG2	1:A:931:ARG:NE	2.33	0.43
2:B:193:VAL:HG11	2:B:470:LEU:HD13	2.01	0.43
2:B:499:ARG:NH1	2:B:518:HIS:O	2.46	0.43
2:B:711:ILE:HG12	2:B:725:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:94:LYS:NZ	7:G:3:TYR:OH	2.47	0.43
14:N:10:DT:H2'	14:N:11:DT:C7	2.48	0.43
14:N:57:DT:C6	14:N:57:DT:P	3.12	0.43
19:T:1:DA:H2"	19:T:2:DC:C6	2.53	0.43
2:B:331:THR:HG23	2:B:334:LYS:H	1.84	0.43
17:Q:723:LEU:O	17:Q:725:ARG:N	2.51	0.43
19:T:25:DA:H2"	19:T:26:DC:C6	2.53	0.43
1:A:88:ILE:HD12	1:A:88:ILE:N	2.34	0.43
1:A:991:GLN:HA	1:A:996:ILE:CG1	2.49	0.43
1:A:1085:GLU:O	1:A:1087:VAL:HG13	2.17	0.43
2:B:741:HIS:CE1	2:B:742:VAL:HG23	2.53	0.43
2:B:854:ILE:O	2:B:907:VAL:HG21	2.19	0.43
14:N:-15:DC:H2'	14:N:-14:DT:C7	2.44	0.43
14:N:8:DT:H2"	14:N:9:DT:C5	2.53	0.43
19:T:-113:DG:H2'	19:T:-112:DT:C7	2.48	0.43
1:A:855:ALA:HA	19:T:-54:DC:O4'	2.19	0.43
1:A:1182:GLN:C	1:A:1182:GLN:OE1	2.57	0.43
2:B:423:ILE:CG2	2:B:424:ASP:N	2.81	0.43
2:B:698:ILE:HG23	2:B:699:HIS:H	1.84	0.43
2:B:859:ARG:NH1	2:B:901:THR:HG23	2.33	0.43
5:E:66:ASP:C	5:E:66:ASP:OD1	2.56	0.43
14:N:7:DG:H8	14:N:7:DG:OP2	2.01	0.43
14:N:34:DT:C5	14:N:35:DT:C4	3.06	0.43
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.99	0.43
2:B:652:SER:N	2:B:655:ASP:OD2	2.50	0.43
14:N:26:DC:H2'	14:N:27:DT:C7	2.49	0.43
14:N:40:DG:N2	19:T:-39:DA:C4	2.86	0.43
19:T:-81:DC:H2"	19:T:-80:DG:C8	2.53	0.43
24:Z:550:ILE:HD12	24:Z:559:GLN:O	2.19	0.43
1:A:260:VAL:HG12	1:A:260:VAL:O	2.18	0.43
1:A:849:ASP:OD1	1:A:849:ASP:N	2.52	0.43
1:A:1374:VAL:CG1	1:A:1411:LEU:HD21	2.49	0.43
2:B:497:LYS:HG2	2:B:498:PRO:HD3	2.01	0.43
14:N:22:DG:H2'	14:N:23:DT:C7	2.47	0.43
14:N:111:DG:H1'	14:N:112:DA:C8	2.54	0.43
19:T:-80:DG:OP2	19:T:-80:DG:H2'	2.18	0.43
19:T:6:DC:H2'	19:T:7:DA:C8	2.54	0.43
24:Z:529:ASP:HB3	24:Z:553:LEU:HD23	1.99	0.43
1:A:991:GLN:HA	1:A:996:ILE:HG12	2.01	0.43
2:B:520:VAL:HG13	2:B:520:VAL:O	2.18	0.43
9:I:39:CYS:SG	9:I:40:ARG:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:-66:DC:H2'	19:T:-65:DT:C6	2.54	0.43
1:A:1301:ILE:HG13	1:A:1304:ILE:HG12	2.01	0.43
2:B:491:ARG:H	2:B:491:ARG:CD	2.32	0.43
3:C:263:LEU:HD22	11:K:87:PHE:CD1	2.54	0.43
5:E:89:VAL:O	5:E:93:ARG:HD2	2.19	0.43
7:G:148:VAL:HG22	7:G:160:ILE:HG23	2.01	0.43
8:H:20:LYS:HE2	8:H:23:ASP:HA	1.99	0.43
11:K:57:LEU:N	11:K:76:GLN:O	2.52	0.43
14:N:85:DG:C8	14:N:86:DT:H72	2.54	0.43
19:T:-75:DC:H2'	19:T:-74:DG:C8	2.53	0.43
19:T:14:DA:H8	19:T:14:DA:OP2	2.01	0.43
1:A:427:ILE:N	1:A:427:ILE:HD12	2.34	0.42
1:A:580:LEU:O	1:A:582:PRO:HD2	2.19	0.42
2:B:545:LEU:O	2:B:550:MET:CB	2.67	0.42
3:C:26:THR:HG22	3:C:27:ASP:N	2.26	0.42
14:N:11:DT:H2"	14:N:12:DT:C6	2.54	0.42
14:N:91:DG:H2"	14:N:92:DC:C6	2.54	0.42
1:A:413:TYR:CD1	1:A:413:TYR:C	2.91	0.42
2:B:786:THR:HG21	2:B:949:TYR:OH	2.19	0.42
3:C:40:ALA:O	3:C:171:LYS:N	2.52	0.42
11:K:93:ASP:OD1	11:K:93:ASP:C	2.56	0.42
14:N:1:DT:H2'	14:N:2:DT:H71	2.00	0.42
14:N:99:DA:H2"	14:N:100:DG:N7	2.34	0.42
19:T:-73:DC:H2"	19:T:-72:DT:C6	2.55	0.42
19:T:-8:DA:C5	19:T:-7:DC:C4	3.08	0.42
24:Z:775:TPO:O2P	24:Z:775:TPO:N	2.52	0.42
1:A:1171:ALA:O	9:I:58:ILE:N	2.53	0.42
2:B:284:ILE:HG22	2:B:285:LEU:H	1.84	0.42
2:B:291:ASP:OD1	2:B:291:ASP:N	2.52	0.42
19:T:-108:DA:C5	19:T:-107:DG:C6	3.07	0.42
19:T:-28:DC:H2'	19:T:-27:DA:C8	2.53	0.42
19:T:4:DG:C4	19:T:5:DC:C5	3.08	0.42
2:B:622:CYS:HB3	2:B:666:ASP:HB3	2.02	0.42
3:C:152:LYS:HB2	10:J:60:LEU:HD11	2.02	0.42
19:T:9:DC:OP2	19:T:9:DC:H6	2.02	0.42
2:B:545:LEU:O	2:B:550:MET:HB3	2.20	0.42
14:N:91:DG:N2	19:T:-90:DT:O2	2.52	0.42
19:T:14:DA:C6	19:T:15:DG:C6	3.07	0.42
1:A:996:ILE:HD13	1:A:996:ILE:HA	1.94	0.42
11:K:53:ASP:HB3	11:K:56:VAL:HG23	2.00	0.42
19:T:-53:DG:C6	19:T:-52:DC:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:-48:DG:H4'	19:T:-48:DG:OP1	2.19	0.42
24:Z:538:GLU:OE2	24:Z:577:ARG:NE	2.48	0.42
1:A:420:ILE:HD11	1:A:447:GLU:OE2	2.20	0.42
1:A:1073:GLU:HG3	1:A:1074:SER:N	2.35	0.42
1:A:1442:ALA:HA	1:A:1447:GLU:HG3	2.01	0.42
3:C:89:THR:HG23	3:C:89:THR:O	2.19	0.42
5:E:93:ARG:HD2	5:E:93:ARG:N	2.34	0.42
14:N:-31:DC:H1'	14:N:-30:DT:C5	2.54	0.42
14:N:9:DT:H1'	14:N:10:DT:C6	2.55	0.42
19:T:-43:DA:H3'	19:T:-42:DA:O4'	2.20	0.42
19:T:23:DA:H2'	19:T:24:DA:C8	2.53	0.42
1:A:413:TYR:HB3	1:A:414:PRO:HD3	2.02	0.42
1:A:1286:ARG:O	1:A:1289:GLU:HG3	2.19	0.42
1:A:1322:ILE:H	1:A:1322:ILE:CD1	2.32	0.42
16:P:44:U:H2'	16:P:45:C:C6	2.54	0.42
1:A:1184:THR:O	1:A:1187:ALA:N	2.48	0.42
7:G:83:GLU:O	7:G:147:ILE:HD12	2.19	0.42
14:N:105:DG:H2'	14:N:106:DT:H72	2.00	0.42
19:T:8:DC:H2"	19:T:9:DC:C5	2.54	0.42
24:Z:603:ILE:HG23	24:Z:604:ASP:H	1.85	0.42
1:A:29:ASP:O	1:A:33:ARG:HG2	2.19	0.41
1:A:589:LYS:HZ3	1:A:625:ASP:CG	2.22	0.41
3:C:64:ILE:CD1	3:C:151:VAL:HG11	2.50	0.41
8:H:27:ARG:HD3	8:H:42:ASP:OD1	2.20	0.41
14:N:-11:DG:H2'	14:N:-10:DT:H71	2.02	0.41
14:N:57:DT:H2'	14:N:58:DT:H71	2.01	0.41
19:T:-73:DC:H2"	19:T:-72:DT:C2	2.54	0.41
24:Z:470:LYS:HB3	24:Z:472:PHE:CE2	2.54	0.41
1:A:120:ASP:OD2	1:A:122:ASN:ND2	2.50	0.41
1:A:379:GLY:HA2	1:A:475:ARG:O	2.20	0.41
1:A:513:ALA:O	1:A:517:GLU:HG2	2.20	0.41
1:A:873:VAL:O	1:A:1084:GLY:N	2.50	0.41
2:B:528:LEU:HD21	2:B:767:LEU:HD21	2.02	0.41
2:B:956:PHE:CZ	2:B:1029:TYR:HB2	2.56	0.41
6:F:57:MET:HB2	6:F:123:LEU:HD13	2.01	0.41
11:K:21:ILE:HD12	11:K:21:ILE:H	1.85	0.41
14:N:-3:DC:H2"	14:N:-2:DG:C8	2.55	0.41
19:T:25:DA:H1'	19:T:26:DC:C6	2.55	0.41
1:A:299:ALA:HB3	1:A:302:VAL:HG12	2.03	0.41
1:A:1262:MET:SD	1:A:1262:MET:N	2.93	0.41
1:A:1484:MET:SD	1:A:1484:MET:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:ALA:HB1	5:E:68:PRO:HA	2.02	0.41
5:E:83:GLY:O	5:E:87:ILE:HG23	2.19	0.41
16:P:43:U:O2'	16:P:44:U:OP2	2.23	0.41
24:Z:489:THR:HG22	24:Z:490:GLY:N	2.34	0.41
24:Z:727:ALA:HA	24:Z:732:ALA:HA	2.02	0.41
1:A:109:CYS:HA	1:A:148:CYS:SG	2.61	0.41
1:A:1030:SER:HB2	5:E:162:ARG:HE	1.86	0.41
1:A:1036:ASN:OD1	5:E:202:ARG:NH1	2.41	0.41
2:B:193:VAL:CG1	2:B:470:LEU:HD13	2.51	0.41
2:B:813:SER:HA	2:B:922:ARG:HA	2.02	0.41
5:E:100:THR:HB	5:E:125:TYR:HA	2.02	0.41
14:N:-19:DG:C2'	14:N:-18:DT:C6	3.03	0.41
14:N:17:DG:C2	19:T:-16:DA:C2	3.08	0.41
19:T:-97:DG:C4	19:T:-96:DC:C5	3.08	0.41
1:A:286:ILE:CD1	1:A:313:HIS:CD2	3.04	0.41
1:A:1321:ILE:O	1:A:1328:PHE:O	2.38	0.41
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.50	0.41
5:E:7:THR:OG1	5:E:46:ASP:OD1	2.39	0.41
5:E:47:LYS:HB3	5:E:51:GLY:HA3	2.02	0.41
9:I:69:ILE:HD12	9:I:69:ILE:O	2.20	0.41
10:J:44:CYS:O	10:J:47:ARG:CD	2.68	0.41
11:K:42:LEU:O	11:K:46:ILE:HG13	2.20	0.41
19:T:-25:DG:H2"	19:T:-24:DC:C5	2.54	0.41
24:Z:603:ILE:CG2	24:Z:604:ASP:H	2.33	0.41
1:A:110:VAL:HG11	1:A:228:ILE:HD11	2.01	0.41
2:B:357:CYS:SG	2:B:361:LYS:HE2	2.60	0.41
2:B:581:GLU:O	2:B:585:ASN:OD1	2.38	0.41
14:N:36:DG:C5	14:N:37:DG:C5	3.08	0.41
14:N:71:DC:H4'	14:N:72:DA:OP1	2.21	0.41
19:T:24:DA:H2"	19:T:25:DA:H5'	2.02	0.41
1:A:832:THR:CG2	1:A:833:PRO:HD2	2.48	0.41
1:A:1457:ASN:O	1:A:1462:GLN:N	2.53	0.41
2:B:756:LYS:HD2	2:B:996:ILE:HD11	2.03	0.41
2:B:818:GLU:OE2	2:B:829:PHE:CD1	2.74	0.41
5:E:124:LYS:HD3	5:E:125:TYR:CE2	2.56	0.41
14:N:31:DG:C2	14:N:32:DT:C2	3.08	0.41
2:B:407:MET:O	2:B:410:ASN:HB2	2.21	0.41
8:H:40:ILE:O	8:H:123:MET:HA	2.21	0.41
9:I:91:HIS:CD2	9:I:116:ALA:HB2	2.55	0.41
14:N:11:DT:H2'	14:N:12:DT:C7	2.49	0.41
24:Z:603:ILE:CG2	24:Z:604:ASP:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PRO:HB2	1:A:200:ALA:HB1	2.03	0.41
1:A:350:VAL:HG23	1:A:351:ARG:N	2.36	0.41
1:A:527:THR:HB	1:A:534:VAL:HG13	2.03	0.41
1:A:600:ILE:HG12	1:A:660:MET:HE1	2.02	0.41
1:A:604:ARG:NH2	1:A:643:LYS:O	2.52	0.41
1:A:927:GLU:HG3	1:A:943:LEU:HD11	2.03	0.41
1:A:1175:ILE:HD13	9:I:54:TYR:HB3	2.03	0.41
1:A:1180:ASN:OD1	1:A:1182:GLN:HG3	2.21	0.41
1:A:1460:LEU:HD22	1:A:1460:LEU:N	2.35	0.41
2:B:185:PHE:O	2:B:191:GLU:HA	2.21	0.41
2:B:190:SER:HB3	2:B:192:LYS:HE2	2.03	0.41
2:B:190:SER:CB	2:B:192:LYS:HE2	2.51	0.41
2:B:425:ARG:CB	2:B:427:LYS:HG3	2.50	0.41
2:B:597:ILE:CG2	2:B:601:VAL:HB	2.51	0.41
2:B:749:HIS:CE1	2:B:810:PHE:CD1	3.09	0.41
2:B:781:ALA:O	2:B:966:ILE:HA	2.21	0.41
2:B:833:THR:HG22	2:B:835:GLU:OE1	2.21	0.41
2:B:1102:PHE:HA	2:B:1105:GLU:HG2	2.02	0.41
3:C:2:PRO:HB3	11:K:54:PRO:HD2	2.02	0.41
4:D:131:LEU:O	4:D:135:GLN:HG2	2.21	0.41
9:I:42:CYS:SG	9:I:44:TYR:HB2	2.61	0.41
9:I:64:GLU:HB2	9:I:111:TYR:CE2	2.55	0.41
9:I:86:CYS:SG	9:I:121:HIS:HB3	2.60	0.41
14:N:-21:DG:H2"	14:N:-20:DT:C6	2.55	0.41
14:N:-11:DG:H2"	14:N:-10:DT:C6	2.56	0.41
14:N:0:DT:H2'	14:N:1:DT:C6	2.56	0.41
14:N:13:DT:H2"	14:N:14:DT:C6	2.56	0.41
14:N:93:DG:C4	14:N:94:DG:C5	3.08	0.41
14:N:96:DG:N1	19:T:-95:DA:C6	2.89	0.41
14:N:105:DG:H8	14:N:105:DG:OP2	2.03	0.41
14:N:119:DG:N2	19:T:-118:DA:C2	2.89	0.41
19:T:-110:DG:H2"	19:T:-109:DT:C5	2.56	0.41
19:T:-78:DA:H2"	19:T:-77:DC:C6	2.56	0.41
19:T:-70:DT:H2"	19:T:-69:DC:C5	2.56	0.41
19:T:10:DA:H2"	19:T:11:DC:C6	2.55	0.41
24:Z:497:GLU:OE1	24:Z:497:GLU:N	2.49	0.41
1:A:419:ILE:HD11	1:A:440:LEU:HB3	2.01	0.41
1:A:467:MET:HG3	1:A:524:MET:HB3	2.03	0.41
1:A:1219:LYS:O	1:A:1223:ASP:OD2	2.39	0.41
2:B:237:VAL:O	2:B:372:LEU:HD22	2.20	0.41
2:B:266:GLU:O	2:B:266:GLU:CD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:848:VAL:O	13:M:883:GLU:N	2.54	0.41
14:N:22:DG:N2	19:T:-21:DG:C2	2.89	0.41
14:N:33:DC:H1'	14:N:34:DT:C7	2.51	0.41
14:N:40:DG:N2	19:T:-39:DA:C5	2.89	0.41
19:T:-76:DG:C4	19:T:-75:DC:C5	3.09	0.41
24:Z:705:LEU:O	24:Z:705:LEU:HG	2.20	0.41
1:A:854:THR:HB	19:T:-54:DC:C4	2.56	0.40
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.22	0.40
14:N:-29:DT:C4	14:N:-28:DG:O6	2.74	0.40
14:N:-26:DG:N1	19:T:27:DA:N1	2.68	0.40
14:N:-20:DT:H2"	14:N:-19:DG:N7	2.36	0.40
14:N:57:DT:P	14:N:57:DT:H72	2.61	0.40
19:T:-59:DA:C6	19:T:-58:DA:C6	3.08	0.40
19:T:-16:DA:C6	19:T:-15:DG:C6	3.09	0.40
1:A:609:HIS:HA	1:A:626:THR:HG21	2.02	0.40
1:A:777:SER:OG	1:A:779:ILE:HG22	2.21	0.40
5:E:92:GLN:O	5:E:96:GLU:OE1	2.40	0.40
19:T:-69:DC:H2'	19:T:-68:DC:C6	2.56	0.40
19:T:-7:DC:H1'	19:T:-6:DA:C8	2.57	0.40
19:T:24:DA:C6	19:T:25:DA:C6	3.09	0.40
20:U:469:ASN:O	20:U:489:LEU:N	2.53	0.40
24:Z:444:ASP:HB3	24:Z:448:ILE:HA	2.02	0.40
7:G:18:PHE:CD1	7:G:18:PHE:N	2.88	0.40
14:N:-18:DT:C2	14:N:-17:DG:N7	2.89	0.40
1:A:496:PHE:CD2	2:B:791:GLU:HB2	2.57	0.40
1:A:527:THR:HB	1:A:534:VAL:CG1	2.52	0.40
2:B:29:VAL:HG12	2:B:30:ILE:H	1.87	0.40
2:B:225:LEU:HA	2:B:350:HIS:HA	2.03	0.40
2:B:403:LEU:HD13	2:B:447:SER:OG	2.22	0.40
2:B:565:THR:HA	2:B:610:ARG:HB3	2.03	0.40
2:B:847:LYS:HG2	2:B:858:VAL:HG11	2.03	0.40
2:B:1038:THR:HA	3:C:195:THR:HA	2.04	0.40
10:J:53:VAL:O	10:J:53:VAL:CG1	2.69	0.40
14:N:-33:DG:H2'	14:N:-32:DT:C5	2.57	0.40
14:N:114:DC:H2'	14:N:115:DA:N7	2.36	0.40
1:A:953:GLU:O	1:A:957:GLU:HG3	2.21	0.40
7:G:109:SER:O	7:G:112:SER:OG	2.34	0.40
14:N:-17:DG:H2'	14:N:-16:DT:H72	2.03	0.40
14:N:85:DG:C2	19:T:-84:DG:C2	3.10	0.40
19:T:13:DC:H1'	19:T:14:DA:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1984 (71%)	1297 (92%)	109 (8%)	2 (0%)	51	85
2	B	1107/1251 (88%)	1022 (92%)	85 (8%)	0	100	100
3	C	254/275 (92%)	241 (95%)	13 (5%)	0	100	100
4	D	124/184 (67%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
6	F	76/127 (60%)	71 (93%)	5 (7%)	0	100	100
7	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
8	H	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	22	60
9	I	114/125 (91%)	100 (88%)	14 (12%)	0	100	100
10	J	64/67 (96%)	60 (94%)	3 (5%)	1 (2%)	9	40
11	K	113/117 (97%)	106 (94%)	7 (6%)	0	100	100
12	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100
13	M	976/1729 (56%)	903 (92%)	72 (7%)	1 (0%)	51	85
15	O	157/304 (52%)	154 (98%)	3 (2%)	0	100	100
17	Q	888/1179 (75%)	832 (94%)	56 (6%)	0	100	100
18	R	240/713 (34%)	227 (95%)	13 (5%)	0	100	100
20	U	98/666 (15%)	87 (89%)	11 (11%)	0	100	100
21	V	236/531 (44%)	200 (85%)	34 (14%)	2 (1%)	19	57
22	W	298/305 (98%)	271 (91%)	27 (9%)	0	100	100
23	X	41/531 (8%)	38 (93%)	3 (7%)	0	100	100
24	Z	300/1087 (28%)	274 (91%)	25 (8%)	1 (0%)	41	76
25	a	95/136 (70%)	90 (95%)	5 (5%)	0	100	100
25	e	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
26	b	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
26	f	76/103 (74%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	c	101/130 (78%)	97 (96%)	4 (4%)	0	100	100
27	g	103/130 (79%)	99 (96%)	4 (4%)	0	100	100
28	d	93/123 (76%)	88 (95%)	5 (5%)	0	100	100
28	h	91/123 (74%)	87 (96%)	4 (4%)	0	100	100
All	All	7797/12749 (61%)	7242 (93%)	547 (7%)	8 (0%)	54	85

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	582	PRO
13	M	1334	ASN
21	V	300	ASN
8	H	77	PRO
1	A	478	PRO
10	J	64	PRO
21	V	301	TYR
24	Z	452	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	1245/1761 (71%)	1226 (98%)	19 (2%)	65	87
2	B	983/1084 (91%)	968 (98%)	15 (2%)	65	87
3	C	235/252 (93%)	231 (98%)	4 (2%)	60	85
4	D	109/160 (68%)	108 (99%)	1 (1%)	78	92
5	E	191/192 (100%)	188 (98%)	3 (2%)	62	86
6	F	68/111 (61%)	66 (97%)	2 (3%)	42	76
7	G	146/153 (95%)	143 (98%)	3 (2%)	53	82
8	H	130/131 (99%)	128 (98%)	2 (2%)	65	87
9	I	104/112 (93%)	102 (98%)	2 (2%)	57	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	55/56 (98%)	54 (98%)	1 (2%)	59	85
11	K	104/106 (98%)	103 (99%)	1 (1%)	76	91
12	L	44/55 (80%)	42 (96%)	2 (4%)	27	64
24	Z	257/939 (27%)	256 (100%)	1 (0%)	91	97
25	a	85/111 (77%)	85 (100%)	0	100	100
25	e	84/111 (76%)	83 (99%)	1 (1%)	71	90
26	b	68/79 (86%)	67 (98%)	1 (2%)	65	87
26	f	63/79 (80%)	63 (100%)	0	100	100
27	c	82/102 (80%)	82 (100%)	0	100	100
27	g	83/102 (81%)	83 (100%)	0	100	100
28	d	81/103 (79%)	79 (98%)	2 (2%)	47	79
28	h	79/103 (77%)	78 (99%)	1 (1%)	69	89
All	All	4296/5902 (73%)	4235 (99%)	61 (1%)	68	88

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	203	LYS
1	A	234	PHE
1	A	294	GLU
1	A	336	LEU
1	A	365	THR
1	A	380	VAL
1	A	483	ARG
1	A	582	PRO
1	A	723	ASN
1	A	931	ARG
1	A	952	LEU
1	A	1030	SER
1	A	1048	THR
1	A	1139	LEU
1	A	1182	GLN
1	A	1212	LEU
1	A	1375	ARG
1	A	1385	VAL
2	B	83	ARG
2	B	332	LYS

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Mol	Chain	Res	Type
2	B	388	TYR
2	B	424	ASP
2	B	453	TRP
2	B	491	ARG
2	B	550	MET
2	B	610	ARG
2	B	650	ASN
2	B	808	SER
2	B	841	ARG
2	B	995	GLU
2	B	1006	VAL
2	B	1150	ARG
2	B	1156	LYS
3	C	13	GLU
3	C	63	PHE
3	C	118	ARG
3	C	228	ARG
4	D	94	LYS
5	E	36	THR
5	E	73	PHE
5	E	141	GLU
6	F	90	LEU
6	F	123	LEU
7	G	44	PHE
7	G	86	ASP
7	G	132	ASP
8	H	38	ASP
8	H	95	LYS
9	I	67	GLN
9	I	100	HIS
10	J	47	ARG
11	K	1	MET
12	L	37	ARG
12	L	58	ARG
24	Z	624	LEU
26	b	92	ARG
28	d	31	LYS
28	d	39	TYR
25	e	39	HIS
28	h	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	562	ASN
1	A	673	GLN
2	B	111	ASN
2	B	452	ASN
2	B	585	ASN
2	B	749	HIS
2	B	1040	GLN
3	C	260	GLN
7	G	4	HIS
9	I	32	ASN
11	K	2	ASN
24	Z	519	GLN
24	Z	642	HIS
26	f	64	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	15/16 (93%)	4 (26%)	2 (13%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	41	U
16	P	42	U
16	P	44	U
16	P	46	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	43	U
16	P	45	C

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	A	1525	1	8,10,11	1.58	1 (12%)	10,14,16	1.89	1 (10%)
24	TPO	Z	775	24	8,10,11	1.60	1 (12%)	10,14,16	1.54	1 (10%)
1	SEP	A	1547	1	8,9,10	1.55	1 (12%)	8,12,14	1.61	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	1525	1	-	2/9/11/13	-
24	TPO	Z	775	24	-	2/9/11/13	-
1	SEP	A	1547	1	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.39	1.61	1.50
24	Z	775	TPO	P-O1P	3.38	1.61	1.50
1	A	1525	TPO	P-O1P	3.36	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1525	TPO	P-OG1-CB	-5.18	107.56	123.21
24	Z	775	TPO	P-OG1-CB	-3.95	111.27	123.21
1	A	1547	SEP	OG-CB-CA	2.94	111.00	108.14
1	A	1547	SEP	P-OG-CB	-2.88	110.36	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	C-CA-CB-CG2
24	Z	775	TPO	CB-OG1-P-O1P

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Mol	Chain	Res	Type	Atoms
24	Z	775	TPO	CB-OG1-P-O2P
1	A	1525	TPO	N-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	775	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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.

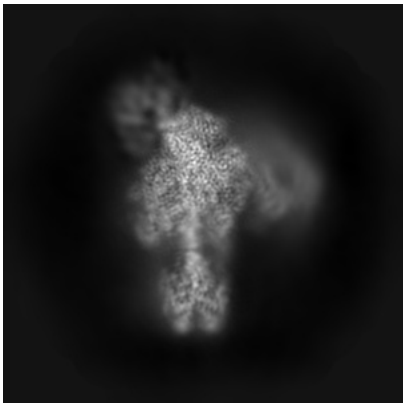
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26620. These allow visual inspection of the internal detail of the map and identification of artifacts.

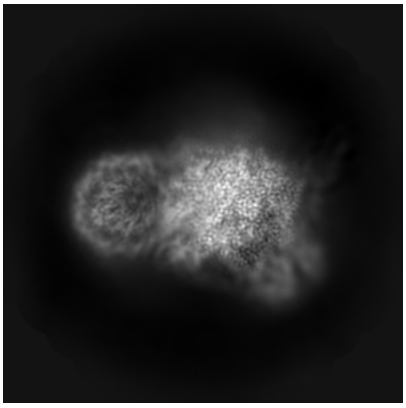
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

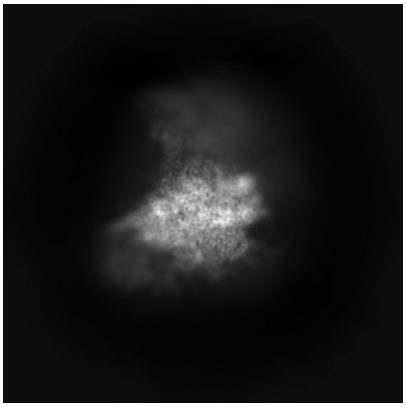
6.1.1 Primary map



X



Y

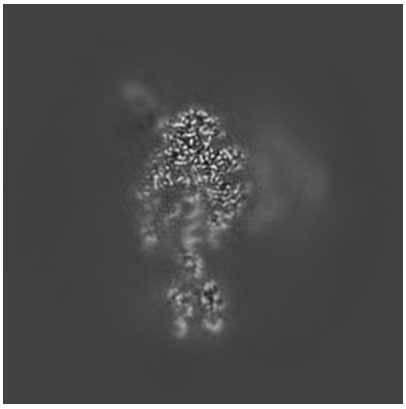


Z

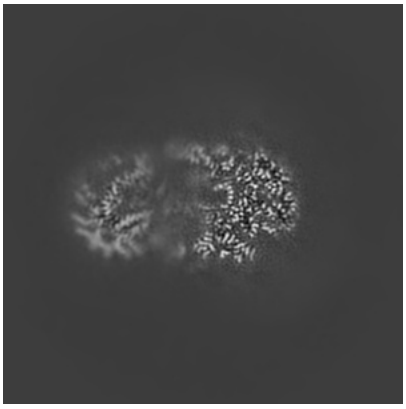
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

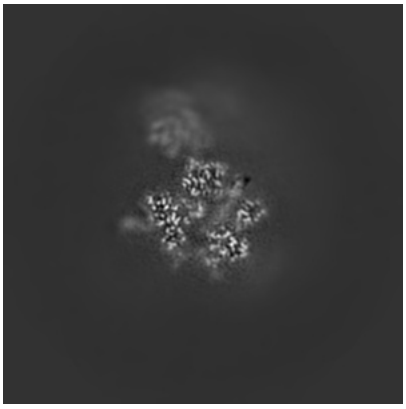
6.2.1 Primary map



X Index: 225



Y Index: 225

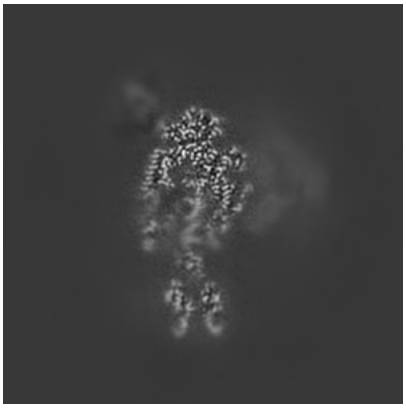


Z Index: 225

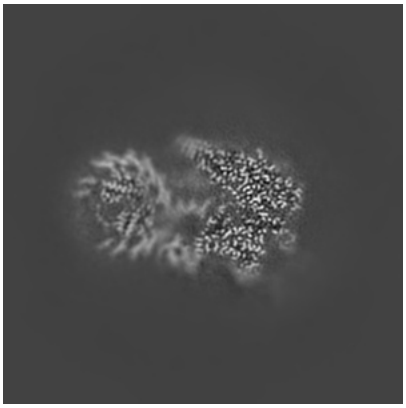
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

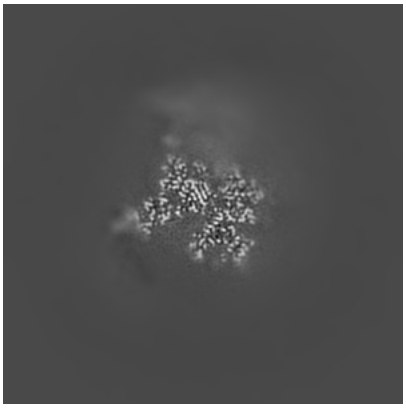
6.3.1 Primary map



X Index: 222



Y Index: 214



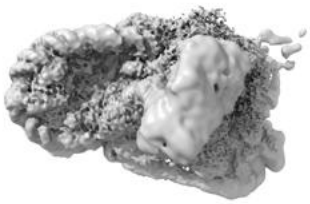
Z Index: 266

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

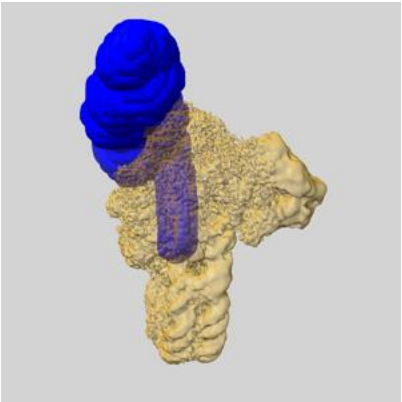
6.5 Mask visualisation (i)

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

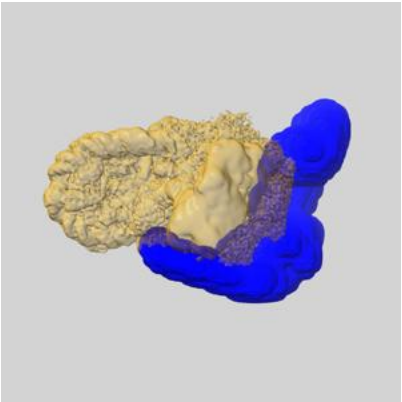
A mask typically either:

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

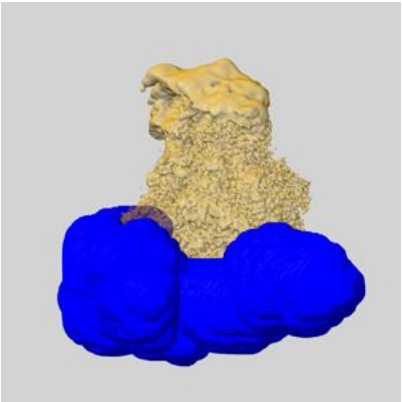
6.5.1 emd_26620_msk_1.map (i)



X

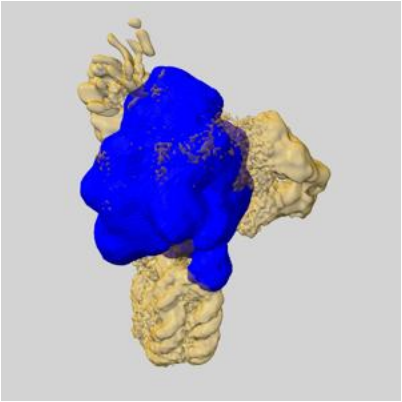


Y

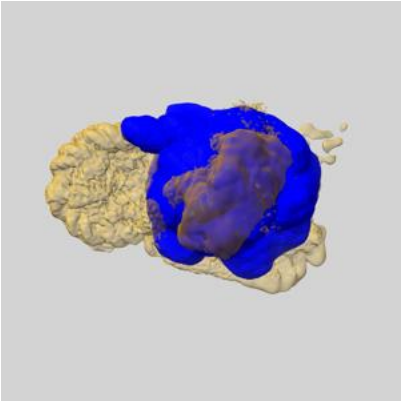


Z

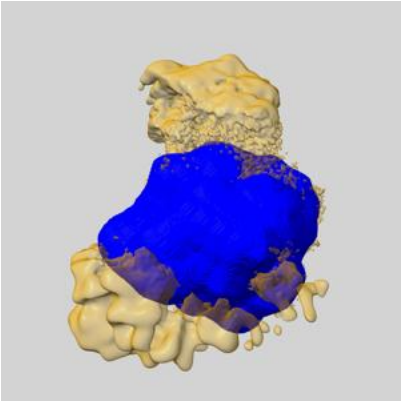
6.5.2 emd_26620_msk_2.map (i)



X

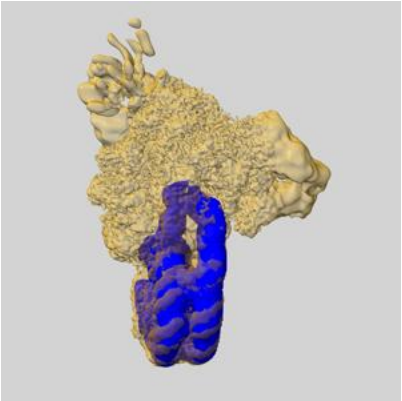


Y

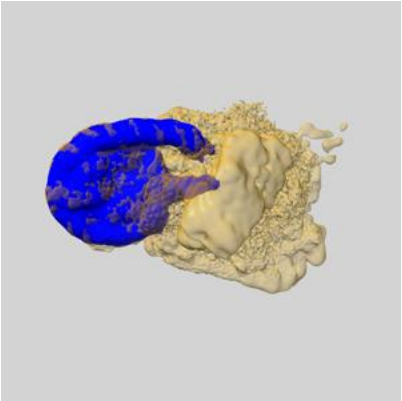


Z

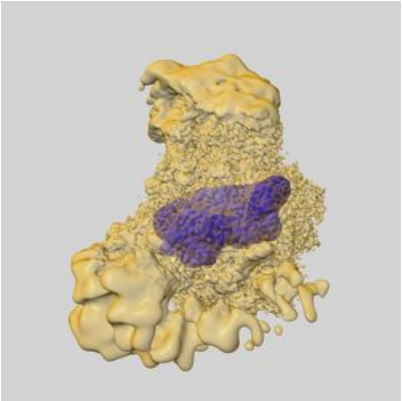
6.5.3 emd_26620_msk_3.map ⓘ



X



Y

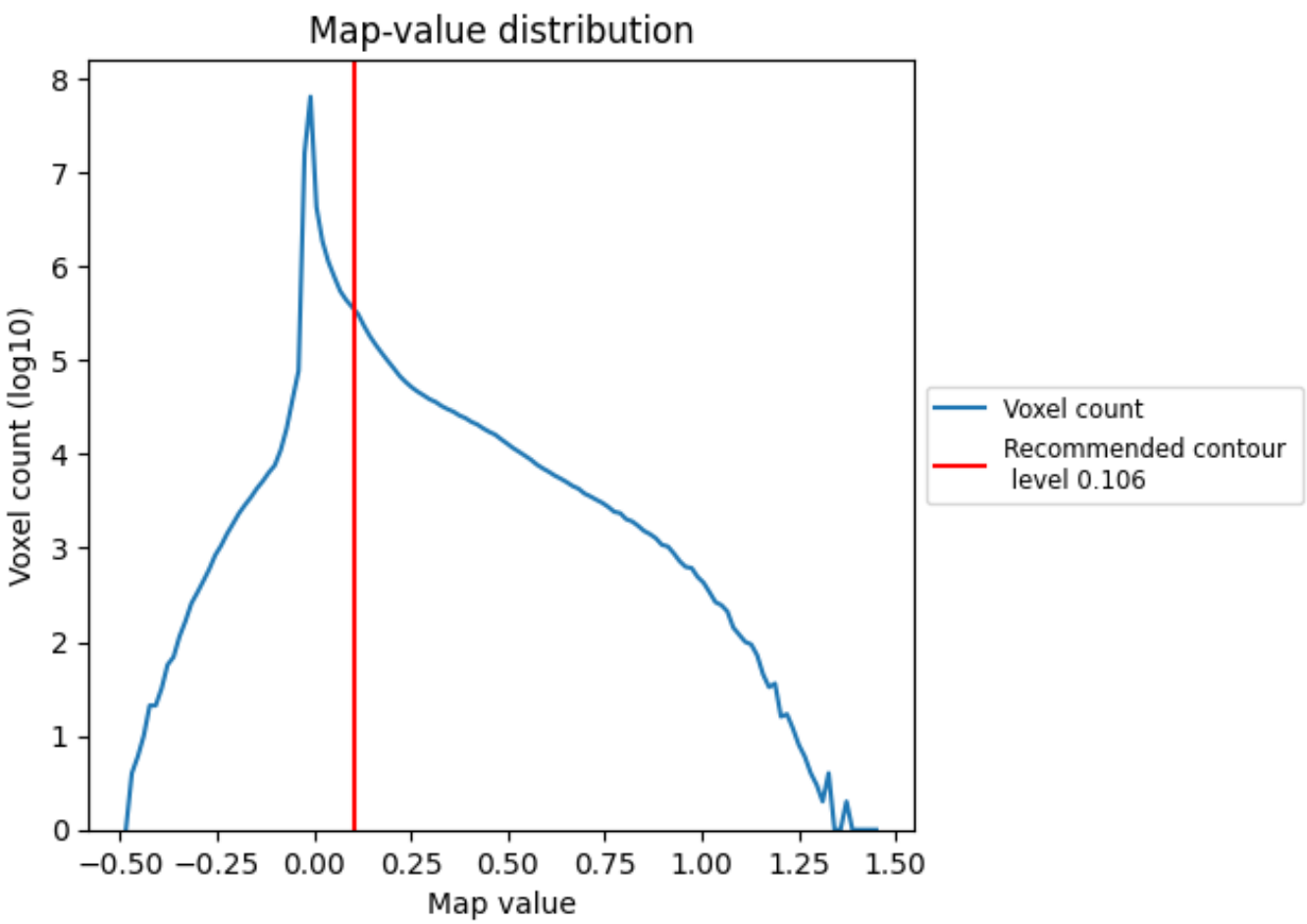


Z

7 Map analysis (i)

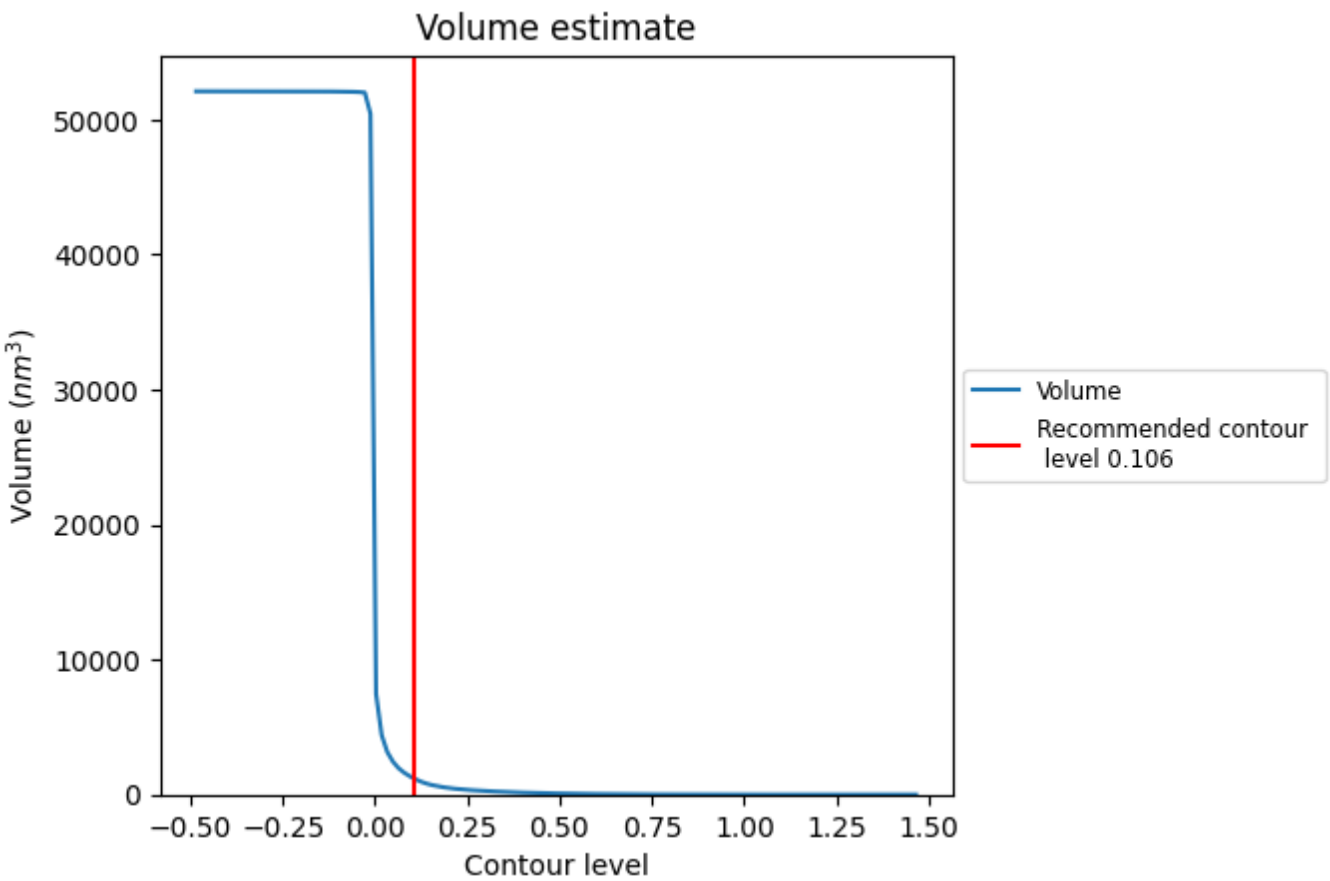
This section contains the results of statistical analysis of the map.

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.

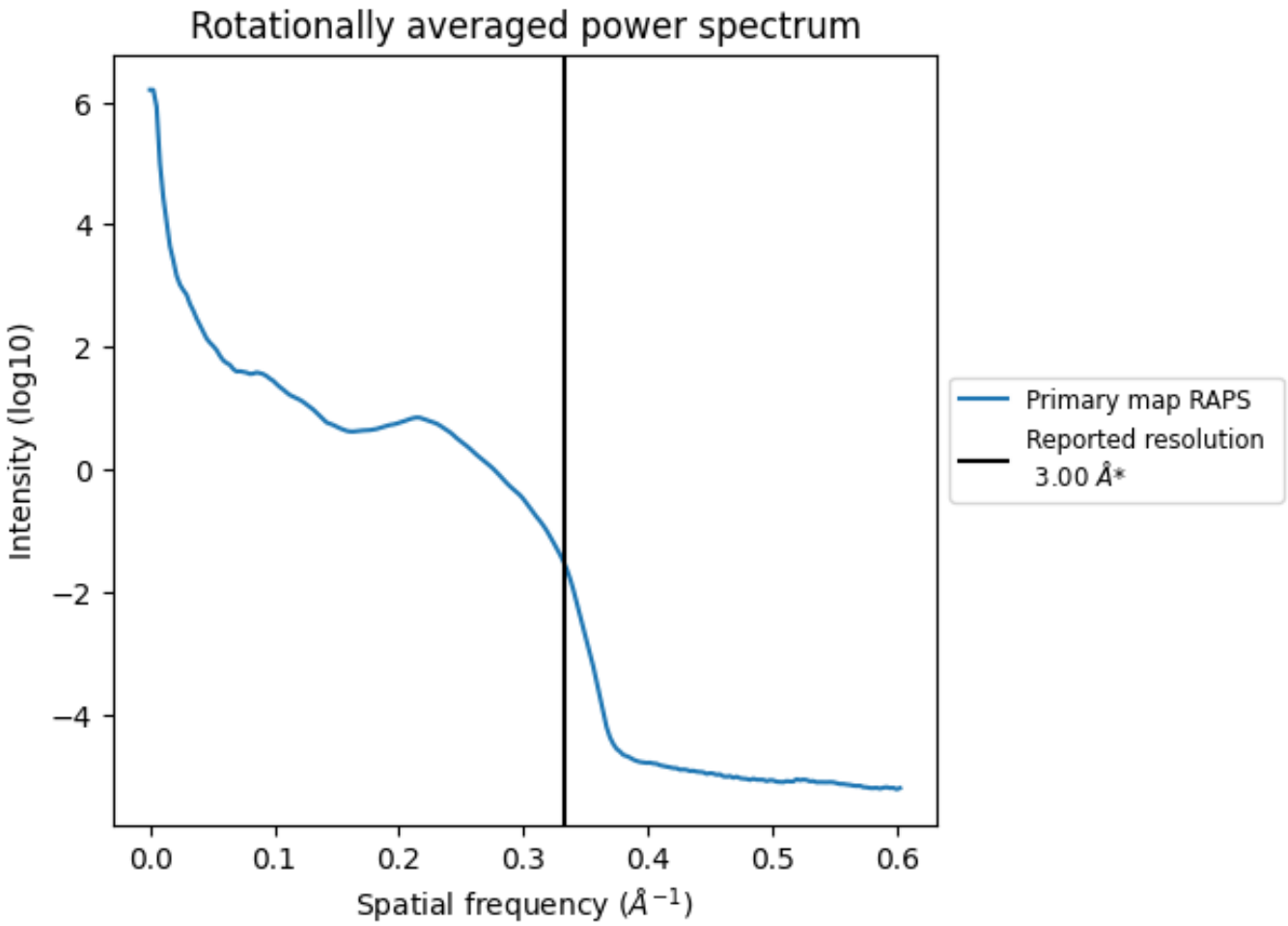
7.2 Volume estimate (i)



The volume at the recommended contour level is 1190 nm^3; this corresponds to an approximate mass of 1075 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



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

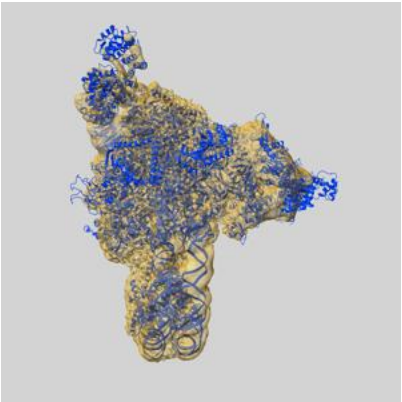
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

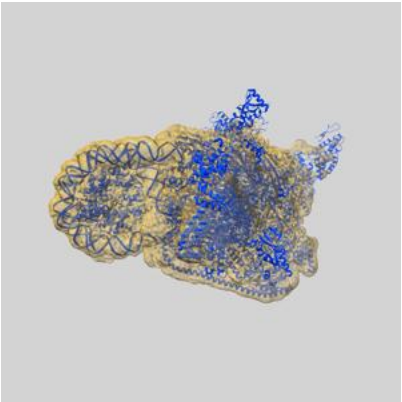
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26620 and PDB model 7UNC. Per-residue inclusion information can be found in section 3 on page 10.

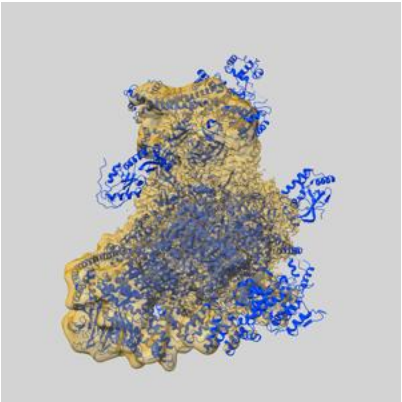
9.1 Map-model overlay (i)



X



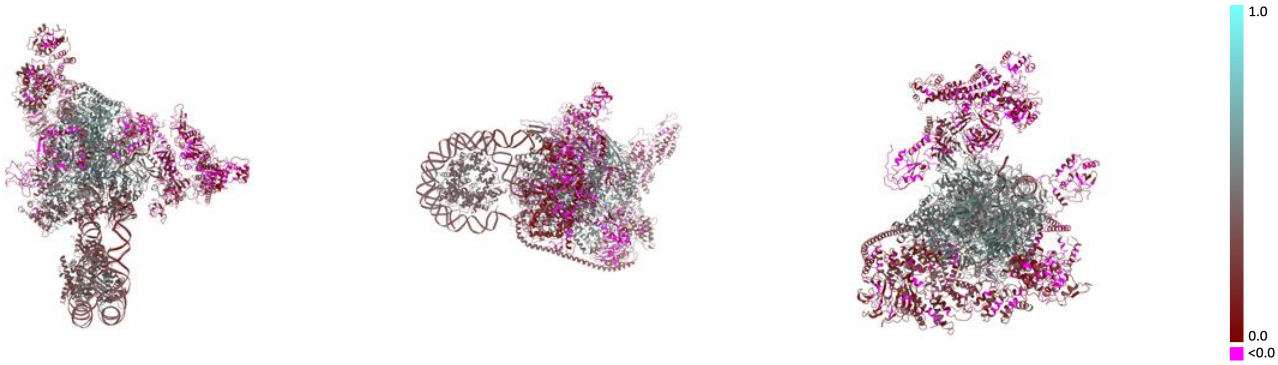
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.106 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.

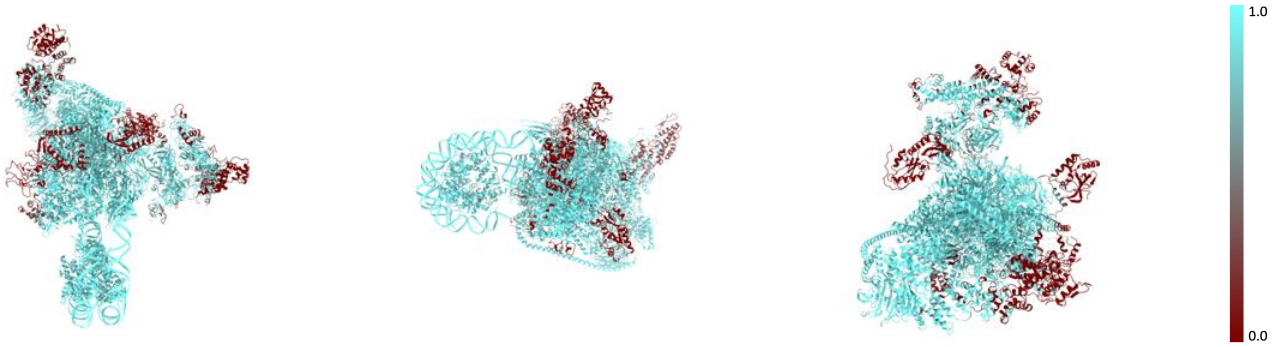
9.2 Q-score mapped to coordinate model (i)



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.

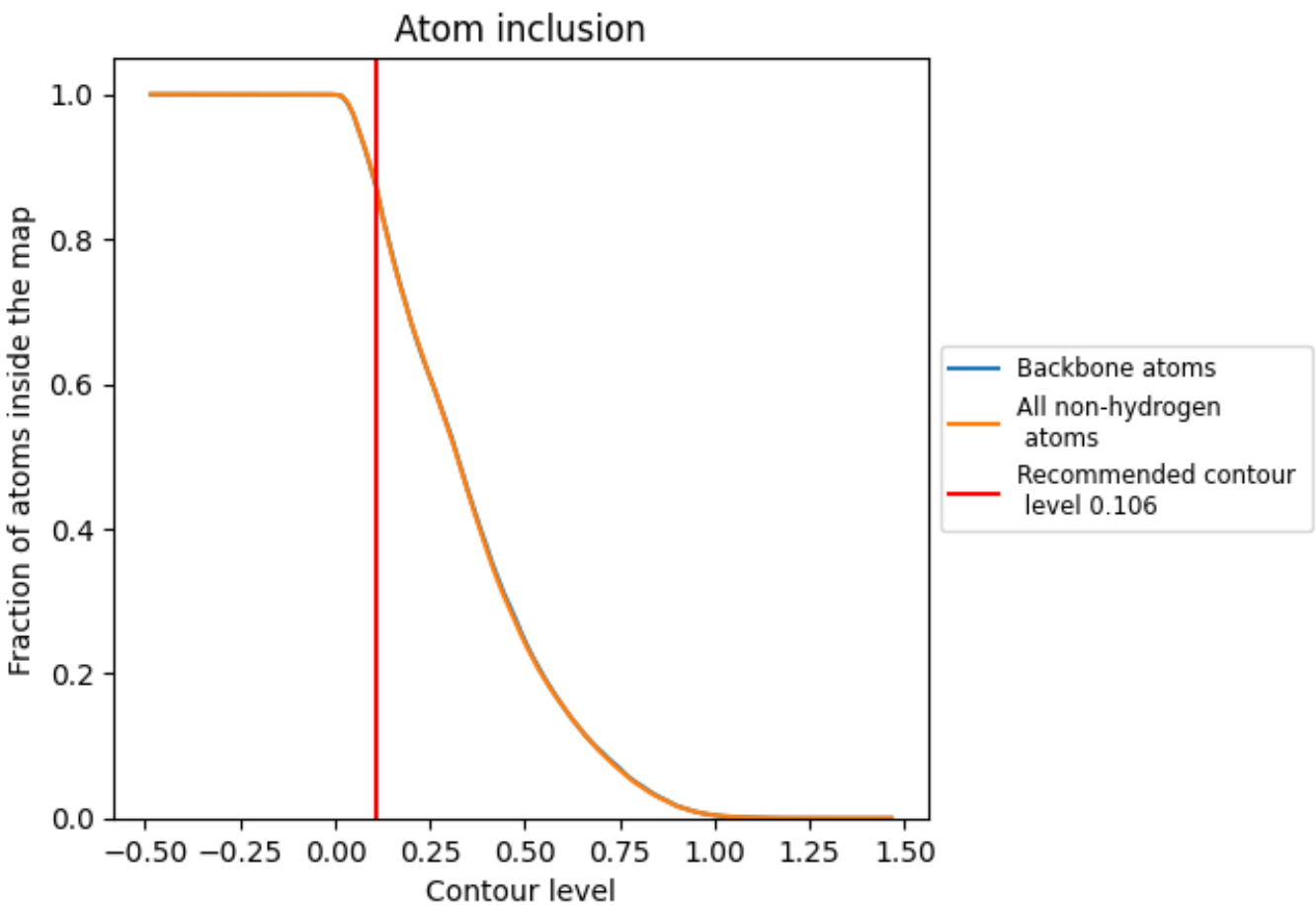
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.106).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8782	0.3440
A	0.9762	0.4790
B	0.9913	0.4950
C	0.9946	0.5280
D	0.9566	0.1580
E	0.9911	0.3560
F	0.9918	0.5280
G	0.9772	0.2300
H	0.9829	0.4160
I	0.9967	0.3840
J	0.9824	0.5340
K	0.9923	0.5250
L	0.9763	0.4380
M	0.4381	0.0470
N	0.9983	0.2890
O	0.2822	0.1330
P	1.0000	0.4100
Q	0.6663	0.1610
R	0.1914	0.0900
T	1.0000	0.3130
U	0.0048	0.0230
V	0.2766	0.1000
W	0.9508	0.1380
X	0.9826	0.2460
Z	0.7625	0.1280
a	0.9870	0.3510
b	0.9890	0.3960
c	0.9701	0.3650
d	0.9739	0.3460
e	0.9727	0.3290
f	0.9832	0.3670
g	0.9745	0.3930
h	0.9887	0.3890