Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 08:30 am BST

PDB ID	:	9GMA / pdb_00009gma
EMDB ID	:	EMD-51446
Title	:	MukBEF in a DNA capture state (dimer)
Authors	:	Burmann, F.; Lowe, J.
Deposited on	:	2024-08-28
Resolution	:	9.10 Å(reported)

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

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

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

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

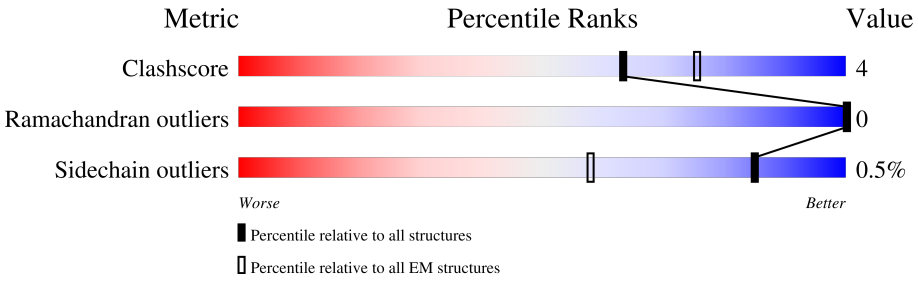
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 9.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1482	92% 7%
1	B	1482	85% 13%
1	O	1482	99% 92% 7%
1	P	1482	96% 84% 15%
2	C	440	87% 12%
2	D	440	29% 87% 12%
3	E	240	68% 20% 12%
3	F	240	62% 19% 18%

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Mol	Chain	Length	Quality of chain
3	Q	240	26% 69% 19% 12%
3	R	240	68% 60% 21% 18%
4	G	78	67% 24% 8%
4	I	78	78% 13% 8%
4	M	78	90% 78% 13% 8%
4	S	78	92% 65% 26% 8%
5	K	2124	97%
6	L	2124	97%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	4HH	G	36	-	-	X	-
4	4HH	S	36	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 130919 atoms, of which 64362 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 Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1467	Total	C	H	N	O	S	0	0
			23547	7298	11707	2188	2314	40		
1	B	1467	Total	C	H	N	O	S	0	0
			23546	7298	11706	2188	2314	40		
1	O	1467	Total	C	H	N	O	S	0	0
			23547	7298	11707	2188	2314	40		
1	P	1467	Total	C	H	N	O	S	0	0
			23546	7298	11706	2188	2314	40		

- Molecule 2 is a protein called Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		
2	D	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		

- Molecule 3 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	F	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		
3	Q	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	R	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		

- Molecule 4 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
4	G	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	I	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	S	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	M	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		

- Molecule 5 is a DNA chain called pFB526.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	73	Total	C	H	N	O	P	0	0
			2311	708	815	285	430	73		

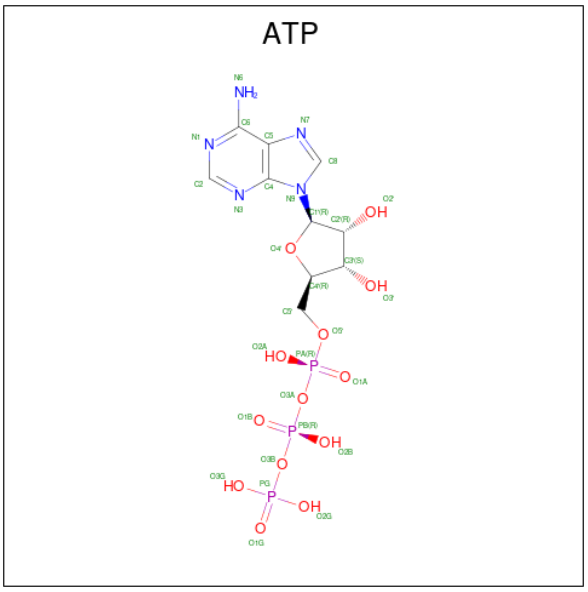
- Molecule 6 is a DNA chain called pFB526.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	73	Total	C	H	N	O	P	0	0
			2320	711	823	267	446	73		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	
7	O	1	Total	Mg	0
			1	1	
7	P	1	Total	Mg	0
			1	1	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



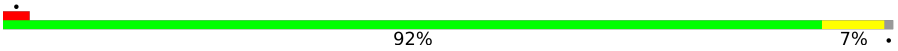
Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	O	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	P	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

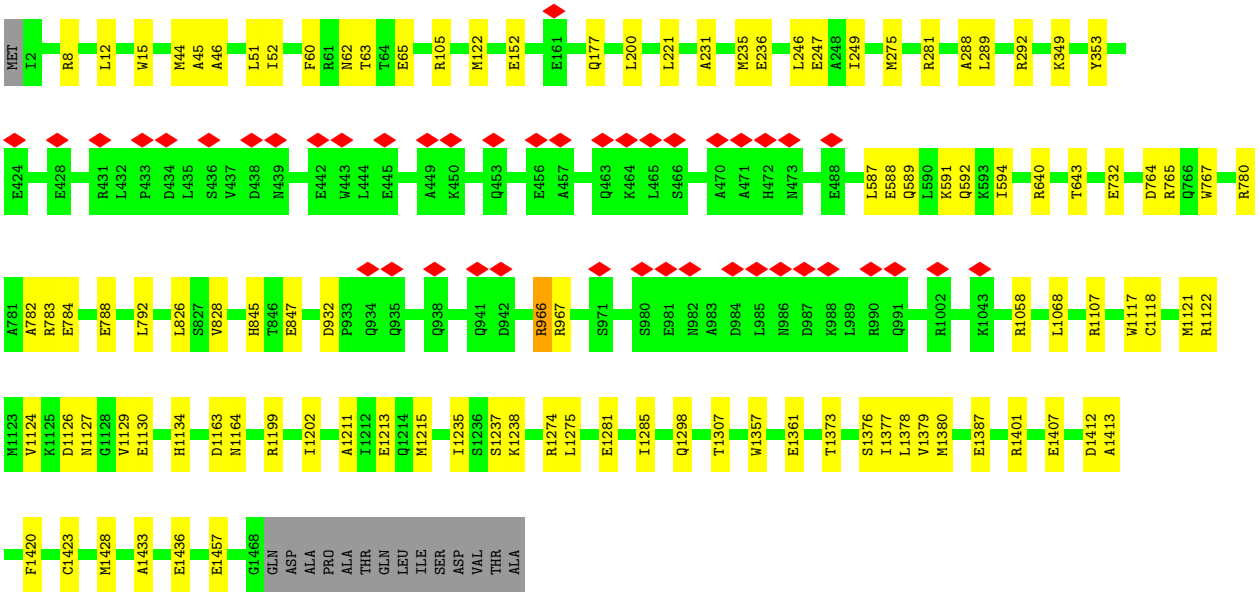
3 Residue-property plots (i)

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: Chromosome partition protein MukB

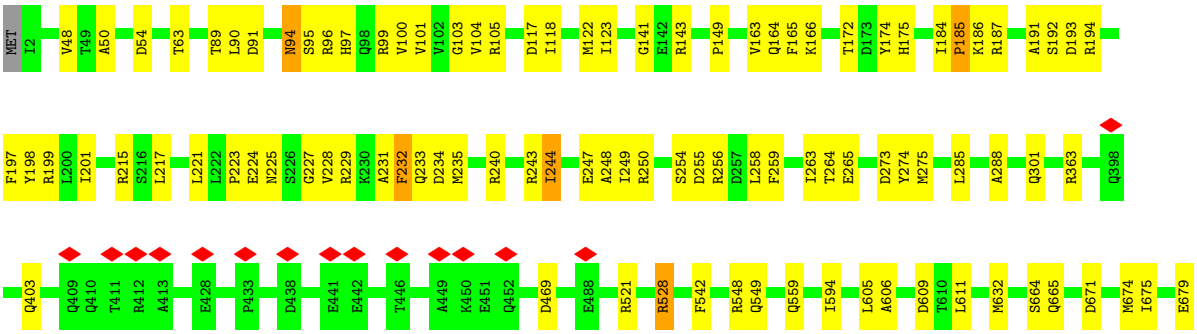
Chain A:

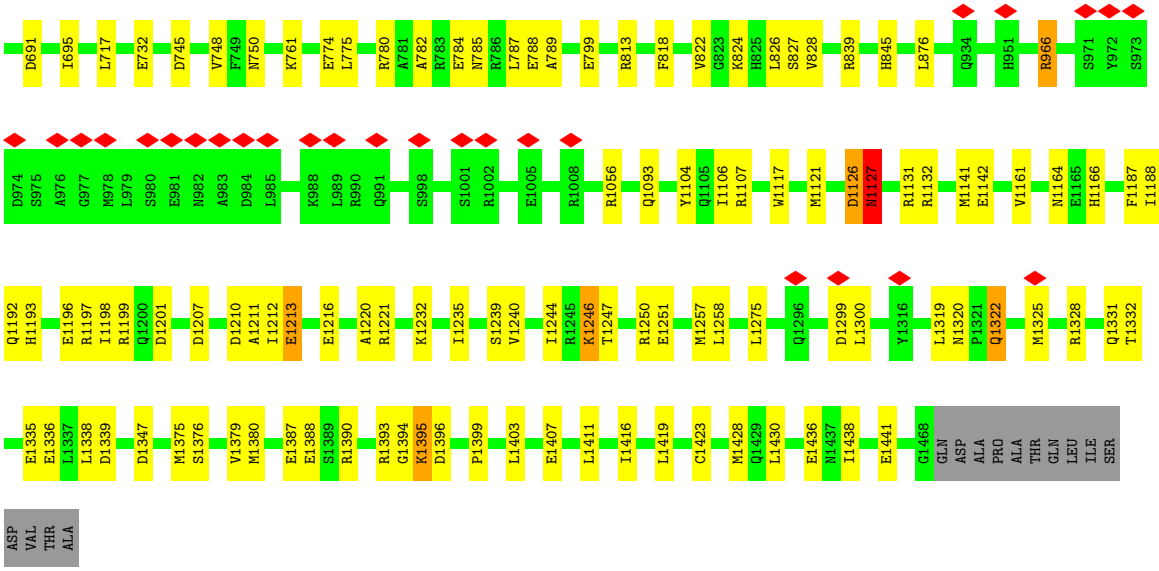




• Molecule 1: Chromosome partition protein MukB

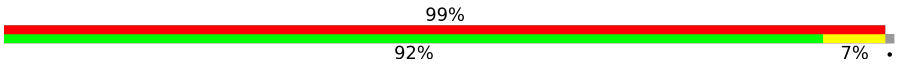
Chain B:

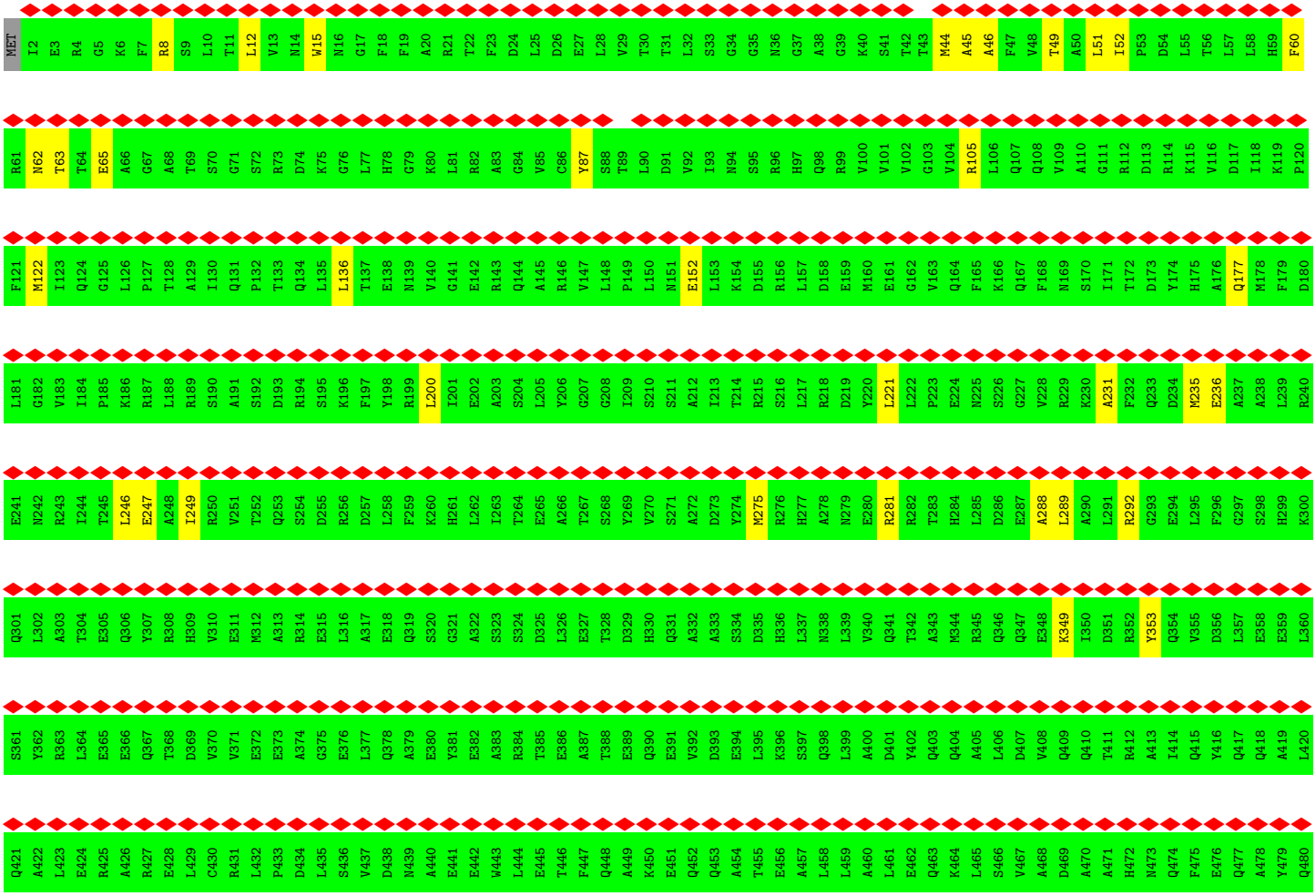


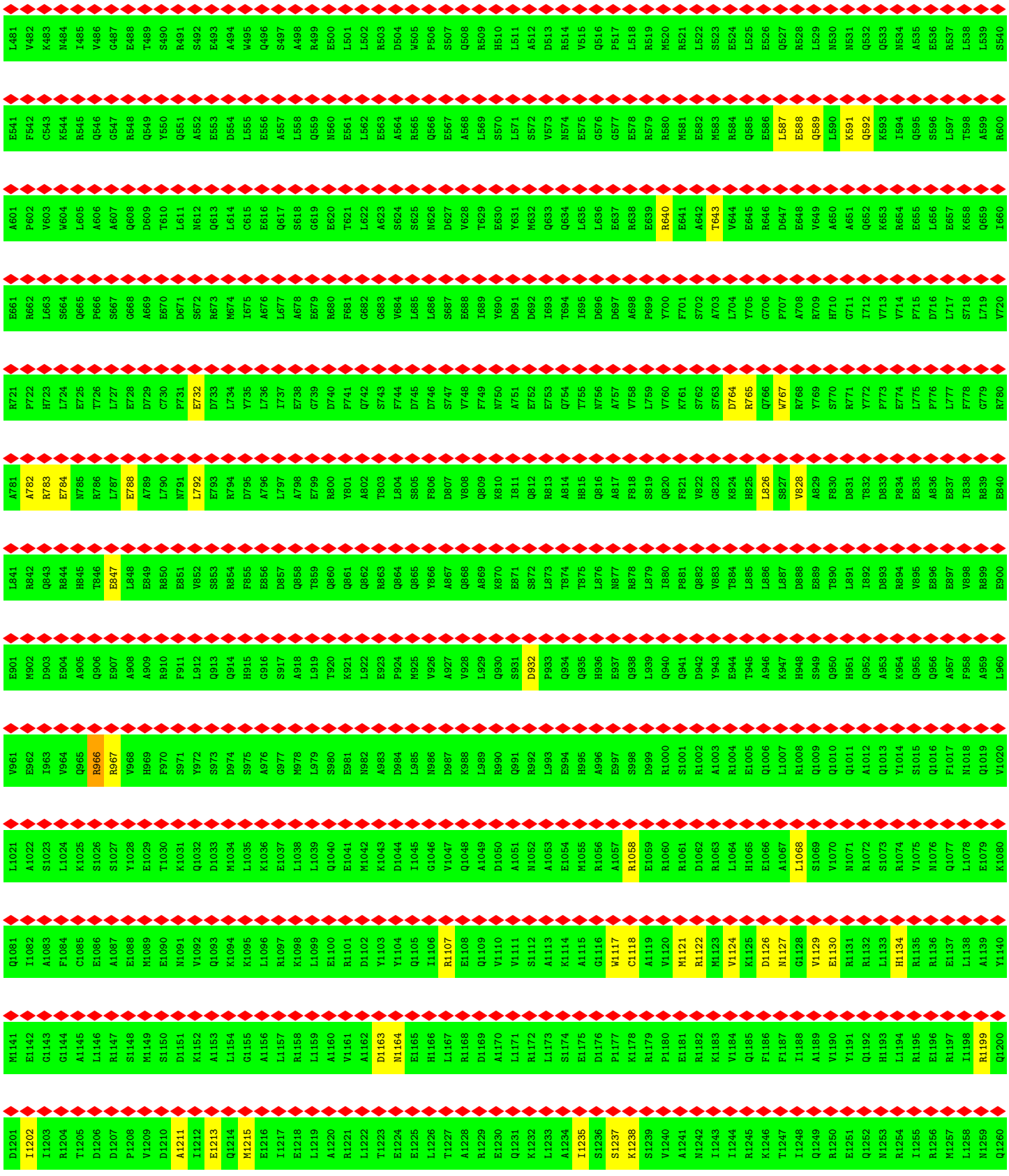


• Molecule 1: Chromosome partition protein MukB

Chain O:



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E541 F542 C543 K544 R545 Q546 G547 R548 Q549 Y550 Q551 A552 E553 D554 L555 E556 A557 L558 Q559 N560 E561 L562 E563 A564 R565 Q566 E567 A568 L569 S570 L571 S572 V573 N574 E575 G576 G577 E578 R579 R580 M581 E582 M583 R584 Q585 E586 L587 E588 Q589 L590 K591 Q592 K593 I594 Q595 S596 L597 T598 A599 R600
A601 P602 V603 W604 L605 A606 A607 Q608 D609 T610 L611 N612 Q613 L614 C615 E616 Q617 S618 G619 E620 T621 L622 A623 S624 S625 N626 D627 V628 T629 E630 Y631 M632 Q633 Q634 L635 L636 E637 R638 E639 R640 E641 A642 T643 V644 E645 R646 D647 E648 V649 A650 A651 Q652 K653 R654 E655 L656 E657 K658 Q659 I660
E661 R662 L663 S664 Q665 P666 S667 G668 A669 E670 D671 S672 R673 M674 I675 A676 L677 A678 E679 R680 F681 G682 G683 V684 L685 L686 S687 E688 I689 Y690 D691 D692 I693 T694 I695 D696 D697 A698 P699 Y700 F701 S702 A703 L704 Y705 G706 P707 A708 R709 H710 G711 I712 V713 V714 P715 D716 L717 S718 L719 V720
R721 P722 H723 L724 E725 T726 L727 E728 D729 C730 P731 E732 D733 L734 Y735 L736 I737 E738 G739 D740 P741 Q742 S743 F744 D745 D746 S747 V748 F749 N750 A751 E752 E753 Q754 T755 N756 A757 V758 L759 V760 K761 S762 S763 D764 R765 Q766 W767 R768 Y769 S770 R771 Y772 P773 E774 L775 P776 L777 F778 G779 R780
A781 A782 R783 E784 N785 R786 L787 E788 A789 L790 N791 L792 E793 R794 D795 A796 L797 A798 E799 R800 Y801 A802 T803 L804 S805 F806 D807 V808 Q809 K810 I811 Q812 R813 A814 H815 Q816 A817 F818 S819 Q820 F821 V822 G823 K824 H825 L826 S827 V828 A829 F830 D831 T832 D833 P834 E835 A836 E837 I838 R839 E840
L841 R842 Q843 R844 H845 T846 E847 L848 E849 R850 E851 V852 S853 R854 F855 E856 D857 Q858 T859 Q860 Q861 Q862 R863 Q864 Q865 Y866 A867 Q868 A869 K870 E871 S872 L873 T874 T875 L876 N877 R878 L879 I880 F881 Q882 V883 T884 L885 L886 L887 D888 E889 T890 L891 I892 D893 R894 V895 E896 E897 V898 R899 E900
E901 M902 D903 E904 A905 Q906 E907 A908 A909 R910 F911 L912 Q913 Q914 H915 G916 S917 A918 L919 T920 K921 L922 E923 P924 M925 V926 A927 V928 L929 Q930 S931 D932 P933 Q934 Q935 H936 E937 Q938 L939 Q940 Q941 D942 Y943 E944 T945 L946 K947 H948 S949 Q950 H951 Q952 A953 K954 Q955 Q956 A957 F958 A959 L960
V961 E962 I963 V964 Q965 R966 R967 V968 H969 F970 S971 Y972 S973 D974 S975 A976 G977 M978 L979 L980 E981 N982 A983 D984 L985 N986 D987 K988 L989 R990 Q991 R992 L993 E994 H995 A996 E997 S998 D999 R1000 S1001 R1002 A1003 R1004 E1005 Q1006 L1007 R1008 Q1009 Q1010 Q1011 A1012 Q1013 Y1014 S1015 Q1016 F1017 N1018 Q1019 V1020
L1021 A1022 S1023 L1024 K1025 S1026 S1027 Y1028 E1029 T1030 K1031 Q1032 D1033 M1034 L1035 K1036 E1037 L1038 L1039 Q1040 E1041 M1042 K1043 D1044 I1045 G1046 V1047 Q1048 A1049 D1050 A1051 N1052 A1053 E1054 M1055 R1056 A1057 R1058 E1059 R1060 R1061 D1062 R1063 L1064 H1065 E1066 A1067 L1068 S1069 V1070 N1071 R1072 S1073 R1074 V1075 N1076 Q1077 L1078 E1079 K1080
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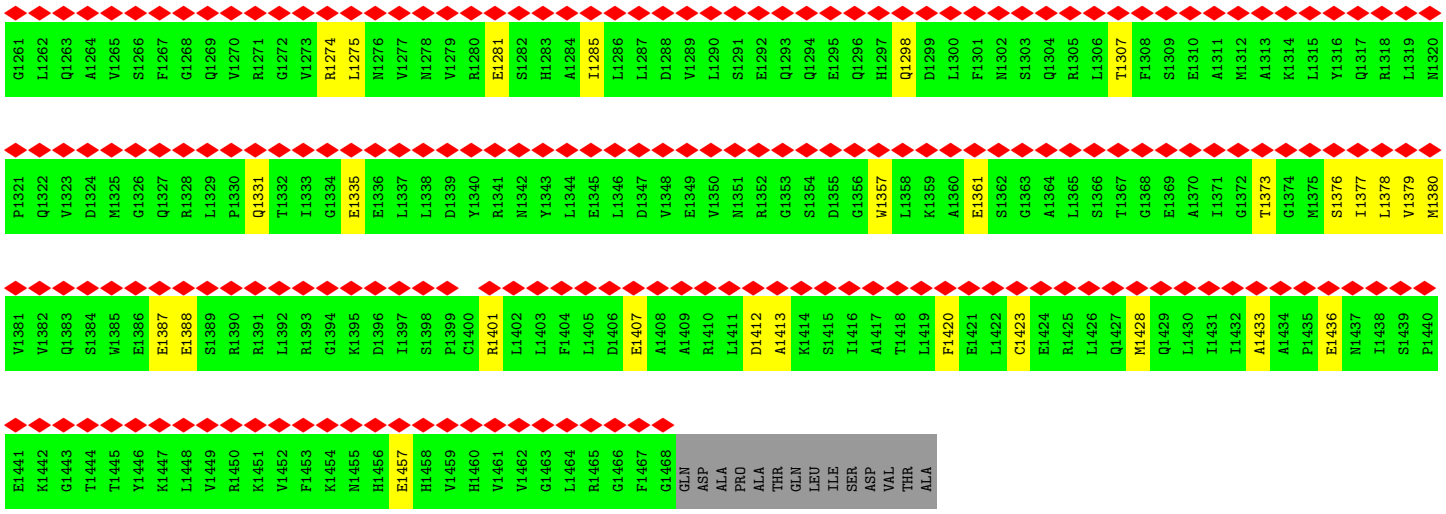
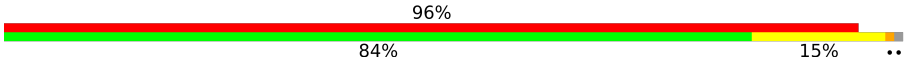
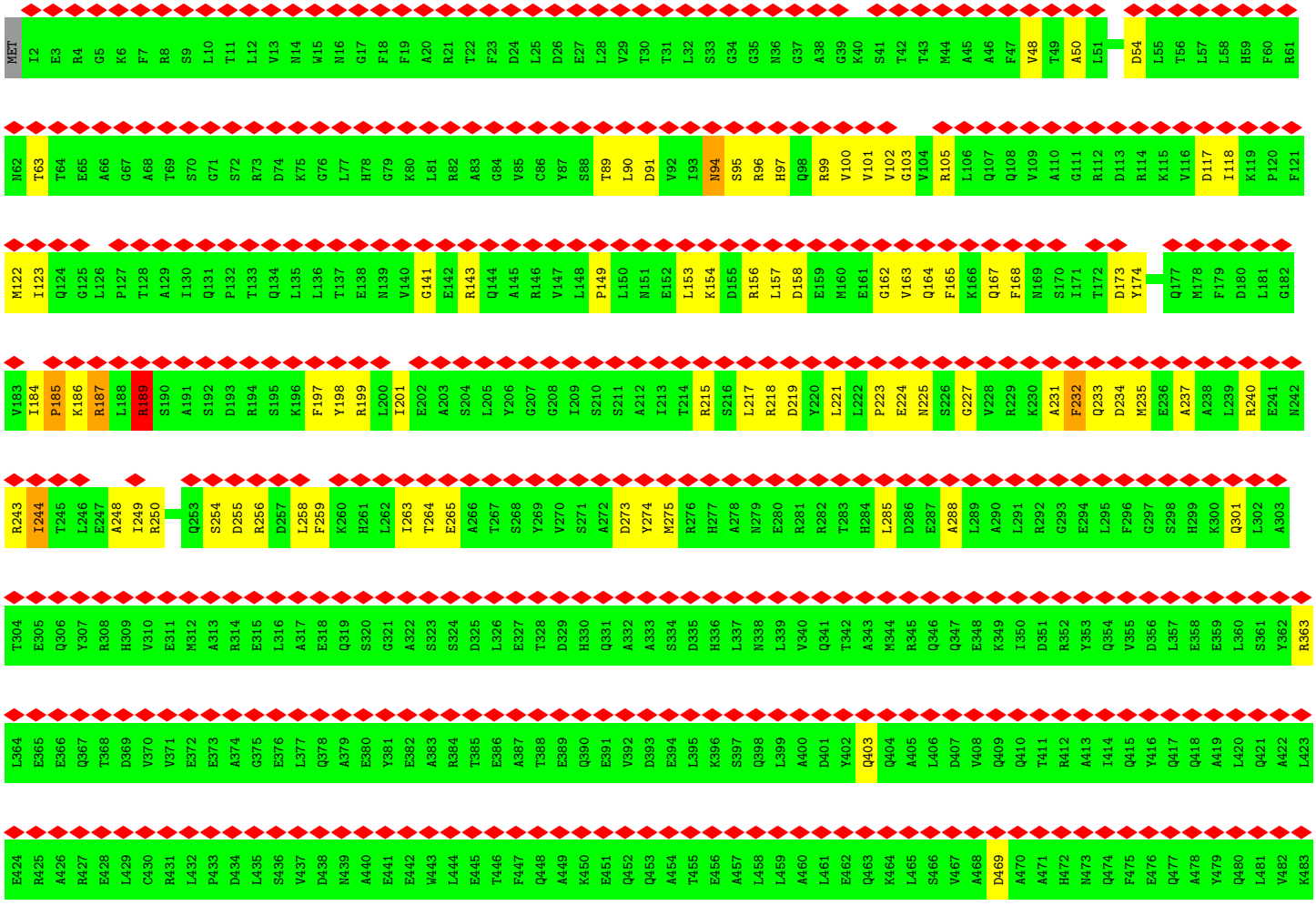
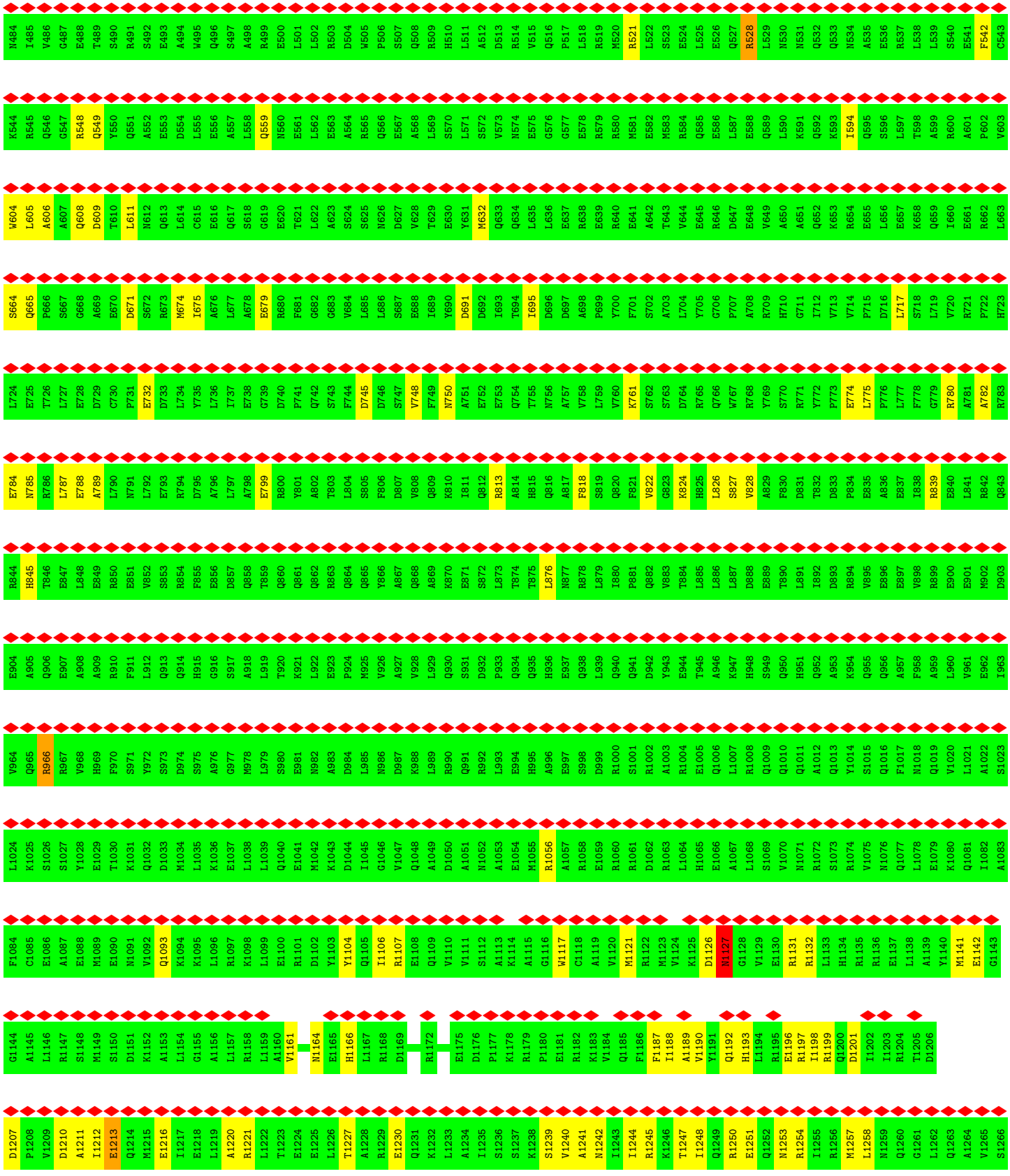


• Molecule 1: Chromosome partition protein MukB

Chain P:



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S664 Q665 P666 S667 G668 A669 E670 D671 S672 R673 M674 I675 A676 L677 A678 E679 R680 F681 G682 G683 V684 L685 L686 S687 E688 I689 Y690 D691 D692 I693 T694 I695 D696 D697 A698 P699 Y700 F701 S702 A703 L704 Y705 G706 P707 A708 R709 H710 G711 I712 V713 V714 P715 D716 L717 S718 L719 V720 R721 P722 H723
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E784 N785 R786 L787 E788 A789 L790 N791 L792 E793 R794 D795 A796 L797 A798 E799 R800 Y801 A802 T803 L804 S805 F806 D807 V808 Q809 K810 I811 Q812 R813 A814 H815 Q816 A817 F818 S819 Q820 F821 V822 G823 K824 H825 L826 S827 V828 A829 F830 D831 T832 D833 P834 E835 A836 E837 I838 R839 E840 L841 R842 Q843
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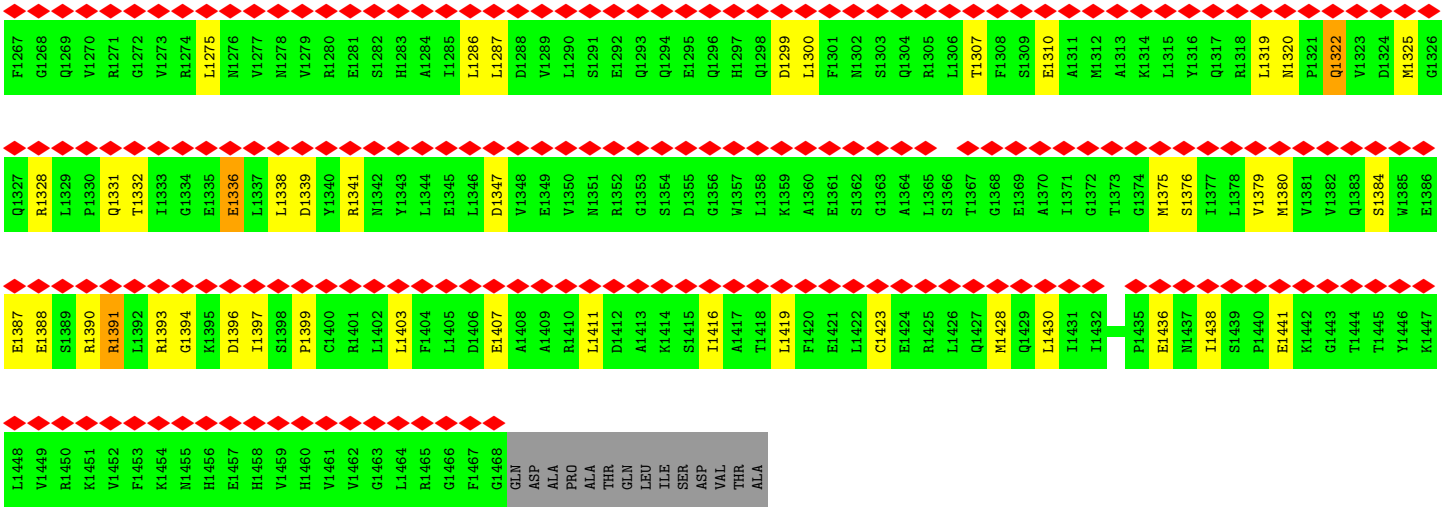
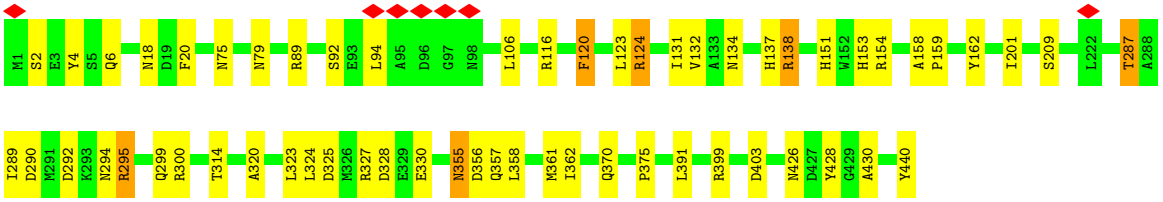
V964 Q965 R966 R967 V968 H969 F970 S971 Y972 S973 D974 S975 A976 G977 M978 L979 S980 E981 N982 A983 D984 L985 N986 D987 K988 L989 R990 Q991 R992 L993 E994 H995 A996 E997 S998 D999 R1000 S1001 R1002 A1003 R1004 E1005 Q1006 L1007 R1008 Q1009 Q1010 Q1011 A1012 Q1013 Y1014 S1015 Q1016 F1017 N1018 Q1019 V1020 L1021 A1022 S1023
L1024 K1025 S1026 S1027 Y1028 E1029 T1030 K1031 Q1032 D1033 M1034 L1035 K1036 E1037 L1038 L1039 Q1040 E1041 M1042 K1043 D1044 I1045 G1046 V1047 Q1048 A1049 D1050 A1051 N1052 A1053 E1054 M1055 R1056 A1057 R1058 E1059 R1060 R1061 D1062 R1063 L1064 H1065 E1066 A1067 L1068 S1069 V1070 N1071 R1072 S1073 R1074 V1075 N1076 Q1077 L1078 E1079 K1080 Q1081 I1082 A1083
F1084 C1085 E1086 A1087 E1088 M1089 E1090 N1091 V1092 Q1093 K1094 K1095 L1096 R1097 K1098 L1099 E1100 R1101 D1102 Y1103 Y1104 Q1105 I1106 R1107 E1108 Q1109 V1110 V1111 S1112 A1113 K1114 A1115 G1116 W1117 C1118 A1119 V1120 M1121 R1122 M1123 V1124 K1125 D1126 N1127 G1128 V1129 E1130 R1131 R1132 L1133 H1134 R1135 R1136 E1137 L1138 A1139 Y1140 M1141 E1142 G1143
G1144 A1145 L1146 R1147 S1148 M1149 S1150 D1151 K1152 A1153 L1154 G1155 A1156 L1157 R1158 L1159 A1160 V1161 N1164 E1165 H1166 L1167 R1168 D1169 R1172 E1175 D1176 P1177 K1178 R1179 P1180 E1181 R1182 K1183 V1184 Q1185 F1186 F1187 I1188 A1189 V1190 Y1191 Q1192 H1193 L1194 R1195 E1196 R1197 I1198 R1199 Q1200 D1201 I1202 I1203 R1204 T1205 D1206
D1207 P1208 V1209 D1210 A1211 I1212 E1213 Q1214 M1215 E1216 I1217 E1218 L1219 A1220 R1221 L1222 T1223 E1224 E1225 L1226 T1227 A1228 R1229 E1230 Q1231 K1232 L1233 A1234 I1235 S1236 S1237 K1238 S1239 V1240 A1241 N1242 I1243 I1244 R1245 K1246 T1247 I1248 Q1249 R1250 E1251 Q1252 N1253 R1254 I1255 R1256 M1257 L1258 N1259 Q1260 G1261 L1262 Q1263 A1264 V1265 S1266



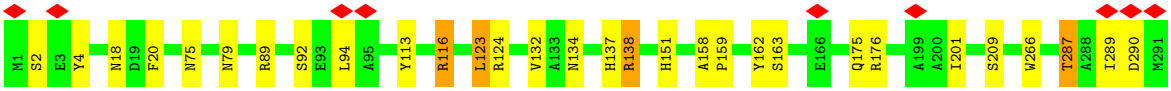
• Molecule 2: Chromosome partition protein MukF

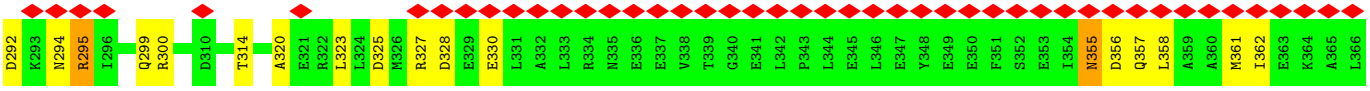
Chain C:



• Molecule 2: Chromosome partition protein MukF

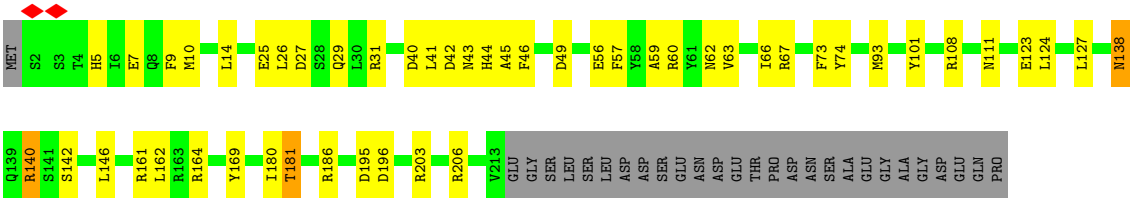
Chain D:



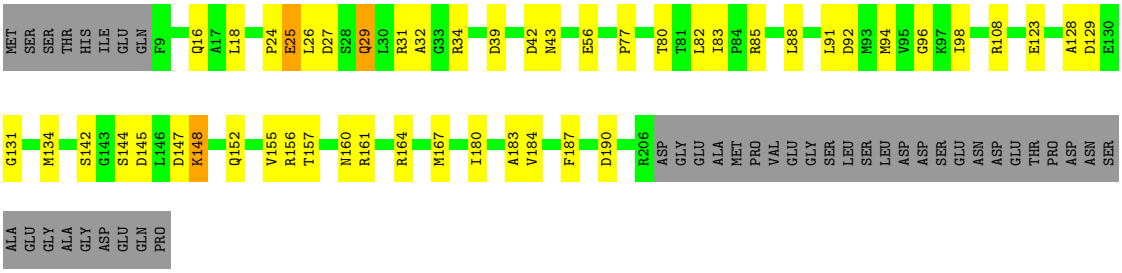


• Molecule 3: Chromosome partition protein MukE

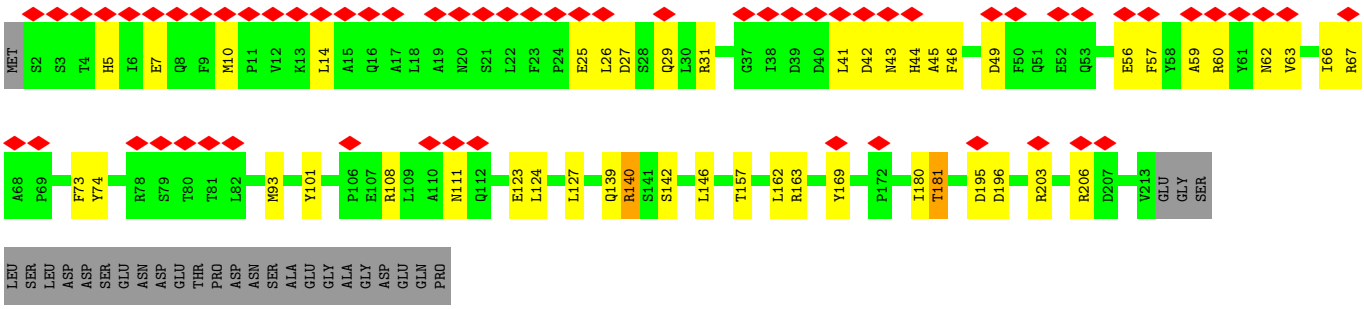
Chain E:



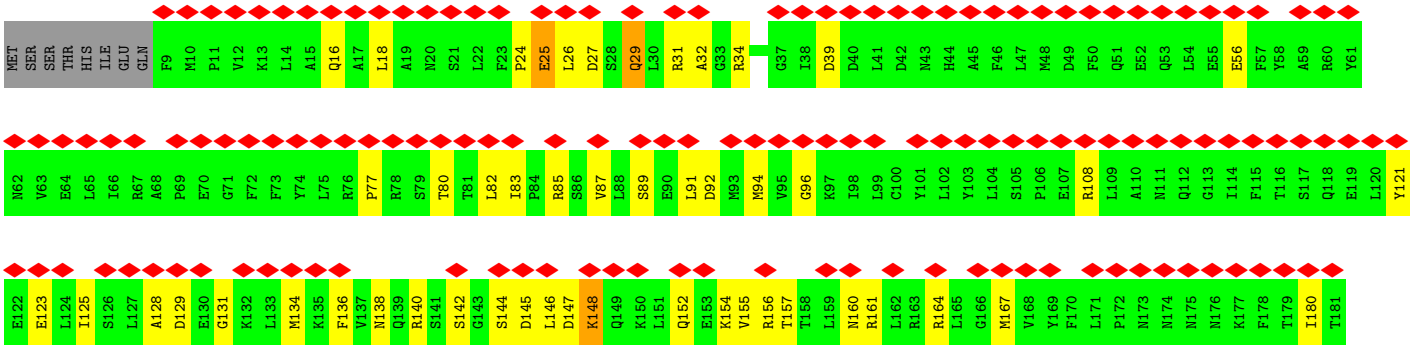
• Molecule 3: Chromosome partition protein MukE

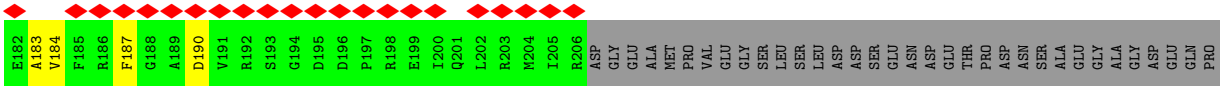


• Molecule 3: Chromosome partition protein MukE



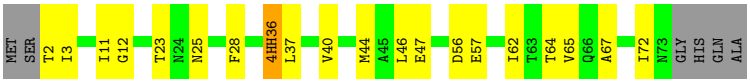
• Molecule 3: Chromosome partition protein MukE





• Molecule 4: Acyl carrier protein

Chain G:

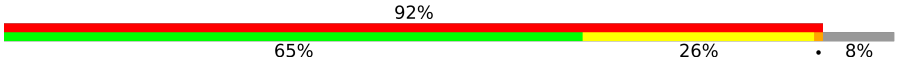


• Molecule 4: Acyl carrier protein

Chain I:

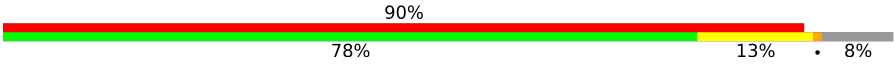
• Molecule 4: Acyl carrier protein

Chain S:



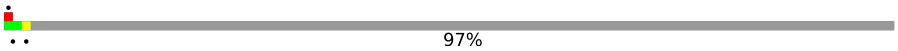
• Molecule 4: Acyl carrier protein

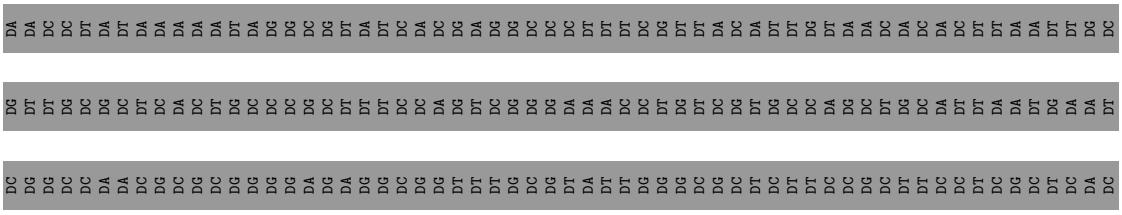
Chain M:

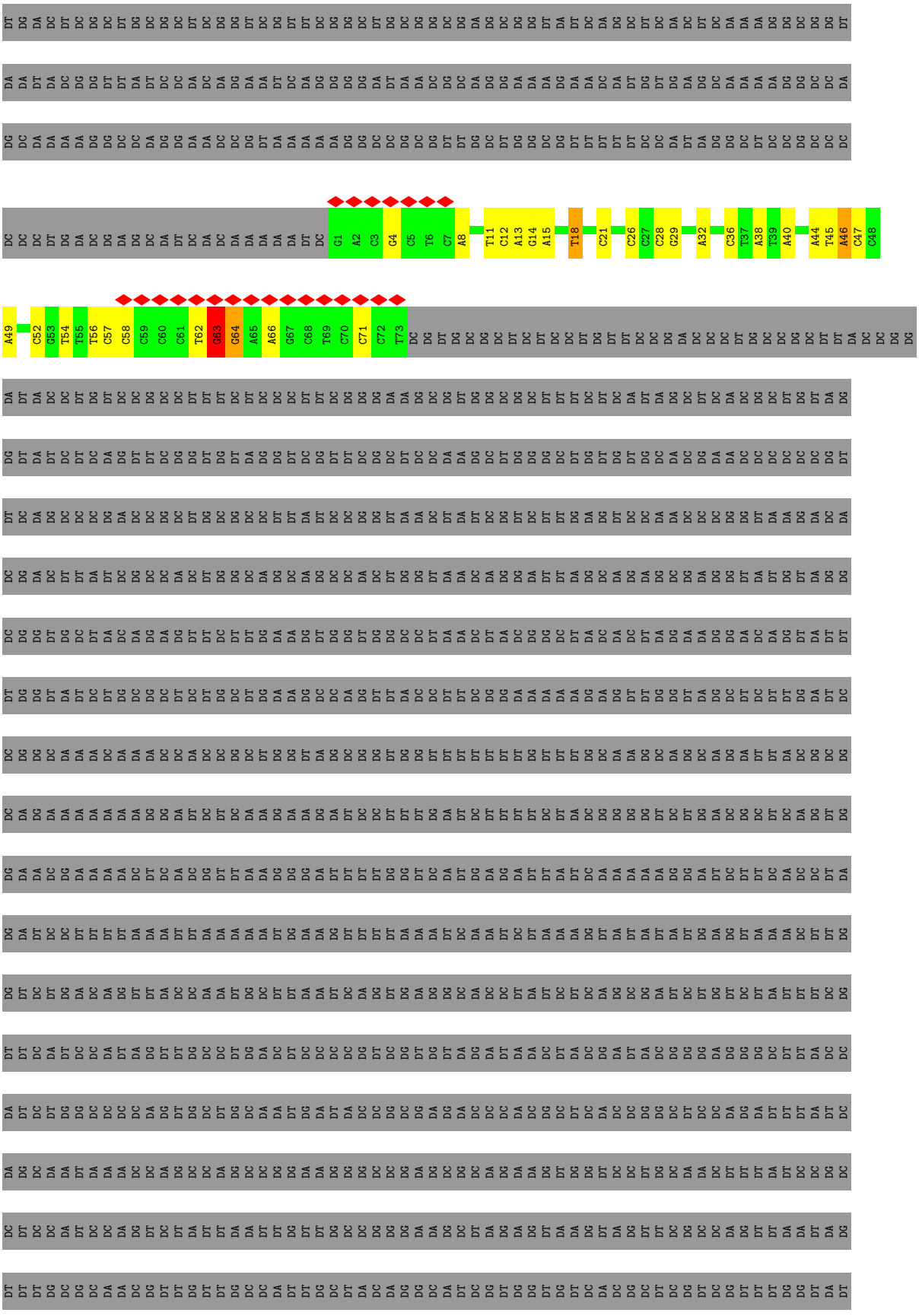


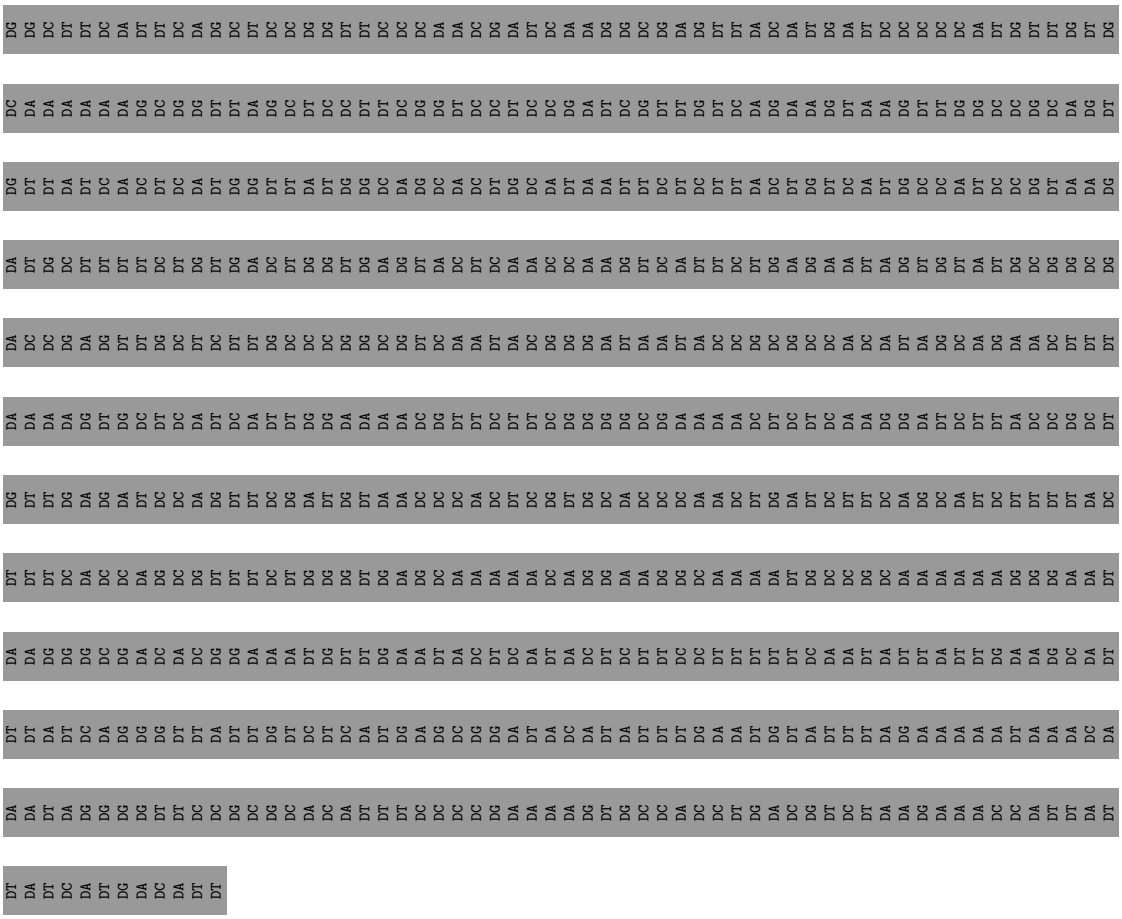
• Molecule 5: pFB526

Chain K:



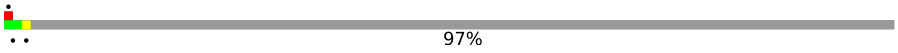


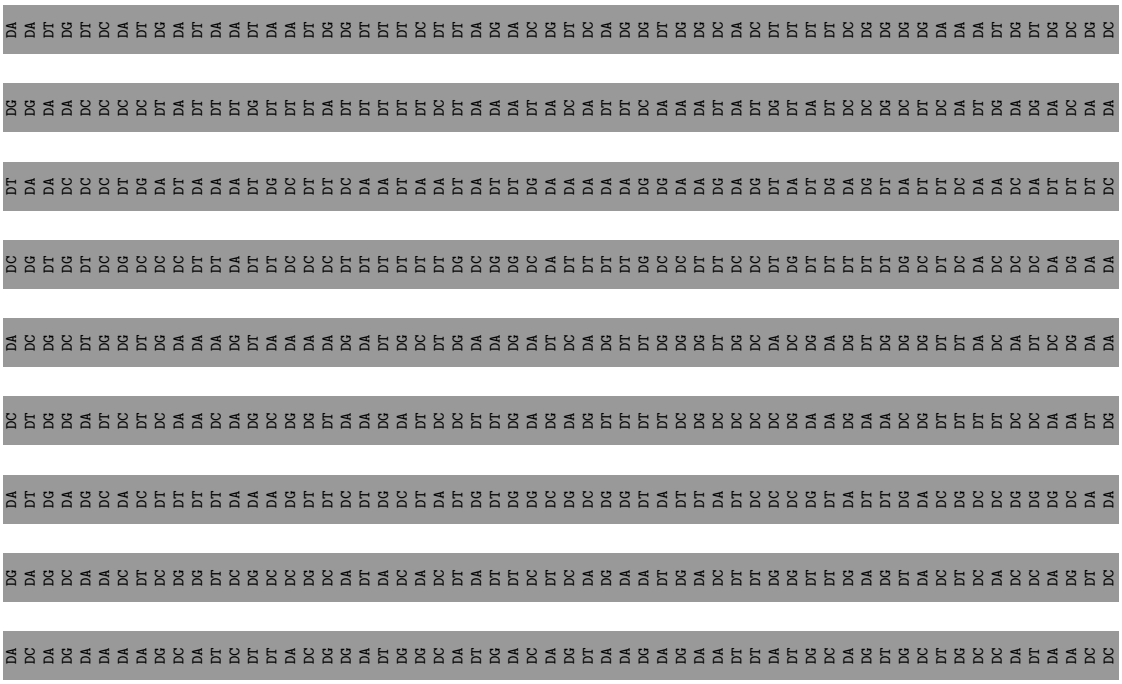

G1 A2 C3 G4 C5 T6 C7 A8 T11 C12 A13 G14 A15 T18 C21 C26 C27 C28 G29 A32 C36 T37 A38 T39 A40 A44 T45 A46 C47 C48
A49 C52 G53 T54 T55 T56 C57 C58 C59 C60 C61 T62 G63 G64 A65 A66 G67 C68 T69 C70 C71 C72 T73

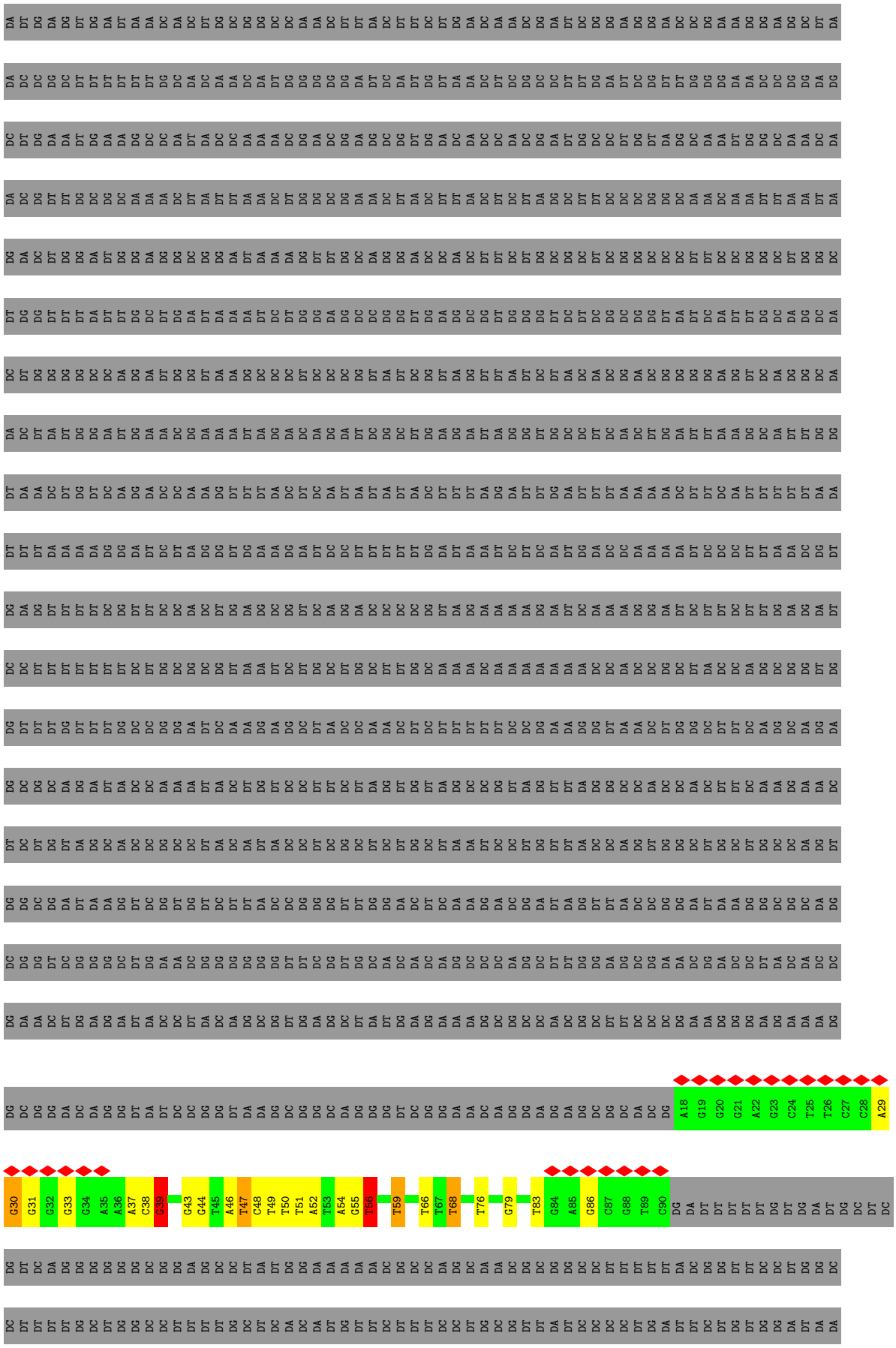


• Molecule 6: pFB526

Chain L:






A18 G19 G20 G21 A22 G23 C24 T25 T26 C27 C28 A29
G30 G31 G32 G33 G34 A35 A36 A37 C38 G39 G43 G44 T45 A46 T47 C48 T49 T50 T51 A52 T53 A54 G55 T56 T59 T66 T67 T68 T76 G79 T83 G84 A85 G86 C87 G88 T89 C90


DC DC DG DT DA DT DT DA DC DC DG DC DC DT DT DT DG DA DG DT DG DA DG DC DT DG DA DT DA DC DC DG DC DT DC DG DC DC DG DC DA DG DC DC DG DA DC DG DA DC DC DG DA DG DC DG DC DA
DC DG DA DG DT DC DA DG DT DG DA DG DC DG DA DG DG DA DA DG DC DG DG DA DA DG DA DG DC DC DG DC DC DC DA DA DT DA DC DG DC DA DA DA DC DC DG DC DT DC DT DC DC DC DC DG DC DG DC
DT DT DG DG DC DC DG DA DT DT DC DA DT DT DA DA DT DG DC DA DG DC DT DG DG DC DA DC DG DA DC DA DG DG DT DT DC DC DC DC DG DA DC DT DG DG DA DA DG DC DG DG DC DA DG DT DG DA
DG DC DG DC DA DA DC DG DC DA DA DA DT DT DA DA DA DG DT DG DT DT DA DA DC DG DA DA DA DG DG DG DC DC DT DC DG DT DG DA DT DA DC DG DC DC DT DA DC DT DA DA DT DT DT DT DT DT
DA DT DA DG DG DT DT

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	720.7206, 720.7206, 720.7206	wwPDB
Map dimensions	166, 166, 166	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.34169, 4.34169, 4.34169	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.53	2/11999 (0.0%)	0.98	5/16166 (0.0%)
1	B	1.09	64/11999 (0.5%)	1.35	147/16166 (0.9%)
1	O	0.53	2/11999 (0.0%)	0.98	5/16166 (0.0%)
1	P	1.14	63/11999 (0.5%)	1.39	165/16166 (1.0%)
2	C	0.83	2/3592 (0.1%)	1.31	23/4862 (0.5%)
2	D	0.84	2/3592 (0.1%)	1.31	22/4862 (0.5%)
3	E	1.50	19/1753 (1.1%)	1.71	45/2361 (1.9%)
3	F	1.64	24/1648 (1.5%)	1.68	50/2218 (2.3%)
3	Q	1.50	19/1753 (1.1%)	1.70	43/2361 (1.8%)
3	R	1.63	23/1648 (1.4%)	1.68	57/2218 (2.6%)
4	G	0.13	0/558	0.28	0/754
4	I	0.13	0/558	0.27	0/754
4	M	0.14	0/558	0.27	0/754
4	S	0.13	0/558	0.28	0/754
5	K	0.69	0/1680	1.66	16/2589 (0.6%)
6	L	0.70	0/1676	1.60	11/2586 (0.4%)
All	All	0.94	220/67570 (0.3%)	1.27	589/91737 (0.6%)

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	3
1	B	0	2
1	O	0	3
1	P	0	3
2	C	0	6
2	D	0	6
3	E	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	Q	0	2
5	K	0	19
6	L	0	17
All	All	0	65

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	295	ARG	C-N	-24.37	1.03	1.33
2	D	295	ARG	C-N	-24.30	1.03	1.33
1	A	589	GLN	C-N	13.59	1.51	1.33
1	O	589	GLN	C-N	13.52	1.51	1.33
3	E	44	HIS	CE1-NE2	-8.96	1.23	1.32
3	Q	44	HIS	CE1-NE2	-8.90	1.23	1.32
1	B	1166	HIS	CE1-NE2	-8.86	1.23	1.32
1	B	1193	HIS	CE1-NE2	-8.86	1.23	1.32
1	P	1193	HIS	CE1-NE2	-8.84	1.23	1.32
1	P	1166	HIS	CE1-NE2	-8.82	1.23	1.32
1	B	175	HIS	CE1-NE2	-8.79	1.23	1.32
1	B	1193	HIS	CD2-NE2	-8.02	1.29	1.37
3	Q	44	HIS	CD2-NE2	-8.00	1.29	1.37
1	P	1166	HIS	CD2-NE2	-7.97	1.29	1.37
1	P	1193	HIS	CD2-NE2	-7.95	1.29	1.37
1	B	175	HIS	CD2-NE2	-7.93	1.29	1.37
1	B	1166	HIS	CD2-NE2	-7.93	1.29	1.37
3	E	44	HIS	CD2-NE2	-7.85	1.29	1.37
3	R	85	ARG	CZ-NH2	-7.79	1.23	1.33
1	P	1341	ARG	CZ-NH2	-7.77	1.23	1.33
1	P	1250	ARG	CZ-NH2	-7.74	1.23	1.33
1	P	1393	ARG	CZ-NH2	-7.72	1.23	1.33
1	P	1245	ARG	CZ-NH2	-7.72	1.23	1.33
3	Q	203	ARG	CZ-NH2	-7.71	1.23	1.33
1	B	1131	ARG	CZ-NH2	-7.71	1.23	1.33
1	P	96	ARG	CZ-NH2	-7.71	1.23	1.33
3	R	34	ARG	CZ-NH2	-7.69	1.23	1.33
1	P	1131	ARG	CZ-NH2	-7.68	1.23	1.33
3	R	161	ARG	CZ-NH2	-7.68	1.23	1.33
1	P	199	ARG	CZ-NH2	-7.67	1.23	1.33
3	E	206	ARG	CZ-NH2	-7.67	1.23	1.33
3	R	156	ARG	CZ-NH2	-7.67	1.23	1.33
1	P	1328	ARG	CZ-NH2	-7.66	1.23	1.33
3	F	31	ARG	CZ-NH2	-7.64	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	206	ARG	CZ-NH2	-7.63	1.23	1.33
1	P	1093	GLN	C-N	7.63	1.44	1.33
1	B	1221	ARG	CZ-NH2	-7.62	1.23	1.33
3	E	31	ARG	CZ-NH2	-7.62	1.23	1.33
1	P	1132	ARG	CZ-NH2	-7.61	1.23	1.33
1	P	1254	ARG	CZ-NH2	-7.61	1.23	1.33
1	B	1197	ARG	CZ-NH2	-7.58	1.23	1.33
3	R	31	ARG	CZ-NH2	-7.56	1.23	1.33
1	B	1199	ARG	CZ-NH2	-7.55	1.23	1.33
1	B	240	ARG	CZ-NH2	-7.55	1.23	1.33
1	P	1221	ARG	CZ-NH2	-7.55	1.23	1.33
1	P	1197	ARG	CZ-NH2	-7.54	1.23	1.33
3	Q	31	ARG	CZ-NH2	-7.54	1.23	1.33
1	B	1093	GLN	C-N	7.53	1.44	1.33
3	E	203	ARG	CZ-NH2	-7.53	1.23	1.33
1	B	1132	ARG	CZ-NH2	-7.53	1.23	1.33
1	B	250	ARG	CZ-NH2	-7.49	1.23	1.33
1	P	1199	ARG	CZ-NH2	-7.48	1.23	1.33
3	F	164	ARG	CZ-NH2	-7.48	1.23	1.33
1	P	240	ARG	CZ-NH2	-7.47	1.23	1.33
3	E	67	ARG	CZ-NH2	-7.45	1.23	1.33
3	Q	67	ARG	CZ-NH2	-7.45	1.23	1.33
1	B	199	ARG	CZ-NH2	-7.45	1.23	1.33
1	P	250	ARG	CZ-NH2	-7.44	1.23	1.33
3	R	164	ARG	CZ-NH2	-7.44	1.23	1.33
1	B	243	ARG	CZ-NH2	-7.42	1.23	1.33
3	F	85	ARG	CZ-NH2	-7.42	1.23	1.33
1	B	1328	ARG	CZ-NH2	-7.40	1.23	1.33
1	B	1393	ARG	CZ-NH2	-7.40	1.23	1.33
1	P	243	ARG	CZ-NH2	-7.38	1.23	1.33
1	B	229	ARG	CZ-NH2	-7.38	1.23	1.33
3	F	34	ARG	CZ-NH2	-7.38	1.23	1.33
3	F	161	ARG	CZ-NH2	-7.36	1.23	1.33
3	Q	60	ARG	CZ-NH2	-7.35	1.23	1.33
1	B	105	ARG	CZ-NH2	-7.33	1.24	1.33
3	E	60	ARG	CZ-NH2	-7.33	1.24	1.33
1	B	1250	ARG	CZ-NH2	-7.32	1.24	1.33
1	B	96	ARG	CZ-NH2	-7.30	1.24	1.33
3	F	156	ARG	CZ-NH2	-7.29	1.24	1.33
1	P	301	GLN	C-N	7.25	1.44	1.34
1	B	1390	ARG	CZ-NH2	-7.22	1.24	1.33
1	B	301	GLN	C-N	7.10	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	1394	GLY	N-CA	-6.80	1.37	1.45
1	B	1394	GLY	N-CA	-6.71	1.37	1.45
1	P	1189	ALA	CA-CB	-6.66	1.43	1.53
1	P	231	ALA	CA-CB	-6.62	1.43	1.53
1	B	1189	ALA	CA-CB	-6.61	1.43	1.53
1	P	248	ALA	CA-CB	-6.58	1.43	1.53
1	A	847	GLU	C-N	6.55	1.42	1.33
1	B	248	ALA	CA-CB	-6.54	1.43	1.53
1	P	237	ALA	CA-CB	-6.50	1.43	1.53
1	O	847	GLU	C-N	6.47	1.42	1.33
1	P	103	GLY	N-CA	-6.40	1.38	1.45
1	P	50	ALA	CA-CB	-6.34	1.43	1.53
3	E	45	ALA	CA-CB	-6.30	1.43	1.53
1	B	103	GLY	N-CA	-6.30	1.38	1.45
3	Q	45	ALA	CA-CB	-6.29	1.43	1.53
3	R	34	ARG	CZ-NH1	-6.29	1.24	1.32
1	P	1250	ARG	CZ-NH1	-6.29	1.24	1.32
1	B	231	ALA	CA-CB	-6.28	1.43	1.53
3	R	161	ARG	CZ-NH1	-6.28	1.24	1.32
1	P	1241	ALA	CA-CB	-6.28	1.43	1.53
1	P	1341	ARG	CZ-NH1	-6.25	1.24	1.32
1	P	1393	ARG	CZ-NH1	-6.25	1.24	1.32
2	C	320	ALA	CA-CB	-6.24	1.43	1.53
1	P	96	ARG	CZ-NH1	-6.23	1.24	1.32
1	B	250	ARG	CZ-NH1	-6.22	1.24	1.32
3	R	156	ARG	CZ-NH1	-6.21	1.24	1.32
1	P	1254	ARG	CZ-NH1	-6.21	1.24	1.32
1	P	1328	ARG	CZ-NH1	-6.21	1.24	1.32
2	D	320	ALA	CA-CB	-6.20	1.43	1.53
1	P	250	ARG	CZ-NH1	-6.16	1.24	1.32
1	B	191	ALA	CA-CB	-6.16	1.43	1.53
1	P	1245	ARG	CZ-NH1	-6.16	1.24	1.32
3	Q	67	ARG	CZ-NH1	-6.13	1.24	1.32
3	Q	31	ARG	CZ-NH1	-6.12	1.24	1.32
1	P	199	ARG	CZ-NH1	-6.11	1.24	1.32
1	B	1199	ARG	CZ-NH1	-6.11	1.24	1.32
3	E	67	ARG	CZ-NH1	-6.10	1.24	1.32
3	R	131	GLY	N-CA	-6.09	1.38	1.45
3	E	31	ARG	CZ-NH1	-6.09	1.24	1.32
3	E	203	ARG	CZ-NH1	-6.09	1.24	1.32
1	B	240	ARG	CZ-NH1	-6.08	1.24	1.32
3	R	31	ARG	CZ-NH1	-6.08	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	203	ARG	CZ-NH1	-6.08	1.24	1.32
3	E	206	ARG	CZ-NH1	-6.07	1.24	1.32
1	P	240	ARG	CZ-NH1	-6.07	1.24	1.32
3	R	164	ARG	CZ-NH1	-6.06	1.24	1.32
3	F	31	ARG	CZ-NH1	-6.06	1.24	1.32
3	F	164	ARG	CZ-NH1	-6.06	1.24	1.32
1	P	1199	ARG	CZ-NH1	-6.06	1.24	1.32
1	B	105	ARG	CZ-NH1	-6.05	1.24	1.32
1	P	243	ARG	CZ-NH1	-6.04	1.24	1.32
3	Q	206	ARG	CZ-NH1	-6.03	1.24	1.32
1	B	50	ALA	CA-CB	-6.03	1.43	1.53
1	B	243	ARG	CZ-NH1	-6.01	1.24	1.32
3	R	96	GLY	N-CA	-6.00	1.38	1.45
3	F	128	ALA	CA-CB	-6.00	1.43	1.53
1	B	1211	ALA	CA-CB	-5.99	1.43	1.53
1	B	1221	ARG	CZ-NH1	-5.99	1.24	1.32
1	P	1211	ALA	CA-CB	-5.98	1.43	1.53
3	R	85	ARG	CZ-NH1	-5.98	1.24	1.32
3	E	60	ARG	CZ-NH1	-5.97	1.24	1.32
3	F	34	ARG	CZ-NH1	-5.96	1.24	1.32
1	B	1132	ARG	CZ-NH1	-5.96	1.24	1.32
1	P	1132	ARG	CZ-NH1	-5.93	1.24	1.32
3	Q	60	ARG	CZ-NH1	-5.93	1.24	1.32
1	P	1131	ARG	CZ-NH1	-5.92	1.24	1.32
1	B	1131	ARG	CZ-NH1	-5.92	1.24	1.32
1	P	1197	ARG	CZ-NH1	-5.91	1.24	1.32
1	P	1221	ARG	CZ-NH1	-5.91	1.24	1.32
3	F	96	GLY	N-CA	-5.91	1.38	1.45
1	B	96	ARG	CZ-NH1	-5.91	1.24	1.32
3	Q	59	ALA	CA-CB	-5.88	1.43	1.53
1	B	1328	ARG	CZ-NH1	-5.86	1.24	1.32
1	B	229	ARG	CZ-NH1	-5.86	1.24	1.32
3	F	156	ARG	CZ-NH1	-5.84	1.24	1.32
1	P	227	GLY	N-CA	-5.83	1.38	1.45
3	F	85	ARG	CZ-NH1	-5.83	1.24	1.32
1	B	1250	ARG	CZ-NH1	-5.81	1.24	1.32
1	B	199	ARG	CZ-NH1	-5.80	1.24	1.32
1	B	1197	ARG	CZ-NH1	-5.79	1.24	1.32
3	F	161	ARG	CZ-NH1	-5.77	1.24	1.32
1	B	1393	ARG	CZ-NH1	-5.77	1.24	1.32
3	F	131	GLY	N-CA	-5.77	1.38	1.45
1	B	227	GLY	N-CA	-5.76	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	83	ILE	N-CA	-5.76	1.42	1.46
3	E	59	ALA	CA-CB	-5.75	1.43	1.53
3	F	83	ILE	N-CA	-5.74	1.42	1.46
3	R	32	ALA	CA-CB	-5.73	1.43	1.53
1	B	1390	ARG	CZ-NH1	-5.72	1.24	1.32
3	F	32	ALA	CA-CB	-5.66	1.43	1.53
3	R	85	ARG	CD-NE	-5.56	1.38	1.46
1	P	199	ARG	CD-NE	-5.55	1.38	1.46
1	P	1245	ARG	CD-NE	-5.51	1.38	1.46
1	B	199	ARG	CD-NE	-5.51	1.38	1.46
1	P	223	PRO	CA-CB	-5.47	1.46	1.53
1	P	240	ARG	CD-NE	-5.44	1.38	1.46
1	B	240	ARG	CD-NE	-5.42	1.38	1.46
1	P	1254	ARG	CD-NE	-5.42	1.38	1.46
3	F	85	ARG	CD-NE	-5.40	1.38	1.46
3	R	34	ARG	CD-NE	-5.36	1.38	1.46
1	P	1250	ARG	CD-NE	-5.35	1.38	1.46
3	R	161	ARG	CD-NE	-5.34	1.38	1.46
3	Q	203	ARG	CD-NE	-5.32	1.38	1.46
1	B	223	PRO	CA-CB	-5.32	1.46	1.53
1	B	1132	ARG	CD-NE	-5.31	1.38	1.46
1	P	250	ARG	CD-NE	-5.31	1.38	1.46
1	P	1132	ARG	CD-NE	-5.31	1.38	1.46
3	R	142	SER	CA-CB	-5.30	1.45	1.52
3	E	203	ARG	CD-NE	-5.29	1.38	1.46
3	F	34	ARG	CD-NE	-5.29	1.38	1.46
1	B	1199	ARG	CD-NE	-5.27	1.38	1.46
3	R	77	PRO	CA-CB	-5.25	1.47	1.53
3	Q	60	ARG	CD-NE	-5.25	1.39	1.46
3	R	164	ARG	CD-NE	-5.24	1.39	1.46
1	P	1341	ARG	CD-NE	-5.23	1.39	1.46
1	P	1199	ARG	CD-NE	-5.22	1.39	1.46
1	B	250	ARG	CD-NE	-5.20	1.39	1.46
1	P	243	ARG	CD-NE	-5.18	1.39	1.46
1	P	1393	ARG	CD-NE	-5.18	1.39	1.46
3	F	164	ARG	CD-NE	-5.17	1.39	1.46
1	B	1221	ARG	CD-NE	-5.16	1.39	1.46
3	F	161	ARG	CD-NE	-5.16	1.39	1.46
1	P	96	ARG	CD-NE	-5.15	1.39	1.46
1	B	1390	ARG	CD-NE	-5.14	1.39	1.46
3	E	60	ARG	CD-NE	-5.13	1.39	1.46
3	E	67	ARG	CD-NE	-5.13	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	ARG	CD-NE	-5.13	1.39	1.46
1	B	1393	ARG	CD-NE	-5.13	1.39	1.46
1	B	96	ARG	CD-NE	-5.13	1.39	1.46
3	F	31	ARG	CD-NE	-5.11	1.39	1.46
1	P	1221	ARG	CD-NE	-5.09	1.39	1.46
3	Q	31	ARG	CD-NE	-5.09	1.39	1.46
3	Q	67	ARG	CD-NE	-5.09	1.39	1.46
1	B	243	ARG	CD-NE	-5.08	1.39	1.46
3	R	31	ARG	CD-NE	-5.08	1.39	1.46
1	B	1250	ARG	CD-NE	-5.08	1.39	1.46
3	F	142	SER	CA-CB	-5.07	1.46	1.52
1	B	229	ARG	CD-NE	-5.07	1.39	1.46
3	Q	206	ARG	CD-NE	-5.06	1.39	1.46
3	E	31	ARG	CD-NE	-5.06	1.39	1.46
1	B	1131	ARG	CD-NE	-5.05	1.39	1.46
1	P	1131	ARG	CD-NE	-5.05	1.39	1.46
3	F	77	PRO	CA-CB	-5.04	1.47	1.53
3	E	206	ARG	CD-NE	-5.03	1.39	1.46

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	295	ARG	CA-C-N	22.15	147.90	120.88
2	C	295	ARG	C-N-CA	22.15	147.90	120.88
2	D	295	ARG	CA-C-N	22.04	147.77	120.88
2	D	295	ARG	C-N-CA	22.04	147.77	120.88
1	O	589	GLN	O-C-N	10.01	132.38	122.07
1	A	589	GLN	O-C-N	9.99	132.35	122.07
3	R	82	LEU	CA-C-N	9.46	129.40	122.59
3	R	82	LEU	C-N-CA	9.46	129.40	122.59
3	F	82	LEU	CA-C-N	9.42	129.37	122.59
3	F	82	LEU	C-N-CA	9.42	129.37	122.59
1	P	469	ASP	CA-CB-CG	8.88	121.48	112.60
1	B	469	ASP	CA-CB-CG	8.79	121.39	112.60
1	B	1127	ASN	CA-CB-CG	8.41	121.01	112.60
1	P	1127	ASN	CA-CB-CG	8.38	120.98	112.60
1	A	589	GLN	CA-C-N	-7.85	109.63	120.38
1	A	589	GLN	C-N-CA	-7.85	109.63	120.38
1	B	259	PHE	CA-CB-CG	7.84	121.64	113.80
1	O	589	GLN	CA-C-N	-7.83	109.66	120.38
1	O	589	GLN	C-N-CA	-7.83	109.66	120.38
1	P	259	PHE	CA-CB-CG	7.81	121.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	63	DG	C4'-C3'-O3'	7.72	121.58	110.00
2	C	120	PHE	CA-CB-CG	-7.54	106.26	113.80
1	P	187	ARG	NE-CZ-NH2	7.50	125.95	119.20
1	P	232	PHE	CA-CB-CG	7.44	121.24	113.80
1	B	232	PHE	CA-CB-CG	7.20	121.00	113.80
5	K	47	DC	O3'-P-O5'	-7.19	93.22	104.00
5	K	64	DG	O5'-C5'-C4'	7.05	121.37	110.80
2	D	294	ASN	N-CA-C	-7.04	103.65	111.82
2	C	294	ASN	N-CA-C	-7.00	103.70	111.82
3	R	160	ASN	CA-CB-CG	6.92	119.52	112.60
3	R	89	SER	CA-C-N	6.91	129.87	120.54
3	R	89	SER	C-N-CA	6.91	129.87	120.54
5	K	62	DT	C4'-C3'-O3'	-6.85	99.72	110.00
1	P	197	PHE	CA-CB-CG	6.81	120.61	113.80
1	P	219	ASP	CA-CB-CG	6.75	119.35	112.60
1	P	225	ASN	CA-CB-CG	6.74	119.34	112.60
1	P	301	GLN	O-C-N	-6.72	115.00	122.12
2	D	176	ARG	CB-CG-CD	6.71	126.74	111.30
3	F	160	ASN	CA-CB-CG	6.71	119.31	112.60
1	P	94	ASN	CA-CB-CG	6.70	119.30	112.60
1	P	1253	ASN	CA-CB-CG	6.68	119.28	112.60
3	R	187	PHE	CA-CB-CG	6.68	120.48	113.80
1	B	197	PHE	CA-CB-CG	6.67	120.47	113.80
1	B	301	GLN	O-C-N	-6.65	115.07	122.12
3	Q	44	HIS	CA-CB-CG	6.65	120.45	113.80
3	E	44	HIS	CA-CB-CG	6.64	120.44	113.80
1	P	158	ASP	CA-CB-CG	6.63	119.23	112.60
3	E	195	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	225	ASN	CA-CB-CG	6.59	119.19	112.60
3	Q	195	ASP	CA-CB-CG	6.55	119.15	112.60
3	E	73	PHE	CA-CB-CG	6.54	120.34	113.80
1	P	1187	PHE	CA-CB-CG	6.51	120.31	113.80
1	P	54	ASP	CA-CB-CG	6.49	119.09	112.60
3	Q	73	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	94	ASN	CA-CB-CG	6.48	119.08	112.60
1	B	1187	PHE	CA-CB-CG	6.48	120.28	113.80
5	K	64	DG	C5'-C4'-O4'	6.47	119.10	109.40
3	Q	43	ASN	CA-CB-CG	6.47	119.07	112.60
3	E	196	ASP	CA-CB-CG	6.47	119.07	112.60
1	P	1207	ASP	CA-CB-CG	6.47	119.07	112.60
3	Q	196	ASP	CA-CB-CG	6.47	119.07	112.60
3	F	187	PHE	CA-CB-CG	6.45	120.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	1164	ASN	CA-CB-CG	6.45	119.05	112.60
3	E	43	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	1164	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	966	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	B	1207	ASP	CA-CB-CG	6.41	119.01	112.60
2	D	325	ASP	CA-CB-CG	6.39	118.99	112.60
6	L	43	DG	C2'-C3'-O3'	-6.38	101.93	111.50
1	B	175	HIS	CA-CB-CG	6.36	120.16	113.80
1	B	1210	ASP	CA-CB-CG	6.33	118.93	112.60
1	P	1201	ASP	N-CA-C	6.33	118.70	111.11
1	B	54	ASP	CA-CB-CG	6.32	118.92	112.60
1	P	1210	ASP	CA-CB-CG	6.32	118.92	112.60
1	P	966	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	B	187	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	B	1201	ASP	N-CA-C	6.30	118.67	111.11
1	B	1193	HIS	CA-CB-CG	6.29	120.09	113.80
1	B	255	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	1131	ARG	CD-NE-CZ	6.28	133.19	124.40
1	P	1131	ARG	CD-NE-CZ	6.28	133.19	124.40
3	R	145	ASP	CA-CB-CG	6.26	118.86	112.60
1	P	1193	HIS	CA-CB-CG	6.25	120.05	113.80
1	P	234	ASP	CA-CB-CG	6.24	118.84	112.60
2	C	325	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	97	HIS	CA-C-N	6.23	131.59	123.00
1	B	97	HIS	C-N-CA	6.23	131.59	123.00
1	P	168	PHE	CA-CB-CG	6.21	120.01	113.80
3	Q	57	PHE	CA-CB-CG	6.21	120.01	113.80
3	E	57	PHE	CA-CB-CG	6.21	120.01	113.80
1	P	255	ASP	CA-CB-CG	6.19	118.79	112.60
5	K	47	DC	C2'-C3'-O3'	-6.19	102.21	111.50
3	R	136	PHE	CA-CB-CG	6.18	119.98	113.80
5	K	46	DA	O3'-P-O5'	6.18	113.27	104.00
1	P	243	ARG	CA-CB-CG	6.17	126.44	114.10
1	P	1242	ASN	CA-CB-CG	6.17	118.77	112.60
1	B	243	ARG	CA-CB-CG	6.17	126.44	114.10
1	B	1132	ARG	CD-NE-CZ	6.15	133.01	124.40
1	B	1221	ARG	CD-NE-CZ	6.14	133.00	124.40
1	P	1221	ARG	CD-NE-CZ	6.14	132.99	124.40
1	B	164	GLN	CA-C-N	6.13	131.46	123.00
1	B	164	GLN	C-N-CA	6.13	131.46	123.00
1	B	234	ASP	CA-CB-CG	6.12	118.72	112.60
1	P	198	TYR	N-CA-CB	6.11	118.87	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	1132	ARG	CD-NE-CZ	6.10	132.94	124.40
1	P	97	HIS	CA-C-N	6.09	131.41	123.00
1	P	97	HIS	C-N-CA	6.09	131.41	123.00
1	P	1339	ASP	CA-CB-CG	6.08	118.68	112.60
3	E	62	ASN	CA-CB-CG	6.08	118.67	112.60
1	P	164	GLN	CA-C-N	6.08	131.38	123.00
1	P	164	GLN	C-N-CA	6.08	131.38	123.00
1	P	1328	ARG	CD-NE-CZ	6.07	132.90	124.40
1	P	1331	GLN	N-CA-C	6.07	123.73	110.80
1	P	201	ILE	N-CA-CB	6.07	117.65	110.55
1	P	243	ARG	CG-CD-NE	6.07	125.35	112.00
1	B	229	ARG	CD-NE-CZ	6.06	132.89	124.40
1	B	201	ILE	N-CA-CB	6.06	117.64	110.55
3	R	27	ASP	CA-CB-CG	6.05	118.66	112.60
1	B	1056	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	B	1328	ARG	CD-NE-CZ	6.05	132.87	124.40
3	Q	62	ASN	CA-CB-CG	6.05	118.65	112.60
1	B	243	ARG	CG-CD-NE	6.04	125.30	112.00
3	R	147	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	105	ARG	CD-NE-CZ	6.04	132.86	124.40
1	B	224	GLU	CA-C-N	6.03	131.50	123.00
1	B	224	GLU	C-N-CA	6.03	131.50	123.00
3	R	156	ARG	CD-NE-CZ	6.03	132.84	124.40
1	P	224	GLU	CA-C-N	6.02	131.48	123.00
1	P	224	GLU	C-N-CA	6.02	131.48	123.00
3	E	138	ASN	CA-CB-CG	6.00	118.61	112.60
1	B	198	TYR	N-CA-CB	6.00	118.71	110.01
3	F	145	ASP	CA-CB-CG	6.00	118.60	112.60
3	E	138	ASN	CB-CA-C	5.99	120.64	109.86
1	B	263	ILE	N-CA-CB	5.98	117.14	110.62
1	P	1056	ARG	NE-CZ-NH2	5.98	124.58	119.20
3	E	42	ASP	CA-C-N	5.97	128.21	120.44
3	E	42	ASP	C-N-CA	5.97	128.21	120.44
1	P	1341	ARG	CD-NE-CZ	5.97	132.76	124.40
1	P	118	ILE	CA-C-N	5.96	130.85	122.74
1	P	118	ILE	C-N-CA	5.96	130.85	122.74
3	F	156	ARG	CD-NE-CZ	5.96	132.75	124.40
3	Q	66	ILE	CA-C-N	5.96	131.78	123.07
3	Q	66	ILE	C-N-CA	5.96	131.78	123.07
1	P	263	ILE	N-CA-CB	5.96	117.12	110.62
3	Q	42	ASP	CA-C-N	5.96	128.19	120.44
3	Q	42	ASP	C-N-CA	5.96	128.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	96	ARG	CD-NE-CZ	5.96	132.74	124.40
3	Q	42	ASP	CA-CB-CG	5.95	118.55	112.60
1	P	103	GLY	N-CA-C	5.95	119.44	110.75
3	E	66	ILE	CA-C-N	5.95	131.75	123.07
3	E	66	ILE	C-N-CA	5.95	131.75	123.07
3	E	42	ASP	CA-CB-CG	5.95	118.55	112.60
1	B	122	MET	CA-C-N	5.94	131.25	122.99
1	B	122	MET	C-N-CA	5.94	131.25	122.99
3	F	27	ASP	CA-CB-CG	5.94	118.54	112.60
1	P	165	PHE	CA-CB-CG	5.93	119.73	113.80
1	B	96	ARG	CD-NE-CZ	5.93	132.70	124.40
1	B	118	ILE	CA-C-N	5.92	130.79	122.74
1	B	118	ILE	C-N-CA	5.92	130.79	122.74
3	E	60	ARG	CD-NE-CZ	5.92	132.68	124.40
3	Q	63	VAL	CA-C-N	5.92	130.29	122.30
3	Q	63	VAL	C-N-CA	5.92	130.29	122.30
1	P	122	MET	CA-C-N	5.91	131.21	122.99
1	P	122	MET	C-N-CA	5.91	131.21	122.99
1	P	1339	ASP	CA-C-N	5.91	128.20	120.28
1	P	1339	ASP	C-N-CA	5.91	128.20	120.28
3	Q	60	ARG	CD-NE-CZ	5.91	132.67	124.40
2	C	124	ARG	CA-CB-CG	5.91	125.92	114.10
3	R	31	ARG	CD-NE-CZ	5.91	132.67	124.40
1	P	1390	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	P	1244	ILE	N-CA-CB	5.90	117.45	110.55
1	P	1250	ARG	CD-NE-CZ	5.89	132.64	124.40
1	B	1339	ASP	CA-C-N	5.88	128.16	120.28
1	B	1339	ASP	C-N-CA	5.88	128.16	120.28
1	B	103	GLY	N-CA-C	5.87	119.16	110.42
3	E	63	VAL	CA-C-N	5.87	130.22	122.30
3	E	63	VAL	C-N-CA	5.87	130.22	122.30
5	K	32	DA	C5'-C4'-C3'	-5.87	106.10	114.90
3	F	31	ARG	CD-NE-CZ	5.86	132.61	124.40
1	B	1244	ILE	N-CA-CB	5.85	117.40	110.55
3	Q	31	ARG	CD-NE-CZ	5.85	132.59	124.40
6	L	30	DG	C4'-C3'-O3'	-5.84	101.24	110.00
1	B	548	ARG	CA-C-N	5.82	130.54	121.76
1	B	548	ARG	C-N-CA	5.82	130.54	121.76
6	L	47	DT	C5'-C4'-O4'	5.81	118.12	109.40
3	E	31	ARG	CD-NE-CZ	5.81	132.53	124.40
3	F	147	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	166	LYS	CA-C-N	5.80	131.18	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	LYS	C-N-CA	5.80	131.18	122.99
1	B	1395	LYS	CA-CB-CG	5.80	125.71	114.10
1	B	1192	GLN	CA-C-N	5.80	128.37	120.54
1	B	1192	GLN	C-N-CA	5.80	128.37	120.54
1	P	548	ARG	CA-C-N	5.80	130.52	121.76
1	P	548	ARG	C-N-CA	5.80	130.52	121.76
3	Q	74	TYR	CA-C-N	5.79	130.71	122.72
3	Q	74	TYR	C-N-CA	5.79	130.71	122.72
2	C	294	ASN	CA-C-N	5.79	130.79	122.40
2	C	294	ASN	C-N-CA	5.79	130.79	122.40
6	L	56	DT	O3'-P-O5'	-5.78	95.33	104.00
1	B	1250	ARG	CD-NE-CZ	5.78	132.49	124.40
1	B	235	MET	CA-C-N	5.77	127.94	120.44
1	B	235	MET	C-N-CA	5.77	127.94	120.44
3	Q	25	GLU	CA-C-N	5.77	127.94	120.44
3	Q	25	GLU	C-N-CA	5.77	127.94	120.44
3	E	25	GLU	CA-C-N	5.77	127.94	120.44
3	E	25	GLU	C-N-CA	5.77	127.94	120.44
3	R	92	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	1197	ARG	CA-C-N	5.76	128.22	120.50
1	B	1197	ARG	C-N-CA	5.76	128.22	120.50
3	F	129	ASP	CA-C-N	5.76	127.99	120.28
3	F	129	ASP	C-N-CA	5.76	127.99	120.28
1	P	153	LEU	CA-C-N	5.75	127.92	120.44
1	P	153	LEU	C-N-CA	5.75	127.92	120.44
1	P	1197	ARG	CA-C-N	5.75	128.20	120.50
1	P	1197	ARG	C-N-CA	5.75	128.20	120.50
1	P	235	MET	CA-C-N	5.75	127.91	120.44
1	P	235	MET	C-N-CA	5.75	127.91	120.44
2	D	294	ASN	CA-C-N	5.74	130.73	122.40
2	D	294	ASN	C-N-CA	5.74	130.73	122.40
1	B	165	PHE	CA-CB-CG	5.73	119.53	113.80
1	P	1192	GLN	CA-C-N	5.72	128.26	120.54
1	P	1192	GLN	C-N-CA	5.72	128.26	120.54
3	E	27	ASP	CA-CB-CG	5.70	118.30	112.60
3	R	161	ARG	N-CA-CB	5.70	118.43	109.94
3	E	74	TYR	CA-C-N	5.70	130.58	122.72
3	E	74	TYR	C-N-CA	5.70	130.58	122.72
3	R	129	ASP	CA-C-N	5.69	127.90	120.28
3	R	129	ASP	C-N-CA	5.69	127.90	120.28
2	C	137	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	B	100	VAL	CA-C-N	5.68	131.05	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	VAL	C-N-CA	5.68	131.05	123.10
3	Q	27	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	103	GLY	CA-C-N	5.67	130.97	122.58
1	B	103	GLY	C-N-CA	5.67	130.97	122.58
3	F	161	ARG	N-CA-CB	5.67	118.39	109.94
3	Q	56	GLU	CA-C-N	5.67	128.13	120.65
3	Q	56	GLU	C-N-CA	5.67	128.13	120.65
1	P	100	VAL	CA-C-N	5.66	131.02	123.10
1	P	100	VAL	C-N-CA	5.66	131.02	123.10
2	C	330	GLU	N-CA-CB	5.66	118.25	109.48
1	P	163	VAL	CA-C-N	5.65	130.97	123.05
1	P	163	VAL	C-N-CA	5.65	130.97	123.05
2	D	330	GLU	N-CA-CB	5.65	118.24	109.48
3	F	26	LEU	CA-C-N	5.65	127.78	120.44
3	F	26	LEU	C-N-CA	5.65	127.78	120.44
1	B	249	ILE	N-CA-CB	5.65	117.16	110.55
1	B	244	ILE	N-CA-CB	5.64	116.55	110.62
1	P	1387	GLU	N-CA-CB	5.64	118.42	110.12
1	P	101	VAL	CA-C-N	5.64	130.18	122.34
1	P	101	VAL	C-N-CA	5.64	130.18	122.34
1	P	1287	LEU	N-CA-CB	5.64	118.19	110.01
1	P	528	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	B	1188	ILE	N-CA-CB	5.63	116.77	110.51
3	E	67	ARG	CG-CD-NE	5.63	124.40	112.00
1	P	244	ILE	N-CA-CB	5.63	116.53	110.62
6	L	33	DG	C4'-C3'-O3'	-5.63	101.56	110.00
3	Q	67	ARG	CG-CD-NE	5.62	124.38	112.00
3	Q	46	PHE	N-CA-CB	5.62	118.32	109.94
3	R	26	LEU	CA-C-N	5.62	127.75	120.44
3	R	26	LEU	C-N-CA	5.62	127.75	120.44
3	E	56	GLU	CA-C-N	5.62	128.07	120.65
3	E	56	GLU	C-N-CA	5.62	128.07	120.65
2	D	137	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	P	256	ARG	CD-NE-CZ	5.62	132.26	124.40
1	B	256	ARG	CD-NE-CZ	5.61	132.26	124.40
3	F	92	ASP	CA-CB-CG	5.61	118.20	112.60
1	B	163	VAL	CA-C-N	5.60	130.90	123.05
1	B	163	VAL	C-N-CA	5.60	130.90	123.05
1	P	1126	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	101	VAL	CA-C-N	5.60	130.13	122.34
1	B	101	VAL	C-N-CA	5.60	130.13	122.34
1	P	249	ILE	N-CA-CB	5.60	117.10	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1387	GLU	N-CA-CB	5.60	118.35	110.12
1	P	1188	ILE	N-CA-CB	5.59	116.72	110.51
3	E	46	PHE	N-CA-CB	5.59	118.27	109.94
3	F	88	LEU	CA-C-N	5.59	130.67	121.39
3	F	88	LEU	C-N-CA	5.59	130.67	121.39
6	L	39	DG	C4'-C3'-O3'	-5.59	101.62	110.00
1	P	103	GLY	CA-C-N	5.58	130.84	122.58
1	P	103	GLY	C-N-CA	5.58	130.84	122.58
5	K	57	DC	C4'-C3'-O3'	-5.57	101.64	110.00
1	B	1126	ASP	CA-CB-CG	5.56	118.16	112.60
1	P	149	PRO	CA-C-N	5.56	127.67	120.44
1	P	149	PRO	C-N-CA	5.56	127.67	120.44
3	F	24	PRO	CA-C-N	5.56	127.67	120.44
3	F	24	PRO	C-N-CA	5.56	127.67	120.44
1	B	104	VAL	CA-C-N	5.56	130.16	122.77
1	B	104	VAL	C-N-CA	5.56	130.16	122.77
1	B	528	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	B	193	ASP	CA-CB-CG	5.56	118.16	112.60
2	D	287	THR	CA-CB-OG1	5.56	117.94	109.60
3	R	148	LYS	CG-CD-CE	5.55	124.08	111.30
2	C	287	THR	CA-CB-OG1	5.55	117.93	109.60
2	C	295	ARG	CB-CA-C	5.55	120.28	111.51
1	P	99	ARG	CA-C-N	5.55	130.71	122.99
1	P	99	ARG	C-N-CA	5.55	130.71	122.99
1	P	186	LYS	CA-CB-CG	5.54	125.19	114.10
3	R	129	ASP	CA-CB-CG	5.54	118.14	112.60
6	L	43	DG	O3'-P-O5'	-5.54	95.69	104.00
1	B	1216	GLU	CA-C-N	5.53	127.53	120.56
1	B	1216	GLU	C-N-CA	5.53	127.53	120.56
1	P	1216	GLU	CA-C-N	5.51	127.51	120.56
1	P	1216	GLU	C-N-CA	5.51	127.51	120.56
1	P	1328	ARG	CB-CG-CD	5.51	123.97	111.30
1	B	99	ARG	CA-C-N	5.50	130.64	122.99
1	B	99	ARG	C-N-CA	5.50	130.64	122.99
1	B	228	VAL	CA-C-N	5.50	127.59	120.44
1	B	228	VAL	C-N-CA	5.50	127.59	120.44
1	B	149	PRO	CA-C-N	5.50	127.59	120.44
1	B	149	PRO	C-N-CA	5.50	127.59	120.44
1	P	167	GLN	CA-C-N	5.50	130.31	122.72
1	P	167	GLN	C-N-CA	5.50	130.31	122.72
1	P	1396	ASP	CA-C-N	5.50	130.26	123.12
1	P	1396	ASP	C-N-CA	5.50	130.26	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	295	ARG	CB-CA-C	5.49	120.19	111.51
1	B	1399	PRO	CA-C-N	5.49	129.04	120.75
1	B	1399	PRO	C-N-CA	5.49	129.04	120.75
1	B	403	GLN	OE1-CD-NE2	-5.49	117.11	122.60
3	R	128	ALA	CA-C-N	5.48	129.26	121.42
3	R	128	ALA	C-N-CA	5.48	129.26	121.42
1	P	117	ASP	CA-C-N	5.48	130.61	122.99
1	P	117	ASP	C-N-CA	5.48	130.61	122.99
1	B	1197	ARG	CD-NE-CZ	5.48	132.07	124.40
1	B	1396	ASP	CA-C-N	5.47	130.23	123.12
1	B	1396	ASP	C-N-CA	5.47	130.23	123.12
3	F	128	ALA	CA-C-N	5.47	129.24	121.42
3	F	128	ALA	C-N-CA	5.47	129.24	121.42
3	Q	44	HIS	CA-C-N	5.46	127.54	120.44
3	Q	44	HIS	C-N-CA	5.46	127.54	120.44
1	B	1212	ILE	N-CA-CB	5.46	116.35	110.62
3	E	44	HIS	CA-C-N	5.46	127.54	120.44
3	E	44	HIS	C-N-CA	5.46	127.54	120.44
1	P	1212	ILE	N-CA-CB	5.46	116.35	110.62
3	E	43	ASN	CA-C-N	5.45	127.53	120.44
3	E	43	ASN	C-N-CA	5.45	127.53	120.44
3	Q	43	ASN	CA-C-N	5.45	127.53	120.44
3	Q	43	ASN	C-N-CA	5.45	127.53	120.44
2	D	323	LEU	CA-C-N	5.45	128.50	120.82
2	D	323	LEU	C-N-CA	5.45	128.50	120.82
1	P	227	GLY	CA-C-N	5.45	127.42	120.56
1	P	227	GLY	C-N-CA	5.45	127.42	120.56
3	R	155	VAL	N-CA-CB	5.45	116.92	110.55
5	K	56	DT	C2'-C3'-O3'	5.44	119.66	111.50
3	Q	46	PHE	CA-CB-CG	5.44	119.24	113.80
1	P	403	GLN	OE1-CD-NE2	-5.43	117.17	122.60
3	E	46	PHE	CA-CB-CG	5.43	119.23	113.80
3	R	24	PRO	CA-C-N	5.43	127.50	120.44
3	R	24	PRO	C-N-CA	5.43	127.50	120.44
3	F	155	VAL	N-CA-CB	5.42	116.90	110.55
1	P	1399	PRO	CA-C-N	5.42	128.94	120.75
1	P	1399	PRO	C-N-CA	5.42	128.94	120.75
2	C	116	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	117	ASP	CA-C-N	5.41	130.51	122.99
1	B	117	ASP	C-N-CA	5.41	130.51	122.99
1	P	218	ARG	CA-C-N	5.40	127.52	120.28
1	P	218	ARG	C-N-CA	5.40	127.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	1197	ARG	CD-NE-CZ	5.40	131.95	124.40
1	P	1384	SER	N-CA-CB	5.39	117.83	110.01
1	B	1221	ARG	CA-CB-CG	5.38	124.87	114.10
2	C	323	LEU	CA-C-N	5.38	128.41	120.82
2	C	323	LEU	C-N-CA	5.38	128.41	120.82
1	P	1221	ARG	CA-CB-CG	5.38	124.86	114.10
1	P	1322	GLN	CA-CB-CG	5.38	124.86	114.10
3	Q	139	GLN	CB-CG-CD	5.38	121.74	112.60
1	B	227	GLY	CA-C-N	5.38	127.33	120.56
1	B	227	GLY	C-N-CA	5.38	127.33	120.56
3	F	91	LEU	CA-C-N	5.37	127.42	120.44
3	F	91	LEU	C-N-CA	5.37	127.42	120.44
1	B	48	VAL	N-CA-CB	5.37	117.84	110.54
1	B	363	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	B	1322	GLN	CA-CB-CG	5.36	124.83	114.10
3	F	129	ASP	CA-CB-CG	5.36	117.96	112.60
1	P	243	ARG	CD-NE-CZ	5.36	131.91	124.40
1	B	250	ARG	CA-C-N	5.36	127.26	120.72
1	B	250	ARG	C-N-CA	5.36	127.26	120.72
3	Q	62	ASN	CA-C-N	5.35	130.41	122.71
3	Q	62	ASN	C-N-CA	5.35	130.41	122.71
1	B	233	GLN	CA-C-N	5.35	127.71	120.65
1	B	233	GLN	C-N-CA	5.35	127.71	120.65
3	R	91	LEU	CA-C-N	5.35	127.39	120.44
3	R	91	LEU	C-N-CA	5.35	127.39	120.44
1	B	194	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	B	186	LYS	CA-CB-CG	5.34	124.78	114.10
1	P	363	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	P	1241	ALA	CA-C-N	5.34	127.70	120.65
1	P	1241	ALA	C-N-CA	5.34	127.70	120.65
1	B	194	ARG	N-CA-CB	-5.34	102.28	110.12
2	C	299	GLN	CA-C-N	5.33	127.74	120.54
2	C	299	GLN	C-N-CA	5.33	127.74	120.54
1	B	243	ARG	CD-NE-CZ	5.33	131.87	124.40
3	F	98	ILE	N-CA-CB	5.33	116.79	110.55
2	D	299	GLN	CA-C-N	5.32	127.72	120.54
2	D	299	GLN	C-N-CA	5.32	127.72	120.54
1	P	233	GLN	CA-C-N	5.32	127.67	120.65
1	P	233	GLN	C-N-CA	5.32	127.67	120.65
3	R	123	GLU	CA-C-N	5.32	127.72	120.54
3	R	123	GLU	C-N-CA	5.32	127.72	120.54
1	P	156	ARG	CA-C-N	5.31	127.67	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	156	ARG	C-N-CA	5.31	127.67	120.44
3	R	34	ARG	N-CA-CB	5.31	117.85	109.83
3	F	148	LYS	CG-CD-CE	5.31	123.52	111.30
3	Q	67	ARG	CD-NE-CZ	5.31	131.84	124.40
1	P	48	VAL	N-CA-CB	5.31	117.76	110.54
3	R	138	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	1328	ARG	CB-CG-CD	5.31	123.50	111.30
3	E	67	ARG	CA-CB-CG	5.30	124.71	114.10
3	F	123	GLU	CA-C-N	5.30	127.70	120.54
3	F	123	GLU	C-N-CA	5.30	127.70	120.54
5	K	56	DT	C4'-C3'-O3'	-5.30	102.05	110.00
3	R	144	SER	CA-C-N	5.30	127.69	120.54
3	R	144	SER	C-N-CA	5.30	127.69	120.54
3	F	161	ARG	CA-C-N	5.29	127.37	120.28
3	F	161	ARG	C-N-CA	5.29	127.37	120.28
1	P	162	GLY	CA-C-N	5.29	128.96	121.66
1	P	162	GLY	C-N-CA	5.29	128.96	121.66
1	B	1220	ALA	CA-C-N	5.29	127.68	120.54
1	B	1220	ALA	C-N-CA	5.29	127.68	120.54
1	P	250	ARG	CA-C-N	5.29	127.17	120.72
1	P	250	ARG	C-N-CA	5.29	127.17	120.72
3	E	67	ARG	CD-NE-CZ	5.29	131.80	124.40
1	B	1188	ILE	CA-C-N	5.29	127.31	120.44
1	B	1188	ILE	C-N-CA	5.29	127.31	120.44
2	D	123	LEU	CB-CG-CD2	-5.29	94.84	110.70
2	C	290	ASP	N-CA-C	5.28	118.88	112.23
1	P	1188	ILE	CA-C-N	5.28	127.30	120.44
1	P	1188	ILE	C-N-CA	5.28	127.30	120.44
2	D	290	ASP	N-CA-C	5.28	118.88	112.23
3	R	85	ARG	CA-CB-CG	5.28	124.65	114.10
3	F	144	SER	CA-C-N	5.27	127.66	120.54
3	F	144	SER	C-N-CA	5.27	127.66	120.54
3	E	62	ASN	CA-C-N	5.27	130.30	122.71
3	E	62	ASN	C-N-CA	5.27	130.30	122.71
3	F	34	ARG	N-CA-CB	5.27	117.79	109.83
3	R	161	ARG	CA-C-N	5.27	127.34	120.28
3	R	161	ARG	C-N-CA	5.27	127.34	120.28
1	P	1248	ILE	N-CA-CB	5.26	117.70	110.54
2	D	116	ARG	NE-CZ-NH2	5.26	123.93	119.20
3	F	94	MET	CA-C-N	5.26	127.19	120.56
3	F	94	MET	C-N-CA	5.26	127.19	120.56
1	P	1164	ASN	N-CA-CB	5.25	117.73	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	147	ASP	CA-C-N	5.25	127.31	120.28
3	F	147	ASP	C-N-CA	5.25	127.31	120.28
3	R	156	ARG	CA-C-N	5.25	127.58	120.65
3	R	156	ARG	C-N-CA	5.25	127.58	120.65
3	Q	67	ARG	CA-CB-CG	5.25	124.59	114.10
3	F	29	GLN	CA-C-N	5.24	127.26	120.44
3	F	29	GLN	C-N-CA	5.24	127.26	120.44
5	K	26	DC	C5'-C4'-O4'	5.24	117.26	109.40
5	K	63	DG	C4-N9-C1'	-5.24	119.14	127.00
3	R	147	ASP	CA-C-N	5.24	127.31	120.28
3	R	147	ASP	C-N-CA	5.24	127.31	120.28
1	P	1254	ARG	N-CA-CB	5.24	117.61	110.01
3	R	29	GLN	CA-C-N	5.24	127.25	120.44
3	R	29	GLN	C-N-CA	5.24	127.25	120.44
1	A	966	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	B	191	ALA	CA-C-N	5.24	127.30	120.28
1	B	191	ALA	C-N-CA	5.24	127.30	120.28
1	P	1220	ALA	CA-C-N	5.24	127.61	120.54
1	P	1220	ALA	C-N-CA	5.24	127.61	120.54
6	L	48	DC	C5'-C4'-O4'	5.23	117.24	109.40
2	C	151	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	P	1397	ILE	CA-C-N	5.22	131.36	122.06
1	P	1397	ILE	C-N-CA	5.22	131.36	122.06
1	B	234	ASP	CA-C-N	5.22	127.27	120.28
1	B	234	ASP	C-N-CA	5.22	127.27	120.28
3	R	94	MET	CA-C-N	5.22	127.13	120.56
3	R	94	MET	C-N-CA	5.22	127.13	120.56
3	E	29	GLN	CA-C-N	5.21	127.21	120.44
3	E	29	GLN	C-N-CA	5.21	127.21	120.44
2	D	320	ALA	CA-C-N	5.20	128.26	120.87
2	D	320	ALA	C-N-CA	5.20	128.26	120.87
1	B	194	ARG	CA-C-N	5.20	127.20	120.44
1	B	194	ARG	C-N-CA	5.20	127.20	120.44
5	K	62	DT	C2'-C3'-O3'	5.20	119.30	111.50
3	F	156	ARG	CA-C-N	5.20	127.51	120.65
3	F	156	ARG	C-N-CA	5.20	127.51	120.65
1	P	173	ASP	CA-C-N	5.20	127.19	120.44
1	P	173	ASP	C-N-CA	5.20	127.19	120.44
1	B	1187	PHE	CA-C-N	5.19	127.30	120.60
1	B	1187	PHE	C-N-CA	5.19	127.30	120.60
3	Q	29	GLN	CA-C-N	5.19	127.18	120.44
3	Q	29	GLN	C-N-CA	5.19	127.18	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	234	ASP	CA-C-N	5.18	127.23	120.28
1	P	234	ASP	C-N-CA	5.18	127.23	120.28
3	F	80	THR	CA-C-N	5.18	128.46	121.05
3	F	80	THR	C-N-CA	5.18	128.46	121.05
1	P	240	ARG	N-CA-CB	5.18	117.52	110.01
1	B	1164	ASN	N-CA-CB	5.18	117.62	110.17
1	P	1250	ARG	N-CA-CB	5.17	117.65	109.94
3	E	206	ARG	N-CA-CB	5.17	117.72	110.12
3	Q	26	LEU	CA-C-N	5.17	127.16	120.44
3	Q	26	LEU	C-N-CA	5.17	127.16	120.44
3	E	26	LEU	CA-C-N	5.17	127.16	120.44
3	E	26	LEU	C-N-CA	5.17	127.16	120.44
2	D	151	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	P	559	GLN	OE1-CD-NE2	-5.17	117.44	122.60
3	Q	206	ARG	N-CA-CB	5.17	117.71	110.12
1	B	1246	LYS	CA-C-N	5.16	127.15	120.44
1	B	1246	LYS	C-N-CA	5.16	127.15	120.44
2	C	6	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	P	1388	GLU	N-CA-CB	5.16	117.50	110.01
1	P	1286	LEU	CA-C-N	5.16	127.15	120.44
1	P	1286	LEU	C-N-CA	5.16	127.15	120.44
3	R	80	THR	CA-C-N	5.16	128.43	121.05
3	R	80	THR	C-N-CA	5.16	128.43	121.05
1	P	1391	ARG	CD-NE-CZ	5.15	131.61	124.40
3	R	154	LYS	CA-C-N	5.15	127.05	120.56
3	R	154	LYS	C-N-CA	5.15	127.05	120.56
1	O	932	ASP	CB-CA-C	5.14	115.64	109.31
1	O	966	ARG	NE-CZ-NH2	5.14	123.83	119.20
6	L	66	DT	C5'-C4'-O4'	5.13	117.10	109.40
6	L	59	DT	C5'-C4'-O4'	5.13	117.09	109.40
1	P	255	ASP	CA-C-N	5.13	127.11	120.44
1	P	255	ASP	C-N-CA	5.13	127.11	120.44
1	P	1187	PHE	CA-C-N	5.12	127.21	120.60
1	P	1187	PHE	C-N-CA	5.12	127.21	120.60
1	P	1190	VAL	N-CA-CB	5.12	116.54	110.55
1	B	192	SER	CA-C-N	5.12	127.09	120.44
1	B	192	SER	C-N-CA	5.12	127.09	120.44
1	P	521	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	240	ARG	N-CA-CB	5.11	117.42	110.01
1	B	521	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	559	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	B	1190	VAL	N-CA-CB	5.11	116.53	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	185	PRO	CA-C-N	5.10	131.07	122.87
1	P	185	PRO	C-N-CA	5.10	131.07	122.87
1	B	185	PRO	CA-C-N	5.09	131.06	122.87
1	B	185	PRO	C-N-CA	5.09	131.06	122.87
1	B	174	TYR	CA-C-N	5.09	127.10	120.28
1	B	174	TYR	C-N-CA	5.09	127.10	120.28
1	P	157	LEU	CA-C-N	5.08	127.09	120.28
1	P	157	LEU	C-N-CA	5.08	127.09	120.28
3	R	148	LYS	CA-C-N	5.08	127.05	120.44
3	R	148	LYS	C-N-CA	5.08	127.05	120.44
3	F	148	LYS	CA-C-N	5.08	127.04	120.44
3	F	148	LYS	C-N-CA	5.08	127.04	120.44
3	E	40	ASP	CA-C-N	5.08	127.39	120.54
3	E	40	ASP	C-N-CA	5.08	127.39	120.54
1	P	123	ILE	CA-C-N	5.08	130.55	122.94
1	P	123	ILE	C-N-CA	5.08	130.55	122.94
3	F	85	ARG	CA-CB-CG	5.07	124.25	114.10
1	P	1239	SER	CA-C-N	5.07	128.67	120.55
1	P	1239	SER	C-N-CA	5.07	128.67	120.55
3	Q	27	ASP	N-CA-CB	5.07	117.36	110.01
1	B	1388	GLU	N-CA-CB	5.07	117.36	110.01
3	E	27	ASP	N-CA-CB	5.07	117.36	110.01
5	K	18	DT	C5'-C4'-O4'	5.07	117.00	109.40
1	P	154	LYS	N-CA-CB	5.07	117.36	110.01
1	A	932	ASP	CB-CA-C	5.07	115.54	109.31
1	B	1250	ARG	N-CA-CB	5.07	117.49	109.94
1	P	174	TYR	CA-CB-CG	5.06	123.01	113.90
1	P	549	GLN	N-CA-C	-5.06	98.81	107.61
3	Q	139	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	1198	ILE	CA-C-N	5.05	128.47	120.89
1	B	1198	ILE	C-N-CA	5.05	128.47	120.89
6	L	68	DT	C5'-C4'-O4'	5.05	116.98	109.40
1	B	123	ILE	CA-C-N	5.04	130.51	122.94
1	B	123	ILE	C-N-CA	5.04	130.51	122.94
2	D	176	ARG	CA-CB-CG	-5.04	104.02	114.10
1	P	1198	ILE	CA-C-N	5.04	128.45	120.89
1	P	1198	ILE	C-N-CA	5.04	128.45	120.89
1	B	1239	SER	CA-C-N	5.04	128.61	120.55
1	B	1239	SER	C-N-CA	5.04	128.61	120.55
3	R	157	THR	CA-C-N	5.03	127.02	120.28
3	R	157	THR	C-N-CA	5.03	127.02	120.28
3	E	186	ARG	NE-CZ-NH2	5.03	123.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	31	ARG	CB-CG-CD	5.03	122.86	111.30
1	P	1336	GLU	CA-C-N	5.02	129.11	120.72
1	P	1336	GLU	C-N-CA	5.02	129.11	120.72
3	R	146	LEU	N-CA-CB	5.02	117.50	110.12
3	R	87	VAL	CA-C-N	5.02	128.82	120.94
3	R	87	VAL	C-N-CA	5.02	128.82	120.94
1	B	255	ASP	CA-C-N	5.02	126.97	120.44
1	B	255	ASP	C-N-CA	5.02	126.97	120.44
1	B	549	GLN	N-CA-C	-5.02	98.88	107.61
3	F	157	THR	CA-C-N	5.02	127.00	120.28
3	F	157	THR	C-N-CA	5.02	127.00	120.28
1	P	102	VAL	CA-C-N	5.02	128.55	120.97
1	P	102	VAL	C-N-CA	5.02	128.55	120.97
1	P	1207	ASP	N-CA-CB	5.02	117.45	110.07
3	Q	163	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	P	548	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	B	247	GLU	N-CA-CB	5.00	117.48	110.12
2	C	324	LEU	CA-C-N	5.00	130.44	122.59
2	C	324	LEU	C-N-CA	5.00	130.44	122.59
3	F	85	ARG	CD-NE-CZ	5.00	131.41	124.40
3	R	85	ARG	CD-NE-CZ	5.00	131.40	124.40
2	C	153	HIS	CB-CG-CD2	-5.00	124.70	131.20
5	K	15	DA	C2'-C3'-O3'	-5.00	104.00	111.50

There are no chirality outliers.

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1058	ARG	Sidechain
1	A	966	ARG	Sidechain
1	A	967	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	966	ARG	Sidechain
2	C	120	PHE	Sidechain
2	C	138	ARG	Sidechain
2	C	300	ARG	Sidechain
2	C	327	ARG	Sidechain
2	C	4	TYR	Sidechain
2	C	89	ARG	Sidechain
2	D	116	ARG	Sidechain
2	D	138	ARG	Sidechain
2	D	300	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	327	ARG	Sidechain
2	D	4	TYR	Sidechain
2	D	89	ARG	Sidechain
3	E	101	TYR	Sidechain
3	E	140	ARG	Sidechain
3	E	161	ARG	Sidechain
3	E	164	ARG	Sidechain
5	K	11	DT	Sidechain
5	K	12	DC	Sidechain
5	K	14	DG	Sidechain
5	K	18	DT	Sidechain
5	K	28	DC	Sidechain
5	K	29	DG	Sidechain
5	K	36	DC	Sidechain
5	K	4	DG	Sidechain
5	K	44	DA	Sidechain
5	K	45	DT	Sidechain
5	K	46	DA	Sidechain
5	K	49	DA	Sidechain
5	K	52	DC	Sidechain
5	K	54	DT	Sidechain
5	K	58	DC	Sidechain
5	K	63	DG	Sidechain
5	K	66	DA	Sidechain
5	K	71	DC	Sidechain
5	K	8	DA	Sidechain
6	L	29	DA	Sidechain
6	L	30	DG	Sidechain
6	L	31	DG	Sidechain
6	L	37	DA	Sidechain
6	L	38	DC	Sidechain
6	L	39	DG	Sidechain
6	L	46	DA	Sidechain
6	L	47	DT	Sidechain
6	L	49	DT	Sidechain
6	L	50	DT	Sidechain
6	L	51	DT	Sidechain
6	L	56	DT	Sidechain
6	L	59	DT	Sidechain
6	L	68	DT	Sidechain
6	L	76	DT	Sidechain
6	L	83	DT	Sidechain

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Mol	Chain	Res	Type	Group
6	L	86	DG	Sidechain
1	O	1058	ARG	Sidechain
1	O	966	ARG	Sidechain
1	O	967	ARG	Sidechain
1	P	189	ARG	Sidechain
1	P	528	ARG	Sidechain
1	P	966	ARG	Sidechain
3	Q	101	TYR	Sidechain
3	Q	140	ARG	Sidechain

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	11840	11707	11705	76	0
1	B	11840	11706	11705	95	0
1	O	11840	11707	11705	79	0
1	P	11840	11706	11705	99	0
2	C	3531	3451	3450	71	0
2	D	3531	3451	3450	71	0
3	E	1722	1719	1718	15	0
3	F	1619	1627	1626	15	0
3	Q	1722	1719	1718	16	0
3	R	1619	1627	1626	15	0
4	G	583	564	563	25	0
4	I	583	564	563	9	0
4	M	583	564	563	9	0
4	S	583	564	563	27	0
5	K	1496	815	816	13	0
6	L	1497	823	822	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	A	31	12	12	0	0
8	B	31	12	12	0	0
8	O	31	12	12	0	0
8	P	31	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	66557	64362	64346	526	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 4.

All (526) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:ALA:HB1	2:D:123:LEU:HG	1.19	1.18
2:C:162:TYR:HB3	2:D:124:ARG:HG3	1.23	1.15
2:C:158:ALA:CB	2:D:123:LEU:HG	1.82	1.10
2:C:131:ILE:HD11	2:D:163:SER:OG	1.56	1.06
4:S:36:4HH:CL3	4:S:40:VAL:HG21	1.87	1.05
4:G:36:4HH:CL3	4:G:40:VAL:HG21	1.87	1.04
1:B:1127:ASN:O	1:B:1127:ASN:ND2	1.91	1.03
1:P:1127:ASN:O	1:P:1127:ASN:ND2	1.91	1.03
2:C:138:ARG:NH1	2:D:134:ASN:ND2	2.10	0.99
2:C:162:TYR:HB3	2:D:124:ARG:CG	1.93	0.98
2:C:134:ASN:HD21	2:D:138:ARG:HH12	1.12	0.93
2:C:131:ILE:CD1	2:D:163:SER:OG	2.18	0.91
1:B:1107:ARG:NE	4:I:48:GLU:OE1	2.04	0.90
1:P:1107:ARG:NE	4:M:48:GLU:OE1	2.04	0.89
1:A:292:ARG:HD3	4:G:36:4HH:SU	2.14	0.88
1:O:292:ARG:HD3	4:S:36:4HH:SU	2.13	0.88
2:C:138:ARG:NH1	2:D:134:ASN:HD21	1.70	0.87
2:C:138:ARG:HH12	2:D:134:ASN:ND2	1.70	0.86
2:C:158:ALA:CB	2:D:123:LEU:CG	2.51	0.86
2:C:162:TYR:CB	2:D:124:ARG:HG3	2.04	0.86
2:C:162:TYR:CG	2:D:124:ARG:HB2	2.12	0.85
1:P:665:GLN:NE2	1:P:671:ASP:OD2	2.11	0.84
1:B:665:GLN:NE2	1:B:671:ASP:OD2	2.11	0.82
2:C:131:ILE:HD11	2:D:163:SER:HG	1.42	0.82
2:C:123:LEU:HG	2:D:158:ALA:HB1	1.61	0.82
1:P:1127:ASN:HD22	1:P:1127:ASN:C	1.88	0.81
2:C:158:ALA:HB2	2:D:123:LEU:CD2	2.13	0.79
2:C:134:ASN:HD21	2:D:138:ARG:NH1	1.80	0.78
2:C:123:LEU:HD21	2:D:158:ALA:HB2	1.67	0.77
4:G:36:4HH:HT3	4:G:56:ASP:OD1	1.85	0.76
1:B:1127:ASN:HD22	1:B:1127:ASN:C	1.88	0.76
4:S:36:4HH:HT3	4:S:56:ASP:OD1	1.85	0.76
1:A:1412:ASP:OD1	1:A:1413:ALA:N	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1412:ASP:OD1	1:O:1413:ALA:N	2.20	0.74
4:G:23:THR:OG1	4:G:25:ASN:OD1	2.04	0.73
2:C:131:ILE:HD11	2:D:163:SER:CB	2.18	0.73
1:B:172:THR:HG21	5:K:21:DC:H5"	1.71	0.72
2:C:124:ARG:HA	2:D:162:TYR:CB	2.20	0.72
4:S:36:4HH:CL3	4:S:40:VAL:CG2	2.68	0.71
1:A:288:ALA:HB1	4:G:44:MET:HE1	1.73	0.71
2:C:124:ARG:HA	2:D:162:TYR:HB3	1.73	0.71
1:O:288:ALA:HB1	4:S:44:MET:HE1	1.73	0.70
4:G:36:4HH:HB2	4:G:36:4HH:HJ2	1.74	0.70
4:S:23:THR:OG1	4:S:25:ASN:OD1	2.04	0.69
4:G:36:4HH:CL3	4:G:40:VAL:CG2	2.68	0.69
4:S:36:4HH:HJ2	4:S:36:4HH:HB2	1.74	0.69
1:P:273:ASP:OD1	1:P:274:TYR:N	2.26	0.69
1:B:273:ASP:OD1	1:B:274:TYR:N	2.26	0.68
1:O:826:LEU:HD21	1:P:827:SER:HA	1.75	0.68
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.26	0.68
1:A:826:LEU:HD21	1:B:827:SER:HA	1.75	0.67
1:A:784:GLU:OE1	1:A:784:GLU:N	2.28	0.67
1:A:1436:GLU:O	1:A:1436:GLU:OE1	2.13	0.67
4:S:36:4HH:HJ2	4:S:36:4HH:CB	2.25	0.67
5:K:63:DG:C3'	1:P:187:ARG:HD3	2.24	0.67
1:O:1436:GLU:O	1:O:1436:GLU:OE1	2.12	0.67
1:O:1298:GLN:N	1:O:1298:GLN:OE1	2.27	0.67
5:K:63:DG:H3'	1:P:187:ARG:HD3	1.77	0.66
1:O:784:GLU:N	1:O:784:GLU:OE1	2.28	0.66
4:S:46:LEU:HD21	4:S:72:ILE:HD11	1.78	0.65
2:C:158:ALA:HB2	2:D:123:LEU:HD21	1.77	0.65
1:B:1332:THR:O	1:B:1336:GLU:N	2.30	0.65
2:C:123:LEU:HG	2:D:158:ALA:CB	2.26	0.65
1:P:1332:THR:O	1:P:1336:GLU:N	2.30	0.65
4:G:46:LEU:HD21	4:G:72:ILE:HD11	1.78	0.64
1:O:1457:GLU:OE1	1:O:1457:GLU:N	2.28	0.63
3:F:167:MET:HE2	3:F:167:MET:HA	1.79	0.63
3:R:167:MET:HE2	3:R:167:MET:HA	1.79	0.63
4:G:36:4HH:HJ2	4:G:36:4HH:CB	2.25	0.63
1:P:1141:MET:HA	1:P:1141:MET:HE3	1.81	0.63
2:D:314:THR:HA	3:Q:93:MET:HE2	1.81	0.62
4:G:36:4HH:ON	4:G:40:VAL:CG2	2.47	0.62
2:C:162:TYR:HB3	2:D:124:ARG:CB	2.29	0.62
4:S:36:4HH:ON	4:S:40:VAL:CG2	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:231:ALA:HB2	1:P:665:GLN:CB	2.30	0.62
1:P:1322:GLN:O	1:P:1322:GLN:CD	2.43	0.62
1:A:1457:GLU:OE1	1:A:1457:GLU:N	2.28	0.61
1:P:254:SER:O	1:P:258:LEU:HD22	2.00	0.61
1:B:1322:GLN:O	1:B:1322:GLN:CD	2.43	0.61
1:A:231:ALA:HB2	1:B:665:GLN:CB	2.30	0.61
1:B:1141:MET:HE3	1:B:1141:MET:HA	1.81	0.61
2:C:124:ARG:HB2	2:D:162:TYR:CD1	2.35	0.61
1:B:254:SER:O	1:B:258:LEU:HD22	2.01	0.61
2:C:314:THR:HA	3:E:93:MET:HE2	1.81	0.61
1:O:289:LEU:HD22	4:S:36:4HH:HS3	1.83	0.60
2:C:138:ARG:NH1	2:D:134:ASN:HD22	2.00	0.60
2:C:123:LEU:CG	2:D:158:ALA:CB	2.79	0.60
1:P:788:GLU:OE1	1:P:789:ALA:N	2.35	0.60
1:A:289:LEU:HD22	4:G:36:4HH:HS3	1.83	0.59
4:M:24:ASN:O	4:M:66:GLN:N	2.35	0.59
1:B:788:GLU:OE1	1:B:789:ALA:N	2.35	0.59
2:C:123:LEU:CG	2:D:158:ALA:HB1	2.30	0.59
2:C:162:TYR:CG	2:D:124:ARG:CB	2.85	0.59
5:K:63:DG:C2'	1:P:187:ARG:HD3	2.33	0.59
2:C:158:ALA:HB3	2:C:159:PRO:HD3	1.85	0.59
3:E:10:MET:SD	3:F:18:LEU:HD11	2.43	0.58
4:I:24:ASN:O	4:I:66:GLN:N	2.35	0.58
3:Q:10:MET:SD	3:R:18:LEU:HD11	2.43	0.58
1:B:1142:GLU:OE1	1:B:1142:GLU:N	2.36	0.58
1:P:674:MET:HE3	1:P:674:MET:HA	1.86	0.58
1:P:1107:ARG:HE	4:M:48:GLU:CD	2.12	0.57
1:B:674:MET:HE3	1:B:674:MET:HA	1.85	0.57
1:P:1142:GLU:N	1:P:1142:GLU:OE1	2.36	0.57
1:B:1107:ARG:HE	4:I:48:GLU:CD	2.12	0.56
2:C:124:ARG:HA	2:D:162:TYR:CG	2.41	0.56
1:P:273:ASP:OD1	1:P:273:ASP:C	2.49	0.55
2:C:131:ILE:CD1	2:D:163:SER:CB	2.83	0.55
4:G:36:4HH:HJ3	4:G:37:LEU:N	2.22	0.55
1:O:231:ALA:HB2	1:P:665:GLN:HB2	1.89	0.55
1:A:231:ALA:HB2	1:B:665:GLN:HB2	1.89	0.55
1:B:273:ASP:OD1	1:B:273:ASP:C	2.49	0.55
2:C:123:LEU:CD2	2:D:158:ALA:HB2	2.36	0.55
2:D:328:ASP:OD1	2:D:328:ASP:O	2.25	0.55
1:P:822:VAL:HA	1:P:826:LEU:HD23	1.88	0.55
1:O:764:ASP:N	1:O:764:ASP:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:36:4HH:HJ3	4:S:37:LEU:N	2.22	0.54
3:F:148:LYS:HD3	3:F:148:LYS:N	2.23	0.54
1:O:236:GLU:OE2	1:O:1307:THR:HG21	2.08	0.54
1:A:764:ASP:N	1:A:764:ASP:OD1	2.40	0.54
1:B:822:VAL:HA	1:B:826:LEU:HD23	1.88	0.54
1:B:1423:CYS:SG	1:B:1430:LEU:HD11	2.48	0.54
1:P:1423:CYS:SG	1:P:1430:LEU:HD11	2.48	0.54
3:E:7:GLU:OE1	3:E:7:GLU:N	2.38	0.54
1:O:1281:GLU:O	1:O:1285:ILE:HD12	2.08	0.54
2:C:79:ASN:CG	3:Q:142:SER:HB3	2.34	0.53
1:A:828:VAL:HG12	1:A:828:VAL:O	2.08	0.53
1:A:1420:PHE:HA	1:A:1423:CYS:SG	2.48	0.53
1:B:1299:ASP:OD1	1:B:1300:LEU:N	2.42	0.53
2:C:328:ASP:OD1	2:C:328:ASP:O	2.25	0.53
1:A:236:GLU:OE2	1:A:1307:THR:HG21	2.08	0.53
1:B:1395:LYS:O	1:B:1395:LYS:HD3	2.09	0.53
3:R:148:LYS:HD3	3:R:148:LYS:N	2.23	0.53
1:A:289:LEU:HD22	4:G:36:4HH:CS	2.39	0.53
1:A:1281:GLU:O	1:A:1285:ILE:HD12	2.08	0.53
1:P:1299:ASP:OD1	1:P:1300:LEU:N	2.42	0.53
1:O:65:GLU:O	1:O:65:GLU:HG3	2.08	0.53
1:O:1420:PHE:HA	1:O:1423:CYS:SG	2.48	0.53
1:P:799:GLU:OE1	1:P:799:GLU:C	2.52	0.53
2:C:123:LEU:HD11	2:D:158:ALA:CB	2.39	0.53
1:O:289:LEU:HD22	4:S:36:4HH:CS	2.39	0.53
1:O:1126:ASP:O	1:O:1127:ASN:OD1	2.27	0.53
1:O:828:VAL:O	1:O:828:VAL:HG12	2.08	0.53
3:Q:124:LEU:C	3:Q:124:LEU:HD23	2.34	0.53
1:A:65:GLU:O	1:A:65:GLU:HG3	2.08	0.53
1:B:799:GLU:C	1:B:799:GLU:OE1	2.52	0.52
1:B:1441:GLU:OE1	1:B:1441:GLU:N	2.37	0.52
1:P:1258:LEU:HD21	1:P:1380:MET:HG2	1.90	0.52
3:E:124:LEU:C	3:E:124:LEU:HD23	2.34	0.52
1:P:1441:GLU:OE1	1:P:1441:GLU:N	2.37	0.52
1:A:1126:ASP:O	1:A:1127:ASN:OD1	2.27	0.52
1:B:1258:LEU:HD21	1:B:1380:MET:HG2	1.90	0.52
2:C:158:ALA:HB2	2:D:123:LEU:CG	2.31	0.52
2:D:79:ASN:CG	3:E:142:SER:HB3	2.34	0.52
1:A:122:MET:HE1	1:A:177:GLN:HB3	1.90	0.52
3:Q:7:GLU:OE1	3:Q:7:GLU:N	2.38	0.52
1:P:217:LEU:HG	1:P:221:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:VAL:HG12	1:B:828:VAL:O	2.10	0.52
1:B:665:GLN:C	1:B:665:GLN:OE1	2.53	0.52
1:O:122:MET:HE1	1:O:177:GLN:HB3	1.90	0.52
2:D:158:ALA:HB3	2:D:159:PRO:HD3	1.91	0.52
1:A:44:MET:HE3	1:A:1433:ALA:HB2	1.92	0.52
1:P:63:THR:HG21	1:P:1407:GLU:HG3	1.92	0.52
1:P:665:GLN:OE1	1:P:665:GLN:C	2.53	0.52
1:P:732:GLU:H	1:P:732:GLU:CD	2.18	0.52
3:E:10:MET:HE3	3:E:14:LEU:HD22	1.92	0.51
1:P:1161:VAL:HG12	1:P:1161:VAL:O	2.10	0.51
1:O:44:MET:HE3	1:O:1433:ALA:HB2	1.92	0.51
1:B:1246:LYS:HD2	1:B:1246:LYS:O	2.11	0.51
1:P:91:ASP:C	1:P:91:ASP:OD1	2.54	0.51
1:B:63:THR:HG21	1:B:1407:GLU:HG3	1.92	0.51
4:G:62:ILE:HG22	4:G:62:ILE:O	2.10	0.51
1:P:828:VAL:HG12	1:P:828:VAL:O	2.10	0.51
2:C:124:ARG:HB2	2:D:162:TYR:CG	2.46	0.51
2:C:134:ASN:ND2	2:D:138:ARG:NH1	2.57	0.51
1:P:1319:LEU:HD12	1:P:1320:ASN:N	2.26	0.51
3:Q:10:MET:HE3	3:Q:14:LEU:HD22	1.92	0.51
1:B:217:LEU:HG	1:B:221:LEU:HD12	1.91	0.51
5:K:63:DG:H4'	1:P:189:ARG:HG3	1.93	0.51
6:L:39:DG:H3'	3:Q:157:THR:HG23	1.93	0.51
1:B:1161:VAL:HG12	1:B:1161:VAL:O	2.09	0.50
1:B:1319:LEU:HD12	1:B:1320:ASN:N	2.26	0.50
2:D:370:GLN:OE1	2:D:370:GLN:O	2.29	0.50
4:S:62:ILE:HG22	4:S:62:ILE:O	2.10	0.50
1:B:1257:MET:SD	1:B:1257:MET:C	2.95	0.50
2:D:358:LEU:HG	2:D:362:ILE:HD11	1.94	0.50
1:B:732:GLU:CD	1:B:732:GLU:H	2.18	0.50
1:O:200:LEU:HD12	1:O:1378:LEU:HD22	1.94	0.50
2:C:370:GLN:OE1	2:C:370:GLN:O	2.29	0.50
1:P:1196:GLU:N	1:P:1196:GLU:OE1	2.45	0.50
1:P:1257:MET:C	1:P:1257:MET:SD	2.95	0.50
1:B:1107:ARG:CZ	4:I:48:GLU:OE1	2.59	0.50
2:C:356:ASP:C	2:C:356:ASP:OD1	2.55	0.50
1:A:1361:GLU:OE1	1:A:1361:GLU:HA	2.12	0.50
2:D:356:ASP:OD1	2:D:356:ASP:C	2.55	0.50
1:A:200:LEU:HD12	1:A:1378:LEU:HD22	1.94	0.50
1:B:91:ASP:C	1:B:91:ASP:OD1	2.54	0.50
2:C:162:TYR:CD1	2:D:124:ARG:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1361:GLU:OE1	1:O:1361:GLU:HA	2.12	0.50
1:P:1107:ARG:CZ	4:M:48:GLU:OE1	2.60	0.50
2:C:134:ASN:ND2	2:D:138:ARG:HH12	1.95	0.49
1:A:1163:ASP:OD1	1:A:1164:ASN:N	2.45	0.49
2:C:358:LEU:HG	2:C:362:ILE:HD11	1.94	0.49
3:F:16:GLN:C	3:F:16:GLN:OE1	2.55	0.49
5:K:63:DG:H3'	1:P:187:ARG:CD	2.41	0.49
1:O:1163:ASP:OD1	1:O:1164:ASN:N	2.45	0.49
1:A:1376:SER:O	1:A:1379:VAL:HG22	2.12	0.49
1:B:1196:GLU:N	1:B:1196:GLU:OE1	2.45	0.49
4:G:36:4HH:CB	4:G:36:4HH:CJ	2.90	0.49
1:P:244:ILE:HD13	3:Q:41:LEU:HD21	1.94	0.49
1:A:235:MET:HA	1:A:235:MET:HE2	1.95	0.49
2:D:75:ASN:HD21	3:E:146:LEU:HB2	1.78	0.49
1:O:732:GLU:N	1:O:732:GLU:OE1	2.46	0.49
3:R:16:GLN:C	3:R:16:GLN:OE1	2.55	0.49
4:S:2:THR:OG1	4:S:3:ILE:N	2.45	0.49
5:K:63:DG:H1'	5:K:64:DG:C8	2.48	0.49
1:A:732:GLU:OE1	1:A:732:GLU:N	2.46	0.49
2:C:124:ARG:CB	2:D:162:TYR:CG	2.96	0.49
4:I:36:4HH:O	4:I:40:VAL:HG23	2.12	0.49
4:M:36:4HH:O	4:M:40:VAL:HG23	2.11	0.49
1:O:1376:SER:O	1:O:1379:VAL:HG22	2.12	0.49
4:S:36:4HH:ON	4:S:40:VAL:HG21	2.06	0.48
1:A:1211:ALA:O	1:A:1215:MET:HG2	2.13	0.48
4:G:36:4HH:ON	4:G:40:VAL:HG23	2.14	0.48
1:O:235:MET:HE2	1:O:235:MET:HA	1.95	0.48
3:R:56:GLU:OE1	3:R:56:GLU:HA	2.13	0.48
1:B:1376:SER:O	1:B:1379:VAL:HG22	2.13	0.48
2:C:123:LEU:CG	2:D:158:ALA:HB2	2.44	0.48
1:O:1237:SER:OG	1:O:1238:LYS:N	2.45	0.48
1:P:782:ALA:O	1:P:785:ASN:N	2.47	0.48
1:B:244:ILE:HD13	3:E:41:LEU:HD21	1.94	0.48
2:C:391:LEU:HD13	2:C:428:TYR:CE2	2.49	0.48
4:G:2:THR:OG1	4:G:3:ILE:N	2.45	0.48
2:C:75:ASN:HD21	3:Q:146:LEU:HB2	1.78	0.48
2:C:106:LEU:HB2	2:D:113:TYR:CD1	2.49	0.48
1:O:1211:ALA:O	1:O:1215:MET:HG2	2.13	0.48
1:P:1376:SER:O	1:P:1379:VAL:HG22	2.13	0.48
3:F:56:GLU:OE1	3:F:56:GLU:HA	2.13	0.48
4:S:11:ILE:HG23	4:S:12:GLY:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:SER:OG	1:A:1238:LYS:N	2.45	0.47
1:B:1161:VAL:O	1:B:1161:VAL:CG1	2.62	0.47
2:D:292:ASP:CG	2:D:295:ARG:HA	2.39	0.47
2:C:292:ASP:CG	2:C:295:ARG:HA	2.39	0.47
4:S:36:4HH:ON	4:S:40:VAL:HG23	2.13	0.47
1:P:1161:VAL:O	1:P:1161:VAL:CG1	2.62	0.47
1:B:1275:LEU:HD12	1:B:1347:ASP:O	2.14	0.47
4:G:11:ILE:HG23	4:G:12:GLY:N	2.29	0.47
1:B:94:ASN:OD1	1:B:95:SER:N	2.47	0.47
1:B:1322:GLN:O	1:B:1322:GLN:OE1	2.32	0.47
2:D:375:PRO:HA	2:D:440:TYR:OH	2.15	0.47
2:D:391:LEU:HD13	2:D:428:TYR:CE2	2.49	0.47
1:A:62:ASN:OD1	1:A:63:THR:N	2.48	0.47
1:B:184:ILE:HG23	1:B:185:PRO:HD2	1.97	0.47
1:B:285:LEU:HD13	4:I:41:GLU:OE2	2.15	0.47
1:B:774:GLU:N	1:B:774:GLU:OE1	2.48	0.47
1:P:774:GLU:N	1:P:774:GLU:OE1	2.48	0.47
1:P:1322:GLN:O	1:P:1322:GLN:OE1	2.31	0.47
1:B:782:ALA:O	1:B:785:ASN:N	2.47	0.47
2:C:162:TYR:CB	2:D:124:ARG:CB	2.93	0.47
2:C:375:PRO:HA	2:C:440:TYR:OH	2.15	0.47
1:P:184:ILE:HG23	1:P:185:PRO:HD2	1.97	0.47
3:R:180:ILE:HG23	3:R:184:VAL:HG21	1.96	0.47
2:D:391:LEU:HD13	2:D:428:TYR:CD2	2.50	0.47
3:F:25:GLU:CD	3:F:25:GLU:H	2.23	0.47
1:O:588:GLU:O	1:O:592:GLN:HG3	2.15	0.47
1:A:588:GLU:O	1:A:592:GLN:HG3	2.15	0.46
1:B:824:LYS:HG2	1:B:824:LYS:O	2.15	0.46
1:P:1117:TRP:O	1:P:1121:MET:HG2	2.14	0.46
1:P:1320:ASN:ND2	3:Q:49:ASP:OD2	2.49	0.46
1:O:62:ASN:OD1	1:O:63:THR:N	2.48	0.46
1:P:1275:LEU:HD12	1:P:1347:ASP:O	2.15	0.46
3:R:25:GLU:CD	3:R:25:GLU:H	2.23	0.46
4:S:28:PHE:CE1	4:S:65:VAL:HG22	2.51	0.46
3:E:5:HIS:CD2	3:E:7:GLU:OE1	2.69	0.46
1:A:12:LEU:HD21	1:A:46:ALA:HB2	1.97	0.46
3:F:39:ASP:OD1	3:F:39:ASP:N	2.49	0.46
3:F:180:ILE:HG23	3:F:184:VAL:HG21	1.96	0.46
4:G:28:PHE:CE1	4:G:65:VAL:HG22	2.51	0.46
1:P:824:LYS:O	1:P:824:LYS:HG2	2.15	0.46
3:Q:140:ARG:HD2	3:Q:140:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:ARG:HH11	2:D:134:ASN:HD21	1.56	0.46
1:P:285:LEU:HD13	4:M:41:GLU:OE2	2.15	0.46
1:B:1117:TRP:O	1:B:1121:MET:HG2	2.14	0.46
1:P:1391:ARG:HA	1:P:1391:ARG:NE	2.30	0.46
4:S:57:GLU:OE1	4:S:57:GLU:N	2.45	0.46
1:O:1285:ILE:HD12	1:O:1285:ILE:H	1.81	0.46
1:B:542:PHE:CD2	1:B:876:LEU:HD21	2.51	0.46
1:B:782:ALA:O	1:B:785:ASN:CB	2.64	0.46
2:C:426:ASN:OD1	2:C:430:ALA:HB3	2.16	0.46
2:D:426:ASN:OD1	2:D:430:ALA:HB3	2.16	0.46
4:G:57:GLU:OE1	4:G:57:GLU:N	2.46	0.46
1:O:349:LYS:HE3	1:O:353:TYR:CZ	2.51	0.46
1:A:8:ARG:HH21	1:A:8:ARG:HG3	1.80	0.46
1:B:664:SER:OG	1:B:665:GLN:HG3	2.15	0.46
2:C:391:LEU:HD13	2:C:428:TYR:CD2	2.50	0.46
3:Q:5:HIS:CD2	3:Q:7:GLU:OE1	2.69	0.46
1:B:1320:ASN:ND2	3:E:49:ASP:OD2	2.49	0.45
1:P:664:SER:OG	1:P:665:GLN:HG3	2.15	0.45
1:P:679:GLU:OE1	1:P:679:GLU:HA	2.16	0.45
1:A:1285:ILE:HD12	1:A:1285:ILE:H	1.81	0.45
2:C:355:ASN:OD1	2:C:355:ASN:N	2.49	0.45
4:G:36:4HH:OM	4:G:37:LEU:HA	2.17	0.45
1:B:679:GLU:OE1	1:B:679:GLU:HA	2.16	0.45
3:R:39:ASP:OD1	3:R:39:ASP:N	2.49	0.45
2:C:106:LEU:HD13	2:D:113:TYR:CG	2.51	0.45
1:O:1275:LEU:HD23	1:O:1380:MET:HE2	1.98	0.45
3:R:121:TYR:CZ	3:R:125:ILE:HD11	2.52	0.45
3:R:190:ASP:C	3:R:190:ASP:OD1	2.59	0.45
1:B:1375:MET:HG2	1:B:1419:LEU:HD11	1.98	0.45
1:O:247:GLU:OE1	1:O:247:GLU:HA	2.17	0.45
1:O:765:ARG:HH11	1:P:748:VAL:HG23	1.81	0.45
1:P:782:ALA:O	1:P:785:ASN:CB	2.65	0.45
1:A:349:LYS:HE3	1:A:353:TYR:CZ	2.51	0.45
1:B:611:LEU:C	1:B:611:LEU:HD23	2.42	0.45
5:K:38:DA:C2	6:L:54:DA:C2	3.05	0.45
1:A:247:GLU:HA	1:A:247:GLU:OE1	2.17	0.45
1:O:1213:GLU:OE1	1:P:813:ARG:NE	2.49	0.45
1:P:542:PHE:CD2	1:P:876:LEU:HD21	2.51	0.45
1:O:8:ARG:HH21	1:O:8:ARG:HG3	1.80	0.45
1:A:640:ARG:O	1:A:643:THR:HG22	2.17	0.45
1:A:1213:GLU:OE1	1:B:813:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:GLU:HA	1:B:787:LEU:HG	1.99	0.45
3:F:134:MET:N	3:F:134:MET:HE2	2.32	0.45
1:O:12:LEU:HD21	1:O:46:ALA:HB2	1.97	0.45
1:A:275:MET:HE1	1:A:1134:HIS:ND1	2.31	0.44
1:A:1127:ASN:OD1	1:A:1127:ASN:C	2.60	0.44
2:D:355:ASN:N	2:D:355:ASN:OD1	2.48	0.44
1:O:640:ARG:O	1:O:643:THR:HG22	2.17	0.44
1:O:1127:ASN:OD1	1:O:1127:ASN:C	2.60	0.44
1:A:765:ARG:HH11	1:B:748:VAL:HG23	1.81	0.44
1:A:1275:LEU:HD23	1:A:1380:MET:HE2	1.98	0.44
1:B:232:PHE:CZ	1:B:1240:VAL:HG11	2.53	0.44
3:F:190:ASP:C	3:F:190:ASP:OD1	2.60	0.44
4:I:58:GLU:OE1	4:I:71:TYR:OH	2.31	0.44
1:O:275:MET:HE1	1:O:1134:HIS:CE1	2.52	0.44
1:P:1375:MET:HG2	1:P:1419:LEU:HD11	1.98	0.44
1:B:750:ASN:HB3	1:B:761:LYS:HB3	2.00	0.44
1:B:839:ARG:HG2	1:B:839:ARG:HH21	1.82	0.44
1:P:691:ASP:OD1	1:P:780:ARG:HB3	2.17	0.44
1:B:1104:TYR:CE1	1:B:1107:ARG:NH1	2.86	0.44
5:K:40:DA:C2	6:L:52:DA:C2	3.05	0.44
1:O:51:LEU:O	1:O:52:ILE:HD13	2.18	0.44
1:P:632:MET:HE1	1:P:818:PHE:HB3	1.99	0.44
1:P:784:GLU:HA	1:P:787:LEU:HG	1.98	0.44
3:R:134:MET:N	3:R:134:MET:HE2	2.32	0.44
4:S:36:4HH:OM	4:S:37:LEU:HA	2.17	0.44
1:O:152:GLU:OE1	1:O:152:GLU:N	2.51	0.44
1:O:275:MET:HE1	1:O:1134:HIS:ND1	2.31	0.44
1:P:611:LEU:HD23	1:P:611:LEU:C	2.42	0.44
1:A:275:MET:HE1	1:A:1134:HIS:CE1	2.52	0.44
1:A:1121:MET:HA	1:A:1124:VAL:HG12	1.99	0.44
1:P:750:ASN:HB3	1:P:761:LYS:HB3	2.00	0.44
1:A:1387:GLU:C	1:A:1387:GLU:OE1	2.61	0.44
2:D:399:ARG:O	2:D:403:ASP:OD2	2.36	0.44
4:I:64:THR:HG22	4:I:65:VAL:N	2.33	0.44
1:P:1213:GLU:H	1:P:1213:GLU:CD	2.26	0.44
3:Q:180:ILE:HG22	3:Q:181:THR:N	2.33	0.44
1:O:1274:ARG:HG3	1:O:1357:TRP:CZ3	2.53	0.43
1:O:1380:MET:HE3	1:O:1380:MET:HB3	1.96	0.43
1:A:51:LEU:O	1:A:52:ILE:HD13	2.18	0.43
1:B:782:ALA:O	1:B:785:ASN:HB3	2.18	0.43
1:O:1401:ARG:HB3	1:O:1428:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:36:4HH:CB	4:S:36:4HH:CJ	2.90	0.43
1:B:215:ARG:HG2	1:B:1325:MET:HE2	2.01	0.43
1:B:89:THR:C	1:B:90:LEU:HD12	2.43	0.43
1:B:632:MET:HE1	1:B:818:PHE:HB3	2.00	0.43
1:B:691:ASP:OD1	1:B:780:ARG:HB3	2.17	0.43
2:D:358:LEU:HA	2:D:361:MET:SD	2.59	0.43
1:P:105:ARG:HD2	1:P:105:ARG:C	2.44	0.43
1:P:1104:TYR:CE1	1:P:1107:ARG:NH1	2.86	0.43
1:P:1338:LEU:N	1:P:1338:LEU:HD23	2.32	0.43
4:M:64:THR:HG22	4:M:65:VAL:N	2.33	0.43
1:A:1401:ARG:HB3	1:A:1428:MET:HE2	1.99	0.43
3:E:180:ILE:HG22	3:E:181:THR:N	2.33	0.43
5:K:63:DG:C5'	1:P:189:ARG:HG3	2.49	0.43
1:O:1121:MET:HA	1:O:1124:VAL:HG12	1.99	0.43
1:P:839:ARG:HG2	1:P:839:ARG:HH21	1.82	0.43
1:A:1285:ILE:HD11	3:F:108:ARG:NH1	2.34	0.43
1:O:1129:VAL:O	1:O:1130:GLU:C	2.61	0.43
1:O:1285:ILE:HD11	3:R:108:ARG:NH1	2.34	0.43
2:C:124:ARG:CA	2:D:162:TYR:CG	3.01	0.43
2:C:358:LEU:HA	2:C:361:MET:SD	2.59	0.43
1:O:782:ALA:C	1:O:783:ARG:HD3	2.43	0.43
1:O:1107:ARG:NH2	4:S:47:GLU:OE2	2.50	0.43
3:Q:127:LEU:HD23	3:Q:127:LEU:C	2.44	0.43
2:C:399:ARG:O	2:C:403:ASP:OD2	2.36	0.43
1:O:105:ARG:HD2	1:O:105:ARG:C	2.44	0.43
1:O:1235:ILE:HG21	1:P:675:ILE:HD13	2.01	0.43
1:P:89:THR:C	1:P:90:LEU:HD12	2.43	0.43
1:P:1436:GLU:O	1:P:1438:ILE:HG23	2.19	0.43
1:P:232:PHE:CZ	1:P:1240:VAL:HG11	2.53	0.43
1:P:775:LEU:HD22	1:P:775:LEU:N	2.34	0.43
2:C:18:ASN:HB3	2:C:20:PHE:CZ	2.53	0.43
2:C:154:ARG:HA	2:D:123:LEU:HD21	2.00	0.43
1:O:782:ALA:O	1:O:783:ARG:HD3	2.19	0.43
1:P:215:ARG:HG2	1:P:1325:MET:HE2	2.00	0.43
1:B:1213:GLU:H	1:B:1213:GLU:CD	2.26	0.42
1:P:782:ALA:O	1:P:785:ASN:HB3	2.18	0.42
3:R:25:GLU:O	3:R:29:GLN:HG3	2.19	0.42
1:A:782:ALA:C	1:A:783:ARG:HD3	2.43	0.42
1:A:1274:ARG:HG3	1:A:1357:TRP:CZ3	2.53	0.42
1:B:1436:GLU:O	1:B:1438:ILE:HG23	2.19	0.42
2:D:175:GLN:HB3	2:D:266:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:594:ILE:HD12	1:P:845:HIS:CE1	2.54	0.42
1:P:1247:THR:O	1:P:1251:GLU:OE1	2.37	0.42
4:I:40:VAL:O	4:I:43:VAL:HG12	2.20	0.42
1:O:1118:CYS:SG	1:O:1122:ARG:NH1	2.92	0.42
1:O:1387:GLU:CD	1:O:1387:GLU:C	2.87	0.42
1:P:605:LEU:O	1:P:609:ASP:OD2	2.37	0.42
1:P:745:ASP:OD1	1:P:745:ASP:N	2.51	0.42
1:B:594:ILE:HD12	1:B:845:HIS:CE1	2.55	0.42
1:B:606:ALA:HA	1:B:609:ASP:OD2	2.20	0.42
2:C:158:ALA:CB	2:D:123:LEU:CD2	2.85	0.42
1:O:1202:ILE:HG22	1:O:1202:ILE:O	2.20	0.42
1:P:606:ALA:HA	1:P:609:ASP:OD2	2.20	0.42
1:A:292:ARG:HD3	4:G:36:4HH:CT	2.49	0.42
1:A:1373:THR:O	1:A:1377:ILE:HG12	2.19	0.42
1:A:1387:GLU:C	1:A:1387:GLU:CD	2.87	0.42
1:O:1387:GLU:C	1:O:1387:GLU:OE1	2.61	0.42
1:P:1325:MET:SD	1:P:1325:MET:N	2.90	0.42
1:A:767:TRP:CE3	1:B:717:LEU:HD13	2.55	0.42
1:A:782:ALA:O	1:A:783:ARG:HD3	2.19	0.42
1:A:1129:VAL:O	1:A:1130:GLU:C	2.61	0.42
1:B:605:LEU:O	1:B:609:ASP:OD2	2.37	0.42
1:B:1247:THR:O	1:B:1251:GLU:OE1	2.37	0.42
2:C:131:ILE:HD13	2:D:163:SER:OG	2.15	0.42
2:D:18:ASN:HB3	2:D:20:PHE:CZ	2.55	0.42
3:E:127:LEU:C	3:E:127:LEU:HD23	2.44	0.42
1:O:12:LEU:HD22	1:O:15:TRP:CG	2.55	0.42
1:O:1373:THR:O	1:O:1377:ILE:HG12	2.19	0.42
1:P:695:ILE:N	1:P:695:ILE:HD12	2.35	0.42
4:M:40:VAL:O	4:M:43:VAL:HG12	2.20	0.42
1:A:105:ARG:HD2	1:A:105:ARG:C	2.44	0.42
1:A:152:GLU:OE1	1:A:152:GLU:N	2.51	0.42
1:A:1235:ILE:HG21	1:B:675:ILE:HD13	2.01	0.42
1:B:1395:LYS:HD3	1:B:1395:LYS:C	2.45	0.42
1:O:292:ARG:HD3	4:S:36:4HH:CT	2.49	0.42
1:O:1331:GLN:NE2	1:O:1335:GLU:OE2	2.48	0.42
4:S:64:THR:HG23	4:S:67:ALA:H	1.85	0.42
1:A:45:ALA:HB1	1:A:60:PHE:CE2	2.55	0.42
1:A:780:ARG:O	1:A:783:ARG:N	2.46	0.42
1:B:775:LEU:N	1:B:775:LEU:HD22	2.34	0.42
5:K:63:DG:C3'	1:P:187:ARG:CD	2.94	0.42
1:O:782:ALA:O	1:O:783:ARG:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:94:ASN:OD1	1:P:95:SER:N	2.53	0.42
1:A:12:LEU:HD22	1:A:15:TRP:CG	2.55	0.41
1:A:1068:LEU:C	1:A:1068:LEU:HD23	2.45	0.41
1:B:695:ILE:HD12	1:B:695:ILE:N	2.35	0.41
2:C:131:ILE:HD11	2:D:163:SER:HB2	1.99	0.41
3:R:167:MET:HE1	3:R:183:ALA:HB1	2.01	0.41
3:F:167:MET:HE1	3:F:183:ALA:HB1	2.01	0.41
1:A:1199:ARG:O	1:A:1199:ARG:HG2	2.19	0.41
1:B:288:ALA:HB2	1:B:1106:ILE:HG22	2.03	0.41
1:B:1142:GLU:CD	1:B:1142:GLU:H	2.28	0.41
1:B:1246:LYS:HD2	1:B:1246:LYS:C	2.45	0.41
6:L:55:DG:H2"	6:L:56:DT:C6	2.56	0.41
1:A:12:LEU:HD21	1:A:46:ALA:CB	2.50	0.41
1:B:264:THR:HG23	1:B:265:GLU:N	2.36	0.41
1:B:1331:GLN:OE1	1:B:1331:GLN:N	2.54	0.41
1:O:1068:LEU:C	1:O:1068:LEU:HD23	2.45	0.41
1:O:1407:GLU:OE1	1:O:1407:GLU:HA	2.21	0.41
1:B:141:GLY:O	1:B:143:ARG:NH1	2.54	0.41
2:C:357:GLN:O	2:C:361:MET:SD	2.78	0.41
5:K:13:DA:C2	6:L:79:DG:C2	3.08	0.41
1:O:767:TRP:CE3	1:P:717:LEU:HD13	2.55	0.41
1:A:587:LEU:HD11	1:A:591:LYS:HE2	2.03	0.41
1:B:745:ASP:OD1	1:B:745:ASP:N	2.51	0.41
1:B:1126:ASP:O	1:B:1127:ASN:HB3	2.21	0.41
3:F:25:GLU:O	3:F:29:GLN:HG3	2.19	0.41
1:O:1199:ARG:O	1:O:1199:ARG:HG2	2.19	0.41
1:P:244:ILE:CD1	3:Q:41:LEU:HD21	2.51	0.41
1:P:141:GLY:O	1:P:143:ARG:NH1	2.54	0.41
1:A:246:LEU:O	1:A:249:ILE:CG2	2.69	0.41
1:B:232:PHE:CZ	1:B:1338:LEU:HA	2.56	0.41
1:B:1403:LEU:HD13	1:B:1428:MET:HE3	2.03	0.41
1:B:1411:LEU:HB2	1:B:1416:ILE:HD11	2.03	0.41
6:L:44:DG:H5"	3:R:140:ARG:CZ	2.51	0.41
1:O:12:LEU:HD21	1:O:46:ALA:CB	2.50	0.41
1:O:46:ALA:O	1:O:49:THR:HG22	2.21	0.41
1:P:264:THR:HG23	1:P:265:GLU:N	2.36	0.41
4:S:7:VAL:O	4:S:11:ILE:HG22	2.21	0.41
1:A:1118:CYS:SG	1:A:1122:ARG:NH1	2.92	0.41
1:B:1232:LYS:O	1:B:1235:ILE:HG22	2.21	0.41
4:G:64:THR:HG23	4:G:67:ALA:H	1.85	0.41
5:K:63:DG:C4'	1:P:189:ARG:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:45:ALA:HB1	1:O:60:PHE:CE2	2.55	0.41
1:O:281:ARG:HD2	1:O:281:ARG:C	2.46	0.41
1:O:1117:TRP:CE3	1:O:1121:MET:HE1	2.56	0.41
1:P:288:ALA:HB2	1:P:1106:ILE:HG22	2.02	0.41
1:P:1142:GLU:H	1:P:1142:GLU:CD	2.28	0.41
1:P:1227:THR:O	1:P:1230:GLU:HG3	2.21	0.41
1:P:1403:LEU:HD13	1:P:1428:MET:HE3	2.03	0.41
3:Q:108:ARG:NH1	3:Q:111:ASN:HD21	2.19	0.41
1:A:1407:GLU:HA	1:A:1407:GLU:OE1	2.21	0.41
1:B:1335:GLU:HA	1:B:1338:LEU:HG	2.03	0.41
1:B:1338:LEU:HD23	1:B:1338:LEU:N	2.36	0.41
3:E:108:ARG:NH1	3:E:111:ASN:HD21	2.19	0.41
1:P:604:TRP:CH2	1:P:608:GLN:HG3	2.56	0.41
4:S:36:4HH:O	4:S:40:VAL:HG23	2.21	0.41
1:A:281:ARG:C	1:A:281:ARG:HD2	2.46	0.40
2:D:357:GLN:O	2:D:361:MET:SD	2.78	0.40
3:E:140:ARG:HD2	3:E:140:ARG:O	2.22	0.40
4:G:36:4HH:O	4:G:40:VAL:HG23	2.21	0.40
4:M:29:VAL:HG13	4:M:30:GLU:N	2.36	0.40
1:A:788:GLU:O	1:A:792:LEU:HD13	2.21	0.40
1:A:1202:ILE:O	1:A:1202:ILE:HG22	2.20	0.40
2:D:201:ILE:HD13	2:D:289:ILE:HD11	2.02	0.40
1:P:1411:LEU:HB2	1:P:1416:ILE:HD11	2.03	0.40
1:A:1107:ARG:NH2	4:G:47:GLU:OE2	2.50	0.40
2:C:162:TYR:CD2	2:D:124:ARG:HB2	2.54	0.40
2:C:440:TYR:CD1	2:C:440:TYR:N	2.90	0.40
1:O:246:LEU:O	1:O:249:ILE:CG2	2.69	0.40
1:O:1387:GLU:OE1	1:O:1388:GLU:N	2.54	0.40
1:P:275:MET:HA	1:P:275:MET:HE3	2.04	0.40
1:A:1117:TRP:CE3	1:A:1121:MET:HE1	2.56	0.40
1:B:1325:MET:SD	1:B:1325:MET:N	2.90	0.40
2:C:124:ARG:CB	2:D:162:TYR:CD1	3.04	0.40
2:C:201:ILE:HD13	2:C:289:ILE:HD11	2.02	0.40
3:E:9:PHE:CE1	3:F:16:GLN:HG2	2.57	0.40
3:F:42:ASP:OD1	3:F:43:ASN:N	2.54	0.40
1:O:87:TYR:CG	1:O:136:LEU:HD23	2.56	0.40
1:O:587:LEU:HD11	1:O:591:LYS:HE2	2.03	0.40
1:O:788:GLU:O	1:O:792:LEU:HD13	2.21	0.40
1:A:594:ILE:HD12	1:A:845:HIS:CE1	2.56	0.40
1:A:782:ALA:O	1:A:783:ARG:C	2.63	0.40
1:B:275:MET:HE3	1:B:275:MET:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1307:THR:OG1	1:P:1310:GLU:HG3	2.22	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	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100	100
1	B	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
1	O	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100	100
1	P	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
2	C	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
2	D	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
3	E	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
3	F	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
3	Q	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
3	R	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
4	G	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
4	I	69/78 (88%)	67 (97%)	2 (3%)	0	100	100
4	M	69/78 (88%)	66 (96%)	3 (4%)	0	100	100
4	S	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
All	All	7824/8080 (97%)	7587 (97%)	237 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1269/1281 (99%)	1268 (100%)	1 (0%)	92 95
1	B	1269/1281 (99%)	1267 (100%)	2 (0%)	92 94
1	O	1269/1281 (99%)	1268 (100%)	1 (0%)	92 95
1	P	1269/1281 (99%)	1266 (100%)	3 (0%)	92 94
2	C	376/376 (100%)	369 (98%)	7 (2%)	52 69
2	D	376/376 (100%)	369 (98%)	7 (2%)	52 69
3	E	189/212 (89%)	184 (97%)	5 (3%)	41 59
3	F	177/212 (84%)	175 (99%)	2 (1%)	70 80
3	Q	189/212 (89%)	185 (98%)	4 (2%)	48 66
3	R	177/212 (84%)	175 (99%)	2 (1%)	70 80
4	G	62/66 (94%)	62 (100%)	0	100 100
4	I	62/66 (94%)	62 (100%)	0	100 100
4	M	62/66 (94%)	62 (100%)	0	100 100
4	S	62/66 (94%)	62 (100%)	0	100 100
All	All	6808/6988 (97%)	6774 (100%)	34 (0%)	85 89

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	B	1127	ASN
1	B	1213	GLU
2	C	2	SER
2	C	92	SER
2	C	94	LEU
2	C	132	VAL
2	C	209	SER
2	C	287	THR
2	C	355	ASN
2	D	2	SER

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Mol	Chain	Res	Type
2	D	92	SER
2	D	94	LEU
2	D	132	VAL
2	D	209	SER
2	D	287	THR
2	D	355	ASN
3	E	123	GLU
3	E	138	ASN
3	E	162	LEU
3	E	169	TYR
3	E	181	THR
3	F	25	GLU
3	F	152	GLN
1	O	221	LEU
1	P	189	ARG
1	P	1127	ASN
1	P	1213	GLU
3	Q	123	GLU
3	Q	162	LEU
3	Q	169	TYR
3	Q	181	THR
3	R	25	GLU
3	R	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	306	GLN
1	A	331	GLN
1	A	367	GLN
1	A	404	GLN
1	A	409	GLN
1	A	472	HIS
1	A	510	HIS
1	A	516	GLN
1	A	652	GLN
1	A	865	GLN
1	A	882	GLN
1	A	930	GLN
1	A	951	HIS
1	A	1077	GLN

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Mol	Chain	Res	Type
1	A	1105	GLN
1	A	1109	GLN
1	A	1242	ASN
1	A	1293	GLN
1	B	62	ASN
1	B	78	HIS
1	B	98	GLN
1	B	175	HIS
1	B	306	GLN
1	B	330	HIS
1	B	398	GLN
1	B	418	GLN
1	B	473	ASN
1	B	531	ASN
1	B	559	GLN
1	B	566	GLN
1	B	766	GLN
1	B	864	GLN
1	B	986	ASN
1	B	1006	GLN
1	B	1013	GLN
1	B	1032	GLN
1	B	1091	ASN
1	B	1166	HIS
1	B	1193	HIS
1	B	1342	ASN
1	B	1437	ASN
2	C	75	ASN
2	C	134	ASN
2	C	198	GLN
2	C	435	HIS
2	D	18	ASN
2	D	75	ASN
2	D	134	ASN
2	D	198	GLN
2	D	435	HIS
3	E	8	GLN
3	E	111	ASN
1	O	242	ASN
1	O	306	GLN
1	O	331	GLN
1	O	367	GLN

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Mol	Chain	Res	Type
1	O	378	GLN
1	O	404	GLN
1	O	409	GLN
1	O	472	HIS
1	O	480	GLN
1	O	510	HIS
1	O	516	GLN
1	O	865	GLN
1	O	882	GLN
1	O	930	GLN
1	O	951	HIS
1	O	1077	GLN
1	O	1105	GLN
1	O	1109	GLN
1	O	1242	ASN
1	O	1293	GLN
1	P	62	ASN
1	P	78	HIS
1	P	97	HIS
1	P	98	GLN
1	P	306	GLN
1	P	330	HIS
1	P	398	GLN
1	P	418	GLN
1	P	473	ASN
1	P	531	ASN
1	P	546	GLN
1	P	559	GLN
1	P	566	GLN
1	P	766	GLN
1	P	864	GLN
1	P	986	ASN
1	P	1006	GLN
1	P	1013	GLN
1	P	1091	ASN
1	P	1342	ASN
1	P	1437	ASN
3	Q	8	GLN
3	Q	111	ASN
3	Q	201	GLN
3	R	139	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\|>2$
4	4HH	I	36	4	21,26,27	0.46	0	27,35,37	1.72	3 (11%)
4	4HH	S	36	4	21,26,27	0.45	0	27,35,37	3.13	4 (14%)
4	4HH	M	36	4	21,26,27	0.47	0	27,35,37	1.73	3 (11%)
4	4HH	G	36	4	21,26,27	0.45	0	27,35,37	3.13	4 (14%)

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
4	4HH	I	36	4	-	6/32/35/37	-
4	4HH	S	36	4	-	5/32/35/37	-
4	4HH	M	36	4	-	6/32/35/37	-
4	4HH	G	36	4	-	5/32/35/37	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	36	4HH	O1P-P-OG	11.65	161.86	107.75
4	S	36	4HH	O1P-P-OG	11.64	161.82	107.75
4	S	36	4HH	OG-P-O2P	-8.87	74.39	109.07
4	G	36	4HH	OG-P-O2P	-8.86	74.46	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	36	4HH	P-OG-CB	6.13	157.62	121.68
4	S	36	4HH	P-OG-CB	6.11	157.50	121.68
4	I	36	4HH	P-OG-CB	-5.41	89.97	121.68
4	M	36	4HH	P-OG-CB	-5.39	90.07	121.68
4	M	36	4HH	O1P-P-OG	4.65	129.33	107.75
4	I	36	4HH	O1P-P-OG	4.64	129.28	107.75
4	M	36	4HH	OG-CB-CA	4.42	112.45	108.14
4	I	36	4HH	OG-CB-CA	4.35	112.38	108.14
4	G	36	4HH	OG-CB-CA	2.86	110.93	108.14
4	S	36	4HH	OG-CB-CA	2.80	110.87	108.14

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	36	4HH	N-CA-CB-OG
4	I	36	4HH	CB-OG-P-O1P
4	M	36	4HH	N-CA-CB-OG
4	M	36	4HH	CB-OG-P-O1P
4	G	36	4HH	CJ-O3P-P-OG
4	S	36	4HH	CJ-O3P-P-OG
4	S	36	4HH	CB-OG-P-O3P
4	G	36	4HH	CB-OG-P-O3P
4	I	36	4HH	CO-CP-CQ-NR
4	M	36	4HH	CO-CP-CQ-NR
4	I	36	4HH	CO-CP-CQ-OR
4	M	36	4HH	CO-CP-CQ-OR
4	I	36	4HH	CB-OG-P-O3P
4	M	36	4HH	CB-OG-P-O3P
4	G	36	4HH	ON-CL3-CM-OM
4	I	36	4HH	ON-CL3-CM-OM
4	S	36	4HH	ON-CL3-CM-OM
4	M	36	4HH	ON-CL3-CM-OM
4	G	36	4HH	CT-CS-NR-CQ
4	S	36	4HH	CT-CS-NR-CQ
4	G	36	4HH	CB-OG-P-O2P
4	S	36	4HH	CB-OG-P-O2P

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	36	4HH	1	0
4	S	36	4HH	16	0
4	M	36	4HH	1	0
4	G	36	4HH	15	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
8	ATP	A	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)
8	ATP	O	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)
8	ATP	P	1502	7	26,33,33	0.63	0	31,52,52	1.12	3 (9%)
8	ATP	B	1502	7	26,33,33	0.63	0	31,52,52	1.12	3 (9%)

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
8	ATP	A	1502	7	-	1/18/38/38	0/3/3/3
8	ATP	O	1502	7	-	1/18/38/38	0/3/3/3
8	ATP	P	1502	7	-	2/18/38/38	0/3/3/3
8	ATP	B	1502	7	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	1502	ATP	C5-C6-N6	2.39	123.99	120.35
8	B	1502	ATP	C5-C6-N6	2.37	123.96	120.35
8	A	1502	ATP	C5-C6-N6	2.35	123.92	120.35
8	A	1502	ATP	O2'-C2'-C3'	-2.32	104.30	111.82
8	O	1502	ATP	O2'-C2'-C3'	-2.31	104.36	111.82
8	O	1502	ATP	C5-C6-N6	2.30	123.85	120.35
8	P	1502	ATP	O2'-C2'-C3'	-2.20	104.72	111.82
8	B	1502	ATP	O2'-C2'-C3'	-2.18	104.77	111.82
8	B	1502	ATP	O3'-C3'-C2'	-2.14	104.90	111.82
8	P	1502	ATP	O3'-C3'-C2'	-2.13	104.93	111.82
8	O	1502	ATP	O3'-C3'-C2'	-2.08	105.10	111.82
8	A	1502	ATP	O3'-C3'-C2'	-2.07	105.12	111.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

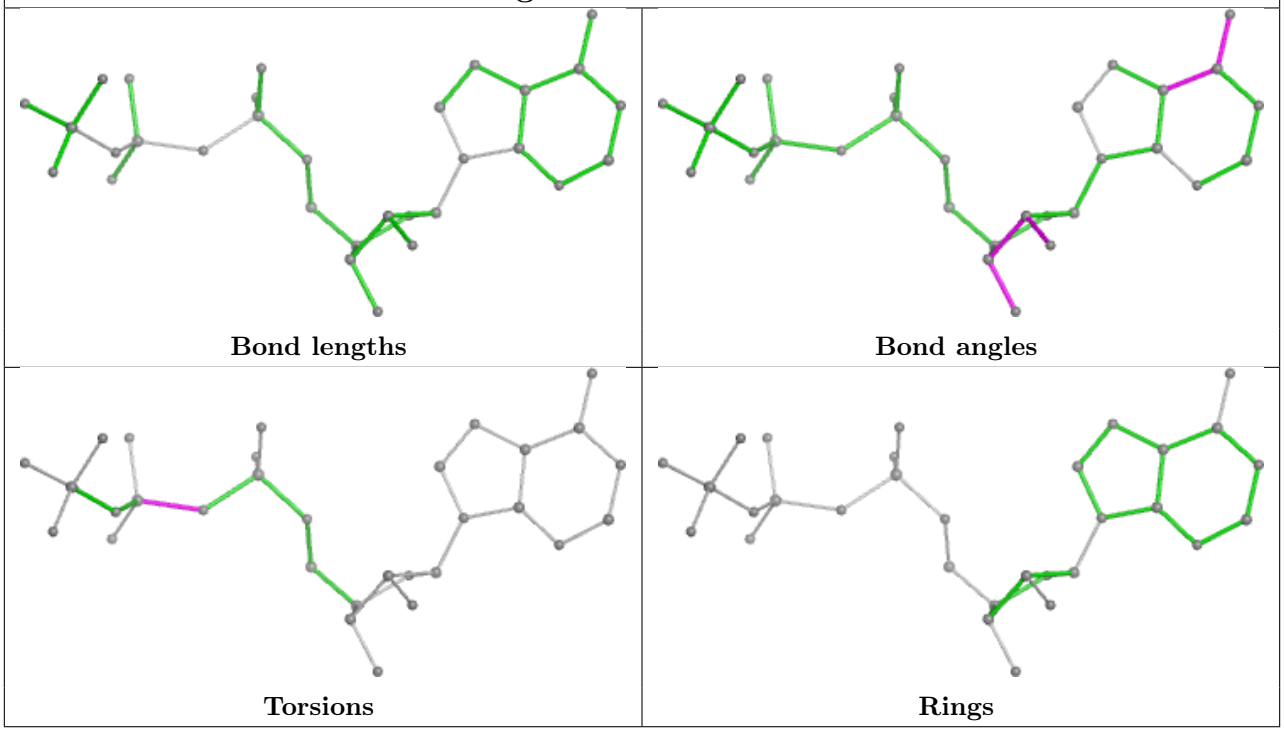
Mol	Chain	Res	Type	Atoms
8	A	1502	ATP	PA-O3A-PB-O2B
8	O	1502	ATP	PA-O3A-PB-O2B
8	B	1502	ATP	PA-O3A-PB-O1B
8	B	1502	ATP	PA-O3A-PB-O2B
8	P	1502	ATP	PA-O3A-PB-O1B
8	P	1502	ATP	PA-O3A-PB-O2B

There are no ring outliers.

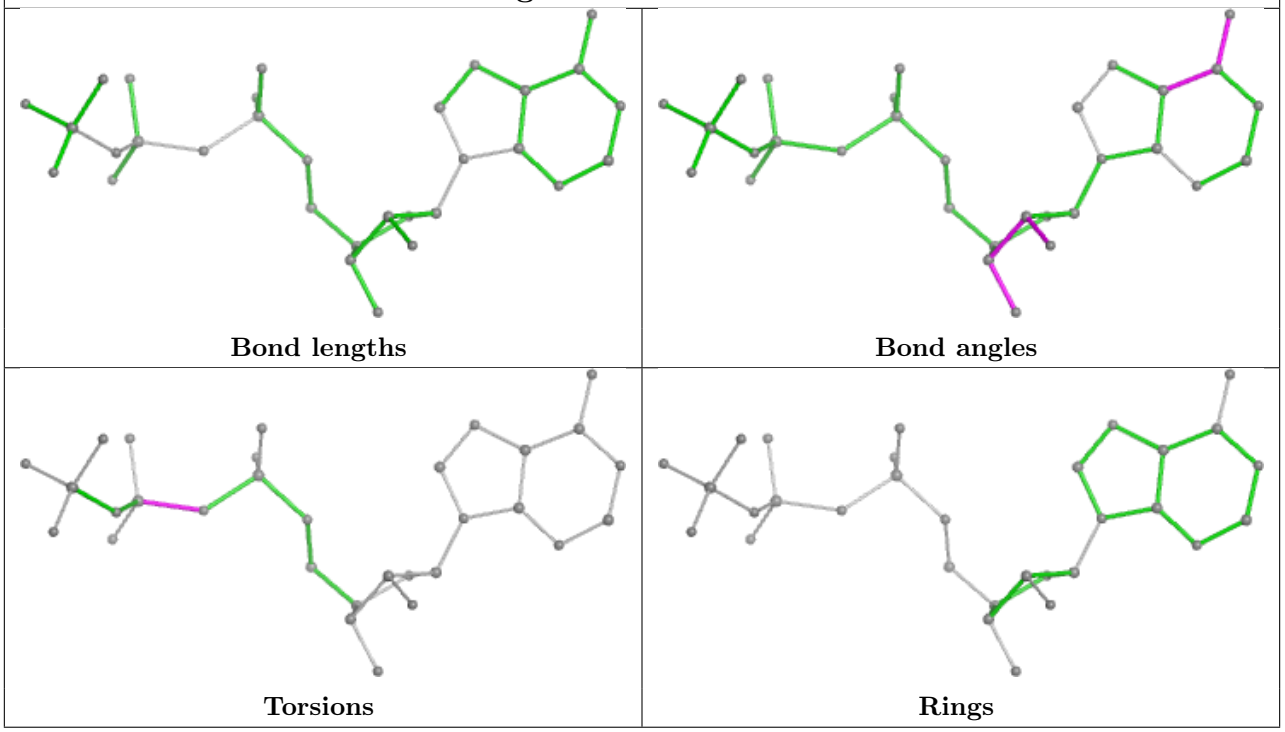
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

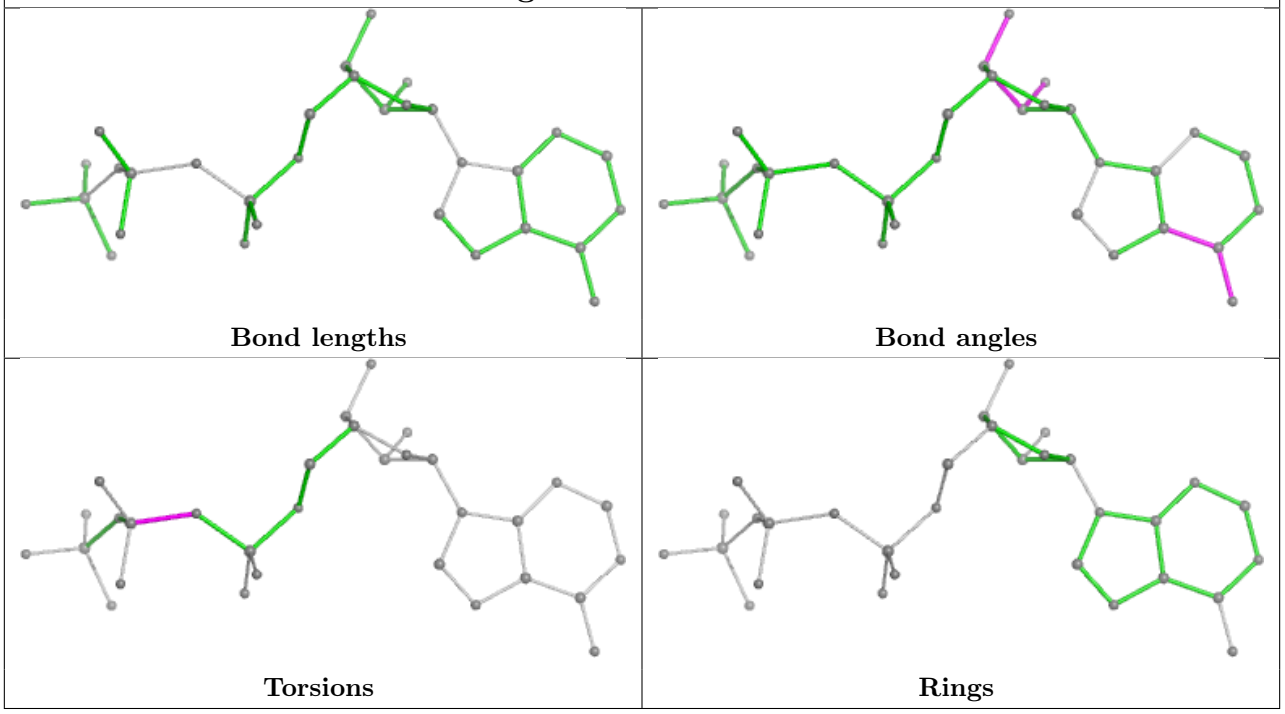
Ligand ATP A 1502



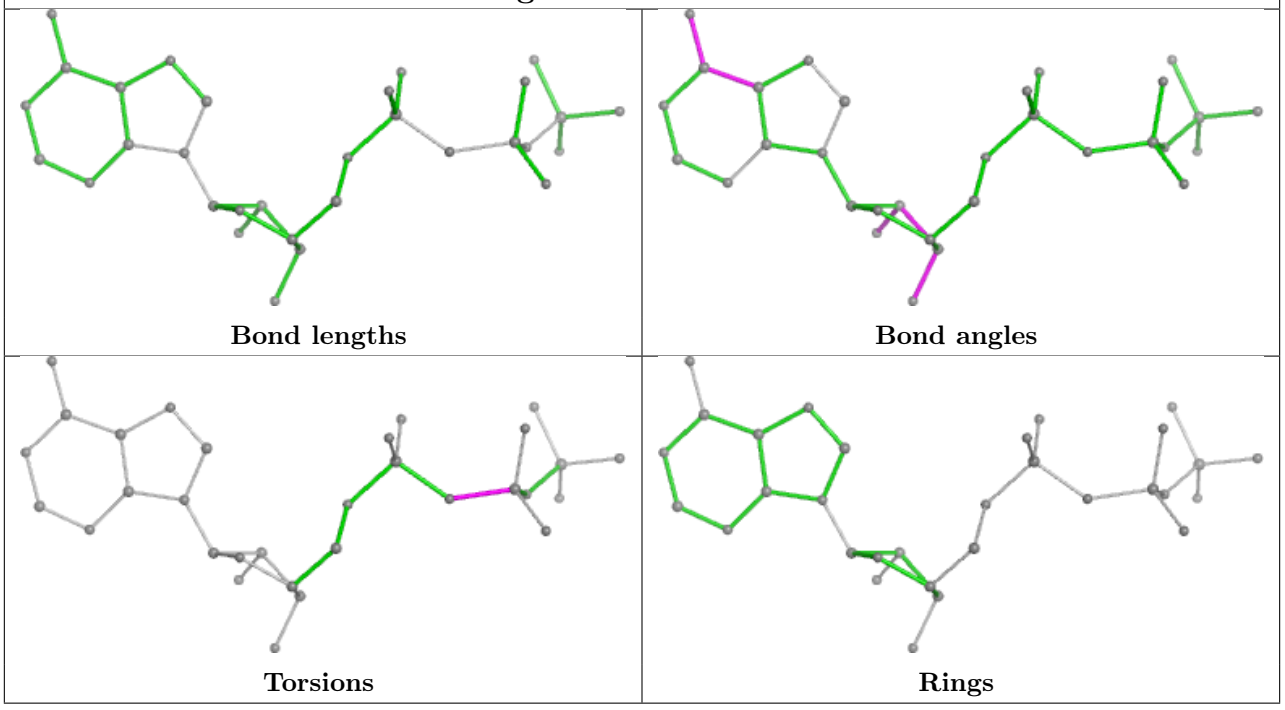
Ligand ATP O 1502



Ligand ATP P 1502



Ligand ATP B 1502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	295:ARG	C	296:ILE	N	1.04
1	C	295:ARG	C	296:ILE	N	1.03

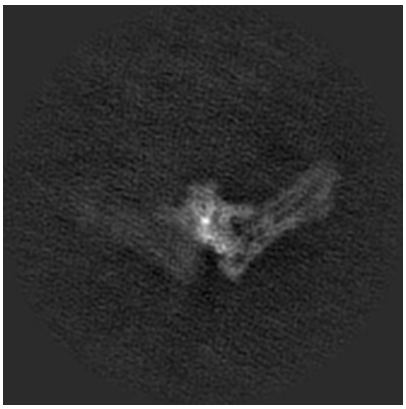
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51446. These allow visual inspection of the internal detail of the map and identification of artifacts.

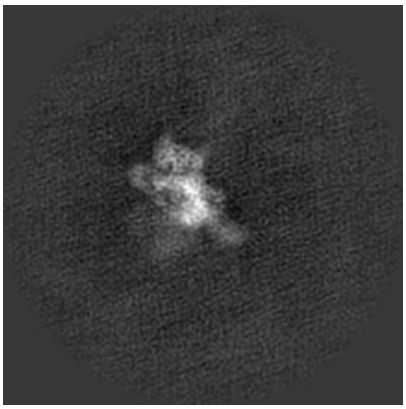
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

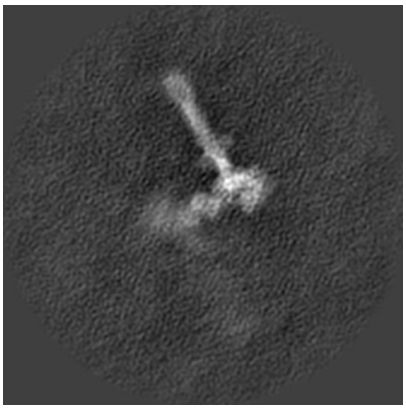
6.1.1 Primary map



X

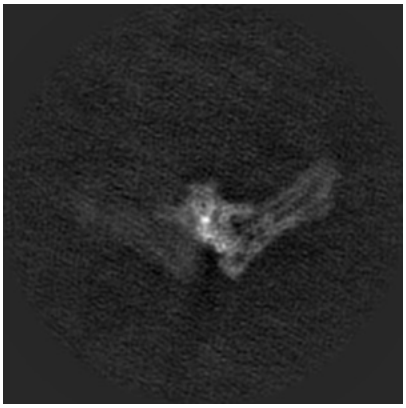


Y

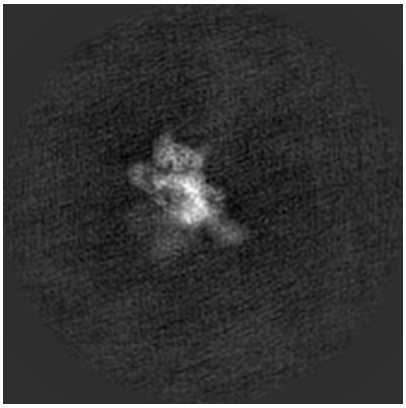


Z

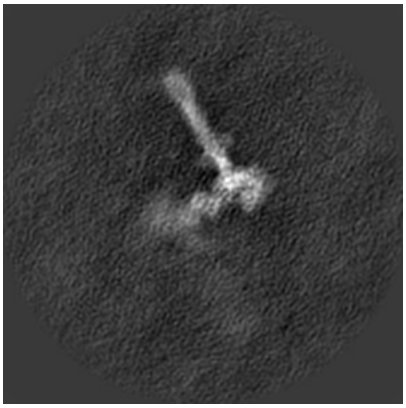
6.1.2 Raw map



X



Y

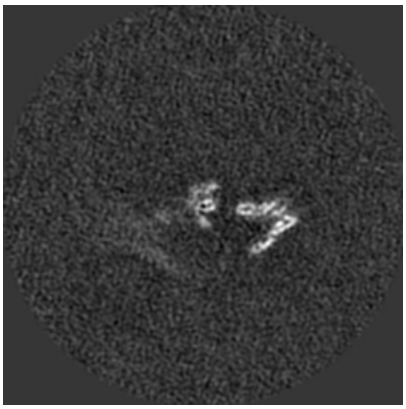


Z

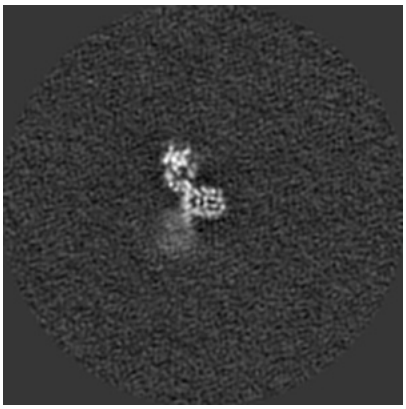
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

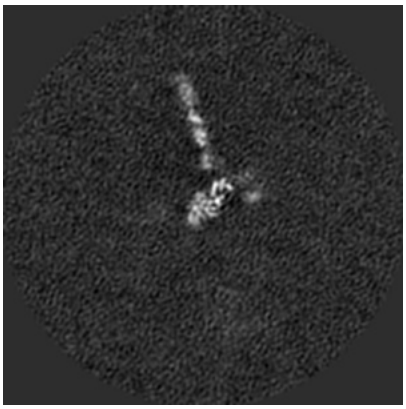
6.2.1 Primary map



X Index: 83

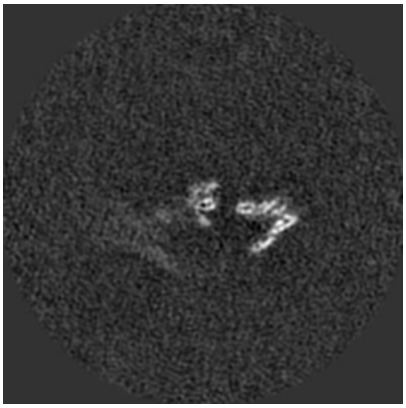


Y Index: 83

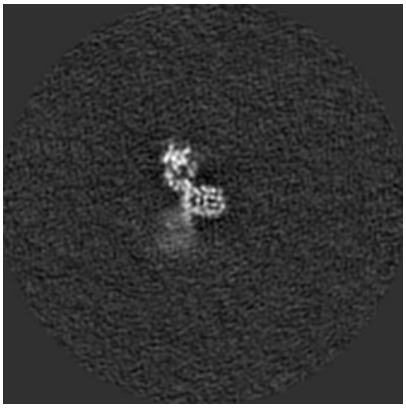


Z Index: 83

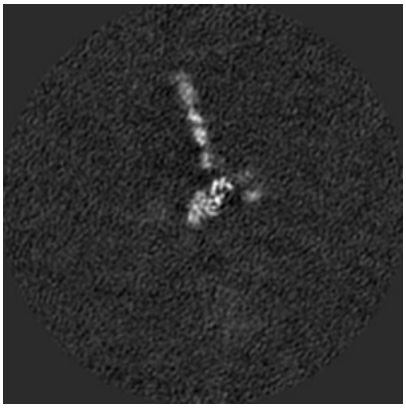
6.2.2 Raw map



X Index: 83



Y Index: 83

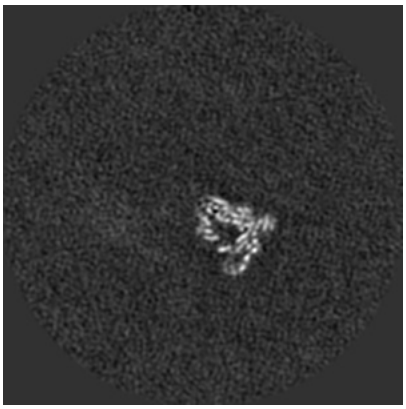


Z Index: 83

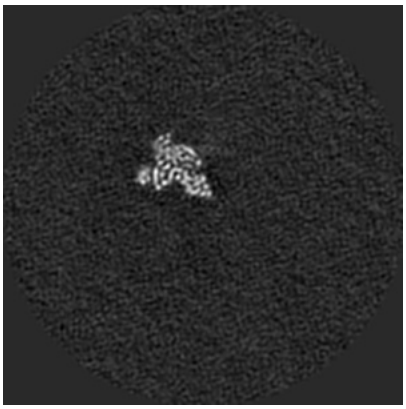
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

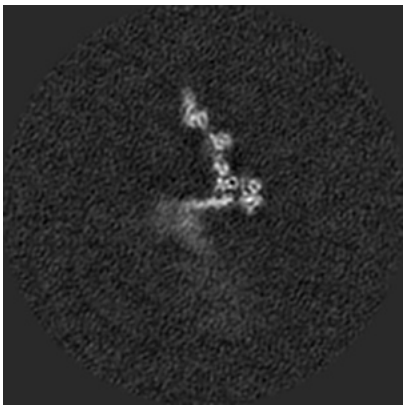
6.3.1 Primary map



X Index: 90

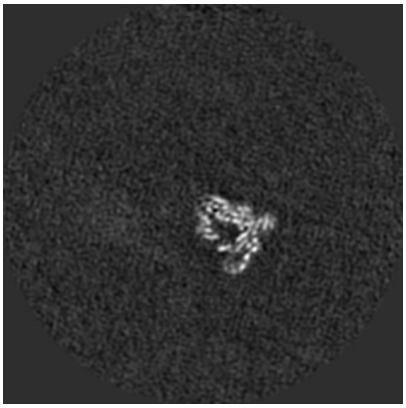


Y Index: 90

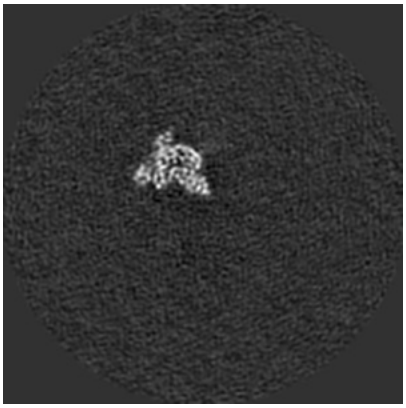


Z Index: 76

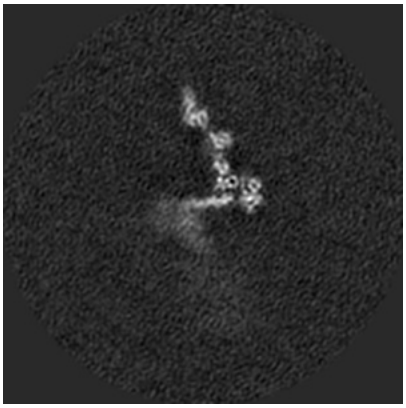
6.3.2 Raw map



X Index: 90



Y Index: 91

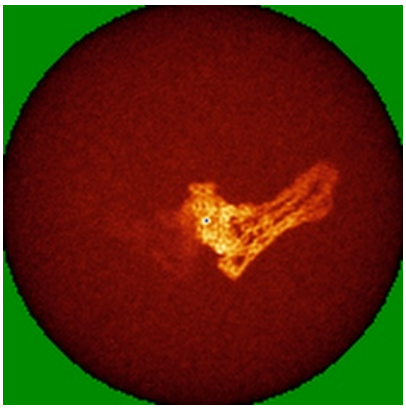


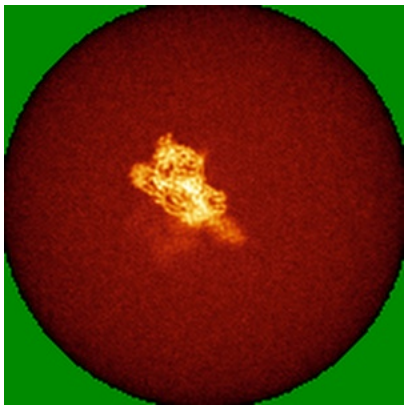
Z Index: 76

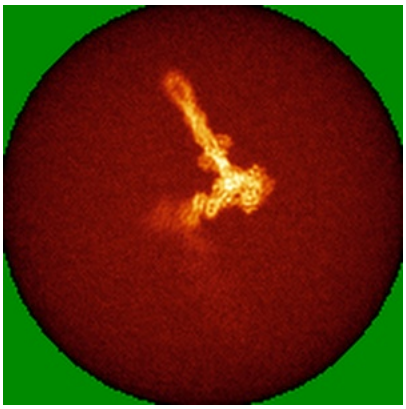
The images above show the largest variance slices of the map in three orthogonal directions.

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

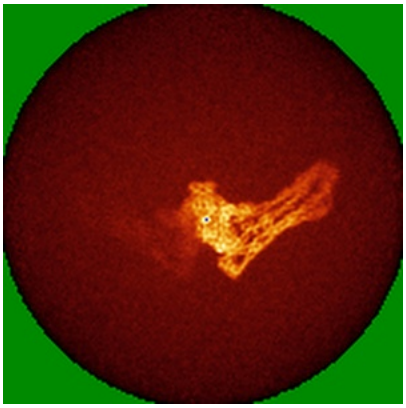
6.4.1 Primary map

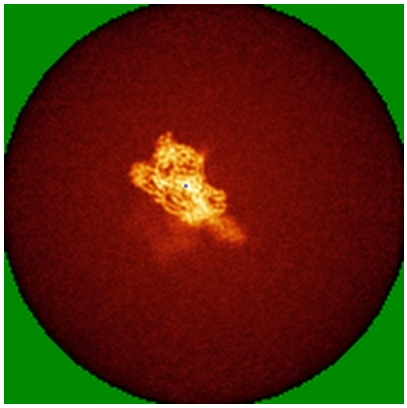

X

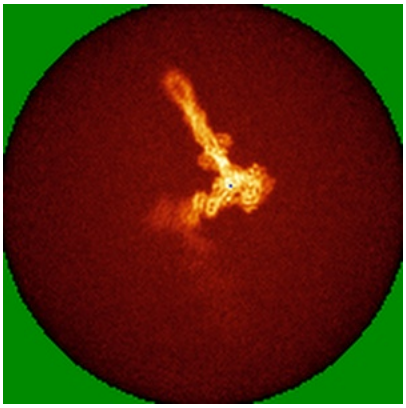

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

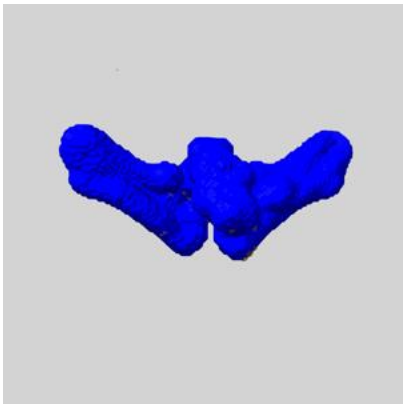
6.6 Mask visualisation

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

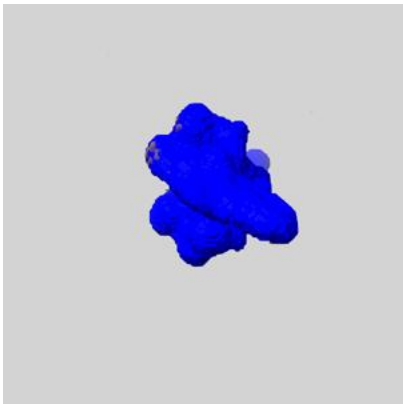
A mask typically either:

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

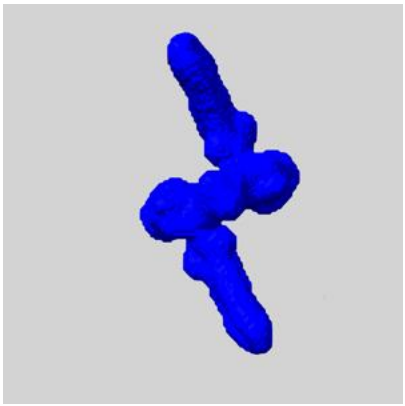
6.6.1 emd_51446_msk_1.map



X



Y

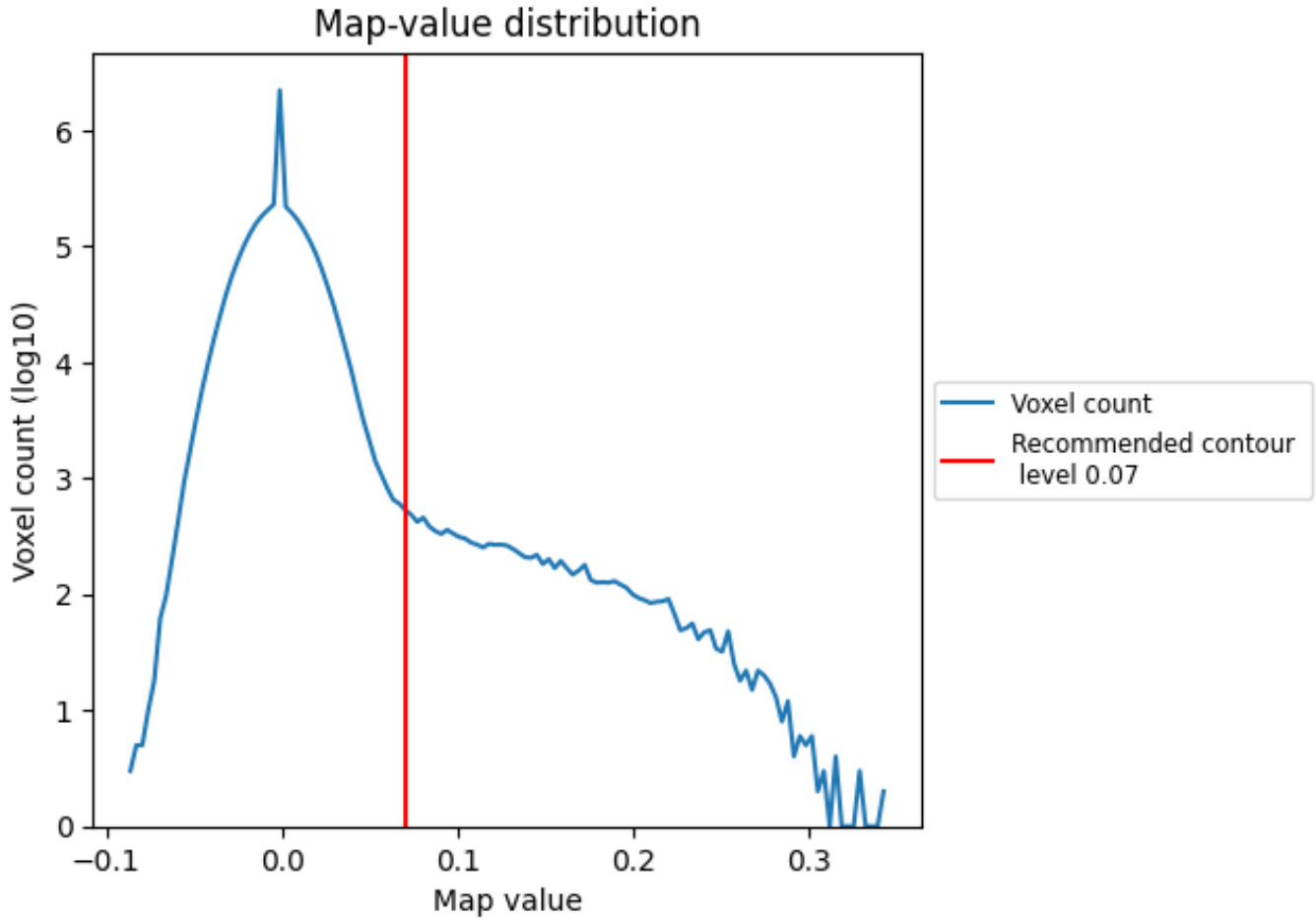


Z

7 Map analysis

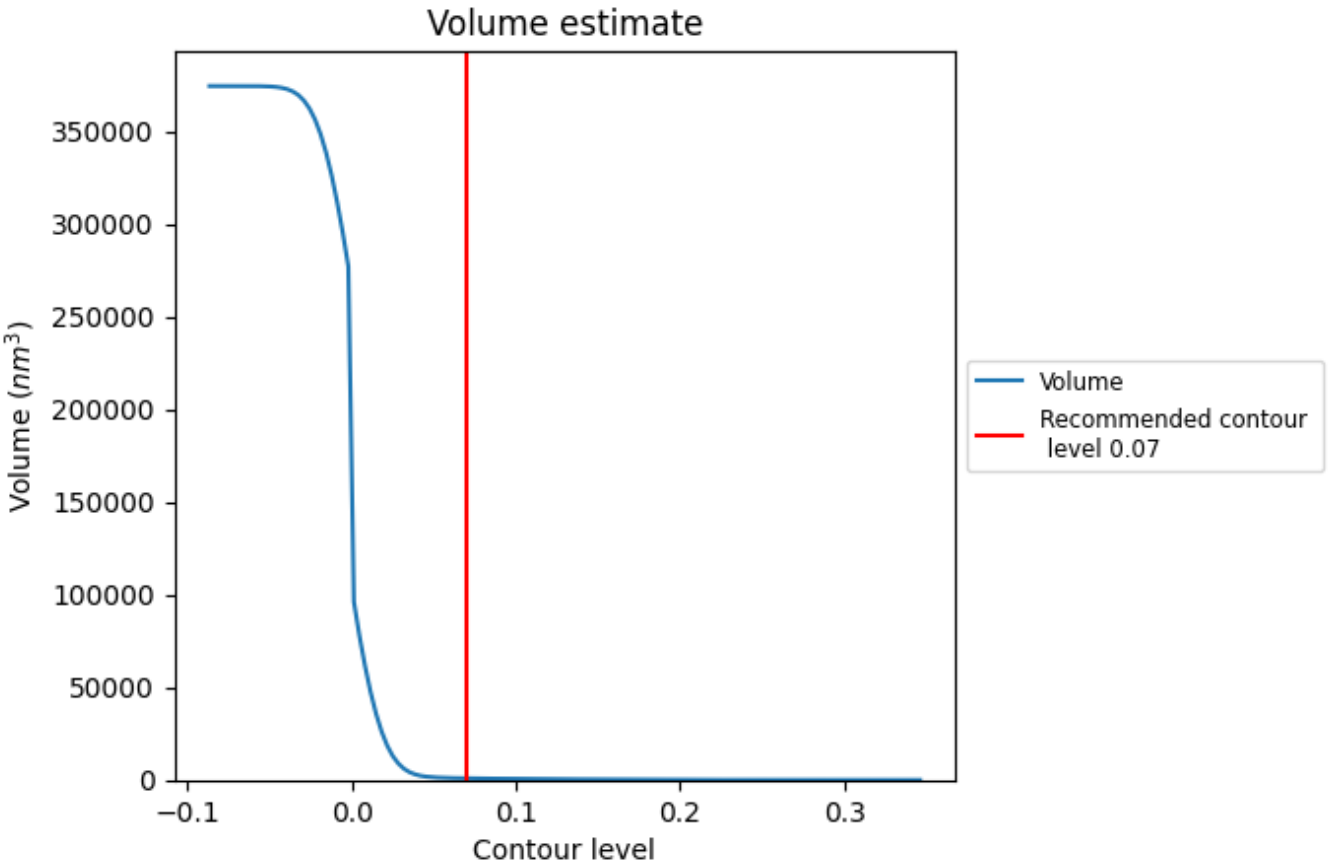
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

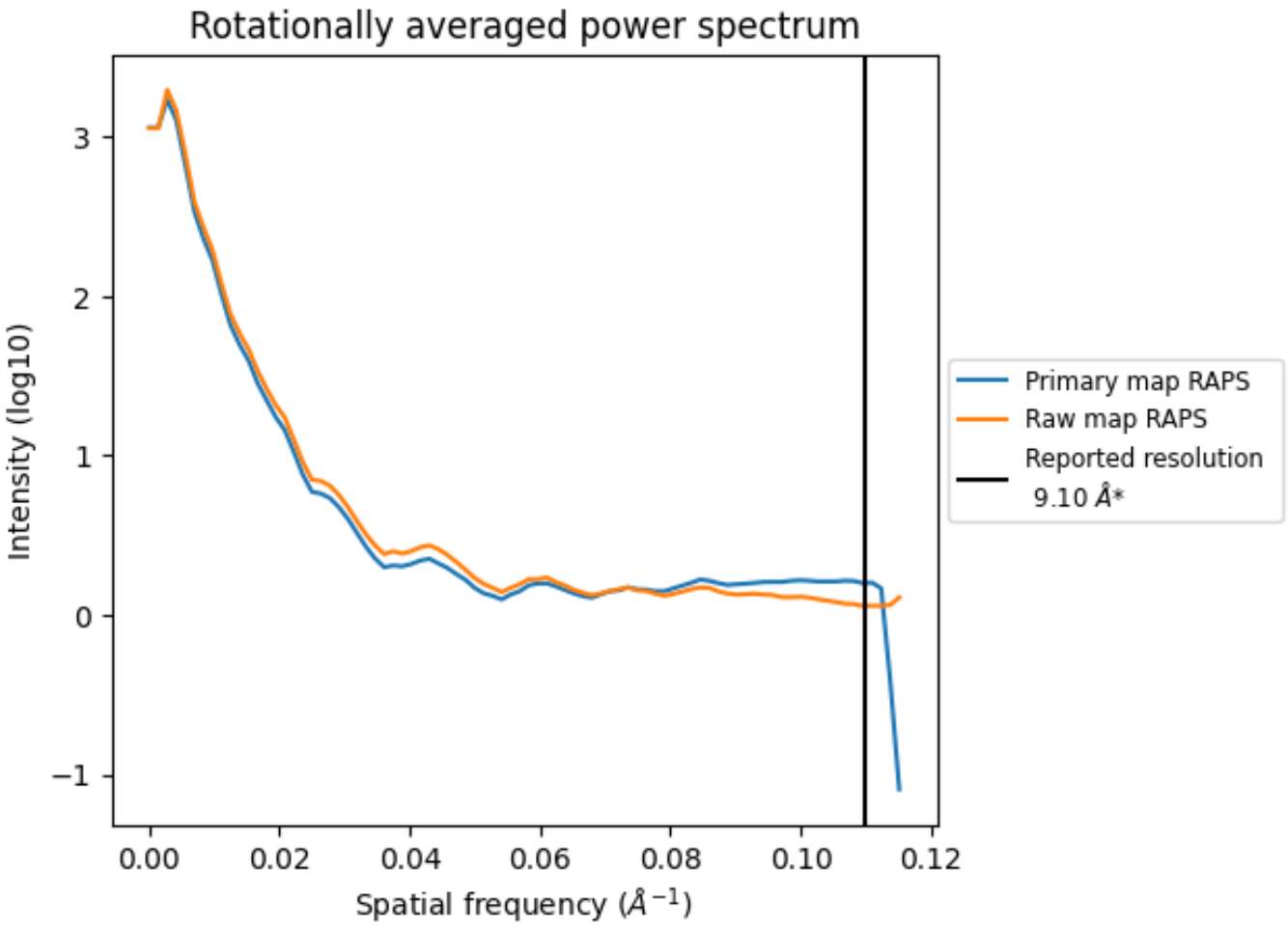
7.2 Volume estimate



The volume at the recommended contour level is 892 nm^3; this corresponds to an approximate mass of 806 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)

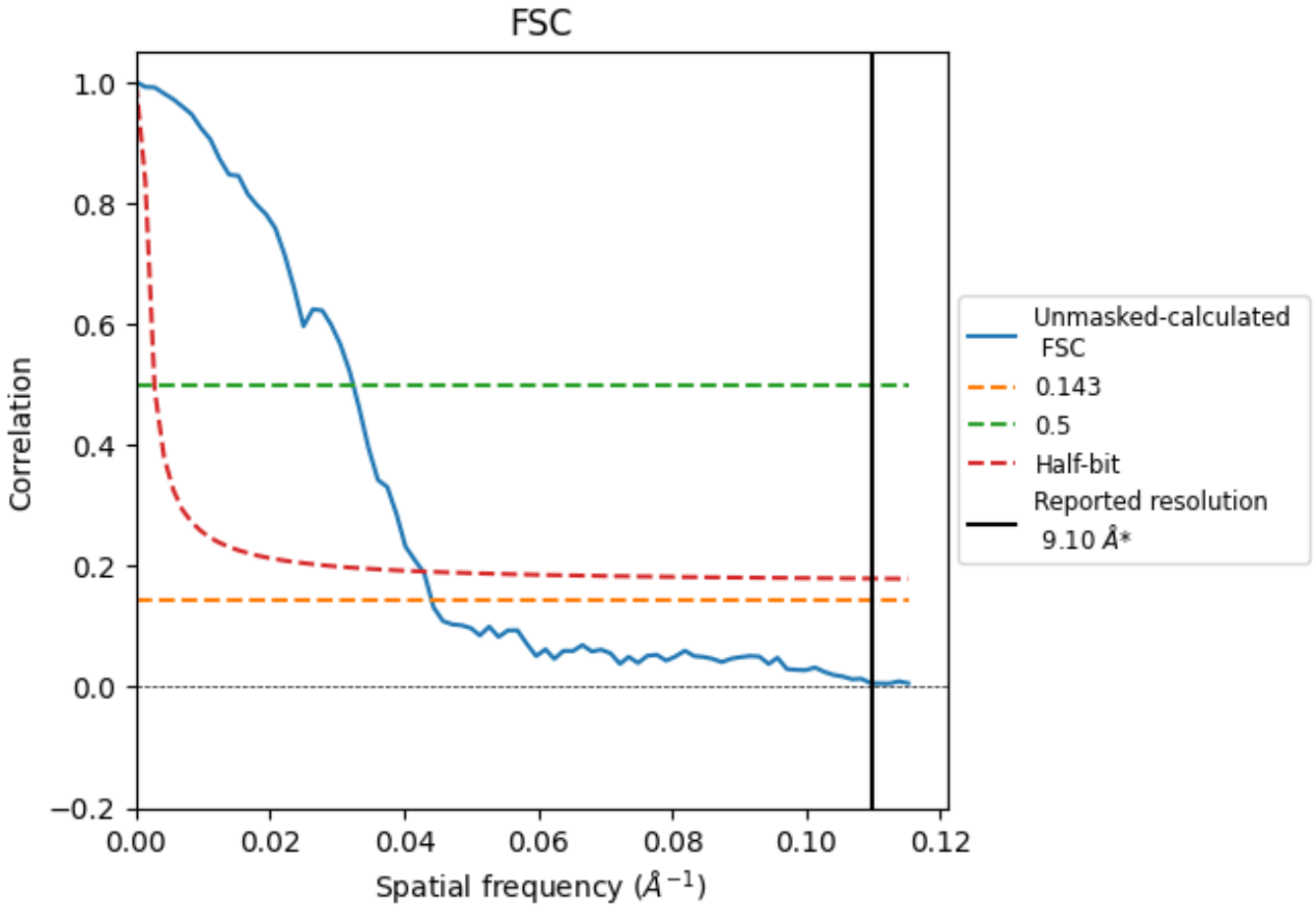


*Reported resolution corresponds to spatial frequency of 0.110 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.110 Å^{-1}

8.2 Resolution estimates (i)

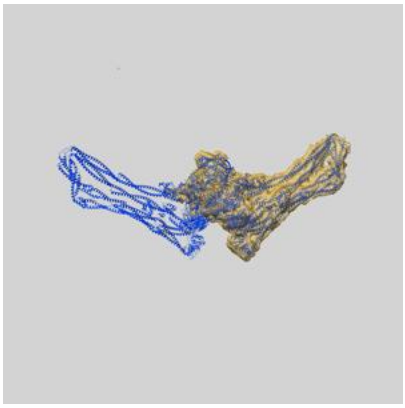
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	22.68	30.86	23.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 22.68 differs from the reported value 9.1 by more than 10 %

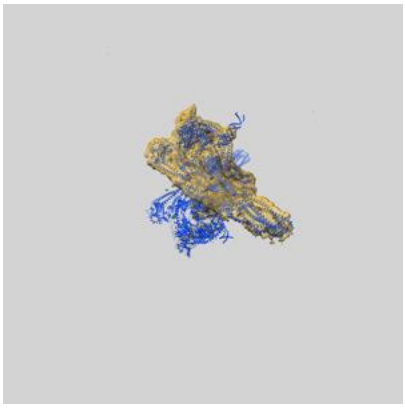
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51446 and PDB model 9GMA. Per-residue inclusion information can be found in section 3 on page 7.

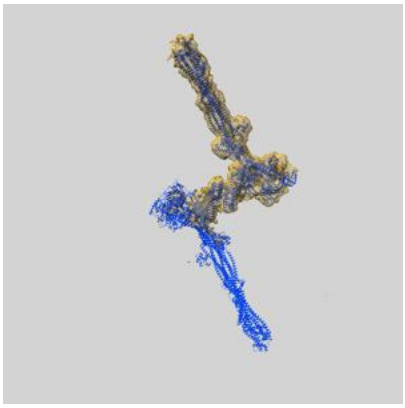
9.1 Map-model overlay



X



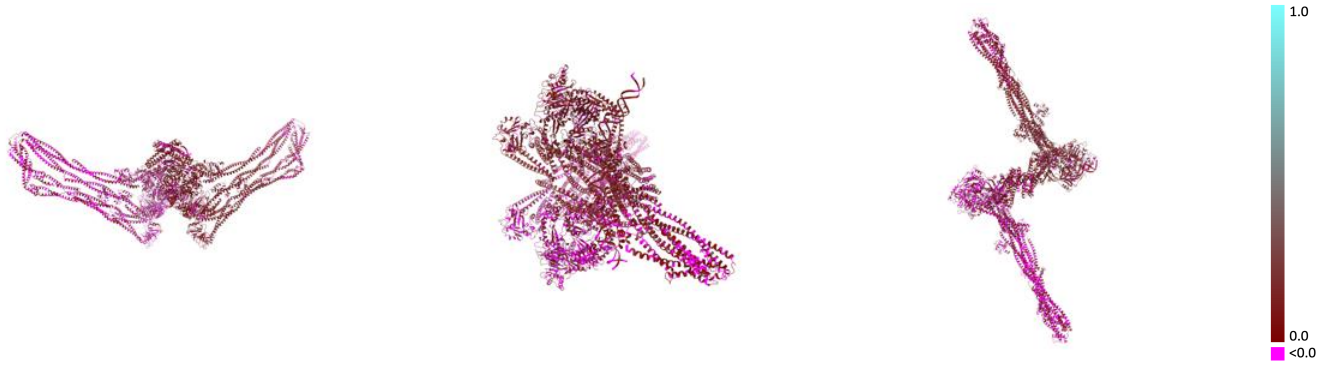
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

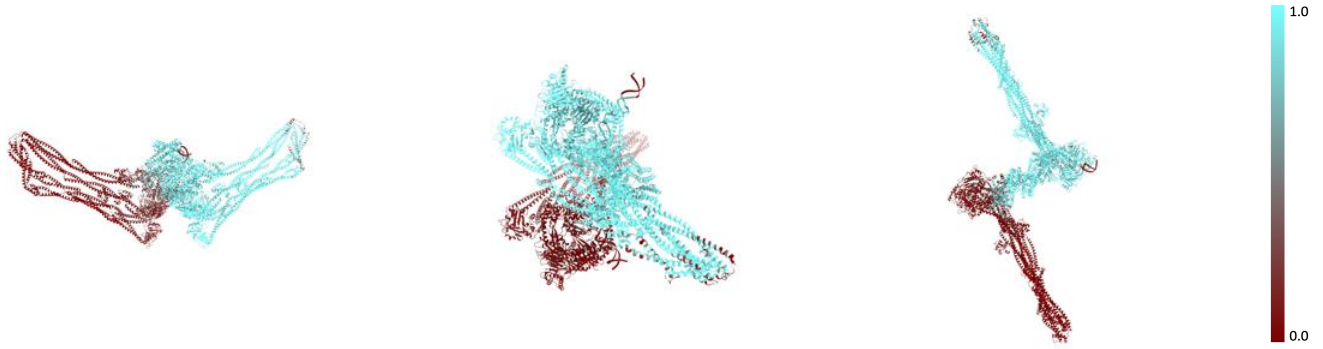
9.2 Q-score mapped to coordinate model (i)



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.

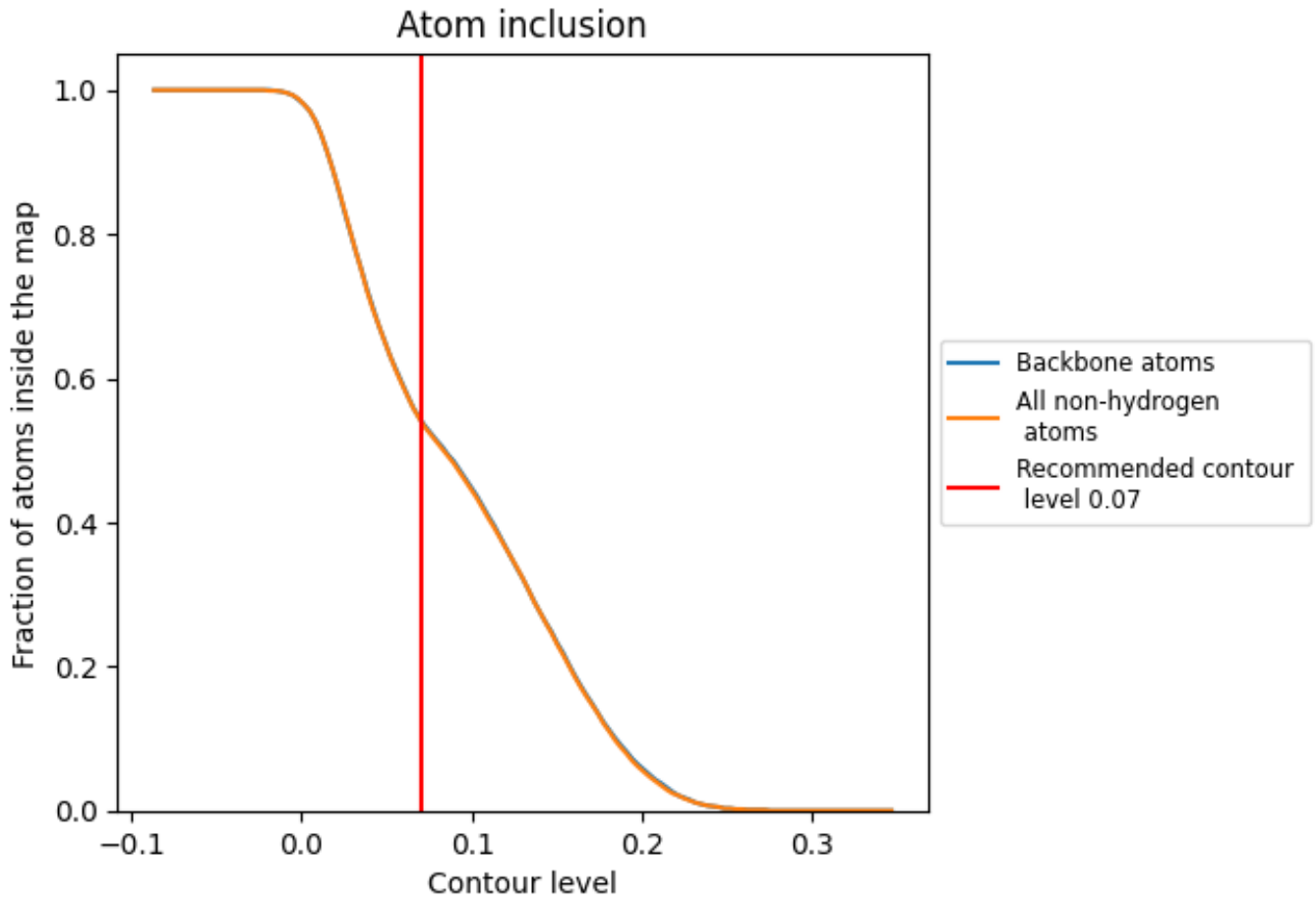
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.0750
A	0.9440	0.1220
B	0.9390	0.1190
C	0.9450	0.1200
D	0.6710	0.0760
E	0.9470	0.1300
F	0.9570	0.1330
G	0.9830	0.1350
I	0.9640	0.1490
K	0.6510	0.1010
L	0.6390	0.0990
M	0.0360	0.0260
O	0.0050	0.0160
P	0.0350	0.0200
Q	0.6600	0.0450
R	0.1760	0.0320
S	0.0000	0.0030