Full wwPDB EM Validation Report ⓘ

Mar 19, 2024 – 02:39 PM JST

PDB ID	:	5X0Y
EMDB ID	:	EMD-6700
Title	:	Complex of Snf2-Nucleosome complex with Snf2 bound to SHL2 of the nucleosome
Authors	:	Li, M.; Liu, X.; Xia, X.; Chen, Z.; Li, X.
Deposited on	:	2017-01-23
Resolution	:	4.69 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:

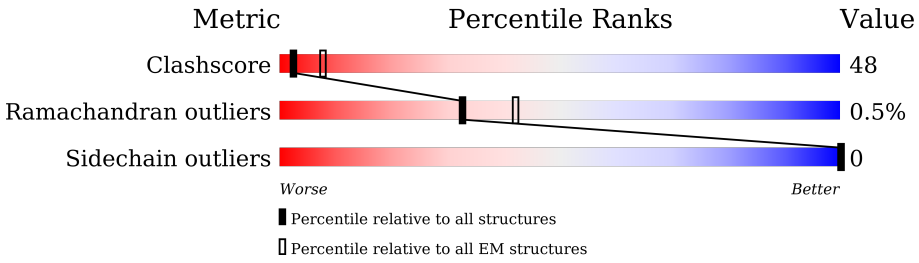
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.69 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	135	22% 30% 42% • 27%
1	E	135	19% 33% 36% • 30%
2	B	102	25% 33% 51% • 15%
2	F	102	23% 46% 38% 16%
3	C	129	35% 40% 42% • 17%
3	G	129	23% 43% 40% • 17%
4	D	122	17% 46% 30% 24%
4	H	122	7% 41% 35% 24%

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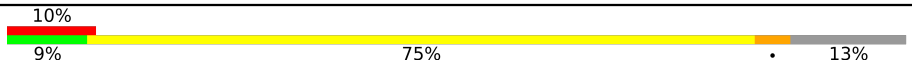
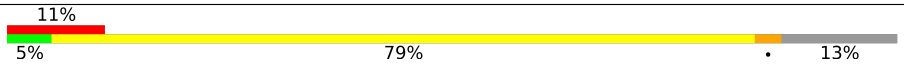
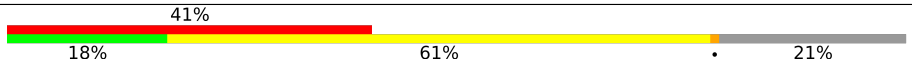
Mol	Chain	Length	Quality of chain
5	I	167	
6	J	167	
7	O	735	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			800	505	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			778	491	148	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			811	510	158	143		
3	G	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	see sequence details	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
H	29	THR	SER	see sequence details	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

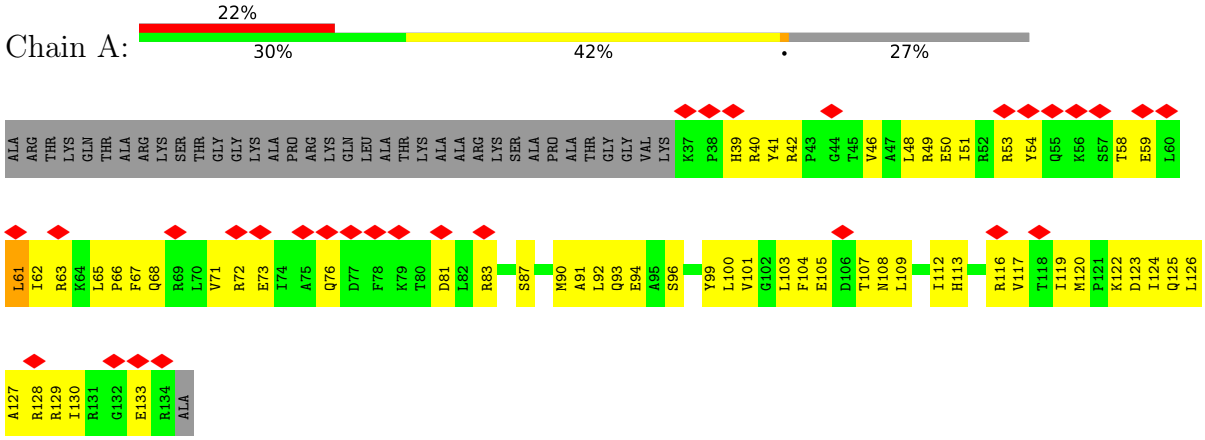
- Molecule 7 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	583	Total	C	N	O	S	0	0
			4789	3045	846	881	17		

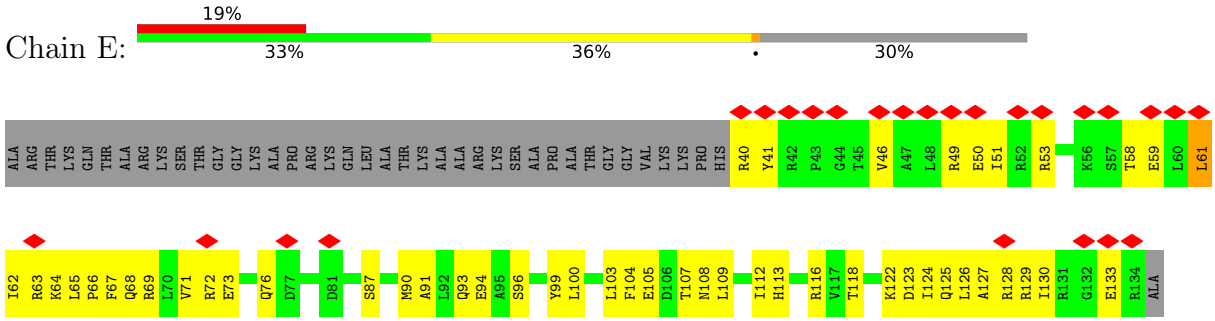
3 Residue-property plots (i)

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.

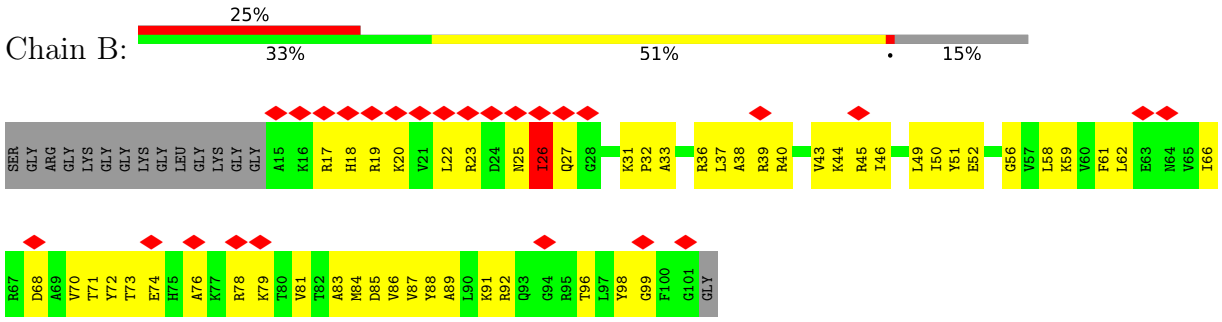
• Molecule 1: Histone H3.2



• Molecule 1: Histone H3.2

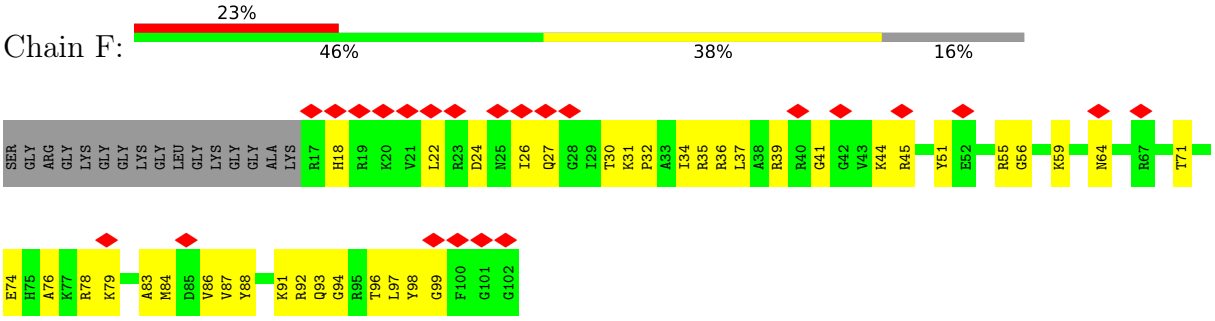


• Molecule 2: Histone H4



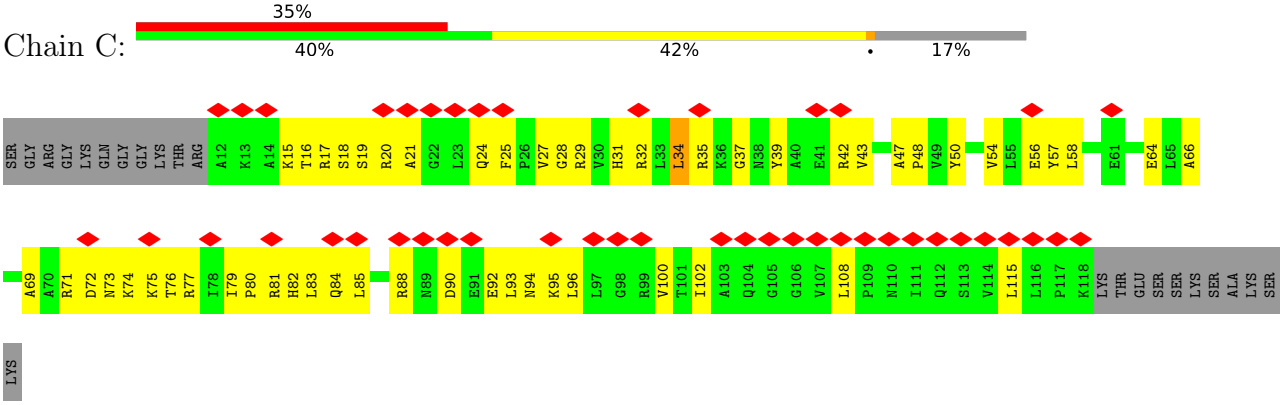
• Molecule 2: Histone H4

Chain F:



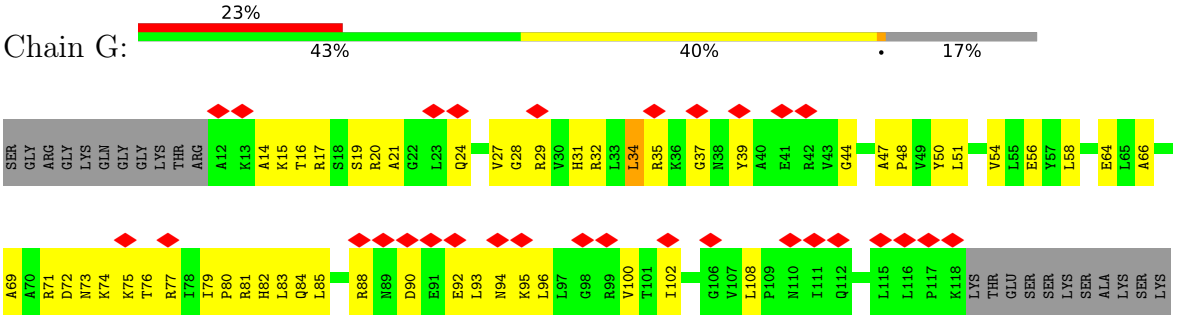
• Molecule 3: Histone H2A

Chain C:



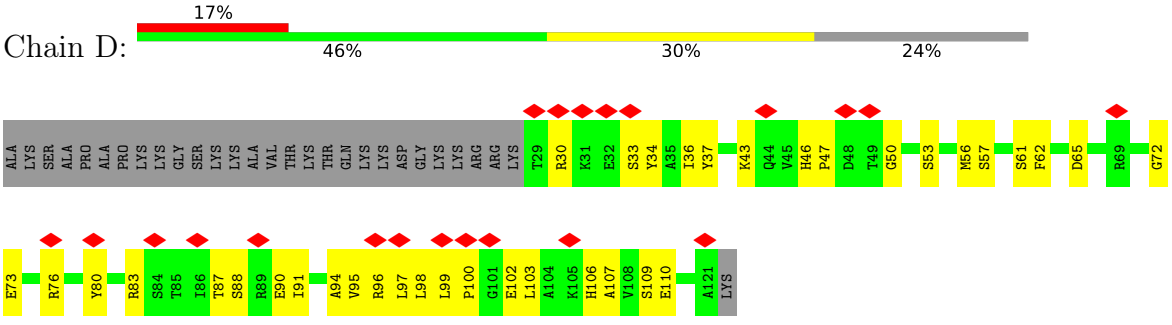
• Molecule 3: Histone H2A

Chain G:



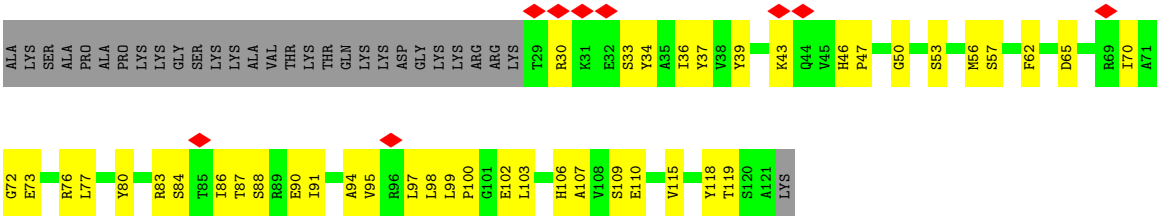
• Molecule 4: Histone H2B 1.1

Chain D:



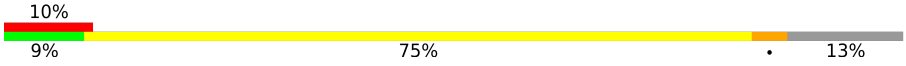
• Molecule 4: Histone H2B 1.1

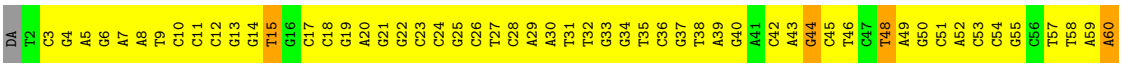
Chain H:

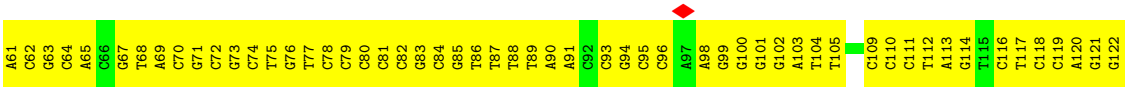


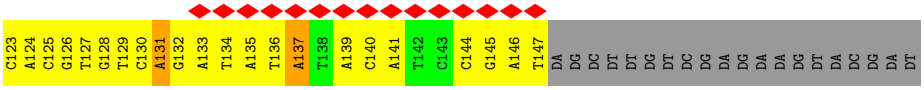
• Molecule 5: DNA (167-MER)

Chain I:



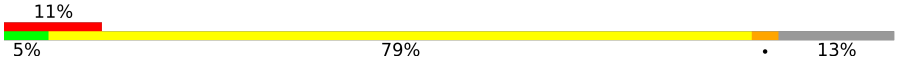


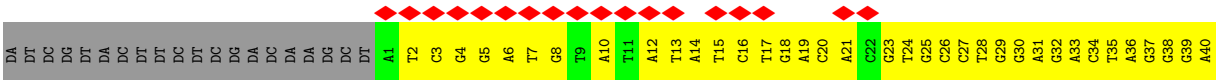


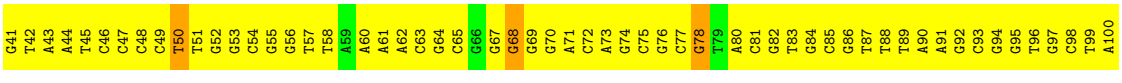


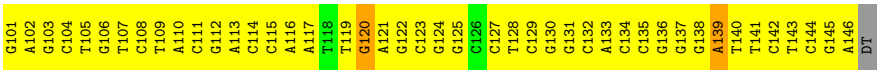
• Molecule 6: DNA (167-MER)

Chain J:



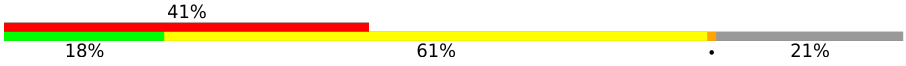


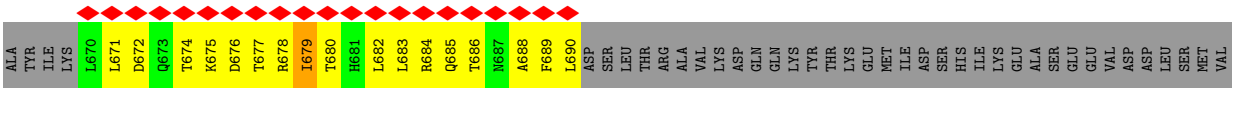


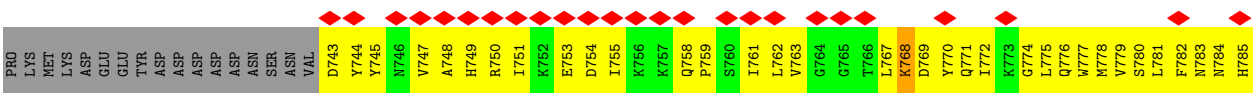


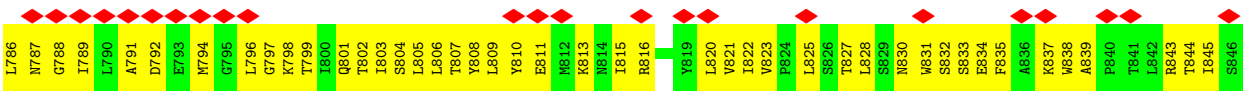
• Molecule 7: Transcription regulatory protein SNF2

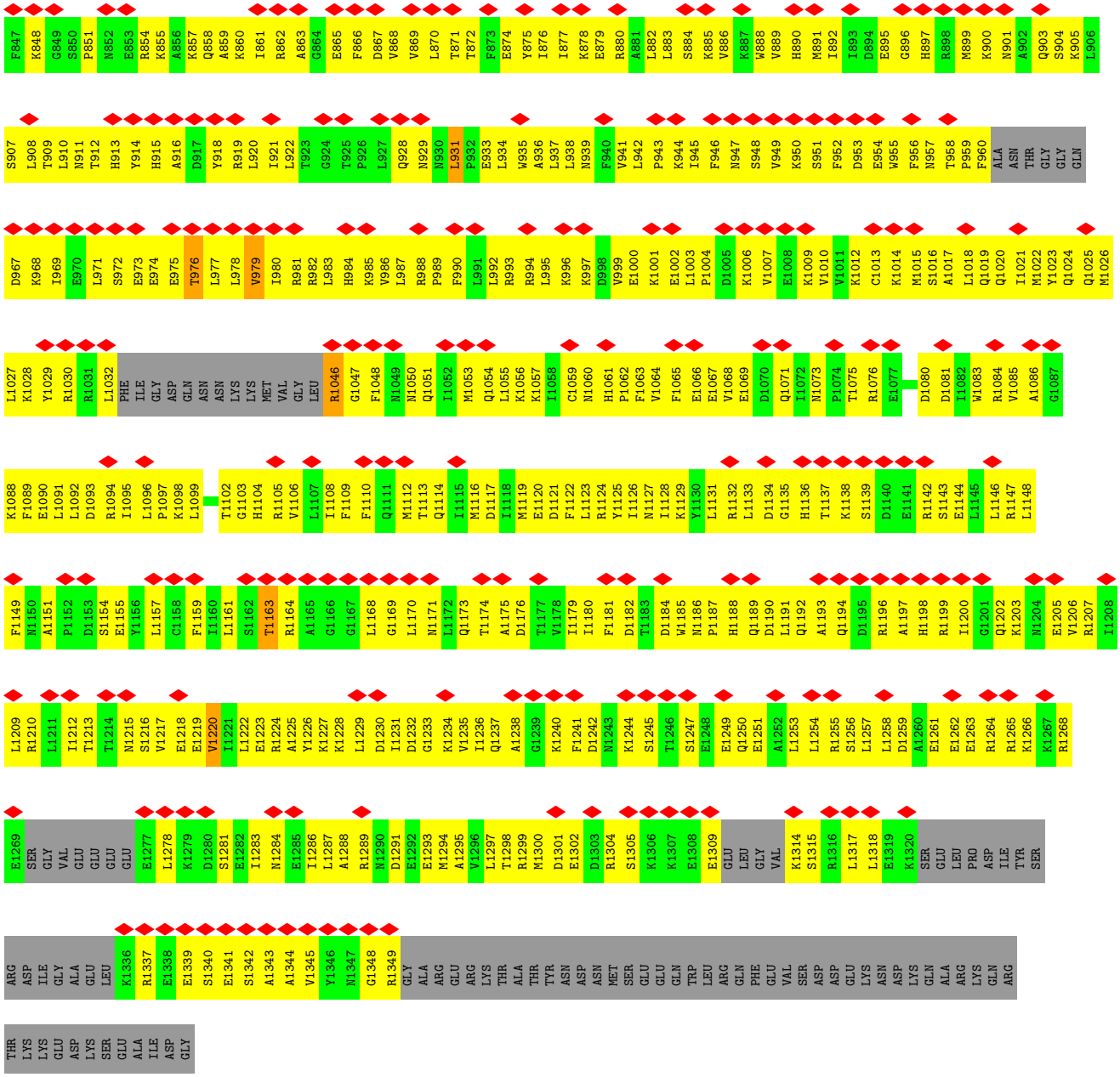
Chain O:










F847 K848 G849 S850 P851 N852 E853 R854 K855 A856 K857 Q858 A859 K860 I861 R862 A863 G864 E865 F866 D867 V868 V869 L870 T871 T872 F873 E874 Y875 I876 I877 K878 E879 R880 A881 L882 L883 S884 K885 V886 K887 W888 V889 H890 M891 I892 I893 D894 E895 G896 H897 R898 M899 K900 N901 A902 Q903 S904 K905 L906
S907 L908 T909 L910 N911 T912 H913 Y914 H915 A916 D917 Y918 R919 L920 I921 L922 T923 G924 T925 P926 L927 Q928 N929 N930 L931 P932 E933 L934 W935 A936 L937 L938 N939 F940 V941 L942 P943 K944 I945 F946 N947 S948 V949 K950 S951 F952 D953 E954 W955 F956 N957 T958 P959 F960 ALA ASN THR GLY GLY GLN
D967 K968 I969 E970 L971 S972 E973 E974 E975 T976 L977 L978 V979 I980 R981 R982 L983 H984 K985 V986 L987 R988 P989 F990 L991 L992 R993 R994 L995 K996 K997 D998 V999 E1000 K1001 E1002 L1003 P1004 D1005 K1006 V1007 E1008 K1009 V1010 V1011 K1012 C1013 K1014 M1015 S1016 A1017 L1018 Q1019 Q1020 I1021 M1022 Y1023 Q1024 Q1025 M1026
L1027 K1028 Y1029 R1030 R1031 L1032 PHE ILE GLY ASP GLN ASN ASN LYS LYS MET VAL GLY LEU R1046 G1047 F1048 N1049 N1050 Q1051 I1052 M1053 Q1054 L1055 K1056 K1057 I1058 C1059 N1060 H1061 P1062 F1063 V1064 F1065 E1066 E1067 V1068 E1069 D1070 Q1071 I1072 N1073 P1074 T1075 R1076 E1077 D1080 D1081 I1082 W1083 R1084 V1085 A1086 G1087
K1088 F1089 E1090 L1091 L1092 D1093 R1094 I1095 L1096 P1097 K1098 L1099 T1102 G1103 H1104 R1105 V1106 L1107 I1108 F1109 F1110 Q1111 M1112 T1113 Q1114 I1115 M1116 D1117 I1118 M1119 E1120 D1121 F1122 L1123 R1124 Y1125 I1126 N1127 I1128 K1129 Y1130 L1131 R1132 L1133 D1134 G1135 H1136 T1137 K1138 S1139 D1140 E1141 R1142 S1143 E1144 L1145 L1146 R1147 L1148
F1149 N1150 A1151 P1152 D1153 S1154 E1155 Y1156 L1157 C1158 F1159 I1160 L1161 S1162 T1163 R1164 A1165 G1166 G1167 L1168 G1169 L1170 N1171 L1172 Q1173 T1174 A1175 D1176 T1177 V1178 I1179 I1180 F1181 D1182 T1183 D1184 W1185 N1186 P1187 H1188 Q1189 D1190 L1191 Q1192 A1193 Q1194 D1195 R1196 A1197 H1198 R1199 I1200 G1201 Q1202 K1203 N1204 E1205 V1206 R1207 I1208
L1209 R1210 L1211 I1212 T1213 T1214 N1215 S1216 V1217 E1218 E1219 V1220 I1221 L1222 E1223 R1224 A1225 Y1226 K1227 K1228 L1229 D1230 I1231 D1232 G1233 K1234 V1235 I1236 Q1237 A1238 G1239 K1240 F1241 D1242 N1243 K1244 S1245 T1246 S1247 E1248 E1249 Q1250 E1251 A1252 L1253 L1254 R1255 S1256 L1257 L1258 D1259 A1260 E1261 E1262 E1263 R1264 R1265 K1266 K1267 R1268
E1269 SER GLY VAL GLU GLU GLU GLU E1277 L1278 K1279 D1280 S1281 E1282 I1283 N1284 E1285 I1286 L1287 A1288 R1289 N1290 D1291 E1292 E1293 M1294 A1295 V1296 L1297 T1298 R1299 M1300 D1301 E1302 D1303 R1304 S1305 K1306 K1307 E1308 E1309 GLU LEU GLY VAL K1314 S1315 R1316 L1317 L1318 E1319 K1320 SER GLU LEU PRO ASP ILE TYR SER
ARG ASP ILE GLY ALA GLU LEU K1336 R1337 E1338 E1339 S1340 E1341 S1342 A1343 A1344 V1345 Y1346 N1347 G1348 R1349 GLY ALA ARG GLU ARG LYS THR ALA THR TYR ASN ASP ASN MET SER GLU GLU GLN TRP LEU ARG GLN PHE GLU VAL SER ASP ASP GLU LYS ASN ASP LYS GLN ALA ARG LYS GLN ARG
THR LYS LYS GLU ASP LYS SER GLU ALA ILE ASP GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0341	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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	0.57	0/812	0.67	1/1091 (0.1%)
1	E	0.57	0/788	0.67	1/1057 (0.1%)
2	B	0.62	0/711	0.68	0/950
2	F	0.62	0/680	0.66	0/912
3	C	0.49	0/821	0.63	1/1112 (0.1%)
3	G	0.48	0/825	0.64	1/1116 (0.1%)
4	D	0.59	0/729	0.61	0/985
4	H	0.59	0/737	0.62	0/993
5	I	1.34	0/3333	1.11	6/5137 (0.1%)
6	J	1.36	1/3381 (0.0%)	1.04	4/5221 (0.1%)
7	O	0.45	0/4864	0.65	2/6536 (0.0%)
All	All	0.93	1/17681 (0.0%)	0.85	16/25110 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
2	B	0	1
7	O	0	5
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	68	DG	C3'-O3'	-5.87	1.36	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	120	DG	O4'-C4'-C3'	-7.85	101.29	106.00
5	I	15	DT	O4'-C4'-C3'	-7.37	101.55	104.50
5	I	48	DT	O4'-C4'-C3'	-7.21	101.61	104.50
5	I	60	DA	O4'-C1'-N9	6.42	112.50	108.00
5	I	44	DG	O4'-C4'-C3'	-6.09	102.06	104.50
7	O	959	PRO	N-CA-CB	5.90	110.38	103.30
1	A	61	LEU	CA-CB-CG	-5.76	102.05	115.30
1	E	61	LEU	CA-CB-CG	-5.75	102.07	115.30
6	J	50	DT	O4'-C4'-C3'	-5.62	102.25	104.50
5	I	137	DA	O4'-C4'-C3'	-5.57	102.27	104.50
6	J	139	DA	O4'-C4'-C3'	-5.24	102.41	104.50
3	G	34	LEU	CA-CB-CG	-5.23	103.28	115.30
3	C	34	LEU	CA-CB-CG	-5.21	103.32	115.30
6	J	78	DG	O4'-C4'-C3'	-5.20	102.42	104.50
5	I	131	DA	O4'-C1'-N9	-5.09	104.43	108.00
7	O	1185	TRP	C-N-CA	5.07	134.37	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	THR	Peptide
2	B	26	ILE	Peptide
1	E	58	THR	Peptide
7	O	1046	ARG	Peptide
7	O	768	LYS	Peptide
7	O	839	ALA	Peptide
7	O	931	LEU	Peptide
7	O	976	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	800	0	829	60	0
1	E	778	0	813	45	0
2	B	703	0	757	74	0
2	F	672	0	698	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	811	0	849	62	0
3	G	815	0	860	51	0
4	D	718	0	725	53	0
4	H	726	0	747	45	0
5	I	2975	0	1639	262	0
6	J	3011	0	1639	309	0
7	O	4789	0	4882	638	0
All	All	16798	0	14438	1477	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 48.

All (1477) 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)
7:O:1233:GLY:O	7:O:1237:GLN:HB2	1.22	1.32
7:O:876:ILE:O	7:O:880:ARG:HB2	1.41	1.17
7:O:1232:ASP:O	7:O:1236:ILE:HB	1.42	1.16
7:O:1301:ASP:O	7:O:1305:SER:HB2	1.60	1.02
5:I:111:DC:O2	6:J:37:DG:N2	1.93	1.01
7:O:807:THR:O	7:O:811:GLU:HB2	1.62	0.99
2:B:71:THR:O	2:B:74:GLU:HB2	1.61	0.98
7:O:1340:SER:O	7:O:1344:ALA:HB2	1.62	0.98
5:I:111:DC:N3	6:J:37:DG:N1	2.14	0.96
5:I:60:DA:N6	6:J:87:DT:O4	1.99	0.95
5:I:28:DC:N4	6:J:119:DT:C4	2.36	0.94
7:O:1129:LYS:HD3	7:O:1155:GLU:HB3	1.51	0.93
7:O:1222:LEU:O	7:O:1226:TYR:HB3	1.68	0.93
5:I:10:DC:N3	6:J:138:DG:N1	2.16	0.93
7:O:977:LEU:O	7:O:981:ARG:HB2	1.68	0.92
7:O:1339:GLU:O	7:O:1343:ALA:HB3	1.69	0.91
7:O:1055:LEU:HB3	7:O:1217:VAL:HG11	1.52	0.91
7:O:1222:LEU:O	7:O:1226:TYR:CB	2.19	0.91
7:O:1233:GLY:O	7:O:1237:GLN:CB	2.17	0.89
7:O:945:ILE:O	7:O:949:VAL:HB	1.69	0.89
7:O:978:LEU:O	7:O:982:ARG:HB2	1.70	0.89
7:O:1018:LEU:HA	7:O:1022:MET:HB2	1.53	0.89
2:F:51:TYR:HB3	2:F:55:ARG:HH12	1.34	0.88
7:O:1055:LEU:O	7:O:1059:CYS:HB2	1.72	0.88
7:O:1173:GLN:NE2	7:O:1199:ARG:O	2.06	0.88
7:O:744:TYR:HE1	7:O:944:LYS:HZ1	1.18	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1255:ARG:O	7:O:1259:ASP:HB2	1.75	0.87
7:O:1004:PRO:HG3	7:O:1203:LYS:HA	1.58	0.86
7:O:1207:ARG:HH12	7:O:1287:LEU:HA	1.39	0.86
7:O:897:HIS:O	7:O:900:LYS:HB3	1.74	0.86
7:O:1228:LYS:HA	7:O:1231:ILE:HB	1.57	0.86
1:E:68:GLN:HE21	1:E:72:ARG:HE	1.24	0.86
7:O:1013:CYS:HB2	7:O:1213:THR:HG22	1.59	0.85
7:O:1105:ARG:NH2	7:O:1149:PHE:O	2.09	0.85
7:O:858:GLN:NE2	7:O:879:GLU:OE2	2.10	0.85
7:O:771:GLN:HA	7:O:994:ARG:HH12	1.40	0.85
7:O:1051:GLN:HA	7:O:1055:LEU:HD12	1.60	0.84
7:O:791:ALA:O	7:O:993:ARG:NH1	2.11	0.84
5:I:10:DC:O2	6:J:138:DG:N2	2.10	0.84
7:O:895:GLU:OE2	7:O:897:HIS:NE2	2.11	0.83
4:D:65:ASP:OD2	2:F:98:TYR:OH	1.96	0.83
1:A:68:GLN:HE21	1:A:72:ARG:HE	1.23	0.83
7:O:1299:ARG:HA	7:O:1302:GLU:HG2	1.60	0.82
7:O:832:SER:HA	7:O:835:PHE:HD2	1.44	0.82
6:J:90:DA:H1'	6:J:91:DA:C8	2.16	0.81
7:O:949:VAL:HA	7:O:952:PHE:HB2	1.61	0.81
7:O:1026:MET:HG2	7:O:1029:TYR:HD2	1.45	0.81
5:I:28:DC:N4	6:J:119:DT:N3	2.29	0.80
7:O:1223:GLU:HA	7:O:1226:TYR:HB3	1.62	0.80
7:O:1020:GLN:O	7:O:1024:GLN:N	2.14	0.80
7:O:1109:PHE:HB3	7:O:1163:THR:HG22	1.64	0.80
5:I:111:DC:C2	6:J:37:DG:N2	2.50	0.79
7:O:931:LEU:HD22	7:O:934:LEU:HG	1.64	0.79
7:O:1301:ASP:O	7:O:1305:SER:CB	2.30	0.79
7:O:1084:ARG:HH21	7:O:1315:SER:HB2	1.46	0.79
7:O:810:TYR:CD1	7:O:816:ARG:HA	2.19	0.78
7:O:1022:MET:O	7:O:1026:MET:N	2.15	0.78
7:O:1116:MET:O	7:O:1119:MET:HB3	1.84	0.78
7:O:1081:ASP:HA	7:O:1084:ARG:HB2	1.66	0.78
7:O:1113:THR:HG22	7:O:1132:ARG:HH21	1.49	0.77
7:O:1063:PHE:HB2	7:O:1066:GLU:HA	1.67	0.77
7:O:1340:SER:O	7:O:1344:ALA:CB	2.32	0.77
7:O:1028:LYS:O	7:O:1032:LEU:N	2.17	0.77
7:O:1055:LEU:HD13	7:O:1217:VAL:HG21	1.65	0.77
7:O:929:ASN:HD21	7:O:1232:ASP:HA	1.49	0.77
7:O:744:TYR:O	7:O:748:ALA:N	2.12	0.77
7:O:1069:GLU:O	7:O:1073:ASN:N	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1135:GLY:O	7:O:1142:ARG:NH2	2.18	0.76
5:I:85:DG:H2'	5:I:86:DT:H71	1.67	0.76
1:A:63:ARG:NH2	6:J:61:DA:OP1	2.19	0.76
2:F:51:TYR:HB3	2:F:55:ARG:NH1	2.01	0.76
7:O:939:ASN:HB3	7:O:946:PHE:HB3	1.65	0.76
7:O:1168:LEU:O	7:O:1196:ARG:NH2	2.19	0.76
3:G:77:ARG:HH21	5:I:20:DA:H4'	1.50	0.75
7:O:843:ARG:HH12	7:O:865:GLU:HB3	1.51	0.75
7:O:671:LEU:HB3	7:O:955:TRP:CH2	2.22	0.75
4:D:53:SER:N	6:J:20:DC:OP1	2.19	0.74
7:O:1212:ILE:HG13	7:O:1222:LEU:HD22	1.68	0.74
7:O:1226:TYR:O	7:O:1264:ARG:NH1	2.20	0.74
7:O:807:THR:O	7:O:811:GLU:CB	2.35	0.74
7:O:952:PHE:HA	7:O:955:TRP:HB2	1.68	0.74
7:O:1212:ILE:HG23	7:O:1218:GLU:HG3	1.69	0.74
5:I:7:DA:H1'	5:I:8:DA:H5'	1.68	0.74
7:O:1023:TYR:HA	7:O:1026:MET:HB2	1.69	0.74
7:O:1255:ARG:HA	7:O:1258:LEU:HG	1.69	0.74
7:O:845:ILE:O	7:O:870:LEU:N	2.20	0.73
7:O:1173:GLN:HE22	7:O:1200:ILE:C	1.91	0.73
1:E:64:LYS:N	6:J:92:DG:OP1	2.19	0.73
5:I:118:DC:H2"	5:I:119:DC:C5	2.24	0.73
7:O:771:GLN:NE2	7:O:796:LEU:O	2.21	0.73
7:O:882:LEU:HD12	7:O:885:LYS:HD2	1.68	0.73
7:O:997:LYS:HA	7:O:1001:LYS:HA	1.70	0.73
7:O:1015:MET:HB2	7:O:1020:GLN:HG3	1.69	0.73
7:O:1099:LEU:O	7:O:1103:GLY:N	2.21	0.73
2:B:45:ARG:HE	5:I:81:DC:H4'	1.54	0.72
7:O:1105:ARG:N	7:O:1176:ASP:OD1	2.21	0.72
7:O:672:ASP:OD2	7:O:982:ARG:NH2	2.22	0.72
7:O:1062:PRO:HG3	7:O:1085:VAL:HG11	1.71	0.72
6:J:58:DT:OP1	7:O:878:LYS:NZ	2.23	0.72
7:O:1026:MET:O	7:O:1030:ARG:HG3	1.89	0.72
2:F:45:ARG:HG3	6:J:82:DG:H5"	1.72	0.72
7:O:891:MET:O	7:O:919:ARG:HA	1.89	0.72
7:O:1230:ASP:OD2	7:O:1264:ARG:NE	2.19	0.72
5:I:28:DC:H4'	5:I:29:DA:H5'	1.70	0.72
7:O:672:ASP:HA	7:O:675:LYS:HD2	1.70	0.71
7:O:1218:GLU:O	7:O:1222:LEU:CB	2.37	0.71
3:C:16:THR:HA	6:J:31:DA:H5"	1.71	0.71
7:O:938:LEU:HG	7:O:945:ILE:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1309:GLU:OE2	7:O:1314:LYS:N	2.22	0.71
7:O:686:THR:HA	7:O:689:PHE:HD2	1.53	0.71
7:O:1113:THR:HG21	7:O:1134:ASP:HB3	1.73	0.71
5:I:10:DC:N4	6:J:138:DG:O6	2.17	0.71
7:O:891:MET:HB3	7:O:919:ARG:HG2	1.71	0.71
4:H:102:GLU:OE1	4:H:106:HIS:NE2	2.24	0.71
7:O:1017:ALA:O	7:O:1022:MET:N	2.24	0.71
7:O:1151:ALA:HB3	7:O:1154:SER:HB2	1.72	0.71
7:O:1207:ARG:HB3	7:O:1209:LEU:HD21	1.72	0.71
7:O:754:ASP:HB3	7:O:776:GLN:HE21	1.55	0.71
7:O:1218:GLU:O	7:O:1222:LEU:HB2	1.91	0.71
4:D:102:GLU:OE1	4:D:106:HIS:NE2	2.24	0.70
5:I:44:DG:H2'	5:I:45:DC:C6	2.25	0.70
7:O:953:ASP:O	7:O:957:ASN:CB	2.39	0.70
7:O:761:ILE:HD11	7:O:807:THR:HB	1.73	0.70
7:O:1083:TRP:HA	7:O:1089:PHE:HB3	1.73	0.70
7:O:1003:LEU:HD12	7:O:1004:PRO:HD2	1.73	0.70
7:O:1232:ASP:O	7:O:1236:ILE:CB	2.33	0.70
3:G:16:THR:HA	5:I:31:DT:H5"	1.73	0.70
5:I:121:DG:H1'	5:I:122:DG:C8	2.26	0.70
7:O:1226:TYR:HD1	7:O:1229:LEU:HD12	1.57	0.70
7:O:1081:ASP:HB3	7:O:1318:LEU:HD21	1.74	0.69
4:D:103:LEU:O	4:D:107:ALA:HB3	1.92	0.69
7:O:919:ARG:HH12	7:O:941:VAL:HA	1.57	0.69
7:O:931:LEU:N	7:O:933:GLU:OE1	2.26	0.69
7:O:1026:MET:HA	7:O:1029:TYR:HB2	1.73	0.69
7:O:1092:LEU:HD23	7:O:1095:ILE:HD11	1.74	0.69
5:I:96:DC:OP2	7:O:901:ASN:ND2	2.23	0.69
2:B:18:HIS:HB3	7:O:1076:ARG:HH21	1.56	0.69
4:D:90:GLU:OE1	4:D:90:GLU:N	2.24	0.69
4:D:103:LEU:O	4:D:107:ALA:CB	2.41	0.69
4:H:103:LEU:O	4:H:107:ALA:HB3	1.92	0.69
7:O:1019:GLN:HE22	7:O:1086:ALA:HB2	1.58	0.69
4:H:103:LEU:O	4:H:107:ALA:CB	2.41	0.69
7:O:1016:SER:O	7:O:1020:GLN:N	2.25	0.69
3:C:90:ASP:OD2	3:C:93:LEU:N	2.20	0.69
2:B:68:ASP:O	2:B:71:THR:HB	1.93	0.68
5:I:99:DG:OP1	7:O:1051:GLN:NE2	2.26	0.68
7:O:1222:LEU:O	7:O:1226:TYR:HB2	1.92	0.68
5:I:87:DT:H2"	5:I:88:DT:H73	1.76	0.68
7:O:982:ARG:HA	7:O:985:LYS:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:ARG:NE	6:J:30:DG:OP1	2.25	0.68
6:J:120:DG:H1'	6:J:121:DA:N7	2.09	0.68
7:O:967:ASP:O	7:O:971:LEU:N	2.27	0.68
2:B:88:TYR:O	2:B:91:LYS:N	2.27	0.67
6:J:44:DA:H2'	6:J:45:DT:C6	2.29	0.67
3:G:92:GLU:HB3	4:H:103:LEU:HD11	1.75	0.67
7:O:1232:ASP:OD1	7:O:1233:GLY:N	2.26	0.67
7:O:952:PHE:HB3	7:O:956:PHE:CD2	2.29	0.67
3:G:32:ARG:HA	3:G:35:ARG:HH21	1.59	0.67
7:O:832:SER:HA	7:O:835:PHE:CD2	2.28	0.67
3:C:92:GLU:HB3	4:D:103:LEU:HD11	1.74	0.67
6:J:27:DC:H1'	6:J:28:DT:C2	2.29	0.67
7:O:969:ILE:HA	7:O:973:GLU:HB3	1.77	0.67
2:B:17:ARG:NH1	7:O:1121:ASP:OD2	2.20	0.67
2:B:70:VAL:O	2:B:74:GLU:N	2.24	0.67
5:I:102:DG:H2"	5:I:103:DA:H8	1.60	0.67
7:O:1063:PHE:HB3	7:O:1068:VAL:HB	1.77	0.67
7:O:1095:ILE:HG13	7:O:1096:LEU:H	1.59	0.67
3:C:16:THR:O	3:C:19:SER:OG	2.10	0.67
7:O:771:GLN:HG2	7:O:801:GLN:HE21	1.60	0.67
5:I:59:DA:H61	6:J:88:DT:H3	1.40	0.67
3:G:90:ASP:OD2	3:G:93:LEU:N	2.20	0.66
5:I:111:DC:H2'	5:I:112:DT:H6	1.60	0.66
7:O:671:LEU:O	7:O:674:THR:OG1	2.14	0.66
7:O:780:SER:OG	7:O:784:ASN:ND2	2.27	0.66
3:G:17:ARG:HH21	3:G:28:GLY:HA2	1.61	0.66
6:J:104:DC:H2'	6:J:105:DT:H71	1.77	0.66
3:C:32:ARG:HA	3:C:35:ARG:HH21	1.59	0.66
7:O:1007:VAL:HG13	7:O:1207:ARG:HD3	1.77	0.66
7:O:1057:LYS:HB3	7:O:1064:VAL:HG11	1.77	0.66
7:O:1081:ASP:OD1	7:O:1084:ARG:HD3	1.93	0.66
1:A:42:ARG:NH2	6:J:69:DG:OP1	2.28	0.66
7:O:910:LEU:HA	7:O:913:HIS:HB3	1.77	0.66
1:A:39:HIS:HE1	1:A:41:TYR:CZ	2.13	0.66
2:F:26:ILE:HD11	2:F:55:ARG:HB3	1.78	0.66
6:J:99:DT:H4'	6:J:100:DA:H5'	1.77	0.66
7:O:676:ASP:HA	7:O:679:ILE:HD12	1.77	0.66
5:I:71:DG:H5'	5:I:71:DG:C8	2.32	0.65
6:J:49:DC:H2"	6:J:50:DT:H73	1.78	0.65
6:J:113:DA:H5'	6:J:113:DA:H8	1.61	0.65
7:O:1046:ARG:HB3	7:O:1048:PHE:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ARG:HH21	3:C:28:GLY:HA2	1.61	0.65
2:F:79:LYS:HG3	6:J:101:DG:H3'	1.79	0.65
6:J:18:DG:H1'	6:J:19:DA:C8	2.32	0.65
5:I:82:DC:H1'	5:I:83:DG:H5'	1.79	0.65
7:O:1265:ARG:O	7:O:1268:ARG:HG2	1.96	0.65
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.30	0.65
6:J:71:DA:H2"	6:J:72:DC:H2'	1.79	0.65
7:O:1215:ASN:N	7:O:1219:GLU:OE2	2.29	0.65
7:O:1289:ARG:N	7:O:1293:GLU:OE1	2.23	0.65
7:O:785:HIS:ND1	7:O:918:TYR:OH	2.30	0.65
7:O:1014:LYS:HB3	7:O:1317:LEU:HD11	1.78	0.65
7:O:1253:LEU:HA	7:O:1256:SER:HB2	1.79	0.65
7:O:1345:VAL:HG12	7:O:1349:ARG:HH22	1.61	0.65
1:A:124:ILE:HD11	2:B:50:ILE:HG23	1.78	0.65
3:C:15:LYS:N	6:J:32:DG:OP1	2.30	0.65
3:C:100:VAL:HG22	2:F:96:THR:HB	1.78	0.65
4:H:90:GLU:OE1	4:H:90:GLU:N	2.24	0.65
5:I:44:DG:H2'	5:I:45:DC:H6	1.60	0.65
5:I:68:DT:H4'	5:I:69:DA:H5'	1.79	0.64
7:O:968:LYS:O	7:O:973:GLU:N	2.27	0.64
7:O:1171:ASN:HD21	7:O:1173:GLN:NE2	1.96	0.64
7:O:1223:GLU:O	7:O:1227:LYS:HG3	1.97	0.64
1:E:40:ARG:HG2	6:J:84:DG:H5'	1.78	0.64
2:F:36:ARG:NH1	5:I:61:DA:OP1	2.30	0.64
6:J:53:DG:H5'	7:O:1112:MET:HA	1.79	0.64
7:O:1105:ARG:HB2	7:O:1175:ALA:HA	1.77	0.64
7:O:1247:SER:O	7:O:1250:GLN:HG2	1.97	0.64
7:O:679:ILE:HG12	7:O:744:TYR:CE2	2.31	0.64
7:O:844:THR:HA	7:O:868:VAL:HB	1.78	0.64
7:O:1207:ARG:HG2	7:O:1289:ARG:HH21	1.62	0.64
3:G:16:THR:O	3:G:19:SER:OG	2.10	0.64
5:I:146:DA:H2'	5:I:147:DT:H71	1.79	0.64
7:O:747:VAL:HA	7:O:750:ARG:HG3	1.80	0.64
7:O:880:ARG:HH22	7:O:912:THR:HG21	1.62	0.64
7:O:935:TRP:HH2	7:O:953:ASP:HA	1.62	0.64
7:O:1255:ARG:HG2	7:O:1258:LEU:HD11	1.79	0.64
7:O:988:ARG:HE	7:O:1241:PHE:HE1	1.46	0.64
7:O:975:GLU:N	7:O:975:GLU:OE1	2.29	0.64
7:O:1251:GLU:HA	7:O:1254:LEU:HG	1.79	0.64
7:O:1175:ALA:O	7:O:1202:GLN:NE2	2.31	0.64
2:B:18:HIS:NE2	7:O:1076:ARG:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:38:DT:H2”	5:I:39:DA:N7	2.13	0.64
7:O:985:LYS:HA	7:O:988:ARG:HG3	1.80	0.64
5:I:125:DC:H2”	5:I:126:DG:H8	1.62	0.63
7:O:1090:GLU:OE2	7:O:1094:ARG:NE	2.18	0.63
7:O:1168:LEU:HG	7:O:1169:GLY:H	1.63	0.63
7:O:1012:LYS:HA	7:O:1212:ILE:O	1.97	0.63
4:D:30:ARG:HB3	5:I:124:DA:H5”	1.80	0.63
5:I:37:DG:H2’	5:I:38:DT:H71	1.79	0.63
7:O:1301:ASP:OD1	7:O:1304:ARG:NH2	2.31	0.63
2:B:18:HIS:CG	7:O:1076:ARG:HD3	2.33	0.63
5:I:59:DA:H8	5:I:59:DA:OP2	1.81	0.63
1:A:50:GLU:O	1:A:53:ARG:N	2.32	0.63
1:E:50:GLU:O	1:E:53:ARG:N	2.32	0.63
6:J:113:DA:H5’	6:J:113:DA:C8	2.33	0.63
2:F:79:LYS:N	6:J:102:DA:OP1	2.29	0.63
7:O:1237:GLN:HE22	7:O:1257:LEU:N	1.96	0.63
7:O:686:THR:HA	7:O:689:PHE:CD2	2.34	0.63
7:O:1023:TYR:O	7:O:1027:LEU:N	2.32	0.63
6:J:34:DC:H2’	6:J:35:DT:H71	1.80	0.62
7:O:1062:PRO:HG2	7:O:1063:PHE:CE2	2.34	0.62
7:O:1198:HIS:HA	7:O:1202:GLN:HB3	1.80	0.62
7:O:1263:GLU:HA	7:O:1266:LYS:HD2	1.80	0.62
7:O:845:ILE:HG21	7:O:861:ILE:HD11	1.79	0.62
7:O:1025:GLN:NE2	7:O:1029:TYR:OH	2.32	0.62
7:O:1188:HIS:HA	7:O:1191:LEU:HD12	1.80	0.62
7:O:1337:ARG:O	7:O:1340:SER:OG	2.13	0.62
7:O:1237:GLN:HG3	7:O:1253:LEU:HD22	1.82	0.62
7:O:755:ILE:H	7:O:776:GLN:HG3	1.64	0.62
7:O:753:GLU:OE1	7:O:783:ASN:ND2	2.33	0.62
1:A:59:GLU:OE1	1:A:59:GLU:N	2.28	0.62
2:B:18:HIS:CE1	7:O:1076:ARG:HB2	2.35	0.62
5:I:34:DG:H3’	5:I:35:DT:H71	1.80	0.62
5:I:11:DC:N4	6:J:136:DG:O6	2.33	0.61
7:O:810:TYR:HD1	7:O:816:ARG:HA	1.64	0.61
7:O:1018:LEU:O	7:O:1023:TYR:N	2.33	0.61
7:O:768:LYS:N	7:O:771:GLN:OE1	2.29	0.61
7:O:928:GLN:HB2	7:O:933:GLU:OE2	2.00	0.61
7:O:743:ASP:OD1	7:O:744:TYR:N	2.33	0.61
7:O:794:MET:HA	7:O:798:LYS:NZ	2.15	0.61
5:I:42:DC:H2”	5:I:43:DA:C8	2.35	0.61
5:I:132:DG:N2	6:J:17:DT:O2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:5:DG:H2”	6:J:6:DA:C8	2.36	0.61
6:J:69:DG:H2”	6:J:70:DG:C8	2.36	0.61
7:O:1112:MET:O	7:O:1114:GLN:N	2.33	0.61
7:O:1113:THR:HG23	7:O:1116:MET:SD	2.41	0.61
5:I:67:DG:H2’	5:I:68:DT:H71	1.83	0.61
6:J:141:DT:H2”	6:J:142:DC:C5	2.36	0.61
7:O:1080:ASP:OD2	7:O:1314:LYS:NZ	2.24	0.61
7:O:1164:ARG:HB2	7:O:1189:GLN:OE1	2.01	0.61
7:O:976:THR:HB	7:O:980:ILE:HB	1.82	0.61
6:J:135:DC:H2”	6:J:136:DG:C8	2.36	0.60
3:C:66:ALA:O	3:C:69:ALA:N	2.35	0.60
7:O:999:VAL:HG23	7:O:1000:GLU:H	1.65	0.60
5:I:18:DC:H2”	5:I:19:DG:N7	2.16	0.60
5:I:84:DC:H2”	5:I:85:DG:H8	1.67	0.60
7:O:1088:LYS:O	7:O:1092:LEU:HG	2.01	0.60
7:O:1117:ASP:OD1	7:O:1132:ARG:NH2	2.30	0.60
3:G:88:ARG:NH1	3:G:94:ASN:OD1	2.34	0.60
7:O:808:TYR:HA	7:O:811:GLU:HB3	1.83	0.60
3:G:66:ALA:O	3:G:69:ALA:N	2.35	0.60
7:O:1137:THR:O	7:O:1142:ARG:NE	2.34	0.60
3:C:93:LEU:O	3:C:96:LEU:N	2.35	0.60
5:I:84:DC:H2”	5:I:85:DG:C8	2.37	0.60
7:O:1088:LYS:HD3	7:O:1181:PHE:HD1	1.65	0.60
7:O:1105:ARG:HG2	7:O:1157:LEU:HA	1.83	0.60
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.35	0.60
2:F:30:THR:HB	2:F:32:PRO:HD2	1.84	0.60
6:J:27:DC:H2”	6:J:28:DT:C5	2.37	0.60
3:C:42:ARG:NH1	6:J:39:DG:H4’	2.17	0.60
4:D:57:SER:OG	2:F:99:GLY:O	2.18	0.60
3:G:88:ARG:HB3	3:G:108:LEU:HD11	1.84	0.60
2:B:25:ASN:C	2:B:27:GLN:H	2.05	0.60
4:H:115:VAL:O	4:H:119:THR:OG1	2.12	0.60
7:O:943:PRO:HA	7:O:946:PHE:CE2	2.36	0.60
7:O:1091:LEU:O	7:O:1094:ARG:N	2.32	0.60
3:C:42:ARG:HH21	5:I:112:DT:H4’	1.67	0.60
1:E:59:GLU:OE1	1:E:59:GLU:N	2.28	0.60
7:O:973:GLU:OE1	7:O:974:GLU:HG3	2.01	0.60
5:I:24:DC:H2”	5:I:25:DG:C8	2.37	0.59
7:O:1017:ALA:O	7:O:1021:ILE:N	2.35	0.59
7:O:1029:TYR:HD1	7:O:1032:LEU:HB2	1.67	0.59
3:G:93:LEU:O	3:G:96:LEU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1084:ARG:NH2	7:O:1317:LEU:O	2.35	0.59
7:O:1234:LYS:O	7:O:1237:GLN:HB3	2.01	0.59
2:B:62:LEU:HD22	2:B:66:ILE:HD11	1.85	0.59
3:C:88:ARG:NH1	3:C:94:ASN:OD1	2.34	0.59
7:O:931:LEU:HD23	7:O:933:GLU:HB2	1.84	0.59
7:O:983:LEU:O	7:O:986:VAL:HB	2.02	0.59
5:I:144:DC:H2"	5:I:145:DG:C8	2.37	0.59
6:J:139:DA:H2'	6:J:140:DT:C6	2.37	0.59
7:O:934:LEU:O	7:O:938:LEU:HB2	2.03	0.59
7:O:1283:ILE:HA	7:O:1286:ILE:HG12	1.85	0.59
7:O:771:GLN:HG2	7:O:801:GLN:NE2	2.18	0.59
7:O:888:TRP:HB3	7:O:916:ALA:HB2	1.85	0.59
7:O:935:TRP:CH2	7:O:953:ASP:HA	2.37	0.59
7:O:1098:LYS:NZ	7:O:1284:ASN:OD1	2.33	0.59
7:O:1278:LEU:HD11	7:O:1283:ILE:HG13	1.85	0.59
5:I:8:DA:H2'	5:I:9:DT:H71	1.85	0.59
5:I:36:DC:H2"	5:I:37:DG:C8	2.37	0.59
7:O:1173:GLN:O	7:O:1202:GLN:NE2	2.36	0.58
3:C:88:ARG:HB3	3:C:108:LEU:HD11	1.84	0.58
7:O:987:LEU:HA	7:O:990:PHE:HD2	1.69	0.58
5:I:99:DG:H2"	5:I:100:DG:OP2	2.03	0.58
7:O:1124:ARG:C	7:O:1127:ASN:H	2.06	0.58
7:O:1237:GLN:NE2	7:O:1253:LEU:O	2.35	0.58
2:B:73:THR:N	2:B:85:ASP:OD2	2.36	0.58
3:C:20:ARG:NH2	6:J:32:DG:OP1	2.29	0.58
5:I:88:DT:H2'	5:I:89:DT:H72	1.84	0.58
7:O:686:THR:HG21	7:O:942:LEU:HD13	1.85	0.58
7:O:1019:GLN:NE2	7:O:1085:VAL:HG22	2.18	0.58
7:O:1095:ILE:HG13	7:O:1096:LEU:N	2.18	0.58
1:A:124:ILE:O	1:A:127:ALA:N	2.37	0.58
6:J:47:DC:H1'	6:J:48:DC:C5	2.38	0.58
7:O:690:LEU:HD21	7:O:785:HIS:HB3	1.84	0.58
1:A:46:VAL:HG21	5:I:83:DG:H3'	1.85	0.58
4:D:62:PHE:HA	2:F:98:TYR:CE1	2.39	0.58
5:I:94:DG:H2'	5:I:95:DC:O4'	2.02	0.58
7:O:859:ALA:O	7:O:863:ALA:N	2.36	0.58
7:O:971:LEU:O	7:O:975:GLU:HB2	2.03	0.58
7:O:1010:VAL:HG12	7:O:1210:ARG:HB3	1.85	0.58
3:G:84:GLN:HA	3:G:102:ILE:HD12	1.86	0.58
7:O:682:LEU:O	7:O:686:THR:HG23	2.04	0.58
7:O:1144:GLU:OE2	7:O:1147:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:MET:O	2:B:87:VAL:N	2.36	0.58
3:C:29:ARG:NH2	5:I:123:DC:OP1	2.33	0.58
5:I:100:DG:H2"	5:I:101:DG:C8	2.39	0.58
7:O:951:SER:O	7:O:955:TRP:HD1	1.86	0.58
7:O:1009:LYS:HE2	7:O:1286:ILE:HD12	1.86	0.58
7:O:1028:LYS:HB3	7:O:1032:LEU:HD12	1.85	0.58
7:O:1108:ILE:HG12	7:O:1179:ILE:HB	1.85	0.58
7:O:1179:ILE:HG12	7:O:1209:LEU:HD12	1.86	0.58
7:O:1295:ALA:O	7:O:1298:THR:OG1	2.20	0.58
7:O:785:HIS:HA	7:O:918:TYR:HE1	1.69	0.58
1:A:40:ARG:HG2	5:I:84:DC:H5'	1.86	0.57
3:C:84:GLN:HA	3:C:102:ILE:HD12	1.86	0.57
6:J:61:DA:H1'	6:J:62:DA:H5'	1.86	0.57
6:J:87:DT:H3'	6:J:88:DT:H71	1.85	0.57
6:J:89:DT:H2"	6:J:90:DA:C8	2.39	0.57
7:O:771:GLN:O	7:O:775:LEU:HB2	2.04	0.57
7:O:802:THR:O	7:O:805:LEU:HB3	2.04	0.57
3:C:92:GLU:OE2	4:D:102:GLU:N	2.37	0.57
3:G:77:ARG:NH2	5:I:20:DA:H4'	2.18	0.57
5:I:132:DG:H1'	5:I:133:DA:N7	2.19	0.57
7:O:843:ARG:N	7:O:867:ASP:OD2	2.29	0.57
5:I:109:DC:H2"	5:I:110:DC:C5	2.39	0.57
5:I:134:DT:H2"	5:I:135:DA:H8	1.69	0.57
6:J:83:DT:H2"	6:J:84:DG:C8	2.38	0.57
7:O:858:GLN:HB3	7:O:862:ARG:NH1	2.19	0.57
7:O:1061:HIS:HE1	7:O:1088:LYS:HB2	1.69	0.57
1:E:124:ILE:O	1:E:127:ALA:N	2.37	0.57
3:G:76:THR:O	4:H:50:GLY:N	2.26	0.57
5:I:72:DC:H2"	5:I:73:DG:C8	2.40	0.57
7:O:1182:ASP:O	7:O:1210:ARG:NH1	2.36	0.57
1:A:65:LEU:O	1:A:68:GLN:N	2.38	0.57
1:E:65:LEU:O	1:E:68:GLN:N	2.37	0.57
7:O:944:LYS:O	7:O:948:SER:OG	2.11	0.57
7:O:1050:ASN:O	7:O:1054:GLN:N	2.37	0.57
1:A:63:ARG:HH21	6:J:61:DA:P	2.27	0.57
5:I:120:DA:H2"	5:I:121:DG:N7	2.20	0.57
7:O:792:ASP:HB2	7:O:798:LYS:HD3	1.86	0.57
5:I:144:DC:H2"	5:I:145:DG:H8	1.70	0.57
7:O:1124:ARG:O	7:O:1127:ASN:N	2.37	0.57
2:F:84:MET:HB3	2:F:88:TYR:HE2	1.69	0.57
5:I:111:DC:H2'	5:I:112:DT:C6	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:130:DG:H2"	6:J:131:DG:N7	2.19	0.57
7:O:913:HIS:O	7:O:913:HIS:ND1	2.38	0.57
6:J:120:DG:OP2	6:J:120:DG:H2'	2.05	0.56
7:O:1084:ARG:NH2	7:O:1315:SER:HB2	2.19	0.56
7:O:1120:GLU:OE2	7:O:1132:ARG:NH1	2.33	0.56
5:I:9:DT:H1'	5:I:10:DC:H5'	1.87	0.56
5:I:17:DC:H2"	5:I:18:DC:C5	2.39	0.56
6:J:145:DG:H2"	6:J:146:DA:C8	2.41	0.56
7:O:1131:LEU:HB2	7:O:1159:PHE:HD1	1.70	0.56
2:B:39:ARG:NH1	2:B:43:VAL:O	2.38	0.56
2:B:71:THR:HA	2:B:74:GLU:CD	2.25	0.56
3:C:17:ARG:NH2	3:C:28:GLY:HA2	2.20	0.56
3:G:15:LYS:HB3	3:G:20:ARG:NH2	2.20	0.56
6:J:35:DT:H2"	6:J:36:DA:C8	2.40	0.56
6:J:41:DG:H2'	6:J:42:DT:H71	1.87	0.56
6:J:105:DT:H2"	6:J:106:DG:N7	2.21	0.56
7:O:976:THR:HA	7:O:979:VAL:HB	1.87	0.56
7:O:983:LEU:O	7:O:987:LEU:HG	2.06	0.56
7:O:1255:ARG:O	7:O:1259:ASP:CB	2.51	0.56
3:C:77:ARG:HH21	6:J:20:DC:H4'	1.70	0.56
5:I:73:DG:H8	5:I:73:DG:OP2	1.89	0.56
6:J:121:DA:H2"	6:J:122:DG:OP2	2.06	0.56
4:H:43:LYS:HA	4:H:47:PRO:HA	1.88	0.56
7:O:751:ILE:HD12	7:O:784:ASN:HA	1.87	0.56
3:C:15:LYS:HB3	3:C:20:ARG:NH2	2.20	0.56
3:G:84:GLN:HE21	3:G:88:ARG:HG3	1.71	0.56
5:I:112:DT:H2'	5:I:113:DA:C8	2.41	0.56
7:O:1090:GLU:O	7:O:1093:ASP:HB3	2.05	0.56
2:F:64:ASN:HB3	2:F:93:GLN:HE22	1.70	0.56
5:I:4:DG:H2"	5:I:5:DA:C8	2.40	0.56
6:J:75:DC:OP2	6:J:75:DC:H2'	2.05	0.56
6:J:139:DA:H2'	6:J:140:DT:H6	1.70	0.56
7:O:679:ILE:HA	7:O:744:TYR:CE1	2.40	0.56
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.32	0.56
4:H:90:GLU:H	4:H:90:GLU:CD	2.08	0.56
5:I:89:DT:H1'	5:I:90:DA:C8	2.41	0.56
7:O:1029:TYR:CD1	7:O:1348:GLY:HA2	2.41	0.56
4:H:106:HIS:O	4:H:110:GLU:HG2	2.06	0.56
7:O:821:VAL:HG23	7:O:870:LEU:HA	1.88	0.56
6:J:116:DA:H2"	6:J:117:DA:H8	1.71	0.56
7:O:794:MET:SD	7:O:798:LYS:NZ	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ASN:O	2:B:26:ILE:HG12	2.07	0.55
7:O:1029:TYR:HA	7:O:1032:LEU:HB2	1.87	0.55
2:B:56:GLY:O	2:B:59:LYS:HB3	2.05	0.55
2:B:96:THR:O	3:G:100:VAL:HG13	2.07	0.55
1:E:128:ARG:NE	1:E:133:GLU:OE1	2.39	0.55
2:F:71:THR:O	2:F:74:GLU:HB2	2.06	0.55
7:O:843:ARG:HH11	7:O:866:PHE:HA	1.71	0.55
6:J:20:DC:H2"	6:J:21:DA:C8	2.42	0.55
6:J:129:DC:H1'	6:J:130:DG:C5	2.41	0.55
7:O:880:ARG:HH11	7:O:913:HIS:HB2	1.72	0.55
7:O:1013:CYS:H	7:O:1213:THR:HA	1.70	0.55
7:O:1121:ASP:O	7:O:1125:TYR:N	2.38	0.55
1:A:128:ARG:NE	1:A:133:GLU:OE1	2.39	0.55
4:D:43:LYS:HA	4:D:47:PRO:HA	1.88	0.55
4:D:99:LEU:HB3	4:D:103:LEU:HB3	1.89	0.55
3:G:17:ARG:NH2	3:G:28:GLY:HA2	2.20	0.55
7:O:979:VAL:O	7:O:983:LEU:HG	2.06	0.55
7:O:1224:ARG:O	7:O:1227:LYS:HB2	2.06	0.55
6:J:145:DG:H2"	6:J:146:DA:H8	1.72	0.55
7:O:785:HIS:HA	7:O:918:TYR:CE1	2.42	0.55
7:O:1217:VAL:O	7:O:1220:VAL:N	2.39	0.55
3:C:84:GLN:OE1	3:C:102:ILE:HB	2.07	0.55
7:O:675:LYS:O	7:O:679:ILE:HG13	2.07	0.55
7:O:1258:LEU:O	7:O:1262:GLU:HG3	2.07	0.55
2:B:31:LYS:HE2	2:B:51:TYR:CE2	2.42	0.55
4:D:90:GLU:H	4:D:90:GLU:CD	2.08	0.55
5:I:28:DC:C4	6:J:119:DT:N3	2.75	0.55
3:C:76:THR:O	4:D:50:GLY:N	2.33	0.55
2:B:33:ALA:HA	2:B:36:ARG:CZ	2.37	0.55
2:B:83:ALA:O	2:B:87:VAL:HG23	2.07	0.55
2:B:92:ARG:NH2	4:D:98:LEU:HD23	2.22	0.55
4:D:106:HIS:O	4:D:110:GLU:HG2	2.06	0.55
4:H:99:LEU:HB3	4:H:103:LEU:HB3	1.88	0.55
7:O:680:THR:O	7:O:684:ARG:HG2	2.07	0.55
7:O:950:LYS:C	7:O:953:ASP:H	2.09	0.55
2:B:92:ARG:HH21	4:D:98:LEU:HD23	1.72	0.55
2:F:71:THR:HA	2:F:74:GLU:CD	2.27	0.55
7:O:1084:ARG:NE	7:O:1315:SER:O	2.26	0.55
7:O:1173:GLN:HG2	7:O:1202:GLN:HB2	1.88	0.55
3:G:84:GLN:OE1	3:G:102:ILE:HB	2.07	0.54
6:J:12:DA:H2'	6:J:13:DT:H71	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:929:ASN:HD21	7:O:1232:ASP:CA	2.20	0.54
1:A:105:GLU:O	1:A:108:ASN:HB3	2.07	0.54
4:D:61:SER:HB3	2:F:98:TYR:HD1	1.73	0.54
1:E:46:VAL:HG22	1:E:49:ARG:HH22	1.72	0.54
5:I:130:DC:H2"	5:I:131:DA:N7	2.23	0.54
6:J:131:DG:H8	6:J:131:DG:P	2.31	0.54
7:O:787:ASN:OD1	7:O:919:ARG:N	2.34	0.54
7:O:1090:GLU:O	7:O:1094:ARG:HG2	2.08	0.54
1:E:105:GLU:O	1:E:108:ASN:HB3	2.07	0.54
6:J:73:DA:H2"	6:J:74:DG:OP2	2.07	0.54
1:A:40:ARG:HG2	5:I:84:DC:C5'	2.38	0.54
5:I:125:DC:H2"	5:I:126:DG:C8	2.42	0.54
7:O:939:ASN:ND2	7:O:946:PHE:HA	2.23	0.54
7:O:1000:GLU:O	7:O:1002:GLU:HG3	2.08	0.54
3:C:84:GLN:HE21	3:C:88:ARG:HG3	1.71	0.54
3:G:31:HIS:HA	3:G:34:LEU:HD12	1.90	0.54
7:O:683:LEU:HG	7:O:944:LYS:NZ	2.22	0.54
7:O:1094:ARG:NH2	7:O:1304:ARG:HD2	2.23	0.54
3:C:27:VAL:HG13	3:C:48:PRO:HB2	1.90	0.54
2:F:79:LYS:NZ	6:J:101:DG:OP1	2.41	0.54
5:I:3:DC:H1'	5:I:4:DG:O5'	2.08	0.54
5:I:60:DA:C4	5:I:61:DA:N7	2.76	0.54
6:J:70:DG:H2"	6:J:71:DA:C8	2.43	0.54
6:J:89:DT:H2"	6:J:90:DA:H8	1.73	0.54
7:O:1121:ASP:HA	7:O:1124:ARG:HB2	1.90	0.54
7:O:1250:GLN:HA	7:O:1253:LEU:HB2	1.89	0.54
2:F:76:ALA:HB1	2:F:78:ARG:HE	1.71	0.53
7:O:914:TYR:CG	7:O:915:HIS:N	2.76	0.53
1:A:46:VAL:HG22	1:A:49:ARG:HH22	1.72	0.53
5:I:129:DT:H2"	5:I:130:DC:C5	2.43	0.53
7:O:769:ASP:HB3	7:O:772:ILE:HD12	1.91	0.53
7:O:891:MET:HB2	7:O:916:ALA:HB3	1.90	0.53
2:B:45:ARG:HE	5:I:81:DC:C4'	2.21	0.53
5:I:90:DA:H1'	5:I:91:DA:C8	2.43	0.53
6:J:138:DG:C2	6:J:139:DA:C4	2.97	0.53
4:H:84:SER:N	5:I:40:DG:OP1	2.32	0.53
6:J:44:DA:H3'	6:J:45:DT:H71	1.89	0.53
7:O:782:PHE:HD1	7:O:918:TYR:CD1	2.26	0.53
7:O:1067:GLU:O	7:O:1071:GLN:HB2	2.08	0.53
7:O:1114:GLN:O	7:O:1117:ASP:HB2	2.08	0.53
7:O:1126:ILE:HD12	7:O:1128:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:HIS:HB3	7:O:1076:ARG:NH2	2.24	0.53
3:C:69:ALA:HA	3:C:72:ASP:OD2	2.08	0.53
4:D:62:PHE:O	4:D:65:ASP:HB3	2.08	0.53
5:I:63:DG:H1'	5:I:64:DC:O4'	2.08	0.53
6:J:54:DC:H2"	6:J:55:DG:C8	2.44	0.53
2:F:91:LYS:O	2:F:94:GLY:N	2.37	0.53
3:G:69:ALA:HA	3:G:72:ASP:OD2	2.08	0.53
4:H:62:PHE:O	4:H:65:ASP:HB3	2.08	0.53
5:I:58:DT:H2"	5:I:59:DA:C8	2.43	0.53
5:I:111:DC:C2	6:J:37:DG:N1	2.76	0.53
7:O:825:LEU:HA	7:O:872:THR:HG21	1.89	0.53
7:O:1164:ARG:HH11	7:O:1189:GLN:HA	1.74	0.53
7:O:1247:SER:O	7:O:1251:GLU:HG3	2.09	0.53
2:B:20:LYS:HD3	7:O:1076:ARG:HH12	1.73	0.53
1:E:63:ARG:NH2	5:I:61:DA:OP1	2.42	0.53
3:G:88:ARG:HD3	3:G:94:ASN:OD1	2.08	0.53
5:I:93:DC:H2"	5:I:94:DG:C8	2.43	0.53
6:J:81:DC:OP2	6:J:81:DC:H2'	2.07	0.53
6:J:122:DG:C4	6:J:123:DC:C5	2.96	0.53
7:O:1102:THR:HB	7:O:1104:HIS:CD2	2.44	0.53
7:O:1258:LEU:HA	7:O:1261:GLU:OE1	2.09	0.53
3:G:27:VAL:HG13	3:G:48:PRO:HB2	1.90	0.53
6:J:18:DG:H1'	6:J:19:DA:N9	2.23	0.53
7:O:769:ASP:O	7:O:772:ILE:HB	2.09	0.53
7:O:809:LEU:HA	7:O:813:LYS:HB2	1.90	0.53
1:A:117:VAL:N	6:J:71:DA:OP1	2.41	0.53
3:C:31:HIS:HA	3:C:34:LEU:HD12	1.90	0.53
4:D:102:GLU:HB3	4:D:106:HIS:CD2	2.44	0.53
6:J:98:DC:H2'	6:J:99:DT:C5	2.44	0.53
6:J:107:DT:H2"	6:J:108:DC:C5	2.43	0.53
7:O:771:GLN:O	7:O:775:LEU:CB	2.57	0.53
7:O:778:MET:HG2	7:O:781:LEU:HD12	1.90	0.53
7:O:1198:HIS:HB3	7:O:1206:VAL:HG21	1.90	0.53
7:O:1344:ALA:O	7:O:1348:GLY:N	2.42	0.53
5:I:111:DC:N4	6:J:36:DA:N1	2.56	0.53
7:O:1138:LYS:O	7:O:1142:ARG:HG3	2.09	0.53
7:O:1250:GLN:HA	7:O:1253:LEU:HD12	1.90	0.53
6:J:86:DG:H1'	6:J:87:DT:O4'	2.08	0.52
6:J:100:DA:C5	6:J:101:DG:C5	2.98	0.52
6:J:124:DG:H8	6:J:124:DG:OP2	1.93	0.52
7:O:1083:TRP:CE2	7:O:1084:ARG:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1238:ALA:HA	7:O:1241:PHE:CE2	2.45	0.52
2:B:25:ASN:O	2:B:27:GLN:N	2.39	0.52
3:C:73:ASN:HB3	3:C:75:LYS:HE2	1.91	0.52
5:I:28:DC:H1'	5:I:29:DA:C8	2.44	0.52
7:O:1015:MET:HE3	7:O:1019:GLN:HB3	1.90	0.52
7:O:782:PHE:CE1	7:O:787:ASN:HA	2.44	0.52
7:O:822:ILE:HA	7:O:871:THR:O	2.09	0.52
5:I:89:DT:C2	5:I:90:DA:C5	2.98	0.52
6:J:43:DA:H2"	6:J:44:DA:C8	2.44	0.52
7:O:1227:LYS:O	7:O:1231:ILE:N	2.42	0.52
2:B:17:ARG:HA	7:O:1117:ASP:HB3	1.92	0.52
2:B:49:LEU:O	2:B:52:GLU:HB3	2.10	0.52
3:C:88:ARG:HD3	3:C:94:ASN:OD1	2.08	0.52
3:C:92:GLU:O	3:C:95:LYS:HB3	2.10	0.52
4:H:106:HIS:O	4:H:109:SER:HB2	2.10	0.52
7:O:777:TRP:CE3	7:O:778:MET:HG3	2.44	0.52
7:O:835:PHE:HE2	7:O:870:LEU:HD22	1.75	0.52
7:O:880:ARG:HA	7:O:883:LEU:HD12	1.92	0.52
7:O:939:ASN:HD22	7:O:945:ILE:HG22	1.74	0.52
4:D:76:ARG:HB3	4:D:80:TYR:CZ	2.45	0.52
4:H:76:ARG:HB3	4:H:80:TYR:CZ	2.45	0.52
4:H:102:GLU:HB3	4:H:106:HIS:CD2	2.44	0.52
7:O:804:SER:O	7:O:807:THR:OG1	2.23	0.52
7:O:1085:VAL:HG13	7:O:1086:ALA:H	1.74	0.52
7:O:1106:VAL:N	7:O:1157:LEU:O	2.29	0.52
7:O:1218:GLU:O	7:O:1222:LEU:HB3	2.10	0.52
1:A:48:LEU:HD21	2:B:44:LYS:HD2	1.90	0.52
3:C:18:SER:OG	3:C:25:PHE:O	2.22	0.52
7:O:896:GLY:O	7:O:899:MET:HB2	2.09	0.52
7:O:942:LEU:HB2	7:O:945:ILE:HG13	1.92	0.52
7:O:982:ARG:O	7:O:986:VAL:HG23	2.10	0.52
7:O:1060:ASN:HB3	7:O:1061:HIS:CD2	2.45	0.52
7:O:1225:ALA:O	7:O:1228:LYS:HB2	2.09	0.52
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.91	0.51
5:I:10:DC:H2"	5:I:11:DC:OP2	2.08	0.51
5:I:13:DG:OP2	5:I:13:DG:H2'	2.10	0.51
6:J:56:DG:H1'	6:J:57:DT:H5'	1.91	0.51
6:J:124:DG:C6	6:J:125:DG:C6	2.98	0.51
7:O:858:GLN:HB3	7:O:862:ARG:HH12	1.74	0.51
7:O:908:LEU:HA	7:O:911:ASN:OD1	2.10	0.51
7:O:939:ASN:ND2	7:O:945:ILE:HG22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1030:ARG:HG2	7:O:1054:GLN:HG3	1.91	0.51
7:O:1131:LEU:HD12	7:O:1149:PHE:HB2	1.92	0.51
6:J:103:DG:C4	6:J:104:DC:C5	2.98	0.51
7:O:827:THR:O	7:O:831:TRP:HD1	1.93	0.51
7:O:1062:PRO:HG3	7:O:1085:VAL:CG1	2.40	0.51
4:D:33:SER:OG	4:D:34:TYR:N	2.43	0.51
5:I:33:DG:H2"	5:I:34:DG:H5"	1.92	0.51
7:O:854:ARG:NH1	7:O:875:TYR:OH	2.43	0.51
7:O:939:ASN:HD22	7:O:945:ILE:C	2.13	0.51
7:O:1027:LEU:O	7:O:1030:ARG:HB2	2.10	0.51
7:O:1173:GLN:NE2	7:O:1200:ILE:O	2.31	0.51
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.43	0.51
6:J:119:DT:H2"	6:J:120:DG:N7	2.25	0.51
5:I:34:DG:C6	5:I:35:DT:C4	2.98	0.51
5:I:132:DG:H1'	5:I:133:DA:C8	2.45	0.51
6:J:53:DG:H8	6:J:53:DG:OP2	1.92	0.51
7:O:855:LYS:HA	7:O:858:GLN:OE1	2.10	0.51
7:O:939:ASN:ND2	7:O:945:ILE:O	2.43	0.51
7:O:1116:MET:HB2	7:O:1132:ARG:NH2	2.25	0.51
7:O:1190:ASP:O	7:O:1194:GLN:HG3	2.10	0.51
5:I:104:DT:H2'	5:I:105:DT:H71	1.93	0.51
7:O:797:GLY:O	7:O:801:GLN:HG3	2.11	0.51
1:E:51:ILE:HG12	2:F:39:ARG:O	2.11	0.51
4:H:76:ARG:HB3	4:H:80:TYR:CE2	2.45	0.51
5:I:77:DT:H2"	5:I:78:DC:C6	2.46	0.51
5:I:101:DG:H2'	5:I:101:DG:OP2	2.10	0.51
6:J:61:DA:C2	6:J:62:DA:C5	2.99	0.51
6:J:97:DG:C4	6:J:98:DC:C5	2.99	0.51
7:O:848:LYS:HA	7:O:875:TYR:HE2	1.74	0.51
7:O:1006:LYS:HA	7:O:1206:VAL:HB	1.93	0.51
7:O:1007:VAL:N	7:O:1206:VAL:O	2.42	0.51
7:O:1083:TRP:HA	7:O:1089:PHE:CB	2.41	0.51
3:G:73:ASN:HB3	3:G:75:LYS:HE2	1.92	0.51
6:J:46:DC:H2"	6:J:47:DC:OP2	2.10	0.51
1:A:40:ARG:NH1	5:I:84:DC:O4'	2.44	0.51
4:D:76:ARG:HB3	4:D:80:TYR:CE2	2.45	0.51
3:G:14:ALA:HA	5:I:32:DT:OP1	2.11	0.51
3:G:17:ARG:HH21	3:G:28:GLY:CA	2.24	0.51
5:I:102:DG:C2'	5:I:103:DA:H8	2.24	0.51
6:J:109:DT:H1'	6:J:110:DA:C8	2.46	0.51
6:J:123:DC:H2"	6:J:124:DG:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:142:DC:C2	6:J:143:DT:C4	2.99	0.51
7:O:837:LYS:HB2	7:O:838:TRP:CD1	2.46	0.51
7:O:843:ARG:HD2	7:O:866:PHE:HA	1.92	0.51
7:O:854:ARG:O	7:O:858:GLN:HG3	2.10	0.51
7:O:945:ILE:O	7:O:949:VAL:CB	2.52	0.51
7:O:978:LEU:HD22	7:O:982:ARG:HH12	1.75	0.51
7:O:980:ILE:HG12	7:O:983:LEU:HD12	1.92	0.51
7:O:1106:VAL:HG11	7:O:1179:ILE:HD12	1.92	0.51
7:O:1159:PHE:CE2	7:O:1161:LEU:HD21	2.46	0.51
3:G:37:GLY:HA3	3:G:39:TYR:CE2	2.46	0.50
3:G:92:GLU:O	3:G:95:LYS:HB3	2.10	0.50
6:J:17:DT:H2"	6:J:18:DG:OP2	2.09	0.50
6:J:63:DC:H2"	6:J:64:DG:H8	1.76	0.50
7:O:928:GLN:HE22	7:O:1228:LYS:HD3	1.76	0.50
7:O:1133:LEU:HD11	7:O:1142:ARG:HG2	1.92	0.50
3:C:17:ARG:HH21	3:C:28:GLY:CA	2.24	0.50
3:C:77:ARG:NE	6:J:20:DC:H5"	2.26	0.50
1:E:72:ARG:O	1:E:76:GLN:HG3	2.11	0.50
4:H:107:ALA:O	4:H:110:GLU:N	2.44	0.50
5:I:111:DC:C2	6:J:37:DG:C2	3.00	0.50
6:J:128:DT:H1'	6:J:129:DC:C2	2.46	0.50
7:O:683:LEU:HD11	7:O:744:TYR:HD1	1.76	0.50
7:O:684:ARG:HH12	7:O:747:VAL:HG21	1.76	0.50
7:O:835:PHE:CG	7:O:844:THR:HG21	2.46	0.50
7:O:1262:GLU:O	7:O:1266:LYS:HG3	2.11	0.50
1:A:72:ARG:O	1:A:76:GLN:HG3	2.11	0.50
4:D:106:HIS:O	4:D:109:SER:HB2	2.10	0.50
5:I:103:DA:H2'	5:I:104:DT:H6	1.76	0.50
6:J:41:DG:C5	6:J:42:DT:C4	2.99	0.50
6:J:71:DA:H1'	6:J:72:DC:H5'	1.93	0.50
6:J:101:DG:H2"	6:J:102:DA:C8	2.46	0.50
6:J:123:DC:C2	6:J:124:DG:C5	2.99	0.50
4:D:107:ALA:O	4:D:110:GLU:N	2.44	0.50
1:E:68:GLN:NE2	1:E:72:ARG:HE	2.03	0.50
4:H:33:SER:OG	4:H:34:TYR:N	2.43	0.50
5:I:90:DA:H1'	5:I:91:DA:N7	2.27	0.50
6:J:42:DT:C2	6:J:43:DA:C8	2.99	0.50
7:O:781:LEU:O	7:O:786:LEU:N	2.45	0.50
7:O:1085:VAL:HA	7:O:1318:LEU:HG	1.94	0.50
7:O:1254:LEU:O	7:O:1257:LEU:HB3	2.10	0.50
3:C:37:GLY:HA3	3:C:39:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:111:DC:O2	6:J:37:DG:C2	2.64	0.50
7:O:1108:ILE:HG23	7:O:1179:ILE:O	2.10	0.50
7:O:1113:THR:HG21	7:O:1134:ASP:CB	2.41	0.50
7:O:1236:ILE:O	7:O:1240:LYS:HG3	2.10	0.50
5:I:64:DC:H2"	5:I:65:DA:N7	2.27	0.50
6:J:37:DG:H1'	6:J:38:DG:C5	2.47	0.50
6:J:73:DA:H2"	6:J:74:DG:H8	1.75	0.50
6:J:76:DG:C4	6:J:77:DC:C4	2.99	0.50
6:J:120:DG:H1'	6:J:121:DA:C5	2.47	0.50
7:O:744:TYR:CE2	7:O:986:VAL:HG13	2.47	0.50
7:O:753:GLU:OE1	7:O:813:LYS:NZ	2.30	0.50
7:O:908:LEU:HD12	7:O:909:THR:HG23	1.94	0.50
5:I:60:DA:OP2	5:I:60:DA:H2'	2.12	0.50
5:I:110:DC:N3	6:J:37:DG:C2	2.80	0.50
5:I:136:DT:H2"	5:I:137:DA:H5'	1.93	0.50
6:J:111:DC:H2"	6:J:112:DG:C8	2.46	0.50
2:B:20:LYS:CD	7:O:1076:ARG:HH12	2.24	0.50
2:B:25:ASN:C	2:B:27:GLN:N	2.65	0.50
3:C:50:TYR:O	3:C:54:VAL:HG23	2.12	0.50
5:I:122:DG:H2'	5:I:122:DG:OP2	2.12	0.50
7:O:1064:VAL:HG23	7:O:1065:PHE:CD2	2.47	0.50
3:C:42:ARG:HH21	5:I:112:DT:C4'	2.25	0.50
3:G:50:TYR:O	3:G:54:VAL:HG23	2.12	0.50
6:J:81:DC:H2"	6:J:82:DG:N7	2.27	0.50
7:O:1237:GLN:NE2	7:O:1256:SER:HB2	2.27	0.50
6:J:142:DC:H1'	6:J:143:DT:H5'	1.93	0.49
7:O:767:LEU:HB3	7:O:771:GLN:HB2	1.94	0.49
7:O:1091:LEU:O	7:O:1095:ILE:HG12	2.11	0.49
2:B:84:MET:HB3	2:B:88:TYR:HE2	1.76	0.49
5:I:20:DA:H1'	5:I:21:DG:O4'	2.12	0.49
6:J:7:DT:H2"	6:J:8:DG:N7	2.27	0.49
6:J:15:DT:H4'	6:J:16:DC:OP1	2.12	0.49
2:B:71:THR:HA	2:B:74:GLU:OE1	2.13	0.49
2:F:88:TYR:O	2:F:92:ARG:CB	2.60	0.49
5:I:59:DA:H2"	5:I:60:DA:O4'	2.13	0.49
5:I:74:DC:C6	5:I:75:DT:H72	2.47	0.49
5:I:145:DG:C6	5:I:146:DA:C6	2.99	0.49
6:J:32:DG:H2"	6:J:33:DA:H8	1.77	0.49
6:J:98:DC:H2'	6:J:99:DT:H72	1.93	0.49
6:J:133:DA:H1'	6:J:134:DC:H5'	1.94	0.49
7:O:1015:MET:SD	7:O:1213:THR:HG21	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:THR:O	3:C:20:ARG:HG3	2.12	0.49
5:I:126:DG:H2'	5:I:127:DT:C6	2.47	0.49
6:J:116:DA:H2"	6:J:117:DA:C8	2.47	0.49
7:O:987:LEU:HA	7:O:990:PHE:CD2	2.47	0.49
7:O:989:PRO:HG2	7:O:990:PHE:CD2	2.48	0.49
3:G:16:THR:O	3:G:20:ARG:HG3	2.12	0.49
5:I:44:DG:OP2	5:I:44:DG:H8	1.95	0.49
5:I:111:DC:N4	6:J:37:DG:O6	2.46	0.49
5:I:121:DG:H2"	5:I:122:DG:OP2	2.12	0.49
7:O:1015:MET:HB2	7:O:1020:GLN:CG	2.39	0.49
7:O:1023:TYR:OH	7:O:1055:LEU:HD23	2.12	0.49
7:O:1340:SER:OG	7:O:1341:GLU:OE1	2.30	0.49
1:A:91:ALA:HB1	2:B:86:VAL:HG11	1.94	0.49
5:I:33:DG:H2"	5:I:34:DG:H8	1.77	0.49
6:J:131:DG:H8	6:J:131:DG:O5'	1.95	0.49
6:J:134:DC:H2"	6:J:135:DC:C6	2.48	0.49
7:O:1084:ARG:NH1	7:O:1318:LEU:HD23	2.27	0.49
1:A:67:PHE:O	1:A:71:VAL:HG23	2.12	0.49
2:B:58:LEU:O	2:B:61:PHE:HB3	2.12	0.49
6:J:98:DC:H2'	6:J:99:DT:C6	2.48	0.49
6:J:142:DC:H1'	6:J:143:DT:C5'	2.42	0.49
7:O:828:LEU:HD11	7:O:870:LEU:HG	1.95	0.49
7:O:909:THR:O	7:O:913:HIS:HB2	2.12	0.49
7:O:921:ILE:HG21	7:O:937:LEU:HD22	1.94	0.49
7:O:939:ASN:HA	7:O:945:ILE:HB	1.95	0.49
6:J:43:DA:C4	6:J:44:DA:N7	2.81	0.49
6:J:72:DC:H1'	6:J:73:DA:C8	2.48	0.49
2:B:91:LYS:HD3	4:D:76:ARG:HH22	1.78	0.49
4:H:72:GLY:O	4:H:76:ARG:HG3	2.13	0.49
5:I:33:DG:C6	5:I:34:DG:C6	3.01	0.49
5:I:50:DG:H2"	5:I:51:DC:H5'	1.95	0.49
6:J:32:DG:H2"	6:J:33:DA:OP2	2.11	0.49
7:O:981:ARG:HD2	7:O:1238:ALA:HB2	1.94	0.49
7:O:1116:MET:HB2	7:O:1132:ARG:HH21	1.78	0.49
7:O:1235:VAL:O	7:O:1238:ALA:HB3	2.12	0.49
2:B:22:LEU:HD12	2:B:23:ARG:H	1.77	0.48
2:B:39:ARG:HH12	2:B:46:ILE:HG13	1.78	0.48
2:B:79:LYS:NZ	5:I:101:DG:OP1	2.45	0.48
5:I:30:DA:H2'	5:I:31:DT:H71	1.94	0.48
7:O:744:TYR:HB2	7:O:989:PRO:HG3	1.94	0.48
7:O:774:GLY:HA3	7:O:992:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:820:LEU:HD12	7:O:821:VAL:N	2.28	0.48
7:O:1016:SER:HB2	7:O:1318:LEU:HB2	1.95	0.48
3:C:64:GLU:HA	4:D:46:HIS:NE2	2.28	0.48
4:H:30:ARG:HE	6:J:123:DC:H4'	1.78	0.48
5:I:54:DC:H2"	5:I:55:DG:C8	2.48	0.48
5:I:95:DC:OP1	7:O:904:SER:HA	2.13	0.48
6:J:30:DG:H2"	6:J:31:DA:H8	1.78	0.48
7:O:889:VAL:C	7:O:916:ALA:HB1	2.32	0.48
7:O:1104:HIS:C	7:O:1157:LEU:HD22	2.34	0.48
7:O:1163:THR:OG1	7:O:1164:ARG:N	2.45	0.48
5:I:103:DA:H2'	5:I:104:DT:C6	2.48	0.48
5:I:122:DG:N2	6:J:27:DC:O2	2.46	0.48
7:O:882:LEU:HA	7:O:885:LYS:HE3	1.95	0.48
7:O:989:PRO:HG2	7:O:990:PHE:CE2	2.48	0.48
7:O:1105:ARG:HD3	7:O:1174:THR:O	2.12	0.48
7:O:1108:ILE:HG22	7:O:1109:PHE:H	1.78	0.48
3:G:21:ALA:HA	4:H:118:TYR:HB2	1.95	0.48
6:J:3:DC:H1'	6:J:4:DG:O4'	2.13	0.48
7:O:1019:GLN:NE2	7:O:1086:ALA:HB2	2.27	0.48
7:O:1055:LEU:O	7:O:1059:CYS:CB	2.54	0.48
4:D:72:GLY:O	4:D:76:ARG:HG3	2.13	0.48
5:I:69:DA:H2"	5:I:70:DC:C5	2.49	0.48
6:J:108:DC:H2'	6:J:108:DC:OP2	2.13	0.48
6:J:136:DG:H2"	6:J:137:DG:OP2	2.13	0.48
7:O:768:LYS:HB3	7:O:770:TYR:CE2	2.49	0.48
7:O:782:PHE:HA	7:O:786:LEU:H	1.79	0.48
7:O:789:ILE:HG12	7:O:921:ILE:HB	1.95	0.48
7:O:860:LYS:O	7:O:863:ALA:HB3	2.13	0.48
5:I:32:DT:C4	5:I:33:DG:C6	3.02	0.48
7:O:794:MET:HA	7:O:798:LYS:HZ1	1.79	0.48
7:O:809:LEU:O	7:O:813:LYS:HB2	2.13	0.48
7:O:845:ILE:N	7:O:868:VAL:O	2.47	0.48
7:O:980:ILE:HA	7:O:983:LEU:HD12	1.95	0.48
7:O:1021:ILE:HA	7:O:1024:GLN:OE1	2.13	0.48
1:E:67:PHE:O	1:E:71:VAL:HG23	2.12	0.48
2:F:18:HIS:NE2	5:I:52:DA:O3'	2.46	0.48
5:I:12:DC:H2"	5:I:13:DG:N7	2.28	0.48
6:J:75:DC:H2"	6:J:76:DG:C8	2.48	0.48
6:J:115:DC:H2"	6:J:116:DA:H8	1.78	0.48
6:J:131:DG:C4	6:J:132:DC:C5	3.02	0.48
7:O:754:ASP:CB	7:O:776:GLN:HE21	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:834:GLU:O	7:O:838:TRP:HD1	1.97	0.48
7:O:984:HIS:O	7:O:988:ARG:N	2.47	0.48
7:O:1051:GLN:O	7:O:1055:LEU:HB2	2.13	0.48
6:J:37:DG:OP2	6:J:37:DG:H8	1.96	0.48
2:B:71:THR:HG21	4:D:97:LEU:HD21	1.95	0.48
6:J:41:DG:C2	6:J:42:DT:C2	3.02	0.48
7:O:671:LEU:HB3	7:O:955:TRP:HH2	1.77	0.48
7:O:672:ASP:O	7:O:675:LYS:HB2	2.14	0.48
7:O:778:MET:HA	7:O:781:LEU:HD12	1.95	0.48
7:O:950:LYS:O	7:O:953:ASP:N	2.46	0.48
5:I:96:DC:N4	6:J:53:DG:O6	2.46	0.48
7:O:778:MET:O	7:O:781:LEU:HB2	2.14	0.48
7:O:1136:HIS:O	7:O:1136:HIS:ND1	2.45	0.48
6:J:64:DG:C5	6:J:65:DC:C4	3.01	0.47
6:J:67:DG:C2	6:J:68:DG:C2	3.02	0.47
6:J:111:DC:OP2	6:J:111:DC:H2'	2.14	0.47
7:O:903:GLN:OE1	7:O:903:GLN:N	2.42	0.47
7:O:951:SER:O	7:O:954:GLU:HB2	2.14	0.47
7:O:1003:LEU:HD13	7:O:1198:HIS:HD2	1.79	0.47
1:E:72:ARG:NH2	5:I:51:DC:OP2	2.48	0.47
6:J:72:DC:C2	6:J:73:DA:C5	3.02	0.47
7:O:675:LYS:HE2	7:O:983:LEU:HD21	1.96	0.47
7:O:823:VAL:HG22	7:O:828:LEU:HD12	1.97	0.47
7:O:929:ASN:ND2	7:O:1231:ILE:HG22	2.29	0.47
7:O:1014:LYS:HE3	7:O:1317:LEU:CD1	2.44	0.47
7:O:1238:ALA:HA	7:O:1241:PHE:CD2	2.49	0.47
7:O:1244:LYS:O	7:O:1245:SER:OG	2.25	0.47
2:F:56:GLY:O	2:F:59:LYS:HB3	2.13	0.47
3:G:14:ALA:HB2	5:I:32:DT:H5"	1.96	0.47
5:I:120:DA:OP2	5:I:120:DA:H8	1.97	0.47
6:J:137:DG:OP2	6:J:137:DG:H8	1.97	0.47
7:O:1096:LEU:HA	7:O:1099:LEU:HD12	1.96	0.47
7:O:1297:LEU:O	7:O:1300:MET:HB2	2.13	0.47
2:B:32:PRO:O	2:B:36:ARG:HG3	2.14	0.47
1:E:69:ARG:HB3	2:F:22:LEU:HD13	1.96	0.47
6:J:82:DG:C4	6:J:83:DT:C5	3.01	0.47
7:O:908:LEU:HD12	7:O:909:THR:N	2.28	0.47
7:O:914:TYR:C	7:O:915:HIS:CG	2.87	0.47
7:O:947:ASN:HA	7:O:950:LYS:NZ	2.30	0.47
7:O:1088:LYS:HD3	7:O:1181:PHE:CD1	2.48	0.47
1:A:109:LEU:HA	1:A:112:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:GLU:O	4:D:76:ARG:HB2	2.15	0.47
2:F:31:LYS:O	2:F:35:ARG:HG3	2.15	0.47
6:J:116:DA:OP2	6:J:116:DA:H2'	2.15	0.47
7:O:1120:GLU:O	7:O:1123:LEU:HB2	2.14	0.47
7:O:1216:SER:O	7:O:1219:GLU:HB2	2.14	0.47
7:O:1226:TYR:CD1	7:O:1229:LEU:HD12	2.46	0.47
1:E:87:SER:O	1:E:90:MET:HB2	2.15	0.47
4:H:87:THR:O	4:H:91:ILE:HG12	2.15	0.47
6:J:52:DG:C2	6:J:53:DG:C5	3.02	0.47
4:D:73:GLU:HA	4:D:76:ARG:HD3	1.97	0.47
1:E:104:PHE:CE2	2:F:37:LEU:HB3	2.50	0.47
6:J:53:DG:H5'	7:O:1112:MET:HG2	1.96	0.47
6:J:63:DC:H2"	6:J:64:DG:C8	2.50	0.47
6:J:68:DG:H2"	6:J:69:DG:C8	2.50	0.47
6:J:98:DC:H2'	6:J:99:DT:C7	2.44	0.47
7:O:759:PRO:HB2	7:O:811:GLU:OE2	2.15	0.47
7:O:771:GLN:HA	7:O:994:ARG:NH1	2.20	0.47
7:O:1025:GLN:HG2	7:O:1029:TYR:CE2	2.49	0.47
4:D:87:THR:O	4:D:91:ILE:HG12	2.15	0.47
4:D:91:ILE:O	4:D:95:VAL:HG23	2.15	0.47
1:E:104:PHE:O	1:E:107:THR:N	2.48	0.47
3:G:17:ARG:O	3:G:21:ALA:N	2.46	0.47
4:H:98:LEU:HA	4:H:98:LEU:HD23	1.74	0.47
5:I:33:DG:O6	6:J:114:DC:N4	2.47	0.47
6:J:73:DA:H2"	6:J:74:DG:C8	2.50	0.47
7:O:780:SER:O	7:O:784:ASN:ND2	2.45	0.47
7:O:872:THR:O	7:O:876:ILE:HG12	2.15	0.47
7:O:1053:MET:HG3	7:O:1054:GLN:NE2	2.30	0.47
7:O:1080:ASP:HA	7:O:1083:TRP:HE1	1.80	0.47
1:A:68:GLN:O	1:A:71:VAL:N	2.48	0.47
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.49	0.47
5:I:95:DC:H2'	5:I:96:DC:C6	2.49	0.47
6:J:37:DG:H2"	6:J:38:DG:N7	2.30	0.47
7:O:968:LYS:HA	7:O:972:SER:H	1.80	0.47
7:O:999:VAL:HG23	7:O:1000:GLU:N	2.28	0.47
7:O:1225:ALA:HA	7:O:1228:LYS:HD2	1.96	0.47
7:O:1226:TYR:O	7:O:1229:LEU:HB2	2.14	0.47
2:B:74:GLU:OE2	4:D:96:ARG:NH2	2.48	0.47
2:B:92:ARG:NH2	4:D:98:LEU:HA	2.30	0.47
6:J:67:DG:H1'	6:J:68:DG:C8	2.50	0.47
1:A:113:HIS:HE1	1:E:122:LYS:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ARG:O	3:C:21:ALA:N	2.46	0.46
2:F:31:LYS:HG3	2:F:51:TYR:CZ	2.50	0.46
3:G:80:PRO:HA	3:G:83:LEU:HD12	1.98	0.46
4:H:91:ILE:O	4:H:95:VAL:HG23	2.15	0.46
5:I:132:DG:H4'	5:I:133:DA:OP1	2.14	0.46
6:J:37:DG:H21	6:J:38:DG:N2	2.13	0.46
7:O:1227:LYS:O	7:O:1231:ILE:HG13	2.15	0.46
1:A:46:VAL:HB	5:I:83:DG:P	2.54	0.46
1:E:68:GLN:O	1:E:71:VAL:N	2.48	0.46
1:E:109:LEU:HA	1:E:112:ILE:HD12	1.97	0.46
5:I:39:DA:H2"	5:I:40:DG:C8	2.50	0.46
5:I:44:DG:C2	5:I:45:DC:C2	3.03	0.46
5:I:127:DT:H2"	5:I:128:DG:N7	2.30	0.46
7:O:897:HIS:O	7:O:900:LYS:CB	2.57	0.46
1:A:87:SER:O	1:A:90:MET:HB2	2.15	0.46
2:F:34:ILE:HA	2:F:37:LEU:HD12	1.96	0.46
4:H:73:GLU:O	4:H:76:ARG:HB2	2.15	0.46
5:I:124:DA:H1'	5:I:125:DC:H5'	1.98	0.46
6:J:53:DG:H2"	6:J:54:DC:H5'	1.96	0.46
7:O:744:TYR:HB3	7:O:748:ALA:HB2	1.97	0.46
7:O:890:HIS:CE1	7:O:892:ILE:HG13	2.50	0.46
7:O:978:LEU:O	7:O:982:ARG:CB	2.54	0.46
7:O:995:LEU:O	7:O:999:VAL:HG22	2.14	0.46
4:H:39:TYR:HE1	5:I:21:DG:OP2	1.97	0.46
5:I:12:DC:C2	5:I:13:DG:C6	3.03	0.46
5:I:119:DC:C2	5:I:120:DA:C5	3.04	0.46
6:J:122:DG:C4	6:J:123:DC:C4	3.03	0.46
6:J:128:DT:H2"	6:J:129:DC:C5	2.51	0.46
7:O:679:ILE:O	7:O:683:LEU:HB2	2.15	0.46
7:O:1288:ALA:HB2	7:O:1294:MET:HG2	1.98	0.46
1:A:91:ALA:CB	2:B:86:VAL:HG11	2.46	0.46
3:C:80:PRO:HA	3:C:83:LEU:HD12	1.98	0.46
1:E:109:LEU:HA	1:E:109:LEU:HD23	1.66	0.46
2:F:24:ASP:HB3	2:F:27:GLN:HG2	1.96	0.46
5:I:13:DG:C4	5:I:14:DG:C5	3.03	0.46
6:J:139:DA:C6	6:J:140:DT:C4	3.03	0.46
7:O:671:LEU:O	7:O:675:LYS:HG3	2.15	0.46
7:O:754:ASP:HB3	7:O:776:GLN:NE2	2.28	0.46
7:O:880:ARG:HH22	7:O:912:THR:CG2	2.26	0.46
7:O:1094:ARG:HH21	7:O:1304:ARG:HD2	1.80	0.46
5:I:20:DA:H5'	5:I:20:DA:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:47:DC:OP2	6:J:47:DC:H2'	2.15	0.46
6:J:121:DA:C4	6:J:122:DG:C5	3.03	0.46
7:O:1067:GLU:OE1	7:O:1067:GLU:N	2.40	0.46
7:O:1223:GLU:HG2	7:O:1226:TYR:HD2	1.80	0.46
1:A:104:PHE:O	1:A:107:THR:N	2.48	0.46
2:B:33:ALA:O	2:B:36:ARG:N	2.48	0.46
5:I:99:DG:C6	5:I:100:DG:C6	3.03	0.46
7:O:931:LEU:HA	7:O:933:GLU:HB2	1.98	0.46
2:F:84:MET:O	2:F:87:VAL:N	2.49	0.46
5:I:46:DT:H6	5:I:46:DT:O5'	1.98	0.46
5:I:57:DT:OP1	5:I:57:DT:H3'	2.15	0.46
5:I:141:DA:C2	6:J:8:DG:C2	3.04	0.46
6:J:83:DT:H2"	6:J:84:DG:N7	2.30	0.46
6:J:136:DG:H1'	6:J:137:DG:O5'	2.16	0.46
7:O:996:LYS:O	7:O:1000:GLU:N	2.49	0.46
7:O:1004:PRO:HG3	7:O:1203:LYS:CA	2.39	0.46
7:O:1020:GLN:O	7:O:1024:GLN:HG3	2.16	0.46
3:C:71:ARG:C	3:C:74:LYS:H	2.19	0.46
3:C:84:GLN:HE21	3:C:88:ARG:CG	2.29	0.46
4:D:83:ARG:HD2	6:J:40:DA:H5"	1.97	0.46
5:I:100:DG:H2"	5:I:101:DG:N7	2.31	0.46
6:J:90:DA:OP2	6:J:90:DA:H2'	2.16	0.46
7:O:920:LEU:HD21	7:O:922:LEU:HD21	1.96	0.46
7:O:943:PRO:HA	7:O:946:PHE:CD2	2.49	0.46
2:B:31:LYS:HG3	2:B:51:TYR:CZ	2.51	0.46
4:H:73:GLU:HA	4:H:76:ARG:HD3	1.97	0.46
5:I:27:DT:H4'	5:I:28:DC:OP1	2.15	0.46
5:I:94:DG:H5"	7:O:905:LYS:CE	2.46	0.46
6:J:39:DG:H1'	6:J:40:DA:O4'	2.16	0.46
7:O:950:LYS:O	7:O:953:ASP:HB3	2.15	0.46
7:O:1026:MET:HG2	7:O:1029:TYR:CD2	2.37	0.46
7:O:1026:MET:HA	7:O:1029:TYR:CB	2.44	0.46
6:J:73:DA:H8	6:J:73:DA:OP2	1.98	0.45
6:J:82:DG:C2	6:J:83:DT:C2	3.04	0.45
6:J:105:DT:H2"	6:J:106:DG:C8	2.51	0.45
7:O:676:ASP:O	7:O:679:ILE:HB	2.16	0.45
7:O:685:GLN:O	7:O:688:ALA:HB3	2.17	0.45
7:O:778:MET:O	7:O:782:PHE:HD2	1.99	0.45
7:O:780:SER:C	7:O:784:ASN:HD22	2.20	0.45
7:O:1053:MET:HG3	7:O:1054:GLN:HE21	1.81	0.45
7:O:1207:ARG:NH2	7:O:1288:ALA:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HD2	6:J:50:DT:H4'	1.98	0.45
3:C:28:GLY:HA3	6:J:30:DG:H3'	1.98	0.45
1:E:73:GLU:HB2	2:F:22:LEU:HB2	1.98	0.45
5:I:22:DG:C6	5:I:23:DC:N4	2.84	0.45
6:J:78:DG:H2'	6:J:78:DG:OP2	2.15	0.45
7:O:1092:LEU:HB3	7:O:1096:LEU:CD1	2.46	0.45
3:G:81:ARG:CZ	3:G:85:LEU:HD21	2.46	0.45
6:J:32:DG:H5'	6:J:32:DG:H8	1.82	0.45
7:O:1080:ASP:OD1	7:O:1125:TYR:OH	2.32	0.45
7:O:1086:ALA:HB3	7:O:1089:PHE:CE2	2.51	0.45
4:D:98:LEU:HD23	4:D:98:LEU:HA	1.74	0.45
3:G:47:ALA:HA	4:H:88:SER:HA	1.98	0.45
5:I:22:DG:C4	5:I:23:DC:C5	3.05	0.45
6:J:62:DA:C4	6:J:63:DC:C5	3.04	0.45
6:J:74:DG:C5	6:J:75:DC:C4	3.04	0.45
2:B:72:TYR:HB2	2:B:85:ASP:CG	2.36	0.45
5:I:61:DA:C4	5:I:62:DC:C5	3.04	0.45
6:J:16:DC:H1'	6:J:17:DT:C2	2.52	0.45
6:J:52:DG:N1	6:J:53:DG:C6	2.85	0.45
6:J:117:DA:H8	6:J:117:DA:OP2	1.99	0.45
6:J:121:DA:C5	6:J:122:DG:C6	3.04	0.45
6:J:133:DA:C4	6:J:134:DC:C5	3.05	0.45
6:J:137:DG:C6	6:J:138:DG:C6	3.04	0.45
6:J:139:DA:OP2	6:J:139:DA:H8	1.99	0.45
7:O:834:GLU:OE1	7:O:838:TRP:NE1	2.50	0.45
7:O:1062:PRO:HG2	7:O:1063:PHE:CD2	2.51	0.45
3:C:81:ARG:CZ	3:C:85:LEU:HD21	2.46	0.45
3:G:71:ARG:C	3:G:74:LYS:H	2.19	0.45
3:G:84:GLN:HE21	3:G:88:ARG:CG	2.29	0.45
5:I:24:DC:H2"	5:I:25:DG:N7	2.31	0.45
6:J:102:DA:H2"	6:J:103:DG:H8	1.82	0.45
7:O:768:LYS:HB2	7:O:770:TYR:CZ	2.52	0.45
7:O:874:GLU:O	7:O:877:ILE:HB	2.16	0.45
7:O:952:PHE:HB3	7:O:956:PHE:CE2	2.52	0.45
7:O:1133:LEU:HB3	7:O:1161:LEU:CD2	2.47	0.45
7:O:1179:ILE:HA	7:O:1209:LEU:HB2	1.99	0.45
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.73	0.45
2:B:99:GLY:O	4:H:57:SER:OG	2.22	0.45
5:I:135:DA:C8	5:I:136:DT:H72	2.52	0.45
6:J:80:DA:OP2	6:J:80:DA:H8	1.99	0.45
7:O:674:THR:O	7:O:677:THR:OG1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:884:SER:HB3	7:O:913:HIS:HA	1.99	0.45
7:O:1237:GLN:HE21	7:O:1253:LEU:HB3	1.82	0.45
4:D:36:ILE:HG13	4:D:37:TYR:N	2.32	0.45
4:D:97:LEU:HD23	4:D:97:LEU:HA	1.74	0.45
5:I:34:DG:H2'	5:I:35:DT:C6	2.52	0.45
6:J:143:DT:C6	6:J:144:DC:C4	3.05	0.45
7:O:907:SER:OG	7:O:908:LEU:N	2.50	0.45
7:O:938:LEU:CG	7:O:945:ILE:HG21	2.45	0.45
7:O:971:LEU:O	7:O:976:THR:HG23	2.17	0.45
7:O:1063:PHE:HB3	7:O:1069:GLU:H	1.82	0.45
2:B:62:LEU:HB3	2:B:66:ILE:HD12	1.98	0.45
1:E:116:ARG:NH2	1:E:122:LYS:HE3	2.32	0.45
5:I:52:DA:H1'	5:I:53:DC:H5'	1.99	0.45
5:I:85:DG:H2"	5:I:86:DT:O5'	2.17	0.45
6:J:74:DG:C4	6:J:75:DC:C4	3.05	0.45
6:J:92:DG:H1'	6:J:93:DC:H5'	1.99	0.45
6:J:138:DG:C4	6:J:139:DA:C5	3.05	0.45
7:O:1025:GLN:HG2	7:O:1029:TYR:CZ	2.51	0.45
4:H:36:ILE:HG13	4:H:37:TYR:N	2.32	0.45
5:I:68:DT:H2"	5:I:69:DA:C8	2.51	0.45
6:J:16:DC:H1'	6:J:17:DT:O4'	2.17	0.45
6:J:44:DA:H2'	6:J:45:DT:H6	1.78	0.45
7:O:682:LEU:C	7:O:944:LYS:HD2	2.37	0.45
7:O:935:TRP:HZ2	7:O:956:PHE:HB2	1.82	0.45
7:O:1016:SER:N	7:O:1019:GLN:HB2	2.32	0.45
7:O:1029:TYR:OH	7:O:1344:ALA:HB1	2.16	0.45
7:O:1093:ASP:OD2	7:O:1094:ARG:CZ	2.65	0.45
7:O:1164:ARG:HH11	7:O:1189:GLN:CA	2.30	0.45
3:C:88:ARG:HB2	3:C:108:LEU:HD21	1.99	0.44
5:I:67:DG:C2'	5:I:68:DT:H71	2.46	0.44
6:J:91:DA:C4	6:J:92:DG:C8	3.05	0.44
7:O:751:ILE:HB	7:O:784:ASN:HA	1.98	0.44
7:O:798:LYS:HA	7:O:801:GLN:OE1	2.17	0.44
7:O:1139:SER:O	7:O:1142:ARG:HB2	2.17	0.44
7:O:1230:ASP:CG	7:O:1264:ARG:HH11	2.19	0.44
7:O:1281:SER:O	7:O:1284:ASN:HB2	2.16	0.44
1:A:48:LEU:HG	2:B:44:LYS:HE3	2.00	0.44
1:A:116:ARG:NH2	1:A:122:LYS:HE3	2.32	0.44
2:B:45:ARG:HH21	5:I:81:DC:C4'	2.30	0.44
1:E:62:ILE:HB	1:E:93:GLN:HE21	1.83	0.44
6:J:74:DG:C2	6:J:75:DC:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:82:DG:C5	6:J:83:DT:C4	3.05	0.44
7:O:876:ILE:O	7:O:880:ARG:CB	2.35	0.44
7:O:883:LEU:O	7:O:886:VAL:HG22	2.16	0.44
7:O:1207:ARG:NH1	7:O:1287:LEU:HA	2.20	0.44
1:A:54:TYR:HB3	2:B:40:ARG:HB2	1.99	0.44
2:F:32:PRO:HA	2:F:35:ARG:HD3	1.98	0.44
3:G:88:ARG:HB2	3:G:108:LEU:HD21	1.99	0.44
5:I:5:DA:H2"	5:I:6:DG:OP2	2.17	0.44
5:I:60:DA:H2"	5:I:61:DA:C8	2.52	0.44
5:I:88:DT:H2"	5:I:89:DT:O5'	2.17	0.44
5:I:96:DC:N3	6:J:53:DG:N1	2.65	0.44
5:I:127:DT:OP2	5:I:127:DT:H2'	2.17	0.44
7:O:1007:VAL:O	7:O:1207:ARG:HA	2.17	0.44
7:O:1063:PHE:CB	7:O:1068:VAL:HB	2.46	0.44
7:O:1096:LEU:HD23	7:O:1099:LEU:HD12	1.98	0.44
7:O:1299:ARG:HG2	7:O:1302:GLU:HG2	1.99	0.44
1:E:50:GLU:O	1:E:53:ARG:HB3	2.18	0.44
1:E:118:THR:HG23	2:F:45:ARG:O	2.17	0.44
5:I:33:DG:C2	5:I:34:DG:C4	3.06	0.44
5:I:79:DC:H2"	5:I:80:DC:C5	2.52	0.44
7:O:976:THR:HG22	7:O:979:VAL:HB	1.99	0.44
7:O:1047:GLY:HA2	7:O:1054:GLN:NE2	2.33	0.44
7:O:1149:PHE:CD1	7:O:1159:PHE:HB2	2.53	0.44
1:A:68:GLN:HE21	1:A:72:ARG:NE	2.04	0.44
1:A:130:ILE:HD13	1:A:130:ILE:HA	1.73	0.44
5:I:8:DA:C4	5:I:9:DT:C5	3.06	0.44
5:I:13:DG:H2"	5:I:14:DG:OP2	2.18	0.44
6:J:8:DG:O5'	6:J:8:DG:H8	2.01	0.44
6:J:139:DA:H2'	6:J:140:DT:O4'	2.18	0.44
7:O:830:ASN:O	7:O:833:SER:HB3	2.17	0.44
7:O:845:ILE:HB	7:O:869:VAL:HA	2.00	0.44
7:O:1086:ALA:HB3	7:O:1089:PHE:CD2	2.53	0.44
7:O:1226:TYR:CD2	7:O:1264:ARG:NH2	2.84	0.44
1:A:62:ILE:HB	1:A:93:GLN:HE21	1.83	0.44
1:A:68:GLN:NE2	1:A:72:ARG:HE	2.03	0.44
5:I:28:DC:H1'	5:I:29:DA:N9	2.32	0.44
5:I:76:DG:H2"	5:I:77:DT:OP2	2.17	0.44
5:I:78:DC:OP2	5:I:78:DC:H2'	2.18	0.44
6:J:38:DG:H1'	6:J:39:DG:H5'	2.00	0.44
6:J:100:DA:H2"	6:J:101:DG:OP2	2.17	0.44
6:J:140:DT:H2'	6:J:141:DT:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:753:GLU:HB3	7:O:783:ASN:HD22	1.81	0.44
7:O:1283:ILE:O	7:O:1286:ILE:HG12	2.17	0.44
1:A:51:ILE:HG12	2:B:39:ARG:O	2.18	0.44
4:D:98:LEU:O	4:D:100:PRO:HD3	2.18	0.44
5:I:14:DG:C4	5:I:15:DT:C6	3.05	0.44
5:I:57:DT:H6	5:I:57:DT:H2'	1.60	0.44
6:J:107:DT:H2"	6:J:108:DC:C6	2.53	0.44
7:O:1062:PRO:HD3	7:O:1089:PHE:HE2	1.83	0.44
7:O:1170:LEU:HB2	7:O:1196:ARG:HD2	2.00	0.44
2:B:83:ALA:O	2:B:86:VAL:HB	2.18	0.44
3:C:100:VAL:HG13	2:F:96:THR:O	2.18	0.44
4:H:94:ALA:O	4:H:97:LEU:HB2	2.18	0.44
4:H:103:LEU:O	4:H:107:ALA:HB2	2.18	0.44
5:I:18:DC:OP2	5:I:18:DC:H2'	2.18	0.44
5:I:49:DA:OP2	5:I:49:DA:H2'	2.18	0.44
6:J:36:DA:C2	6:J:37:DG:C6	3.06	0.44
7:O:799:THR:HG21	7:O:834:GLU:HG3	2.00	0.44
7:O:805:LEU:O	7:O:808:TYR:HB3	2.18	0.44
7:O:935:TRP:HB3	7:O:939:ASN:OD1	2.18	0.44
7:O:1171:ASN:HB2	7:O:1199:ARG:HD2	1.98	0.44
4:D:103:LEU:O	4:D:107:ALA:HB2	2.18	0.44
4:H:83:ARG:HE	5:I:40:DG:H3'	1.82	0.44
5:I:4:DG:N1	6:J:145:DG:C6	2.86	0.44
5:I:43:DA:C4	5:I:44:DG:C8	3.06	0.44
5:I:59:DA:H2'	5:I:60:DA:H8	1.83	0.44
5:I:78:DC:H2"	5:I:79:DC:C5	2.53	0.44
5:I:88:DT:C2	5:I:89:DT:C4	3.06	0.44
5:I:124:DA:H1'	5:I:125:DC:O4'	2.18	0.44
6:J:50:DT:H2'	6:J:51:DT:C6	2.53	0.44
6:J:82:DG:C2	6:J:83:DT:N3	2.86	0.44
7:O:903:GLN:H	7:O:903:GLN:CD	2.21	0.44
7:O:938:LEU:HG	7:O:945:ILE:HD13	2.00	0.44
7:O:1061:HIS:CE1	7:O:1088:LYS:HD2	2.53	0.44
1:A:104:PHE:CE1	2:B:38:ALA:HB2	2.53	0.43
1:A:122:LYS:HA	1:A:125:GLN:NE2	2.33	0.43
1:E:122:LYS:HA	1:E:125:GLN:NE2	2.33	0.43
5:I:26:DC:C4	6:J:121:DA:N6	2.86	0.43
5:I:38:DT:H2"	5:I:39:DA:C8	2.52	0.43
5:I:139:DA:H1'	5:I:140:DC:C6	2.52	0.43
6:J:42:DT:N3	6:J:43:DA:C5	2.86	0.43
6:J:57:DT:H6	6:J:57:DT:H2'	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:678:ARG:O	7:O:682:LEU:HB2	2.18	0.43
7:O:910:LEU:O	7:O:914:TYR:N	2.50	0.43
7:O:981:ARG:CD	7:O:1238:ALA:HB2	2.48	0.43
7:O:1109:PHE:CB	7:O:1163:THR:HG22	2.43	0.43
7:O:1237:GLN:HE21	7:O:1253:LEU:CA	2.31	0.43
5:I:75:DT:H2"	5:I:76:DG:C8	2.53	0.43
6:J:69:DG:H2"	6:J:70:DG:N7	2.33	0.43
7:O:679:ILE:HG12	7:O:744:TYR:CZ	2.52	0.43
7:O:745:TYR:O	7:O:749:HIS:HD2	2.01	0.43
7:O:761:ILE:O	7:O:763:VAL:HG23	2.18	0.43
7:O:845:ILE:HB	7:O:869:VAL:HG22	1.99	0.43
7:O:981:ARG:HE	7:O:1241:PHE:HE2	1.66	0.43
7:O:1105:ARG:HG2	7:O:1157:LEU:HD23	2.00	0.43
1:A:40:ARG:NH2	5:I:83:DG:O4'	2.51	0.43
2:B:92:ARG:O	2:B:92:ARG:HG2	2.17	0.43
4:D:76:ARG:HB3	4:D:80:TYR:OH	2.18	0.43
5:I:12:DC:H2'	5:I:12:DC:OP2	2.18	0.43
5:I:80:DC:H1'	5:I:81:DC:C5	2.53	0.43
6:J:53:DG:C5'	7:O:1112:MET:HG2	2.48	0.43
6:J:84:DG:C4	6:J:85:DC:C4	3.07	0.43
6:J:100:DA:C6	6:J:101:DG:C2	3.07	0.43
7:O:843:ARG:HB2	7:O:867:ASP:H	1.83	0.43
7:O:857:LYS:O	7:O:860:LYS:HB3	2.18	0.43
7:O:907:SER:O	7:O:910:LEU:HB2	2.18	0.43
7:O:1021:ILE:O	7:O:1024:GLN:HB2	2.17	0.43
7:O:1113:THR:O	7:O:1132:ARG:NH2	2.51	0.43
7:O:1207:ARG:CG	7:O:1289:ARG:HH21	2.28	0.43
4:H:76:ARG:HB3	4:H:80:TYR:OH	2.18	0.43
5:I:35:DT:OP2	5:I:35:DT:H6	2.01	0.43
6:J:74:DG:OP2	6:J:74:DG:H2'	2.18	0.43
7:O:767:LEU:HD22	7:O:771:GLN:HB3	2.00	0.43
7:O:776:GLN:O	7:O:779:VAL:HB	2.17	0.43
7:O:1216:SER:H	7:O:1219:GLU:CD	2.22	0.43
1:A:50:GLU:O	1:A:53:ARG:HB3	2.18	0.43
1:A:81:ASP:OD1	7:O:1046:ARG:HG2	2.18	0.43
3:C:85:LEU:HD23	3:C:108:LEU:HD23	2.00	0.43
4:D:94:ALA:O	4:D:97:LEU:HB2	2.18	0.43
6:J:32:DG:C2	6:J:33:DA:C5	3.07	0.43
6:J:97:DG:H2"	6:J:98:DC:H6	1.83	0.43
7:O:929:ASN:O	7:O:931:LEU:HG	2.18	0.43
7:O:1056:LYS:O	7:O:1060:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1291:ASP:O	7:O:1294:MET:HB2	2.19	0.43
3:G:85:LEU:HD23	3:G:108:LEU:HD23	2.00	0.43
4:H:98:LEU:O	4:H:100:PRO:HD3	2.18	0.43
5:I:18:DC:OP2	5:I:18:DC:H6	2.01	0.43
6:J:25:DG:H1'	6:J:26:DC:C6	2.54	0.43
6:J:91:DA:C6	6:J:92:DG:C6	3.07	0.43
6:J:100:DA:C4	6:J:101:DG:C4	3.06	0.43
7:O:1099:LEU:HD13	7:O:1106:VAL:HG21	1.99	0.43
7:O:1302:GLU:O	7:O:1305:SER:HB3	2.18	0.43
5:I:48:DT:H1'	5:I:49:DA:O4'	2.19	0.43
5:I:68:DT:H2"	5:I:69:DA:N7	2.33	0.43
5:I:87:DT:C6	5:I:88:DT:H72	2.52	0.43
6:J:95:DG:H2"	6:J:96:DT:OP2	2.19	0.43
6:J:113:DA:C4	6:J:114:DC:C5	3.07	0.43
6:J:115:DC:H2"	6:J:116:DA:C8	2.54	0.43
7:O:1184:ASP:HB3	7:O:1186:ASN:O	2.19	0.43
7:O:1187:PRO:O	7:O:1191:LEU:HG	2.18	0.43
2:B:73:THR:HG21	2:B:81:VAL:HG22	2.00	0.43
5:I:52:DA:C4	5:I:53:DC:C5	3.07	0.43
6:J:40:DA:H2"	6:J:41:DG:H8	1.83	0.43
6:J:74:DG:H2'	6:J:74:DG:P	2.57	0.43
6:J:90:DA:H4'	6:J:91:DA:H5'	2.01	0.43
6:J:133:DA:O5'	6:J:133:DA:H8	2.02	0.43
7:O:1192:GLN:HB3	7:O:1196:ARG:NH2	2.33	0.43
1:A:39:HIS:CD2	5:I:7:DA:H5'	2.53	0.43
1:A:104:PHE:O	1:A:105:GLU:C	2.57	0.43
6:J:2:DT:C2	6:J:3:DC:C5	3.07	0.43
6:J:101:DG:H2"	6:J:102:DA:OP2	2.19	0.43
6:J:121:DA:H2"	6:J:122:DG:C8	2.54	0.43
7:O:956:PHE:CZ	7:O:983:LEU:HD13	2.54	0.43
7:O:1227:LYS:O	7:O:1230:ASP:N	2.52	0.43
2:B:76:ALA:O	2:B:78:ARG:HG3	2.18	0.43
2:B:84:MET:HB3	2:B:88:TYR:CE2	2.54	0.43
3:G:32:ARG:CA	3:G:35:ARG:HH21	2.28	0.43
4:H:77:LEU:HD23	4:H:77:LEU:HA	1.79	0.43
5:I:79:DC:N4	6:J:68:DG:O6	2.52	0.43
6:J:32:DG:H2"	6:J:33:DA:C8	2.54	0.43
7:O:744:TYR:O	7:O:747:VAL:N	2.52	0.43
7:O:886:VAL:HG23	7:O:888:TRP:NE1	2.34	0.43
7:O:1025:GLN:NE2	7:O:1344:ALA:HB1	2.33	0.43
5:I:44:DG:N2	6:J:105:DT:C2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:71:DG:C2	6:J:78:DG:C2	3.07	0.42
5:I:72:DC:H2"	5:I:73:DG:H8	1.83	0.42
5:I:90:DA:H4'	5:I:91:DA:OP1	2.19	0.42
5:I:110:DC:H1'	5:I:111:DC:O4'	2.18	0.42
5:I:128:DG:C8	5:I:129:DT:H72	2.53	0.42
6:J:3:DC:P	6:J:3:DC:H3'	2.58	0.42
6:J:104:DC:C2'	6:J:105:DT:H71	2.48	0.42
7:O:803:ILE:O	7:O:806:LEU:N	2.51	0.42
1:E:65:LEU:HG	6:J:92:DG:OP2	2.19	0.42
2:F:79:LYS:HG3	6:J:101:DG:O5'	2.19	0.42
2:F:97:LEU:HG	2:F:98:TYR:N	2.34	0.42
5:I:8:DA:C2	6:J:141:DT:N3	2.88	0.42
5:I:32:DT:C2	5:I:33:DG:C4	3.07	0.42
5:I:135:DA:H2'	5:I:136:DT:C7	2.49	0.42
6:J:91:DA:C6	6:J:92:DG:C5	3.07	0.42
6:J:124:DG:C4	6:J:125:DG:N7	2.88	0.42
6:J:139:DA:C2	6:J:140:DT:C2	3.07	0.42
7:O:788:GLY:O	7:O:920:LEU:HD12	2.19	0.42
2:B:88:TYR:O	2:B:89:ALA:C	2.58	0.42
3:C:24:GLN:HG2	3:C:56:GLU:OE2	2.19	0.42
4:D:87:THR:H	4:D:90:GLU:CD	2.23	0.42
5:I:98:DA:C6	5:I:99:DG:C6	3.08	0.42
6:J:61:DA:C4	6:J:62:DA:N7	2.88	0.42
6:J:69:DG:OP2	6:J:69:DG:H2'	2.19	0.42
6:J:96:DT:C2	6:J:97:DG:C4	3.07	0.42
6:J:124:DG:C4	6:J:125:DG:C5	3.07	0.42
7:O:1283:ILE:O	7:O:1287:LEU:HG	2.18	0.42
3:C:32:ARG:CA	3:C:35:ARG:HH21	2.28	0.42
1:E:41:TYR:OH	6:J:7:DT:H4'	2.19	0.42
1:E:104:PHE:O	1:E:105:GLU:C	2.57	0.42
5:I:13:DG:C6	5:I:14:DG:C6	3.07	0.42
5:I:111:DC:N4	6:J:36:DA:C6	2.88	0.42
6:J:45:DT:C2	6:J:46:DC:C5	3.07	0.42
6:J:82:DG:H2'	6:J:83:DT:H71	2.01	0.42
7:O:948:SER:O	7:O:952:PHE:HD2	2.02	0.42
7:O:972:SER:HA	7:O:976:THR:CG2	2.49	0.42
7:O:1024:GLN:HA	7:O:1027:LEU:HG	2.01	0.42
7:O:1025:GLN:O	7:O:1028:LYS:HB2	2.19	0.42
1:A:42:ARG:HG2	6:J:144:DC:O5'	2.19	0.42
2:F:88:TYR:O	2:F:92:ARG:HB3	2.19	0.42
3:G:64:GLU:HA	4:H:46:HIS:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:3:DC:H2”	5:I:4:DG:OP2	2.19	0.42
5:I:58:DT:C4	5:I:59:DA:C6	3.07	0.42
6:J:19:DA:H2”	6:J:20:DC:OP2	2.20	0.42
6:J:23:DG:C4	6:J:24:DT:C5	3.08	0.42
6:J:37:DG:OP2	6:J:37:DG:H2’	2.19	0.42
6:J:41:DG:C4	6:J:42:DT:C4	3.07	0.42
6:J:63:DC:C2	6:J:64:DG:N7	2.88	0.42
6:J:91:DA:C5	6:J:92:DG:C5	3.07	0.42
6:J:124:DG:C4	6:J:125:DG:C8	3.07	0.42
7:O:1073:ASN:OD1	7:O:1075:THR:OG1	2.25	0.42
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.70	0.42
1:A:119:ILE:HG13	2:B:50:ILE:HG13	2.00	0.42
5:I:53:DC:C2	5:I:54:DC:C4	3.07	0.42
5:I:59:DA:C6	5:I:60:DA:C6	3.07	0.42
5:I:88:DT:N3	5:I:89:DT:C4	2.88	0.42
5:I:136:DT:C4	5:I:137:DA:N6	2.88	0.42
7:O:929:ASN:C	7:O:931:LEU:HG	2.40	0.42
7:O:1259:ASP:O	7:O:1262:GLU:HB2	2.20	0.42
2:B:37:LEU:HA	2:B:37:LEU:HD23	1.62	0.42
4:D:30:ARG:HD3	5:I:123:DC:H4’	2.02	0.42
3:G:51:LEU:HD13	4:H:70:ILE:HG21	2.02	0.42
6:J:38:DG:H2”	6:J:39:DG:N7	2.35	0.42
6:J:132:DC:H2”	6:J:133:DA:N7	2.34	0.42
6:J:138:DG:C6	6:J:139:DA:C6	3.08	0.42
7:O:973:GLU:O	7:O:977:LEU:HG	2.19	0.42
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.55	0.42
5:I:101:DG:H2”	5:I:102:DG:C8	2.55	0.42
5:I:123:DC:H2”	5:I:124:DA:C8	2.54	0.42
5:I:139:DA:C4	5:I:140:DC:C4	3.07	0.42
6:J:29:DG:H1’	6:J:30:DG:C8	2.54	0.42
6:J:138:DG:H2”	6:J:139:DA:OP2	2.19	0.42
7:O:745:TYR:O	7:O:749:HIS:CD2	2.72	0.42
3:C:64:GLU:HA	4:D:46:HIS:CD2	2.54	0.42
5:I:34:DG:H5”	5:I:34:DG:H8	1.84	0.42
5:I:126:DG:N1	6:J:23:DG:C6	2.87	0.42
6:J:74:DG:H2”	6:J:75:DC:OP2	2.20	0.42
6:J:112:DG:C4	6:J:113:DA:N7	2.88	0.42
7:O:684:ARG:HH12	7:O:747:VAL:CG2	2.32	0.42
7:O:1098:LYS:HB3	7:O:1297:LEU:HD13	2.02	0.42
7:O:1258:LEU:HD12	7:O:1259:ASP:N	2.35	0.42
1:A:91:ALA:O	1:A:94:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:O	2:B:19:ARG:HG2	2.20	0.42
2:B:88:TYR:O	2:B:91:LYS:HB3	2.20	0.42
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.55	0.42
1:E:126:LEU:O	1:E:129:ARG:HB3	2.20	0.42
5:I:9:DT:C2	5:I:10:DC:C5	3.08	0.42
5:I:116:DC:H1'	5:I:117:DT:H5'	2.02	0.42
6:J:39:DG:C6	6:J:40:DA:C6	3.08	0.42
7:O:1230:ASP:O	7:O:1234:LYS:HB2	2.20	0.42
7:O:1293:GLU:O	7:O:1297:LEU:HG	2.20	0.42
3:C:43:VAL:N	5:I:113:DA:OP1	2.39	0.41
5:I:33:DG:H2"	5:I:34:DG:C8	2.55	0.41
5:I:81:DC:H5'	5:I:81:DC:C6	2.55	0.41
6:J:102:DA:C6	6:J:103:DG:C6	3.08	0.41
6:J:127:DC:H2'	6:J:128:DT:H72	2.02	0.41
7:O:1190:ASP:HA	7:O:1193:ALA:HB3	2.02	0.41
7:O:1253:LEU:HA	7:O:1256:SER:CB	2.49	0.41
1:E:103:LEU:HA	1:E:103:LEU:HD12	1.75	0.41
2:F:76:ALA:O	2:F:78:ARG:HG3	2.20	0.41
5:I:102:DG:C4	5:I:103:DA:C8	3.08	0.41
6:J:87:DT:H5"	6:J:88:DT:H71	2.01	0.41
6:J:112:DG:C2	6:J:113:DA:C5	3.08	0.41
7:O:679:ILE:HG23	7:O:744:TYR:CD1	2.56	0.41
7:O:938:LEU:CD1	7:O:945:ILE:HD13	2.50	0.41
7:O:1022:MET:O	7:O:1026:MET:HG3	2.21	0.41
7:O:1244:LYS:HB2	7:O:1249:GLU:HG3	2.02	0.41
2:B:71:THR:HG21	4:D:97:LEU:CD2	2.50	0.41
2:B:73:THR:OG1	2:B:85:ASP:OD2	2.20	0.41
3:G:24:GLN:HG2	3:G:56:GLU:OE2	2.19	0.41
5:I:8:DA:C2'	5:I:9:DT:H71	2.50	0.41
5:I:13:DG:H1'	5:I:14:DG:C8	2.55	0.41
5:I:63:DG:C5	5:I:64:DC:C4	3.08	0.41
6:J:46:DC:C2	6:J:47:DC:C4	3.08	0.41
7:O:890:HIS:HE1	7:O:892:ILE:HG13	1.85	0.41
7:O:901:ASN:HB3	7:O:904:SER:OG	2.19	0.41
7:O:1084:ARG:O	7:O:1317:LEU:HA	2.20	0.41
7:O:1119:MET:O	7:O:1120:GLU:C	2.58	0.41
7:O:1180:ILE:N	7:O:1209:LEU:O	2.52	0.41
7:O:1237:GLN:HA	7:O:1240:LYS:CE	2.50	0.41
1:E:63:ARG:O	1:E:66:PRO:HD2	2.20	0.41
2:F:83:ALA:O	2:F:86:VAL:HB	2.21	0.41
4:H:97:LEU:HD23	4:H:97:LEU:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:14:DG:C5	5:I:15:DT:C5	3.09	0.41
6:J:18:DG:C2	6:J:19:DA:C2	3.09	0.41
6:J:49:DC:H2"	6:J:50:DT:OP2	2.21	0.41
6:J:57:DT:H2"	6:J:58:DT:C6	2.55	0.41
6:J:94:DG:C4	6:J:95:DG:C8	3.08	0.41
7:O:851:PRO:O	7:O:854:ARG:HB2	2.20	0.41
7:O:1016:SER:HB3	7:O:1085:VAL:O	2.20	0.41
7:O:1092:LEU:HA	7:O:1095:ILE:CG1	2.51	0.41
7:O:1117:ASP:HA	7:O:1132:ARG:HH12	1.84	0.41
3:C:47:ALA:HA	4:D:88:SER:HA	2.02	0.41
6:J:13:DT:O4	6:J:14:DA:N6	2.53	0.41
6:J:68:DG:C2	6:J:69:DG:C2	3.09	0.41
6:J:124:DG:C2	6:J:125:DG:C4	3.08	0.41
7:O:835:PHE:CD1	7:O:844:THR:HG21	2.55	0.41
7:O:905:LYS:O	7:O:909:THR:OG1	2.39	0.41
7:O:934:LEU:HD23	7:O:934:LEU:HA	1.88	0.41
7:O:935:TRP:O	7:O:936:ALA:C	2.58	0.41
7:O:1018:LEU:CA	7:O:1022:MET:HB2	2.38	0.41
7:O:1121:ASP:HA	7:O:1124:ARG:HD2	2.02	0.41
1:A:63:ARG:O	1:A:66:PRO:HD2	2.20	0.41
2:B:79:LYS:HZ2	5:I:101:DG:P	2.43	0.41
3:C:57:TYR:OH	4:D:106:HIS:HB2	2.19	0.41
3:C:64:GLU:HA	4:D:46:HIS:HE2	1.85	0.41
5:I:10:DC:H1'	5:I:11:DC:O5'	2.21	0.41
5:I:34:DG:C5	5:I:35:DT:C4	3.08	0.41
5:I:46:DT:H73	5:I:46:DT:OP2	2.21	0.41
6:J:13:DT:C4	6:J:14:DA:N6	2.88	0.41
7:O:1093:ASP:O	7:O:1097:PRO:HG2	2.20	0.41
1:E:91:ALA:O	1:E:94:GLU:HB2	2.20	0.41
3:G:44:GLY:N	4:H:86:ILE:O	2.36	0.41
5:I:20:DA:OP2	5:I:20:DA:H2'	2.20	0.41
5:I:49:DA:H2"	5:I:50:DG:OP2	2.20	0.41
5:I:139:DA:C2	6:J:10:DA:C2	3.09	0.41
6:J:42:DT:H2"	6:J:43:DA:O5'	2.19	0.41
6:J:45:DT:H2"	6:J:46:DC:C6	2.56	0.41
6:J:86:DG:H2"	6:J:87:DT:O5'	2.21	0.41
6:J:144:DC:C4	6:J:145:DG:O6	2.74	0.41
7:O:678:ARG:HD3	7:O:948:SER:HB2	2.01	0.41
7:O:791:ALA:HB1	7:O:993:ARG:HH11	1.85	0.41
7:O:1053:MET:O	7:O:1057:LYS:HB2	2.20	0.41
7:O:1080:ASP:HA	7:O:1083:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1099:LEU:HD23	7:O:1099:LEU:HA	1.88	0.41
7:O:1241:PHE:HB3	7:O:1253:LEU:HD12	2.01	0.41
3:C:81:ARG:NE	3:C:85:LEU:HD11	2.36	0.41
3:C:93:LEU:HD23	3:C:93:LEU:HA	1.81	0.41
5:I:6:DG:C6	5:I:7:DA:C6	3.08	0.41
6:J:73:DA:C2	6:J:74:DG:C5	3.09	0.41
7:O:960:PHE:HA	7:O:972:SER:HB3	2.02	0.41
7:O:1027:LEU:HA	7:O:1030:ARG:HD3	2.03	0.41
7:O:1217:VAL:HA	7:O:1220:VAL:HG23	2.03	0.41
1:A:39:HIS:CE1	5:I:7:DA:H4'	2.55	0.41
1:A:120:MET:C	2:B:50:ILE:HD11	2.42	0.41
1:A:126:LEU:O	1:A:129:ARG:HB3	2.20	0.41
4:D:53:SER:O	4:D:56:MET:N	2.54	0.41
1:E:61:LEU:HA	1:E:61:LEU:HD23	1.74	0.41
3:G:93:LEU:HD23	3:G:93:LEU:HA	1.81	0.41
4:H:43:LYS:NZ	4:H:47:PRO:O	2.33	0.41
4:H:87:THR:H	4:H:90:GLU:CD	2.23	0.41
5:I:49:DA:H1'	5:I:50:DG:C8	2.56	0.41
5:I:59:DA:C2'	5:I:60:DA:C8	3.04	0.41
5:I:101:DG:H2"	5:I:102:DG:H8	1.85	0.41
5:I:113:DA:C4	5:I:114:DG:C8	3.08	0.41
6:J:89:DT:H2"	6:J:90:DA:OP2	2.21	0.41
6:J:92:DG:C6	6:J:93:DC:C4	3.09	0.41
6:J:113:DA:H1'	6:J:114:DC:H5'	2.03	0.41
6:J:124:DG:H2"	6:J:125:DG:H8	1.85	0.41
6:J:128:DT:OP2	6:J:128:DT:H2'	2.20	0.41
6:J:137:DG:C2	6:J:138:DG:C4	3.09	0.41
7:O:948:SER:O	7:O:951:SER:OG	2.16	0.41
7:O:1062:PRO:HB3	7:O:1085:VAL:HG21	2.03	0.41
7:O:1110:PHE:O	7:O:1163:THR:HG23	2.20	0.41
7:O:1171:ASN:HD21	7:O:1173:GLN:CD	2.24	0.41
7:O:1229:LEU:HD23	7:O:1229:LEU:HA	1.86	0.41
3:C:115:LEU:HD13	2:F:44:LYS:HB2	2.03	0.41
1:E:96:SER:O	1:E:99:TYR:HB3	2.21	0.41
5:I:25:DG:O5'	5:I:25:DG:H8	2.04	0.41
5:I:100:DG:N2	6:J:49:DC:C2	2.89	0.41
6:J:46:DC:H1'	6:J:47:DC:O5'	2.21	0.41
6:J:110:DA:C4	6:J:111:DC:C5	3.09	0.41
7:O:995:LEU:HD23	7:O:995:LEU:HA	1.84	0.41
7:O:1122:PHE:O	7:O:1125:TYR:HB3	2.21	0.41
7:O:1126:ILE:HB	7:O:1128:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1205:GLU:OE1	7:O:1289:ARG:HG2	2.21	0.41
5:I:21:DG:H2"	5:I:22:DG:C8	2.56	0.40
5:I:39:DA:N6	6:J:108:DC:C4	2.89	0.40
5:I:86:DT:H2"	5:I:87:DT:C6	2.55	0.40
6:J:31:DA:C2	6:J:32:DG:C5	3.09	0.40
6:J:134:DC:C2	6:J:135:DC:C4	3.09	0.40
7:O:751:ILE:N	7:O:784:ASN:OD1	2.54	0.40
7:O:835:PHE:CE2	7:O:870:LEU:HD22	2.56	0.40
7:O:1143:SER:HA	7:O:1146:LEU:HD12	2.02	0.40
1:A:96:SER:O	1:A:99:TYR:HB3	2.21	0.40
1:E:65:LEU:HB3	1:E:69:ARG:NH1	2.37	0.40
3:G:54:VAL:O	3:G:58:LEU:HG	2.20	0.40
5:I:37:DG:H8	5:I:37:DG:OP2	2.04	0.40
5:I:60:DA:H2"	5:I:61:DA:H8	1.85	0.40
6:J:56:DG:H1'	6:J:57:DT:C5'	2.51	0.40
7:O:767:LEU:HD12	7:O:772:ILE:HG13	2.03	0.40
7:O:828:LEU:HG	7:O:870:LEU:HD21	2.02	0.40
7:O:1143:SER:O	7:O:1146:LEU:HB2	2.21	0.40
1:A:100:LEU:O	1:A:101:VAL:C	2.60	0.40
3:C:34:LEU:HD23	3:C:34:LEU:HA	1.72	0.40
3:C:54:VAL:O	3:C:58:LEU:HG	2.20	0.40
4:D:43:LYS:O	4:D:47:PRO:HG3	2.22	0.40
1:E:105:GLU:HG2	2:F:41:GLY:O	2.22	0.40
4:H:43:LYS:O	4:H:47:PRO:HG3	2.22	0.40
5:I:110:DC:N3	6:J:37:DG:N2	2.69	0.40
5:I:123:DC:C4	5:I:124:DA:N6	2.89	0.40
6:J:71:DA:C4	6:J:72:DC:C6	3.09	0.40
6:J:142:DC:N3	6:J:143:DT:C4	2.89	0.40
7:O:787:ASN:HB2	7:O:941:VAL:HG13	2.04	0.40
7:O:813:LYS:HB3	7:O:815:ILE:HG13	2.03	0.40
7:O:929:ASN:CG	7:O:1231:ILE:HG22	2.42	0.40
7:O:988:ARG:HA	7:O:1242:ASP:OD1	2.22	0.40
7:O:1184:ASP:OD1	7:O:1190:ASP:HB2	2.21	0.40
7:O:1339:GLU:HA	7:O:1342:SER:OG	2.20	0.40
2:B:50:ILE:O	2:B:51:TYR:C	2.60	0.40
1:E:130:ILE:HD13	1:E:130:ILE:HA	1.73	0.40
4:H:53:SER:O	4:H:56:MET:N	2.54	0.40
5:I:23:DC:H6	5:I:23:DC:O5'	2.03	0.40
5:I:102:DG:C2'	5:I:103:DA:C8	3.04	0.40
5:I:110:DC:C4	6:J:37:DG:N1	2.90	0.40
6:J:60:DA:H2"	6:J:61:DA:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:134:DC:C4	6:J:135:DC:N4	2.89	0.40
7:O:770:TYR:CE1	7:O:771:GLN:HG3	2.56	0.40
7:O:775:LEU:O	7:O:779:VAL:HG23	2.21	0.40
7:O:1148:LEU:HA	7:O:1148:LEU:HD23	1.87	0.40
7:O:1173:GLN:HG2	7:O:1197:ALA:O	2.21	0.40
1:A:103:LEU:HD12	1:A:103:LEU:HA	1.75	0.40
1:E:100:LEU:O	1:E:103:LEU:N	2.55	0.40
3:G:14:ALA:CB	5:I:32:DT:H5"	2.51	0.40
3:G:29:ARG:HG3	3:G:32:ARG:NH2	2.36	0.40
6:J:128:DT:C4'	6:J:129:DC:H5'	2.51	0.40
7:O:678:ARG:CZ	7:O:952:PHE:CE2	3.04	0.40
7:O:758:GLN:HB2	7:O:762:LEU:HD22	2.04	0.40
7:O:884:SER:HB3	7:O:913:HIS:CD2	2.56	0.40
7:O:935:TRP:N	7:O:935:TRP:CD1	2.87	0.40
7:O:981:ARG:NE	7:O:1238:ALA:HB2	2.37	0.40
7:O:1117:ASP:HA	7:O:1132:ARG:NH1	2.36	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	96/135 (71%)	88 (92%)	8 (8%)	0	100	100
1	E	93/135 (69%)	85 (91%)	8 (9%)	0	100	100
2	B	85/102 (83%)	69 (81%)	15 (18%)	1 (1%)	13	50
2	F	84/102 (82%)	81 (96%)	3 (4%)	0	100	100
3	C	105/129 (81%)	99 (94%)	6 (6%)	0	100	100
3	G	105/129 (81%)	99 (94%)	6 (6%)	0	100	100
4	D	91/122 (75%)	83 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	91/122 (75%)	83 (91%)	8 (9%)	0	100	100
7	O	569/735 (77%)	483 (85%)	81 (14%)	5 (1%)	17	56
All	All	1319/1711 (77%)	1170 (89%)	143 (11%)	6 (0%)	32	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	26	ILE
7	O	1163	THR
7	O	958	THR
7	O	979	VAL
7	O	679	ILE
7	O	1220	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/110 (76%)	84 (100%)	0	100	100
1	E	82/110 (74%)	82 (100%)	0	100	100
2	B	72/78 (92%)	72 (100%)	0	100	100
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	82/101 (81%)	82 (100%)	0	100	100
4	D	77/102 (76%)	77 (100%)	0	100	100
4	H	79/102 (78%)	79 (100%)	0	100	100
7	O	525/667 (79%)	525 (100%)	0	100	100
All	All	1149/1449 (79%)	1149 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	GLN
3	C	38	ASN
3	C	84	GLN
4	D	79	HIS
1	E	68	GLN
2	F	93	GLN
3	G	38	ASN
3	G	84	GLN
4	H	79	HIS
7	O	749	HIS
7	O	784	ASN
7	O	801	GLN
7	O	928	GLN
7	O	929	ASN
7	O	939	ASN
7	O	1025	GLN
7	O	1051	GLN
7	O	1054	GLN
7	O	1111	GLN
7	O	1171	ASN
7	O	1198	HIS
7	O	1237	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

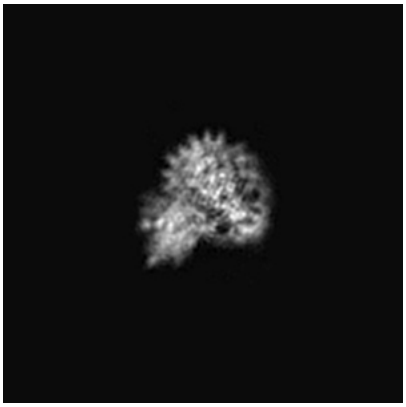
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6700. These allow visual inspection of the internal detail of the map and identification of artifacts.

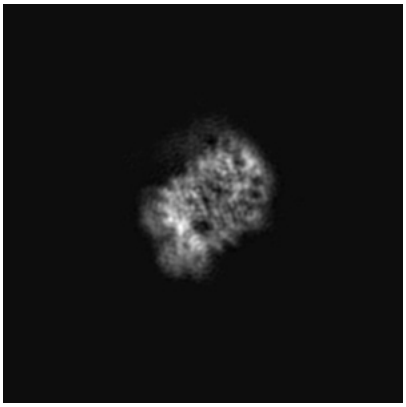
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

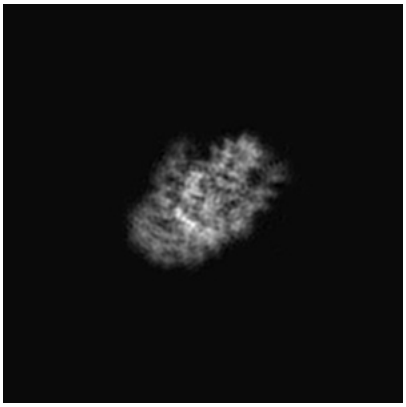
6.1.1 Primary map



X



Y

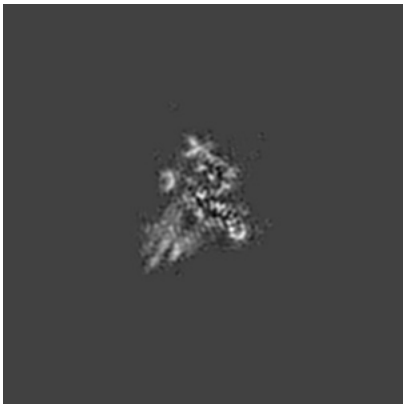


Z

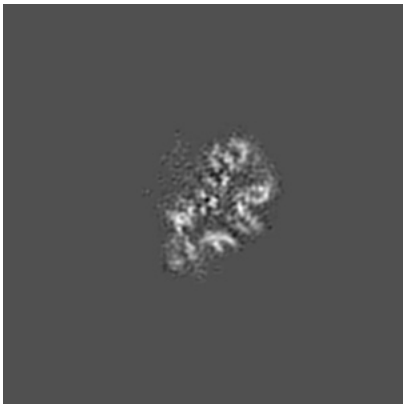
The images above show the map projected in three orthogonal directions.

6.2 Central slices

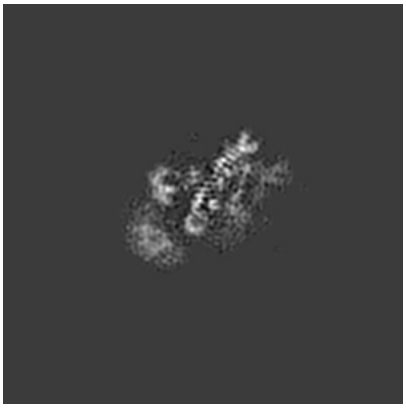
6.2.1 Primary map



X Index: 128



Y Index: 128

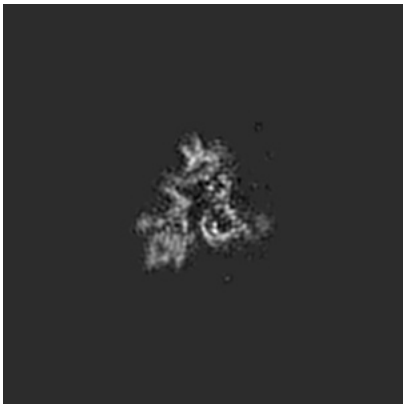


Z Index: 128

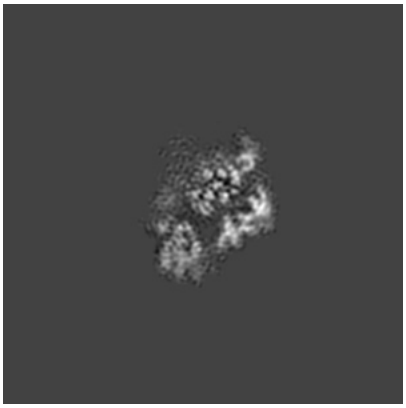
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

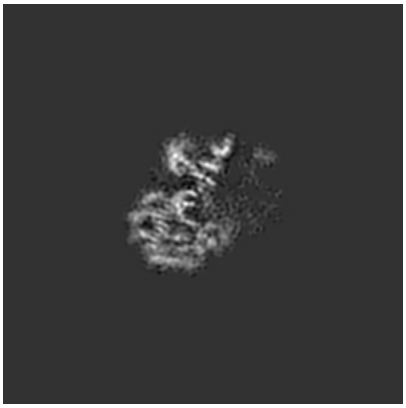
6.3.1 Primary map



X Index: 118



Y Index: 122

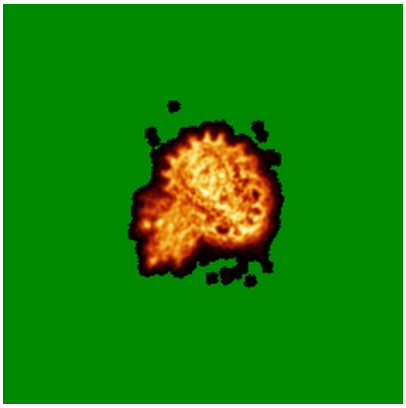


Z Index: 113

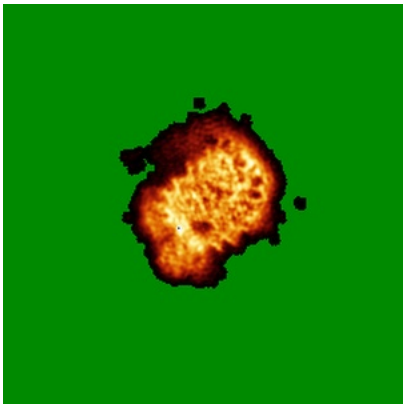
The images above show the largest variance slices of the map in three orthogonal directions.

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

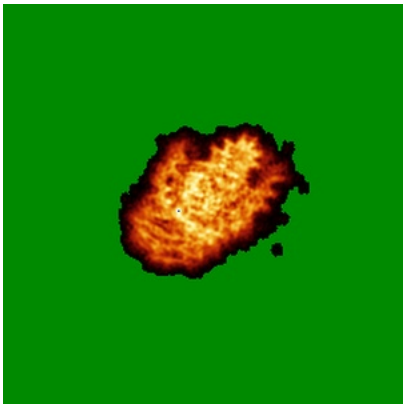
6.4.1 Primary map



X



Y



Z

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 0.0341. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

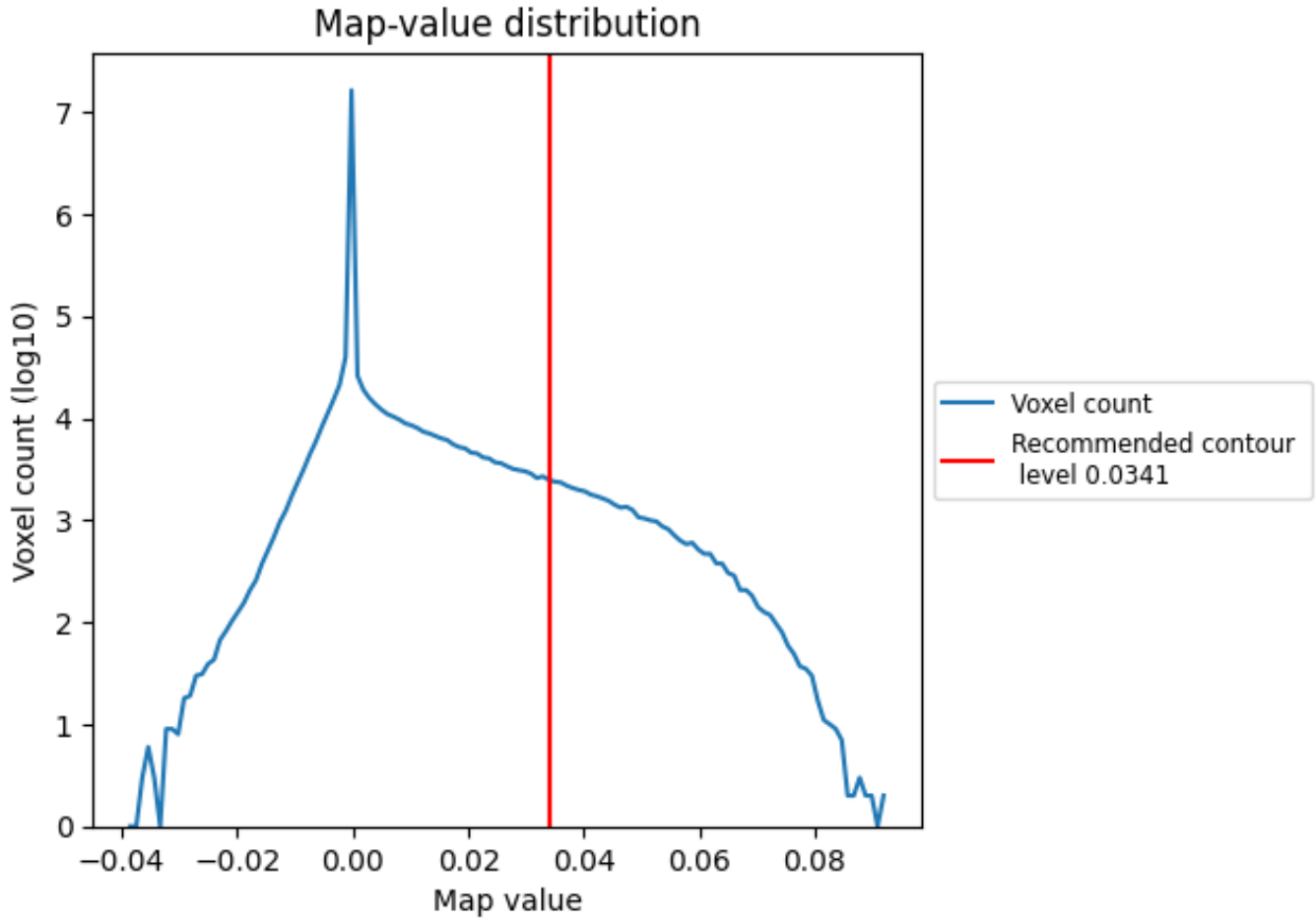
6.6 Mask visualisation (i)

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

7 Map analysis

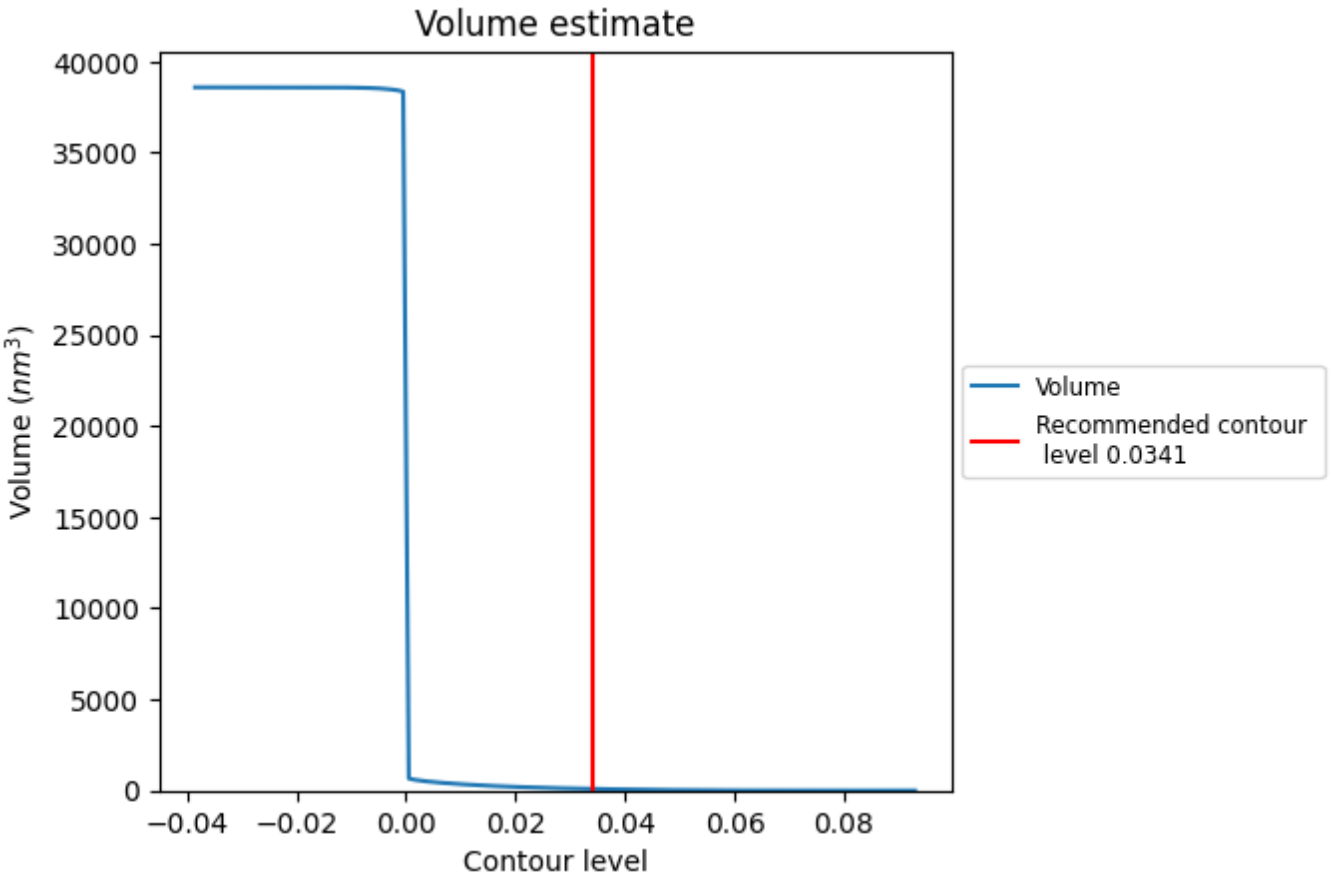
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

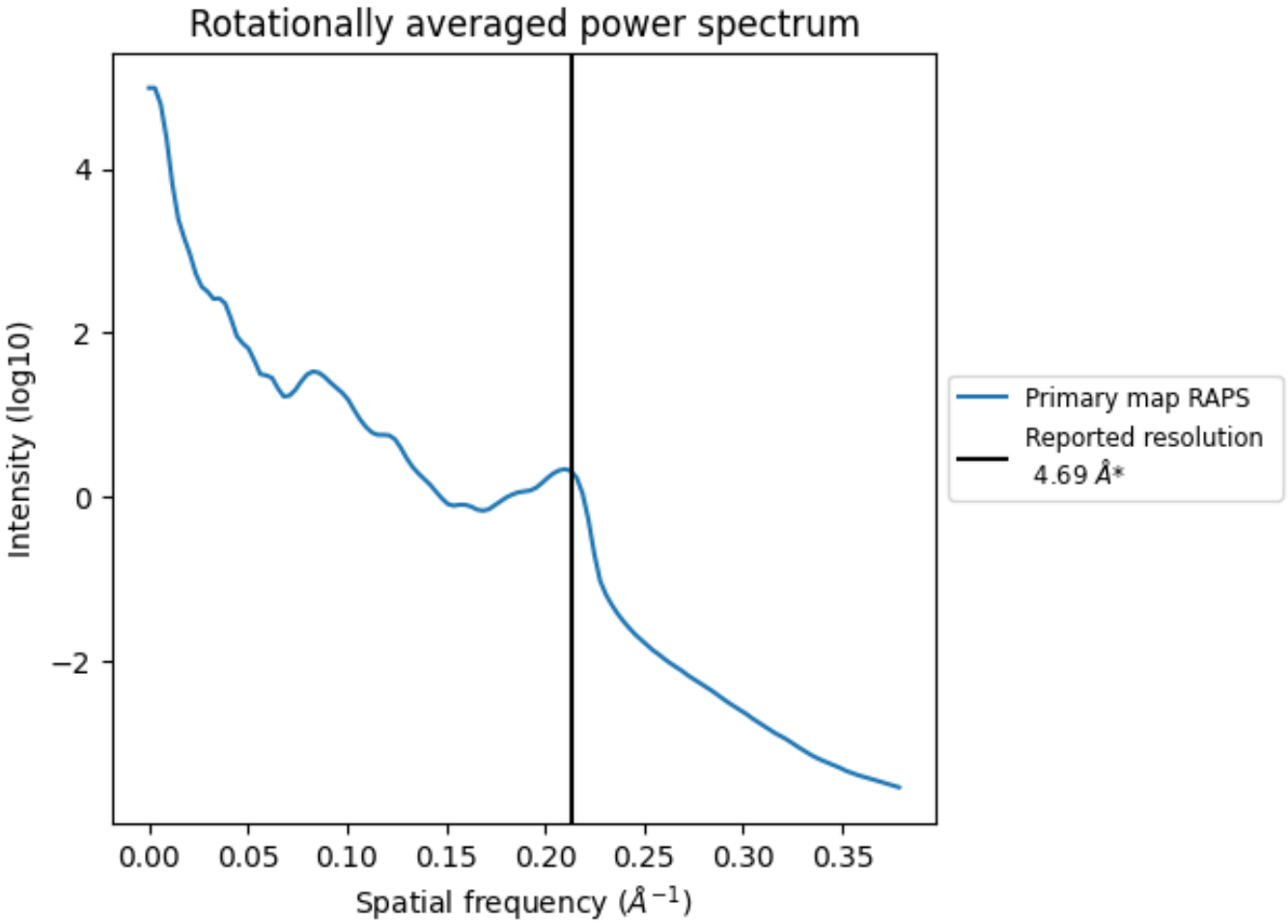
7.2 Volume estimate



The volume at the recommended contour level is 91 nm^3; this corresponds to an approximate mass of 82 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 0.213 Å^{-1}

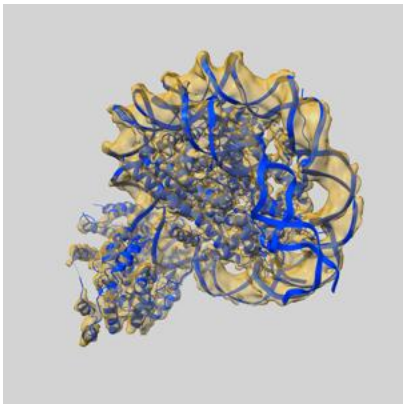
8 Fourier-Shell correlation

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

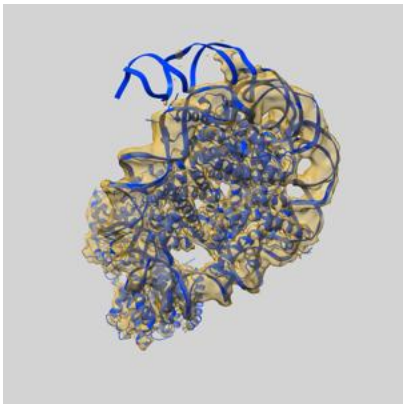
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6700 and PDB model 5X0Y. Per-residue inclusion information can be found in section 3 on page 6.

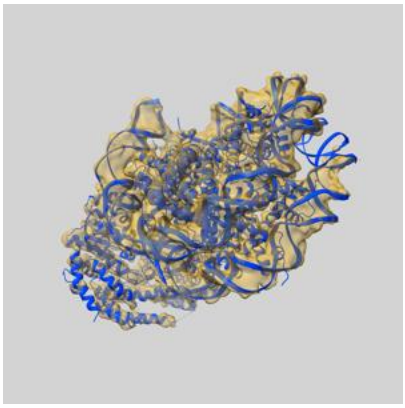
9.1 Map-model overlay



X



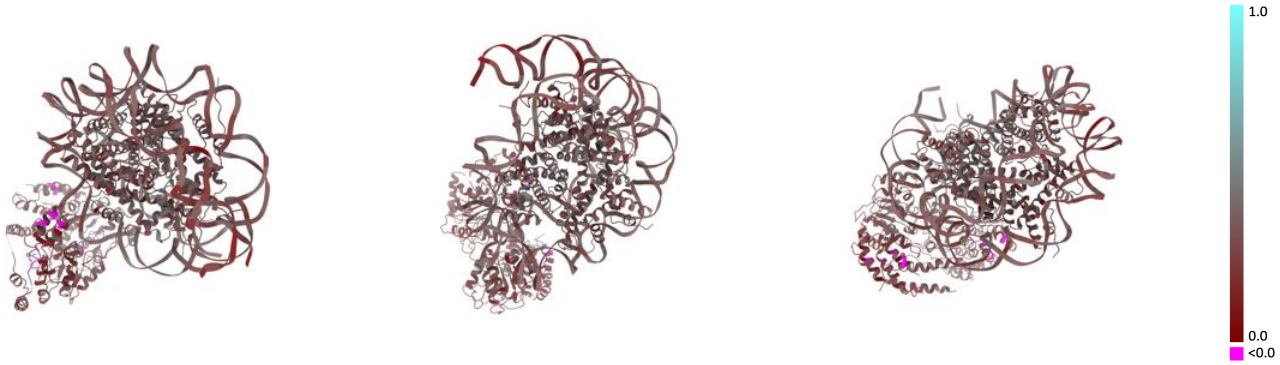
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0341 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.

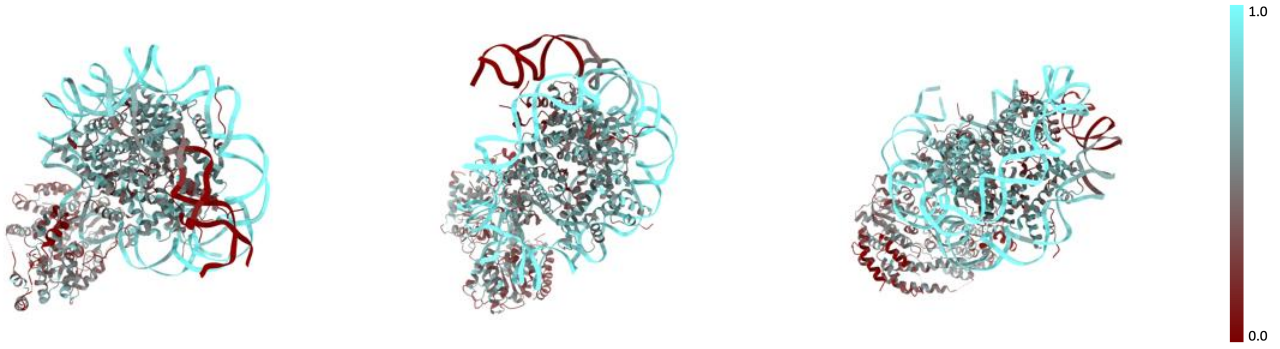
9.2 Q-score mapped to coordinate model (i)



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.

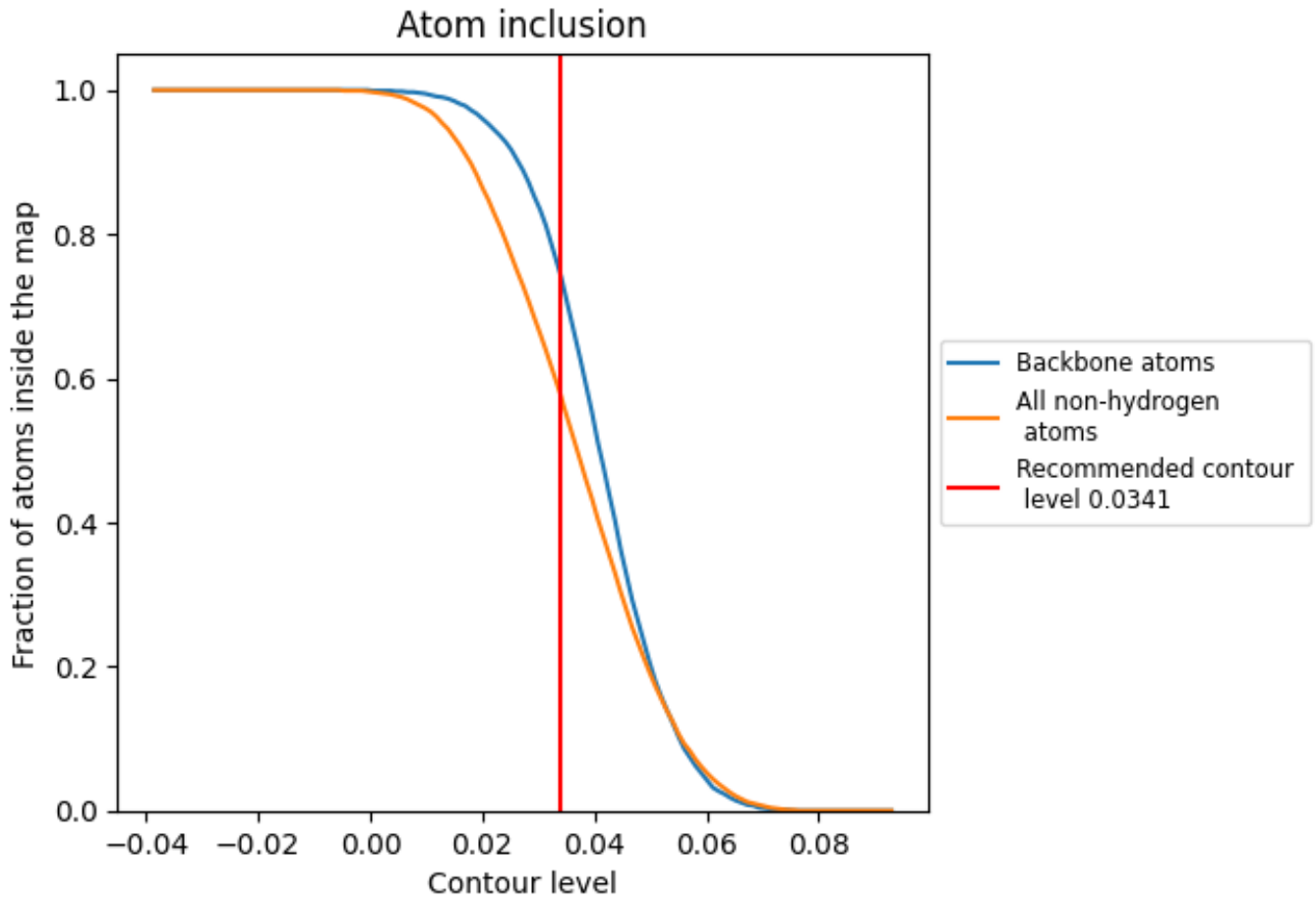
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0341).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 57% 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 (0.0341) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5740	0.3150
A	0.5320	0.3630
B	0.5200	0.3700
C	0.4380	0.3190
D	0.5490	0.3320
E	0.5070	0.3590
F	0.5290	0.3620
G	0.5440	0.3520
H	0.6010	0.3590
I	0.7780	0.3240
J	0.7810	0.3270
O	0.3690	0.2570