Full wwPDB EM Validation Report ⓘ

Jul 11, 2024 – 12:14 PM JST

PDB ID	:	8XOM
EMDB ID	:	EMD-38534
Title	:	Cryo-EM structure of human ABCC4 in complex with ANP-bound in NBD1 and METHOTREXATE
Authors	:	Zhang, P.F.; Liu, Z.
Deposited on	:	2024-01-01
Resolution	:	3.05 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:

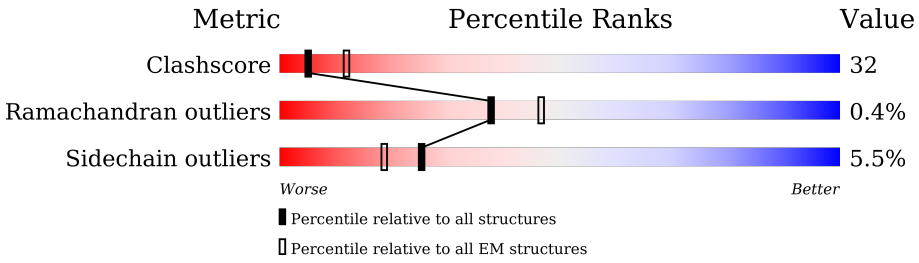
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 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	1325	7%, 46%, 39%, 5%, 10%

2 Entry composition

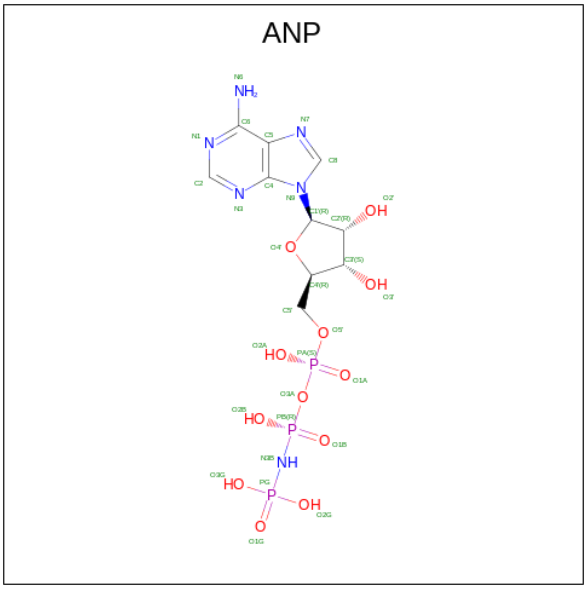
There are 6 unique types of molecules in this entry. The entry contains 10150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-binding cassette sub-family C member 4.

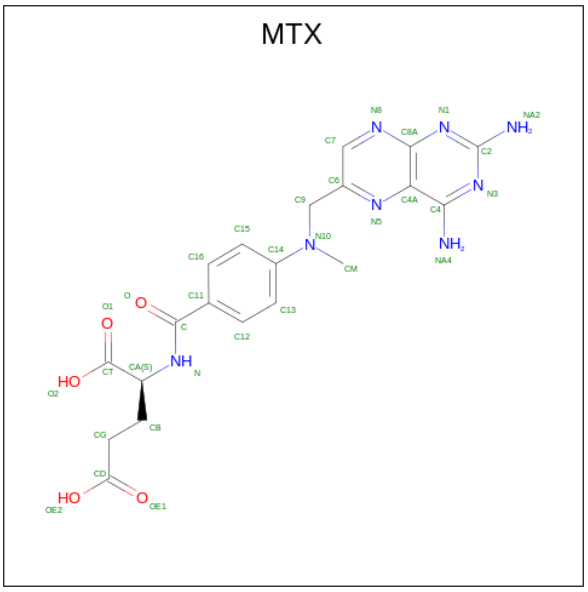
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1197	9549	6197	1608	1701	43	1	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



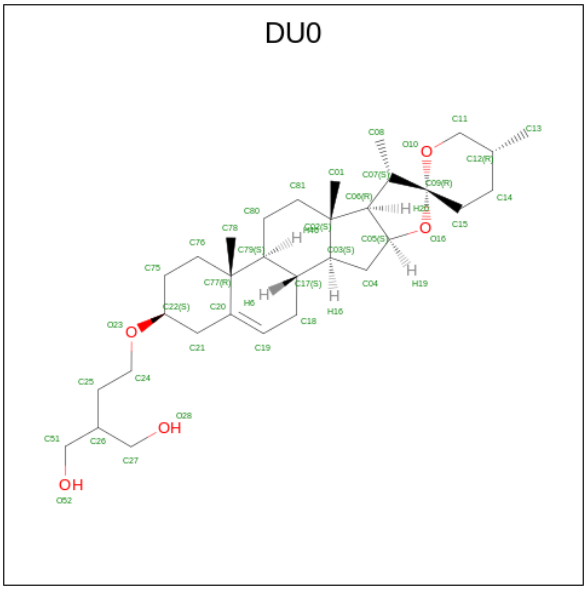
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	6	12	3	0

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			33	20	8	5	

- Molecule 4 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]icos-18-ene-6 ,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (three-letter code: DU0) (formula: $C_{32}H_{52}O_5$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O		0
			37	32	5		
4	A	1	Total	C	O		0
			37	32	5		

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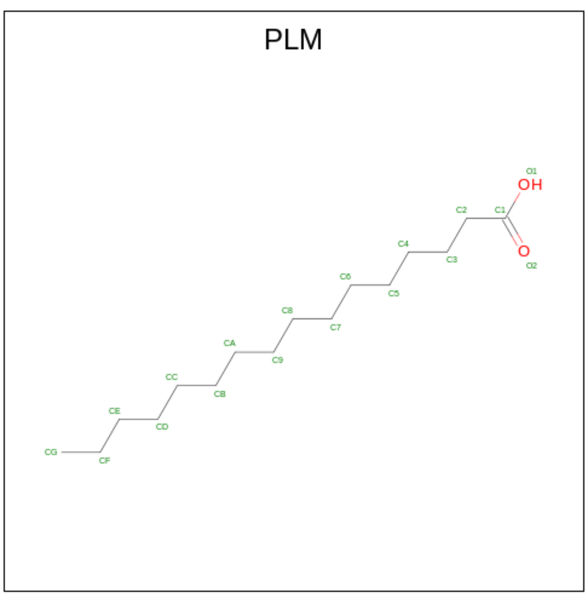
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0
4	A	1	Total C O 37 32 5	0

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			18	16	2	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

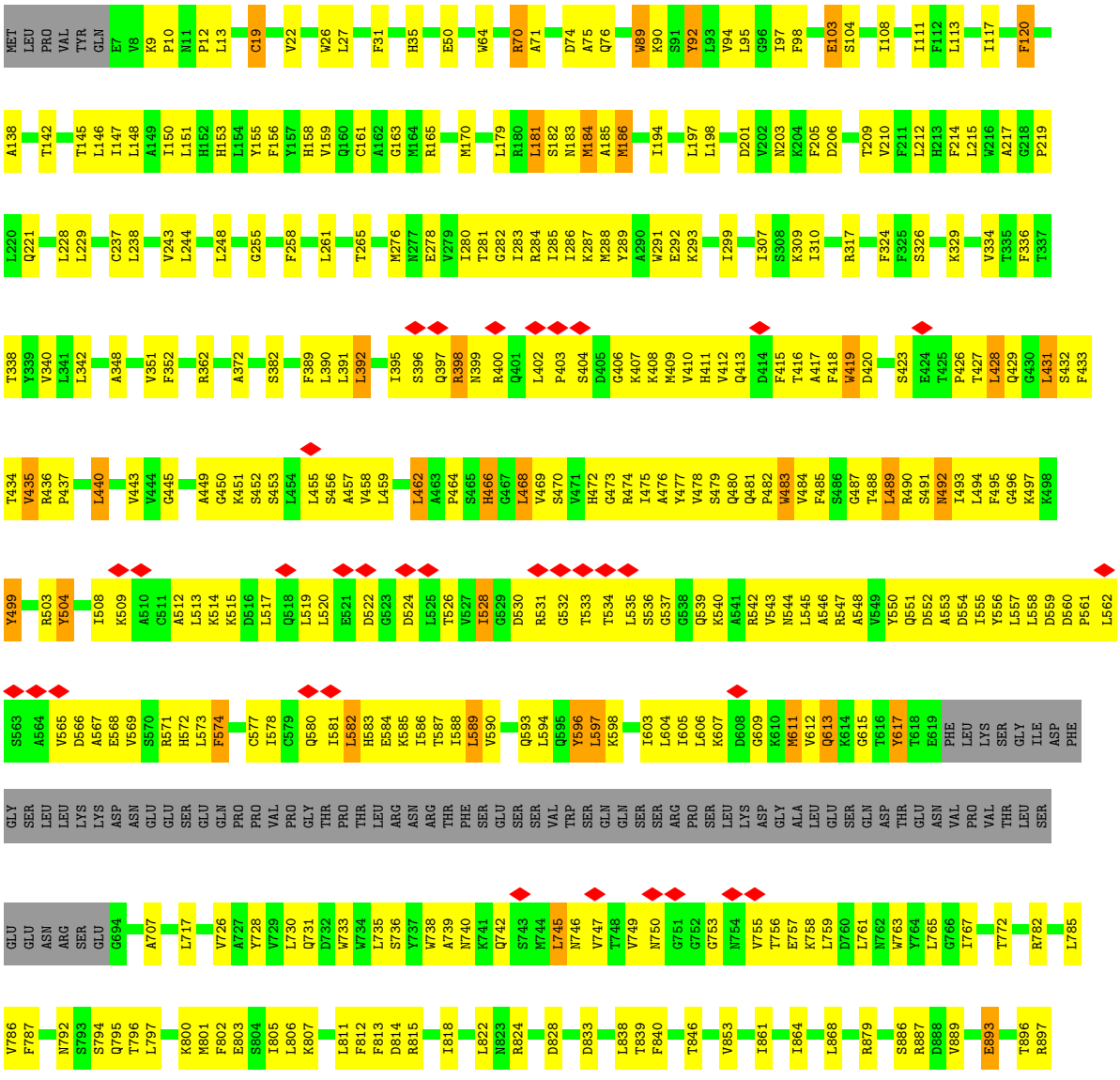
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	

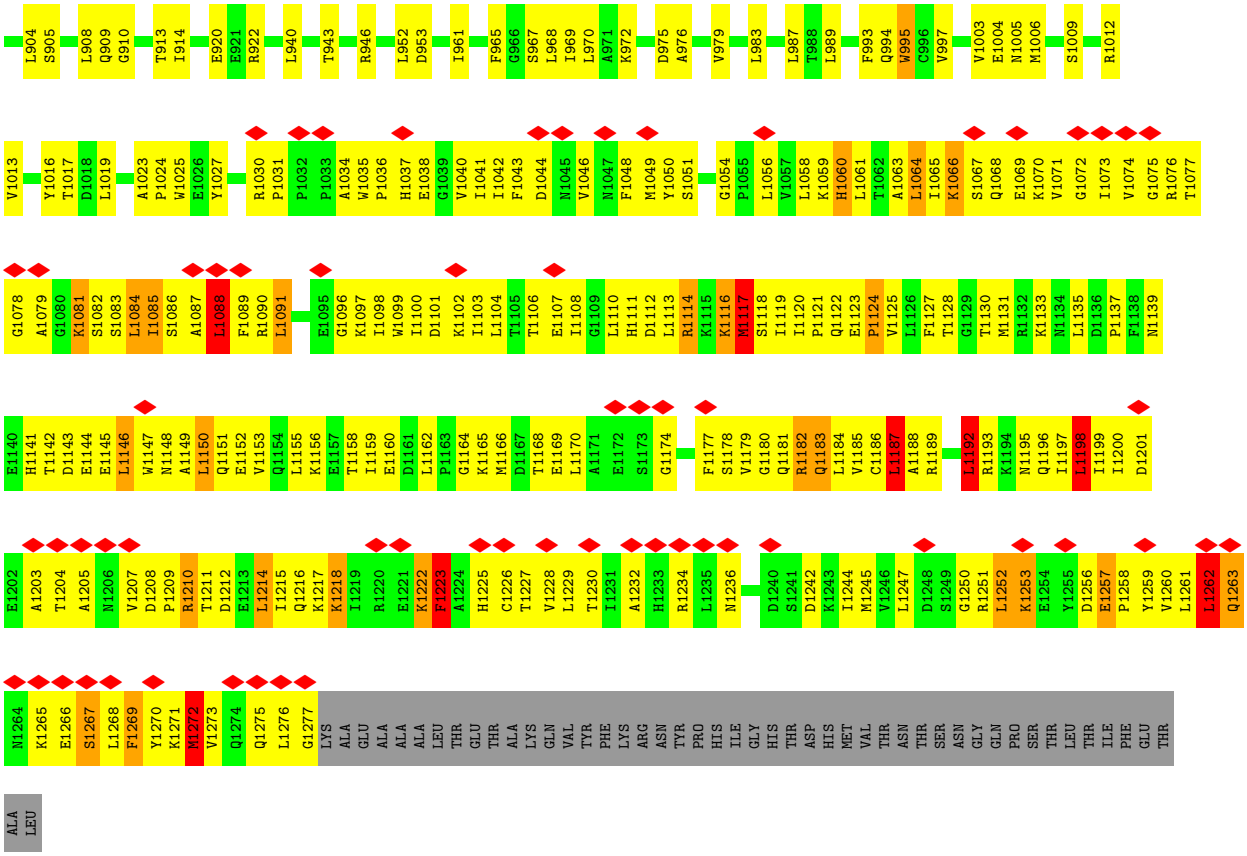
3 Residue-property plots (i)

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: ATP-binding cassette sub-family C member 4

Chain A:




L904 S905 L908 Q909 G910 T913 I914 E920 E921 R922 L940 T943 R946 L952 D953 I961 F965 G966 S967 L968 I969 L970 A971 K972 D975 A976 V979 L983 L987 T988 L989 F993 Q994 W995 C996 V997 V1003 E1004 N1005 M1006 S1009 R1012
V1013 Y1016 T1017 D1018 L1019 A1023 P1024 W1025 E1026 Y1027 R1030 P1031 P1032 P1033 A1034 W1035 P1036 H1037 E1038 G1039 V1040 I1041 I1042 F1043 D1044 N1045 V1046 N1047 F1048 M1049 Y1050 S1051 G1054 P1055 L1056 V1057 L1058 K1059 H1060 L1061 T1062 A1063 L1064 I1065 K1066 S1067 Q1068 E1069 K1070 V1071 G1072 I1073 V1074 G1075 R1076 T1077
G1078 A1079 G1080 K1081 S1082 S1083 L1084 I1085 S1086 A1087 L1088 F1089 R1090 L1091 E1095 G1096 K1097 I1098 W1099 I1100 D1101 K1102 I1103 L1104 T1105 T1106 E1107 I1108 G1109 L1110 H1111 D1112 L1113 R1114 K1115 K1116 M1117 S1118 I1119 I1120 P1121 Q1122 E1123 P1124 V1125 L1126 F1127 T1128 G1129 T1130 M1131 R1132 K1133 N1134 L1135 D1136 P1137 F1138 N1139
E1140 H1141 T1142 D1143 E1144 E1145 L1146 W1147 N1148 A1149 L1150 Q1151 E1152 V1153 Q1154 L1155 K1156 E1157 T1158 I1159 E1160 D1161 L1162 P1163 G1164 K1165 M1166 D1167 T1168 E1169 L1170 A1171 E1172 S1173 G1174 F1177 S1178 V1179 G1180 Q1181 R1182 Q1183 L1184 V1185 C1186 L1187 A1188 R1189 L1192 R1193 K1194 N1195 Q1196 I1197 L1198 I1199 I1200 D1201
E1202 A1203 T1204 A1205 N1206 V1207 D1208 P1209 R1210 T1211 D1212 E1213 L1214 I1215 Q1216 K1217 K1218 I1219 R1220 E1221 K1222 F1223 A1224 H1225 C1226 T1227 V1228 L1229 T1230 I1231 A1232 H1233 R1234 L1235 N1236 D1240 S1241 D1242 K1243 I1244 M1245 V1246 L1247 D1248 S1249 G1250 R1251 L1252 K1253 E1254 Y1255 D1256 E1257 P1258 Y1259 V1260 L1261 L1262 Q1263
N1264 K1265 E1266 S1267 L1268 F1269 Y1270 K1271 M1272 V1273 Q1274 Q1275 L1276 G1277 LYS ALA GLU ALA ALA ALA LEU THR GLU THR ALA LYS GLN VAL TYR PHE LYS ARG ASN TYR PRO HIS ILE GLY HIS THR ASP HIS MET VAL THR ASN THR SER ASN GLY GLN PRO SER THR LEU THR ILE PHE GLU THR
ALA LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1283813	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.194	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0505	Depositor
Map size (Å)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MG, PLM, MTX, DU0

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	0.37	0/9757	0.83	34/13227 (0.3%)

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	5

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1198	LEU	CA-CB-CG	11.58	141.94	115.30
1	A	1146	LEU	CA-CB-CG	9.52	137.19	115.30
1	A	597	LEU	CA-CB-CG	9.48	137.11	115.30
1	A	589	LEU	CA-CB-CG	8.74	135.40	115.30
1	A	1272	MET	CA-CB-CG	8.68	128.05	113.30
1	A	435	VAL	C-N-CA	8.54	143.04	121.70
1	A	1187	LEU	CA-CB-CG	8.41	134.63	115.30
1	A	468	LEU	CA-CB-CG	7.78	133.19	115.30
1	A	1091	LEU	CA-CB-CG	7.28	132.04	115.30
1	A	582	LEU	CA-CB-CG	7.08	131.57	115.30
1	A	1064	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	1084	LEU	CB-CG-CD1	-6.78	99.47	111.00
1	A	1150	LEU	CA-CB-CG	6.72	130.75	115.30
1	A	428	LEU	CA-CB-CG	6.56	130.39	115.30
1	A	1222	LYS	C-N-CA	-6.37	105.77	121.70
1	A	1192	LEU	CA-CB-CG	6.17	129.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	745	LEU	CA-CB-CG	6.10	129.32	115.30
1	A	1223	PHE	N-CA-CB	6.09	121.56	110.60
1	A	1085	ILE	CG1-CB-CG2	5.91	124.39	111.40
1	A	1262	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	489	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	1114	ARG	CA-CB-CG	5.68	125.91	113.40
1	A	528	ILE	CG1-CB-CG2	-5.50	99.30	111.40
1	A	431	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	440	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	1214	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	462	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	1218	LYS	CA-CB-CG	5.21	124.86	113.40
1	A	1088	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	181	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	1117	MET	CA-CB-CG	5.13	122.02	113.30
1	A	13	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	392	LEU	CA-CB-CG	5.02	126.86	115.30
1	A	1252	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	LEU	Mainchain
1	A	150	ILE	Mainchain
1	A	219	PRO	Mainchain
1	A	396	SER	Peptide
1	A	893	GLU	Mainchain

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	9549	0	9801	649	0
2	A	31	0	13	2	0
3	A	33	0	19	2	0
4	A	518	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	18	0	31	1	0
6	A	1	0	0	0	0
All	All	10150	0	9864	649	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 32.

All (649) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:VAL:O	1:A:432:SER:HA	1.35	1.24
1:A:1066:LYS:HG3	1:A:1069:GLU:HG3	1.41	0.99
1:A:490:ARG:O	1:A:494:LEU:HB2	1.65	0.96
1:A:1082:SER:HA	1:A:1085:ILE:HD12	1.50	0.94
1:A:98:PHE:HZ	1:A:151:LEU:HB3	1.35	0.92
1:A:1124:PRO:HG2	1:A:1182:ARG:HG3	1.51	0.90
1:A:457:ALA:HA	1:A:462:LEU:HD11	1.54	0.89
1:A:594:LEU:HA	1:A:597:LEU:HG	1.53	0.89
1:A:1041:ILE:HD11	1:A:1098:ILE:HG22	1.55	0.89
1:A:1041:ILE:HA	1:A:1099:TRP:O	1.72	0.89
1:A:1025:TRP:HA	1:A:1110:LEU:HB2	1.53	0.89
1:A:1085:ILE:O	1:A:1090:ARG:N	2.08	0.86
1:A:1253:LYS:NZ	1:A:1267:SER:OG	2.09	0.85
1:A:409:MET:HA	1:A:435:VAL:O	1.79	0.83
1:A:285:ILE:HD11	1:A:1121:PRO:HB3	1.61	0.83
1:A:975:ASP:OD1	1:A:976:ALA:N	2.11	0.83
1:A:1118:SER:O	1:A:1198:LEU:HA	1.77	0.83
1:A:455:LEU:HA	1:A:557:LEU:HD12	1.62	0.82
1:A:1043:PHE:HB2	1:A:1061:LEU:O	1.80	0.81
1:A:1075:GLY:H	1:A:1084:LEU:HD11	1.45	0.81
1:A:415:PHE:CE1	1:A:417:ALA:HB3	2.16	0.80
1:A:1070:LYS:HZ3	1:A:1196:GLN:HA	1.47	0.80
1:A:577:CYS:O	1:A:582:LEU:N	2.15	0.79
1:A:740:ASN:ND2	1:A:975:ASP:OD2	2.14	0.79
1:A:412:VAL:O	1:A:432:SER:CA	2.26	0.79
1:A:1086:SER:HA	1:A:1090:ARG:HA	1.64	0.79
1:A:801:MET:HE3	1:A:1013:VAL:HG13	1.63	0.78
1:A:329:LYS:NZ	1:A:728:TYR:O	2.17	0.78
1:A:455:LEU:HD11	1:A:559:ASP:HB2	1.66	0.78
1:A:547:ARG:O	1:A:551:GLN:HB3	1.84	0.77
1:A:1116:LYS:HE3	1:A:1196:GLN:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:CYS:HA	1:A:581:ILE:HB	1.65	0.77
1:A:560:ASP:HB3	1:A:590:VAL:HG13	1.66	0.77
1:A:1200:ILE:HD12	1:A:1204:THR:HB	1.67	0.77
1:A:1223:PHE:O	1:A:1226:CYS:N	2.18	0.76
1:A:1146:LEU:O	1:A:1150:LEU:HD12	1.86	0.76
1:A:1085:ILE:HG23	1:A:1089:PHE:CB	2.15	0.76
1:A:573:LEU:O	1:A:578:ILE:N	2.17	0.76
1:A:201:ASP:O	1:A:382:SER:OG	2.02	0.76
1:A:1035:TRP:O	1:A:1037:HIS:N	2.18	0.75
1:A:398:ARG:NH1	1:A:459:LEU:O	2.20	0.75
1:A:407:LYS:O	1:A:472:HIS:HB2	1.86	0.75
1:A:1078:GLY:HA2	1:A:1081:LYS:HE3	1.69	0.75
1:A:520:LEU:HD22	1:A:526:THR:HG21	1.67	0.74
1:A:1036:PRO:CG	1:A:1116:LYS:HG2	2.17	0.74
1:A:1088:LEU:HA	1:A:1113:LEU:HD11	1.69	0.74
1:A:738:TRP:O	1:A:742:GLN:HB3	1.88	0.73
1:A:512:ALA:O	1:A:542:ARG:NH2	2.21	0.73
1:A:578:ILE:HD13	1:A:582:LEU:HD13	1.71	0.73
1:A:411:HIS:ND1	1:A:434:THR:OG1	2.21	0.73
1:A:490:ARG:NH1	1:A:524:ASP:O	2.23	0.72
1:A:1048:PHE:HB2	1:A:1058:LEU:HG	1.71	0.72
1:A:508:ILE:HD13	1:A:513:LEU:HD12	1.73	0.71
1:A:182:SER:HB2	1:A:395:ILE:HA	1.73	0.71
1:A:1188:ALA:O	1:A:1192:LEU:HD12	1.91	0.71
1:A:1120:ILE:HD12	1:A:1121:PRO:HD2	1.73	0.71
1:A:443:VAL:HG23	1:A:604:LEU:HB2	1.73	0.71
1:A:1205:ALA:HB2	1:A:1232:ALA:HB1	1.71	0.71
1:A:98:PHE:CZ	1:A:151:LEU:HB3	2.22	0.70
1:A:409:MET:O	1:A:470:SER:OG	2.10	0.70
1:A:1074:VAL:HG22	1:A:1229:LEU:HD23	1.72	0.70
1:A:1088:LEU:HG	1:A:1117:MET:HG3	1.73	0.70
1:A:528:ILE:HG13	1:A:532:GLY:HA2	1.73	0.69
1:A:1116:LYS:CE	1:A:1196:GLN:H	2.06	0.69
1:A:198:LEU:HD22	1:A:904:LEU:HD22	1.74	0.69
1:A:287:LYS:HA	1:A:292:GLU:OE2	1.93	0.69
1:A:481:GLN:NE2	1:A:482:PRO:O	2.26	0.69
1:A:1085:ILE:O	1:A:1089:PHE:N	2.25	0.69
1:A:1218:LYS:HD2	1:A:1222:LYS:HB3	1.75	0.69
1:A:530:ASP:OD2	1:A:531:ARG:NH1	2.26	0.69
1:A:742:GLN:HA	1:A:745:LEU:HB3	1.75	0.69
1:A:410:VAL:HG22	1:A:435:VAL:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:THR:HG21	1:A:1230:THR:HB	1.74	0.69
1:A:474:ARG:H	1:A:554:ASP:HB2	1.58	0.68
1:A:1077:THR:O	1:A:1081:LYS:HG3	1.94	0.68
1:A:284:ARG:NH2	1:A:814:ASP:OD1	2.27	0.67
1:A:1118:SER:OG	1:A:1197:ILE:O	2.12	0.67
1:A:194:ILE:HG22	1:A:904:LEU:HD21	1.75	0.67
1:A:494:LEU:HA	1:A:550:TYR:HE2	1.58	0.67
1:A:1089:PHE:CD1	1:A:1117:MET:HG2	2.30	0.67
1:A:1160:GLU:OE2	1:A:1165:LYS:NZ	2.25	0.67
1:A:1090:ARG:HB3	1:A:1114:ARG:NE	2.10	0.66
1:A:1185:VAL:HG22	1:A:1189:ARG:HH21	1.59	0.66
1:A:504:TYR:CE1	1:A:508:ILE:HD11	2.30	0.66
1:A:1085:ILE:CG2	1:A:1091:LEU:HB3	2.26	0.66
1:A:504:TYR:O	1:A:508:ILE:HG12	1.94	0.66
1:A:1119:ILE:HD12	1:A:1199:ILE:O	1.96	0.66
1:A:1142:THR:OG1	1:A:1144:GLU:OE2	2.12	0.66
1:A:1082:SER:HA	1:A:1085:ILE:CD1	2.25	0.66
1:A:458:VAL:HG11	1:A:475:ILE:HG21	1.78	0.65
1:A:27:LEU:HD22	1:A:943:THR:HG22	1.77	0.65
1:A:1184:LEU:O	1:A:1187:LEU:HD12	1.96	0.65
1:A:811:LEU:HD21	1:A:815:ARG:HH21	1.61	0.65
1:A:794:SER:OG	1:A:833:ASP:OD1	2.11	0.65
1:A:1013:VAL:O	1:A:1017:THR:OG1	2.15	0.65
1:A:1089:PHE:O	1:A:1114:ARG:NH1	2.29	0.65
1:A:1263:GLN:OE1	1:A:1263:GLN:N	2.20	0.65
1:A:731:GLN:HE21	1:A:772:THR:HB	1.60	0.64
1:A:1186:CYS:O	1:A:1189:ARG:HG2	1.97	0.64
1:A:449:ALA:HA	2:A:1401:ANP:H4'	1.79	0.64
1:A:920:GLU:OE1	1:A:920:GLU:N	2.28	0.64
1:A:1155:LEU:HD21	1:A:1184:LEU:HB3	1.78	0.64
1:A:738:TRP:O	1:A:742:GLN:CB	2.45	0.64
1:A:1036:PRO:HG2	1:A:1116:LYS:HG2	1.80	0.64
1:A:485:PHE:O	1:A:492:ASN:ND2	2.30	0.64
1:A:289:TYR:O	1:A:1193:ARG:NH2	2.31	0.64
1:A:1215:ILE:HA	1:A:1218:LYS:HG2	1.80	0.64
1:A:568:GLU:O	1:A:572:HIS:ND1	2.32	0.63
1:A:1117:MET:SD	1:A:1117:MET:N	2.71	0.63
1:A:420:ASP:OD2	1:A:423:SER:HB3	1.98	0.63
1:A:761:LEU:O	1:A:765:LEU:HB2	1.98	0.63
1:A:1048:PHE:CE2	1:A:1079:ALA:HB1	2.33	0.63
1:A:147:ILE:O	1:A:151:LEU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ILE:O	1:A:1103:ILE:HG12	1.99	0.63
1:A:431:LEU:HD13	1:A:611:MET:HB2	1.81	0.62
1:A:1244:ILE:HG12	1:A:1269:PHE:HE1	1.64	0.62
1:A:558:LEU:HB3	1:A:561:PRO:HG2	1.81	0.62
1:A:995:TRP:CD1	3:A:1402:MTX:H92	2.35	0.62
1:A:229:LEU:HB3	1:A:237:CYS:HB2	1.80	0.62
1:A:418:PHE:CZ	1:A:426:PRO:HA	2.34	0.62
1:A:404:SER:HA	1:A:472:HIS:HB3	1.81	0.62
1:A:556:TYR:HB3	1:A:558:LEU:HD11	1.81	0.62
1:A:1218:LYS:O	1:A:1223:PHE:N	2.33	0.62
1:A:1247:LEU:HD12	1:A:1250:GLY:HA2	1.81	0.62
1:A:1272:MET:HA	1:A:1276:LEU:HD13	1.81	0.61
1:A:1144:GLU:HA	1:A:1147:TRP:HD1	1.65	0.61
1:A:1156:LYS:HZ3	1:A:1159:ILE:HD11	1.64	0.61
1:A:1209:PRO:HA	1:A:1212:ASP:OD2	2.00	0.61
1:A:351:VAL:HG21	1:A:735:LEU:HG	1.82	0.61
1:A:455:LEU:HD23	1:A:557:LEU:HB3	1.81	0.61
1:A:1180:GLY:HA2	1:A:1183:GLN:HE21	1.65	0.61
1:A:1059:LYS:HG2	1:A:1251:ARG:HD3	1.81	0.61
1:A:1085:ILE:HA	1:A:1088:LEU:HD23	1.82	0.61
1:A:415:PHE:CZ	1:A:462:LEU:HB2	2.35	0.61
1:A:1067:SER:O	1:A:1069:GLU:HG2	2.00	0.61
1:A:886:SER:O	1:A:889:VAL:HG12	2.01	0.60
1:A:1040:VAL:HG11	1:A:1102:LYS:HD3	1.83	0.60
1:A:1058:LEU:HD22	1:A:1061:LEU:HD22	1.83	0.60
1:A:1037:HIS:O	1:A:1068:GLN:HG2	2.00	0.60
1:A:487:GLY:O	1:A:528:ILE:HG22	2.00	0.60
1:A:535:LEU:HD22	1:A:539:GLN:HB3	1.82	0.60
1:A:408:LYS:NZ	1:A:584:GLU:O	2.35	0.60
1:A:1098:ILE:O	1:A:1104:LEU:HA	2.02	0.60
1:A:487:GLY:C	1:A:528:ILE:HG22	2.22	0.60
1:A:1072:GLY:O	1:A:1229:LEU:HD21	2.02	0.60
1:A:1211:THR:O	1:A:1215:ILE:HG12	2.01	0.60
1:A:95:LEU:HD11	1:A:158:HIS:HB3	1.84	0.60
1:A:1143:ASP:O	1:A:1146:LEU:HD23	2.01	0.60
1:A:746:ASN:OD1	1:A:747:VAL:N	2.34	0.59
1:A:451:LYS:N	2:A:1401:ANP:O1A	2.35	0.59
1:A:574:PHE:HZ	1:A:596:TYR:HD1	1.50	0.59
1:A:1200:ILE:HD11	1:A:1230:THR:HA	1.83	0.59
1:A:530:ASP:O	1:A:531:ARG:HG2	2.02	0.59
1:A:1025:TRP:CD2	1:A:1111:HIS:CE1	2.89	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PHE:HE1	1:A:417:ALA:HB3	1.68	0.59
1:A:445:GLY:O	1:A:451:LYS:NZ	2.34	0.59
1:A:544:ASN:OD1	1:A:547:ARG:NH1	2.36	0.59
1:A:113:LEU:HD22	1:A:987:LEU:HD12	1.85	0.59
1:A:92:TYR:OH	1:A:209:THR:O	2.21	0.59
1:A:489:LEU:HD23	1:A:526:THR:HG22	1.84	0.59
1:A:496:GLY:HA3	1:A:922:ARG:CZ	2.33	0.59
1:A:1031:PRO:HB2	1:A:1035:TRP:CD1	2.38	0.59
1:A:449:ALA:H	1:A:606:LEU:HD11	1.68	0.59
1:A:1043:PHE:HB3	1:A:1046:VAL:HG21	1.85	0.58
1:A:489:LEU:O	1:A:493:ILE:HG12	2.03	0.58
1:A:1072:GLY:C	1:A:1229:LEU:HD21	2.24	0.58
1:A:1035:TRP:HA	1:A:1037:HIS:CE1	2.39	0.58
1:A:1121:PRO:HG2	1:A:1124:PRO:HA	1.84	0.58
1:A:1198:LEU:HD21	1:A:1228:VAL:HG12	1.85	0.58
1:A:1179:VAL:O	1:A:1182:ARG:HG2	2.03	0.58
1:A:1098:ILE:O	1:A:1104:LEU:HD12	2.04	0.58
1:A:1174:GLY:O	1:A:1182:ARG:NH2	2.37	0.58
1:A:50:GLU:OE2	1:A:50:GLU:N	2.24	0.58
1:A:556:TYR:HB2	1:A:586:ILE:O	2.04	0.58
1:A:555:ILE:HG13	1:A:586:ILE:HG13	1.86	0.58
1:A:1085:ILE:HG23	1:A:1089:PHE:HB2	1.85	0.58
1:A:1085:ILE:HG22	1:A:1091:LEU:HB3	1.86	0.57
1:A:1153:VAL:HG13	1:A:1155:LEU:HD23	1.84	0.57
1:A:336:PHE:O	1:A:340:VAL:HG23	2.03	0.57
1:A:503:ARG:HE	1:A:550:TYR:HD1	1.52	0.57
1:A:558:LEU:HB3	1:A:561:PRO:CG	2.33	0.57
1:A:1048:PHE:HE2	1:A:1079:ALA:HB1	1.67	0.57
1:A:411:HIS:HA	1:A:433:PHE:O	2.05	0.57
1:A:582:LEU:HD21	1:A:587:THR:HG22	1.85	0.57
1:A:893:GLU:HA	1:A:896:THR:HG22	1.86	0.57
1:A:428:LEU:HD11	1:A:450:GLY:HA3	1.86	0.57
1:A:488:THR:HA	1:A:528:ILE:H	1.68	0.57
1:A:598:LYS:HG2	1:A:617:TYR:OH	2.04	0.57
1:A:1259:TYR:HA	1:A:1262:LEU:HG	1.84	0.57
1:A:470:SER:HB2	1:A:472:HIS:CE1	2.40	0.57
1:A:255:GLY:O	1:A:258:PHE:HB3	2.04	0.57
1:A:717:LEU:HD13	1:A:785:LEU:HD23	1.87	0.57
1:A:1079:ALA:HA	1:A:1082:SER:HB3	1.85	0.57
1:A:904:LEU:O	1:A:908:LEU:HD23	2.05	0.56
1:A:1180:GLY:O	1:A:1184:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:LEU:HD23	1:A:1227:THR:O	2.06	0.56
1:A:181:LEU:HD22	1:A:186:MET:HG2	1.87	0.56
1:A:1089:PHE:CE1	1:A:1117:MET:HG2	2.39	0.56
1:A:1149:ALA:O	1:A:1153:VAL:HG12	2.05	0.56
1:A:182:SER:HB2	1:A:395:ILE:CA	2.36	0.56
1:A:1205:ALA:HB1	1:A:1234:ARG:HG2	1.88	0.56
1:A:431:LEU:HA	1:A:611:MET:HB2	1.86	0.56
1:A:1275:GLN:HG2	1:A:1276:LEU:HD12	1.88	0.56
1:A:554:ASP:HA	1:A:585:LYS:HD2	1.87	0.56
1:A:1165:LYS:HG3	1:A:1166:MET:H	1.70	0.56
1:A:214:PHE:HA	1:A:217:ALA:HB3	1.86	0.56
1:A:756:THR:O	1:A:758:LYS:N	2.36	0.56
1:A:1005:ASN:OD1	1:A:1006:MET:N	2.38	0.56
1:A:1130:THR:HG23	1:A:1133:LYS:H	1.71	0.56
1:A:1046:VAL:HG13	1:A:1096:GLY:H	1.71	0.56
1:A:1071:VAL:C	1:A:1227:THR:HG21	2.25	0.56
1:A:1110:LEU:HD12	1:A:1114:ARG:HH21	1.71	0.56
1:A:965:PHE:O	1:A:969:ILE:HG12	2.06	0.55
1:A:1044:ASP:HB2	1:A:1097:LYS:HB3	1.88	0.55
1:A:1046:VAL:HG22	1:A:1096:GLY:HA3	1.88	0.55
1:A:95:LEU:HD13	1:A:159:VAL:HG23	1.88	0.55
1:A:582:LEU:CD2	1:A:587:THR:HG22	2.36	0.55
1:A:1156:LYS:HA	1:A:1159:ILE:HG12	1.86	0.55
1:A:593:GLN:OE1	1:A:593:GLN:N	2.34	0.55
1:A:730:LEU:HA	1:A:733:TRP:HB3	1.87	0.55
1:A:828:ASP:HB3	1:A:1009:SER:HB3	1.87	0.55
1:A:1120:ILE:CG2	1:A:1200:ILE:HG22	2.37	0.55
1:A:508:ILE:HG22	1:A:514:LYS:HG3	1.88	0.55
1:A:1272:MET:O	1:A:1277:GLY:N	2.40	0.55
1:A:587:THR:O	1:A:589:LEU:HD22	2.07	0.55
1:A:594:LEU:HD13	1:A:597:LEU:HD21	1.87	0.55
1:A:763:TRP:O	1:A:767:ILE:HD12	2.07	0.55
1:A:1208:ASP:HB2	1:A:1210:ARG:NH1	2.22	0.55
1:A:89:TRP:CD1	1:A:90:LYS:HG2	2.42	0.55
1:A:1081:LYS:O	1:A:1085:ILE:HD12	2.07	0.55
1:A:1268:LEU:HA	1:A:1271:LYS:HG2	1.87	0.55
1:A:456:SER:C	1:A:458:VAL:H	2.11	0.55
1:A:594:LEU:O	1:A:598:LYS:HG3	2.07	0.55
1:A:1038:GLU:O	1:A:1067:SER:HA	2.07	0.55
1:A:476:ALA:N	1:A:555:ILE:O	2.35	0.54
1:A:1131:MET:HB3	1:A:1166:MET:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:MET:SD	1:A:1245:MET:N	2.80	0.54
1:A:429:GLN:NE2	1:A:609:GLY:HA3	2.22	0.54
1:A:801:MET:HE1	1:A:1013:VAL:HA	1.89	0.54
1:A:1079:ALA:O	1:A:1083:SER:OG	2.21	0.54
1:A:183:ASN:OD1	1:A:183:ASN:N	2.37	0.54
1:A:428:LEU:HA	1:A:609:GLY:HA2	1.89	0.54
1:A:1085:ILE:HG21	1:A:1091:LEU:HB3	1.89	0.54
1:A:1075:GLY:N	1:A:1084:LEU:HD11	2.18	0.54
1:A:1153:VAL:O	1:A:1155:LEU:HD22	2.07	0.54
1:A:1131:MET:N	1:A:1168:THR:O	2.40	0.54
1:A:1023:ALA:HB1	1:A:1027:TYR:HE1	1.73	0.54
1:A:1257:GLU:OE2	1:A:1260:VAL:N	2.38	0.54
1:A:104:SER:O	1:A:108:ILE:HG23	2.08	0.54
1:A:161:CYS:SG	1:A:165:ARG:NH1	2.81	0.54
1:A:184:MET:SD	1:A:185:ALA:N	2.81	0.54
1:A:403:PRO:O	1:A:472:HIS:ND1	2.41	0.54
1:A:1203:ALA:O	1:A:1207:VAL:HG23	2.08	0.54
1:A:410:VAL:HB	1:A:469:VAL:HG13	1.90	0.54
1:A:573:LEU:O	1:A:578:ILE:HG12	2.08	0.54
1:A:280:ILE:HD12	1:A:822:LEU:HD13	1.90	0.53
1:A:993:PHE:O	1:A:997:VAL:HG22	2.08	0.53
1:A:244:LEU:HD21	1:A:362:ARG:HA	1.89	0.53
1:A:475:ILE:HD12	1:A:475:ILE:H	1.73	0.53
1:A:571:ARG:HA	1:A:574:PHE:CD1	2.43	0.53
1:A:1048:PHE:O	1:A:1056:LEU:HD13	2.08	0.53
1:A:1089:PHE:CZ	1:A:1119:ILE:HB	2.44	0.53
1:A:482:PRO:HB2	1:A:540:LYS:HB2	1.89	0.53
1:A:1142:THR:O	1:A:1145:GLU:HB2	2.09	0.53
1:A:1087:ALA:O	1:A:1113:LEU:HD11	2.09	0.53
1:A:307:ILE:HD12	1:A:310:ILE:HG21	1.90	0.53
1:A:450:GLY:H	1:A:606:LEU:HD11	1.72	0.53
1:A:550:TYR:C	1:A:552:ASP:H	2.11	0.53
1:A:1064:LEU:HD12	1:A:1064:LEU:O	2.08	0.53
1:A:504:TYR:HE1	1:A:508:ILE:HD11	1.70	0.53
1:A:1088:LEU:HA	1:A:1113:LEU:CD1	2.38	0.53
1:A:194:ILE:HG12	1:A:389:PHE:HE1	1.73	0.53
1:A:443:VAL:O	1:A:590:VAL:HA	2.09	0.53
1:A:1119:ILE:HD13	1:A:1199:ILE:HB	1.91	0.53
1:A:478:VAL:HB	1:A:558:LEU:HA	1.91	0.53
1:A:792:ASN:O	1:A:796:THR:HG22	2.09	0.53
1:A:1036:PRO:HG3	1:A:1116:LYS:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:VAL:HA	1:A:1084:LEU:CD1	2.38	0.53
1:A:398:ARG:NH2	1:A:399:ASN:OD1	2.42	0.53
1:A:1085:ILE:HG23	1:A:1089:PHE:HB3	1.88	0.52
1:A:1158:THR:HG21	1:A:1181:GLN:OE1	2.09	0.52
1:A:490:ARG:HE	1:A:493:ILE:HD11	1.75	0.52
1:A:726:VAL:O	1:A:730:LEU:HD23	2.10	0.52
1:A:1088:LEU:HD23	1:A:1089:PHE:H	1.73	0.52
1:A:746:ASN:HA	1:A:750:ASN:HB2	1.91	0.52
1:A:1061:LEU:HG	1:A:1252:LEU:HD23	1.91	0.52
1:A:398:ARG:HH12	1:A:459:LEU:HB2	1.74	0.52
1:A:839:THR:HG22	1:A:1003:VAL:HG23	1.92	0.52
1:A:1119:ILE:CD1	1:A:1199:ILE:HB	2.39	0.52
1:A:1179:VAL:HA	1:A:1182:ARG:HD2	1.91	0.52
1:A:338:THR:O	1:A:342:LEU:HD23	2.10	0.52
1:A:1059:LYS:HB2	1:A:1060:HIS:CE1	2.45	0.52
1:A:307:ILE:HG12	1:A:795:GLN:HB2	1.92	0.52
1:A:846:THR:HG21	1:A:995:TRP:HB3	1.92	0.52
1:A:1165:LYS:CG	1:A:1166:MET:H	2.23	0.52
1:A:477:TYR:HD2	1:A:913:THR:HG22	1.74	0.51
1:A:569:VAL:O	1:A:573:LEU:HG	2.10	0.51
1:A:1179:VAL:HA	1:A:1182:ARG:CD	2.40	0.51
1:A:1048:PHE:HB3	1:A:1058:LEU:H	1.75	0.51
1:A:1181:GLN:O	1:A:1185:VAL:HG12	2.11	0.51
1:A:853:VAL:HG11	1:A:989:LEU:HB2	1.91	0.51
1:A:490:ARG:NH2	1:A:504:TYR:OH	2.44	0.51
1:A:508:ILE:HD12	1:A:513:LEU:HB2	1.91	0.51
1:A:1081:LYS:HA	1:A:1084:LEU:HG	1.92	0.51
1:A:1123:GLU:N	1:A:1123:GLU:OE1	2.43	0.51
1:A:103:GLU:OE2	1:A:221:GLN:HA	2.10	0.51
1:A:568:GLU:OE2	1:A:569:VAL:HG23	2.11	0.51
1:A:1043:PHE:HD1	1:A:1098:ILE:HD12	1.76	0.51
1:A:1089:PHE:O	1:A:1114:ARG:HD2	2.11	0.51
1:A:497:LYS:HZ3	1:A:503:ARG:NH2	2.09	0.51
1:A:533:THR:O	1:A:535:LEU:N	2.39	0.51
1:A:1153:VAL:HG23	1:A:1218:LYS:HE3	1.92	0.51
1:A:185:ALA:HB1	1:A:392:LEU:HD21	1.92	0.51
1:A:197:LEU:HA	1:A:201:ASP:HB2	1.93	0.51
1:A:551:GLN:OE1	1:A:553:ALA:HB2	2.11	0.51
1:A:742:GLN:NE2	1:A:746:ASN:HB3	2.26	0.51
1:A:1198:LEU:HD22	1:A:1226:CYS:HB3	1.94	0.51
1:A:1116:LYS:HE3	1:A:1196:GLN:N	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:ARG:NE	1:A:1012:ARG:HB3	2.25	0.50
1:A:1046:VAL:O	1:A:1059:LYS:HA	2.11	0.50
1:A:203:ASN:OD1	1:A:897:ARG:NH2	2.45	0.50
1:A:292:GLU:OE1	1:A:292:GLU:N	2.39	0.50
1:A:1023:ALA:HB1	1:A:1027:TYR:CE1	2.45	0.50
1:A:1211:THR:HA	1:A:1214:LEU:HB3	1.92	0.50
1:A:499:TYR:CE1	1:A:504:TYR:HD2	2.28	0.50
1:A:170:MET:HG3	1:A:205:PHE:CE2	2.46	0.50
1:A:745:LEU:O	1:A:749:VAL:N	2.45	0.50
1:A:1049:MET:SD	1:A:1054:GLY:N	2.85	0.50
1:A:74:ASP:HB3	1:A:76:GLN:OE1	2.12	0.49
1:A:707:ALA:O	1:A:796:THR:HG21	2.11	0.49
1:A:1046:VAL:HG13	1:A:1096:GLY:N	2.27	0.49
1:A:142:THR:HA	1:A:145:THR:HG22	1.93	0.49
1:A:566:ASP:OD1	1:A:567:ALA:N	2.38	0.49
1:A:887:ARG:NH2	1:A:1004:GLU:OE2	2.46	0.49
1:A:426:PRO:HB2	1:A:429:GLN:OE1	2.12	0.49
1:A:408:LYS:HB2	1:A:437:PRO:HA	1.94	0.49
1:A:582:LEU:HD23	1:A:585:LYS:HB2	1.95	0.49
1:A:1041:ILE:HD11	1:A:1098:ILE:CG2	2.35	0.49
1:A:491:SER:O	1:A:495:PHE:N	2.35	0.49
1:A:1025:TRP:CE2	1:A:1111:HIS:HE1	2.31	0.49
1:A:1074:VAL:HG12	1:A:1199:ILE:HG23	1.95	0.49
1:A:142:THR:O	1:A:146:LEU:HD22	2.13	0.49
1:A:477:TYR:CD2	1:A:913:THR:HG22	2.48	0.48
1:A:504:TYR:CD1	1:A:508:ILE:HD11	2.48	0.48
1:A:513:LEU:CD2	1:A:542:ARG:HE	2.26	0.48
1:A:440:LEU:HG	1:A:587:THR:HG21	1.94	0.48
1:A:968:LEU:HD23	1:A:968:LEU:HA	1.67	0.48
1:A:1086:SER:O	1:A:1090:ARG:NE	2.42	0.48
1:A:536:SER:OG	1:A:537:GLY:N	2.47	0.48
1:A:1272:MET:HA	1:A:1276:LEU:HB2	1.96	0.48
1:A:416:THR:HB	1:A:466:HIS:HE1	1.78	0.48
1:A:1038:GLU:HB2	1:A:1040:VAL:HG12	1.94	0.48
1:A:1150:LEU:HA	1:A:1153:VAL:HG12	1.95	0.48
1:A:402:LEU:H	1:A:402:LEU:HD22	1.78	0.48
1:A:1210:ARG:H	1:A:1210:ARG:HD3	1.79	0.48
1:A:562:LEU:HA	1:A:565:VAL:HG12	1.95	0.48
1:A:1070:LYS:NZ	1:A:1196:GLN:HA	2.24	0.48
1:A:1085:ILE:CB	1:A:1089:PHE:HB2	2.43	0.48
1:A:1117:MET:HB3	1:A:1117:MET:HE3	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:PHE:HA	1:A:1272:MET:SD	2.54	0.48
1:A:450:GLY:N	1:A:606:LEU:HD11	2.29	0.47
1:A:478:VAL:HG22	1:A:544:ASN:HB3	1.96	0.47
1:A:803:GLU:OE2	1:A:807:LYS:HE2	2.13	0.47
1:A:153:HIS:NE2	1:A:953:ASP:OD2	2.47	0.47
1:A:182:SER:OG	1:A:183:ASN:N	2.47	0.47
1:A:455:LEU:CD2	1:A:557:LEU:HB3	2.45	0.47
1:A:558:LEU:HB3	1:A:561:PRO:CD	2.44	0.47
1:A:733:TRP:HA	1:A:736:SER:OG	2.14	0.47
1:A:812:PHE:HZ	1:A:1016:TYR:CE2	2.31	0.47
1:A:1046:VAL:HA	1:A:1096:GLY:HA3	1.95	0.47
1:A:749:VAL:CG1	1:A:757:GLU:HB2	2.45	0.47
1:A:348:ALA:HA	1:A:351:VAL:HG12	1.96	0.47
1:A:404:SER:CB	1:A:473:GLY:H	2.26	0.47
1:A:1035:TRP:CZ2	1:A:1103:ILE:HD11	2.50	0.47
1:A:742:GLN:HE22	1:A:750:ASN:ND2	2.13	0.47
1:A:905:SER:O	1:A:909:GLN:OE1	2.33	0.47
1:A:528:ILE:HD12	1:A:534:THR:OG1	2.14	0.47
1:A:536:SER:H	1:A:539:GLN:HB2	1.79	0.47
1:A:824:ARG:HA	1:A:828:ASP:OD1	2.14	0.47
1:A:1091:LEU:HD12	1:A:1091:LEU:O	2.15	0.47
1:A:1179:VAL:HA	1:A:1182:ARG:HG2	1.96	0.47
1:A:1215:ILE:HG22	1:A:1223:PHE:HZ	1.79	0.47
1:A:194:ILE:HG12	1:A:389:PHE:CE1	2.50	0.47
1:A:307:ILE:HA	1:A:310:ILE:HG22	1.97	0.47
1:A:497:LYS:NZ	1:A:552:ASP:OD2	2.42	0.47
1:A:1089:PHE:CE2	1:A:1119:ILE:HB	2.50	0.47
1:A:413:GLN:O	1:A:413:GLN:HG2	2.14	0.47
1:A:1123:GLU:O	1:A:1125:VAL:N	2.48	0.47
1:A:265:THR:HG22	1:A:309:LYS:HB3	1.96	0.46
1:A:1069:GLU:HB3	1:A:1071:VAL:HG23	1.96	0.46
1:A:1155:LEU:HD11	1:A:1184:LEU:HD12	1.97	0.46
1:A:1214:LEU:HA	1:A:1217:LYS:HE2	1.97	0.46
1:A:336:PHE:CZ	1:A:351:VAL:HA	2.50	0.46
1:A:1071:VAL:CA	1:A:1227:THR:HG21	2.46	0.46
1:A:1085:ILE:HG23	1:A:1089:PHE:C	2.35	0.46
1:A:1170:LEU:N	1:A:1170:LEU:HD22	2.30	0.46
1:A:1186:CYS:HA	1:A:1189:ARG:NE	2.31	0.46
1:A:9:LYS:HD3	1:A:10:PRO:HD2	1.97	0.46
1:A:408:LYS:HD3	1:A:586:ILE:HD11	1.97	0.46
1:A:1024:PRO:HG2	1:A:1027:TYR:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:LYS:H	1:A:1066:LYS:HG2	1.53	0.46
1:A:1153:VAL:HG23	1:A:1218:LYS:CE	2.45	0.46
1:A:1218:LYS:C	1:A:1223:PHE:H	2.18	0.46
1:A:26:TRP:CH2	1:A:943:THR:HG21	2.51	0.46
1:A:605:ILE:HG22	1:A:607:LYS:HZ1	1.81	0.46
1:A:94:VAL:O	1:A:97:ILE:HB	2.16	0.46
1:A:1025:TRP:CE2	1:A:1111:HIS:CE1	3.04	0.46
1:A:429:GLN:C	1:A:431:LEU:H	2.19	0.46
1:A:468:LEU:O	1:A:468:LEU:HD12	2.15	0.46
1:A:508:ILE:CD1	1:A:513:LEU:HD12	2.43	0.46
1:A:571:ARG:HA	1:A:574:PHE:HD1	1.81	0.46
1:A:970:LEU:C	1:A:972:LYS:H	2.19	0.46
1:A:1165:LYS:HD3	1:A:1166:MET:N	2.30	0.46
1:A:237:CYS:SG	1:A:238:LEU:N	2.88	0.46
1:A:317:ARG:HD2	1:A:838:LEU:HD22	1.98	0.46
1:A:427:THR:O	1:A:428:LEU:HD22	2.16	0.46
1:A:497:LYS:HE3	1:A:551:GLN:HA	1.96	0.46
1:A:1207:VAL:HG13	1:A:1211:THR:HB	1.98	0.46
1:A:558:LEU:HB2	1:A:589:LEU:HD13	1.98	0.46
1:A:1077:THR:C	1:A:1079:ALA:H	2.18	0.46
1:A:103:GLU:CG	1:A:221:GLN:HB2	2.46	0.46
1:A:280:ILE:HG22	1:A:818:ILE:HD12	1.97	0.46
1:A:612:VAL:HG23	1:A:613:GLN:OE1	2.16	0.46
1:A:1035:TRP:C	1:A:1037:HIS:N	2.69	0.46
1:A:1040:VAL:O	1:A:1101:ASP:N	2.47	0.46
1:A:1116:LYS:HE2	1:A:1195:ASN:HB3	1.98	0.46
1:A:1118:SER:OG	1:A:1198:LEU:HB3	2.16	0.46
1:A:555:ILE:HG13	1:A:586:ILE:CG1	2.46	0.45
1:A:584:GLU:O	1:A:585:LYS:HD3	2.15	0.45
1:A:1041:ILE:HG21	1:A:1073:ILE:HG21	1.98	0.45
1:A:1063:ALA:HB3	1:A:1073:ILE:HD11	1.98	0.45
1:A:1085:ILE:HA	1:A:1089:PHE:H	1.81	0.45
1:A:1178:SER:OG	1:A:1181:GLN:HG3	2.15	0.45
1:A:547:ARG:O	1:A:551:GLN:CB	2.59	0.45
1:A:1025:TRP:CG	1:A:1111:HIS:ND1	2.84	0.45
1:A:1253:LYS:HE2	1:A:1268:LEU:HG	1.99	0.45
1:A:156:PHE:CE1	1:A:210:VAL:HG13	2.51	0.45
1:A:398:ARG:HH12	1:A:459:LEU:CB	2.29	0.45
1:A:415:PHE:CE1	1:A:464:PRO:HA	2.52	0.45
1:A:940:LEU:HD23	1:A:940:LEU:HA	1.80	0.45
1:A:1263:GLN:H	1:A:1263:GLN:CD	2.12	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:HD2	1:A:946:ARG:CZ	2.29	0.45
1:A:1068:GLN:OE1	1:A:1068:GLN:HA	2.15	0.45
1:A:1204:THR:CG2	1:A:1232:ALA:HB2	2.47	0.45
1:A:111:ILE:HD11	1:A:228:LEU:HD13	1.98	0.45
1:A:515:LYS:HE3	1:A:542:ARG:HH22	1.82	0.45
1:A:1097:LYS:HD2	1:A:1104:LEU:CD1	2.47	0.45
1:A:605:ILE:HG22	1:A:607:LYS:NZ	2.32	0.45
1:A:735:LEU:HD12	1:A:735:LEU:HA	1.74	0.45
1:A:1187:LEU:HD22	1:A:1223:PHE:HE1	1.81	0.45
1:A:113:LEU:O	1:A:117:ILE:HG12	2.17	0.45
1:A:597:LEU:HD12	1:A:598:LYS:HG3	1.98	0.45
1:A:352:PHE:HZ	1:A:736:SER:HB3	1.81	0.45
1:A:970:LEU:O	1:A:972:LYS:N	2.50	0.45
1:A:1183:GLN:NE2	1:A:1208:ASP:OD2	2.50	0.45
1:A:1271:LYS:HB3	1:A:1275:GLN:NE2	2.32	0.45
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.75	0.45
1:A:400:ARG:NH2	1:A:403:PRO:HD3	2.32	0.45
1:A:952:LEU:HA	1:A:952:LEU:HD23	1.67	0.45
1:A:1043:PHE:CE2	1:A:1073:ILE:HD11	2.52	0.45
1:A:1059:LYS:HG3	1:A:1251:ARG:NE	2.32	0.45
1:A:1059:LYS:CG	1:A:1251:ARG:HD3	2.47	0.45
1:A:1133:LYS:HD3	1:A:1137:PRO:HB3	1.98	0.45
1:A:483:TRP:CZ2	1:A:485:PHE:HB3	2.52	0.44
1:A:512:ALA:HA	1:A:514:LYS:NZ	2.31	0.44
1:A:1122:GLN:HB3	1:A:1123:GLU:OE1	2.17	0.44
1:A:1133:LYS:HD3	1:A:1137:PRO:HA	1.99	0.44
1:A:413:GLN:HA	1:A:432:SER:OG	2.17	0.44
1:A:416:THR:HB	1:A:466:HIS:CE1	2.52	0.44
1:A:1074:VAL:HA	1:A:1084:LEU:HD11	1.99	0.44
1:A:1085:ILE:CG2	1:A:1089:PHE:HB2	2.46	0.44
1:A:1097:LYS:NZ	1:A:1104:LEU:HD13	2.32	0.44
1:A:1185:VAL:CG2	1:A:1189:ARG:HH21	2.27	0.44
1:A:1251:ARG:CZ	1:A:1251:ARG:HB3	2.45	0.44
1:A:285:ILE:HD13	1:A:285:ILE:HA	1.73	0.44
1:A:574:PHE:HZ	1:A:596:TYR:CD1	2.32	0.44
1:A:746:ASN:HA	1:A:750:ASN:CB	2.47	0.44
1:A:215:LEU:HD22	1:A:372:ALA:HB1	1.99	0.44
1:A:717:LEU:HD11	1:A:786:VAL:HG23	2.00	0.44
1:A:983:LEU:HD23	1:A:983:LEU:HA	1.79	0.44
1:A:995:TRP:CE3	1:A:995:TRP:HA	2.52	0.44
1:A:1143:ASP:HA	1:A:1146:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PHE:CE2	1:A:462:LEU:HB2	2.53	0.44
1:A:1050:TYR:CD1	1:A:1079:ALA:HB2	2.53	0.44
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.84	0.44
1:A:508:ILE:HG22	1:A:514:LYS:CG	2.48	0.44
1:A:594:LEU:HA	1:A:597:LEU:CG	2.36	0.44
1:A:1214:LEU:HG	1:A:1218:LYS:HZ2	1.83	0.44
1:A:1273:VAL:HA	1:A:1277:GLY:O	2.17	0.44
1:A:1204:THR:HG23	1:A:1232:ALA:HB2	1.99	0.44
1:A:455:LEU:HD13	1:A:477:TYR:CZ	2.53	0.44
1:A:1024:PRO:HG2	1:A:1027:TYR:CD1	2.53	0.44
1:A:1130:THR:CG2	1:A:1133:LYS:H	2.30	0.44
1:A:1143:ASP:HA	1:A:1146:LEU:HD23	1.99	0.44
1:A:1162:LEU:HD13	1:A:1168:THR:HG21	1.99	0.44
1:A:243:VAL:HG21	1:A:334:VAL:HG11	1.99	0.44
1:A:480:GLN:HG2	1:A:559:ASP:CG	2.37	0.44
1:A:1025:TRP:CG	1:A:1111:HIS:CE1	3.06	0.44
1:A:1269:PHE:O	1:A:1272:MET:SD	2.75	0.44
1:A:163:GLY:HA3	1:A:209:THR:HG21	1.98	0.43
1:A:1223:PHE:C	1:A:1225:HIS:N	2.70	0.43
1:A:120:PHE:CE2	1:A:979:VAL:HG21	2.53	0.43
1:A:555:ILE:N	1:A:555:ILE:HD12	2.33	0.43
1:A:746:ASN:HA	1:A:750:ASN:CG	2.39	0.43
1:A:1218:LYS:HB2	1:A:1223:PHE:CE2	2.53	0.43
1:A:310:ILE:HA	1:A:310:ILE:HD12	1.77	0.43
1:A:562:LEU:HA	1:A:565:VAL:CG1	2.49	0.43
1:A:910:GLY:O	1:A:914:ILE:HG12	2.17	0.43
1:A:1074:VAL:HA	1:A:1084:LEU:HD13	1.99	0.43
1:A:244:LEU:HD12	1:A:244:LEU:HA	1.83	0.43
1:A:489:LEU:HD13	1:A:528:ILE:HD13	1.99	0.43
1:A:1049:MET:SD	1:A:1051:SER:O	2.76	0.43
1:A:1170:LEU:HD22	1:A:1170:LEU:H	1.83	0.43
1:A:1256:ASP:OD1	1:A:1256:ASP:N	2.51	0.43
1:A:419:TRP:HH2	1:A:452:SER:HG	1.65	0.43
1:A:428:LEU:HD21	1:A:450:GLY:HA3	2.00	0.43
1:A:429:GLN:O	1:A:431:LEU:HD22	2.18	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.84	0.43
1:A:453:SER:HA	1:A:456:SER:OG	2.18	0.43
1:A:603:ILE:HG12	1:A:615:GLY:O	2.18	0.43
1:A:749:VAL:HG13	1:A:757:GLU:HB2	2.01	0.43
1:A:1031:PRO:CB	1:A:1035:TRP:CD1	3.02	0.43
1:A:1041:ILE:HG23	1:A:1073:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1257:GLU:OE2	1:A:1260:VAL:HG13	2.18	0.43
1:A:582:LEU:CD2	1:A:585:LYS:HB2	2.48	0.43
1:A:443:VAL:HG12	1:A:588:ILE:HG23	2.01	0.43
1:A:824:ARG:HG3	1:A:1016:TYR:CE1	2.54	0.43
1:A:1072:GLY:CA	1:A:1229:LEU:HD11	2.49	0.43
1:A:285:ILE:HA	1:A:288:MET:HB2	2.01	0.42
1:A:436:ARG:HA	1:A:437:PRO:HD3	1.90	0.42
1:A:1049:MET:HE2	1:A:1049:MET:HA	2.01	0.42
1:A:1108:ILE:HD12	1:A:1108:ILE:N	2.34	0.42
1:A:64:TRP:HH2	1:A:391:LEU:HD21	1.83	0.42
1:A:281:THR:HG22	1:A:818:ILE:HG21	2.01	0.42
1:A:558:LEU:HD23	1:A:561:PRO:HG2	2.01	0.42
1:A:515:LYS:O	1:A:519:LEU:HG	2.18	0.42
1:A:580:GLN:O	1:A:583:HIS:HB3	2.19	0.42
1:A:483:TRP:CH2	1:A:914:ILE:HD11	2.54	0.42
1:A:542:ARG:HA	1:A:545:LEU:HG	2.02	0.42
1:A:1034:ALA:O	1:A:1037:HIS:CD2	2.73	0.42
1:A:476:ALA:HB1	1:A:548:ALA:CB	2.49	0.42
1:A:802:PHE:HA	1:A:805:ILE:HG22	2.01	0.42
1:A:1148:ASN:HA	1:A:1151:GLN:CG	2.50	0.42
1:A:1148:ASN:HA	1:A:1151:GLN:HG3	2.01	0.42
1:A:1229:LEU:N	1:A:1229:LEU:HD12	2.34	0.42
1:A:138:ALA:O	1:A:142:THR:HG22	2.19	0.42
1:A:522:ASP:HB3	1:A:526:THR:OG1	2.19	0.42
1:A:1030:ARG:CZ	1:A:1112:ASP:OD2	2.67	0.42
1:A:1148:ASN:O	1:A:1151:GLN:HG3	2.18	0.42
1:A:1162:LEU:HD23	1:A:1162:LEU:HA	1.88	0.42
1:A:282:GLY:O	1:A:286:ILE:HG13	2.19	0.42
1:A:742:GLN:CA	1:A:745:LEU:HB3	2.46	0.42
1:A:879:ARG:NH1	5:A:1417:PLM:HB1	2.35	0.42
1:A:1088:LEU:HB2	1:A:1117:MET:HE2	2.01	0.42
1:A:1104:LEU:HG	1:A:1106:THR:HG23	2.00	0.42
1:A:1261:LEU:HD22	1:A:1266:GLU:CD	2.40	0.42
1:A:117:ILE:CD1	1:A:979:VAL:HG13	2.50	0.42
1:A:474:ARG:NH2	1:A:552:ASP:O	2.46	0.42
1:A:1072:GLY:HA3	1:A:1229:LEU:CD1	2.50	0.42
1:A:1152:GLU:O	1:A:1222:LYS:NZ	2.21	0.42
1:A:1164:GLY:HA3	1:A:1168:THR:HA	2.02	0.42
1:A:1198:LEU:HD22	1:A:1226:CYS:CB	2.50	0.42
1:A:429:GLN:HE22	1:A:609:GLY:HA3	1.83	0.42
1:A:1120:ILE:CG2	1:A:1200:ILE:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1236:ASN:OD1	1:A:1236:ASN:N	2.51	0.42
1:A:307:ILE:HD12	1:A:310:ILE:CG2	2.50	0.42
1:A:329:LYS:HE3	1:A:728:TYR:CZ	2.55	0.42
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.90	0.42
1:A:1123:GLU:O	1:A:1123:GLU:HG2	2.20	0.42
1:A:1251:ARG:NH1	1:A:1252:LEU:H	2.18	0.42
1:A:499:TYR:HE1	1:A:504:TYR:HD2	1.68	0.41
1:A:546:ALA:O	1:A:550:TYR:HB3	2.19	0.41
1:A:742:GLN:NE2	1:A:742:GLN:O	2.53	0.41
1:A:1082:SER:OG	1:A:1091:LEU:HG	2.20	0.41
1:A:1177:PHE:O	1:A:1182:ARG:NH2	2.52	0.41
1:A:1242:ASP:O	1:A:1258:PRO:HD2	2.20	0.41
1:A:542:ARG:O	1:A:545:LEU:HG	2.19	0.41
1:A:1247:LEU:HA	1:A:1251:ARG:O	2.20	0.41
1:A:1262:LEU:HD12	1:A:1263:GLN:OE1	2.20	0.41
1:A:484:VAL:HG22	1:A:532:GLY:HA3	2.02	0.41
1:A:560:ASP:N	1:A:561:PRO:HD3	2.35	0.41
1:A:745:LEU:HD11	1:A:759:LEU:HD21	2.03	0.41
1:A:1089:PHE:CZ	1:A:1117:MET:O	2.73	0.41
1:A:1131:MET:SD	1:A:1135:LEU:HD23	2.61	0.41
1:A:71:ALA:O	1:A:75:ALA:N	2.53	0.41
1:A:513:LEU:HD23	1:A:542:ARG:HE	1.85	0.41
1:A:1070:LYS:HE3	1:A:1225:HIS:HA	2.03	0.41
1:A:1096:GLY:O	1:A:1098:ILE:HG12	2.21	0.41
1:A:411:HIS:HD2	1:A:413:GLN:OE1	2.03	0.41
1:A:1118:SER:O	1:A:1198:LEU:CA	2.59	0.41
1:A:1120:ILE:HG23	1:A:1200:ILE:HA	2.01	0.41
1:A:70:ARG:NH2	1:A:71:ALA:HA	2.35	0.41
1:A:142:THR:OG1	1:A:961:ILE:HG12	2.21	0.41
1:A:565:VAL:HG22	1:A:566:ASP:N	2.36	0.41
1:A:797:LEU:HD23	1:A:797:LEU:HA	1.89	0.41
1:A:1049:MET:HA	1:A:1049:MET:CE	2.51	0.41
1:A:276:MET:SD	1:A:299:ILE:HD11	2.61	0.41
1:A:293:LYS:HA	1:A:293:LYS:HD2	1.74	0.41
1:A:1025:TRP:O	1:A:1110:LEU:N	2.54	0.41
1:A:1072:GLY:HA3	1:A:1229:LEU:HD11	2.01	0.41
1:A:1085:ILE:HG22	1:A:1091:LEU:N	2.35	0.41
1:A:1212:ASP:O	1:A:1216:GLN:HG2	2.21	0.41
1:A:1261:LEU:O	1:A:1269:PHE:HB3	2.21	0.41
1:A:952:LEU:CD1	1:A:997:VAL:HG21	2.51	0.41
1:A:1107:GLU:HG2	1:A:1108:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD23	1:A:31:PHE:HE2	1.86	0.41
1:A:31:PHE:O	1:A:35:HIS:N	2.53	0.41
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.86	0.41
1:A:278:GLU:CD	1:A:1128:THR:H	2.24	0.41
1:A:428:LEU:HD21	1:A:450:GLY:CA	2.50	0.41
1:A:440:LEU:HD11	1:A:578:ILE:HG22	2.02	0.41
1:A:497:LYS:CE	1:A:551:GLN:HA	2.50	0.41
1:A:765:LEU:HD12	1:A:765:LEU:HA	1.71	0.41
1:A:800:LYS:HD2	1:A:1017:THR:CG2	2.51	0.41
1:A:861:ILE:O	1:A:864:ILE:HB	2.21	0.41
1:A:868:LEU:HA	1:A:868:LEU:HD12	1.74	0.41
1:A:995:TRP:CE2	3:A:1402:MTX:H15	2.55	0.41
1:A:1059:LYS:HB3	1:A:1059:LYS:HE3	1.81	0.41
1:A:1187:LEU:HD22	1:A:1223:PHE:CE1	2.55	0.41
1:A:1189:ARG:O	1:A:1193:ARG:HB2	2.20	0.41
1:A:1266:GLU:O	1:A:1270:TYR:HB3	2.20	0.41
1:A:12:PRO:HG2	1:A:26:TRP:CE3	2.56	0.41
1:A:515:LYS:HE3	1:A:542:ARG:HH12	1.85	0.41
1:A:584:GLU:C	1:A:585:LYS:HD3	2.41	0.41
1:A:1208:ASP:HB2	1:A:1210:ARG:HH12	1.84	0.41
1:A:1259:TYR:O	1:A:1263:GLN:OE1	2.38	0.41
1:A:19:CYS:HA	1:A:22:VAL:HG12	2.03	0.40
1:A:212:LEU:O	1:A:215:LEU:HD23	2.21	0.40
1:A:291:TRP:CH2	1:A:1189:ARG:HD3	2.56	0.40
1:A:749:VAL:O	1:A:753:GLY:HA2	2.21	0.40
1:A:1041:ILE:O	1:A:1042:ILE:HD13	2.21	0.40
1:A:1063:ALA:HB3	1:A:1073:ILE:CD1	2.51	0.40
1:A:1144:GLU:HA	1:A:1147:TRP:CD1	2.51	0.40
1:A:1150:LEU:HB2	1:A:1156:LYS:HE2	2.03	0.40
1:A:283:ILE:HG12	1:A:813:PHE:CZ	2.57	0.40
1:A:517:LEU:HD23	1:A:517:LEU:HA	1.87	0.40
1:A:543:VAL:HA	1:A:546:ALA:HB3	2.02	0.40
1:A:994:GLN:OE1	1:A:994:GLN:HA	2.21	0.40
1:A:455:LEU:HB3	1:A:477:TYR:CE1	2.56	0.40
1:A:479:SER:OG	1:A:480:GLN:N	2.55	0.40
1:A:739:ALA:HA	1:A:742:GLN:HB3	2.03	0.40
1:A:755:VAL:O	1:A:756:THR:OG1	2.30	0.40
1:A:975:ASP:CG	1:A:976:ALA:N	2.74	0.40
1:A:1040:VAL:HA	1:A:1065:ILE:O	2.21	0.40
1:A:1082:SER:CA	1:A:1085:ILE:HD12	2.34	0.40
1:A:1267:SER:O	1:A:1271:LYS:HE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ALA:HA	1:A:514:LYS:HZ1	1.85	0.40
1:A:1031:PRO:HB2	1:A:1035:TRP:HD1	1.86	0.40
1:A:1198:LEU:CD2	1:A:1228:VAL:HG12	2.50	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	1194/1325 (90%)	1117 (94%)	72 (6%)	5 (0%)	34 64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1267	SER
1	A	1263	GLN
1	A	1201	ASP
1	A	406	GLY
1	A	1124	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1045/1159 (90%)	987 (94%)	58 (6%)	21 49

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	CYS
1	A	70	ARG
1	A	89	TRP
1	A	92	TYR
1	A	103	GLU
1	A	120	PHE
1	A	155	TYR
1	A	184	MET
1	A	186	MET
1	A	206	ASP
1	A	324[A]	PHE
1	A	324[B]	PHE
1	A	326	SER
1	A	397	GLN
1	A	398	ARG
1	A	419	TRP
1	A	466	HIS
1	A	483	TRP
1	A	492	ASN
1	A	499	TYR
1	A	504	TYR
1	A	509	LYS
1	A	574	PHE
1	A	596	TYR
1	A	611	MET
1	A	613	GLN
1	A	617	TYR
1	A	782	ARG
1	A	787	PHE
1	A	806	LEU
1	A	840	PHE
1	A	967	SER
1	A	995	TRP
1	A	1019	LEU
1	A	1060	HIS
1	A	1066	LYS
1	A	1076	ARG
1	A	1081	LYS
1	A	1088	LEU
1	A	1116	LYS
1	A	1117	MET
1	A	1127	PHE

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Mol	Chain	Res	Type
1	A	1139	ASN
1	A	1141	HIS
1	A	1169	GLU
1	A	1182	ARG
1	A	1183	GLN
1	A	1187	LEU
1	A	1192	LEU
1	A	1198	LEU
1	A	1210	ARG
1	A	1223	PHE
1	A	1253	LYS
1	A	1257	GLU
1	A	1262	LEU
1	A	1265	LYS
1	A	1269	PHE
1	A	1272	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	742	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DU0	A	1415	-	42,42,42	0.47	0	66,66,66	0.65	2 (3%)
4	DU0	A	1414	-	42,42,42	0.49	0	66,66,66	0.79	2 (3%)
4	DU0	A	1413	-	42,42,42	0.47	0	66,66,66	1.24	6 (9%)
4	DU0	A	1416	-	42,42,42	0.47	0	66,66,66	0.86	2 (3%)
3	MTX	A	1402	-	35,35,35	0.92	0	46,49,49	2.27	10 (21%)
4	DU0	A	1408	-	42,42,42	0.49	0	66,66,66	1.00	3 (4%)
5	PLM	A	1417	-	17,17,17	0.66	0	17,17,17	0.67	1 (5%)
4	DU0	A	1403	-	42,42,42	0.46	0	66,66,66	0.80	2 (3%)
4	DU0	A	1404	-	42,42,42	0.46	0	66,66,66	0.67	0
4	DU0	A	1406	-	42,42,42	0.48	0	66,66,66	0.99	4 (6%)
4	DU0	A	1409	-	42,42,42	0.50	0	66,66,66	1.25	5 (7%)
4	DU0	A	1411	-	42,42,42	0.47	0	66,66,66	1.01	3 (4%)
4	DU0	A	1410	-	42,42,42	0.47	0	66,66,66	0.81	2 (3%)
4	DU0	A	1412	-	42,42,42	0.47	0	66,66,66	0.78	2 (3%)
2	ANP	A	1401	6	29,33,33	2.45	6 (20%)	31,52,52	1.54	3 (9%)
4	DU0	A	1407	-	42,42,42	0.53	0	66,66,66	0.80	2 (3%)
4	DU0	A	1405	-	42,42,42	0.45	0	66,66,66	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DU0	A	1415	-	-	2/10/98/98	0/6/6/6
4	DU0	A	1414	-	-	1/10/98/98	0/6/6/6
4	DU0	A	1413	-	-	3/10/98/98	0/6/6/6
4	DU0	A	1416	-	-	2/10/98/98	0/6/6/6
3	MTX	A	1402	-	-	17/25/25/25	0/3/3/3
4	DU0	A	1408	-	-	2/10/98/98	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PLM	A	1417	-	-	5/15/15/15	-
4	DU0	A	1403	-	-	3/10/98/98	0/6/6/6
4	DU0	A	1404	-	-	2/10/98/98	0/6/6/6
4	DU0	A	1406	-	-	7/10/98/98	0/6/6/6
4	DU0	A	1409	-	-	4/10/98/98	0/6/6/6
4	DU0	A	1411	-	-	5/10/98/98	0/6/6/6
4	DU0	A	1410	-	-	3/10/98/98	0/6/6/6
4	DU0	A	1412	-	-	5/10/98/98	0/6/6/6
2	ANP	A	1401	6	-	6/14/38/38	0/3/3/3
4	DU0	A	1407	-	-	1/10/98/98	0/6/6/6
4	DU0	A	1405	-	-	3/10/98/98	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	ANP	PB-O3A	8.73	1.70	1.59
2	A	1401	ANP	PG-N3B	6.39	1.80	1.63
2	A	1401	ANP	PG-O1G	4.47	1.53	1.46
2	A	1401	ANP	PB-O1B	2.64	1.50	1.46
2	A	1401	ANP	C8-N7	-2.37	1.30	1.34
2	A	1401	ANP	PB-O2B	-2.10	1.51	1.56

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1402	MTX	CA-N-C	8.89	143.36	121.60
3	A	1402	MTX	C11-C-N	6.97	130.42	117.06
4	A	1409	DU0	O10-C09-C15	6.03	116.38	110.77
4	A	1411	DU0	O10-C09-C15	5.69	116.06	110.77
4	A	1408	DU0	O10-C09-C15	5.21	115.61	110.77
2	A	1401	ANP	O2B-PB-O1B	4.72	119.81	109.92
3	A	1402	MTX	O-C-C11	-4.37	113.15	120.94
4	A	1413	DU0	O10-C09-C15	4.35	114.81	110.77
2	A	1401	ANP	O1G-PG-N3B	-4.31	105.42	111.77
4	A	1409	DU0	C11-O10-C09	3.70	120.73	113.72
4	A	1413	DU0	C14-C15-C09	3.57	118.11	111.93
4	A	1410	DU0	O10-C09-C15	3.51	114.04	110.77
4	A	1409	DU0	C14-C15-C09	3.38	117.78	111.93
4	A	1413	DU0	C22-C21-C20	3.36	116.74	111.52
3	A	1402	MTX	O-C-N	-3.27	116.42	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1402	MTX	C6-C9-N10	3.19	119.06	113.60
4	A	1408	DU0	C11-O10-C09	3.13	119.65	113.72
4	A	1411	DU0	C14-C15-C09	3.11	117.31	111.93
4	A	1406	DU0	C79-C17-C03	-3.08	104.97	109.09
2	A	1401	ANP	PB-O3A-PA	-3.02	121.99	132.62
4	A	1416	DU0	C22-C21-C20	2.89	116.00	111.52
4	A	1409	DU0	C03-C04-C05	-2.82	96.95	102.37
4	A	1403	DU0	O10-C09-C15	2.81	113.39	110.77
4	A	1411	DU0	C11-O10-C09	2.72	118.86	113.72
4	A	1406	DU0	C18-C17-C79	2.67	112.94	109.71
4	A	1406	DU0	C03-C04-C05	-2.66	97.25	102.37
3	A	1402	MTX	C15-C16-C11	2.65	123.86	120.78
3	A	1402	MTX	C16-C11-C12	-2.61	114.87	118.59
4	A	1407	DU0	C22-C21-C20	2.55	115.49	111.52
3	A	1402	MTX	OE1-CD-CG	-2.49	115.07	123.08
4	A	1407	DU0	C21-C20-C19	-2.46	117.06	120.61
4	A	1415	DU0	C11-O10-C09	2.41	118.28	113.72
4	A	1416	DU0	C21-C20-C19	-2.40	117.15	120.61
3	A	1402	MTX	CB-CA-N	-2.35	106.12	110.88
4	A	1413	DU0	C03-C04-C05	-2.34	97.87	102.37
4	A	1406	DU0	C76-C75-C22	2.27	114.20	110.33
4	A	1413	DU0	C11-O10-C09	2.17	117.83	113.72
4	A	1408	DU0	C14-C15-C09	2.17	115.68	111.93
3	A	1402	MTX	CT-CA-N	2.14	115.63	110.55
4	A	1412	DU0	C03-C04-C05	-2.14	98.25	102.37
4	A	1414	DU0	C79-C17-C03	-2.14	106.22	109.09
4	A	1412	DU0	C22-C21-C20	2.13	114.83	111.52
4	A	1413	DU0	C76-C75-C22	2.12	113.94	110.33
4	A	1414	DU0	C09-C07-C06	-2.08	99.98	103.37
4	A	1410	DU0	C11-O10-C09	2.07	117.64	113.72
4	A	1409	DU0	C75-C22-C21	-2.07	107.90	110.99
4	A	1403	DU0	C75-C76-C77	2.07	117.22	112.74
4	A	1415	DU0	O10-C11-C12	2.07	115.16	112.18
5	A	1417	PLM	O2-C1-C2	-2.05	116.51	123.08

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	ANP	PG-N3B-PB-O1B
2	A	1401	ANP	C5'-O5'-PA-O3A
3	A	1402	MTX	C11-C-N-CA

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Mol	Chain	Res	Type	Atoms
3	A	1402	MTX	O-C-N-CA
3	A	1402	MTX	CT-CA-N-C
3	A	1402	MTX	N-CA-CB-CG
4	A	1403	DU0	C75-C22-O23-C24
4	A	1403	DU0	C25-C26-C51-O52
4	A	1404	DU0	C21-C22-O23-C24
4	A	1406	DU0	C21-C22-O23-C24
4	A	1409	DU0	C25-C26-C27-O28
4	A	1409	DU0	C51-C26-C27-O28
4	A	1410	DU0	C75-C22-O23-C24
4	A	1410	DU0	C25-C26-C27-O28
4	A	1413	DU0	C25-C26-C51-O52
4	A	1413	DU0	C27-C26-C51-O52
4	A	1415	DU0	C21-C22-O23-C24
3	A	1402	MTX	O-C-C11-C12
3	A	1402	MTX	N-C-C11-C12
3	A	1402	MTX	O-C-C11-C16
3	A	1402	MTX	N-C-C11-C16
3	A	1402	MTX	CB-CA-CT-O1
3	A	1402	MTX	CB-CA-CT-O2
4	A	1405	DU0	C21-C22-O23-C24
4	A	1408	DU0	C21-C22-O23-C24
4	A	1408	DU0	C75-C22-O23-C24
4	A	1412	DU0	C21-C22-O23-C24
4	A	1412	DU0	C75-C22-O23-C24
5	A	1417	PLM	CB-CC-CD-CE
5	A	1417	PLM	C1-C2-C3-C4
3	A	1402	MTX	CT-CA-CB-CG
4	A	1406	DU0	C24-C25-C26-C27
4	A	1409	DU0	O23-C24-C25-C26
3	A	1402	MTX	CA-CB-CG-CD
5	A	1417	PLM	CA-CB-CC-CD
2	A	1401	ANP	C3'-C4'-C5'-O5'
4	A	1405	DU0	C75-C22-O23-C24
4	A	1411	DU0	C21-C22-O23-C24
4	A	1411	DU0	C75-C22-O23-C24
4	A	1406	DU0	C25-C24-O23-C22
4	A	1410	DU0	C51-C26-C27-O28
4	A	1412	DU0	C27-C26-C51-O52
4	A	1416	DU0	C27-C26-C51-O52
3	A	1402	MTX	N-CA-CT-O2
4	A	1406	DU0	C25-C26-C51-O52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1412	DU0	C25-C26-C51-O52
4	A	1416	DU0	C25-C26-C51-O52
4	A	1406	DU0	C24-C25-C26-C51
3	A	1402	MTX	N-CA-CT-O1
4	A	1406	DU0	O23-C24-C25-C26
4	A	1406	DU0	C75-C22-O23-C24
4	A	1415	DU0	C75-C22-O23-C24
2	A	1401	ANP	C4'-C5'-O5'-PA
2	A	1401	ANP	C5'-O5'-PA-O1A
3	A	1402	MTX	C6-C9-N10-CM
4	A	1409	DU0	C21-C22-O23-C24
4	A	1405	DU0	C25-C24-O23-C22
4	A	1411	DU0	C25-C24-O23-C22
4	A	1403	DU0	C27-C26-C51-O52
5	A	1417	PLM	O1-C1-C2-C3
2	A	1401	ANP	PB-O3A-PA-O1A
4	A	1411	DU0	C24-C25-C26-C27
5	A	1417	PLM	O2-C1-C2-C3
4	A	1404	DU0	C25-C24-O23-C22
4	A	1412	DU0	C25-C24-O23-C22
4	A	1413	DU0	C25-C24-O23-C22
4	A	1414	DU0	C25-C24-O23-C22
3	A	1402	MTX	OE2-CD-CG-CB
3	A	1402	MTX	OE1-CD-CG-CB
4	A	1407	DU0	C24-C25-C26-C27
4	A	1411	DU0	C24-C25-C26-C51

There are no ring outliers.

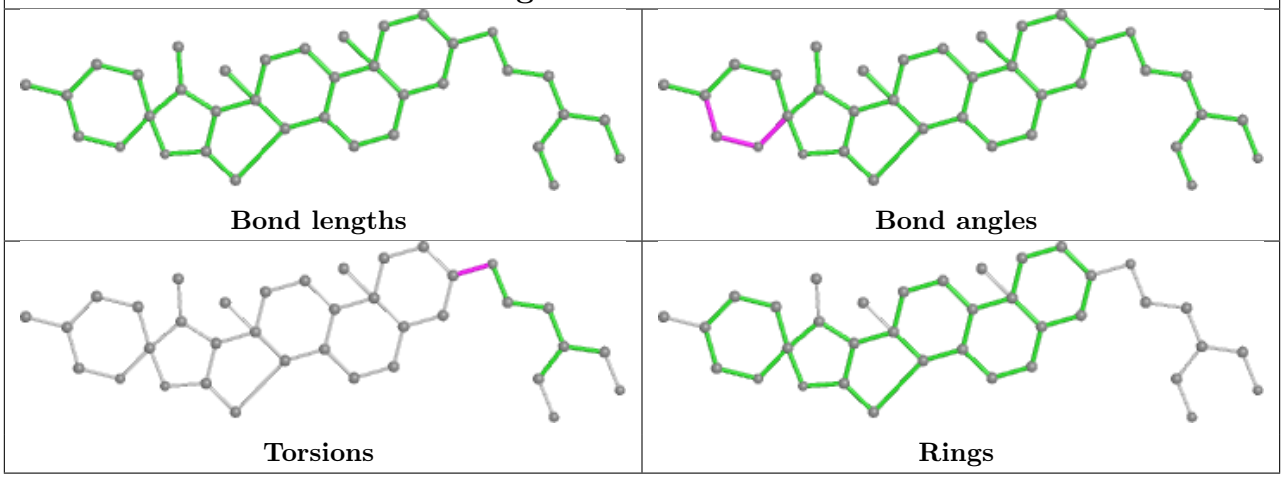
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	MTX	2	0
5	A	1417	PLM	1	0
2	A	1401	ANP	2	0

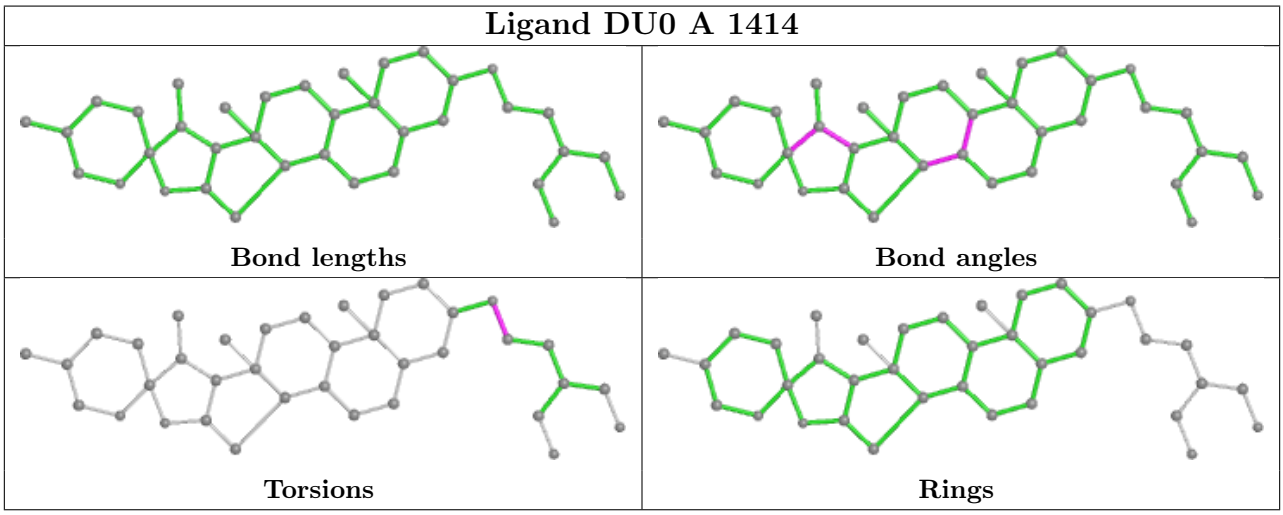
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

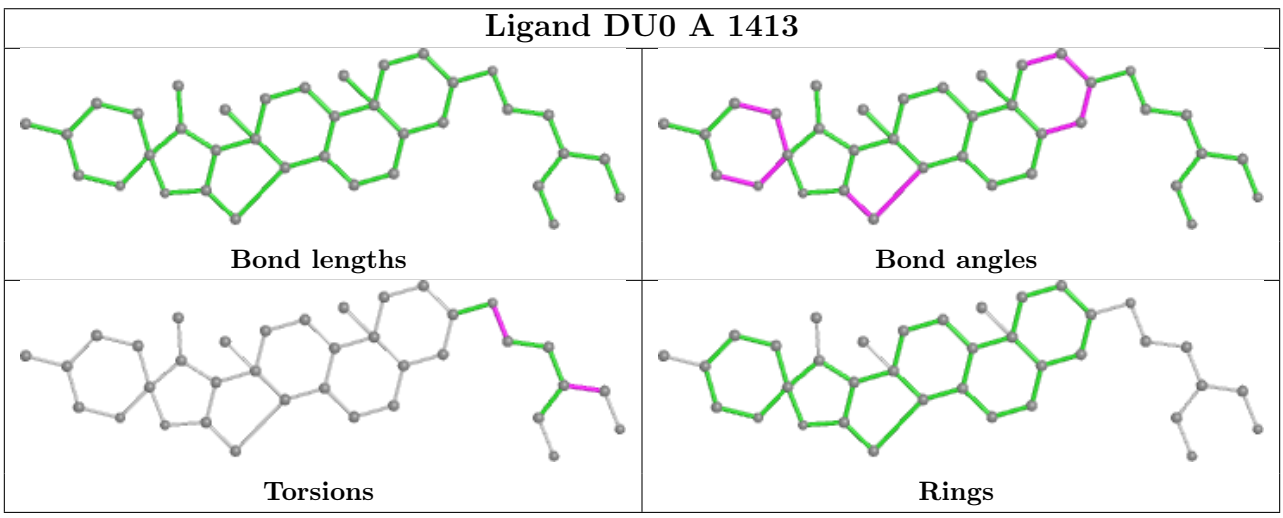
Ligand DU0 A 1415



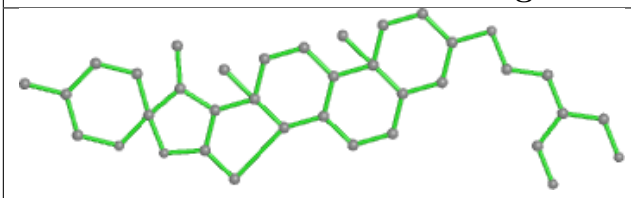
Ligand DU0 A 1414



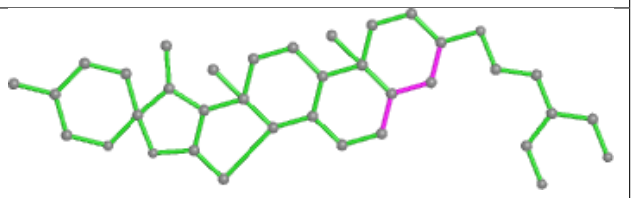
Ligand DU0 A 1413



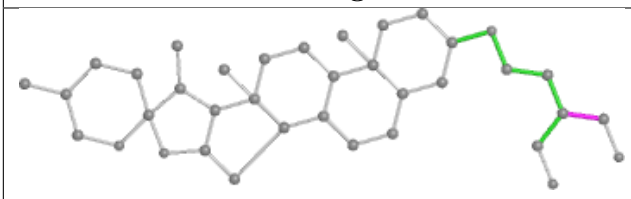
Ligand DU0 A 1416



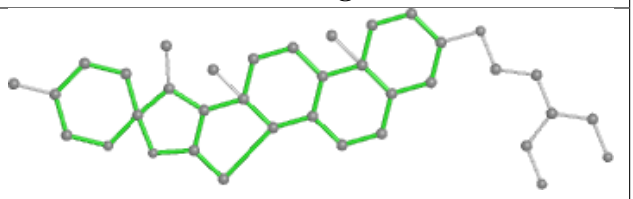
Bond lengths



Bond angles

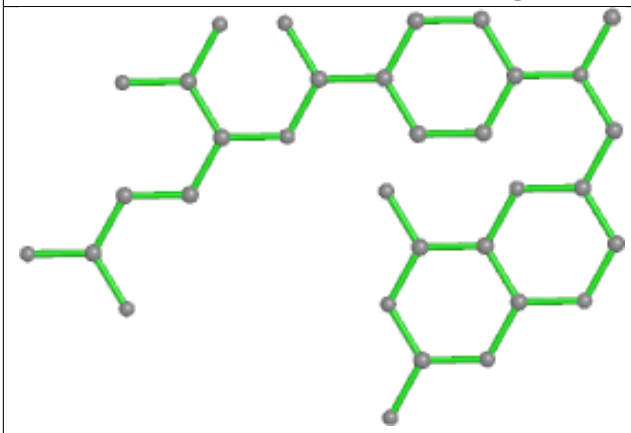


Torsions

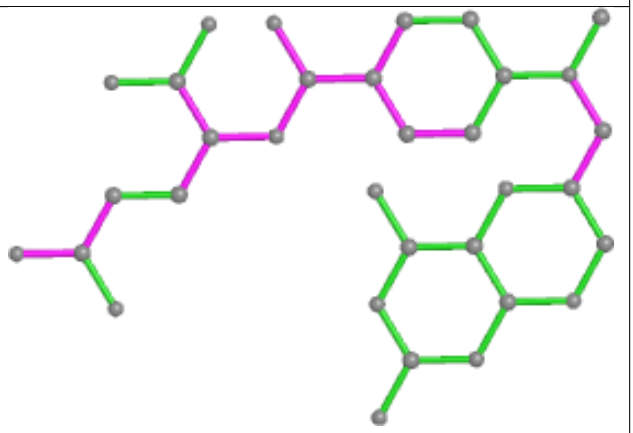


Rings

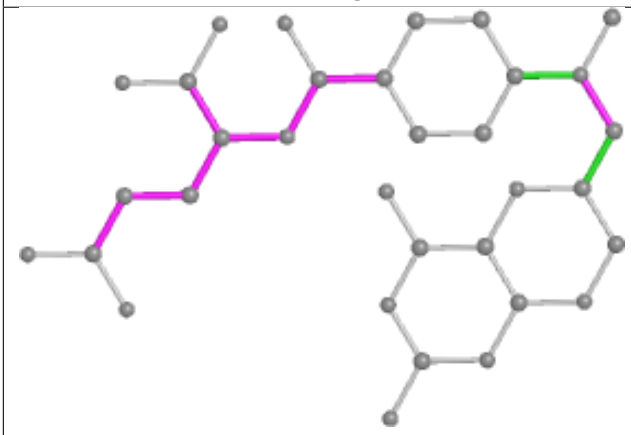
Ligand MTX A 1402



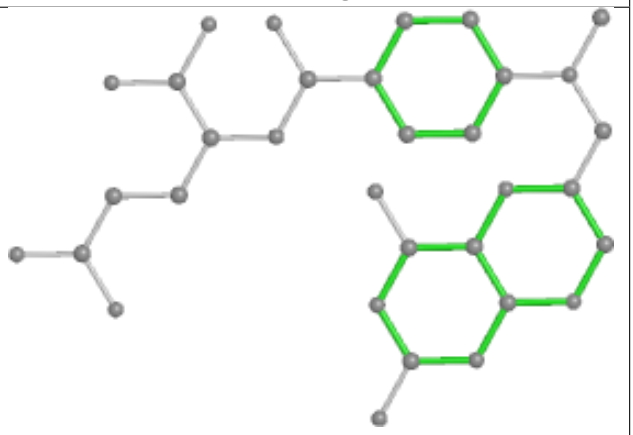
Bond lengths



Bond angles

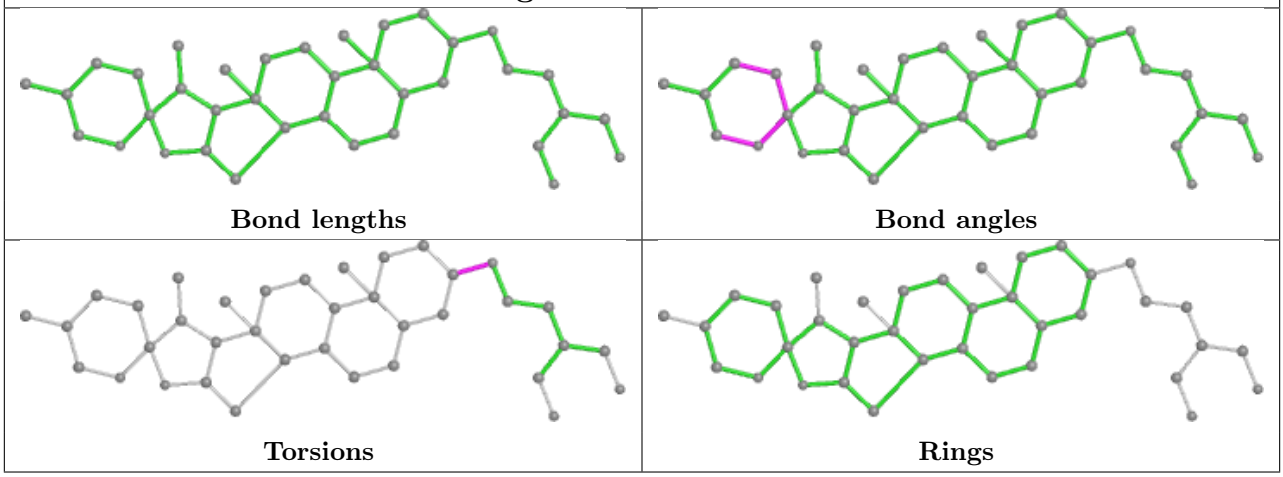


Torsions

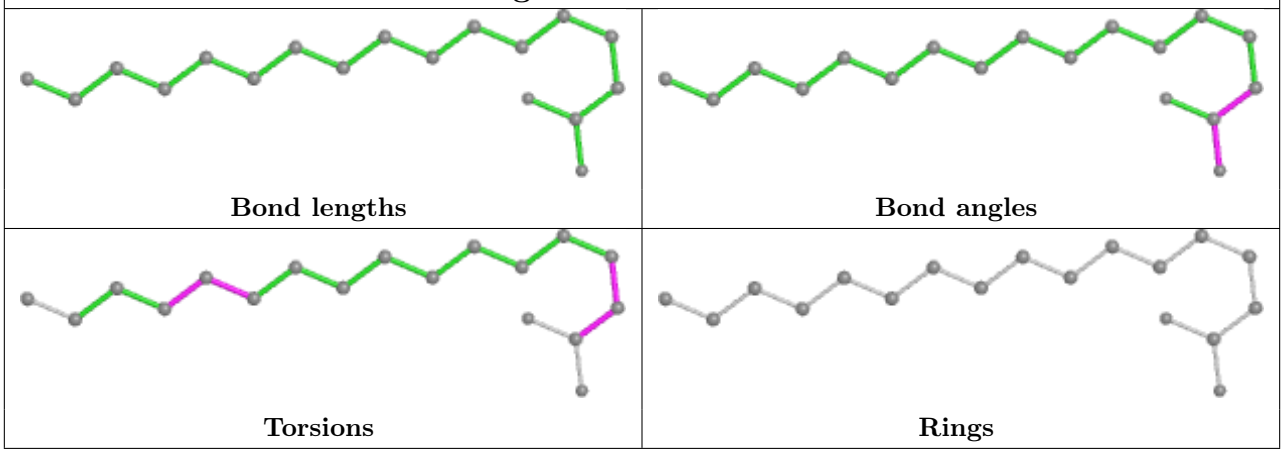


Rings

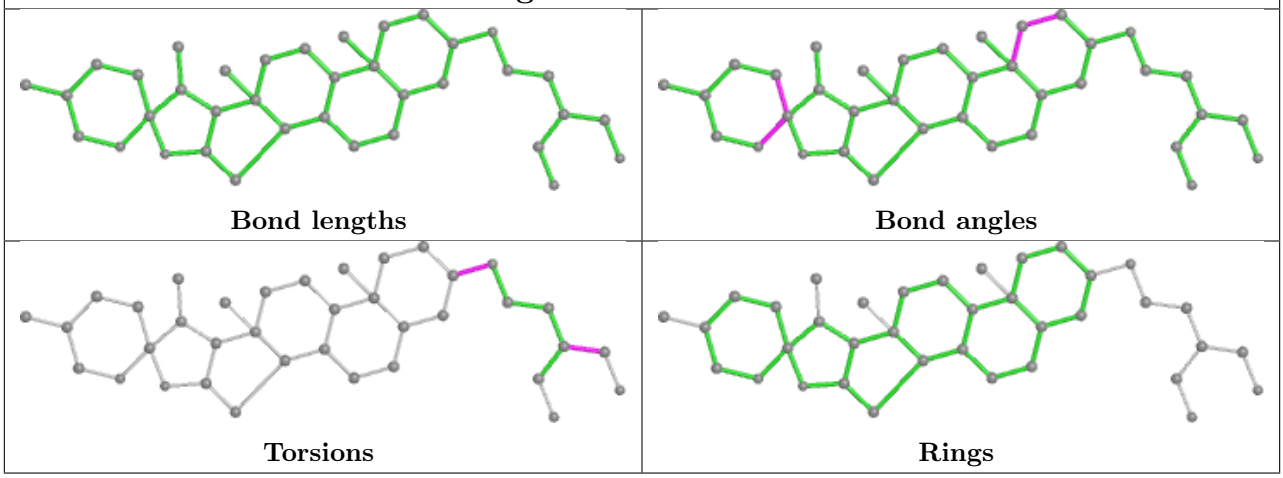
Ligand DU0 A 1408



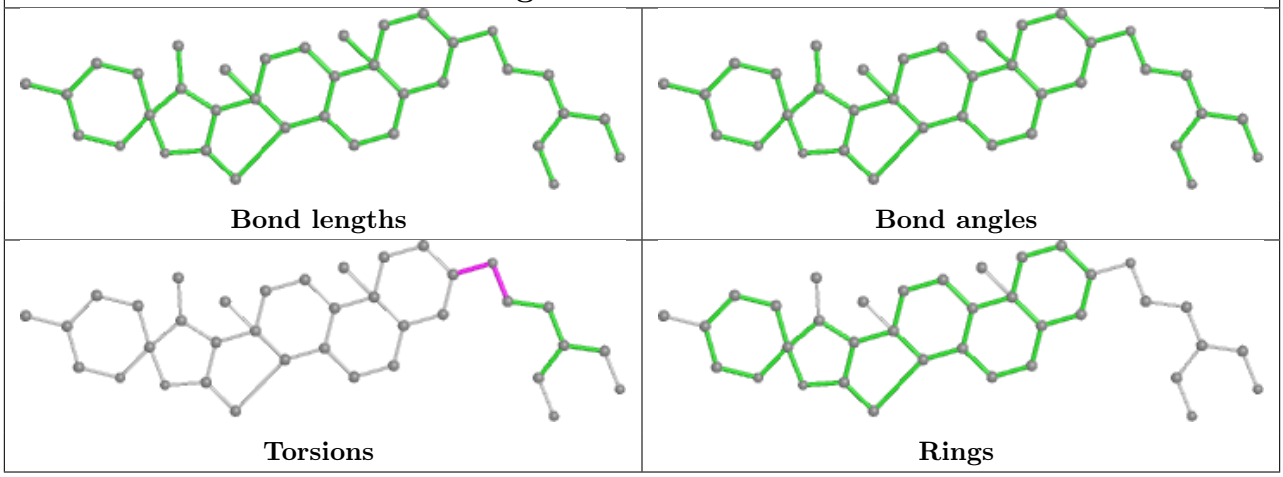
Ligand PLM A 1417



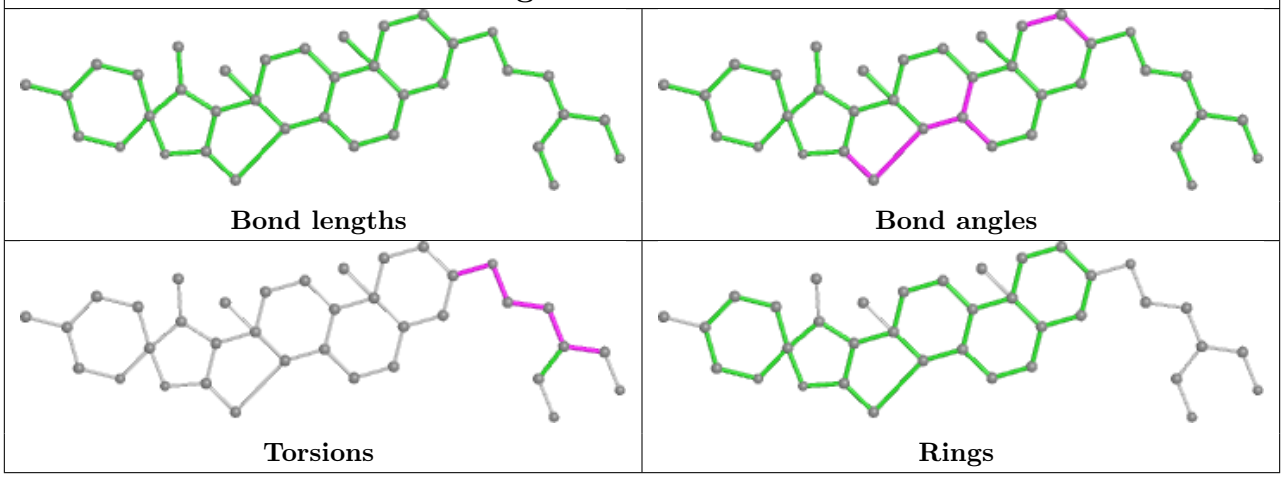
Ligand DU0 A 1403



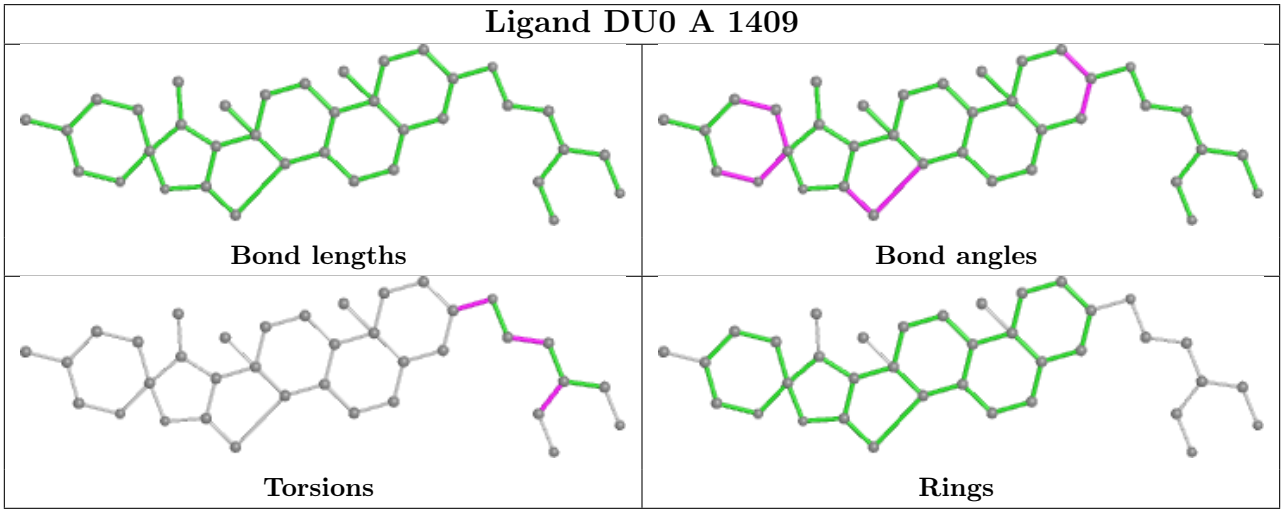
Ligand DU0 A 1404



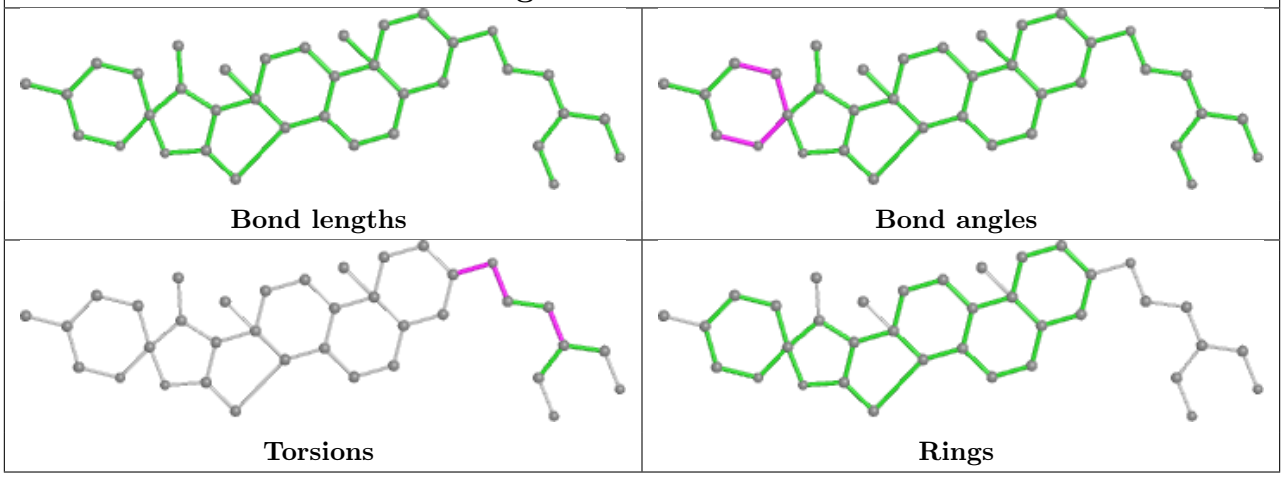
Ligand DU0 A 1406



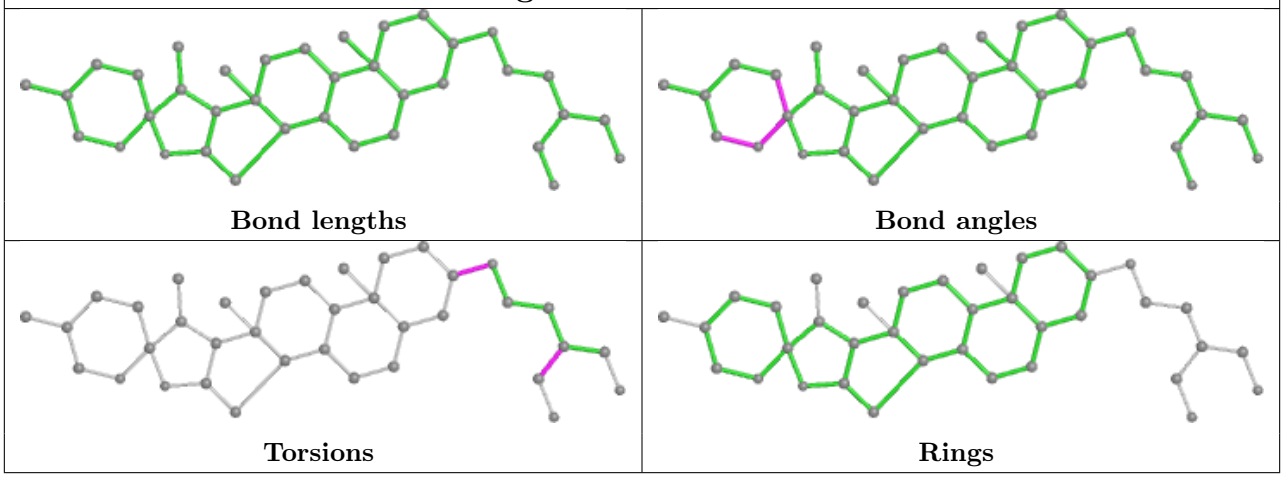
Ligand DU0 A 1409



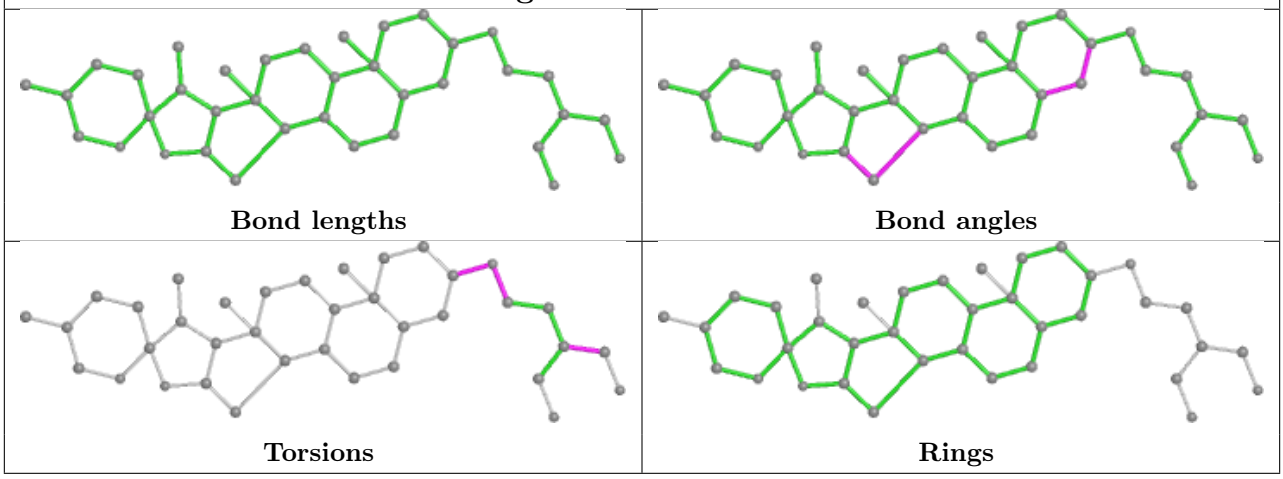
Ligand DU0 A 1411



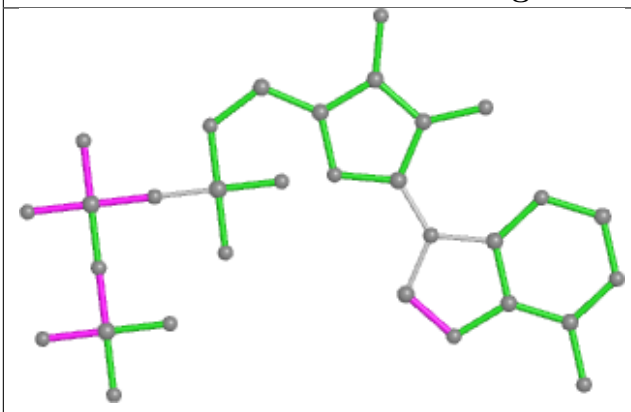
Ligand DU0 A 1410



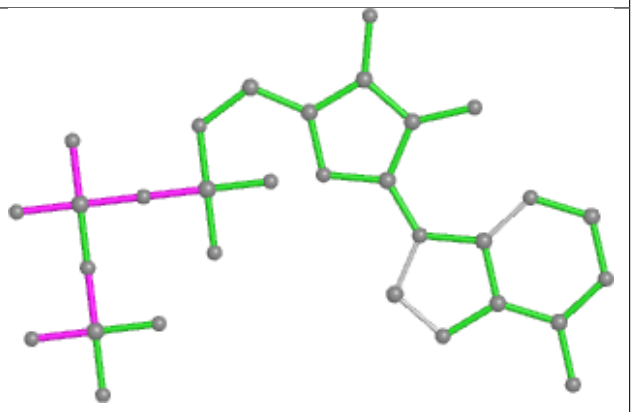
Ligand DU0 A 1412



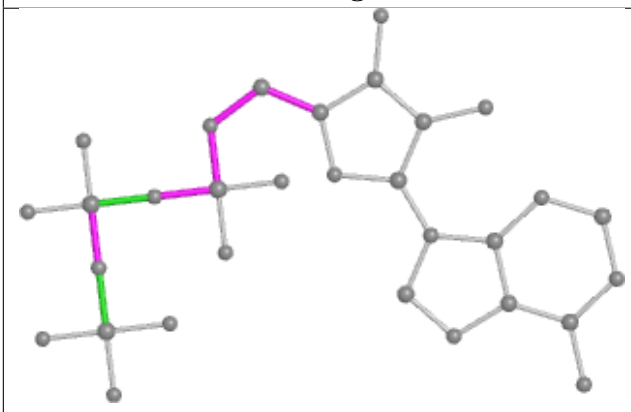
Ligand ANP A 1401



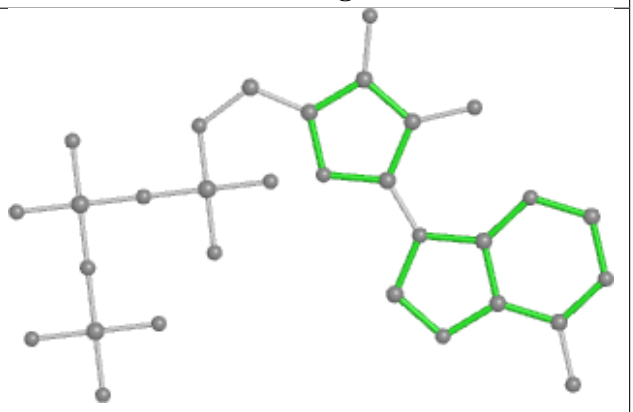
Bond lengths



Bond angles

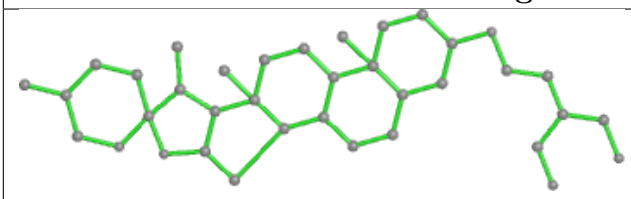


Torsions

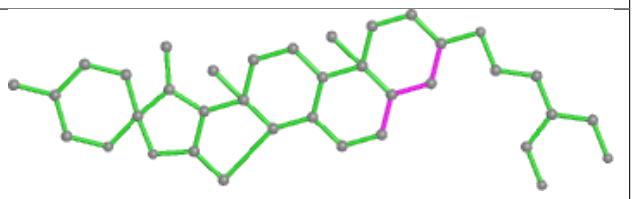


Rings

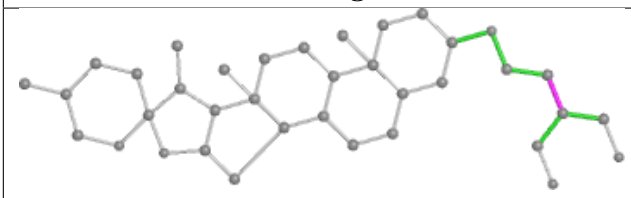
Ligand DU0 A 1407



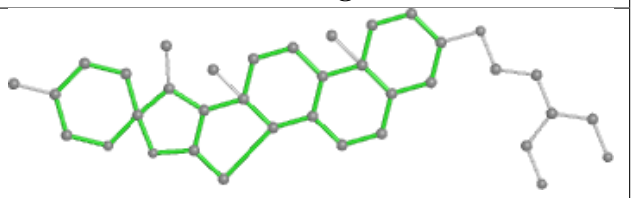
Bond lengths



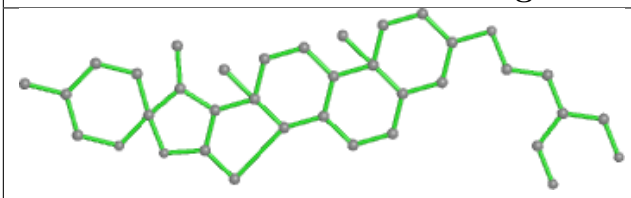
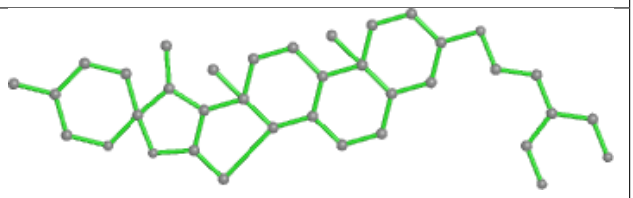
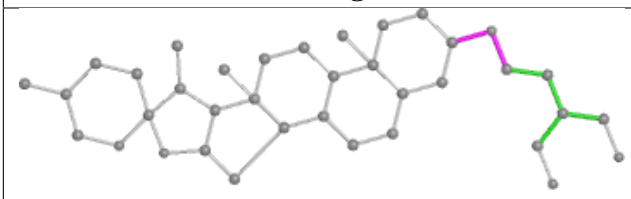
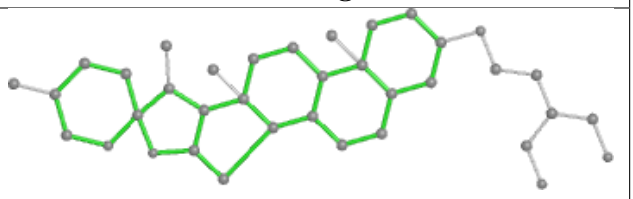
Bond angles



Torsions



Rings

Ligand DU0 A 1405	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

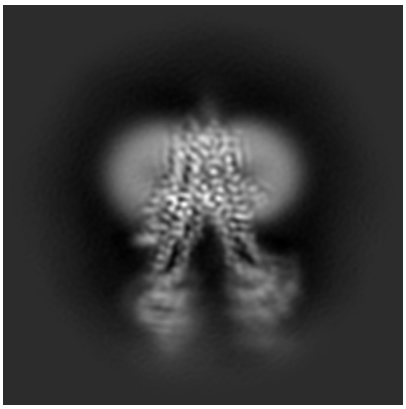
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38534. These allow visual inspection of the internal detail of the map and identification of artifacts.

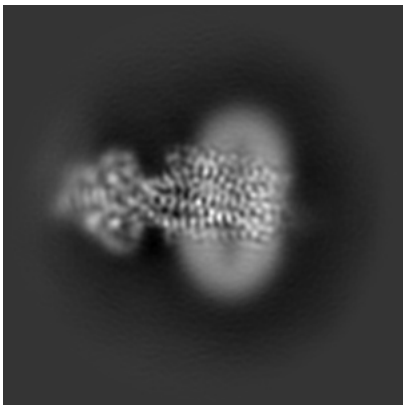
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

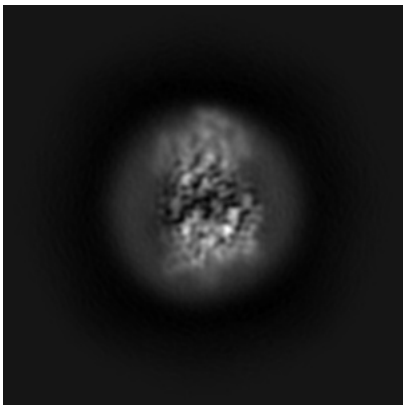
6.1.1 Primary map



X

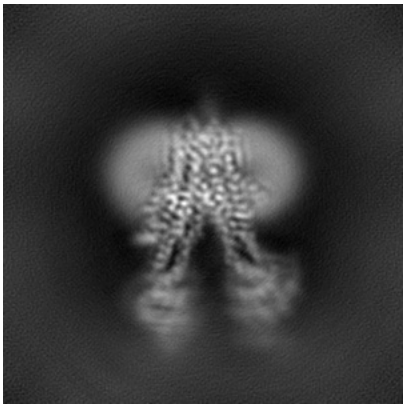


Y

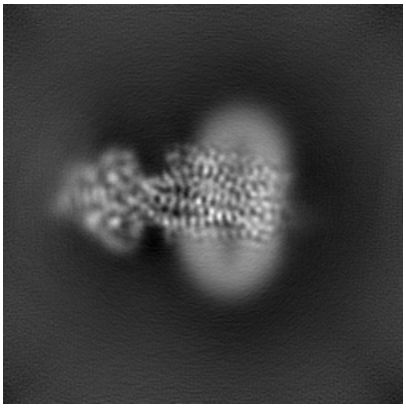


Z

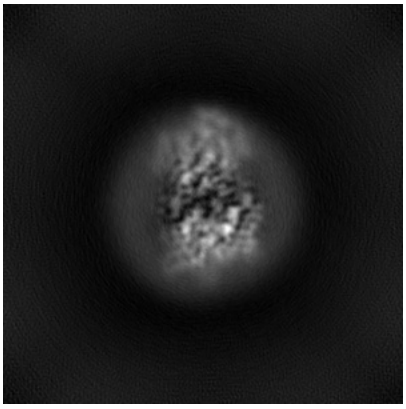
6.1.2 Raw map



X



Y

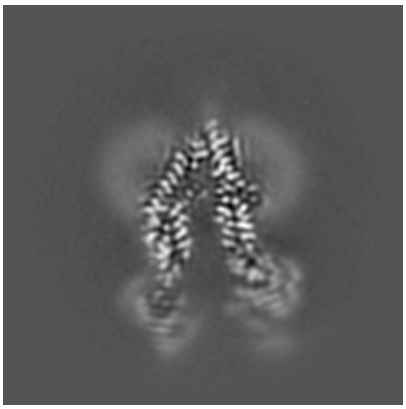


Z

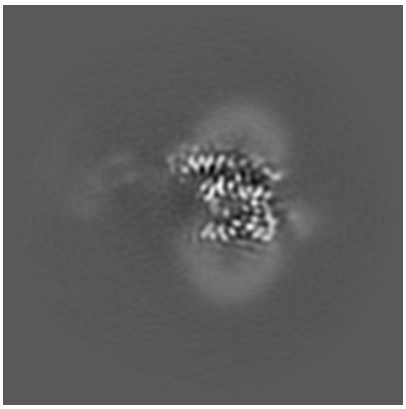
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

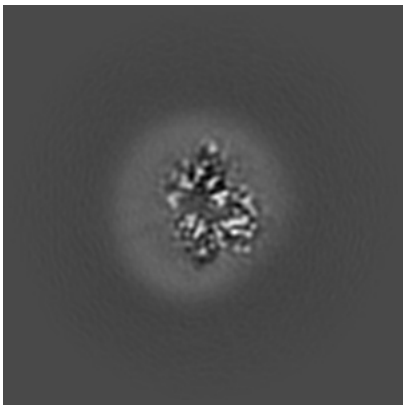
6.2.1 Primary map



X Index: 128

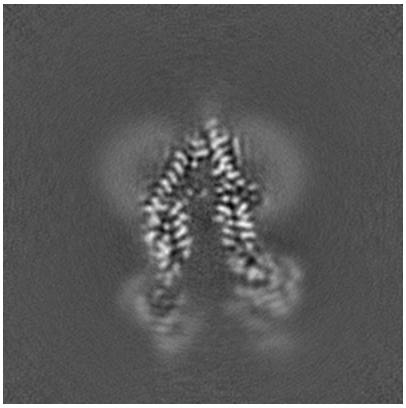


Y Index: 128

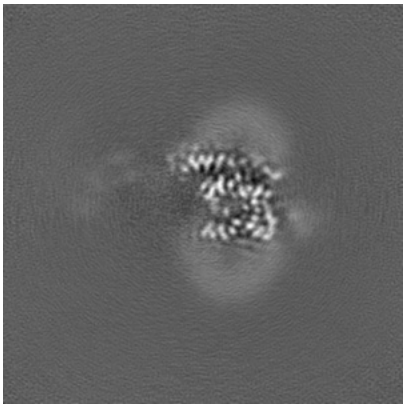


Z Index: 128

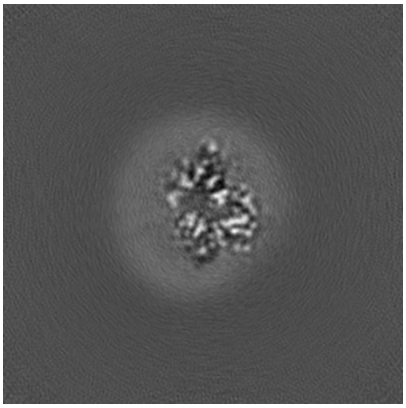
6.2.2 Raw map



X Index: 128



Y Index: 128

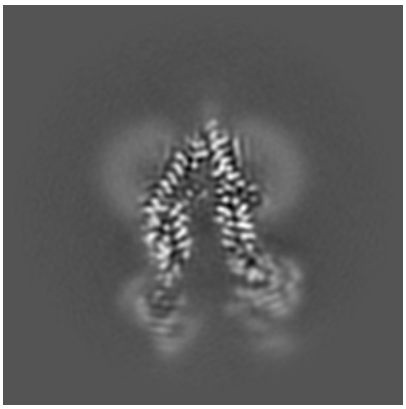


Z Index: 128

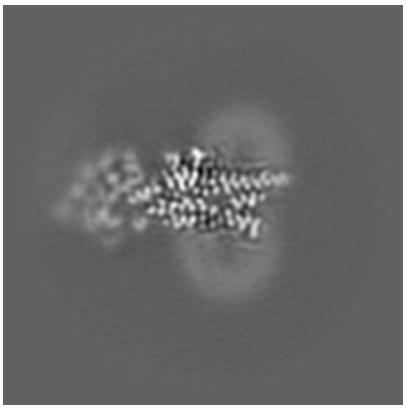
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

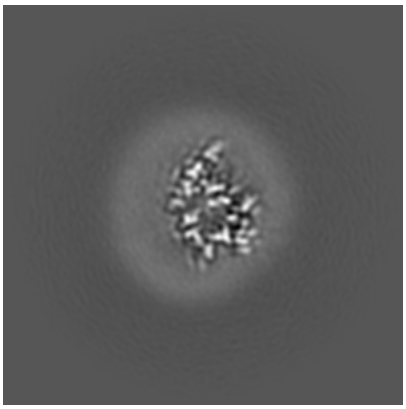
6.3.1 Primary map



X Index: 128

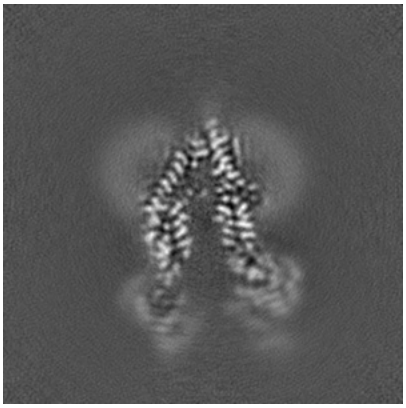


Y Index: 113

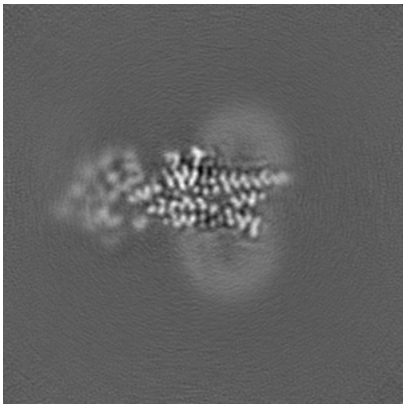


Z Index: 132

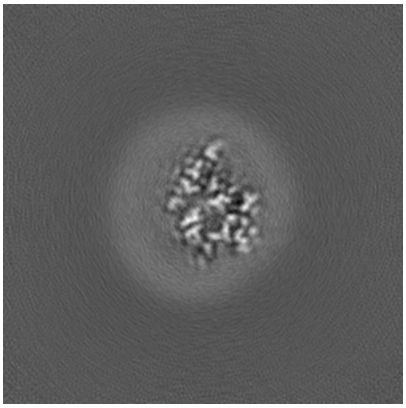
6.3.2 Raw map



X Index: 128



Y Index: 113

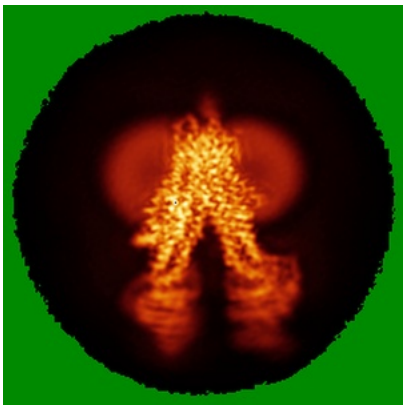


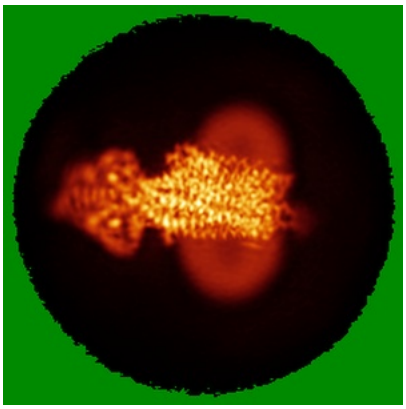
Z Index: 133

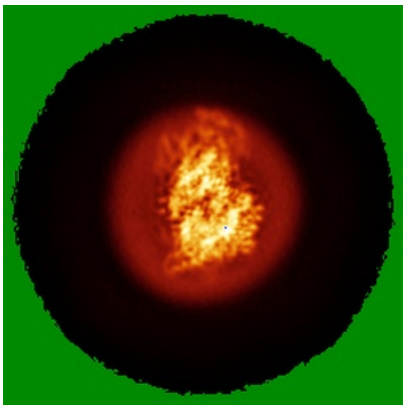
The images above show the largest variance slices of the map in three orthogonal directions.

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

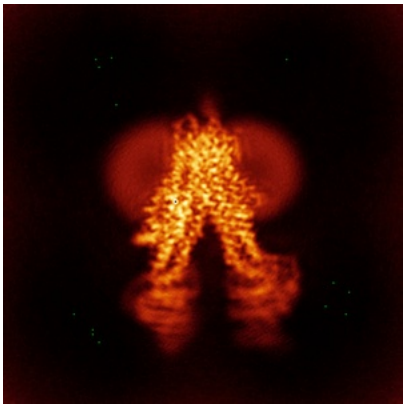
6.4.1 Primary map

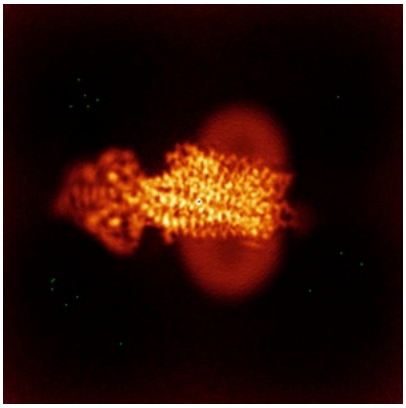

X

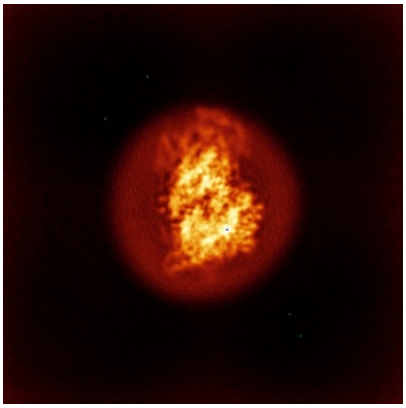

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0505. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

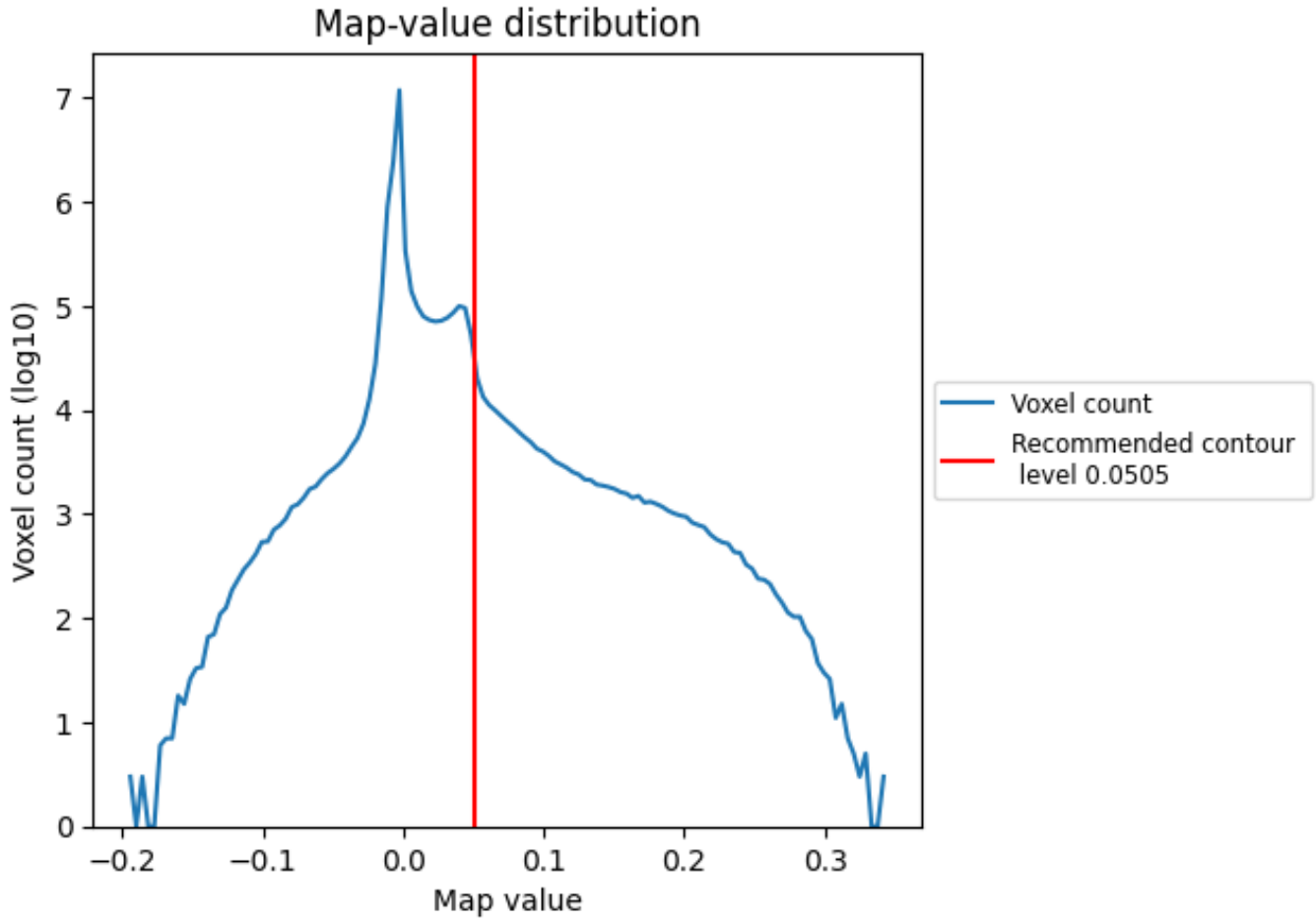
6.6 Mask visualisation (i)

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

7 Map analysis

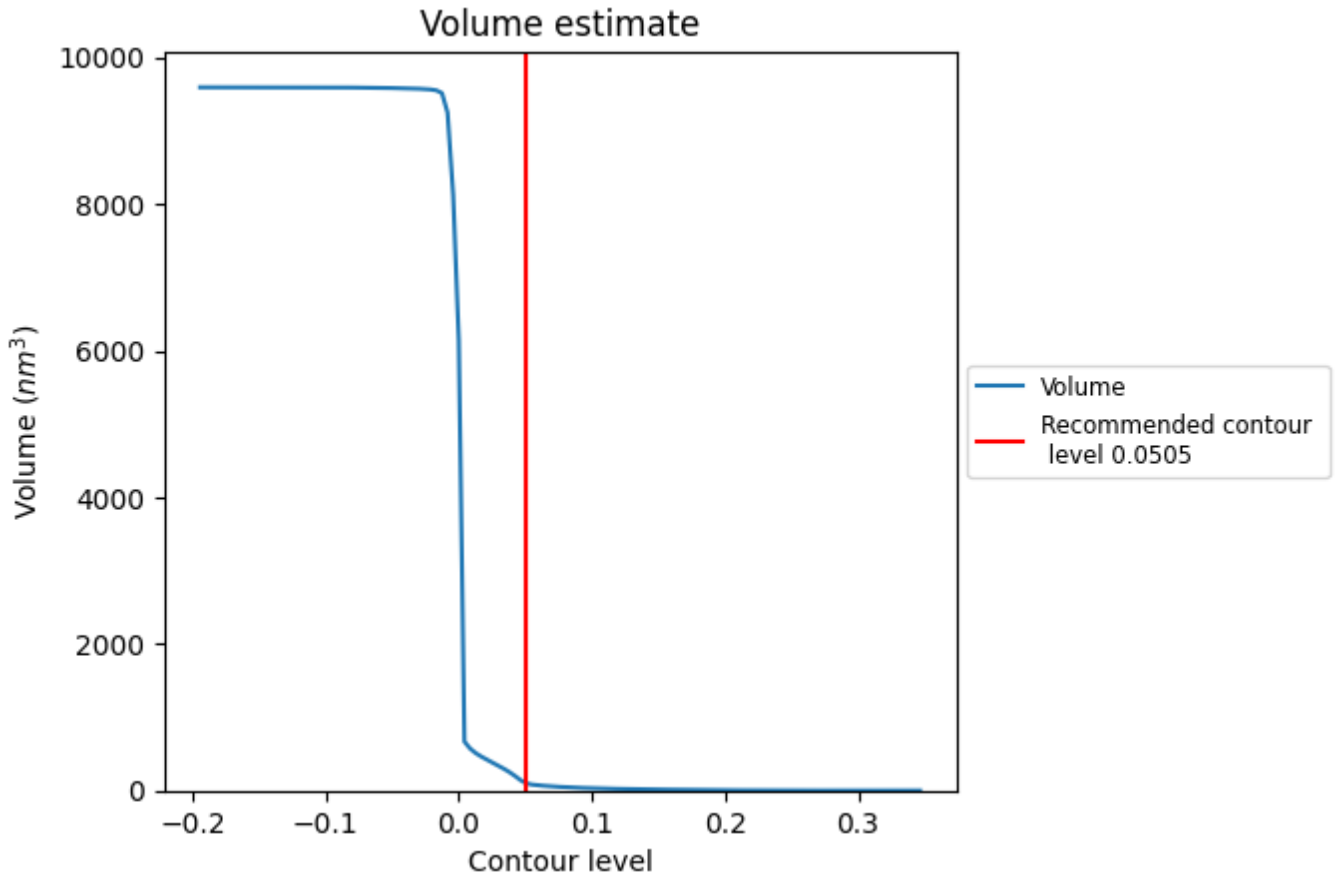
This section contains the results of statistical analysis of the map.

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.

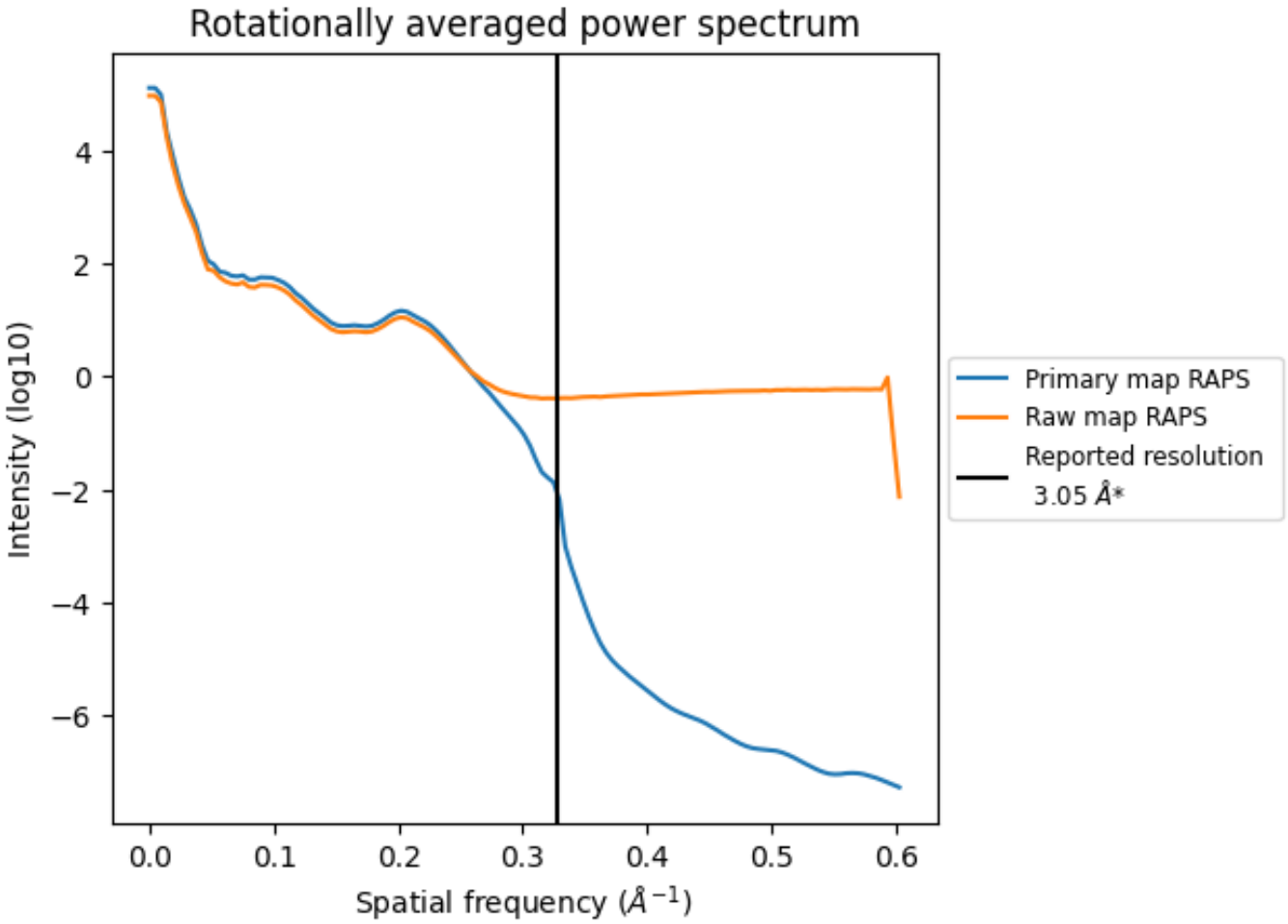
7.2 Volume estimate



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 91 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)

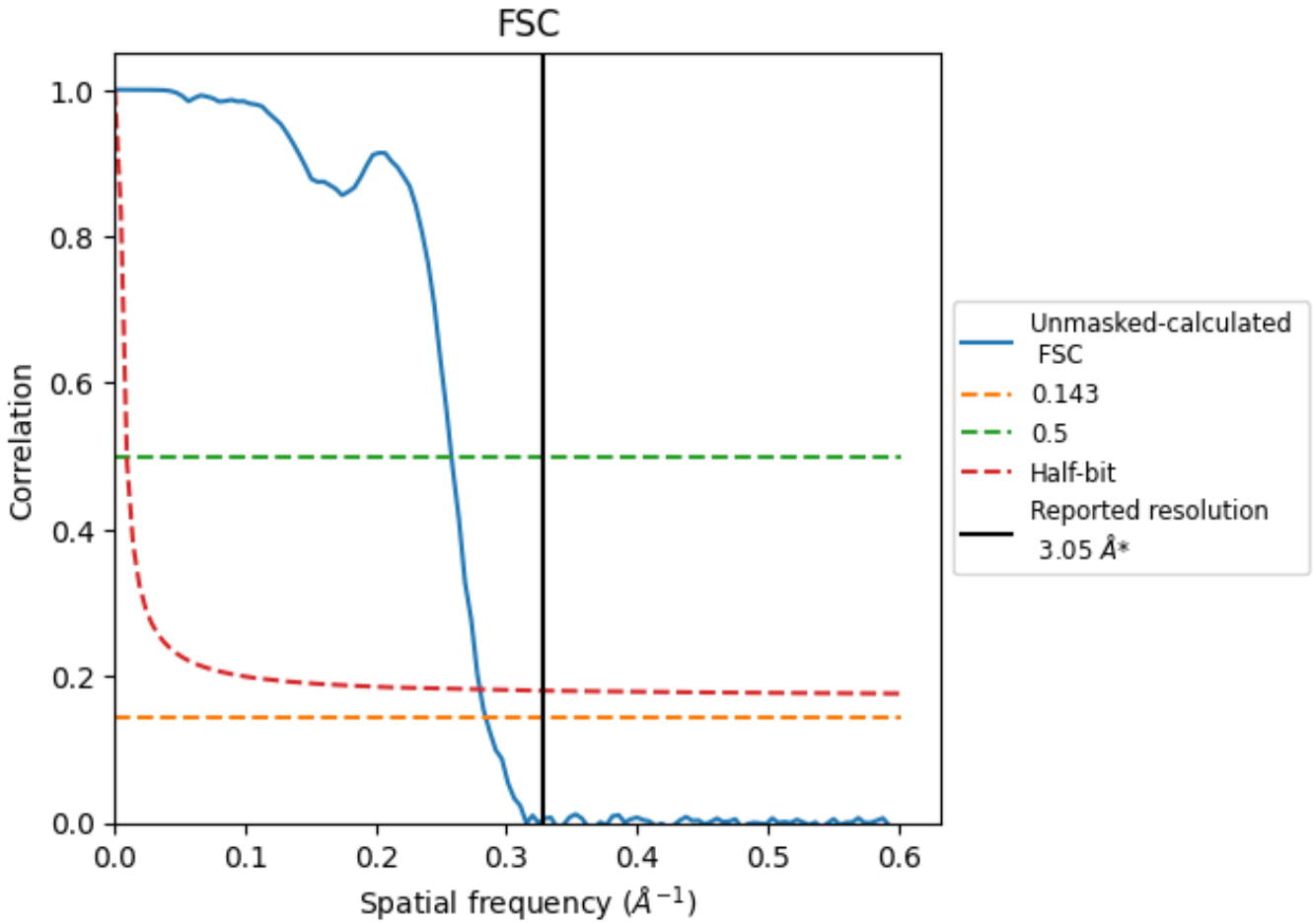


*Reported resolution corresponds to spatial frequency of 0.328 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.328 Å^{-1}

8.2 Resolution estimates (i)

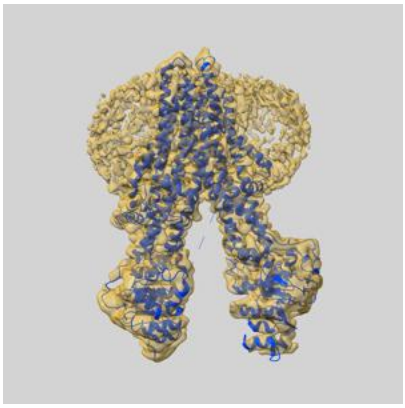
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.52	3.88	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.52 differs from the reported value 3.05 by more than 10 %

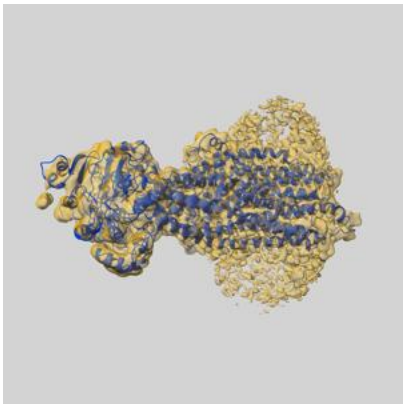
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38534 and PDB model 8XOM. Per-residue inclusion information can be found in section 3 on page 7.

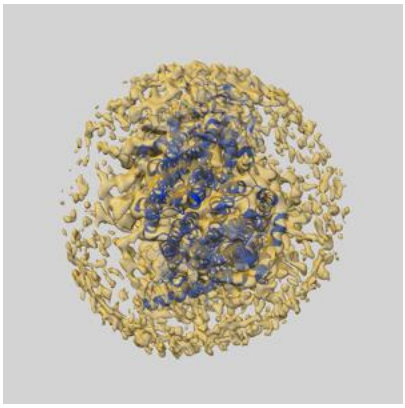
9.1 Map-model overlay



X



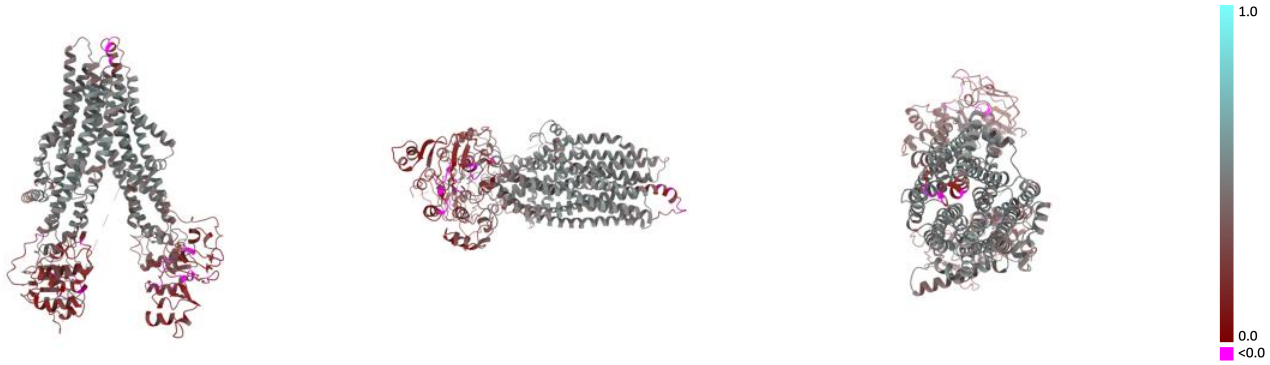
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0505 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.

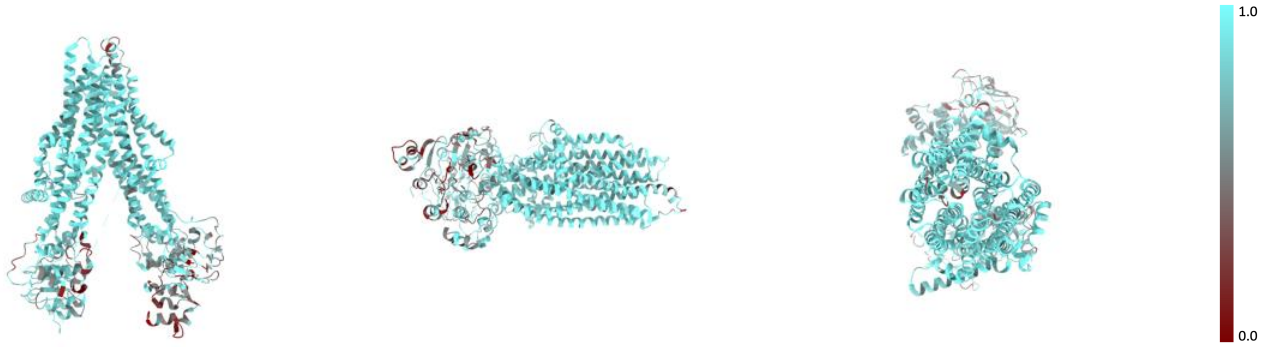
9.2 Q-score mapped to coordinate model (i)



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.

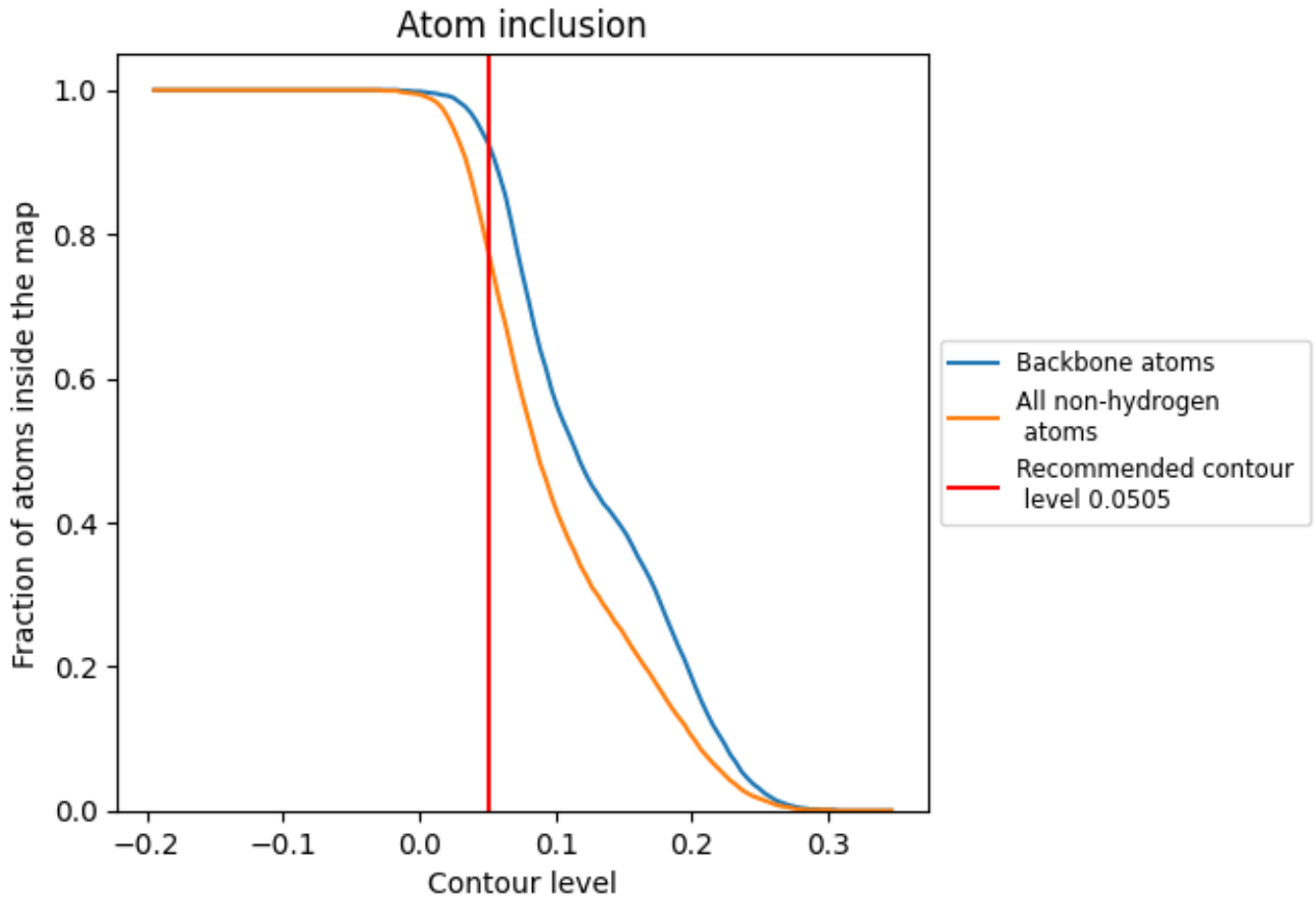
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0505).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0505) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.3650
A	0.7770	0.3650