Full wwPDB EM Validation Report ⓘ

Oct 25, 2026 – 02:17 PM JST

PDB ID	:	9UV7 / pdb_00009uv7
EMDB ID	:	EMD-64527
Title	:	Single-subunit apo Escherichia coli nicotinamide nucleotide transhydrogenase
Authors	:	Zhu, J.; Gennis, R.B.; Zhang, K.; Li, J.
Deposited on	:	2025-05-09
Resolution	:	3.43 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:

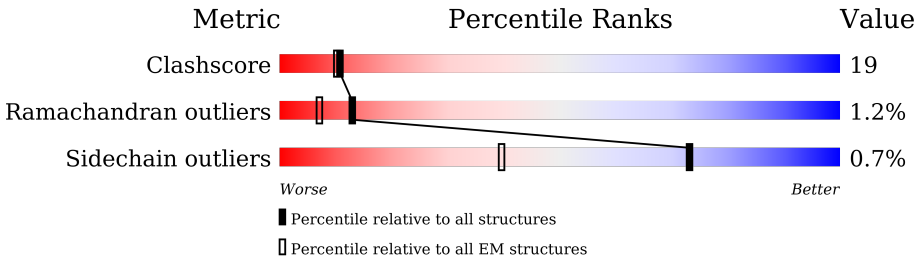
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

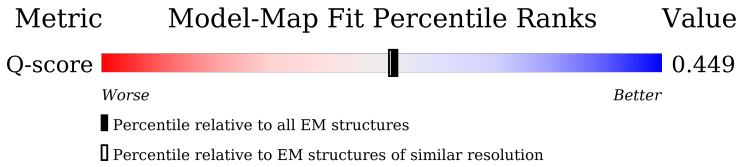
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.43 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.





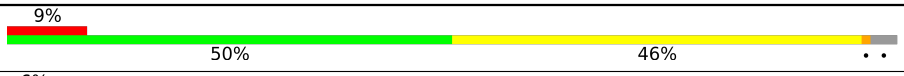
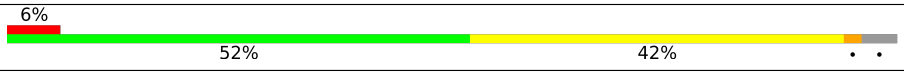
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13927 (2.93 - 3.93)

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	462	60% 35%
1	B	462	64% 31%
2	C	99	56% 44%
2	D	99	66% 32%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	377	
3	F	377	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13802 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 NAD(P) transhydrogenase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	444	Total	C	N	O	S	0	0
			3304	2142	549	591	22		
1	B	444	Total	C	N	O	S	0	0
			3304	2142	549	591	22		

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	99	Total	C	N	O	S	0	0
			758	510	121	122	5		
2	D	97	Total	C	N	O	S	0	0
			742	498	119	120	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	508	LYS	-	expression tag	UNP P07001
C	509	ASN	-	expression tag	UNP P07001
D	508	LYS	-	expression tag	UNP P07001
D	509	ASN	-	expression tag	UNP P07001

- Molecule 3 is a protein called NAD(P) transhydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	367	Total	C	N	O	S	0	0
			2739	1738	464	525	12		
3	F	361	Total	C	N	O	S	0	0
			2703	1713	461	518	11		

There are 6 discrepancies between the modelled and reference sequences:

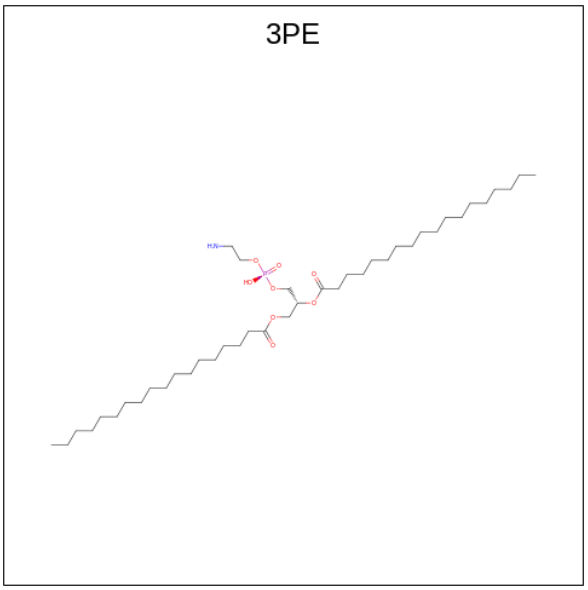
Chain	Residue	Modelled	Actual	Comment	Reference
E	999	HIS	-	expression tag	UNP P07001

Continued on next page...

Continued from previous page...

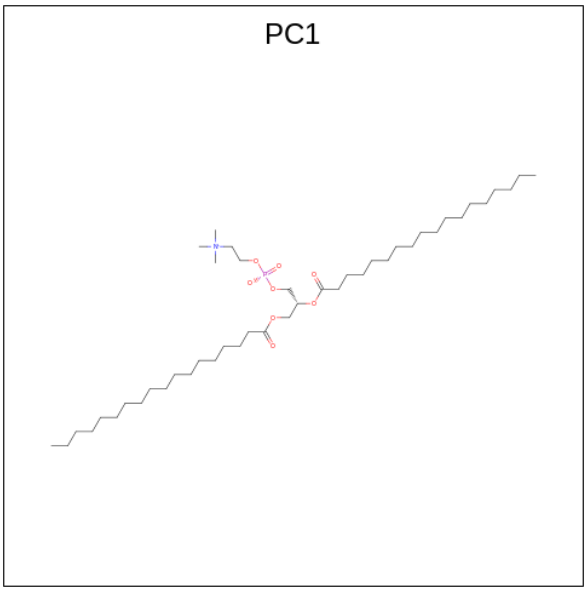
Chain	Residue	Modelled	Actual	Comment	Reference
E	1000	HIS	-	expression tag	UNP P07001
E	1001	GLY	-	expression tag	UNP P07001
F	999	HIS	-	expression tag	UNP P07001
F	1000	HIS	-	expression tag	UNP P07001
F	1001	GLY	-	expression tag	UNP P07001

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
4	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
4	D	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



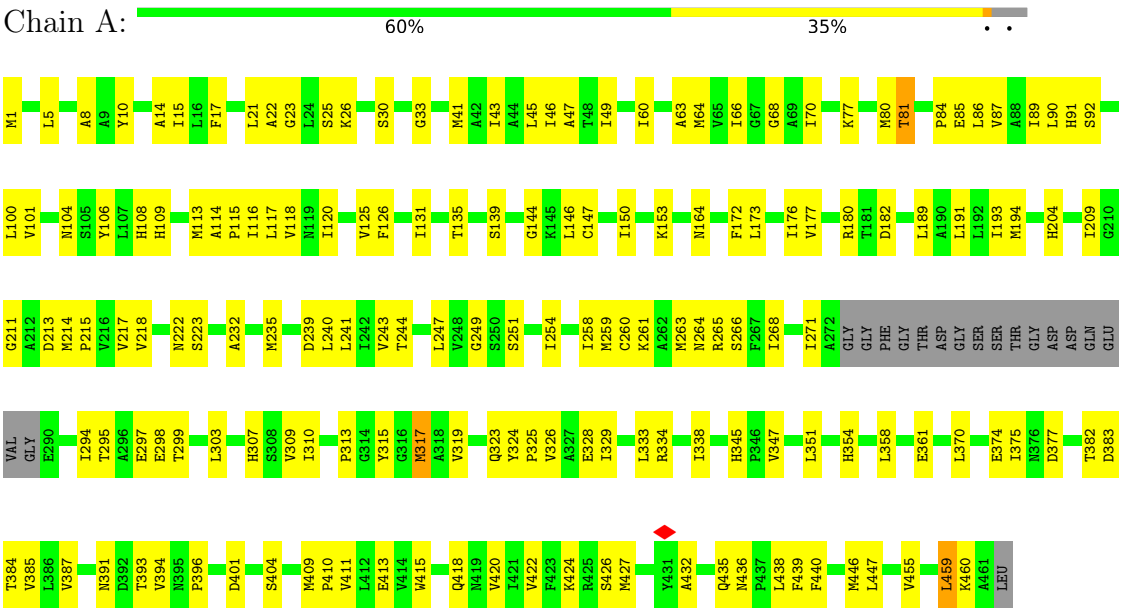
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			36	26	1	8	1	

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.

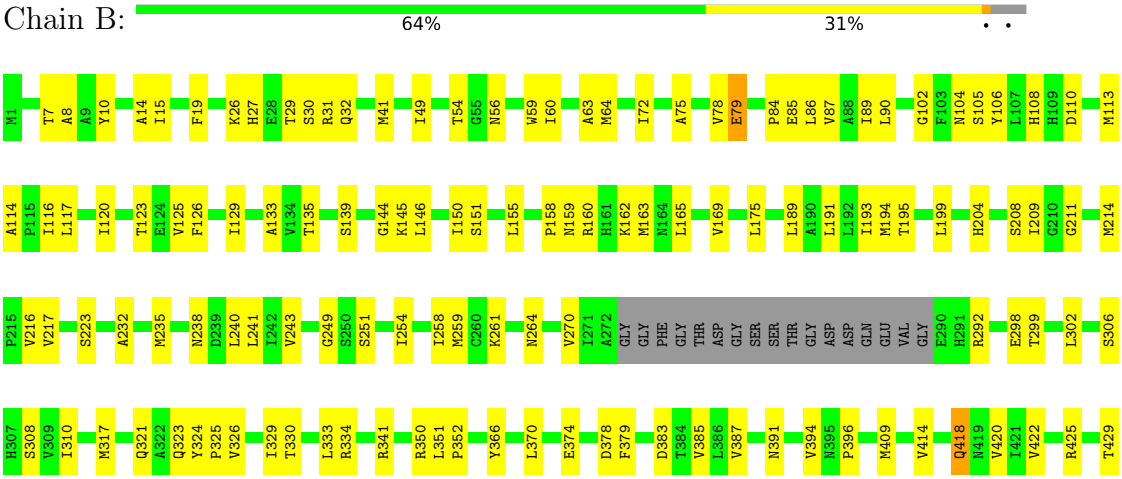
• Molecule 1: NAD(P) transhydrogenase subunit beta

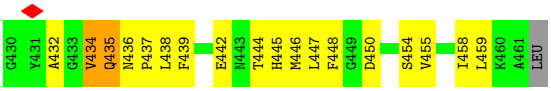
Chain A:



• Molecule 1: NAD(P) transhydrogenase subunit beta

Chain B:





• Molecule 2: NAD(P) transhydrogenase subunit alpha

Chain C:

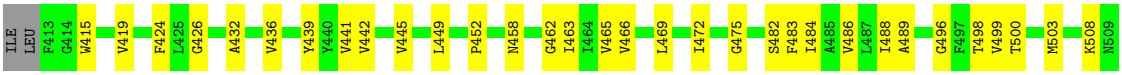




• Molecule 2: NAD(P) transhydrogenase subunit alpha

Chain D:

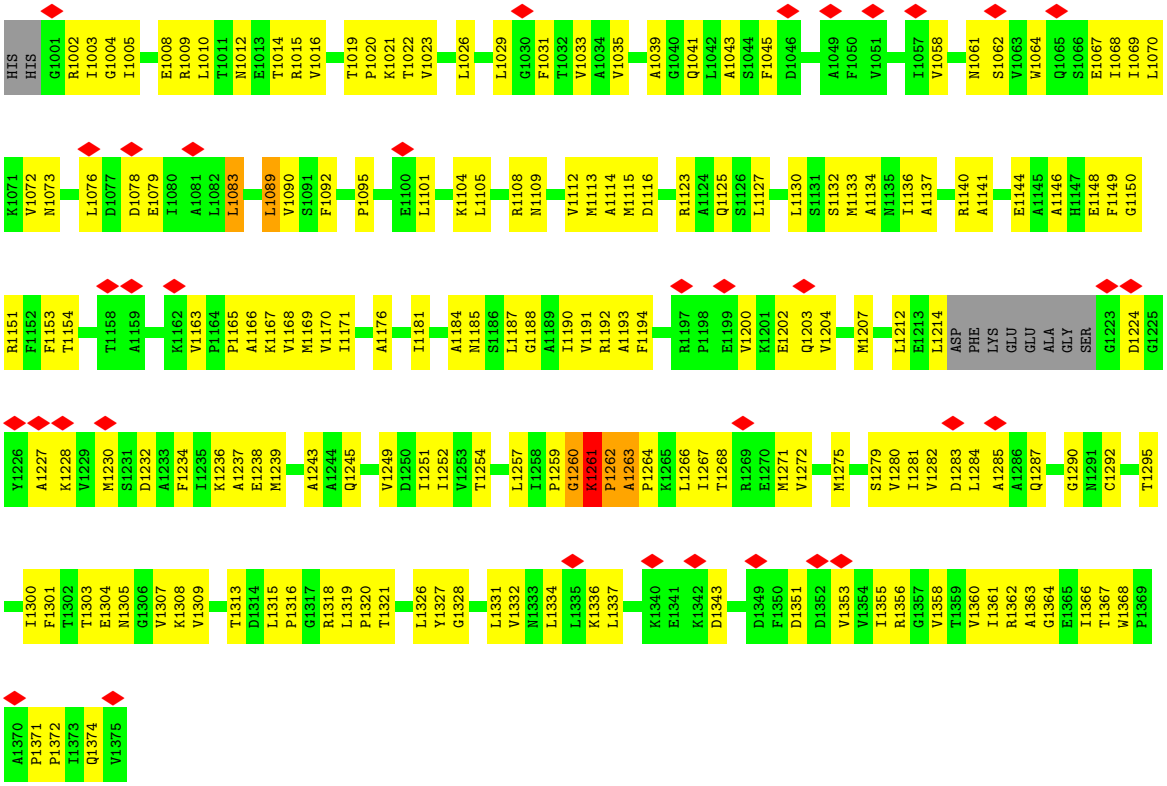




• Molecule 3: NAD(P) transhydrogenase subunit alpha

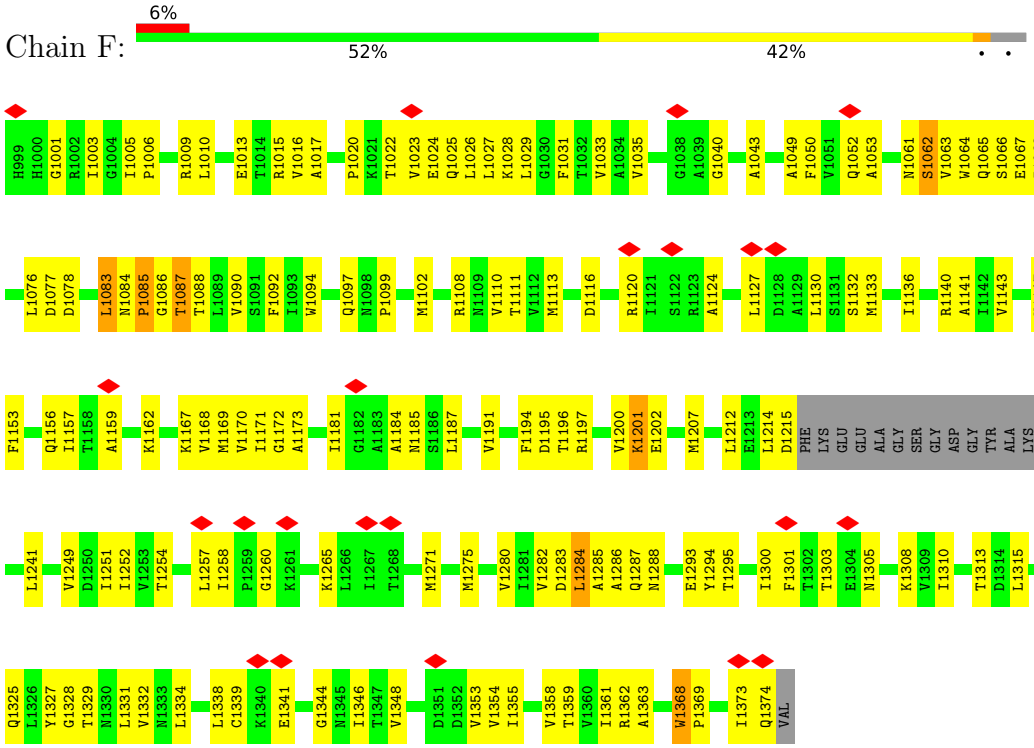
Chain E:





• Molecule 3: NAD(P) transhydrogenase subunit alpha

Chain F:


6%
52%
42%
H999 H1000 G1001 R1002 I1003 G1004 I1005 P1006 R1009 L1010 E1013 T1014 R1015 V1016 A1017 P1020 K1021 T1022 V1023 E1024 Q1025 L1026 L1027 K1028 L1029 G1030 F1031 T1032 V1033 A1034 V1035 G1038 A1039 G1040 A1043 A1049 F1050 V1051 Q1052 A1053 N1061 S1062 V1063 W1064 Q1065 S1066 E1067 I1068 I1069 L1070 K1071 V1072 N1073
L1076 D1077 D1078 L1083 N1084 P1085 G1086 T1087 T1088 L1089 V1090 S1091 F1092 T1093 W1094 Q1097 N1098 P1099 M1102 R1108 N1109 V1110 T1111 V1112 M1113 D1116 R1120 I1121 S1122 R1123 A1124 L1127 D1128 A1129 L1130 S1131 S1132 M1133 I1136 R1140 A1141 I1142 V1143 H1147 E1148 F1149 G1150 R1151 F1152
F1153 Q1156 I1157 T1158 A1159 K1162 K1167 V1168 M1169 V1170 I1171 G1172 A1173 I1181 G1182 A1183 A1184 N1185 S1186 L1187 V1191 F1194 D1195 T1196 R1197 V1200 K1201 E1202 M1207 L1212 E1213 L1214 D1215 PHE LYS GLU GLU ALA GLY SER GLY ASP GLY TYR ALA LYS VAL MET S1231 E1238
L1241 V1249 D1250 I1251 I1252 V1253 T1254 L1257 I1258 P1259 G1260 K1261 K1265 L1266 I1267 T1268 M1271 M1275 V1280 I1281 V1282 D1283 L1284 A1285 A1286 Q1287 N1288 E1293 Y1294 T1295 I1300 F1301 T1302 T1303 E1304 N1305 K1308 V1309 I1310 T1313 D1314 L1315 L1319 P1320 T1321 Q1322 S1323 S1324
Q1325 L1326 Y1327 G1328 T1329 N1330 L1331 V1332 N1333 L1334 L1338 C1339 K1340 E1341 G1344 N1345 I1346 T1347 V1348 D1351 D1352 V1353 V1354 I1355 V1358 T1359 V1360 I1361 R1362 A1363 W1368 P1369 I1373 Q1374 VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42826	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.443	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, 3PE

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	0.20	0/3367	0.41	0/4575
1	B	0.19	0/3367	0.37	0/4575
2	C	0.22	0/779	0.44	0/1060
2	D	0.20	0/763	0.38	0/1038
3	E	0.16	0/2781	0.37	0/3777
3	F	0.15	0/2746	0.38	0/3731
All	All	0.18	0/13803	0.39	0/18756

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
3	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	THR	Peptide
3	F	1368	TRP	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	3304	0	3415	129	0
1	B	3304	0	3415	104	0
2	C	758	0	781	43	0
2	D	742	0	759	29	0
3	E	2739	0	2799	148	0
3	F	2703	0	2753	121	0
4	A	112	0	152	4	0
4	B	31	0	36	3	0
4	C	31	0	36	1	0
4	D	42	0	61	4	0
5	B	36	0	46	3	0
All	All	13802	0	14253	521	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 19.

All (521) 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:391:ASN:O	1:A:436:ASN:ND2	2.10	0.84
3:F:1090:VAL:HG12	3:F:1113:MET:HB3	1.60	0.81
1:B:330:THR:O	1:B:334:ARG:HB2	1.83	0.79
3:F:1099:PRO:HA	3:F:1102:MET:HE1	1.68	0.76
3:E:1061:ASN:HA	3:E:1064:TRP:HD1	1.50	0.76
3:E:1073:ASN:HA	3:E:1092:PHE:HB2	1.67	0.75
3:E:1133:MET:HE3	3:E:1133:MET:HA	1.68	0.75
3:F:1169:MET:HB2	3:F:1249:VAL:HG11	1.68	0.75
1:A:309:VAL:HG22	1:A:384:THR:HB	1.72	0.71
3:F:1353:VAL:HG11	3:F:1373:ILE:HD12	1.72	0.70
3:E:1154:THR:OG1	3:E:1187:LEU:O	2.08	0.70
1:A:104:ASN:HB2	2:C:478:VAL:HG13	1.71	0.70
1:A:80:MET:HG3	1:A:81:THR:HG23	1.72	0.70
3:F:1157:ILE:HG23	3:F:1162:LYS:HB2	1.74	0.70
3:F:1294:TYR:HB3	3:F:1301:PHE:HB3	1.74	0.70
1:A:345:HIS:NE2	1:A:410:PRO:O	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1026:LEU:HG	3:E:1332:VAL:HG22	1.74	0.69
3:E:1132:SER:HB2	3:E:1326:LEU:HD11	1.73	0.69
3:F:1295:THR:HA	3:F:1300:ILE:HG23	1.75	0.68
3:E:1252:ILE:HB	3:E:1281:ILE:HG22	1.75	0.68
3:F:1084:ASN:HB2	3:F:1087:THR:HG23	1.75	0.68
1:B:329:ILE:HG13	1:B:459:LEU:HD13	1.76	0.67
3:E:1004:GLY:HA3	3:E:1069:ILE:HD13	1.76	0.67
1:A:401:ASP:HB3	1:A:404:SER:HB2	1.77	0.67
3:E:1202:GLU:N	3:E:1202:GLU:OE1	2.27	0.67
1:B:78:VAL:O	1:B:79:GLU:HB2	1.94	0.66
1:B:232:ALA:HA	1:B:235:MET:HE3	1.76	0.66
3:F:1102:MET:HB2	3:F:1361:ILE:HD11	1.77	0.66
3:E:1125:GLN:HE21	3:F:1159:ALA:HB1	1.61	0.66
1:A:309:VAL:HG23	1:A:338:ILE:HD11	1.78	0.66
1:B:385:VAL:HG11	1:B:414:VAL:HB	1.77	0.66
1:B:110:ASP:HB3	1:B:113:MET:HE2	1.77	0.65
1:A:328:GLU:HG2	1:A:459:LEU:HD21	1.78	0.65
3:F:1068:ILE:HG23	3:F:1088:THR:HB	1.78	0.65
2:C:465:VAL:HG23	2:C:486:VAL:HA	1.78	0.65
2:C:468:ALA:O	2:C:482:SER:OG	2.14	0.64
3:E:1328:GLY:HA2	3:E:1331:LEU:HD12	1.78	0.64
3:E:1154:THR:HG23	3:E:1188:GLY:HA3	1.77	0.64
3:F:1020:PRO:HA	3:F:1023:VAL:HB	1.80	0.64
3:E:1287:GLN:NE2	3:E:1313:THR:O	2.30	0.64
1:A:385:VAL:HB	1:A:420:VAL:HG22	1.80	0.64
3:E:1090:VAL:HG12	3:E:1113:MET:HB2	1.80	0.64
3:F:1185:ASN:ND2	3:F:1207:MET:O	2.30	0.64
1:A:240:LEU:HD21	2:C:463:ILE:HD11	1.79	0.64
2:D:465:VAL:HG13	2:D:489:ALA:HB3	1.80	0.64
2:D:452:PRO:HG3	2:D:503:MET:HG3	1.79	0.63
3:E:1281:ILE:HD11	3:E:1309:VAL:HG12	1.80	0.63
1:B:155:LEU:H	1:B:208:SER:HA	1.63	0.63
1:B:105:SER:OG	1:B:235:MET:SD	2.54	0.62
3:E:1095:PRO:HB2	3:E:1368:TRP:CE2	2.35	0.62
3:E:1239:MET:HE2	3:E:1266:LEU:HD13	1.82	0.62
3:E:1003:ILE:HG22	3:E:1033:VAL:HA	1.80	0.62
1:B:144:GLY:HA3	1:B:150:ILE:HD12	1.81	0.62
3:F:1196:THR:HB	3:F:1197:ARG:HH21	1.65	0.62
3:E:1133:MET:HE2	3:E:1316:PRO:HB3	1.82	0.62
3:E:1141:ALA:HB1	3:E:1282:VAL:HG11	1.81	0.62
5:B:501:PC1:H231	4:D:601:3PE:H342	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG13	2:C:458:ASN:HD21	1.64	0.61
1:B:108:HIS:HE1	2:D:475:GLY:H	1.47	0.61
3:E:1334:LEU:HD11	3:E:1358:VAL:HG11	1.82	0.61
1:B:204:HIS:O	1:B:208:SER:OG	2.13	0.61
2:D:465:VAL:HG12	2:D:486:VAL:HA	1.80	0.61
1:A:241:LEU:HD22	2:C:463:ILE:HG23	1.83	0.61
1:A:427:MET:O	1:A:427:MET:HG3	2.01	0.61
3:F:1120:ARG:HD3	3:F:1130:LEU:HD11	1.82	0.61
3:F:1354:VAL:O	3:F:1358:VAL:HG12	1.99	0.61
3:F:1005:ILE:HG12	3:F:1070:LEU:HD11	1.82	0.60
3:E:1136:ILE:HG23	3:E:1319:LEU:HD23	1.82	0.60
3:F:1238:GLU:HA	3:F:1241:LEU:HG	1.83	0.60
1:A:241:LEU:HD21	2:C:466:VAL:HG22	1.84	0.60
3:E:1116:ASP:HA	3:E:1130:LEU:HD21	1.84	0.60
2:C:445:VAL:HG11	2:C:453:LEU:HD22	1.84	0.60
3:E:1134:ALA:HB1	3:E:1176:ALA:HB2	1.84	0.60
3:F:1066:SER:O	3:F:1087:THR:HG22	2.02	0.60
3:F:1085:PRO:HA	3:F:1108:ARG:O	2.02	0.60
3:E:1003:ILE:HG12	3:E:1026:LEU:HD13	1.83	0.59
3:F:1133:MET:HE2	3:F:1133:MET:HA	1.84	0.59
3:E:1112:VAL:C	3:E:1113:MET:HE2	2.26	0.59
3:E:1151:ARG:HH21	3:E:1163:VAL:HB	1.67	0.59
2:C:414:GLY:O	2:C:418:SER:N	2.34	0.59
3:E:1257:LEU:HD12	3:E:1285:ALA:HA	1.84	0.59
3:F:1152:PHE:HE2	3:F:1156:GLN:HE21	1.51	0.59
3:F:1265:LYS:HD2	3:F:1293:GLU:HA	1.83	0.59
4:A:503:3PE:H362	4:D:601:3PE:H352	1.84	0.59
2:D:496:GLY:O	2:D:500:THR:OG1	2.20	0.59
3:F:1025:GLN:HA	3:F:1028:LYS:HD2	1.85	0.59
2:C:501:GLN:O	2:C:505:LYS:HE3	2.02	0.58
1:A:418:GLN:NE2	3:F:1157:ILE:HG21	2.18	0.58
3:F:1133:MET:HE1	3:F:1323:SER:HA	1.84	0.58
1:A:370:LEU:HD23	1:A:374:GLU:HG2	1.85	0.58
3:E:1353:VAL:HA	3:E:1356:ARG:HH21	1.69	0.58
1:B:135:THR:O	1:B:139:SER:OG	2.16	0.58
3:E:1140:ARG:HH12	3:F:1147:HIS:HA	1.68	0.58
1:B:425:ARG:NH1	1:B:425:ARG:HB2	2.19	0.58
3:E:1003:ILE:HD11	3:E:1070:LEU:HD21	1.86	0.58
1:A:108:HIS:CD2	2:C:478:VAL:HG21	2.38	0.58
1:A:268:ILE:HD12	1:A:268:ILE:H	1.69	0.58
3:F:1303:THR:OG1	3:F:1305:ASN:OD1	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1009:ARG:HD2	3:F:1076:LEU:HD22	1.86	0.57
3:F:1113:MET:SD	3:F:1358:VAL:HG13	2.43	0.57
1:A:81:THR:HB	1:A:354:HIS:HE2	1.70	0.57
3:E:1263:ALA:HB3	3:E:1290:GLY:H	1.68	0.57
3:F:1325:GLN:O	3:F:1329:THR:HG23	2.05	0.57
2:C:465:VAL:O	2:C:469:LEU:HG	2.05	0.56
3:F:1005:ILE:HB	3:F:1035:VAL:HG13	1.87	0.56
1:A:240:LEU:O	1:A:244:THR:HG23	2.04	0.56
1:A:307:HIS:C	1:A:338:ILE:HG13	2.30	0.56
1:B:114:ALA:HB3	1:B:117:LEU:HG	1.88	0.56
1:A:294:ILE:HG13	1:A:298:GLU:HB2	1.88	0.56
3:E:1061:ASN:HA	3:E:1064:TRP:CD1	2.37	0.56
3:F:1132:SER:O	3:F:1136:ILE:HG12	2.05	0.56
1:A:14:ALA:HB1	1:A:243:VAL:HG11	1.88	0.56
3:E:1140:ARG:HE	3:E:1318:ARG:HG2	1.71	0.56
3:E:1167:LYS:HB2	3:E:1249:VAL:HA	1.87	0.56
1:A:182:ASP:OD1	1:A:182:ASP:N	2.34	0.56
3:F:1020:PRO:O	3:F:1024:GLU:HG3	2.06	0.56
3:E:1019:THR:H	3:E:1022:THR:HG1	1.54	0.56
1:A:232:ALA:HA	1:A:235:MET:HE3	1.86	0.55
1:B:366:TYR:CE2	2:D:508:LYS:HB3	2.41	0.55
1:B:216:VAL:HG21	1:B:270:VAL:HG11	1.88	0.55
3:E:1243:ALA:HA	3:E:1271:MET:HE1	1.88	0.55
3:F:1025:GLN:OE1	3:F:1332:VAL:HG11	2.06	0.55
3:F:1148:GLU:OE1	3:F:1308:LYS:HG2	2.07	0.55
1:A:15:ILE:HD11	2:D:432:ALA:HB1	1.89	0.55
1:A:126:PHE:CZ	1:A:194:MET:HG3	2.42	0.55
3:E:1292:CYS:O	3:E:1295:THR:OG1	2.20	0.55
1:A:17:PHE:HE2	2:C:463:ILE:HD13	1.71	0.55
3:F:1212:LEU:H	3:F:1212:LEU:HD23	1.71	0.55
1:B:216:VAL:HG12	1:B:259:MET:HB2	1.89	0.54
3:E:1070:LEU:HB3	3:E:1331:LEU:HD13	1.89	0.54
3:E:1116:ASP:OD1	3:E:1116:ASP:N	2.40	0.54
3:F:1113:MET:HG2	3:F:1334:LEU:HD21	1.89	0.54
1:B:84:PRO:HB2	1:B:146:LEU:HD13	1.89	0.54
1:A:1:MET:N	1:A:1:MET:SD	2.80	0.54
3:F:1031:PHE:HE1	3:F:1344:GLY:HA2	1.71	0.54
3:E:1123:ARG:HH21	3:E:1337:LEU:HD11	1.72	0.54
1:A:21:LEU:HD12	1:A:247:LEU:HD22	1.88	0.54
1:A:80:MET:HA	2:C:502:ARG:HH12	1.73	0.54
1:A:383:ASP:OD1	1:A:418:GLN:NE2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:3PE:H291	4:D:601:3PE:H391	1.90	0.54
3:E:1005:ILE:HB	3:E:1035:VAL:HG22	1.89	0.54
3:E:1132:SER:O	3:E:1136:ILE:HG12	2.08	0.54
3:F:1017:ALA:HB1	3:F:1331:LEU:HD11	1.88	0.54
3:F:1148:GLU:HG2	3:F:1310:ILE:HG13	1.90	0.54
1:B:104:ASN:ND2	2:D:482:SER:OG	2.40	0.54
1:B:158:PRO:O	1:B:163:MET:HE3	2.08	0.54
1:B:41:MET:HE1	2:D:463:ILE:HA	1.89	0.53
3:E:1008:GLU:HG2	3:E:1010:LEU:H	1.74	0.53
3:E:1010:LEU:HD13	3:E:1076:LEU:HD21	1.91	0.53
3:F:1023:VAL:O	3:F:1027:LEU:HD12	2.08	0.53
1:B:391:ASN:O	1:B:436:ASN:ND2	2.41	0.53
3:E:1002:ARG:NH2	3:E:1062:SER:O	2.41	0.53
3:F:1200:VAL:C	3:F:1201:LYS:HG2	2.32	0.53
1:A:115:PRO:HA	1:A:118:VAL:HB	1.91	0.53
1:A:251:SER:HB2	2:C:442:VAL:HG11	1.88	0.53
1:B:434:VAL:HG13	1:B:435:GLN:H	1.72	0.53
3:E:1151:ARG:HD2	3:F:1322:GLN:HG2	1.90	0.53
1:B:325:PRO:HB2	1:B:455:VAL:HG12	1.91	0.53
3:F:1023:VAL:HG21	3:F:1050:PHE:HE1	1.74	0.53
1:A:45:LEU:O	1:A:46:ILE:HB	2.09	0.53
1:B:15:ILE:HD11	2:C:432:ALA:HB1	1.89	0.53
3:E:1151:ARG:HA	3:F:1322:GLN:HG2	1.91	0.53
3:E:1200:VAL:HB	3:E:1203:GLN:HE22	1.73	0.53
1:A:80:MET:HG2	1:A:361:GLU:HB2	1.91	0.53
3:E:1372:PRO:HD2	3:E:1374:GLN:HE22	1.74	0.53
3:E:1140:ARG:NH2	3:F:1147:HIS:O	2.42	0.52
1:B:450:ASP:OD1	1:B:450:ASP:N	2.42	0.52
1:A:81:THR:HG21	1:A:358:LEU:HD23	1.90	0.52
1:B:7:THR:HB	2:C:425:LEU:HD13	1.91	0.52
3:E:1320:PRO:HD2	3:F:1150:GLY:HA3	1.91	0.52
3:F:1035:VAL:HG21	3:F:1050:PHE:CE1	2.44	0.52
3:F:1113:MET:HA	3:F:1113:MET:HE2	1.92	0.52
1:B:391:ASN:OD1	1:B:436:ASN:ND2	2.35	0.52
3:E:1170:VAL:HG21	3:E:1181:ILE:HD11	1.91	0.52
1:B:75:ALA:HB1	2:D:499:VAL:HB	1.92	0.52
3:E:1181:ILE:HD13	3:E:1204:VAL:HG13	1.91	0.52
3:F:1016:VAL:N	3:F:1324:SER:OG	2.41	0.52
1:B:87:VAL:HG13	2:D:458:ASN:HD21	1.76	0.51
3:E:1149:PHE:HD1	3:E:1150:GLY:H	1.58	0.51
1:B:14:ALA:HB1	1:B:243:VAL:HG11	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:499:VAL:O	2:C:503:MET:HG3	2.10	0.51
1:B:145:LYS:NZ	1:B:151:SER:O	2.36	0.51
3:E:1284:LEU:HD23	3:E:1315:LEU:HD13	1.92	0.51
3:E:1321:THR:OG1	3:F:1150:GLY:O	2.20	0.51
3:F:1153:PHE:CZ	3:F:1251:ILE:HG13	2.46	0.51
3:E:1144:GLU:OE2	3:F:1147:HIS:ND1	2.40	0.51
1:A:43:ILE:O	1:A:47:ALA:CB	2.58	0.51
3:E:1343:ASP:N	3:E:1343:ASP:OD1	2.44	0.51
3:F:1173:ALA:H	3:F:1195:ASP:HB2	1.76	0.51
3:E:1070:LEU:HA	3:E:1090:VAL:HG23	1.93	0.51
3:E:1327:TYR:O	3:E:1331:LEU:HG	2.11	0.51
1:A:100:LEU:HD22	2:C:481:LEU:HD22	1.94	0.50
1:A:387:VAL:HG11	1:A:394:VAL:HG21	1.92	0.50
3:F:1072:VAL:HG23	3:F:1327:TYR:CZ	2.47	0.50
1:A:10:TYR:HB3	1:A:240:LEU:HB2	1.92	0.50
1:B:383:ASP:O	1:B:418:GLN:HB3	2.11	0.50
3:F:1214:LEU:HG	3:F:1215:ASP:H	1.77	0.50
1:A:313:PRO:HB3	1:A:317:MET:SD	2.51	0.50
1:B:264:ASN:HB2	1:B:409:MET:HA	1.92	0.50
3:F:1171:ILE:HD13	3:F:1254:THR:HG22	1.94	0.50
3:F:1258:ILE:O	3:F:1288:ASN:ND2	2.44	0.50
1:B:396:PRO:HD3	1:B:438:LEU:HB2	1.92	0.50
1:A:383:ASP:HA	1:A:418:GLN:HB2	1.93	0.50
3:E:1332:VAL:HG12	3:E:1336:LYS:HD2	1.93	0.50
3:F:1149:PHE:HB2	3:F:1280:VAL:HB	1.94	0.50
1:A:22:ALA:O	1:A:25:SER:OG	2.22	0.49
1:A:126:PHE:CE1	1:A:194:MET:HG3	2.47	0.49
3:E:1016:VAL:HG11	3:E:1039:ALA:HA	1.94	0.49
3:F:1061:ASN:O	3:F:1063:VAL:N	2.45	0.49
3:F:1353:VAL:CG1	3:F:1373:ILE:HD12	2.40	0.49
1:A:17:PHE:HD2	1:A:244:THR:HG21	1.77	0.49
1:A:106:TYR:HB2	1:A:125:VAL:HG11	1.95	0.49
1:A:351:LEU:HB3	1:A:354:HIS:HB2	1.94	0.49
3:E:1010:LEU:HB2	3:E:1076:LEU:HD11	1.94	0.49
1:B:29:THR:O	1:B:32:GLN:N	2.38	0.49
2:D:463:ILE:O	2:D:466:VAL:HG22	2.13	0.49
3:E:1285:ALA:HB3	3:E:1290:GLY:HA2	1.95	0.49
1:B:129:ILE:HD12	1:B:191:LEU:HD11	1.94	0.49
2:D:462:GLY:O	2:D:465:VAL:HG22	2.13	0.49
3:F:1001:GLY:HA2	3:F:1067:GLU:HG2	1.94	0.49
1:A:114:ALA:O	1:A:116:ILE:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:TYR:HB2	1:B:125:VAL:HG11	1.94	0.49
3:E:1058:VAL:HB	3:E:1062:SER:HB2	1.95	0.49
3:E:1170:VAL:HG22	3:E:1193:ALA:HA	1.93	0.49
3:E:1185:ASN:ND2	3:E:1207:MET:O	2.45	0.49
3:F:1308:LYS:HG3	3:F:1310:ILE:HG12	1.94	0.49
3:F:1124:ALA:HA	3:F:1127:LEU:HD12	1.94	0.49
1:A:60:ILE:HG13	2:C:472:ILE:HG21	1.95	0.49
1:B:108:HIS:CE1	2:D:475:GLY:H	2.30	0.48
2:C:445:VAL:HG21	2:C:453:LEU:HD13	1.95	0.48
3:E:1280:VAL:HG13	3:E:1308:LYS:HB2	1.94	0.48
3:F:1061:ASN:O	3:F:1064:TRP:N	2.38	0.48
3:E:1192:ARG:HH22	3:E:1212:LEU:HD21	1.76	0.48
3:E:1303:THR:O	3:E:1305:ASN:N	2.46	0.48
1:B:29:THR:O	1:B:31:ARG:N	2.46	0.48
1:B:387:VAL:HG11	1:B:394:VAL:HG21	1.96	0.48
3:E:1136:ILE:HD11	3:E:1326:LEU:HD13	1.95	0.48
3:E:1153:PHE:HA	3:E:1166:ALA:HB3	1.95	0.48
1:B:223:SER:HA	1:B:249:GLY:HA2	1.94	0.48
3:E:1101:LEU:HA	3:E:1104:LYS:HB3	1.95	0.48
3:E:1112:VAL:H	3:E:1361:ILE:HG22	1.79	0.48
3:F:1111:THR:HG23	3:F:1362:ARG:HA	1.96	0.48
2:C:465:VAL:HG11	2:C:493:ILE:HD11	1.95	0.48
3:F:1003:ILE:HG23	3:F:1033:VAL:HG23	1.94	0.48
3:F:1013:GLU:HG2	3:F:1073:ASN:HD22	1.78	0.48
3:F:1283:ASP:O	3:F:1285:ALA:N	2.47	0.48
1:A:295:THR:O	1:A:299:THR:HG22	2.14	0.48
1:A:436:ASN:O	1:A:439:PHE:N	2.45	0.48
1:A:172:PHE:O	1:A:176:ILE:HG12	2.14	0.48
2:C:442:VAL:HA	2:C:445:VAL:HG23	1.96	0.48
3:E:1356:ARG:NH1	3:E:1371:PRO:O	2.47	0.48
1:A:113:MET:O	1:A:117:LEU:HB2	2.14	0.48
1:B:10:TYR:HB3	1:B:240:LEU:HB2	1.96	0.48
3:E:1290:GLY:HA3	3:E:1295:THR:HG21	1.96	0.48
1:B:420:VAL:O	1:B:445:HIS:N	2.35	0.47
1:A:460:LYS:HA	1:A:460:LYS:HD2	1.71	0.47
1:B:165:LEU:O	1:B:169:VAL:HG13	2.13	0.47
1:B:195:THR:O	1:B:199:LEU:HG	2.13	0.47
3:F:1169:MET:HB3	3:F:1252:ILE:HD13	1.95	0.47
1:B:429:THR:HA	1:B:435:GLN:HG2	1.96	0.47
1:B:189:LEU:O	1:B:193:ILE:HG12	2.14	0.47
1:B:366:TYR:CZ	2:D:508:LYS:HB3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1019:THR:HG23	3:E:1021:LYS:H	1.80	0.47
3:F:1201:LYS:HG3	3:F:1202:GLU:OE2	2.15	0.47
1:A:92:SER:HB3	1:A:139:SER:HB2	1.97	0.47
1:B:123:THR:HG23	1:B:175:LEU:HD11	1.96	0.47
3:E:1168:VAL:HG11	3:E:1184:ALA:HB1	1.96	0.47
3:F:1094:TRP:HB3	3:F:1097:GLN:HG3	1.97	0.47
1:B:160:ARG:HG3	1:B:204:HIS:NE2	2.29	0.47
1:B:333:LEU:O	1:B:333:LEU:HD12	2.15	0.47
3:E:1137:ALA:HB2	3:E:1316:PRO:HG3	1.97	0.47
3:F:1362:ARG:HG3	3:F:1363:ALA:N	2.30	0.47
1:A:418:GLN:HE22	3:F:1157:ILE:HG21	1.79	0.47
3:E:1151:ARG:HD3	3:F:1321:THR:HG22	1.97	0.47
3:E:1267:ILE:HB	3:E:1292:CYS:HA	1.96	0.47
1:A:258:ILE:HG22	1:A:259:MET:HE2	1.96	0.46
3:E:1181:ILE:HG23	3:E:1191:VAL:HG11	1.98	0.46
3:F:1006:PRO:HG3	3:F:1069:ILE:HD11	1.97	0.46
1:B:370:LEU:HD23	1:B:374:GLU:HG2	1.96	0.46
1:B:420:VAL:HB	1:B:444:THR:HA	1.96	0.46
1:B:436:ASN:O	1:B:438:LEU:N	2.48	0.46
3:F:1092:PHE:CG	3:F:1116:ASP:HB3	2.50	0.46
1:A:424:LYS:HD3	1:A:446:MET:HE1	1.97	0.46
3:F:1140:ARG:HD2	3:F:1140:ARG:HA	1.64	0.46
3:E:1069:ILE:O	3:E:1089:LEU:HA	2.16	0.46
3:F:1257:LEU:HB2	3:F:1285:ALA:HB2	1.96	0.46
1:A:41:MET:HE1	2:C:463:ILE:HD12	1.98	0.46
1:A:422:VAL:HG11	1:A:439:PHE:CE1	2.51	0.46
2:C:490:SER:HA	2:C:493:ILE:HD12	1.96	0.46
2:D:465:VAL:HB	2:D:469:LEU:HD23	1.97	0.46
3:E:1267:ILE:HG23	3:E:1271:MET:HB3	1.98	0.46
1:B:292:ARG:NH1	1:B:442:GLU:O	2.45	0.46
1:B:85:GLU:OE2	1:B:350:ARG:NH2	2.49	0.46
1:B:102:GLY:HA2	1:B:235:MET:SD	2.56	0.46
4:B:502:3PE:H362	4:C:601:3PE:H261	1.98	0.46
1:B:298:GLU:O	1:B:302:LEU:HG	2.16	0.46
3:F:1339:CYS:O	3:F:1341:GLU:N	2.45	0.46
1:A:264:ASN:HB2	1:A:409:MET:HA	1.97	0.46
3:E:1305:ASN:HD21	3:E:1307:VAL:HG23	1.80	0.46
1:B:321:GLN:OE1	1:B:321:GLN:HA	2.14	0.46
3:E:1165:PRO:HB2	3:E:1190:ILE:HG12	1.97	0.46
3:E:1361:ILE:HG23	3:E:1363:ALA:H	1.81	0.46
1:A:260:CYS:HB3	1:A:265:ARG:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1227:ALA:HA	3:E:1230:MET:HG3	1.99	0.45
3:F:1149:PHE:CG	3:F:1251:ILE:HD11	2.52	0.45
1:A:345:HIS:ND1	1:A:347:VAL:HG12	2.30	0.45
1:B:89:ILE:HD12	1:B:89:ILE:HA	1.83	0.45
1:B:317:MET:HE2	1:B:323:GLN:HA	1.98	0.45
3:F:1338:LEU:HD22	3:F:1355:ILE:HD13	1.98	0.45
1:A:218:VAL:HG12	2:C:454:MET:HE1	1.98	0.45
1:A:413:GLU:HG3	1:A:415:TRP:CZ2	2.51	0.45
1:B:422:VAL:HG11	1:B:439:PHE:HE1	1.80	0.45
3:E:1268:THR:H	3:E:1271:MET:HB2	1.80	0.45
3:F:1286:ALA:HB3	3:F:1313:THR:HG22	1.98	0.45
1:A:120:ILE:HG12	4:A:502:3PE:H331	1.98	0.45
3:E:1194:PHE:HE2	3:E:1238:GLU:HG2	1.80	0.45
3:E:1261:LYS:HB3	3:E:1261:LYS:HE3	1.63	0.45
3:F:1368:TRP:CD1	3:F:1369:PRO:HD3	2.52	0.45
1:A:310:ILE:HD13	1:A:375:ILE:HD11	1.98	0.45
1:A:409:MET:O	1:A:411:VAL:HG13	2.17	0.45
3:E:1083:LEU:HB3	3:E:1108:ARG:NH2	2.32	0.45
3:F:1083:LEU:HD13	3:F:1110:VAL:HG11	1.97	0.45
3:F:1355:ILE:O	3:F:1359:THR:OG1	2.19	0.45
1:B:49:ILE:HD11	1:B:64:MET:HE1	1.97	0.45
3:E:1127:LEU:HD22	3:E:1337:LEU:HD23	1.99	0.45
3:E:1151:ARG:HD2	3:E:1151:ARG:HA	1.68	0.45
3:E:1224:ASP:HB2	3:E:1227:ALA:HB3	1.98	0.45
3:E:1228:LYS:HB3	3:E:1234:PHE:CE2	2.52	0.45
1:A:144:GLY:HA3	1:A:150:ILE:HG13	1.99	0.45
1:A:209:ILE:HD13	1:A:217:VAL:HG22	1.99	0.45
1:A:325:PRO:O	1:A:329:ILE:HG13	2.16	0.45
1:A:25:SER:HA	2:C:444:ASN:O	2.17	0.45
1:B:126:PHE:CZ	1:B:194:MET:HG3	2.52	0.45
3:E:1261:LYS:CE	3:E:1262:PRO:HD2	2.47	0.45
1:A:324:TYR:HB2	1:A:325:PRO:HD3	2.00	0.44
1:A:396:PRO:HD3	1:A:438:LEU:HB2	2.00	0.44
2:C:446:SER:O	2:C:448:ALA:N	2.50	0.44
3:E:1009:ARG:NH1	3:E:1078:ASP:OD2	2.44	0.44
3:E:1109:ASN:OD1	3:E:1363:ALA:HB1	2.17	0.44
1:B:454:SER:O	1:B:458:ILE:HG12	2.16	0.44
2:D:441:VAL:O	2:D:445:VAL:HG23	2.17	0.44
3:F:1086:GLY:O	3:F:1088:THR:N	2.50	0.44
1:A:91:HIS:CE1	1:A:222:ASN:HB2	2.52	0.44
1:B:56:ASN:HB3	1:B:59:TRP:HD1	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1092:PHE:CE1	3:E:1115:MET:HB2	2.52	0.44
3:F:1015:ARG:NH1	3:F:1133:MET:SD	2.90	0.44
1:B:258:ILE:HG22	1:B:259:MET:HE2	2.00	0.44
3:E:1281:ILE:O	3:E:1281:ILE:HG13	2.17	0.44
1:A:43:ILE:O	1:A:47:ALA:HB2	2.18	0.44
1:A:131:ILE:O	1:A:135:THR:HG22	2.17	0.44
1:B:330:THR:HG23	1:B:334:ARG:HD3	1.98	0.44
3:E:1212:LEU:HD22	3:E:1245:GLN:NE2	2.32	0.44
3:F:1005:ILE:HD12	3:F:1035:VAL:HG22	2.00	0.44
1:A:30:SER:HB2	2:C:504:LEU:HD22	1.98	0.44
1:A:45:LEU:HD13	1:A:64:MET:HE1	1.99	0.44
1:A:310:ILE:HD12	1:A:382:THR:HG21	1.99	0.44
3:E:1015:ARG:HG2	3:E:1072:VAL:HG11	1.99	0.44
3:F:1130:LEU:HD23	3:F:1130:LEU:H	1.82	0.44
3:F:1141:ALA:HB1	3:F:1282:VAL:HG11	1.99	0.44
1:A:84:PRO:HB2	1:A:146:LEU:HD13	1.98	0.44
1:A:109:HIS:NE2	1:A:118:VAL:HG13	2.32	0.44
3:E:1064:TRP:CE3	3:E:1083:LEU:HD13	2.53	0.44
3:F:1284:LEU:HD23	3:F:1315:LEU:HD13	1.99	0.44
1:A:261:LYS:HE3	1:A:261:LYS:HB3	1.82	0.44
3:E:1029:LEU:HD22	3:E:1031:PHE:HE1	1.83	0.44
3:E:1092:PHE:HE1	3:E:1115:MET:HB2	1.83	0.44
3:E:1362:ARG:C	3:E:1364:GLY:H	2.26	0.44
3:F:1140:ARG:HD3	3:F:1319:LEU:HD13	1.99	0.44
1:A:317:MET:HE2	1:A:323:GLN:HA	2.00	0.44
3:E:1315:LEU:HB2	3:E:1316:PRO:HD3	1.99	0.44
3:F:1170:VAL:HG21	3:F:1181:ILE:HG13	2.00	0.44
3:F:1287:GLN:N	3:F:1287:GLN:OE1	2.50	0.44
1:B:254:ILE:HD11	2:D:439:TYR:HA	2.00	0.43
3:E:1148:GLU:HB2	3:E:1280:VAL:HG21	2.00	0.43
3:E:1252:ILE:HD13	3:E:1275:MET:HE3	1.99	0.43
1:A:345:HIS:CD2	1:A:393:THR:HB	2.53	0.43
2:D:424:PHE:C	2:D:426:GLY:H	2.26	0.43
3:E:1259:PRO:O	3:E:1260:GLY:C	2.61	0.43
1:A:66:ILE:O	1:A:70:ILE:HG12	2.18	0.43
1:A:85:GLU:HG2	1:A:147:CYS:HB3	1.99	0.43
1:A:303:LEU:HD23	1:A:309:VAL:HG21	2.00	0.43
1:A:333:LEU:HB3	1:A:338:ILE:HG23	2.01	0.43
1:B:434:VAL:HG13	1:B:435:GLN:N	2.33	0.43
3:F:1140:ARG:HA	3:F:1143:VAL:HG12	1.99	0.43
1:A:334:ARG:HH11	1:A:334:ARG:HG2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:501:PC1:H221	5:B:501:PC1:H2	1.64	0.43
3:E:1144:GLU:O	3:E:1148:GLU:HG2	2.18	0.43
3:E:1263:ALA:HB3	3:E:1290:GLY:N	2.32	0.43
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.90	0.43
4:A:503:3PE:H252	2:D:436:VAL:HG22	2.00	0.43
1:B:63:ALA:HB2	2:D:483:PHE:CE1	2.53	0.43
2:C:505:LYS:HD3	2:C:505:LYS:N	2.33	0.43
3:F:1065:GLN:HB3	3:F:1084:ASN:HD21	1.83	0.43
3:F:1167:LYS:HE2	3:F:1167:LYS:HB3	1.75	0.43
1:B:133:ALA:HB1	1:B:199:LEU:HD23	2.00	0.43
3:E:1153:PHE:CZ	3:E:1251:ILE:HG13	2.53	0.43
2:D:484:ILE:O	2:D:488:ILE:HG12	2.19	0.43
3:E:1361:ILE:HG13	3:E:1366:ILE:HA	2.01	0.43
3:E:1371:PRO:HA	3:E:1372:PRO:HD3	1.91	0.43
1:A:84:PRO:HB2	1:A:146:LEU:HD22	2.01	0.43
1:B:56:ASN:O	1:B:60:ILE:HG13	2.18	0.43
1:B:72:ILE:HG12	2:D:498:THR:HG21	2.01	0.43
3:E:1020:PRO:HA	3:E:1023:VAL:HB	2.00	0.43
1:A:23:GLY:HA3	1:A:33:GLY:HA3	2.00	0.43
1:A:297:GLU:CD	1:A:297:GLU:H	2.26	0.43
1:B:126:PHE:CE2	1:B:194:MET:HG3	2.54	0.43
2:C:419:VAL:HG13	2:C:419:VAL:O	2.19	0.43
1:A:173:LEU:O	1:A:177:VAL:HG23	2.19	0.43
1:B:8:ALA:HB2	2:C:417:ALA:CB	2.49	0.43
1:B:306:SER:HB2	1:B:383:ASP:HB2	2.00	0.43
1:A:209:ILE:HD11	1:A:271:ILE:HG22	2.00	0.42
1:A:424:LYS:HE3	1:A:426:SER:O	2.18	0.42
3:F:1062:SER:OG	3:F:1063:VAL:N	2.52	0.42
3:F:1323:SER:O	3:F:1327:TYR:HB2	2.18	0.42
1:A:8:ALA:HB1	2:D:415:TRP:HE3	1.85	0.42
1:B:308:SER:OG	1:B:383:ASP:OD1	2.38	0.42
1:A:77:LYS:HD3	1:A:77:LYS:HA	1.64	0.42
1:A:108:HIS:NE2	2:C:474:GLN:O	2.52	0.42
1:B:310:ILE:O	1:B:385:VAL:HA	2.19	0.42
3:F:1010:LEU:HD22	3:F:1073:ASN:HB2	2.01	0.42
1:A:63:ALA:HB2	2:C:483:PHE:CE1	2.55	0.42
3:E:1014:THR:HG23	3:E:1043:ALA:HA	2.00	0.42
3:E:1272:VAL:HG21	3:E:1303:THR:HG21	2.01	0.42
3:E:1351:ASP:HB2	3:E:1355:ILE:HB	2.02	0.42
1:B:116:ILE:HG12	2:D:419:VAL:O	2.18	0.42
1:B:160:ARG:HD2	1:B:208:SER:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:465:VAL:O	2:D:469:LEU:N	2.43	0.42
3:F:1049:ALA:O	3:F:1053:ALA:N	2.46	0.42
3:F:1373:ILE:HG23	3:F:1374:GLN:O	2.19	0.42
1:A:254:ILE:HD11	2:C:439:TYR:CD2	2.54	0.42
1:A:239:ASP:OD1	2:C:427:HIS:ND1	2.51	0.42
1:A:251:SER:HA	2:C:442:VAL:HG21	2.01	0.42
3:E:1279:SER:HB2	3:E:1307:VAL:HG22	2.00	0.42
3:F:1009:ARG:NH1	3:F:1078:ASP:HB3	2.35	0.42
3:F:1254:THR:O	3:F:1284:LEU:HB2	2.20	0.42
1:A:49:ILE:HG12	2:C:469:LEU:HD13	2.02	0.42
3:F:1049:ALA:HA	3:F:1052:GLN:HB3	2.02	0.42
3:F:1140:ARG:HG2	3:F:1315:LEU:O	2.19	0.42
3:E:1012:ASN:HB2	3:E:1015:ARG:HE	1.85	0.42
3:F:1031:PHE:HE2	3:F:1346:ILE:HD11	1.85	0.42
1:A:101:VAL:HG21	2:C:464:ILE:HG22	2.02	0.42
5:B:501:PC1:H31	4:D:601:3PE:H221	2.01	0.42
3:E:1072:VAL:HG23	3:E:1073:ASN:H	1.85	0.42
3:E:1133:MET:HA	3:E:1133:MET:CE	2.46	0.42
3:F:1184:ALA:HA	3:F:1187:LEU:HB2	2.02	0.42
1:A:299:THR:HG21	1:A:447:LEU:HD22	2.02	0.41
3:E:1146:ALA:HA	3:E:1153:PHE:HE1	1.85	0.41
3:E:1146:ALA:HA	3:E:1153:PHE:CE1	2.55	0.41
1:A:211:GLY:C	1:A:213:ASP:H	2.28	0.41
1:B:129:ILE:HB	1:B:194:MET:HE1	2.02	0.41
1:B:261:LYS:HE2	1:B:261:LYS:HB3	1.64	0.41
3:E:1089:LEU:HD21	3:E:1105:LEU:HD22	2.02	0.41
3:E:1301:PHE:CE2	3:E:1303:THR:HG22	2.55	0.41
1:A:26:LYS:HE3	1:A:26:LYS:HB3	1.75	0.41
1:A:191:LEU:HD12	1:A:194:MET:HE3	2.03	0.41
3:E:1171:ILE:HB	3:E:1254:THR:HA	2.02	0.41
3:E:1275:MET:O	3:E:1305:ASN:ND2	2.53	0.41
3:F:1022:THR:HG21	3:F:1328:GLY:HA3	2.02	0.41
1:A:326:VAL:HG23	1:A:455:VAL:HG11	2.01	0.41
1:B:436:ASN:O	1:B:437:PRO:C	2.63	0.41
3:E:1254:THR:OG1	3:E:1283:ASP:OD1	2.29	0.41
3:E:1361:ILE:HA	3:E:1367:THR:HG23	2.02	0.41
1:A:176:ILE:O	1:A:180:ARG:HB2	2.20	0.41
1:A:259:MET:O	1:A:263:MET:HG2	2.20	0.41
1:B:211:GLY:HA2	1:B:214:MET:HG2	2.03	0.41
1:B:446:MET:HB3	1:B:448:PHE:CE1	2.55	0.41
3:E:1114:ALA:HB1	3:E:1116:ASP:OD1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1232:ASP:O	3:E:1236:LYS:HG3	2.21	0.41
1:A:244:THR:OG1	2:C:463:ILE:HG21	2.20	0.41
1:A:377:ASP:OD1	1:A:377:ASP:N	2.35	0.41
1:B:251:SER:HA	2:D:442:VAL:HG11	2.02	0.41
1:B:341:ARG:HH22	1:B:378:ASP:HB3	1.85	0.41
2:C:438:GLY:HA2	2:C:441:VAL:HG22	2.02	0.41
3:E:1003:ILE:HD12	3:E:1003:ILE:HA	1.83	0.41
1:A:90:LEU:HB3	2:C:492:ASN:ND2	2.36	0.41
1:B:27:HIS:HA	2:D:449:LEU:HD11	2.01	0.41
1:B:84:PRO:HB3	1:B:351:LEU:HD13	2.02	0.41
1:B:159:ASN:HB3	1:B:162:LYS:HB2	2.01	0.41
1:A:86:LEU:O	1:A:90:LEU:HG	2.21	0.41
1:B:60:ILE:HG12	2:D:472:ILE:HG21	2.03	0.41
1:B:351:LEU:HG	1:B:352:PRO:HD2	2.02	0.41
3:F:1260:GLY:H	3:F:1288:ASN:HD21	1.68	0.41
1:A:214:MET:N	1:A:215:PRO:HD2	2.36	0.41
1:A:315:TYR:O	1:A:319:VAL:HG13	2.21	0.41
1:A:435:GLN:HB3	1:A:440:PHE:CE2	2.56	0.41
1:B:238:ASN:HB3	1:B:241:LEU:HB2	2.01	0.41
1:B:321:GLN:OE1	1:B:323:GLN:NE2	2.54	0.41
1:B:324:TYR:HB2	1:B:325:PRO:HD3	2.03	0.41
3:E:1079:GLU:H	3:E:1079:GLU:HG2	1.71	0.41
3:E:1125:GLN:NE2	3:F:1159:ALA:HB1	2.32	0.41
3:E:1214:LEU:HD13	3:E:1237:ALA:HB3	2.02	0.41
3:E:1261:LYS:NZ	3:E:1262:PRO:HD2	2.35	0.41
3:E:1360:VAL:O	3:E:1367:THR:N	2.54	0.41
3:F:1172:GLY:N	3:F:1194:PHE:O	2.44	0.41
3:F:1348:VAL:HG21	3:F:1362:ARG:CZ	2.51	0.41
1:B:19:PHE:CD1	4:B:502:3PE:H32	2.55	0.41
1:B:86:LEU:O	1:B:90:LEU:HG	2.21	0.41
1:B:299:THR:HG21	1:B:447:LEU:HD11	2.02	0.41
3:E:1169:MET:HG2	3:E:1192:ARG:O	2.21	0.41
1:A:164:ASN:OD1	1:A:204:HIS:ND1	2.49	0.40
1:A:435:GLN:HB3	1:A:440:PHE:HE2	1.85	0.40
1:B:209:ILE:HG21	1:B:217:VAL:HG21	2.02	0.40
3:F:1026:LEU:O	3:F:1029:LEU:HB2	2.20	0.40
3:E:1151:ARG:HD3	3:F:1321:THR:CG2	2.50	0.40
3:E:1319:LEU:HD12	3:F:1150:GLY:HA2	2.02	0.40
3:F:1040:GLY:HA2	3:F:1043:ALA:HB3	2.03	0.40
3:F:1168:VAL:HB	3:F:1191:VAL:HG22	2.02	0.40
1:A:68:GLY:HA2	2:C:494:PHE:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:O	1:A:89:ILE:HG22	2.21	0.40
1:A:89:ILE:HD12	1:A:89:ILE:HA	1.88	0.40
1:A:189:LEU:O	1:A:193:ILE:HG13	2.22	0.40
1:A:223:SER:HA	1:A:249:GLY:HA2	2.02	0.40
3:E:1067:GLU:HG2	3:E:1068:ILE:HG13	2.02	0.40
3:E:1300:ILE:HG23	3:E:1309:VAL:H	1.85	0.40
3:F:1271:MET:O	3:F:1275:MET:HB3	2.21	0.40
1:A:153:LYS:HD2	1:A:153:LYS:HA	1.90	0.40
1:B:26:LYS:HE3	4:B:502:3PE:H111	2.02	0.40
1:B:326:VAL:HG23	1:B:455:VAL:HG11	2.03	0.40
1:B:379:PHE:CE1	1:B:414:VAL:HG12	2.57	0.40
3:E:1041:GLN:HA	3:E:1045:PHE:O	2.20	0.40
3:E:1101:LEU:O	3:E:1105:LEU:HD12	2.21	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	440/462 (95%)	415 (94%)	24 (6%)	1 (0%)	43 73
1	B	440/462 (95%)	409 (93%)	26 (6%)	5 (1%)	11 40
2	C	97/99 (98%)	91 (94%)	3 (3%)	3 (3%)	3 22
2	D	95/99 (96%)	87 (92%)	8 (8%)	0	100 100
3	E	363/377 (96%)	319 (88%)	38 (10%)	6 (2%)	7 32
3	F	357/377 (95%)	322 (90%)	29 (8%)	6 (2%)	7 32
All	All	1792/1876 (96%)	1643 (92%)	128 (7%)	21 (1%)	13 38

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	SER
2	C	451	THR
3	F	1062	SER
1	B	79	GLU
1	B	434	VAL
3	F	1077	ASP
3	F	1087	THR
3	F	1201	LYS
3	F	1284	LEU
1	B	432	ALA
3	E	1264	PRO
3	E	1304	GLU
2	C	447	HIS
3	E	1262	PRO
1	A	432	ALA
1	B	54	THR
2	C	507	PHE
3	F	1085	PRO
3	E	1261	LYS
3	E	1263	ALA
3	E	1260	GLY

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	348/360 (97%)	345 (99%)	3 (1%)	70	76
1	B	348/360 (97%)	345 (99%)	3 (1%)	70	76
2	C	80/80 (100%)	80 (100%)	0	100	100
2	D	78/80 (98%)	78 (100%)	0	100	100
3	E	290/298 (97%)	287 (99%)	3 (1%)	68	75
3	F	287/298 (96%)	286 (100%)	1 (0%)	86	84
All	All	1431/1476 (97%)	1421 (99%)	10 (1%)	73	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	SER
1	A	317	MET
1	A	459	LEU
1	B	120	ILE
1	B	418	GLN
1	B	435	GLN
3	E	1083	LEU
3	E	1089	LEU
3	E	1261	LYS
3	F	1083	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	HIS
1	A	399	GLN
1	A	418	GLN
1	B	91	HIS
1	B	418	GLN
2	C	458	ASN
2	D	474	GLN
3	E	1125	GLN
3	E	1185	ASN
3	E	1305	ASN
3	F	1065	GLN
3	F	1135	ASN
3	F	1288	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	3PE	C	601	-	30,30,50	0.63	0	33,35,55	0.64	1 (3%)
5	PC1	B	501	-	35,35,53	0.57	0	41,43,61	0.60	1 (2%)
4	3PE	A	501	-	28,28,50	0.66	0	31,33,55	0.65	1 (3%)
4	3PE	B	502	-	30,30,50	0.65	0	33,35,55	0.63	1 (3%)
4	3PE	A	503	-	31,31,50	0.65	0	34,36,55	0.59	1 (2%)
4	3PE	A	502	-	50,50,50	0.51	0	53,55,55	0.49	1 (1%)
4	3PE	D	601	-	41,41,50	0.56	0	44,46,55	0.57	1 (2%)

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	3PE	C	601	-	-	16/34/34/54	-
5	PC1	B	501	-	-	17/39/39/57	-
4	3PE	A	501	-	-	17/32/32/54	-
4	3PE	B	502	-	-	15/34/34/54	-
4	3PE	A	503	-	-	16/35/35/54	-
4	3PE	A	502	-	-	20/54/54/54	-
4	3PE	D	601	-	-	17/45/45/54	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	601	3PE	O12-P-O14	2.42	124.22	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	3PE	O12-P-O14	2.35	123.83	112.24
4	A	502	3PE	O12-P-O14	2.32	123.73	112.24
4	A	503	3PE	O12-P-O14	2.32	123.72	112.24
5	B	501	PC1	O12-P-O14	2.32	123.71	112.24
4	B	502	3PE	O12-P-O14	2.32	123.69	112.24
4	D	601	3PE	O12-P-O14	2.31	123.68	112.24

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	3PE	C1-O11-P-O14
4	A	501	3PE	C11-O13-P-O11
4	A	501	3PE	C11-O13-P-O12
4	A	501	3PE	C11-O13-P-O14
4	A	501	3PE	O13-C11-C12-N
4	A	501	3PE	O22-C21-O21-C2
4	A	501	3PE	C22-C21-O21-C2
4	A	502	3PE	C1-O11-P-O14
4	A	502	3PE	C11-O13-P-O11
4	A	502	3PE	C11-O13-P-O12
4	A	502	3PE	C11-O13-P-O14
4	A	503	3PE	C1-O11-P-O14
4	A	503	3PE	C11-O13-P-O14
4	A	503	3PE	O13-C11-C12-N
4	B	502	3PE	C1-O11-P-O14
4	B	502	3PE	C11-O13-P-O11
4	B	502	3PE	C11-O13-P-O12
4	B	502	3PE	C11-O13-P-O14
4	C	601	3PE	C1-O11-P-O12
4	D	601	3PE	C1-O11-P-O12
4	D	601	3PE	C1-O11-P-O13
4	D	601	3PE	C1-O11-P-O14
5	B	501	PC1	C11-O13-P-O14
5	B	501	PC1	C1-O11-P-O12
5	B	501	PC1	C1-O11-P-O14
5	B	501	PC1	C1-O11-P-O13
5	B	501	PC1	O22-C21-O21-C2
5	B	501	PC1	C22-C21-O21-C2
5	B	501	PC1	C2-C3-O31-C31
4	A	503	3PE	O32-C31-O31-C3
5	B	501	PC1	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	501	3PE	O32-C31-O31-C3
4	D	601	3PE	O32-C31-O31-C3
4	A	503	3PE	C32-C31-O31-C3
4	D	601	3PE	C32-C31-O31-C3
5	B	501	PC1	C32-C31-O31-C3
4	A	501	3PE	C32-C31-O31-C3
4	D	601	3PE	C21-C22-C23-C24
4	A	501	3PE	C31-C32-C33-C34
4	A	503	3PE	C31-C32-C33-C34
4	A	503	3PE	C21-C22-C23-C24
4	A	502	3PE	C21-C22-C23-C24
4	D	601	3PE	C22-C21-O21-C2
4	A	502	3PE	C1-O11-P-O13
4	A	503	3PE	C1-O11-P-O13
4	B	502	3PE	C1-O11-P-O13
4	C	601	3PE	C1-O11-P-O13
5	B	501	PC1	C11-O13-P-O11
4	D	601	3PE	O22-C21-O21-C2
4	D	601	3PE	C33-C34-C35-C36
4	D	601	3PE	C37-C38-C39-C3A
4	C	601	3PE	O13-C11-C12-N
4	C	601	3PE	C33-C34-C35-C36
4	C	601	3PE	C22-C23-C24-C25
4	A	503	3PE	C33-C34-C35-C36
4	A	503	3PE	C32-C33-C34-C35
4	A	501	3PE	C32-C33-C34-C35
4	C	601	3PE	C22-C21-O21-C2
4	A	502	3PE	O11-C1-C2-O21
4	C	601	3PE	O22-C21-O21-C2
4	A	503	3PE	C11-O13-P-O11
4	D	601	3PE	C35-C36-C37-C38
4	A	501	3PE	C33-C34-C35-C36
5	B	501	PC1	C37-C38-C39-C3A
4	C	601	3PE	C32-C33-C34-C35
4	A	502	3PE	C2C-C2D-C2E-C2F
4	A	502	3PE	C2F-C2G-C2H-C2I
4	A	502	3PE	C3B-C3C-C3D-C3E
4	B	502	3PE	O13-C11-C12-N
4	A	501	3PE	C1-C2-C3-O31
4	B	502	3PE	O31-C31-C32-C33
4	A	501	3PE	C1-O11-P-O13
4	C	601	3PE	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	502	3PE	C32-C31-O31-C3
4	D	601	3PE	C36-C37-C38-C39
4	A	501	3PE	O21-C2-C3-O31
4	C	601	3PE	O21-C2-C3-O31
4	C	601	3PE	C2-C1-O11-P
4	A	502	3PE	C32-C33-C34-C35
4	A	502	3PE	O11-C1-C2-C3
4	B	502	3PE	O11-C1-C2-C3
4	B	502	3PE	C34-C35-C36-C37
4	D	601	3PE	C1-C2-C3-O31
4	B	502	3PE	O32-C31-O31-C3
4	A	501	3PE	O11-C1-C2-O21
4	A	502	3PE	C1-O11-P-O12
4	A	503	3PE	C1-O11-P-O12
4	B	502	3PE	C1-O11-P-O12
5	B	501	PC1	C11-O13-P-O12
4	D	601	3PE	C34-C35-C36-C37
4	A	501	3PE	O11-C1-C2-C3
4	A	503	3PE	O11-C1-C2-C3
4	A	502	3PE	C12-C11-O13-P
5	B	501	PC1	C12-C11-O13-P
4	A	503	3PE	O11-C1-C2-O21
4	B	502	3PE	O11-C1-C2-O21
4	C	601	3PE	C1-C2-C3-O31
4	B	502	3PE	C31-C32-C33-C34
4	D	601	3PE	C38-C39-C3A-C3B
4	A	503	3PE	O21-C2-C3-O31
4	D	601	3PE	O21-C2-C3-O31
4	C	601	3PE	C11-O13-P-O11
4	C	601	3PE	C31-C32-C33-C34
4	C	601	3PE	C24-C25-C26-C27
4	D	601	3PE	C26-C27-C28-C29
4	C	601	3PE	O11-C1-C2-C3
4	A	502	3PE	C2E-C2F-C2G-C2H
4	A	502	3PE	C3E-C3F-C3G-C3H
5	B	501	PC1	C33-C34-C35-C36
4	A	502	3PE	C34-C35-C36-C37
4	A	502	3PE	C27-C28-C29-C2A
4	A	502	3PE	O21-C21-C22-C23
4	B	502	3PE	O32-C31-C32-C33
5	B	501	PC1	O21-C21-C22-C23
4	A	502	3PE	O22-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	503	3PE	C11-O13-P-O12
5	B	501	PC1	O22-C21-C22-C23
5	B	501	PC1	C35-C36-C37-C38

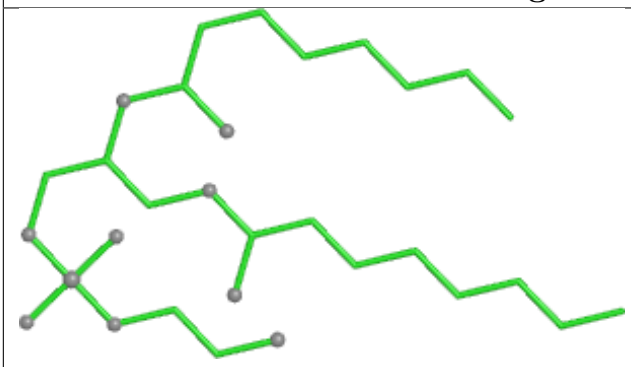
There are no ring outliers.

6 monomers are involved in 10 short contacts:

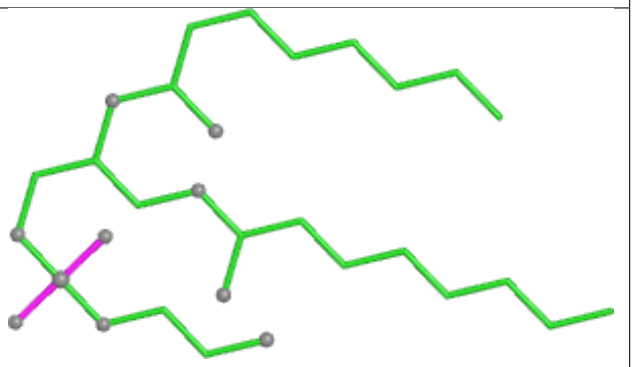
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	3PE	1	0
5	B	501	PC1	3	0
4	B	502	3PE	3	0
4	A	503	3PE	3	0
4	A	502	3PE	1	0
4	D	601	3PE	4	0

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.

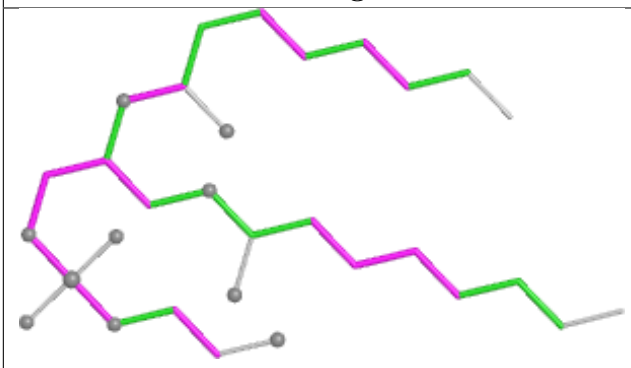
Ligand 3PE C 601



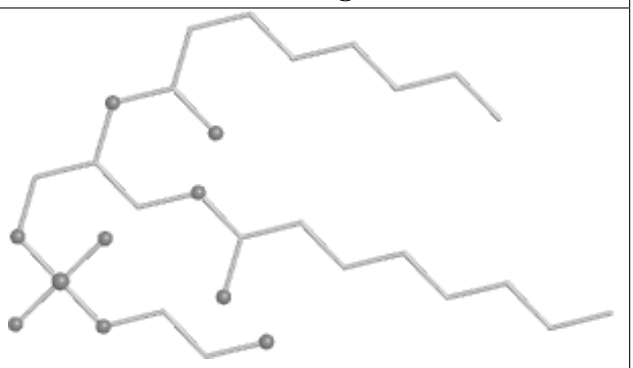
Bond lengths



Bond angles

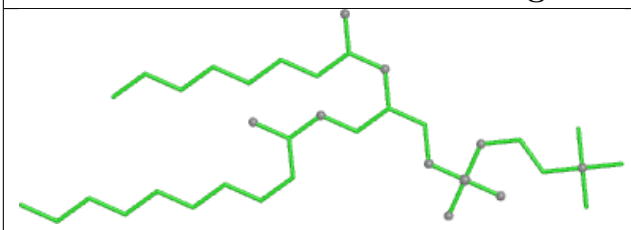


Torsions

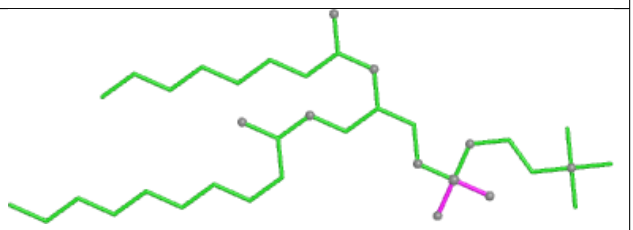


Rings

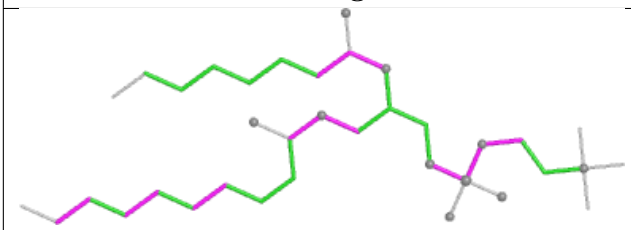
Ligand PC1 B 501



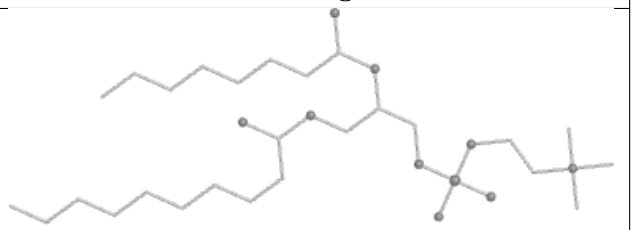
Bond lengths



Bond angles

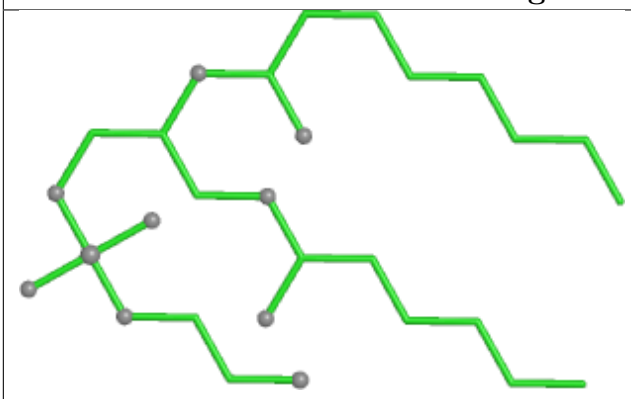


Torsions

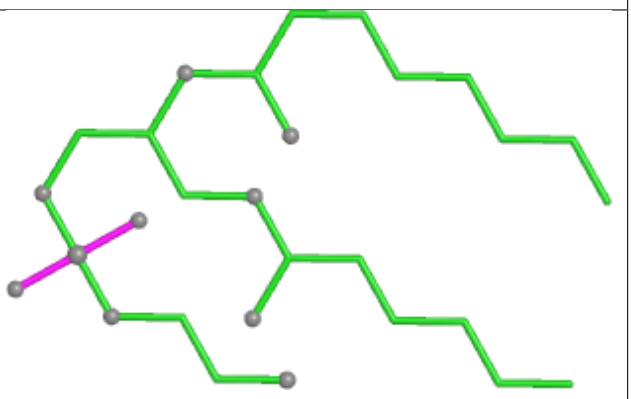


Rings

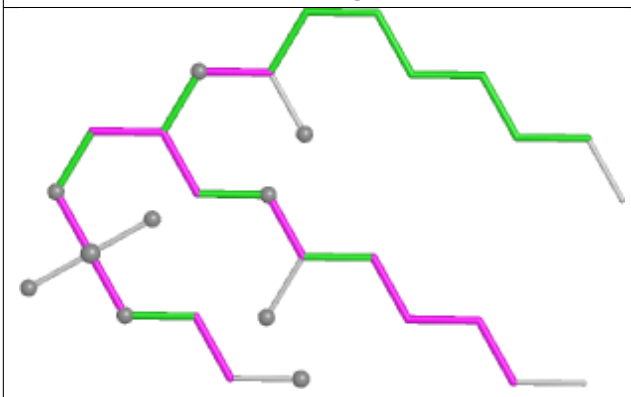
Ligand 3PE A 501



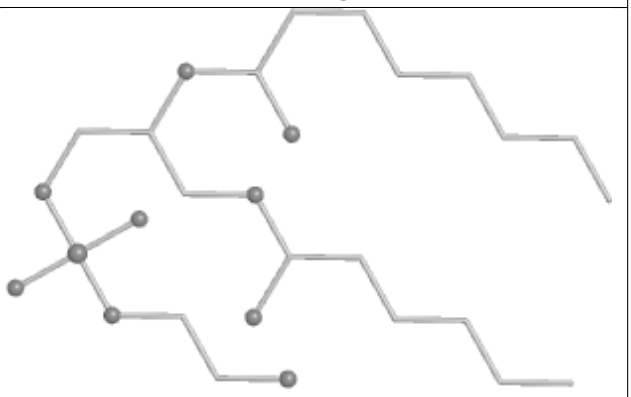
Bond lengths



Bond angles

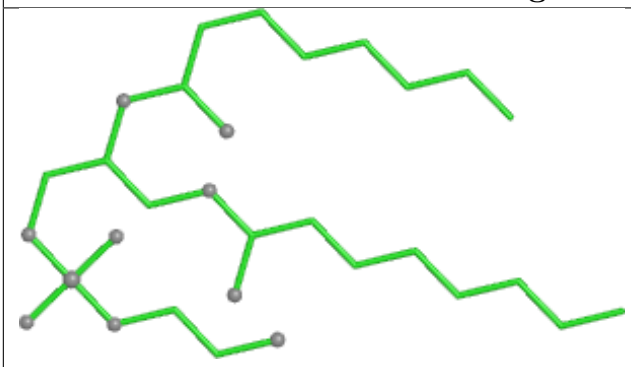


Torsions

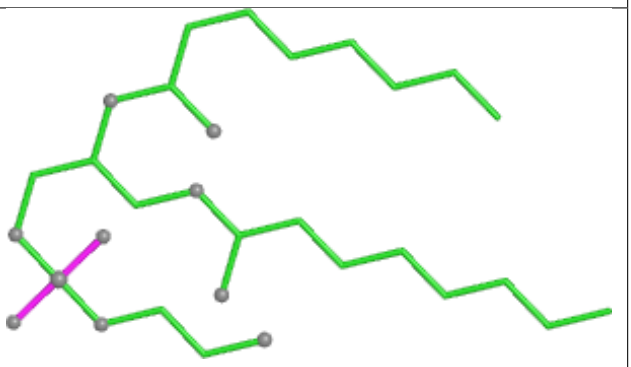


Rings

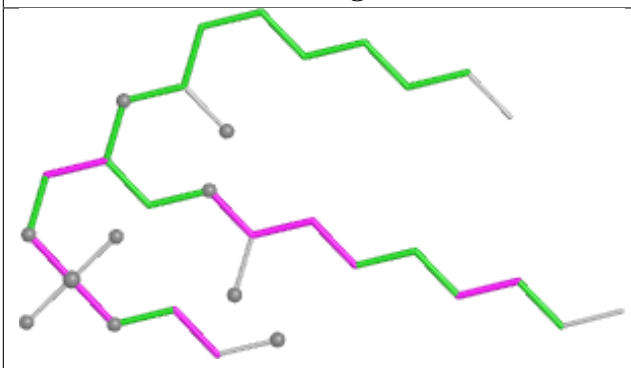
Ligand 3PE B 502



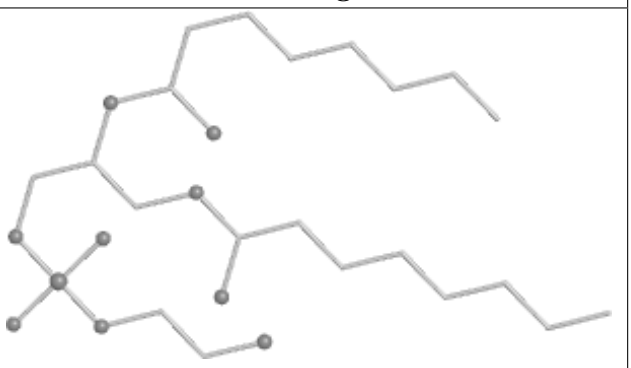
Bond lengths



Bond angles

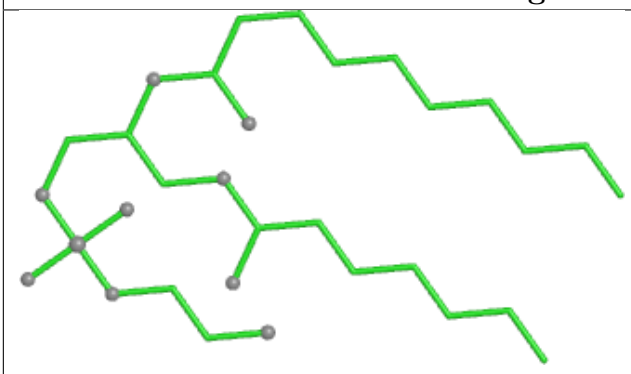


Torsions

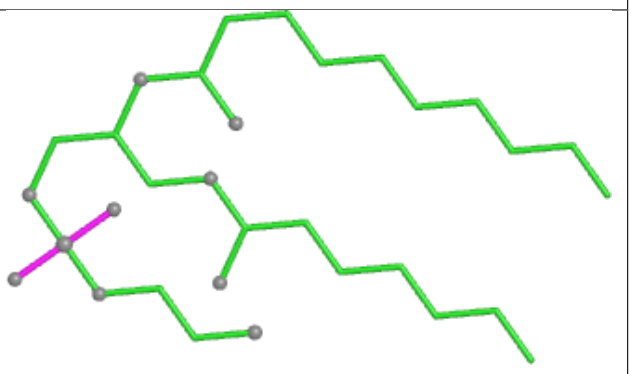


Rings

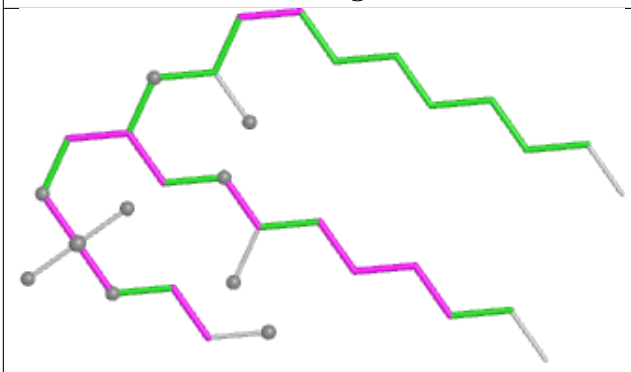
Ligand 3PE A 503



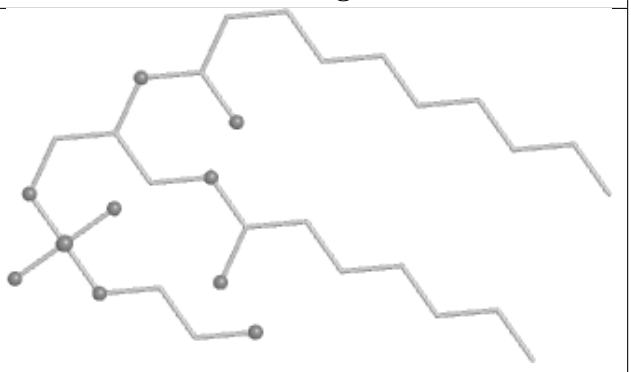
Bond lengths



Bond angles

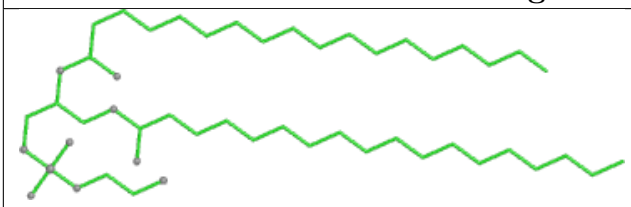


Torsions

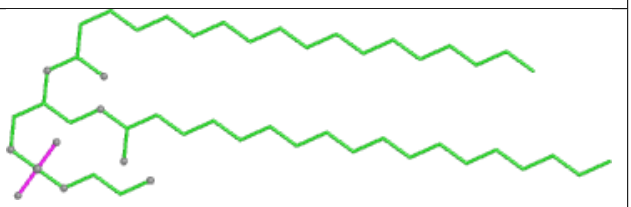


Rings

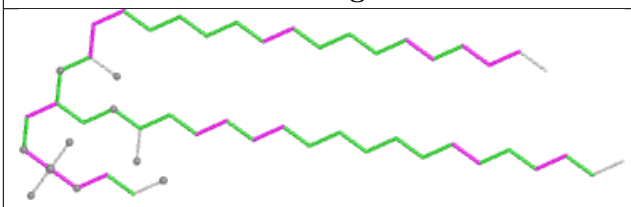
Ligand 3PE A 502



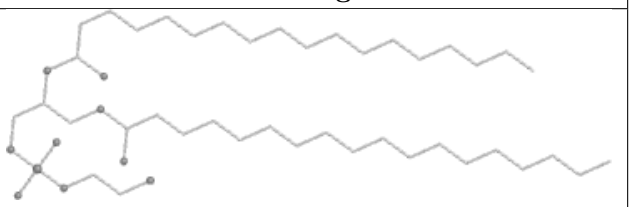
Bond lengths



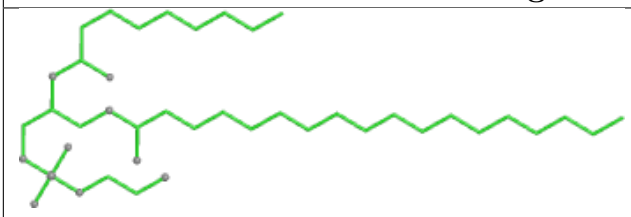
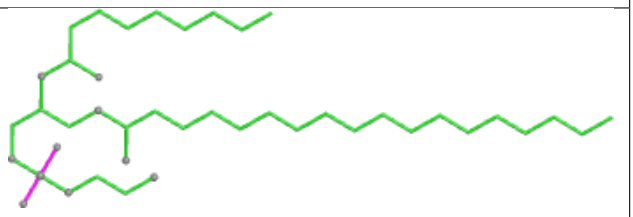
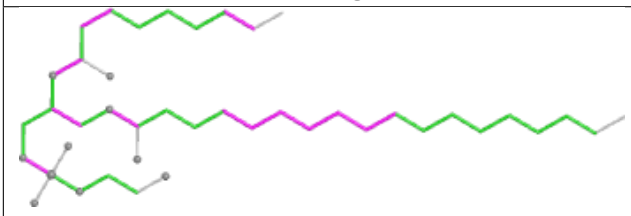
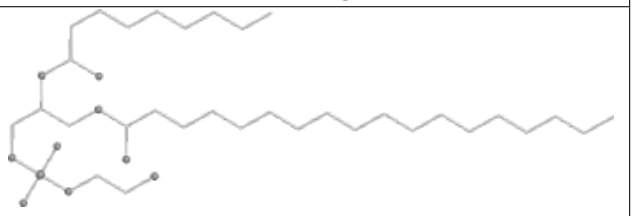
Bond angles



Torsions



Rings

Ligand 3PE D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

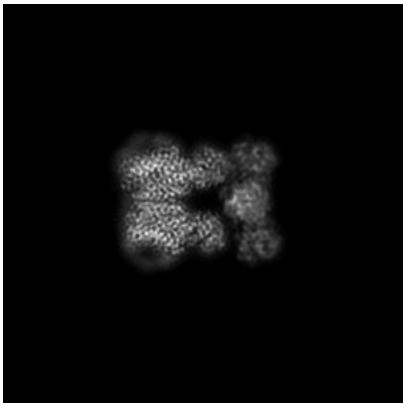
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64527. These allow visual inspection of the internal detail of the map and identification of artifacts.

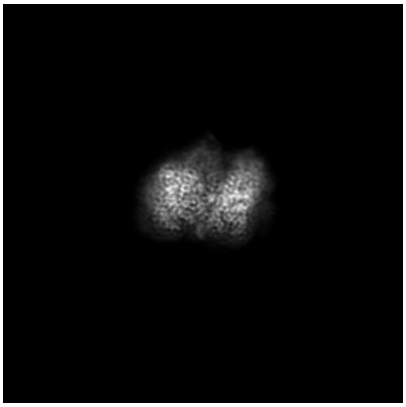
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

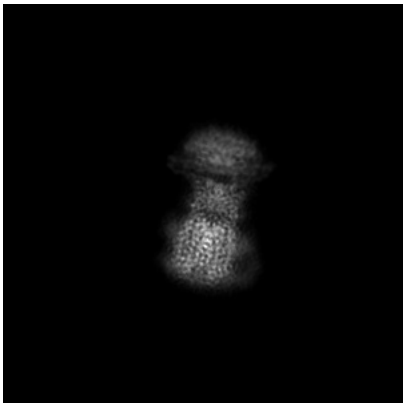
6.1.1 Primary map



X



Y

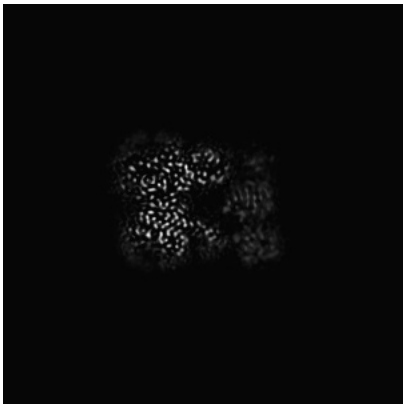


Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

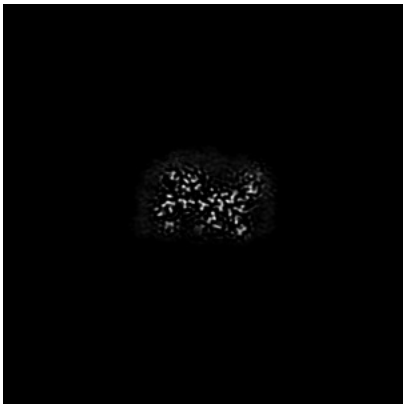
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 186



Y Index: 141

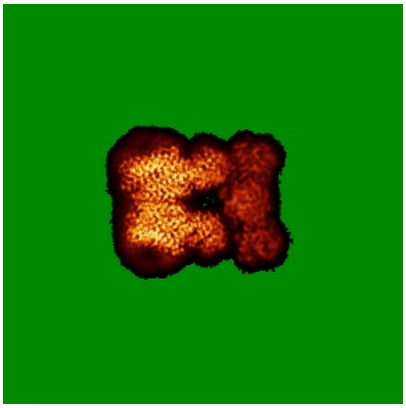


Z Index: 212

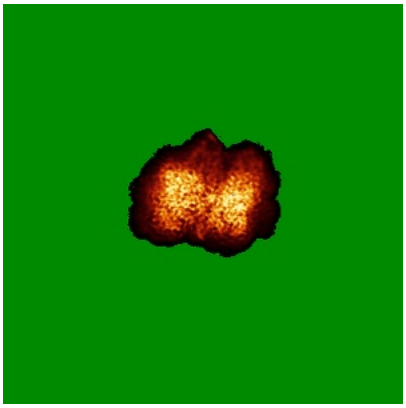
The images above show the largest variance slices of the map in three orthogonal directions.

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

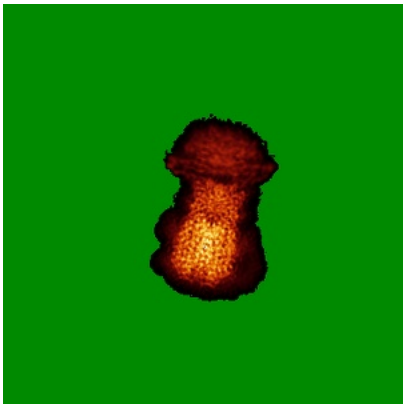
6.4.1 Primary map



X



Y

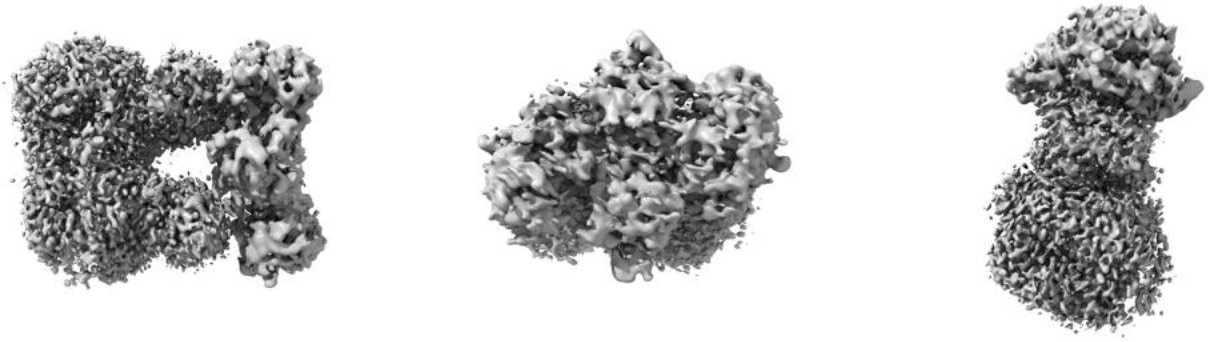


Z

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

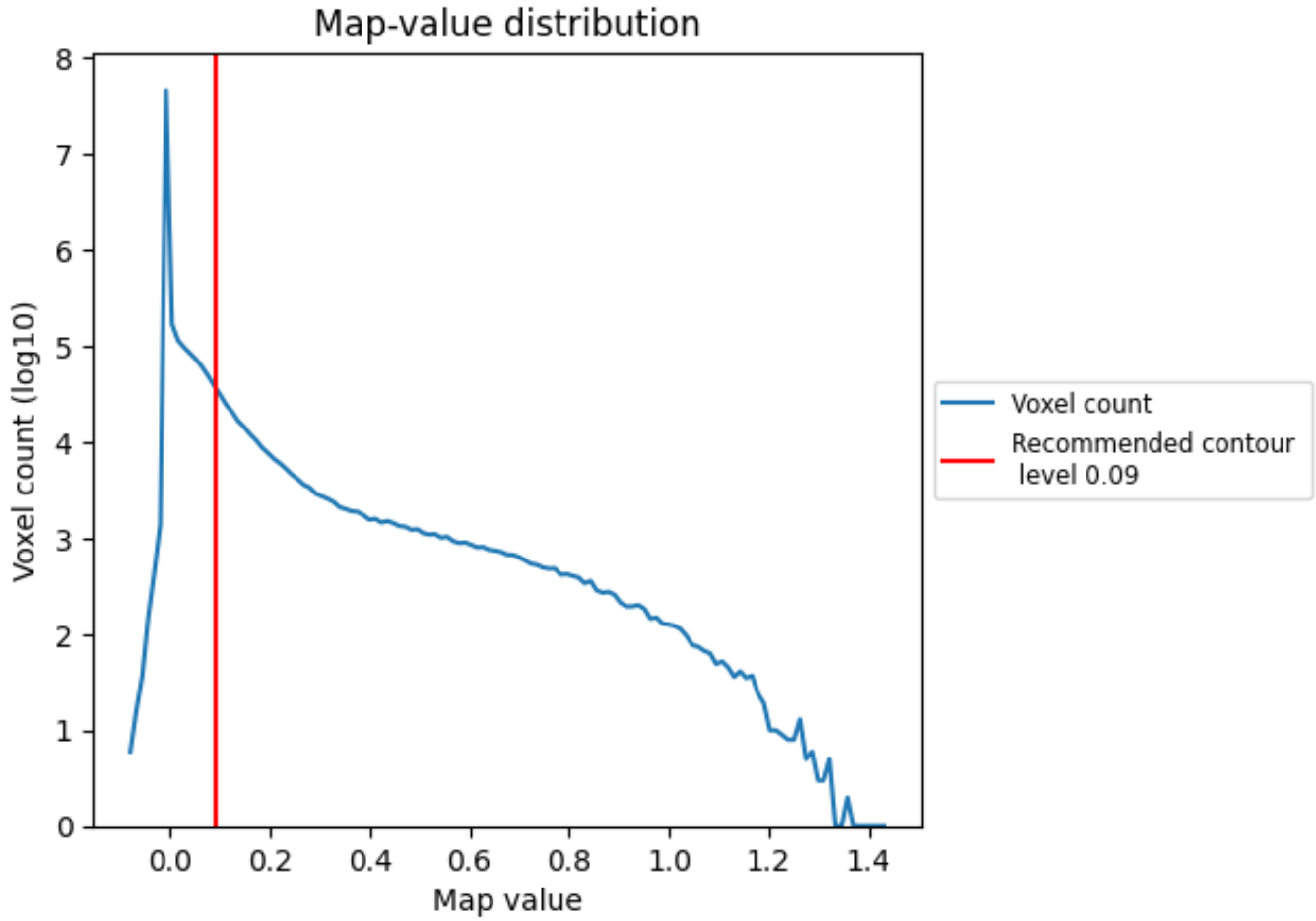
6.6 Mask visualisation (i)

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

7 Map analysis

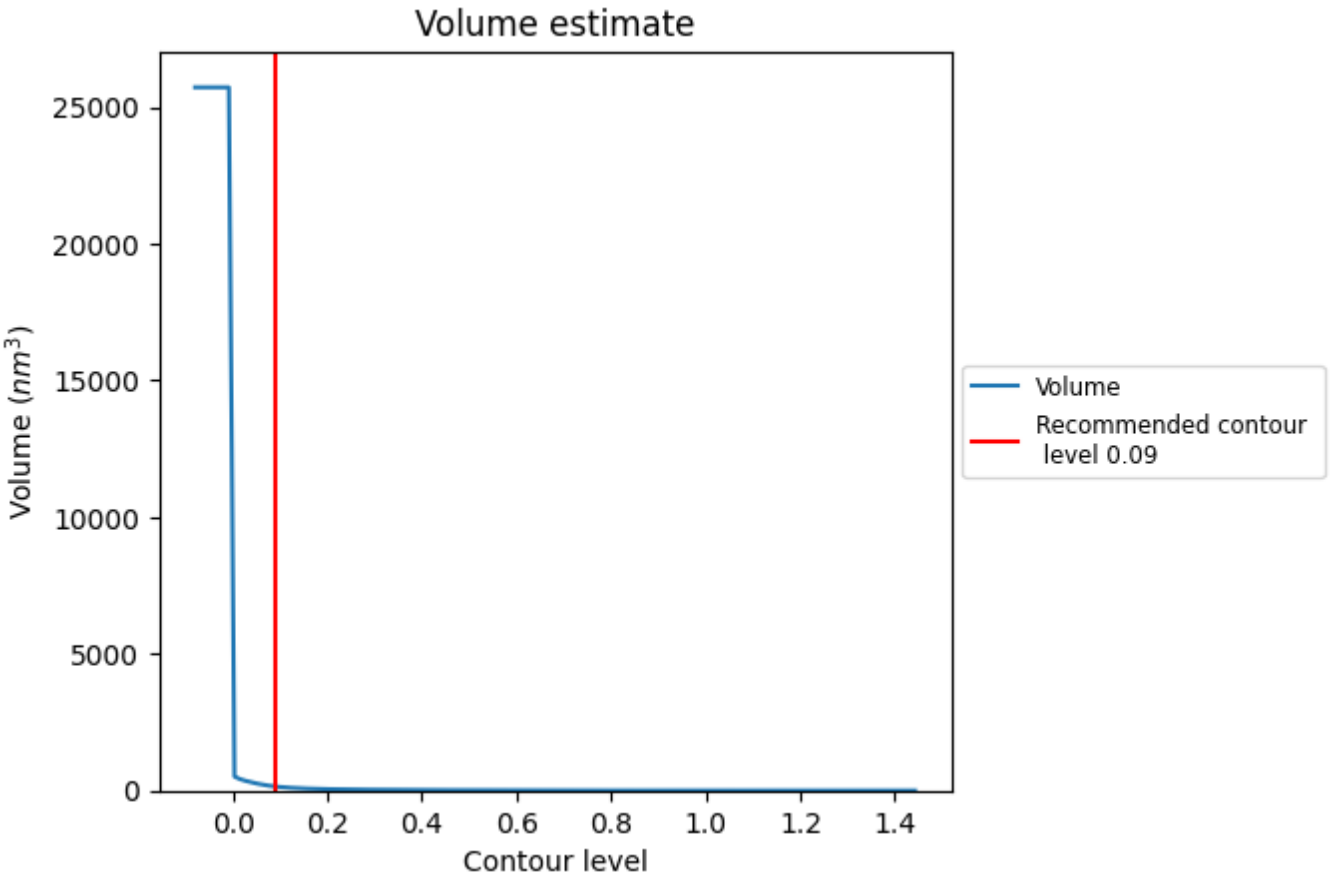
This section contains the results of statistical analysis of the map.

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.

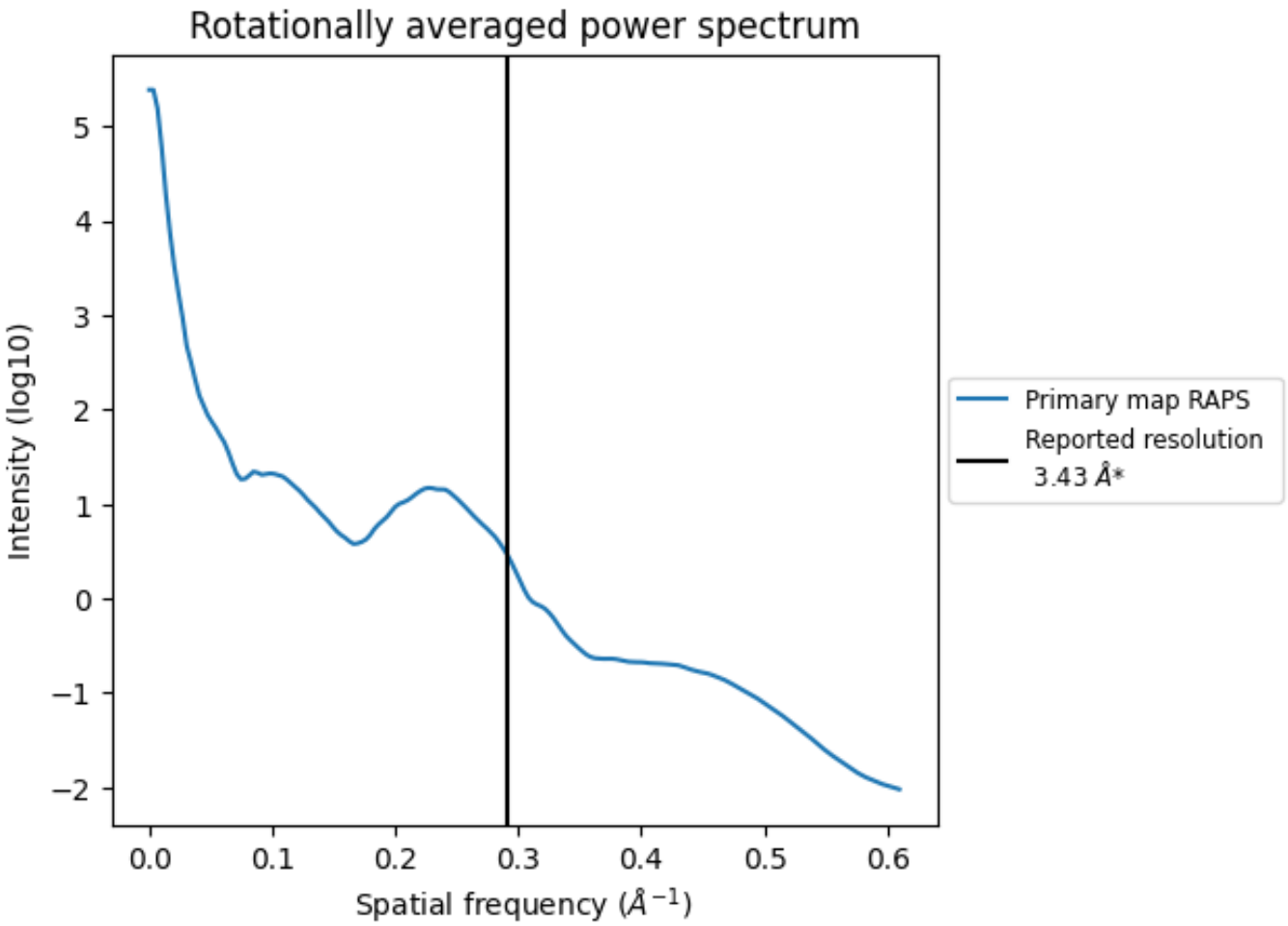
7.2 Volume estimate



The volume at the recommended contour level is 148 nm^3; this corresponds to an approximate mass of 134 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 0.292 Å^{-1}

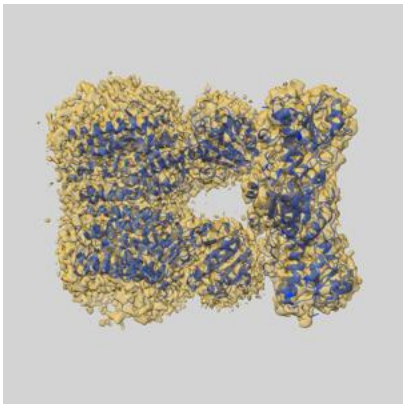
8 Fourier-Shell correlation (i)

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

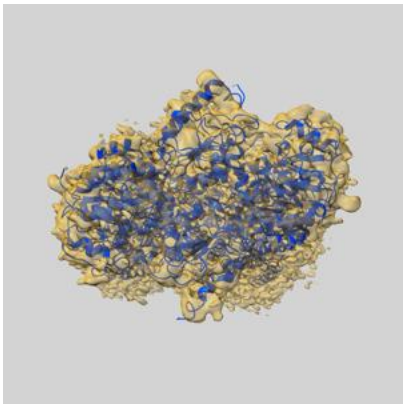
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64527 and PDB model 9UV7. Per-residue inclusion information can be found in section 3 on page 7.

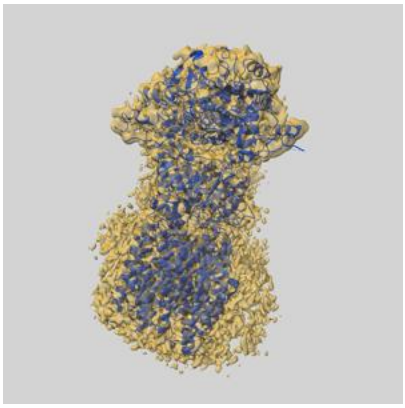
9.1 Map-model overlay



X



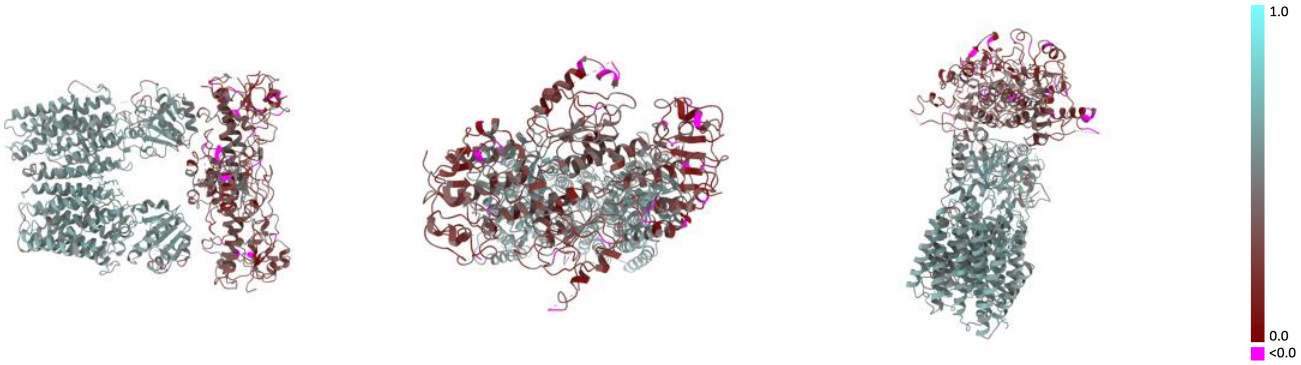
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

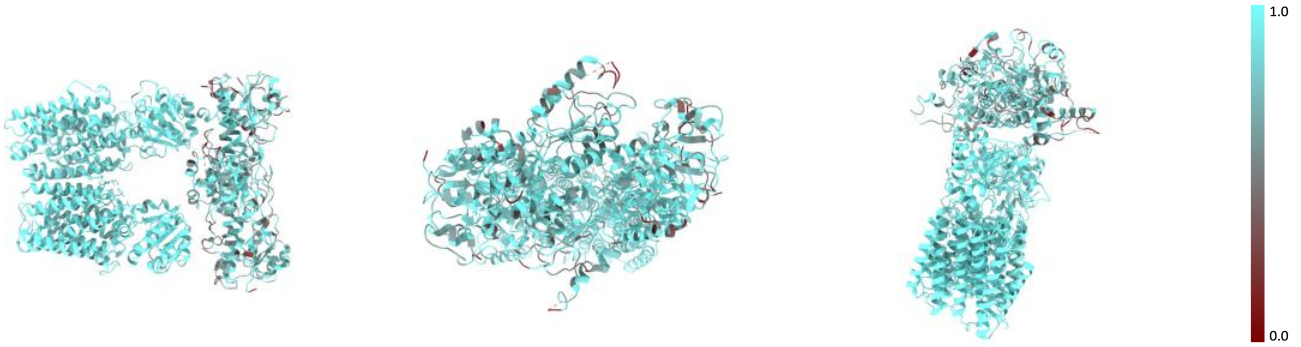
9.2 Q-score mapped to coordinate model (i)



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.

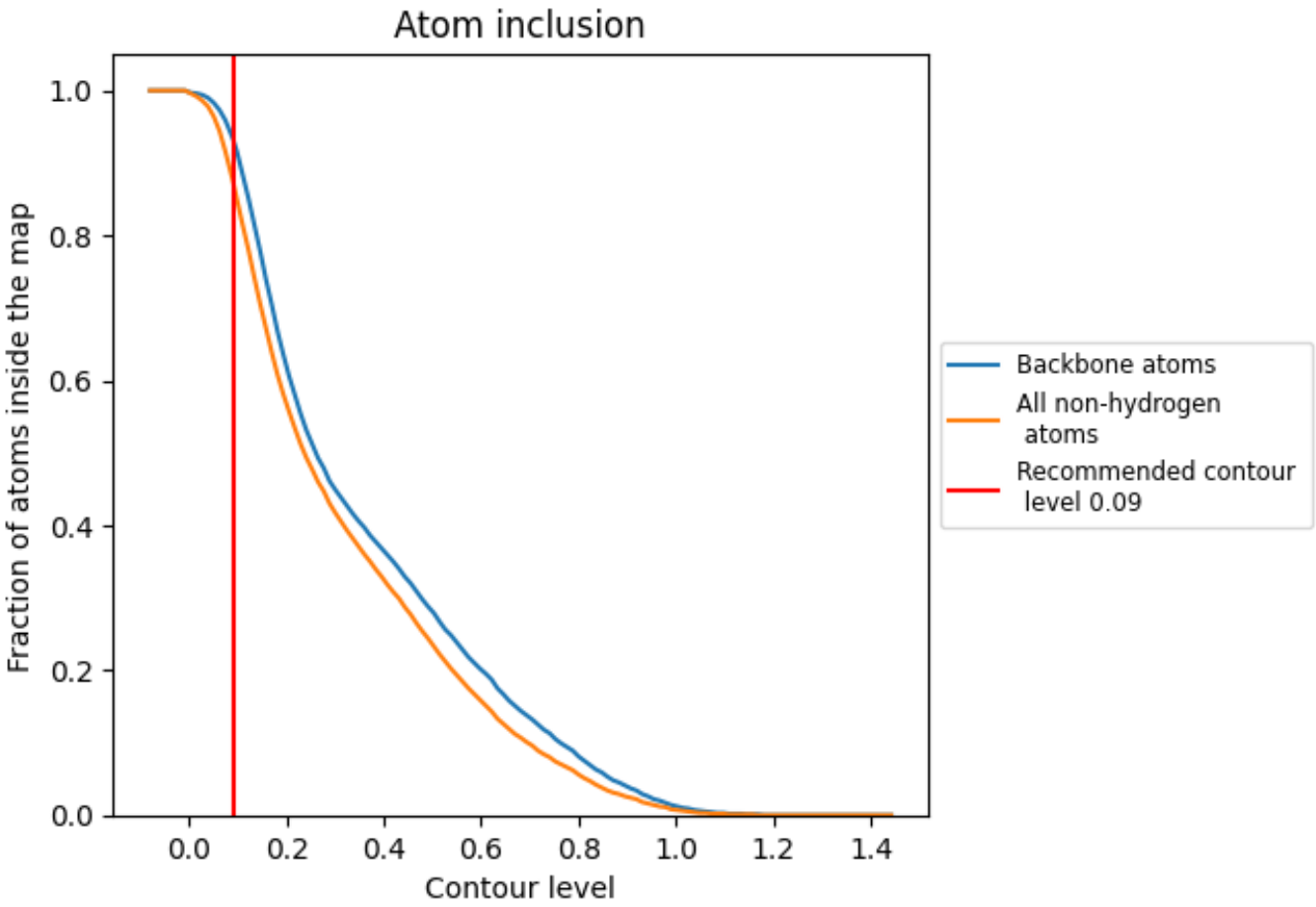
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8760	0.4490
A	0.9680	0.5570
B	0.9610	0.5550
C	0.9710	0.5670
D	0.9820	0.5720
E	0.7340	0.2740
F	0.7400	0.2870

