Full wwPDB EM Validation Report

Mar 10, 2025 – 05:36 PM EDT

PDB ID	:	8V0G
EMDB ID	:	EMD-42854
Title	:	plasmodium falciparum Niemann-Pick type C1-related protein form I
Authors	:	Zhang, Z.; Lyu, M.
Deposited on	:	2023-11-17
Resolution	:	3.11 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:

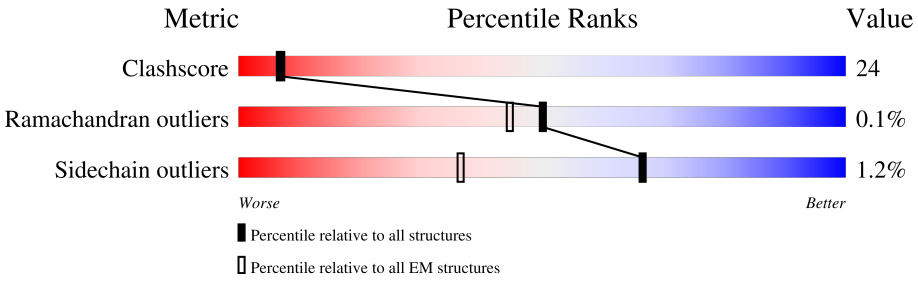
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.11 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1470	35% 31% 33%

2 Entry composition

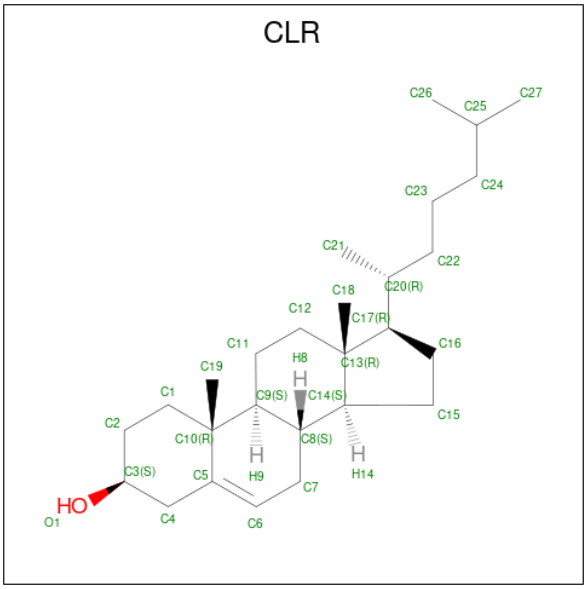
There are 3 unique types of molecules in this entry. The entry contains 8106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Niemann-Pick type C1-related protein.

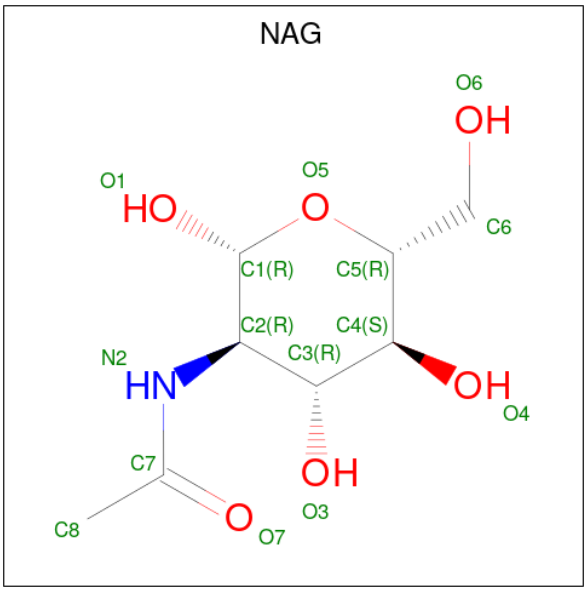
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	985	8050	5285	1266	1454	45	0	0

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
2	A	1	28	27	1		0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



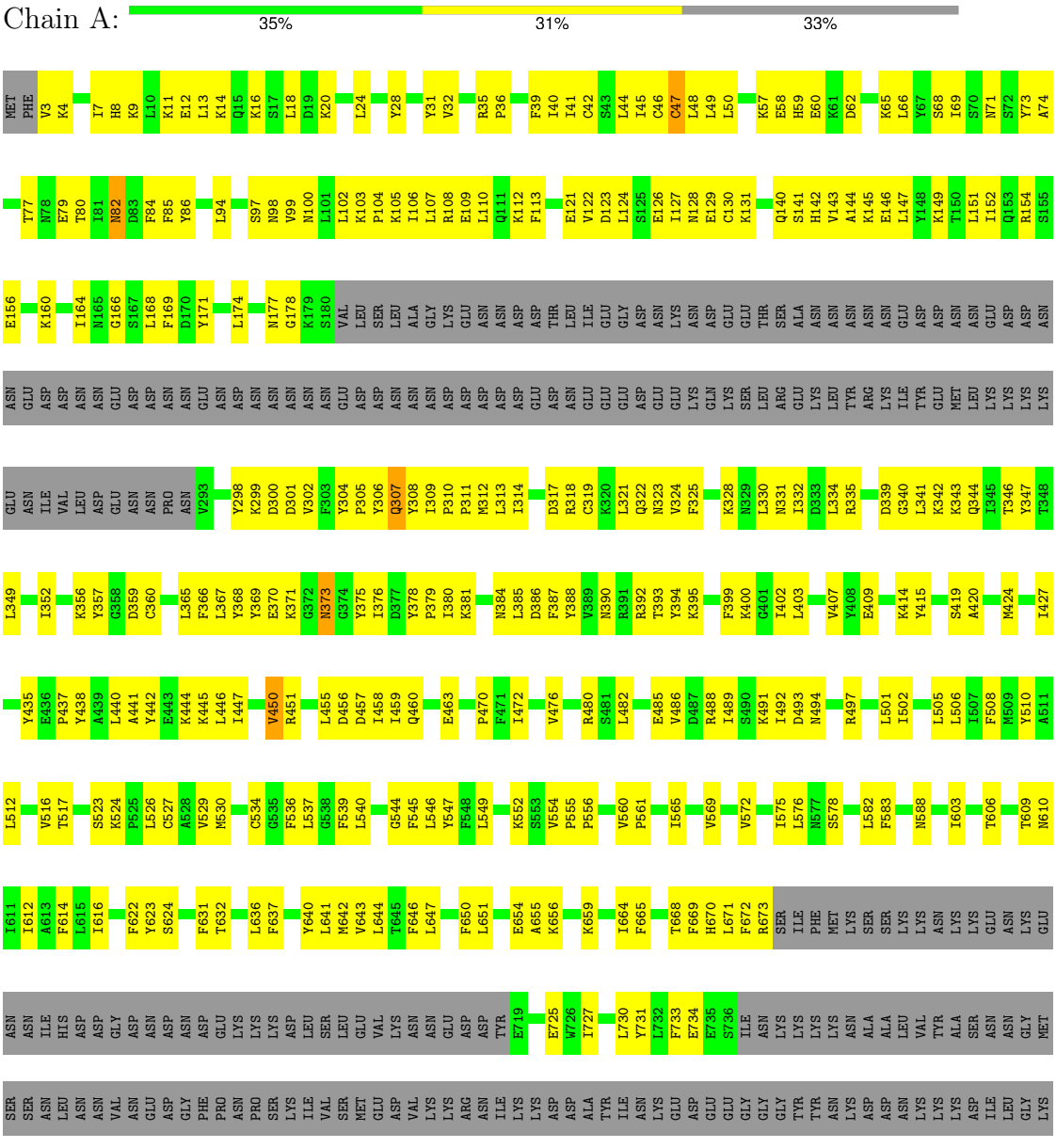
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

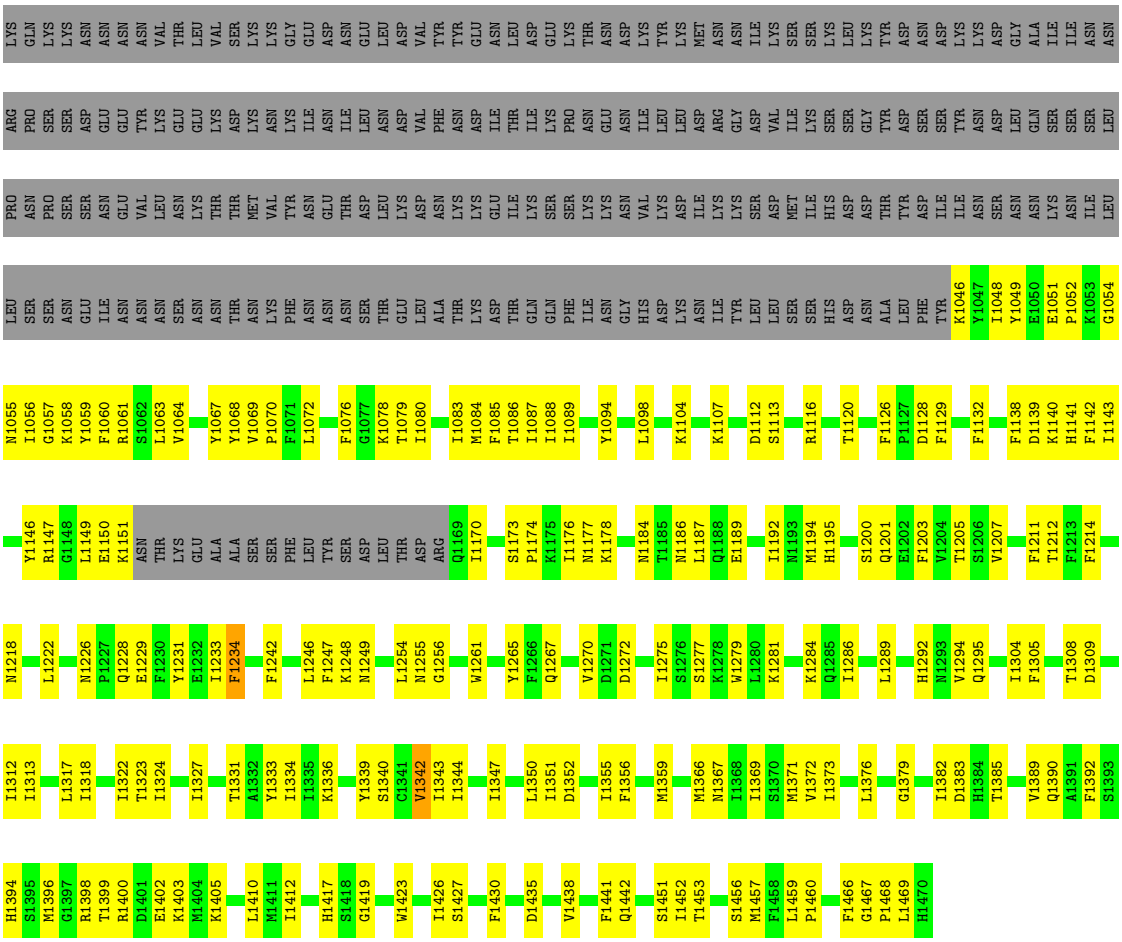
3 Residue-property plots (i)

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: Niemann-Pick type C1-related protein

Chain A:




LYS GLN LYS LYS ASN ASN ASN VAL THR LEU VAL SER LYS LYS GLY GLU ASP ASN GLU LEU ASP VAL TYR TYR GLU ASN GLU ASP LYS TYR LYS MET ASN ASN ILE LYS SER SER LYS LEU LYS ASP GLY ALA ILE ILE ASN ASN
ARG PRO SER SER ASP GLU GLU TYR LYS GLU GLU LYS ASP LYS ASN LYS ILE ASN ILE LEU ASN ASP VAL PHE ASN ASP ILE THR ILE LYS PRO ASN GLU ASN ILE LEU LEU ASP ARG GLY ASP VAL ILE LYS SER SER GLY TYR ASP SER SER TYR ASN ASP LEU GLN SER ASN SER SER ASN
PRO ASN PRO SER SER ASN GLU VAL LEU ASN LYS THR THR MET VAL TYR ASN GLU THR ASP LEU LYS ASP ASN LYS LYS GLU LEU ASN ASP VAL LEU LYS LYS SER ASP MET ILE HIS ASP ASP THR TYR ASP ILE ILE ASN SER ASN LYS SER ASN ILE LEU
LEU SER SER ASN GLU ILE ASN ASN ASN SER ASN ASN ASN THR ASN LYS PHE ASN ASN ASN SER THR GLU LEU ALA THR LYS ASP THR GLN GLN PHE ILE ASN GLY HIS ASP LYS ASN ILE TYR LEU LEU SER SER HIS ASP ASN ALA LEU PHE TYR K1046 Y1047 I1048 Y1049 E1050 E1051 P1052 K1053 G1054
N1055 I1056 G1057 K1058 Y1059 F1060 R1061 S1062 L1063 V1064 Y1067 Y1068 V1069 P1070 F1071 L1072 F1076 G1077 K1078 T1079 I1080 I1083 M1084 F1085 T1086 I1087 I1088 I1089 Y1094 L1098 K1104 K1107 D1112 S1113 R1116 T1120 F1126 P1127 D1128 F1129 F1132 F1138 D1139 K1140 H1141 F1142 I1143
Y1146 R1147 G1148 L1149 E1150 K1151 ASN THR LYS GLU ALA ALA SER SER PHE LEU TYR SER ASP LEU THR ASP ARG Q1169 I1170 S1173 P1174 K1175 I1176 N1177 K1178 N1184 T1185 N1186 L1187 Q1188 E1189 I1192 N1193 M1194 H1195 S1200 Q1201 E1202 F1203 V1204 T1205 S1206 V1207 F1211 T1212 F1213 F1214
N1218 L1222 N1226 P1227 Q1228 E1229 F1230 Y1231 E1232 I1233 F1234 F1242 L1246 F1247 K1248 N1249 L1254 N1255 G1256 W1261 Y1265 F1266 Q1267 V1270 D1271 D1272 I1275 S1276 S1277 K1278 W1279 L1280 K1281 K1284 Q1285 I1286 L1289 H1292 N1293 V1294 Q1295 I1304 F1305 T1308 D1309
I1312 I1313 L1317 I1318 I1322 T1323 I1324 I1327 T1331 A1332 Y1333 I1334 I1335 K1336 Y1339 S1340 C1341 V1342 I1343 I1344 I1347 L1350 I1351 D1352 I1355 F1356 M1359 M1366 N1367 I1368 I1369 S1370 M1371 V1372 I1373 L1376 G1379 I1382 D1383 H1384 T1385 V1389 Q1390 A1391 F1392 S1393
H1394 S1395 M1396 G1397 R1398 T1399 R1400 D1401 E1402 K1403 M1404 K1405 L1410 M1411 I1412 H1417 S1418 G1419 W1423 I1426 S1427 F1430 D1435 V1438 F1441 Q1442 S1451 I1452 T1453 S1456 M1457 F1458 L1459 P1460 F1466 G1467 P1468 L1469 H1470

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63097	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 ($e^-/Å^2$)	35.86	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.535	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, NAG

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	0.33	0/8239	0.41	0/11120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8050	0	8078	391	0
2	A	28	0	46	7	0
3	A	28	0	26	1	0
All	All	8106	0	8150	392	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 24.

All (392) 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:530:MET:HB3	1:A:646:PHE:HE1	1.22	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:ARG:HD3	1:A:1467:GLY:H	1.34	0.92
1:A:1177:ASN:HD21	1:A:1295:GLN:H	1.15	0.91
1:A:80:THR:HA	1:A:1147:ARG:HH21	1.36	0.91
1:A:517:THR:HG22	1:A:523:SER:HB3	1.57	0.85
1:A:530:MET:HB3	1:A:646:PHE:CE1	2.10	0.82
1:A:322:GLN:HB2	1:A:331:ASN:HA	1.60	0.82
1:A:312:MET:HG3	1:A:313:LEU:HD12	1.64	0.80
1:A:1128:ASP:HB3	1:A:1205:THR:HG21	1.62	0.80
1:A:609:THR:HG21	1:A:1382:ILE:HG21	1.63	0.79
1:A:69:ILE:HG13	1:A:1308:THR:HG22	1.64	0.78
1:A:313:LEU:HD11	1:A:1149:LEU:HD21	1.66	0.78
1:A:140:GLN:HB3	1:A:145:LYS:HD3	1.66	0.75
1:A:1055:ASN:HB2	1:A:1058:LYS:HB2	1.72	0.72
1:A:536:PHE:CE2	1:A:540:LEU:HD11	2.24	0.72
1:A:640:TYR:CE2	1:A:644:LEU:HD11	2.25	0.71
1:A:637:PHE:CE2	1:A:641:LEU:HD11	2.25	0.71
1:A:730:LEU:HD13	1:A:1049:TYR:HB3	1.73	0.71
1:A:328:LYS:HB3	1:A:330:LEU:HG	1.74	0.70
1:A:637:PHE:CZ	1:A:641:LEU:HD11	2.26	0.70
1:A:108:ARG:HG2	1:A:376:ILE:HG21	1.72	0.70
1:A:1052:PRO:HD2	1:A:1055:ASN:HD21	1.56	0.70
1:A:1173:SER:HB3	1:A:1176:ILE:HG12	1.73	0.69
1:A:556:PRO:HG2	1:A:624:SER:HB2	1.73	0.69
1:A:168:LEU:HD21	3:A:1502:NAG:H62	1.73	0.69
1:A:1402:GLU:O	1:A:1405:LYS:HG2	1.92	0.69
1:A:727:ILE:HG21	1:A:1410:LEU:HD11	1.76	0.68
1:A:640:TYR:CZ	1:A:644:LEU:HD11	2.28	0.68
1:A:446:LEU:O	1:A:450:VAL:HG12	1.93	0.68
1:A:31:TYR:HB3	1:A:35:ARG:NH2	2.09	0.68
1:A:1214:PHE:CE2	1:A:1222:LEU:HD21	2.30	0.67
1:A:1046:LYS:HG3	1:A:1048:ILE:HG22	1.76	0.67
1:A:609:THR:HG23	1:A:1327:ILE:HD12	1.77	0.67
1:A:575:ILE:HD11	1:A:603:ILE:HD13	1.76	0.67
1:A:1289:LEU:HB2	1:A:1294:VAL:HB	1.76	0.66
1:A:1170:ILE:HG23	1:A:1176:ILE:HG21	1.77	0.66
1:A:310:PRO:HB2	1:A:313:LEU:HD13	1.78	0.66
1:A:1399:THR:HB	1:A:1402:GLU:HG3	1.78	0.66
1:A:1419:GLY:HA3	1:A:1452:ILE:HD11	1.77	0.65
1:A:668:THR:O	1:A:671:LEU:HG	1.95	0.65
1:A:122:VAL:HG22	1:A:445:LYS:HG3	1.78	0.65
1:A:330:LEU:HB3	1:A:332:ILE:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:CYS:O	1:A:45:ILE:HG12	1.98	0.64
1:A:109:GLU:O	1:A:112:LYS:HG2	1.98	0.64
1:A:486:VAL:O	1:A:489:ILE:HG12	1.99	0.63
1:A:725:GLU:HA	1:A:1396:MET:SD	2.38	0.63
1:A:71:ASN:HD21	1:A:74:ALA:H	1.47	0.63
1:A:1056:ILE:HD12	1:A:1056:ILE:H	1.61	0.62
1:A:1369:ILE:H	1:A:1369:ILE:HD12	1.63	0.62
1:A:147:LEU:HD22	1:A:298:TYR:HB3	1.80	0.62
1:A:321:LEU:HD13	1:A:330:LEU:HD12	1.82	0.62
1:A:609:THR:HG21	1:A:1382:ILE:CG2	2.30	0.62
1:A:104:PRO:O	1:A:108:ARG:HG3	1.99	0.62
1:A:1272:ASP:HB3	1:A:1275:ILE:HG22	1.81	0.61
1:A:44:LEU:O	1:A:48:LEU:HD23	2.00	0.61
1:A:367:LEU:HA	1:A:370:GLU:HG2	1.82	0.61
1:A:1194:MET:HG3	1:A:1286:ILE:HG22	1.82	0.61
1:A:301:ASP:HB3	1:A:1254:LEU:HD21	1.83	0.60
1:A:107:LEU:HD23	1:A:376:ILE:HG23	1.83	0.60
1:A:1435:ASP:O	1:A:1438:VAL:HG12	2.02	0.60
1:A:47:CYS:SG	1:A:537:LEU:HD12	2.41	0.60
1:A:357:TYR:CD2	1:A:395:LYS:HG2	2.36	0.60
1:A:517:THR:HG21	1:A:1054:GLY:O	2.01	0.60
1:A:1076:PHE:CE2	1:A:1080:ILE:HD11	2.37	0.59
1:A:375:TYR:HB2	1:A:378:TYR:CD2	2.37	0.59
1:A:1177:ASN:ND2	1:A:1295:GLN:H	1.95	0.59
1:A:1347:ILE:HG13	1:A:1459:LEU:HD13	1.84	0.59
1:A:31:TYR:HB3	1:A:35:ARG:HH22	1.66	0.59
1:A:1094:TYR:CE2	1:A:1098:LEU:HD11	2.38	0.59
1:A:643:VAL:HG13	1:A:647:LEU:HD23	1.85	0.59
1:A:324:VAL:HG21	1:A:438:TYR:CE1	2.37	0.59
1:A:1146:TYR:O	1:A:1149:LEU:HG	2.03	0.59
1:A:28:TYR:HA	1:A:31:TYR:HD2	1.67	0.59
1:A:1356:PHE:O	1:A:1359:MET:HG2	2.02	0.59
1:A:127:ILE:HD11	1:A:347:TYR:HE2	1.67	0.58
1:A:304:TYR:HA	1:A:305:PRO:C	2.22	0.58
1:A:1064:VAL:HG12	1:A:1069:VAL:HG23	1.85	0.58
1:A:1339:TYR:O	1:A:1342:VAL:HG22	2.03	0.58
1:A:1060:PHE:HE2	1:A:1412:ILE:HG23	1.69	0.58
1:A:142:HIS:O	1:A:146:GLU:HG3	2.02	0.58
1:A:1344:ILE:HG12	1:A:1389:VAL:HG21	1.85	0.58
1:A:407:VAL:HB	1:A:419:SER:HB3	1.86	0.58
1:A:166:GLY:HA2	1:A:169:PHE:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:O	1:A:491:LYS:HG2	2.04	0.57
1:A:1247:PHE:CZ	2:A:1501:CLR:H14	2.39	0.57
1:A:103:LYS:HD3	1:A:105:LYS:NZ	2.19	0.57
1:A:28:TYR:HA	1:A:31:TYR:CD2	2.39	0.57
1:A:301:ASP:HA	1:A:1255:ASN:HD21	1.69	0.57
1:A:84:PHE:HA	1:A:311:PRO:HD2	1.88	0.56
1:A:123:ASP:OD1	1:A:126:GLU:HG3	2.04	0.56
1:A:50:LEU:HD12	1:A:545:PHE:HB2	1.88	0.56
1:A:508:PHE:CZ	1:A:529:VAL:HG22	2.41	0.56
1:A:82:ASN:HD22	1:A:82:ASN:N	2.03	0.56
1:A:510:TYR:OH	1:A:1417:HIS:HA	2.05	0.56
1:A:366:PHE:HA	1:A:369:TYR:HD2	1.71	0.56
1:A:1150:GLU:O	1:A:1151:LYS:C	2.43	0.55
1:A:669:PHE:O	1:A:673:ARG:HG3	2.07	0.55
1:A:1207:VAL:HG12	1:A:1265:TYR:HB2	1.89	0.55
1:A:1336:LYS:HD2	1:A:1394:HIS:CE1	2.42	0.55
1:A:152:ILE:HA	1:A:309:ILE:HD11	1.89	0.55
1:A:32:VAL:HA	1:A:39:PHE:CE1	2.42	0.55
1:A:545:PHE:CE2	1:A:549:LEU:HD11	2.42	0.55
1:A:502:ILE:O	1:A:506:LEU:HG	2.07	0.54
1:A:1392:PHE:HZ	1:A:1400:ARG:HG3	1.73	0.54
1:A:8:HIS:CE1	1:A:11:LYS:HZ1	2.25	0.54
1:A:1063:LEU:HD12	1:A:1067:TYR:CD1	2.43	0.54
1:A:1379:GLY:O	1:A:1382:ILE:HG22	2.07	0.54
1:A:14:LYS:HE3	1:A:1333:TYR:O	2.07	0.54
1:A:151:LEU:HD23	1:A:154:ARG:HH11	1.71	0.54
1:A:1226:ASN:HB3	1:A:1229:GLU:HB3	1.90	0.54
1:A:387:PHE:CD2	2:A:1501:CLR:H231	2.42	0.54
1:A:1218:ASN:O	1:A:1222:LEU:HD13	2.08	0.54
1:A:31:TYR:HB3	1:A:35:ARG:CZ	2.37	0.54
1:A:384:ASN:HD21	1:A:386:ASP:HB2	1.72	0.54
1:A:730:LEU:CD1	1:A:1049:TYR:HB3	2.38	0.54
1:A:1400:ARG:HD3	1:A:1467:GLY:N	2.13	0.54
1:A:129:GLU:HG3	1:A:437:PRO:HB3	1.89	0.54
1:A:1141:HIS:NE2	1:A:1178:LYS:HG3	2.23	0.53
1:A:1214:PHE:CE1	1:A:1234:PHE:HA	2.43	0.53
1:A:1456:SER:O	1:A:1460:PRO:HG2	2.07	0.53
1:A:459:ILE:HD13	1:A:472:ILE:HG22	1.90	0.53
1:A:1149:LEU:CD1	1:A:1150:GLU:HG2	2.38	0.53
1:A:13:LEU:HA	1:A:16:LYS:HE2	1.90	0.53
1:A:731:TYR:CE1	1:A:1405:LYS:HE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ILE:O	1:A:310:PRO:C	2.48	0.52
1:A:455:LEU:O	1:A:458:ILE:HG22	2.09	0.52
1:A:447:ILE:O	1:A:451:ARG:HG3	2.10	0.52
1:A:365:LEU:HD13	1:A:403:LEU:HD11	1.91	0.52
1:A:1423:TRP:HA	1:A:1426:ILE:HG12	1.90	0.52
1:A:3:VAL:O	1:A:7:ILE:HG13	2.10	0.52
1:A:485:GLU:O	1:A:489:ILE:HG23	2.08	0.52
1:A:1390:GLN:HG3	1:A:1394:HIS:HD2	1.75	0.52
1:A:545:PHE:O	1:A:549:LEU:HG	2.10	0.52
1:A:140:GLN:HB3	1:A:145:LYS:CD	2.39	0.51
1:A:371:LYS:CB	1:A:392:ARG:HB2	2.40	0.51
1:A:1331:THR:O	1:A:1334:ILE:HG13	2.10	0.51
1:A:1052:PRO:HD2	1:A:1055:ASN:ND2	2.25	0.51
1:A:94:LEU:HD13	1:A:424:MET:HB2	1.92	0.51
1:A:123:ASP:HA	1:A:346:THR:HG22	1.92	0.51
1:A:1184:ASN:HB3	1:A:1186:ASN:OD1	2.11	0.51
1:A:31:TYR:HB3	1:A:35:ARG:NH1	2.25	0.51
1:A:516:VAL:HA	1:A:523:SER:HB2	1.92	0.51
1:A:390:ASN:HB3	1:A:393:THR:OG1	2.11	0.51
1:A:357:TYR:HD2	1:A:395:LYS:HG2	1.72	0.51
1:A:1289:LEU:H	1:A:1289:LEU:HD22	1.76	0.51
1:A:147:LEU:HD23	1:A:313:LEU:HD21	1.91	0.51
1:A:373:ASN:HA	1:A:392:ARG:CZ	2.41	0.51
1:A:103:LYS:HD3	1:A:105:LYS:HZ3	1.74	0.50
1:A:384:ASN:HA	1:A:415:TYR:HE2	1.75	0.50
1:A:140:GLN:HG2	1:A:144:ALA:HB3	1.93	0.50
1:A:1076:PHE:O	1:A:1080:ILE:HG13	2.11	0.50
1:A:71:ASN:ND2	1:A:74:ALA:H	2.10	0.50
1:A:80:THR:CA	1:A:1147:ARG:HH21	2.16	0.50
1:A:583:PHE:CE2	1:A:1051:GLU:HG2	2.47	0.50
1:A:385:LEU:HG	1:A:415:TYR:CD2	2.47	0.50
1:A:1390:GLN:HG3	1:A:1394:HIS:CD2	2.46	0.50
1:A:325:PHE:CE1	1:A:352:ILE:HG23	2.47	0.49
1:A:546:LEU:CD1	1:A:631:PHE:HA	2.42	0.49
1:A:588:ASN:OD1	1:A:659:LYS:HB2	2.12	0.49
1:A:1277:SER:O	1:A:1281:LYS:HG3	2.12	0.49
1:A:1339:TYR:CE2	1:A:1343:ILE:HD11	2.47	0.49
1:A:1084:MET:O	1:A:1087:ILE:HG22	2.12	0.49
1:A:1132:PHE:CZ	2:A:1501:CLR:H21	2.47	0.49
1:A:1267:GLN:NE2	1:A:1279:TRP:HE3	2.09	0.49
1:A:1366:MET:HB2	1:A:1371:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1339:TYR:O	1:A:1343:ILE:HG13	2.13	0.49
1:A:373:ASN:OD1	1:A:390:ASN:HA	2.13	0.49
1:A:527:CYS:SG	1:A:651:LEU:HA	2.53	0.49
1:A:622:PHE:HZ	1:A:1308:THR:HB	1.76	0.49
1:A:1084:MET:O	1:A:1088:ILE:HG13	2.13	0.49
1:A:50:LEU:O	1:A:544:GLY:HA3	2.12	0.49
1:A:123:ASP:CG	1:A:126:GLU:HG3	2.33	0.49
1:A:124:LEU:HA	1:A:127:ILE:HD13	1.94	0.49
1:A:390:ASN:HB3	1:A:393:THR:HG1	1.77	0.49
1:A:35:ARG:HG3	1:A:39:PHE:CE1	2.48	0.49
1:A:41:ILE:HG13	1:A:42:CYS:N	2.27	0.49
1:A:1189:GLU:O	1:A:1192:ILE:HG22	2.12	0.49
1:A:1242:PHE:O	1:A:1246:LEU:HG	2.12	0.49
1:A:106:ILE:HG22	1:A:110:LEU:HD23	1.95	0.48
1:A:1126:PHE:HB3	1:A:1129:PHE:HD2	1.78	0.48
1:A:1339:TYR:CD2	1:A:1468:PRO:HG3	2.48	0.48
1:A:1459:LEU:HB3	1:A:1460:PRO:HD3	1.94	0.48
1:A:1085:PHE:CZ	1:A:1453:THR:HG22	2.47	0.48
1:A:131:LYS:O	1:A:335:ARG:HA	2.13	0.48
1:A:1270:VAL:HG21	1:A:1275:ILE:HG21	1.95	0.48
1:A:339:ASP:HB3	1:A:343:LYS:NZ	2.29	0.48
1:A:390:ASN:O	1:A:394:TYR:N	2.45	0.48
1:A:1057:GLY:O	1:A:1061:ARG:HG3	2.13	0.48
1:A:41:ILE:O	1:A:45:ILE:HG23	2.13	0.48
1:A:572:VAL:HG22	1:A:647:LEU:HD22	1.95	0.48
1:A:1229:GLU:O	1:A:1233:ILE:HG12	2.13	0.48
1:A:1385:THR:HG23	1:A:1459:LEU:HD22	1.96	0.48
1:A:1142:PHE:CD1	1:A:1254:LEU:HD12	2.48	0.48
1:A:1352:ASP:HA	1:A:1355:ILE:HG12	1.95	0.48
1:A:58:GLU:OE1	1:A:552:LYS:HE2	2.14	0.48
1:A:105:LYS:HE2	1:A:458:ILE:HG13	1.96	0.48
1:A:98:ASN:HD21	1:A:470:PRO:HA	1.77	0.48
1:A:612:ILE:O	1:A:616:ILE:HG12	2.14	0.47
1:A:441:ALA:O	1:A:445:LYS:HG2	2.14	0.47
1:A:1318:ILE:O	1:A:1322:ILE:HG13	2.13	0.47
1:A:1132:PHE:HZ	2:A:1501:CLR:H21	1.80	0.47
1:A:71:ASN:ND2	1:A:73:TYR:HB3	2.29	0.47
1:A:508:PHE:CZ	1:A:529:VAL:HG13	2.49	0.47
1:A:727:ILE:HD12	1:A:730:LEU:HD23	1.97	0.47
1:A:97:SER:OG	1:A:99:VAL:HG22	2.14	0.47
1:A:302:VAL:H	1:A:1255:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:TYR:C	1:A:308:TYR:H	2.17	0.47
1:A:508:PHE:HZ	1:A:529:VAL:HG13	1.80	0.47
1:A:174:LEU:HB3	1:A:178:GLY:HA2	1.95	0.47
1:A:1176:ILE:HG23	1:A:1295:GLN:HB3	1.97	0.47
1:A:141:SER:O	1:A:144:ALA:HB3	2.15	0.47
1:A:1104:LYS:HD3	1:A:1107:LYS:HZ3	1.80	0.47
1:A:575:ILE:HD11	1:A:603:ILE:HG21	1.97	0.47
1:A:1174:PRO:O	1:A:1178:LYS:HD3	2.15	0.47
1:A:9:LYS:O	1:A:12:GLU:HB3	2.15	0.46
1:A:45:ILE:HG13	1:A:46:CYS:N	2.30	0.46
1:A:110:LEU:O	1:A:113:PHE:HB3	2.16	0.46
1:A:156:GLU:O	1:A:160:LYS:HG3	2.15	0.46
1:A:546:LEU:HD12	1:A:631:PHE:HA	1.96	0.46
1:A:1076:PHE:CZ	1:A:1080:ILE:HD11	2.50	0.46
1:A:8:HIS:HA	1:A:11:LYS:HD3	1.97	0.46
1:A:444:LYS:O	1:A:447:ILE:HG12	2.16	0.46
1:A:402:ILE:HB	1:A:403:LEU:HD12	1.97	0.46
1:A:539:PHE:HD2	1:A:540:LEU:HD23	1.81	0.46
1:A:578:SER:O	1:A:582:LEU:HD23	2.14	0.46
1:A:456:ASP:O	1:A:459:ILE:HG12	2.15	0.46
1:A:1313:ILE:O	1:A:1317:LEU:HG	2.15	0.46
1:A:319:CYS:SG	1:A:335:ARG:HD3	2.56	0.46
1:A:130:CYS:SG	1:A:319:CYS:HA	2.56	0.46
1:A:530:MET:HG3	1:A:650:PHE:CD2	2.51	0.46
1:A:637:PHE:CE1	1:A:641:LEU:HD21	2.50	0.46
1:A:457:ASP:HA	1:A:460:GLN:NE2	2.31	0.46
1:A:517:THR:OG1	1:A:1054:GLY:HA2	2.16	0.46
1:A:1139:ASP:O	1:A:1143:ILE:HG12	2.16	0.46
1:A:65:LYS:HE2	1:A:623:TYR:CG	2.51	0.46
1:A:122:VAL:HG13	1:A:126:GLU:OE1	2.15	0.46
1:A:339:ASP:O	1:A:343:LYS:HG3	2.15	0.46
1:A:546:LEU:HD12	1:A:631:PHE:CD1	2.50	0.46
1:A:606:THR:HG23	1:A:1383:ASP:CG	2.36	0.46
1:A:57:LYS:HE2	1:A:59:HIS:CE1	2.51	0.46
1:A:20:LYS:O	1:A:24:LEU:HG	2.15	0.46
1:A:371:LYS:CG	1:A:393:THR:HG22	2.46	0.46
1:A:1398:ARG:HG3	1:A:1402:GLU:OE1	2.16	0.45
1:A:40:ILE:HD13	1:A:650:PHE:CE1	2.50	0.45
1:A:121:GLU:HG2	1:A:346:THR:HB	1.98	0.45
1:A:440:LEU:HB3	1:A:480:ARG:NH1	2.32	0.45
1:A:1068:TYR:OH	1:A:1457:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:PHE:CZ	1:A:650:PHE:CE1	3.04	0.45
1:A:1201:GLN:HB3	1:A:1203:PHE:CE1	2.51	0.45
1:A:378:TYR:HB3	1:A:379:PRO:HD2	1.99	0.45
1:A:554:VAL:HB	1:A:556:PRO:HD2	1.99	0.45
1:A:1138:PHE:HB3	1:A:1143:ILE:HG13	1.99	0.45
1:A:632:THR:O	1:A:636:LEU:HG	2.17	0.45
1:A:1116:ARG:O	1:A:1120:THR:HG23	2.16	0.45
1:A:1457:MET:C	1:A:1460:PRO:HD2	2.37	0.45
1:A:60:GLU:HG3	1:A:62:ASP:OD1	2.16	0.45
1:A:60:GLU:HB3	1:A:66:LEU:HD21	1.98	0.45
1:A:385:LEU:HD21	1:A:415:TYR:HB2	1.98	0.45
1:A:4:LYS:HD3	1:A:4:LYS:C	2.37	0.45
1:A:349:LEU:HD13	1:A:442:TYR:CE2	2.52	0.45
1:A:1367:ASN:O	1:A:1371:MET:HG2	2.16	0.45
1:A:1309:ASP:O	1:A:1312:ILE:HG22	2.17	0.44
1:A:321:LEU:CD2	1:A:328:LYS:HG3	2.47	0.44
1:A:365:LEU:HD11	1:A:380:ILE:HD13	1.99	0.44
1:A:1231:TYR:CD1	1:A:1256:GLY:HA2	2.53	0.44
1:A:501:LEU:O	1:A:505:LEU:HD13	2.18	0.44
1:A:1089:ILE:HD11	1:A:1350:LEU:HD21	2.00	0.44
1:A:1149:LEU:HD11	1:A:1150:GLU:HG2	1.99	0.44
1:A:1312:ILE:HD13	1:A:1366:MET:O	2.18	0.44
1:A:100:ASN:C	1:A:102:LEU:N	2.71	0.44
1:A:539:PHE:CD2	1:A:540:LEU:HD23	2.52	0.44
1:A:340:GLY:O	1:A:344:GLN:HG2	2.18	0.44
1:A:368:TYR:O	1:A:373:ASN:HB3	2.18	0.44
1:A:409:GLU:O	1:A:415:TYR:HA	2.18	0.44
1:A:492:ILE:N	1:A:492:ILE:HD12	2.31	0.44
1:A:305:PRO:HB2	1:A:307:GLN:CD	2.37	0.44
1:A:671:LEU:HD12	1:A:672:PHE:N	2.32	0.44
1:A:1140:LYS:NZ	1:A:1176:ILE:HB	2.32	0.44
1:A:1438:VAL:O	1:A:1442:GLN:HG3	2.18	0.44
1:A:1068:TYR:CZ	1:A:1072:LEU:HD11	2.53	0.44
1:A:1369:ILE:O	1:A:1373:ILE:HG12	2.18	0.44
1:A:321:LEU:HD22	1:A:328:LYS:HG3	2.00	0.43
1:A:1399:THR:H	1:A:1402:GLU:CD	2.20	0.43
1:A:325:PHE:HE1	1:A:352:ILE:HG23	1.83	0.43
1:A:370:GLU:HB2	1:A:393:THR:HG21	1.99	0.43
1:A:371:LYS:HB3	1:A:392:ARG:HB2	2.00	0.43
1:A:456:ASP:O	1:A:460:GLN:HG3	2.18	0.43
1:A:572:VAL:O	1:A:576:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:ILE:O	1:A:1086:THR:HB	2.18	0.43
1:A:1242:PHE:CE2	1:A:1246:LEU:HD11	2.54	0.43
1:A:1369:ILE:HD12	1:A:1369:ILE:N	2.32	0.43
1:A:45:ILE:O	1:A:49:LEU:HG	2.17	0.43
1:A:68:SER:HB2	1:A:1304:ILE:HG13	2.00	0.43
1:A:1112:ASP:O	1:A:1113:SER:C	2.56	0.43
1:A:1389:VAL:HG23	1:A:1459:LEU:HD21	2.00	0.43
1:A:664:ILE:HG23	1:A:665:PHE:N	2.33	0.43
1:A:1078:LYS:O	1:A:1079:THR:C	2.57	0.43
1:A:387:PHE:CG	2:A:1501:CLR:H231	2.54	0.43
1:A:730:LEU:O	1:A:734:GLU:HG3	2.19	0.43
1:A:1430:PHE:HB2	1:A:1441:PHE:CE2	2.53	0.43
1:A:85:PHE:HZ	1:A:1261:TRP:HA	1.83	0.43
1:A:352:ILE:HG22	1:A:435:TYR:HD1	1.84	0.43
1:A:555:PRO:HB2	1:A:556:PRO:HD3	2.00	0.43
1:A:1340:SER:O	1:A:1344:ILE:HG13	2.18	0.43
1:A:84:PHE:HZ	1:A:1147:ARG:HG2	1.84	0.43
1:A:86:TYR:OH	1:A:314:ILE:HG13	2.18	0.43
1:A:341:LEU:HA	1:A:344:GLN:HG2	2.01	0.43
1:A:1351:ILE:HD13	1:A:1451:SER:HA	2.01	0.43
1:A:80:THR:HA	1:A:1147:ARG:NH2	2.17	0.42
1:A:317:ASP:N	1:A:317:ASP:OD1	2.52	0.42
1:A:1323:THR:O	1:A:1324:ILE:C	2.57	0.42
1:A:1069:VAL:HB	1:A:1070:PRO:HD3	1.99	0.42
1:A:35:ARG:HG3	1:A:39:PHE:HE1	1.85	0.42
1:A:62:ASP:CG	1:A:65:LYS:HB3	2.40	0.42
1:A:328:LYS:C	1:A:330:LEU:N	2.72	0.42
1:A:368:TYR:HB2	1:A:399:PHE:HZ	1.84	0.42
1:A:727:ILE:O	1:A:730:LEU:HB3	2.19	0.42
1:A:1046:LYS:CG	1:A:1048:ILE:HG22	2.46	0.42
1:A:1369:ILE:O	1:A:1372:VAL:HG12	2.18	0.42
1:A:1284:LYS:HB2	1:A:1284:LYS:HE3	1.80	0.42
1:A:493:ASP:O	1:A:497:ARG:HG3	2.19	0.42
1:A:1149:LEU:C	1:A:1149:LEU:HD12	2.40	0.42
1:A:1289:LEU:N	1:A:1294:VAL:O	2.53	0.42
1:A:102:LEU:HG	1:A:420:ALA:HB3	2.01	0.42
1:A:317:ASP:OD1	1:A:323:ASN:ND2	2.53	0.42
1:A:565:ILE:O	1:A:569:VAL:HG23	2.19	0.42
1:A:13:LEU:O	1:A:14:LYS:C	2.58	0.42
1:A:99:VAL:HG12	1:A:463:GLU:O	2.20	0.42
1:A:1403:LYS:HE2	1:A:1469:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:HA	1:A:149:LYS:HE3	2.00	0.42
1:A:1170:ILE:O	1:A:1176:ILE:HG13	2.20	0.42
1:A:1331:THR:HG21	1:A:1382:ILE:HG12	2.02	0.42
1:A:57:LYS:HE2	1:A:59:HIS:NE2	2.34	0.42
1:A:57:LYS:HG3	1:A:547:TYR:CE1	2.55	0.42
1:A:388:TYR:HB3	1:A:399:PHE:CE1	2.54	0.42
1:A:400:LYS:HE3	1:A:400:LYS:HB2	1.79	0.42
1:A:450:VAL:HG11	1:A:476:VAL:HB	2.02	0.42
1:A:130:CYS:HB3	1:A:334:LEU:HB2	2.02	0.42
1:A:367:LEU:HA	1:A:370:GLU:CG	2.50	0.42
1:A:560:VAL:HB	1:A:561:PRO:HD3	2.02	0.42
1:A:1248:LYS:HG3	1:A:1249:ASN:OD1	2.20	0.42
1:A:11:LYS:HG2	1:A:12:GLU:N	2.34	0.41
1:A:610:ASN:O	1:A:614:PHE:HD2	2.03	0.41
1:A:614:PHE:CE1	1:A:1376:LEU:HD13	2.55	0.41
1:A:143:VAL:HA	1:A:146:GLU:CD	2.41	0.41
1:A:151:LEU:HA	1:A:154:ARG:HG2	2.02	0.41
1:A:318:ARG:HD2	1:A:437:PRO:HG2	2.01	0.41
1:A:128:ASN:OD1	1:A:131:LYS:HD3	2.20	0.41
1:A:349:LEU:HD22	1:A:442:TYR:OH	2.20	0.41
1:A:371:LYS:HB2	1:A:392:ARG:HB2	2.01	0.41
1:A:381:LYS:HZ1	1:A:414:LYS:HB2	1.85	0.41
1:A:349:LEU:HD21	1:A:427:ILE:HG21	2.03	0.41
1:A:359:ASP:O	1:A:360:CYS:C	2.58	0.41
1:A:387:PHE:CE2	2:A:1501:CLR:H272	2.55	0.41
1:A:539:PHE:CZ	1:A:561:PRO:HG3	2.55	0.41
1:A:1059:TYR:O	1:A:1060:PHE:C	2.59	0.41
1:A:1226:ASN:HB3	1:A:1229:GLU:CB	2.50	0.41
1:A:339:ASP:HA	1:A:342:LYS:HE2	2.01	0.41
1:A:1149:LEU:HD12	1:A:1150:GLU:N	2.35	0.41
1:A:1200:SER:O	1:A:1201:GLN:C	2.59	0.41
1:A:299:LYS:HG2	1:A:300:ASP:OD1	2.20	0.41
1:A:14:LYS:O	1:A:18:LEU:HG	2.21	0.41
1:A:140:GLN:O	1:A:141:SER:C	2.58	0.41
1:A:356:LYS:HG2	1:A:357:TYR:CD2	2.55	0.41
1:A:526:LEU:HB3	1:A:654:GLU:OE1	2.20	0.41
1:A:534:CYS:SG	1:A:642:MET:CB	3.09	0.41
1:A:1176:ILE:HD13	1:A:1176:ILE:HA	1.93	0.41
1:A:124:LEU:HB2	1:A:342:LYS:O	2.20	0.41
1:A:164:ILE:N	1:A:164:ILE:HD12	2.36	0.41
1:A:171:TYR:CE2	1:A:1228:GLN:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LYS:HB3	1:A:330:LEU:CG	2.48	0.41
1:A:664:ILE:HG23	1:A:665:PHE:H	1.85	0.41
1:A:1339:TYR:HD2	1:A:1468:PRO:HG3	1.86	0.41
1:A:154:ARG:NH2	1:A:300:ASP:HA	2.36	0.41
1:A:347:TYR:OH	1:A:441:ALA:HB3	2.21	0.41
1:A:482:LEU:O	1:A:486:VAL:HG23	2.20	0.41
1:A:512:LEU:O	1:A:516:VAL:HG22	2.21	0.41
1:A:670:HIS:HA	1:A:673:ARG:HH11	1.85	0.41
1:A:1187:LEU:HB2	1:A:1292:HIS:CD2	2.56	0.41
1:A:1173:SER:HB3	1:A:1176:ILE:CG1	2.47	0.41
1:A:1195:HIS:CD2	1:A:1212:THR:HG21	2.55	0.41
1:A:74:ALA:O	1:A:77:THR:HB	2.21	0.40
1:A:1304:ILE:HG23	1:A:1305:PHE:N	2.35	0.40
1:A:349:LEU:HB2	1:A:442:TYR:CZ	2.56	0.40
1:A:388:TYR:HB3	1:A:399:PHE:HE1	1.86	0.40
1:A:494:ASN:HA	1:A:497:ARG:HD2	2.04	0.40
1:A:1427:SER:HA	1:A:1441:PHE:CE1	2.55	0.40
1:A:36:PRO:HG3	1:A:656:LYS:NZ	2.36	0.40
1:A:524:LYS:HZ1	1:A:655:ALA:HA	1.86	0.40
1:A:84:PHE:CE2	1:A:1143:ILE:HG23	2.56	0.40
1:A:1069:VAL:O	1:A:1070:PRO:C	2.59	0.40
2:A:1501:CLR:H162	2:A:1501:CLR:H222	1.89	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	975/1470 (66%)	931 (96%)	43 (4%)	1 (0%)	48 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	GLN

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	905/1371 (66%)	894 (99%)	11 (1%)	67 82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	CYS
1	A	79	GLU
1	A	82	ASN
1	A	177	ASN
1	A	373	ASN
1	A	450	VAL
1	A	733	PHE
1	A	1211	PHE
1	A	1234	PHE
1	A	1342	VAL
1	A	1466	PHE

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

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	23	ASN
1	A	82	ASN
1	A	140	GLN
1	A	431	ASN
1	A	514	ASN
1	A	577	ASN
1	A	1177	ASN
1	A	1184	ASN

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Mol	Chain	Res	Type
1	A	1228	GLN
1	A	1255	ASN
1	A	1269	ASN
1	A	1291	ASN
1	A	1293	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)

3 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	$\#\|Z\| > 2$
3	NAG	A	1503	1	14,14,15	0.33	0	17,19,21	1.47	2 (11%)
3	NAG	A	1502	1	14,14,15	0.30	0	17,19,21	0.63	0
2	CLR	A	1501	-	31,31,31	0.88	2 (6%)	48,48,48	1.36	8 (16%)

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
3	NAG	A	1503	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1502	1	-	2/6/23/26	0/1/1/1
2	CLR	A	1501	-	-	0/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	CLR	C13-C14	-2.17	1.51	1.55
2	A	1501	CLR	C10-C9	-2.14	1.52	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1503	NAG	C1-O5-C5	4.95	118.82	112.19
2	A	1501	CLR	C13-C14-C8	-3.16	109.92	114.41
2	A	1501	CLR	C11-C12-C13	-2.89	107.87	112.74
2	A	1501	CLR	C8-C7-C6	-2.86	108.79	112.76
2	A	1501	CLR	C17-C13-C14	2.85	103.37	100.10
2	A	1501	CLR	C13-C17-C20	-2.76	115.23	119.50
2	A	1501	CLR	C11-C9-C10	-2.47	110.04	113.08
2	A	1501	CLR	C3-C4-C5	-2.15	108.62	112.05
2	A	1501	CLR	C19-C10-C9	-2.15	109.25	111.66
3	A	1503	NAG	C4-C3-C2	-2.01	108.07	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1502	NAG	C8-C7-N2-C2
3	A	1502	NAG	O7-C7-N2-C2
3	A	1503	NAG	C8-C7-N2-C2
3	A	1503	NAG	O7-C7-N2-C2

There are no ring outliers.

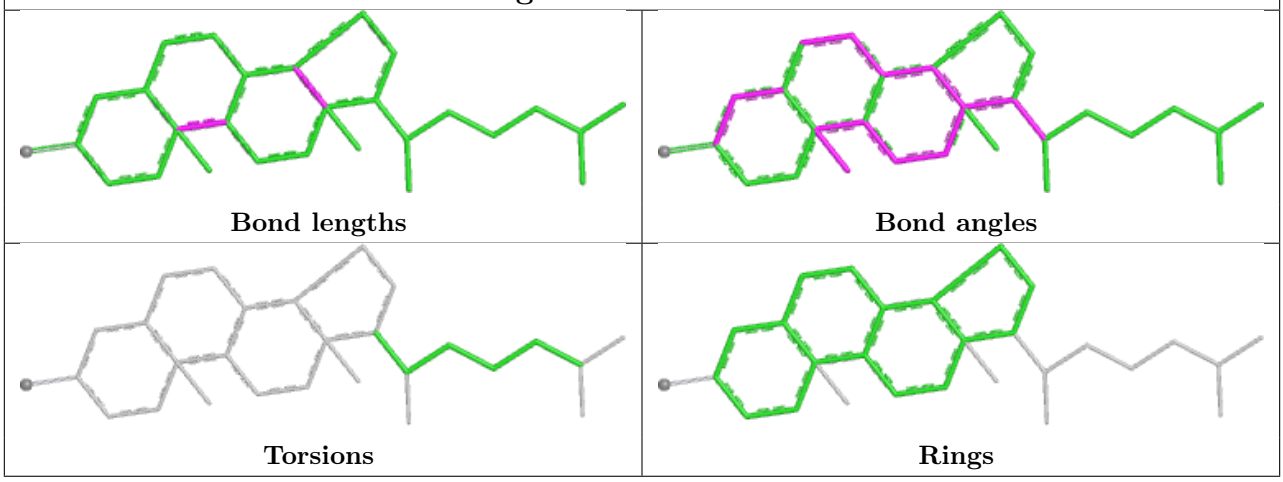
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	NAG	1	0
2	A	1501	CLR	7	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 CLR A 1501



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.

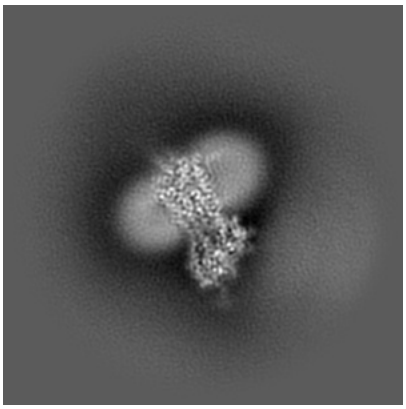
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42854. These allow visual inspection of the internal detail of the map and identification of artifacts.

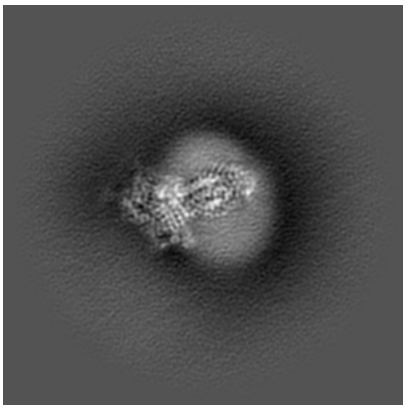
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

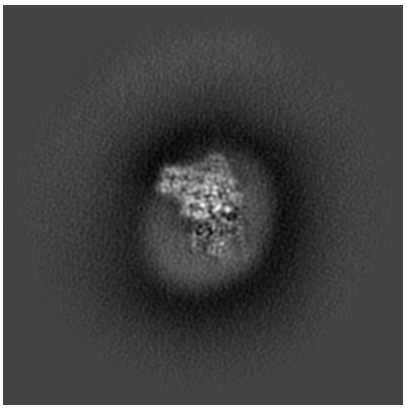
6.1.1 Primary map



X

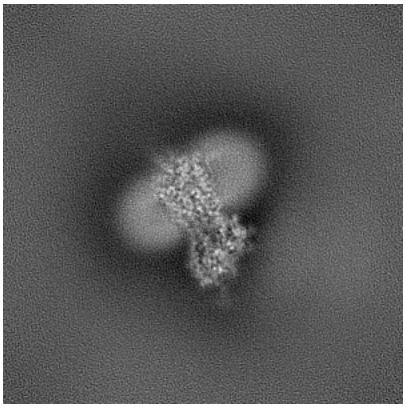


Y

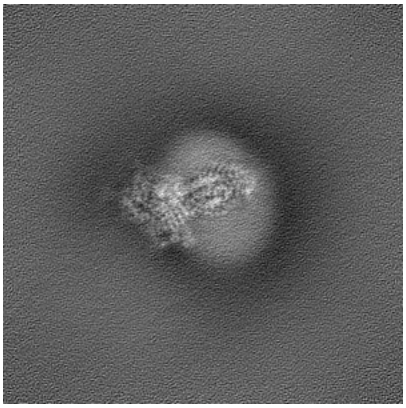


Z

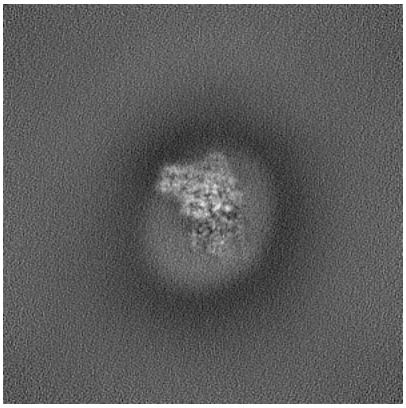
6.1.2 Raw map



X



Y

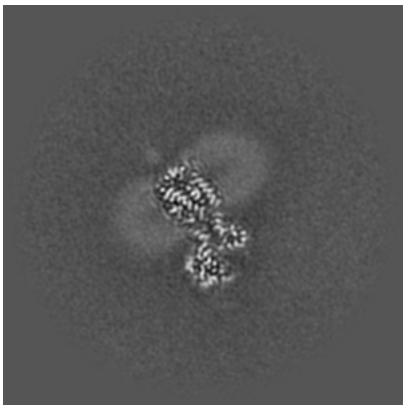


Z

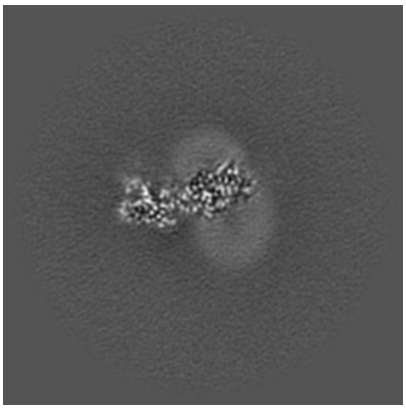
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

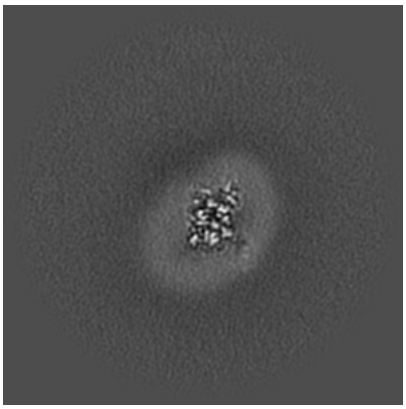
6.2.1 Primary map



X Index: 150

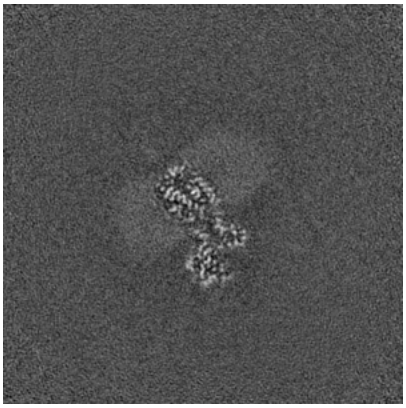


Y Index: 150

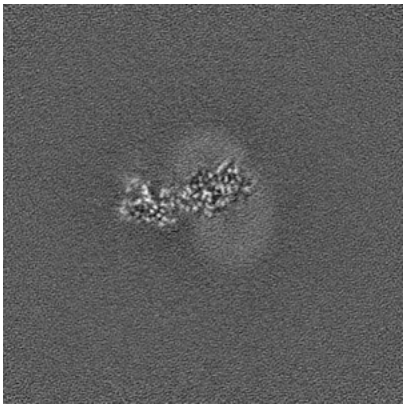


Z Index: 150

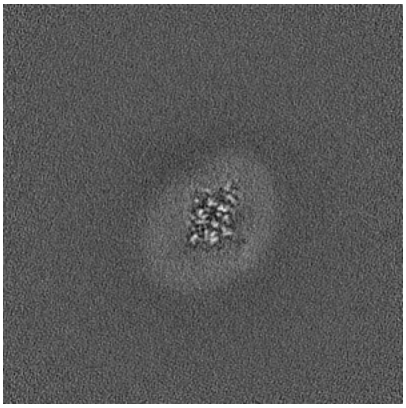
6.2.2 Raw map



X Index: 150



Y Index: 150

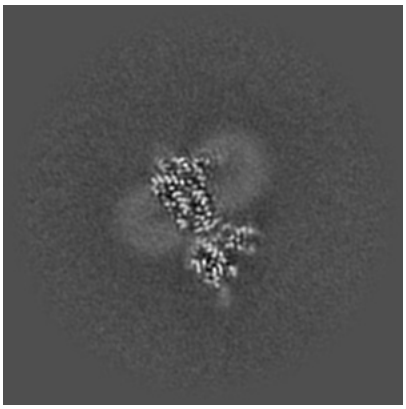


Z Index: 150

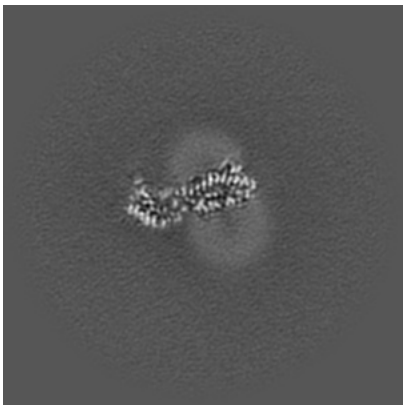
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

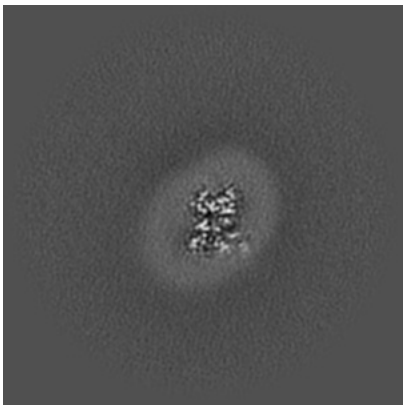
6.3.1 Primary map



X Index: 158

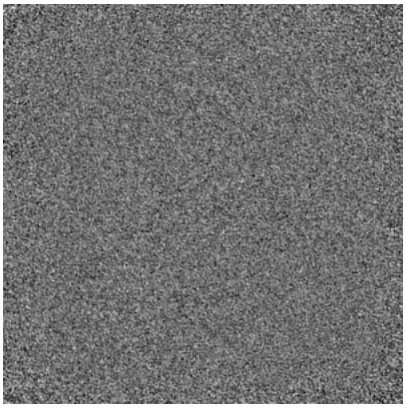


Y Index: 145

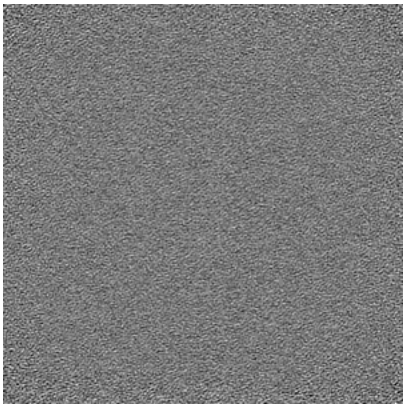


Z Index: 155

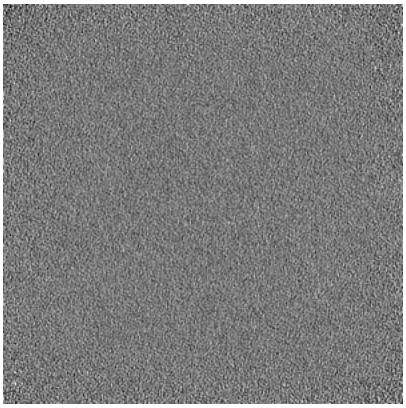
6.3.2 Raw map



X Index: 0



Y Index: 0

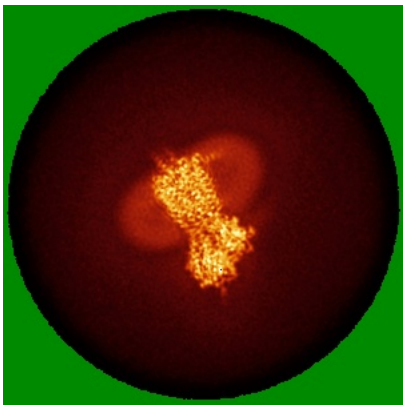


Z Index: 0

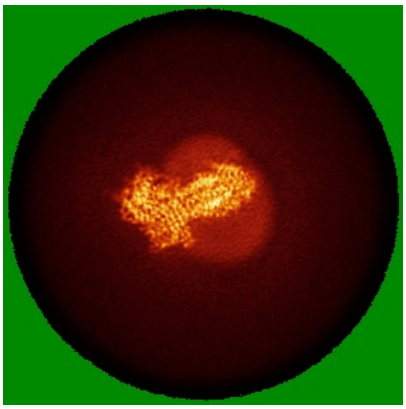
The images above show the largest variance slices of the map in three orthogonal directions.

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

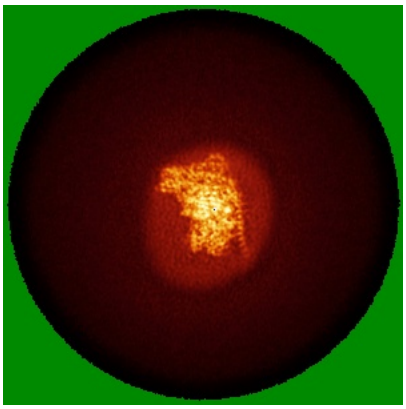
6.4.1 Primary map



X

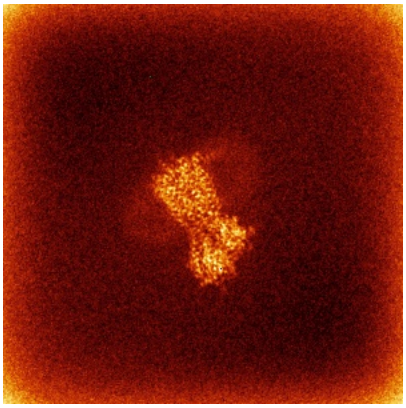


Y

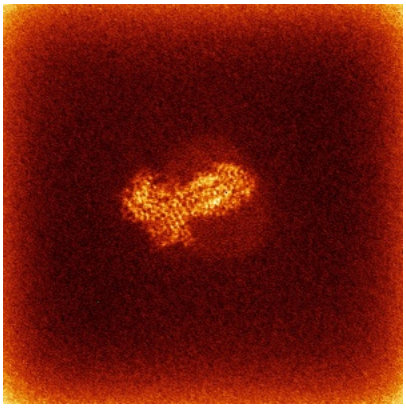


Z

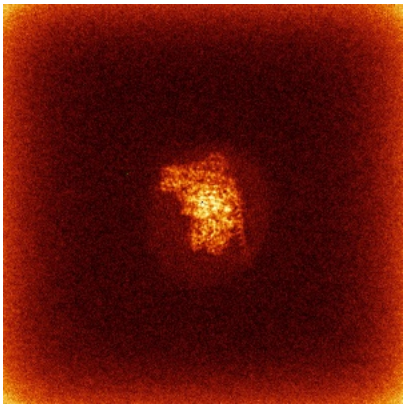
6.4.2 Raw map



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 0.1. 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.

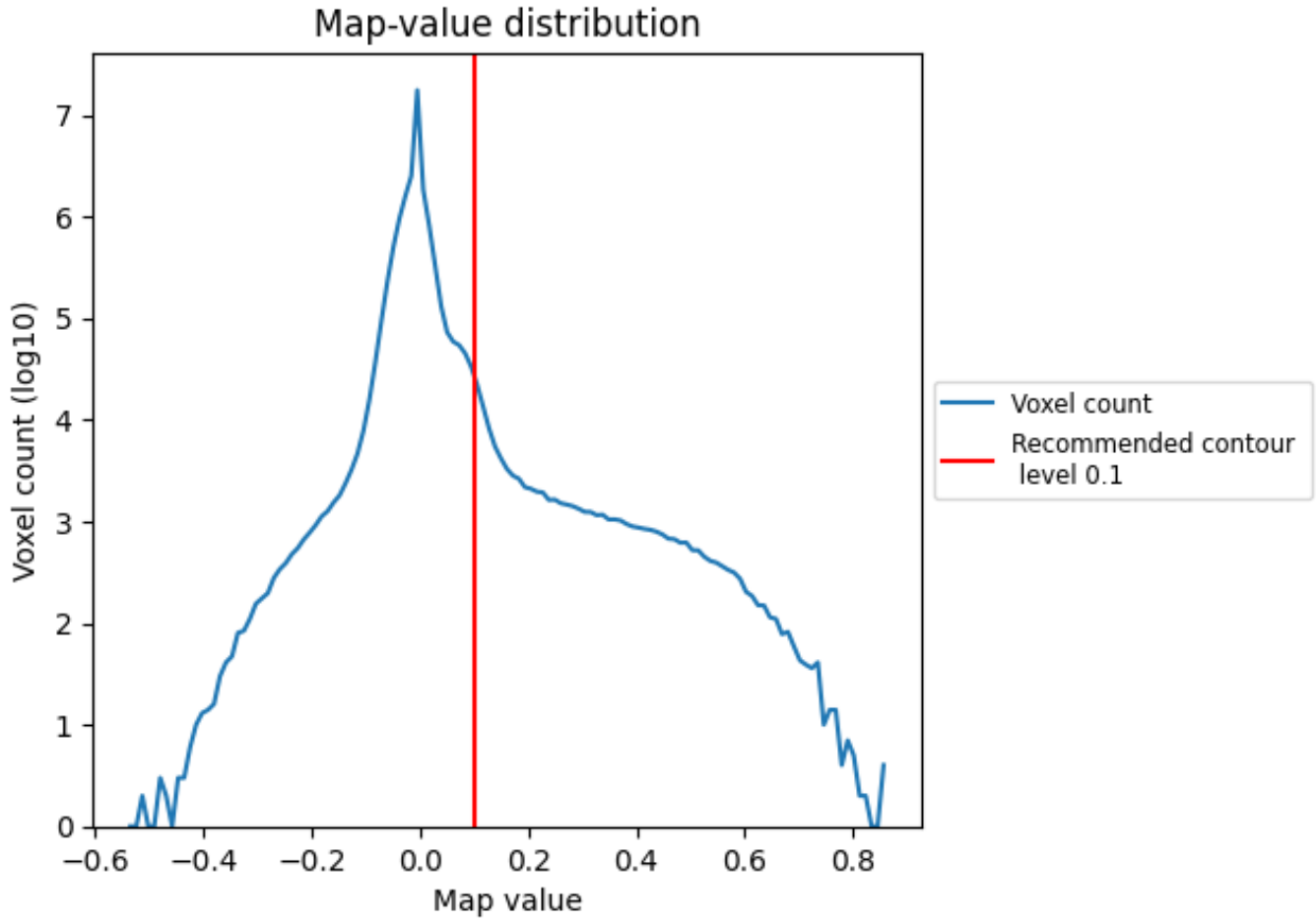
6.6 Mask visualisation (i)

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

7 Map analysis

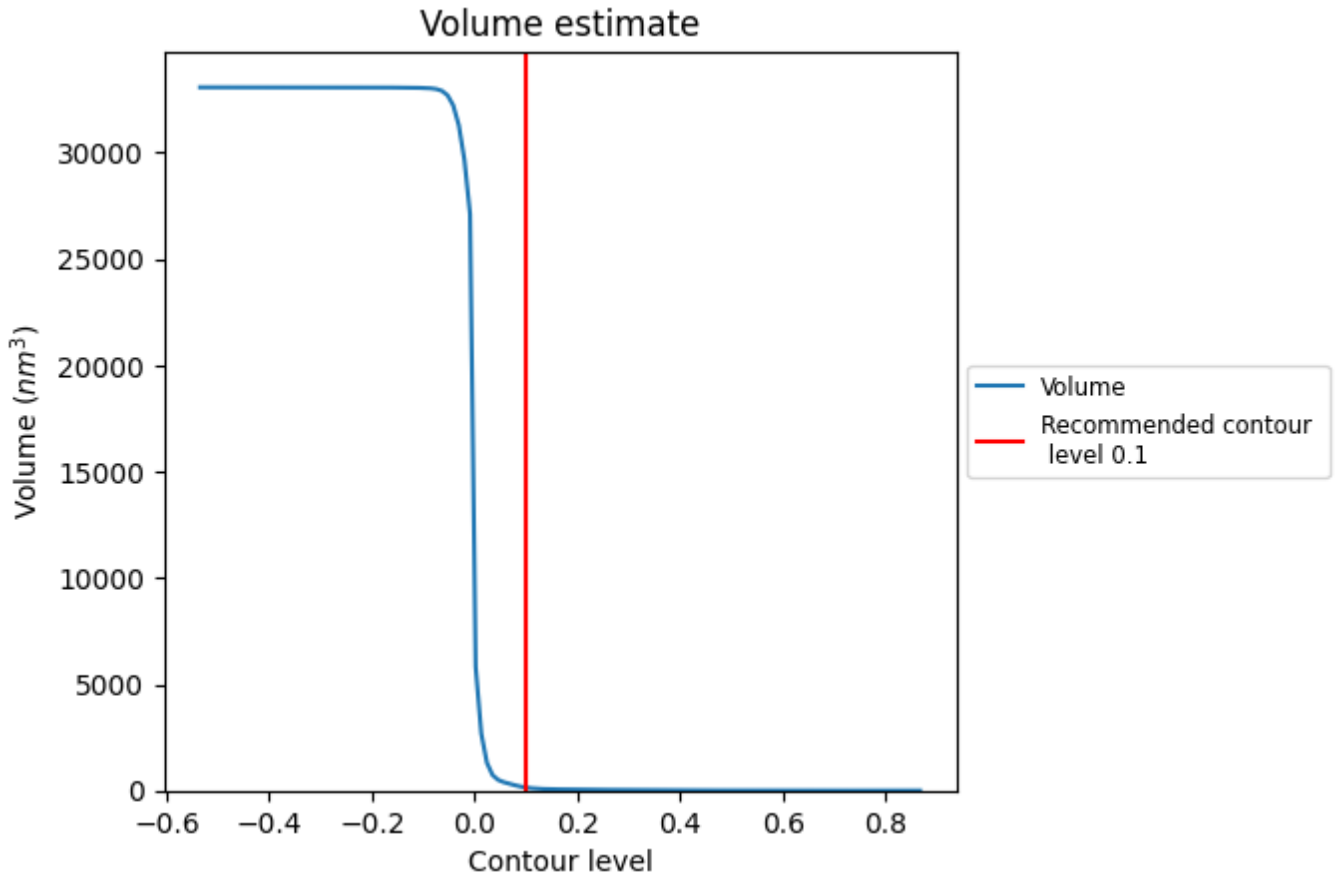
This section contains the results of statistical analysis of the map.

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.

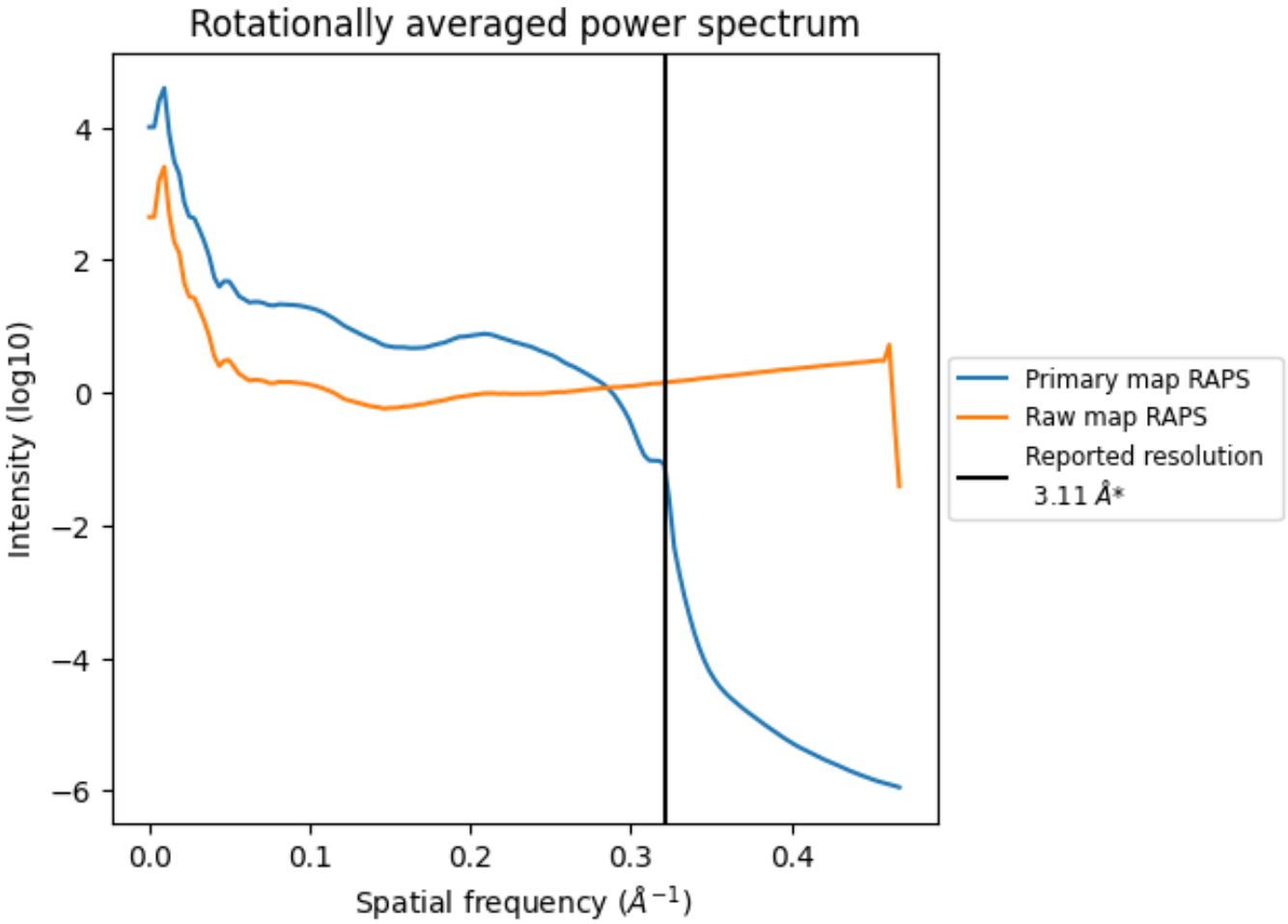
7.2 Volume estimate



The volume at the recommended contour level is 144 nm^3; this corresponds to an approximate mass of 130 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)

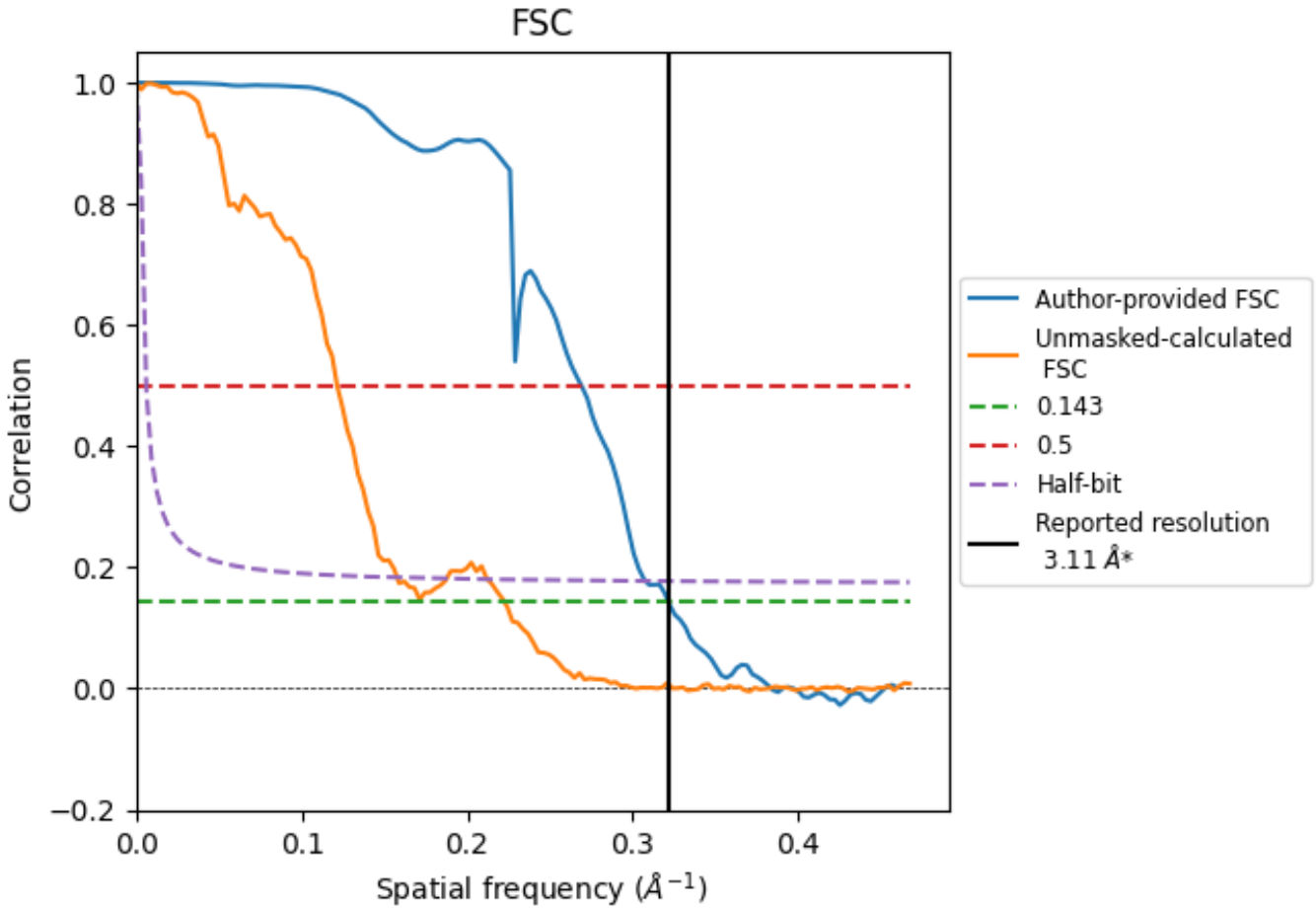


*Reported resolution corresponds to spatial frequency of 0.322 Å^{-1}

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 0.322 Å^{-1}

8.2 Resolution estimates (i)

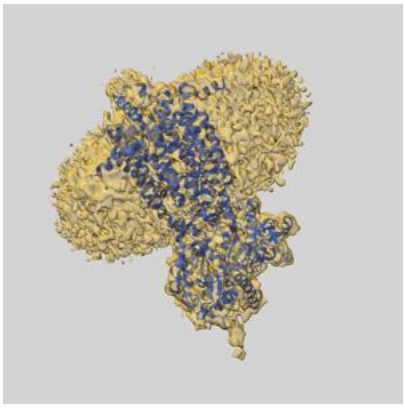
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.72	3.25
Unmasked-calculated*	4.50	8.24	6.34

*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 4.50 differs from the reported value 3.11 by more than 10 %

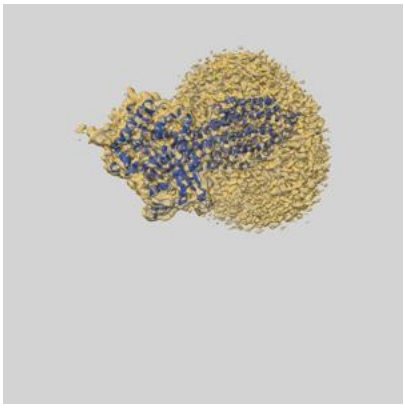
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42854 and PDB model 8V0G. Per-residue inclusion information can be found in section 3 on page 5.

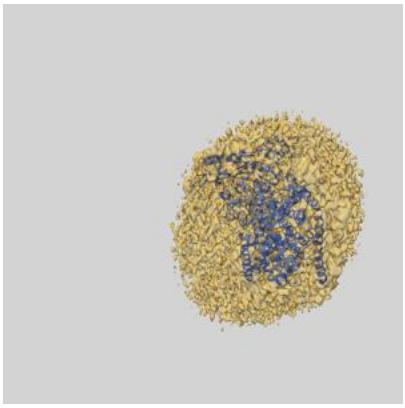
9.1 Map-model overlay



X



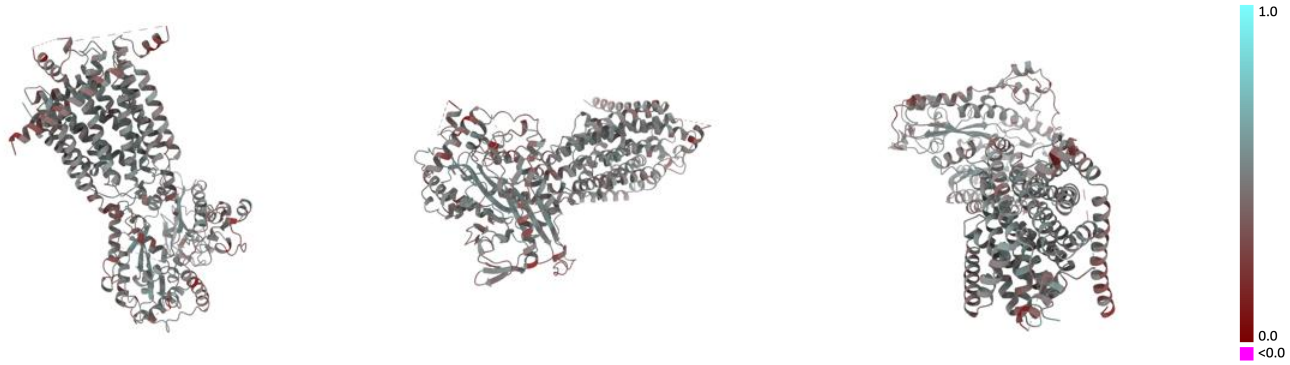
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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

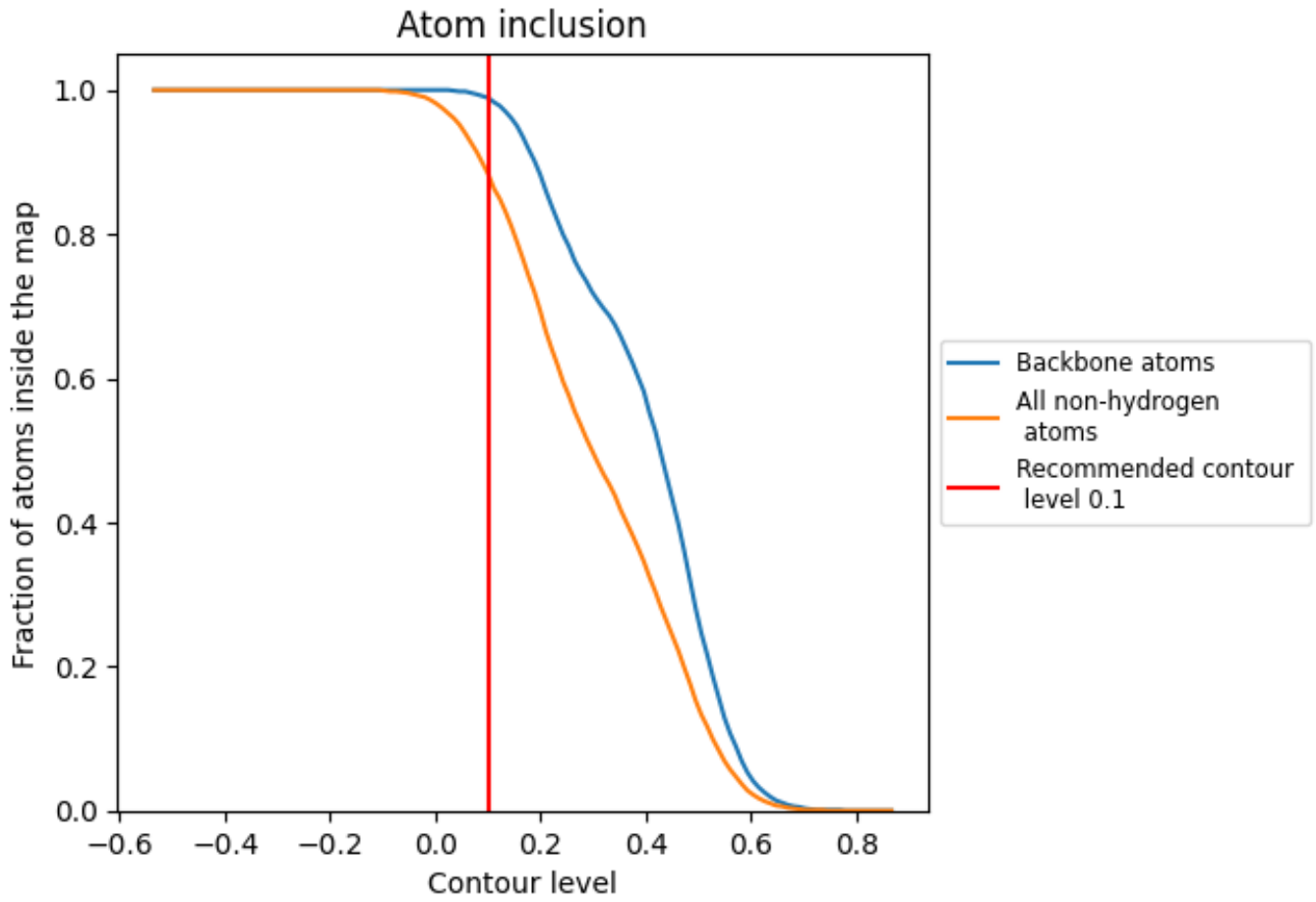
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.4580
A	0.8840	0.4580