Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 05:01 PM JST

PDB ID	:	5YW7
EMDB ID	:	EMD-6847
Title	:	Structure of pancreatic ATP-sensitive potassium channel bound with glibenclamide and ATPgammaS (focused refinement on SUR1 ABC transporter module at 4.4A)
Authors	:	Chen, L.; Wu, J.X.
Deposited on	:	2017-11-29
Resolution	:	4.40 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 (i) 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 (1)) were used in the production of this report:

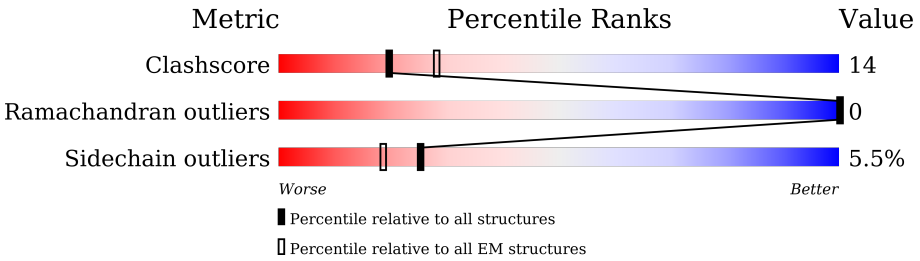
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	1582	

2 Entry composition (i)

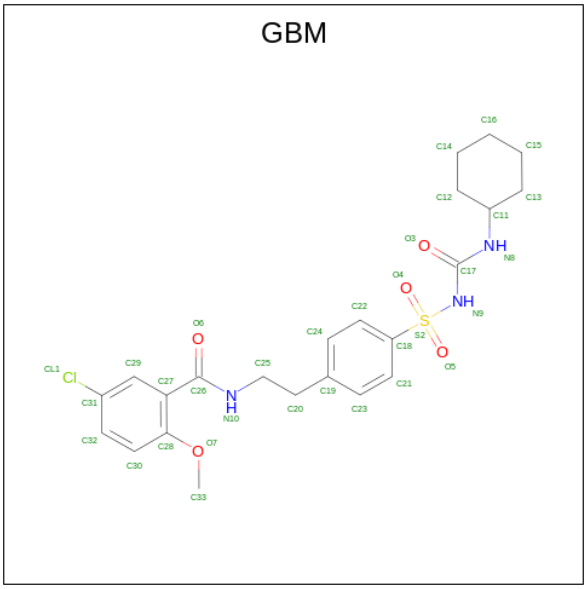
There are 3 unique types of molecules in this entry. The entry contains 8944 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

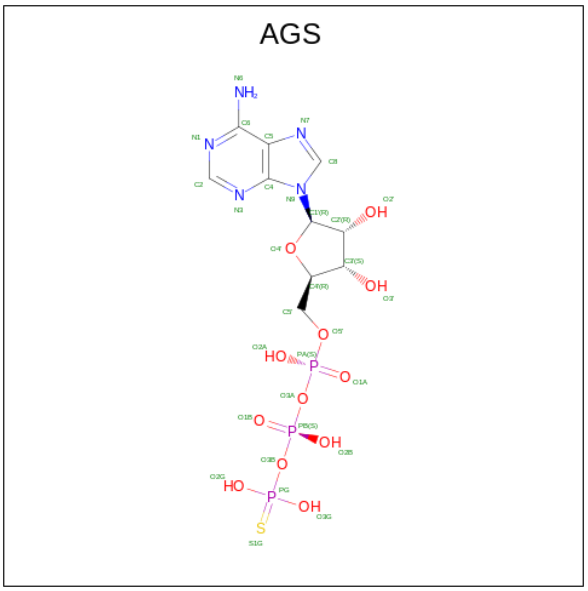
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1140	8880	5752	1516	1565	47	0	0

- Molecule 2 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxybenzamide (three-letter code: GBM) (formula: $C_{23}H_{28}ClN_3O_5S$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	N	O	S	
2	B	1	33	23	1	3	5	1	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



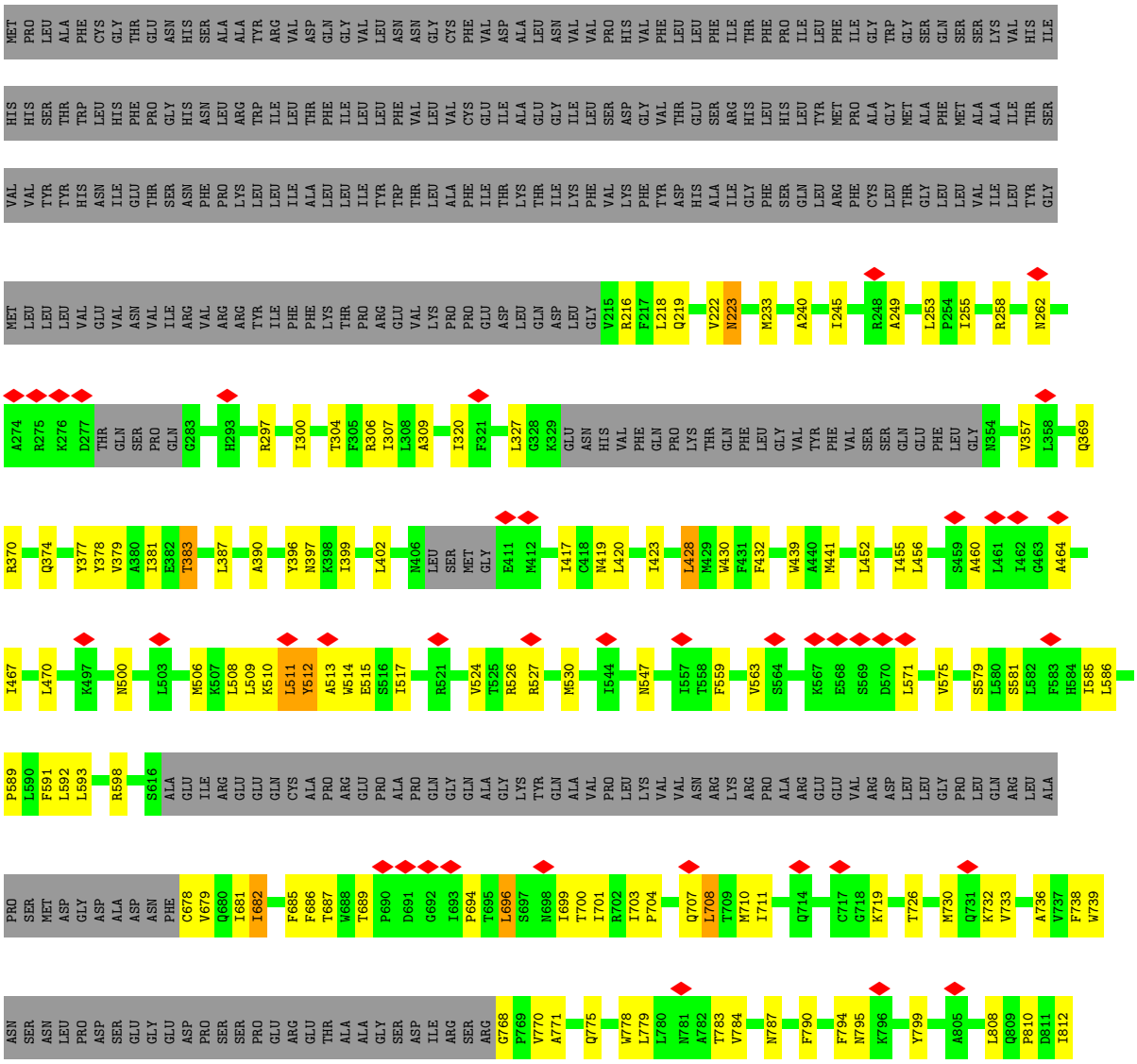
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	B	1	31	10	5	12	3	1	0

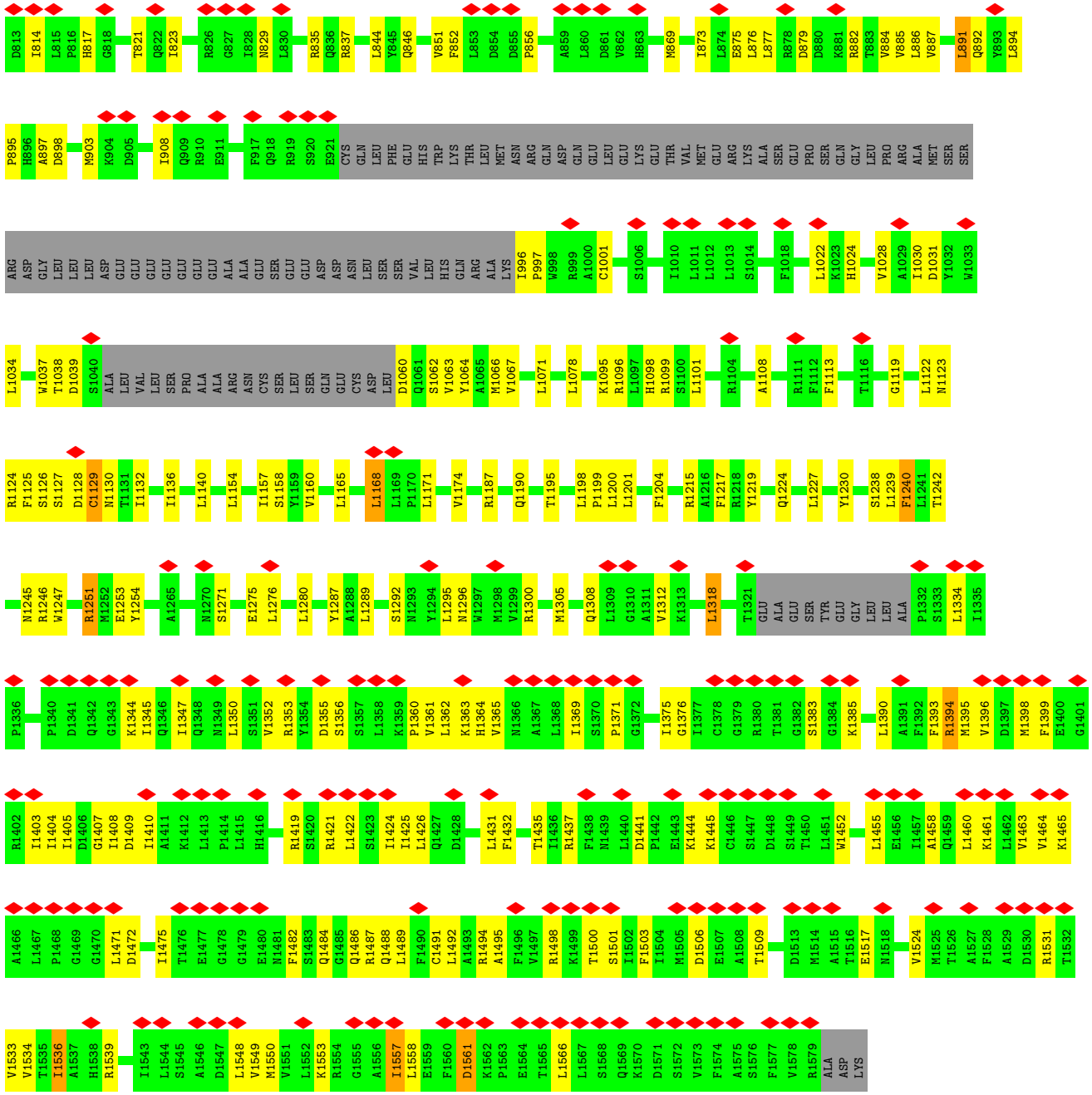
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-binding cassette sub-family C member 8 isoform X2

Chain B: 14% 51% 20% 28%




D813 I814 L815 P816 H817 G818 T821 Q822 I823 R826 G827 I828 N829 L830 R835 Q836 R837 L844 Y845 Q846 V851 F852 L853 D854 D855 P856 A859 L860 D861 V862 H863 M869 I873 L874 E875 L876 L877 R878 D879 D880 K881 R882 T883 V884 V885 L886 V887 L891 Q892 Y893 L894
P895 H896 A897 D898 M903 K904 D905 I908 Q909 R910 E911 F917 Q918 R919 S920 E921 CYS GLN LEU LEU PHE GLU HIS TRP LYS THR LEU MET ASN ARG GLN ASP GLN GLU LEU GLU LYS GLU THR VAL MET GLU ARG LYS ALA SER GLU PRO SER GLN GLY LEU PRO ARG ALA MET SER SER
ARG ASP GLY LEU LEU LEU ASP GLU GLU GLU GLU GLU GLU GLU ALA ALA ARG GLU GLU SER GLU GLU GLU ASP ASP ASN LEU SER SER VAL LEU HIS GLN ARG ALA LYS I996 P997 W998 R999 A1000 C1001 S1006 I1010 L1011 L1012 L1013 S1014 F1018 L1022 K1023 H1024 V1028 A1029 I1030 D1031 Y1032 W1033
L1034 W1037 T1038 D1039 S1040 ALA LEU VAL LEU SER PRO ALA ALA ARG ASN CYS SER LEU SER GLN GLU CYS ASP LEU D1060 Q1061 S1062 V1063 Y1064 A1065 M1066 V1067 L1071 L1078 K1095 R1096 L1097 H1098 R1099 S1100 L1101 R1104 A1108 R1111 F1112 F1113 T1116 G1119 L1122 N1123
R1124 F1125 S1126 S1127 D1128 C1129 N1130 T1131 I1132 I1136 L1140 L1154 I1157 S1158 Y1159 V1160 L1165 L1168 L1169 P1170 L1171 V1174 R1187 Q1190 T1195 L1198 P1199 L1200 L1201 F1204 R1215 A1216 F1217 R1218 Y1219 Q1224 L1227 Y1230 S1238 L1239 F1240 L1241 T1242
N1245 R1246 W1247 R1251 M1252 E1253 Y1254 A1265 N1270 S1271 E1275 L1276 L1280 Y1287 A1288 L1289 S1292 N1293 Y1294 L1295 N1296 W1297 M1298 V1299 R1300 M1305 Q1308 L1309 G1310 A1311 V1312 K1313 L1318 T1321 GLU ALA GLU SER TYR GLU GLY LEU LEU ALA P1332 S1333 L1334 I1335
P1336 P1340 D1341 Q1342 G1343 K1344 I1345 Q1346 I1347 Q1348 N1349 L1350 S1351 V1352 R1353 Y1354 D1355 S1356 S1357 L1358 K1359 P1360 V1361 L1362 K1363 H1364 V1365 N1366 A1367 L1368 I1369 S1370 P1371 G1372 I1375 G1376 I1377 C1378 G1379 R1380 T1381 G1382 S1383 G1384 K1385 L1390 A1391 F1392 F1393 R1394 M1395 V1396 D1397 M1398 F1399 E1400 G1401
R1402 I1403 I1404 I1405 D1406 G1407 I1408 D1409 I1410 A1411 K1412 L1413 P1414 L1415 H1416 R1419 S1420 R1421 L1422 S1423 I1424 I1425 L1426 Q1427 D1428 L1431 F1432 T1435 I1436 R1437 F1438 N1439 L1440 D1441 P1442 E1443 K1444 K1445 C1446 S1447 D1448 S1449 T1450 L1451 W1452 L1455 E1456 I1457 A1458 Q1459 L1460 K1461 L1462 V1463 V1464 K1465
A1466 L1467 P1468 G1469 G1470 L1471 D1472 I1475 T1476 E1477 G1478 G1479 E1480 N1481 F1482 S1483 Q1484 G1485 Q1486 R1487 Q1488 L1489 F1490 C1491 L1492 A1493 R1494 A1495 F1496 V1497 R1498 K1499 T1500 S1501 I1502 F1503 I1504 M1505 D1506 E1507 A1508 T1509 D1513 M1514 A1515 T1516 E1517 N1518 V1524 M1525 T1526 A1527 F1528 A1529 D1530 R1531 T1532
V1533 V1534 T1535 I1536 A1537 H1538 R1539 I1543 L1544 S1545 A1546 D1547 L1548 V1549 M1550 V1551 L1552 K1553 R1554 G1555 A1556 I1557 L1558 E1559 F1560 D1561 K1562 P1563 E1564 T1565 L1566 L1567 S1568 Q1569 K1570 D1571 S1572 V1573 F1574 A1575 S1576 F1577 V1578 R1579 ALA ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	348180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.141	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	329.15997, 329.15997, 329.15997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	B	0.27	0/9046	0.44	0/12269

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 (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	B	8880	0	9202	250	0
2	B	33	0	28	4	0
3	B	31	0	12	2	0
All	All	8944	0	9242	252	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 14.

All (252) 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:B:1350:LEU:HD11	1:B:1403:ILE:HD11	1.20	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:TYR:CB	1:B:1498:ARG:HH12	1.65	1.10
1:B:512:TYR:HB3	1:B:1498:ARG:NH1	1.67	1.08
1:B:1125:PHE:HA	1:B:1129:CYS:SG	1.95	1.06
1:B:1350:LEU:HD13	1:B:1403:ILE:CG1	1.85	1.06
1:B:1350:LEU:HD13	1:B:1403:ILE:HG12	1.35	1.05
1:B:1494:ARG:O	1:B:1498:ARG:HG3	1.59	1.02
1:B:1124:ARG:HD2	1:B:1318:LEU:HD12	1.41	0.99
1:B:1350:LEU:CD1	1:B:1403:ILE:HD11	1.92	0.99
1:B:512:TYR:CB	1:B:1498:ARG:NH1	2.27	0.94
1:B:1350:LEU:HD11	1:B:1403:ILE:CD1	2.00	0.92
1:B:500:ASN:OD1	1:B:1122:LEU:HD21	1.70	0.92
1:B:512:TYR:HB3	1:B:1498:ARG:CZ	2.03	0.89
1:B:512:TYR:CB	1:B:1498:ARG:HH22	1.87	0.87
1:B:1350:LEU:CD1	1:B:1403:ILE:CG1	2.52	0.86
1:B:1350:LEU:CD1	1:B:1403:ILE:CD1	2.57	0.82
1:B:1101:LEU:HD23	1:B:1125:PHE:CE1	2.16	0.81
1:B:512:TYR:CB	1:B:1498:ARG:NH2	2.44	0.81
1:B:512:TYR:HB2	1:B:1498:ARG:HH12	1.42	0.80
1:B:512:TYR:CD2	1:B:1498:ARG:NH2	2.49	0.80
1:B:1037:TRP:CD1	1:B:1064:TYR:HB3	2.18	0.78
1:B:1132:ILE:HD11	1:B:1312:VAL:HG22	1.67	0.77
1:B:1124:ARG:CD	1:B:1318:LEU:HD12	2.15	0.77
1:B:456:LEU:HB2	1:B:460:ALA:HB2	1.70	0.73
1:B:1125:PHE:CA	1:B:1129:CYS:SG	2.76	0.73
1:B:512:TYR:CB	1:B:1498:ARG:CZ	2.67	0.72
1:B:1422:LEU:C	1:B:1500:THR:HG21	2.10	0.72
1:B:1441:ASP:OD2	1:B:1444:LYS:HA	1.90	0.72
1:B:1124:ARG:HD2	1:B:1318:LEU:CD1	2.21	0.71
1:B:1125:PHE:O	1:B:1129:CYS:SG	2.50	0.69
1:B:1353:ARG:HH11	1:B:1398:MET:HE3	1.59	0.68
1:B:687:THR:HB	1:B:694:PRO:HA	1.75	0.68
1:B:1345:ILE:HD11	1:B:1369:ILE:HD12	1.76	0.68
1:B:1421:ARG:HG3	1:B:1422:LEU:HG	1.76	0.68
1:B:1101:LEU:HG	1:B:1125:PHE:CZ	2.29	0.68
1:B:512:TYR:CG	1:B:1498:ARG:NH2	2.62	0.67
1:B:530:MET:HG3	1:B:1095:LYS:HE2	1.77	0.67
1:B:1509:THR:HG23	1:B:1517:GLU:HG2	1.75	0.67
1:B:1165:LEU:HA	1:B:1168:LEU:HD23	1.76	0.67
1:B:1126:SER:O	1:B:1130:ASN:ND2	2.28	0.67
1:B:1136:ILE:HD11	1:B:1308:GLN:HB3	1.77	0.66
1:B:512:TYR:HB2	1:B:1498:ARG:HH22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1441:ASP:OD2	1:B:1444:LYS:CA	2.43	0.65
1:B:1122:LEU:HD12	1:B:1122:LEU:O	1.96	0.65
1:B:1491:CYS:HA	1:B:1494:ARG:HD2	1.79	0.64
1:B:1404:ILE:HG23	1:B:1408:ILE:N	2.11	0.64
1:B:530:MET:CE	1:B:1095:LYS:HG2	2.28	0.64
1:B:1503:PHE:HB2	1:B:1533:VAL:HG22	1.79	0.64
1:B:846:GLN:O	1:B:882:ARG:NH1	2.31	0.63
1:B:1352:VAL:HA	1:B:1399:PHE:HA	1.79	0.63
1:B:1404:ILE:HG23	1:B:1408:ILE:H	1.64	0.63
1:B:262:ASN:HB3	1:B:390:ALA:HB2	1.80	0.63
1:B:771:ALA:HB3	1:B:851:VAL:HG12	1.82	0.62
1:B:873:ILE:HA	1:B:877:LEU:HD12	1.81	0.62
1:B:682:ILE:HG23	1:B:736:ALA:HB3	1.82	0.62
1:B:1198:LEU:HB3	1:B:1199:PRO:HD3	1.82	0.62
1:B:1404:ILE:CG2	1:B:1405:ILE:N	2.63	0.62
1:B:452:LEU:HD11	1:B:464:ALA:HB2	1.80	0.61
1:B:686:PHE:HB2	1:B:732:LYS:HA	1.82	0.61
1:B:1347:ILE:CG2	1:B:1403:ILE:HG12	2.30	0.61
1:B:1506:ASP:HA	1:B:1536:ILE:HG13	1.83	0.61
1:B:387:LEU:HD21	1:B:428:LEU:HD22	1.81	0.61
1:B:1101:LEU:CD2	1:B:1125:PHE:CE1	2.83	0.61
1:B:1157:ILE:HD11	1:B:1168:LEU:HD22	1.82	0.61
1:B:1245:ASN:OD1	1:B:1300:ARG:NH2	2.33	0.61
1:B:530:MET:HE2	1:B:1095:LYS:HG2	1.82	0.61
1:B:1096:ARG:HG2	1:B:1099:ARG:HH12	1.66	0.60
1:B:377:TYR:O	1:B:381:ILE:HG12	2.02	0.60
1:B:1347:ILE:HG23	1:B:1403:ILE:HG23	1.83	0.60
1:B:547:ASN:HA	1:B:591:PHE:HZ	1.66	0.60
1:B:399:ILE:HD11	1:B:417:ILE:HD13	1.82	0.60
1:B:563:VAL:HG21	1:B:1037:TRP:HH2	1.67	0.60
1:B:783:THR:O	1:B:787:ASN:ND2	2.31	0.59
1:B:1124:ARG:HA	1:B:1128:ASP:OD2	2.03	0.59
1:B:1501:SER:HA	1:B:1531:ARG:HD3	1.85	0.59
1:B:1125:PHE:HA	1:B:1129:CYS:HG	1.66	0.58
1:B:1344:LYS:HB2	1:B:1371:PRO:HG3	1.83	0.58
1:B:510:LYS:O	1:B:1419:ARG:NH1	2.36	0.58
1:B:1345:ILE:HG12	1:B:1369:ILE:HB	1.85	0.58
1:B:304:THR:HA	1:B:307:ILE:HG22	1.85	0.58
1:B:399:ILE:HA	1:B:402:LEU:HD23	1.85	0.58
1:B:686:PHE:HD1	1:B:733:VAL:HG23	1.69	0.58
1:B:1352:VAL:HG13	1:B:1361:VAL:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1362:LEU:HD13	1:B:1365:VAL:HG21	1.85	0.58
1:B:1119:GLY:O	1:B:1123:ASN:HB2	2.04	0.57
1:B:1334:LEU:HD13	1:B:1408:ILE:HG12	1.86	0.57
1:B:1393:PHE:CZ	1:B:1422:LEU:HB2	2.39	0.57
1:B:1271:SER:HA	1:B:1275:GLU:HB3	1.85	0.57
1:B:1390:LEU:HB3	1:B:1395:MET:HB2	1.86	0.56
1:B:1125:PHE:C	1:B:1129:CYS:HG	2.09	0.56
1:B:1344:LYS:HA	1:B:1369:ILE:O	2.06	0.56
1:B:1548:LEU:HG	1:B:1561:ASP:HA	1.86	0.56
1:B:467:ILE:HD12	1:B:586:LEU:HD22	1.88	0.56
1:B:1251:ARG:HH11	1:B:1251:ARG:HB2	1.71	0.56
1:B:1422:LEU:O	1:B:1500:THR:HG21	2.05	0.55
1:B:1495:ALA:HB1	1:B:1503:PHE:HE2	1.72	0.55
1:B:681:ILE:O	1:B:700:THR:HA	2.07	0.55
1:B:512:TYR:HB2	1:B:1498:ARG:NH1	2.11	0.55
1:B:844:LEU:HD21	1:B:876:LEU:HD23	1.87	0.55
1:B:1125:PHE:CA	1:B:1129:CYS:HG	2.19	0.54
1:B:514:TRP:CZ2	1:B:1498:ARG:NH2	2.75	0.54
1:B:559:PHE:HE2	1:B:1034:LEU:HD11	1.71	0.54
1:B:1435:THR:HB	1:B:1472:ASP:HA	1.88	0.54
1:B:1292:SER:HA	1:B:1295:LEU:HD12	1.90	0.54
1:B:707:GLN:HG3	1:B:898:ASP:HB2	1.90	0.54
1:B:397:ASN:OD1	1:B:1224:GLN:NE2	2.41	0.54
1:B:699:ILE:HG23	1:B:908:ILE:HD11	1.89	0.54
1:B:1353:ARG:HG2	1:B:1360:PRO:HA	1.90	0.54
1:B:1158:SER:HB2	1:B:1165:LEU:HD12	1.88	0.54
1:B:1461:LYS:HE2	1:B:1465:LYS:HE2	1.89	0.53
1:B:589:PRO:HA	1:B:592:LEU:HD12	1.90	0.53
1:B:1347:ILE:HG23	1:B:1403:ILE:HG12	1.90	0.53
1:B:1347:ILE:HG21	1:B:1350:LEU:HD22	1.89	0.53
1:B:456:LEU:HD11	1:B:579:SER:HB3	1.91	0.53
1:B:524:VAL:HG22	1:B:527:ARG:HH12	1.74	0.53
1:B:686:PHE:CD2	1:B:730:MET:HB3	2.43	0.53
1:B:419:ASN:O	1:B:423:ILE:HG13	2.09	0.53
1:B:1345:ILE:HG22	1:B:1405:ILE:HA	1.91	0.53
1:B:1350:LEU:HB3	1:B:1365:VAL:HB	1.90	0.53
1:B:686:PHE:H	1:B:696:LEU:HB3	1.74	0.52
1:B:1246:ARG:HA	1:B:1246:ARG:HH11	1.74	0.52
1:B:441:MET:HG2	1:B:593:LEU:HD12	1.92	0.52
1:B:1160:VAL:HG13	1:B:1280:LEU:HB3	1.91	0.51
1:B:1350:LEU:CD1	1:B:1403:ILE:HG13	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1404:ILE:HG12	1:B:1409:ASP:HB3	1.93	0.51
1:B:685:PHE:HD2	1:B:733:VAL:HB	1.75	0.51
1:B:1022:LEU:HB3	1:B:1078:LEU:HD21	1.93	0.51
1:B:1217:PHE:HB3	1:B:1219:TYR:HD2	1.75	0.51
1:B:808:LEU:HD13	1:B:837:ARG:HE	1.75	0.51
1:B:1463:VAL:HG21	1:B:1486:GLN:HE22	1.74	0.51
1:B:1484:GLN:OE1	1:B:1487:ARG:NH2	2.43	0.51
1:B:223:ASN:OD1	1:B:223:ASN:N	2.41	0.50
1:B:233:MET:HB2	1:B:1247:TRP:CD1	2.47	0.50
1:B:1455:LEU:HD13	1:B:1464:VAL:HG21	1.94	0.50
1:B:1127:SER:O	1:B:1128:ASP:C	2.50	0.50
1:B:1404:ILE:HG22	1:B:1405:ILE:N	2.26	0.50
1:B:784:VAL:HG22	1:B:823:ILE:HD11	1.94	0.50
1:B:508:LEU:HD12	1:B:1426:LEU:HD23	1.94	0.50
1:B:513:ALA:HB2	1:B:1419:ARG:HG3	1.94	0.49
1:B:370:ARG:HB3	1:B:1253:GLU:HG2	1.94	0.49
1:B:869:MET:HA	1:B:873:ILE:HD12	1.94	0.49
3:B:2002:AGS:O2A	3:B:2002:AGS:S1G	2.70	0.49
1:B:1385:LYS:HB2	1:B:1536:ILE:HG21	1.94	0.49
1:B:711:ILE:HB	1:B:887:VAL:HG13	1.95	0.49
1:B:1024:HIS:O	1:B:1028:VAL:HG12	2.13	0.48
1:B:563:VAL:HG21	1:B:1037:TRP:CH2	2.47	0.48
1:B:1132:ILE:CD1	1:B:1312:VAL:HG22	2.41	0.48
1:B:779:LEU:HD11	1:B:835:ARG:HG2	1.95	0.48
1:B:1171:LEU:O	1:B:1174:VAL:HB	2.13	0.48
1:B:1495:ALA:HB1	1:B:1503:PHE:CE2	2.48	0.48
1:B:255:ILE:HA	1:B:258:ARG:HE	1.77	0.48
1:B:320:ILE:HD11	1:B:1289:LEU:HD13	1.95	0.48
1:B:455:ILE:HG22	1:B:575:VAL:HG13	1.96	0.48
1:B:1125:PHE:C	1:B:1129:CYS:SG	2.92	0.47
1:B:1404:ILE:HG21	1:B:1407:GLY:CA	2.44	0.47
1:B:1553:LYS:HE3	1:B:1558:LEU:HB2	1.96	0.47
1:B:396:TYR:HE2	1:B:1224:GLN:HG3	1.80	0.47
1:B:1431:LEU:HD23	1:B:1494:ARG:HH21	1.79	0.47
1:B:1030:ILE:HA	1:B:1071:LEU:HD13	1.96	0.47
1:B:1441:ASP:OD2	1:B:1444:LYS:C	2.53	0.47
1:B:1187:ARG:O	1:B:1190:GLN:HB3	2.15	0.47
1:B:559:PHE:CE2	1:B:1034:LEU:HD11	2.49	0.47
1:B:1561:ASP:N	1:B:1561:ASP:OD1	2.47	0.47
1:B:240:ALA:HB1	1:B:245:ILE:HD11	1.97	0.46
1:B:775:GLN:OE1	3:B:2002:AGS:S1G	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1458:ALA:O	1:B:1489:LEU:HG	2.15	0.46
1:B:846:GLN:HG3	1:B:1217:PHE:HE2	1.80	0.46
1:B:506:MET:SD	1:B:1113:PHE:HB3	2.55	0.46
1:B:1246:ARG:NH2	2:B:2001:GBM:H18	2.31	0.46
1:B:1404:ILE:HG23	1:B:1408:ILE:O	2.16	0.46
1:B:679:VAL:HB	1:B:703:ILE:HB	1.97	0.46
1:B:1034:LEU:O	1:B:1038:THR:HG23	2.16	0.46
1:B:1375:ILE:HB	1:B:1534:VAL:HG22	1.98	0.46
1:B:739:TRP:HE1	1:B:768:GLY:N	2.15	0.45
2:B:2001:GBM:H20	2:B:2001:GBM:H22	1.75	0.45
1:B:678:CYS:HB3	1:B:704:PRO:HA	1.99	0.45
1:B:808:LEU:HG	1:B:812:ILE:HG12	1.98	0.45
1:B:996:ILE:HD12	1:B:997:PRO:HD2	1.98	0.45
1:B:1246:ARG:HH21	2:B:2001:GBM:H18	1.82	0.45
1:B:875:GLU:O	1:B:879:ASP:HB2	2.17	0.45
1:B:1460:LEU:HD13	1:B:1489:LEU:HD23	1.99	0.45
1:B:379:VAL:O	1:B:383:THR:OG1	2.35	0.45
1:B:1376:GLY:O	1:B:1549:VAL:HA	2.16	0.45
1:B:1039:ASP:OD1	1:B:1039:ASP:N	2.50	0.45
1:B:790:PHE:HB3	1:B:846:GLN:HE21	1.83	0.44
1:B:581:SER:O	1:B:585:ILE:HG12	2.17	0.44
1:B:1154:LEU:HD22	1:B:1168:LEU:HD13	2.00	0.44
1:B:216:ARG:NH1	1:B:249:ALA:O	2.51	0.44
1:B:1375:ILE:HD12	1:B:1548:LEU:HB2	2.00	0.44
1:B:511:LEU:HG	1:B:1424:ILE:HG21	1.98	0.44
1:B:1393:PHE:O	1:B:1394:ARG:HG3	2.18	0.44
1:B:297:ARG:O	1:B:300:ILE:HG13	2.18	0.44
1:B:509:LEU:HD11	1:B:515:GLU:HA	2.00	0.44
1:B:856:PRO:HD2	1:B:886:LEU:HD21	1.99	0.44
1:B:512:TYR:HB2	1:B:1498:ARG:NH2	2.24	0.43
1:B:1246:ARG:HA	1:B:1246:ARG:HD3	1.71	0.43
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.86	0.43
1:B:810:PRO:O	1:B:814:ILE:HG13	2.18	0.43
1:B:396:TYR:CE2	1:B:1224:GLN:HG3	2.54	0.43
1:B:891:LEU:HD23	1:B:891:LEU:H	1.81	0.43
1:B:894:LEU:HB2	1:B:895:PRO:HD3	1.99	0.43
1:B:1369:ILE:HD13	1:B:1375:ILE:HG13	1.99	0.43
1:B:511:LEU:HD23	1:B:1426:LEU:HD21	2.01	0.43
1:B:511:LEU:HD13	1:B:511:LEU:HA	1.85	0.43
1:B:681:ILE:HD11	1:B:726:THR:HG22	1.99	0.43
1:B:1140:LEU:HB2	1:B:1305:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:PHE:HD1	1:B:1240:PHE:HA	1.66	0.43
1:B:530:MET:CE	1:B:1095:LYS:CG	2.96	0.43
1:B:512:TYR:HB3	1:B:1498:ARG:NH2	2.16	0.43
1:B:1200:LEU:HD13	1:B:1230:TYR:HB3	2.01	0.43
1:B:1355:ASP:OD1	1:B:1356:SER:N	2.50	0.43
1:B:514:TRP:HA	1:B:517:ILE:HD13	2.01	0.43
1:B:530:MET:HE3	1:B:1095:LYS:CG	2.49	0.42
1:B:686:PHE:CE2	1:B:730:MET:HB3	2.54	0.42
1:B:1201:LEU:HD23	1:B:1201:LEU:HA	1.84	0.42
1:B:1124:ARG:O	1:B:1128:ASP:HB2	2.19	0.42
1:B:1452:TRP:CE3	1:B:1461:LYS:HE3	2.55	0.42
1:B:219:GLN:HG2	1:B:378:TYR:OH	2.20	0.42
1:B:1437:ARG:HG3	1:B:1471:LEU:O	2.20	0.42
1:B:719:LYS:HB3	1:B:887:VAL:HG11	2.01	0.42
1:B:710:MET:HG2	1:B:897:ALA:HB2	2.02	0.42
1:B:1475:ILE:HD12	1:B:1482:PHE:HE2	1.84	0.42
1:B:1425:ILE:HD13	1:B:1492:LEU:HD12	2.02	0.42
1:B:817:HIS:O	1:B:821:THR:OG1	2.38	0.41
1:B:1127:SER:O	1:B:1130:ASN:N	2.53	0.41
1:B:1347:ILE:HG22	1:B:1350:LEU:HB2	2.01	0.41
1:B:852:PHE:CD1	1:B:885:VAL:HB	2.55	0.41
1:B:877:LEU:HB3	1:B:884:VAL:HG21	2.02	0.41
1:B:1108:ALA:HB3	1:B:1113:PHE:CE2	2.55	0.41
1:B:1365:VAL:HG22	1:B:1557:ILE:HG13	2.01	0.41
1:B:1441:ASP:OD2	1:B:1445:LYS:N	2.53	0.41
1:B:306:ARG:NH2	2:B:2001:GBM:CL1	2.72	0.41
1:B:402:LEU:O	1:B:1215:ARG:NH1	2.50	0.41
1:B:708:LEU:HB3	1:B:897:ALA:HA	2.02	0.41
1:B:795:ASN:O	1:B:799:TYR:HB3	2.21	0.41
1:B:1239:LEU:O	1:B:1242:THR:HG22	2.21	0.41
1:B:812:ILE:HD13	1:B:812:ILE:HA	1.84	0.41
1:B:1404:ILE:HG21	1:B:1407:GLY:HA2	2.02	0.41
1:B:1060:ASP:OD1	1:B:1060:ASP:N	2.53	0.41
1:B:309:ALA:O	1:B:369:GLN:HG3	2.21	0.40
1:B:1062:SER:O	1:B:1066:MET:HG2	2.21	0.40
1:B:1405:ILE:HD13	1:B:1422:LEU:HD21	2.03	0.40
1:B:370:ARG:HG3	1:B:1253:GLU:CD	2.42	0.40
1:B:571:LEU:HD12	1:B:571:LEU:HA	1.94	0.40
1:B:1132:ILE:HA	1:B:1136:ILE:HD13	2.02	0.40
1:B:903:MET:SD	1:B:908:ILE:HG12	2.60	0.40
1:B:1363:LYS:HE3	1:B:1364:HIS:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:ARG:NH1	1:B:1098:HIS:ND1	2.68	0.40
1:B:1031:ASP:OD2	1:B:1287:TYR:OH	2.25	0.40
1:B:1063:VAL:O	1:B:1067:VAL:HG23	2.21	0.40
1:B:1251:ARG:HB2	1:B:1251:ARG:NH1	2.36	0.40
1:B:1394:ARG:HG2	1:B:1410:ILE:HG21	2.03	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	B	1122/1582 (71%)	1074 (96%)	48 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	970/1371 (71%)	917 (94%)	53 (6%)	21 49

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	218	LEU

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Mol	Chain	Res	Type
1	B	222	VAL
1	B	223	ASN
1	B	327	LEU
1	B	357	VAL
1	B	374	GLN
1	B	383	THR
1	B	420	LEU
1	B	428	LEU
1	B	430	TRP
1	B	432	PHE
1	B	439	TRP
1	B	470	LEU
1	B	511	LEU
1	B	512	TYR
1	B	598	ARG
1	B	682	ILE
1	B	689	THR
1	B	696	LEU
1	B	701	ILE
1	B	708	LEU
1	B	738	PHE
1	B	770	VAL
1	B	778	TRP
1	B	794	PHE
1	B	829	ASN
1	B	891	LEU
1	B	892	GLN
1	B	1001	CYS
1	B	1129	CYS
1	B	1168	LEU
1	B	1195	THR
1	B	1204	PHE
1	B	1227	LEU
1	B	1238	SER
1	B	1240	PHE
1	B	1251	ARG
1	B	1254	TYR
1	B	1276	LEU
1	B	1296	ASN
1	B	1318	LEU
1	B	1383	SER
1	B	1394	ARG

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Mol	Chain	Res	Type
1	B	1396	VAL
1	B	1432	PHE
1	B	1488	GLN
1	B	1524	VAL
1	B	1536	ILE
1	B	1539	ARG
1	B	1550	MET
1	B	1557	ILE
1	B	1561	ASP
1	B	1566	LEU

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

Mol	Chain	Res	Type
1	B	485	GLN
1	B	1135	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	GBM	B	2001	-	35,35,35	2.03	4 (11%)	48,48,48	1.87	7 (14%)
3	AGS	B	2002	-	26,33,33	1.89	3 (11%)	26,52,52	1.47	4 (15%)

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
2	GBM	B	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	B	2002	-	-	2/17/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	GBM	C18-S2	-10.13	1.60	1.76
3	B	2002	AGS	PG-S1G	7.95	2.08	1.90
2	B	2001	GBM	C27-C28	4.64	1.49	1.40
2	B	2001	GBM	C31-CL1	2.56	1.80	1.74
3	B	2002	AGS	C5-C4	2.48	1.47	1.40
2	B	2001	GBM	C17-N9	-2.20	1.34	1.39
3	B	2002	AGS	PG-O2G	2.03	1.61	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	GBM	O5-S2-O4	-9.70	107.62	119.55
2	B	2001	GBM	O7-C28-C27	3.76	122.02	116.55
3	B	2002	AGS	C3'-C2'-C1'	3.43	106.14	100.98
2	B	2001	GBM	C18-S2-N9	3.26	110.91	105.97
3	B	2002	AGS	PA-O3A-PB	-3.23	121.74	132.83
3	B	2002	AGS	N3-C2-N1	-3.16	123.74	128.68
2	B	2001	GBM	O7-C28-C30	-2.90	119.40	124.37
3	B	2002	AGS	C4-C5-N7	-2.58	106.71	109.40
2	B	2001	GBM	C25-C20-C19	-2.26	107.64	112.87
2	B	2001	GBM	C28-C27-C26	-2.06	122.41	126.16
2	B	2001	GBM	C33-O7-C28	2.04	120.61	117.53

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	GBM	C27-C26-N10-C25
3	B	2002	AGS	PB-O3B-PG-O2G
3	B	2002	AGS	PB-O3B-PG-O3G
2	B	2001	GBM	O6-C26-N10-C25
2	B	2001	GBM	O3-C17-N8-C11
2	B	2001	GBM	C30-C28-O7-C33
2	B	2001	GBM	C27-C28-O7-C33
2	B	2001	GBM	N9-C17-N8-C11
2	B	2001	GBM	C24-C19-C20-C25
2	B	2001	GBM	C23-C19-C20-C25

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	GBM	4	0
3	B	2002	AGS	2	0

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

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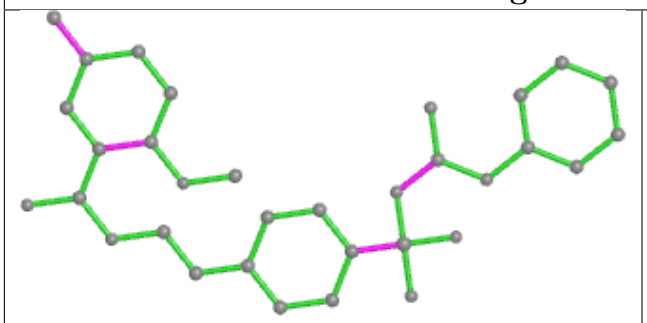
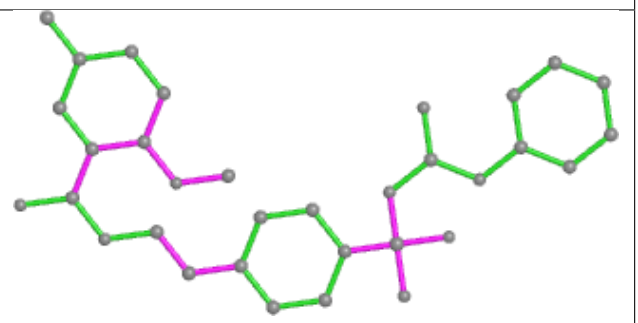
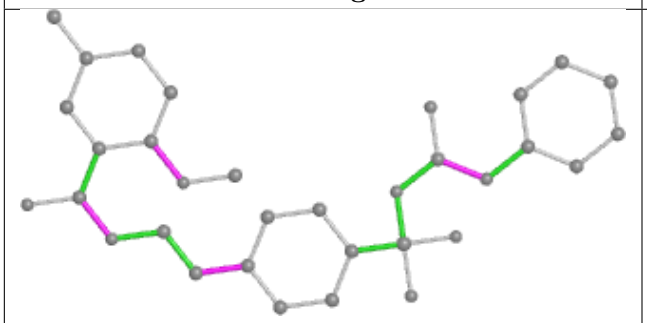


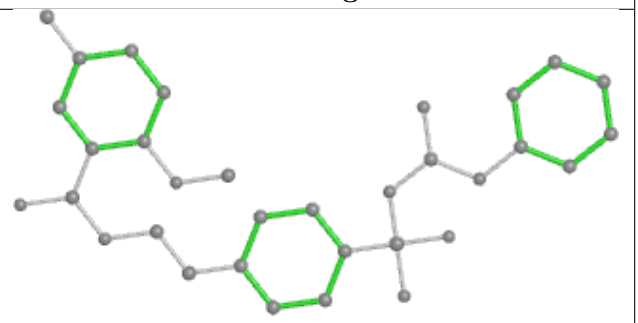
Bond lengths



Bond angles

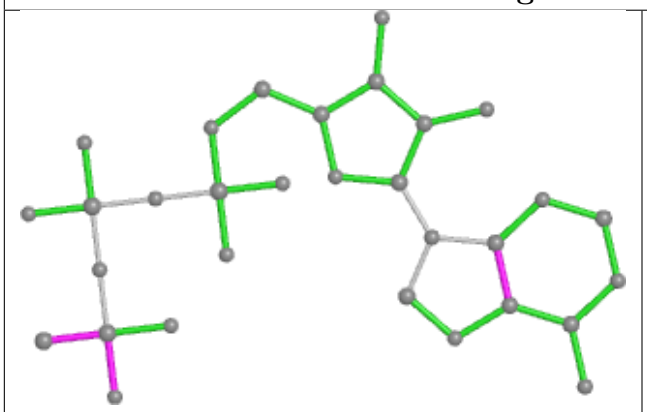


Torsions

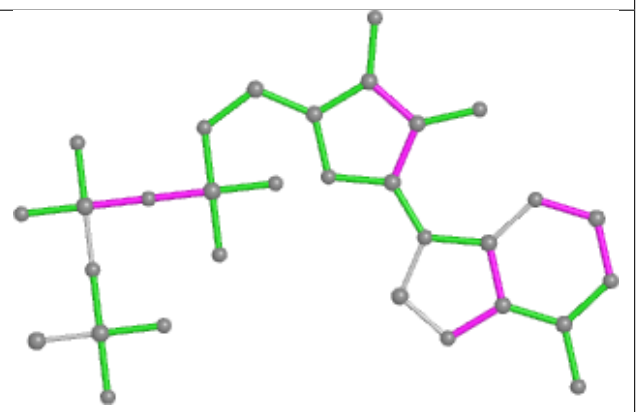


Rings

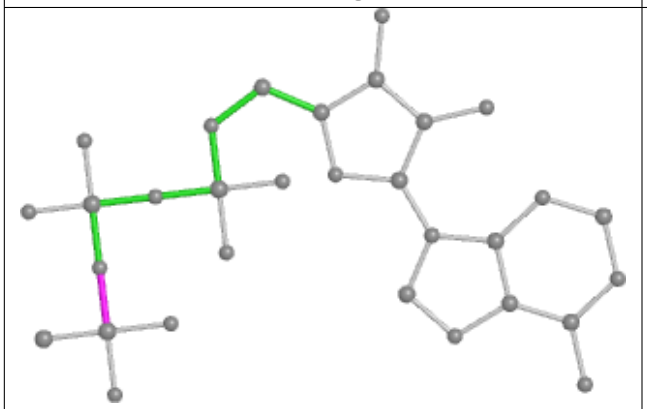
Ligand AGS B 2002



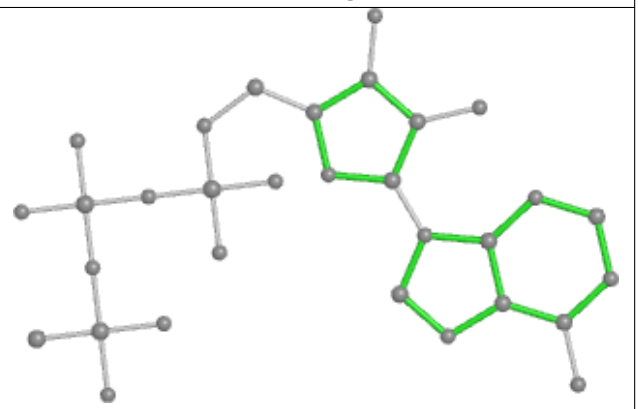
Bond lengths



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.

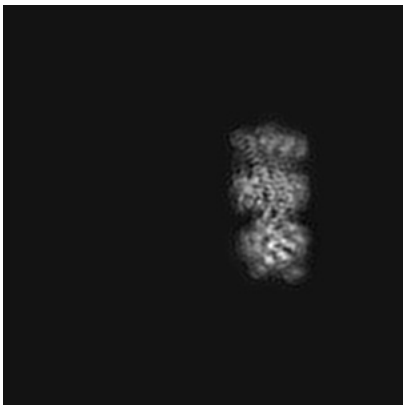
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6847. These allow visual inspection of the internal detail of the map and identification of artifacts.

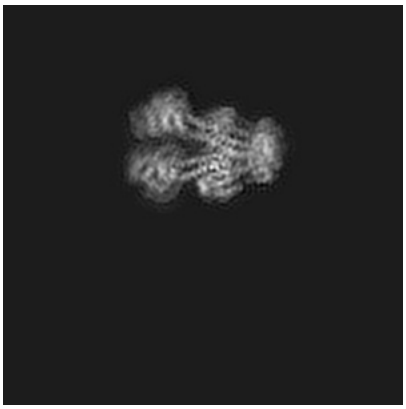
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

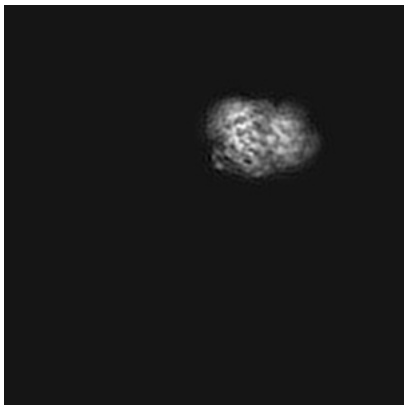
6.1.1 Primary map



X

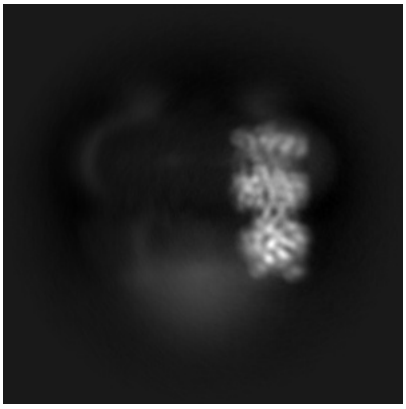


Y

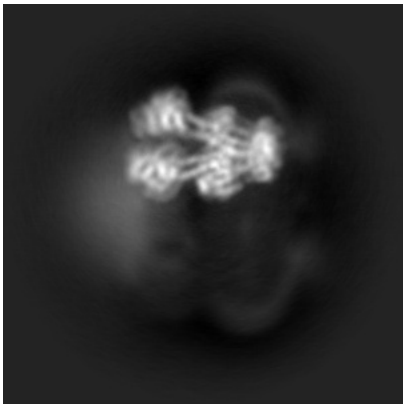


Z

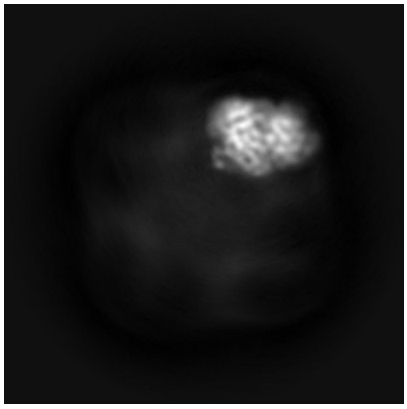
6.1.2 Raw map



X



Y

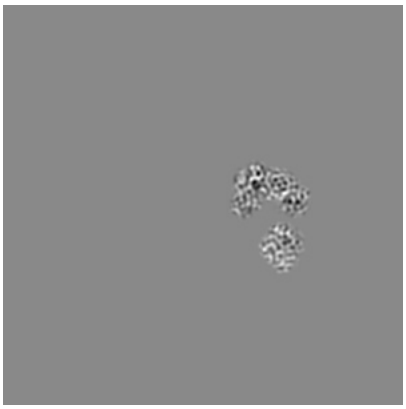


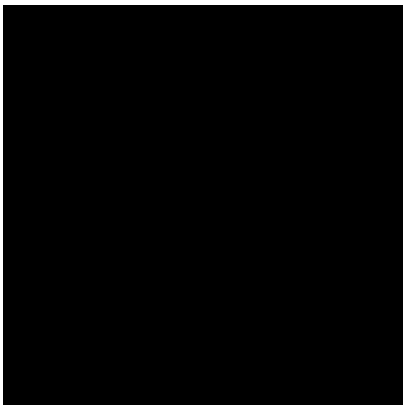
Z

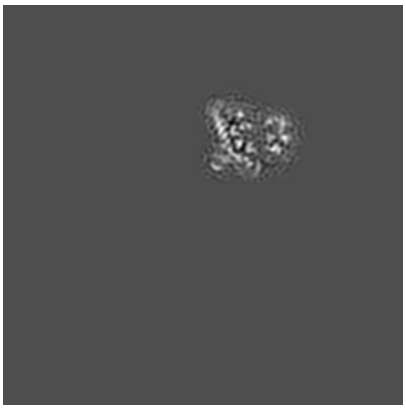
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

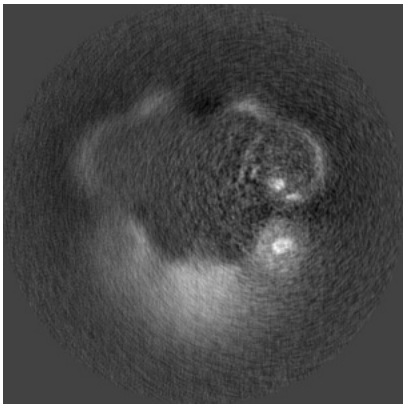
6.2.1 Primary map

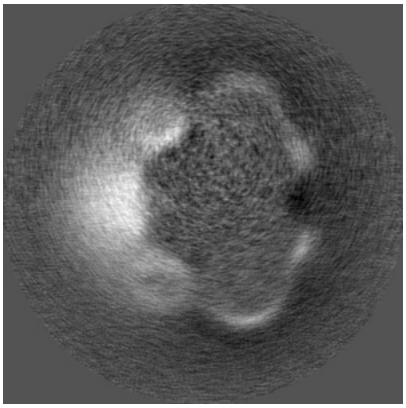

X Index: 156

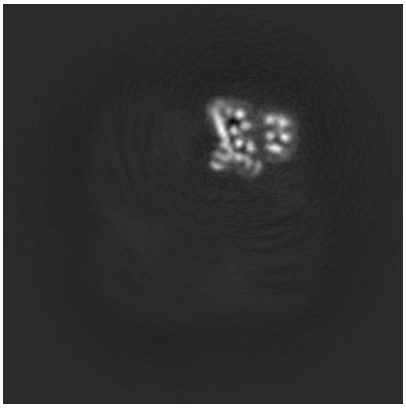

Y Index: 156


Z Index: 156

6.2.2 Raw map


X Index: 156


Y Index: 156


Z Index: 156

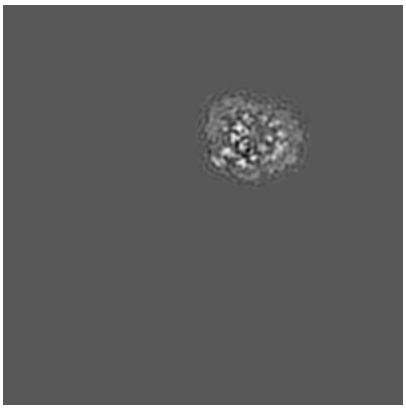
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

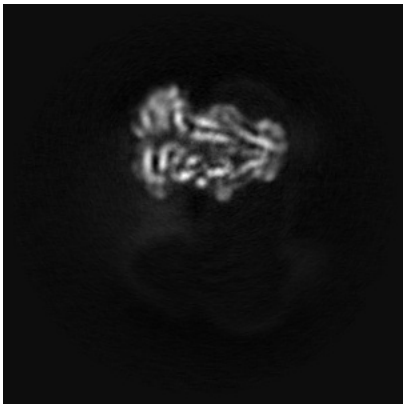
X Index: 183

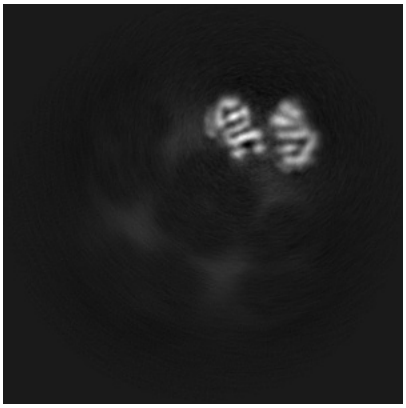
Y Index: 208


Z Index: 166

6.3.2 Raw map

X Index: 182

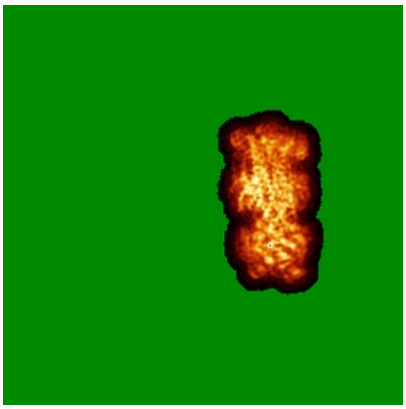

Y Index: 208

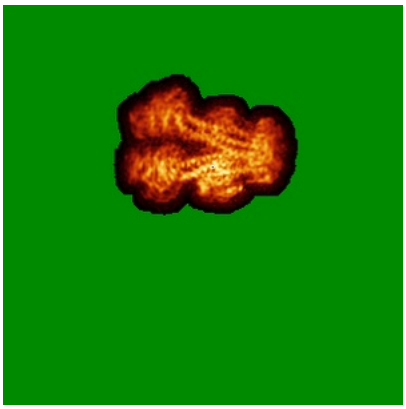

Z Index: 125

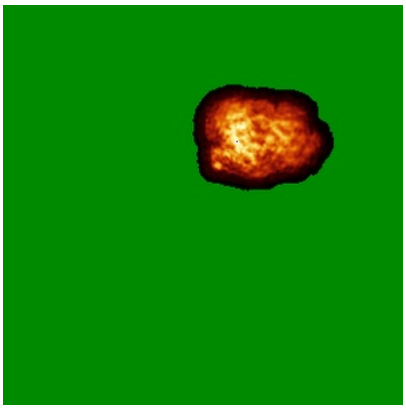
The images above show the largest variance slices of the map in three orthogonal directions.

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

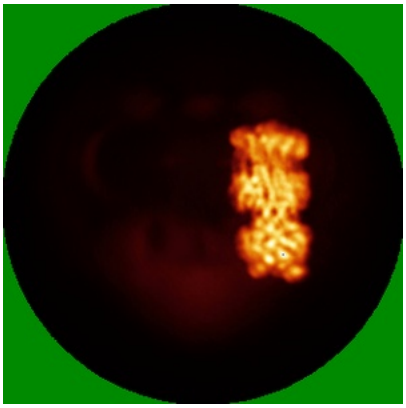
6.4.1 Primary map

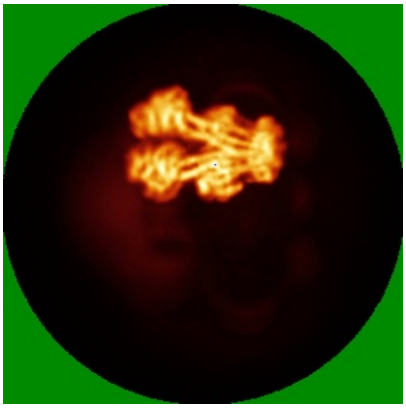

X

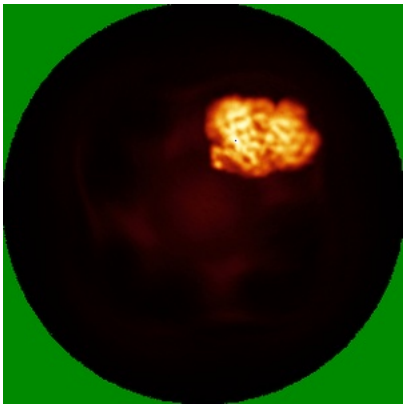

Y


Z

6.4.2 Raw map


X

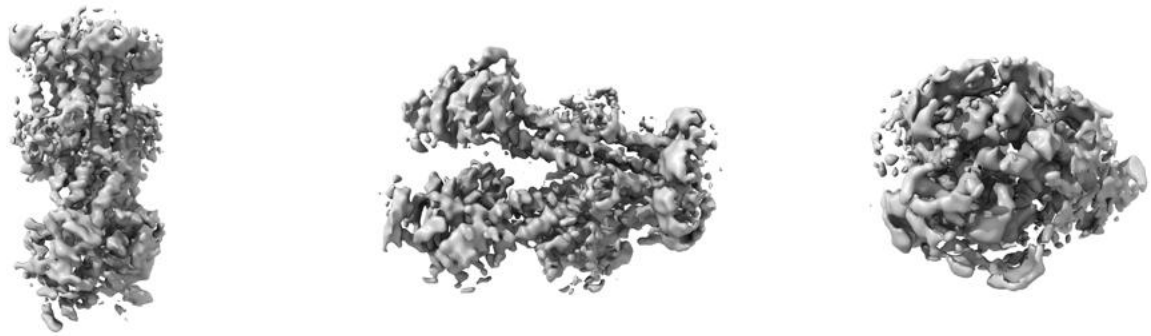

Y


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)

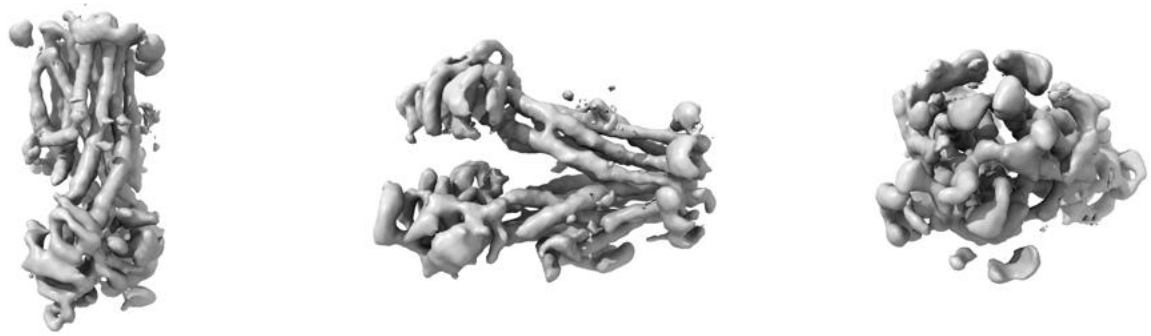
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

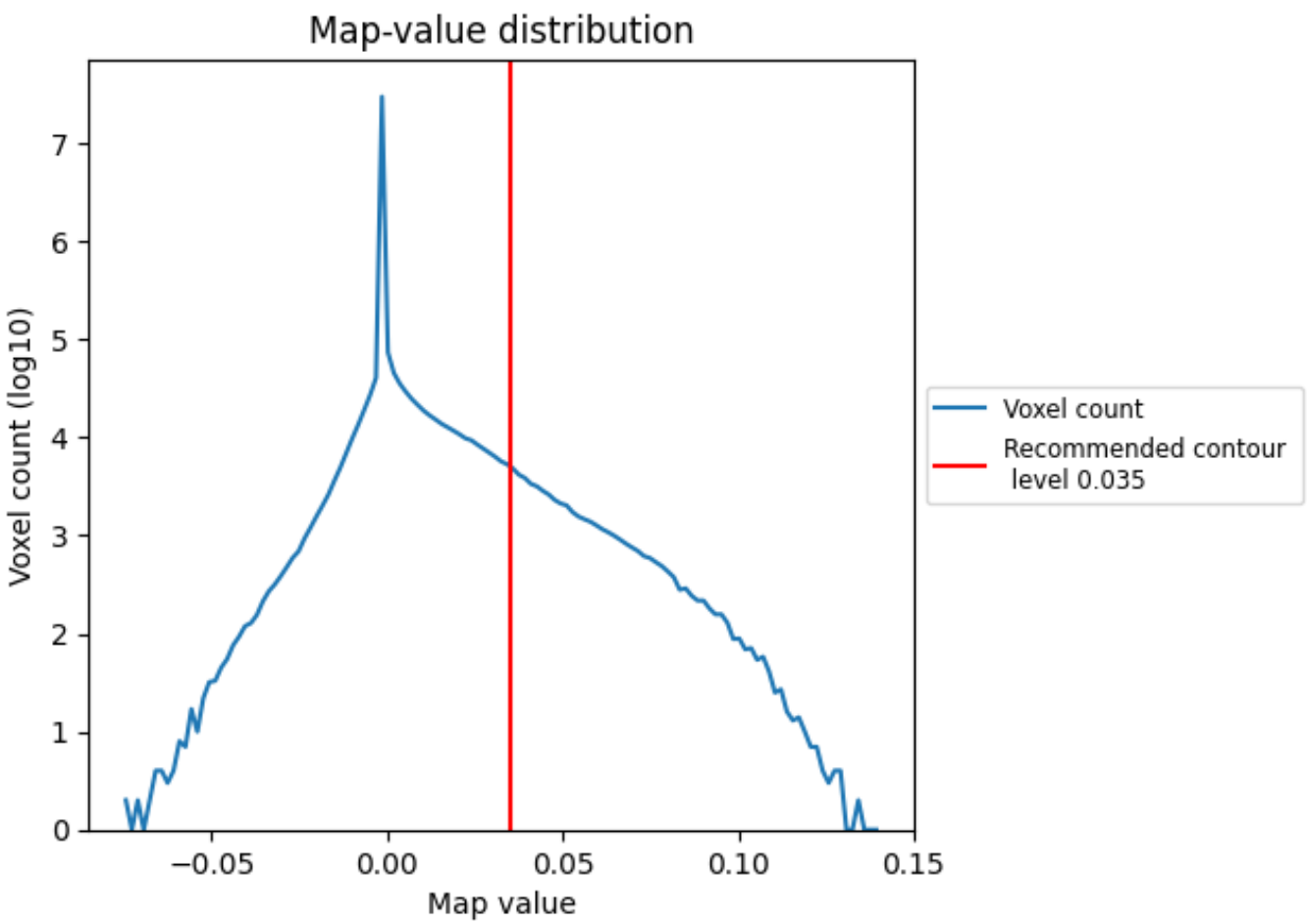
6.6 Mask visualisation (i)

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

7 Map analysis (i)

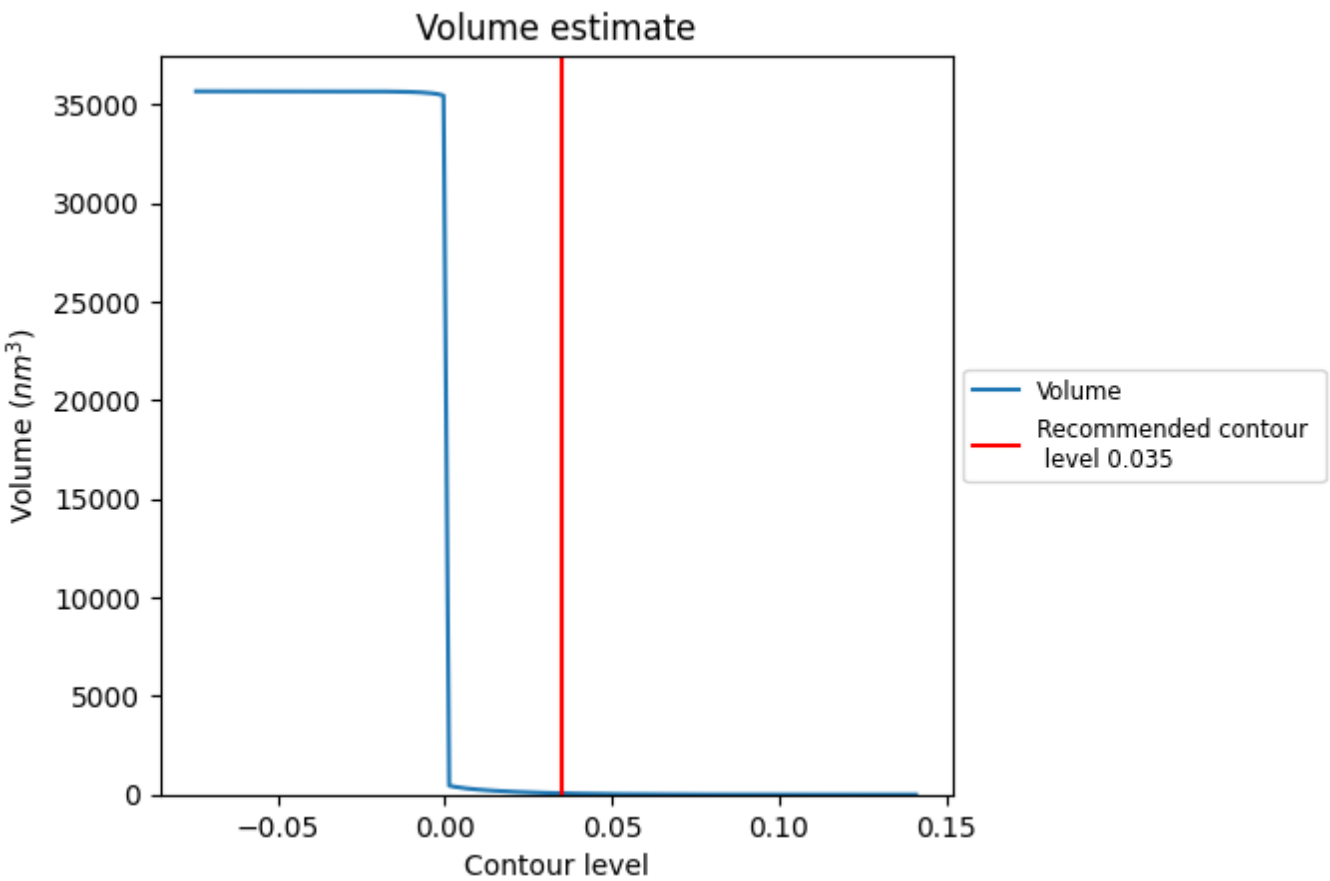
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

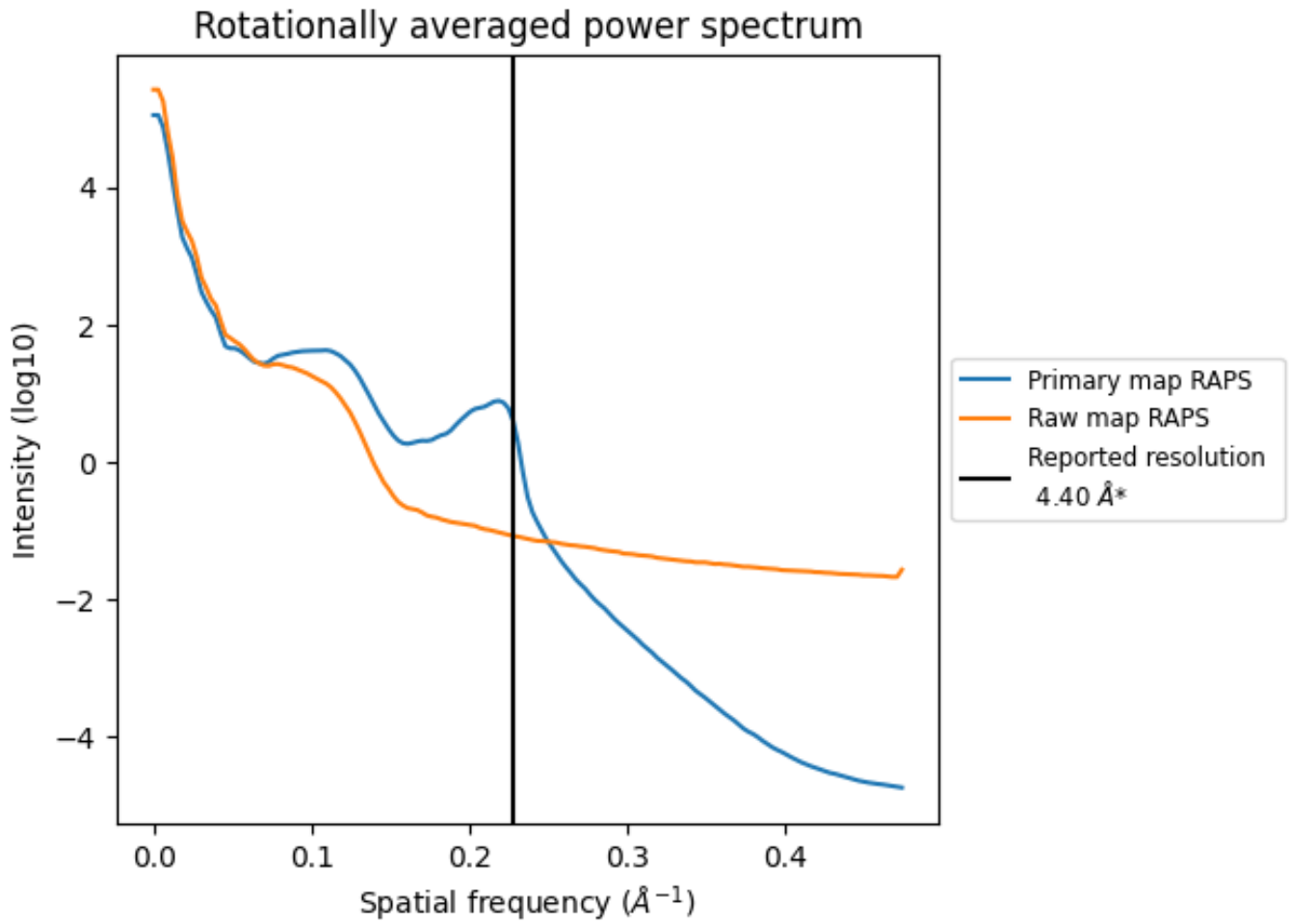
7.2 Volume estimate (i)



The volume at the recommended contour level is 63 nm^3; this corresponds to an approximate mass of 57 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)

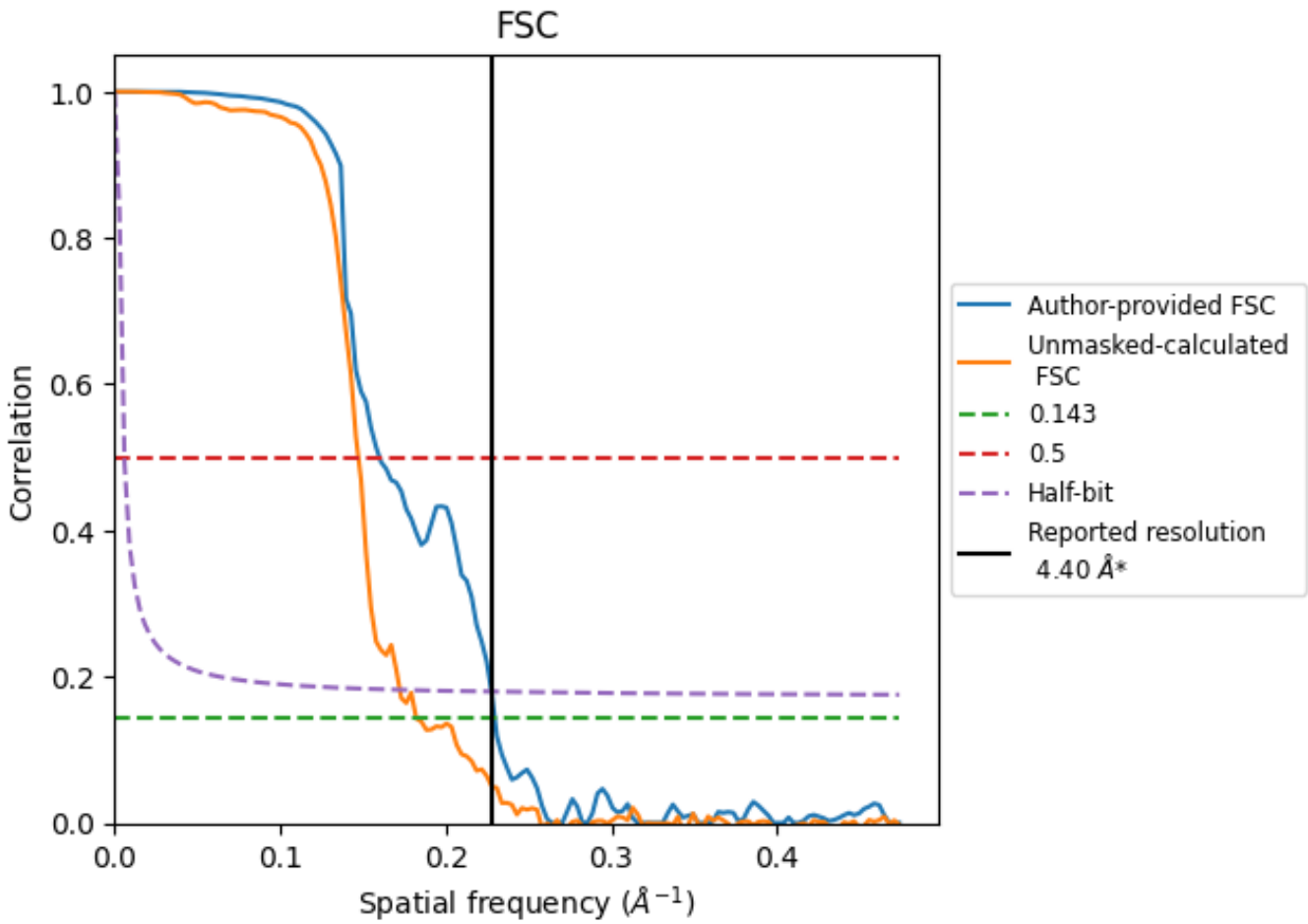


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

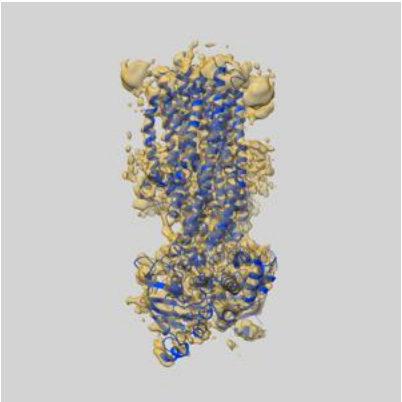
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.36	6.25	4.39
Unmasked-calculated*	5.49	6.79	5.80

*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 5.49 differs from the reported value 4.4 by more than 10 %

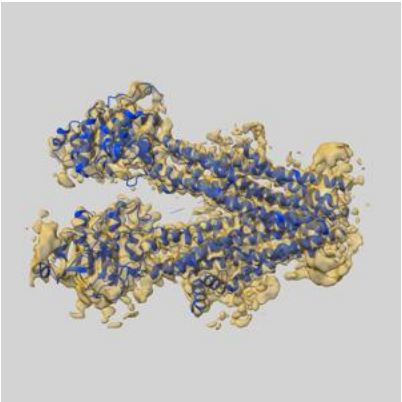
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6847 and PDB model 5YW7. Per-residue inclusion information can be found in section 3 on page 5.

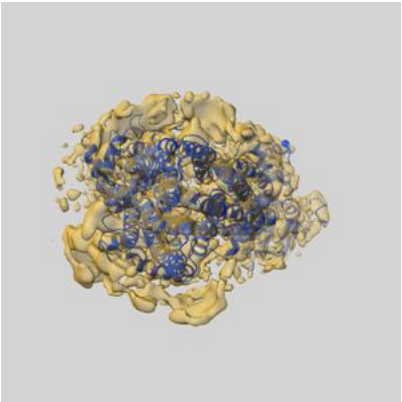
9.1 Map-model overlay (i)



X



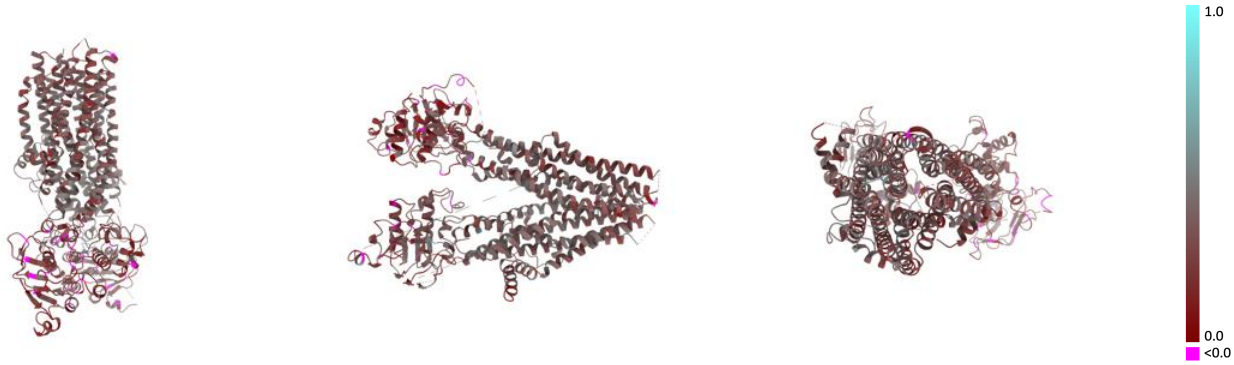
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

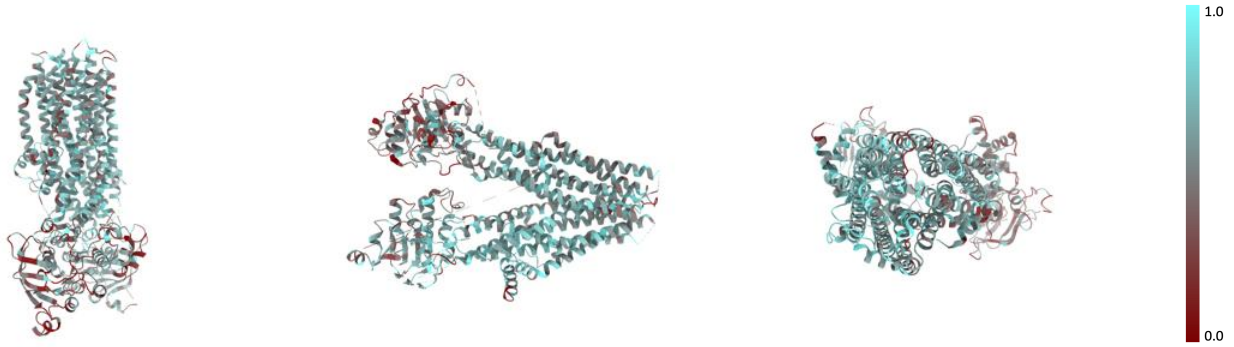
9.2 Q-score mapped to coordinate model (i)



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.

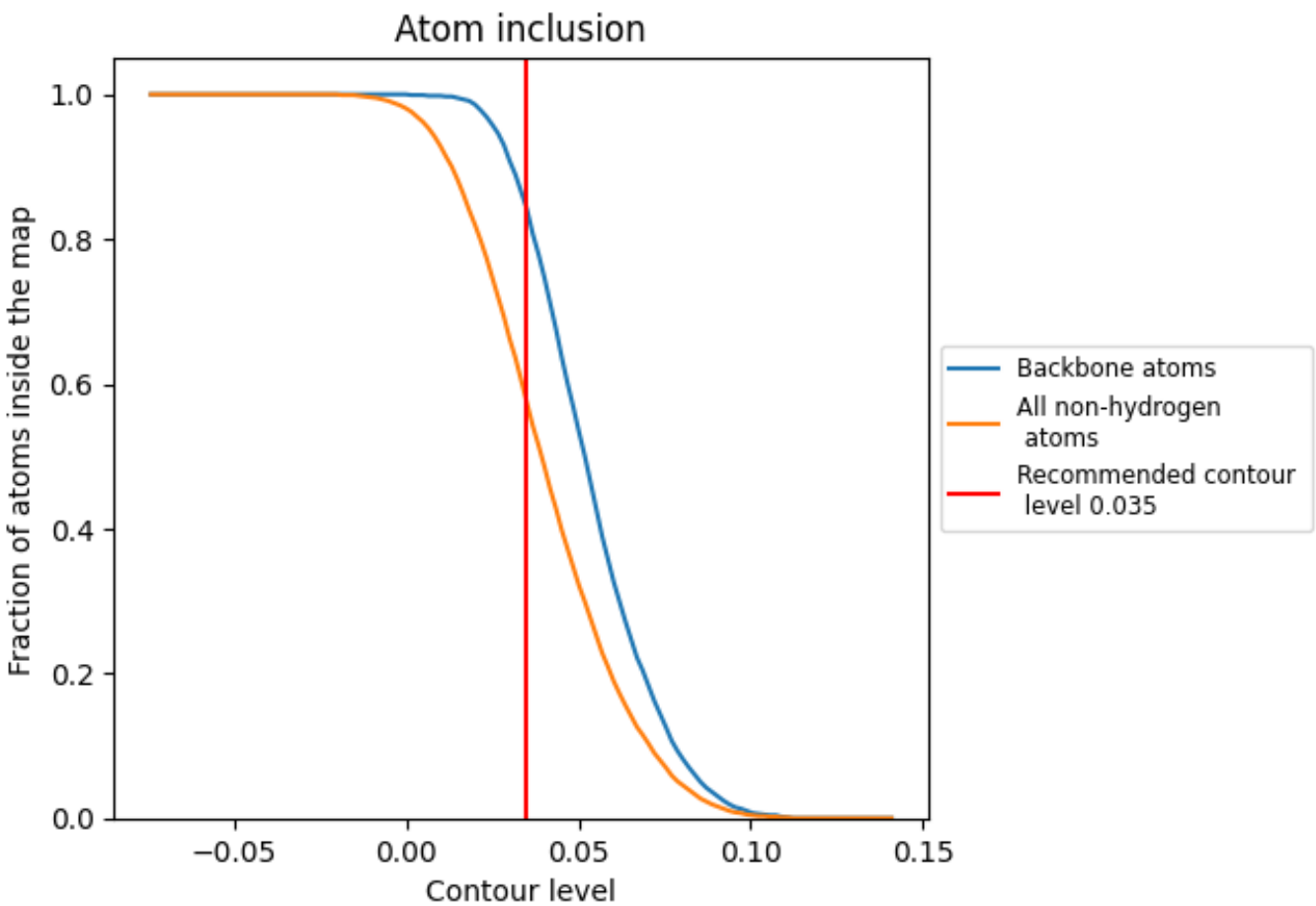
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 57% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5740	0.3050
B	0.5740	0.3050