Full wwPDB EM Validation Report

Nov 7, 2022 – 03:41 PM JST

PDB ID	:	5XSY
EMDB ID	:	EMD-6770
Title	:	Structure of the Nav1.4-beta1 complex from electric eel
Authors	:	Yan, Z.; Zhou, Q.; Wu, J.P.; Yan, N.
Deposited on	:	2017-06-15
Resolution	:	4.00 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:

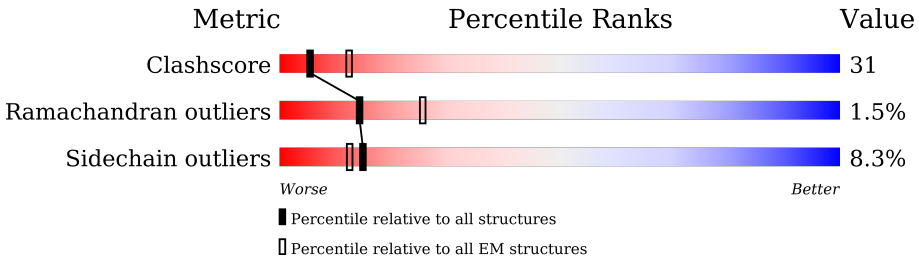
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1820	25% 40% 19% • 37%
2	B	209	31% 41% 32% 7% • 18%
3	C	5	20% 20% 60% 20%
4	D	3	67% 33% 67%
4	E	3	67% 67% 33%
4	F	3	67% 33% 67%
5	G	2	100% 50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10634 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.

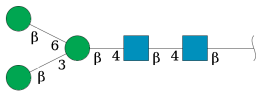
- Molecule 1 is a protein called Sodium channel protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1140	9057	5992	1436	1551	78	0	0

- Molecule 2 is a protein called Voltage-gated sodium channel beta subunit 1.

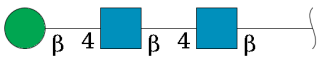
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	172	1371	874	223	261	13	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	5	61	34	2	25	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	3	39	22	2	15	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

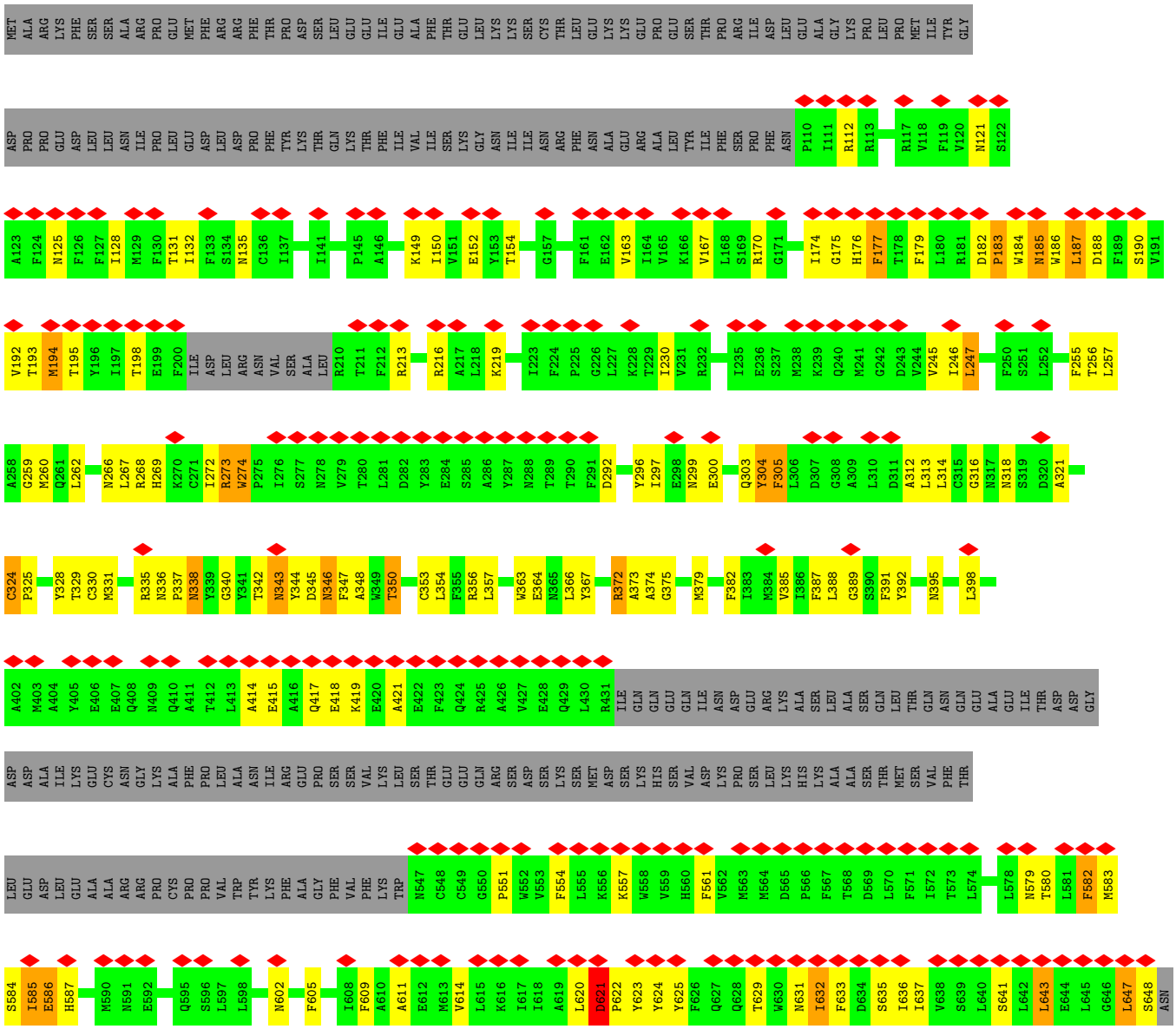
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

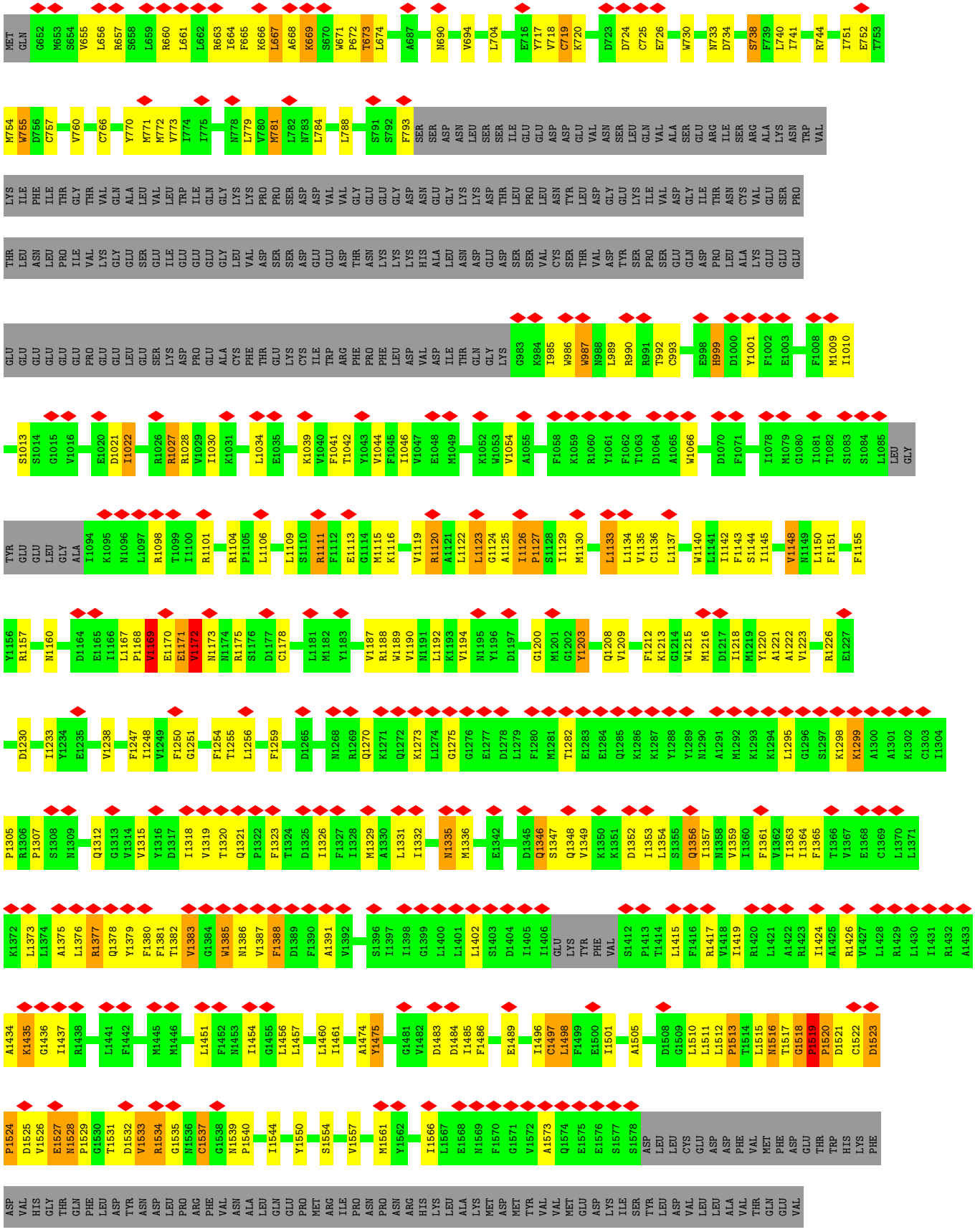
3 Residue-property plots (i)

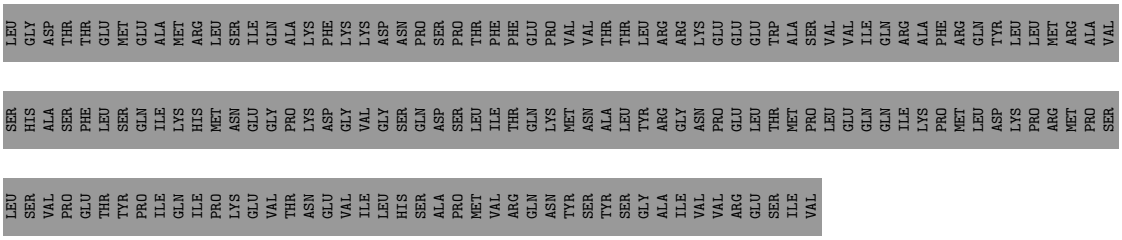
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium channel protein

Chain A:

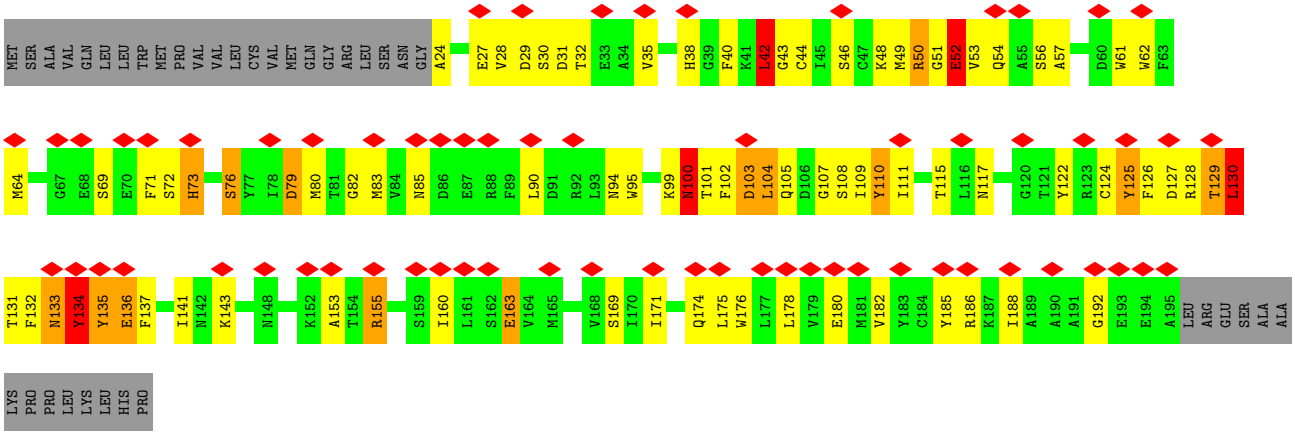



MET GLN G652 M653 S654 V655 L656 R657 S658 L659 R660 L661 L662 R663 I664 F665 K666 L667 A668 K669 S670 W671 P672 T673 L674 A687 N690 V694 L704 E716 Y717 V718 C719 K720 D723 D724 C725 E726 W730 N733 D734 S738 F739 L740 I741 R744 I751 E752 T753
M754 W755 D756 C757 V760 C766 Y770 M771 M772 V773 I774 L775 N778 L779 V780 M781 L782 N783 L784 L788 S791 S792 F793 SER SER ASP ASN LEU SER SER ILE GLU GLU ASP ASP GLU VAL ASN SER LEU GLN VAL ALA SER GLU ARG ILE SER ARG ALA LYS ASN TRP VAL
LYS ILE PHE ILE THR GLY THR VAL GLN ALA LEU VAL LEU TRP ILE GLN GLY LYS LYS PRO PRO SER ASP ASP VAL VAL GLY GLU GLU GLY ASP ASN GLU GLY LYS LYS ASP THR LEU PRO LEU ASN TYR LEU ASP GLY GLU LYS ILE VAL ASP GLY ILE THR ASN CYS VAL GLU SER PRO
THR LEU ASN LEU PRO ILE VAL LYS GLY GLU SER GLU ILE GLU GLU GLU GLY LEU VAL ASP SER SER ASP GLU GLU ASP THR ASN LYS LYS LYS HIS ALA LEU ASN ASP GLU ASP SER SER VAL CYS SER THR VAL ASP TYR SER PRO SER GLU GLN ASP PRO LEU ALA LYS GLU GLU GLU
GLU GLU GLU GLU GLU GLU PRO GLU GLU LEU GLU SER LYS ASP PRO GLU ALA CYS PHE THR GLU LYS CYS ILE TRP ARG PHE PRO PHE LEU ASP VAL ASP ILE THR GLN GLY LYS G983 K984 I985 W986 W987 N988 L989 R990 R991 T992 C993 E998 H999 D1000 Y1001 F1002 E1003 F1008 M1009 I1010
S1013 S1014 G1015 V1016 E1020 D1021 I1022 R1026 R1027 R1028 V1029 I1030 K1031 L1034 E1035 K1039 V1040 F1041 T1042 Y1043 V1044 F1045 I1046 V1047 E1048 M1049 K1052 W1053 V1054 A1055 F1058 K1059 R1060 Y1061 F1062 T1063 D1064 A1065 W1066 D1070 F1071 I1078 M1079 G1080 I1081 T1082 S1083 S1084 L1085 LEU GLY
TYR GLU GLU LEU GLY ALA I1094 K1095 N1096 L1097 R1098 T1099 I1100 R1101 R1104 P1105 L1106 L1109 S1110 R1111 F1112 E1113 G1114 M1115 K1116 V1119 R1120 A1121 L1122 L1123 G1124 A1125 I1126 P1127 S1128 I1129 M1130 L1133 L1134 V1135 C1136 L1137 W1140 L1141 I1142 F1143 S1144 I1145 V1148 N1149 L1150 F1151 F1155
Y1156 R1157 N1160 D1164 E1165 I1166 L1167 P1168 V1169 E1170 E1171 V1172 N1173 N1174 R1175 S1176 D1177 C1178 L1181 M1182 Y1183 V1187 R1188 W1189 V1190 N1191 L1192 K1193 V1194 N1195 Y1196 D1197 G1200 M1201 G1202 Y1203 Q1208 V1209 F1212 K1213 G1214 W1215 M1216 D1217 I1218 M1219 Y1220 A1221 A1222 V1223 R1226 E1227
D1230 I1233 Y1234 E1235 V1238 F1247 I1248 V1249 F1250 G1251 F1254 T1255 L1256 F1259 D1265 N1268 R1269 Q1270 K1271 Q1272 K1273 L1274 G1275 G1276 E1277 D1278 L1279 F1280 M1281 T1282 E1283 E1284 Q1285 K1286 K1287 Y1288 Y1289 N1290 A1291 M1292 K1293 K1294 L1295 G1296 S1297 K1298 K1299 A1300 A1301 K1302 C1303 I1304
P1305 R1306 P1307 S1308 N1309 Q1312 G1313 V1314 V1315 Y1316 D1317 I1318 V1319 T1320 Q1321 P1322 F1323 T1324 D1325 I1326 F1327 I1328 M1329 A1330 L1331 I1332 N1335 M1336 E1342 D1345 Q1346 S1347 Q1348 V1349 K1350 K1351 D1352 I1353 L1354 S1355 Q1356 I1357 N1358 V1359 I1360 F1361 V1362 I1363 I1364 F1365 T1366 V1367 E1368 C1369 L1370 L1371
K1372 L1373 L1374 A1375 L1376 R1377 Q1378 Y1379 F1380 F1381 T1382 V1383 G1384 W1385 N1386 V1387 F1388 D1389 F1390 A1391 V1392 S1396 I1397 I1398 G1399 L1400 L1401 L1402 S1403 D1404 I1405 I1406 GLU LYS TYR PHE VAL S1412 P1413 T1414 L1415 F1416 R1417 V1418 I1419 R1420 L1421 A1422 R1423 I1424 A1425 R1426 V1427 L1428 R1429 L1430 I1431 R1432 A1433
A1434 K1435 G1436 I1437 R1438 L1441 F1442 M1445 M1446 L1451 F1452 N1453 I1454 G1455 L1456 L1457 L1460 I1461 A1474 Y1475 G1481 V1482 D1483 D1484 I1485 F1486 E1489 I1496 C1497 L1498 F1499 E1500 I1501 A1505 D1508 G1509 L1510 L1511 L1512 P1513 T1514 L1515 N1516 T1517 G1518 P1519 P1520 D1521 C1522 D1523
P1524 D1525 V1526 E1527 N1528 P1529 G1530 T1531 D1532 V1533 R1534 G1535 N1536 C1537 G1538 N1539 P1540 I1544 Y1550 S1554 V1557 M1561 Y1562 I1566 L1567 E1568 N1569 F1570 G1571 V1572 A1573 Q1574 E1575 E1576 S1577 S1578 ASP LEU LEU CYS GLU ASP ASP PHE VAL MET PHE ASP GLU THR TRP HIS LYS PHE
ASP VAL HIS GLY THR GLN PHE LEU ASP TYR ASN ASP LEU PRO ARG PHE VAL ASN ALA LEU GLN GLU PRO MET ARG ILE PRO ASN PRO ASN ARG HIS LYS LEU ALA LYS MET ASP MET TYR VAL VAL MET GLU ASP LYS ILE SER TYR LEU ASP VAL LEU LEU ALA VAL THR GLN GLU VAL



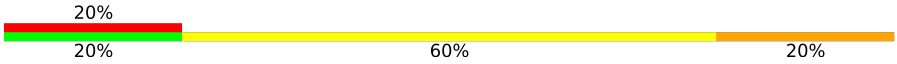
• Molecule 2: Voltage-gated sodium channel beta subunit 1

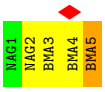
Chain B:



• Molecule 3: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:





• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

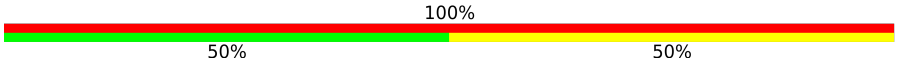
Chain E:

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123431	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 ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.334	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	267.6, 267.6, 267.6	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.54	6/9269 (0.1%)	0.67	11/12571 (0.1%)
2	B	0.51	1/1399 (0.1%)	1.07	12/1894 (0.6%)
All	All	0.54	7/10668 (0.1%)	0.73	23/14465 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	136	GLU	CA-C	6.02	1.68	1.52
1	A	1520	PRO	N-CD	5.70	1.55	1.47
1	A	183	PRO	N-CD	5.43	1.55	1.47
1	A	1519	PRO	N-CD	5.27	1.55	1.47
1	A	622	PRO	N-CD	5.15	1.55	1.47
1	A	1513	PRO	N-CD	5.10	1.54	1.47
1	A	1127	PRO	N-CD	5.05	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	76	SER	CB-CA-C	-14.61	82.35	110.10
2	B	110	TYR	CB-CA-C	-13.68	83.04	110.40
2	B	130	LEU	CB-CA-C	12.86	134.63	110.20
2	B	130	LEU	N-CA-C	-11.00	81.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	83	MET	CB-CA-C	-9.08	92.25	110.40
2	B	129	THR	N-CA-C	-7.96	89.52	111.00
2	B	125	TYR	N-CA-C	-6.52	93.40	111.00
2	B	54	GLN	CB-CA-C	-6.51	97.37	110.40
1	A	1528	ASN	C-N-CD	6.28	141.59	128.40
2	B	29	ASP	CB-CA-C	-6.08	98.24	110.40
1	A	1383	VAL	C-N-CA	-5.98	109.75	122.30
1	A	1518	GLY	C-N-CD	5.97	140.95	128.40
1	A	1126	ILE	C-N-CD	5.76	140.50	128.40
1	A	621	ASP	C-N-CD	5.73	140.42	128.40
2	B	42	LEU	N-CA-C	-5.71	95.59	111.00
1	A	1512	LEU	C-N-CD	5.68	140.33	128.40
1	A	586	GLU	N-CA-C	-5.61	95.85	111.00
1	A	1256	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	335	ARG	C-N-CA	5.54	135.55	121.70
2	B	136	GLU	C-N-CA	5.45	135.34	121.70
2	B	32	THR	CB-CA-C	-5.36	97.12	111.60
1	A	1106	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	1573	ALA	CB-CA-C	5.11	117.77	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1524	PRO	Peptide
1	A	213	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	726	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9057	0	9064	559	0
2	B	1371	0	1326	121	0
3	C	61	0	52	1	0
4	D	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	39	0	34	0	0
4	F	39	0	34	0	0
5	G	28	0	25	0	0
All	All	10634	0	10569	663	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 31.

All (663) 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:1383:VAL:CG1	1:A:1386:ASN:HB2	1.64	1.28
2:B:76:SER:O	2:B:82:GLY:HA3	1.33	1.23
1:A:324:CYS:SG	1:A:325:PRO:HD2	1.83	1.17
1:A:664:ILE:HD12	1:A:1142:ILE:HD11	1.27	1.16
1:A:1376:LEU:CB	1:A:1380:PHE:HB3	1.76	1.16
1:A:273:ARG:HG2	1:A:328:TYR:CE1	1.80	1.14
1:A:1022:ILE:HD13	2:B:24:ALA:HB3	1.28	1.14
1:A:1383:VAL:HG12	1:A:1386:ASN:HB2	1.19	1.13
1:A:629:THR:O	1:A:632:ILE:HG22	1.47	1.13
1:A:661:LEU:O	1:A:664:ILE:HG13	1.47	1.13
1:A:247:LEU:HD23	1:A:1437:ILE:HG13	1.14	1.12
1:A:1522:CYS:C	1:A:1524:PRO:CD	2.18	1.11
1:A:1376:LEU:CD1	1:A:1380:PHE:HB3	1.81	1.11
1:A:1188:ARG:HH21	1:A:1190:VAL:HG21	1.10	1.09
2:B:43:GLY:HA2	2:B:108:SER:HB3	1.31	1.09
1:A:1123:LEU:O	1:A:1126:ILE:HG22	1.51	1.08
1:A:247:LEU:CD2	1:A:1437:ILE:HG13	1.83	1.07
1:A:1383:VAL:CG1	1:A:1386:ASN:CB	2.33	1.07
1:A:1383:VAL:HG13	1:A:1386:ASN:H	1.18	1.06
2:B:35:VAL:CG2	2:B:153:ALA:HB2	1.86	1.05
1:A:629:THR:C	1:A:632:ILE:HG22	1.76	1.05
1:A:1522:CYS:O	1:A:1524:PRO:HD2	1.54	1.04
1:A:304:TYR:HD1	1:A:305:PHE:N	1.55	1.03
1:A:629:THR:CA	1:A:632:ILE:HG22	1.87	1.03
1:A:1188:ARG:HD2	1:A:1190:VAL:CG2	1.89	1.03
1:A:1376:LEU:CD1	1:A:1380:PHE:CB	2.36	1.02
1:A:1376:LEU:HD12	1:A:1380:PHE:CB	1.90	1.02
1:A:629:THR:HA	1:A:632:ILE:HG22	1.43	1.01
1:A:1522:CYS:C	1:A:1524:PRO:HD3	1.81	1.01
1:A:1188:ARG:CD	1:A:1190:VAL:CG2	2.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:SER:O	1:A:193:THR:HG22	1.61	1.00
1:A:273:ARG:HG2	1:A:328:TYR:HE1	1.17	0.99
1:A:671:TRP:HD1	1:A:672:PRO:N	1.61	0.98
1:A:643:LEU:HD22	1:A:656:LEU:HD13	1.44	0.98
1:A:1522:CYS:HB3	1:A:1524:PRO:HD3	1.44	0.98
1:A:247:LEU:HD23	1:A:1437:ILE:CG1	1.92	0.97
1:A:1188:ARG:HD2	1:A:1190:VAL:HG23	1.44	0.97
1:A:1346:GLN:H	1:A:1346:GLN:HE21	1.09	0.96
2:B:43:GLY:CA	2:B:108:SER:HB3	1.95	0.96
1:A:1188:ARG:HD3	1:A:1190:VAL:HG22	1.43	0.96
1:A:629:THR:O	1:A:632:ILE:CG2	2.14	0.96
1:A:583:MET:HE1	1:A:661:LEU:HG	1.46	0.95
2:B:35:VAL:HG21	2:B:153:ALA:HB2	1.48	0.95
1:A:176:HIS:O	1:A:179:PHE:HB3	1.63	0.95
1:A:1376:LEU:HB3	1:A:1380:PHE:HB3	1.46	0.95
1:A:1522:CYS:C	1:A:1524:PRO:HD2	1.83	0.95
1:A:367:TYR:HD1	1:A:382:PHE:CD2	1.85	0.95
1:A:1434:ALA:CB	1:A:1437:ILE:HG22	1.97	0.95
1:A:1402:LEU:HD23	1:A:1419:ILE:HG13	1.47	0.94
1:A:1171:GLU:O	1:A:1172:VAL:HB	1.64	0.94
1:A:1529:PRO:CG	2:B:105:GLN:HE21	1.81	0.93
1:A:1383:VAL:HG12	1:A:1386:ASN:CB	1.98	0.92
1:A:629:THR:HA	1:A:632:ILE:CG2	1.98	0.92
1:A:1315:VAL:HG12	1:A:1375:ALA:HB2	1.50	0.92
1:A:1172:VAL:HG13	1:A:1172:VAL:O	1.65	0.92
1:A:1529:PRO:HG3	2:B:105:GLN:HE21	1.35	0.92
1:A:367:TYR:CD1	1:A:382:PHE:HD2	1.87	0.91
1:A:664:ILE:HA	1:A:667:LEU:HD12	1.52	0.91
1:A:784:LEU:O	1:A:788:LEU:HD23	1.70	0.91
1:A:1066:TRP:CH2	1:A:1119:VAL:HG11	2.06	0.90
1:A:325:PRO:HG2	1:A:328:TYR:HD2	1.36	0.90
2:B:43:GLY:HA2	2:B:108:SER:CB	2.00	0.90
1:A:321:ALA:HB2	1:A:375:GLY:HA2	1.54	0.90
1:A:1522:CYS:HB3	1:A:1524:PRO:CD	2.01	0.90
1:A:367:TYR:HD1	1:A:382:PHE:HD2	1.19	0.90
2:B:134:TYR:HB2	2:B:135:TYR:CD1	2.06	0.90
1:A:1113:GLU:CG	1:A:1282:THR:HG21	2.02	0.89
1:A:1376:LEU:HD12	1:A:1380:PHE:HB2	1.50	0.89
1:A:583:MET:HE1	1:A:661:LEU:CG	2.01	0.89
1:A:1515:LEU:HD11	1:A:1544:ILE:HD11	1.53	0.89
1:A:1529:PRO:CG	2:B:105:GLN:NE2	2.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:ARG:HH21	1:A:1190:VAL:CG2	1.87	0.88
1:A:1498:LEU:O	1:A:1501:ILE:HG22	1.72	0.88
1:A:1527:GLU:OE1	1:A:1534:ARG:HG3	1.73	0.88
1:A:1346:GLN:O	1:A:1347:SER:OG	1.92	0.88
1:A:187:LEU:HD23	1:A:188:ASP:N	1.89	0.87
1:A:643:LEU:CD2	1:A:656:LEU:HD13	2.03	0.87
1:A:671:TRP:CD1	1:A:672:PRO:HD2	2.09	0.87
2:B:134:TYR:HB2	2:B:135:TYR:CE1	2.07	0.87
2:B:42:LEU:HD13	2:B:122:TYR:CE2	2.08	0.87
1:A:643:LEU:CD2	1:A:656:LEU:CD1	2.52	0.87
1:A:174:ILE:HG23	1:A:177:PHE:CE2	2.10	0.87
1:A:1475:TYR:OH	1:A:1533:VAL:HG21	1.75	0.86
1:A:664:ILE:HD12	1:A:1142:ILE:CD1	2.06	0.86
1:A:1169:VAL:HG21	1:A:1226:ARG:NH1	1.90	0.86
1:A:1361:PHE:O	1:A:1364:ILE:HG22	1.76	0.85
1:A:1188:ARG:HD3	1:A:1190:VAL:CG2	2.05	0.85
1:A:1524:PRO:HA	1:A:1535:GLY:HA2	1.59	0.85
1:A:1529:PRO:HG3	2:B:105:GLN:NE2	1.92	0.85
1:A:195:THR:O	1:A:198:THR:HG22	1.77	0.85
1:A:1402:LEU:CD2	1:A:1419:ILE:HD12	2.06	0.85
1:A:661:LEU:O	1:A:664:ILE:CG1	2.24	0.84
2:B:35:VAL:HG22	2:B:153:ALA:HB2	1.58	0.84
1:A:1123:LEU:O	1:A:1123:LEU:HD22	1.78	0.84
2:B:57:ALA:HB1	2:B:104:LEU:HD12	1.58	0.83
1:A:1523:ASP:N	1:A:1524:PRO:CD	2.40	0.83
2:B:42:LEU:HD11	2:B:111:ILE:HD11	1.58	0.83
1:A:324:CYS:SG	1:A:325:PRO:CD	2.67	0.83
1:A:1383:VAL:HG11	1:A:1386:ASN:ND2	1.93	0.83
1:A:174:ILE:HG23	1:A:177:PHE:HE2	1.42	0.82
1:A:367:TYR:CD1	1:A:382:PHE:CD2	2.66	0.82
1:A:989:LEU:O	1:A:992:THR:HG22	1.79	0.82
1:A:1022:ILE:HD13	2:B:24:ALA:CB	2.07	0.82
1:A:1383:VAL:HG13	1:A:1386:ASN:N	1.95	0.82
1:A:1379:TYR:O	1:A:1382:THR:HG23	1.80	0.81
1:A:305:PHE:HB3	1:A:312:ALA:HA	1.60	0.81
1:A:632:ILE:HD13	1:A:632:ILE:O	1.79	0.81
1:A:1346:GLN:HE21	1:A:1346:GLN:N	1.78	0.81
1:A:1383:VAL:CG1	1:A:1386:ASN:ND2	2.43	0.81
1:A:357:LEU:HD21	1:A:366:LEU:HD23	1.61	0.81
1:A:1123:LEU:O	1:A:1127:PRO:HD3	1.81	0.81
1:A:1188:ARG:NH2	1:A:1190:VAL:HG21	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:LEU:HD23	1:A:1419:ILE:CG1	2.11	0.81
1:A:1066:TRP:CZ2	1:A:1119:VAL:HG11	2.16	0.80
1:A:1312:GLN:NE2	1:A:1375:ALA:HA	1.96	0.80
1:A:1434:ALA:HB1	1:A:1437:ILE:HG22	1.63	0.80
1:A:304:TYR:CD1	1:A:305:PHE:N	2.45	0.80
1:A:1353:ILE:O	1:A:1357:ILE:HG13	1.82	0.80
1:A:300:GLU:HA	1:A:303:GLN:HE21	1.46	0.80
1:A:671:TRP:CD1	1:A:672:PRO:N	2.48	0.80
1:A:1516:ASN:HD22	1:A:1517:THR:N	1.80	0.80
1:A:273:ARG:HA	1:A:328:TYR:HD1	1.46	0.80
1:A:620:LEU:O	1:A:621:ASP:O	1.99	0.80
1:A:1434:ALA:HB3	1:A:1437:ILE:HG22	1.62	0.80
1:A:1522:CYS:CB	1:A:1524:PRO:HD3	2.11	0.80
1:A:583:MET:HE3	1:A:661:LEU:HD11	1.63	0.79
1:A:1402:LEU:CD2	1:A:1419:ILE:CD1	2.59	0.79
1:A:1517:THR:HG21	1:A:1540:PRO:HD3	1.64	0.79
1:A:664:ILE:CD1	1:A:1142:ILE:HD11	2.09	0.79
1:A:582:PHE:HD2	1:A:605:PHE:CE2	2.01	0.79
1:A:1113:GLU:HG3	1:A:1282:THR:HG21	1.63	0.78
1:A:1113:GLU:HG2	1:A:1282:THR:HG21	1.65	0.78
1:A:1188:ARG:HG2	1:A:1189:TRP:N	1.99	0.78
1:A:1515:LEU:HD11	1:A:1544:ILE:CD1	2.14	0.78
1:A:1383:VAL:HG13	1:A:1386:ASN:HB2	1.60	0.78
1:A:671:TRP:HD1	1:A:672:PRO:CD	1.96	0.78
1:A:671:TRP:CD1	1:A:672:PRO:CD	2.66	0.78
2:B:50:ARG:HH11	2:B:50:ARG:HG2	1.49	0.77
1:A:583:MET:CE	1:A:661:LEU:HD11	2.14	0.77
1:A:1172:VAL:O	1:A:1172:VAL:CG1	2.30	0.77
1:A:582:PHE:HD2	1:A:605:PHE:HE2	1.32	0.77
1:A:1526:VAL:HG12	1:A:1535:GLY:CA	2.15	0.77
1:A:1113:GLU:HG3	1:A:1282:THR:CG2	2.15	0.77
1:A:1376:LEU:CG	1:A:1380:PHE:HB3	2.14	0.77
1:A:1376:LEU:HD13	1:A:1380:PHE:CB	2.15	0.76
1:A:1383:VAL:HG11	1:A:1386:ASN:CG	2.05	0.76
1:A:274:TRP:CZ3	1:A:331:MET:CE	2.68	0.76
1:A:602:ASN:HB3	1:A:660:ARG:HH12	1.50	0.76
1:A:664:ILE:HG22	1:A:667:LEU:HD13	1.67	0.76
1:A:1511:LEU:HG	1:A:1515:LEU:HD13	1.67	0.76
1:A:1335:ASN:HB2	1:A:1361:PHE:CE1	2.21	0.76
2:B:42:LEU:CD1	2:B:122:TYR:CE2	2.69	0.76
1:A:1129:ILE:HD12	1:A:1259:PHE:HE1	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:TYR:CE1	1:A:631:ASN:HB3	2.20	0.75
1:A:247:LEU:O	1:A:247:LEU:HD22	1.85	0.75
1:A:304:TYR:CE2	1:A:325:PRO:HG3	2.21	0.75
1:A:1526:VAL:HG12	1:A:1535:GLY:HA2	1.68	0.75
1:A:1022:ILE:CD1	2:B:24:ALA:HB3	2.14	0.74
1:A:1434:ALA:HB3	1:A:1437:ILE:CG2	2.16	0.74
2:B:62:TRP:CH2	2:B:73:HIS:HD2	2.05	0.74
1:A:738:SER:O	1:A:741:ILE:HG22	1.87	0.74
1:A:1383:VAL:CG1	1:A:1386:ASN:CG	2.55	0.74
2:B:42:LEU:HD13	2:B:122:TYR:CD2	2.20	0.74
1:A:195:THR:HG21	1:A:216:ARG:HH21	1.53	0.74
1:A:345:ASP:O	1:A:346:ASN:HB3	1.85	0.74
2:B:130:LEU:O	2:B:130:LEU:HD23	1.86	0.74
1:A:1523:ASP:HB3	1:A:1526:VAL:HB	1.69	0.74
1:A:1501:ILE:HD12	1:A:1510:LEU:HD12	1.69	0.74
1:A:987:TRP:CE3	1:A:987:TRP:HA	2.23	0.74
1:A:1529:PRO:HG2	2:B:105:GLN:NE2	2.01	0.73
1:A:274:TRP:HA	1:A:274:TRP:CE3	2.24	0.73
1:A:629:THR:CA	1:A:632:ILE:CG2	2.62	0.73
1:A:1124:GLY:O	1:A:1127:PRO:HD2	1.88	0.73
1:A:1111:ARG:N	1:A:1111:ARG:HD2	2.02	0.73
1:A:379:MET:SD	1:A:1496:ILE:HD13	2.29	0.72
1:A:751:ILE:HG23	1:A:755:TRP:CZ2	2.24	0.72
2:B:61:TRP:CZ3	2:B:124:CYS:HB3	2.23	0.72
1:A:986:TRP:HH2	1:A:990:ARG:HH11	1.36	0.72
1:A:1188:ARG:HG2	1:A:1189:TRP:H	1.55	0.72
1:A:1517:THR:CG2	1:A:1540:PRO:HD3	2.20	0.72
1:A:583:MET:CE	1:A:661:LEU:HD21	2.20	0.71
1:A:379:MET:SD	1:A:1496:ILE:CD1	2.78	0.71
1:A:1434:ALA:CB	1:A:1437:ILE:CG2	2.68	0.71
1:A:1113:GLU:CG	1:A:1282:THR:CG2	2.68	0.71
1:A:1349:VAL:O	1:A:1353:ILE:HG13	1.91	0.71
1:A:1376:LEU:HB2	1:A:1380:PHE:HB3	1.72	0.71
1:A:1516:ASN:HD22	1:A:1517:THR:H	1.38	0.71
1:A:987:TRP:HA	1:A:987:TRP:HE3	1.55	0.71
1:A:1415:LEU:O	1:A:1419:ILE:HG12	1.90	0.71
2:B:99:LYS:O	2:B:100:ASN:CB	2.39	0.71
1:A:273:ARG:HA	1:A:328:TYR:CD1	2.27	0.70
1:A:620:LEU:O	1:A:624:TYR:HB2	1.92	0.70
1:A:664:ILE:CA	1:A:667:LEU:HD12	2.22	0.70
1:A:1123:LEU:HD13	1:A:1124:GLY:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1475:TYR:HB3	2:B:24:ALA:N	2.07	0.69
1:A:1376:LEU:HD13	1:A:1380:PHE:CA	2.22	0.69
2:B:57:ALA:HB3	2:B:104:LEU:HG	1.73	0.69
1:A:751:ILE:CG2	1:A:755:TRP:CZ2	2.75	0.69
2:B:99:LYS:O	2:B:100:ASN:HB3	1.90	0.69
1:A:657:ARG:O	1:A:660:ARG:HG3	1.92	0.69
1:A:273:ARG:CG	1:A:328:TYR:HE1	2.01	0.69
1:A:321:ALA:CB	1:A:375:GLY:HA2	2.23	0.69
1:A:1125:ALA:O	1:A:1129:ILE:HG12	1.93	0.69
1:A:1522:CYS:CA	1:A:1524:PRO:HD3	2.23	0.69
1:A:1523:ASP:N	1:A:1524:PRO:HD3	2.06	0.69
1:A:174:ILE:HA	1:A:177:PHE:HD2	1.58	0.69
1:A:664:ILE:CG2	1:A:667:LEU:HD13	2.22	0.68
1:A:1315:VAL:CG1	1:A:1375:ALA:HB2	2.21	0.68
1:A:584:SER:HA	1:A:1145:ILE:HD12	1.75	0.68
1:A:1510:LEU:O	1:A:1513:PRO:HD2	1.91	0.68
1:A:247:LEU:CD2	1:A:1437:ILE:CG1	2.64	0.68
1:A:664:ILE:HA	1:A:667:LEU:CD1	2.23	0.68
1:A:1066:TRP:HH2	1:A:1119:VAL:HG11	1.54	0.67
1:A:999:HIS:CE1	1:A:1001:TYR:HD2	2.12	0.67
1:A:1116:LYS:CE	1:A:1120:ARG:HE	2.08	0.67
1:A:1123:LEU:HD13	1:A:1123:LEU:C	2.15	0.67
1:A:1475:TYR:CZ	1:A:1533:VAL:HG21	2.30	0.67
1:A:664:ILE:O	1:A:667:LEU:HB2	1.94	0.67
1:A:666:LYS:O	1:A:669:LYS:HD3	1.95	0.67
1:A:304:TYR:HE2	1:A:325:PRO:HG3	1.58	0.67
1:A:262:LEU:O	1:A:1417:ARG:HD2	1.95	0.67
2:B:57:ALA:CB	2:B:104:LEU:HD12	2.25	0.67
1:A:1319:VAL:HG13	1:A:1320:THR:HG23	1.76	0.67
1:A:272:ILE:HD12	1:A:331:MET:HB2	1.75	0.67
1:A:986:TRP:HH2	1:A:990:ARG:NH1	1.92	0.66
1:A:1133:LEU:O	1:A:1137:LEU:HD13	1.93	0.66
2:B:50:ARG:O	2:B:52:GLU:N	2.29	0.66
1:A:643:LEU:HD22	1:A:656:LEU:CD1	2.17	0.66
1:A:347:PHE:O	1:A:350:THR:HG23	1.96	0.66
1:A:187:LEU:HD23	1:A:187:LEU:C	2.15	0.66
1:A:318:ASN:ND2	1:A:374:ALA:O	2.29	0.66
1:A:247:LEU:C	1:A:247:LEU:HD13	2.16	0.65
1:A:274:TRP:CZ3	1:A:331:MET:HE1	2.31	0.65
1:A:1115:MET:HE2	1:A:1456:LEU:HG	1.79	0.65
1:A:190:SER:C	1:A:193:THR:HG22	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:ILE:CD1	2:B:24:ALA:CB	2.74	0.65
1:A:1486:PHE:HB3	1:A:1497:CYS:SG	2.36	0.65
1:A:1188:ARG:CD	1:A:1190:VAL:HG23	2.13	0.65
1:A:744:ARG:NH1	1:A:752:GLU:OE1	2.29	0.64
1:A:1123:LEU:O	1:A:1126:ILE:CG2	2.37	0.64
1:A:1376:LEU:O	1:A:1377:ARG:C	2.36	0.64
1:A:1376:LEU:HB3	1:A:1380:PHE:CB	2.25	0.64
1:A:1376:LEU:HD13	1:A:1380:PHE:HB3	1.76	0.64
1:A:1157:ARG:HH11	1:A:1192:LEU:CD2	2.11	0.64
1:A:329:THR:HG22	1:A:330:CYS:N	2.12	0.64
1:A:673:THR:CG2	1:A:1135:VAL:HG21	2.27	0.64
1:A:663:ARG:O	1:A:666:LYS:HB3	1.97	0.64
1:A:1523:ASP:CB	1:A:1526:VAL:HB	2.28	0.64
1:A:1383:VAL:HG12	1:A:1386:ASN:HD22	1.63	0.64
1:A:300:GLU:HA	1:A:303:GLN:NE2	2.13	0.63
1:A:583:MET:CE	1:A:661:LEU:CG	2.77	0.63
1:A:274:TRP:CZ3	1:A:331:MET:HE3	2.33	0.63
1:A:337:PRO:O	1:A:338:ASN:HB2	1.96	0.63
1:A:582:PHE:CD2	1:A:605:PHE:HE2	2.17	0.62
1:A:1402:LEU:HD22	1:A:1419:ILE:HD12	1.81	0.62
1:A:1529:PRO:HG2	2:B:105:GLN:HE21	1.58	0.62
1:A:1483:ASP:O	1:A:1484:ASP:OD1	2.18	0.62
2:B:104:LEU:O	2:B:105:GLN:HB2	1.99	0.62
1:A:1145:ILE:O	1:A:1148:VAL:CG2	2.48	0.62
1:A:1522:CYS:HB3	1:A:1524:PRO:CG	2.29	0.62
1:A:1379:TYR:O	1:A:1382:THR:CG2	2.48	0.62
1:A:187:LEU:O	1:A:190:SER:N	2.33	0.61
1:A:256:THR:HG23	1:A:354:LEU:HD23	1.80	0.61
1:A:342:THR:HG22	1:A:342:THR:O	2.00	0.61
1:A:1194:VAL:HG13	1:A:1515:LEU:CD2	2.30	0.61
1:A:625:TYR:CD1	1:A:631:ASN:HB3	2.36	0.61
1:A:1168:PRO:O	1:A:1169:VAL:HG12	2.01	0.61
2:B:132:PHE:O	2:B:133:ASN:HB2	2.01	0.61
1:A:1364:ILE:HG23	1:A:1365:PHE:CD1	2.36	0.61
2:B:103:ASP:O	2:B:104:LEU:HB2	2.00	0.61
1:A:1169:VAL:HG21	1:A:1226:ARG:HH11	1.65	0.60
1:A:1519:PRO:HA	1:A:1520:PRO:C	2.22	0.60
1:A:190:SER:O	1:A:193:THR:CG2	2.44	0.60
2:B:62:TRP:CH2	2:B:73:HIS:CD2	2.89	0.60
1:A:357:LEU:CD2	1:A:366:LEU:HD23	2.30	0.60
1:A:625:TYR:CE1	1:A:631:ASN:CB	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1501:ILE:CD1	1:A:1510:LEU:HD12	2.32	0.60
2:B:46:SER:HB2	2:B:126:PHE:CD2	2.36	0.60
2:B:155:ARG:HH11	2:B:155:ARG:CG	2.15	0.60
1:A:274:TRP:HZ3	1:A:331:MET:CE	2.14	0.59
1:A:1352:ASP:O	1:A:1356:GLN:HG2	2.01	0.59
1:A:1376:LEU:CB	1:A:1380:PHE:CB	2.69	0.59
1:A:1518:GLY:C	1:A:1522:CYS:HB2	2.23	0.59
1:A:1534:ARG:H	1:A:1534:ARG:CD	2.15	0.59
1:A:183:PRO:O	1:A:186:TRP:HB3	2.02	0.59
1:A:585:ILE:HG13	1:A:585:ILE:O	2.02	0.59
1:A:1383:VAL:HG12	1:A:1386:ASN:ND2	2.15	0.59
1:A:1511:LEU:HD11	1:A:1544:ILE:HD13	1.83	0.59
1:A:272:ILE:HD13	1:A:297:ILE:HB	1.85	0.59
1:A:999:HIS:CE1	1:A:1001:TYR:CD2	2.90	0.59
1:A:1376:LEU:HD12	1:A:1380:PHE:HB3	1.60	0.59
1:A:266:ASN:O	1:A:269:HIS:HD2	1.84	0.59
1:A:583:MET:CE	1:A:661:LEU:CD1	2.80	0.59
1:A:1312:GLN:HE21	1:A:1375:ALA:HA	1.65	0.59
1:A:602:ASN:HB3	1:A:660:ARG:NH1	2.18	0.59
1:A:256:THR:CG2	1:A:354:LEU:HD23	2.33	0.58
1:A:1373:LEU:HD12	1:A:1380:PHE:CE1	2.38	0.58
1:A:1511:LEU:CG	1:A:1515:LEU:HD13	2.33	0.58
2:B:42:LEU:HD13	2:B:122:TYR:HE2	1.67	0.58
1:A:661:LEU:O	1:A:664:ILE:CD1	2.51	0.58
1:A:1348:GLN:O	1:A:1352:ASP:N	2.32	0.58
1:A:1376:LEU:HD13	1:A:1380:PHE:HA	1.84	0.58
2:B:40:PHE:HD2	2:B:42:LEU:CD2	2.15	0.58
1:A:1101:ARG:O	1:A:1104:ARG:HG2	2.03	0.58
1:A:1383:VAL:CG1	1:A:1386:ASN:HD22	2.13	0.58
1:A:1385:TRP:HA	1:A:1385:TRP:CE3	2.38	0.58
1:A:1383:VAL:CG1	1:A:1386:ASN:H	2.04	0.58
2:B:132:PHE:HE1	2:B:137:PHE:HB3	1.68	0.58
1:A:1145:ILE:O	1:A:1148:VAL:HG23	2.04	0.58
1:A:245:VAL:HG12	1:A:246:ILE:N	2.18	0.58
1:A:188:ASP:OD2	1:A:219:LYS:NZ	2.36	0.58
1:A:255:PHE:CB	1:A:354:LEU:HD21	2.33	0.58
2:B:178:LEU:O	2:B:182:VAL:HG23	2.03	0.58
2:B:100:ASN:C	2:B:100:ASN:HD22	2.06	0.58
1:A:1169:VAL:HG21	1:A:1226:ARG:HH12	1.68	0.57
1:A:673:THR:HG22	1:A:1135:VAL:HG21	1.84	0.57
1:A:1511:LEU:CD1	1:A:1515:LEU:HD13	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:SER:OG	2:B:31:ASP:N	2.37	0.57
1:A:305:PHE:O	1:A:305:PHE:HD1	1.87	0.57
1:A:316:GLY:HA3	1:A:373:ALA:O	2.04	0.57
2:B:35:VAL:HG21	2:B:153:ALA:CB	2.30	0.57
1:A:632:ILE:O	1:A:636:ILE:HG12	2.05	0.57
1:A:1208:GLN:OE1	1:A:1218:ILE:HD11	2.03	0.57
1:A:1009:MET:HG3	1:A:1044:VAL:HG11	1.85	0.57
1:A:1377:ARG:O	1:A:1380:PHE:CD1	2.57	0.57
1:A:1123:LEU:HD22	1:A:1123:LEU:C	2.24	0.57
1:A:673:THR:HG22	1:A:1135:VAL:CG2	2.35	0.57
1:A:1194:VAL:CG1	1:A:1515:LEU:HD21	2.34	0.57
2:B:62:TRP:CZ2	2:B:73:HIS:HD2	2.23	0.56
2:B:134:TYR:CB	2:B:135:TYR:CE1	2.85	0.56
1:A:347:PHE:O	1:A:350:THR:CG2	2.53	0.56
1:A:1373:LEU:HD12	1:A:1380:PHE:CZ	2.41	0.56
1:A:1385:TRP:HA	1:A:1385:TRP:HE3	1.69	0.56
1:A:1402:LEU:HD23	1:A:1419:ILE:CD1	2.31	0.56
2:B:62:TRP:CZ2	2:B:73:HIS:CD2	2.93	0.56
2:B:125:TYR:CE2	2:B:127:ASP:HB2	2.41	0.56
2:B:50:ARG:HH11	2:B:50:ARG:CG	2.15	0.56
2:B:57:ALA:HB2	2:B:128:ARG:HG2	1.88	0.56
1:A:1550:TYR:O	1:A:1554:SER:N	2.39	0.56
1:A:1129:ILE:HD12	1:A:1259:PHE:CE1	2.38	0.56
1:A:1373:LEU:HA	1:A:1380:PHE:CE1	2.40	0.56
2:B:180:GLU:OE2	2:B:180:GLU:HA	2.03	0.56
1:A:1116:LYS:HG2	1:A:1120:ARG:HD2	1.87	0.56
2:B:48:LYS:O	2:B:50:ARG:N	2.39	0.56
1:A:273:ARG:HH12	2:B:135:TYR:HB2	1.70	0.55
1:A:313:LEU:HD13	1:A:313:LEU:C	2.26	0.55
1:A:256:THR:O	1:A:260:MET:N	2.39	0.55
1:A:367:TYR:HA	1:A:382:PHE:CE2	2.41	0.55
1:A:1194:VAL:CG1	1:A:1515:LEU:CD2	2.84	0.55
1:A:625:TYR:CE1	1:A:631:ASN:CG	2.80	0.55
1:A:751:ILE:HG23	1:A:755:TRP:CH2	2.41	0.55
2:B:43:GLY:HA3	2:B:108:SER:HB3	1.86	0.55
1:A:299:ASN:O	1:A:303:GLN:HG2	2.07	0.55
1:A:325:PRO:HG2	1:A:328:TYR:CD2	2.27	0.55
1:A:346:ASN:O	1:A:350:THR:HG22	2.06	0.55
1:A:1522:CYS:HB3	1:A:1524:PRO:HG3	1.86	0.55
1:A:1377:ARG:HG3	1:A:1378:GLN:H	1.71	0.55
1:A:343:ASN:ND2	1:A:345:ASP:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ARG:NH1	2:B:155:ARG:HG2	2.20	0.54
2:B:35:VAL:O	2:B:38:HIS:HB3	2.06	0.54
1:A:583:MET:HE1	1:A:661:LEU:CD1	2.36	0.54
1:A:664:ILE:CG2	1:A:667:LEU:CD1	2.86	0.54
1:A:583:MET:CE	1:A:661:LEU:CD2	2.85	0.54
1:A:1454:ILE:HG21	1:A:1561:MET:HB2	1.88	0.54
2:B:64:MET:HB2	2:B:71:PHE:HE1	1.73	0.54
1:A:551:PRO:HA	1:A:554:PHE:HB3	1.88	0.53
1:A:1335:ASN:HB2	1:A:1361:PHE:CD1	2.43	0.53
2:B:42:LEU:N	2:B:42:LEU:HD23	2.23	0.53
1:A:1115:MET:CE	1:A:1456:LEU:HG	2.37	0.53
1:A:1170:GLU:OE1	1:A:1170:GLU:HA	2.08	0.53
1:A:1373:LEU:HA	1:A:1380:PHE:CZ	2.43	0.53
1:A:1434:ALA:O	1:A:1435:LYS:HB3	2.08	0.53
1:A:602:ASN:CB	1:A:660:ARG:HH12	2.18	0.53
1:A:273:ARG:HH12	2:B:135:TYR:CB	2.22	0.53
2:B:40:PHE:CD2	2:B:42:LEU:CD2	2.92	0.53
1:A:163:VAL:CG2	1:A:188:ASP:OD1	2.57	0.52
1:A:274:TRP:HZ3	1:A:331:MET:HE1	1.74	0.52
1:A:1457:LEU:O	1:A:1461:ILE:HG13	2.09	0.52
1:A:1534:ARG:NH1	1:A:1534:ARG:HG2	2.23	0.52
1:A:167:VAL:HG11	1:A:176:HIS:ND1	2.25	0.52
1:A:1116:LYS:HE2	1:A:1120:ARG:HE	1.72	0.52
1:A:1136:CYS:SG	1:A:1255:THR:HG23	2.50	0.52
1:A:1116:LYS:HE2	1:A:1120:ARG:NE	2.25	0.52
1:A:1169:VAL:HG11	1:A:1233:ILE:HG13	1.92	0.52
1:A:1534:ARG:CD	1:A:1534:ARG:N	2.73	0.52
1:A:343:ASN:HB2	1:A:345:ASP:OD2	2.10	0.52
1:A:993:CYS:SG	1:A:1054:VAL:CG2	2.98	0.52
1:A:344:TYR:HA	1:A:350:THR:HB	1.91	0.52
2:B:132:PHE:HB3	2:B:134:TYR:CE1	2.45	0.52
1:A:417:GLN:O	1:A:421:ALA:N	2.43	0.51
1:A:1377:ARG:O	1:A:1380:PHE:CE1	2.63	0.51
1:A:1116:LYS:HE3	1:A:1120:ARG:HE	1.73	0.51
2:B:79:ASP:O	2:B:80:MET:HG3	2.10	0.51
2:B:115:THR:HG23	2:B:117:ASN:H	1.74	0.51
1:A:304:TYR:HD1	1:A:305:PHE:H	1.49	0.51
1:A:990:ARG:HG3	1:A:1054:VAL:O	2.10	0.51
1:A:580:THR:HG23	1:A:661:LEU:HD22	1.92	0.51
1:A:632:ILE:HD13	1:A:632:ILE:C	2.30	0.51
1:A:1173:ASN:H	4:D:1:NAG:H82	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:PHE:HE1	1:A:1248:ILE:HD11	1.76	0.51
1:A:1383:VAL:O	1:A:1387:VAL:HG23	2.10	0.51
1:A:1273:LYS:N	1:A:1273:LYS:CD	2.73	0.51
1:A:1534:ARG:HG2	1:A:1534:ARG:HH11	1.75	0.51
1:A:1120:ARG:CG	1:A:1120:ARG:HH11	2.22	0.51
1:A:1247:PHE:O	1:A:1251:GLY:N	2.38	0.51
1:A:353:CYS:O	1:A:356:ARG:HB3	2.11	0.51
2:B:104:LEU:O	2:B:105:GLN:CB	2.60	0.50
1:A:150:ILE:O	1:A:154:THR:N	2.44	0.50
1:A:625:TYR:O	1:A:631:ASN:HB2	2.11	0.50
1:A:664:ILE:O	1:A:667:LEU:HD12	2.11	0.50
2:B:50:ARG:CG	2:B:50:ARG:NH1	2.73	0.50
1:A:329:THR:CG2	1:A:330:CYS:N	2.74	0.50
1:A:128:ILE:HA	1:A:131:THR:HG22	1.93	0.50
1:A:1250:PHE:HA	1:A:1254:PHE:HD2	1.75	0.50
1:A:1359:VAL:O	1:A:1363:ILE:HG12	2.11	0.50
2:B:134:TYR:C	2:B:135:TYR:CG	2.85	0.50
1:A:1013:SER:HB3	1:A:1041:PHE:CD1	2.47	0.50
1:A:1483:ASP:N	1:A:1483:ASP:OD1	2.44	0.50
2:B:133:ASN:C	2:B:134:TYR:CG	2.85	0.50
1:A:121:ASN:O	1:A:125:ASN:ND2	2.44	0.50
1:A:347:PHE:CD1	1:A:347:PHE:C	2.85	0.50
1:A:757:CYS:SG	1:A:770:TYR:HE2	2.34	0.50
1:A:1527:GLU:OE1	1:A:1534:ARG:CG	2.55	0.50
1:A:751:ILE:CG2	1:A:755:TRP:CE2	2.95	0.50
1:A:1388:PHE:C	1:A:1388:PHE:CD1	2.85	0.50
1:A:1273:LYS:N	1:A:1273:LYS:HD3	2.26	0.50
1:A:1516:ASN:OD1	1:A:1521:ASP:HB3	2.12	0.50
1:A:1528:ASN:HB3	2:B:24:ALA:O	2.11	0.50
2:B:76:SER:O	2:B:82:GLY:CA	2.28	0.49
2:B:133:ASN:C	2:B:134:TYR:CD1	2.85	0.49
1:A:304:TYR:CD2	1:A:325:PRO:HG3	2.46	0.49
1:A:1332:ILE:O	1:A:1336:MET:N	2.45	0.49
1:A:346:ASN:ND2	1:A:348:ALA:N	2.60	0.49
1:A:367:TYR:CE1	1:A:382:PHE:HD2	2.29	0.49
1:A:985:ILE:HG23	2:B:185:TYR:OH	2.11	0.49
1:A:1027:ARG:HG3	1:A:1030:ILE:HD12	1.94	0.49
1:A:1489:GLU:HG2	2:B:24:ALA:HB2	1.95	0.49
1:A:1534:ARG:H	1:A:1534:ARG:HD2	1.77	0.49
1:A:149:LYS:HG2	1:A:152:GLU:OE1	2.12	0.49
2:B:124:CYS:SG	2:B:143:LYS:HB2	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:TYR:CD1	1:A:304:TYR:C	2.86	0.49
1:A:255:PHE:HB3	1:A:354:LEU:HD21	1.95	0.49
1:A:1377:ARG:HG3	1:A:1378:GLN:N	2.28	0.49
2:B:57:ALA:HB3	2:B:104:LEU:CG	2.42	0.49
1:A:602:ASN:HB3	1:A:660:ARG:HH22	1.78	0.49
1:A:170:ARG:O	1:A:175:GLY:C	2.51	0.49
1:A:1120:ARG:HH11	1:A:1120:ARG:CB	2.26	0.49
1:A:629:THR:O	1:A:633:PHE:N	2.44	0.48
1:A:1157:ARG:HH11	1:A:1192:LEU:HD23	1.77	0.48
1:A:643:LEU:CD2	1:A:656:LEU:HD12	2.41	0.48
2:B:57:ALA:CB	2:B:104:LEU:CD1	2.90	0.48
1:A:583:MET:HE3	1:A:661:LEU:HD21	1.93	0.48
2:B:61:TRP:CH2	2:B:124:CYS:HB3	2.47	0.48
1:A:314:LEU:O	1:A:372:ARG:CG	2.62	0.48
1:A:1483:ASP:C	1:A:1484:ASP:OD1	2.52	0.48
1:A:177:PHE:CD1	1:A:177:PHE:C	2.85	0.48
1:A:247:LEU:CD2	1:A:1437:ILE:CD1	2.91	0.48
1:A:1039:LYS:O	1:A:1042:THR:OG1	2.25	0.48
1:A:1534:ARG:N	1:A:1534:ARG:HD2	2.28	0.48
1:A:1402:LEU:HD21	1:A:1419:ILE:CD1	2.41	0.48
2:B:43:GLY:HA2	2:B:108:SER:CA	2.43	0.48
2:B:130:LEU:HD23	2:B:130:LEU:C	2.34	0.48
2:B:171:ILE:O	2:B:175:LEU:HG	2.13	0.47
1:A:179:PHE:CE1	1:A:185:ASN:OD1	2.67	0.47
1:A:255:PHE:O	1:A:259:GLY:N	2.45	0.47
1:A:1376:LEU:HB2	1:A:1380:PHE:CD1	2.49	0.47
1:A:267:LEU:HG	1:A:344:TYR:CD2	2.49	0.47
1:A:1373:LEU:CD1	1:A:1380:PHE:HZ	2.27	0.47
1:A:583:MET:HE1	1:A:661:LEU:CD2	2.44	0.47
1:A:1524:PRO:HA	1:A:1535:GLY:CA	2.38	0.47
1:A:163:VAL:HG21	1:A:192:VAL:HG21	1.95	0.47
1:A:346:ASN:ND2	1:A:348:ALA:H	2.12	0.47
1:A:755:TRP:CE3	1:A:755:TRP:CA	2.97	0.47
1:A:582:PHE:CD2	1:A:605:PHE:CE2	2.92	0.47
2:B:155:ARG:CG	2:B:155:ARG:NH1	2.73	0.47
1:A:167:VAL:CG1	1:A:176:HIS:ND1	2.78	0.47
1:A:643:LEU:HD21	1:A:656:LEU:CD1	2.41	0.47
1:A:717:TYR:HB2	1:A:760:VAL:HG23	1.97	0.47
1:A:755:TRP:CE3	1:A:755:TRP:HA	2.49	0.47
1:A:1326:ILE:O	1:A:1329:MET:HB2	2.15	0.47
2:B:107:GLY:H	2:B:126:PHE:HZ	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1356:GLN:N	1:A:1356:GLN:OE1	2.48	0.47
1:A:267:LEU:HD12	1:A:342:THR:O	2.15	0.47
1:A:415:GLU:O	1:A:419:LYS:N	2.47	0.47
1:A:671:TRP:CD1	1:A:671:TRP:C	2.88	0.47
1:A:1298:LYS:O	1:A:1299:LYS:CB	2.63	0.47
1:A:1383:VAL:HG13	1:A:1386:ASN:CB	2.25	0.47
1:A:1520:PRO:O	1:A:1521:ASP:HB2	2.15	0.47
2:B:188:ILE:O	2:B:192:GLY:N	2.47	0.47
1:A:609:PHE:CD1	1:A:663:ARG:CZ	2.98	0.46
2:B:50:ARG:HG2	2:B:50:ARG:NH1	2.24	0.46
1:A:663:ARG:O	1:A:666:LYS:CB	2.63	0.46
2:B:155:ARG:HH11	2:B:155:ARG:HG2	1.79	0.46
1:A:1373:LEU:CD1	1:A:1380:PHE:CZ	2.98	0.46
1:A:364:GLU:O	1:A:367:TYR:HB3	2.16	0.46
1:A:255:PHE:HZ	1:A:388:LEU:HD22	1.81	0.46
1:A:372:ARG:HH21	1:A:1485:ILE:HD13	1.79	0.46
1:A:664:ILE:CD1	1:A:1142:ILE:CD1	2.81	0.46
1:A:1021:ASP:OD1	1:A:1022:ILE:N	2.49	0.46
2:B:160:ILE:O	2:B:163:GLU:HB3	2.15	0.46
1:A:273:ARG:HH21	1:A:273:ARG:HG3	1.81	0.46
1:A:1022:ILE:HG23	1:A:1531:THR:HG21	1.97	0.46
1:A:1212:PHE:CE1	1:A:1248:ILE:HD11	2.51	0.46
1:A:1160:ASN:HA	1:A:1187:VAL:HG23	1.98	0.46
2:B:174:GLN:HA	2:B:174:GLN:NE2	2.31	0.46
1:A:273:ARG:HG3	1:A:273:ARG:NH2	2.32	0.45
1:A:655:VAL:HG12	1:A:655:VAL:O	2.16	0.45
1:A:754:MET:HA	1:A:757:CYS:HB3	1.97	0.45
1:A:719:CYS:O	1:A:720:LYS:C	2.54	0.45
1:A:1209:VAL:HG12	1:A:1215:TRP:HB2	1.98	0.45
3:C:5:BMA:O6	3:C:5:BMA:O4	2.28	0.45
1:A:724:ASP:O	1:A:725:CYS:HB2	2.14	0.45
1:A:1098:ARG:HD2	1:A:1101:ARG:NH1	2.32	0.45
1:A:1376:LEU:CB	1:A:1380:PHE:CD1	3.00	0.45
1:A:193:THR:HG23	1:A:194:MET:N	2.31	0.45
1:A:1066:TRP:HZ2	1:A:1119:VAL:HG11	1.78	0.45
1:A:1134:LEU:HD23	1:A:1134:LEU:HA	1.72	0.45
1:A:1171:GLU:O	1:A:1172:VAL:CB	2.51	0.45
1:A:1388:PHE:C	1:A:1388:PHE:HD1	2.19	0.45
1:A:1511:LEU:HD11	1:A:1515:LEU:CD1	2.47	0.45
1:A:1376:LEU:HB3	1:A:1380:PHE:H	1.82	0.45
1:A:1518:GLY:O	1:A:1522:CYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518:GLY:N	1:A:1537:CYS:SG	2.83	0.45
2:B:131:THR:O	2:B:131:THR:OG1	2.29	0.45
1:A:584:SER:O	1:A:586:GLU:N	2.50	0.45
1:A:718:VAL:HG13	1:A:719:CYS:N	2.32	0.45
1:A:1021:ASP:CG	1:A:1022:ILE:H	2.20	0.45
1:A:163:VAL:HG22	1:A:188:ASP:OD1	2.17	0.45
1:A:1387:VAL:O	1:A:1391:ALA:N	2.46	0.45
1:A:1435:LYS:CD	1:A:1435:LYS:C	2.85	0.45
1:A:313:LEU:C	1:A:313:LEU:CD1	2.85	0.45
1:A:647:LEU:HD23	1:A:647:LEU:HA	1.78	0.45
1:A:346:ASN:HD21	1:A:348:ALA:H	1.64	0.45
1:A:584:SER:CB	1:A:1145:ILE:HD11	2.47	0.45
1:A:1200:GLY:HA2	1:A:1203:TYR:HB2	1.99	0.45
2:B:46:SER:OG	2:B:141:ILE:HD13	2.17	0.45
1:A:580:THR:HA	1:A:661:LEU:HD21	1.99	0.44
1:A:664:ILE:HD11	1:A:1142:ILE:HG12	1.99	0.44
1:A:1216:MET:HB3	1:A:1220:TYR:CZ	2.53	0.44
1:A:1475:TYR:CZ	1:A:1533:VAL:CG2	2.98	0.44
2:B:134:TYR:CD1	2:B:134:TYR:N	2.85	0.44
1:A:174:ILE:O	1:A:177:PHE:CD2	2.70	0.44
1:A:367:TYR:HA	1:A:382:PHE:HE2	1.82	0.44
1:A:398:LEU:HD11	1:A:1566:ILE:HG12	1.99	0.44
1:A:664:ILE:HG23	1:A:667:LEU:CD1	2.47	0.44
1:A:1380:PHE:C	1:A:1382:THR:N	2.68	0.44
2:B:102:PHE:O	2:B:102:PHE:CG	2.70	0.44
1:A:770:TYR:HA	1:A:773:VAL:HG12	2.00	0.44
1:A:1167:LEU:HD23	1:A:1167:LEU:HA	1.87	0.44
1:A:1120:ARG:CG	1:A:1120:ARG:NH1	2.79	0.44
1:A:387:PHE:HZ	1:A:1451:LEU:HD21	1.83	0.44
1:A:1321:GLN:HG2	1:A:1323:PHE:H	1.83	0.44
2:B:132:PHE:CE1	2:B:137:PHE:HB3	2.52	0.44
1:A:292:ASP:O	1:A:296:TYR:N	2.50	0.44
2:B:40:PHE:CD2	2:B:42:LEU:HD23	2.52	0.44
2:B:57:ALA:CB	2:B:128:ARG:HG2	2.46	0.44
2:B:95:TRP:HE3	2:B:109:ILE:HG22	1.82	0.44
2:B:102:PHE:O	2:B:102:PHE:CD2	2.70	0.44
2:B:134:TYR:O	2:B:135:TYR:CD2	2.71	0.44
2:B:101:THR:O	2:B:102:PHE:CD1	2.70	0.44
1:A:184:TRP:HA	1:A:184:TRP:CE3	2.52	0.44
1:A:1010:ILE:HD11	1:A:1111:ARG:HH11	1.83	0.44
1:A:1223:VAL:HG13	1:A:1238:VAL:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:SER:OG	2:B:141:ILE:HG21	2.17	0.44
2:B:48:LYS:C	2:B:50:ARG:H	2.21	0.44
2:B:130:LEU:O	2:B:137:PHE:O	2.35	0.44
1:A:247:LEU:HD11	1:A:392:TYR:CE1	2.53	0.43
1:A:336:ASN:HB2	1:A:340:GLY:HA2	1.99	0.43
1:A:1213:LYS:HE2	1:A:1505:ALA:HA	2.00	0.43
1:A:391:PHE:O	1:A:395:ASN:ND2	2.51	0.43
1:A:664:ILE:HG13	1:A:664:ILE:H	1.62	0.43
1:A:986:TRP:CH2	1:A:990:ARG:NH1	2.73	0.43
1:A:1155:PHE:HD1	1:A:1221:ALA:HB1	1.83	0.43
1:A:629:THR:HA	1:A:632:ILE:HG21	1.91	0.43
1:A:1140:TRP:O	1:A:1143:PHE:N	2.51	0.43
1:A:1522:CYS:CB	1:A:1524:PRO:CD	2.80	0.43
1:A:1022:ILE:HG23	1:A:1531:THR:CG2	2.47	0.43
1:A:1373:LEU:HD13	1:A:1380:PHE:HZ	1.84	0.43
2:B:94:ASN:HB3	2:B:110:TYR:HD2	1.84	0.43
1:A:305:PHE:O	1:A:305:PHE:CD1	2.70	0.43
1:A:637:ILE:O	1:A:641:SER:N	2.48	0.43
1:A:1122:LEU:HD23	1:A:1122:LEU:HA	1.81	0.43
1:A:1168:PRO:HB2	1:A:1170:GLU:HG2	2.00	0.43
2:B:85:ASN:HA	2:B:90:LEU:HD13	1.99	0.43
1:A:629:THR:O	1:A:632:ILE:HG23	2.08	0.43
2:B:42:LEU:CD1	2:B:122:TYR:HE2	2.26	0.43
2:B:56:SER:OG	2:B:102:PHE:HE2	2.02	0.43
1:A:273:ARG:NH1	2:B:135:TYR:HB2	2.32	0.43
1:A:704:LEU:HD23	1:A:704:LEU:HA	1.87	0.43
1:A:1046:ILE:HD13	1:A:1046:ILE:HA	1.92	0.43
1:A:664:ILE:O	1:A:667:LEU:N	2.50	0.43
1:A:1109:LEU:HD21	1:A:1460:LEU:HD23	2.01	0.43
1:A:357:LEU:HD23	1:A:363:TRP:HB2	2.01	0.42
2:B:28:VAL:HG13	2:B:28:VAL:O	2.18	0.42
1:A:273:ARG:CA	1:A:328:TYR:HD1	2.25	0.42
1:A:1140:TRP:O	1:A:1143:PHE:HB2	2.19	0.42
1:A:1315:VAL:HA	1:A:1318:ILE:HD12	2.02	0.42
1:A:1364:ILE:HG23	1:A:1365:PHE:N	2.34	0.42
2:B:42:LEU:CD1	2:B:122:TYR:CD2	2.95	0.42
2:B:85:ASN:OD1	2:B:85:ASN:N	2.52	0.42
2:B:129:THR:HG22	2:B:136:GLU:HG3	2.00	0.42
1:A:187:LEU:HD23	1:A:188:ASP:CA	2.48	0.42
1:A:230:ILE:HG21	1:A:694:VAL:HG21	2.02	0.42
1:A:346:ASN:HD21	1:A:348:ALA:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:TYR:O	1:A:631:ASN:CB	2.67	0.42
1:A:671:TRP:HA	1:A:672:PRO:HD3	1.82	0.42
1:A:1331:LEU:HD23	1:A:1331:LEU:HA	1.88	0.42
2:B:43:GLY:HA2	2:B:108:SER:HA	2.00	0.42
1:A:1034:LEU:HD12	1:A:1034:LEU:HA	1.86	0.42
1:A:1167:LEU:HB3	1:A:1168:PRO:HD2	2.01	0.42
1:A:1516:ASN:OD1	1:A:1521:ASP:CB	2.68	0.42
2:B:43:GLY:CA	2:B:108:SER:CB	2.78	0.42
1:A:247:LEU:O	1:A:247:LEU:HD13	2.20	0.42
1:A:665:PHE:O	1:A:668:ALA:HB3	2.20	0.42
1:A:1167:LEU:HD11	1:A:1187:VAL:HG21	2.01	0.42
1:A:1270:GLN:O	1:A:1275:GLY:N	2.53	0.42
1:A:1145:ILE:O	1:A:1148:VAL:HG22	2.20	0.42
1:A:343:ASN:ND2	1:A:343:ASN:O	2.52	0.42
2:B:44:CYS:HB2	2:B:61:TRP:HH2	1.85	0.42
1:A:1028:ARG:NH2	2:B:31:ASP:OD1	2.53	0.41
1:A:1120:ARG:NH1	1:A:1120:ARG:HG2	2.35	0.41
1:A:1123:LEU:C	1:A:1126:ILE:HG22	2.32	0.41
1:A:1498:LEU:HD12	1:A:1498:LEU:HA	1.76	0.41
1:A:1511:LEU:CD1	1:A:1515:LEU:CD1	2.98	0.41
2:B:42:LEU:HD21	2:B:111:ILE:HD12	2.01	0.41
1:A:257:LEU:HB3	1:A:1424:ILE:HD12	2.01	0.41
1:A:300:GLU:CA	1:A:303:GLN:HE21	2.26	0.41
1:A:346:ASN:ND2	1:A:346:ASN:C	2.73	0.41
1:A:730:TRP:HZ3	1:A:740:LEU:HB3	1.85	0.41
1:A:1151:PHE:CE1	1:A:1222:ALA:HB1	2.55	0.41
2:B:48:LYS:C	2:B:50:ARG:N	2.73	0.41
1:A:379:MET:SD	1:A:1496:ILE:HD12	2.56	0.41
1:A:611:ALA:HA	1:A:614:VAL:HG12	2.02	0.41
1:A:621:ASP:OD2	1:A:624:TYR:CE2	2.73	0.41
1:A:1248:ILE:HD13	1:A:1248:ILE:HG21	1.87	0.41
1:A:1126:ILE:CG2	1:A:1127:PRO:HD3	2.50	0.41
2:B:126:PHE:HB2	2:B:141:ILE:HG22	2.02	0.41
1:A:583:MET:HG2	1:A:1145:ILE:CG2	2.51	0.41
1:A:655:VAL:HG21	1:A:1150:LEU:HD11	2.01	0.41
1:A:665:PHE:HD1	1:A:674:LEU:HD21	1.86	0.41
1:A:1123:LEU:C	1:A:1123:LEU:CD1	2.86	0.41
1:A:1474:ALA:O	1:A:1475:TYR:CD1	2.73	0.41
1:A:414:ALA:O	1:A:418:GLU:N	2.44	0.41
1:A:1434:ALA:O	1:A:1436:GLY:N	2.44	0.41
1:A:262:LEU:O	1:A:1417:ARG:CD	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HG2	1:A:328:TYR:CD1	2.48	0.41
1:A:385:VAL:O	1:A:389:GLY:N	2.47	0.41
1:A:557:LYS:O	1:A:561:PHE:N	2.51	0.41
1:A:1335:ASN:OD1	1:A:1426:ARG:NH1	2.53	0.41
1:A:132:ILE:HD11	1:A:219:LYS:HB3	2.02	0.41
1:A:1122:LEU:HD11	1:A:1557:VAL:HG22	2.03	0.41
1:A:1388:PHE:HD1	1:A:1388:PHE:O	2.03	0.41
1:A:314:LEU:HD23	1:A:373:ALA:HB2	2.02	0.40
1:A:398:LEU:HA	1:A:398:LEU:HD23	1.87	0.40
1:A:781:MET:HE3	1:A:781:MET:HB3	1.90	0.40
2:B:100:ASN:C	2:B:100:ASN:ND2	2.73	0.40
2:B:64:MET:HG3	2:B:69:SER:HA	2.03	0.40
1:A:766:CYS:O	1:A:770:TYR:HD2	2.04	0.40
1:A:1066:TRP:CE3	1:A:1066:TRP:HA	2.56	0.40
1:A:1098:ARG:HD2	1:A:1101:ARG:HH12	1.86	0.40
1:A:734:ASP:O	1:A:738:SER:HB2	2.22	0.40
1:A:1216:MET:HB3	1:A:1220:TYR:OH	2.20	0.40
1:A:582:PHE:HD1	1:A:582:PHE:HA	1.72	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	1126/1820 (62%)	1041 (92%)	73 (6%)	12 (1%)	14 51
2	B	170/209 (81%)	149 (88%)	13 (8%)	8 (5%)	2 23
All	All	1296/2029 (64%)	1190 (92%)	86 (7%)	20 (2%)	14 45

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1169	VAL
1	A	1172	VAL
1	A	1299	LYS
1	A	1305	PRO
1	A	1307	PRO
2	B	51	GLY
2	B	100	ASN
2	B	133	ASN
1	A	1022	ILE
2	B	79	ASP
1	A	338	ASN
1	A	621	ASP
1	A	1377	ARG
2	B	49	MET
2	B	104	LEU
2	B	134	TYR
1	A	585	ILE
2	B	52	GLU
1	A	1523	ASP
1	A	1519	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	965/1628 (59%)	889 (92%)	76 (8%)	12 39
2	B	149/181 (82%)	132 (89%)	17 (11%)	5 25
All	All	1114/1809 (62%)	1021 (92%)	93 (8%)	15 38

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	135	ASN
1	A	177	PHE
1	A	182	ASP

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Mol	Chain	Res	Type
1	A	185	ASN
1	A	187	LEU
1	A	194	MET
1	A	247	LEU
1	A	273	ARG
1	A	274	TRP
1	A	304	TYR
1	A	305	PHE
1	A	324	CYS
1	A	343	ASN
1	A	346	ASN
1	A	350	THR
1	A	372	ARG
1	A	579	ASN
1	A	582	PHE
1	A	587	HIS
1	A	623	TYR
1	A	632	ILE
1	A	635	SER
1	A	643	LEU
1	A	647	LEU
1	A	648	SER
1	A	667	LEU
1	A	669	LYS
1	A	673	THR
1	A	690	ASN
1	A	719	CYS
1	A	733	ASN
1	A	738	SER
1	A	755	TRP
1	A	771	MET
1	A	772	MET
1	A	779	LEU
1	A	781	MET
1	A	793	PHE
1	A	987	TRP
1	A	999	HIS
1	A	1027	ARG
1	A	1111	ARG
1	A	1120	ARG
1	A	1123	LEU
1	A	1130	MET

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Mol	Chain	Res	Type
1	A	1133	LEU
1	A	1144	SER
1	A	1148	VAL
1	A	1169	VAL
1	A	1171	GLU
1	A	1172	VAL
1	A	1175	ARG
1	A	1178	CYS
1	A	1203	TYR
1	A	1230	ASP
1	A	1295	LEU
1	A	1335	ASN
1	A	1346	GLN
1	A	1354	LEU
1	A	1356	GLN
1	A	1381	PHE
1	A	1385	TRP
1	A	1388	PHE
1	A	1435	LYS
1	A	1475	TYR
1	A	1497	CYS
1	A	1498	LEU
1	A	1516	ASN
1	A	1525	ASP
1	A	1527	GLU
1	A	1532	ASP
1	A	1533	VAL
1	A	1534	ARG
1	A	1537	CYS
1	A	1539	ASN
2	B	27	GLU
2	B	42	LEU
2	B	50	ARG
2	B	52	GLU
2	B	53	VAL
2	B	72	SER
2	B	73	HIS
2	B	100	ASN
2	B	103	ASP
2	B	130	LEU
2	B	134	TYR
2	B	135	TYR

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Mol	Chain	Res	Type
2	B	155	ARG
2	B	163	GLU
2	B	169	SER
2	B	176	TRP
2	B	186	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	269	HIS
1	A	303	GLN
1	A	343	ASN
1	A	346	ASN
1	A	365	ASN
1	A	395	ASN
1	A	409	ASN
1	A	587	HIS
1	A	628	GLN
1	A	690	ASN
1	A	999	HIS
1	A	1312	GLN
1	A	1346	GLN
1	A	1386	ASN
1	A	1516	ASN
1	A	1528	ASN
2	B	73	HIS
2	B	100	ASN
2	B	105	GLN
2	B	174	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

16 monosaccharides 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	C	1	1,3	14,14,15	0.47	0	17,19,21	0.64	0
3	NAG	C	2	3	14,14,15	0.46	0	17,19,21	1.02	1 (5%)
3	BMA	C	3	3	11,11,12	0.84	0	15,15,17	2.11	3 (20%)
3	BMA	C	4	3	11,11,12	0.79	0	15,15,17	1.42	3 (20%)
3	BMA	C	5	3	11,11,12	0.86	1 (9%)	15,15,17	0.84	0
4	NAG	D	1	1,4	14,14,15	0.46	0	17,19,21	0.59	0
4	NAG	D	2	4	14,14,15	0.21	0	17,19,21	0.54	0
4	BMA	D	3	4	11,11,12	0.58	0	15,15,17	1.29	2 (13%)
4	NAG	E	1	1,4	14,14,15	0.41	0	17,19,21	0.60	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.62	0
4	BMA	E	3	4	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
4	NAG	F	1	4,2	14,14,15	1.26	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	F	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.57	0
4	BMA	F	3	4	11,11,12	0.94	0	15,15,17	0.82	0
5	NAG	G	1	5,2	14,14,15	0.64	1 (7%)	17,19,21	0.69	0
5	NAG	G	2	5	14,14,15	0.53	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	BMA	C	4	3	-	2/2/19/22	0/1/1/1
3	BMA	C	5	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	-4.45	1.36	1.43
4	F	2	NAG	O5-C1	2.31	1.47	1.43
5	G	1	NAG	O5-C1	-2.13	1.40	1.43
3	C	5	BMA	C1-C2	2.11	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	BMA	C1-O5-C5	5.80	120.05	112.19
4	D	3	BMA	C1-O5-C5	3.92	117.50	112.19
4	F	1	NAG	C4-C3-C2	3.75	116.52	111.02
3	C	3	BMA	C3-C4-C5	-3.67	103.69	110.24
3	C	4	BMA	C1-O5-C5	3.54	116.99	112.19
3	C	2	NAG	C1-O5-C5	3.51	116.95	112.19
3	C	3	BMA	O2-C2-C3	-2.95	104.22	110.14
4	E	3	BMA	C1-O5-C5	2.47	115.53	112.19
3	C	4	BMA	O2-C2-C3	-2.37	105.40	110.14
4	F	1	NAG	O3-C3-C2	-2.15	105.02	109.47
4	D	3	BMA	O2-C2-C3	-2.09	105.96	110.14
3	C	4	BMA	C3-C4-C5	-2.06	106.56	110.24
4	E	3	BMA	O2-C2-C3	-2.06	106.01	110.14

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	5	BMA	O5-C5-C6-O6
3	C	4	BMA	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	4	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7

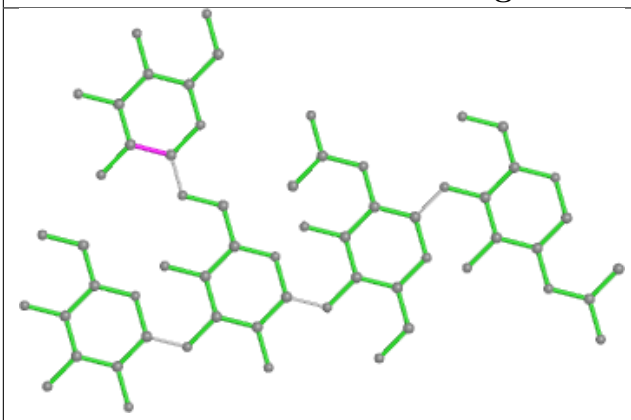
There are no ring outliers.

2 monomers are involved in 2 short contacts:

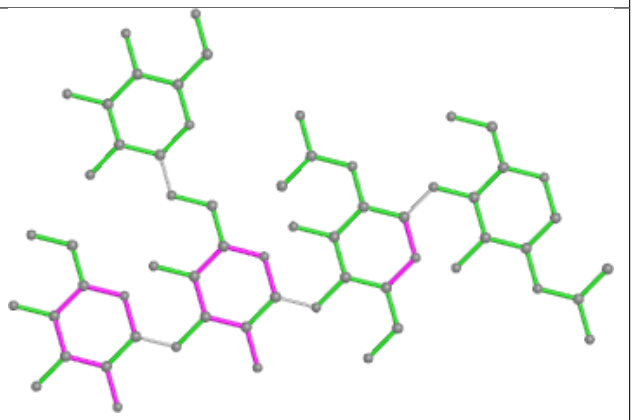
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5	BMA	1	0
4	D	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

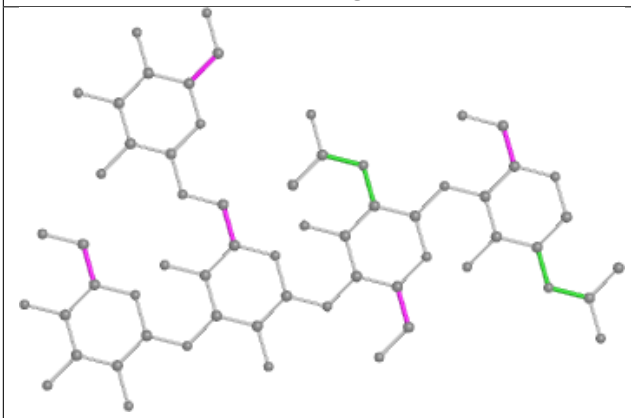
Oligosaccharide Chain C



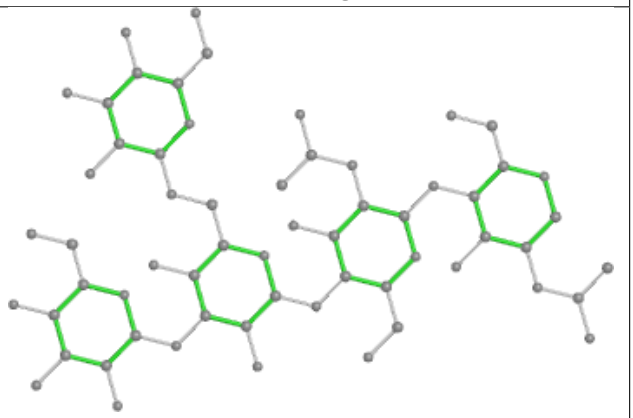
Bond lengths



Bond angles

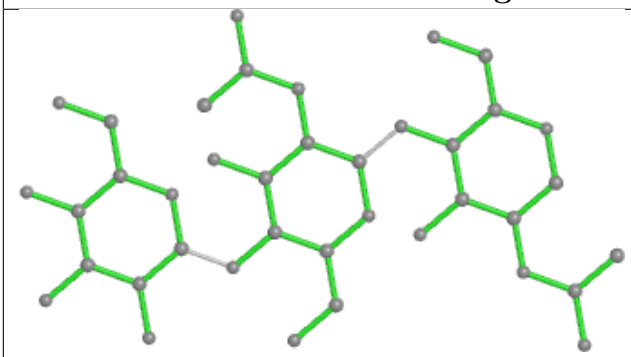


Torsions

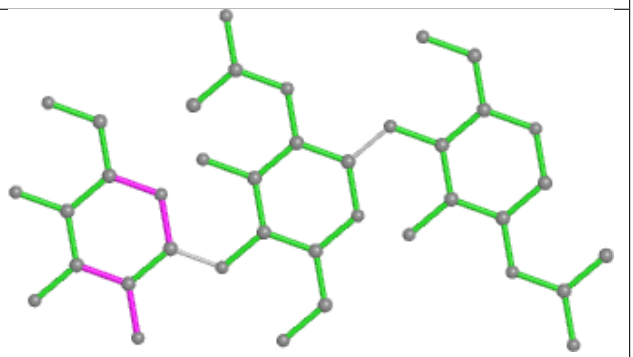


Rings

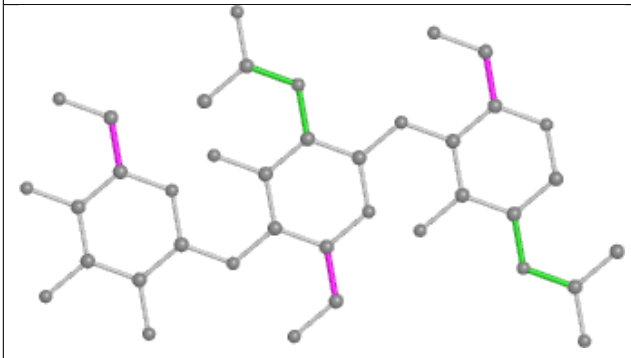
Oligosaccharide Chain D



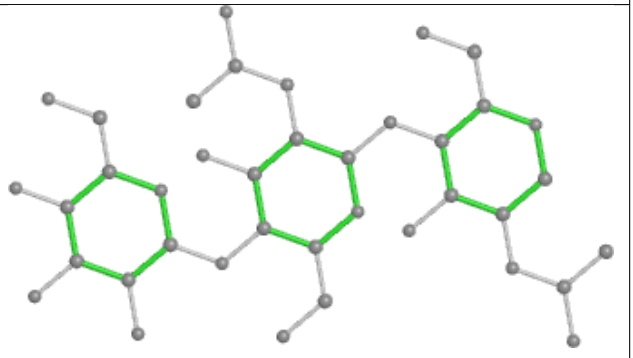
Bond lengths



Bond angles

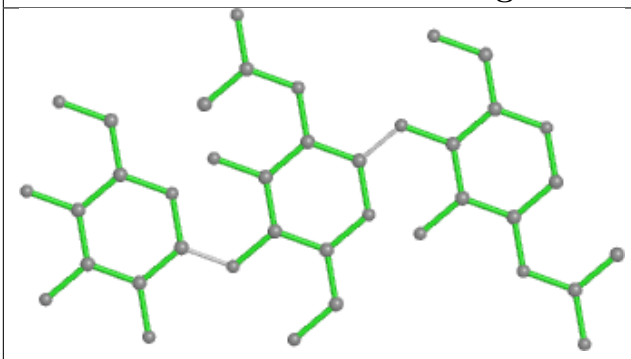


Torsions

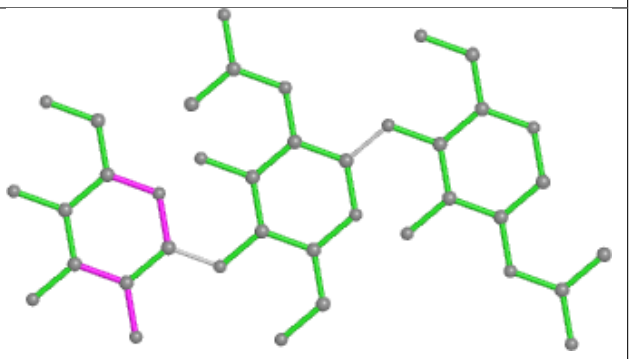


Rings

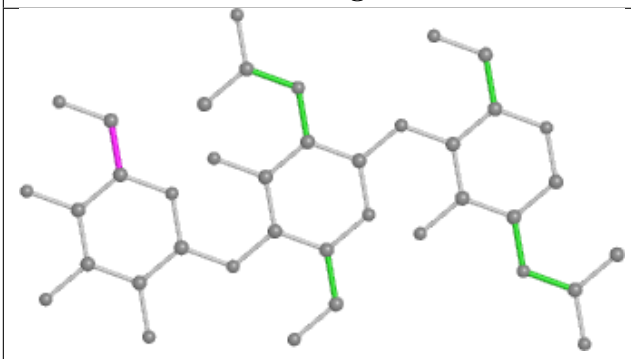
Oligosaccharide Chain E



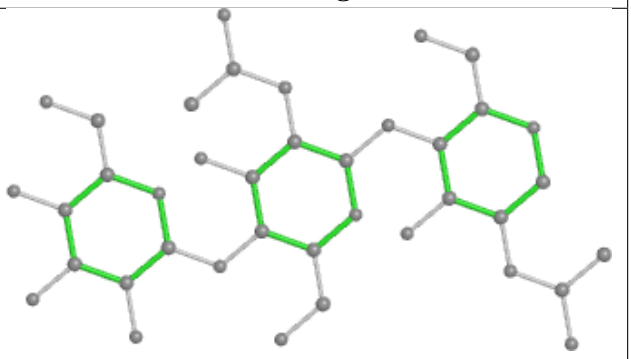
Bond lengths



Bond angles

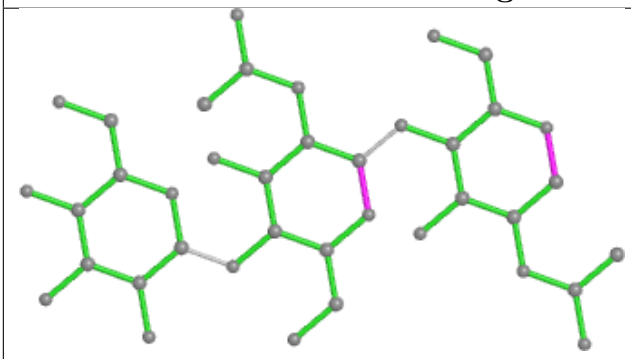


Torsions

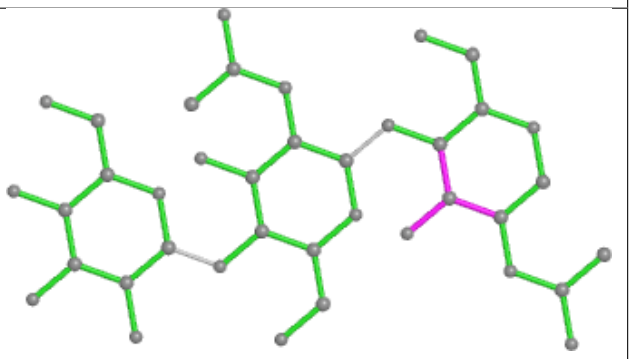


Rings

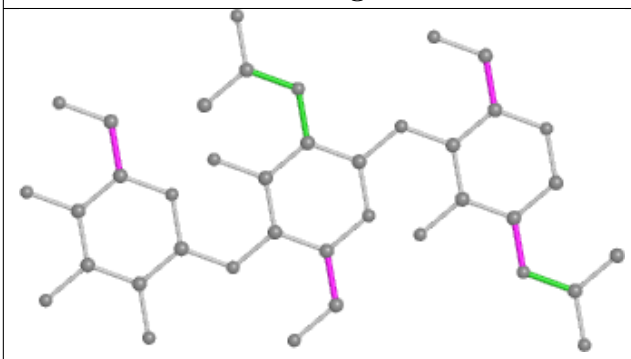
Oligosaccharide Chain F



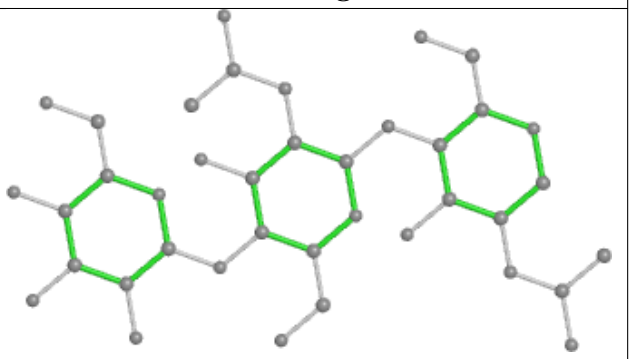
Bond lengths



Bond angles

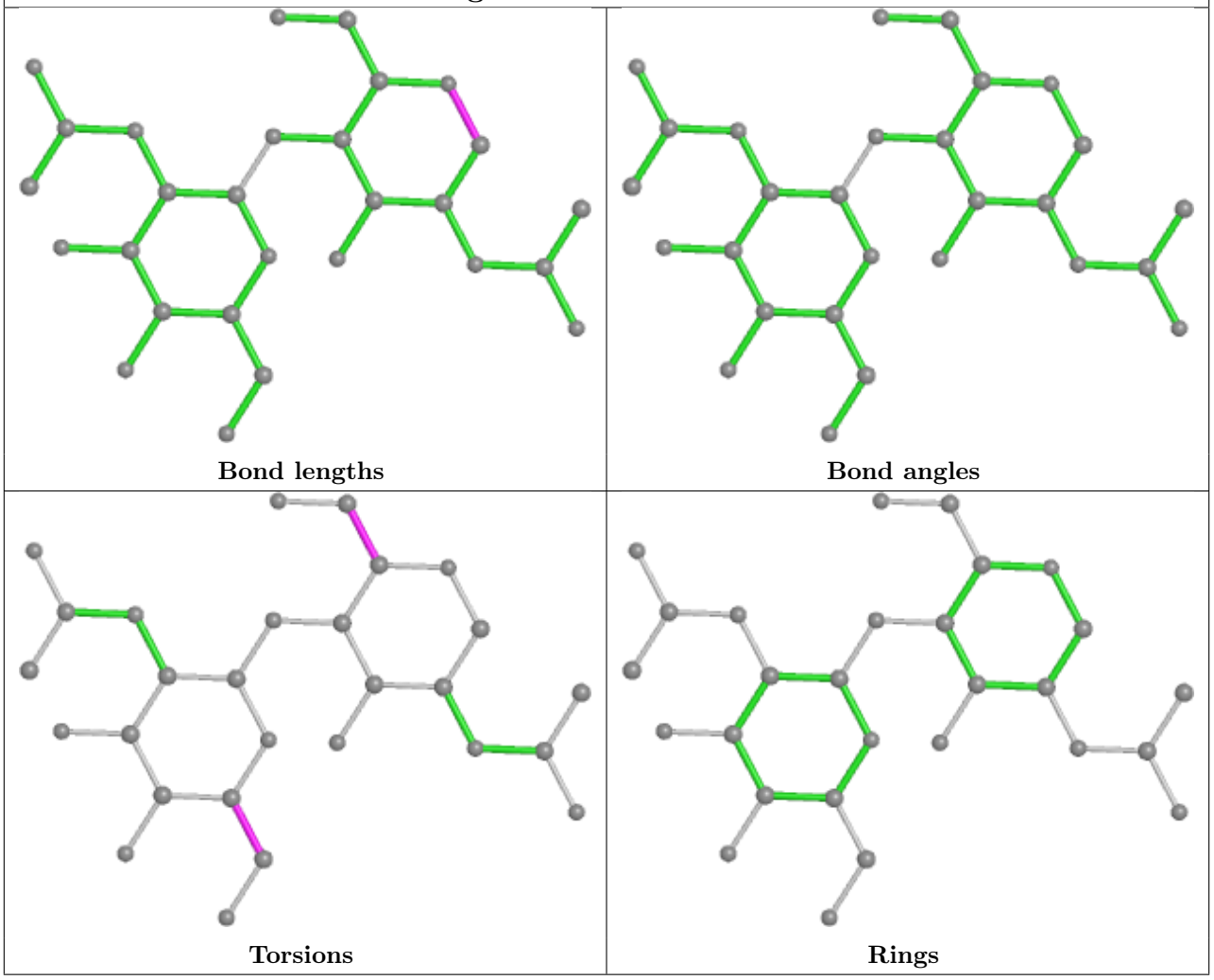


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

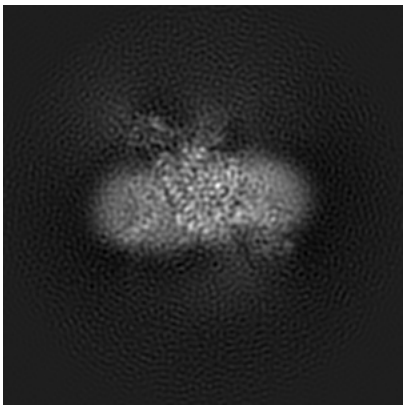
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6770. These allow visual inspection of the internal detail of the map and identification of artifacts.

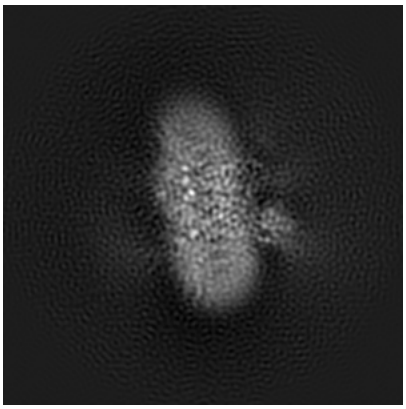
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

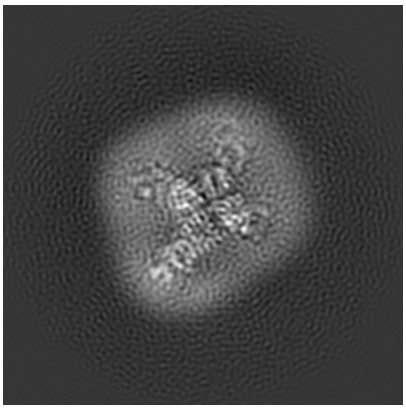
6.1.1 Primary map



X

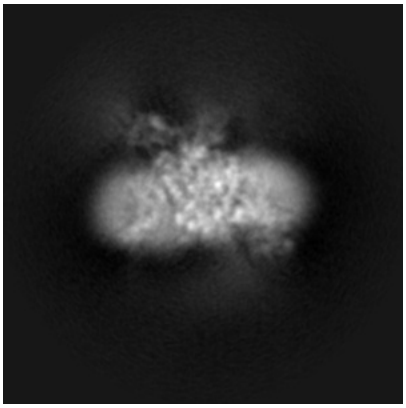


Y

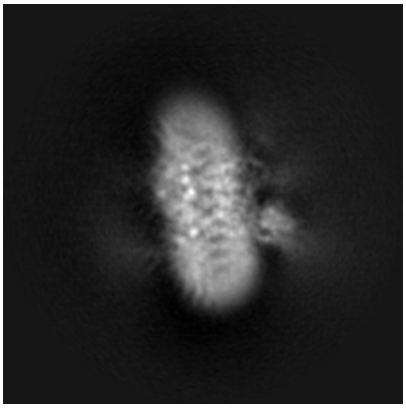


Z

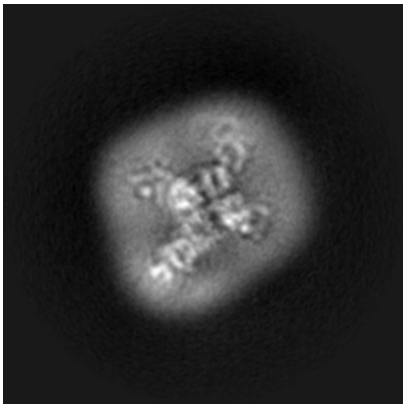
6.1.2 Raw map



X



Y

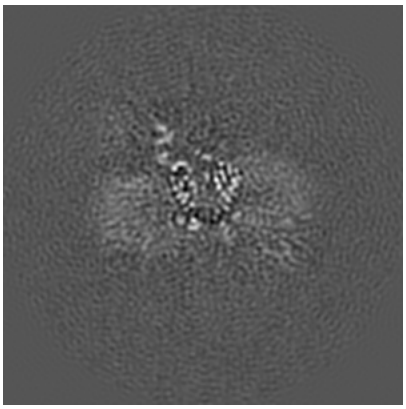


Z

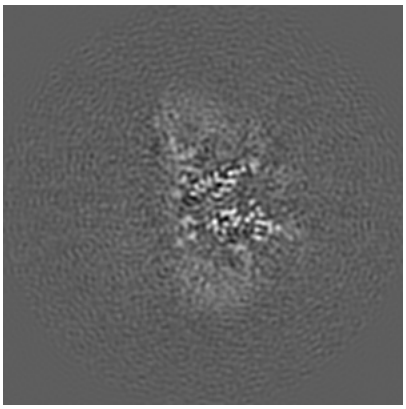
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

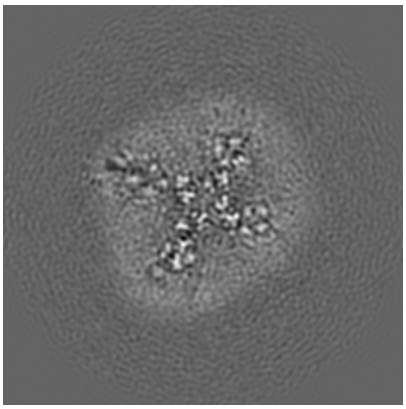
6.2.1 Primary map



X Index: 100

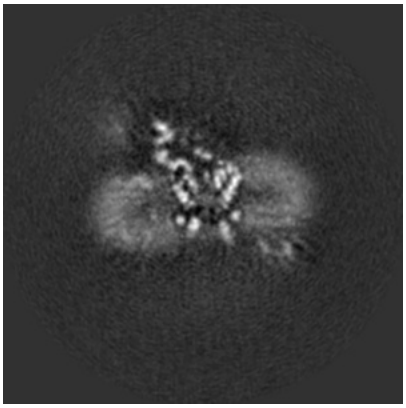


Y Index: 100

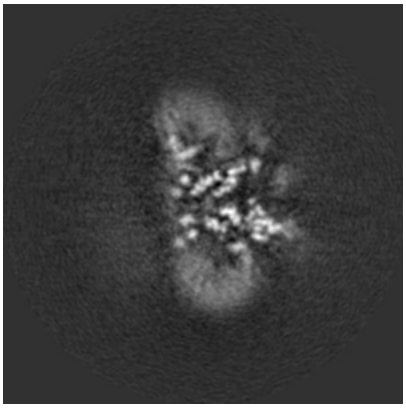


Z Index: 100

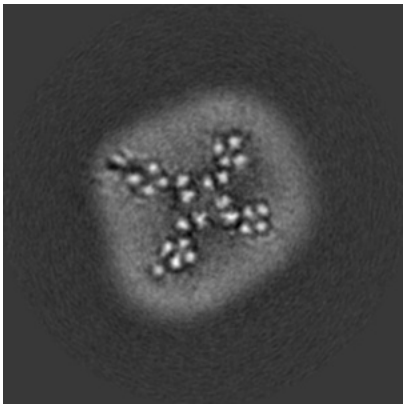
6.2.2 Raw map



X Index: 100



Y Index: 100

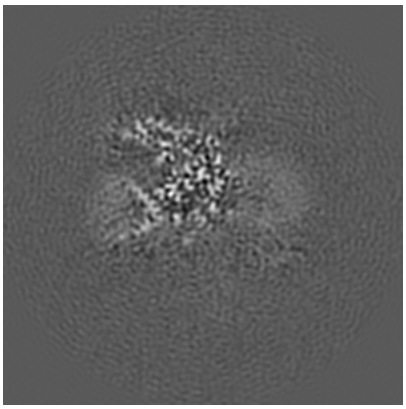


Z Index: 100

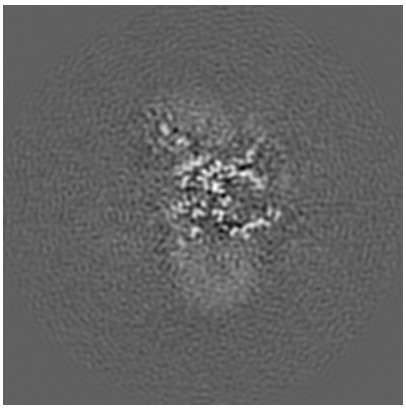
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

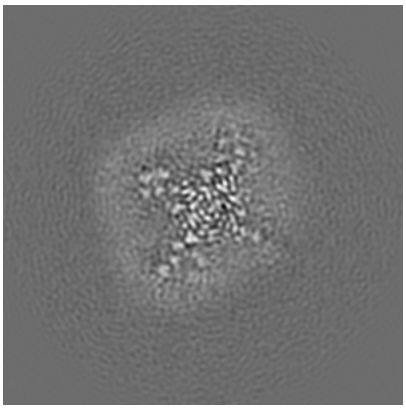
6.3.1 Primary map



X Index: 93

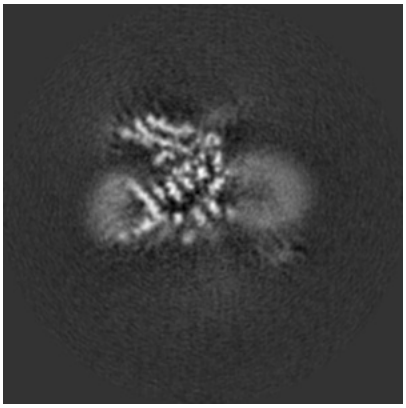


Y Index: 94

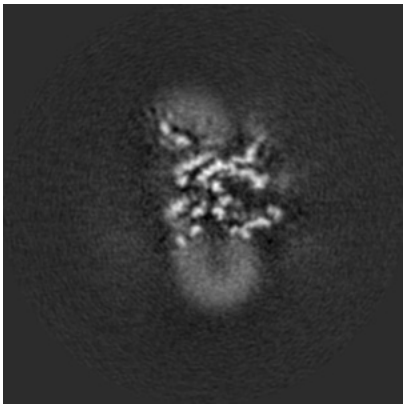


Z Index: 109

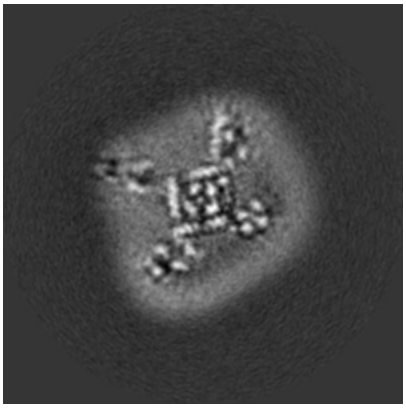
6.3.2 Raw map



X Index: 93



Y Index: 94



Z Index: 94

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

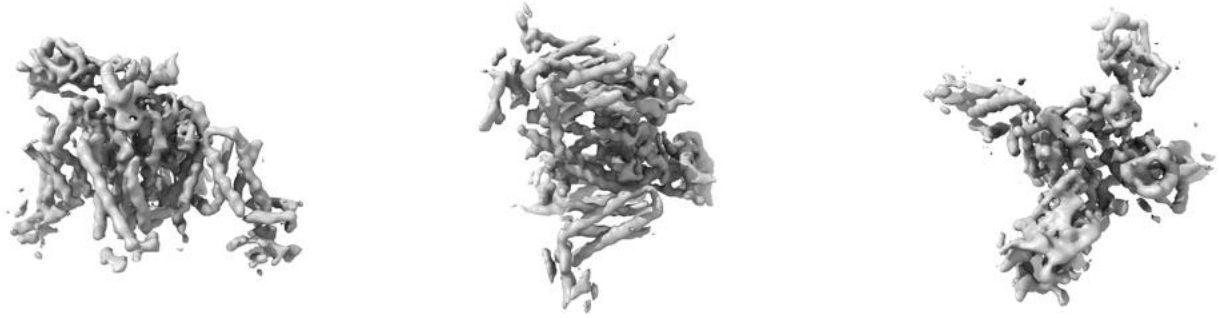
6.4 Orthogonal surface views (i)

6.4.1 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.

6.4.2 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.

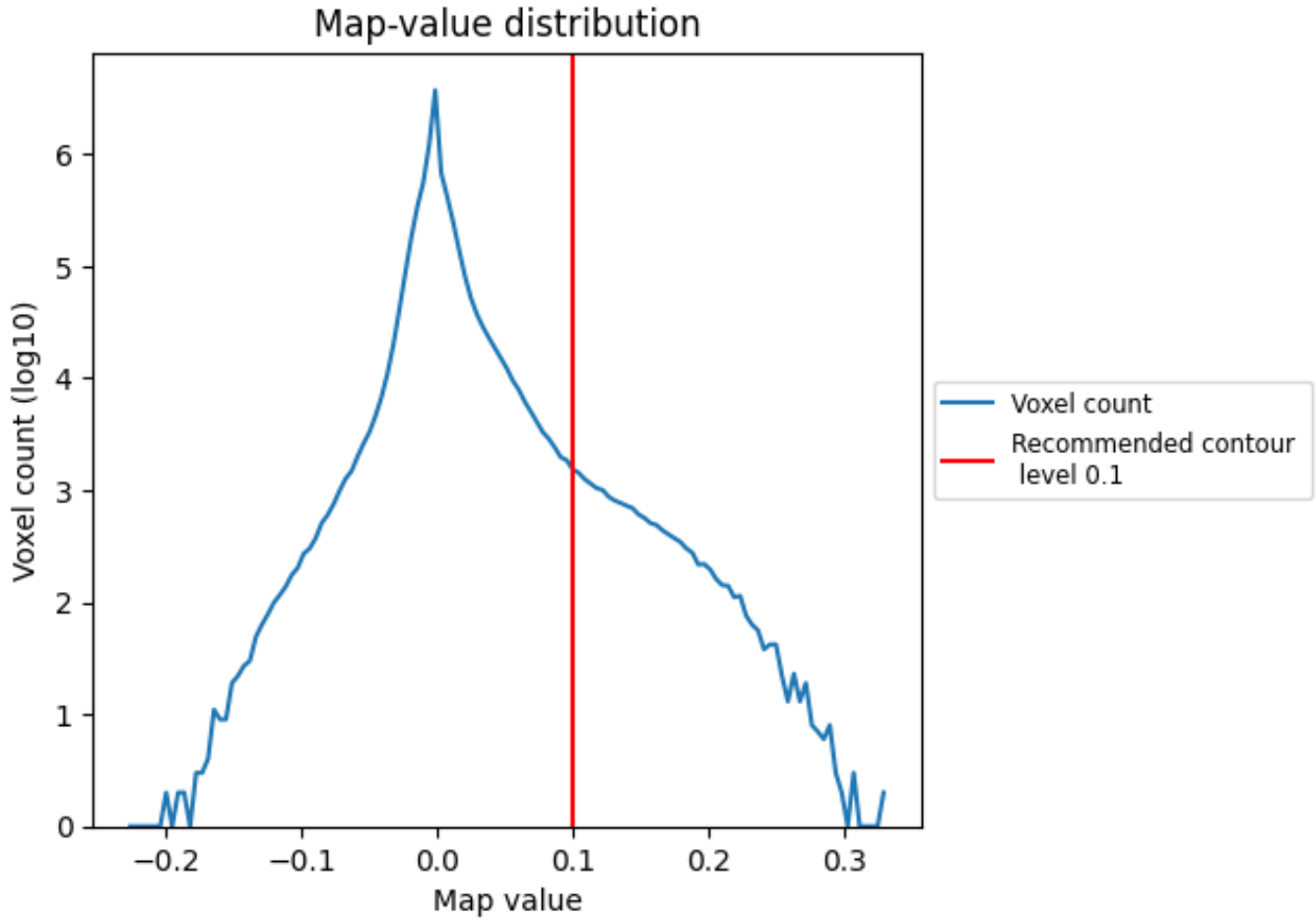
6.5 Mask visualisation (i)

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

7 Map analysis

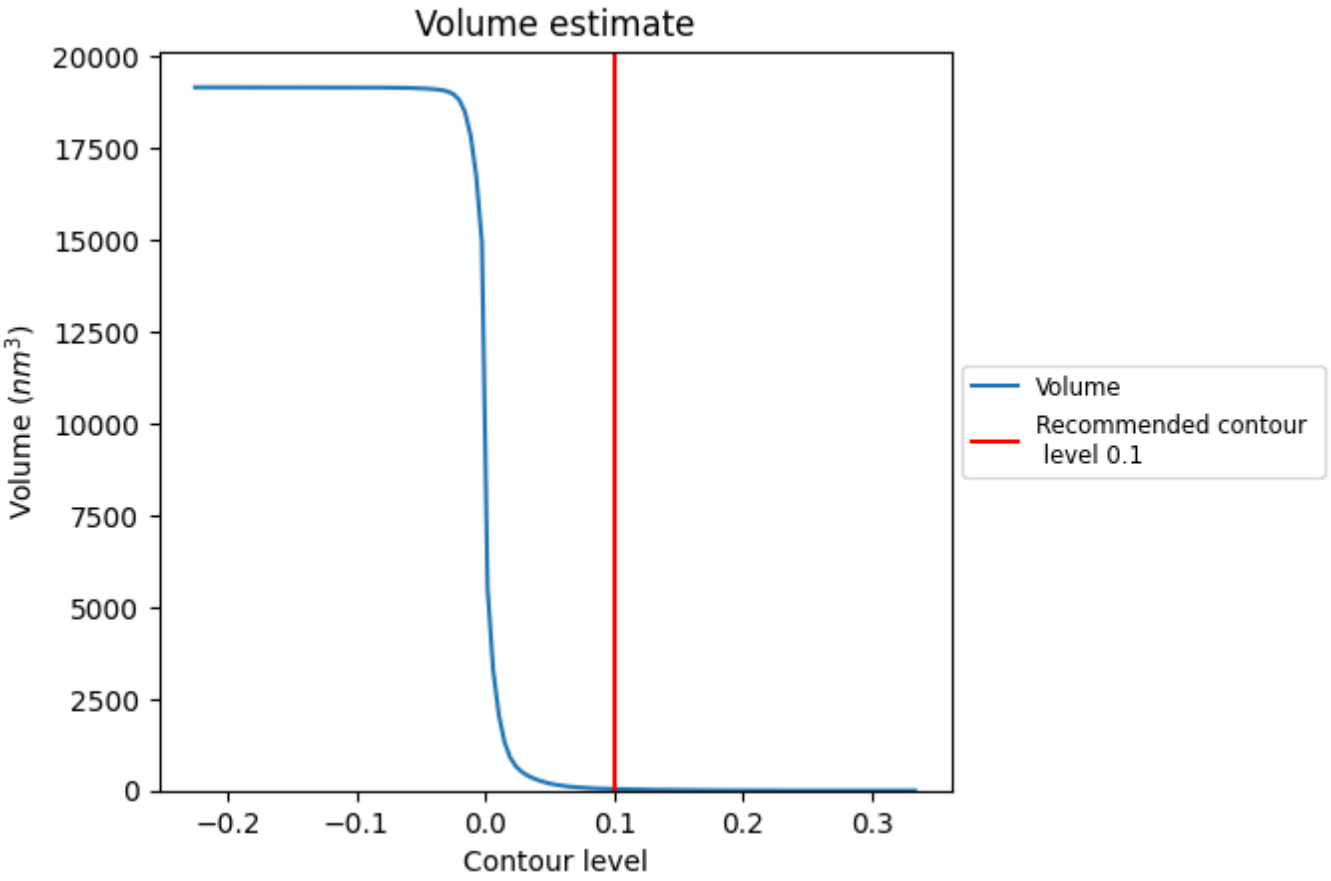
This section contains the results of statistical analysis of the map.

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.

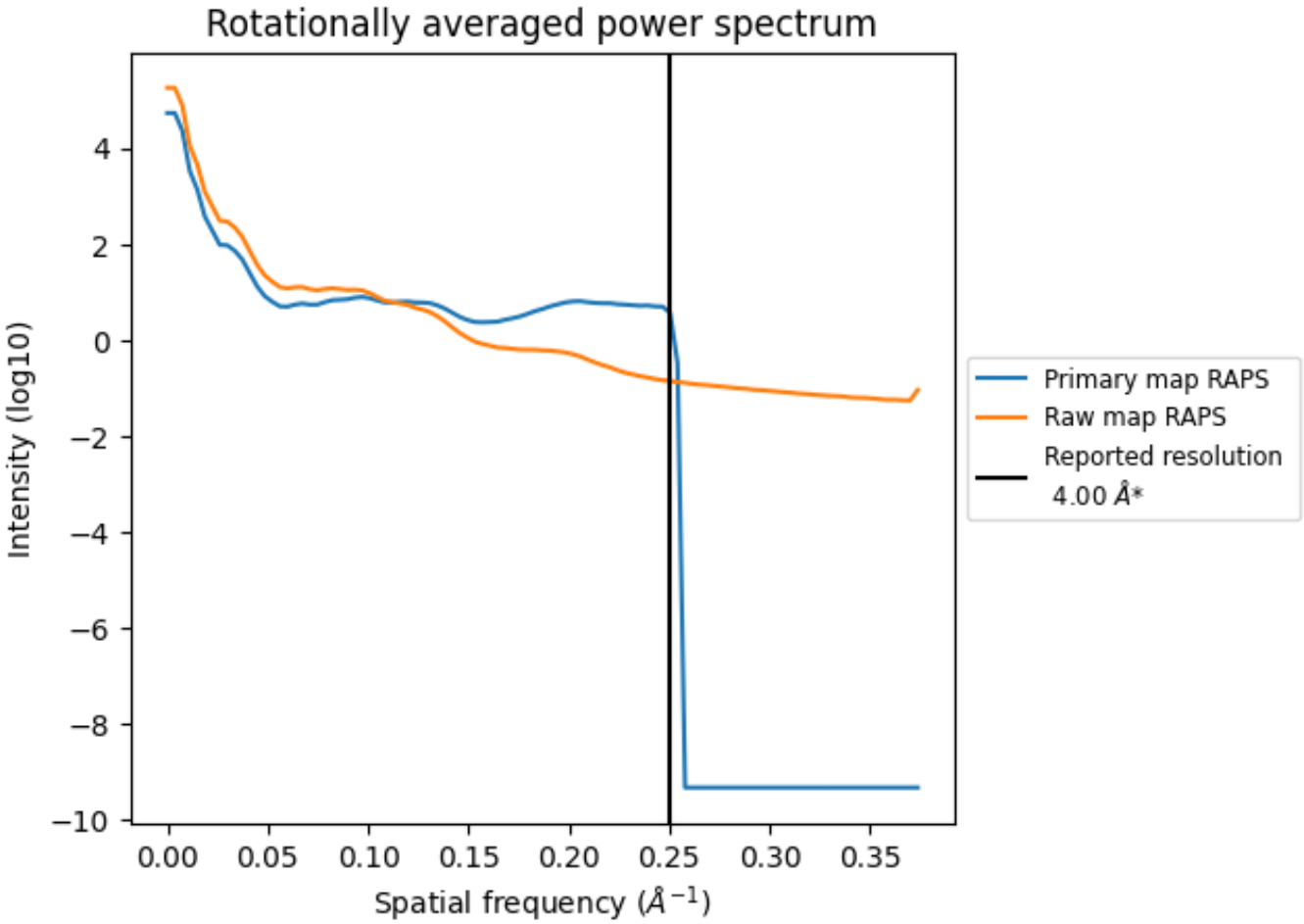
7.2 Volume estimate



The volume at the recommended contour level is 42 nm^3; this corresponds to an approximate mass of 38 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)

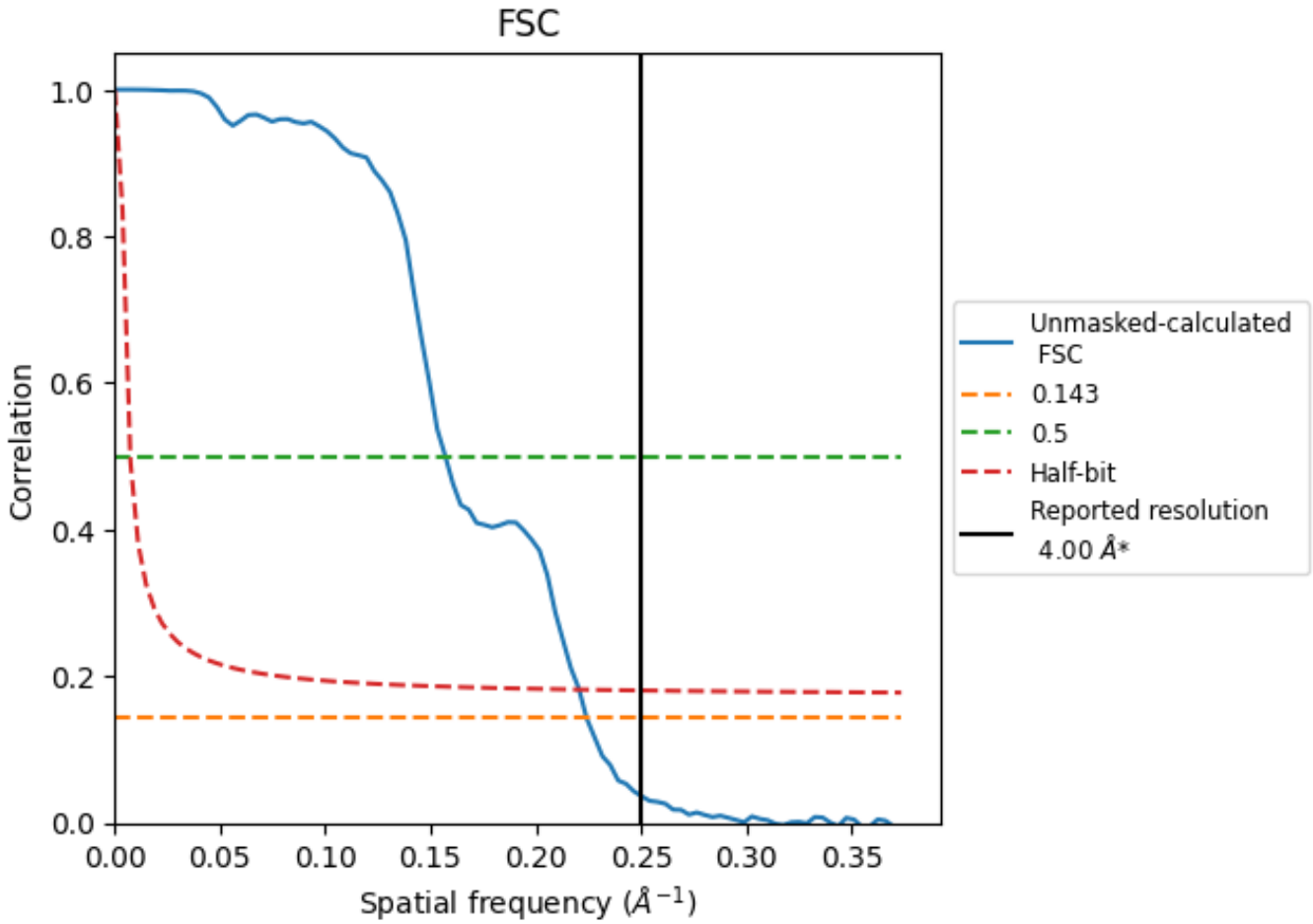


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

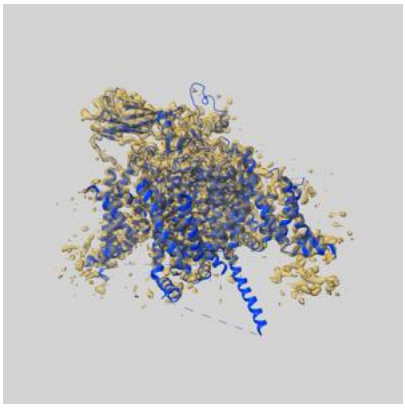
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.46	6.37	4.53

*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 4.46 differs from the reported value 4.0 by more than 10 %

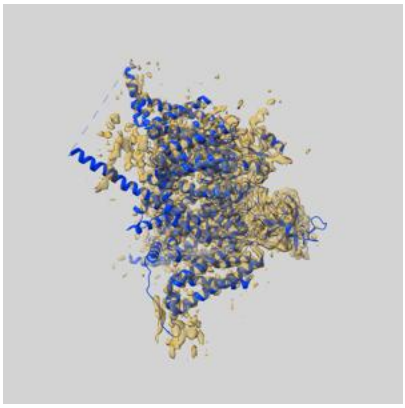
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6770 and PDB model 5XSY. Per-residue inclusion information can be found in section 3 on page 5.

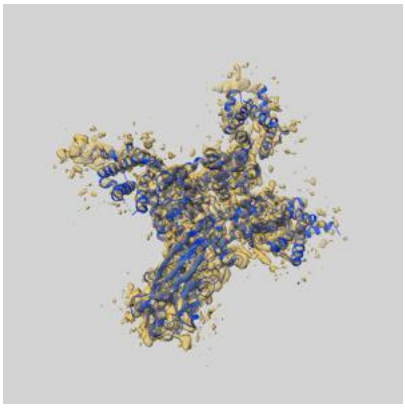
9.1 Map-model overlay



X



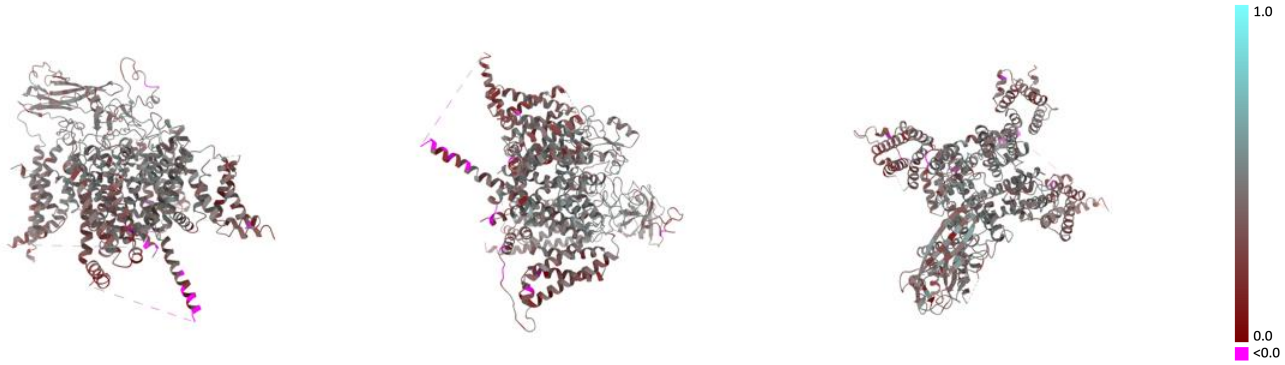
Y



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.

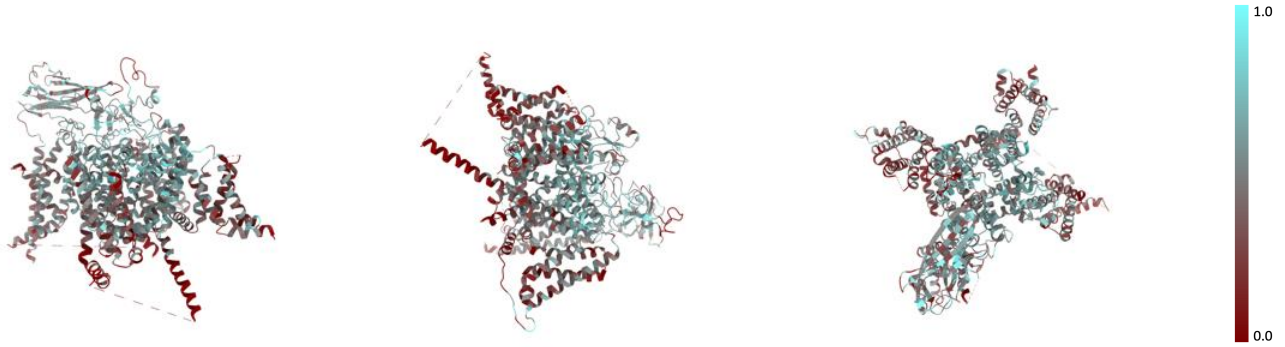
9.2 Q-score mapped to coordinate model (i)



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.

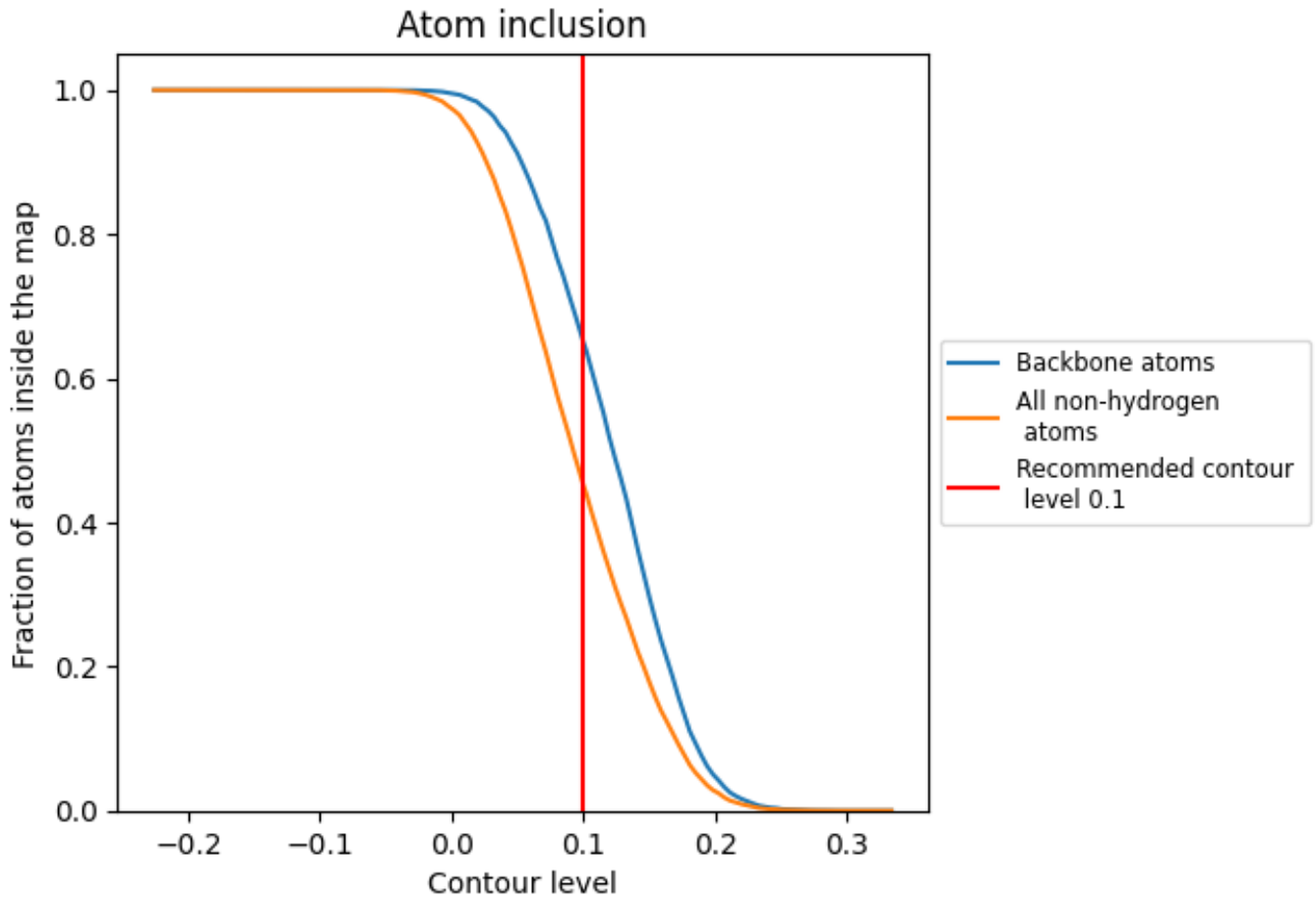
9.3 Atom inclusion mapped to coordinate model (i)



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, 65% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.4514	0.4030
A	0.4511	0.4030
B	0.4735	0.4040
C	0.5410	0.4620
D	0.3590	0.3830
E	0.2308	0.3220
F	0.1538	0.2480
G	0.1429	0.3210