Full wwPDB EM Validation Report

Nov 29, 2022 – 12:50 PM JST

PDB ID	:	7WFW
EMDB ID	:	EMD-32476
Title	:	Apo human Nav1.8
Authors	:	Yan, N.; Pan, X.J.; Huang, X.S.; Huang, G.X.
Deposited on	:	2021-12-27
Resolution	:	3.10 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:

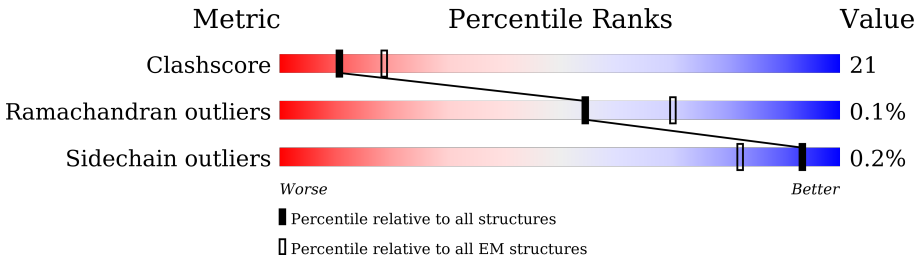
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1956	5%, 32%, 19%, 49%
2	B	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8689 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 type 10 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	998	8064	5360	1282	1364	58	1	0

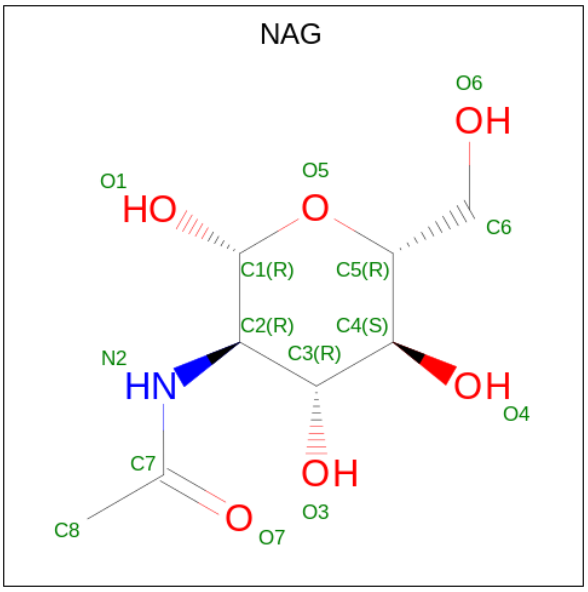
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	894	PHE	SER	conflict	UNP Q9Y5Y9

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

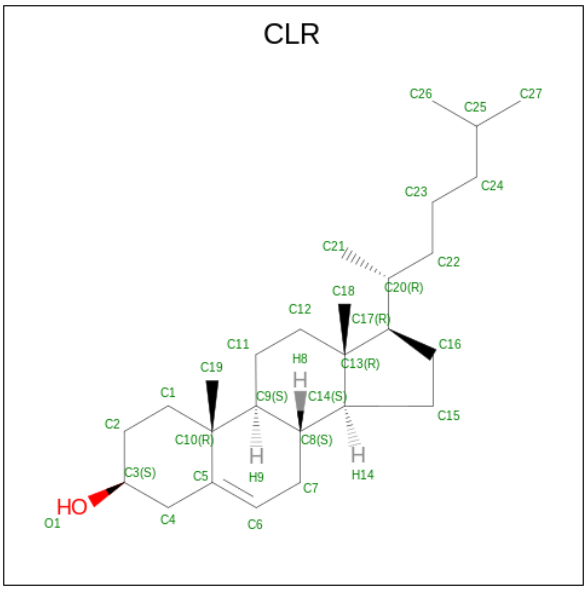
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0

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



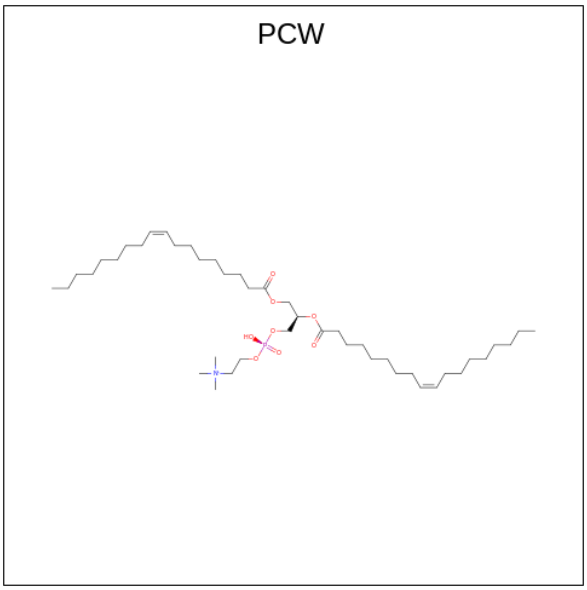
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



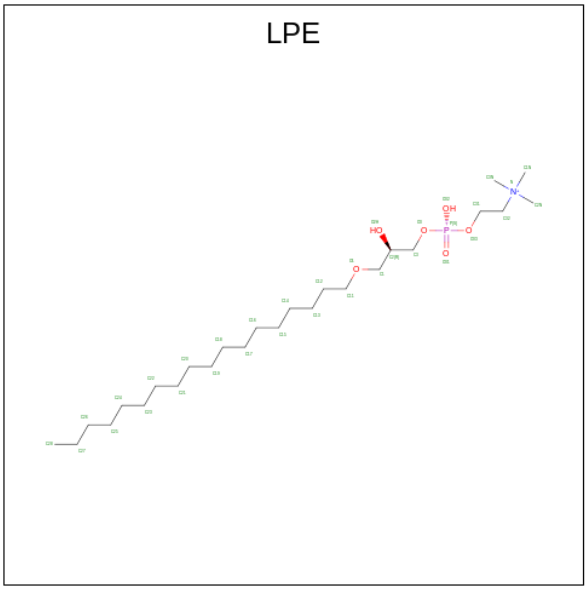
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 112	C 108	O 4	0
4	A	1	Total 112	C 108	O 4	0
4	A	1	Total 112	C 108	O 4	0
4	A	1	Total 112	C 108	O 4	0

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



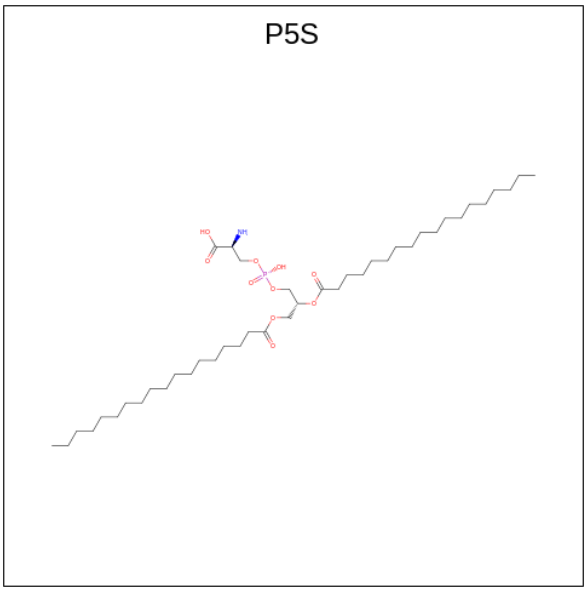
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 136	C 107	N 2	O 24	P 3	0
5	A	1	Total 136	C 107	N 2	O 24	P 3	0
5	A	1	Total 136	C 107	N 2	O 24	P 3	0

- Molecule 6 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O P 200 136 8 48 8	0
6	A	1	Total C N O P 200 136 8 48 8	0
6	A	1	Total C N O P 200 136 8 48 8	0
6	A	1	Total C N O P 200 136 8 48 8	0
6	A	1	Total C N O P 200 136 8 48 8	0
6	A	1	Total C N O P 200 136 8 48 8	0
6	A	1	Total C N O P 200 136 8 48 8	0
6	A	1	Total C N O P 200 136 8 48 8	0

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



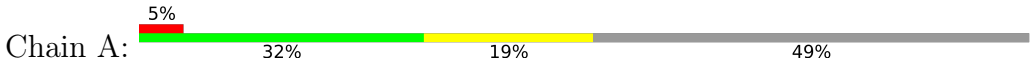
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			93	69	2	20	2	
7	A	1	Total	C	N	O	P	0
			93	69	2	20	2	

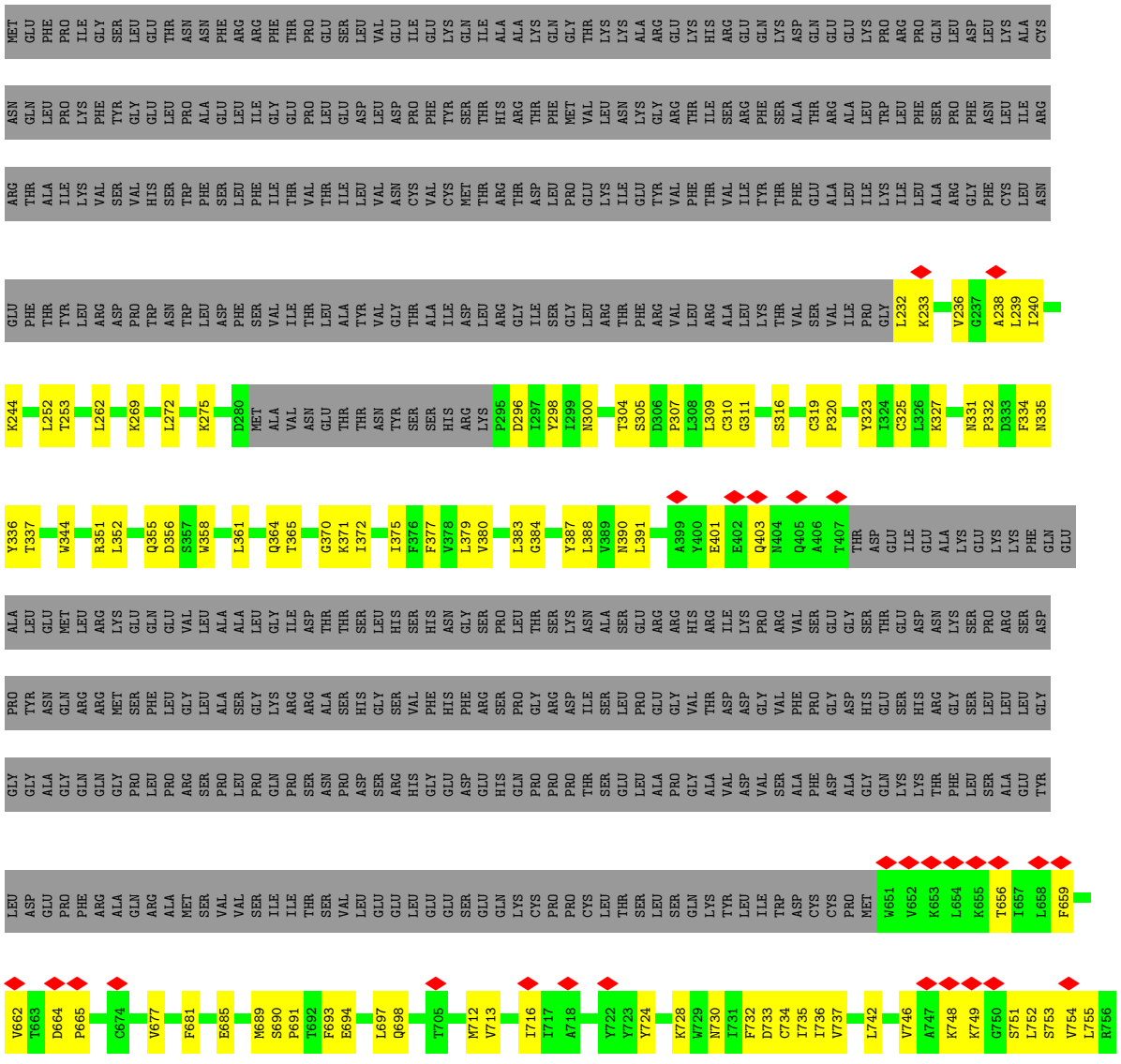
3 Residue-property plots (i)

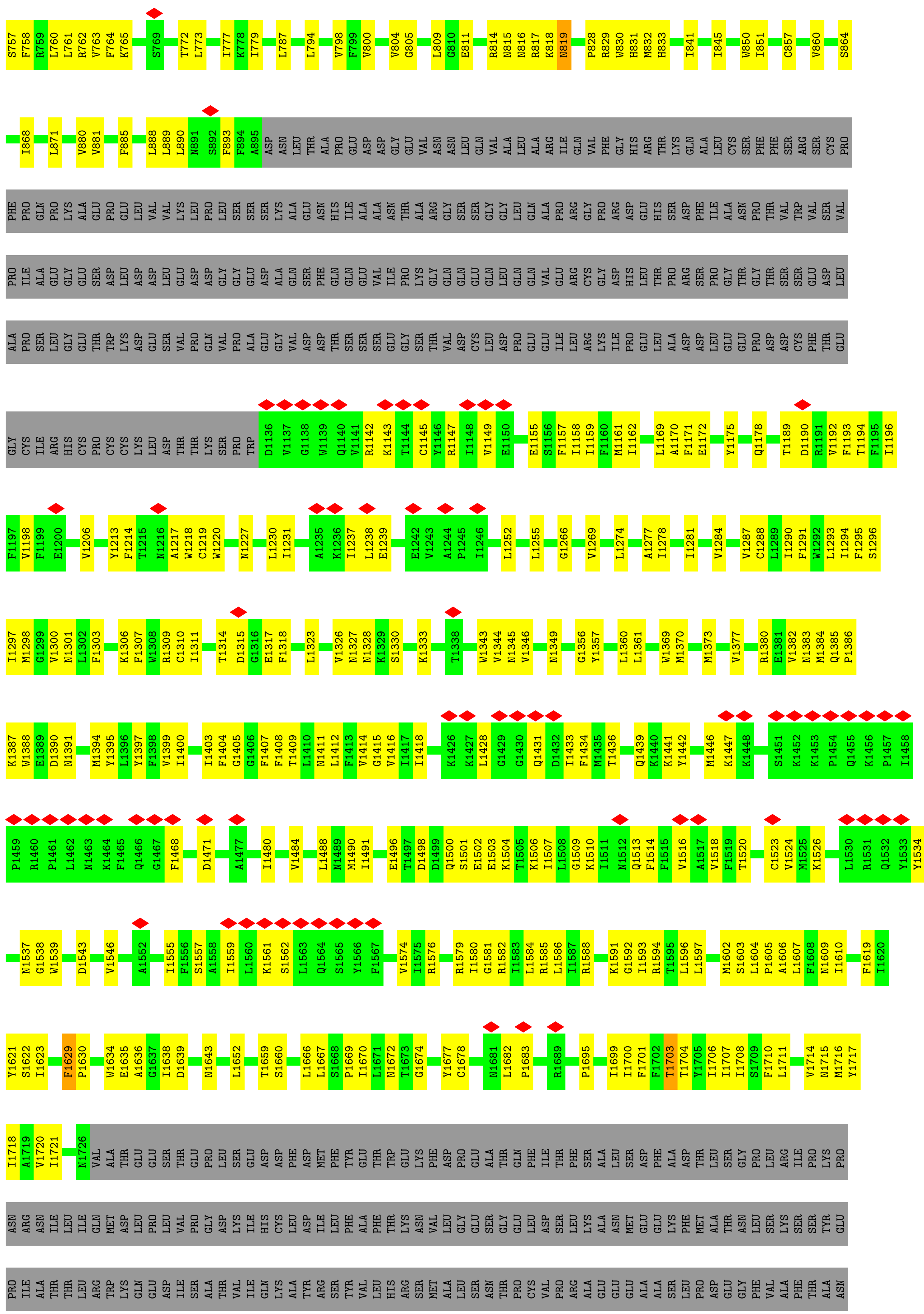
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 type 10 subunit alpha

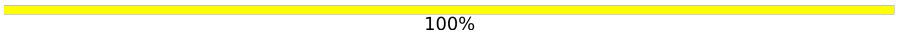
Chain A:






S757 F758 R759 L760 L761 R762 V763 F764 K765 S769 T772 L773 I777 K778 I779 L787 L794 V798 F799 V800 V804 G805 L809 G810 E811 R814 N815 N816 R817 K818 N819 P828 R829 W830 H831 M832 H833 I841 I845 W850 I851 C857 V860 S864
I868 L871 V880 V881 F885 L888 L889 L890 N891 S892 F893 F894 A895 ASP ASN LEU THR ALA PRO GLU ASP ASP GLY GLU VAL ASN ASN LEU GLN VAL ALA LEU ALA ARG ILE GLN VAL PHE GLY HIS ARG THR LYS GLN ALA LEU CYS SER PHE PHE SER ARG SER CYS PRO
PHE PRO GLN PRO LYS ALA GLU PRO GLU LEU VAL VAL LYS LEU PRO LEU SER SER SER LYS ALA GLU ASN HIS ILE ALA ALA ASN THR ALA ARG GLY SER SER GLY GLY LEU GLN ALA PRO ARG GLY PRO ARG ASP GLU HIS SER ASP PHE ILE ALA ASN PRO THR VAL TRP VAL SER VAL
PRO ILE ALA GLU GLY GLU SER ASP LEU ASP ASP LEU GLU ASP ASP GLY GLY GLU ASP ALA GLN SER PHE GLN GLN GLU VAL ILE PRO LYS GLY GLN GLN GLU GLN LEU GLN GLN VAL GLU ARG CYS GLY ASP HIS LEU THR PRO ARG SER PRO GLY THR GLY THR SER SER GLU ASP LEU
ALA PRO SER LEU GLY GLU THR TRP LYS ASP GLU SER VAL PRO GLN VAL PRO ALA GLU GLY VAL ASP ASP THR SER SER SER GLU GLY SER THR VAL ASP CYS LEU ASP PRO GLU GLU ILE LEU ARG LYS ILE PRO GLU LEU ALA ASP ASP LEU GLU GLU PRO ASP ASP CYS PHE THR GLU
GLY CYS ILE ARG HIS CYS PRO CYS CYS LYS LEU ASP THR THR LYS SER PRO TRP D1136 V1137 G1138 W1139 Q1140 V1141 R1142 K1143 T1144 C1145 Y1146 R1147 I1148 V1149 E1150 E1155 S1156 F1157 I1158 I1159 F1160 M1161 I1162 L1169 A1170 F1171 E1172 Y1175 Q1178 T1189 D1190 R1191 V1192 F1193 T1194 F1195 I1196
F1197 V1198 F1199 E1200 V1206 Y1213 F1214 T1215 N1216 A1217 W1218 C1219 W1220 N1227 L1230 I1231 A1235 K1236 I1237 L1238 E1239 E1242 V1243 A1244 P1245 I1246 L1252 L1255 G1266 V1269 L1274 A1277 I1278 I1281 V1284 V1287 C1288 L1289 I1290 F1291 W1292 L1293 I1294 F1295 S1296
I1297 M1298 G1299 V1300 N1301 L1302 F1303 K1306 F1307 W1308 R1309 C1310 I1311 T1314 D1315 G1316 E1317 F1318 L1323 V1326 N1327 N1328 K1329 S1330 K1333 T1338 W1343 V1344 N1345 V1346 N1349 G1356 Y1357 L1360 L1361 W1369 M1370 M1373 V1377 R1380 E1381 V1382 N1383 M1384 Q1385 P1386
K1387 W1388 E1389 D1390 N1391 M1394 Y1395 L1396 Y1397 F1398 V1399 I1400 I1403 F1404 G1405 G1406 F1407 F1408 T1409 L1410 N1411 L1412 F1413 V1414 G1415 V1416 I1417 I1418 K1426 K1427 L1428 G1429 G1430 Q1431 D1432 I1433 F1434 M1435 T1436 Q1439 K1440 K1441 Y1442 M1446 K1447 K1448 S1451 K1452 K1453 P1454 Q1455 K1456 P1457 I1458
P1459 R1460 P1461 L1462 N1463 K1464 F1465 Q1466 G1467 F1468 D1471 A1477 I1480 V1484 L1488 N1489 M1490 I1491 E1496 T1497 D1498 D1499 Q1500 S1501 E1502 E1503 K1504 T1505 K1506 I1507 L1508 G1509 K1510 I1511 N1512 Q1513 F1514 F1515 V1516 A1517 V1518 F1519 T1520 C1523 V1524 M1525 K1526 L1530 R1531 Q1532 Y1533 Y1534
N1537 G1538 W1539 D1543 V1546 A1552 I1555 F1556 S1557 A1558 I1559 L1560 K1561 S1562 L1563 Q1564 S1565 Y1566 F1567 V1574 I1575 R1576 R1579 I1580 G1581 R1582 I1583 L1584 R1585 L1586 I1587 R1588 K1591 G1592 I1593 R1594 T1595 L1596 L1597 M1602 S1603 L1604 P1605 A1606 L1607 F1608 N1609 I1610 F1619 I1620
Y1621 S1622 I1623 F1629 P1630 W1634 E1635 A1636 G1637 I1638 D1639 N1643 L1652 T1659 S1660 L1666 L1667 S1668 P1669 I1670 L1671 N1672 T1673 G1674 Y1677 C1678 N1681 L1682 P1683 R1689 P1695 I1699 I1700 F1701 F1702 T1703 T1704 Y1705 I1706 I1707 I1708 S1709 F1710 L1711 V1714 N1715 M1716 Y1717
I1718 A1719 V1720 I1721 N1726 VAL ALA THR GLU GLU SER THR GLU PRO LEU SER GLU ASP ASP PHE ASP MET PHE TYR GLU THR TRP GLU LYS PHE ASP PRO GLU ALA THR GLN PHE ILE THR PHE SER ALA LEU SER ASP PHE ALA ASP THR LEU SER GLY PRO LEU ARG ILE PRO LYS PRO
ASN ARG ASN ILE LEU ILE GLN MET ASP LEU PRO LEU VAL PRO GLY ASP LYS ILE HIS CYS LEU ASP ILE LEU PHE ALA PHE THR LYS ASN VAL LEU GLY GLU SER GLY GLU LEU ASP SER LEU LYS ALA ASN MET GLU GLU LYS PHE MET ALA THR ASN LEU SER LYS SER SER TYR GLU
PRO ILE ALA THR THR LEU ARG TRP LYS GLN GLU ASP ILE SER ALA THR VAL ILE GLN LYS ALA TYR ARG SER TYR VAL LEU HIS ARG SER MET ALA LEU SER ASN THR PRO CYS VAL PRO ARG ALA GLU GLU GLU ALA ALA SER LEU PRO ASP GLU GLY PHE VAL ALA PHE THR ALA ASN

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

Chain B: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	410478	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.225	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0249	Depositor
Map size (Å)	277.12, 277.12, 277.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	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, P5S, PCW, LPE, CLR

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	0.51	1/8269 (0.0%)	0.61	0/11206

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1630	PRO	C-N	5.85	1.47	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8064	0	8231	332	0
2	B	28	0	25	2	0
3	A	56	0	52	4	0
4	A	112	0	184	23	0
5	A	136	0	187	24	0
6	A	200	0	286	39	0
7	A	93	0	121	14	0
All	All	8689	0	9086	371	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 21.

All (371) 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:809:LEU:HD12	1:A:832:MET:SD	1.67	1.33
1:A:1619:PHE:CE2	6:A:2015:LPE:H131	1.75	1.21
1:A:1619:PHE:CD2	6:A:2015:LPE:H131	1.75	1.19
1:A:761:LEU:HD11	4:A:2012:CLR:H272	1.23	1.16
4:A:2005:CLR:H152	6:A:2018:LPE:H262	1.23	1.12
1:A:1330:SER:HB2	3:A:2003:NAG:H82	1.34	1.09
1:A:761:LEU:HD11	4:A:2012:CLR:C27	1.89	1.01
5:A:2007:PCW:H332	5:A:2007:PCW:H32	1.46	0.96
1:A:1303:PHE:HE2	1:A:1397:TYR:CE2	1.85	0.95
1:A:809:LEU:CD1	1:A:832:MET:SD	2.55	0.94
1:A:1716:MET:HE3	6:A:2008:LPE:C16	1.97	0.94
5:A:2007:PCW:H32	5:A:2007:PCW:C33	1.98	0.92
1:A:1716:MET:CE	6:A:2008:LPE:C16	2.48	0.91
4:A:2005:CLR:C15	6:A:2018:LPE:H262	2.03	0.89
5:A:2011:PCW:H412	4:A:2012:CLR:H211	1.55	0.88
1:A:1311:ILE:HG21	1:A:1318:PHE:HB2	1.56	0.87
1:A:1619:PHE:CE2	6:A:2015:LPE:C13	2.60	0.83
1:A:1405:GLY:O	1:A:1409:THR:HG23	1.79	0.83
1:A:1619:PHE:CD2	6:A:2015:LPE:C13	2.59	0.83
1:A:1330:SER:HB2	3:A:2003:NAG:C8	2.10	0.82
5:A:2007:PCW:H32	5:A:2007:PCW:C32	2.08	0.81
1:A:728:LYS:HG3	5:A:2011:PCW:O4P	1.83	0.79
1:A:1169:LEU:HD23	1:A:1172:GLU:OE1	1.85	0.77
1:A:1284:VAL:HG21	1:A:1416:VAL:HG21	1.65	0.77
1:A:1303:PHE:HE2	1:A:1397:TYR:CD2	2.04	0.76
1:A:1361:LEU:HD12	7:A:2021:P5S:H27	1.67	0.76
1:A:352:LEU:HD21	1:A:361:LEU:HD23	1.68	0.75
1:A:1537:ASN:OD1	1:A:1538:GLY:N	2.19	0.75
1:A:1674:GLY:N	1:A:1678:CYS:SG	2.60	0.75
6:A:2016:LPE:H322	7:A:2021:P5S:C	2.18	0.74
1:A:1303:PHE:CE2	1:A:1397:TYR:CD2	2.75	0.73
1:A:1288:CYS:SG	7:A:2021:P5S:C30	2.76	0.73
1:A:757:SER:HB2	1:A:1301:ASN:HD22	1.53	0.73
6:A:2016:LPE:H322	7:A:2021:P5S:O	1.87	0.73
1:A:1252:LEU:O	1:A:1252:LEU:HD23	1.89	0.72
1:A:1704:THR:O	1:A:1708:ILE:HG13	1.89	0.72
1:A:377:PHE:HA	1:A:380:VAL:HG12	1.73	0.71
1:A:1255:LEU:HD11	6:A:2013:LPE:H222	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:GLY:O	1:A:809:LEU:HB2	1.92	0.70
1:A:1382:VAL:HG12	1:A:1383:ASN:OD1	1.93	0.69
1:A:1303:PHE:CE2	1:A:1397:TYR:CE2	2.75	0.69
1:A:841:ILE:O	1:A:845:ILE:HG13	1.92	0.69
1:A:1502:GLU:N	1:A:1502:GLU:OE1	2.27	0.68
1:A:736:ILE:HD13	1:A:758:PHE:CE1	2.29	0.67
1:A:1695:PRO:O	1:A:1699:ILE:HG13	1.95	0.67
1:A:390:ASN:HD22	1:A:1720:VAL:HG11	1.60	0.67
1:A:1716:MET:HE1	6:A:2008:LPE:C16	2.23	0.67
1:A:1155:GLU:O	1:A:1159:ILE:HG13	1.95	0.67
1:A:1377:VAL:HG11	1:A:1395:TYR:CE1	2.30	0.66
1:A:857:CYS:HA	1:A:860:VAL:HG12	1.78	0.65
1:A:1484:VAL:O	1:A:1488:LEU:HG	1.97	0.65
1:A:757:SER:HB2	1:A:1301:ASN:ND2	2.13	0.64
1:A:1218:TRP:HE1	6:A:2013:LPE:H32	1.63	0.64
1:A:1306:LYS:CD	1:A:1380:ARG:O	2.46	0.64
1:A:1326:VAL:HG23	1:A:1327:ASN:H	1.63	0.64
1:A:1296:SER:O	1:A:1300:VAL:HG23	1.97	0.63
1:A:361:LEU:O	1:A:365:THR:HG23	1.98	0.63
1:A:656:THR:HA	1:A:659:PHE:CE2	2.34	0.63
1:A:1404:PHE:HA	1:A:1408:PHE:HD1	1.63	0.63
1:A:387:TYR:CZ	1:A:391:LEU:HD21	2.34	0.63
1:A:1672:ASN:ND2	1:A:1677:TYR:HB3	2.13	0.63
1:A:1707:ILE:O	1:A:1711:LEU:HG	1.99	0.62
1:A:864:SER:O	1:A:868:ILE:HG13	2.00	0.62
1:A:253:THR:HG23	1:A:388:LEU:HD13	1.82	0.62
1:A:1214:PHE:HB3	1:A:1220:TRP:HE1	1.64	0.62
1:A:1442:TYR:HE1	6:A:2009:LPE:H2N3	1.64	0.62
1:A:758:PHE:HE2	4:A:2012:CLR:H261	1.64	0.61
1:A:779:ILE:HD11	1:A:893:PHE:CE2	2.35	0.61
1:A:1395:TYR:O	1:A:1399:VAL:HG23	2.00	0.61
1:A:1606:ALA:O	1:A:1610:ILE:HD12	2.00	0.61
1:A:748:LYS:HD3	1:A:749:LYS:H	1.66	0.61
1:A:811:GLU:OE1	1:A:811:GLU:HA	2.00	0.60
5:A:2007:PCW:H82	5:A:2007:PCW:O1P	2.01	0.60
1:A:748:LYS:HB3	1:A:751:SER:HB2	1.82	0.60
1:A:1158:ILE:O	1:A:1162:ILE:HG13	2.01	0.60
1:A:1175:TYR:HB3	1:A:1178:GLN:NE2	2.17	0.60
1:A:1682:LEU:HD12	1:A:1683:PRO:HD2	1.84	0.60
1:A:787:LEU:HD22	1:A:888:LEU:HD12	1.84	0.59
4:A:2014:CLR:O1	4:A:2014:CLR:H192	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1361:LEU:HD21	1:A:1706:ILE:HD11	1.82	0.59
5:A:2007:PCW:H332	5:A:2007:PCW:C3	2.26	0.59
1:A:1619:PHE:O	1:A:1623:ILE:HD12	2.02	0.59
1:A:1491:ILE:HG12	4:A:2019:CLR:H211	1.84	0.59
1:A:1310:CYS:SG	1:A:1343:TRP:HE3	2.25	0.59
1:A:888:LEU:HB3	1:A:1411:ASN:HD21	1.66	0.59
1:A:1290:ILE:CD1	4:A:2005:CLR:H25	2.33	0.59
5:A:2006:PCW:H372	5:A:2007:PCW:H131	1.84	0.59
1:A:311:GLY:N	1:A:325:CYS:SG	2.76	0.59
1:A:1717:TYR:O	1:A:1721:ILE:HG12	2.01	0.58
1:A:1604:LEU:HD22	6:A:2008:LPE:H111	1.86	0.58
1:A:1237:ILE:HG22	1:A:1238:LEU:HD12	1.85	0.58
1:A:1619:PHE:HD2	6:A:2015:LPE:C14	2.16	0.58
1:A:296:ASP:HB3	1:A:298:TYR:HE1	1.68	0.58
5:A:2011:PCW:C41	4:A:2012:CLR:H211	2.32	0.58
1:A:1714:VAL:O	1:A:1718:ILE:HG13	2.03	0.57
1:A:344:TRP:HH2	7:A:2020:P5S:H3	1.68	0.57
1:A:1707:ILE:HD12	7:A:2021:P5S:H51	1.87	0.57
1:A:272:LEU:HD23	1:A:332:PRO:HG2	1.87	0.57
1:A:1290:ILE:HD12	4:A:2005:CLR:H25	1.86	0.57
1:A:401:GLU:HG2	1:A:890:LEU:HD11	1.86	0.57
1:A:829:ARG:HG2	1:A:1388:TRP:HH2	1.68	0.57
1:A:1361:LEU:HD12	7:A:2021:P5S:C27	2.35	0.56
1:A:1699:ILE:O	1:A:1703:THR:HB	2.05	0.56
1:A:889:LEU:HD21	1:A:1418:ILE:HD12	1.86	0.56
1:A:1506:LYS:O	1:A:1510:LYS:HG2	2.06	0.56
1:A:355:GLN:HG2	1:A:358:TRP:CD1	2.40	0.56
1:A:814:ARG:HD3	1:A:833:HIS:CE1	2.40	0.56
1:A:1503:GLU:O	1:A:1507:ILE:HG12	2.05	0.56
1:A:1604:LEU:HD11	5:A:2006:PCW:C19	2.36	0.56
1:A:888:LEU:HB3	1:A:1411:ASN:ND2	2.20	0.55
1:A:1252:LEU:HD21	1:A:1255:LEU:HD12	1.88	0.55
1:A:753:SER:HB3	1:A:1301:ASN:HB3	1.88	0.55
1:A:871:LEU:HB3	7:A:2020:P5S:H31A	1.87	0.55
1:A:1309:ARG:HH12	1:A:1346:VAL:CG1	2.19	0.55
1:A:1306:LYS:HG2	1:A:1380:ARG:O	2.07	0.55
1:A:1490:MET:HE1	1:A:1586:LEU:HD11	1.87	0.55
1:A:1574:VAL:HG21	6:A:2010:LPE:O31	2.06	0.55
1:A:1619:PHE:CD2	6:A:2015:LPE:C14	2.90	0.55
1:A:1703:THR:O	1:A:1707:ILE:HG13	2.07	0.55
1:A:296:ASP:HB3	1:A:298:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:ASN:HB2	1:A:860:VAL:HG23	1.89	0.55
1:A:814:ARG:HG2	1:A:814:ARG:HH11	1.72	0.54
1:A:1171:PHE:CD1	6:A:2015:LPE:C2N	2.91	0.54
1:A:1142:ARG:HG2	1:A:1206:VAL:O	2.08	0.54
1:A:748:LYS:HA	1:A:748:LYS:HE2	1.89	0.53
1:A:1604:LEU:HD22	6:A:2008:LPE:C11	2.38	0.53
1:A:1190:ASP:O	1:A:1194:THR:HG23	2.07	0.53
1:A:1543:ASP:OD2	1:A:1588:ARG:NH1	2.41	0.53
7:A:2021:P5S:H44	7:A:2021:P5S:H22	1.91	0.53
1:A:1227:ASN:O	1:A:1231:ILE:HG13	2.09	0.53
1:A:881:VAL:HG13	1:A:1407:PHE:HE1	1.74	0.53
1:A:320:PRO:HG2	1:A:323:TYR:CD2	2.44	0.53
1:A:1171:PHE:CE1	6:A:2015:LPE:H2N3	2.43	0.53
1:A:1404:PHE:HA	1:A:1408:PHE:CD1	2.42	0.53
1:A:893:PHE:CZ	1:A:1412:LEU:HA	2.44	0.53
1:A:327:LYS:NZ	1:A:1498:ASP:OD2	2.42	0.53
1:A:1538:GLY:HA2	5:A:2007:PCW:O31	2.09	0.53
1:A:1714:VAL:HA	1:A:1717:TYR:HD1	1.74	0.53
1:A:1433:ILE:HG22	1:A:1434:PHE:H	1.73	0.53
1:A:694:GLU:O	1:A:698:GLN:HG2	2.09	0.52
1:A:1145:CYS:O	1:A:1149:VAL:HG23	2.09	0.52
1:A:1597:LEU:HB3	5:A:2006:PCW:H122	1.91	0.52
1:A:356:ASP:OD2	1:A:851:ILE:HB	2.10	0.52
1:A:1170:ALA:CB	6:A:2015:LPE:O32	2.58	0.52
1:A:1619:PHE:CE1	1:A:1623:ILE:HD11	2.43	0.52
4:A:2014:CLR:H212	4:A:2014:CLR:H183	1.92	0.52
1:A:1716:MET:CE	6:A:2008:LPE:C15	2.87	0.52
1:A:1439:GLN:OE1	1:A:1605:PRO:HB3	2.09	0.52
1:A:304:THR:HG22	1:A:305:SER:H	1.74	0.52
1:A:734:CYS:O	1:A:737:VAL:HG12	2.10	0.52
1:A:1414:VAL:O	1:A:1418:ILE:HG13	2.09	0.52
4:A:2005:CLR:H121	4:A:2005:CLR:H212	1.92	0.52
6:A:2009:LPE:H2N2	6:A:2009:LPE:O31	2.09	0.52
5:A:2011:PCW:H381	5:A:2011:PCW:H152	1.91	0.52
1:A:814:ARG:HD3	1:A:833:HIS:HE1	1.73	0.51
1:A:1604:LEU:HD11	5:A:2006:PCW:C20	2.40	0.51
1:A:1377:VAL:HG11	1:A:1395:TYR:CD1	2.45	0.51
1:A:380:VAL:O	1:A:380:VAL:HG22	2.10	0.51
1:A:724:TYR:CE1	1:A:730:ASN:HB3	2.44	0.51
1:A:1579:ARG:HG2	1:A:1582:ARG:NH2	2.25	0.51
1:A:1666:LEU:O	1:A:1669:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2014:CLR:H212	4:A:2014:CLR:H121	1.93	0.51
1:A:1290:ILE:HD11	4:A:2005:CLR:H231	1.93	0.51
1:A:830:TRP:HZ2	1:A:1370:MET:HE1	1.75	0.51
5:A:2011:PCW:H461	4:A:2012:CLR:H241	1.92	0.51
1:A:244:LYS:HD2	1:A:244:LYS:O	2.11	0.51
1:A:1309:ARG:HH12	1:A:1346:VAL:HG12	1.75	0.51
1:A:1629:PHE:CD1	1:A:1670:ILE:HD12	2.46	0.51
1:A:690:SER:OG	1:A:691:PRO:HD2	2.11	0.50
1:A:1391:ASN:HB3	1:A:1394:MET:HG2	1.92	0.50
1:A:1500:GLN:HG3	1:A:1501:SER:H	1.75	0.50
1:A:1543:ASP:HA	1:A:1546:VAL:HG12	1.93	0.50
1:A:316:SER:HA	1:A:370:GLY:HA2	1.92	0.50
1:A:331:ASN:HB2	1:A:335:ASN:HA	1.93	0.50
1:A:1514:PHE:O	1:A:1518:VAL:HG23	2.12	0.50
1:A:1526:LYS:HG2	1:A:1534:TYR:CD2	2.46	0.50
4:A:2012:CLR:H121	4:A:2012:CLR:H212	1.93	0.50
1:A:829:ARG:HG2	1:A:1388:TRP:CH2	2.46	0.50
1:A:1345:ASN:OD1	1:A:1346:VAL:N	2.44	0.50
1:A:1579:ARG:O	1:A:1582:ARG:HB2	2.11	0.50
1:A:269:LYS:HE2	1:A:1496:GLU:OE1	2.11	0.50
1:A:728:LYS:HG3	5:A:2011:PCW:P	2.51	0.50
1:A:1311:ILE:HD13	1:A:1318:PHE:HD1	1.76	0.50
1:A:1380:ARG:NH1	1:A:1385:GLN:O	2.44	0.50
5:A:2011:PCW:H412	4:A:2012:CLR:C21	2.35	0.50
1:A:1306:LYS:HD2	1:A:1380:ARG:O	2.12	0.50
1:A:1311:ILE:CG2	1:A:1318:PHE:HB2	2.35	0.50
1:A:765:LYS:HD2	1:A:765:LYS:O	2.12	0.50
1:A:712:MET:CE	1:A:733:ASP:HB3	2.42	0.49
1:A:760:LEU:HD11	1:A:1297:ILE:HD13	1.94	0.49
1:A:1635:GLU:HB2	1:A:1669:PRO:HB3	1.94	0.49
1:A:760:LEU:O	1:A:763:VAL:HG12	2.12	0.49
1:A:1307:PHE:HD1	1:A:1346:VAL:HG21	1.76	0.49
1:A:390:ASN:HD22	1:A:1720:VAL:CG1	2.25	0.49
1:A:818:LYS:HD3	1:A:818:LYS:O	2.12	0.49
1:A:1491:ILE:HG12	4:A:2019:CLR:C21	2.42	0.49
1:A:1592:GLY:O	1:A:1596:LEU:HG	2.12	0.49
2:B:1:NAG:H61	2:B:2:NAG:C7	2.42	0.49
1:A:1143:LYS:HE3	1:A:1147:ARG:NH2	2.28	0.49
1:A:1591:LYS:HZ3	1:A:1594:ARG:HH21	1.60	0.49
1:A:1446:MET:HB3	1:A:1602:MET:SD	2.52	0.49
1:A:800:VAL:O	1:A:804:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:GLY:O	1:A:1409:THR:CG2	2.57	0.49
1:A:1526:LYS:HG2	1:A:1534:TYR:HD2	1.78	0.49
1:A:758:PHE:CE2	4:A:2012:CLR:H261	2.45	0.49
1:A:850:TRP:CZ3	1:A:851:ILE:HG13	2.47	0.49
1:A:1387:LYS:HB3	1:A:1390:ASP:HB2	1.94	0.49
1:A:1157:PHE:CZ	1:A:1196:ILE:HD11	2.47	0.48
1:A:1303:PHE:CZ	1:A:1397:TYR:CD2	3.01	0.48
1:A:1436:THR:HG23	1:A:1439:GLN:HG3	1.95	0.48
5:A:2007:PCW:H32	5:A:2007:PCW:H321	1.91	0.48
1:A:1333:LYS:HE2	2:B:1:NAG:H81	1.94	0.48
1:A:893:PHE:HZ	1:A:1412:LEU:HA	1.78	0.48
1:A:236:VAL:O	1:A:240:ILE:HG12	2.13	0.48
1:A:1700:ILE:O	1:A:1704:THR:HG23	2.14	0.48
1:A:300:ASN:HD22	1:A:305:SER:HA	1.79	0.48
1:A:1591:LYS:NZ	1:A:1594:ARG:HH21	2.12	0.48
1:A:1193:PHE:HA	1:A:1196:ILE:HG22	1.96	0.47
1:A:1277:ALA:O	1:A:1281:ILE:HG13	2.14	0.47
1:A:1434:PHE:CE1	1:A:1715:ASN:ND2	2.78	0.47
1:A:816:ASN:O	1:A:819:ASN:HB2	2.13	0.47
1:A:1314:THR:HG21	3:A:2004:NAG:O6	2.14	0.47
1:A:693:PHE:CD2	6:A:2018:LPE:O32	2.67	0.47
1:A:1576:ARG:HD2	1:A:1579:ARG:NH2	2.29	0.47
1:A:1161:MET:HG3	1:A:1196:ILE:HD13	1.96	0.47
6:A:2016:LPE:H322	7:A:2021:P5S:OXT	2.14	0.47
1:A:889:LEU:HD11	1:A:1414:VAL:HG12	1.97	0.47
1:A:1442:TYR:CE1	6:A:2009:LPE:H2N3	2.45	0.47
1:A:1369:TRP:O	1:A:1373:MET:HG3	2.15	0.47
1:A:1513:GLN:HA	1:A:1516:VAL:HG12	1.97	0.47
1:A:319:CYS:HB3	1:A:323:TYR:HB2	1.97	0.47
1:A:889:LEU:HD11	1:A:1414:VAL:CG1	2.45	0.47
1:A:732:PHE:O	1:A:735:ILE:HG22	2.16	0.46
1:A:893:PHE:HZ	1:A:1412:LEU:HD12	1.79	0.46
1:A:1441:LYS:HA	1:A:1441:LYS:HD3	1.77	0.46
1:A:712:MET:O	1:A:716:ILE:HG23	2.15	0.46
1:A:1213:TYR:CZ	1:A:1219:CYS:HB3	2.51	0.46
1:A:344:TRP:CH2	7:A:2020:P5S:C3	2.98	0.46
1:A:893:PHE:CE2	1:A:1415:GLY:HA3	2.50	0.46
1:A:1582:ARG:HA	1:A:1585:ARG:CD	2.44	0.46
1:A:1217:ALA:HB3	6:A:2013:LPE:O2H	2.16	0.46
1:A:1520:THR:O	1:A:1524:VAL:HG12	2.16	0.46
1:A:772:THR:HG22	1:A:1287:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:ARG:HG2	1:A:814:ARG:NH1	2.30	0.46
1:A:1291:PHE:HE1	1:A:1295:PHE:HE2	1.64	0.46
1:A:1603:SER:O	1:A:1607:LEU:HD23	2.15	0.46
1:A:252:LEU:HD13	1:A:1593:ILE:HG12	1.98	0.45
1:A:344:TRP:HH2	7:A:2020:P5S:C3	2.28	0.45
6:A:2016:LPE:H122	6:A:2016:LPE:H151	1.71	0.45
1:A:752:LEU:O	1:A:754:VAL:N	2.50	0.45
1:A:1189:THR:O	1:A:1192:VAL:HG12	2.17	0.45
1:A:1480:ILE:O	1:A:1484:VAL:HG12	2.17	0.45
7:A:2021:P5S:H42	7:A:2021:P5S:H20	1.98	0.45
1:A:814:ARG:HB2	1:A:833:HIS:CE1	2.52	0.45
1:A:1539:TRP:CH2	5:A:2006:PCW:H381	2.52	0.45
1:A:1634:TRP:HD1	1:A:1638:ILE:HG22	1.81	0.45
6:A:2013:LPE:H2N3	6:A:2013:LPE:H311	1.68	0.45
1:A:1580:ILE:O	1:A:1584:LEU:HG	2.17	0.45
1:A:1303:PHE:HB3	1:A:1307:PHE:CE2	2.51	0.45
1:A:1330:SER:CB	3:A:2003:NAG:C8	2.90	0.45
1:A:1434:PHE:O	1:A:1609:ASN:ND2	2.49	0.45
1:A:238:ALA:HB1	1:A:403:GLN:OE1	2.17	0.45
1:A:850:TRP:CE3	1:A:851:ILE:HG13	2.51	0.45
1:A:681:PHE:HB3	1:A:697:LEU:CD1	2.47	0.45
1:A:1434:PHE:HE1	1:A:1715:ASN:HD22	1.57	0.45
1:A:1399:VAL:O	1:A:1403:ILE:HG13	2.16	0.45
1:A:1400:ILE:O	1:A:1404:PHE:HD2	2.00	0.44
1:A:232:LEU:HD23	1:A:232:LEU:HA	1.69	0.44
1:A:716:ILE:HG22	1:A:724:TYR:CE2	2.51	0.44
1:A:816:ASN:HB2	1:A:860:VAL:CG2	2.47	0.44
6:A:2018:LPE:H311	6:A:2018:LPE:H2N2	1.75	0.44
1:A:1315:ASP:O	1:A:1317:GLU:HG2	2.18	0.44
1:A:1619:PHE:HE2	6:A:2015:LPE:H122	1.82	0.44
6:A:2008:LPE:H312	6:A:2008:LPE:H3N3	1.63	0.44
1:A:275:LYS:HD2	1:A:307:PRO:HB2	1.98	0.44
1:A:372:ILE:O	1:A:375:ILE:HG13	2.16	0.44
1:A:659:PHE:O	1:A:662:VAL:HG22	2.18	0.44
1:A:1500:GLN:HB2	1:A:1504:LYS:HE2	1.98	0.44
1:A:1555:ILE:O	1:A:1559:ILE:HG12	2.17	0.44
1:A:1468:PHE:HA	1:A:1471:ASP:OD2	2.17	0.44
1:A:664:ASP:HB2	1:A:665:PRO:HD2	1.99	0.44
1:A:748:LYS:HD3	1:A:749:LYS:N	2.30	0.44
1:A:1369:TRP:CE3	1:A:1373:MET:HE3	2.53	0.44
1:A:1672:ASN:HD21	1:A:1677:TYR:HB3	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:LYS:CG	1:A:1380:ARG:O	2.65	0.44
1:A:1266:GLY:O	1:A:1269:VAL:HG12	2.18	0.43
1:A:1290:ILE:O	1:A:1293:LEU:HB3	2.18	0.43
1:A:1659:THR:O	1:A:1660:SER:OG	2.35	0.43
1:A:1311:ILE:HD13	1:A:1318:PHE:CD1	2.53	0.43
1:A:1327:ASN:HA	1:A:1385:GLN:HB3	1.99	0.43
1:A:1557:SER:O	1:A:1561:LYS:HB2	2.18	0.43
5:A:2006:PCW:H42	5:A:2006:PCW:H72	1.52	0.43
5:A:2011:PCW:C41	4:A:2012:CLR:C21	2.96	0.43
1:A:1293:LEU:HB2	1:A:1357:TYR:OH	2.18	0.43
1:A:677:VAL:HG12	1:A:681:PHE:HE1	1.83	0.43
1:A:1323:LEU:HD11	1:A:1386:PRO:O	2.18	0.43
1:A:1509:GLY:O	1:A:1513:GLN:HG3	2.19	0.43
1:A:693:PHE:O	1:A:697:LEU:HD23	2.18	0.43
1:A:736:ILE:HG22	1:A:762:ARG:HH21	1.83	0.43
1:A:1198:VAL:HG21	1:A:1230:LEU:HD11	2.00	0.43
1:A:1239:GLU:N	1:A:1239:GLU:OE1	2.51	0.43
5:A:2006:PCW:H341	5:A:2006:PCW:H371	1.60	0.43
1:A:337:THR:HG21	1:A:351:ARG:NH2	2.34	0.43
1:A:384:GLY:O	1:A:388:LEU:HB2	2.19	0.43
1:A:693:PHE:HD2	6:A:2018:LPE:O32	2.00	0.43
1:A:1193:PHE:O	1:A:1196:ILE:HG22	2.19	0.43
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.81	0.43
1:A:712:MET:HE2	1:A:733:ASP:HB3	2.01	0.43
1:A:383:LEU:O	1:A:387:TYR:HB3	2.19	0.42
1:A:1303:PHE:CZ	1:A:1397:TYR:HD2	2.36	0.42
1:A:1311:ILE:HD12	1:A:1344:VAL:HG21	2.01	0.42
1:A:1638:ILE:HG23	1:A:1643:ASN:HB3	1.99	0.42
1:A:233:LYS:HB3	1:A:233:LYS:HE3	1.78	0.42
1:A:1171:PHE:CE1	6:A:2015:LPE:C2N	3.02	0.42
6:A:2010:LPE:H312	6:A:2010:LPE:H2N3	1.75	0.42
1:A:310:CYS:C	1:A:325:CYS:SG	2.98	0.42
1:A:773:LEU:HD23	1:A:773:LEU:O	2.20	0.42
1:A:1428:LEU:HB3	1:A:1431:GLN:HE21	1.83	0.42
1:A:1434:PHE:HE1	1:A:1715:ASN:ND2	2.16	0.42
1:A:1326:VAL:C	1:A:1328:ASN:H	2.23	0.42
4:A:2012:CLR:H8	4:A:2012:CLR:H182	1.76	0.42
1:A:685:GLU:HA	1:A:689:MET:CE	2.49	0.42
1:A:1639:ASP:OD2	1:A:1639:ASP:N	2.53	0.42
1:A:1635:GLU:HB3	1:A:1636:ALA:H	1.68	0.42
1:A:817:ARG:HB2	1:A:828:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:HIS:HD2	1:A:833:HIS:H	1.66	0.42
1:A:331:ASN:HB3	1:A:332:PRO:CD	2.49	0.41
1:A:371:LYS:HD3	1:A:1652:LEU:HD21	2.01	0.41
1:A:1380:ARG:HB3	1:A:1384:MET:HE3	2.02	0.41
1:A:1591:LYS:NZ	1:A:1594:ARG:NH2	2.68	0.41
4:A:2012:CLR:H211	4:A:2012:CLR:H232	1.54	0.41
1:A:239:LEU:HD21	1:A:880:VAL:HG22	2.01	0.41
1:A:1356:GLY:O	1:A:1360:LEU:HD13	2.21	0.41
1:A:1490:MET:CE	1:A:1586:LEU:HD11	2.49	0.41
1:A:764:PHE:CE2	1:A:777:ILE:HD11	2.55	0.41
1:A:1171:PHE:CD1	6:A:2015:LPE:H2N2	2.55	0.41
1:A:1716:MET:CE	6:A:2008:LPE:H152	2.50	0.41
1:A:742:LEU:O	1:A:746:VAL:HG12	2.21	0.41
1:A:757:SER:OG	1:A:1298:MET:HG2	2.21	0.41
1:A:1447:LYS:HB2	1:A:1447:LYS:HE2	1.78	0.41
1:A:1621:TYR:CD1	1:A:1701:PHE:CE2	3.09	0.41
1:A:755:LEU:HA	1:A:755:LEU:HD23	1.77	0.41
1:A:1345:ASN:OD1	1:A:1349:ASN:ND2	2.49	0.41
1:A:1581:GLY:O	1:A:1585:ARG:HG3	2.20	0.41
1:A:334:PHE:HB3	1:A:336:TYR:HE2	1.86	0.41
1:A:379:LEU:O	1:A:383:LEU:HD12	2.20	0.41
1:A:1294:ILE:O	1:A:1298:MET:HG3	2.21	0.41
1:A:1523:CYS:SG	1:A:1524:VAL:N	2.93	0.41
1:A:1561:LYS:CG	1:A:1562:SER:N	2.83	0.41
1:A:1619:PHE:O	1:A:1622:SER:HB2	2.21	0.41
1:A:304:THR:HG22	1:A:305:SER:N	2.35	0.41
1:A:713:VAL:HA	1:A:716:ILE:HG12	2.03	0.41
1:A:1291:PHE:HE1	1:A:1295:PHE:CE2	2.39	0.41
5:A:2007:PCW:C33	5:A:2007:PCW:C3	2.86	0.41
1:A:238:ALA:HB1	1:A:403:GLN:CD	2.41	0.41
1:A:309:LEU:HD22	1:A:364:GLN:HG2	2.03	0.41
1:A:344:TRP:CH2	7:A:2020:P5S:H3A	2.56	0.41
1:A:1561:LYS:CG	1:A:1562:SER:H	2.34	0.41
1:A:1710:PHE:O	1:A:1714:VAL:HG23	2.21	0.41
5:A:2007:PCW:H63	5:A:2007:PCW:H41	1.85	0.41
6:A:2010:LPE:O31	6:A:2010:LPE:H21	2.20	0.41
1:A:815:ASN:OD1	1:A:815:ASN:N	2.53	0.40
1:A:1391:ASN:HB3	1:A:1394:MET:CG	2.51	0.40
1:A:794:LEU:O	1:A:798:VAL:HG23	2.21	0.40
1:A:1274:LEU:O	1:A:1278:ILE:HG12	2.20	0.40
1:A:1400:ILE:HG23	1:A:1404:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1667:LEU:O	1:A:1667:LEU:HD23	2.21	0.40
1:A:724:TYR:HE1	1:A:730:ASN:OD1	2.03	0.40
1:A:885:PHE:CE2	1:A:889:LEU:HD12	2.56	0.40
1:A:685:GLU:HA	1:A:689:MET:HE3	2.04	0.40
1:A:1327:ASN:OD1	1:A:1380:ARG:NH2	2.55	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	991/1956 (51%)	907 (92%)	83 (8%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1629	PHE

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	886/1727 (51%)	884 (100%)	2 (0%)	93 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	819	ASN
1	A	1703	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	355	GLN
1	A	390	ASN
1	A	730	ASN
1	A	831	HIS
1	A	833	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)

2 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	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	B	2	2	14,14,15	0.29	0	17,19,21	0.61	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
2	NAG	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

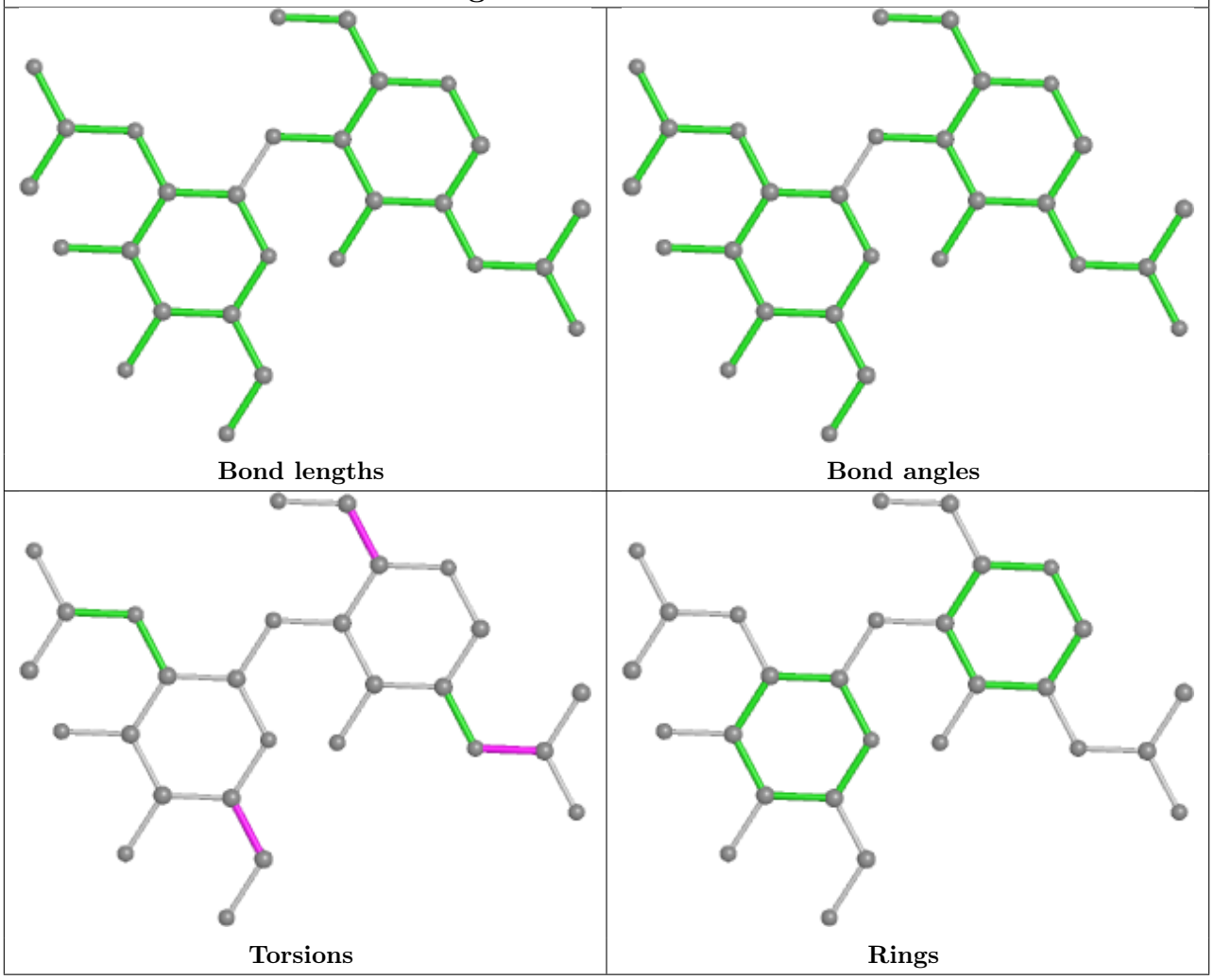
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	2	0
2	B	2	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 B



5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CLR	A	2019	-	31,31,31	0.91	2 (6%)	48,48,48	1.38	7 (14%)
6	LPE	A	2009	-	21,21,33	0.57	0	25,27,39	0.58	0
3	NAG	A	2001	1	14,14,15	0.29	0	17,19,21	1.63	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CLR	A	2014	-	31,31,31	0.80	0	48,48,48	1.54	8 (16%)
3	NAG	A	2004	1	14,14,15	0.53	0	17,19,21	1.66	2 (11%)
6	LPE	A	2018	-	33,33,33	0.48	0	37,39,39	0.60	0
5	PCW	A	2006	-	47,47,53	0.97	2 (4%)	52,55,61	1.16	4 (7%)
3	NAG	A	2002	1	14,14,15	0.49	0	17,19,21	1.49	3 (17%)
6	LPE	A	2016	-	21,21,33	0.57	0	25,27,39	0.70	0
3	NAG	A	2003	1	14,14,15	0.33	0	17,19,21	1.13	1 (5%)
6	LPE	A	2008	-	21,21,33	0.57	0	25,27,39	0.53	0
5	PCW	A	2011	-	40,40,53	1.06	2 (5%)	43,45,61	1.14	4 (9%)
4	CLR	A	2005	-	31,31,31	0.70	0	48,48,48	1.16	5 (10%)
5	PCW	A	2007	-	46,46,53	1.00	2 (4%)	52,54,61	1.04	2 (3%)
7	P5S	A	2021	-	42,43,53	0.96	3 (7%)	46,50,60	1.48	8 (17%)
6	LPE	A	2010	-	22,22,33	0.54	0	26,28,39	0.60	0
4	CLR	A	2012	-	31,31,31	0.79	0	48,48,48	1.51	7 (14%)
6	LPE	A	2017	-	20,20,33	0.58	0	24,26,39	0.60	0
6	LPE	A	2013	-	33,33,33	0.47	0	37,39,39	0.62	0
7	P5S	A	2020	-	47,48,53	1.00	2 (4%)	51,55,60	1.40	5 (9%)
6	LPE	A	2015	-	21,21,33	0.67	0	25,27,39	0.78	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	A	2019	-	-	6/10/68/68	0/4/4/4
6	LPE	A	2009	-	-	13/22/22/34	-
3	NAG	A	2001	1	-	3/6/23/26	0/1/1/1
4	CLR	A	2014	-	-	2/10/68/68	0/4/4/4
3	NAG	A	2004	1	-	2/6/23/26	0/1/1/1
6	LPE	A	2018	-	-	18/34/34/34	-
5	PCW	A	2006	-	-	21/51/51/57	-
3	NAG	A	2002	1	-	0/6/23/26	0/1/1/1
6	LPE	A	2016	-	-	4/22/22/34	-
3	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
6	LPE	A	2008	-	-	13/22/22/34	-
5	PCW	A	2011	-	-	11/42/42/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	A	2005	-	-	3/10/68/68	0/4/4/4
5	PCW	A	2007	-	-	33/50/50/57	-
7	P5S	A	2021	-	-	12/49/49/59	-
6	LPE	A	2010	-	-	8/23/23/34	-
4	CLR	A	2012	-	-	4/10/68/68	0/4/4/4
6	LPE	A	2017	-	-	6/21/21/34	-
6	LPE	A	2013	-	-	4/34/34/34	-
7	P5S	A	2020	-	-	8/54/54/59	-
6	LPE	A	2015	-	-	10/22/22/34	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2020	P5S	O37-C38	4.40	1.46	1.34
7	A	2020	P5S	O19-C17	4.39	1.46	1.33
5	A	2011	PCW	O3-C11	4.30	1.45	1.33
5	A	2007	PCW	O3-C11	4.24	1.45	1.33
5	A	2006	PCW	O2-C31	4.14	1.46	1.34
5	A	2007	PCW	O2-C31	4.12	1.45	1.34
5	A	2011	PCW	O2-C31	4.08	1.45	1.34
5	A	2006	PCW	O3-C11	3.81	1.44	1.33
7	A	2021	P5S	O19-C17	3.77	1.44	1.33
7	A	2021	P5S	O37-C38	3.64	1.44	1.34
4	A	2019	CLR	C10-C9	-2.38	1.52	1.56
4	A	2019	CLR	C13-C14	-2.09	1.51	1.55
7	A	2021	P5S	O37-C2	-2.03	1.41	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2020	P5S	OG-CB-CA	5.61	112.95	108.06
7	A	2021	P5S	OG-CB-CA	4.97	112.39	108.06
4	A	2014	CLR	C13-C17-C20	-4.83	111.92	119.49
4	A	2012	CLR	C13-C17-C20	-4.81	111.95	119.49
3	A	2004	NAG	C4-C3-C2	-4.57	104.32	111.02
3	A	2001	NAG	C4-C3-C2	-4.23	104.81	111.02
4	A	2014	CLR	C13-C14-C8	-4.13	108.26	114.38
4	A	2012	CLR	C13-C14-C8	-4.06	108.37	114.38
7	A	2021	P5S	O37-C38-C39	3.97	120.06	111.50
3	A	2002	NAG	O5-C1-C2	-3.96	105.03	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2020	P5S	O37-C38-C39	3.92	119.94	111.50
5	A	2007	PCW	O2-C31-C32	3.84	119.78	111.50
3	A	2003	NAG	C4-C3-C2	-3.83	105.40	111.02
3	A	2004	NAG	C6-C5-C4	-3.69	104.37	113.00
5	A	2006	PCW	O2-C31-C32	3.68	119.42	111.50
4	A	2019	CLR	C11-C12-C13	-3.56	106.68	112.78
4	A	2019	CLR	C13-C17-C20	-3.53	113.96	119.49
4	A	2012	CLR	C17-C13-C14	3.52	104.24	100.07
4	A	2014	CLR	C17-C13-C14	3.52	104.24	100.07
5	A	2011	PCW	O2-C31-C32	3.45	118.94	111.50
4	A	2019	CLR	C16-C17-C20	3.41	117.42	112.15
4	A	2005	CLR	C13-C17-C20	-3.31	114.31	119.49
7	A	2021	P5S	O19-C17-C20	3.20	121.94	111.91
5	A	2006	PCW	O3-C11-C12	3.18	121.89	111.91
3	A	2001	NAG	C2-N2-C7	3.16	127.41	122.90
5	A	2011	PCW	O3-C11-C12	2.97	121.22	111.91
3	A	2002	NAG	C4-C3-C2	-2.84	106.86	111.02
7	A	2020	P5S	OXT-C-O	-2.79	117.77	124.09
4	A	2014	CLR	C11-C12-C13	-2.76	108.05	112.78
5	A	2007	PCW	O3-C11-C12	2.73	120.49	111.91
4	A	2012	CLR	C11-C12-C13	-2.72	108.11	112.78
4	A	2019	CLR	C21-C20-C17	-2.70	108.79	112.92
7	A	2020	P5S	OXT-C-CA	2.68	122.50	113.38
4	A	2019	CLR	C22-C20-C17	2.56	115.58	110.28
7	A	2021	P5S	OXT-C-O	-2.56	118.27	124.09
4	A	2019	CLR	C11-C9-C10	-2.54	109.73	113.08
4	A	2005	CLR	C11-C12-C13	-2.54	108.43	112.78
5	A	2006	PCW	C3-C2-C1	-2.51	105.85	111.79
4	A	2005	CLR	C13-C14-C8	-2.47	110.72	114.38
4	A	2014	CLR	C8-C7-C6	-2.45	109.21	112.73
5	A	2011	PCW	O1P-P-O2P	2.40	120.06	110.68
3	A	2001	NAG	C1-C2-N2	-2.39	106.40	110.49
7	A	2020	P5S	O19-C17-C20	2.38	119.37	111.91
5	A	2006	PCW	O3-C11-O11	-2.34	117.69	123.59
4	A	2014	CLR	C7-C6-C5	-2.31	120.81	125.06
6	A	2015	LPE	C3-C2-C1	-2.30	106.03	112.79
7	A	2021	P5S	OXT-C-CA	2.29	121.20	113.38
4	A	2005	CLR	C4-C5-C10	2.27	119.44	116.42
7	A	2021	P5S	O37-C38-O47	-2.26	118.25	123.70
4	A	2012	CLR	C4-C5-C10	2.24	119.39	116.42
4	A	2005	CLR	C17-C13-C14	2.20	102.68	100.07
7	A	2021	P5S	C2-O37-C38	-2.19	112.40	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2014	CLR	C1-C2-C3	2.16	113.23	110.47
4	A	2014	CLR	C3-C4-C5	-2.14	108.39	112.03
4	A	2019	CLR	C23-C22-C20	-2.09	109.02	115.03
7	A	2021	P5S	O19-C17-O18	-2.08	118.35	123.59
4	A	2012	CLR	C10-C9-C8	-2.06	109.64	112.73
5	A	2011	PCW	C2-O2-C31	-2.05	112.75	117.79
3	A	2002	NAG	C3-C4-C5	-2.04	106.60	110.24
4	A	2012	CLR	C7-C8-C9	2.02	112.17	109.71

There are no chirality outliers.

All (183) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	NAG	C3-C2-N2-C7
3	A	2001	NAG	C8-C7-N2-C2
3	A	2001	NAG	O7-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	A	2004	NAG	C8-C7-N2-C2
3	A	2004	NAG	O7-C7-N2-C2
5	A	2006	PCW	O4P-C4-C5-N
5	A	2006	PCW	C4-O4P-P-O2P
5	A	2007	PCW	O4P-C4-C5-N
5	A	2007	PCW	C32-C31-O2-C2
5	A	2011	PCW	C1-O3P-P-O1P
5	A	2011	PCW	C1-O3P-P-O4P
6	A	2008	LPE	C3-O3-P-O32
6	A	2008	LPE	C31-O33-P-O3
6	A	2008	LPE	C31-O33-P-O31
6	A	2008	LPE	C31-O33-P-O32
6	A	2009	LPE	O1-C1-C2-O2H
6	A	2009	LPE	O1-C1-C2-C3
6	A	2009	LPE	C31-O33-P-O31
6	A	2009	LPE	C31-O33-P-O32
6	A	2009	LPE	O33-C31-C32-N
6	A	2010	LPE	O1-C1-C2-O2H
6	A	2010	LPE	O1-C1-C2-C3
6	A	2010	LPE	C2-C3-O3-P
6	A	2010	LPE	C3-O3-P-O32
6	A	2013	LPE	C31-O33-P-O31
6	A	2015	LPE	C3-O3-P-O32
6	A	2015	LPE	C31-O33-P-O32
6	A	2016	LPE	O33-C31-C32-N

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Mol	Chain	Res	Type	Atoms
6	A	2018	LPE	O1-C1-C2-O2H
6	A	2018	LPE	O1-C1-C2-C3
6	A	2018	LPE	C1-C2-C3-O3
6	A	2018	LPE	C3-O3-P-O31
6	A	2018	LPE	C3-O3-P-O32
6	A	2018	LPE	C3-O3-P-O33
7	A	2021	P5S	O-C-CA-N
7	A	2021	P5S	O47-C38-O37-C2
5	A	2007	PCW	O31-C31-O2-C2
3	A	2003	NAG	C8-C7-N2-C2
7	A	2021	P5S	C39-C38-O37-C2
4	A	2019	CLR	C16-C17-C20-C21
4	A	2019	CLR	C13-C17-C20-C21
4	A	2019	CLR	C13-C17-C20-C22
5	A	2006	PCW	C12-C11-O3-C3
4	A	2019	CLR	C16-C17-C20-C22
6	A	2018	LPE	O2H-C2-C3-O3
5	A	2006	PCW	O11-C11-O3-C3
4	A	2012	CLR	C21-C20-C22-C23
7	A	2021	P5S	OXT-C-CA-N
6	A	2009	LPE	C1-C2-C3-O3
5	A	2011	PCW	C31-C32-C33-C34
4	A	2012	CLR	C20-C22-C23-C24
5	A	2006	PCW	C4-C5-N-C7
6	A	2008	LPE	C3-O3-P-O33
6	A	2009	LPE	C31-O33-P-O3
6	A	2010	LPE	C3-O3-P-O33
6	A	2015	LPE	C3-O3-P-O33
6	A	2015	LPE	C31-O33-P-O3
6	A	2016	LPE	C31-O33-P-O3
6	A	2017	LPE	C31-O33-P-O3
7	A	2020	P5S	C44-C45-C46-C48
6	A	2018	LPE	C23-C24-C25-C26
5	A	2007	PCW	C33-C34-C35-C36
6	A	2015	LPE	C2-C3-O3-P
5	A	2006	PCW	C35-C36-C37-C38
6	A	2009	LPE	O2H-C2-C3-O3
4	A	2005	CLR	C23-C24-C25-C27
5	A	2007	PCW	C13-C14-C15-C16
7	A	2020	P5S	C21-C22-C23-C24
5	A	2007	PCW	C31-C32-C33-C34
4	A	2005	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
6	A	2018	LPE	C24-C25-C26-C27
6	A	2018	LPE	C22-C23-C24-C25
5	A	2007	PCW	C35-C36-C37-C38
4	A	2005	CLR	C23-C24-C25-C26
6	A	2018	LPE	C21-C22-C23-C24
5	A	2006	PCW	C4-C5-N-C6
5	A	2006	PCW	C4-C5-N-C8
5	A	2006	PCW	C15-C16-C17-C18
6	A	2018	LPE	C13-C14-C15-C16
6	A	2018	LPE	C20-C21-C22-C23
5	A	2011	PCW	C32-C31-O2-C2
5	A	2006	PCW	C34-C35-C36-C37
5	A	2011	PCW	O31-C31-O2-C2
6	A	2018	LPE	O1-C11-C12-C13
6	A	2018	LPE	C11-C12-C13-C14
5	A	2007	PCW	C43-C44-C45-C46
6	A	2009	LPE	C11-C12-C13-C14
5	A	2006	PCW	C40-C41-C42-C43
6	A	2008	LPE	C2-C1-O1-C11
6	A	2010	LPE	C2-C1-O1-C11
6	A	2009	LPE	C13-C14-C15-C16
4	A	2014	CLR	C22-C23-C24-C25
6	A	2018	LPE	C14-C15-C16-C17
5	A	2007	PCW	O2-C2-C3-O3
6	A	2009	LPE	O1-C11-C12-C13
5	A	2007	PCW	C44-C45-C46-C47
5	A	2007	PCW	C32-C33-C34-C35
5	A	2011	PCW	C12-C11-O3-C3
7	A	2020	P5S	O19-C1-C2-C3
6	A	2013	LPE	C31-O33-P-O3
7	A	2021	P5S	O37-C2-C3-O16
4	A	2012	CLR	C23-C24-C25-C26
5	A	2006	PCW	C19-C20-C21-C22
5	A	2011	PCW	C19-C20-C21-C22
5	A	2007	PCW	O3P-C1-C2-C3
7	A	2021	P5S	C1-C2-C3-O16
6	A	2010	LPE	C12-C11-O1-C1
5	A	2007	PCW	C15-C16-C17-C18
5	A	2007	PCW	C1-C2-C3-O3
6	A	2009	LPE	C2-C3-O3-P
5	A	2006	PCW	O3P-C1-C2-O2
7	A	2020	P5S	O19-C1-C2-O37

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Mol	Chain	Res	Type	Atoms
5	A	2011	PCW	O11-C11-O3-C3
5	A	2007	PCW	C45-C46-C47-C48
7	A	2020	P5S	N-CA-CB-OG
7	A	2021	P5S	N-CA-CB-OG
5	A	2006	PCW	C16-C17-C18-C19
5	A	2006	PCW	C4-O4P-P-O3P
6	A	2009	LPE	C3-O3-P-O33
6	A	2010	LPE	C31-O33-P-O3
5	A	2007	PCW	C42-C43-C44-C45
5	A	2006	PCW	C4-O4P-P-O1P
6	A	2016	LPE	C31-O33-P-O31
6	A	2017	LPE	C31-O33-P-O31
6	A	2008	LPE	O1-C1-C2-C3
6	A	2017	LPE	C32-C31-O33-P
5	A	2006	PCW	C32-C33-C34-C35
6	A	2008	LPE	C1-C2-C3-O3
6	A	2016	LPE	C2-C1-O1-C11
6	A	2008	LPE	O2H-C2-C3-O3
6	A	2013	LPE	O33-C31-C32-N
6	A	2015	LPE	O33-C31-C32-N
6	A	2017	LPE	O33-C31-C32-N
5	A	2007	PCW	C16-C17-C18-C19
4	A	2012	CLR	C23-C24-C25-C27
5	A	2011	PCW	O2-C31-C32-C33
6	A	2013	LPE	C12-C11-O1-C1
6	A	2015	LPE	O1-C1-C2-C3
5	A	2007	PCW	C3-C2-O2-C31
4	A	2019	CLR	C20-C22-C23-C24
5	A	2006	PCW	O2-C2-C3-O3
5	A	2007	PCW	C14-C15-C16-C17
5	A	2007	PCW	C1-O3P-P-O4P
5	A	2007	PCW	C4-O4P-P-O3P
6	A	2017	LPE	C3-O3-P-O33
7	A	2020	P5S	C3-O16-P12-OG
5	A	2007	PCW	C40-C41-C42-C43
5	A	2007	PCW	C41-C42-C43-C44
6	A	2018	LPE	C16-C17-C18-C19
5	A	2007	PCW	C36-C37-C38-C39
7	A	2021	P5S	C45-C46-C48-C49
4	A	2014	CLR	C20-C22-C23-C24
6	A	2015	LPE	C11-C12-C13-C14
6	A	2018	LPE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
5	A	2011	PCW	C32-C33-C34-C35
5	A	2006	PCW	O3P-C1-C2-C3
5	A	2007	PCW	C2-C1-O3P-P
6	A	2015	LPE	C12-C13-C14-C15
4	A	2019	CLR	C23-C24-C25-C26
5	A	2006	PCW	C39-C40-C41-C42
5	A	2007	PCW	O3P-C1-C2-O2
6	A	2008	LPE	C31-C32-N-C3N
6	A	2008	LPE	O1-C1-C2-O2H
7	A	2020	P5S	C17-C20-C21-C22
5	A	2006	PCW	C17-C18-C19-C20
7	A	2021	P5S	O37-C38-C39-C40
7	A	2020	P5S	OXT-C-CA-N
5	A	2007	PCW	O2-C31-C32-C33
5	A	2007	PCW	C39-C40-C41-C42
5	A	2007	PCW	O3-C11-C12-C13
7	A	2021	P5S	C39-C40-C41-C42
5	A	2007	PCW	C1-O3P-P-O2P
6	A	2008	LPE	C31-C32-N-C1N
6	A	2008	LPE	C31-C32-N-C2N
6	A	2015	LPE	C31-C32-N-C2N
6	A	2017	LPE	C3-O3-P-O31
7	A	2021	P5S	CB-OG-P12-O13
7	A	2021	P5S	O47-C38-C39-C40
5	A	2007	PCW	O31-C31-C32-C33
5	A	2007	PCW	C11-C12-C13-C14
5	A	2007	PCW	O11-C11-C12-C13
5	A	2011	PCW	C33-C34-C35-C36

There are no ring outliers.

18 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2019	CLR	2	0
6	A	2009	LPE	3	0
4	A	2014	CLR	3	0
3	A	2004	NAG	1	0
6	A	2018	LPE	5	0
5	A	2006	PCW	7	0
6	A	2016	LPE	4	0
3	A	2003	NAG	3	0
6	A	2008	LPE	8	0

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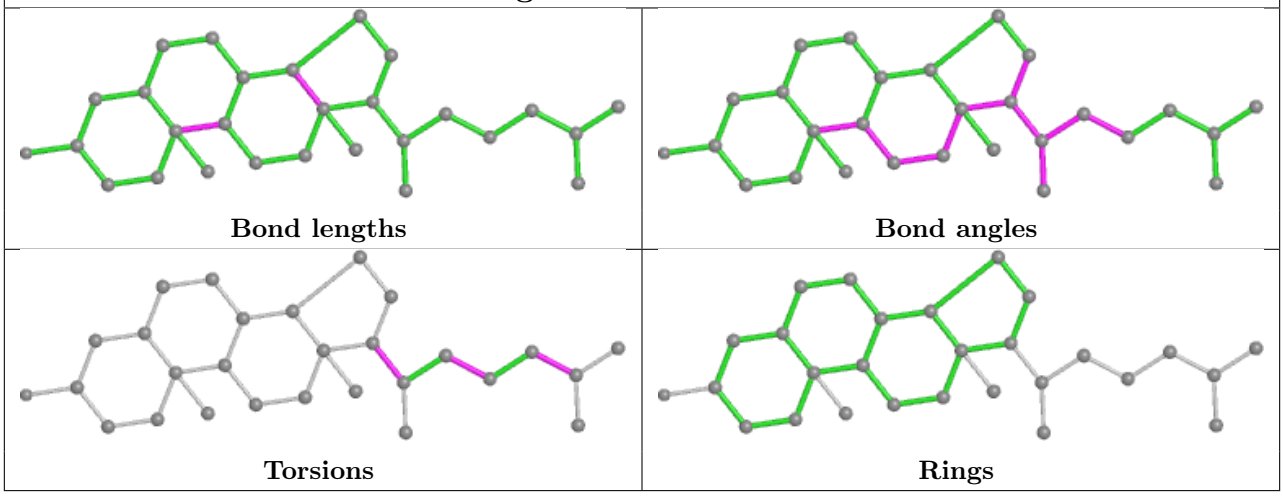
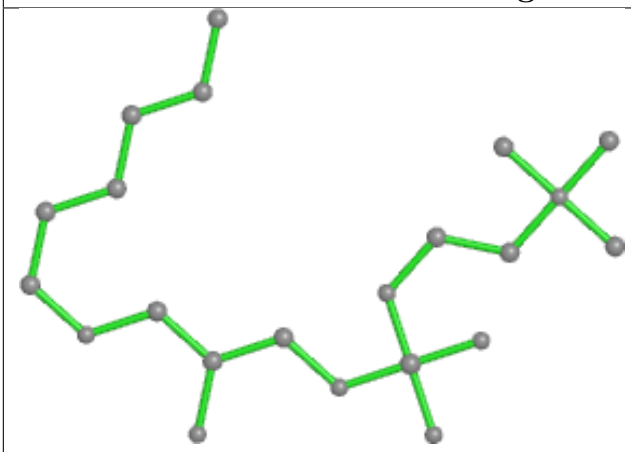
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2011	PCW	8	0
4	A	2005	CLR	6	0
5	A	2007	PCW	10	0
7	A	2021	P5S	9	0
6	A	2010	LPE	3	0
4	A	2012	CLR	12	0
6	A	2013	LPE	4	0
7	A	2020	P5S	5	0
6	A	2015	LPE	12	0

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

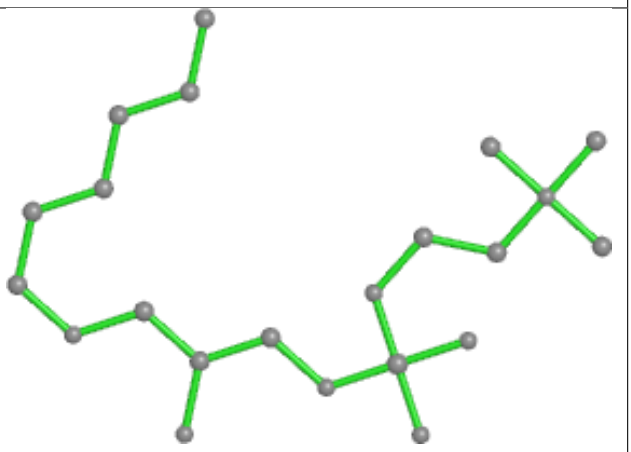
Ligand CLR A 2019



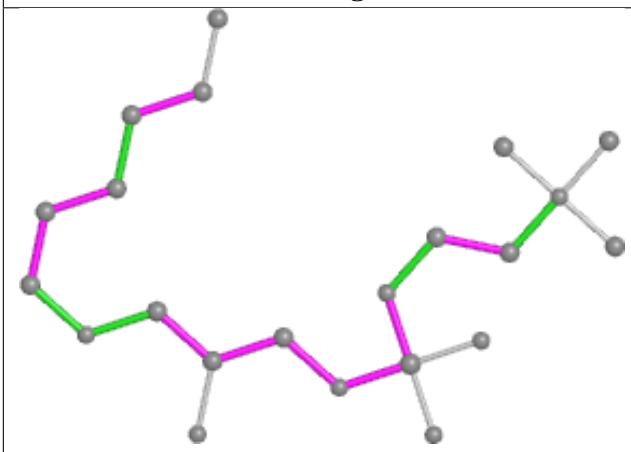
Ligand LPE A 2009



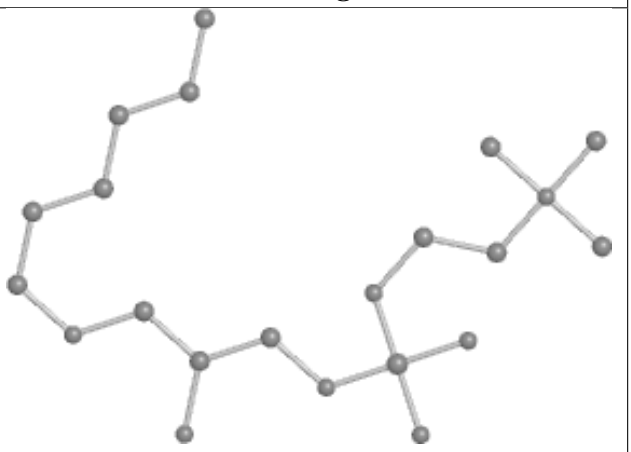
Bond lengths



Bond angles

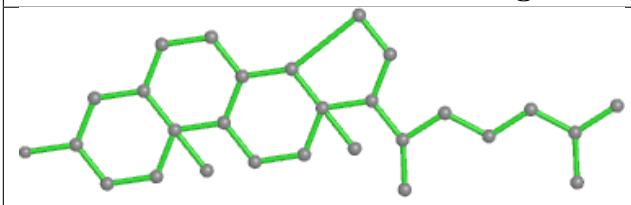


Torsions

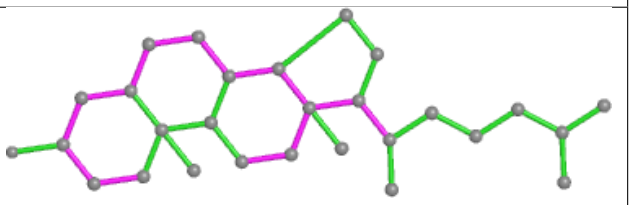


Rings

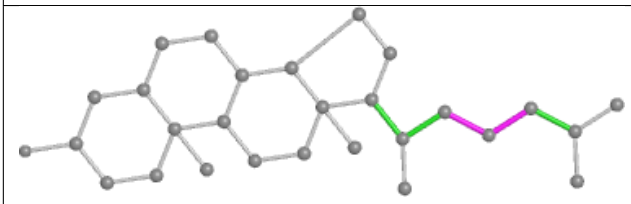
Ligand CLR A 2014



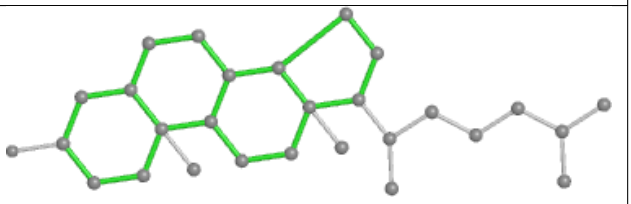
Bond lengths



Bond angles

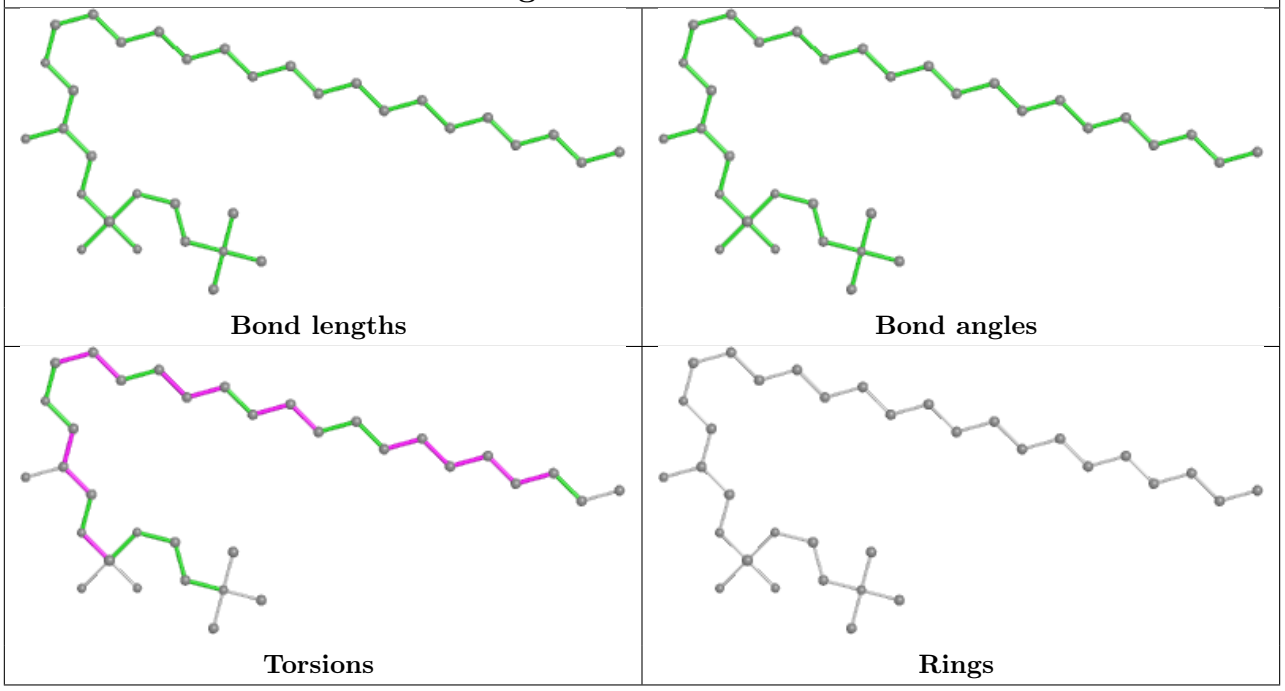


Torsions

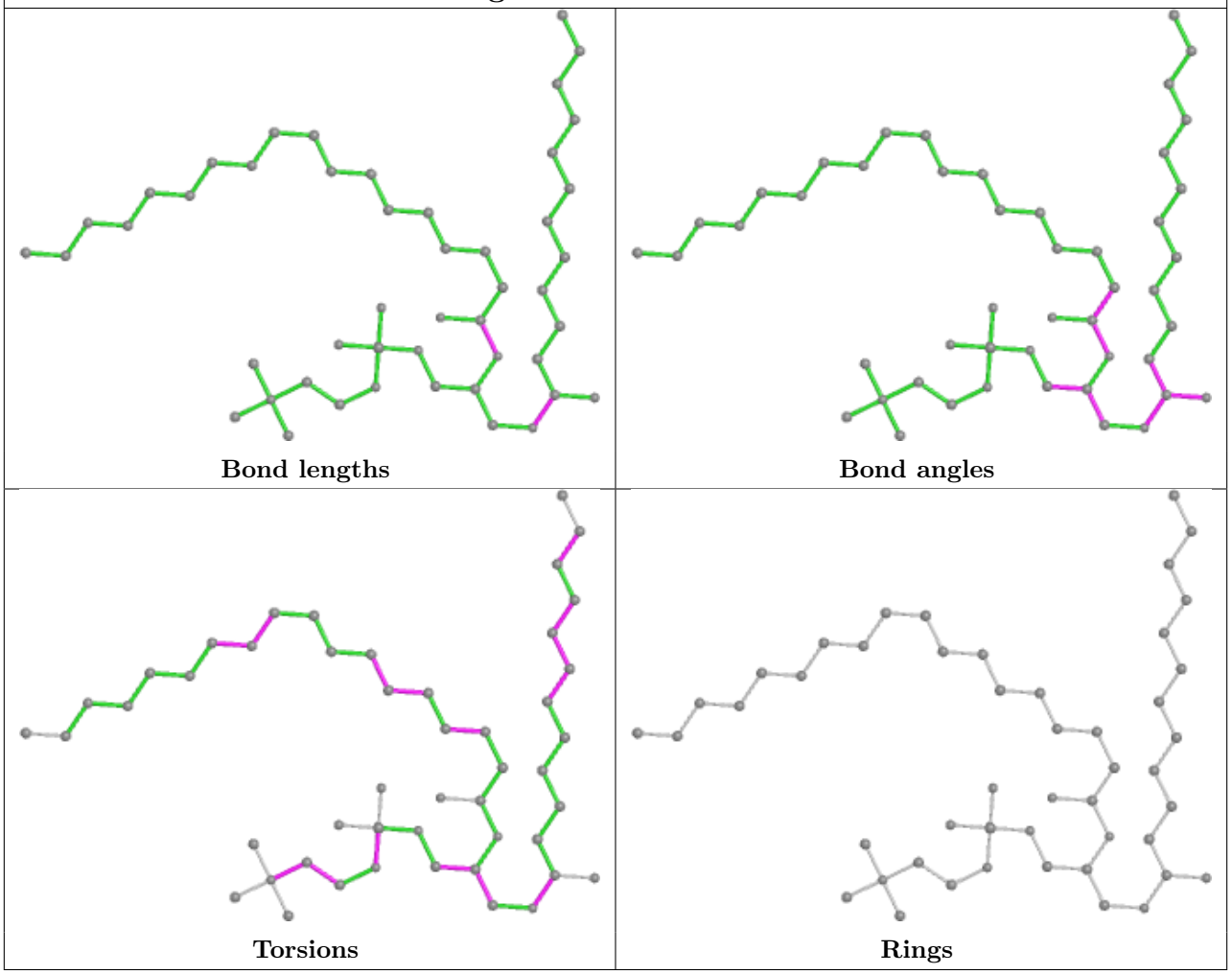


Rings

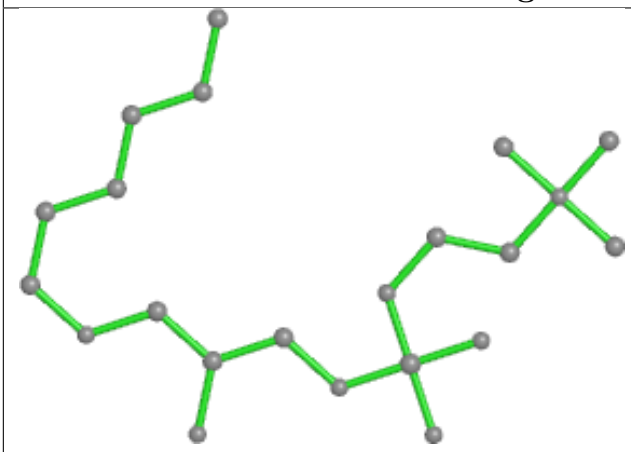
Ligand LPE A 2018



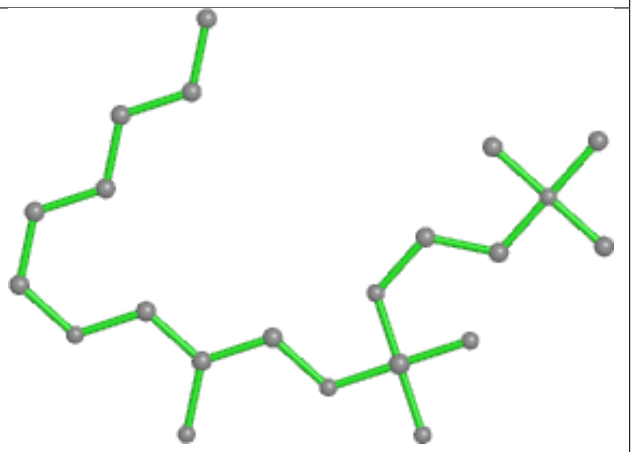
Ligand PCW A 2006



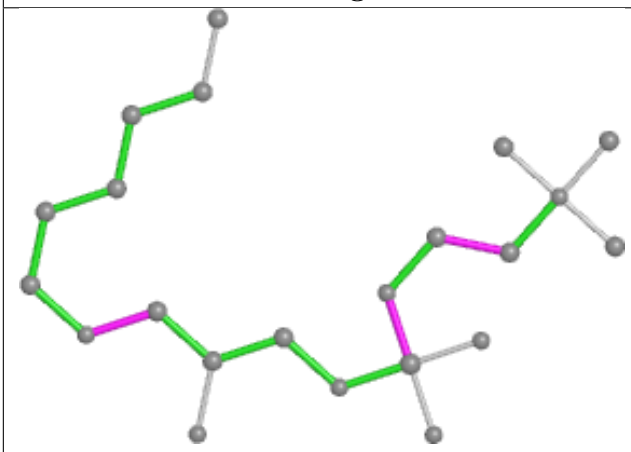
Ligand LPE A 2016



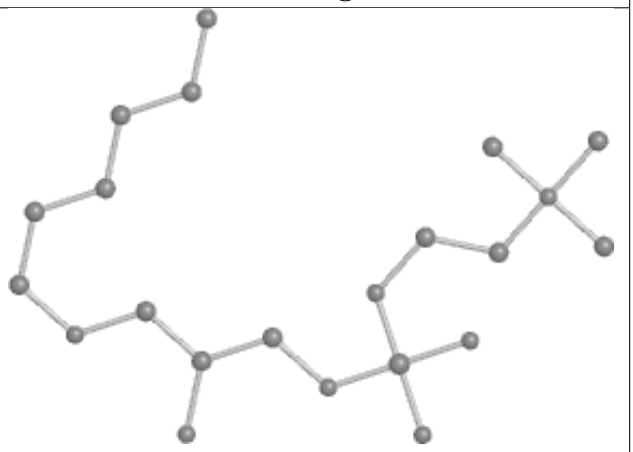
Bond lengths



Bond angles

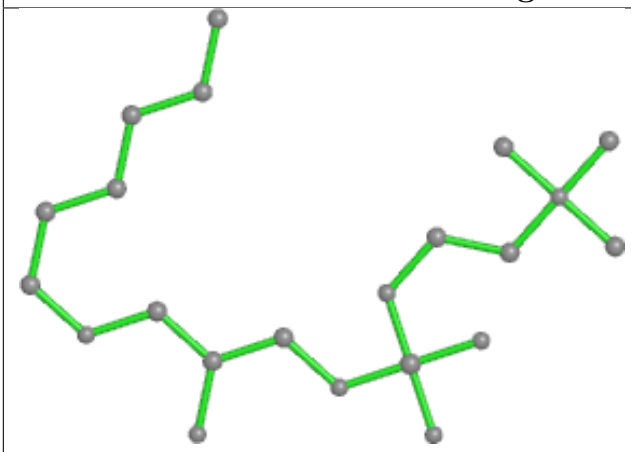


Torsions

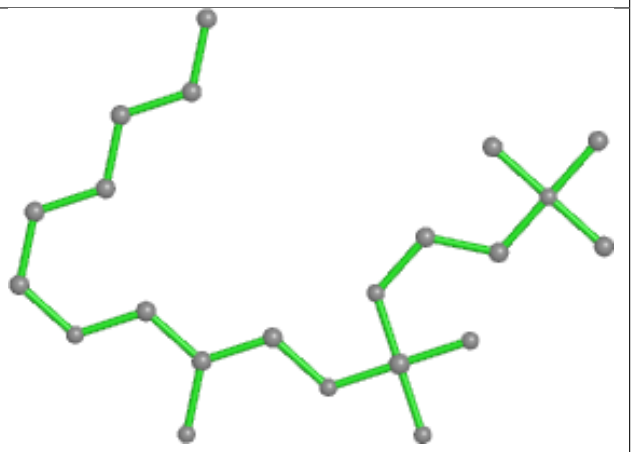


Rings

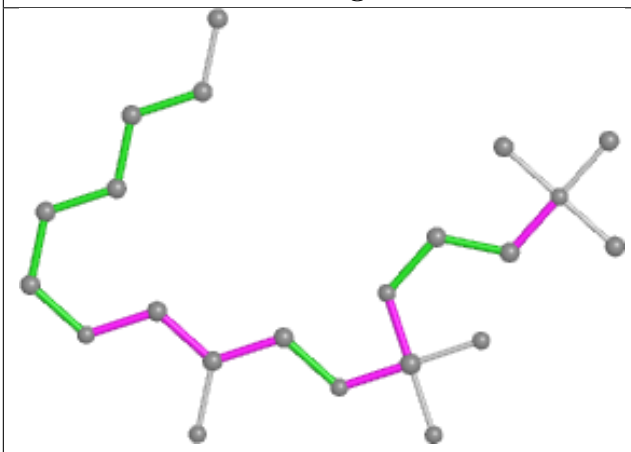
Ligand LPE A 2008



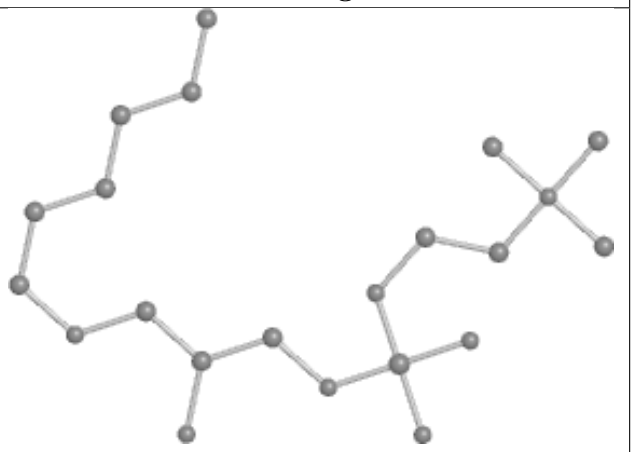
Bond lengths



Bond angles

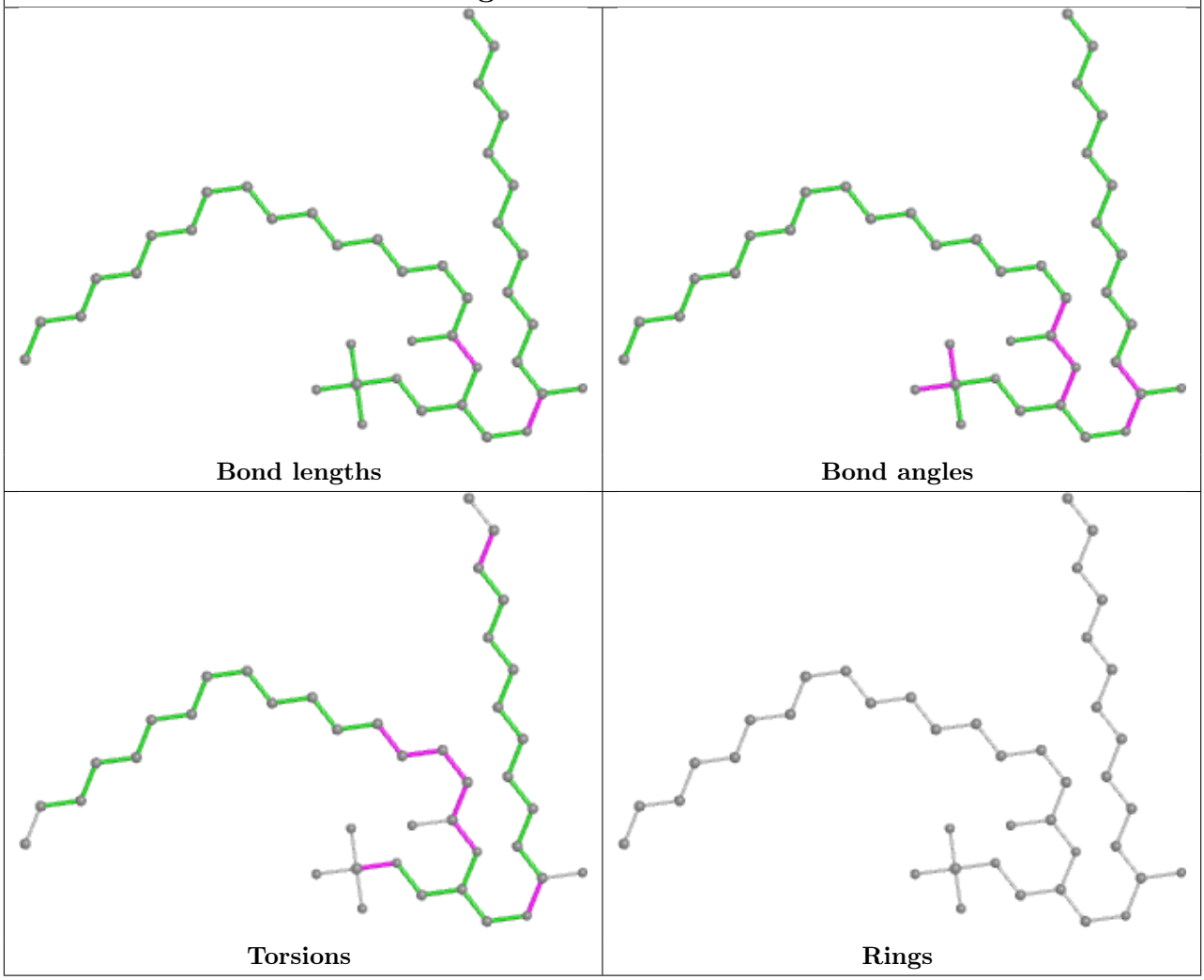


Torsions

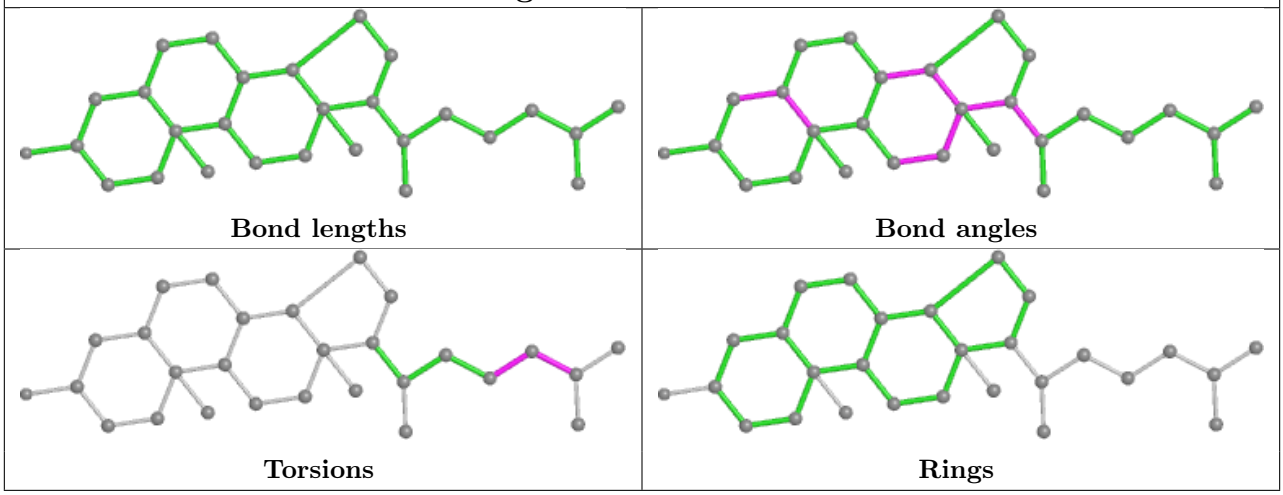


Rings

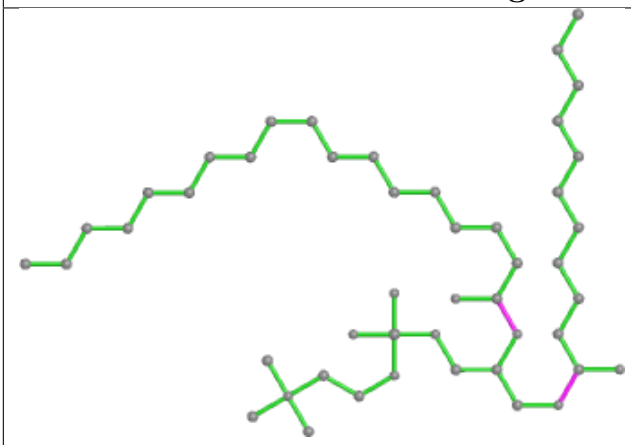
Ligand PCW A 2011



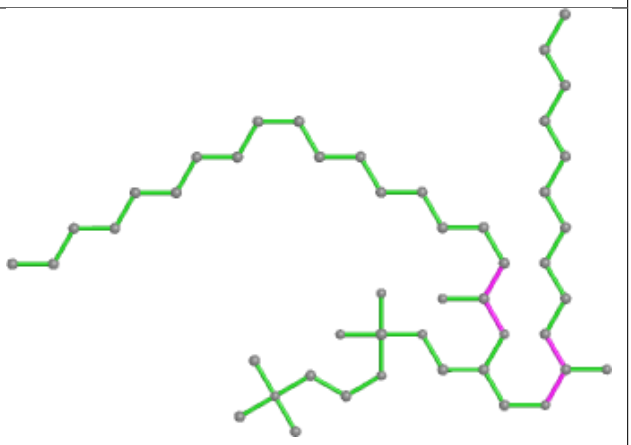
Ligand CLR A 2005



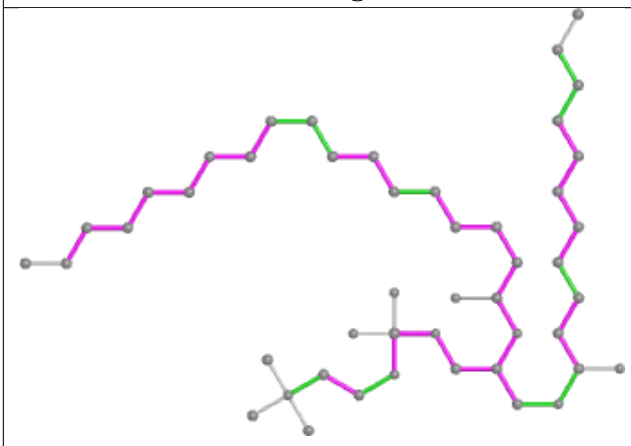
Ligand PCW A 2007



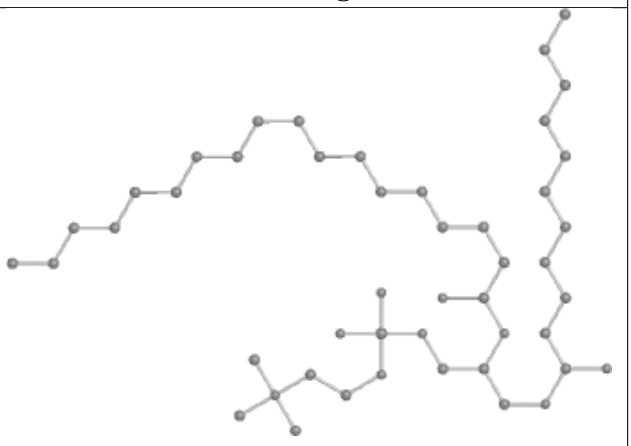
Bond lengths



Bond angles

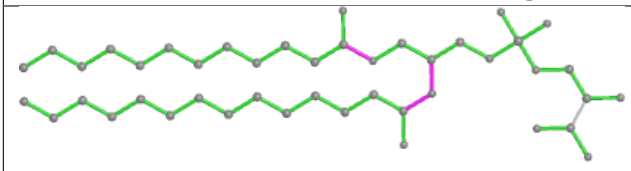


Torsions

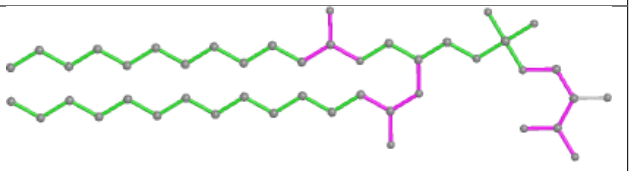


Rings

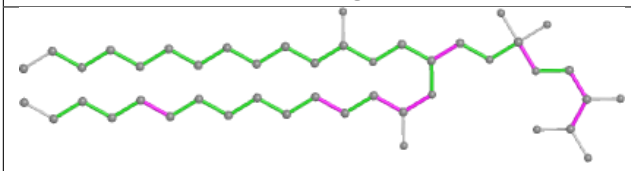
Ligand P5S A 2021



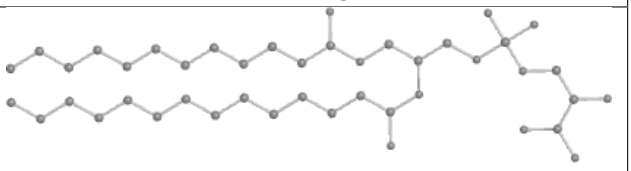
Bond lengths



Bond angles

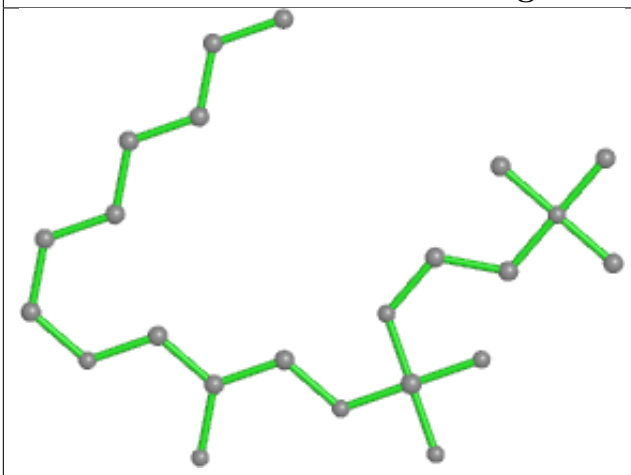


Torsions

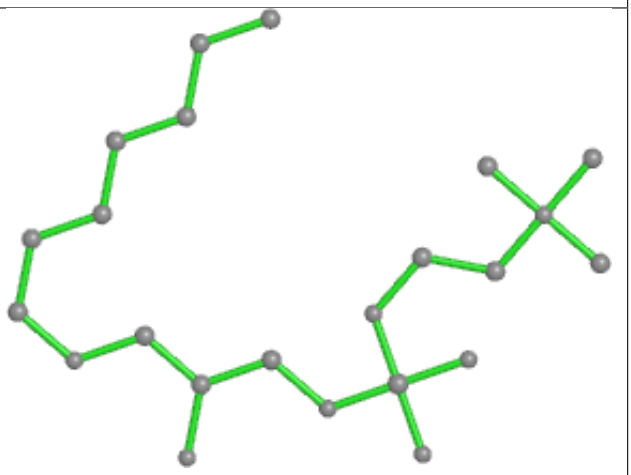


Rings

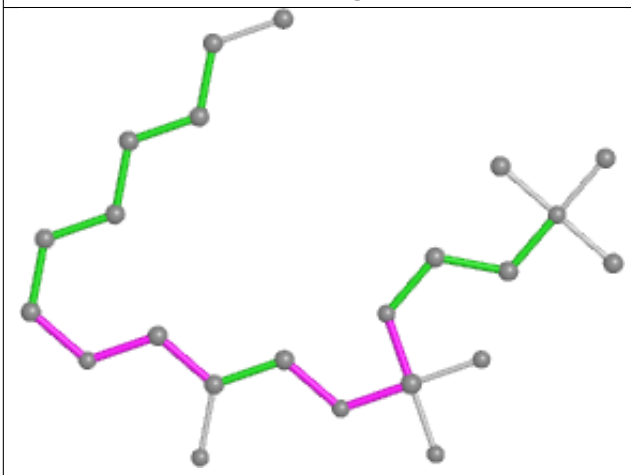
Ligand LPE A 2010



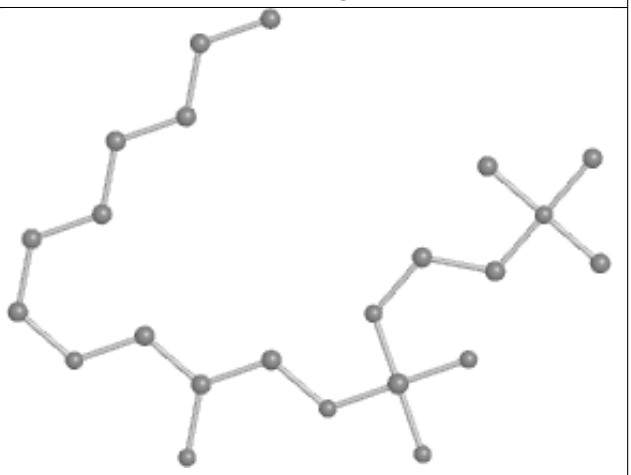
Bond lengths



Bond angles

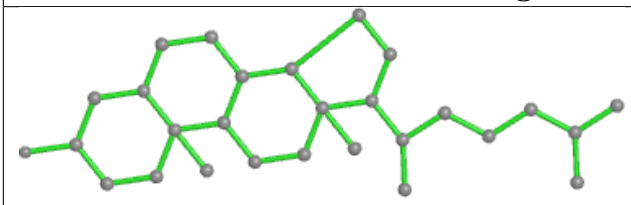


Torsions

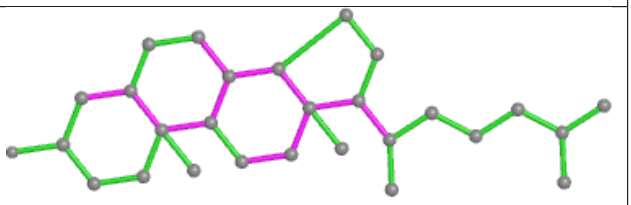


Rings

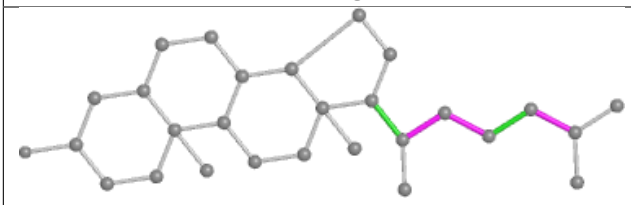
Ligand CLR A 2012



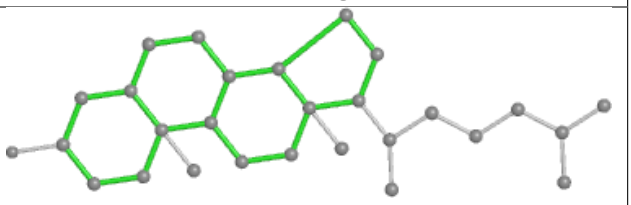
Bond lengths



Bond angles

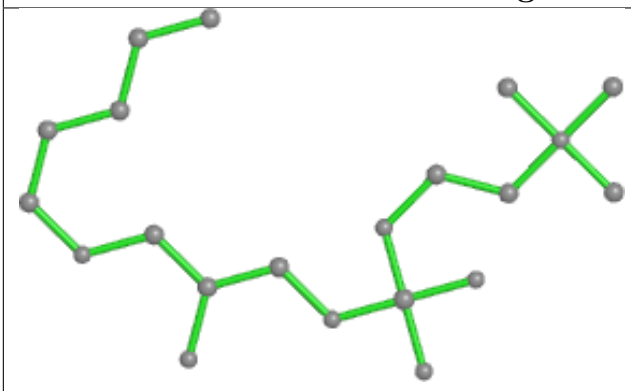


Torsions

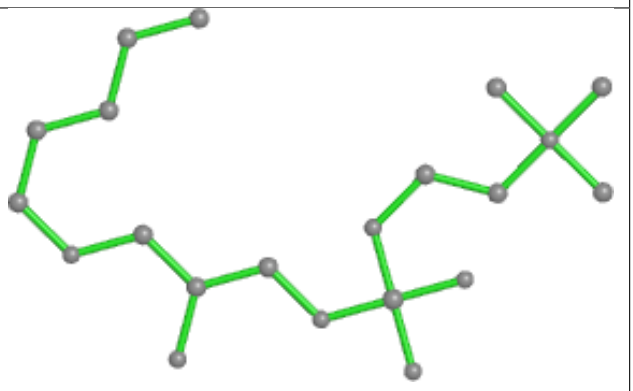


Rings

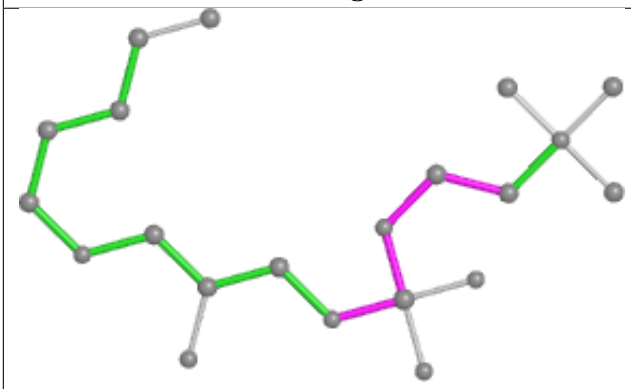
Ligand LPE A 2017



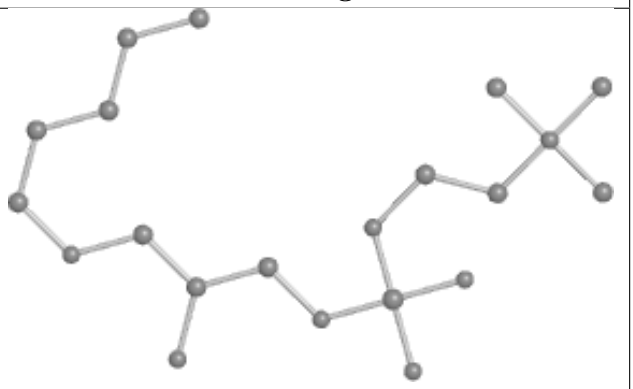
Bond lengths



Bond angles

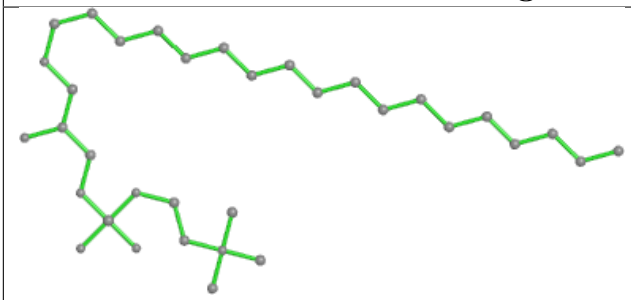


Torsions

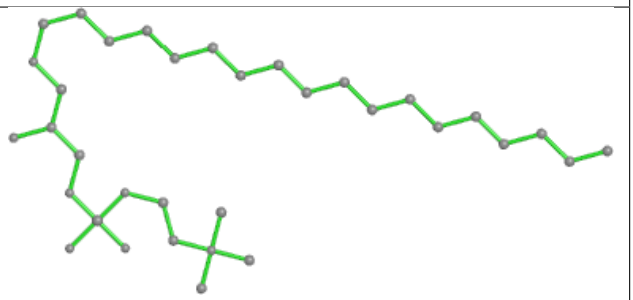


Rings

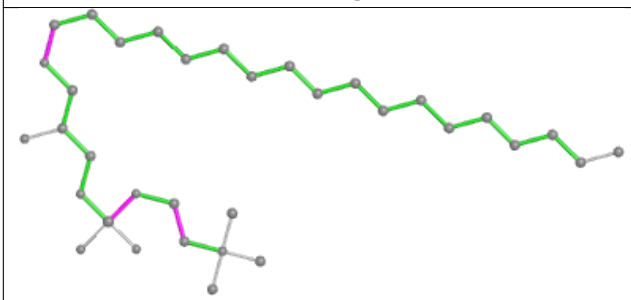
Ligand LPE A 2013



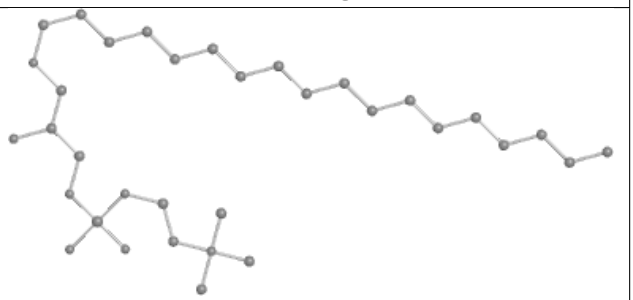
Bond lengths



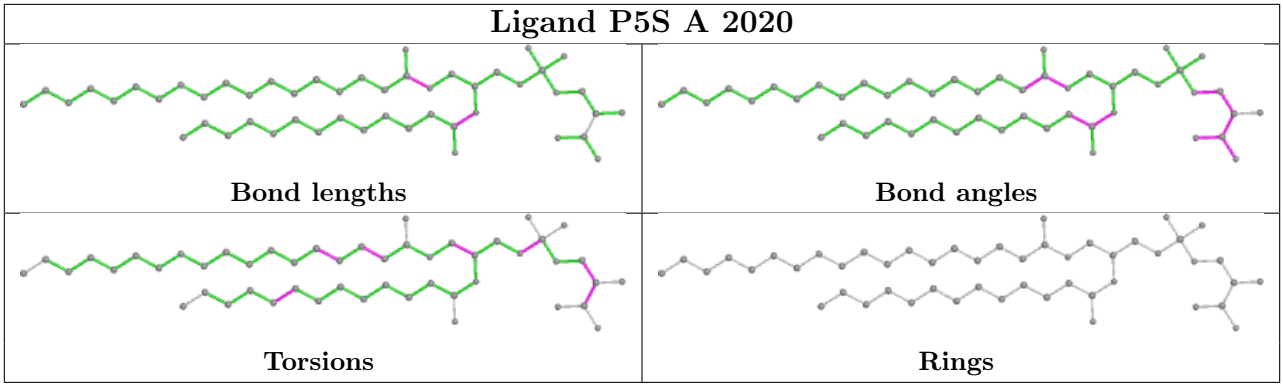
Bond angles

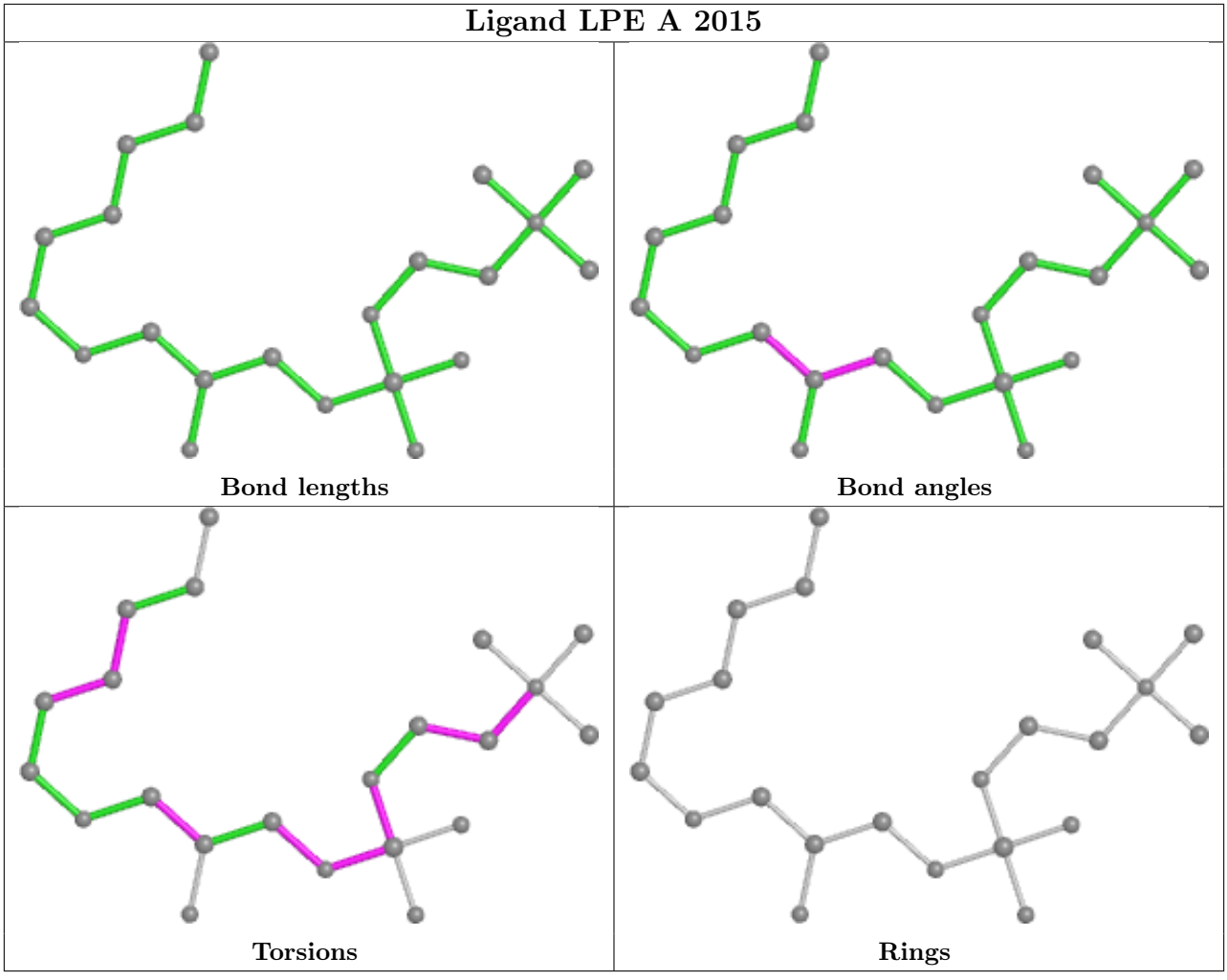


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

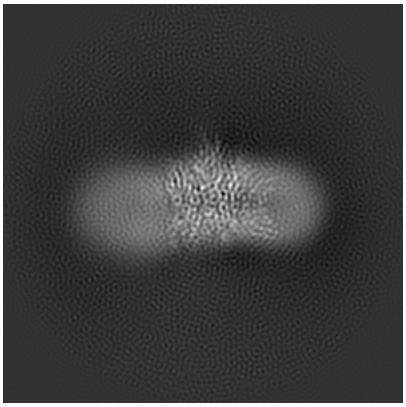
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32476. These allow visual inspection of the internal detail of the map and identification of artifacts.

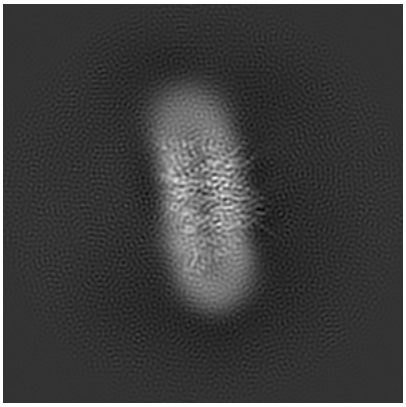
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

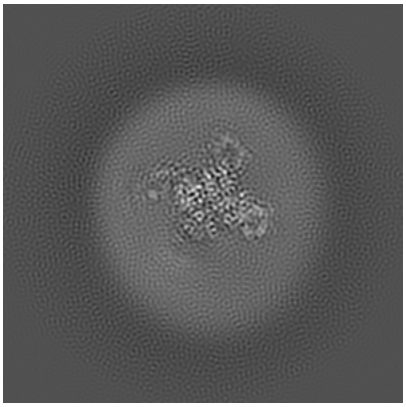
6.1.1 Primary map



X



Y

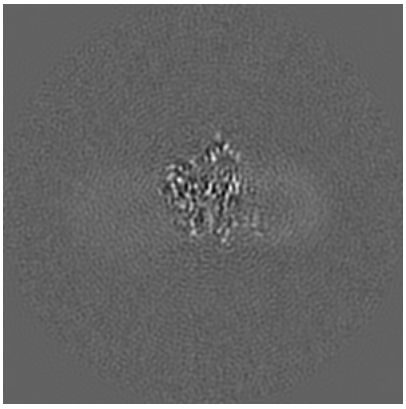


Z

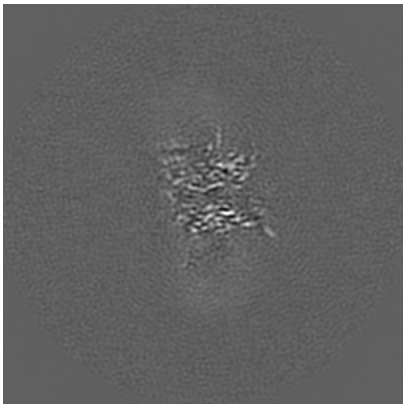
The images above show the map projected in three orthogonal directions.

6.2 Central slices

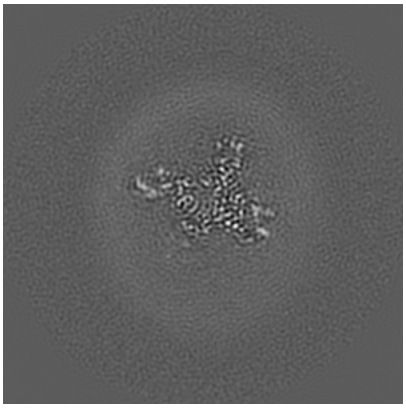
6.2.1 Primary map



X Index: 128



Y Index: 128

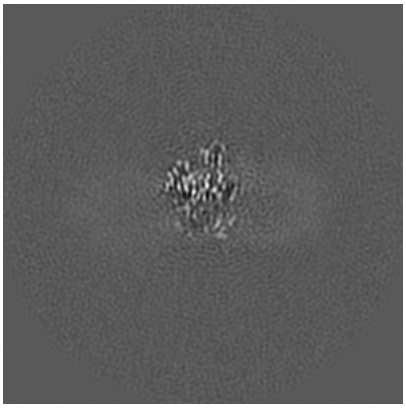


Z Index: 128

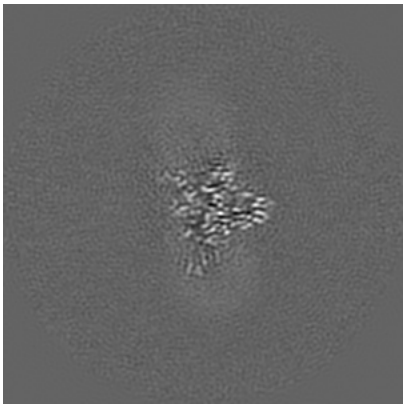
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

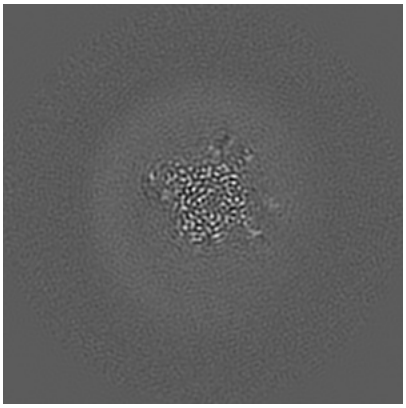
6.3.1 Primary map



X Index: 125



Y Index: 137



Z Index: 139

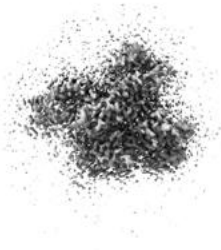
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0249. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

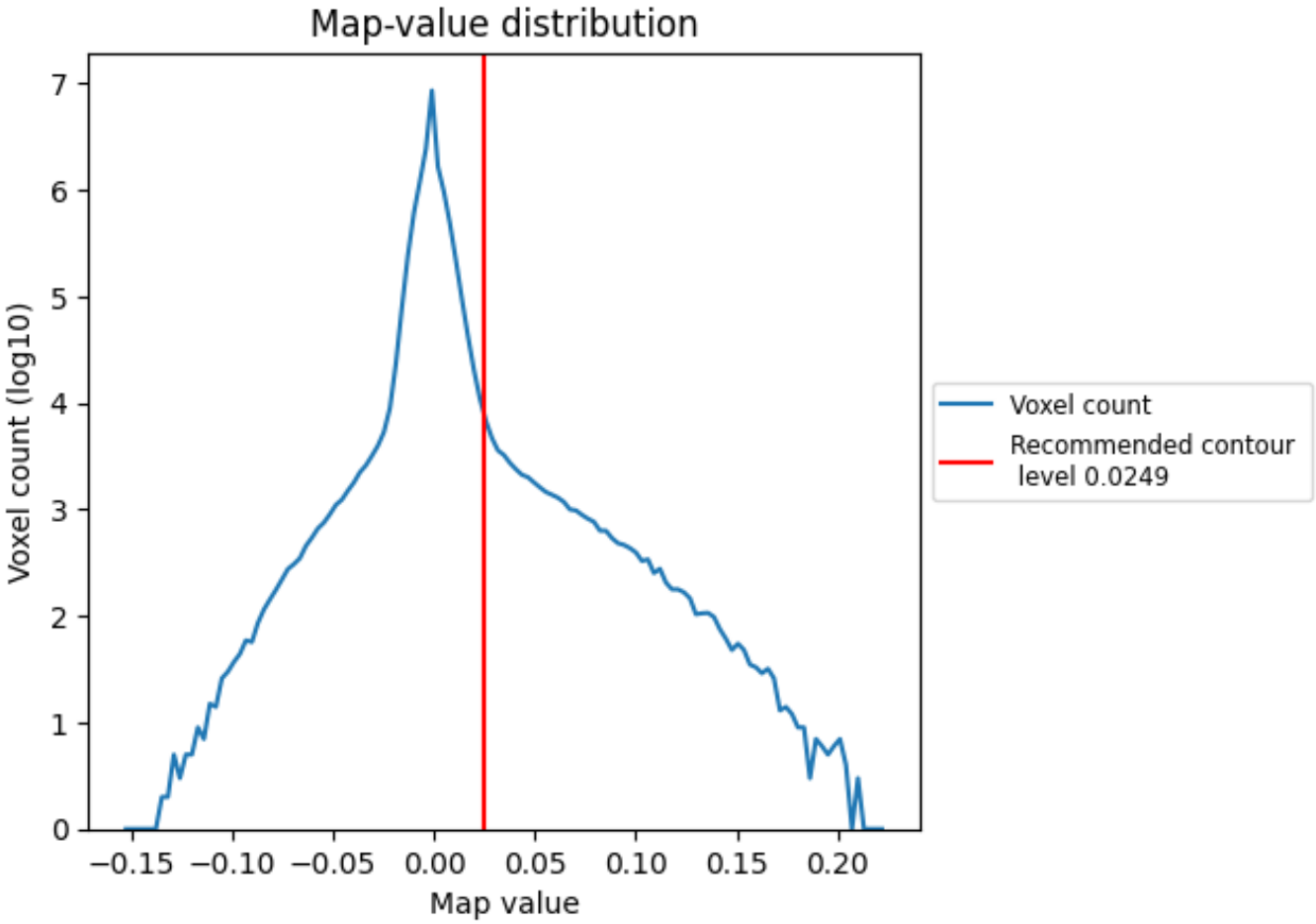
6.5 Mask visualisation (i)

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

7 Map analysis

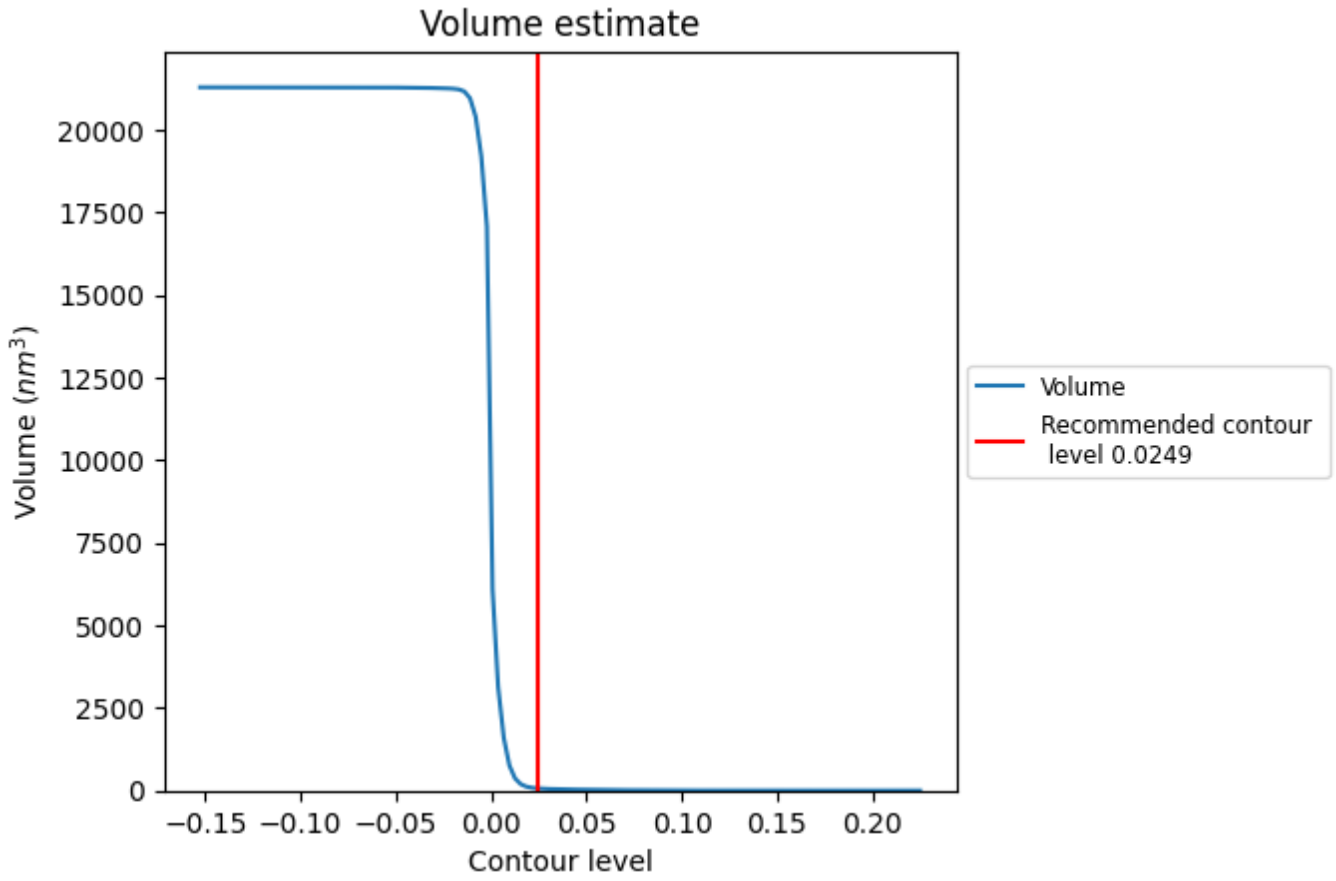
This section contains the results of statistical analysis of the map.

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.

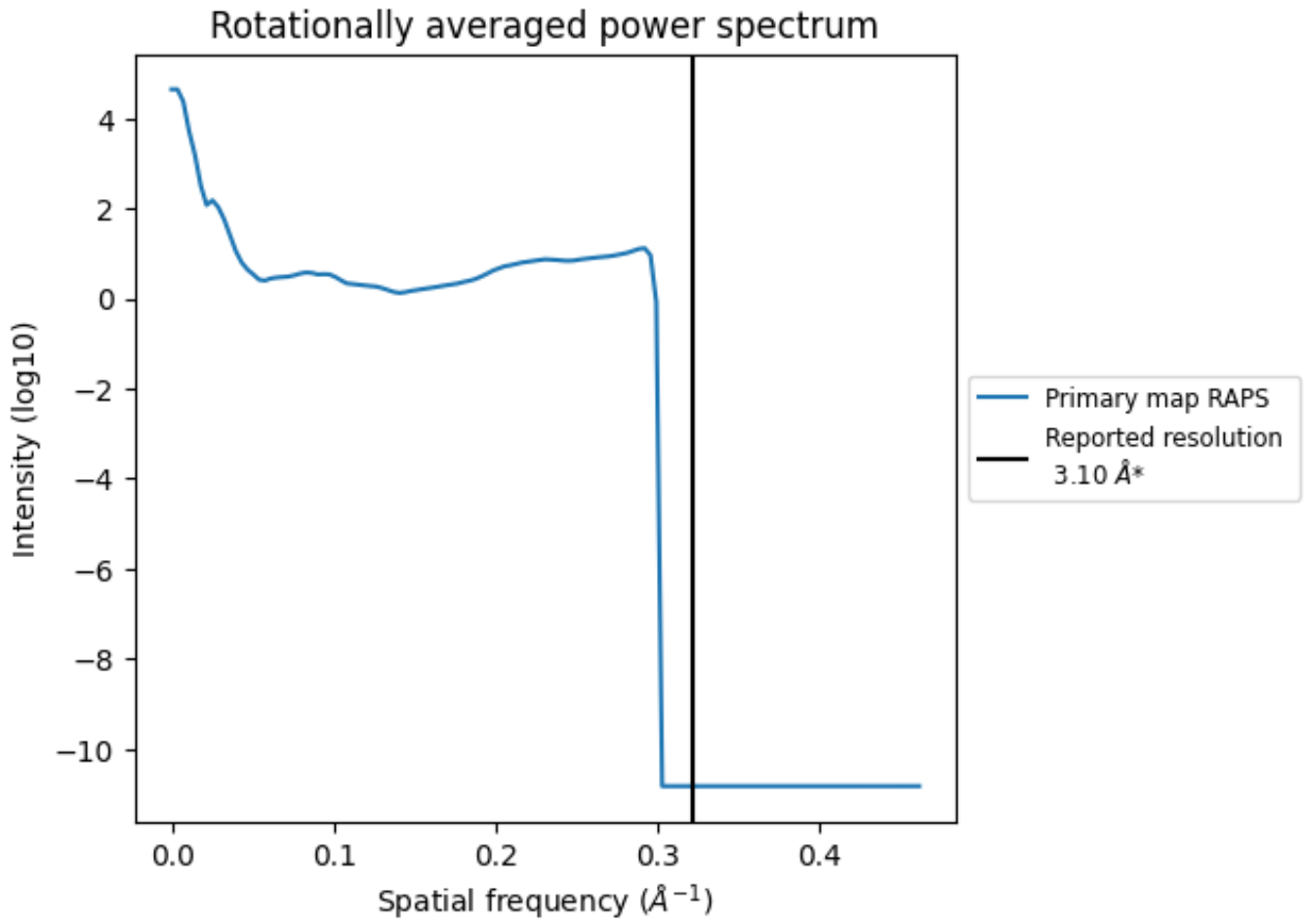
7.2 Volume estimate (i)



The volume at the recommended contour level is 64 nm^3; this corresponds to an approximate mass of 58 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 0.323 Å^{-1}

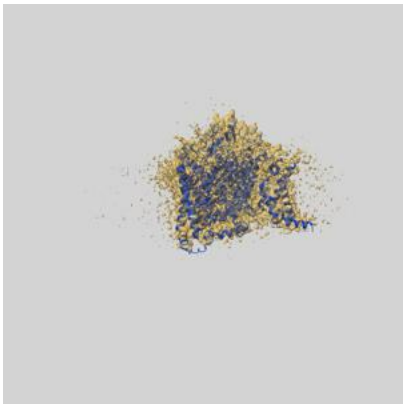
8 Fourier-Shell correlation

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

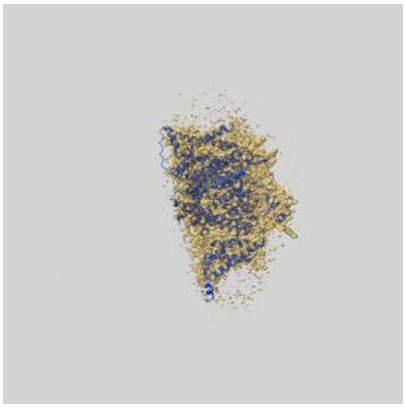
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32476 and PDB model 7WFW. Per-residue inclusion information can be found in section 3 on page 8.

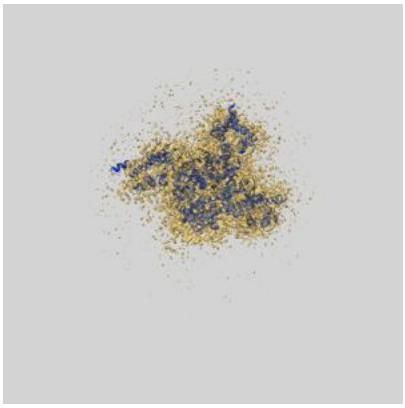
9.1 Map-model overlay



X



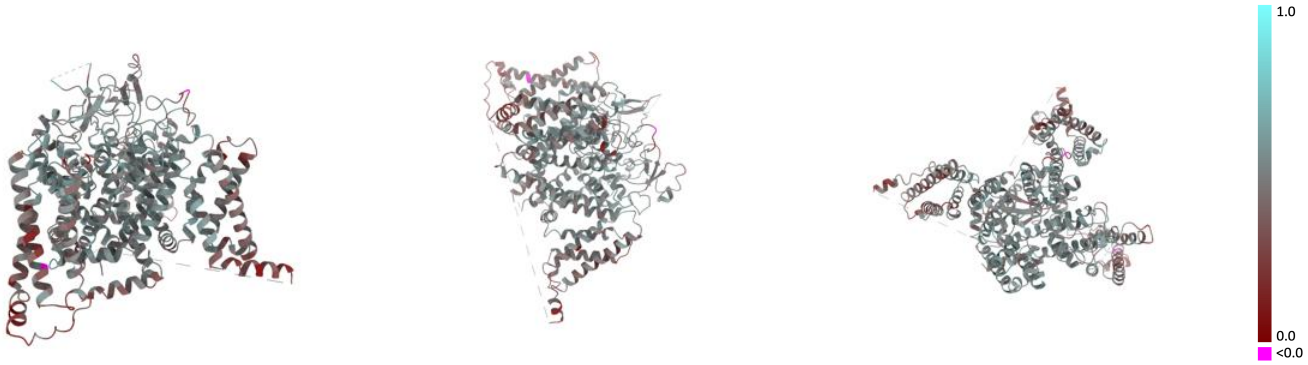
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0249 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.

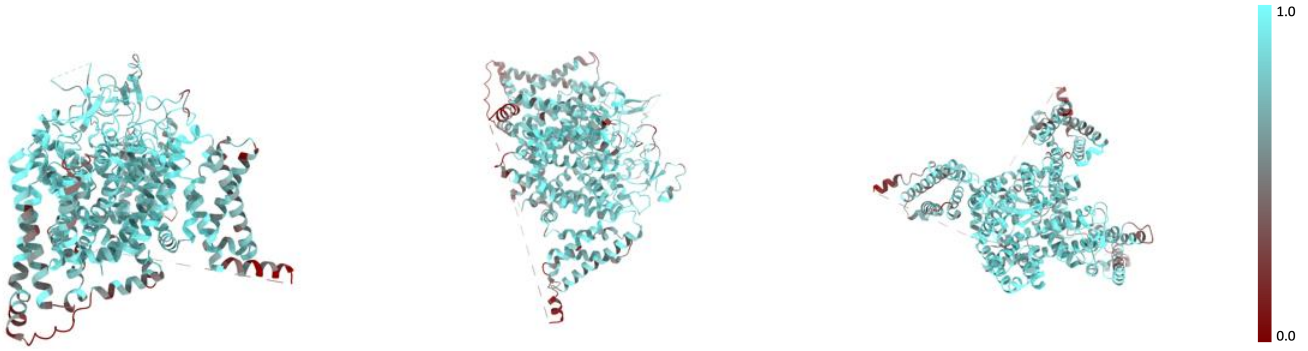
9.2 Q-score mapped to coordinate model



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.

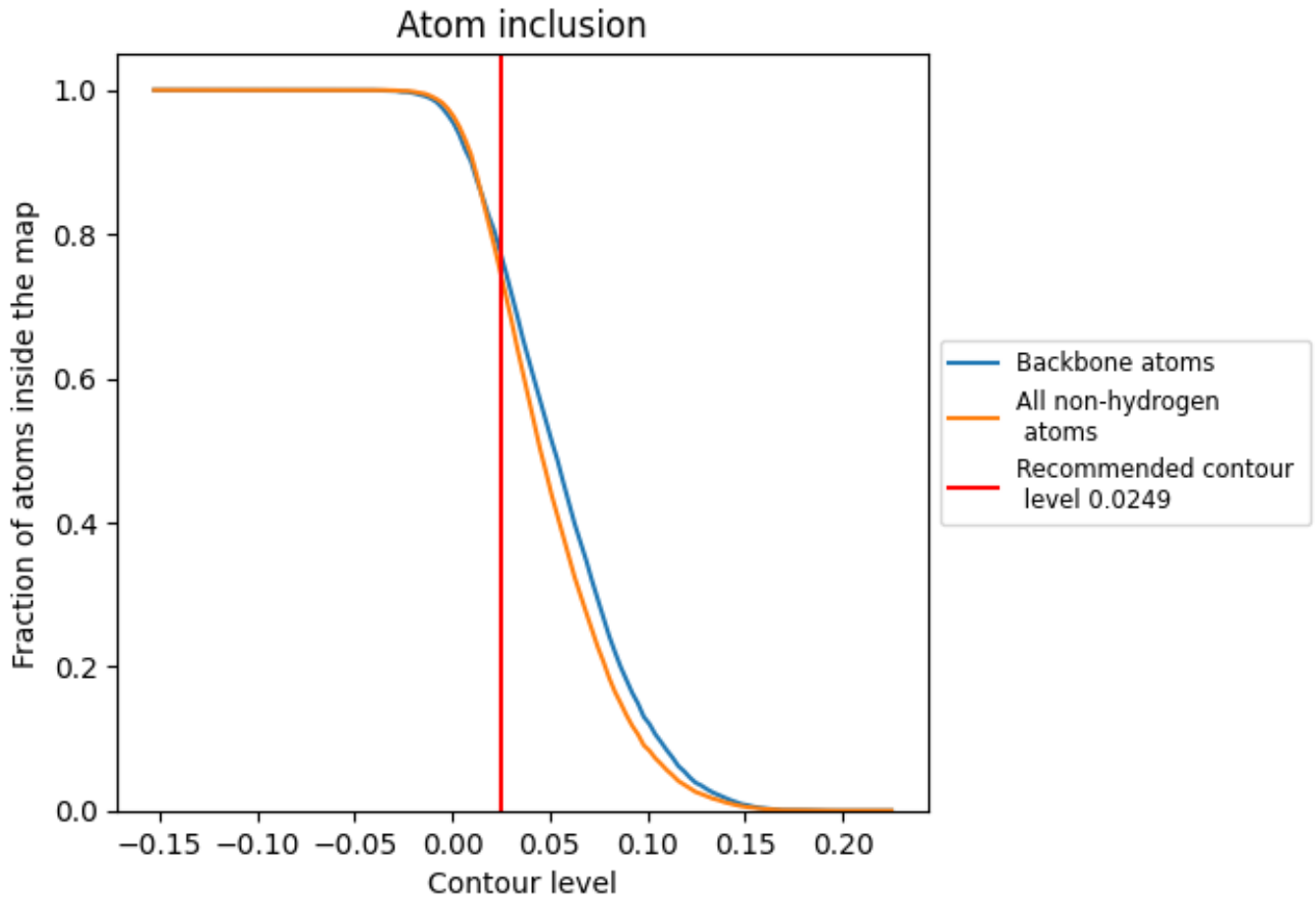
9.3 Atom inclusion mapped to coordinate model



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 (0.0249).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 74% 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 (0.0249) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.4710
A	0.7452	0.4710
B	0.6786	0.3680