



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:20 AM UTC

PDB ID : 7WFW / pdb_00007wfw
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.

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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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

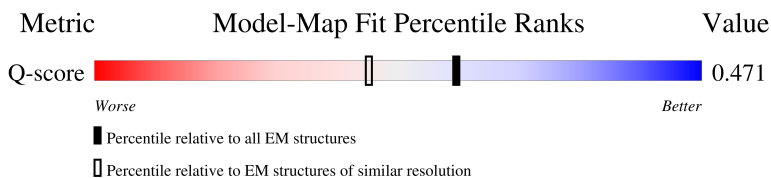
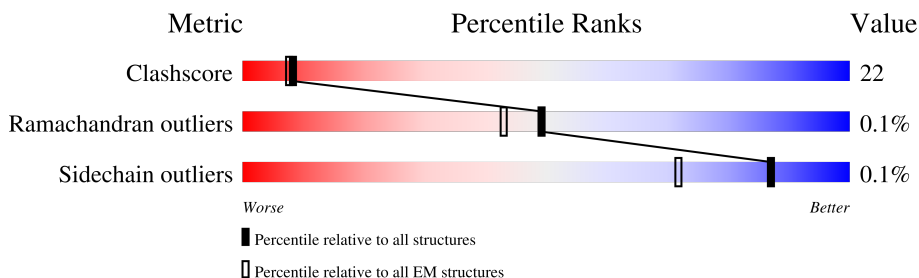
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. 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	
2	B	2	

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.

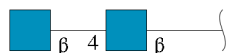
- Molecule 1 is a protein called Sodium channel protein type 10 subunit alpha.

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.



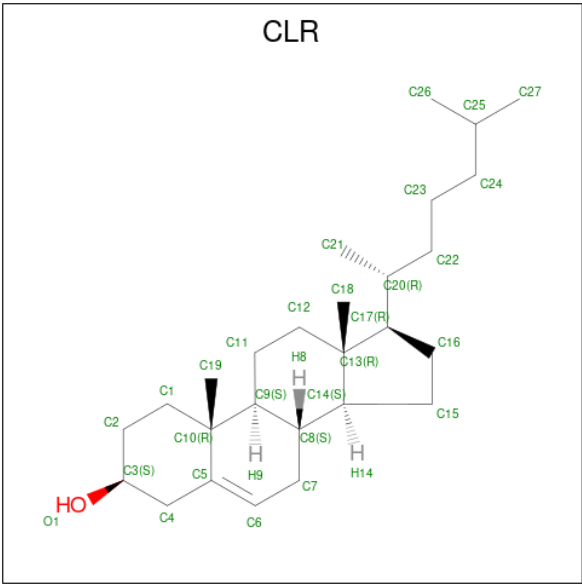
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



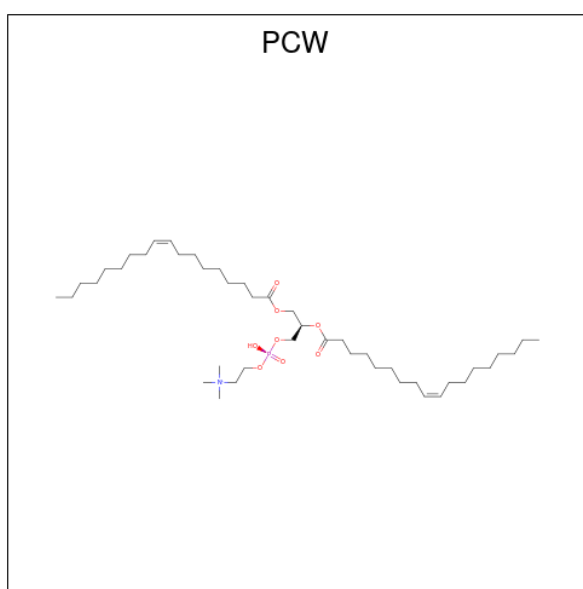
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



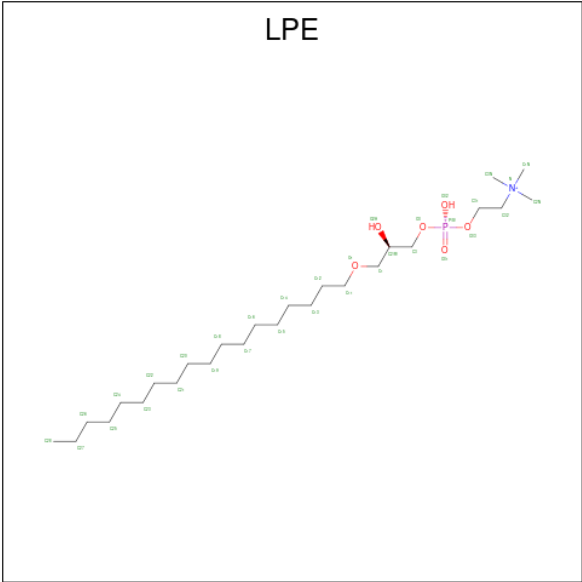
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	

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



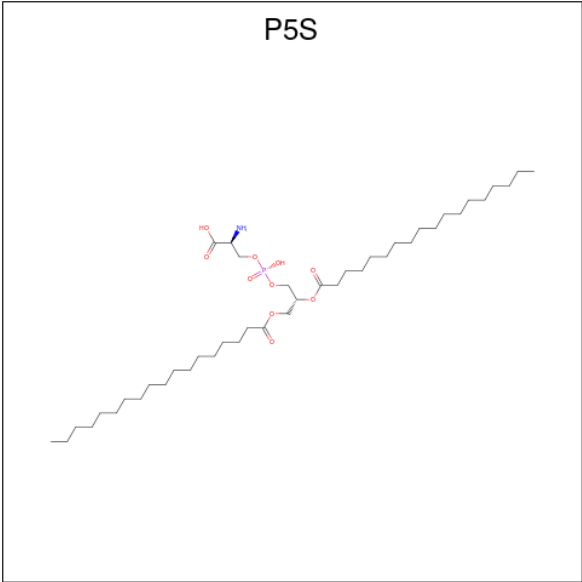
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
5	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
5	A	1	Total	C	O	P		0
			41	32	8	1		

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



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
6	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
6	A	1	Total	C	N	O	P	0
			23	15	1	6	1	
6	A	1	Total	C	N	O	P	0
			34	26	1	6	1	
6	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
6	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
6	A	1	Total	C	N	O	P	0
			21	13	1	6	1	
6	A	1	Total	C	N	O	P	0
			34	26	1	6	1	

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).

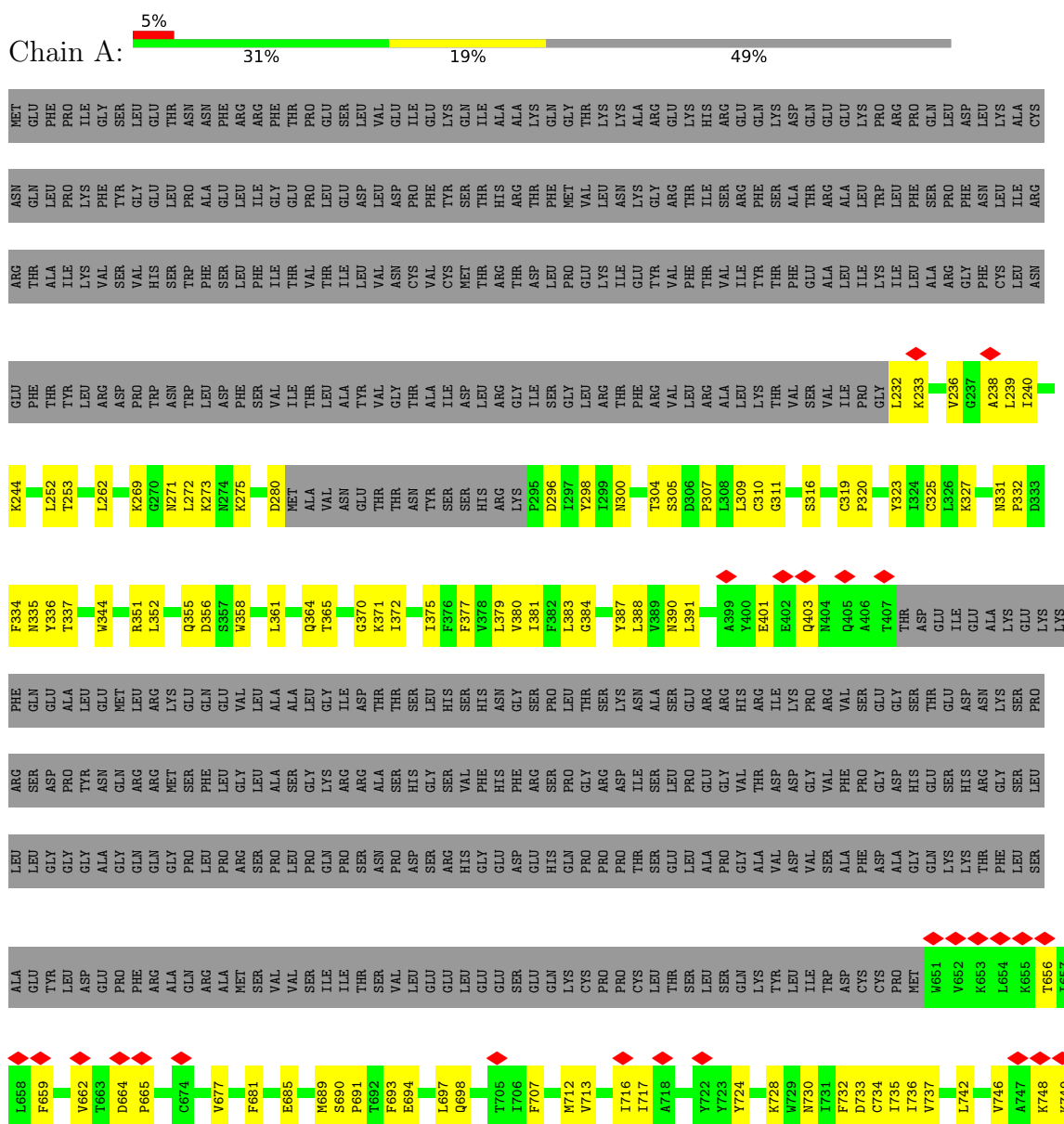


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			49	37	1	10	1	
7	A	1	Total	C	N	O	P	0
			44	32	1	10	1	

3 Residue-property plots

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



L752	S753	V754	L755	F756	S757	F759	L760	L761	L762	L763	F764	K765	S769	L772	L773	L777	K778	L779	L787	L794	V798	F799	V800	V804	G805	L809	G810	E811	R814	N815	N816	K817	N819	P828	R829	W830	H831	M832	H833	I841	I845	W850	I851						
M854	C857	V860	S864	I868	L871	V880	V881	F885	L888	L889	L890	N891	S892	F894	ASP	ASN	ASN	THR	THR	ALA	ALA	THR	ALA	GLU	ASP	ASP	GLY	GLU	VAL	ASN	ASN	R814	N815	N816	K817	N819	P828	R829	W830	H831	M832	H833	I841	I845	W850	I851			
PHE	PHE	SER	ARG	SER	VAL	THR	PRO	PHE	PRO	PRO	ALA	GLN	PRO	GLY	LYS	ALA	GLU	PRO	ASP	GLU	GLY	VAL	VAL	ASP	ASP	GLY	GLU	VAL	ASN	ASN	R814	N815	N816	K817	N819	P828	R829	W830	H831	M832	H833	I841	I845	W850	I851				
PRO	THR	VAL	TRP	GLU	VAL	SER	VAL	PRO	ILE	ALA	GLN	PRO	GLY	GLY	GLY	ALA	GLU	PRO	ASP	ALA	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN				
GLY	THR	SER	SER	GLU	VAL	ASP	LEU	ALA	SER	GLN	SER	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR			
PRO	ASP	CYS	THR	PHE	THR	GLY	CYS	ILE	ARG	GLN	THR	CYS	PRO	CYS	LYS	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR			
D1190	R1191	V1192	F1193	T1194	L1195	I1196	F1197	V1198	F1199	E1200	V1206	V1213	F1214	T1215	N1216	A1217	W1218	C1219	W1220	M1227	L1230	I1231	A1235	K1236	I1237	L1238	E1239	E1242	V1243	A1244	P1245	I1246	L1252	R1253	L1255	L1261	G1266	M1267	R1268	V1269	L1274	A1277	I1278	I1281	M1282	N1283			
PRO	ASP	CYS	CYS	THR	THR	GLU	GLY	CYS	ILE	ARG	GLN	CYS	LYS	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
V1284	V1287	C1288	L1289	F1291	W1292	L1293	L1294	F1295	S1296	I1297	M1298	G1299	V1300	N1301	F1302	F1303	K1306	F1307	W1308	C1309	R1310	I1311	T1314	D1315	G1316	E1317	F1318	L1323	V1326	N1327	N1328	K1329	S1330	K1333	T1338	W1343	V1344	N1345	V1346	N1349	G1356	V1357	L1360	L1361	W1369	M1370			
M1373	V1377	R1380	F1381	V1382	M1383	M1384	Q1385	P1386	K1387	W1388	E1389	D1390	N1391	M1394	Y1395	L1396	Y1397	F1398	V1399	I1400	I1403	F1404	G1405	G1406	F1407	F1408	T1409	N1411	L1412	F1413	V1414	G1415	V1416	I1417	I1418	K1426	K1427	L1428	G1429	G1430	Q1431	D1432	I1433	F1434	T1436	Q1439	K1440	K1441	Y1442
M1446	K1447	K1448	S1451	K1452	P1454	Q1455	K1456	P1457	I1458	P1459	R1460	P1461	L1462	M1463	K1464	F1465	Q1466	G1467	F1468	D1471	A1477	I1480	V1484	L1488	M1489	N1490	I1491	E1496	T1497	D1498	Q1500	S1501	E1502	E1503	K1504	T1505	K1506	I1507	L1508	G1509	K1510	I1511	N1512	Q1513	F1514	V1516	A1517	F1519	
T1520	C1523	V1524	W1525	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	I1582	I1583	L1584	R1585	L1586	I1587	R1588	K1591	G1592	I1593	R1594	I1595	L1596	L1597	
M1602	S1603	L1604	P1605	A1606	L1607	F1608	N1609	L1610	L1616	F1619	Y1621	S1622	I1623	F1629	W1634	E1635	A1636	G1637	I1638	D1639	I1640	M1641	F1642	N1643	L1652	L1666	L1667	S1668	P1669	I1670	L1671	N1672	T1673	Q1674	Y1677	C1678	N1681	L1682	P1683	G1687	T1688	R1689	P1695	I1699	I1700	F1701	F1702		
T1703	T1704	Y1705	L1706	I1707	L1708	S1709	F1710	L1711	V1714	N1715	M1716	Y1717	I1718	I1719	VAL	ALA	THR	THR	GLY	GLU	SER	THR	THR	THR	GLU	ASP	ASP	ASP	ASP	MET	PHE	THR	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
PHE	ALA	ASP	THR	ALA	LEU	THR	ASN	GLY	PRO	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	
GLU	LYS	PHE	NET	THR	ALA	THR	ASN	GLY	PRO	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU

ALA
SER
LEU
PRO
ASP
GLU
GLY
PHE
VAL
ALA
PHE
THR
ALA
ASN
GLU
ASN
CYS
VAL
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ALA
THR
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PHE
PRO
PRO
SER
TYR
GLU
SER
VAL
THR
ARG
GLY
LEU
SER
ASP
ARG
VAL
ASN
MET
ARG
THR
SER
SER
ILE
GLN
ASN
GLU
ASP
GLU
ALA

THR
SER
MET
GLU
LEU
ILE
ALA
PRO
GLY
PRO

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

Chain B:

100%

MAG1
MAG2

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	277.12, 277.12, 277.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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, PCW, LPE, P5S, 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	0.46	0/8269	0.72	12/11206 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ILE	N-CA-C	-11.10	102.26	111.81
1	A	810	GLY	N-CA-C	9.69	124.35	112.73
1	A	817	ARG	N-CA-C	9.54	124.02	112.38
1	A	1329	LYS	N-CA-C	-7.12	103.25	112.23
1	A	809	LEU	N-CA-C	6.97	118.96	111.36
1	A	1455	GLN	N-CA-C	-6.01	99.91	109.23
1	A	1253	ARG	N-CA-C	-5.83	106.02	113.01
1	A	1326	VAL	N-CA-C	5.70	121.20	109.34
1	A	717	ILE	N-CA-C	-5.50	107.02	111.91
1	A	1629	PHE	N-CA-C	5.46	121.88	109.81
1	A	1328	ASN	N-CA-C	5.21	117.10	109.24
1	A	1218	TRP	N-CA-C	-5.15	107.02	113.72

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	347	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	38	0
7	A	93	0	121	14	0
All	All	8689	0	9086	386	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 22.

All (386) 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:1716:MET:HE1	6:A:2008:LPE:C16	1.71	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:685:GLU:HA	1:A:689:MET:HE3	1.77	0.66
1:A:857:CYS:HA	1:A:860:VAL:HG12	1.78	0.65
1:A:1261:LEU:HD23	1:A:1267:MET:HE2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:830:TRP:HZ2	1:A:1370:MET:HE1	1.65	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
1:A:712:MET:HE1	1:A:733:ASP:HB3	1.83	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
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:1294:ILE:HG22	1:A:1298:MET:HE3	1.87	0.57
1:A:1391:ASN:HD22	1:A:1394:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:816:ASN:HB2	1:A:860:VAL:HG23	1.89	0.55
1:A:830:TRP:CZ2	1:A:1370:MET:HE1	2.42	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1282:MET:HE3	1:A:1282:MET:HA	1.92	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
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
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:689:MET:HE2	1:A:693:PHE:HD1	1.76	0.50
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:1490:MET:HE1	1:A:1586:LEU:HD11	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:712:MET:CE	1:A:733:ASP:HB3	2.42	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:310:CYS:C	1:A:325:CYS:SG	2.98	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:1326:VAL:C	1:A:1328:ASN:H	2.23	0.46
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:1369:TRP:CE3	1:A:1373:MET:HE3	2.50	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
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
1:A:238:ALA:HB1	1:A:403:GLN:CD	2.41	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:1267:MET:HE1	1:A:1616:LEU:HD22	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1345:ASN:CG	1:A:1349:ASN:HD22	2.26	0.44
1:A:1672:ASN:HD21	1:A:1677:TYR:HB3	1.79	0.44
1:A:1306:LYS:CG	1:A:1380:ARG:O	2.65	0.44
1:A:1391:ASN:ND2	1:A:1394:MET:HE2	2.31	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: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:1687:GLY:C	1:A:1689:ARG:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1591:LYS:HZ1	1:A:1594:ARG:NH2	2.17	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:370:GLY:O	1:A:371:LYS:C	2.62	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
4:A:2012:CLR:H8	4:A:2012:CLR:H182	1.76	0.42
1:A:271:ASN:C	1:A:273:LYS:H	2.28	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:1641:MET:HE2	1:A:1641:MET:HB3	1.82	0.42
1:A:817:ARG:HB2	1:A:828:PRO:HD3	2.02	0.42
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: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:850:TRP:HZ3	1:A:854:MET:HE1	1.85	0.41
1:A:1356:GLY:O	1:A:1360:LEU:HD13	2.21	0.41
1:A:1370:MET:HE3	1:A:1370:MET:HA	2.01	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:280:ASP:C	1:A:280:ASP:OD1	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:LEU:HA	1:A:755:LEU:HD23	1.77	0.41
1:A:707:PHE:CD2	1:A:707:PHE:C	2.99	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:1195:PHE:CD1	1:A:1195:PHE:C	2.98	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: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:818:LYS:HD3	1:A:818:LYS:C	2.47	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
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: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%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1629	PHE

5.3.2 Protein sidechains ⓘ

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%)	885 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1703	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	A	274	ASN
1	A	355	GLN
1	A	390	ASN
1	A	687	HIS
1	A	730	ASN
1	A	831	HIS
1	A	833	HIS
1	A	853	ASN
1	A	1349	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	2,1	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	B	2	2	14,14,15	0.29	0	17,19,21	0.56	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	2,1	-	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

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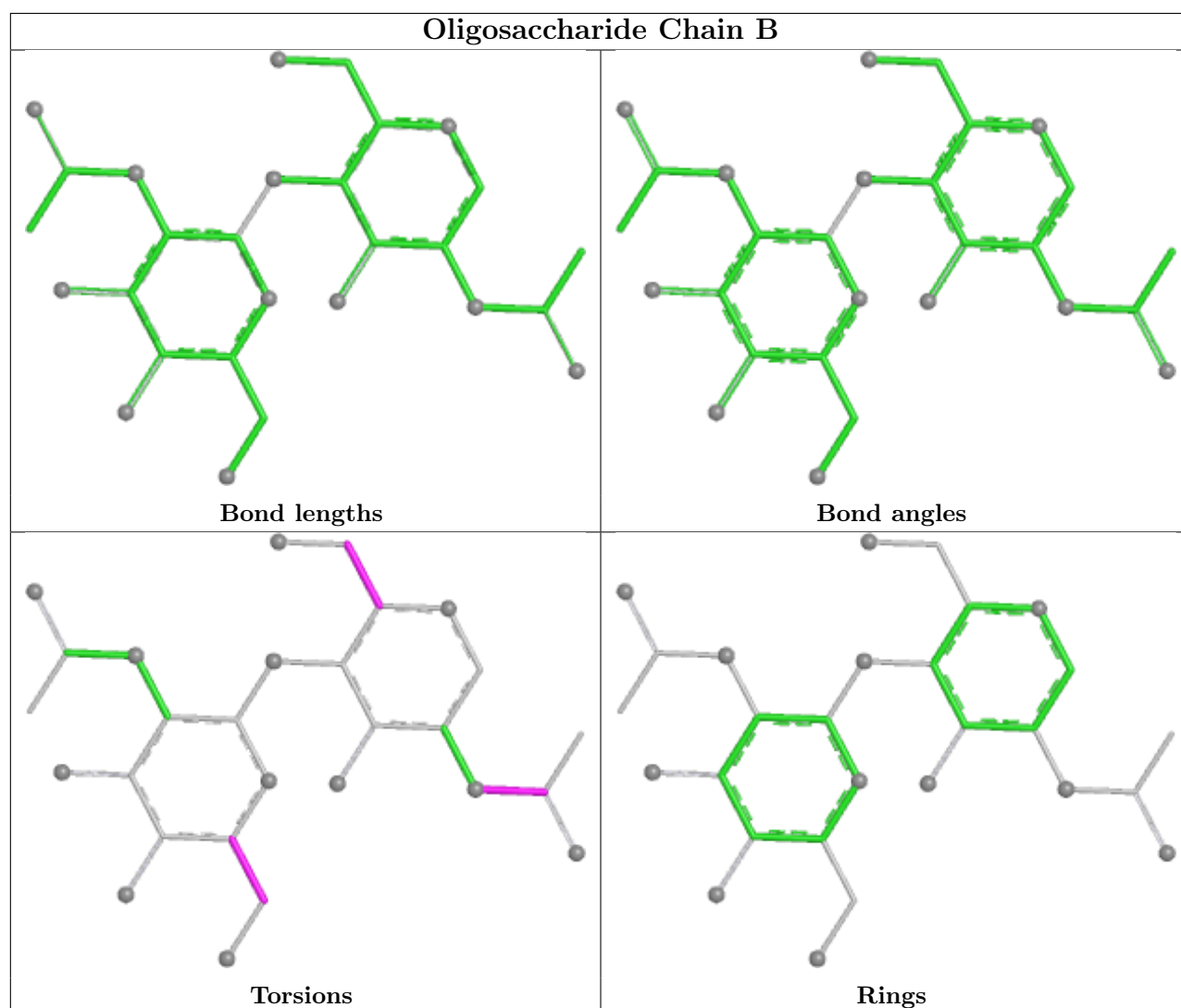
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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



5.6 Ligand geometry

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
5	PCW	A	2007	-	46,46,53	1.01	2 (4%)	52,54,61	1.05	2 (3%)
6	LPE	A	2018	-	33,33,33	0.48	0	37,39,39	0.60	0
6	LPE	A	2009	-	21,21,33	0.59	0	25,27,39	0.59	0
7	P5S	A	2021	-	42,43,53	0.96	3 (7%)	44,50,60	1.49	7 (15%)
6	LPE	A	2016	-	21,21,33	0.58	0	25,27,39	0.71	0
3	NAG	A	2002	1	14,14,15	0.48	0	17,19,21	1.51	3 (17%)
7	P5S	A	2020	-	47,48,53	1.00	2 (4%)	49,55,60	1.38	4 (8%)
4	CLR	A	2005	-	31,31,31	0.73	0	48,48,48	1.20	5 (10%)
6	LPE	A	2010	-	22,22,33	0.55	0	26,28,39	0.61	0
5	PCW	A	2006	-	47,47,53	0.98	2 (4%)	53,55,61	1.17	5 (9%)
6	LPE	A	2017	-	20,20,33	0.59	0	24,26,39	0.62	0
4	CLR	A	2014	-	31,31,31	0.83	2 (6%)	48,48,48	1.59	8 (16%)
3	NAG	A	2004	1	14,14,15	0.56	0	17,19,21	1.62	2 (11%)
5	PCW	A	2011	-	40,40,53	1.06	2 (5%)	43,45,61	1.16	4 (9%)
6	LPE	A	2015	-	21,21,33	0.68	0	25,27,39	0.79	1 (4%)
3	NAG	A	2001	1	14,14,15	0.31	0	17,19,21	1.67	4 (23%)
6	LPE	A	2013	-	33,33,33	0.48	0	37,39,39	0.63	0
3	NAG	A	2003	1	14,14,15	0.33	0	17,19,21	1.11	1 (5%)
4	CLR	A	2012	-	31,31,31	0.82	2 (6%)	48,48,48	1.56	7 (14%)
6	LPE	A	2008	-	21,21,33	0.58	0	25,27,39	0.54	0
4	CLR	A	2019	-	31,31,31	0.94	2 (6%)	48,48,48	1.42	7 (14%)

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
5	PCW	A	2007	-	-	30/50/50/57	-
6	LPE	A	2018	-	-	18/34/34/34	-
6	LPE	A	2009	-	-	12/22/22/34	-
7	P5S	A	2021	-	-	11/49/49/59	-
6	LPE	A	2016	-	-	4/22/22/34	-
3	NAG	A	2002	1	-	1/6/23/26	0/1/1/1
7	P5S	A	2020	-	-	7/54/54/59	-
4	CLR	A	2005	-	-	3/10/68/68	0/4/4/4
6	LPE	A	2010	-	-	7/23/23/34	-
5	PCW	A	2006	-	-	21/51/51/57	-
6	LPE	A	2017	-	-	5/21/21/34	-
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
5	PCW	A	2011	-	-	10/42/42/57	-
6	LPE	A	2015	-	-	10/22/22/34	-
3	NAG	A	2001	1	-	3/6/23/26	0/1/1/1
6	LPE	A	2013	-	-	4/34/34/34	-
3	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
4	CLR	A	2012	-	-	4/10/68/68	0/4/4/4
6	LPE	A	2008	-	-	13/22/22/34	-
4	CLR	A	2019	-	-	6/10/68/68	0/4/4/4

All (17) 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	4.40	1.46	1.33
5	A	2011	PCW	O3-C11	4.31	1.45	1.33
5	A	2007	PCW	O3-C11	4.25	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	3.82	1.44	1.33
7	A	2021	P5S	O19-C17	3.78	1.44	1.33
7	A	2021	P5S	O37-C38	3.64	1.44	1.34
4	A	2019	CLR	C10-C9	-2.52	1.52	1.56
4	A	2019	CLR	C13-C14	-2.16	1.51	1.55
7	A	2021	P5S	O37-C2	-2.16	1.41	1.46
4	A	2012	CLR	C10-C9	-2.11	1.52	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2014	CLR	C13-C14	-2.04	1.51	1.55
4	A	2014	CLR	C10-C9	-2.03	1.52	1.56
4	A	2012	CLR	C13-C14	-2.01	1.51	1.55

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	-4.90	111.92	119.50
4	A	2012	CLR	C13-C17-C20	-4.88	111.95	119.50
3	A	2004	NAG	C4-C3-C2	-4.57	104.32	111.02
4	A	2014	CLR	C13-C14-C8	-4.33	108.26	114.41
4	A	2012	CLR	C13-C14-C8	-4.26	108.37	114.41
3	A	2001	NAG	C4-C3-C2	-4.23	104.81	111.02
3	A	2002	NAG	O5-C1-C2	-4.04	105.03	111.29
7	A	2021	P5S	O37-C38-C39	3.97	120.06	111.48
7	A	2020	P5S	O37-C38-C39	3.91	119.94	111.48
5	A	2007	PCW	O2-C31-C32	3.84	119.78	111.48
3	A	2003	NAG	C4-C3-C2	-3.83	105.40	111.02
5	A	2006	PCW	O2-C31-C32	3.67	119.42	111.48
4	A	2012	CLR	C17-C13-C14	3.61	104.24	100.10
4	A	2014	CLR	C17-C13-C14	3.61	104.24	100.10
4	A	2019	CLR	C11-C12-C13	-3.59	106.68	112.74
4	A	2019	CLR	C13-C17-C20	-3.58	113.96	119.50
3	A	2004	NAG	C6-C5-C4	-3.52	104.37	113.02
4	A	2019	CLR	C16-C17-C20	3.46	117.42	112.18
5	A	2011	PCW	O2-C31-C32	3.45	118.94	111.48
3	A	2001	NAG	C2-N2-C7	3.36	127.41	122.90
4	A	2005	CLR	C13-C17-C20	-3.36	114.31	119.50
7	A	2021	P5S	O19-C17-C20	3.31	121.94	111.83
5	A	2006	PCW	O3-C11-C12	3.30	121.89	111.83
5	A	2011	PCW	O3-C11-C12	3.08	121.22	111.83
3	A	2002	NAG	C4-C3-C2	-2.84	106.86	111.02
5	A	2007	PCW	O3-C11-C12	2.84	120.49	111.83
7	A	2020	P5S	OXT-C-O	-2.78	117.77	124.08
4	A	2014	CLR	C11-C12-C13	-2.78	108.05	112.74
4	A	2012	CLR	C11-C12-C13	-2.74	108.11	112.74
4	A	2019	CLR	C21-C20-C17	-2.72	108.79	112.88
4	A	2019	CLR	C11-C9-C10	-2.72	109.73	113.08
4	A	2005	CLR	C13-C14-C8	-2.60	110.72	114.41
4	A	2014	CLR	C8-C7-C6	-2.56	109.21	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2021	P5S	OXT-C-O	-2.56	118.27	124.08
3	A	2001	NAG	C1-C2-N2	-2.56	106.40	110.43
4	A	2005	CLR	C11-C12-C13	-2.56	108.43	112.74
5	A	2006	PCW	C3-C2-C1	-2.55	105.85	111.78
4	A	2019	CLR	C22-C20-C17	2.53	115.58	110.33
4	A	2014	CLR	C7-C6-C5	-2.50	120.81	125.02
7	A	2020	P5S	O19-C17-C20	2.47	119.37	111.83
5	A	2006	PCW	O3-C11-O11	-2.37	117.69	123.63
5	A	2011	PCW	O1P-P-O2P	2.37	120.06	110.83
4	A	2005	CLR	C4-C5-C10	2.36	119.44	116.42
7	A	2021	P5S	O37-C38-O47	-2.33	118.25	123.70
4	A	2012	CLR	C4-C5-C10	2.32	119.39	116.42
6	A	2015	LPE	C3-C2-C1	-2.30	106.03	112.65
4	A	2014	CLR	C3-C4-C5	-2.30	108.39	112.05
7	A	2021	P5S	C2-O37-C38	-2.25	112.40	117.80
4	A	2005	CLR	C17-C13-C14	2.25	102.68	100.10
4	A	2019	CLR	C23-C22-C20	-2.17	109.02	115.08
4	A	2012	CLR	C7-C8-C9	2.11	112.17	109.72
7	A	2021	P5S	O19-C17-O18	-2.11	118.35	123.63
5	A	2011	PCW	C2-O2-C31	-2.11	112.75	117.80
4	A	2012	CLR	C10-C9-C8	-2.10	109.64	112.71
4	A	2014	CLR	C1-C2-C3	2.08	113.23	110.48
3	A	2001	NAG	O3-C3-C2	2.01	113.57	109.40
3	A	2002	NAG	C3-C4-C5	-2.00	106.60	110.23
5	A	2006	PCW	C2-O2-C31	-2.00	113.00	117.80

There are no chirality outliers.

All (175) 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

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Mol	Chain	Res	Type	Atoms
6	A	2008	LPE	C3-O3-P-O32
6	A	2008	LPE	C3-O3-P-O33
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-O3
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	2010	LPE	C3-O3-P-O33
6	A	2013	LPE	C31-O33-P-O31
6	A	2015	LPE	C3-O3-P-O32
6	A	2015	LPE	C3-O3-P-O33
6	A	2015	LPE	C31-O33-P-O3
6	A	2015	LPE	C31-O33-P-O32
6	A	2016	LPE	C31-O33-P-O3
6	A	2016	LPE	O33-C31-C32-N
6	A	2017	LPE	C31-O33-P-O3
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
5	A	2006	PCW	C12-C11-O3-C3
4	A	2019	CLR	C16-C17-C20-C22
4	A	2019	CLR	C13-C17-C20-C22
6	A	2018	LPE	O2H-C2-C3-O3
4	A	2019	CLR	C13-C17-C20-C21
5	A	2006	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
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	2009	LPE	O2H-C2-C3-O3
6	A	2015	LPE	C2-C3-O3-P
4	A	2005	CLR	C23-C24-C25-C27
7	A	2020	P5S	C44-C45-C46-C48
5	A	2007	PCW	C33-C34-C35-C36
6	A	2018	LPE	C23-C24-C25-C26
4	A	2005	CLR	C23-C24-C25-C26
5	A	2006	PCW	C35-C36-C37-C38
5	A	2007	PCW	C31-C32-C33-C34
4	A	2005	CLR	C22-C23-C24-C25
5	A	2007	PCW	C13-C14-C15-C16
7	A	2020	P5S	C21-C22-C23-C24
5	A	2006	PCW	C4-C5-N-C6
5	A	2006	PCW	C4-C5-N-C8
6	A	2018	LPE	C24-C25-C26-C27
5	A	2007	PCW	C35-C36-C37-C38
5	A	2011	PCW	C32-C31-O2-C2
6	A	2018	LPE	C22-C23-C24-C25
5	A	2011	PCW	O31-C31-O2-C2
6	A	2018	LPE	O1-C11-C12-C13
6	A	2018	LPE	C11-C12-C13-C14
6	A	2018	LPE	C21-C22-C23-C24
5	A	2006	PCW	C15-C16-C17-C18
5	A	2006	PCW	C34-C35-C36-C37
6	A	2018	LPE	C13-C14-C15-C16
6	A	2009	LPE	C11-C12-C13-C14
6	A	2018	LPE	C20-C21-C22-C23
5	A	2006	PCW	C40-C41-C42-C43
6	A	2008	LPE	C2-C1-O1-C11
6	A	2010	LPE	C2-C1-O1-C11
5	A	2007	PCW	C43-C44-C45-C46
5	A	2007	PCW	O2-C2-C3-O3
6	A	2009	LPE	C13-C14-C15-C16
5	A	2011	PCW	C12-C11-O3-C3
6	A	2009	LPE	O1-C11-C12-C13
4	A	2014	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
5	A	2007	PCW	C44-C45-C46-C47
6	A	2018	LPE	C14-C15-C16-C17
5	A	2007	PCW	C32-C33-C34-C35
7	A	2020	P5S	O19-C1-C2-C3
4	A	2012	CLR	C23-C24-C25-C26
7	A	2021	P5S	O37-C2-C3-O16
5	A	2006	PCW	C19-C20-C21-C22
7	A	2021	P5S	C1-C2-C3-O16
6	A	2009	LPE	C2-C3-O3-P
5	A	2011	PCW	O11-C11-O3-C3
5	A	2006	PCW	O3P-C1-C2-O2
5	A	2007	PCW	C1-C2-C3-O3
6	A	2010	LPE	C12-C11-O1-C1
6	A	2017	LPE	C32-C31-O33-P
7	A	2020	P5S	O19-C1-C2-O37
5	A	2007	PCW	C15-C16-C17-C18
6	A	2013	LPE	O33-C31-C32-N
6	A	2015	LPE	O33-C31-C32-N
6	A	2017	LPE	O33-C31-C32-N
7	A	2020	P5S	N-CA-CB-OG
7	A	2021	P5S	N-CA-CB-OG
5	A	2007	PCW	O3P-C1-C2-C3
4	A	2012	CLR	C23-C24-C25-C27
6	A	2008	LPE	O2H-C2-C3-O3
5	A	2007	PCW	C42-C43-C44-C45
5	A	2007	PCW	C45-C46-C47-C48
5	A	2007	PCW	C16-C17-C18-C19
5	A	2006	PCW	C32-C33-C34-C35
5	A	2006	PCW	C16-C17-C18-C19
5	A	2006	PCW	C4-O4P-P-O1P
5	A	2006	PCW	C4-O4P-P-O3P
5	A	2007	PCW	C1-O3P-P-O2P
6	A	2013	LPE	C31-O33-P-O3
6	A	2016	LPE	C31-O33-P-O31
6	A	2017	LPE	C3-O3-P-O31
6	A	2017	LPE	C31-O33-P-O31
6	A	2016	LPE	C2-C1-O1-C11
6	A	2013	LPE	C12-C11-O1-C1
5	A	2007	PCW	C3-C2-O2-C31
4	A	2019	CLR	C20-C22-C23-C24
6	A	2008	LPE	O1-C1-C2-C3
6	A	2008	LPE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	2011	PCW	O2-C31-C32-C33
5	A	2006	PCW	O2-C2-C3-O3
5	A	2011	PCW	C19-C20-C21-C22
5	A	2007	PCW	C36-C37-C38-C39
5	A	2007	PCW	C40-C41-C42-C43
6	A	2015	LPE	O1-C1-C2-C3
5	A	2007	PCW	C14-C15-C16-C17
5	A	2007	PCW	C41-C42-C43-C44
6	A	2018	LPE	C16-C17-C18-C19
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
5	A	2011	PCW	C32-C33-C34-C35
6	A	2008	LPE	O1-C1-C2-O2H
3	A	2002	NAG	C1-C2-N2-C7
5	A	2007	PCW	O3P-C1-C2-O2
6	A	2015	LPE	C12-C13-C14-C15
4	A	2019	CLR	C23-C24-C25-C26
5	A	2006	PCW	O3P-C1-C2-C3
5	A	2006	PCW	C39-C40-C41-C42
5	A	2007	PCW	C2-C1-O3P-P
6	A	2008	LPE	C31-C32-N-C3N
5	A	2006	PCW	C17-C18-C19-C20
5	A	2007	PCW	C39-C40-C41-C42
7	A	2020	P5S	C17-C20-C21-C22
6	A	2008	LPE	C31-C32-N-C1N
7	A	2020	P5S	OXT-C-CA-N
7	A	2021	P5S	O37-C38-C39-C40
5	A	2007	PCW	O2-C31-C32-C33
7	A	2021	P5S	C39-C40-C41-C42
6	A	2015	LPE	C31-C32-N-C2N
5	A	2007	PCW	O3-C11-C12-C13
6	A	2008	LPE	C31-C32-N-C2N
5	A	2007	PCW	O31-C31-C32-C33
7	A	2021	P5S	O47-C38-C39-C40
5	A	2007	PCW	C11-C12-C13-C14

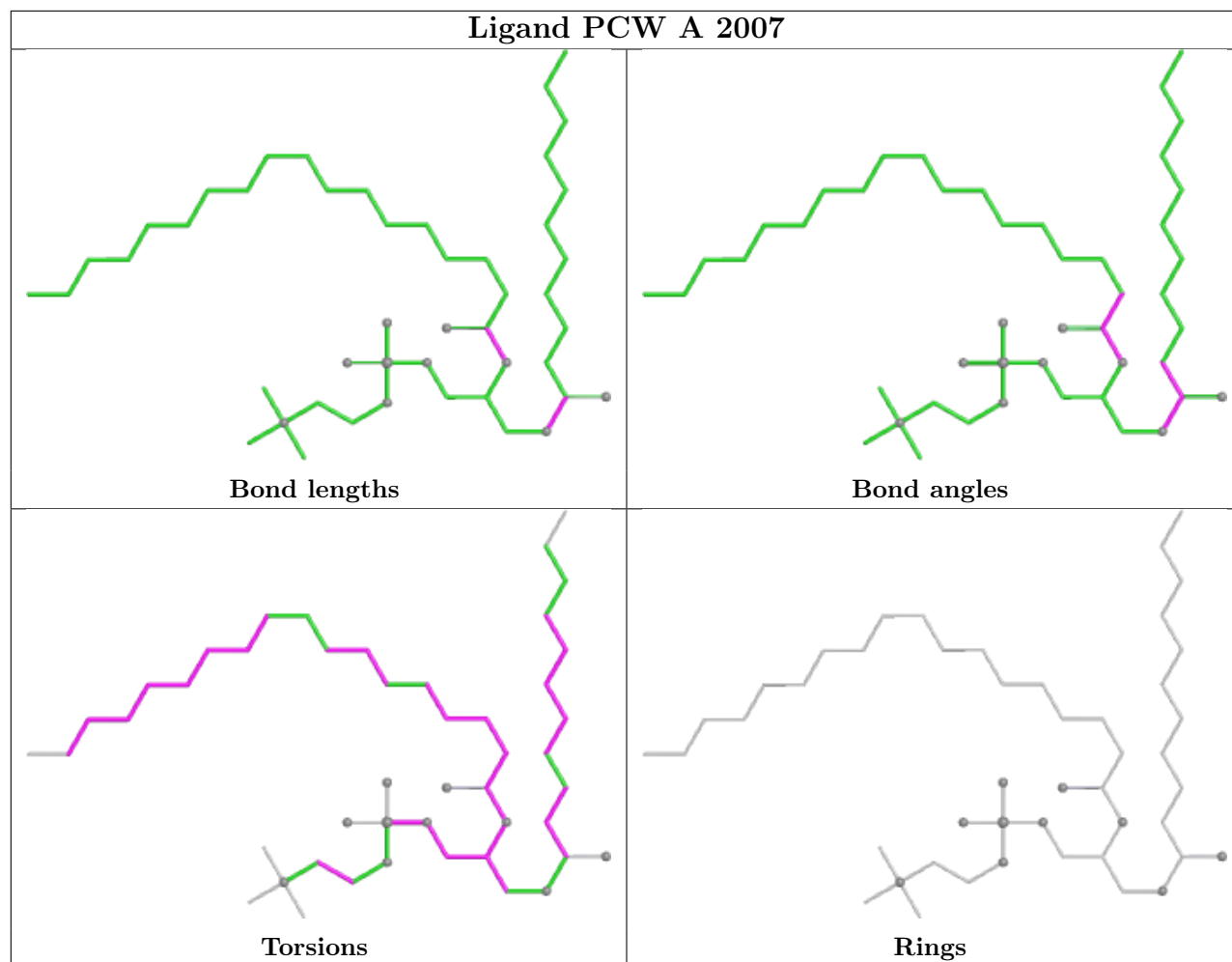
There are no ring outliers.

18 monomers are involved in 93 short contacts:

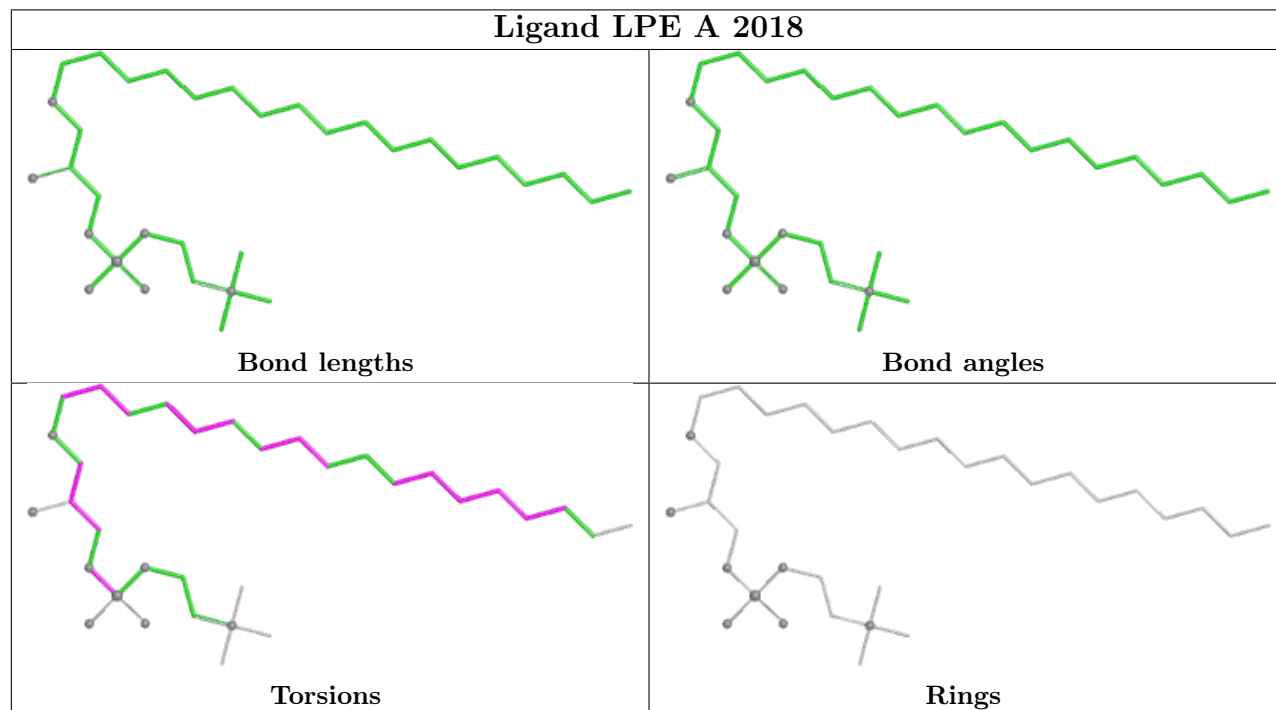
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2007	PCW	10	0
6	A	2018	LPE	5	0
6	A	2009	LPE	3	0
7	A	2021	P5S	9	0
6	A	2016	LPE	4	0
7	A	2020	P5S	5	0
4	A	2005	CLR	6	0
6	A	2010	LPE	3	0
5	A	2006	PCW	7	0
4	A	2014	CLR	3	0
3	A	2004	NAG	1	0
5	A	2011	PCW	8	0
6	A	2015	LPE	12	0
6	A	2013	LPE	4	0
3	A	2003	NAG	3	0
4	A	2012	CLR	12	0
6	A	2008	LPE	7	0
4	A	2019	CLR	2	0

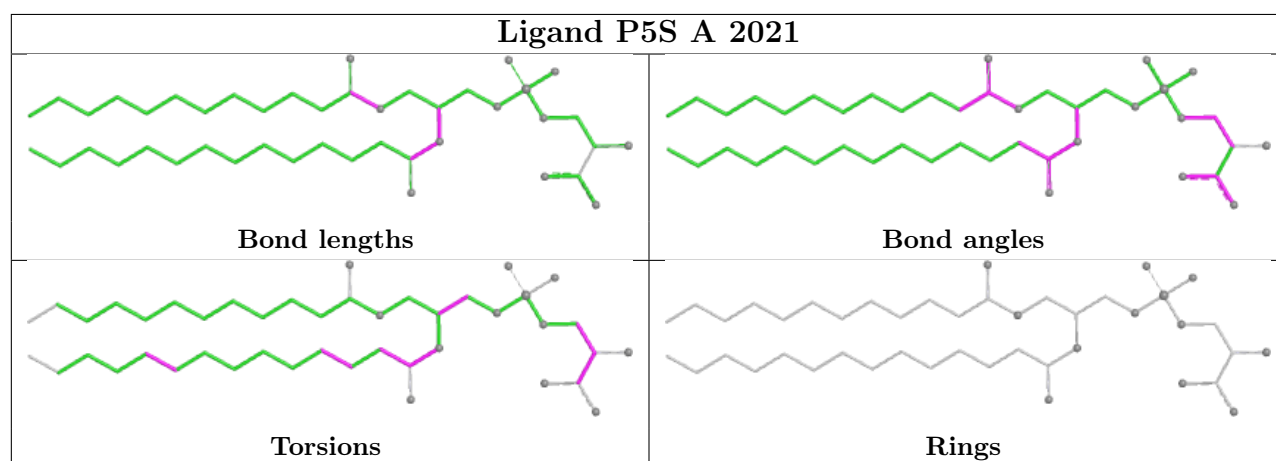
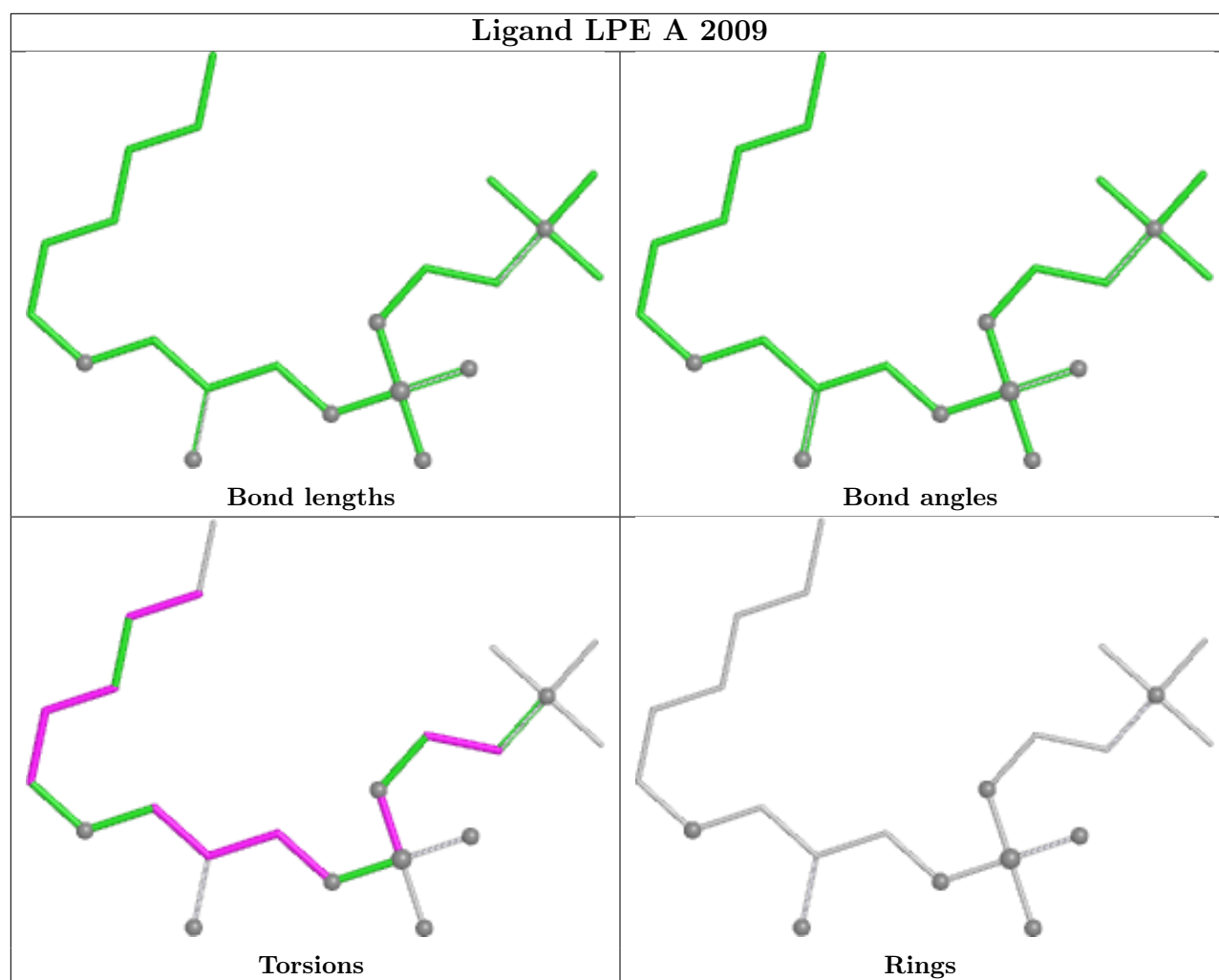
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

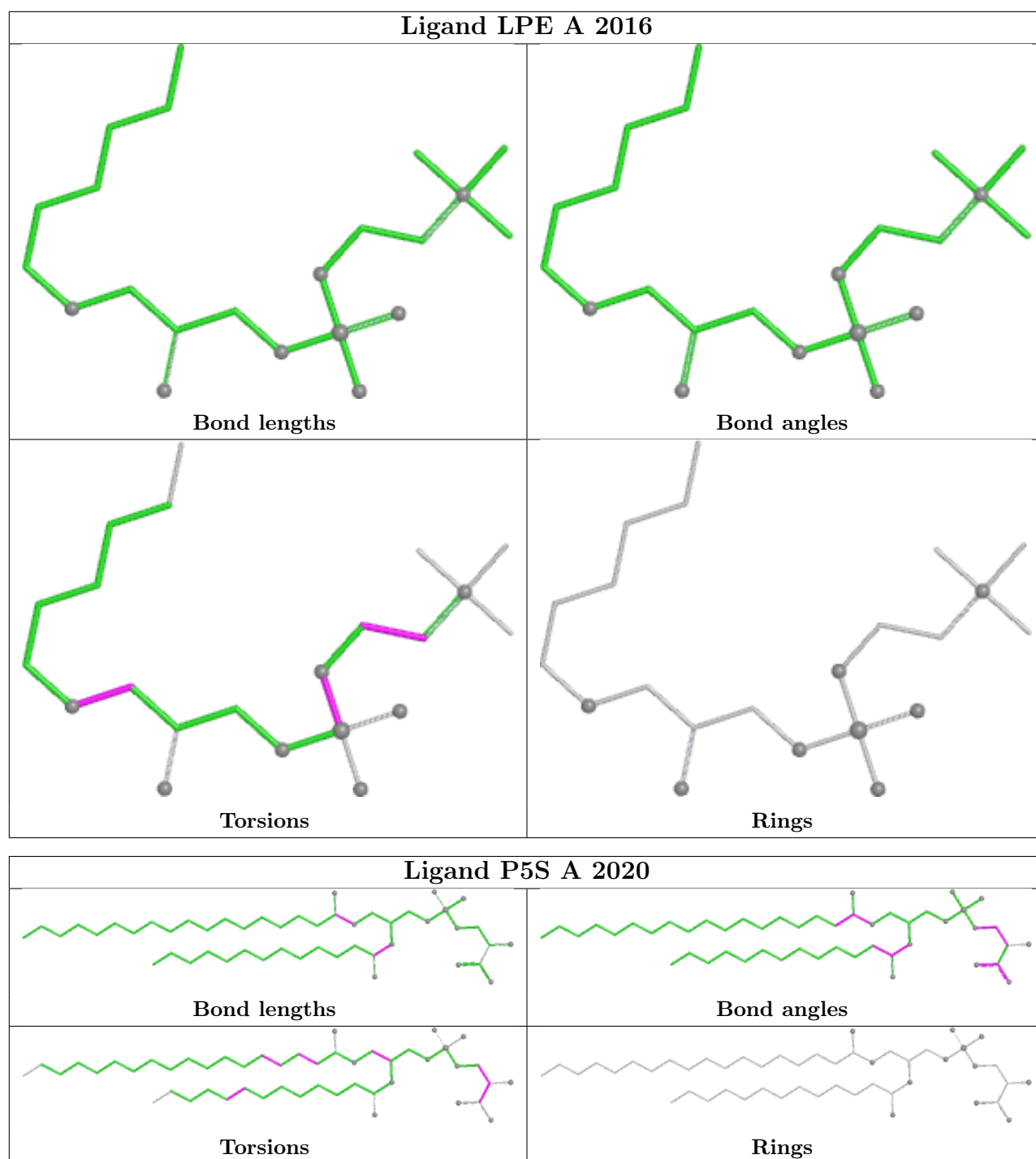
Ligand PCW A 2007

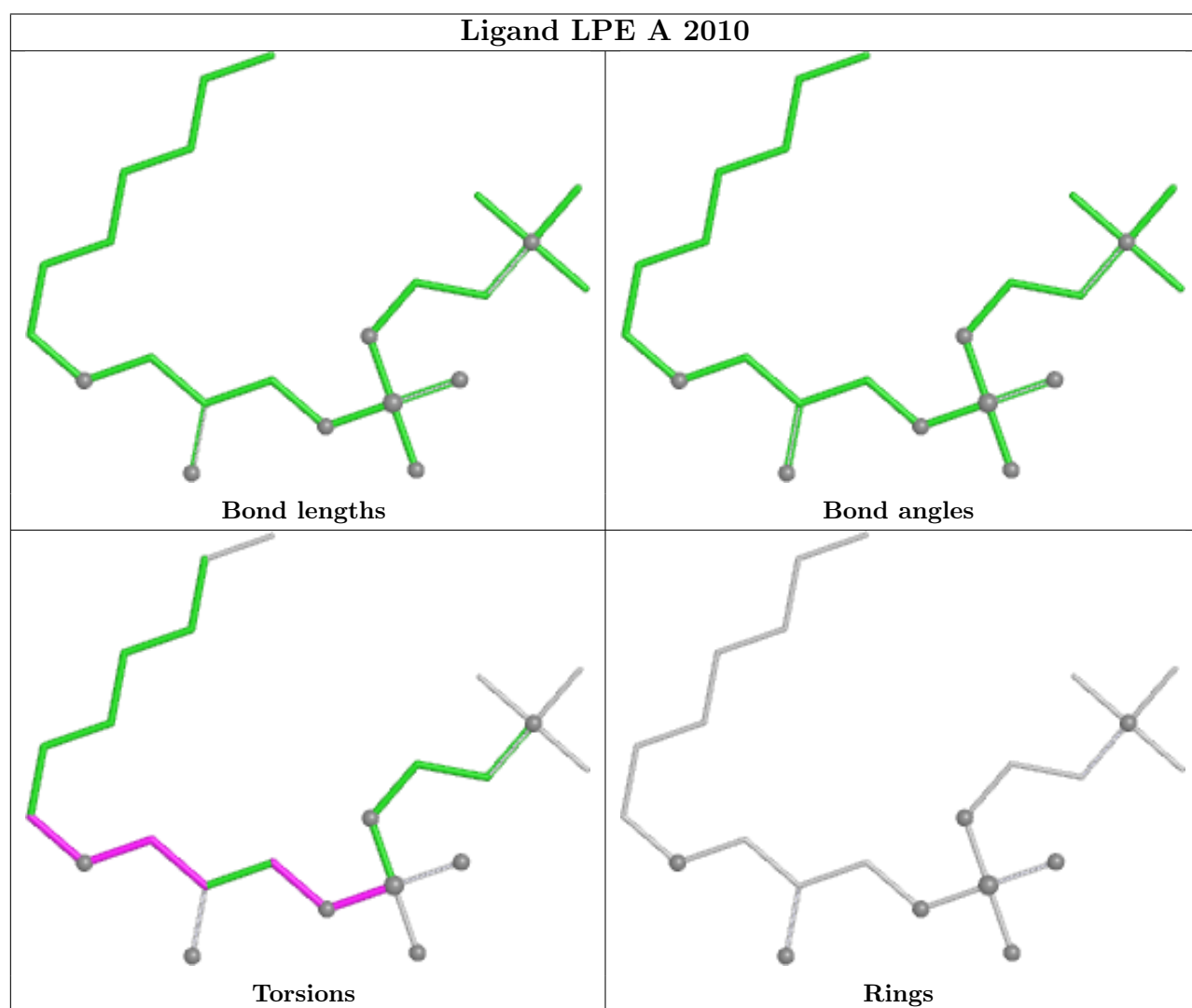
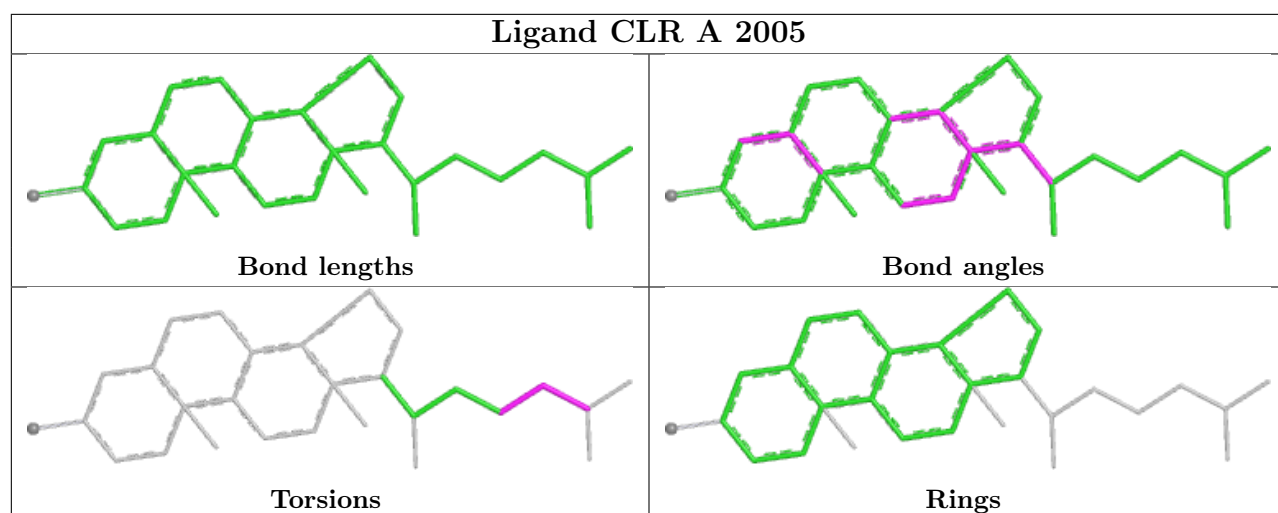


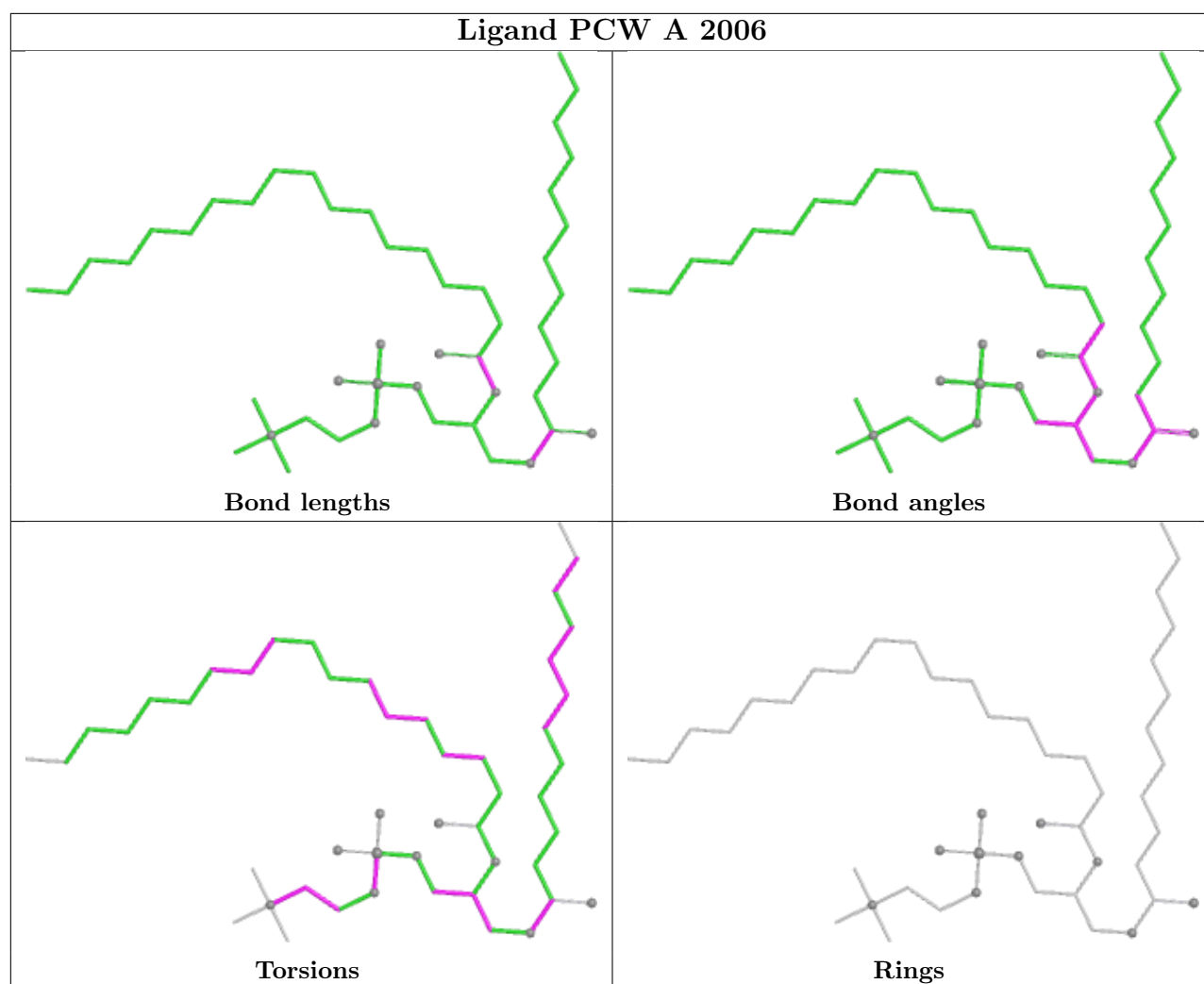
Ligand LPE A 2018

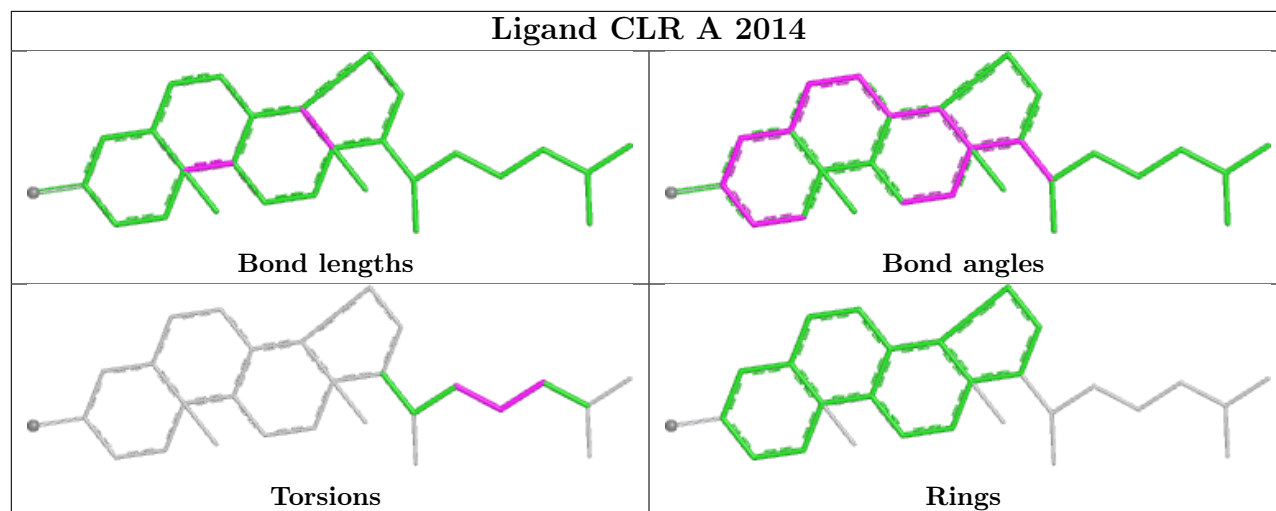
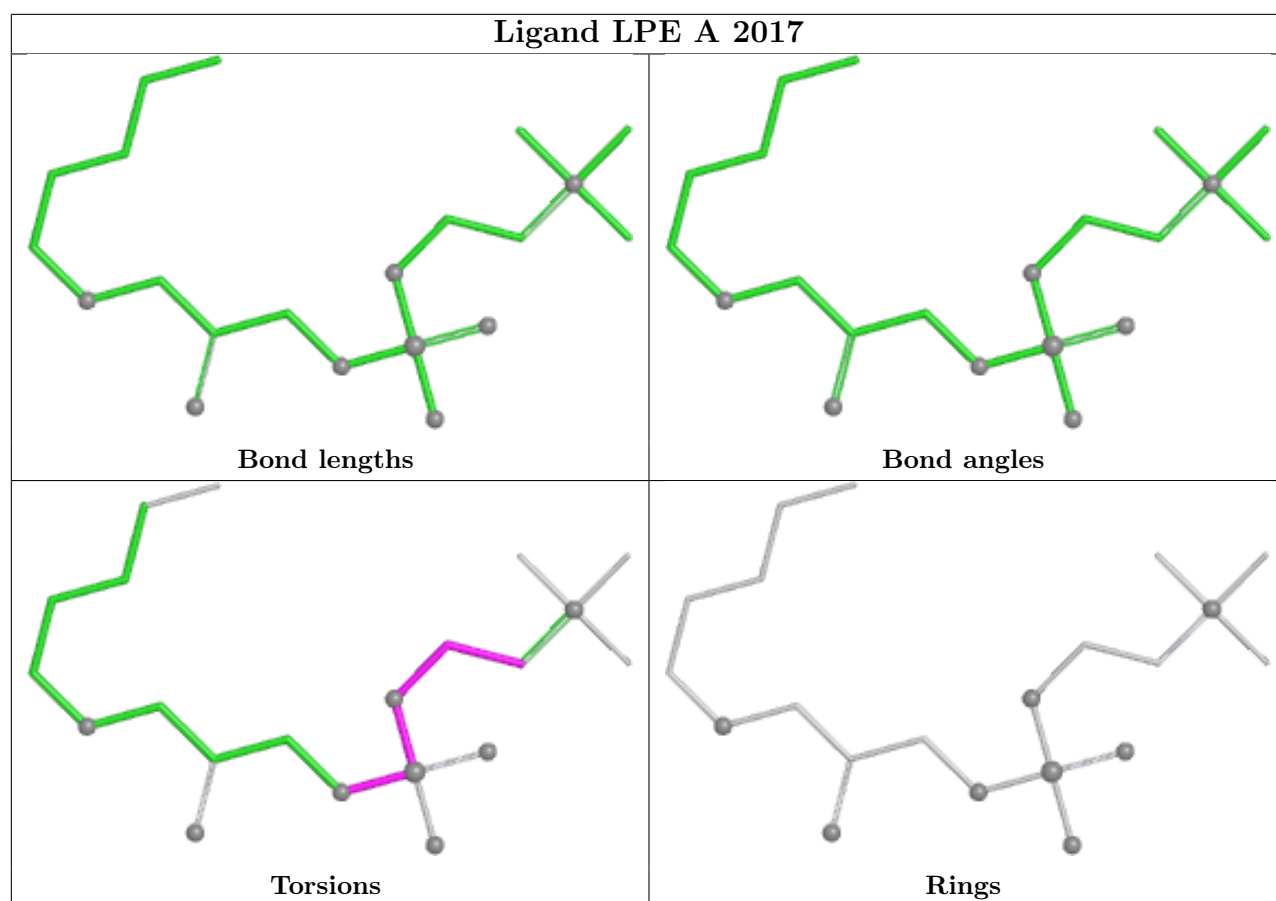


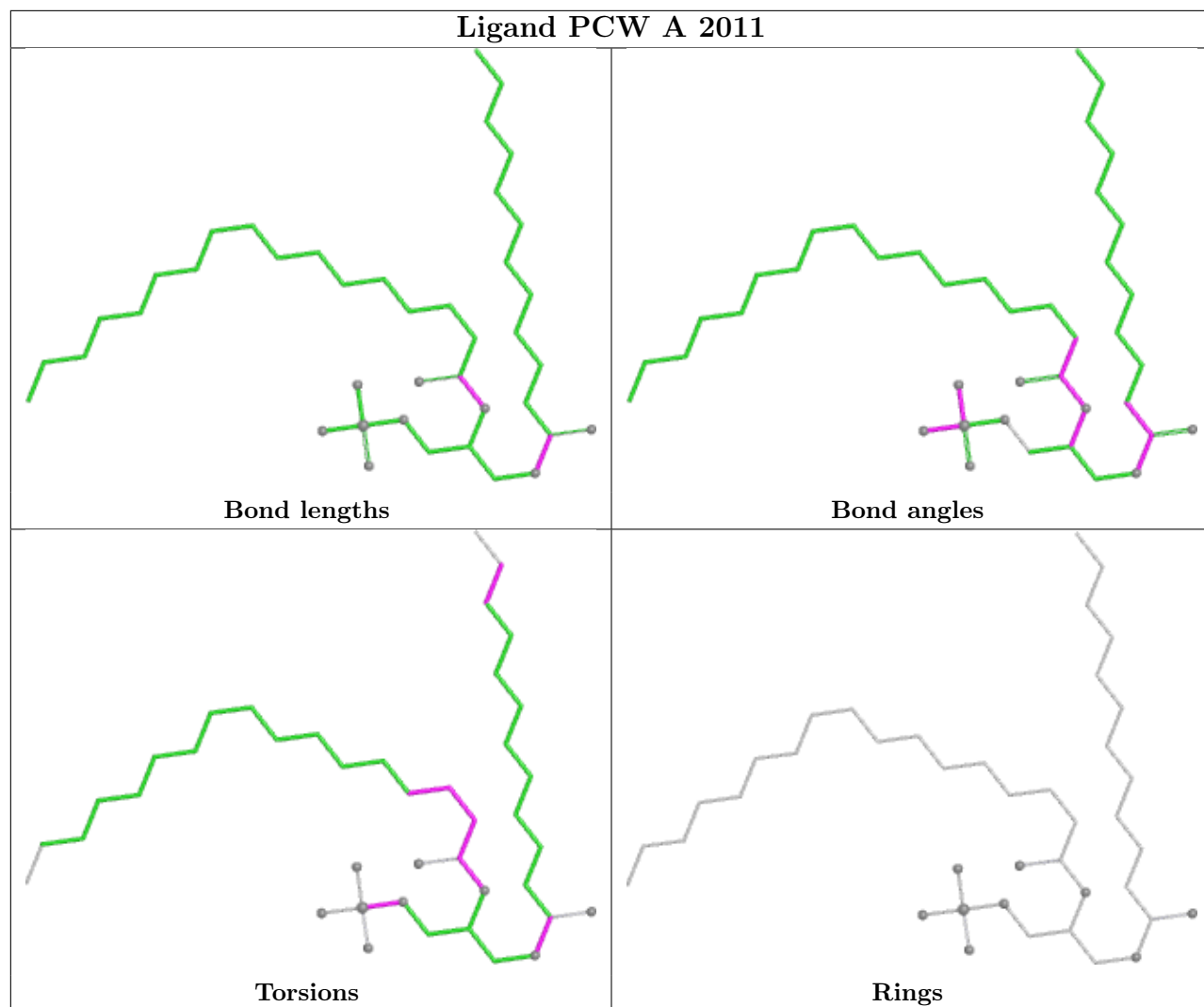


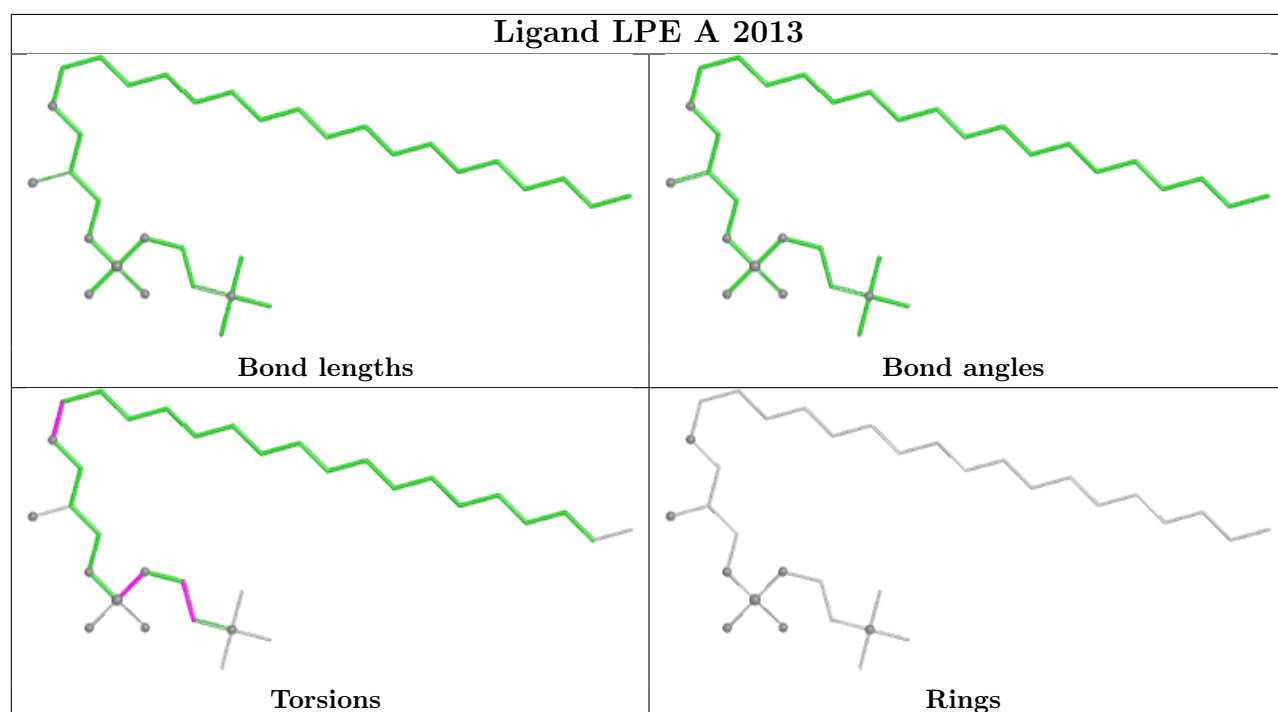
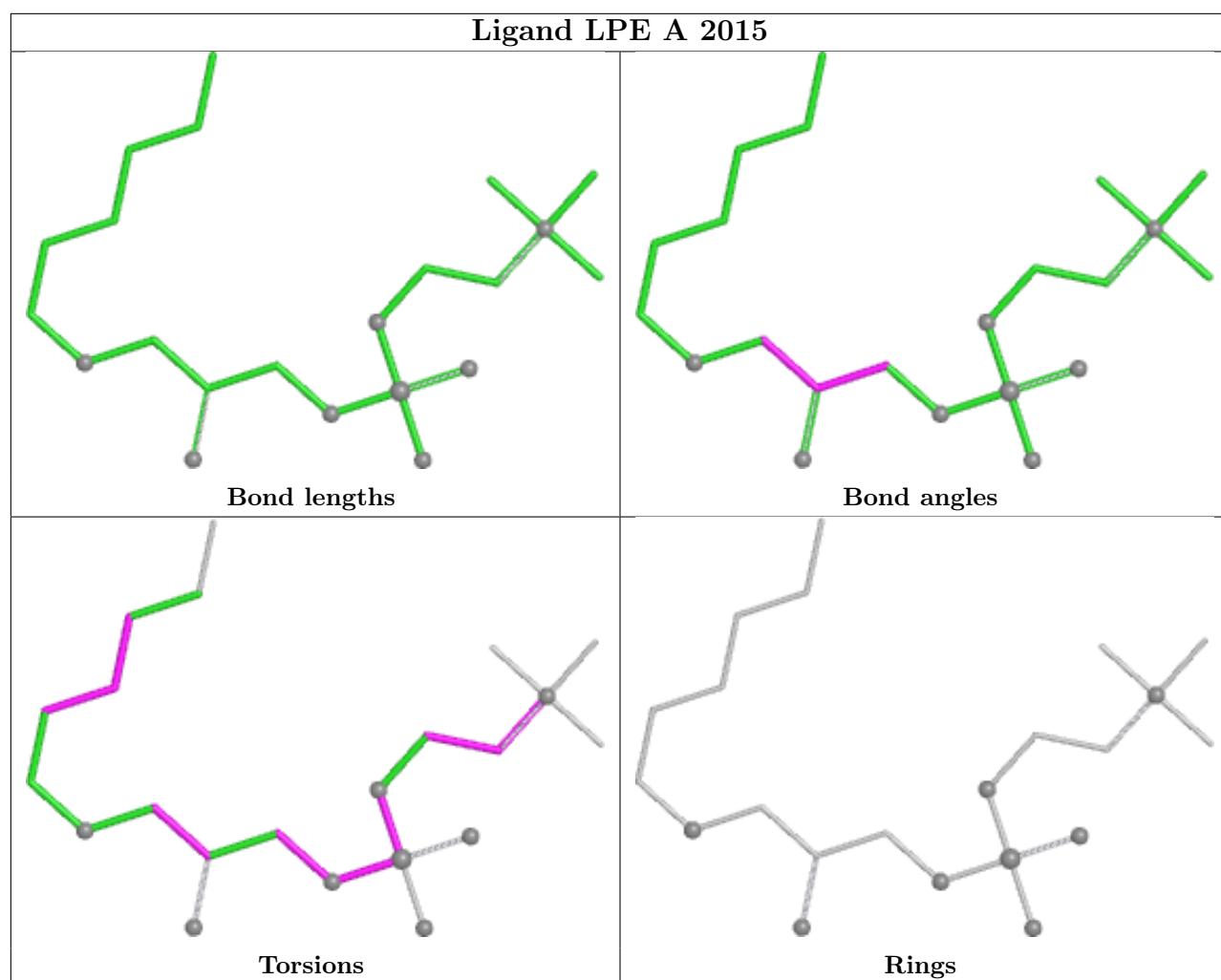


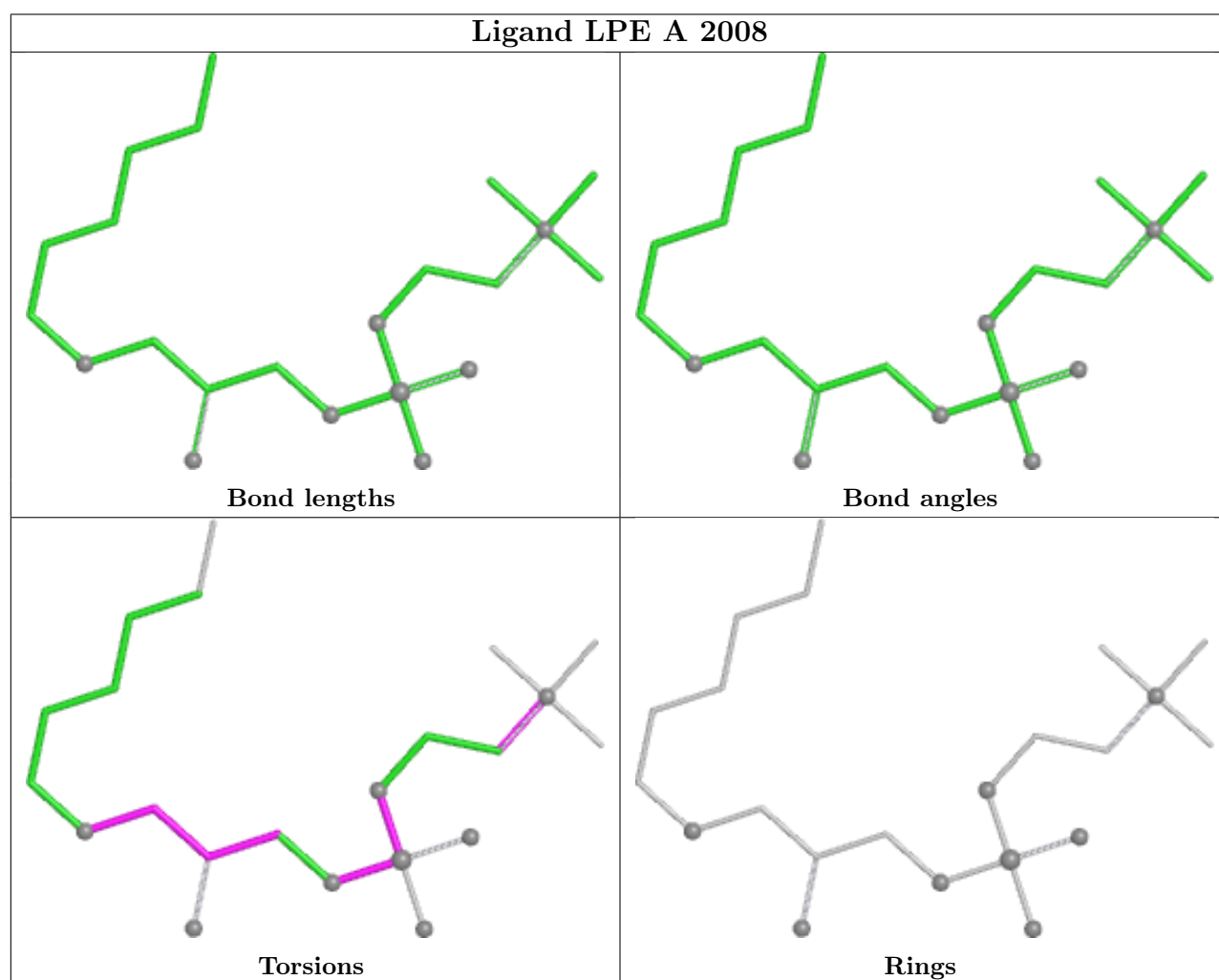
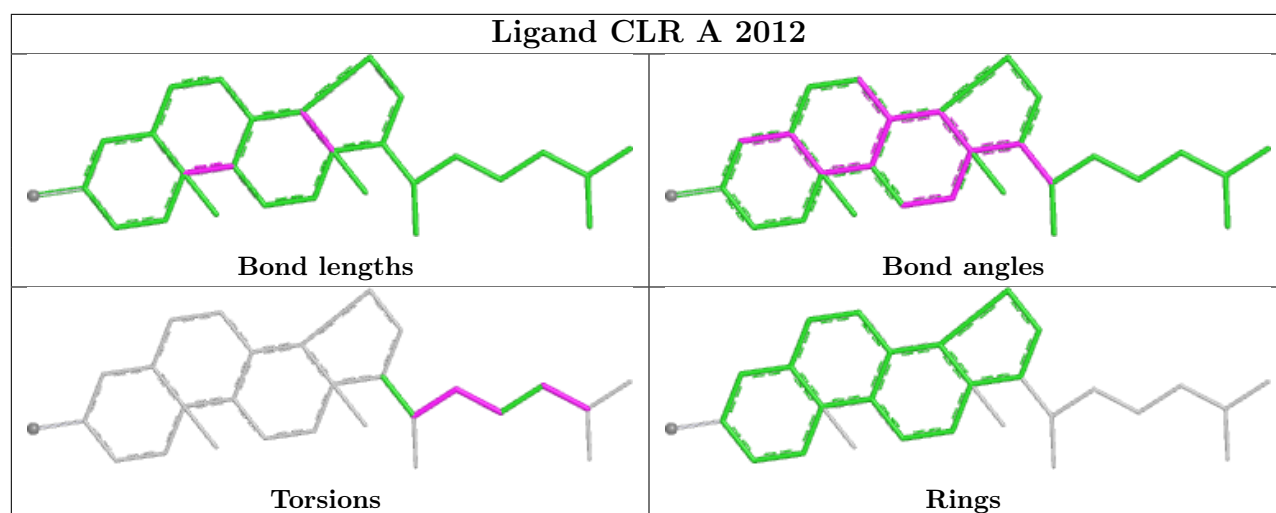


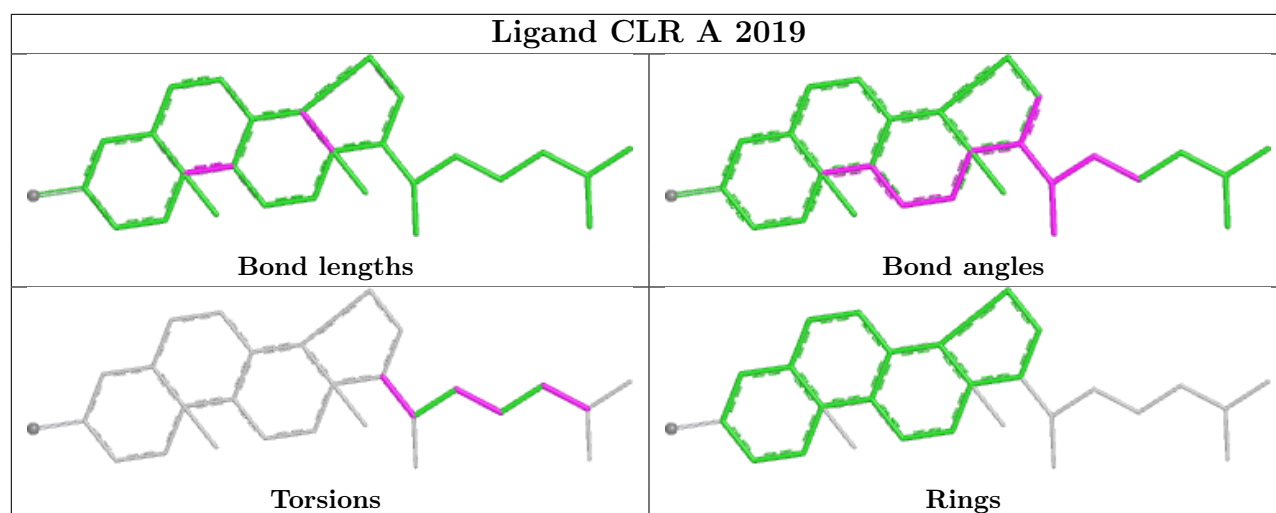












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

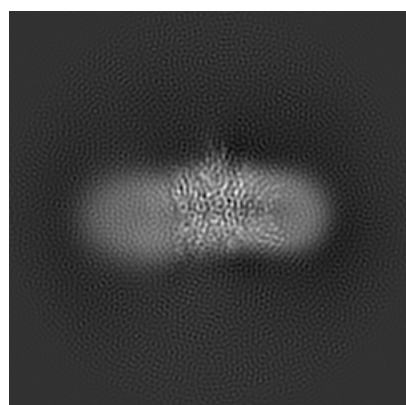
6 Map visualisation [i](#)

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

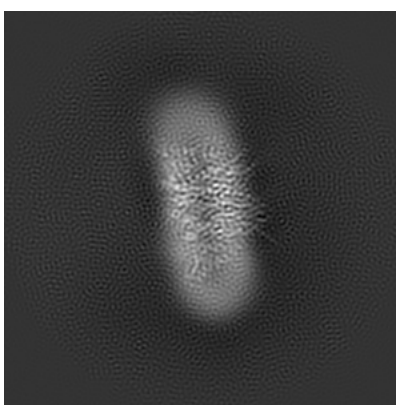
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

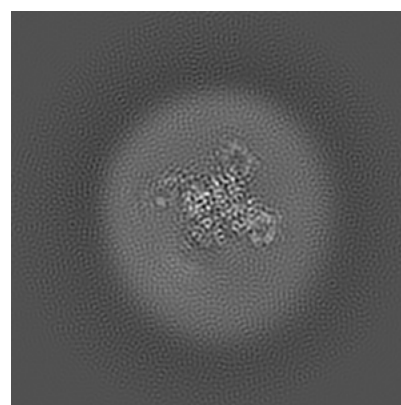
6.1.1 Primary map



X



Y

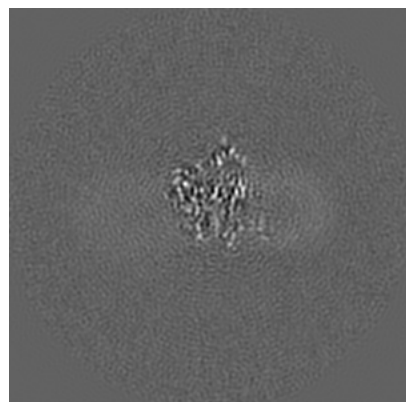


Z

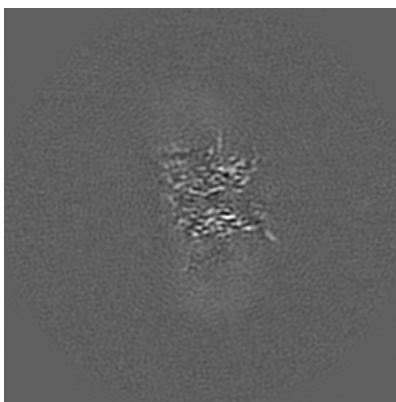
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

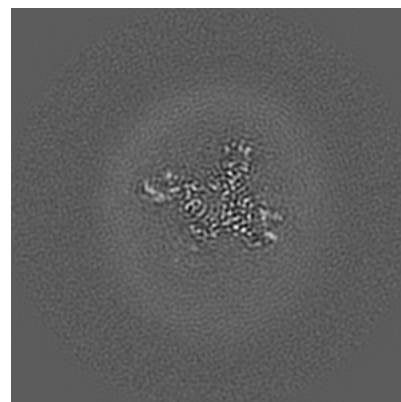
6.2.1 Primary map



X Index: 128



Y Index: 128

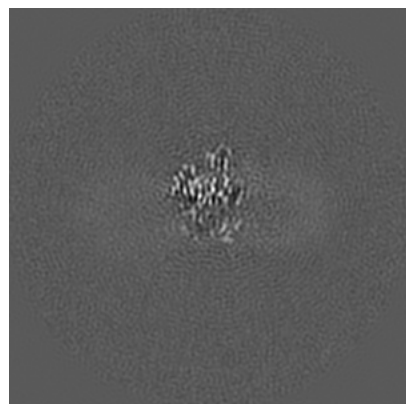


Z Index: 128

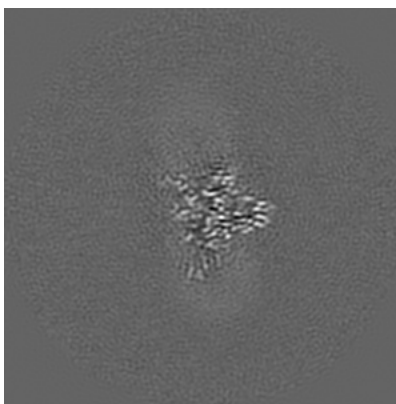
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

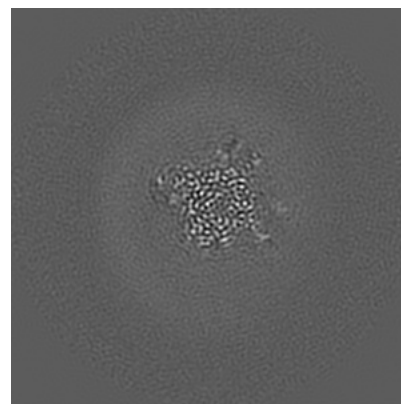
6.3.1 Primary map



X Index: 125



Y Index: 137

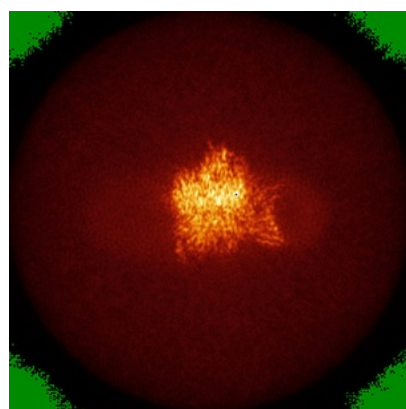


Z Index: 139

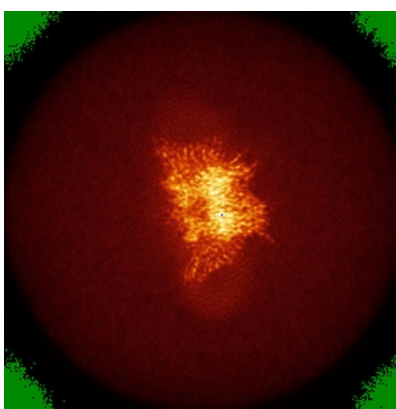
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

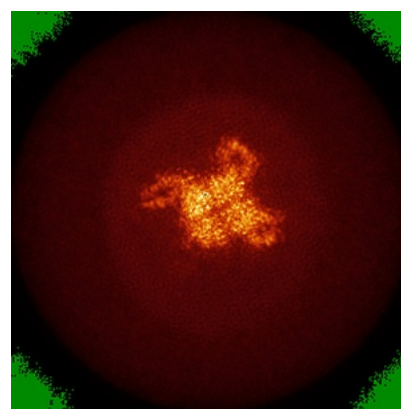
6.4.1 Primary map



X



Y

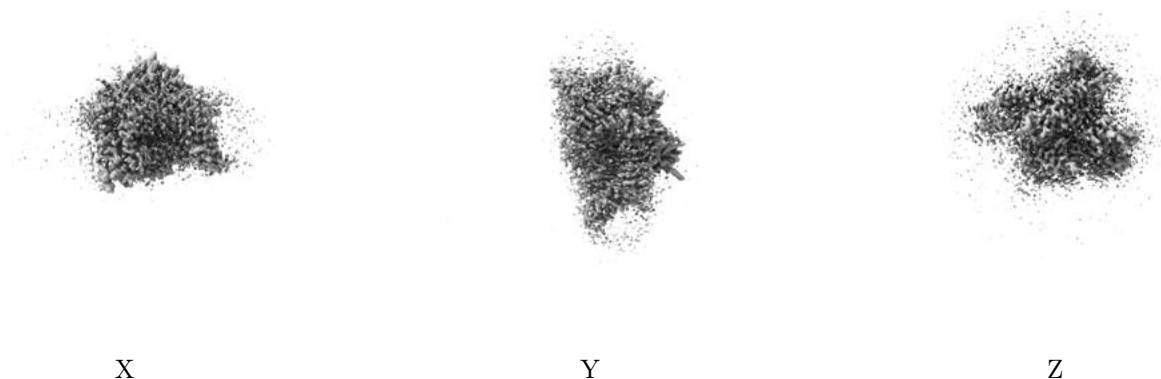


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

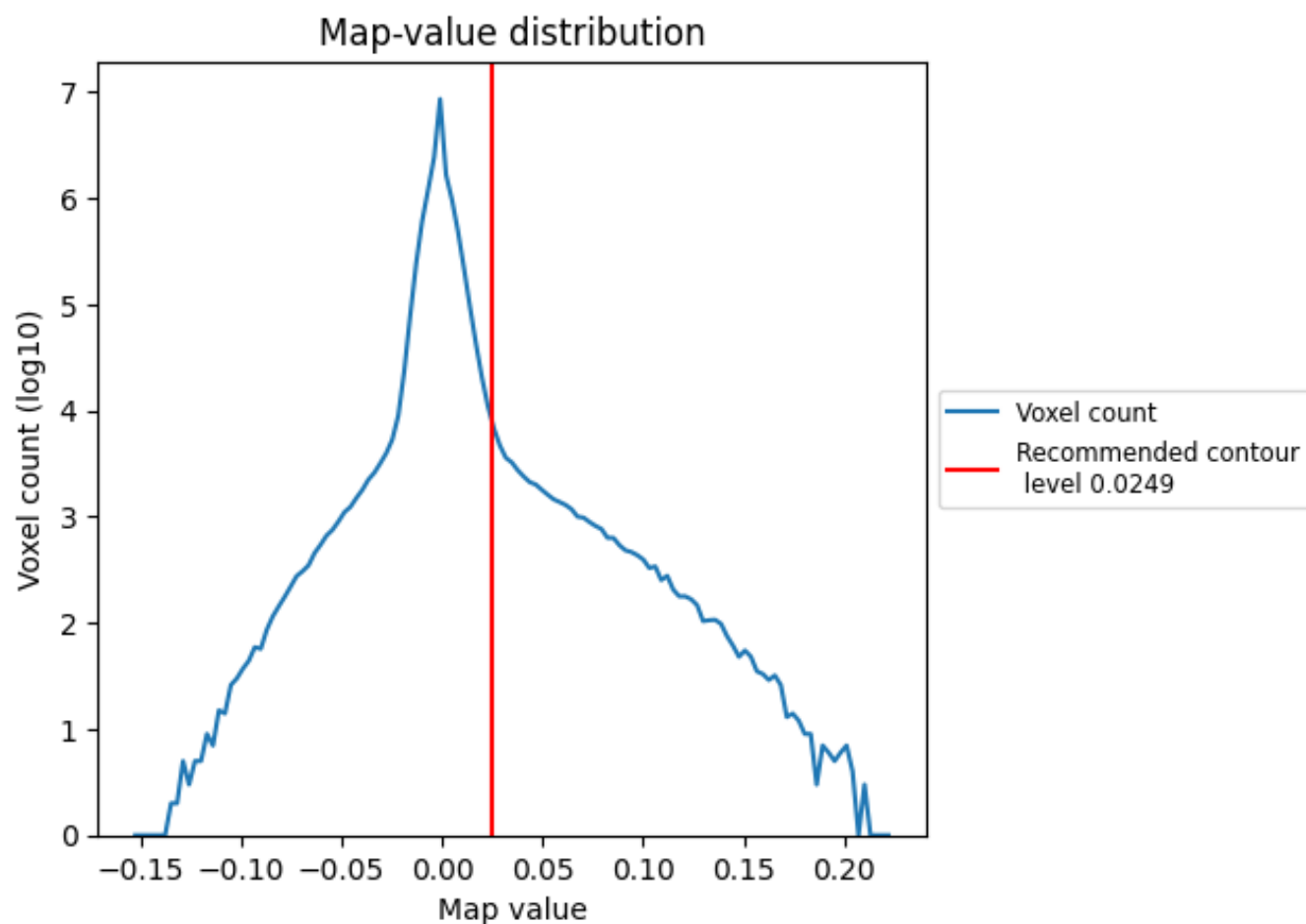
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

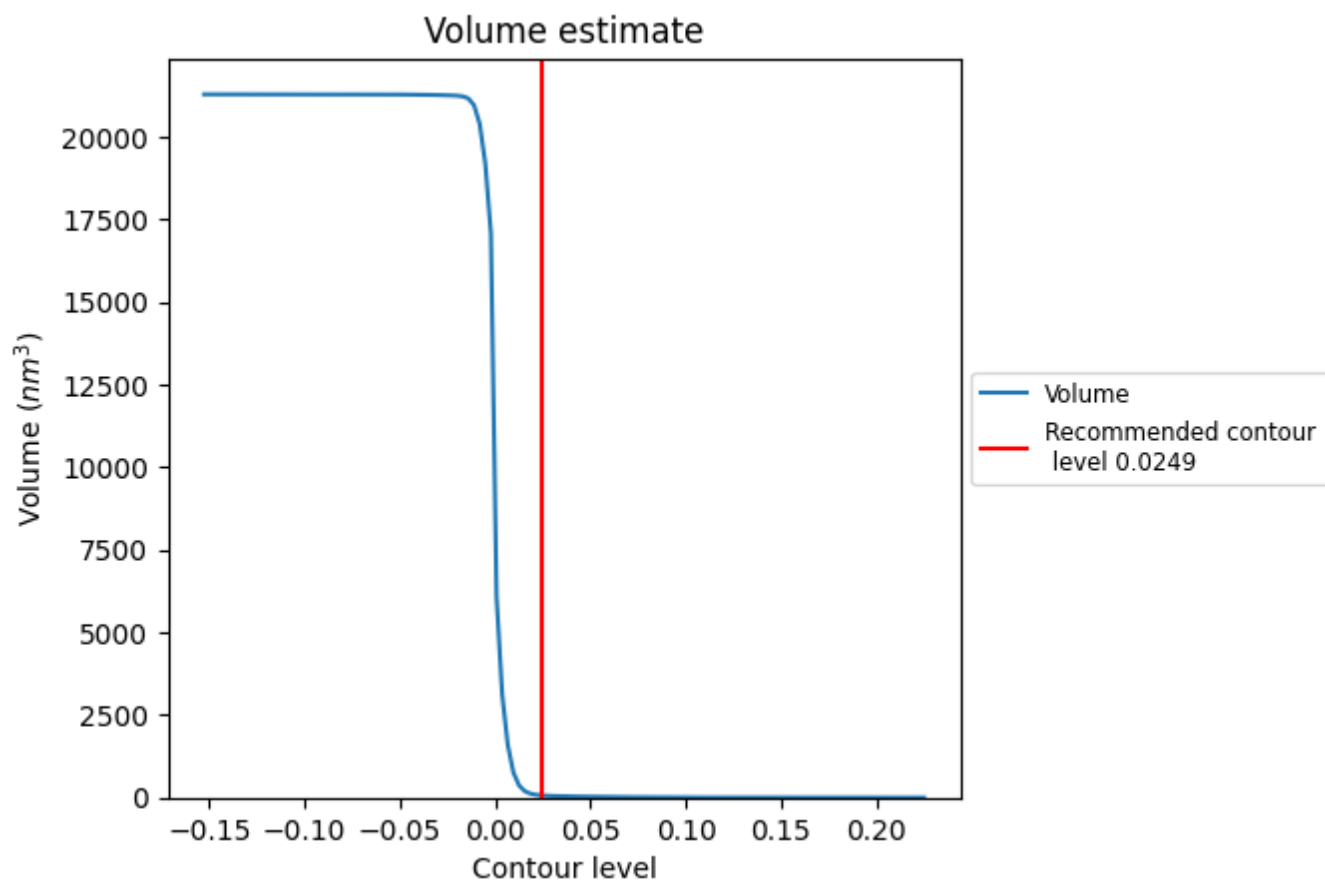
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

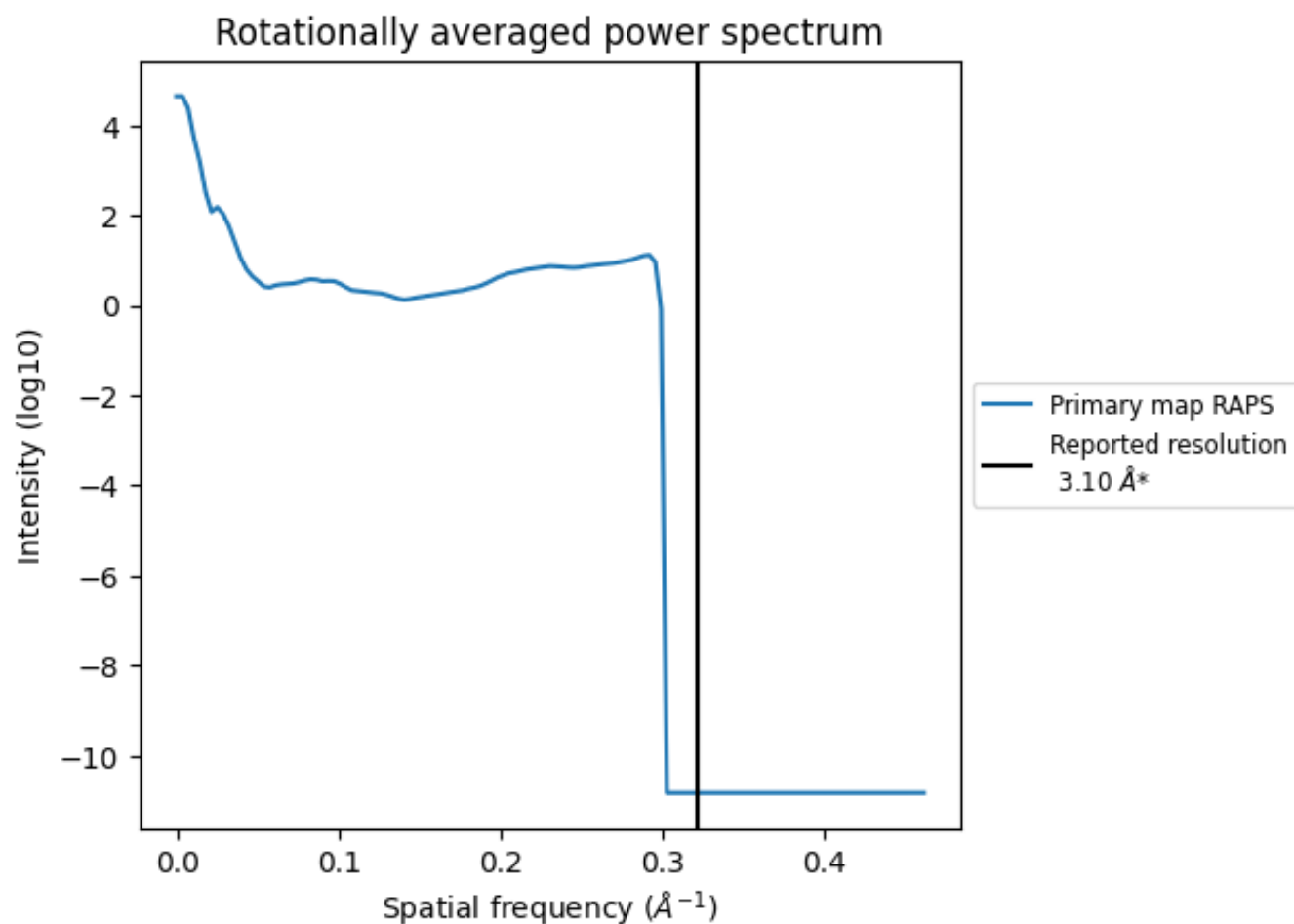
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

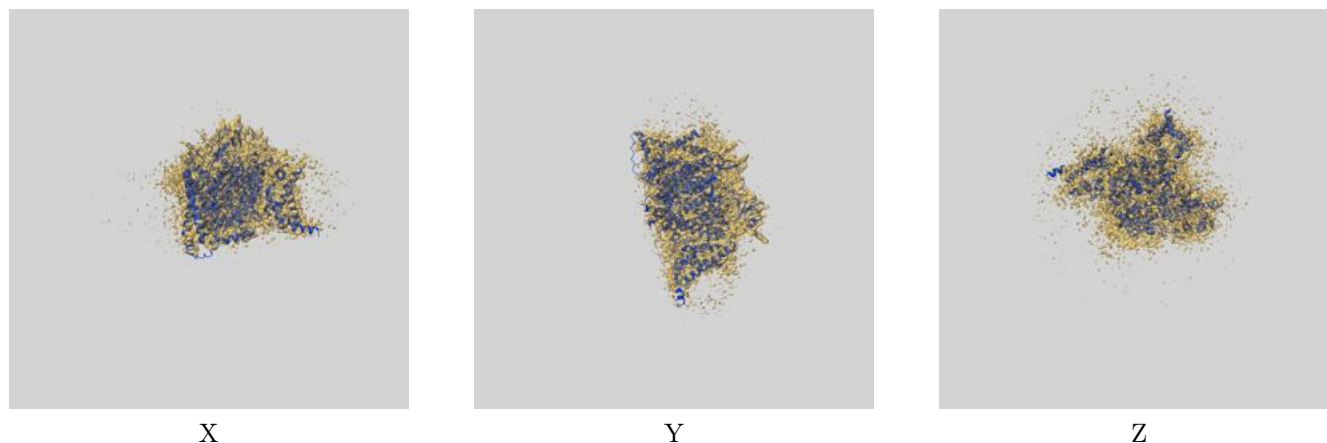
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

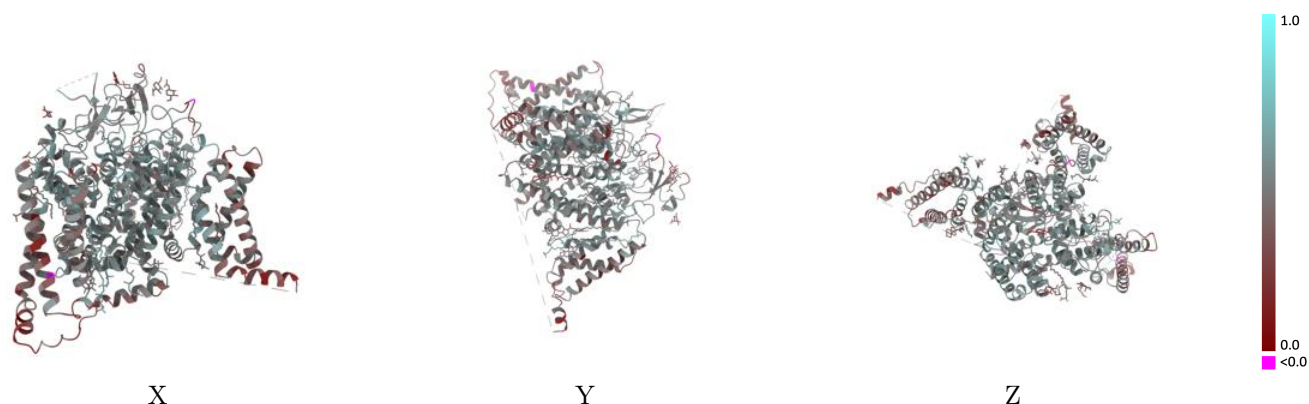
This section contains information regarding the fit between EMDB map EMD-32476 and PDB model 7WFW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



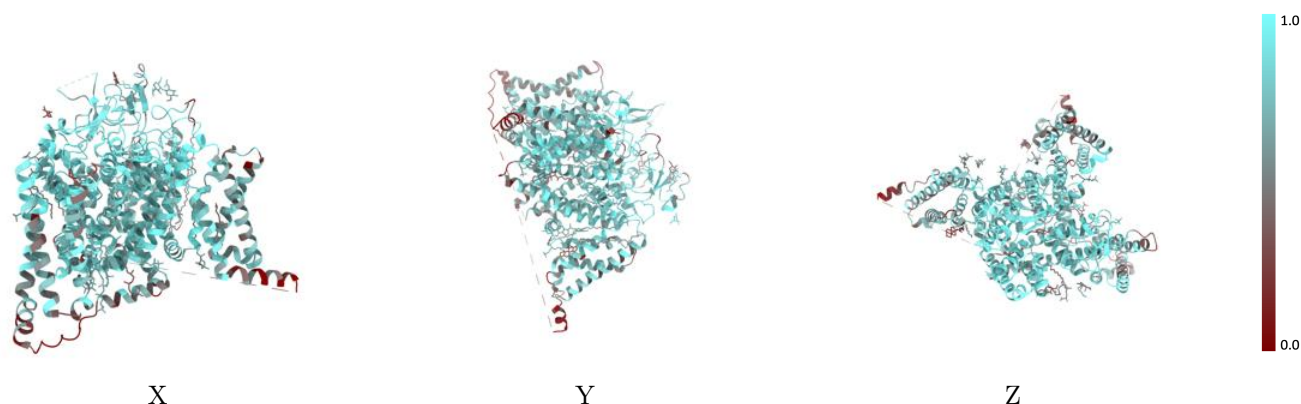
The images above show the 3D surface view of the map at the recommended contour level 0.0249 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



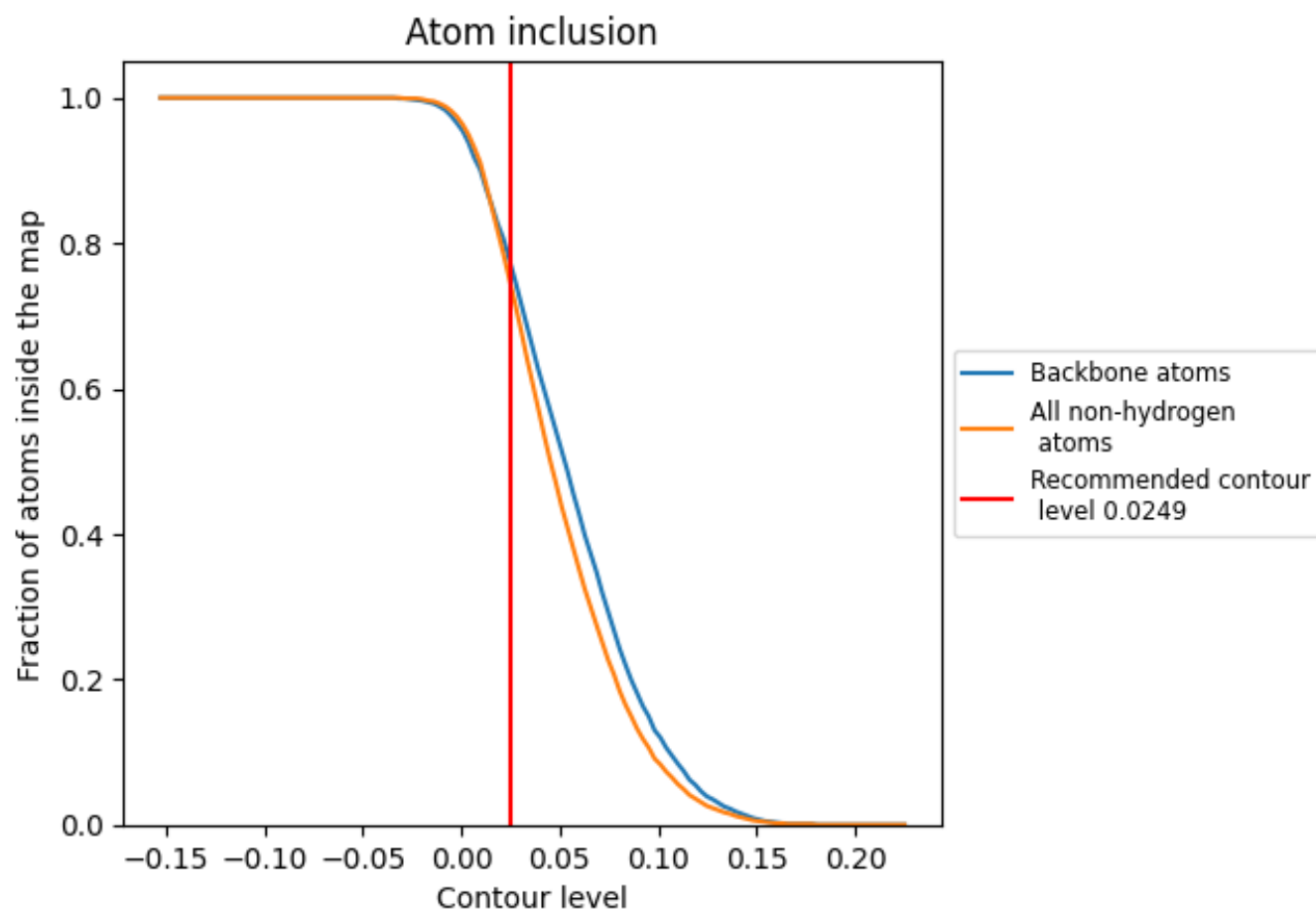
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	0.7450	0.4710
B	0.6790	0.3680

