



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:40 PM UTC

PDB ID : 7W9K / pdb_00007w9k
EMDB ID : EMD-32368
Title : Cryo-EM structure of human Nav1.7-beta1-beta2 complex at 2.2 angstrom resolution
Authors : Yan, N.; Huang, G.; Liu, D.; Wei, P.; Shen, H.
Deposited on : 2021-12-09
Resolution : 2.20 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.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

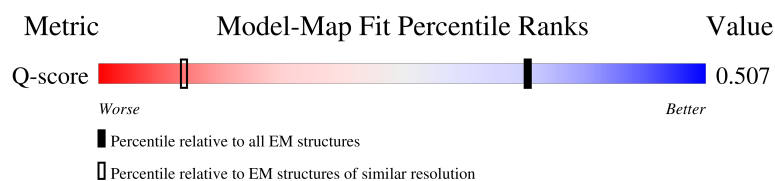
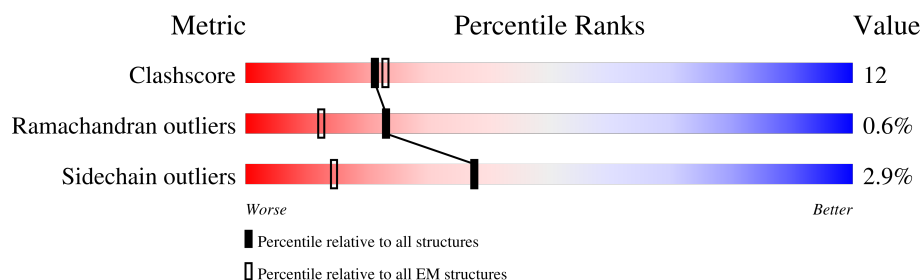
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	2031	
2	B	218	
3	C	215	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 100%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 14933 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 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1413	Total	C	N	O	S	1	0
			11412	7534	1796	1997	85		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	4	0
			980	615	172	183	10		

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



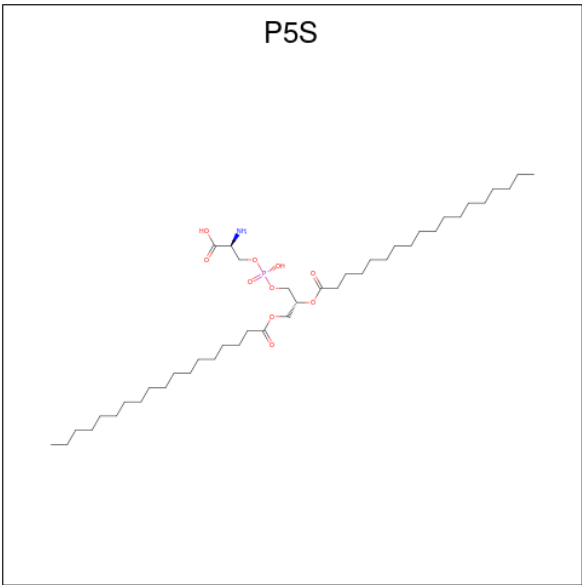
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	2	Total	C	N	O		0	0
			28	16	2	10			
4	E	2	Total	C	N	O		0	0
			28	16	2	10			
4	F	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



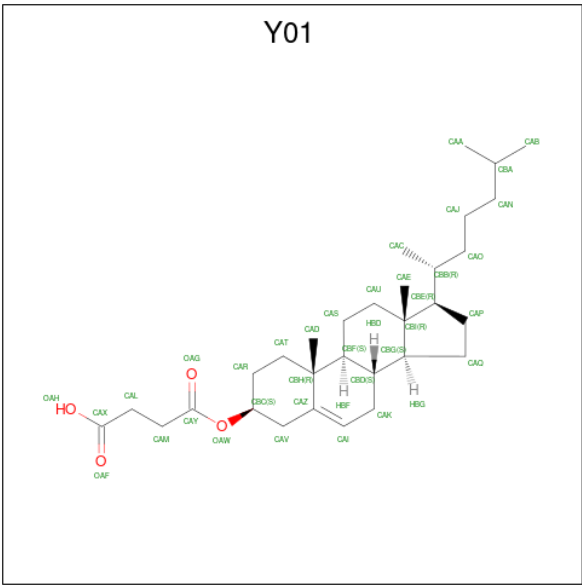
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			35	24	1	9	1	
6	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
6	A	1	Total	C	N	O	P	0
			34	22	1	10	1	

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



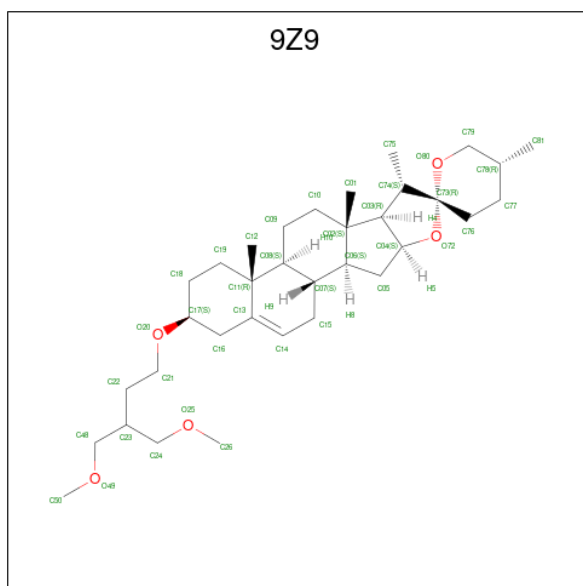
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			35	31	4	

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Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			35	31	4	
7	A	1	Total	C	O	0
			35	31	4	
7	A	1	Total	C	O	0
			35	31	4	
7	A	1	Total	C	O	0
			35	31	4	
7	A	1	Total	C	O	0
			35	31	4	

- Molecule 8 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).

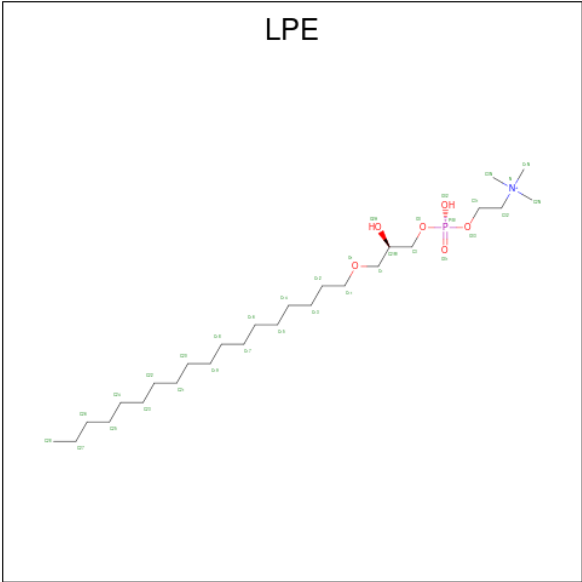


Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			39	34	5	

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Na	0
			1	1	

- Molecule 10 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: C₂₆H₅₇NO₆P).



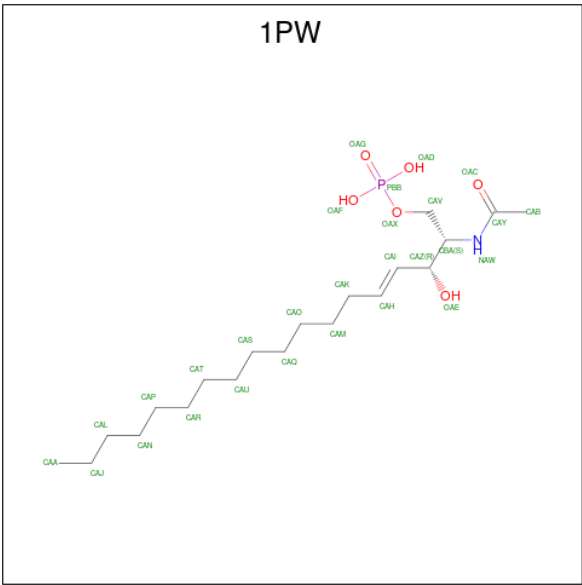
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
10	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
10	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			17	9	1	6	1	
10	A	1	Total	C	N	O	P	0
			17	9	1	6	1	

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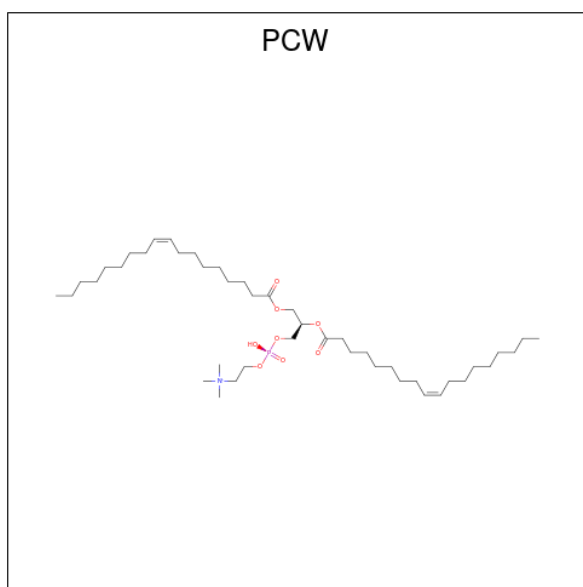
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	N	O	P	0
			17	9	1	6	1	

- Molecule 11 is (2S,3R,4E)-2-(acetylamino)-3-hydroxyoctadec-4-en-1-yl dihydrogen phosphate (CCD ID: 1PW) (formula: C₂₀H₄₀NO₆P).



Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			24	18	5	1	

- Molecule 12 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
12	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
12	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
12	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
12	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 13 is water.

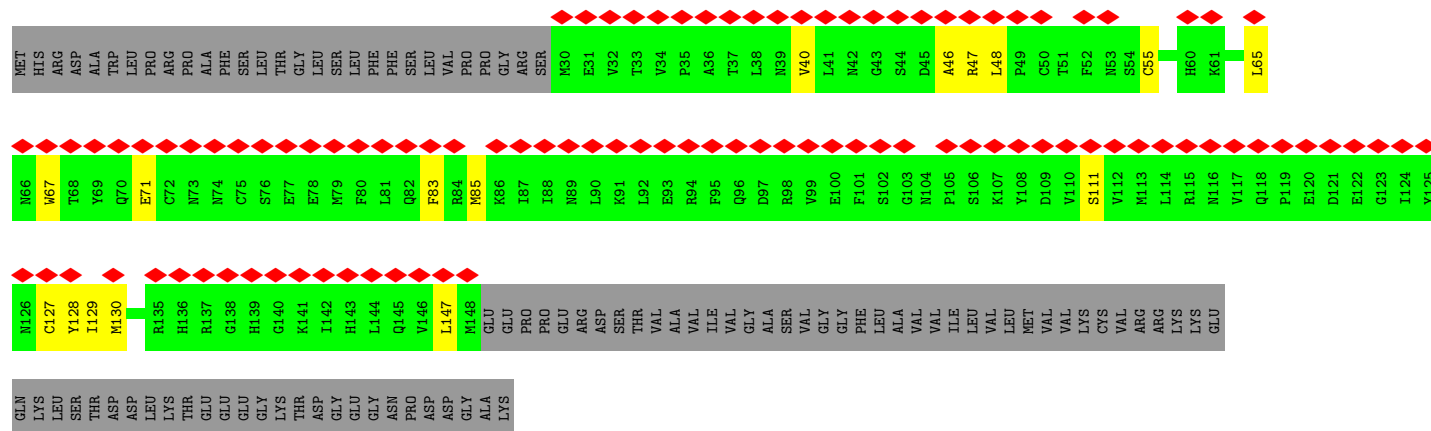
Mol	Chain	Residues	Atoms		AltConf
13	A	9	Total	O	0
			9	9	

T1794	P1722	M1543	F1443	F1347	I1224	MET	THR	GLN	L964	L869	M763	SER
Q1795	N1732	V1546	T1448	Y1348	I1225	ASN	VAL	ALA	A965	L865	E764	ARG
F1796	G1736	L1547	T1449	I1351	L1239	ASP	VAL	ASP	L966	I876	H765	ALA
I1797	V1552	V1553	N1450	T1353	G1249	GLU	PRO	LEU	L968	I879	P767	ILE
E1798	F1553	F1554	V1455	R1358	Y1250	GLU	ALA	ASN	F971	F880	M768	LEU
F1799	I1555	I1556	I1456	F1359	K1251	ALA	PRO	LYS	S972	L887	K773	THR
S1800	M1639	I1556	D1458	P1360	Y1252	CYS	GLY	GLU	S973	L776	L776	THR
K1801	M1639	I1556	D1458	A1361	Y1253	PHE	GLU	ASN	D974	V896	V896	VAL
L1802	S1741	G1560	F1460	Q1362	A1257	THR	SER	ASN	H975	A789	A789	GLU
S1803	Y1743	T1569	F1461	Q1363	Y1257	ASP	LEU	ILE	L976	E790	E790	LEU
S1804	I1744	G1560	H1461	Q1363	Y1257	GLY	ASP	LEU	L976	E790	E790	LEU
F1805	F1748	E1561	Q1462	V1364	W1260	CYS	GLU	SER	T977	P906	D799	GLU
F1806	L1749	C1562	K1465	P1365	L1261	VAL	ASN	ASN	T977	P906	D799	GLU
A1807	V1750	V1563	K1466	E1369	D1262	THR	MET	HIS	A978	M910	P800	SER
L1808	V1751	K1565	K1466	E1369	F1263	ARG	ASN	THR	T979	M910	P800	ARG
A1808	V1752	L1566	L1373	H1374	L1264	PHE	ALA	LEU	E980	Y801	Y801	GLN
L1809	M1753	I1567	H1373	H1374	I1265	SER	GLU	ALA	E980	Y801	Y801	LYS
D1810	N1754	T1567	M1375	M1375	L1283	CYS	GLU	GLU	E981	F913	Q805	CYS
P1811	I1755	R1570	M1474	Q1378	S1288	CYS	LEU	MET	D982	F914	Q805	PRO
F1812	I1756	H1571	Q1478	N1379	L1289	GLN	SER	SER	P983	H915	V808	PRO
F1812	A1757	Y1572	K1479	N1379	R1290	VAL	SER	LYS	P983	S916	G807	TRP
L1813	V1758	Y1573	V1380	V1380	T1291	ILE	ASP	GLY	D984	F917	D812	TRP
L1814	I1759	Y1481	M1384	M1384	L1292	GLU	ASP	HIS	A985	I919	D812	TVR
L1814	L1760	Y1482	L1385	L1385	L1292	SER	SER	ASN	N986	V920	F924	ARG
A1816	G1577	Y1482	L1385	L1385	L1292	GLY	GLU	PHE	N987	R921	L825	PHE
K1817	V1578	Y1482	L1385	L1385	L1292	LYS	TYR	LEU	L988	R922	L825	ALA
P1818	K1670	M1485	M1388	M1388	L1295	GLU	TYR	GLU	Q989	E927	ASP	HIS
N1819	D1677	K1486	M1388	M1388	L1295	GLU	TYR	GLU	Q989	E927	ASP	LYS
K1820	M1678	K1487	L1394	L1394	R1296	LYS	VAL	GLU	V928	V928	VAL	LYS
V1821	F1679	L1488	G1395	G1395	L1300	ASP	ARG	GLY	I929	I929	GLU	PHE
Q1822	F1681	D1592	Y1396	Y1396	L1301	ILE	LEU	SER	E930	E930	GLY	LEU
L1823	E1682	F1583	Y1396	Y1396	L1301	ASN	ASN	ASN	L831	L831	S932	TRP
I1824	F1684	F1494	K1406	K1406	F1304	ARG	ARG	GLY	S932	S932	S932	ASN
A1825	F1684	F1494	K1406	K1406	F1304	GLY	SER	PHE	M936	M936	S836	CYS
M1826	S1687	F1496	G1407	G1407	M1307	SER	SER	GLY	E937	E937	F837	SER
D1827	I1599	R1499	Y1421	Y1421	M1307	SER	SER	GLY	V938	V938	F837	SER
L1828	I1599	R1499	Y1421	Y1421	M1307	SER	SER	GLY	V938	V938	F837	SER
P1829	S1697	P1500	Q1424	Q1424	V1324	SER	SER	SER	G998	G998	R838	P728
M1830	A1698	P1500	Q1424	Q1424	L1325	VAL	VAL	VAL	C998	C998	R838	Y729
V1831	G1699	Q1505	Y1432	Y1432	L1326	GLU	GLU	GLU	V999	V999	L839	W730
V1831	W1700	Q1505	Y1432	Y1432	L1326	CYS	CYS	ASP	M1000	M1000	L840	W730
S1832	D1701	V1512	L1431	L1431	V1327	SER	SER	LYS	Y1001	Y1001	R841	I731
G1833	L1704	Q1515	M1433	M1433	C1328	THR	THR	HIS	V1002	V1002	F843	K732
D1834	M1709	Q1515	M1433	M1433	L1334	LEU	VAL	LEU	V1002	V1002	M943	F733
R1835	S1710	D1518	Y1436	Y1436	I1337	ASP	ASP	GLY	K1003	K1003	V947	K734
I1836	K1711	D1518	Y1436	Y1436	I1337	ASP	ASP	GLY	V950	V950	A846	K734
I1836	P1712	M1529	F1437	F1437	V1340	PRO	PRO	GLU	V951	V951	K847	K735
H1837	P1713	M1529	F1437	F1437	V1340	PRO	PRO	GLU	V952	V952	W849	K735
C1838	D1714	M1533	V1439	V1439	L1342	GLY	GLY	GLY	V953	V953	P850	I737
L1839	A1627	W1534	F1440	F1440	F1343	GLU	ALA	GLU	E1008	E1008	T851	I740
D1840	K1628	E1536	I1441	I1441	A1344	GLU	GLU	ASN	F1009	F1009	L852	V741
I1841	H1721	E1536	I1442	I1442	K1346	PRO	PRO	ASN	I1010	I1010	K857	W742
L1842	F1789	E1537	I1442	I1442	K1346	PRO	PRO	ASN	I1011	I1011	I858	D743
F1843	D1790	E1537	I1442	I1442	K1346	PRO	PRO	ASN	K1012	K1012	V859	P744
A1844	P1791	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1013	F1013	G860	F745
F1845	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	T758
T1846	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	L759
K1847	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	W760
E1848	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	M761
V1849	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	A762
L1850	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	A762
G1851	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	A762
E1852	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	A762
S1853	D1792	E1537	I1442	I1442	K1346	PRO	PRO	ASN	F1014	F1014	V863	A762

- Molecule 2: Sodium channel subunit beta-1



- Molecule 3: Sodium channel subunit beta-2



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



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	785228	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	0.145	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	421.59363, 421.59363, 421.59363	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, 1PW, NAG, NA, PCW, P5S, LPE, 9Z9

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	1.34	115/11686 (1.0%)	1.30	106/15823 (0.7%)
2	B	1.59	24/1442 (1.7%)	1.34	16/1949 (0.8%)
3	C	0.34	0/1011	0.59	1/1367 (0.1%)
All	All	1.32	139/14139 (1.0%)	1.27	123/19139 (0.6%)

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

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

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1388	ASN	C-O	-9.26	1.17	1.24
1	A	1437	PHE	C-O	-8.38	1.14	1.24
1	A	1442	ILE	C-O	-8.34	1.14	1.24
1	A	1416	VAL	CA-CB	8.29	1.65	1.54
1	A	919	ILE	CA-CB	8.26	1.64	1.54
2	B	139	VAL	C-O	-8.20	1.15	1.24
1	A	1743	TYR	C-O	-8.16	1.14	1.24
1	A	1621	LEU	CA-C	-7.94	1.42	1.52
2	B	115	HIS	CA-C	-7.92	1.42	1.52
1	A	1697	SER	C-O	-7.67	1.14	1.24
1	A	1643	ALA	C-O	-7.66	1.15	1.24
1	A	1340	VAL	CA-CB	7.41	1.63	1.54
1	A	1563	VAL	C-O	-7.28	1.15	1.24
1	A	1262	ASP	CA-C	-7.27	1.43	1.52
1	A	972	SER	CA-C	-7.24	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	THR	C-O	-7.17	1.14	1.24
1	A	1761	GLU	C-O	-7.12	1.15	1.24
2	B	126	LEU	C-O	-6.99	1.15	1.24
1	A	328	TYR	C-O	-6.96	1.15	1.23
2	B	102	GLN	C-O	-6.94	1.14	1.24
2	B	128	PHE	C-O	-6.93	1.15	1.23
2	B	125	ARG	C-O	-6.93	1.15	1.24
1	A	936	MET	C-O	-6.86	1.15	1.24
2	B	103	ASP	C-O	-6.76	1.16	1.24
1	A	291	ASN	CA-C	6.76	1.61	1.52
1	A	916	SER	CA-C	6.72	1.61	1.52
2	B	22	VAL	C-O	-6.72	1.16	1.24
1	A	349	TRP	C-O	-6.71	1.16	1.24
1	A	920	VAL	CA-CB	6.69	1.62	1.54
1	A	371	LEU	C-O	-6.68	1.16	1.24
1	A	370	THR	CA-C	6.66	1.61	1.52
1	A	1583	PHE	C-N	-6.58	1.25	1.33
1	A	338	ASP	CA-CB	6.52	1.62	1.53
1	A	1591	VAL	CA-C	-6.50	1.44	1.53
1	A	1701	ASP	C-O	-6.47	1.16	1.24
1	A	1698	ALA	C-O	-6.46	1.16	1.24
1	A	914	PHE	C-O	-6.43	1.16	1.24
1	A	929	ILE	CA-CB	6.40	1.61	1.54
1	A	938	VAL	C-O	-6.38	1.16	1.24
1	A	301	LYS	C-O	-6.38	1.16	1.23
1	A	57	LYS	CA-C	-6.33	1.44	1.52
1	A	857	LYS	C-O	-6.30	1.16	1.24
1	A	1197	PHE	C-O	-6.24	1.16	1.24
1	A	1534	VAL	C-O	-6.21	1.16	1.24
1	A	369	GLN	N-CA	6.18	1.53	1.46
2	B	51	ALA	C-O	-6.17	1.16	1.23
1	A	1353	THR	CA-C	6.17	1.60	1.52
1	A	198	PHE	C-O	-6.15	1.17	1.24
1	A	932	MET	C-O	-6.12	1.17	1.24
1	A	1741	VAL	CA-CB	6.12	1.62	1.54
1	A	1701	ASP	N-CA	-6.10	1.38	1.46
1	A	336	ASN	C-O	-6.09	1.15	1.23
1	A	365	ASN	C-O	-6.07	1.17	1.24
1	A	953	VAL	CA-CB	6.07	1.62	1.54
1	A	1205	SER	CA-C	6.06	1.60	1.52
1	A	276	PHE	C-O	-6.06	1.16	1.24
1	A	1555	ILE	N-CA	-6.06	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1721	HIS	C-O	-6.03	1.17	1.24
1	A	349	TRP	N-CA	5.96	1.53	1.46
2	B	31	VAL	C-O	-5.96	1.17	1.24
1	A	942	ALA	C-O	-5.94	1.17	1.24
2	B	22	VAL	CA-CB	5.93	1.62	1.54
1	A	958	VAL	CA-C	5.91	1.60	1.52
1	A	1660	ILE	CA-CB	5.89	1.61	1.54
1	A	1414	ALA	C-O	-5.88	1.17	1.24
1	A	1592	GLY	CA-C	-5.87	1.45	1.52
1	A	1457	ILE	N-CA	-5.86	1.39	1.46
1	A	376	LYS	C-O	-5.85	1.16	1.24
1	A	1698	ALA	CA-CB	-5.84	1.45	1.53
2	B	154	MET	C-O	-5.81	1.17	1.24
1	A	1443	PHE	C-O	-5.79	1.16	1.23
1	A	311	ASP	CA-C	-5.78	1.45	1.52
1	A	1440	PHE	C-O	-5.76	1.17	1.24
2	B	155	ALA	C-O	-5.75	1.17	1.24
1	A	931	THR	C-O	-5.71	1.17	1.24
1	A	1325	LEU	N-CA	-5.69	1.39	1.46
1	A	1583	PHE	C-O	-5.67	1.16	1.24
1	A	414	GLU	N-CA	-5.67	1.39	1.46
1	A	1441	ILE	C-O	-5.66	1.17	1.24
1	A	1700	TRP	C-O	-5.66	1.17	1.24
1	A	965	ALA	N-CA	-5.65	1.39	1.46
1	A	1664	SER	CA-C	5.59	1.60	1.52
1	A	761	MET	C-O	-5.58	1.16	1.24
1	A	913	PHE	CA-C	5.58	1.59	1.52
1	A	1421	VAL	CA-CB	5.53	1.60	1.53
1	A	1438	VAL	CA-CB	5.52	1.61	1.54
1	A	1683	THR	CA-CB	5.52	1.63	1.53
1	A	910	MET	N-CA	5.51	1.52	1.46
1	A	1342	LEU	C-O	-5.50	1.17	1.24
1	A	953	VAL	C-O	-5.50	1.17	1.24
1	A	260	ALA	C-O	-5.49	1.17	1.24
1	A	914	PHE	CA-CB	5.47	1.61	1.53
2	B	78	LEU	CA-C	-5.47	1.46	1.52
1	A	134	CYS	CA-C	-5.47	1.45	1.52
1	A	262	ILE	C-O	-5.47	1.18	1.24
1	A	1738	PHE	C-O	-5.43	1.17	1.24
1	A	863	VAL	N-CA	-5.42	1.39	1.46
2	B	162	MET	N-CA	-5.42	1.39	1.46
1	A	1687	SER	C-O	-5.41	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	ILE	C-O	-5.41	1.18	1.24
1	A	131	LEU	N-CA	-5.41	1.39	1.46
1	A	1324	VAL	CA-C	-5.40	1.45	1.52
1	A	1482	TYR	CA-C	-5.39	1.46	1.52
1	A	913	PHE	C-O	-5.38	1.18	1.24
1	A	1757	ALA	C-O	5.38	1.30	1.24
1	A	275	CYS	C-O	-5.37	1.17	1.24
2	B	103	ASP	CA-C	-5.32	1.46	1.52
1	A	334	GLY	C-O	-5.31	1.16	1.23
1	A	337	PRO	C-O	-5.29	1.17	1.23
1	A	140	CYS	C-O	5.27	1.30	1.24
1	A	860	GLY	C-O	-5.26	1.17	1.23
1	A	1352	ASN	CA-CB	-5.22	1.46	1.53
2	B	107	PHE	CA-C	-5.21	1.46	1.52
1	A	1735	VAL	CA-CB	5.19	1.60	1.54
2	B	134	HIS	C-O	-5.17	1.18	1.24
1	A	1388	ASN	CA-C	5.17	1.59	1.53
1	A	373	ALA	C-O	-5.14	1.17	1.24
1	A	1554	PHE	C-O	-5.14	1.18	1.24
1	A	345	ASP	N-CA	5.14	1.52	1.46
1	A	1249	GLY	CA-C	-5.13	1.46	1.51
1	A	1180	ASN	N-CA	-5.12	1.40	1.46
1	A	1681	PHE	CA-CB	5.11	1.60	1.53
1	A	156	GLU	CA-C	-5.08	1.45	1.52
1	A	1337	ILE	CA-CB	5.07	1.60	1.54
1	A	338	ASP	N-CA	5.07	1.54	1.46
2	B	31	VAL	CA-C	-5.06	1.46	1.52
1	A	1562	CYS	C-O	-5.06	1.17	1.24
2	B	83	ASP	CA-C	-5.06	1.46	1.52
1	A	1264	LEU	N-CA	-5.06	1.40	1.46
1	A	1334	ILE	C-O	-5.04	1.18	1.24
1	A	1744	ILE	CA-CB	5.04	1.60	1.54
2	B	84	GLU	CA-C	-5.04	1.46	1.52
1	A	239	ILE	C-O	-5.03	1.17	1.24
1	A	1183	LYS	CA-C	-5.03	1.45	1.52
1	A	1332	TRP	C-O	-5.02	1.17	1.24
2	B	50	ASN	CA-CB	5.01	1.61	1.53
2	B	46	ARG	C-O	-5.01	1.18	1.23
1	A	1559	THR	C-N	-5.01	1.28	1.34
1	A	313	LEU	N-CA	-5.00	1.39	1.46

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	955	GLY	N-CA-C	10.28	125.08	112.64
1	A	1353	THR	N-CA-C	10.12	122.31	111.28
1	A	388	LEU	N-CA-C	9.97	122.10	111.03
2	B	99	LYS	N-CA-C	-8.85	102.49	113.38
2	B	47	SER	N-CA-C	8.77	120.84	111.28
1	A	335	ARG	N-CA-C	8.66	121.50	110.24
2	B	144	ILE	N-CA-C	8.34	119.92	107.75
2	B	111	VAL	N-CA-C	8.27	119.76	108.84
1	A	1775	SER	N-CA-C	8.26	121.27	108.96
1	A	1301	LEU	N-CA-C	8.15	121.19	111.33
1	A	355	PHE	N-CA-C	-8.05	102.46	111.07
1	A	806	VAL	N-CA-C	7.96	119.25	109.30
1	A	246	SER	N-CA-C	7.85	119.84	111.28
1	A	267	PHE	N-CA-C	7.79	122.93	112.88
1	A	178	VAL	N-CA-C	7.74	118.49	110.36
1	A	1342	LEU	N-CA-C	7.69	119.44	111.14
1	A	1424	GLN	N-CA-C	7.67	119.00	109.57
1	A	929	ILE	N-CA-C	7.66	117.77	110.42
1	A	1631	ARG	N-CA-C	-7.58	102.15	111.40
2	B	90	VAL	N-CA-C	7.49	118.59	108.11
1	A	299	PHE	N-CA-C	-7.44	103.19	111.82
1	A	51	SER	N-CA-C	-7.37	103.39	112.38
1	A	1563	VAL	N-CA-C	7.31	118.08	110.62
1	A	852	LEU	N-CA-C	-7.26	103.09	112.23
1	A	745	PHE	N-CA-C	7.20	122.11	111.96
1	A	1201	MET	N-CA-C	7.14	119.06	111.28
2	B	66	GLU	N-CA-C	7.12	120.54	109.07
1	A	286	LEU	N-CA-C	-7.05	102.65	111.11
1	A	896	VAL	N-CA-C	7.00	117.76	110.62
1	A	118	ILE	N-CA-C	6.98	117.77	110.72
2	B	51	ALA	N-CA-C	6.97	120.00	109.41
1	A	344	PHE	N-CA-C	-6.96	102.06	111.87
1	A	1324	VAL	N-CA-C	-6.95	103.70	110.72
1	A	292	THR	N-CA-C	6.81	121.98	112.72
1	A	144	THR	CA-C-N	6.74	130.45	120.87
1	A	144	THR	C-N-CA	6.74	130.45	120.87
1	A	1283	LEU	N-CA-C	-6.74	100.06	110.10
1	A	942	ALA	N-CA-C	6.71	119.16	111.11
3	C	85	MET	N-CA-C	-6.69	105.25	113.41
1	A	1630	ILE	N-CA-C	-6.65	106.18	113.43
1	A	1561	GLU	N-CA-C	-6.62	103.99	111.07
1	A	940	GLY	N-CA-C	6.61	120.48	112.48
1	A	947	VAL	N-CA-C	6.59	116.75	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1188	ILE	N-CA-C	6.49	116.59	110.30
1	A	1198	ILE	N-CA-C	6.44	116.58	110.53
1	A	1677	ASP	N-CA-C	6.43	120.23	112.38
1	A	291	ASN	CB-CA-C	6.38	120.09	109.56
1	A	173	ALA	N-CA-C	6.37	119.17	111.40
1	A	119	SER	N-CA-C	-6.33	104.38	111.28
1	A	189	ASN	N-CA-C	-6.32	105.05	112.89
1	A	1625	LYS	N-CA-C	-6.29	104.48	111.71
1	A	1465	LYS	N-CA-C	6.24	117.75	111.07
1	A	228	ILE	N-CA-C	-6.21	103.24	109.02
1	A	1666	PHE	N-CA-C	6.21	120.56	112.92
1	A	1667	ALA	N-CA-C	6.18	120.68	113.20
1	A	850	PRO	N-CA-C	6.18	121.58	113.86
1	A	1442	ILE	N-CA-C	6.14	116.32	110.42
1	A	1603	PHE	N-CA-C	-6.12	98.99	108.42
1	A	1722	PRO	CA-C-O	-6.11	114.85	121.27
1	A	1737	ILE	N-CA-C	-5.99	104.90	110.53
2	B	125	ARG	N-CA-C	5.92	118.38	108.73
1	A	343	SER	N-CA-C	5.89	117.49	108.42
1	A	1630	ILE	CB-CA-C	5.89	118.20	110.84
1	A	915	HIS	N-CA-C	-5.88	104.96	111.36
1	A	1670	LYS	N-CA-C	5.84	118.52	110.35
1	A	345	ASP	N-CA-C	5.80	119.53	112.23
2	B	101	LEU	N-CA-C	5.78	119.05	109.46
1	A	291	ASN	N-CA-C	-5.78	105.90	113.12
2	B	65	GLU	N-CA-C	5.77	120.48	113.38
1	A	415	GLU	N-CA-C	-5.68	106.19	113.23
1	A	1362	SER	N-CA-C	-5.67	105.00	111.07
2	B	153	ASP	N-CA-C	5.64	119.12	110.20
1	A	1663	MET	N-CA-C	5.64	118.15	111.33
1	A	1756	ILE	CB-CA-C	-5.63	104.49	111.70
1	A	1184	THR	N-CA-C	-5.62	104.78	111.69
1	A	144	THR	N-CA-C	5.60	119.21	112.38
2	B	97	GLY	N-CA-C	5.60	123.08	115.30
1	A	836	SER	N-CA-C	5.59	120.10	113.16
1	A	125	HIS	N-CA-C	-5.58	100.64	108.96
1	A	12	PHE	CB-CA-C	-5.58	103.04	110.79
1	A	984	ASP	N-CA-C	-5.57	100.03	108.67
1	A	265	GLN	N-CA-C	5.56	117.02	111.07
1	A	296	GLU	N-CA-C	-5.56	106.50	113.28
1	A	1699	GLY	N-CA-C	5.56	123.46	114.90
1	A	292	THR	CB-CA-C	-5.55	104.39	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	LEU	N-CA-CB	-5.55	101.96	110.01
1	A	1534	VAL	CA-C-N	5.54	128.58	120.71
1	A	1534	VAL	C-N-CA	5.54	128.58	120.71
1	A	918	LEU	N-CA-C	5.51	117.29	111.28
1	A	369	GLN	N-CA-C	5.49	117.26	111.28
1	A	957	LEU	N-CA-C	5.48	116.94	111.07
1	A	971	PHE	CB-CA-C	-5.47	102.48	110.95
1	A	1626	GLY	N-CA-C	5.46	119.76	112.77
1	A	1290	ARG	O-C-N	-5.45	116.34	122.12
1	A	917	PHE	CA-C-N	5.45	127.58	120.28
1	A	917	PHE	C-N-CA	5.45	127.58	120.28
1	A	807	GLY	N-CA-C	5.45	120.37	113.24
2	B	64	THR	N-CA-C	-5.44	100.53	109.40
1	A	971	PHE	CA-C-N	-5.37	113.81	122.24
1	A	971	PHE	C-N-CA	-5.37	113.81	122.24
1	A	408	GLN	N-CA-C	5.36	117.13	111.28
2	B	139	VAL	N-CA-C	5.33	115.66	107.77
1	A	183	PHE	N-CA-C	5.32	117.49	111.11
1	A	13	VAL	N-CA-C	5.30	115.34	108.35
2	B	52	GLU	CB-CA-C	5.29	118.61	110.62
1	A	129	SER	N-CA-C	5.29	117.80	111.71
1	A	932	MET	CA-C-O	-5.27	114.96	120.55
1	A	1581	PHE	N-CA-C	-5.21	105.28	111.69
1	A	1552	VAL	CB-CA-C	5.20	118.84	112.02
1	A	366	LEU	N-CA-C	5.20	116.64	111.07
1	A	1437	PHE	N-CA-C	5.20	117.03	111.36
1	A	282	ASN	N-CA-CB	-5.14	104.36	112.13
1	A	1768	GLU	N-CA-C	5.14	117.45	108.76
1	A	1209	LEU	N-CA-C	5.14	117.62	111.71
2	B	55	THR	N-CA-C	5.12	117.58	109.50
1	A	248	VAL	N-CA-C	-5.09	105.45	111.00
1	A	1499	ARG	CA-C-N	-5.09	113.97	120.23
1	A	1499	ARG	C-N-CA	-5.09	113.97	120.23
1	A	409	ASN	N-CA-C	-5.07	105.76	111.28
1	A	1300	ALA	N-CA-C	5.07	117.53	111.71
1	A	1704	LEU	N-CA-C	5.07	116.80	111.28
1	A	1753	ASN	N-CA-C	5.04	116.78	111.28
1	A	730	TRP	N-CA-C	-5.02	105.50	110.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1712	PRO	Peptide

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	11412	0	11617	268	0
2	B	1416	0	1380	27	0
3	C	980	0	935	5	0
4	D	28	0	25	2	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	28	0	26	1	0
5	B	42	0	39	7	0
6	A	110	0	130	9	0
7	A	210	0	294	72	0
8	A	39	0	0	14	0
9	A	1	0	0	0	0
10	A	329	0	445	37	0
10	B	17	0	19	0	0
11	A	24	0	33	2	0
12	A	232	0	323	29	0
13	A	9	0	0	0	0
All	All	14933	0	15316	357	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 12.

All (357) 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:89:ILE:HD11	1:A:99:ARG:NH1	1.60	1.16
2:B:112:THR:HG21	5:B:303:NAG:C8	1.84	1.06
1:A:1250:TYR:HB3	7:A:2004:Y01:HAU1	1.36	1.03
1:A:1485:MET:HB3	1:A:1639:MET:HE1	1.43	0.98
1:A:1324:VAL:HG21	1:A:1455:VAL:HG21	1.47	0.96
1:A:1759:ILE:HG21	8:A:2006:9Z9:C09	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:THR:HG21	5:B:303:NAG:H81	1.49	0.93
1:A:964:LEU:HD11	8:A:2006:9Z9:C04	2.00	0.92
1:A:398:LEU:HD13	8:A:2006:9Z9:C75	2.02	0.89
1:A:182:THR:HG22	1:A:185:ARG:HD3	1.57	0.87
2:B:112:THR:HG21	5:B:303:NAG:H82	1.57	0.86
1:A:268:MET:HG2	1:A:1537:GLU:HG2	1.56	0.86
1:A:964:LEU:HD11	8:A:2006:9Z9:C05	2.08	0.84
12:A:2015:PCW:H372	7:A:2032:Y01:CAQ	2.10	0.81
1:A:950:MET:HE1	7:A:2007:Y01:HAU2	1.62	0.81
1:A:950:MET:CE	7:A:2007:Y01:HAU2	2.11	0.81
12:A:2015:PCW:H372	7:A:2032:Y01:HAQ2	1.63	0.81
1:A:1224:ILE:HD11	2:B:155:ALA:HB1	1.62	0.79
2:B:51:ALA:HB2	2:B:127:LEU:HD13	1.64	0.78
1:A:858:ILE:HG21	1:A:1450:ASN:HD22	1.48	0.76
1:A:1759:ILE:HG13	8:A:2006:9Z9:C10	2.16	0.76
1:A:950:MET:HE1	7:A:2007:Y01:CAS	2.16	0.75
1:A:963:PHE:CE2	8:A:2006:9Z9:C81	2.69	0.75
2:B:85:ARG:O	2:B:115:HIS:HE1	1.71	0.74
2:B:125:ARG:HG2	2:B:127:LEU:CD2	2.18	0.74
1:A:1485:MET:CB	1:A:1639:MET:HE1	2.16	0.73
12:A:2015:PCW:C37	7:A:2032:Y01:CAQ	2.66	0.73
1:A:849:TRP:HB2	7:A:2005:Y01:HAD3	1.71	0.73
12:A:2015:PCW:H81	7:A:2032:Y01:OAF	1.89	0.73
1:A:1460:PHE:CD2	1:A:1756:ILE:HG13	2.24	0.72
1:A:950:MET:HE1	7:A:2007:Y01:CAU	2.18	0.72
10:A:2033:LPE:H3N1	2:B:181:CYS:SG	2.30	0.72
1:A:60:PRO:HB2	1:A:62:ILE:HG12	1.70	0.71
2:B:112:THR:CG2	5:B:303:NAG:H82	2.20	0.71
1:A:101:ASN:ND2	1:A:103:THR:HB	2.06	0.70
1:A:1301:LEU:HD21	10:A:2016:LPE:H152	1.74	0.70
1:A:47:PRO:HB2	1:A:81:TYR:CE2	2.27	0.69
1:A:943:MET:HE1	7:A:2007:Y01:HAR1	1.73	0.69
2:B:125:ARG:HG2	2:B:127:LEU:HD21	1.75	0.69
1:A:91:LEU:HD23	1:A:97:ILE:HA	1.74	0.69
1:A:426:MET:O	1:A:430:LEU:HG	1.91	0.69
1:A:1224:ILE:CD1	2:B:155:ALA:HB1	2.23	0.69
1:A:1250:TYR:CB	7:A:2004:Y01:HAU1	2.19	0.68
1:A:1328:CYS:HB3	12:A:2015:PCW:H281	1.75	0.68
1:A:1640:SER:HB3	1:A:1761:GLU:HG3	1.74	0.68
1:A:67:PRO:HB2	1:A:70:MET:HG3	1.75	0.67
1:A:1432:TYR:CD2	7:A:2009:Y01:HBF	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1533:MET:HE1	10:A:2026:LPE:H122	1.76	0.67
1:A:59:LEU:HD22	1:A:91:LEU:HD13	1.76	0.67
2:B:57:TRP:HB2	2:B:71:LEU:HG	1.76	0.67
1:A:1627:ALA:HA	10:A:2026:LPE:H1N2	1.76	0.66
1:A:398:LEU:CD1	8:A:2006:9Z9:C75	2.73	0.66
1:A:30:ARG:NH2	1:A:84:ASP:OD2	2.29	0.65
1:A:89:ILE:HD11	1:A:99:ARG:HH11	1.59	0.65
1:A:1328:CYS:SG	1:A:1448:THR:HG23	2.37	0.65
1:A:1577:GLY:H	12:A:2020:PCW:H51	1.62	0.65
6:A:2019:P5S:H22	12:A:2020:PCW:H131	1.79	0.65
1:A:1330:ILE:HG13	7:A:2005:Y01:HAB2	1.77	0.65
1:A:963:PHE:CZ	8:A:2006:9Z9:C81	2.80	0.65
1:A:964:LEU:CD1	8:A:2006:9Z9:C05	2.74	0.64
1:A:413:ILE:HB	1:A:417:LYS:HE3	1.80	0.64
1:A:1478:GLN:HG2	10:A:2021:LPE:H311	1.79	0.64
12:A:2015:PCW:C8	7:A:2032:Y01:HAM2	2.28	0.63
1:A:1478:GLN:HE22	1:A:1646:ASN:HD21	1.47	0.63
1:A:271:LEU:HD12	1:A:343:SER:HA	1.81	0.62
1:A:1432:TYR:CE2	7:A:2009:Y01:HBFB	2.34	0.62
1:A:1571:HIS:HB3	6:A:2031:P5S:N	2.15	0.62
1:A:139:ASN:HD21	1:A:220:ARG:HD3	1.64	0.62
12:A:2015:PCW:H371	7:A:2032:Y01:HAP1	1.81	0.61
1:A:139:ASN:ND2	1:A:220:ARG:HD3	2.16	0.61
7:A:2003:Y01:HAE2	7:A:2003:Y01:HAC1	1.83	0.60
1:A:1653:LEU:HD13	10:A:2025:LPE:H162	1.82	0.60
1:A:887:LEU:HD11	7:A:2007:Y01:HAT1	1.84	0.60
7:A:2004:Y01:HAC1	7:A:2004:Y01:HAE2	1.84	0.60
1:A:120:ILE:HD13	1:A:173:ALA:HB1	1.84	0.60
7:A:2005:Y01:HAE2	7:A:2005:Y01:HAC1	1.84	0.60
1:A:1295:LEU:HD21	10:A:2017:LPE:H192	1.83	0.60
1:A:9:PRO:HB3	1:A:63:TYR:O	2.00	0.60
7:A:2009:Y01:HAC1	7:A:2009:Y01:HAE2	1.84	0.60
7:A:2007:Y01:HAE2	7:A:2007:Y01:HAC1	1.84	0.59
1:A:50:SER:HB2	1:A:53:LEU:HB2	1.83	0.59
1:A:1661:PHE:CD2	10:A:2016:LPE:H3N3	2.36	0.59
1:A:1478:GLN:HE22	1:A:1646:ASN:ND2	2.00	0.59
1:A:1478:GLN:HG2	10:A:2021:LPE:C31	2.33	0.58
1:A:1331:PHE:CZ	1:A:1443:PHE:HB3	2.38	0.58
1:A:761:MET:SD	1:A:838:ARG:HD2	2.43	0.58
1:A:187:PRO:HA	1:A:190[B]:TRP:HD1	1.67	0.58
1:A:858:ILE:CG2	1:A:1450:ASN:HD22	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2012:LPE:H21	12:A:2015:PCW:H131	1.84	0.58
10:A:2014:LPE:H112	7:A:2032:Y01:HAO1	1.84	0.58
1:A:963:PHE:CE2	8:A:2006:9Z9:C77	2.86	0.58
1:A:1325:LEU:HD13	11:A:2013:1PW:H16	1.85	0.58
1:A:47:PRO:HB2	1:A:81:TYR:CD2	2.39	0.57
2:B:112:THR:CB	5:B:303:NAG:H82	2.35	0.57
1:A:880:PHE:HE1	7:A:2007:Y01:HAC2	1.70	0.57
1:A:1249:GLY:HA2	6:A:2002:P5S:H48A	1.86	0.57
1:A:1636:ALA:HB2	1:A:1765:VAL:HG11	1.86	0.57
1:A:1641:LEU:HB3	10:A:2021:LPE:H11	1.85	0.56
1:A:293:LEU:HD22	1:A:298:ASP:HB3	1.86	0.56
1:A:1288:SER:O	1:A:1291:THR:HG22	2.05	0.56
1:A:1347:PHE:HB3	1:A:1385:LEU:HD13	1.87	0.56
1:A:1373:LEU:HG	1:A:1380:VAL:HG21	1.87	0.56
1:A:1533:MET:HE1	10:A:2026:LPE:C12	2.34	0.56
1:A:89:ILE:CD1	1:A:99:ARG:NH1	2.51	0.56
12:A:2015:PCW:H82	7:A:2032:Y01:HAM2	1.87	0.56
1:A:1329:LEU:HD23	12:A:2015:PCW:H271	1.87	0.56
1:A:1364:VAL:HG21	1:A:1373:LEU:HD22	1.88	0.56
6:A:2019:P5S:C35	6:A:2019:P5S:C46	2.83	0.56
1:A:1571:HIS:HB3	6:A:2031:P5S:HN	1.71	0.56
1:A:1458:ASP:O	1:A:1462:GLN:HG2	2.06	0.56
1:A:1460:PHE:CE2	1:A:1756:ILE:HG13	2.41	0.56
1:A:1570:ARG:HG3	6:A:2031:P5S:H1	1.88	0.56
1:A:89:ILE:HG12	1:A:99:ARG:HG3	1.86	0.55
1:A:1474:MET:HE3	1:A:1479:LYS:HG2	1.89	0.55
1:A:1512:VAL:CG1	1:A:1565:LYS:HG2	2.36	0.55
1:A:357:LEU:HD23	1:A:363:TRP:HB2	1.88	0.55
1:A:1219:LYS:HE3	1:A:1222:ILE:HD11	1.89	0.55
1:A:950:MET:HE1	7:A:2007:Y01:HAS2	1.89	0.55
1:A:851:THR:HG23	1:A:1327:VAL:HG21	1.89	0.55
1:A:1301:LEU:HA	1:A:1307:MET:HE3	1.89	0.55
1:A:1324:VAL:CG2	1:A:1455:VAL:HG21	2.30	0.55
1:A:1224:ILE:HD12	1:A:1225:ILE:N	2.21	0.54
2:B:33:GLY:O	5:B:302:NAG:H82	2.07	0.54
1:A:194:VAL:HA	1:A:197:VAL:HG22	1.89	0.54
1:A:92:ASN:C	1:A:94:GLY:H	2.15	0.54
1:A:224:THR:HA	1:A:227:VAL:HG22	1.90	0.54
1:A:91:LEU:CD2	1:A:97:ILE:HA	2.37	0.54
1:A:1460:PHE:HD2	1:A:1756:ILE:HG13	1.71	0.54
1:A:150:ASP:C	1:A:152:THR:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1552:VAL:HG22	1:A:1593:MET:SD	2.47	0.54
1:A:139:ASN:ND2	1:A:143:MET:HE2	2.22	0.54
1:A:1553:VAL:HA	1:A:1556:ILE:HG13	1.88	0.54
1:A:1628:LYS:HG3	1:A:1631:ARG:HH12	1.73	0.54
1:A:92:ASN:HB2	1:A:124:VAL:HG22	1.89	0.53
1:A:836:SER:O	1:A:839:LEU:HB2	2.09	0.53
1:A:1638:MET:HB2	6:A:2019:P5S:H44A	1.90	0.53
1:A:950:MET:HE3	7:A:2007:Y01:HAU2	1.88	0.53
1:A:1748:PHE:HB2	11:A:2013:1PW:H30	1.90	0.53
1:A:812:ASP:HB2	1:A:844:LYS:NZ	2.23	0.53
1:A:1588:ILE:HD13	12:A:2020:PCW:H221	1.90	0.53
1:A:849:TRP:CZ3	7:A:2005:Y01:HAE3	2.43	0.53
1:A:966:LEU:HB3	1:A:1450:ASN:HD21	1.74	0.53
2:B:35:THR:HG22	2:B:109:THR:O	2.08	0.53
1:A:1396:TYR:OH	7:A:2032:Y01:HAA2	2.09	0.52
1:A:1500:PRO:HB2	1:A:1505:GLN:HB3	1.91	0.52
1:A:1627:ALA:HA	10:A:2026:LPE:C1N	2.39	0.52
12:A:2015:PCW:H371	7:A:2032:Y01:CAP	2.39	0.52
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.45	0.52
1:A:182:THR:CG2	1:A:185:ARG:HD3	2.35	0.52
1:A:1331:PHE:HZ	1:A:1443:PHE:HB3	1.75	0.52
1:A:1661:PHE:CZ	10:A:2016:LPE:H3N1	2.45	0.52
1:A:768:MET:HE3	1:A:773:LYS:HE2	1.92	0.52
3:C:47:ARG:NH2	3:C:111[B]:SER:OG	2.43	0.52
1:A:1406:LYS:HD2	1:A:1698:ALA:HA	1.92	0.52
1:A:984:ASP:O	1:A:985:ALA:C	2.53	0.51
1:A:1348:TYR:CE1	1:A:1384:ASN:HB2	2.45	0.51
12:A:2015:PCW:H61	7:A:2032:Y01:CAX	2.39	0.51
1:A:848:SER:HB3	1:A:986:ASN:HD21	1.74	0.51
1:A:1188:ILE:HG13	10:A:2033:LPE:H3N3	1.91	0.51
1:A:1257:ALA:HB1	10:A:2017:LPE:H31	1.92	0.51
12:A:2015:PCW:H371	7:A:2032:Y01:CAQ	2.39	0.51
1:A:1351:ILE:HG22	1:A:1358:ARG:HA	1.93	0.51
1:A:899:ILE:HD12	1:A:906:PRO:HG3	1.93	0.50
7:A:2007:Y01:HAE2	7:A:2007:Y01:CAC	2.41	0.50
4:D:1:NAG:C3	4:D:2:NAG:O7	2.59	0.50
10:A:2033:LPE:H21	2:B:173:TRP:CZ3	2.47	0.50
12:A:2015:PCW:C37	7:A:2032:Y01:CAP	2.90	0.50
1:A:1481:TYR:CE1	10:A:2021:LPE:H1N3	2.46	0.50
1:A:981:GLU:OE2	7:A:2005:Y01:OAF	2.30	0.50
1:A:1406:LYS:HD2	1:A:1697:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:SER:CB	1:A:986:ASN:HD21	2.25	0.50
7:A:2003:Y01:HAE2	7:A:2003:Y01:CAC	2.41	0.50
7:A:2005:Y01:HAE2	7:A:2005:Y01:CAC	2.41	0.50
2:B:125:ARG:CG	2:B:127:LEU:CD2	2.89	0.50
1:A:59:LEU:HD22	1:A:91:LEU:CD1	2.41	0.50
1:A:1478:GLN:NE2	1:A:1646:ASN:HD21	2.10	0.50
1:A:1512:VAL:HG13	1:A:1565:LYS:HG2	1.95	0.49
1:A:971:PHE:HD1	1:A:972:SER:HB2	1.78	0.49
1:A:858:ILE:HG21	1:A:1450:ASN:ND2	2.24	0.49
1:A:1177:ILE:O	1:A:1181:ILE:HG12	2.13	0.49
1:A:228:ILE:HB	1:A:231:LEU:HD22	1.93	0.49
1:A:379:MET:HE1	10:A:2023:LPE:H151	1.95	0.49
1:A:1325:LEU:O	1:A:1329:LEU:HG	2.13	0.49
10:A:2014:LPE:H3N2	7:A:2032:Y01:HAV1	1.93	0.49
1:A:849:TRP:CZ2	1:A:1327:VAL:HG23	2.48	0.49
1:A:1343:PHE:HB3	1:A:1347:PHE:CE1	2.48	0.49
1:A:268:MET:CG	1:A:1537:GLU:HG2	2.33	0.48
1:A:968:LEU:HD21	8:A:2006:9Z9:C14	2.43	0.48
1:A:1654:VAL:HG22	10:A:2016:LPE:H141	1.94	0.48
1:A:275:CYS:SG	1:A:315:CYS:HB3	2.52	0.48
1:A:368:GLN:HG2	1:A:1679:PHE:CZ	2.48	0.48
1:A:876:ILE:O	1:A:879:ILE:HG13	2.13	0.48
1:A:60:PRO:CB	1:A:62:ILE:HG12	2.42	0.48
7:A:2005:Y01:HAV2	7:A:2005:Y01:OAG	2.14	0.48
1:A:273:HIS:CE1	1:A:317:PHE:HE2	2.32	0.48
7:A:2009:Y01:OAG	7:A:2009:Y01:HAV2	2.14	0.48
12:A:2015:PCW:H61	7:A:2032:Y01:OAF	2.14	0.48
2:B:34:MET:O	2:B:111:VAL:HG23	2.14	0.48
1:A:845:LEU:HD11	7:A:2005:Y01:HAA1	1.94	0.48
1:A:1251:LYS:C	1:A:1253:TYR:H	2.22	0.48
7:A:2007:Y01:HAU2	7:A:2007:Y01:HAC1	1.96	0.48
1:A:120:ILE:CD1	1:A:173:ALA:HB1	2.43	0.48
7:A:2005:Y01:HAC1	7:A:2005:Y01:HAU2	1.96	0.47
7:A:2009:Y01:HAC1	7:A:2009:Y01:HAU2	1.96	0.47
1:A:1375:ASN:HD22	1:A:1375:ASN:HA	1.52	0.47
1:A:240:GLN:O	1:A:244:LYS:HD2	2.14	0.47
1:A:851:THR:HG23	1:A:1327:VAL:CG2	2.45	0.47
7:A:2004:Y01:HAC1	7:A:2004:Y01:HAU2	1.96	0.47
2:B:174:LEU:HG	2:B:178:MET:HE3	1.95	0.47
1:A:985:ALA:O	1:A:986:ASN:C	2.57	0.47
7:A:2003:Y01:HAC1	7:A:2003:Y01:HAU2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:O	1:A:17:LYS:C	2.57	0.47
1:A:273:HIS:CE1	1:A:332:LYS:HB2	2.50	0.46
1:A:89:ILE:HD11	1:A:99:ARG:HH12	1.66	0.46
1:A:961:ASN:HD22	1:A:961:ASN:N	2.13	0.46
1:A:1358:ARG:HG2	1:A:1359:PHE:O	2.16	0.46
4:D:1:NAG:H3	4:D:2:NAG:O7	2.14	0.46
1:A:133:MET:HE2	1:A:228:ILE:HG12	1.96	0.46
1:A:737:ILE:HD13	1:A:740:ILE:HD12	1.97	0.46
1:A:1304:PHE:HB2	1:A:1307:MET:HE2	1.98	0.46
1:A:1732:ASN:HD22	1:A:1735:VAL:HG23	1.80	0.46
7:A:2004:Y01:HAE2	7:A:2004:Y01:CAC	2.41	0.46
7:A:2009:Y01:HAE2	7:A:2009:Y01:CAC	2.41	0.46
12:A:2029:PCW:H341	12:A:2029:PCW:H371	1.56	0.46
1:A:92:ASN:HB2	1:A:124:VAL:CG2	2.46	0.46
1:A:423:PHE:O	1:A:427:LEU:HG	2.15	0.46
10:A:2023:LPE:H3N2	10:A:2024:LPE:H31	1.97	0.46
1:A:758:THR:HG21	7:A:2005:Y01:HBA	1.98	0.46
1:A:1003:LYS:HE2	1:A:1007:ARG:HH21	1.80	0.46
12:A:2015:PCW:C37	7:A:2032:Y01:HAQ1	2.43	0.46
1:A:849:TRP:HB2	7:A:2005:Y01:CAD	2.43	0.45
1:A:1651:LEU:HD13	1:A:1750:VAL:HG21	1.98	0.45
12:A:2020:PCW:H31	12:A:2029:PCW:H31	1.98	0.45
1:A:101:ASN:HD21	1:A:103:THR:HB	1.80	0.45
1:A:1571:HIS:C	1:A:1573:TYR:N	2.73	0.45
7:A:2032:Y01:HBB	7:A:2032:Y01:HAE2	1.60	0.45
2:B:71:LEU:HB3	2:B:80:LEU:HD12	1.97	0.45
1:A:1365:PRO:HD2	1:A:1369:GLU:HG3	1.99	0.45
1:A:858:ILE:CG2	1:A:1450:ASN:ND2	2.80	0.45
1:A:1653:LEU:HD22	10:A:2025:LPE:H182	1.99	0.45
10:A:2028:LPE:H3N2	10:A:2028:LPE:H312	1.72	0.45
1:A:348:SER:HB2	12:A:2018:PCW:H332	1.99	0.45
1:A:1301:LEU:HD21	10:A:2016:LPE:C15	2.44	0.45
1:A:1488:LEU:C	1:A:1490:SER:H	2.25	0.45
1:A:1251:LYS:C	1:A:1253:TYR:N	2.74	0.45
2:B:125:ARG:CG	2:B:127:LEU:HD22	2.47	0.45
1:A:1430:SER:HB3	1:A:1433:MET:HG2	1.98	0.44
1:A:842:VAL:HG13	7:A:2005:Y01:HAA2	1.99	0.44
1:A:866:LEU:HD12	1:A:966:LEU:HD23	1.99	0.44
1:A:104:PRO:HB2	1:A:107:TYR:HA	1.98	0.44
1:A:736:CYS:O	1:A:740:ILE:HG13	2.17	0.44
1:A:1197:PHE:O	1:A:1201:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1529:MET:HG2	1:A:1533:MET:HE3	1.99	0.44
2:B:162:MET:HA	2:B:165:VAL:HG22	1.99	0.44
1:A:80:PRO:O	1:A:81:TYR:C	2.60	0.44
1:A:760:PHE:CE2	1:A:776:LEU:HA	2.52	0.44
1:A:849:TRP:CE3	7:A:2005:Y01:HAE3	2.53	0.44
1:A:187:PRO:HA	1:A:190[B]:TRP:CD1	2.51	0.44
1:A:272:LYS:HB2	1:A:332:LYS:HG3	2.00	0.44
1:A:1361:ALA:O	1:A:1365:PRO:HB3	2.17	0.44
7:A:2007:Y01:HAS2	7:A:2007:Y01:HAE1	1.81	0.44
1:A:1219:LYS:HB3	1:A:1222:ILE:HG13	1.99	0.44
1:A:1261:LEU:O	1:A:1265:ILE:HG13	2.18	0.44
1:A:1543:MET:HA	1:A:1546:VAL:HG22	2.00	0.44
1:A:1624:VAL:HG13	1:A:1630:ILE:HD12	2.00	0.44
10:A:2021:LPE:H311	10:A:2021:LPE:H2N3	1.61	0.44
1:A:850:PRO:HD3	7:A:2005:Y01:HAV1	1.99	0.44
7:A:2005:Y01:HAN2	7:A:2005:Y01:HAC3	2.00	0.44
1:A:1250:TYR:OH	10:A:2027:LPE:H172	2.18	0.44
1:A:1260:TRP:CE3	7:A:2003:Y01:CAE	3.01	0.43
1:A:1571:HIS:C	1:A:1573:TYR:H	2.25	0.43
1:A:1774:LEU:HD21	1:A:1849:VAL:HG11	2.00	0.43
2:B:112:THR:H	2:B:115:HIS:CD2	2.36	0.43
1:A:16:THR:C	1:A:18:GLN:N	2.76	0.43
1:A:1583:PHE:HA	1:A:1586:VAL:HG22	2.00	0.43
1:A:812:ASP:HB2	1:A:844:LYS:HZ3	1.82	0.43
1:A:1394:LEU:HG	12:A:2015:PCW:H121	2.00	0.43
1:A:1435:ILE:O	1:A:1436:TYR:C	2.62	0.43
1:A:1487:LYS:O	1:A:1488:LEU:C	2.58	0.43
2:B:44:LYS:HG2	2:B:102:GLN:OE1	2.18	0.43
1:A:89:ILE:CG1	1:A:99:ARG:HG3	2.48	0.43
1:A:981:GLU:CG	7:A:2005:Y01:OAF	2.65	0.43
1:A:1652:PHE:HE1	10:A:2023:LPE:H141	1.84	0.43
1:A:733:PHE:O	1:A:737:ILE:HG12	2.19	0.43
1:A:880:PHE:CG	1:A:951:VAL:HG22	2.54	0.43
12:A:2020:PCW:H73	12:A:2020:PCW:H41	1.57	0.43
1:A:952:MET:HE2	1:A:952:MET:HB3	1.83	0.43
1:A:789:ALA:O	1:A:790:GLU:C	2.62	0.43
3:C:128:TYR:C	3:C:129:ILE:HG13	2.44	0.43
1:A:259:PHE:HZ	1:A:388:LEU:HD12	1.84	0.42
1:A:1296:ARG:HG2	1:A:1297:PRO:HD3	2.01	0.42
7:A:2032:Y01:HAS2	7:A:2032:Y01:HAE1	1.81	0.42
1:A:372:ARG:HA	1:A:1678:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:THR:HB	5:B:303:NAG:H82	2.01	0.42
1:A:1641:LEU:HD23	10:A:2021:LPE:H12	2.01	0.42
12:A:2015:PCW:H81	7:A:2032:Y01:HAM2	2.01	0.42
1:A:91:LEU:HD21	1:A:97:ILE:HG12	2.01	0.42
1:A:1563:VAL:O	1:A:1567:ILE:HG13	2.19	0.42
1:A:1577:GLY:N	12:A:2020:PCW:H51	2.32	0.42
1:A:50:SER:N	1:A:79:ASP:OD2	2.48	0.42
1:A:150:ASP:C	1:A:152:THR:N	2.78	0.42
1:A:198:PHE:HD1	1:A:198:PHE:HA	1.77	0.42
1:A:1488:LEU:O	1:A:1490:SER:N	2.52	0.42
7:A:2009:Y01:HAS2	7:A:2009:Y01:HAE1	1.81	0.42
1:A:236:GLY:O	1:A:240:GLN:HG2	2.19	0.42
1:A:922:ARG:HG2	1:A:927:GLU:HB2	2.02	0.42
6:A:2002:P5S:H56A	6:A:2002:P5S:H53	1.86	0.42
7:A:2009:Y01:HAN2	7:A:2009:Y01:HAC3	2.00	0.42
1:A:1751:VAL:O	1:A:1755:TYR:HD1	2.01	0.42
3:C:65:LEU:HB3	3:C:83:PHE:HB3	2.02	0.42
1:A:766:HIS:CD2	1:A:1345:GLY:HA3	2.54	0.42
1:A:215:THR:HB	7:A:2007:Y01:HAK2	2.02	0.41
1:A:283:ASN:HB2	5:A:2001:NAG:H2	2.02	0.41
1:A:981:GLU:HG3	7:A:2005:Y01:OAF	2.19	0.41
1:A:1289:LEU:O	1:A:1292:LEU:HB2	2.20	0.41
1:A:264:LEU:O	1:A:268:MET:HB2	2.20	0.41
1:A:332:LYS:HB3	1:A:332:LYS:HE3	1.92	0.41
1:A:1570:ARG:HB3	1:A:1571:HIS:H	1.56	0.41
2:B:174:LEU:O	2:B:178:MET:HG3	2.20	0.41
3:C:40:VAL:HG11	3:C:46:ALA:HB2	2.03	0.41
1:A:23:ILE:HG23	1:A:84:ASP:O	2.20	0.41
1:A:763:MET:O	1:A:765:HIS:HD2	2.03	0.41
1:A:968:LEU:HD21	8:A:2006:9Z9:C15	2.49	0.41
1:A:1759:ILE:HG23	1:A:1763:PHE:CE1	2.55	0.41
1:A:1216:ILE:HA	1:A:1219:LYS:HE2	2.03	0.41
12:A:2029:PCW:H63	12:A:2029:PCW:H42	1.59	0.41
1:A:238:LEU:HD23	1:A:961:ASN:OD1	2.20	0.41
1:A:963:PHE:CD2	8:A:2006:9Z9:C81	3.03	0.41
1:A:993:THR:HG22	1:A:997:LYS:HE3	2.02	0.41
7:A:2005:Y01:HAS2	7:A:2005:Y01:HAE1	1.81	0.41
1:A:1684:PHE:HD2	10:A:2024:LPE:H141	1.85	0.41
10:A:2017:LPE:H311	10:A:2017:LPE:H2N2	1.87	0.41
10:A:2022:LPE:H112	10:A:2022:LPE:H142	1.98	0.41
7:A:2032:Y01:HAP1	7:A:2032:Y01:HAO2	1.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ALA:HB1	8:A:2006:9Z9:C15	2.51	0.41
1:A:869:LEU:HD22	1:A:962:LEU:HD13	2.03	0.41
1:A:1481:TYR:CD1	10:A:2021:LPE:H1N3	2.56	0.41
7:A:2004:Y01:HAS2	7:A:2004:Y01:HAE1	1.81	0.41
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.59	0.41
1:A:1325:LEU:HD11	12:A:2015:PCW:C47	2.51	0.41
1:A:1432:TYR:CE2	7:A:2009:Y01:HAT1	2.57	0.41
1:A:1576:VAL:HB	1:A:1579:ASN:HB2	2.03	0.41
1:A:1561:GLU:O	1:A:1562:CYS:C	2.62	0.40
1:A:1709:ASN:ND2	1:A:1714:ASP:HB3	2.36	0.40
10:A:2027:LPE:H312	10:A:2027:LPE:H2N2	1.81	0.40
1:A:1408:TRP:H	1:A:1408:TRP:CD1	2.38	0.40
1:A:1617:ILE:HB	12:A:2020:PCW:H261	2.03	0.40
10:A:2023:LPE:H311	10:A:2023:LPE:H2N3	1.78	0.40
1:A:85:LYS:HE2	1:A:85:LYS:HB2	1.87	0.40
1:A:399:ALA:HB2	1:A:1759:ILE:HD12	2.04	0.40
2:B:37:LYS:HE3	2:B:93:ASN:HB3	2.03	0.40
1:A:845:LEU:CD1	7:A:2005:Y01:HAA1	2.51	0.40
1:A:1492:LYS:HD3	1:A:1493:PRO:HD2	2.03	0.40
1:A:1512:VAL:HG11	1:A:1565:LYS:HG2	2.03	0.40
1:A:1581:PHE:CD1	6:A:2019:P5S:H24A	2.56	0.40
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.86	0.40
1:A:1179:TRP:HZ3	10:A:2027:LPE:O31	2.04	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	1402/2031 (69%)	1318 (94%)	75 (5%)	9 (1%)	21 23
2	B	171/218 (78%)	167 (98%)	3 (2%)	1 (1%)	21 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	120/215 (56%)	117 (98%)	3 (2%)	0	100	100
All	All	1693/2464 (69%)	1602 (95%)	81 (5%)	10 (1%)	23	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1773	PRO
2	B	150	ALA
1	A	15	PHE
1	A	93	LYS
1	A	953	VAL
1	A	1572	TYR
1	A	52	ASP
1	A	199	ALA
1	A	1360	PRO
1	A	1818	PRO

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	1265/1809 (70%)	1232 (97%)	33 (3%)	40	55
2	B	157/190 (83%)	150 (96%)	7 (4%)	24	33
3	C	114/193 (59%)	109 (96%)	5 (4%)	25	34
All	All	1536/2192 (70%)	1491 (97%)	45 (3%)	38	51

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	57	LYS
1	A	124	VAL
1	A	155	VAL
1	A	253	VAL

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Mol	Chain	Res	Type
1	A	289	ILE
1	A	379	MET
1	A	380	ILE
1	A	840	LEU
1	A	844	LYS
1	A	847	LYS
1	A	929	ILE
1	A	964	LEU
1	A	968	LEU
1	A	1187	LYS
1	A	1195	GLU
1	A	1222	ILE
1	A	1239	LEU
1	A	1375	ASN
1	A	1406	LYS
1	A	1435	ILE
1	A	1492	LYS
1	A	1512	VAL
1	A	1534	VAL
1	A	1535	GLU
1	A	1547	LEU
1	A	1553	VAL
1	A	1587	ILE
1	A	1599	ILE
1	A	1620	ILE
1	A	1633	LEU
1	A	1641	LEU
1	A	1711	LYS
2	B	31	VAL
2	B	85	ARG
2	B	90	VAL
2	B	93	ASN
2	B	104	LEU
2	B	138	VAL
2	B	190	GLU
3	C	48	LEU
3	C	55	CYS
3	C	71	GLU
3	C	130	MET
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	58	GLN
1	A	139	ASN
1	A	273	HIS
1	A	278	ASN
1	A	412	ASN
1	A	765	HIS
1	A	766	HIS
1	A	886	GLN
1	A	909	HIS
1	A	986	ASN
1	A	1276	ASN
1	A	1323	ASN
1	A	1341	ASN
1	A	1378	GLN
1	A	1384	ASN
1	A	1450	ASN
1	A	1459	ASN
1	A	1461	ASN
1	A	1462	GLN
1	A	1463	GLN
1	A	1478	GLN
1	A	1494	GLN
1	A	1721	HIS
1	A	1732	ASN
1	A	1837	HIS
2	B	115	HIS
2	B	122	HIS
2	B	143	HIS
3	C	53	ASN
3	C	82	GLN
3	C	145	GLN

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

6 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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.35	0	17,19,21	0.53	0
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.73	0
4	NAG	E	1	1,4	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.67	0
4	NAG	F	1	2,4	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.21	1 (5%)

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	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.78	115.92	112.19
4	F	1	NAG	C3-C4-C5	-2.60	105.52	110.23
4	F	2	NAG	C4-C3-C2	-2.40	107.50	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

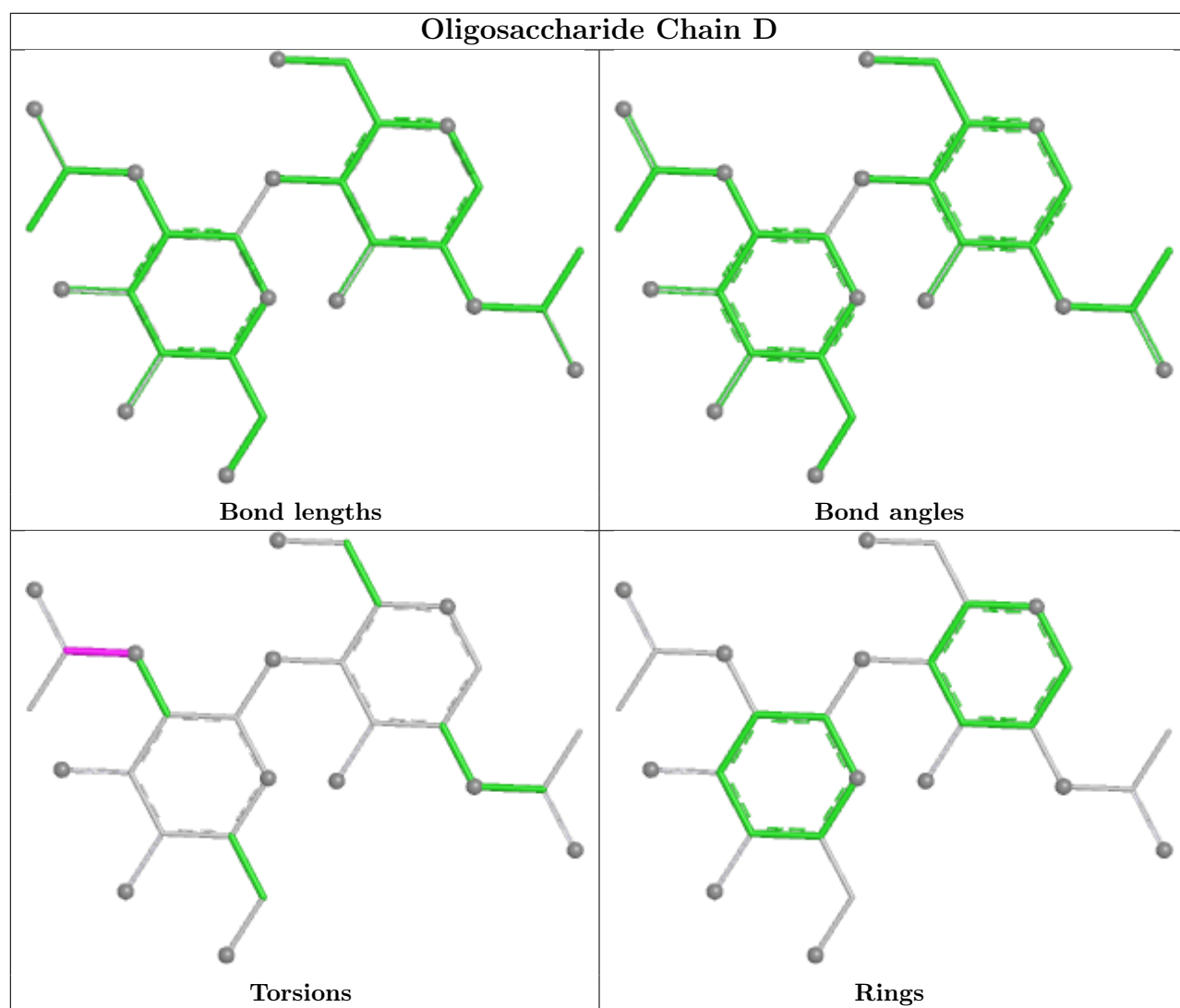
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

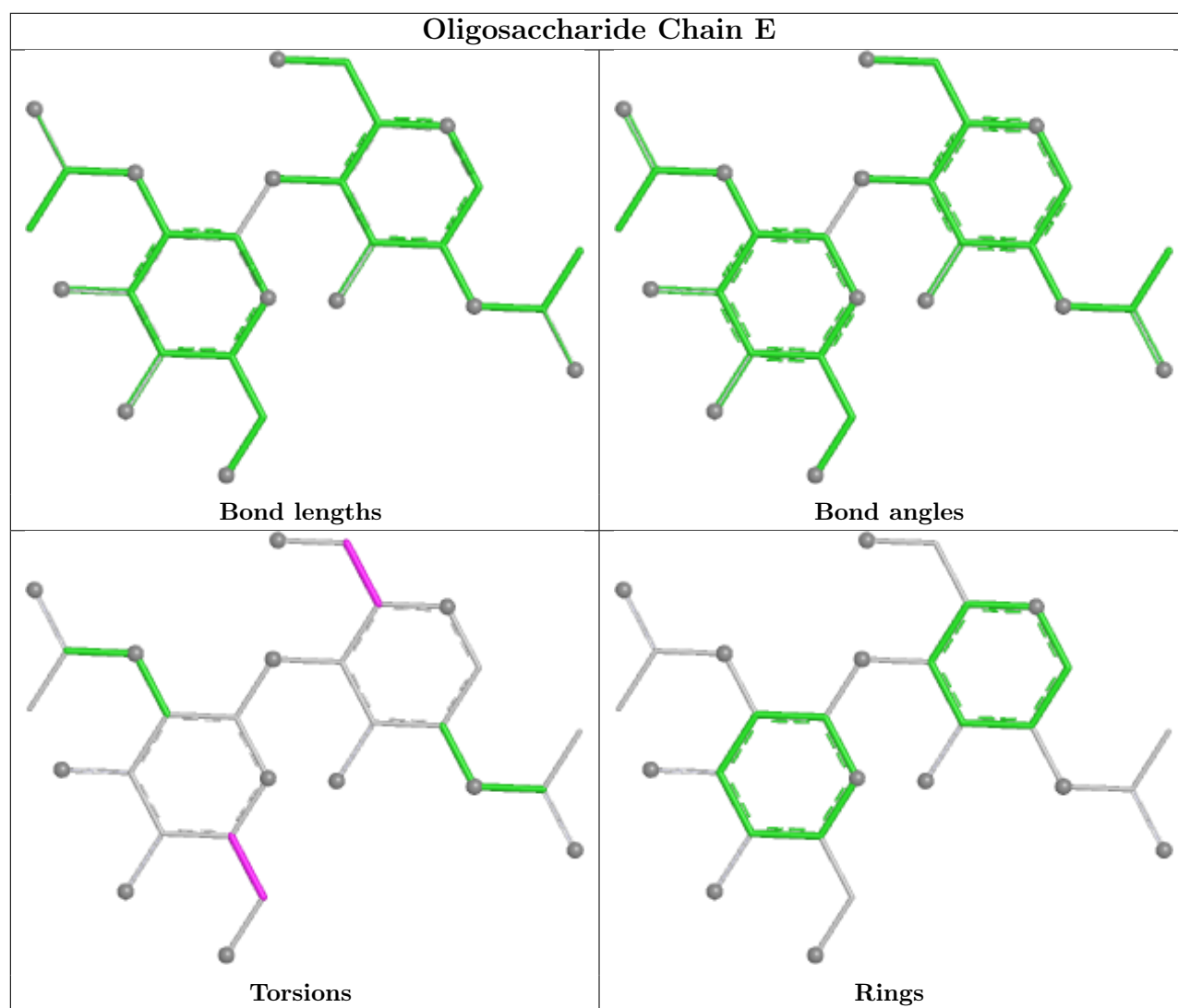
There are no ring outliers.

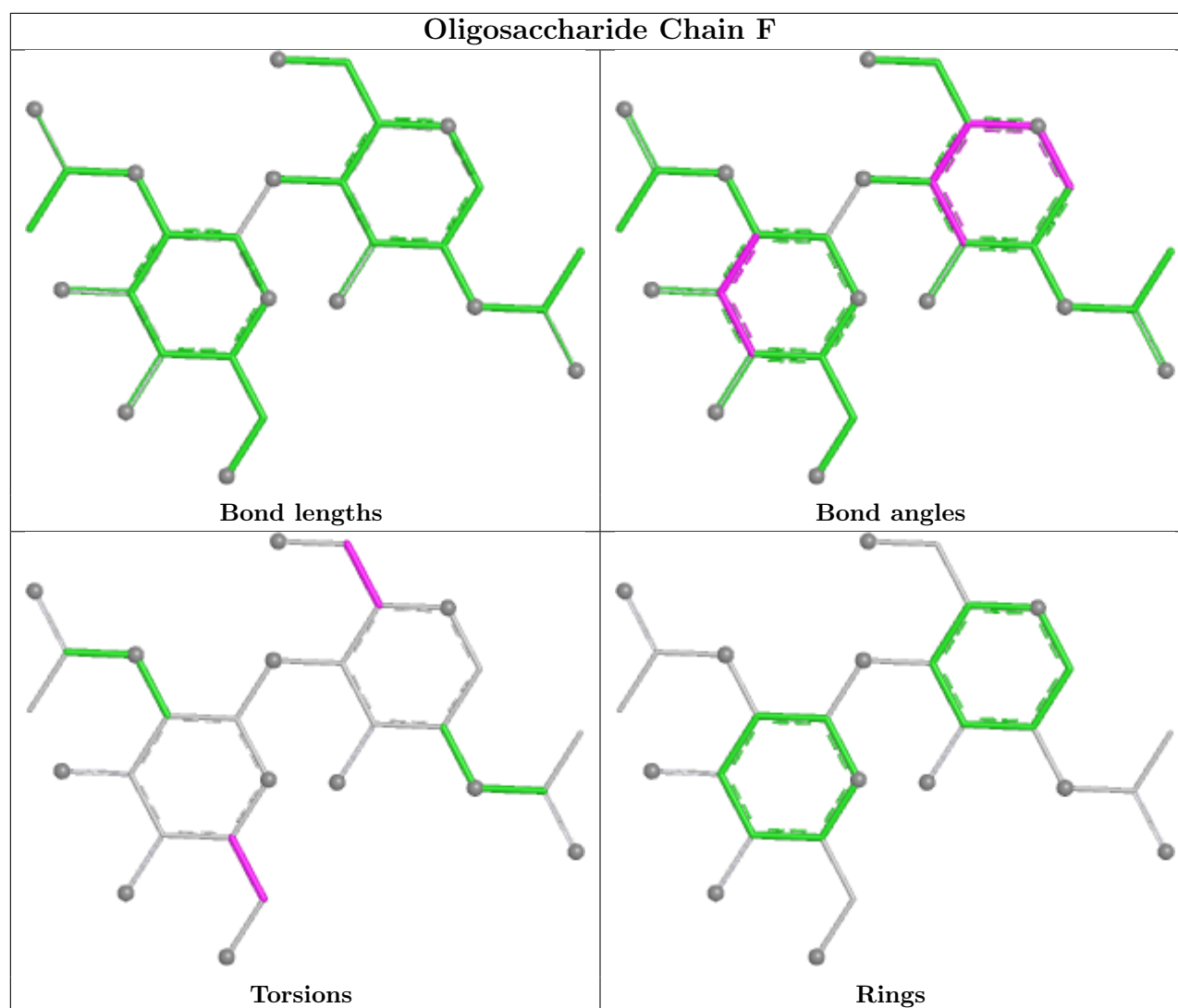
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
4	D	2	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 [i](#)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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	$\# Z > 2$
7	Y01	A	2004	-	38,38,38	0.68	1 (2%)	57,57,57	1.83	13 (22%)
7	Y01	A	2005	-	38,38,38	1.17	4 (10%)	57,57,57	1.79	12 (21%)
5	NAG	B	302	2	14,14,15	0.19	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.97	0
7	Y01	A	2009	-	38,38,38	1.17	4 (10%)	57,57,57	1.79	12 (21%)
11	1PW	A	2013	-	23,23,27	0.44	0	24,26,32	0.54	0
10	LPE	A	2011	-	24,24,33	0.52	0	28,30,39	0.61	0
10	LPE	A	2016	-	21,21,33	0.70	0	25,27,39	1.05	2 (8%)
10	LPE	A	2024	-	24,24,33	0.54	0	28,30,39	0.65	0
10	LPE	A	2014	-	19,19,33	0.63	0	23,25,39	0.53	0
10	LPE	A	2025	-	24,24,33	0.54	0	28,30,39	0.54	0
5	NAG	B	303	2	14,14,15	0.26	0	17,19,21	0.44	0
10	LPE	A	2023	-	24,24,33	0.55	0	28,30,39	0.69	1 (3%)
7	Y01	A	2007	-	38,38,38	0.69	1 (2%)	57,57,57	1.83	12 (21%)
12	PCW	A	2030	-	43,43,53	1.04	2 (4%)	49,51,61	1.01	2 (4%)
12	PCW	A	2018	-	46,46,53	1.00	3 (6%)	52,54,61	1.19	4 (7%)
7	Y01	A	2032	-	38,38,38	1.66	7 (18%)	57,57,57	1.68	12 (21%)
12	PCW	A	2029	-	43,43,53	1.04	2 (4%)	49,51,61	0.95	2 (4%)
10	LPE	A	2021	-	24,24,33	0.61	0	28,30,39	0.91	1 (3%)
5	NAG	A	2008	1	14,14,15	0.40	0	17,19,21	0.88	1 (5%)
10	LPE	A	2033	-	16,16,33	0.69	0	20,22,39	0.68	0
6	P5S	A	2031	-	32,33,53	1.19	4 (12%)	34,40,60	1.02	2 (5%)
12	PCW	A	2020	-	43,43,53	1.02	2 (4%)	49,51,61	1.13	5 (10%)
7	Y01	A	2003	-	38,38,38	0.69	1 (2%)	57,57,57	1.83	12 (21%)
10	LPE	A	2022	-	24,24,33	0.88	0	28,30,39	0.91	1 (3%)
10	LPE	A	2012	-	24,24,33	0.33	0	25,27,39	0.61	0
10	LPE	A	2027	-	24,24,33	0.56	0	28,30,39	0.50	0
10	LPE	A	2017	-	27,27,33	0.55	0	31,33,39	0.62	0
5	NAG	A	2001	1	14,14,15	0.36	0	17,19,21	0.46	0
12	PCW	A	2015	-	52,52,53	0.94	2 (3%)	58,60,61	0.99	2 (3%)
6	P5S	A	2019	-	40,40,53	1.17	3 (7%)	43,45,60	1.38	3 (6%)
10	LPE	A	2028	-	16,16,33	0.71	0	20,22,39	0.69	0
8	9Z9	A	2006	-	44,44,44	0.73	1 (2%)	64,68,68	1.51	11 (17%)
10	LPE	B	304	-	16,16,33	0.68	0	20,22,39	0.61	0
10	LPE	A	2026	-	24,24,33	0.52	0	28,30,39	0.63	0
6	P5S	A	2002	-	33,34,53	0.77	1 (3%)	34,40,60	1.80	4 (11%)

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
7	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
7	Y01	A	2005	-	-	4/19/77/77	0/4/4/4
5	NAG	B	302	2	-	0/6/23/26	0/1/1/1
5	NAG	B	301	2	-	0/6/23/26	0/1/1/1
7	Y01	A	2009	-	-	4/19/77/77	0/4/4/4
11	1PW	A	2013	-	-	4/22/22/29	-
10	LPE	A	2011	-	-	8/25/25/34	-
10	LPE	A	2016	-	-	15/22/22/34	-
10	LPE	A	2024	-	-	3/25/25/34	-
10	LPE	A	2014	-	-	8/20/20/34	-
10	LPE	A	2025	-	-	7/25/25/34	-
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
10	LPE	A	2023	-	-	2/25/25/34	-
7	Y01	A	2007	-	-	0/19/77/77	0/4/4/4
12	PCW	A	2030	-	-	11/47/47/57	-
12	PCW	A	2018	-	-	12/50/50/57	-
7	Y01	A	2032	-	-	7/19/77/77	0/4/4/4
12	PCW	A	2029	-	-	15/47/47/57	-
10	LPE	A	2021	-	-	5/25/25/34	-
5	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
10	LPE	A	2033	-	-	8/17/17/34	-
6	P5S	A	2031	-	-	18/39/39/59	-
12	PCW	A	2020	-	-	10/47/47/57	-
7	Y01	A	2003	-	-	0/19/77/77	0/4/4/4
10	LPE	A	2022	-	-	11/25/25/34	-
10	LPE	A	2012	-	-	8/25/25/34	-
10	LPE	A	2027	-	-	10/25/25/34	-
10	LPE	A	2017	-	-	8/28/28/34	-
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
12	PCW	A	2015	-	-	16/56/56/57	-
6	P5S	A	2019	-	-	8/44/44/59	-
10	LPE	A	2028	-	-	6/17/17/34	-
8	9Z9	A	2006	-	-	0/12/100/100	0/6/6/6
10	LPE	B	304	-	-	9/17/17/34	-
10	LPE	A	2026	-	-	4/25/25/34	-
6	P5S	A	2002	-	-	27/39/39/59	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2032	Y01	CBB-CBE	-4.44	1.46	1.54
12	A	2029	PCW	O3-C11	4.41	1.46	1.33
6	A	2019	P5S	O37-C38	4.40	1.46	1.34
12	A	2030	PCW	O3-C11	4.27	1.45	1.33
7	A	2032	Y01	CAR-CBC	-4.24	1.39	1.51
12	A	2030	PCW	O2-C31	4.20	1.46	1.34
12	A	2015	PCW	O2-C31	4.19	1.46	1.34
12	A	2015	PCW	O3-C11	4.14	1.45	1.33
12	A	2020	PCW	O2-C31	3.93	1.45	1.34
6	A	2019	P5S	O19-C17	3.93	1.44	1.33
12	A	2018	PCW	O3-C11	3.89	1.44	1.33
12	A	2020	PCW	O3-C11	3.89	1.44	1.33
12	A	2029	PCW	O2-C31	3.89	1.45	1.34
6	A	2019	P5S	C28-C27	-3.81	1.32	1.51
7	A	2032	Y01	OAW-CAY	3.70	1.44	1.34
12	A	2018	PCW	O2-C31	3.66	1.44	1.34
7	A	2009	Y01	OAW-CAY	3.63	1.44	1.34
7	A	2005	Y01	OAW-CAY	3.62	1.44	1.34
6	A	2002	P5S	O37-C38	3.41	1.43	1.34
7	A	2032	Y01	CAV-CBC	3.15	1.59	1.52
6	A	2031	P5S	O19-C17	2.74	1.41	1.33
6	A	2031	P5S	O37-C2	-2.68	1.40	1.46
7	A	2032	Y01	CAM-CAY	2.41	1.57	1.50
7	A	2005	Y01	CAM-CAY	2.39	1.57	1.50
7	A	2009	Y01	CAM-CAY	2.38	1.57	1.50
7	A	2003	Y01	CBH-CBF	-2.35	1.52	1.56
6	A	2031	P5S	O19-C1	-2.34	1.39	1.45
7	A	2032	Y01	CBH-CBF	-2.32	1.52	1.56
8	A	2006	9Z9	C11-C08	-2.32	1.52	1.56
7	A	2005	Y01	CBH-CBF	-2.31	1.52	1.56
7	A	2007	Y01	CBH-CBF	-2.28	1.52	1.56
6	A	2031	P5S	O37-C38	2.28	1.40	1.34
7	A	2009	Y01	CAL-CAX	2.26	1.55	1.50
7	A	2009	Y01	CBH-CBF	-2.25	1.52	1.56
7	A	2004	Y01	CBH-CBF	-2.25	1.52	1.56
7	A	2005	Y01	CAL-CAX	2.24	1.55	1.50
7	A	2032	Y01	CAL-CAX	2.18	1.55	1.50
12	A	2018	PCW	C6-N	-2.15	1.43	1.50

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2002	P5S	OG-CB-CA	7.10	114.25	108.06
7	A	2009	Y01	CBI-CBE-CBB	-6.03	110.19	119.50
7	A	2005	Y01	CBI-CBE-CBB	-6.01	110.21	119.50
7	A	2004	Y01	CBI-CBE-CBB	-6.00	110.23	119.50
7	A	2007	Y01	CBI-CBE-CBB	-6.00	110.23	119.50
7	A	2003	Y01	CBI-CBE-CBB	-5.99	110.24	119.50
6	A	2019	P5S	O37-C38-C39	5.46	123.29	111.48
7	A	2004	Y01	CBI-CBG-CBD	-5.05	107.25	114.41
7	A	2007	Y01	CBI-CBG-CBD	-5.04	107.26	114.41
7	A	2003	Y01	CBI-CBG-CBD	-5.00	107.32	114.41
7	A	2032	Y01	CBI-CBG-CBD	-4.96	107.37	114.41
7	A	2005	Y01	CBI-CBG-CBD	-4.96	107.38	114.41
7	A	2009	Y01	CBI-CBG-CBD	-4.95	107.39	114.41
12	A	2018	PCW	O2-C31-C32	4.82	121.92	111.48
8	A	2006	9Z9	C02-C06-C07	-4.60	107.89	114.41
7	A	2032	Y01	CBI-CBE-CBB	-4.22	112.98	119.50
6	A	2002	P5S	OXT-C-O	-4.06	114.87	124.08
7	A	2004	Y01	OAW-CAY-CAM	3.98	120.08	111.48
7	A	2003	Y01	OAW-CAY-CAM	3.96	120.06	111.48
7	A	2007	Y01	OAW-CAY-CAM	3.95	120.02	111.48
12	A	2030	PCW	O2-C31-C32	3.93	119.98	111.48
12	A	2015	PCW	O2-C31-C32	3.86	119.83	111.48
10	A	2022	LPE	C3N-N-C2N	3.84	119.06	108.98
7	A	2009	Y01	OAW-CAY-CAM	3.74	119.58	111.48
7	A	2005	Y01	OAW-CAY-CAM	3.73	119.56	111.48
8	A	2006	9Z9	C02-C03-C74	-3.71	109.53	120.50
6	A	2002	P5S	O37-C38-C39	3.69	119.46	111.48
7	A	2032	Y01	OAW-CAY-CAM	3.58	119.23	111.48
6	A	2031	P5S	O37-C38-C39	3.43	118.90	111.48
7	A	2009	Y01	CAS-CAU-CBI	-3.35	107.08	112.74
7	A	2032	Y01	CAS-CAU-CBI	-3.34	107.10	112.74
7	A	2003	Y01	CAS-CAU-CBI	-3.34	107.10	112.74
7	A	2005	Y01	CAS-CAU-CBI	-3.34	107.11	112.74
7	A	2004	Y01	CAS-CAU-CBI	-3.34	107.11	112.74
7	A	2007	Y01	CAS-CAU-CBI	-3.32	107.14	112.74
8	A	2006	9Z9	C09-C10-C02	-3.31	107.16	112.74
12	A	2029	PCW	O2-C31-C32	3.24	118.49	111.48
12	A	2018	PCW	O3-C11-C12	3.17	121.51	111.83
8	A	2006	9Z9	C76-C73-C74	-3.14	109.98	115.66
7	A	2003	Y01	CAD-CBH-CBF	-3.10	108.19	111.66
7	A	2009	Y01	CAD-CBH-CBF	-3.09	108.19	111.66
7	A	2004	Y01	CAD-CBH-CBF	-3.07	108.22	111.66
7	A	2005	Y01	CAD-CBH-CBF	-3.07	108.22	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2007	Y01	CAD-CBH-CBF	-3.04	108.25	111.66
7	A	2032	Y01	CAD-CBH-CBF	-3.03	108.26	111.66
8	A	2006	9Z9	C12-C11-C08	-3.02	108.28	111.66
12	A	2020	PCW	C3-C2-C1	-2.93	104.95	111.78
10	A	2016	LPE	C3-C2-C1	-2.88	104.37	112.65
8	A	2006	9Z9	C75-C74-C73	-2.87	110.32	114.94
12	A	2020	PCW	O2-C31-C32	2.81	117.55	111.48
12	A	2030	PCW	O3-C11-C12	2.80	120.36	111.83
7	A	2007	Y01	CBG-CBI-CBE	2.79	103.30	100.10
7	A	2032	Y01	CBG-CBI-CBE	2.78	103.28	100.10
7	A	2005	Y01	CBG-CBI-CBE	2.77	103.28	100.10
7	A	2003	Y01	CBG-CBI-CBE	2.77	103.28	100.10
7	A	2009	Y01	CBG-CBI-CBE	2.77	103.28	100.10
7	A	2007	Y01	CAS-CBF-CBH	-2.76	109.69	113.08
7	A	2004	Y01	CBG-CBI-CBE	2.76	103.26	100.10
7	A	2004	Y01	CAS-CBF-CBH	-2.72	109.73	113.08
7	A	2032	Y01	CAS-CBF-CBH	-2.71	109.74	113.08
5	A	2008	NAG	C1-O5-C5	2.67	115.77	112.19
7	A	2009	Y01	CAS-CBF-CBH	-2.67	109.79	113.08
10	A	2016	LPE	C31-C32-N	-2.67	107.27	115.82
7	A	2003	Y01	CAS-CBF-CBH	-2.67	109.80	113.08
7	A	2005	Y01	CAS-CBF-CBH	-2.66	109.81	113.08
8	A	2006	9Z9	C09-C08-C11	-2.63	109.84	113.08
12	A	2020	PCW	O3-C11-C12	2.60	119.75	111.83
7	A	2003	Y01	CBD-CAK-CAI	-2.58	109.18	112.76
7	A	2009	Y01	CBD-CAK-CAI	-2.58	109.19	112.76
7	A	2005	Y01	CBD-CAK-CAI	-2.56	109.22	112.76
12	A	2015	PCW	O3-C11-C12	2.55	119.60	111.83
7	A	2032	Y01	CBD-CAK-CAI	-2.54	109.24	112.76
7	A	2007	Y01	CBD-CAK-CAI	-2.54	109.24	112.76
7	A	2004	Y01	CBD-CAK-CAI	-2.54	109.25	112.76
6	A	2031	P5S	O19-C17-C20	2.53	119.54	111.83
8	A	2006	9Z9	C07-C15-C14	-2.52	109.28	112.76
7	A	2003	Y01	CBF-CBH-CAZ	2.51	113.33	109.65
7	A	2005	Y01	CBF-CBH-CAZ	2.49	113.29	109.65
7	A	2032	Y01	CBF-CBH-CAZ	2.48	113.28	109.65
7	A	2007	Y01	CBF-CBH-CAZ	2.47	113.28	109.65
7	A	2009	Y01	CBF-CBH-CAZ	2.47	113.27	109.65
8	A	2006	9Z9	C08-C11-C13	2.44	113.23	109.65
7	A	2004	Y01	CBF-CBH-CAZ	2.43	113.21	109.65
12	A	2029	PCW	O3-C11-C12	2.41	119.17	111.83
6	A	2002	P5S	C2-O37-C38	-2.36	112.16	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2019	P5S	C41-C40-C39	-2.31	104.64	113.13
7	A	2007	Y01	CAC-CBB-CBE	-2.29	109.44	112.88
10	A	2023	LPE	C31-C32-N	-2.27	108.53	115.82
8	A	2006	9Z9	O80-C79-C78	-2.27	109.26	112.17
7	A	2004	Y01	CAC-CBB-CBE	-2.26	109.50	112.88
7	A	2005	Y01	CAC-CBB-CBE	-2.24	109.52	112.88
7	A	2003	Y01	CAC-CBB-CBE	-2.24	109.53	112.88
7	A	2009	Y01	CAC-CBB-CBE	-2.23	109.54	112.88
10	A	2021	LPE	C31-C32-N	-2.23	108.67	115.82
6	A	2019	P5S	O15-P12-O13	2.19	122.65	112.44
12	A	2018	PCW	O2-C31-O31	-2.18	118.61	123.70
7	A	2004	Y01	CAQ-CBG-CBD	-2.13	115.70	119.10
7	A	2003	Y01	CAQ-CBG-CBD	-2.11	115.73	119.10
7	A	2005	Y01	CAQ-CBG-CBD	-2.11	115.73	119.10
12	A	2020	PCW	C34-C33-C32	-2.11	105.39	113.13
12	A	2020	PCW	O3-C3-C2	2.10	114.45	108.40
7	A	2009	Y01	CAQ-CBG-CBD	-2.09	115.76	119.10
12	A	2018	PCW	O3-C11-O11	-2.08	118.41	123.63
8	A	2006	9Z9	C17-C16-C13	-2.08	108.37	111.45
7	A	2032	Y01	CAQ-CBG-CBD	-2.07	115.79	119.10
7	A	2007	Y01	CAQ-CBG-CBD	-2.07	115.79	119.10
7	A	2005	Y01	CBC-CAV-CAZ	-2.06	108.41	111.45
7	A	2032	Y01	CAT-CAR-CBC	2.05	113.68	110.33
7	A	2007	Y01	CBC-CAV-CAZ	-2.05	108.43	111.45
7	A	2032	Y01	CAR-CBC-CAV	2.04	113.81	110.97
7	A	2003	Y01	CBC-CAV-CAZ	-2.04	108.44	111.45
7	A	2004	Y01	CBC-CAV-CAZ	-2.04	108.44	111.45
7	A	2009	Y01	CBC-CAV-CAZ	-2.03	108.45	111.45
7	A	2004	Y01	CAJ-CAO-CBB	-2.01	109.44	115.08

There are no chirality outliers.

All (252) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2002	P5S	C-CA-CB-OG
6	A	2002	P5S	N-CA-CB-OG
6	A	2002	P5S	CB-OG-P12-O13
6	A	2002	P5S	CB-OG-P12-O16
6	A	2002	P5S	C3-O16-P12-OG
6	A	2002	P5S	C3-O16-P12-O13
6	A	2002	P5S	C3-O16-P12-O15
6	A	2019	P5S	CB-OG-P12-O15

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Mol	Chain	Res	Type	Atoms
6	A	2019	P5S	C3-O16-P12-OG
6	A	2019	P5S	C3-O16-P12-O13
6	A	2019	P5S	C3-O16-P12-O15
6	A	2031	P5S	O-C-CA-CB
6	A	2031	P5S	OXT-C-CA-CB
6	A	2031	P5S	C3-O16-P12-O13
10	A	2011	LPE	C3-O3-P-O31
10	A	2012	LPE	C3-O3-P-O31
10	A	2012	LPE	C31-O33-P-O3
10	A	2014	LPE	C3-O3-P-O32
10	A	2014	LPE	C3-O3-P-O33
10	A	2014	LPE	C31-O33-P-O31
10	A	2016	LPE	O1-C1-C2-C3
10	A	2016	LPE	C3-O3-P-O32
10	A	2016	LPE	C3-O3-P-O33
10	A	2016	LPE	C31-O33-P-O3
10	A	2016	LPE	C31-O33-P-O31
10	A	2016	LPE	C32-C31-O33-P
10	A	2016	LPE	O33-C31-C32-N
10	A	2017	LPE	C3-O3-P-O32
10	A	2017	LPE	C3-O3-P-O33
10	A	2021	LPE	C31-O33-P-O31
10	A	2021	LPE	O33-C31-C32-N
10	A	2022	LPE	C31-O33-P-O31
10	A	2023	LPE	C31-O33-P-O31
10	A	2024	LPE	C3-O3-P-O33
10	A	2025	LPE	C31-O33-P-O3
10	A	2025	LPE	C31-O33-P-O32
10	A	2026	LPE	C31-O33-P-O31
10	A	2027	LPE	O1-C1-C2-C3
10	A	2027	LPE	C3-O3-P-O32
10	A	2027	LPE	C3-O3-P-O33
10	A	2027	LPE	C31-O33-P-O3
10	A	2027	LPE	C31-O33-P-O31
10	A	2027	LPE	C31-O33-P-O32
10	A	2028	LPE	C31-O33-P-O3
10	A	2033	LPE	C3-O3-P-O32
10	A	2033	LPE	C3-O3-P-O33
10	A	2033	LPE	C31-O33-P-O3
10	A	2033	LPE	C31-O33-P-O31
10	A	2033	LPE	C31-O33-P-O32
10	B	304	LPE	C3-O3-P-O31

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Mol	Chain	Res	Type	Atoms
10	B	304	LPE	C3-O3-P-O32
10	B	304	LPE	C3-O3-P-O33
10	B	304	LPE	C31-O33-P-O3
11	A	2013	1PW	CAH-CAI-CAZ-OAE
11	A	2013	1PW	CAH-CAI-CAZ-CBA
12	A	2015	PCW	C4-O4P-P-O3P
12	A	2018	PCW	O4P-C4-C5-N
12	A	2018	PCW	C4-O4P-P-O3P
12	A	2020	PCW	C32-C31-O2-C2
12	A	2020	PCW	C4-O4P-P-O3P
12	A	2029	PCW	O4P-C4-C5-N
12	A	2029	PCW	C1-O3P-P-O2P
12	A	2029	PCW	C4-O4P-P-O2P
12	A	2030	PCW	C1-O3P-P-O4P
12	A	2030	PCW	C4-O4P-P-O1P
12	A	2030	PCW	C4-O4P-P-O3P
6	A	2031	P5S	O18-C17-O19-C1
6	A	2031	P5S	C20-C17-O19-C1
7	A	2032	Y01	CAC-CBB-CBE-CAP
7	A	2032	Y01	CAC-CBB-CBE-CBI
12	A	2020	PCW	O31-C31-O2-C2
7	A	2032	Y01	CAJ-CAO-CBB-CAC
7	A	2032	Y01	CAO-CBB-CBE-CBI
12	A	2029	PCW	O11-C11-O3-C3
12	A	2029	PCW	C12-C11-O3-C3
5	A	2008	NAG	C8-C7-N2-C2
5	A	2008	NAG	O7-C7-N2-C2
5	A	2001	NAG	O5-C5-C6-O6
10	A	2027	LPE	O1-C1-C2-O2H
7	A	2032	Y01	CAO-CBB-CBE-CAP
5	A	2001	NAG	C4-C5-C6-O6
12	A	2030	PCW	C12-C11-O3-C3
7	A	2005	Y01	CAR-CBC-OAW-CAY
10	A	2025	LPE	C31-C32-N-C2N
10	A	2025	LPE	C31-C32-N-C3N
12	A	2018	PCW	C4-C5-N-C8
12	A	2020	PCW	C4-C5-N-C7
7	A	2032	Y01	CAJ-CAO-CBB-CBE
7	A	2009	Y01	CAR-CBC-OAW-CAY
10	A	2016	LPE	O1-C1-C2-O2H
10	A	2028	LPE	C31-C32-N-C3N
12	A	2018	PCW	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
12	A	2030	PCW	O11-C11-O3-C3
6	A	2002	P5S	C38-C39-C40-C41
10	A	2016	LPE	O1-C11-C12-C13
10	A	2022	LPE	O1-C1-C2-O2H
7	A	2005	Y01	CAV-CBC-OAW-CAY
7	A	2009	Y01	CAV-CBC-OAW-CAY
10	A	2016	LPE	C31-C32-N-C1N
10	A	2016	LPE	C31-C32-N-C2N
10	A	2016	LPE	C31-C32-N-C3N
12	A	2020	PCW	C4-C5-N-C6
10	A	2011	LPE	O1-C11-C12-C13
10	A	2022	LPE	O1-C1-C2-C3
10	A	2025	LPE	C31-C32-N-C1N
10	A	2012	LPE	O1-C11-C12-C13
6	A	2031	P5S	C17-C20-C21-C22
6	A	2019	P5S	C25-C26-C27-C28
6	A	2002	P5S	C46-C48-C49-C50
6	A	2019	P5S	C27-C28-C29-C30
12	A	2018	PCW	C4-C5-N-C6
12	A	2020	PCW	C4-C5-N-C8
10	A	2022	LPE	C12-C13-C14-C15
12	A	2015	PCW	C32-C31-O2-C2
6	A	2002	P5S	C41-C42-C43-C44
6	A	2031	P5S	C42-C43-C44-C45
12	A	2029	PCW	C33-C34-C35-C36
6	A	2002	P5S	C52-C53-C54-C55
6	A	2031	P5S	C21-C22-C23-C24
12	A	2015	PCW	C32-C33-C34-C35
10	A	2028	LPE	C31-C32-N-C1N
10	A	2028	LPE	C31-C32-N-C2N
6	A	2002	P5S	C39-C38-O37-C2
12	A	2029	PCW	C31-C32-C33-C34
6	A	2002	P5S	C51-C52-C53-C54
10	A	2022	LPE	C14-C15-C16-C17
12	A	2015	PCW	C24-C25-C26-C27
12	A	2015	PCW	O31-C31-O2-C2
10	A	2011	LPE	C2-C1-O1-C11
6	A	2002	P5S	C48-C49-C50-C51
6	A	2031	P5S	C43-C44-C45-C46
6	A	2031	P5S	C40-C41-C42-C43
10	A	2026	LPE	C13-C14-C15-C16
6	A	2031	P5S	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
7	A	2032	Y01	CAN-CAJ-CAO-CBB
10	A	2012	LPE	C13-C14-C15-C16
12	A	2018	PCW	C35-C36-C37-C38
12	A	2018	PCW	C34-C35-C36-C37
10	A	2017	LPE	O1-C1-C2-O2H
10	B	304	LPE	C2-C3-O3-P
12	A	2015	PCW	C41-C42-C43-C44
6	A	2002	P5S	C1-C2-C3-O16
6	A	2002	P5S	O47-C38-O37-C2
6	A	2002	P5S	C2-C3-O16-P12
10	A	2028	LPE	C2-C1-O1-C11
10	A	2022	LPE	C11-C12-C13-C14
10	A	2017	LPE	O1-C1-C2-C3
10	A	2022	LPE	C16-C17-C18-C19
10	A	2021	LPE	C2-C1-O1-C11
11	A	2013	1PW	CAK-CAM-CAO-CAQ
10	B	304	LPE	C2-C1-O1-C11
7	A	2009	Y01	CAO-CAJ-CAN-CBA
7	A	2005	Y01	CAO-CAJ-CAN-CBA
6	A	2002	P5S	O37-C2-C3-O16
6	A	2031	P5S	C39-C38-O37-C2
10	A	2012	LPE	C32-C31-O33-P
10	A	2033	LPE	C32-C31-O33-P
10	B	304	LPE	C32-C31-O33-P
12	A	2015	PCW	C4-C5-N-C7
10	A	2022	LPE	C12-C11-O1-C1
10	A	2033	LPE	C2-C1-O1-C11
10	A	2011	LPE	O33-C31-C32-N
10	A	2014	LPE	O33-C31-C32-N
10	A	2017	LPE	O33-C31-C32-N
10	A	2022	LPE	O33-C31-C32-N
10	A	2023	LPE	O33-C31-C32-N
10	A	2024	LPE	O33-C31-C32-N
10	A	2025	LPE	O33-C31-C32-N
10	A	2026	LPE	O33-C31-C32-N
10	A	2027	LPE	O33-C31-C32-N
10	A	2033	LPE	O33-C31-C32-N
10	B	304	LPE	O33-C31-C32-N
12	A	2030	PCW	O4P-C4-C5-N
6	A	2002	P5S	C40-C41-C42-C43
6	A	2031	P5S	CA-CB-OG-P12
10	A	2014	LPE	C12-C11-O1-C1

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Mol	Chain	Res	Type	Atoms
10	A	2016	LPE	C12-C11-O1-C1
12	A	2015	PCW	C4-C5-N-C6
12	A	2029	PCW	O31-C31-O2-C2
10	A	2021	LPE	C12-C11-O1-C1
6	A	2031	P5S	O47-C38-O37-C2
12	A	2030	PCW	C4-C5-N-C6
12	A	2029	PCW	C34-C35-C36-C37
10	A	2011	LPE	C11-C12-C13-C14
6	A	2002	P5S	CB-OG-P12-O15
6	A	2019	P5S	CB-OG-P12-O16
6	A	2031	P5S	C3-O16-P12-OG
6	A	2031	P5S	C3-O16-P12-O15
10	A	2012	LPE	C3-O3-P-O32
10	A	2012	LPE	C3-O3-P-O33
10	A	2012	LPE	C31-O33-P-O31
10	A	2014	LPE	C3-O3-P-O31
10	A	2017	LPE	C31-O33-P-O31
10	A	2021	LPE	C3-O3-P-O31
10	A	2022	LPE	C3-O3-P-O32
10	A	2024	LPE	C3-O3-P-O31
10	A	2025	LPE	C31-O33-P-O31
10	A	2027	LPE	C3-O3-P-O31
10	A	2028	LPE	C31-O33-P-O31
10	B	304	LPE	C31-O33-P-O31
12	A	2015	PCW	C4-C5-N-C8
12	A	2015	PCW	C4-O4P-P-O2P
12	A	2018	PCW	C1-O3P-P-O2P
12	A	2018	PCW	C4-O4P-P-O2P
12	A	2020	PCW	C1-O3P-P-O2P
12	A	2020	PCW	C4-O4P-P-O2P
12	A	2030	PCW	C1-O3P-P-O2P
12	A	2030	PCW	C4-O4P-P-O2P
10	A	2026	LPE	C2-C1-O1-C11
6	A	2031	P5S	C2-C3-O16-P12
10	A	2011	LPE	C2-C3-O3-P
12	A	2020	PCW	C2-C1-O3P-P
10	A	2016	LPE	C13-C14-C15-C16
6	A	2002	P5S	C50-C51-C52-C53
12	A	2018	PCW	C17-C18-C19-C20
12	A	2018	PCW	C37-C38-C39-C40
12	A	2029	PCW	C32-C31-O2-C2
10	A	2017	LPE	C12-C11-O1-C1

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Mol	Chain	Res	Type	Atoms
12	A	2030	PCW	C4-C5-N-C8
10	A	2014	LPE	C2-C3-O3-P
10	A	2027	LPE	C2-C1-O1-C11
12	A	2015	PCW	C23-C24-C25-C26
10	A	2016	LPE	C11-C12-C13-C14
12	A	2029	PCW	C11-C12-C13-C14
11	A	2013	1PW	CAN-CAP-CAR-CAT
12	A	2015	PCW	C44-C45-C46-C47
6	A	2002	P5S	C43-C44-C45-C46
12	A	2030	PCW	C4-C5-N-C7
6	A	2002	P5S	O19-C1-C2-O37
12	A	2029	PCW	C21-C22-C23-C24
6	A	2002	P5S	C39-C40-C41-C42
12	A	2015	PCW	C17-C18-C19-C20
6	A	2031	P5S	C41-C42-C43-C44
6	A	2002	P5S	C53-C54-C55-C56
10	A	2017	LPE	C2-C3-O3-P
12	A	2015	PCW	C13-C14-C15-C16
12	A	2018	PCW	C39-C40-C41-C42
12	A	2015	PCW	C39-C40-C41-C42
12	A	2020	PCW	O3-C11-C12-C13
12	A	2015	PCW	C19-C20-C21-C22
10	A	2011	LPE	C31-C32-N-C2N
10	A	2022	LPE	C13-C14-C15-C16
12	A	2029	PCW	C4-C5-N-C6
10	A	2011	LPE	C16-C17-C18-C19
10	A	2014	LPE	C31-C32-N-C2N
12	A	2029	PCW	C4-C5-N-C7
7	A	2005	Y01	CAN-CAJ-CAO-CBB
7	A	2009	Y01	CAN-CAJ-CAO-CBB
6	A	2002	P5S	C49-C50-C51-C52
12	A	2029	PCW	O3-C11-C12-C13
6	A	2019	P5S	C39-C38-O37-C2
6	A	2002	P5S	O37-C38-C39-C40

There are no ring outliers.

31 monomers are involved in 153 short contacts:

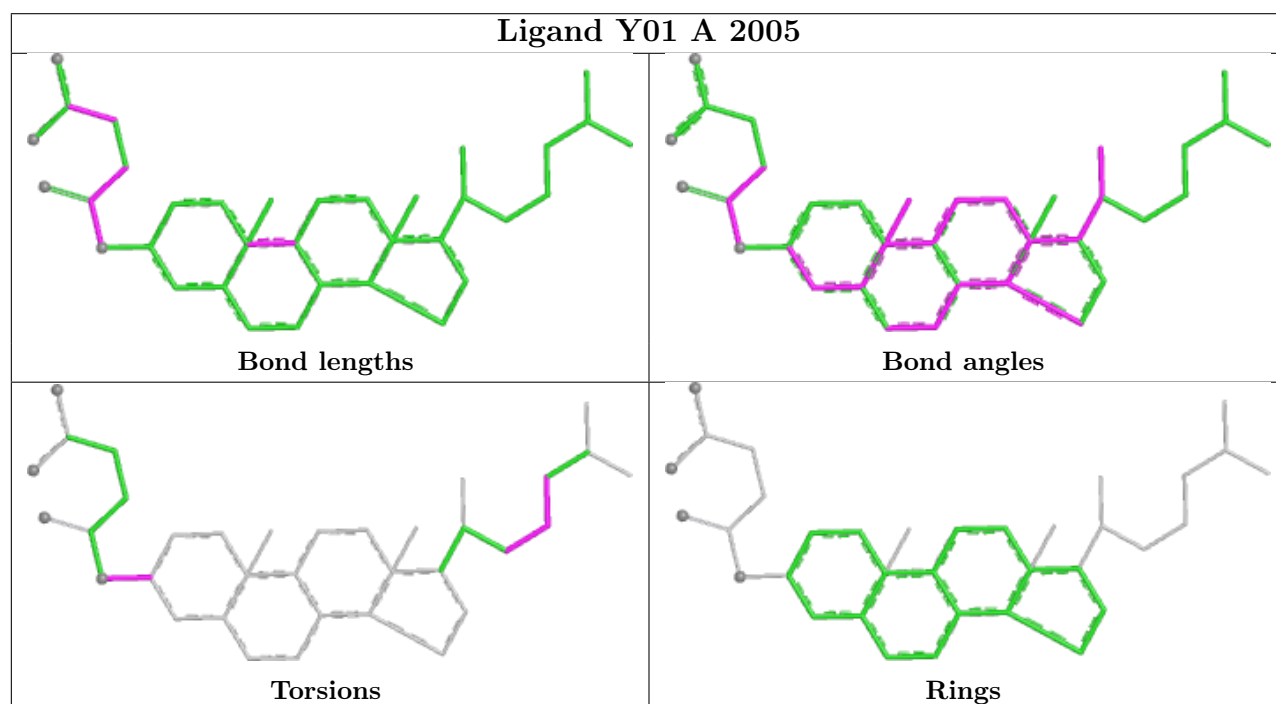
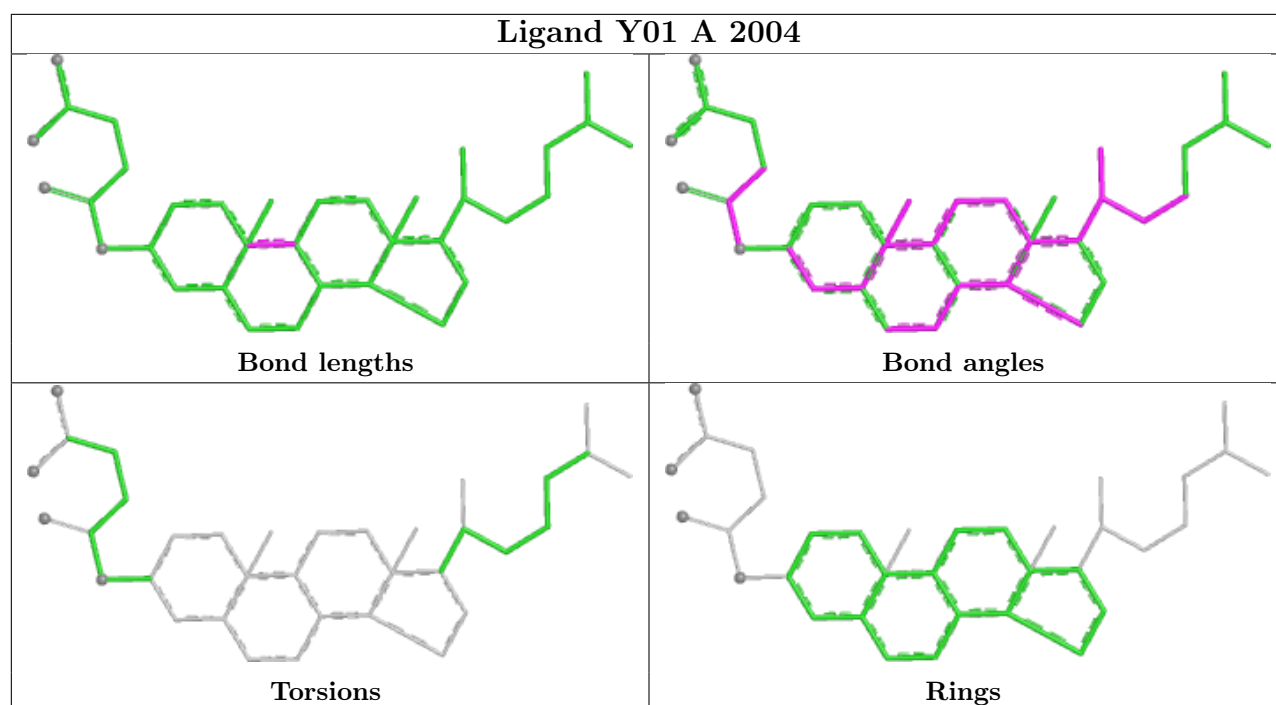
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2004	Y01	6	0
7	A	2005	Y01	19	0
5	B	302	NAG	1	0

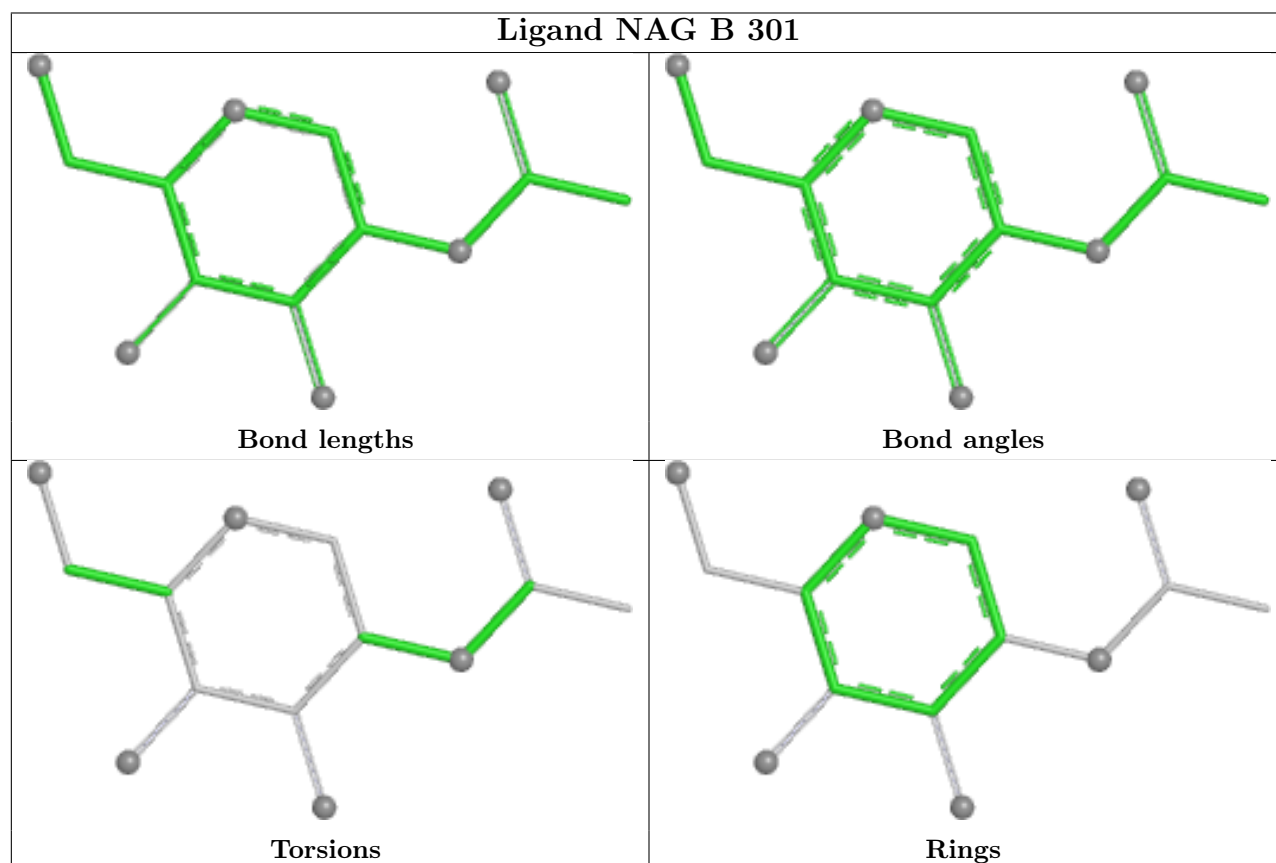
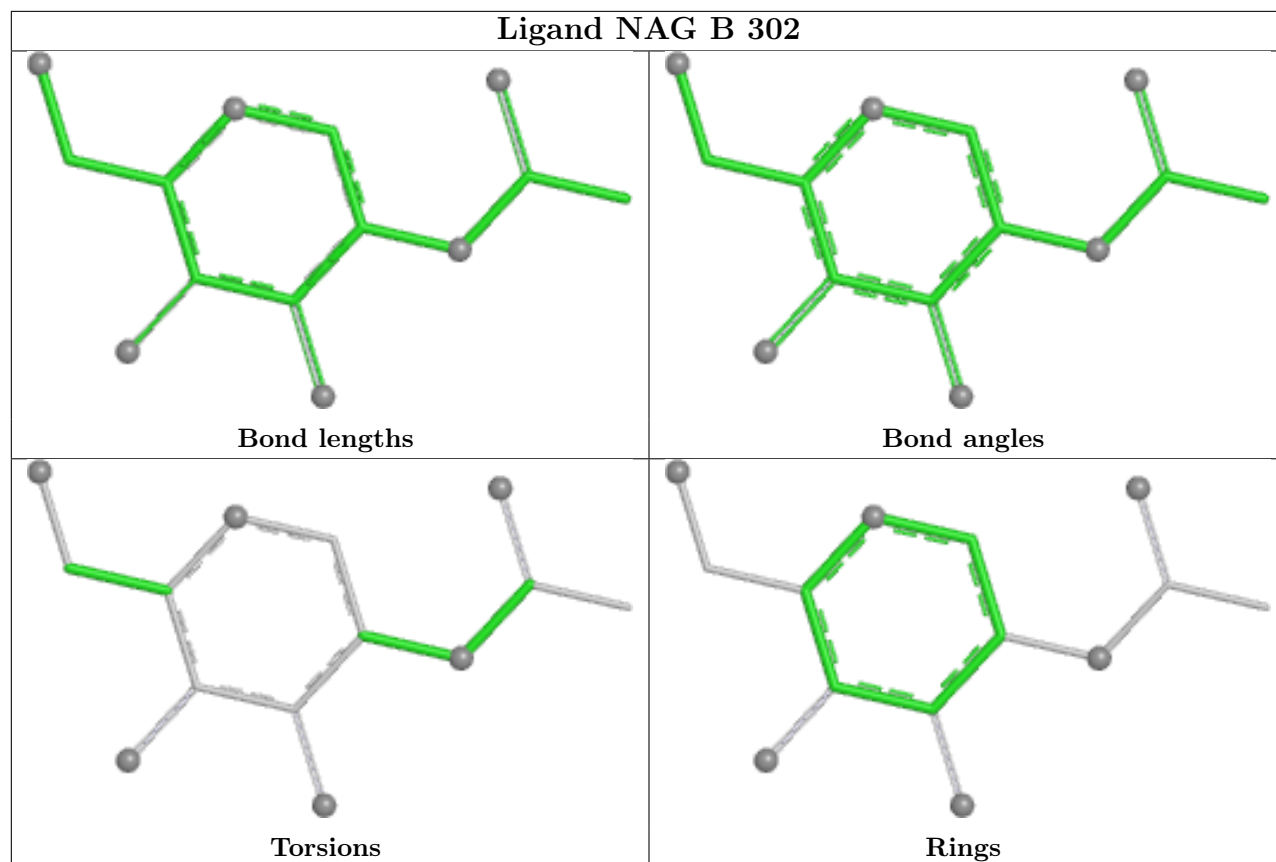
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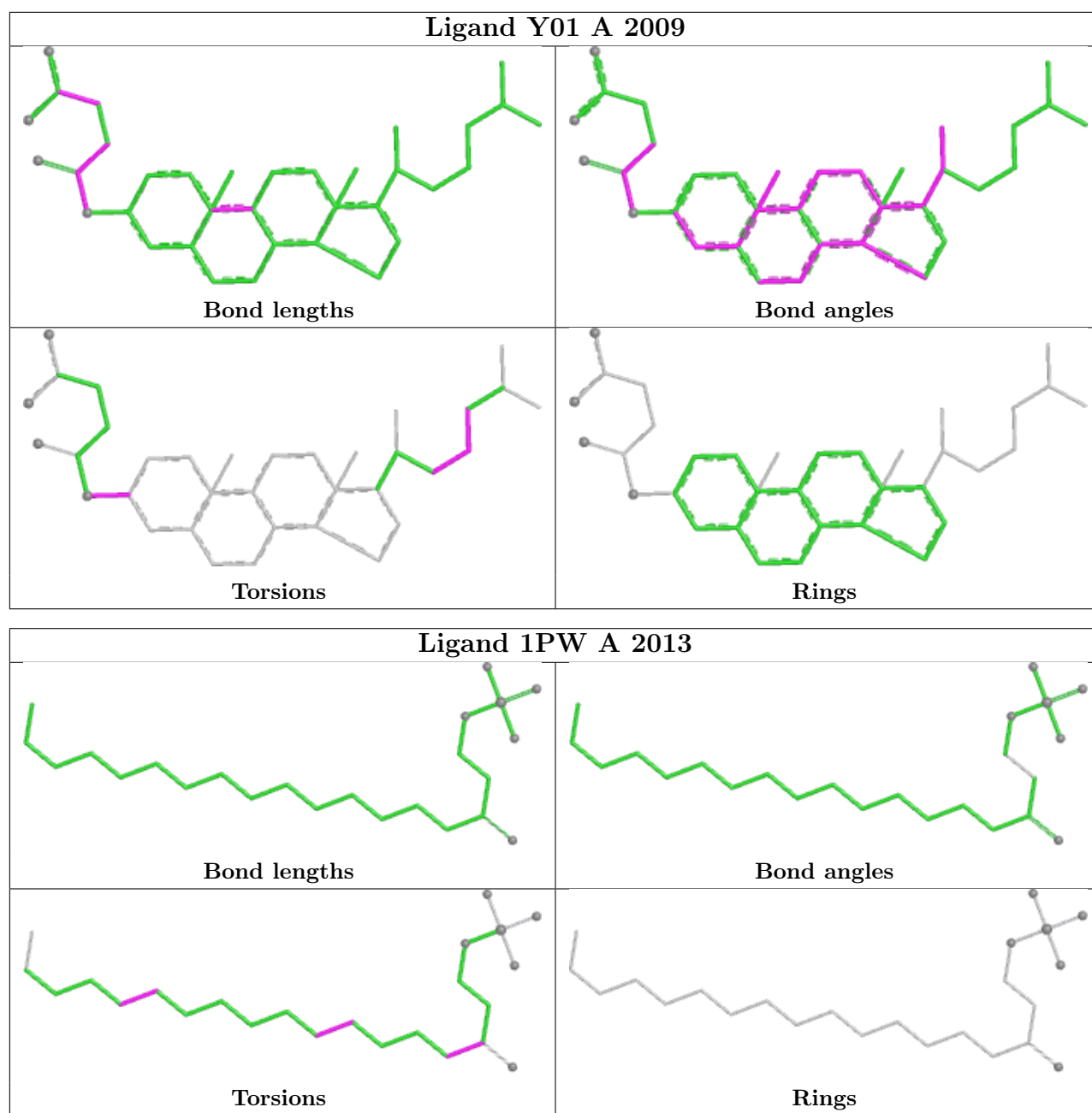
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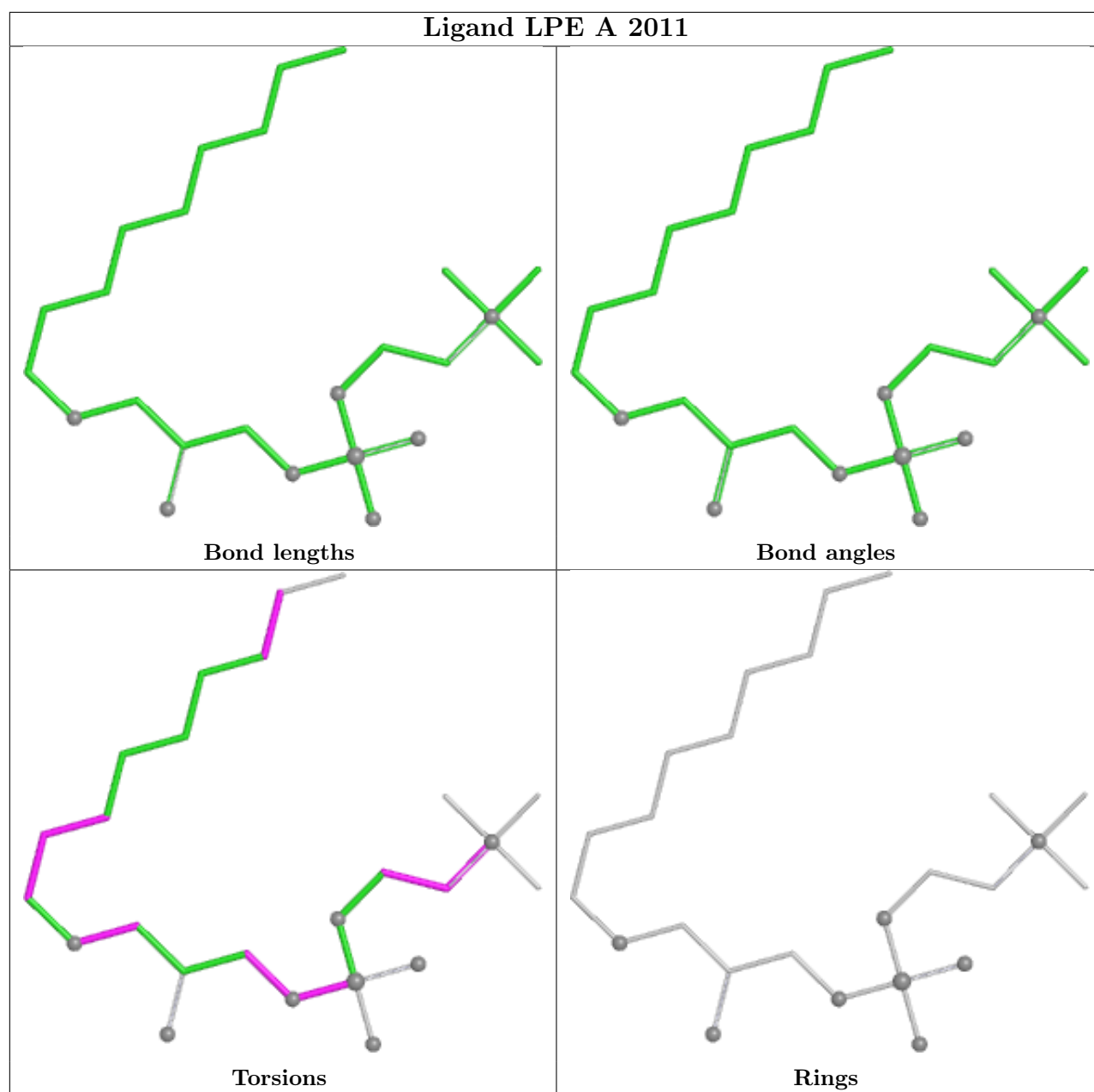
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2009	Y01	9	0
11	A	2013	1PW	2	0
10	A	2016	LPE	5	0
10	A	2024	LPE	2	0
10	A	2014	LPE	2	0
10	A	2025	LPE	2	0
5	B	303	NAG	6	0
10	A	2023	LPE	4	0
7	A	2007	Y01	14	0
12	A	2018	PCW	1	0
7	A	2032	Y01	20	0
12	A	2029	PCW	3	0
10	A	2021	LPE	7	0
10	A	2033	LPE	3	0
6	A	2031	P5S	3	0
12	A	2020	PCW	7	0
7	A	2003	Y01	4	0
10	A	2022	LPE	1	0
10	A	2012	LPE	1	0
10	A	2027	LPE	3	0
10	A	2017	LPE	3	0
5	A	2001	NAG	1	0
12	A	2015	PCW	19	0
6	A	2019	P5S	4	0
10	A	2028	LPE	1	0
8	A	2006	9Z9	14	0
10	A	2026	LPE	4	0
6	A	2002	P5S	2	0

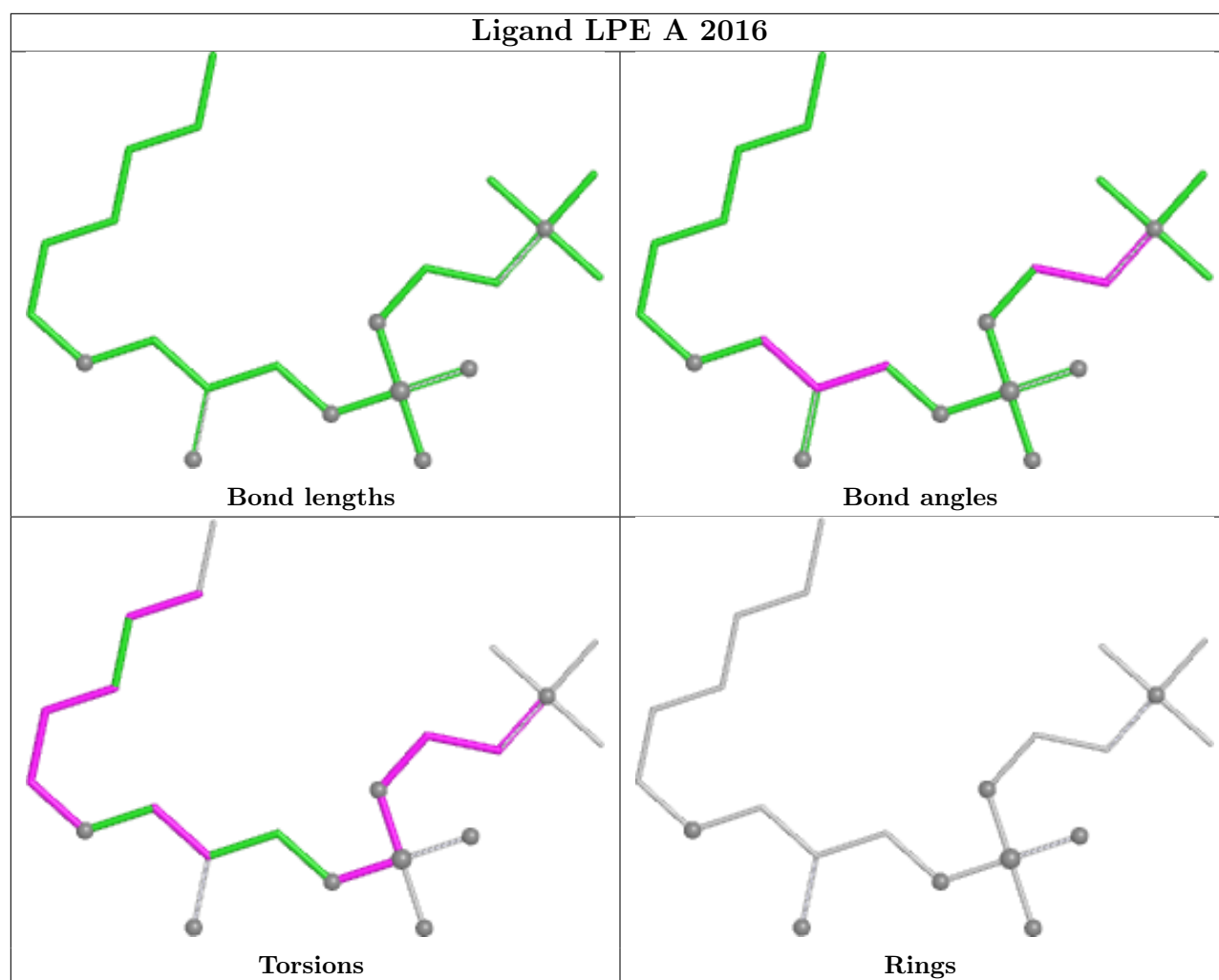
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

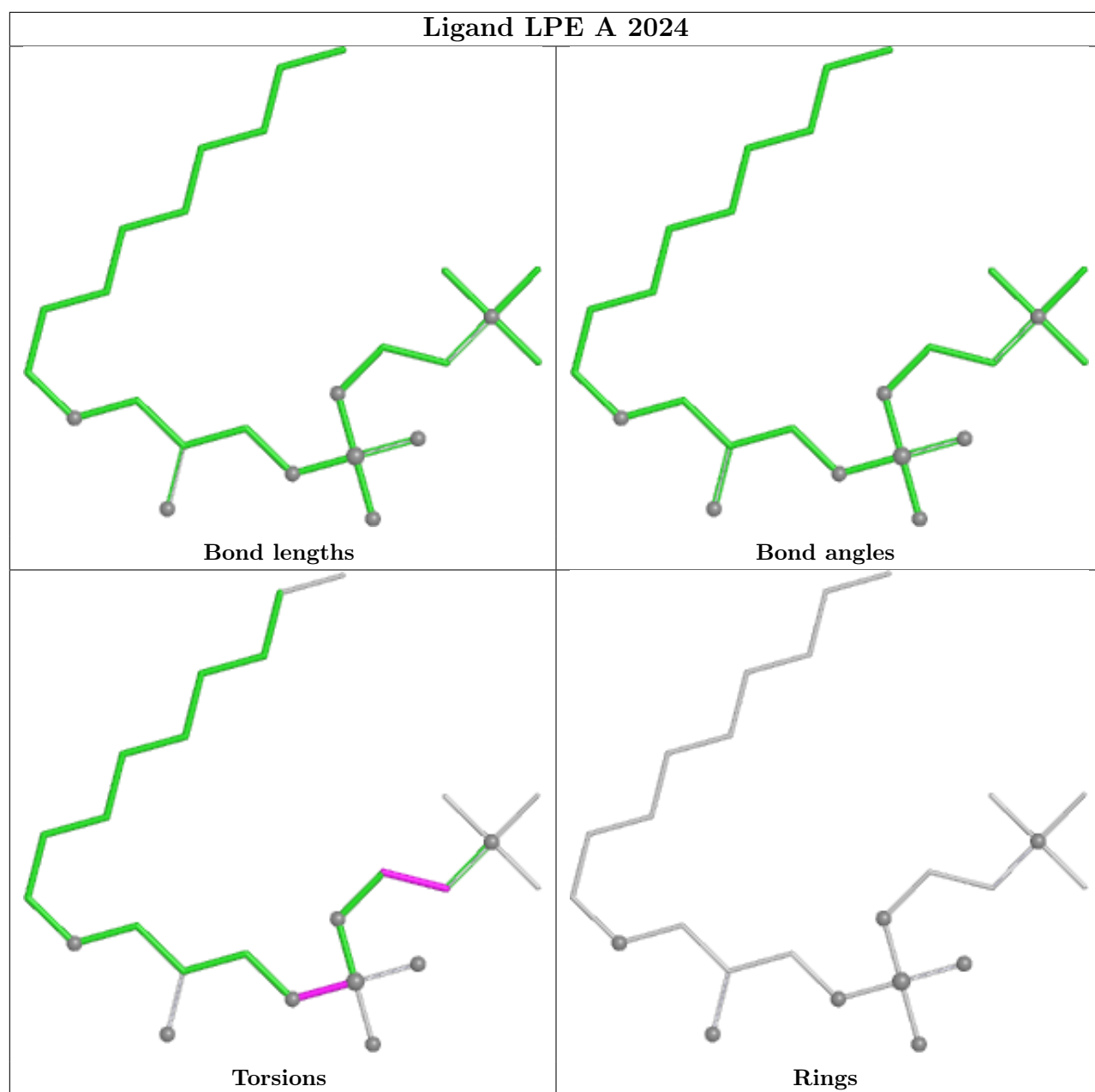


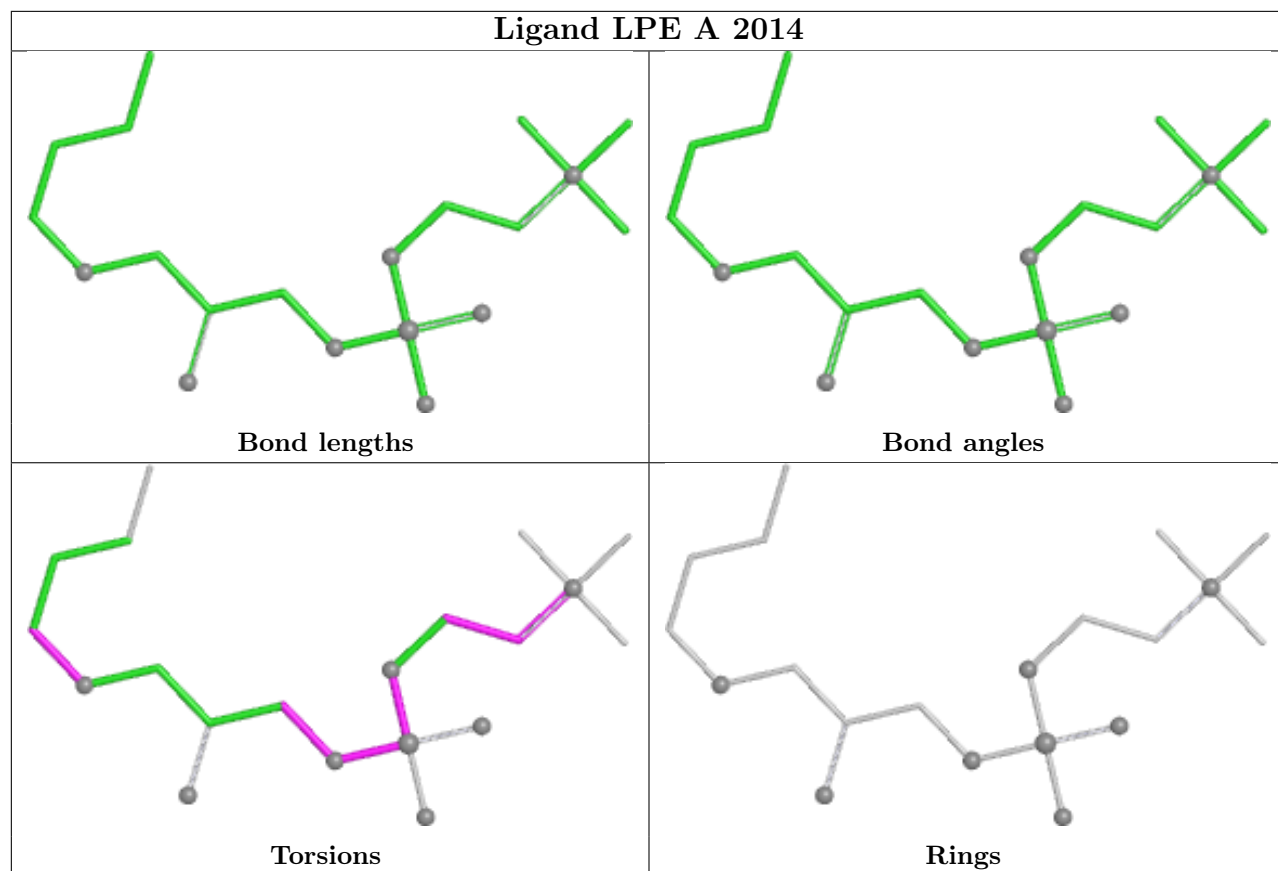


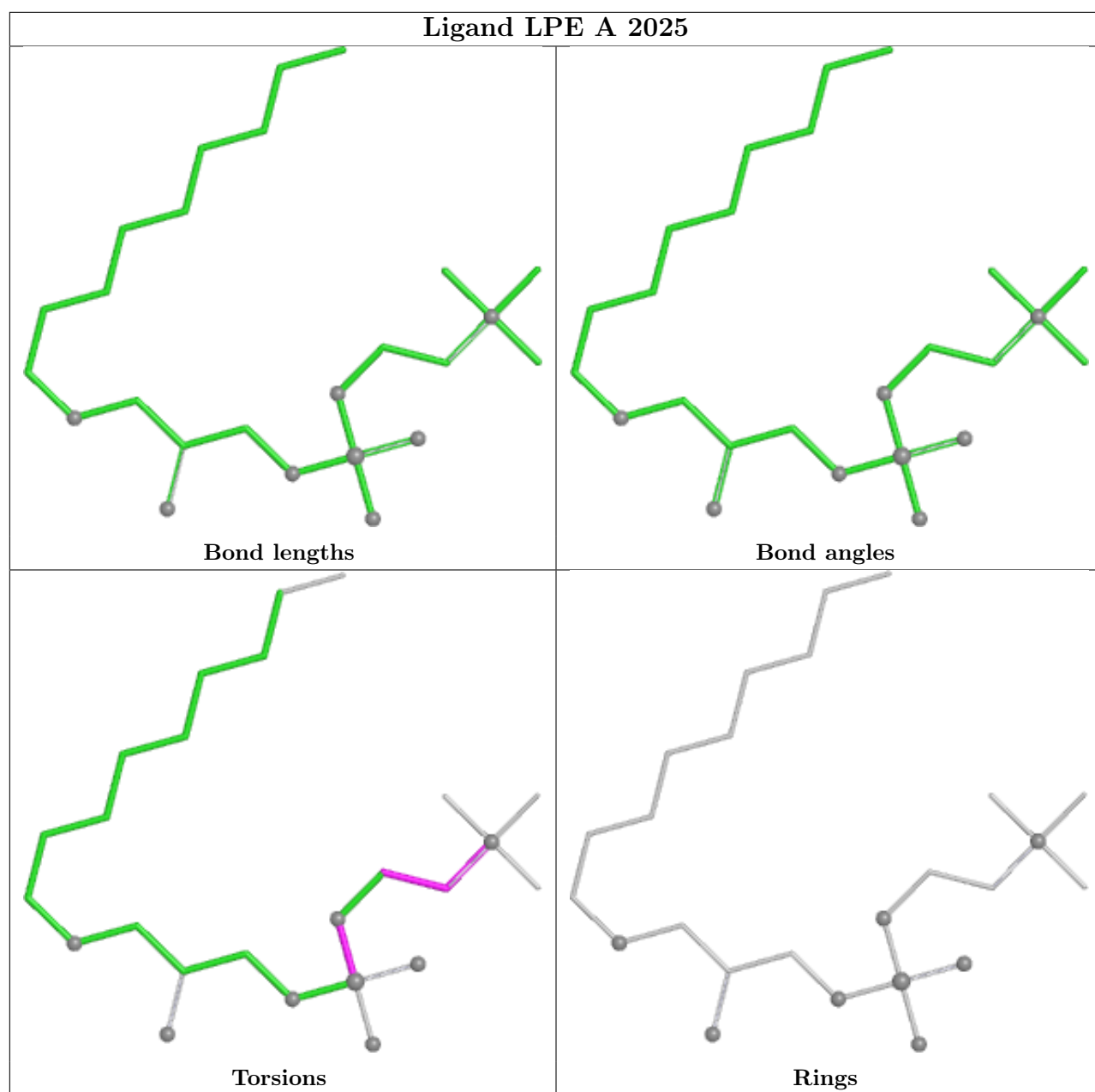


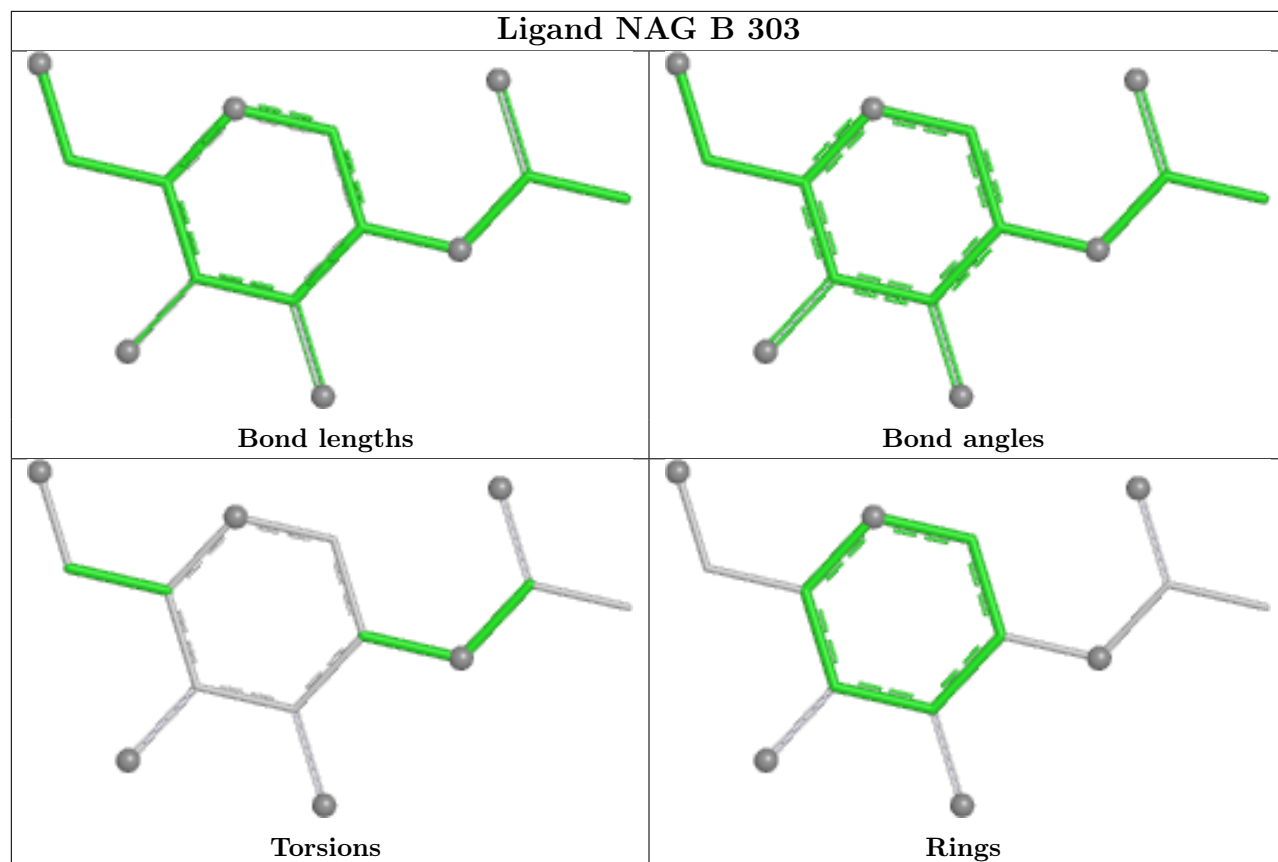


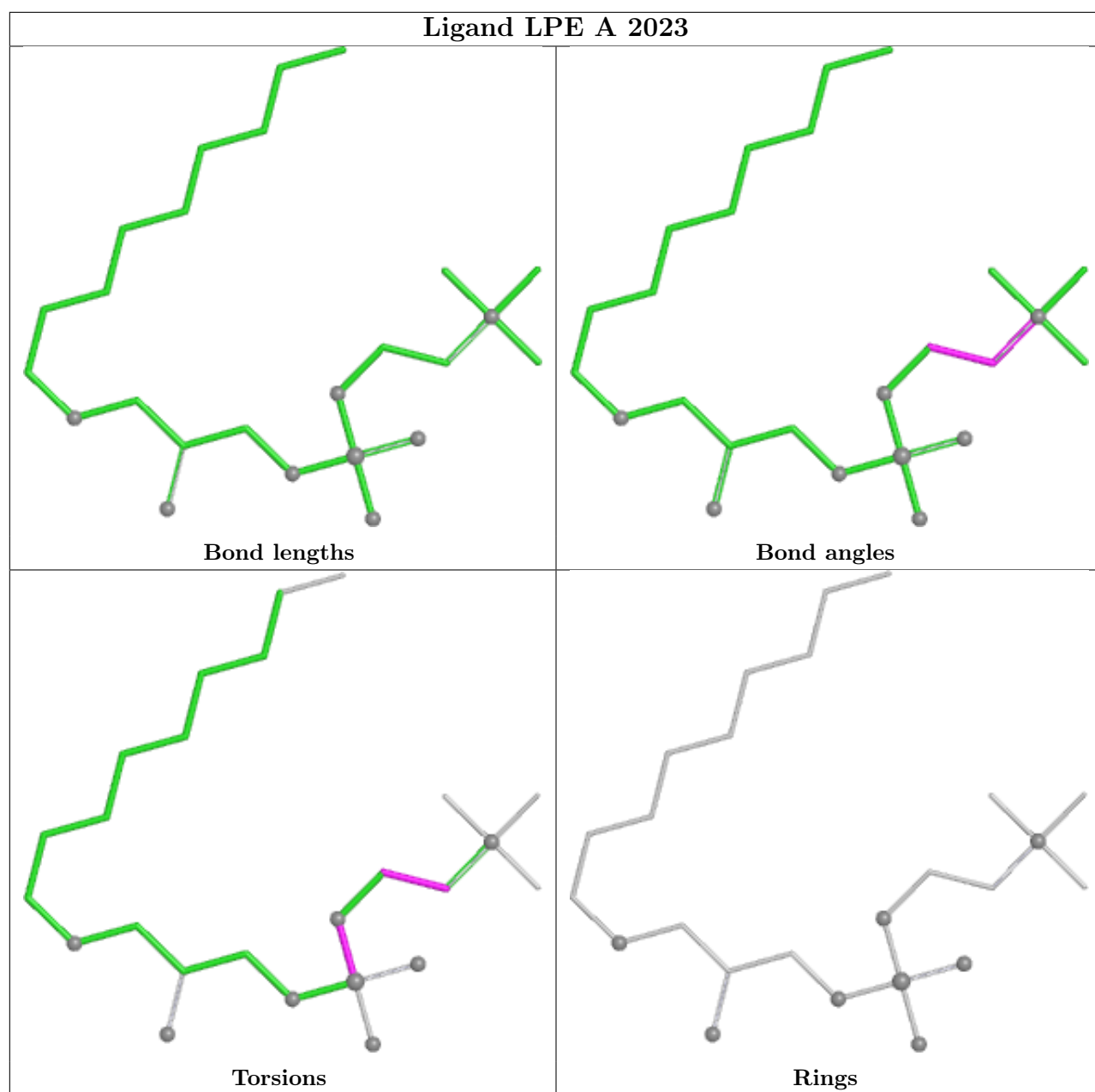


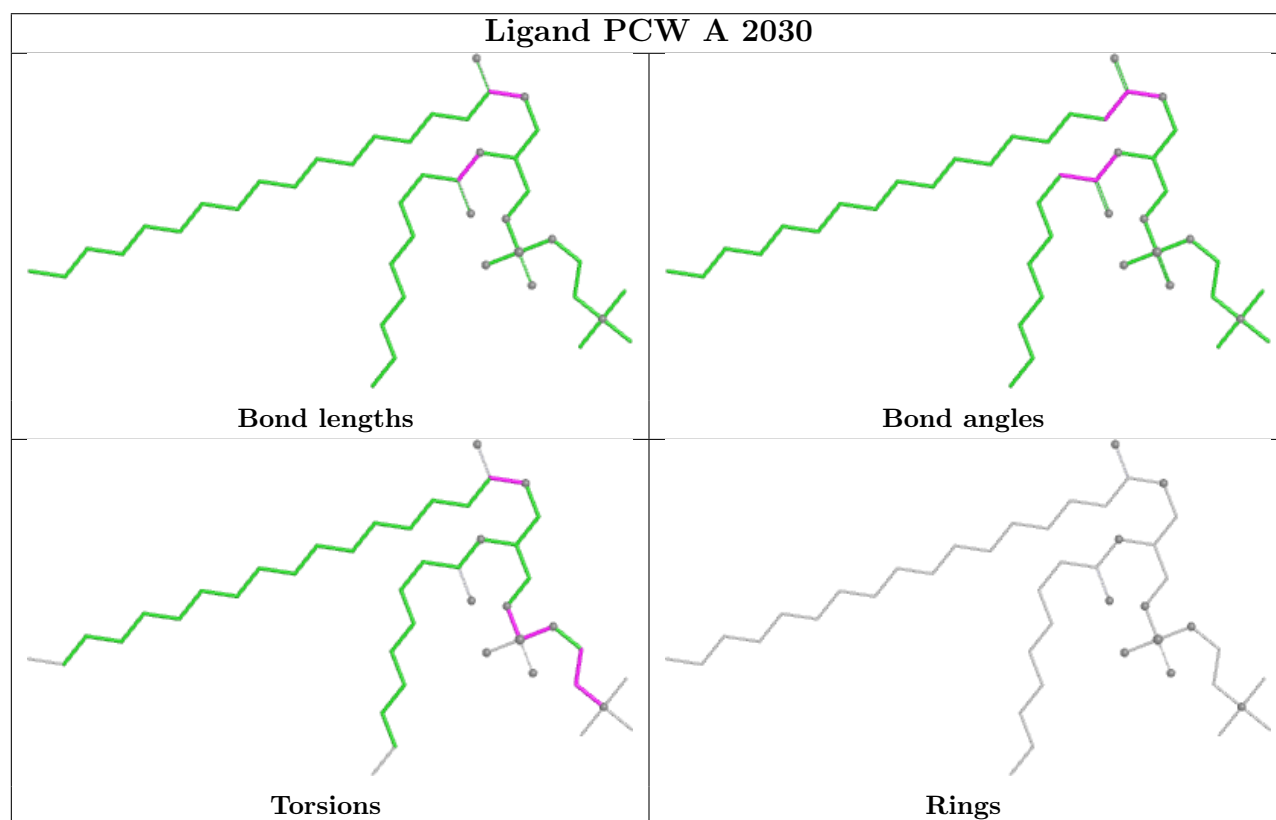
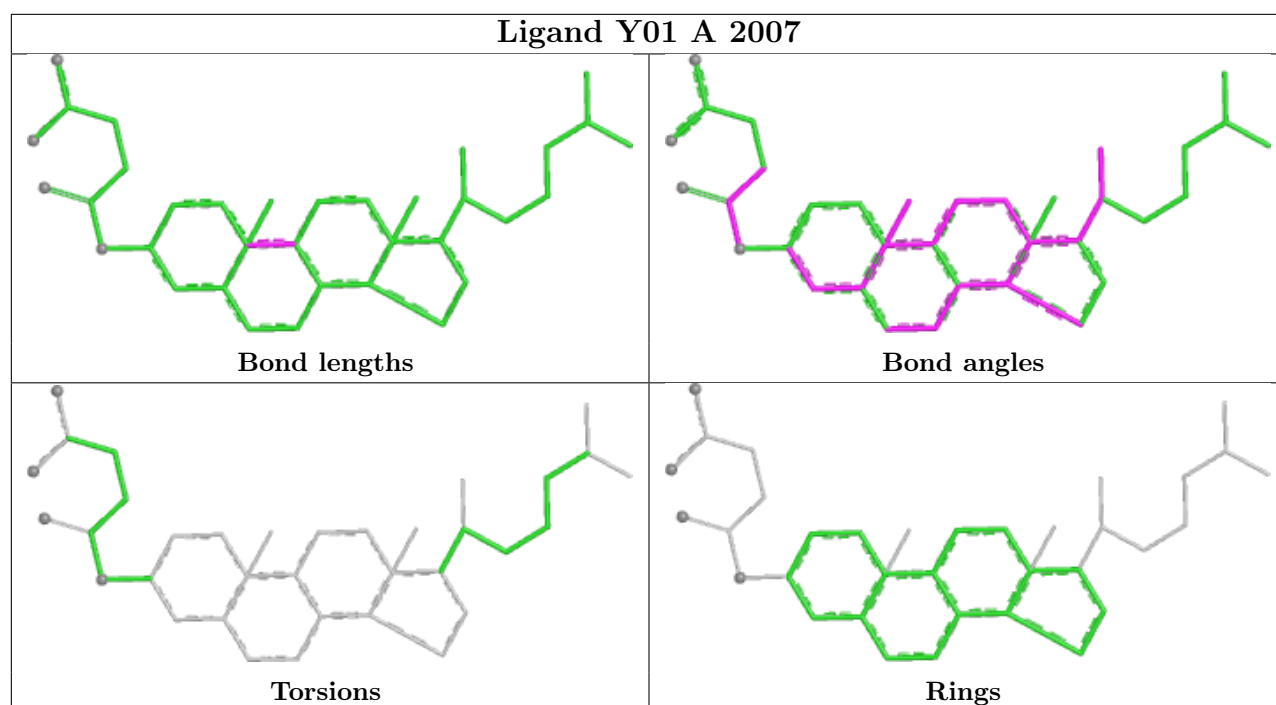


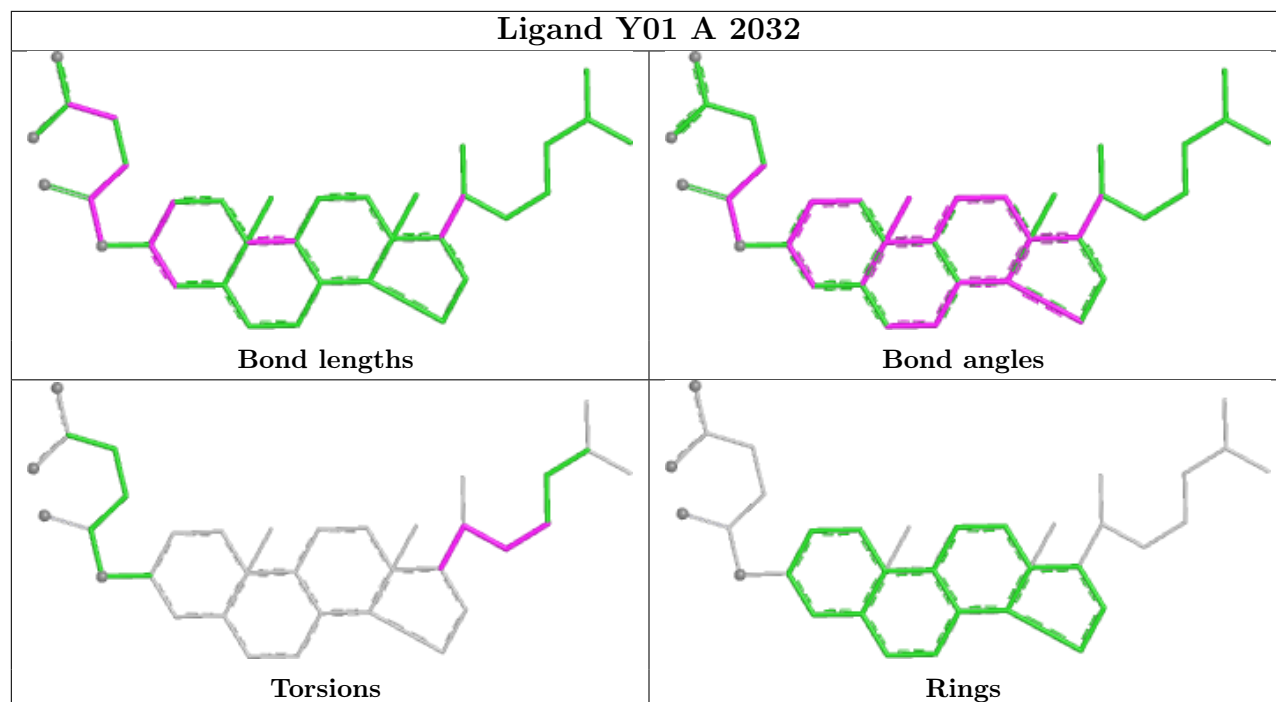
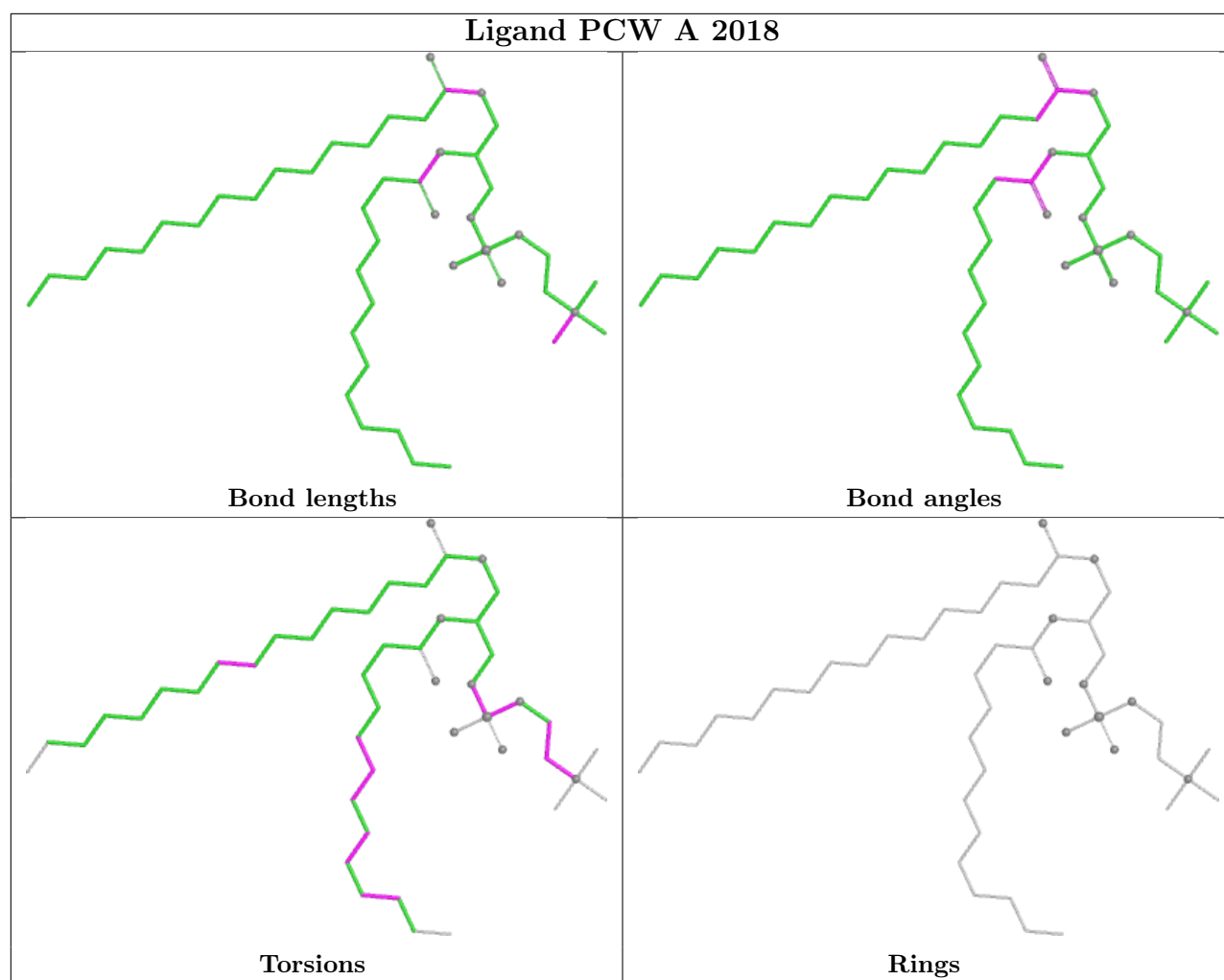


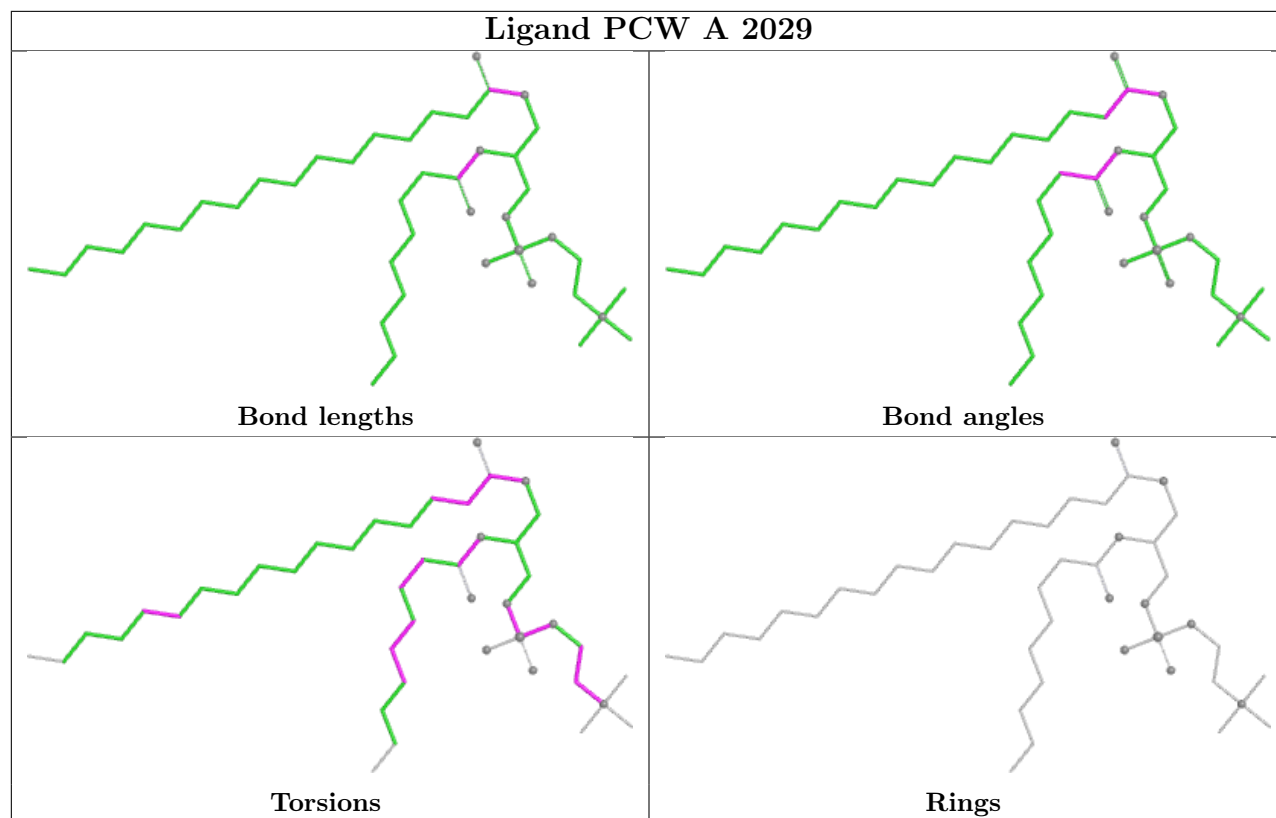


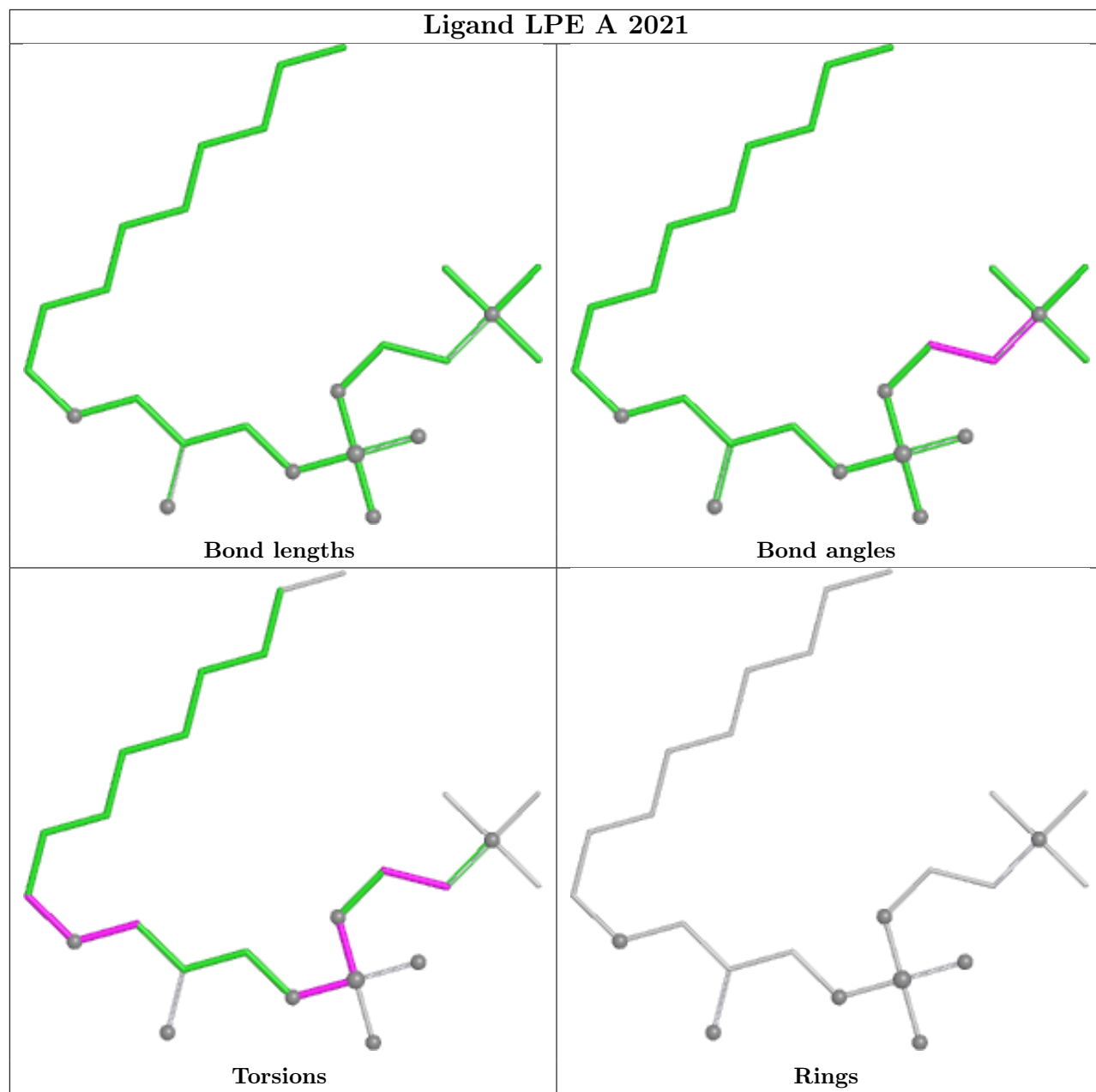




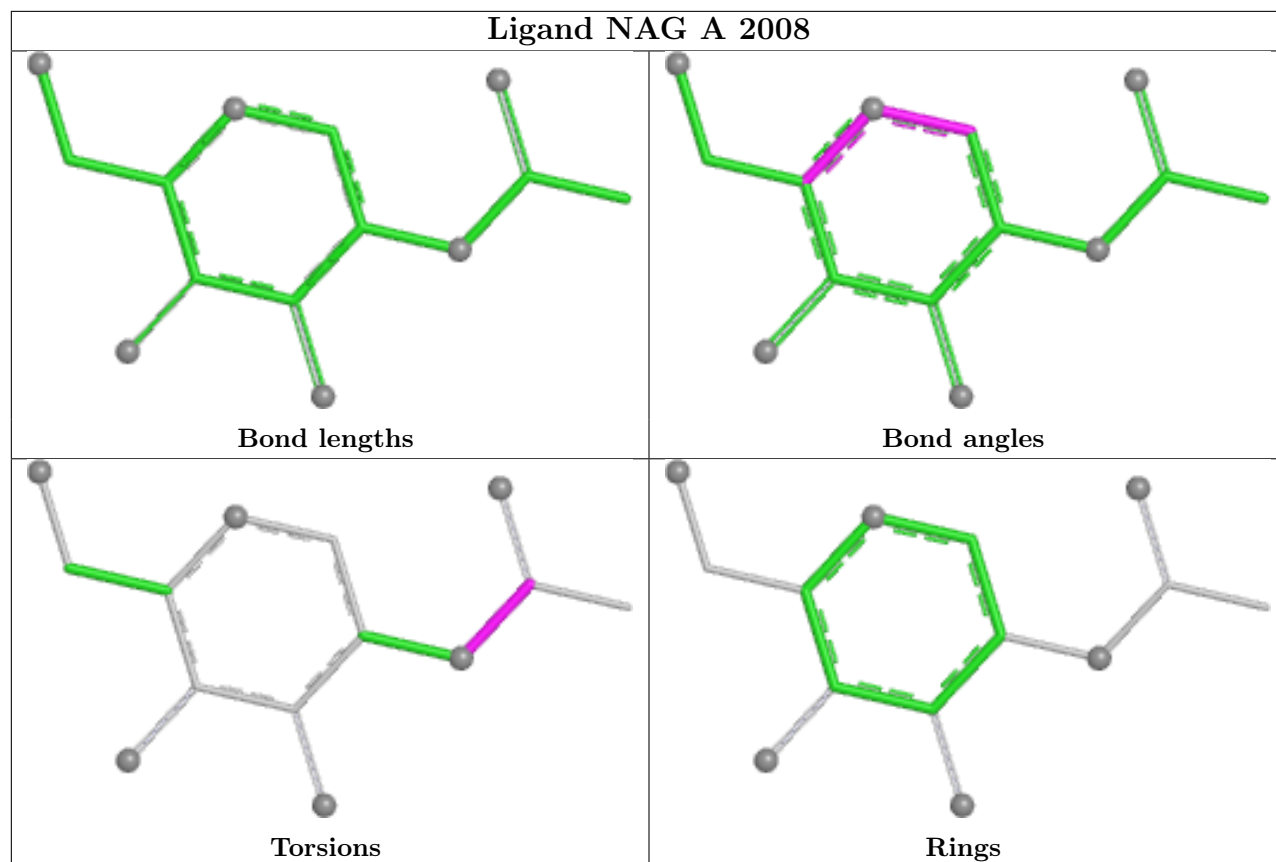




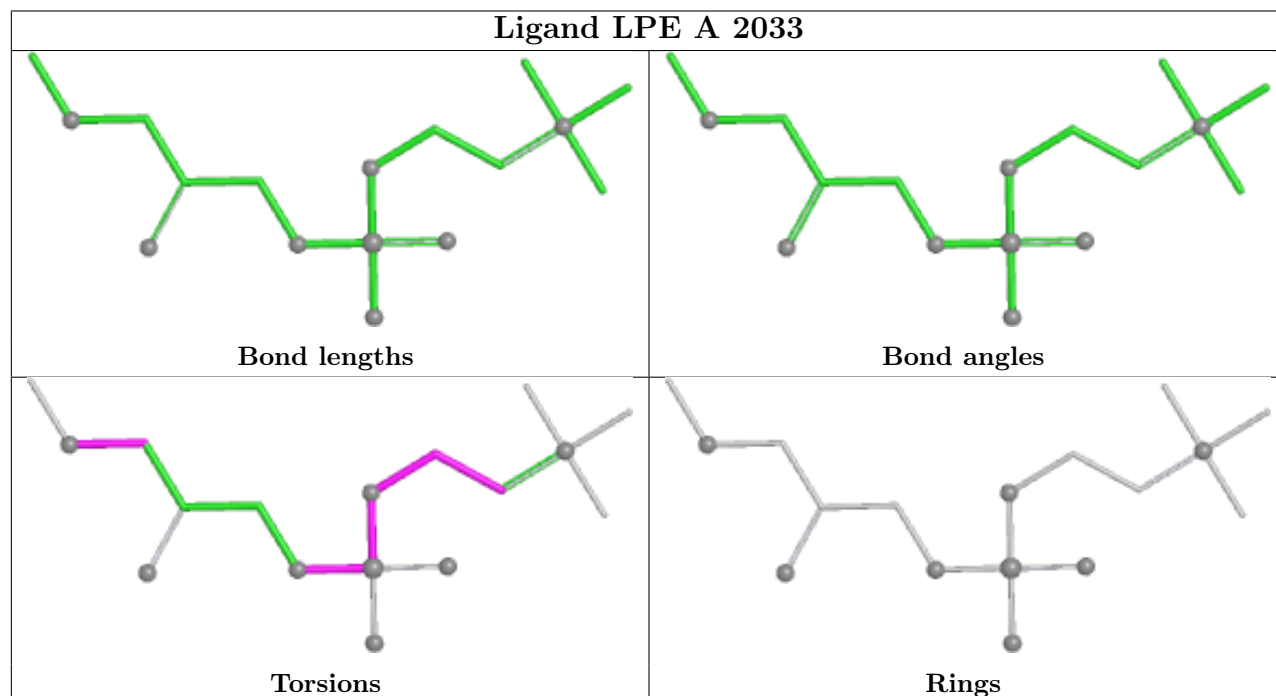


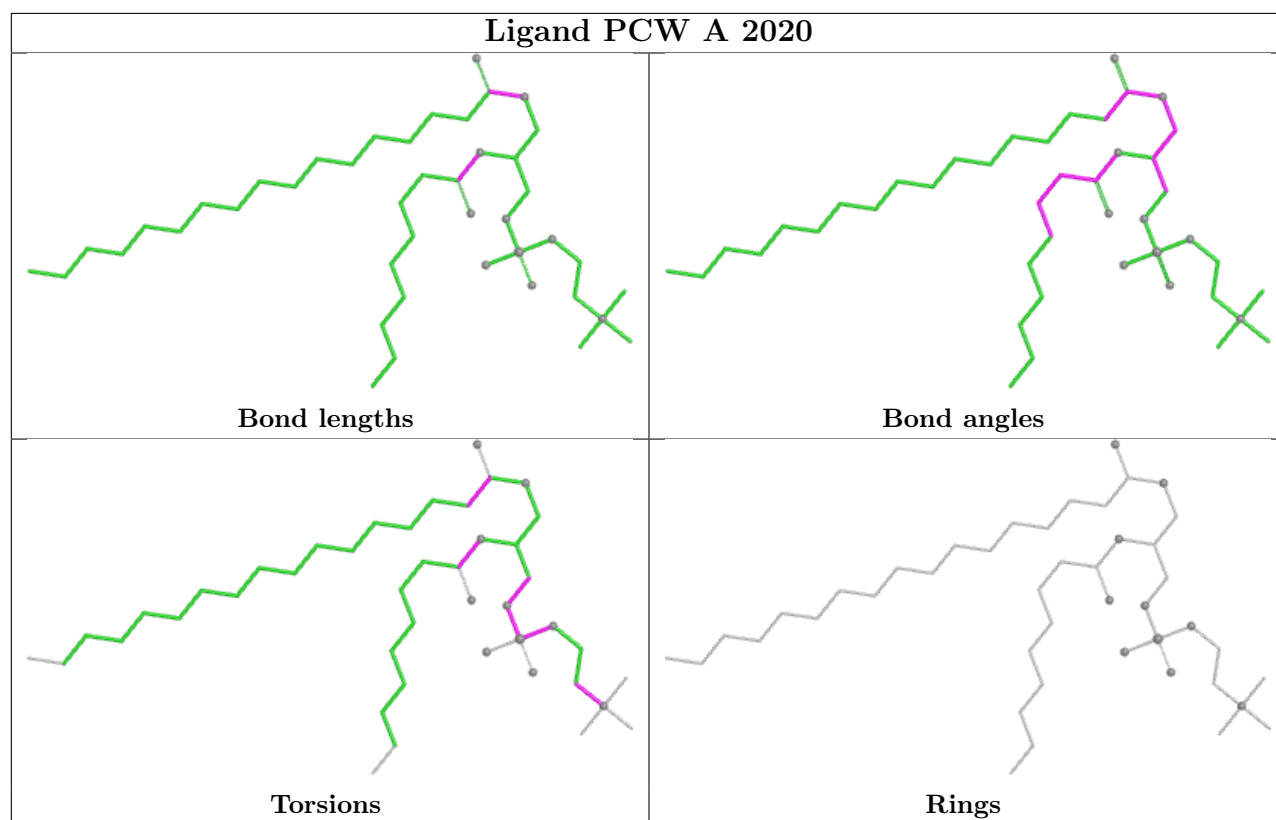
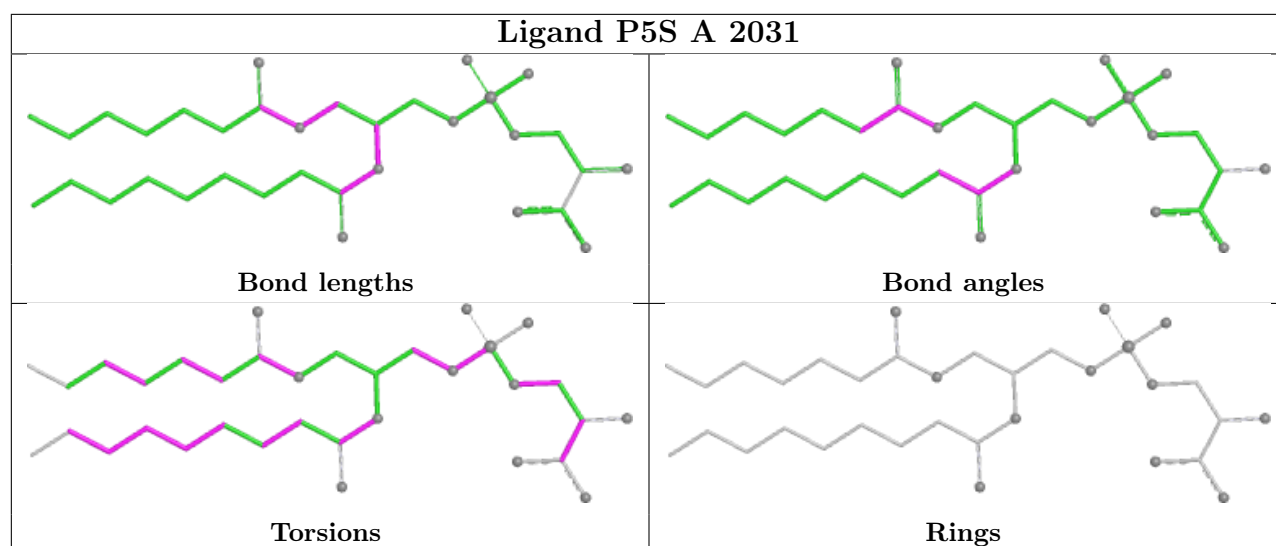


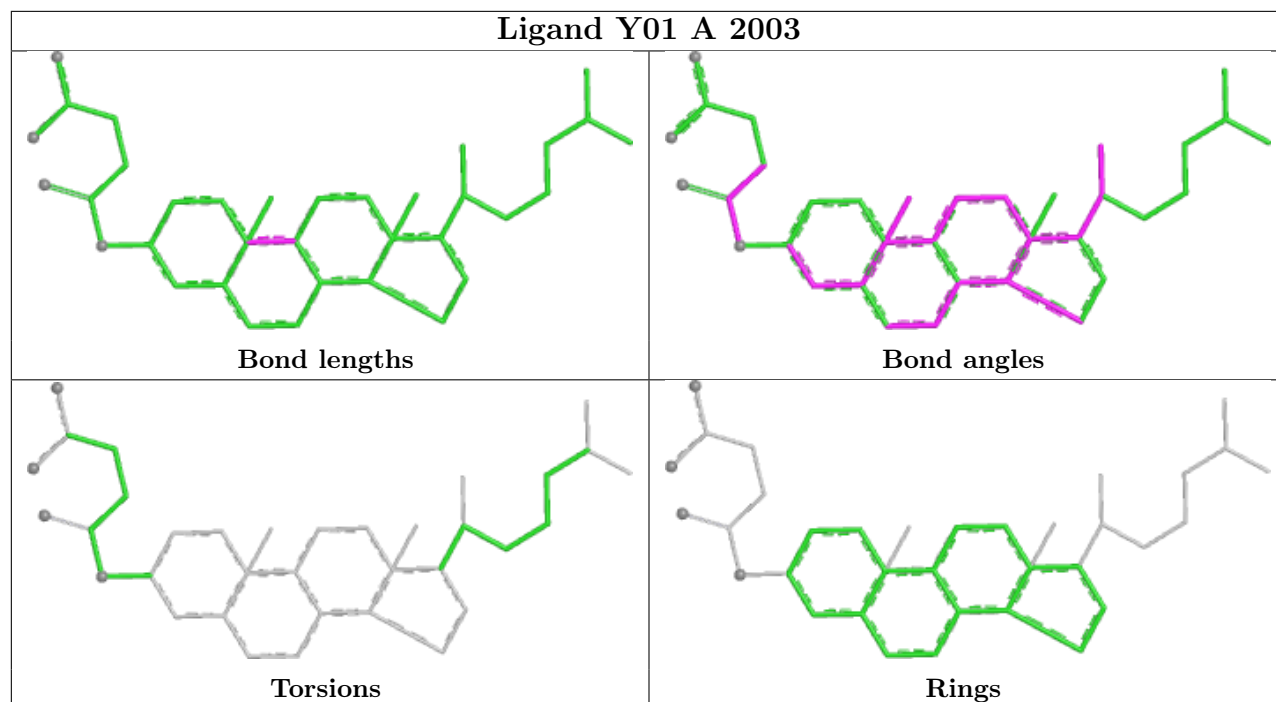
Ligand NAG A 2008

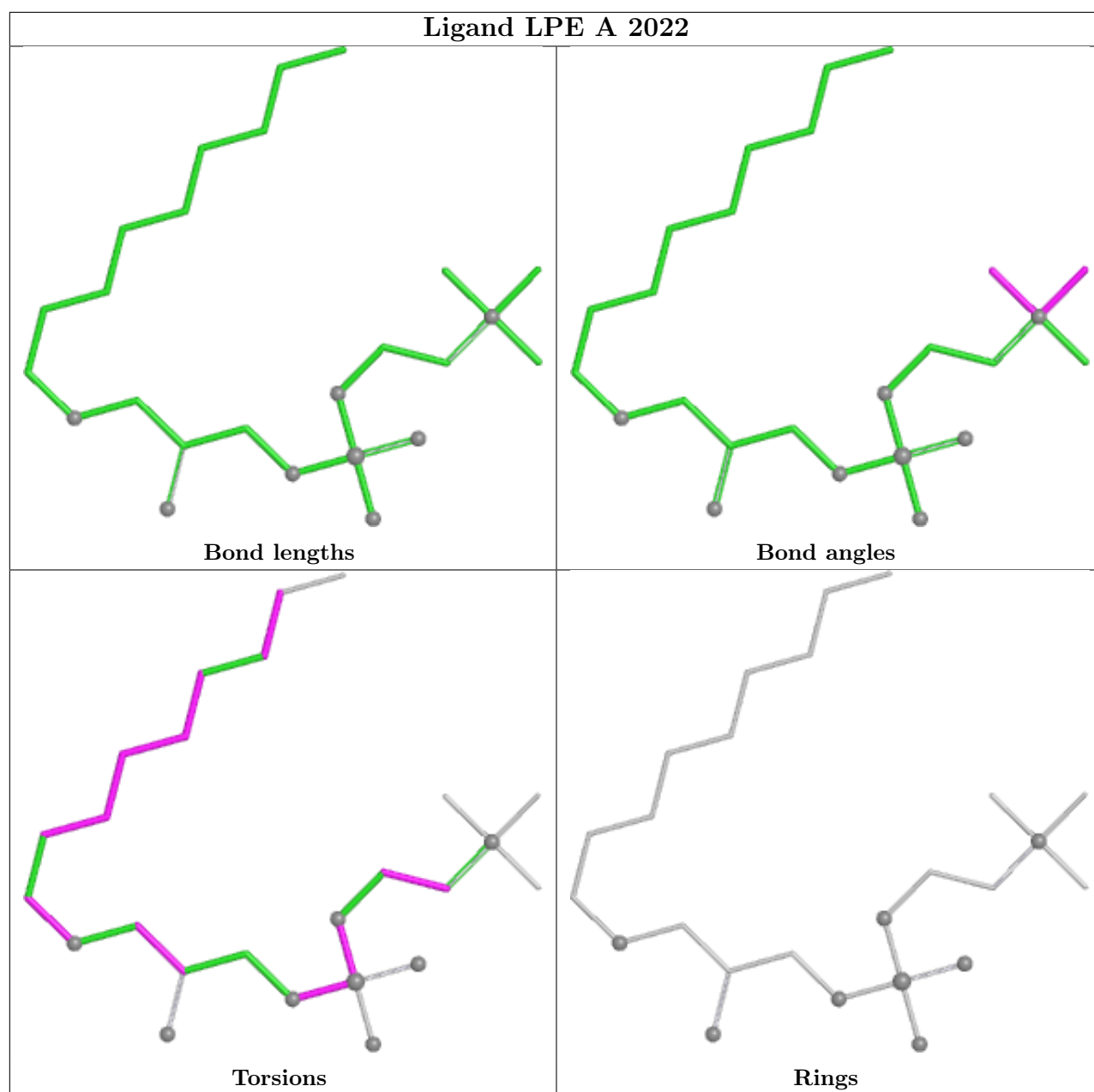


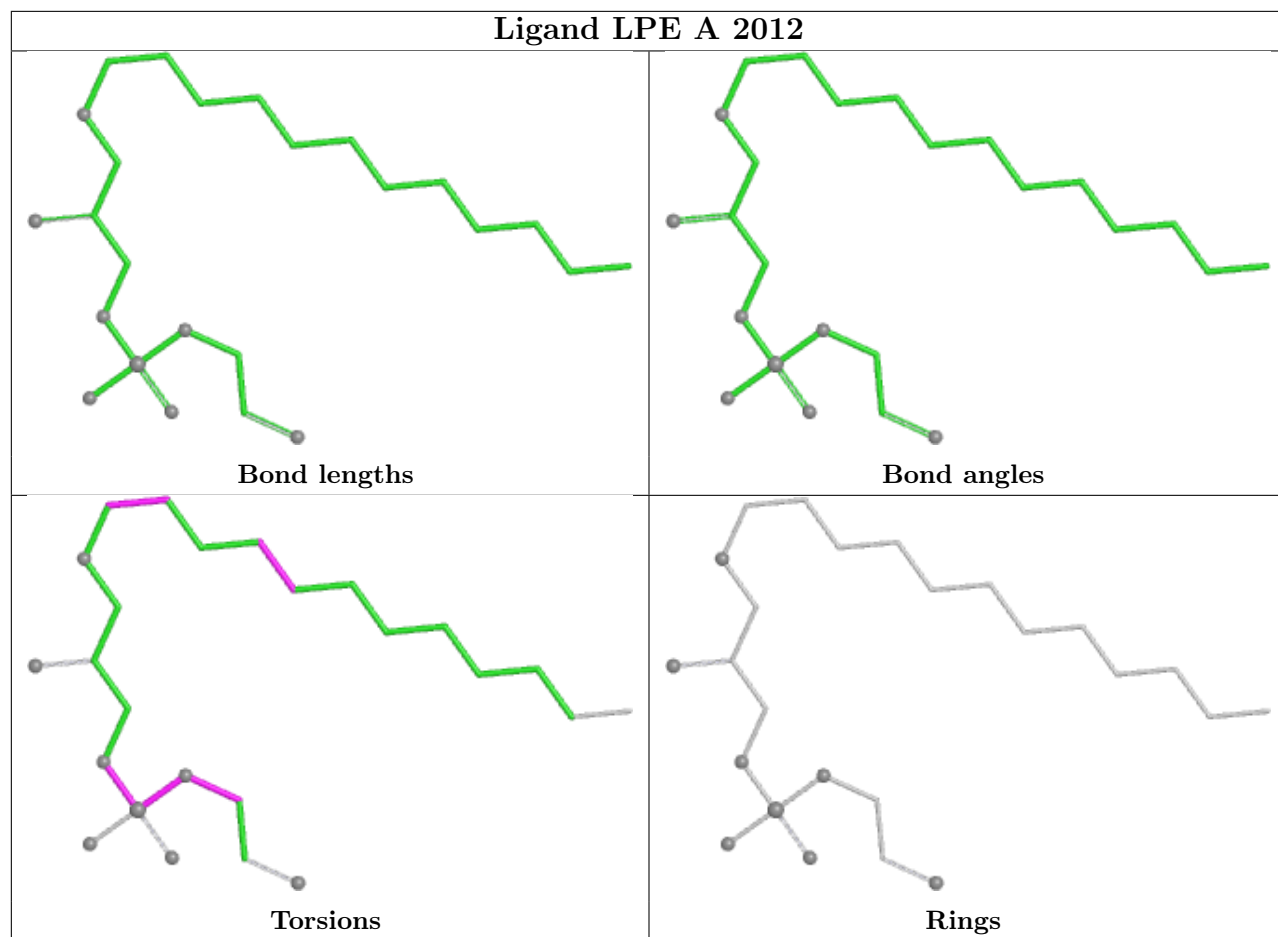
Ligand LPE A 2033

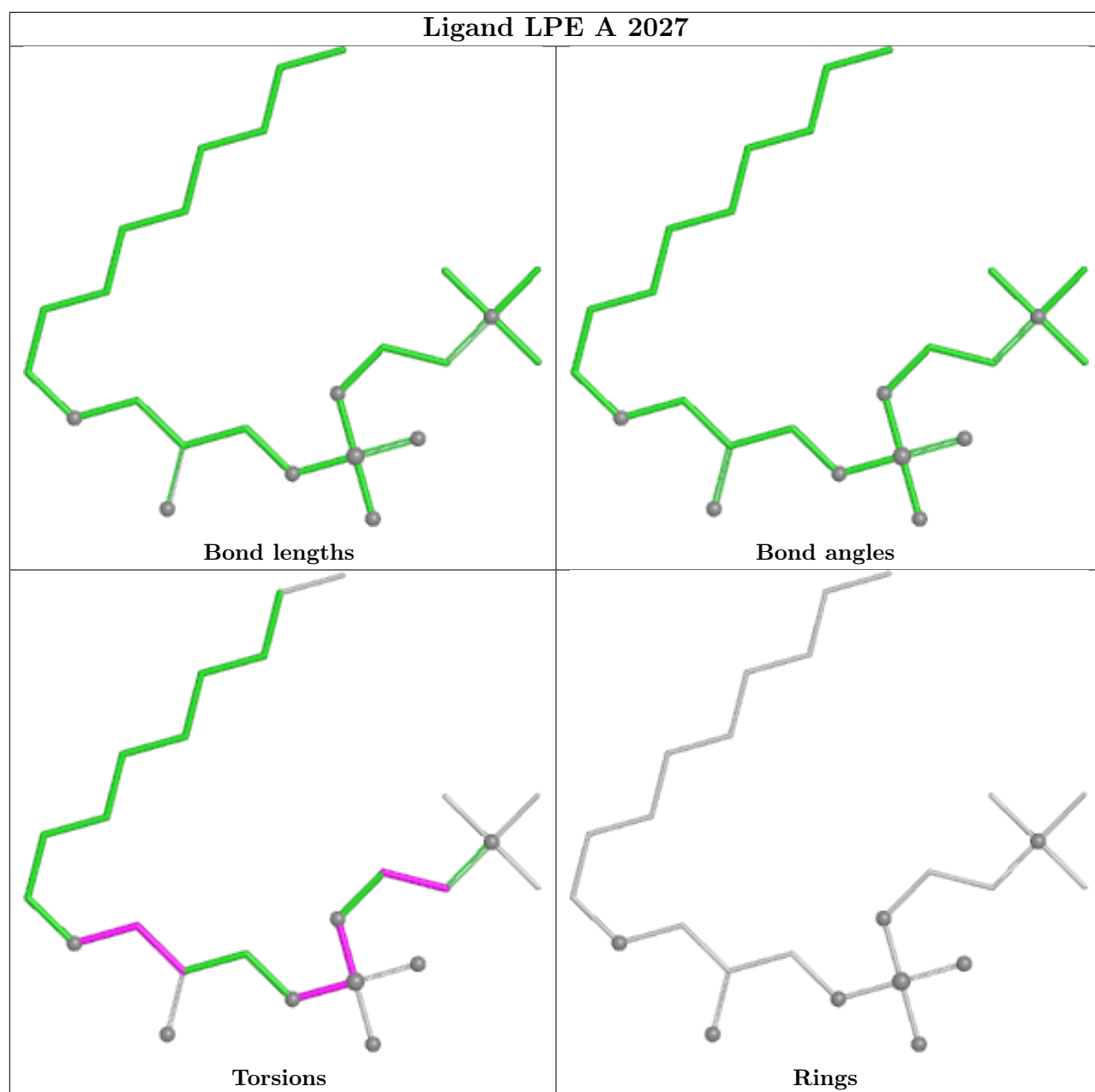


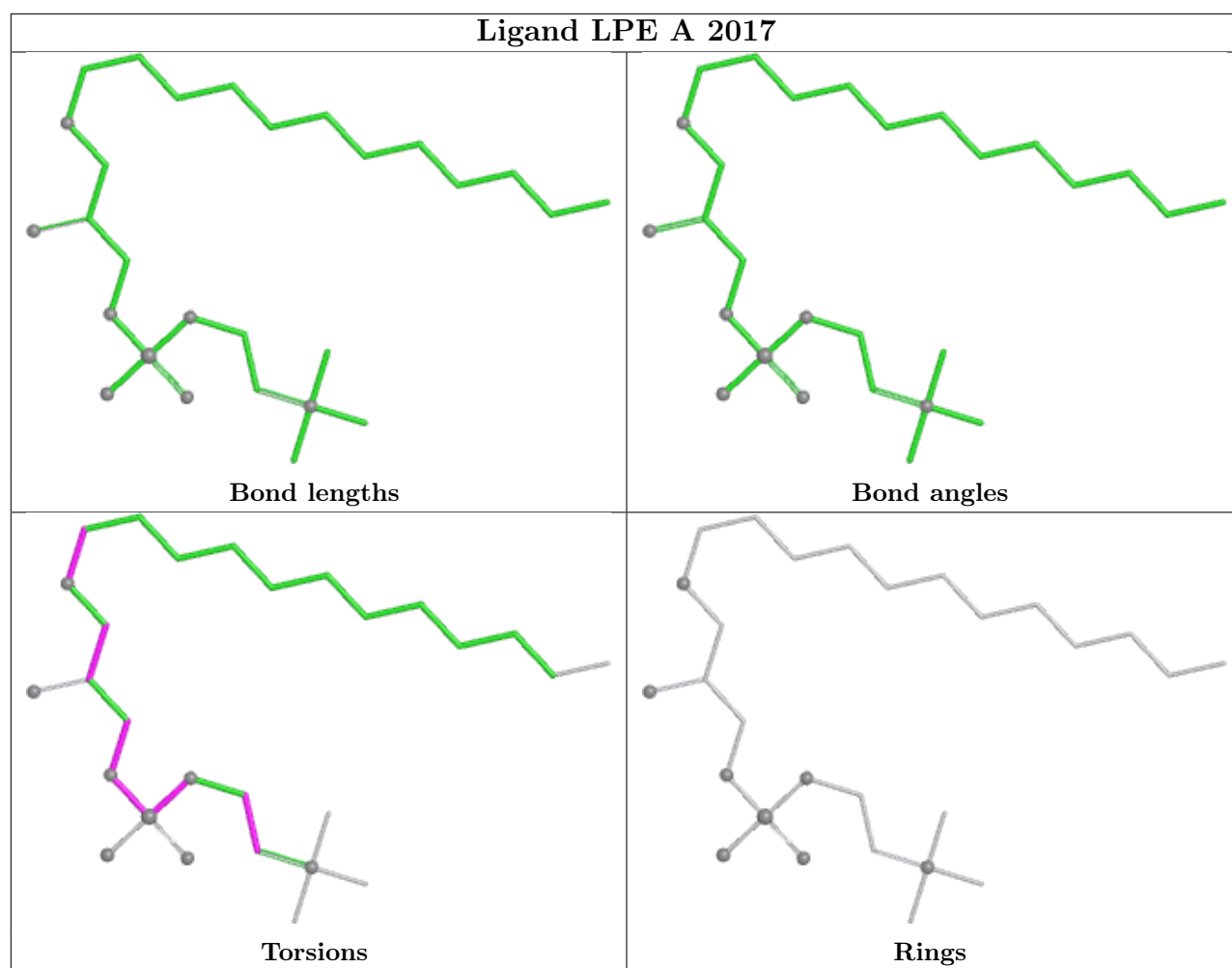


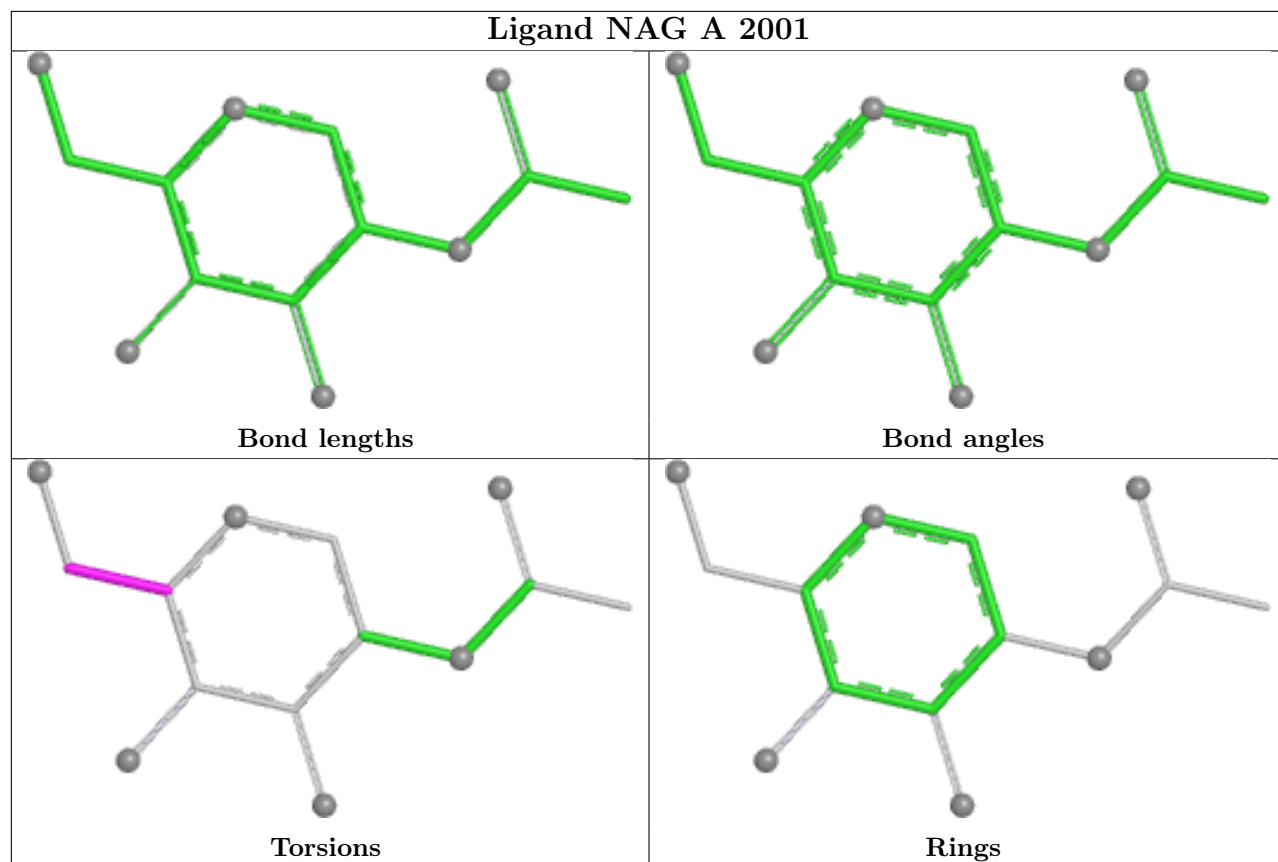


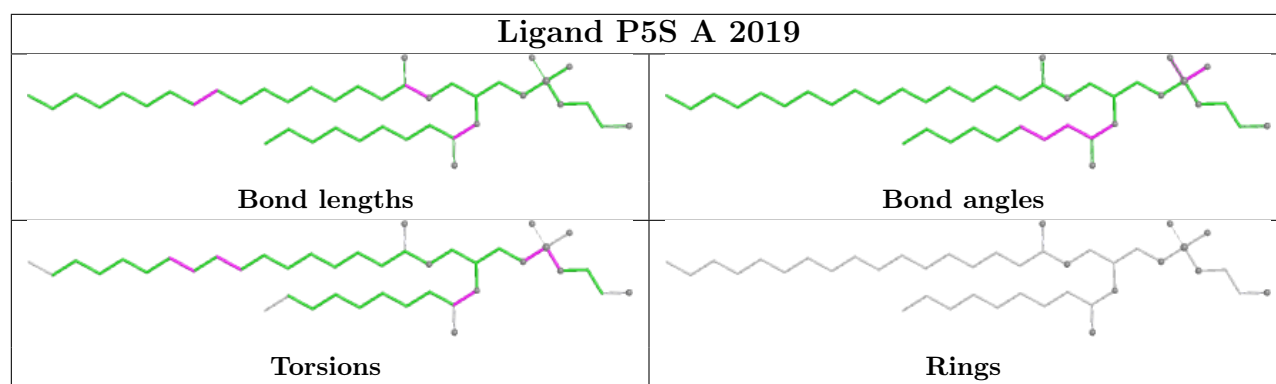
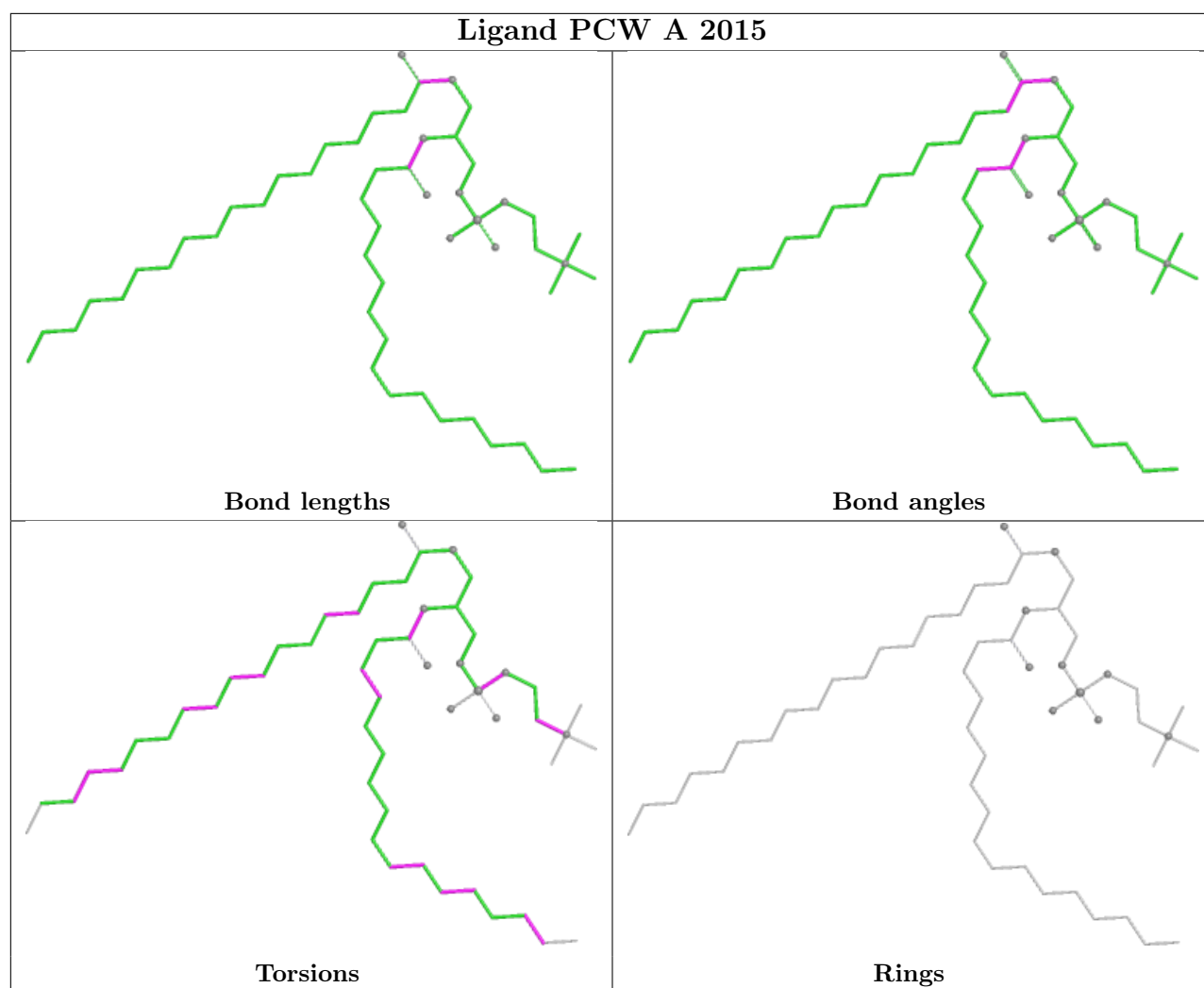


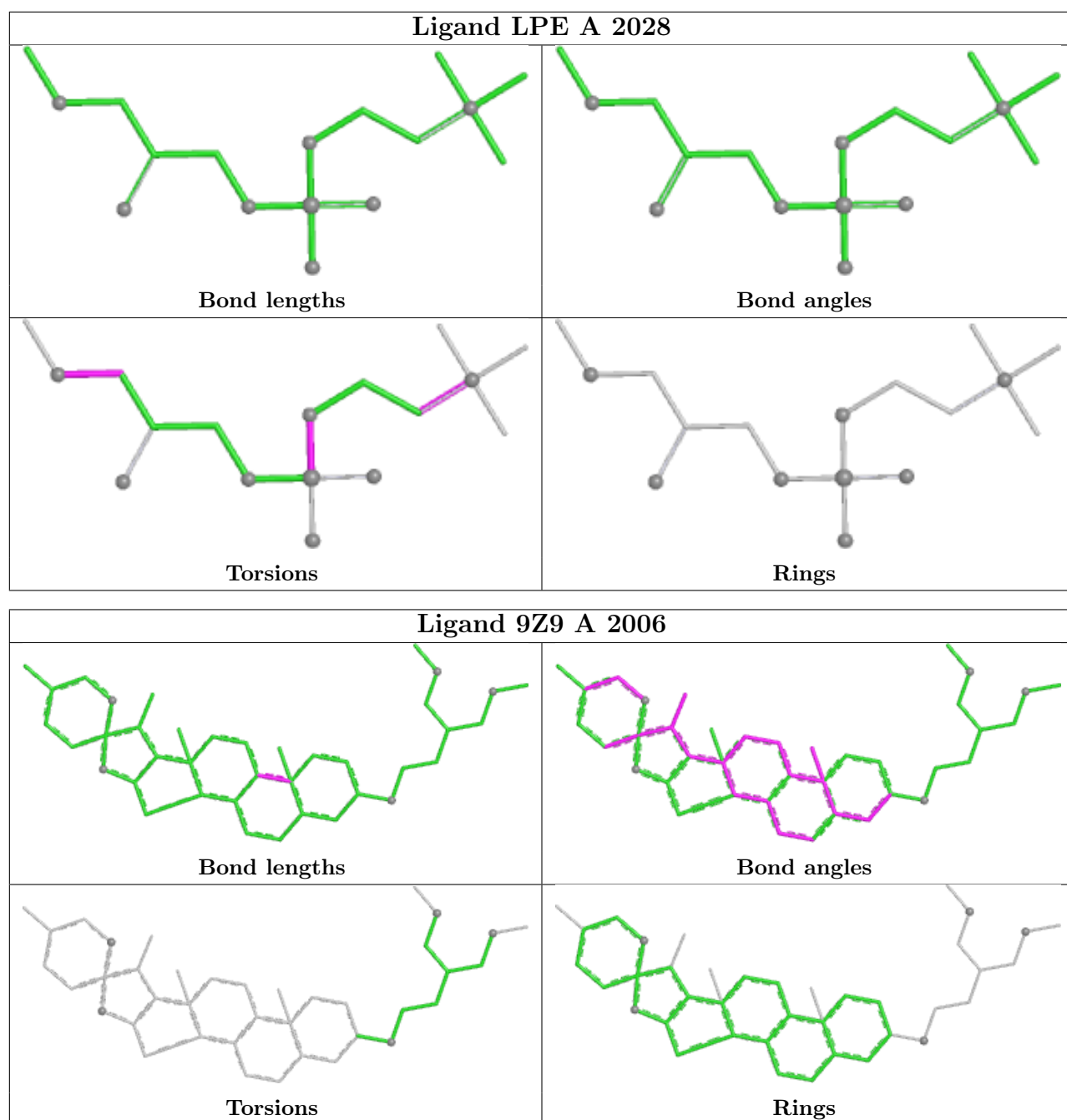


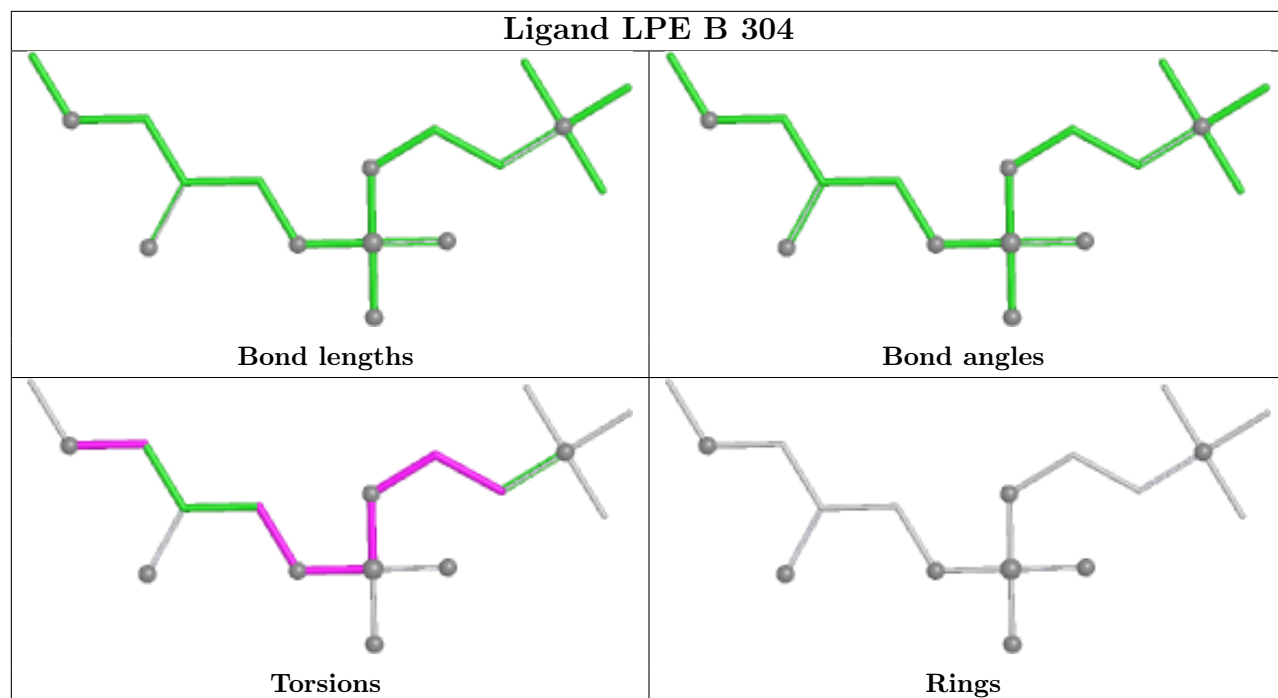


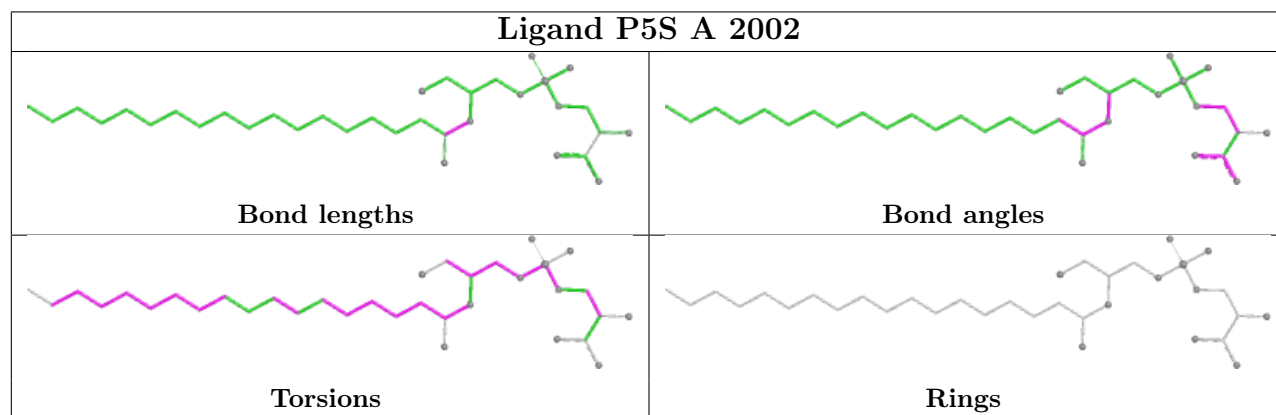
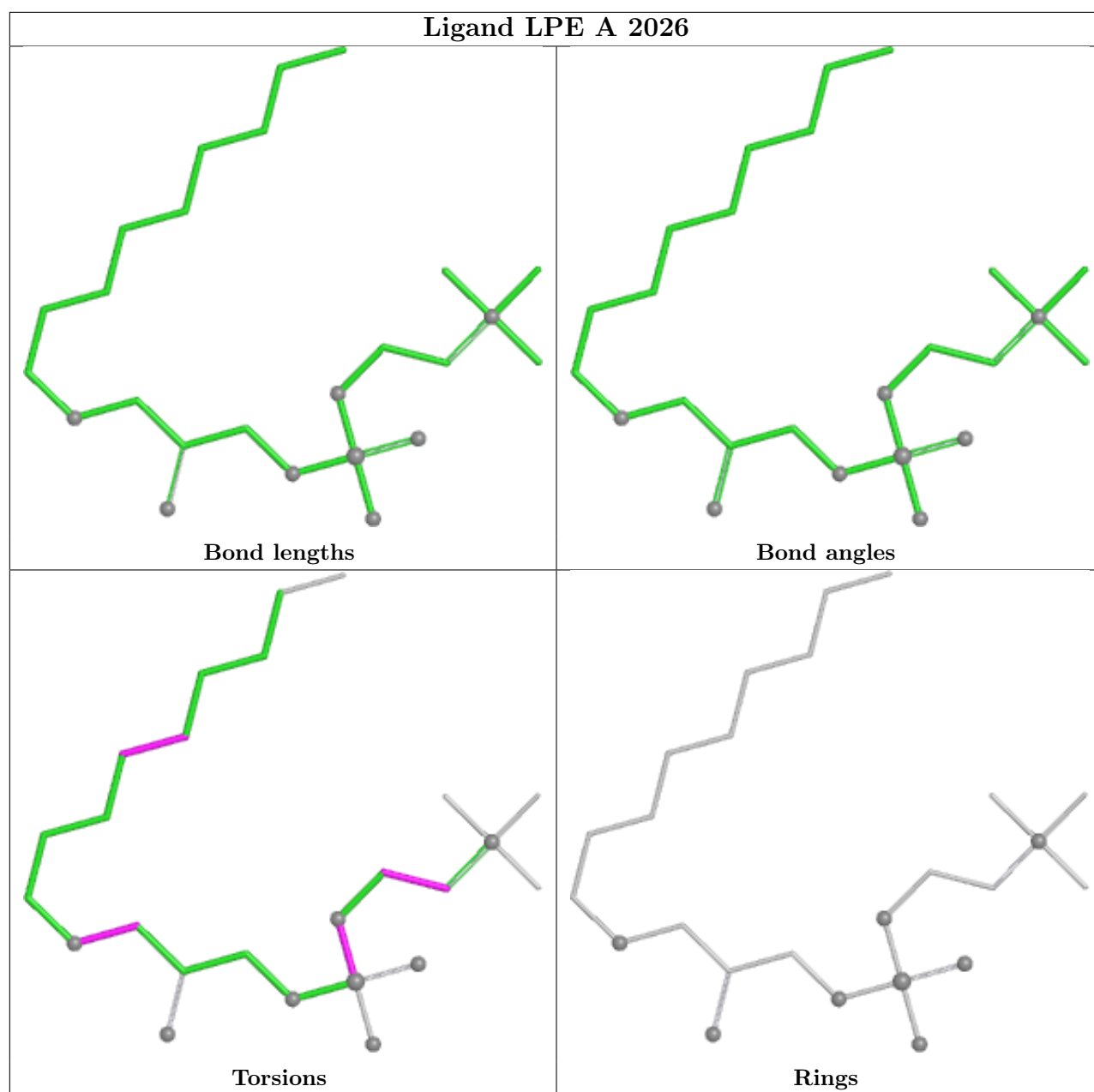












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

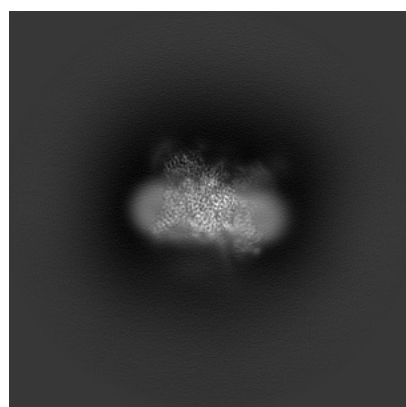
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32368. These allow visual inspection of the internal detail of the map and identification of artifacts.

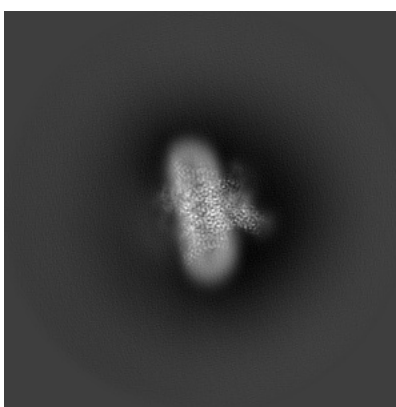
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

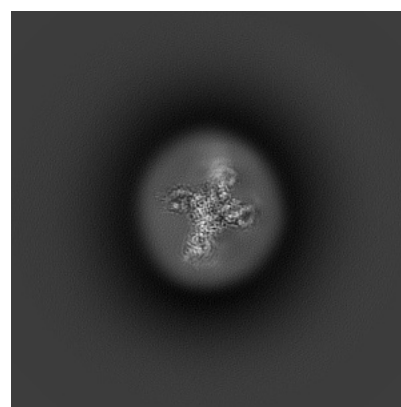
6.1.1 Primary map



X



Y

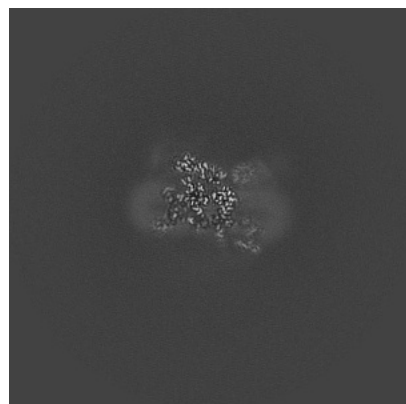


Z

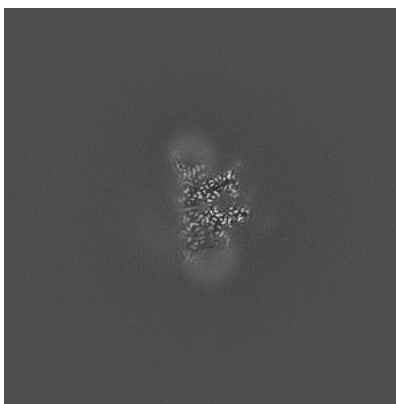
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

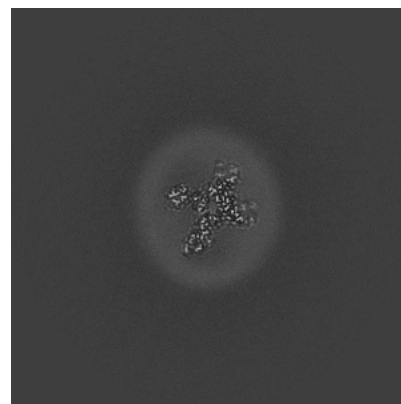
6.2.1 Primary map



X Index: 192



Y Index: 192

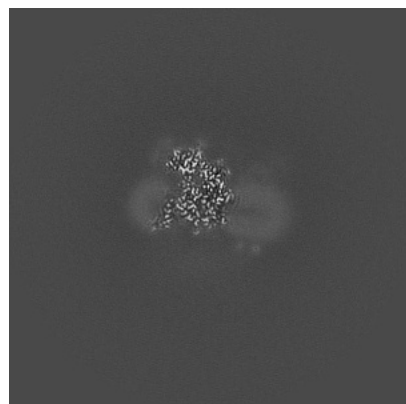


Z Index: 192

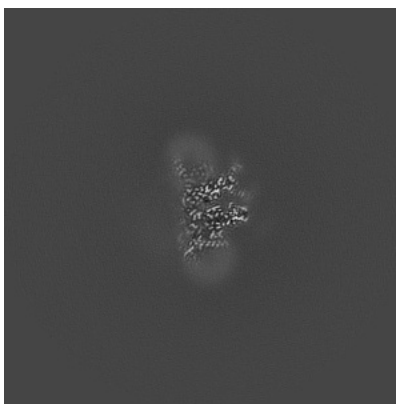
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

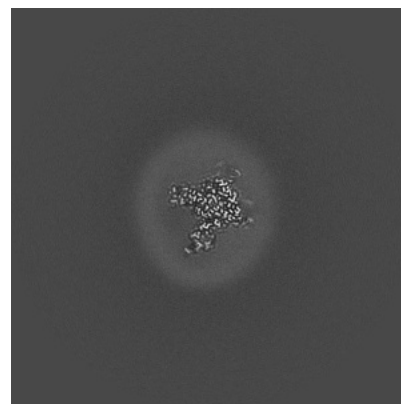
6.3.1 Primary map



X Index: 183



Y Index: 196

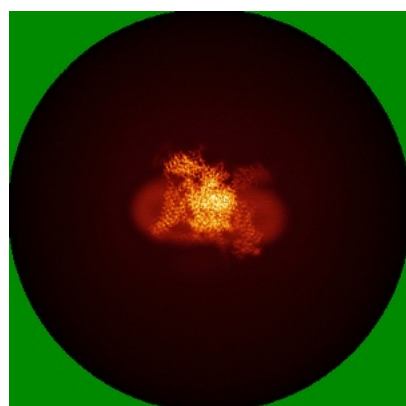


Z Index: 198

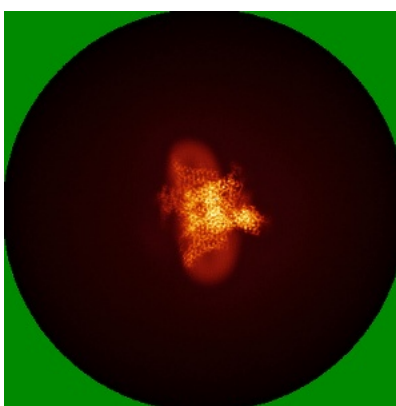
The images above show the largest variance slices of the map in three orthogonal directions.

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

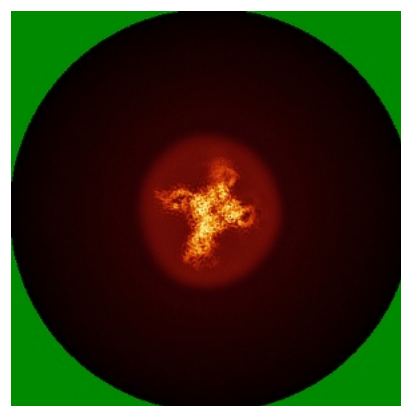
6.4.1 Primary map



X



Y

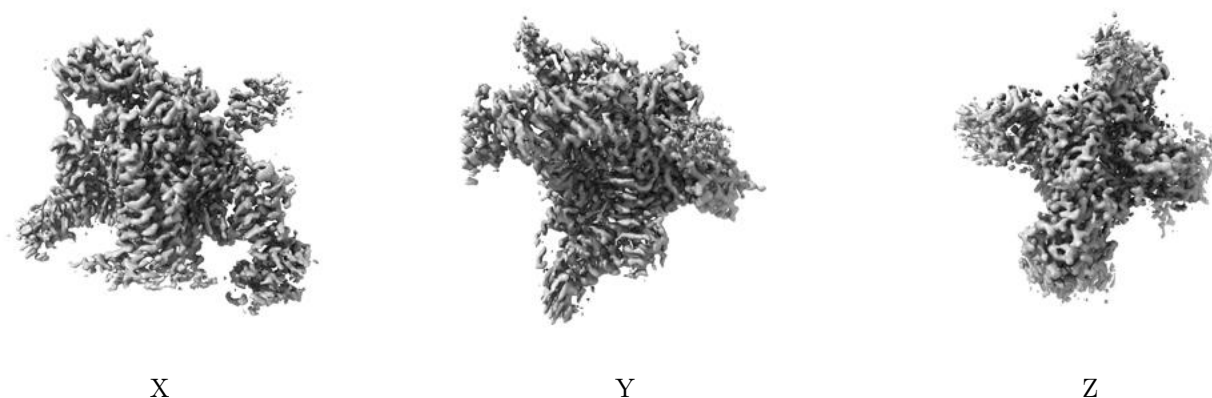


Z

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

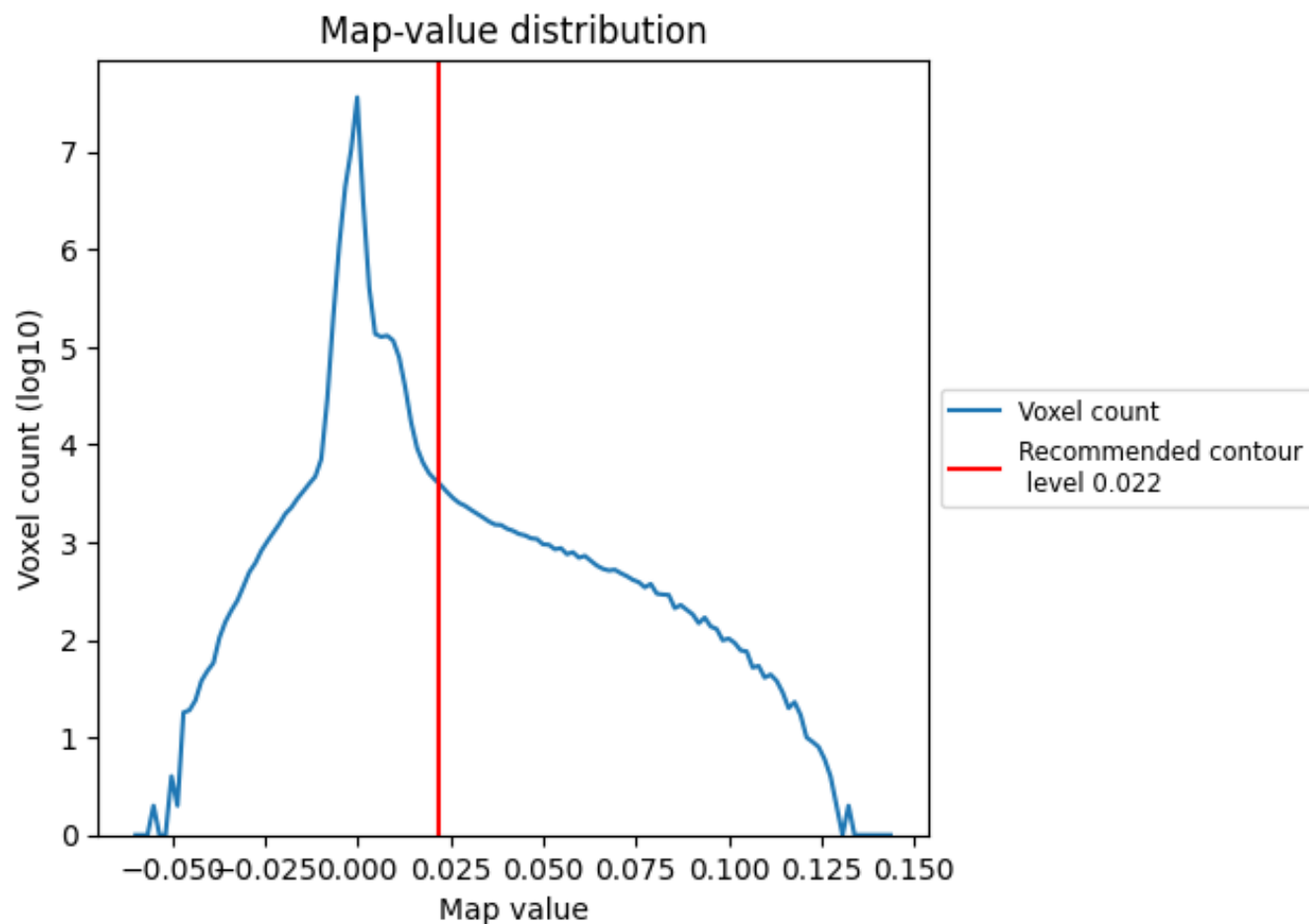
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

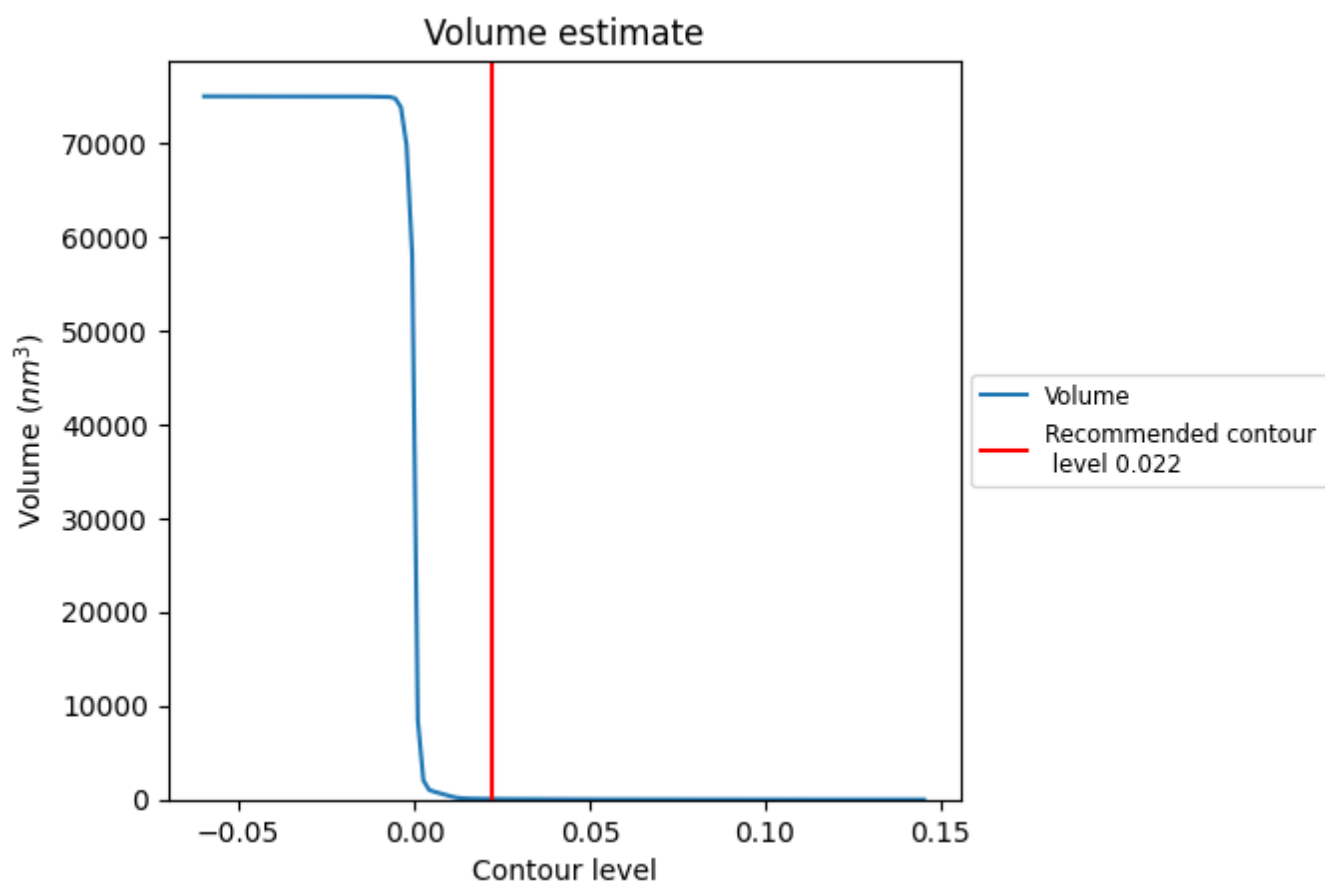
This section contains the results of statistical analysis of the map.

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.

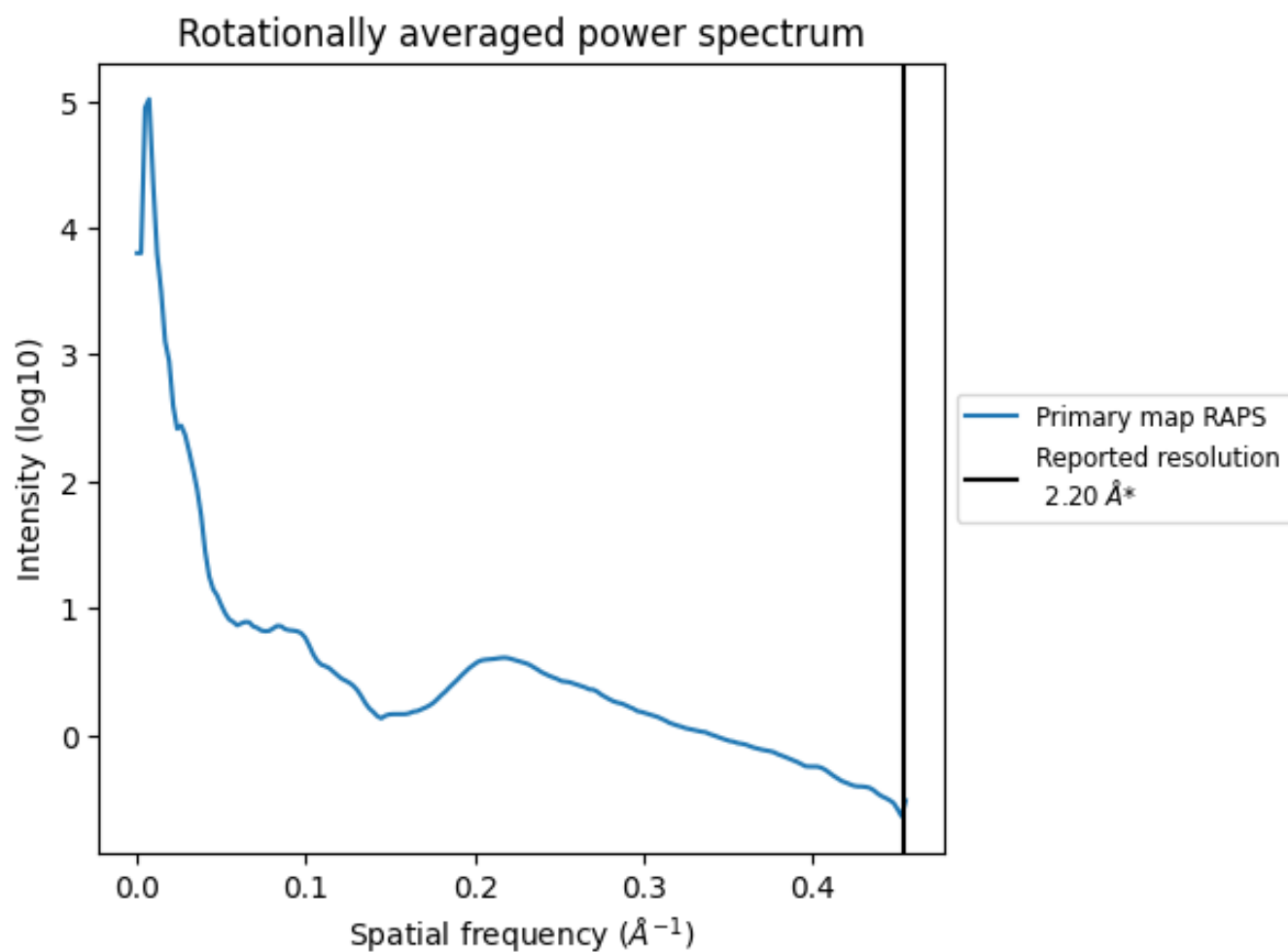
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 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 0.455 Å⁻¹

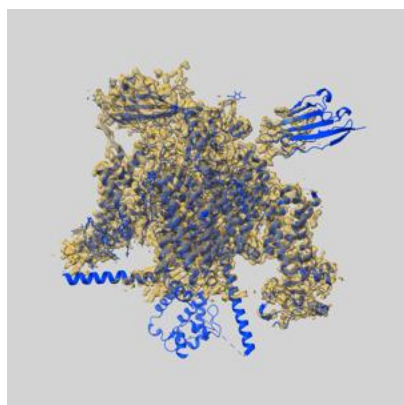
8 Fourier-Shell correlation ⓘ

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

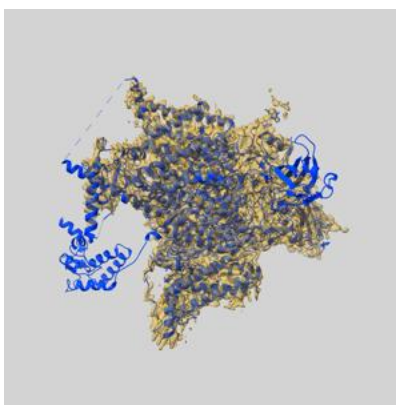
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32368 and PDB model 7W9K. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

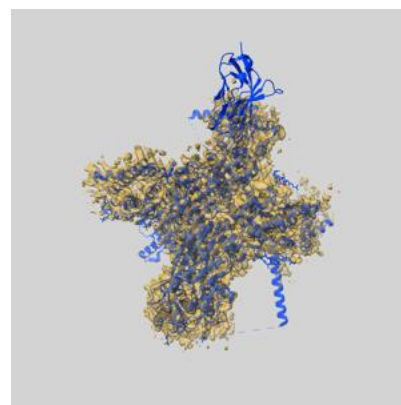
9.1 Map-model overlay [i](#)



X



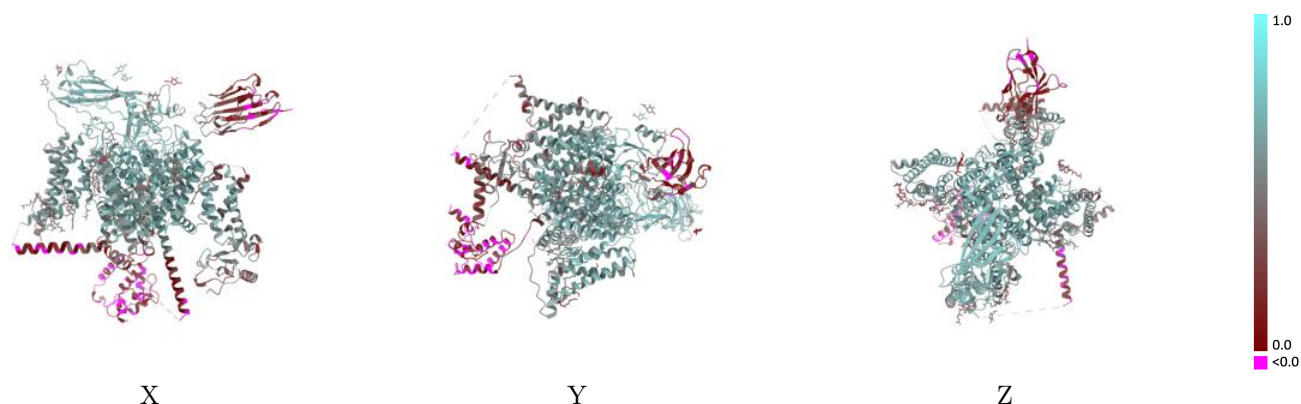
Y



Z

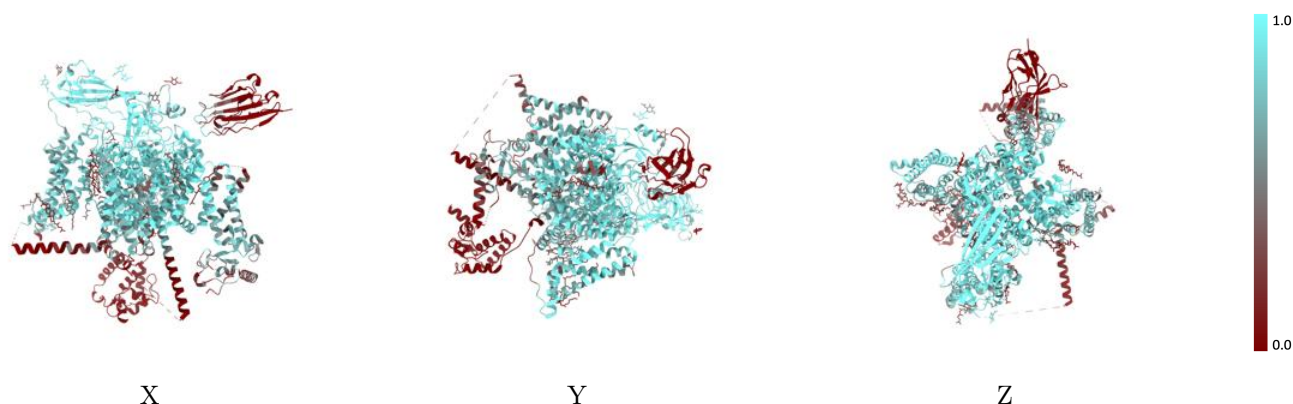
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



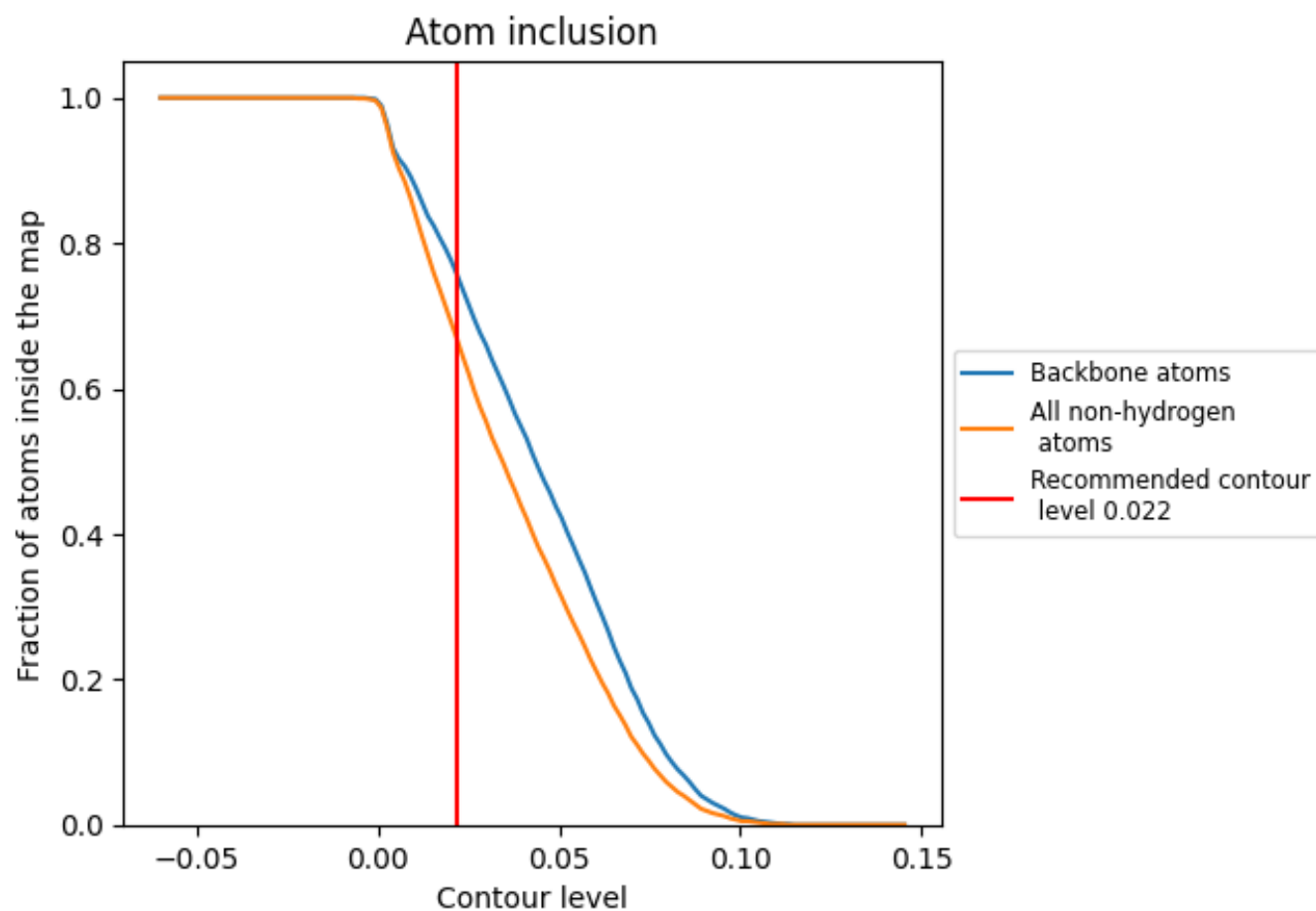
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6660	0.5070
A	0.6840	0.5180
B	0.8590	0.6100
C	0.1440	0.2110
D	0.5000	0.4100
E	0.7140	0.4790
F	0.9290	0.6380

1.0

0.0

<0.0