Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 11:52 am GMT

PDB ID	:	6SCJ
EMDB ID	:	EMD-10141
Title	:	The structure of human thyroglobulin
Authors	:	Coscia, F.; Turk, D.; Lowe, J.
Deposited on	:	2019-07-24
Resolution	:	3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

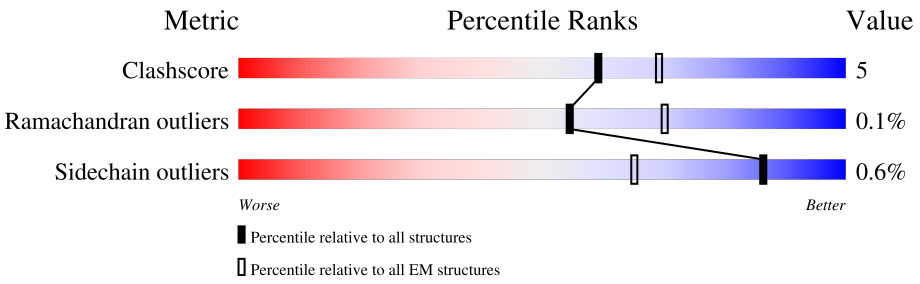
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2768	6% 79% 13% 8%
1	B	2768	6% 79% 13% 8%
2	C	3	67% 33%
2	D	3	67% 33%

2 Entry composition (i)

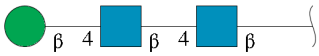
There are 3 unique types of molecules in this entry. The entry contains 39884 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thyroglobulin.

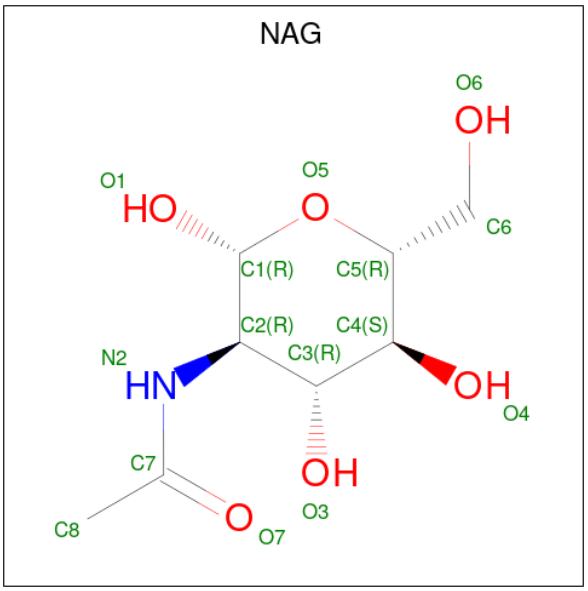
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2551	19693	12350	3428	3759	156	0	0
1	B	2551	19693	12350	3428	3759	156	0	0

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0
3	A	1	210	120	15	75	0

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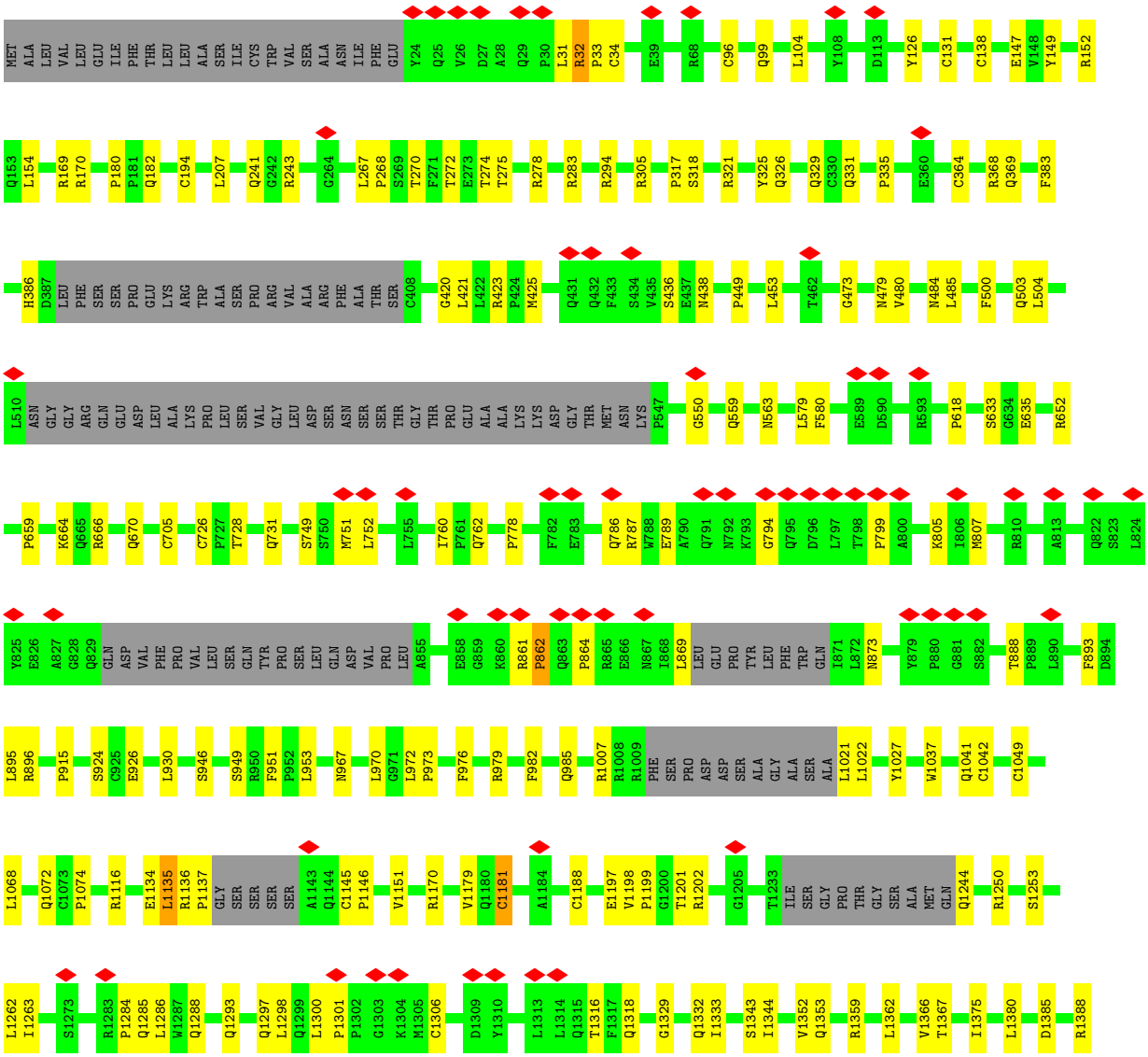
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0
3	B	1	210	120	15	75	0

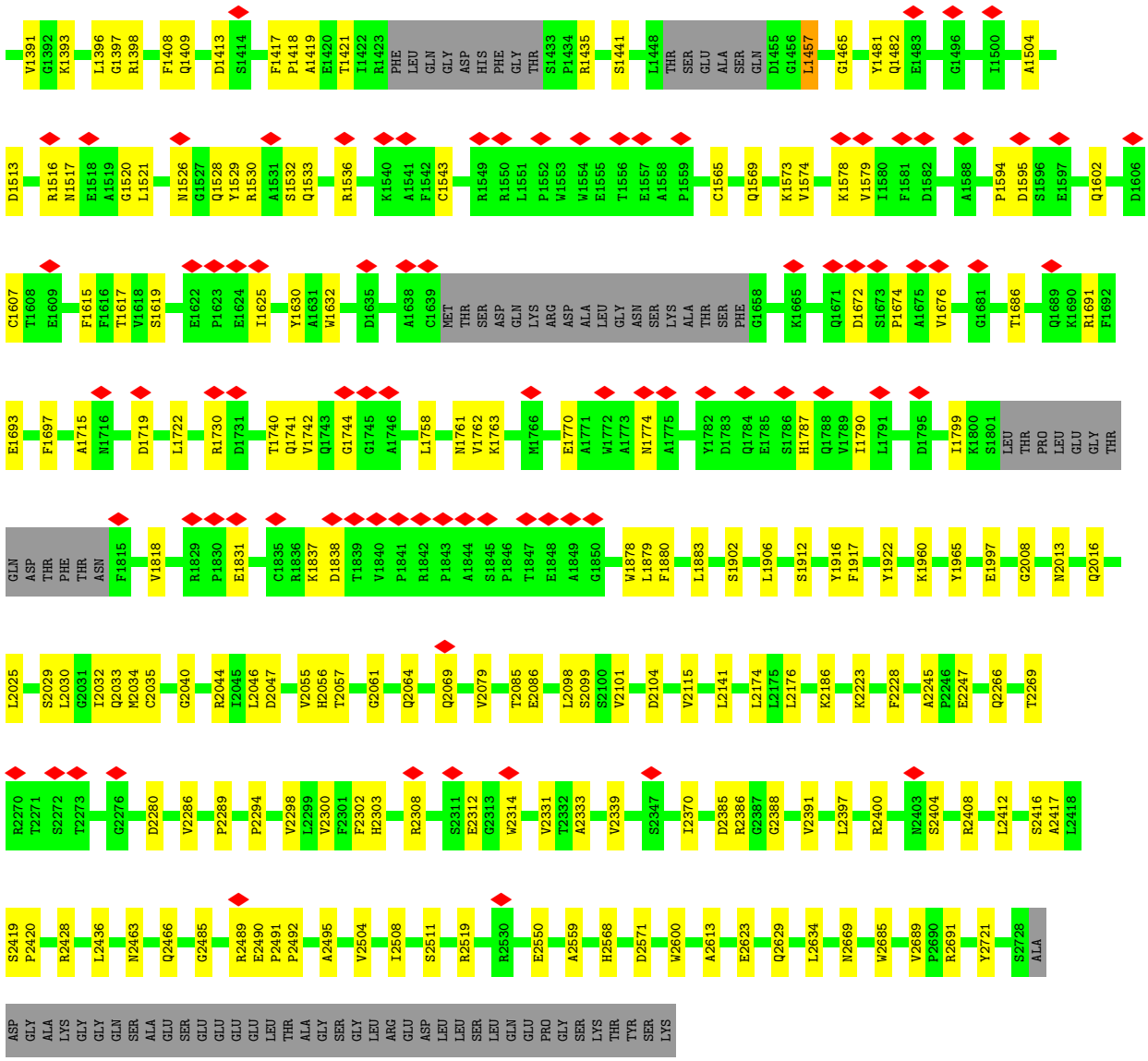
3 Residue-property plots (i)

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

- Molecule 1: Thyroglobulin

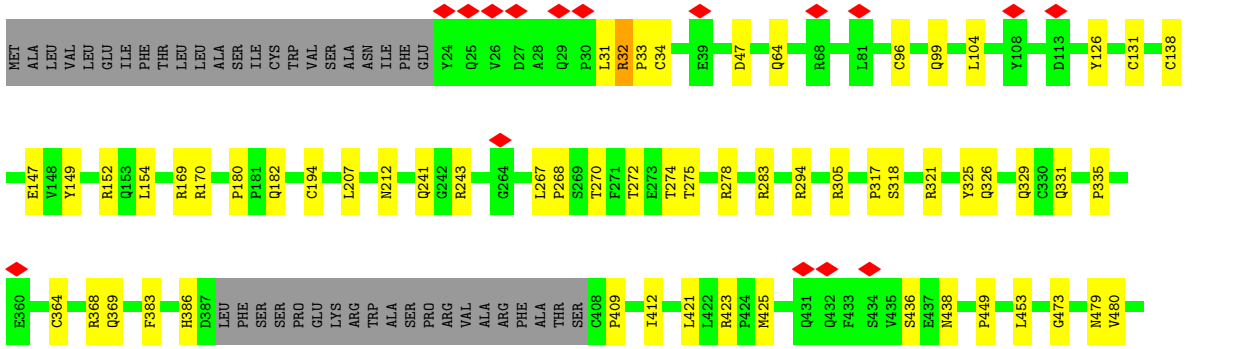
Chain A:

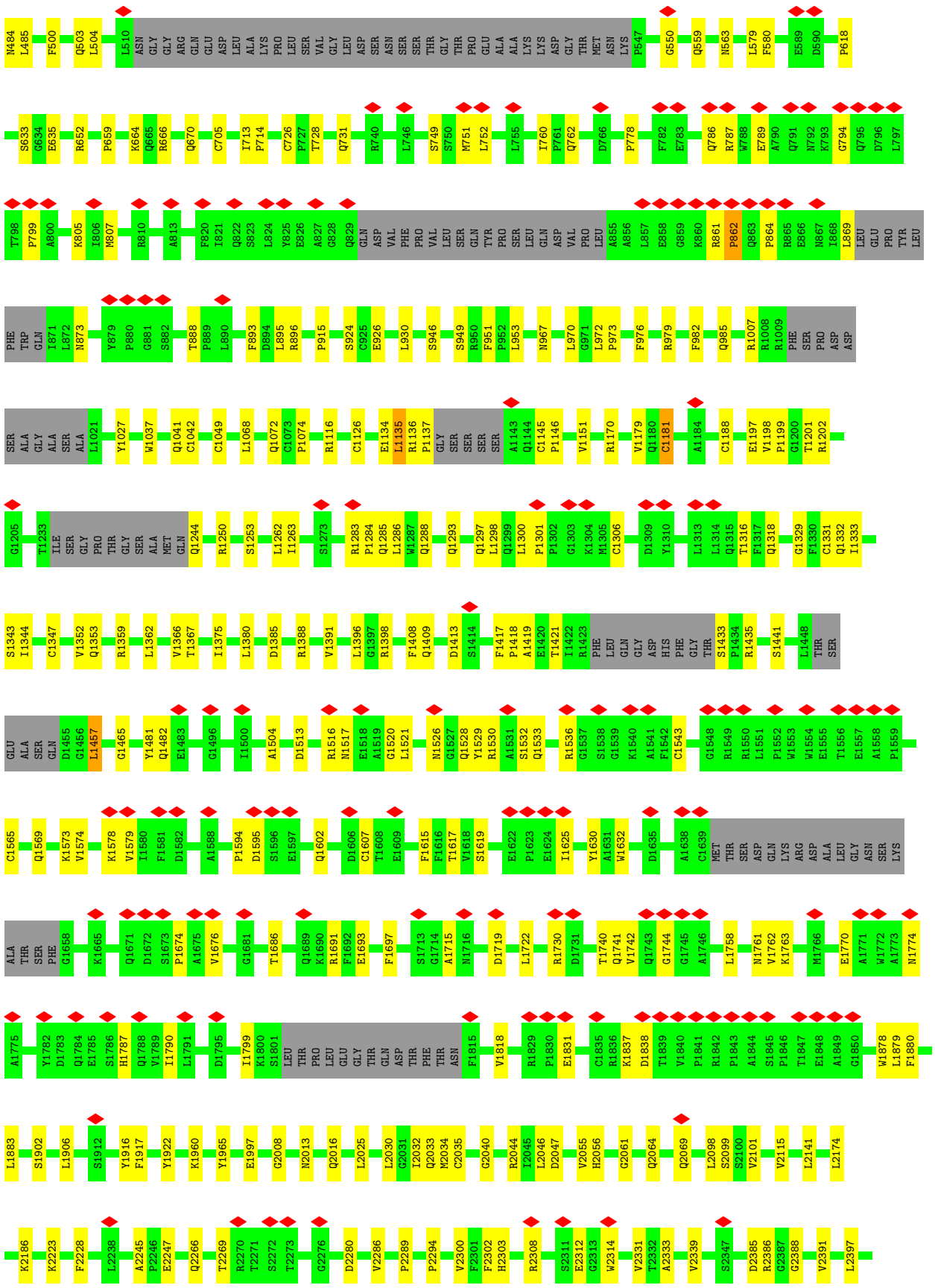


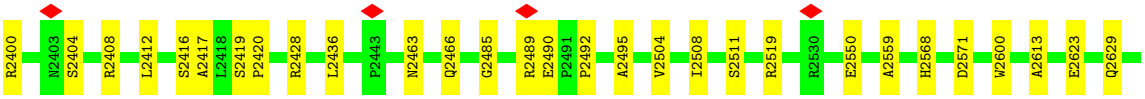


- Molecule 1: Thyroglobulin

Chain B:




N484 L485 F500 Q503 L504 L510 ASN GLY GLY ARG GLN GLU ASP LEU ALA LYS PRO LEU SER VAL GLY LEU ASP SER ASN SER SER THR GLY THR PRO GLU ALA ALA LYS LYS ASP GLY THR MET ASN LYS P547 G550 Q559 N563 L579 F580 E589 D590 P618
S633 G634 E635 R652 P659 K664 Q665 R666 Q670 C705 I713 P714 C726 P727 T728 Q731 R740 L746 S749 S750 M751 L752 L755 I760 P761 Q762 D766 P778 F782 E783 Q786 R787 W788 E789 A790 Q791 N792 K793 G794 Q795 D796 L797
T798 P799 A800 K805 I806 M807 R810 A813 F820 I821 Q822 S823 L824 Y825 E826 A827 G828 Q829 GLN ASP VAL PHE PRO VAL LEU SER GLN TYR PRO SER LEU GLN ASP VAL PRO LEU A855 A856 L857 E858 G859 K860 R861 P862 Q863 P864 R865 E866 N867 I868 L869 LEU GLU PRO TYR LEU
PHE TRP GLN I871 L872 N873 Y879 P880 G881 S882 T888 P889 L890 F893 D894 L895 R896 P915 S924 C925 E926 L930 S946 S949 R950 F951 P952 L953 N967 L970 G971 L972 P973 F976 R979 F982 Q985 R1007 R1008 R1009 PHE SER PRO ASP ASP
SER ALA GLY ALA SER ALA L1021 Y1027 W1037 Q1041 C1042 C1049 L1068 Q1072 C1073 P1074 R1116 C1126 E1134 L1135 R1136 P1137 GLY SER SER SER SER A1143 Q1144 C1145 P1146 V1151 R1170 V1179 Q1180 C1181 A1184 C1188 E1197 V1198 P1199 G1200 T1201 R1202
G1205 T1233 ILE SER GLY PRO THR GLY SER ALA MET GLN Q1244 R1250 S1253 L1262 I1263 S1273 R1283 P1284 Q1285 L1286 W1287 Q1288 Q1293 Q1297 L1298 Q1299 L1300 P1301 P1302 G1303 K1304 M1305 C1306 D1309 Y1310 L1313 L1314 Q1315 T1316 F1317 Q1318 G1329 F1330 C1331 Q1332 I1333
S1343 I1344 C1347 V1352 Q1353 R1359 L1362 V1366 T1367 I1375 L1380 D1385 R1388 V1391 L1396 G1397 R1398 F1408 Q1409 D1413 S1414 F1417 P1418 A1419 E1420 T1421 I1422 R1423 PHE LEU GLN GLY ASP HIS PHE GLY THR S1433 P1434 R1435 S1441 L1448 THR SER
GLU ALA SER GLN D1455 G1456 L1457 G1465 Y1481 Q1482 E1483 G1496 I1500 A1504 D1513 R1516 N1517 E1518 A1519 G1520 L1521 N1526 G1527 Q1528 Y1529 R1530 A1531 S1532 Q1533 R1536 G1537 S1538 G1539 K1540 A1541 F1542 C1543 G1548 R1549 R1550 L1551 P1552 W1553 W1554 E1555 T1556 E1557 A1558 P1559
C1565 Q1569 K1573 V1574 K1578 V1579 I1580 F1581 D1582 A1588 P1594 D1595 S1596 E1597 Q1602 D1606 C1607 T1608 E1609 F1615 F1616 T1617 V1618 S1619 E1622 P1623 E1624 I1625 Y1630 A1631 W1632 D1635 A1638 C1639 MET THR SER ASP GLN LYS ARG ASP ALA LEU GLY ASN SER LYS
ALA THR SER PHE G1658 K1665 Q1671 D1672 S1673 P1674 A1675 V1676 G1681 T1686 Q1689 K1690 R1691 F1692 E1693 F1697 S1713 G1714 A1715 M1716 D1719 L1722 R1730 D1731 T1740 Q1741 V1742 Q1743 G1744 G1745 A1746 L1758 M1761 V1762 K1763 M1766 E1770 A1771 W1772 A1773 M1774
A1775 Y1782 D1783 Q1784 E1785 S1786 H1787 Q1788 V1789 I1790 L1791 D1795 I1799 K1800 S1801 LEU THR PRO LEU GLU GLY THR GLN ASP THR PHE THR ASN F1815 V1818 R1829 P1830 E1831 C1835 R1836 K1837 D1838 T1839 V1840 P1841 R1842 P1843 A1844 S1845 P1846 T1847 E1848 A1849 G1850 W1878 L1879 F1880
L1883 S1902 L1906 S1912 Y1916 F1917 Y1922 K1960 Y1965 E1997 G2008 N2013 Q2016 L2025 L2030 G2031 I2032 Q2033 M2034 C2035 G2040 R2044 I2045 L2046 D2047 V2055 H2056 G2061 Q2064 Q2069 L2098 S2099 S2100 V2101 V2115 L2141 L2174
K2186 K2223 F2228 L2238 A2245 P2246 E2247 Q2266 T2269 R2270 T2271 S2272 T2273 G2276 D2280 V2286 P2289 P2294 V2300 F2301 F2302 H2303 R2308 S2311 E2312 G2313 W2314 V2331 T2332 A2333 V2339 S2347 D2385 R2386 G2387 G2388 V2391 L2397



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

Chain C:

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

Chain D:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	151601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	417.19998, 417.19998, 417.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.043, 1.043, 1.043	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.29	0/20154	0.59	8/27350 (0.0%)
1	B	0.29	0/20154	0.59	8/27350 (0.0%)
All	All	0.29	0/40308	0.59	16/54700 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	864	PRO	N-CA-CB	5.87	110.35	103.30
1	B	864	PRO	N-CA-CB	5.84	110.31	103.30
1	B	1135	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	1135	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	2025	LEU	CA-CB-CG	5.71	128.43	115.30
1	B	2025	LEU	CA-CB-CG	5.69	128.40	115.30
1	B	862	PRO	N-CA-CB	5.68	110.12	103.30
1	A	862	PRO	N-CA-CB	5.68	110.12	103.30
1	A	2035	CYS	CA-CB-SG	5.35	123.64	114.00
1	B	2035	CYS	CA-CB-SG	5.33	123.60	114.00
1	B	1413	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	1413	ASP	CB-CG-OD1	5.26	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1457	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	1457	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	1198	VAL	C-N-CD	-5.11	109.36	120.60
1	A	1198	VAL	C-N-CD	-5.11	109.37	120.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1902	SER	Peptide
1	A	32	ARG	Peptide
1	A	33	PRO	Peptide
1	A	799	PRO	Peptide
1	B	1902	SER	Peptide
1	B	32	ARG	Peptide
1	B	33	PRO	Peptide
1	B	799	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19693	0	18886	204	0
1	B	19693	0	18886	205	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	210	0	195	1	0
3	B	210	0	195	1	0
All	All	39884	0	38230	377	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 5.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1615:PHE:HB2	1:B:1630:TYR:HB2	1.74	0.70
1:A:1615:PHE:HB2	1:A:1630:TYR:HB2	1.74	0.70
1:A:2669:ASN:HD21	1:A:2685:TRP:H	1.38	0.69
1:A:2339:VAL:HG12	1:A:2466:GLN:HE21	1.58	0.69
1:B:2669:ASN:HD21	1:B:2685:TRP:H	1.38	0.69
1:B:2339:VAL:HG12	1:B:2466:GLN:HE21	1.58	0.68
1:A:1301:PRO:HG2	1:A:1417:PHE:HB2	1.78	0.66
1:B:1288:GLN:HE21	1:B:1441:SER:H	1.44	0.66
1:B:2228:PHE:HB2	1:B:2286:VAL:HG13	1.78	0.66
1:B:1301:PRO:HG2	1:B:1417:PHE:HB2	1.78	0.65
1:A:633:SER:O	1:B:652:ARG:NH2	2.30	0.65
1:A:2228:PHE:HB2	1:A:2286:VAL:HG13	1.78	0.64
1:A:1288:GLN:HE21	1:A:1441:SER:H	1.44	0.63
1:A:2056:HIS:NE2	1:B:267:LEU:O	2.29	0.62
1:A:652:ARG:NH2	1:B:633:SER:O	2.33	0.62
1:B:294:ARG:HH22	1:B:321:ARG:HH11	1.48	0.62
1:A:294:ARG:HH22	1:A:321:ARG:HH11	1.48	0.62
1:A:2101:VAL:HG12	1:A:2174:LEU:HB2	1.83	0.60
1:B:924:SER:O	1:B:1037:TRP:NE1	2.35	0.60
1:A:1306:CYS:HB2	1:A:1359:ARG:HA	1.83	0.60
1:A:2223:LYS:HD3	1:A:2289:PRO:HB3	1.83	0.60
1:A:924:SER:O	1:A:1037:TRP:NE1	2.35	0.60
1:A:1481:TYR:HA	1:A:1504:ALA:HB1	1.84	0.60
1:B:2223:LYS:HD3	1:B:2289:PRO:HB3	1.83	0.59
1:A:1740:THR:HG22	1:A:1818:VAL:HG13	1.84	0.59
1:B:728:THR:HG23	1:B:731:GLN:H	1.68	0.59
1:B:1306:CYS:HB2	1:B:1359:ARG:HA	1.83	0.59
1:A:1912:SER:HG	1:A:1916:TYR:HH	1.50	0.59
1:B:2101:VAL:HG12	1:B:2174:LEU:HB2	1.83	0.59
1:B:1740:THR:HG22	1:B:1818:VAL:HG13	1.84	0.58
1:A:728:THR:HG23	1:A:731:GLN:H	1.68	0.58
1:B:1481:TYR:HA	1:B:1504:ALA:HB1	1.84	0.58
1:A:1517:ASN:ND2	1:A:1520:GLY:O	2.36	0.58
1:B:1741:GLN:HE21	1:B:1744:GLY:HA2	1.69	0.58
1:A:480:VAL:HG23	1:A:485:LEU:HD13	1.85	0.58
1:B:480:VAL:HG23	1:B:485:LEU:HD13	1.85	0.57
1:B:967:ASN:HD22	1:B:972:LEU:HD21	1.69	0.57
1:A:1298:LEU:HD13	1:A:1362:LEU:HD23	1.86	0.57
1:A:786:GLN:HG2	1:A:787:ARG:HE	1.68	0.57
1:B:1517:ASN:ND2	1:B:1520:GLY:O	2.36	0.57
1:B:1632:TRP:NE1	1:B:1686:THR:O	2.36	0.57
1:A:154:LEU:O	1:B:2069:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:GLY:O	1:A:1398:ARG:NH2	2.37	0.57
1:A:1632:TRP:NE1	1:A:1686:THR:O	2.36	0.57
1:B:786:GLN:HG2	1:B:787:ARG:HE	1.68	0.57
1:B:1298:LEU:HD13	1:B:1362:LEU:HD23	1.86	0.57
1:A:2069:GLN:NE2	1:B:154:LEU:O	2.36	0.57
1:B:2308:ARG:HH11	1:B:2623:GLU:HG2	1.70	0.57
1:A:182:GLN:HE22	1:A:194:CYS:H	1.52	0.57
1:A:1741:GLN:HE21	1:A:1744:GLY:HA2	1.69	0.57
1:A:967:ASN:HD22	1:A:972:LEU:HD21	1.69	0.56
1:B:1329:GLY:O	1:B:1398:ARG:NH2	2.37	0.56
1:A:1715:ALA:HA	3:A:2805:NAG:H82	1.87	0.56
1:B:331:GLN:HE21	1:B:335:PRO:HD2	1.70	0.56
1:A:2308:ARG:HH11	1:A:2623:GLU:HG2	1.70	0.56
1:A:331:GLN:HE21	1:A:335:PRO:HD2	1.70	0.56
1:A:2055:VAL:HG13	1:A:2061:GLY:HA2	1.87	0.56
1:B:1116:ARG:NH1	1:B:1146:PRO:O	2.34	0.56
1:B:2055:VAL:HG13	1:B:2061:GLY:HA2	1.87	0.56
1:B:2492:PRO:HA	1:B:2495:ALA:HB3	1.88	0.56
1:A:268:PRO:HD2	1:A:274:THR:HG22	1.88	0.56
1:A:1072:GLN:HE21	1:A:2098:LEU:HD22	1.70	0.56
1:A:2485:GLY:O	1:A:2489:ARG:NH2	2.39	0.56
1:A:949:SER:HB3	1:B:949:SER:HB3	1.87	0.56
1:A:2492:PRO:HA	1:A:2495:ALA:HB3	1.88	0.56
1:B:182:GLN:HE22	1:B:194:CYS:H	1.52	0.55
1:B:268:PRO:HD2	1:B:274:THR:HG22	1.88	0.55
1:B:1715:ALA:HA	3:B:2805:NAG:H82	1.87	0.55
1:B:2485:GLY:O	1:B:2489:ARG:NH2	2.39	0.55
1:A:2721:TYR:HH	1:B:2721:TYR:HH	1.49	0.55
1:B:32:ARG:O	1:B:34:CYS:N	2.36	0.55
1:A:1530:ARG:O	1:A:1533:GLN:NE2	2.39	0.55
1:B:1072:GLN:HE21	1:B:2098:LEU:HD22	1.70	0.55
1:B:99:GLN:OE1	1:B:126:TYR:OH	2.25	0.55
1:A:760:ILE:HG13	1:A:778:PRO:HG3	1.89	0.55
1:A:982:PHE:HA	1:A:985:GLN:HE21	1.72	0.55
1:B:436:SER:OG	1:B:438:ASN:OD1	2.24	0.55
1:B:1116:ARG:NH1	1:B:1145:CYS:SG	2.79	0.55
1:B:1068:LEU:O	1:B:1285:GLN:NE2	2.40	0.55
1:A:436:SER:OG	1:A:438:ASN:OD1	2.24	0.55
1:A:2300:VAL:HA	1:A:2331:VAL:HG23	1.89	0.54
1:B:1530:ARG:O	1:B:1533:GLN:NE2	2.39	0.54
1:A:1617:THR:HB	1:A:1676:VAL:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:ILE:HG13	1:B:778:PRO:HG3	1.89	0.54
1:B:982:PHE:HA	1:B:985:GLN:HE21	1.72	0.54
1:B:2300:VAL:HA	1:B:2331:VAL:HG23	1.89	0.54
1:A:32:ARG:O	1:A:34:CYS:N	2.37	0.54
1:A:1906:LEU:HB2	1:A:1922:TYR:HB2	1.90	0.54
1:A:2032:ILE:HG22	1:A:2115:VAL:HG22	1.90	0.54
1:B:1617:THR:HB	1:B:1676:VAL:HA	1.89	0.54
1:B:2032:ILE:HG22	1:B:2115:VAL:HG22	1.90	0.54
1:A:99:GLN:OE1	1:A:126:TYR:OH	2.25	0.53
1:A:1116:ARG:NH1	1:A:1146:PRO:O	2.34	0.53
1:B:1253:SER:HA	1:B:1284:PRO:HD3	1.91	0.53
1:B:1543:CYS:O	1:B:1569:GLN:NE2	2.42	0.53
1:A:1543:CYS:O	1:A:1569:GLN:NE2	2.42	0.53
1:B:1879:LEU:HB2	1:B:1917:PHE:HB2	1.90	0.53
1:A:1879:LEU:HB2	1:A:1917:PHE:HB2	1.90	0.53
1:A:926:GLU:O	1:A:930:LEU:N	2.42	0.52
1:A:1116:ARG:NH1	1:A:1145:CYS:SG	2.79	0.52
1:A:1068:LEU:O	1:A:1285:GLN:NE2	2.40	0.52
1:B:1906:LEU:HB2	1:B:1922:TYR:HB2	1.90	0.52
1:A:368:ARG:NH1	1:A:618:PRO:O	2.42	0.52
1:A:1253:SER:HA	1:A:1284:PRO:HD3	1.91	0.52
1:A:1758:LEU:HB2	1:A:1878:TRP:HD1	1.75	0.52
1:B:2339:VAL:HG21	1:B:2436:LEU:HD22	1.92	0.52
1:A:1344:ILE:HD13	1:A:1375:ILE:HG12	1.92	0.52
1:A:278:ARG:HD2	1:A:453:LEU:HD21	1.92	0.52
1:B:278:ARG:HD2	1:B:453:LEU:HD21	1.92	0.52
1:B:895:LEU:HA	1:B:915:PRO:HB3	1.92	0.52
1:A:1332:GLN:NE2	1:A:1343:SER:OG	2.43	0.51
1:A:2339:VAL:HG21	1:A:2436:LEU:HD22	1.92	0.51
1:A:1742:VAL:HG11	1:A:1799:ILE:HG21	1.92	0.51
1:A:1960:LYS:HE2	1:B:149:TYR:HB3	1.91	0.51
1:B:368:ARG:NH1	1:B:618:PRO:O	2.42	0.51
1:A:2428:ARG:NH2	1:A:2550:GLU:O	2.44	0.51
1:B:1332:GLN:NE2	1:B:1343:SER:OG	2.43	0.51
1:B:2428:ARG:NH2	1:B:2550:GLU:O	2.44	0.51
1:B:1879:LEU:O	1:B:1917:PHE:N	2.44	0.51
1:B:1027:TYR:OH	1:B:1041:GLN:OE1	2.29	0.51
1:B:1344:ILE:HD13	1:B:1375:ILE:HG12	1.92	0.51
1:A:1595:ASP:OD1	1:A:1602:GLN:NE2	2.38	0.51
1:A:2386:ARG:O	1:A:2519:ARG:NH1	2.43	0.51
1:B:1742:VAL:HG11	1:B:1799:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1758:LEU:HB2	1:B:1878:TRP:HD1	1.75	0.51
1:A:149:TYR:HB3	1:B:1960:LYS:HE2	1.92	0.50
1:B:1197:GLU:HG2	1:B:1199:PRO:HA	1.93	0.50
1:A:762:GLN:HA	1:A:888:THR:HG21	1.93	0.50
1:A:895:LEU:HA	1:A:915:PRO:HB3	1.92	0.50
1:B:659:PRO:O	1:B:664:LYS:NZ	2.44	0.50
1:B:2386:ARG:O	1:B:2519:ARG:NH1	2.43	0.50
1:B:762:GLN:HA	1:B:888:THR:HG21	1.93	0.50
1:B:1595:ASP:OD1	1:B:1602:GLN:NE2	2.38	0.50
1:B:180:PRO:HD2	1:B:207:LEU:HD23	1.94	0.50
1:B:926:GLU:O	1:B:930:LEU:N	2.42	0.50
1:A:147:GLU:OE2	1:A:152:ARG:NH1	2.41	0.50
1:A:1027:TYR:OH	1:A:1041:GLN:OE1	2.28	0.50
1:B:1244:GLN:NE2	1:B:1262:LEU:O	2.45	0.50
1:B:970:LEU:HD12	1:B:979:ARG:HH22	1.76	0.50
1:A:267:LEU:O	1:B:2056:HIS:NE2	2.32	0.50
1:A:180:PRO:HD2	1:A:207:LEU:HD23	1.94	0.50
1:A:1879:LEU:O	1:A:1917:PHE:N	2.44	0.50
1:A:659:PRO:O	1:A:664:LYS:NZ	2.44	0.49
1:A:1197:GLU:HG2	1:A:1199:PRO:HA	1.93	0.49
1:A:1578:LYS:HG2	1:A:1579:VAL:HG23	1.95	0.49
1:A:666:ARG:O	1:A:670:GLN:N	2.43	0.49
1:A:1565:CYS:O	1:A:1569:GLN:N	2.39	0.49
1:A:1762:VAL:HG23	1:A:1763:LYS:HG3	1.93	0.49
1:A:970:LEU:HD12	1:A:979:ARG:HH22	1.76	0.49
1:A:2629:GLN:HA	1:A:2634:LEU:HD13	1.94	0.49
1:B:1578:LYS:HG2	1:B:1579:VAL:HG23	1.95	0.49
1:B:2412:LEU:HB2	1:B:2508:ILE:HG13	1.95	0.49
1:A:1244:GLN:NE2	1:A:1262:LEU:O	2.45	0.49
1:B:1762:VAL:HG23	1:B:1763:LYS:HG3	1.94	0.49
1:B:32:ARG:HH22	1:B:241:GLN:HE21	1.61	0.49
1:B:131:CYS:HB3	1:B:138:CYS:HA	1.95	0.49
1:B:147:GLU:OE2	1:B:152:ARG:NH1	2.41	0.49
1:B:1409:GLN:HE22	1:B:1418:PRO:HG3	1.77	0.49
1:A:1352:VAL:HG12	1:A:1366:VAL:HG22	1.94	0.49
1:A:2412:LEU:HB2	1:A:2508:ILE:HG13	1.95	0.49
1:A:1385:ASP:OD1	1:B:369:GLN:NE2	2.45	0.49
1:B:318:SER:OG	1:B:326:GLN:OE1	2.28	0.48
1:A:32:ARG:HH22	1:A:241:GLN:HE21	1.60	0.48
1:A:1573:LYS:HG3	1:A:1574:VAL:HG23	1.95	0.48
1:A:318:SER:OG	1:A:326:GLN:OE1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:ARG:NH1	1:A:1532:SER:O	2.46	0.48
1:A:652:ARG:NH2	1:B:635:GLU:OE1	2.46	0.48
1:B:1333:ILE:HB	1:B:1344:ILE:HB	1.96	0.48
1:A:1965:TYR:O	1:B:169:ARG:NH1	2.47	0.48
1:B:2266:GLN:O	1:B:2269:THR:OG1	2.30	0.48
1:A:1316:THR:H	1:B:104:LEU:HD21	1.79	0.48
1:A:1409:GLN:HE22	1:A:1418:PRO:HG3	1.77	0.48
1:B:1352:VAL:HG12	1:B:1366:VAL:HG22	1.94	0.48
1:A:131:CYS:HB3	1:A:138:CYS:HA	1.95	0.48
1:A:893:PHE:H	1:A:896:ARG:HE	1.62	0.48
1:B:2629:GLN:HA	1:B:2634:LEU:HD13	1.94	0.48
1:B:2013:ASN:HD22	1:B:2016:GLN:HE22	1.62	0.47
1:A:2312:GLU:HG3	1:A:2314:TRP:H	1.78	0.47
1:B:1530:ARG:NH1	1:B:1532:SER:O	2.46	0.47
1:B:1573:LYS:HG3	1:B:1574:VAL:HG23	1.95	0.47
1:A:1293:GLN:HG2	1:A:1367:THR:HG22	1.96	0.47
1:B:666:ARG:O	1:B:670:GLN:N	2.43	0.47
1:B:893:PHE:H	1:B:896:ARG:HE	1.62	0.47
1:A:270:THR:HG23	1:A:272:THR:H	1.80	0.47
1:A:1333:ILE:HB	1:A:1344:ILE:HB	1.96	0.47
1:A:2721:TYR:HE1	1:B:2559:ALA:HA	1.78	0.47
1:B:479:ASN:HD22	1:B:484:ASN:HB2	1.80	0.47
1:B:869:LEU:O	1:B:873:ASN:ND2	2.48	0.47
1:B:1298:LEU:HD22	1:B:1300:LEU:HD23	1.96	0.47
1:B:1565:CYS:O	1:B:1569:GLN:N	2.39	0.47
1:B:2312:GLU:HG3	1:B:2314:TRP:H	1.78	0.47
1:A:283:ARG:NH2	1:A:473:GLY:O	2.48	0.47
1:A:869:LEU:O	1:A:873:ASN:ND2	2.48	0.47
1:B:283:ARG:NH2	1:B:473:GLY:O	2.48	0.47
1:A:2559:ALA:HA	1:B:2721:TYR:HE1	1.79	0.47
1:A:2141:LEU:HD23	1:A:2186:LYS:HD2	1.97	0.46
1:B:270:THR:HG23	1:B:272:THR:H	1.79	0.46
1:B:1293:GLN:HG2	1:B:1367:THR:HG22	1.96	0.46
1:A:635:GLU:OE1	1:B:652:ARG:NH2	2.48	0.46
1:A:2013:ASN:HD22	1:A:2016:GLN:HE22	1.62	0.46
1:A:1298:LEU:HD22	1:A:1300:LEU:HD23	1.96	0.46
1:B:1297:GLN:N	1:B:1421:THR:OG1	2.46	0.46
1:B:2141:LEU:HD23	1:B:2186:LYS:HD2	1.97	0.46
1:A:149:TYR:O	1:A:170:ARG:NH1	2.49	0.46
1:A:951:PHE:HB2	1:B:953:LEU:HD21	1.97	0.46
1:A:953:LEU:HD21	1:B:951:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HB3	1:A:580:PHE:HD1	1.80	0.46
1:A:479:ASN:HD22	1:A:484:ASN:HB2	1.80	0.46
1:B:421:LEU:HB3	1:B:580:PHE:HD1	1.80	0.46
1:A:369:GLN:NE2	1:B:1385:ASP:OD1	2.47	0.46
1:A:1318:GLN:HG2	1:A:1353:GLN:HA	1.98	0.46
1:A:449:PRO:HD2	1:A:453:LEU:HD22	1.97	0.45
1:A:2303:HIS:ND1	1:A:2385:ASP:OD2	2.39	0.45
1:A:2388:GLY:HA2	1:A:2391:VAL:HG22	1.99	0.45
1:B:1331:CYS:HB3	1:B:1347:CYS:HB2	1.87	0.45
1:B:2040:GLY:O	1:B:2044:ARG:NH2	2.49	0.45
1:A:104:LEU:HD21	1:B:1316:THR:H	1.81	0.45
1:A:169:ARG:NH1	1:B:1965:TYR:O	2.50	0.45
1:A:1297:GLN:N	1:A:1421:THR:OG1	2.46	0.45
1:A:423:ARG:HB2	1:B:2691:ARG:HH22	1.80	0.45
1:A:2040:GLY:O	1:A:2044:ARG:NH2	2.49	0.45
1:B:149:TYR:O	1:B:170:ARG:NH1	2.49	0.45
1:A:1719:ASP:HA	1:A:1722:LEU:HB2	1.99	0.45
1:B:449:PRO:HD2	1:B:453:LEU:HD22	1.97	0.45
1:B:1719:ASP:HA	1:B:1722:LEU:HB2	1.99	0.45
1:A:946:SER:HA	1:B:953:LEU:HD13	1.98	0.45
1:A:2511:SER:HA	1:A:2613:ALA:HB3	1.98	0.45
1:B:364:CYS:O	1:B:368:ARG:N	2.48	0.45
1:B:2511:SER:HA	1:B:2613:ALA:HB3	1.98	0.45
1:B:1465:GLY:H	1:B:1482:GLN:HB3	1.83	0.44
1:A:305:ARG:HA	1:A:317:PRO:HD2	2.00	0.44
1:A:751:MET:HG3	1:A:752:LEU:H	1.83	0.44
1:A:1408:PHE:HD2	1:A:1419:ALA:HB3	1.82	0.44
1:A:2419:SER:HA	1:A:2420:PRO:HD3	1.86	0.44
1:B:2034:MET:HB2	1:B:2046:LEU:HD13	2.00	0.44
1:B:2141:LEU:HD11	1:B:2294:PRO:HG2	2.00	0.44
1:A:2568:HIS:NE2	1:A:2571:ASP:OD1	2.51	0.44
1:B:1136:ARG:HD3	1:B:1137:PRO:HD2	1.99	0.44
1:B:2504:VAL:HG13	1:B:2600:TRP:HZ2	1.82	0.44
1:A:1074:PRO:HD3	1:A:2099:SER:HB2	1.99	0.44
1:A:1594:PRO:HD2	1:A:1625:ILE:HG13	1.99	0.44
1:B:705:CYS:HB2	1:B:726:CYS:HB2	1.93	0.44
1:B:1318:GLN:HG2	1:B:1353:GLN:HA	1.98	0.44
1:B:2388:GLY:HA2	1:B:2391:VAL:HG22	1.99	0.44
1:A:325:TYR:HD1	1:A:329:GLN:HE22	1.66	0.44
1:A:1136:ARG:HD3	1:A:1137:PRO:HD2	1.99	0.44
1:B:325:TYR:HD1	1:B:329:GLN:HE22	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1770:GLU:OE2	1:A:1774:ASN:N	2.44	0.44
1:B:751:MET:HG3	1:B:752:LEU:H	1.83	0.44
1:B:1116:ARG:NE	1:B:1126:CYS:SG	2.77	0.44
1:B:1594:PRO:HD2	1:B:1625:ILE:HG13	1.99	0.44
1:A:2280:ASP:OD1	1:A:2280:ASP:N	2.51	0.43
1:B:2385:ASP:OD1	1:B:2385:ASP:N	2.46	0.43
1:A:2034:MET:HB2	1:A:2046:LEU:HD13	2.00	0.43
1:A:2397:LEU:HD11	1:A:2417:ALA:HB1	1.99	0.43
1:B:1408:PHE:HD2	1:B:1419:ALA:HB3	1.82	0.43
1:B:1831:GLU:H	1:B:1837:LYS:HE3	1.82	0.43
1:A:1787:HIS:CE1	1:A:1790:ILE:HB	2.53	0.43
1:B:1074:PRO:HD3	1:B:2099:SER:HB2	1.99	0.43
1:A:500:PHE:HE1	1:A:550:GLY:HA2	1.83	0.43
1:A:1135:LEU:HB2	1:A:1151:VAL:HG21	2.00	0.43
1:A:1244:GLN:HE22	1:A:1263:ILE:HG13	1.82	0.43
1:A:1831:GLU:H	1:A:1837:LYS:HE3	1.83	0.43
1:B:973:PRO:HB2	1:B:976:PHE:HB2	2.01	0.43
1:B:1135:LEU:HB2	1:B:1151:VAL:HG21	2.00	0.43
1:B:1528:GLN:NE2	1:B:1529:TYR:O	2.51	0.43
1:B:2397:LEU:HD11	1:B:2417:ALA:HB1	1.99	0.43
1:B:2568:HIS:NE2	1:B:2571:ASP:OD1	2.51	0.43
1:A:789:GLU:O	1:A:794:GLY:N	2.52	0.43
1:A:425:MET:SD	1:A:425:MET:N	2.92	0.43
1:A:2008:GLY:HA3	1:A:2064:GLN:HA	2.01	0.43
1:B:305:ARG:HA	1:B:317:PRO:HD2	2.00	0.43
1:B:1433:SER:OG	1:B:1435:ARG:NH1	2.45	0.43
1:A:2691:ARG:HH22	1:B:423:ARG:HB2	1.83	0.43
1:B:425:MET:SD	1:B:425:MET:N	2.92	0.43
1:B:1513:ASP:HA	1:B:1516:ARG:HB2	2.00	0.43
1:B:1619:SER:HA	1:B:1674:PRO:HB3	2.00	0.43
1:A:364:CYS:O	1:A:368:ARG:N	2.48	0.43
1:A:1465:GLY:H	1:A:1482:GLN:HB3	1.83	0.43
1:A:1528:GLN:NE2	1:A:1529:TYR:O	2.51	0.43
1:B:1134:GLU:OE2	1:B:1136:ARG:NH1	2.52	0.43
1:B:1880:PHE:HA	1:B:1916:TYR:HA	2.01	0.43
1:A:2504:VAL:HG13	1:A:2600:TRP:HZ2	1.82	0.42
1:B:500:PHE:HE1	1:B:550:GLY:HA2	1.83	0.42
1:B:751:MET:H	1:B:805:LYS:HE2	1.84	0.42
1:B:1181:CYS:HB3	1:B:1188:CYS:HA	2.01	0.42
1:B:1787:HIS:CE1	1:B:1790:ILE:HB	2.54	0.42
1:A:973:PRO:HB2	1:A:976:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1388:ARG:HA	1:A:1391:VAL:HG22	2.01	0.42
1:A:1513:ASP:HA	1:A:1516:ARG:HB2	2.00	0.42
1:B:503:GLN:HG3	1:B:504:LEU:HD12	2.01	0.42
1:B:2286:VAL:HB	1:B:2331:VAL:HG12	2.01	0.42
1:A:953:LEU:HD13	1:B:946:SER:HA	2.01	0.42
1:A:2490:GLU:HB3	1:A:2495:ALA:HB2	2.00	0.42
1:B:2490:GLU:HB3	1:B:2495:ALA:HB2	2.00	0.42
1:A:559:GLN:HE21	1:A:563:ASN:HD21	1.67	0.42
1:A:2085:THR:OG1	1:A:2086:GLU:OE1	2.32	0.42
1:A:2141:LEU:HD11	1:A:2294:PRO:HG2	2.00	0.42
1:B:1380:LEU:HD22	1:B:1385:ASP:HB3	2.01	0.42
1:B:2008:GLY:HA3	1:B:2064:GLN:HA	2.01	0.42
1:B:2030:LEU:HB3	1:B:2033:GLN:HE21	1.83	0.42
1:A:751:MET:H	1:A:805:LYS:HE2	1.84	0.42
1:A:2030:LEU:HB3	1:A:2033:GLN:HE21	1.83	0.42
1:A:169:ARG:NH2	1:B:1997:GLU:OE2	2.53	0.42
1:A:503:GLN:HG3	1:A:504:LEU:HD12	2.01	0.42
1:A:1286:LEU:HA	1:A:1457:LEU:HA	2.02	0.42
1:A:2302:PHE:HA	1:A:2333:ALA:HB3	2.02	0.42
1:B:1838:ASP:HB2	1:B:1883:LEU:HD13	2.02	0.42
1:B:2400:ARG:NH2	1:B:2404:SER:O	2.42	0.42
1:A:1619:SER:HA	1:A:1674:PRO:HB3	2.00	0.42
1:B:383:PHE:O	1:B:386:HIS:N	2.49	0.42
1:B:1244:GLN:HE22	1:B:1263:ILE:HG13	1.83	0.42
1:B:2302:PHE:HA	1:B:2333:ALA:HB3	2.02	0.42
1:A:2057:THR:HG21	1:B:212:ASN:HA	2.01	0.42
1:B:713:ILE:HA	1:B:714:PRO:HD3	1.91	0.42
1:B:2303:HIS:ND1	1:B:2385:ASP:OD2	2.39	0.42
1:A:383:PHE:O	1:A:386:HIS:N	2.49	0.42
1:B:749:SER:O	1:B:805:LYS:NZ	2.53	0.42
1:B:789:GLU:O	1:B:794:GLY:N	2.52	0.42
1:B:1770:GLU:OE2	1:B:1774:ASN:N	2.44	0.42
1:B:2386:ARG:NH1	1:B:2511:SER:OG	2.53	0.42
1:A:1380:LEU:HD22	1:A:1385:ASP:HB3	2.02	0.42
1:B:1283:ARG:HA	1:B:1284:PRO:HD3	1.93	0.42
1:A:2400:ARG:NH2	1:A:2404:SER:O	2.42	0.41
1:B:31:LEU:HD12	1:B:243:ARG:HH22	1.85	0.41
1:A:1134:GLU:OE2	1:A:1136:ARG:NH1	2.52	0.41
1:A:1997:GLU:OE2	1:B:169:ARG:NH2	2.52	0.41
1:B:47:ASP:OD2	1:B:64:GLN:NE2	2.53	0.41
1:A:1880:PHE:HA	1:A:1916:TYR:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2286:VAL:HB	1:A:2331:VAL:HG12	2.01	0.41
1:B:1396:LEU:HD21	1:B:1435:ARG:HH22	1.85	0.41
1:A:705:CYS:HB2	1:A:726:CYS:HB2	1.93	0.41
1:A:1181:CYS:HB3	1:A:1188:CYS:HA	2.01	0.41
1:A:2689:VAL:HG12	1:B:579:LEU:HD23	2.01	0.41
1:B:275:THR:HG22	1:B:278:ARG:HH21	1.85	0.41
1:B:2665:SER:OG	1:B:2670:TYR:O	2.32	0.41
1:A:749:SER:O	1:A:805:LYS:NZ	2.53	0.41
1:A:1021:LEU:HB3	1:A:1022:LEU:H	1.56	0.41
1:A:2104:ASP:N	1:A:2176:LEU:O	2.48	0.41
1:A:579:LEU:HD23	1:B:2689:VAL:HG12	2.02	0.41
1:A:1396:LEU:HD21	1:A:1435:ARG:HH22	1.85	0.41
1:B:1388:ARG:HA	1:B:1391:VAL:HG22	2.01	0.41
1:B:2416:SER:OG	1:B:2417:ALA:N	2.54	0.41
1:A:1691:ARG:NE	1:A:1693:GLU:OE2	2.53	0.41
1:A:1838:ASP:HB2	1:A:1883:LEU:HD13	2.02	0.41
1:B:1691:ARG:NE	1:B:1693:GLU:OE2	2.53	0.41
1:A:1201:THR:O	1:A:1202:ARG:NE	2.54	0.41
1:B:96:CYS:HA	1:B:126:TYR:HE1	1.85	0.41
1:B:1042:CYS:HA	1:B:1049:CYS:HA	2.02	0.41
1:A:1697:PHE:HA	1:A:1761:ASN:HA	2.02	0.41
1:B:409:PRO:HB2	1:B:412:ILE:HD12	2.03	0.41
1:B:559:GLN:HE21	1:B:563:ASN:HD21	1.67	0.41
1:A:2491:PRO:HA	1:A:2492:PRO:HD3	1.89	0.41
1:B:559:GLN:O	1:B:563:ASN:ND2	2.54	0.41
1:B:1286:LEU:HA	1:B:1457:LEU:HA	2.02	0.41
1:B:1697:PHE:HA	1:B:1761:ASN:HA	2.02	0.41
1:B:2280:ASP:N	1:B:2280:ASP:OD1	2.51	0.41
1:A:31:LEU:HD12	1:A:243:ARG:HH22	1.85	0.40
1:A:275:THR:HG22	1:A:278:ARG:HH21	1.85	0.40
1:A:420:GLY:O	1:B:2691:ARG:NH2	2.46	0.40
1:A:1393:LYS:HA	1:A:1397:GLY:HA3	2.03	0.40
1:A:2298:VAL:HG21	1:A:2370:ILE:HG12	2.03	0.40
1:B:1201:THR:O	1:B:1202:ARG:NE	2.54	0.40
1:B:2245:ALA:HB3	1:B:2247:GLU:HG3	2.04	0.40
1:B:1517:ASN:HD22	1:B:1521:LEU:HB2	1.85	0.40
1:A:559:GLN:O	1:A:563:ASN:ND2	2.54	0.40
1:A:2047:ASP:N	1:A:2047:ASP:OD1	2.55	0.40
1:A:2266:GLN:O	1:A:2269:THR:OG1	2.30	0.40
1:B:2419:SER:HA	1:B:2420:PRO:HD3	1.86	0.40
1:A:1042:CYS:HA	1:A:1049:CYS:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1672:ASP:HB3	1:A:1674:PRO:HD2	2.03	0.40
1:A:2245:ALA:HB3	1:A:2247:GLU:HG3	2.04	0.40
1:B:2047:ASP:N	1:B:2047:ASP:OD1	2.55	0.40
1:A:96:CYS:HA	1:A:126:TYR:HE1	1.85	0.40
1:A:1517:ASN:HD22	1:A:1521:LEU:HB2	1.85	0.40
1:A:2029:SER:HB2	1:A:2079:VAL:HG11	2.03	0.40
1:A:2416:SER:OG	1:A:2417:ALA:N	2.54	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	2529/2768 (91%)	2189 (87%)	338 (13%)	2 (0%)	51 83
1	B	2529/2768 (91%)	2190 (87%)	337 (13%)	2 (0%)	51 83
All	All	5058/5536 (91%)	4379 (87%)	675 (13%)	4 (0%)	54 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	862	PRO
1	B	862	PRO
1	A	861	ARG
1	B	861	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2164/2360 (92%)	2152 (99%)	12 (1%)	86 94
1	B	2164/2360 (92%)	2152 (99%)	12 (1%)	86 94
All	All	4328/4720 (92%)	4304 (99%)	24 (1%)	86 94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	807	MET
1	A	1007	ARG
1	A	1170	ARG
1	A	1179	VAL
1	A	1181	CYS
1	A	1250	ARG
1	A	1526	ASN
1	A	1536	ARG
1	A	1607	CYS
1	A	1730	ARG
1	A	2408	ARG
1	A	2463	ASN
1	B	807	MET
1	B	1007	ARG
1	B	1170	ARG
1	B	1179	VAL
1	B	1181	CYS
1	B	1250	ARG
1	B	1526	ASN
1	B	1536	ARG
1	B	1607	CYS
1	B	1730	ARG
1	B	2408	ARG
1	B	2463	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	241	GLN
1	A	331	GLN

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Mol	Chain	Res	Type
1	A	479	ASN
1	A	563	ASN
1	A	878	GLN
1	A	892	HIS
1	A	985	GLN
1	A	1072	GLN
1	A	1091	GLN
1	A	1244	GLN
1	A	1288	GLN
1	A	1295	HIS
1	A	1332	GLN
1	A	1509	HIS
1	A	1522	GLN
1	A	1526	ASN
1	A	1741	GLN
1	A	1787	HIS
1	A	2016	GLN
1	A	2033	GLN
1	A	2463	ASN
1	A	2466	GLN
1	A	2629	GLN
1	A	2669	ASN
1	B	168	ASN
1	B	241	GLN
1	B	331	GLN
1	B	479	ASN
1	B	563	ASN
1	B	878	GLN
1	B	892	HIS
1	B	985	GLN
1	B	1072	GLN
1	B	1091	GLN
1	B	1244	GLN
1	B	1288	GLN
1	B	1295	HIS
1	B	1332	GLN
1	B	1509	HIS
1	B	1522	GLN
1	B	1526	ASN
1	B	1741	GLN
1	B	2016	GLN
1	B	2033	GLN

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Mol	Chain	Res	Type
1	B	2463	ASN
1	B	2466	GLN
1	B	2629	GLN
1	B	2669	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.31	0	17,19,21	0.73	1 (5%)
2	NAG	C	2	2	14,14,15	0.27	0	17,19,21	0.38	0
2	BMA	C	3	2	11,11,12	0.26	0	15,15,17	0.53	0
2	NAG	D	1	1,2	14,14,15	0.31	0	17,19,21	0.73	1 (5%)
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.39	0
2	BMA	D	3	2	11,11,12	0.27	0	15,15,17	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	2.55	115.65	112.19
2	C	1	NAG	C1-O5-C5	2.54	115.64	112.19

There are no chirality outliers.

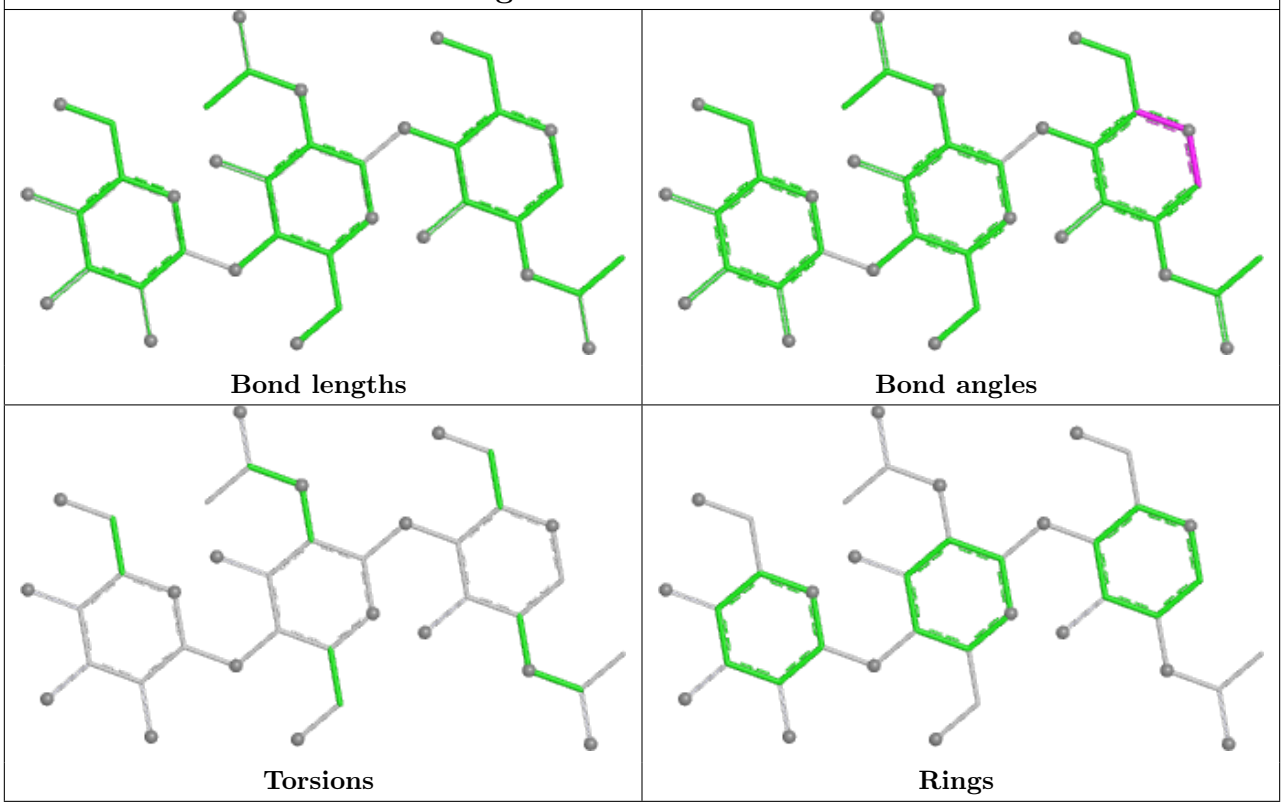
There are no torsion outliers.

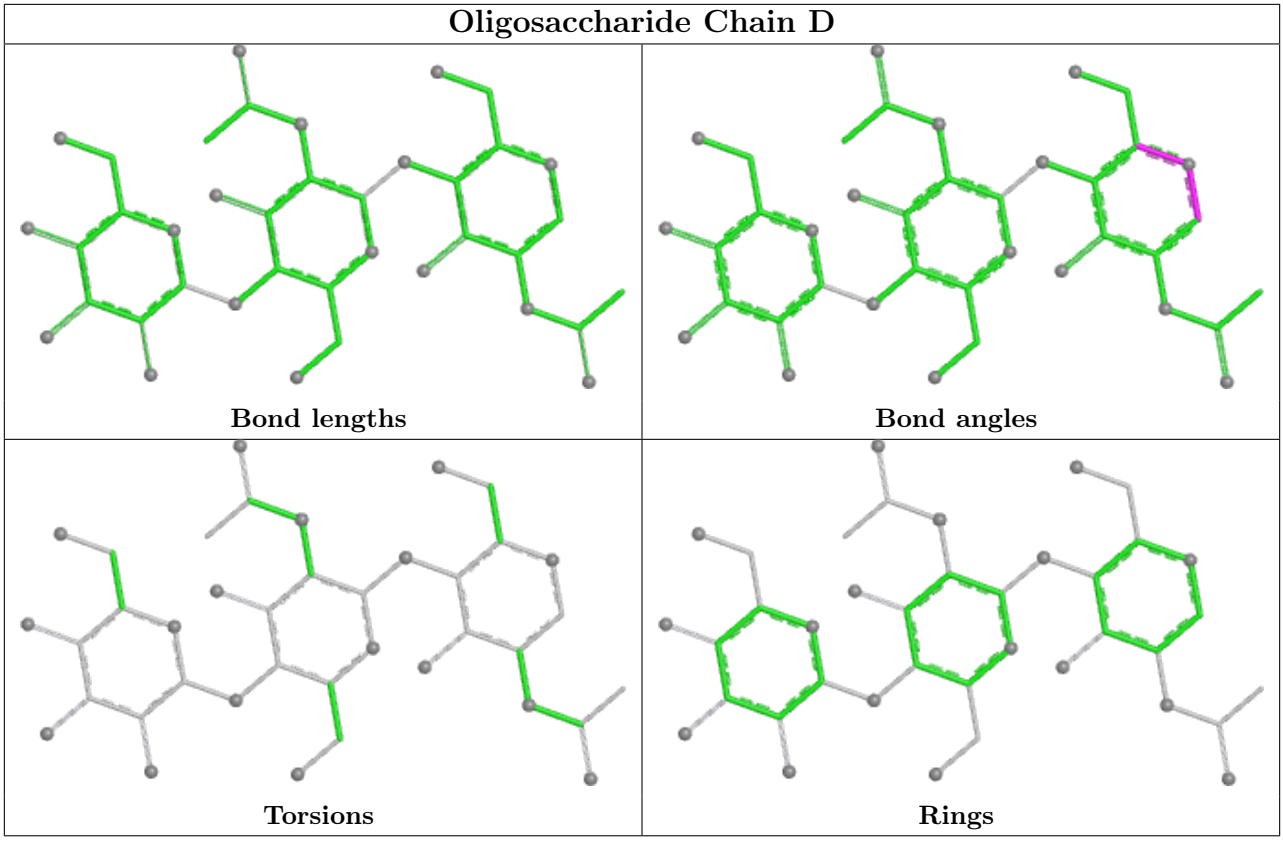
There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain C





5.6 Ligand geometry (i)

30 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	$\#\|Z\| > 2$
3	NAG	A	2809	1	14,14,15	0.25	0	17,19,21	0.52	0
3	NAG	B	2804	1	14,14,15	0.31	0	17,19,21	1.14	2 (11%)
3	NAG	A	2804	1	14,14,15	0.30	0	17,19,21	1.13	2 (11%)
3	NAG	B	2813	1	14,14,15	0.26	0	17,19,21	0.59	0
3	NAG	A	2813	1	14,14,15	0.26	0	17,19,21	0.59	0
3	NAG	A	2805	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	A	2816	1	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	B	2802	1	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
3	NAG	A	2817	1	14,14,15	0.43	0	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	2802	1	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
3	NAG	B	2815	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
3	NAG	B	2809	1	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	A	2815	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
3	NAG	A	2812	1	14,14,15	0.28	0	17,19,21	0.66	1 (5%)
3	NAG	B	2818	1	14,14,15	0.34	0	17,19,21	1.00	1 (5%)
3	NAG	A	2814	1	14,14,15	0.27	0	17,19,21	0.59	0
3	NAG	B	2801	1	14,14,15	0.29	0	17,19,21	0.95	1 (5%)
3	NAG	A	2801	1	14,14,15	0.31	0	17,19,21	0.96	1 (5%)
3	NAG	B	2817	1	14,14,15	0.42	0	17,19,21	0.85	1 (5%)
3	NAG	B	2810	1	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
3	NAG	A	2818	1	14,14,15	0.35	0	17,19,21	1.00	1 (5%)
3	NAG	B	2811	1	14,14,15	0.34	0	17,19,21	0.77	1 (5%)
3	NAG	B	2812	1	14,14,15	0.26	0	17,19,21	0.66	1 (5%)
3	NAG	B	2803	1	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	A	2803	1	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	A	2810	1	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
3	NAG	B	2814	1	14,14,15	0.26	0	17,19,21	0.60	0
3	NAG	A	2811	1	14,14,15	0.34	0	17,19,21	0.76	1 (5%)
3	NAG	B	2816	1	14,14,15	0.27	0	17,19,21	0.52	0
3	NAG	B	2805	1	14,14,15	0.25	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2809	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2804	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2804	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2813	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2813	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2805	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2816	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2802	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2817	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2802	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2815	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	2809	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2815	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2812	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2818	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2814	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2801	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2817	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2810	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2818	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2811	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2812	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2810	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2814	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2811	1	-	1/6/23/26	0/1/1/1
3	NAG	B	2816	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2805	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2815	NAG	C1-O5-C5	3.19	116.52	112.19
3	B	2815	NAG	C1-O5-C5	3.18	116.50	112.19
3	A	2802	NAG	C2-N2-C7	3.07	127.27	122.90
3	B	2802	NAG	C2-N2-C7	3.05	127.24	122.90
3	B	2804	NAG	C2-N2-C7	3.02	127.20	122.90
3	B	2818	NAG	C2-N2-C7	3.01	127.19	122.90
3	A	2801	NAG	C2-N2-C7	3.01	127.19	122.90
3	A	2804	NAG	C2-N2-C7	3.00	127.18	122.90
3	A	2818	NAG	C2-N2-C7	2.99	127.16	122.90
3	B	2801	NAG	C2-N2-C7	2.98	127.14	122.90
3	B	2804	NAG	C1-O5-C5	2.87	116.07	112.19
3	A	2804	NAG	C1-O5-C5	2.86	116.07	112.19
3	B	2817	NAG	C1-O5-C5	2.85	116.05	112.19
3	A	2817	NAG	C1-O5-C5	2.83	116.03	112.19
3	B	2811	NAG	C1-O5-C5	2.60	115.71	112.19
3	A	2811	NAG	C1-O5-C5	2.57	115.68	112.19
3	B	2810	NAG	C1-O5-C5	2.39	115.44	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2810	NAG	C1-O5-C5	2.39	115.43	112.19
3	B	2812	NAG	C1-O5-C5	2.30	115.31	112.19
3	A	2812	NAG	C1-O5-C5	2.30	115.31	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2815	NAG	O5-C5-C6-O6
3	B	2815	NAG	O5-C5-C6-O6
3	A	2811	NAG	O5-C5-C6-O6
3	B	2811	NAG	O5-C5-C6-O6
3	A	2809	NAG	O5-C5-C6-O6
3	B	2809	NAG	O5-C5-C6-O6
3	A	2818	NAG	O5-C5-C6-O6
3	B	2818	NAG	O5-C5-C6-O6
3	A	2810	NAG	O5-C5-C6-O6
3	B	2810	NAG	O5-C5-C6-O6
3	A	2801	NAG	C3-C2-N2-C7
3	A	2804	NAG	C3-C2-N2-C7
3	A	2818	NAG	C3-C2-N2-C7
3	B	2801	NAG	C3-C2-N2-C7
3	B	2804	NAG	C3-C2-N2-C7
3	B	2818	NAG	C3-C2-N2-C7
3	A	2802	NAG	C3-C2-N2-C7
3	B	2802	NAG	C3-C2-N2-C7
3	A	2801	NAG	C1-C2-N2-C7
3	B	2801	NAG	C1-C2-N2-C7

There are no ring outliers.

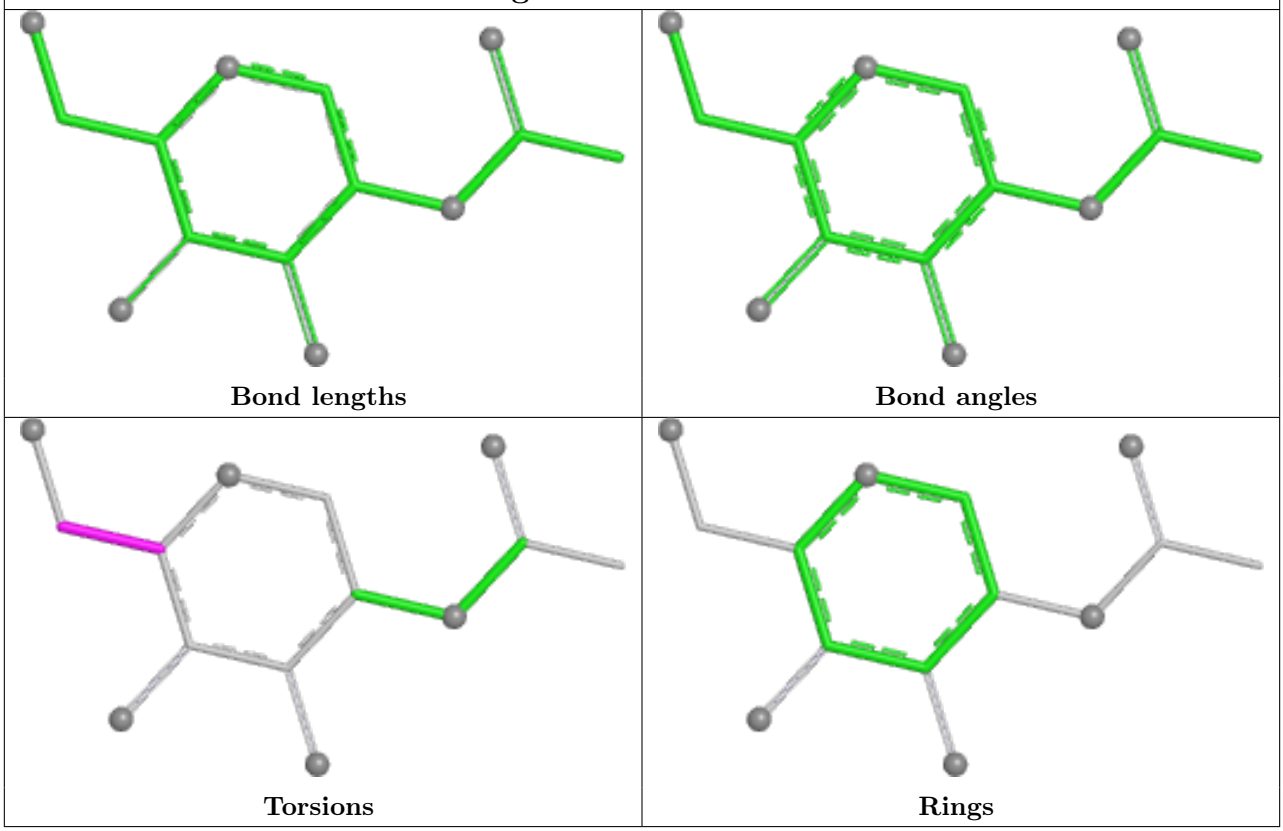
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2805	NAG	1	0
3	B	2805	NAG	1	0

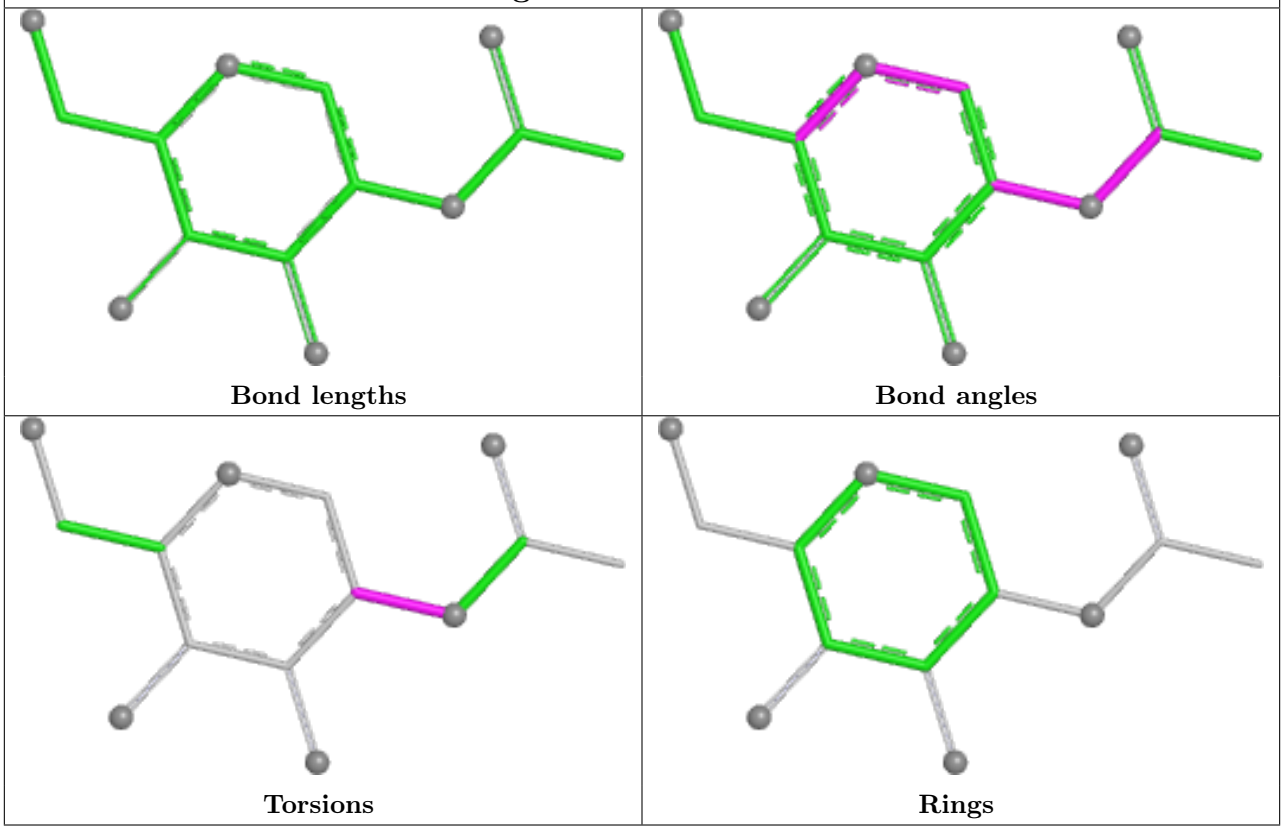
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

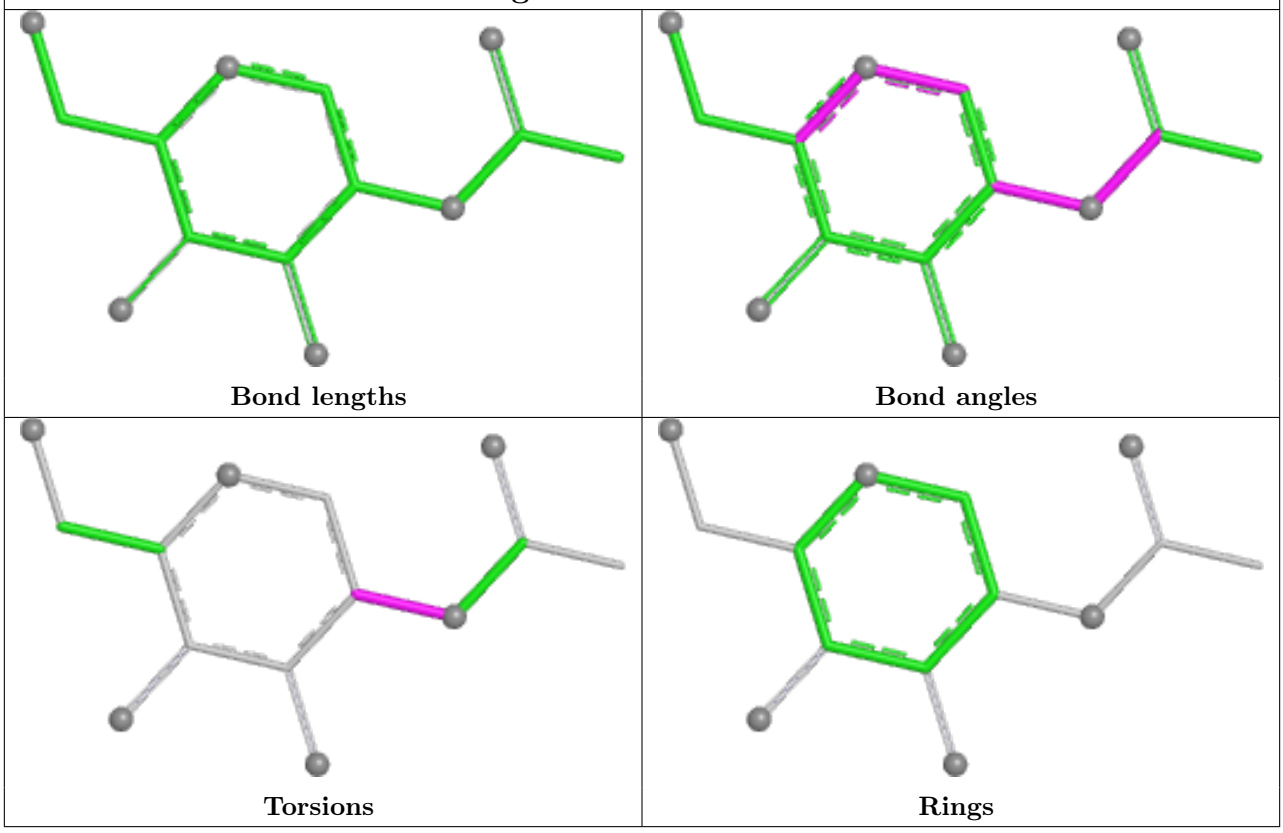
Ligand NAG A 2809



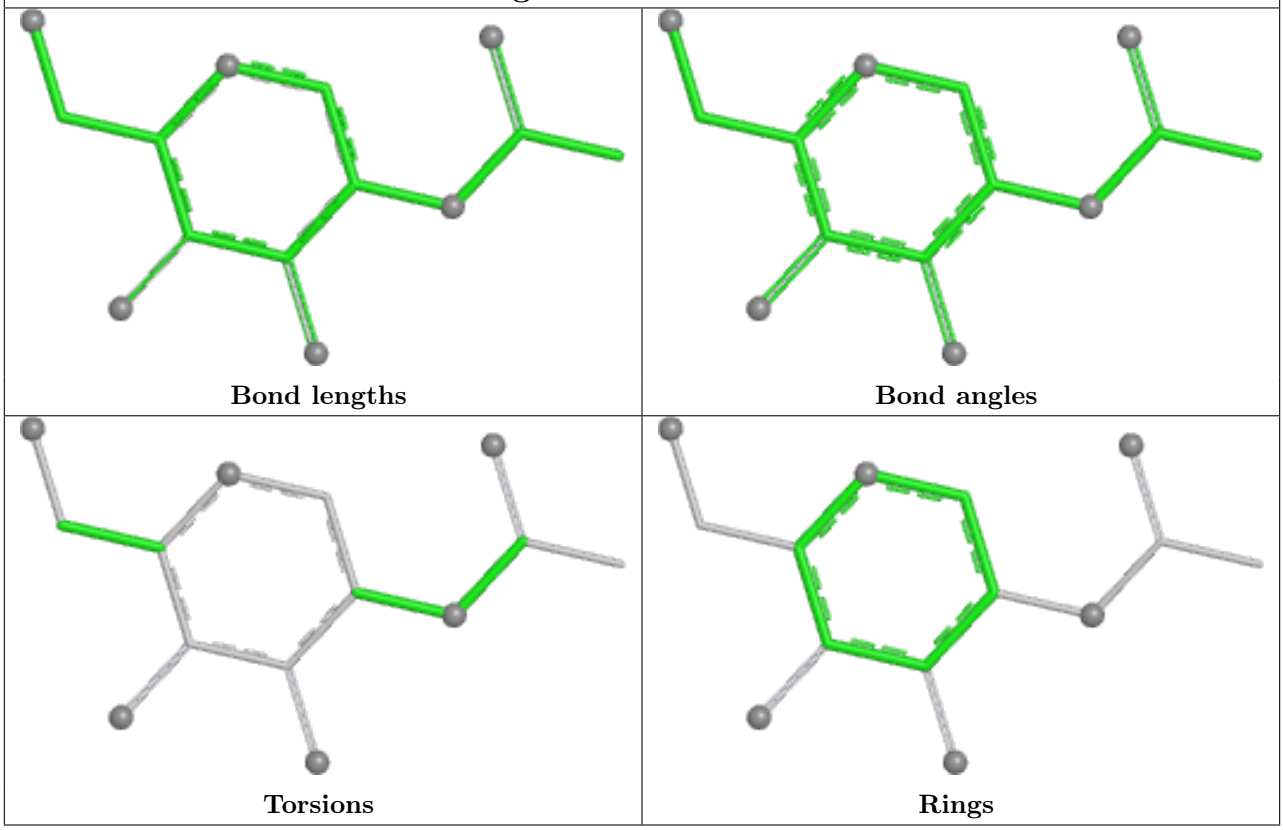
Ligand NAG B 2804



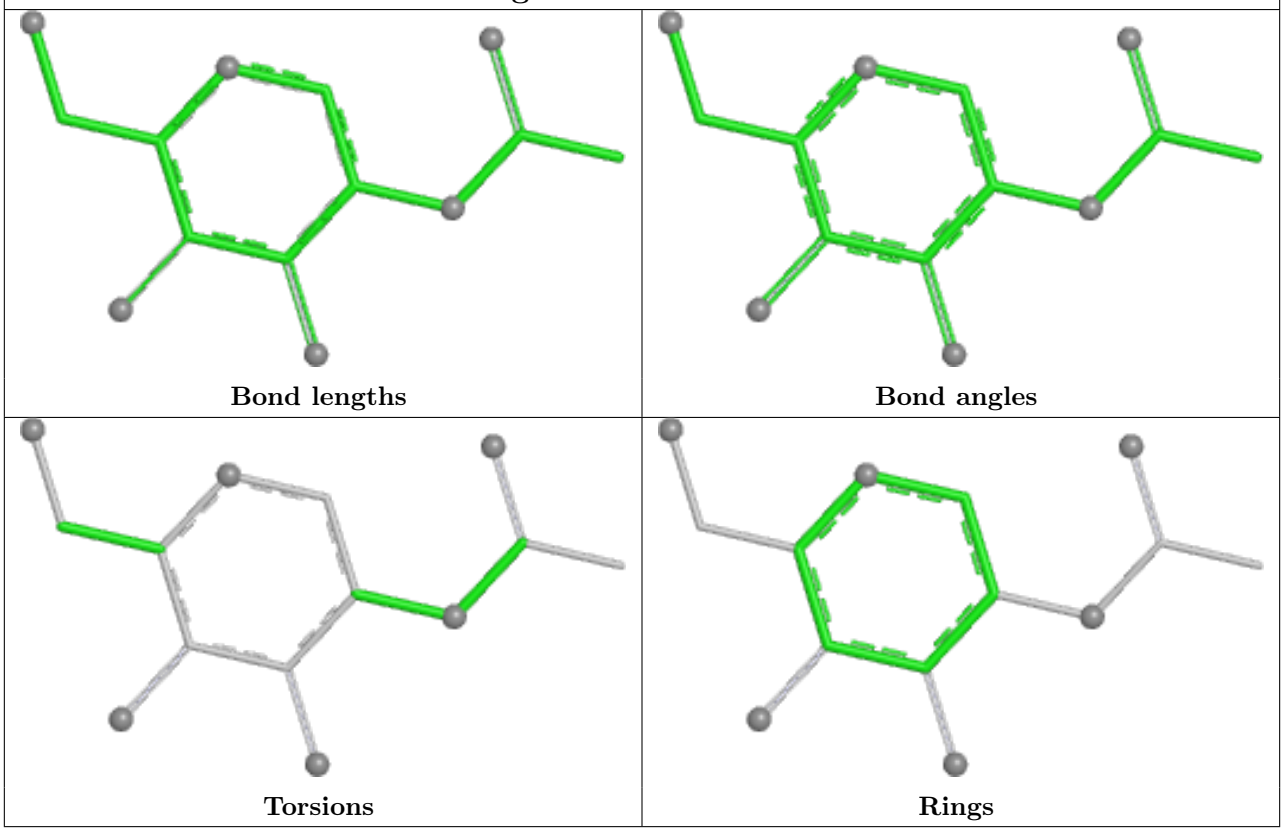
Ligand NAG A 2804



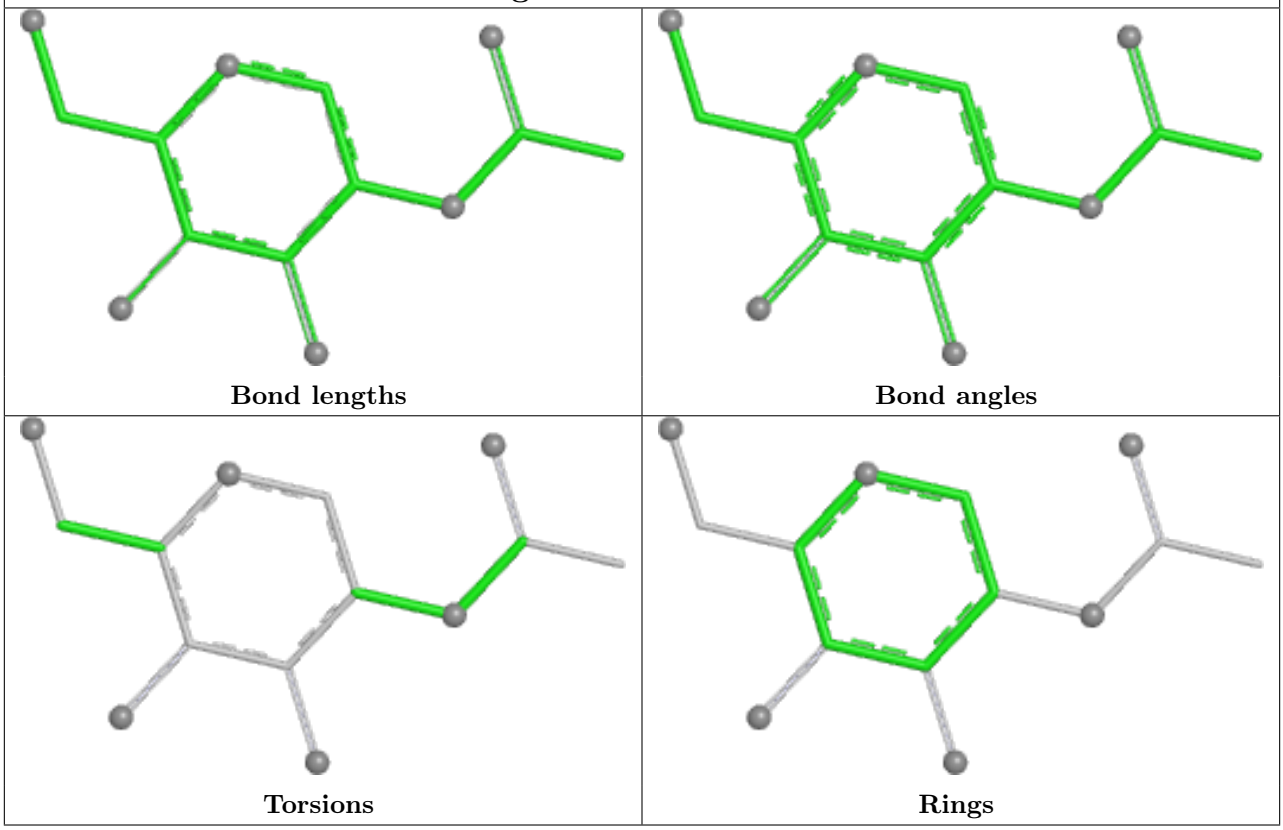
Ligand NAG B 2813



Ligand NAG A 2813



Ligand NAG A 2805



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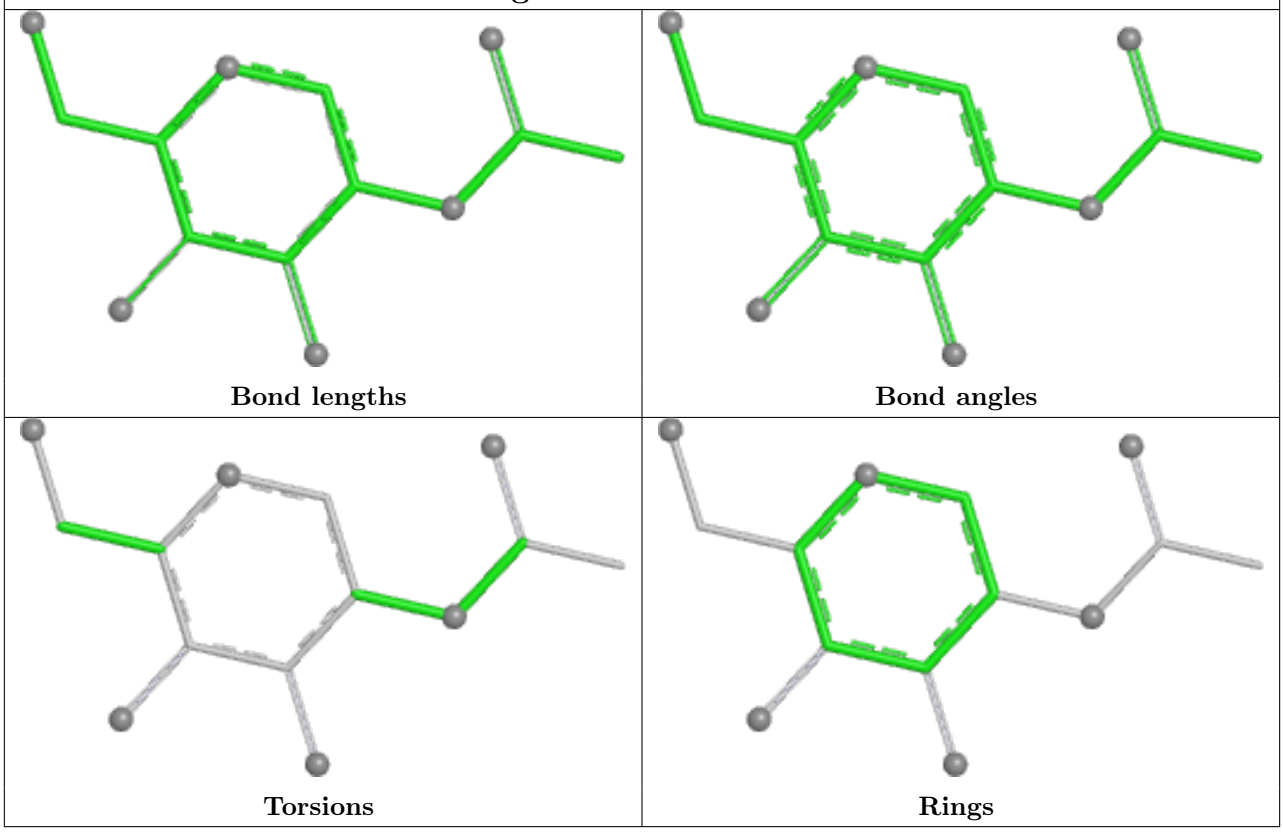
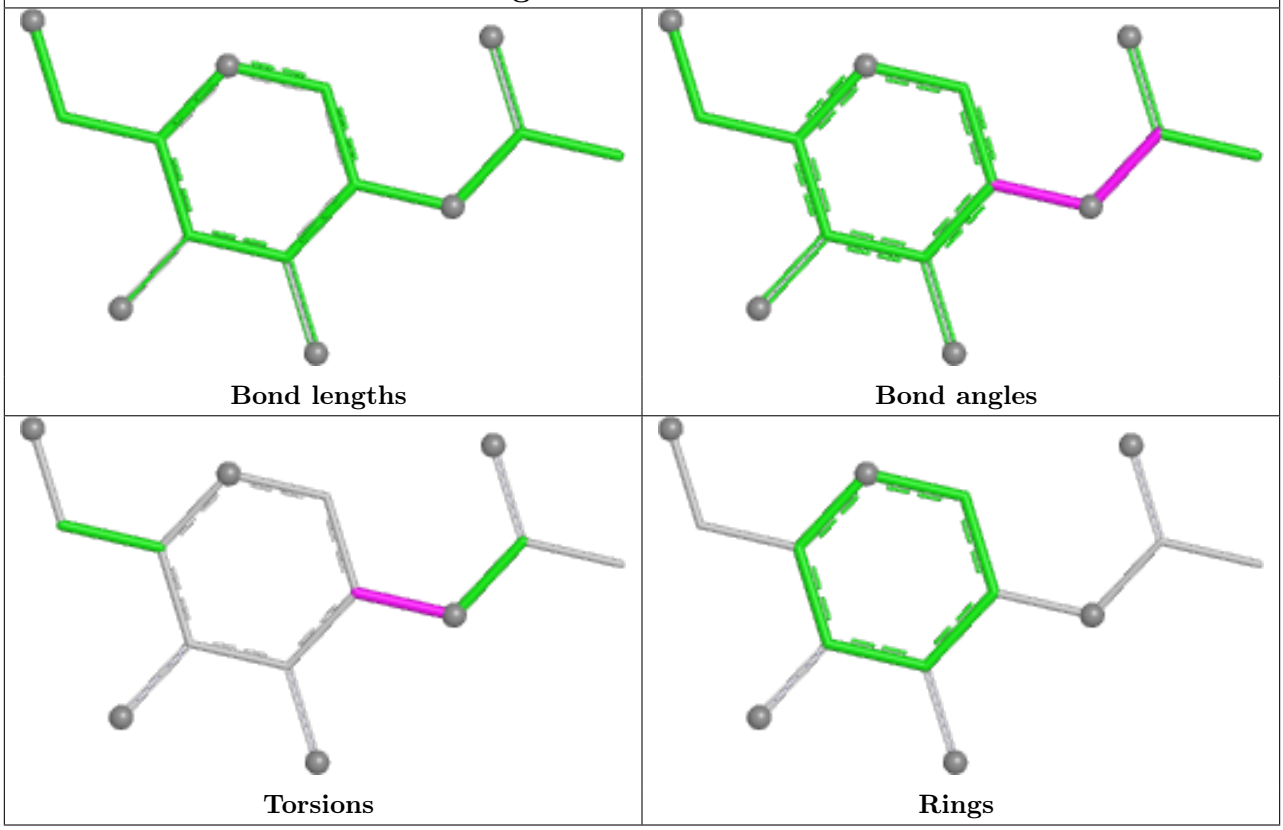
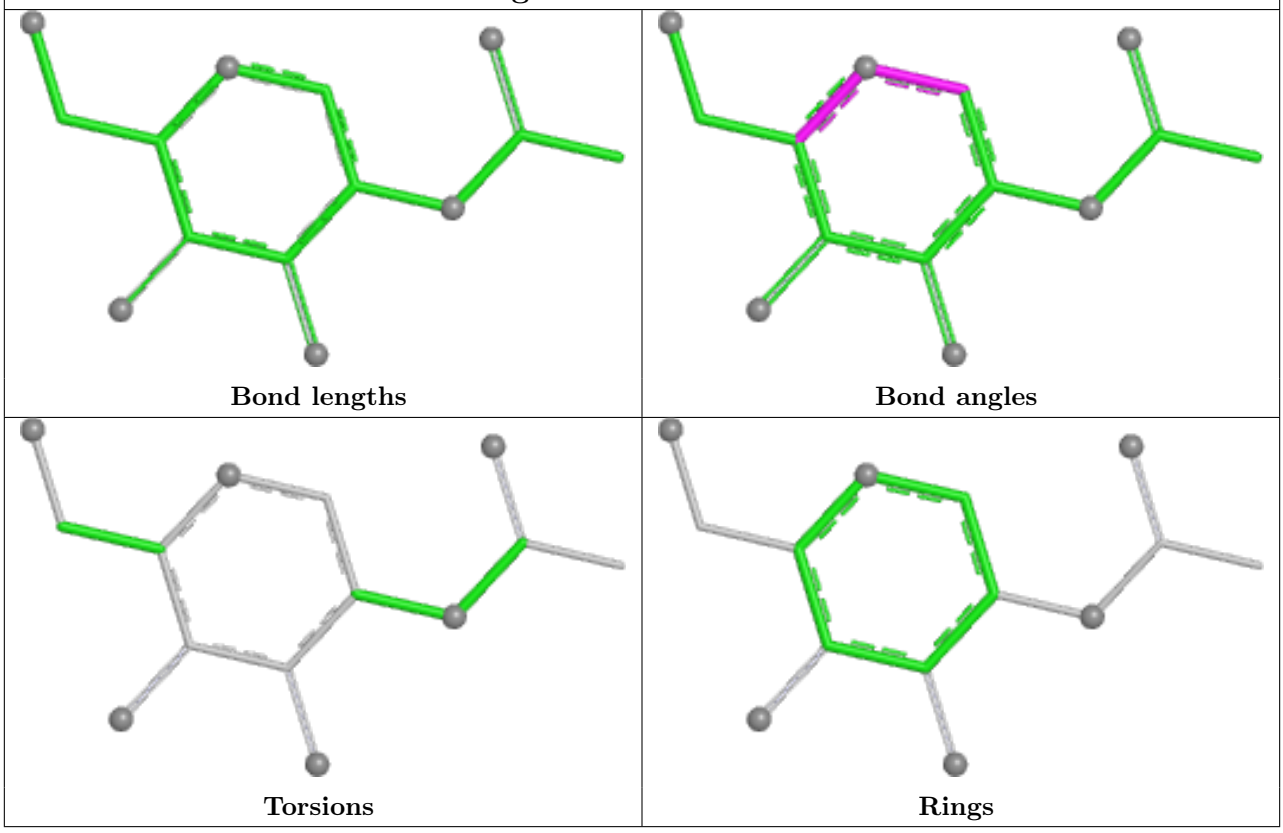


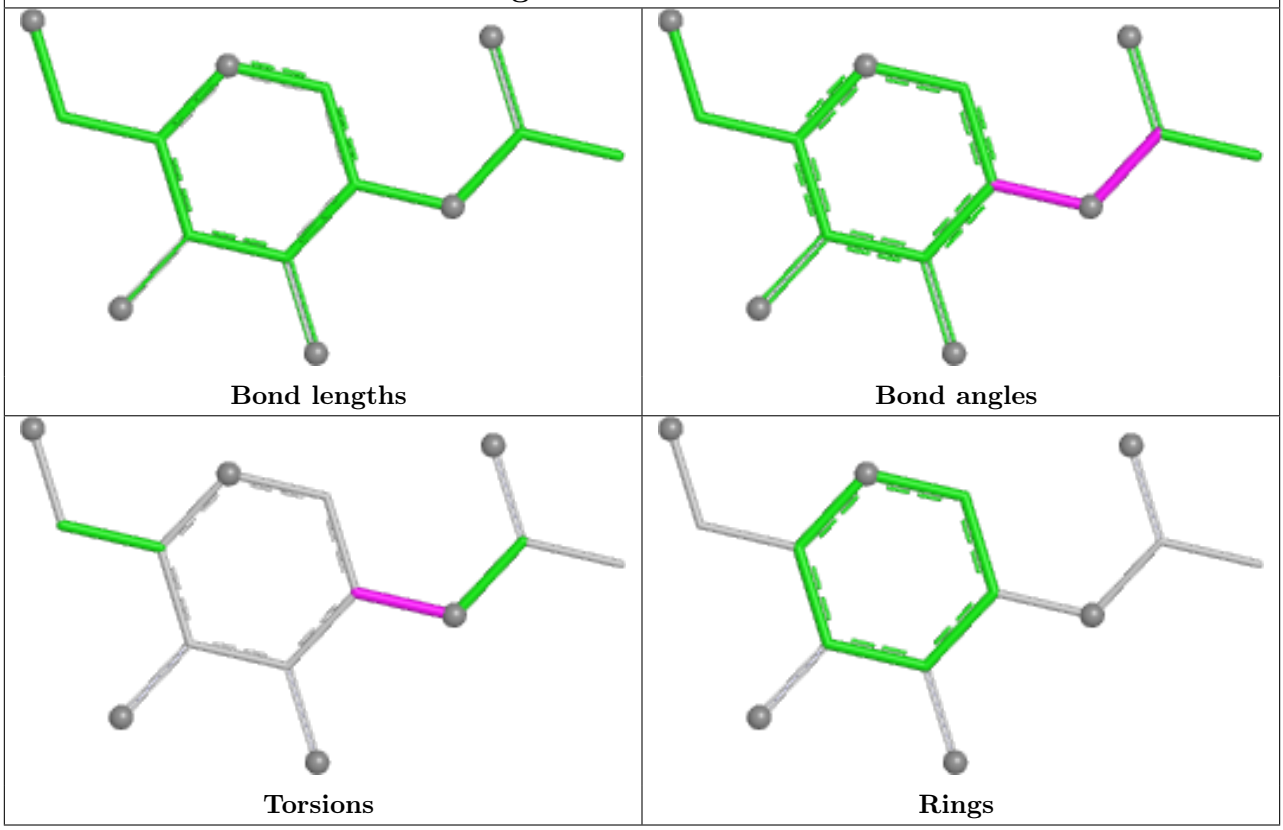
Ligand NAG B 2802



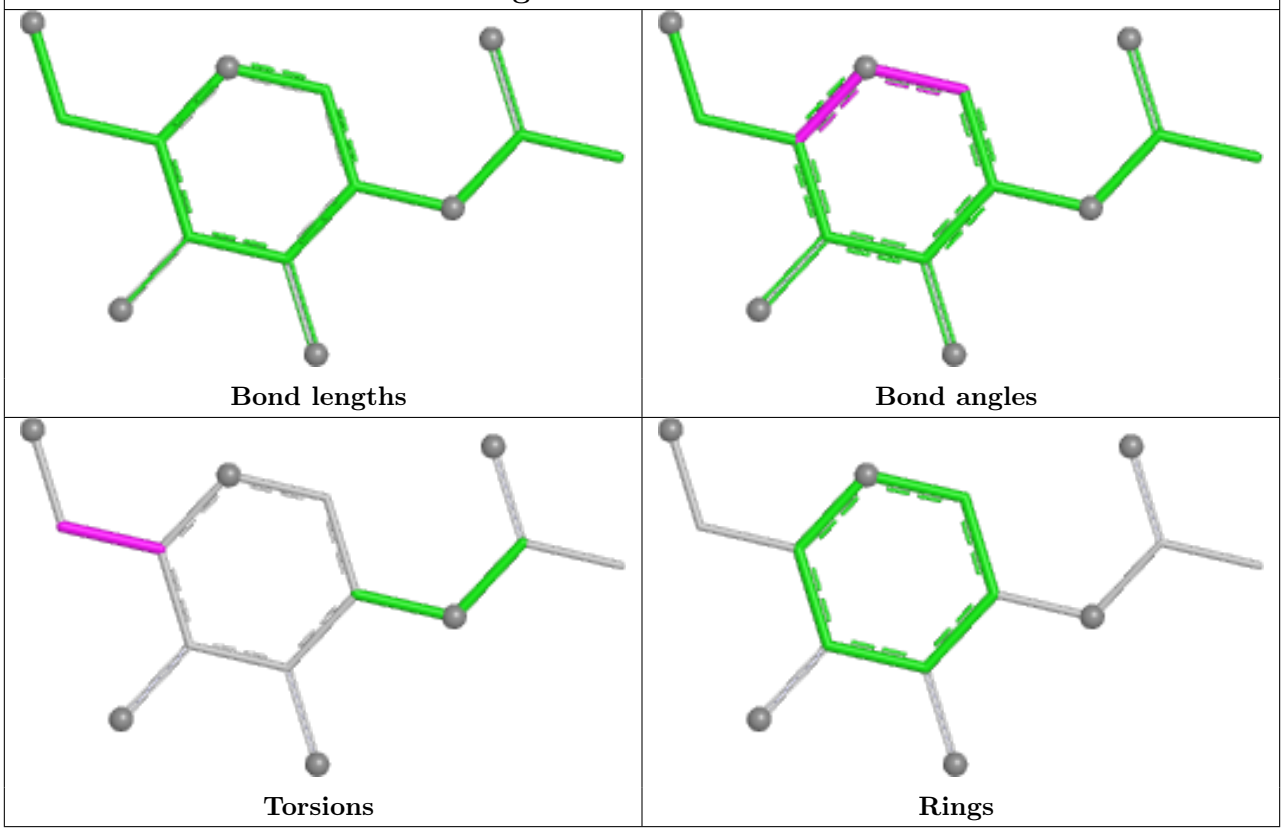
Ligand NAG A 2817



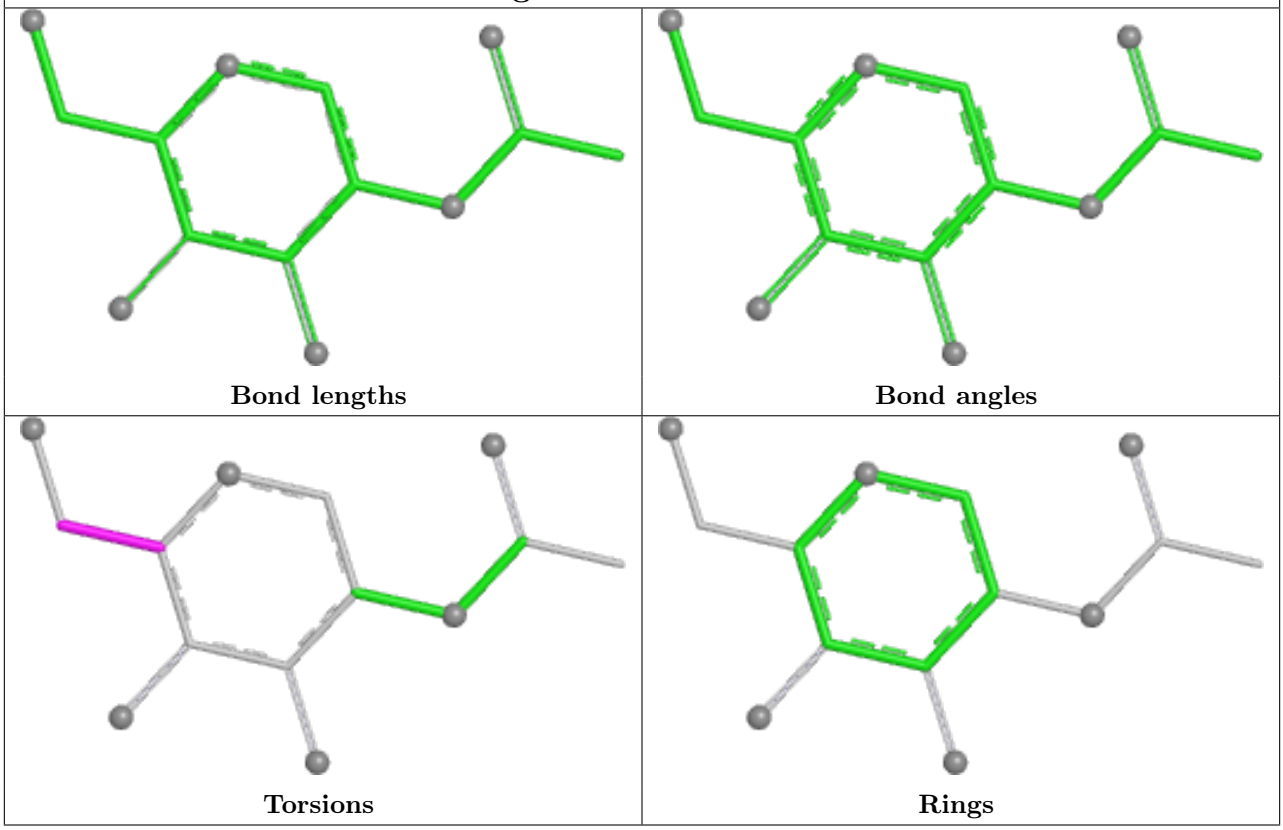
Ligand NAG A 2802



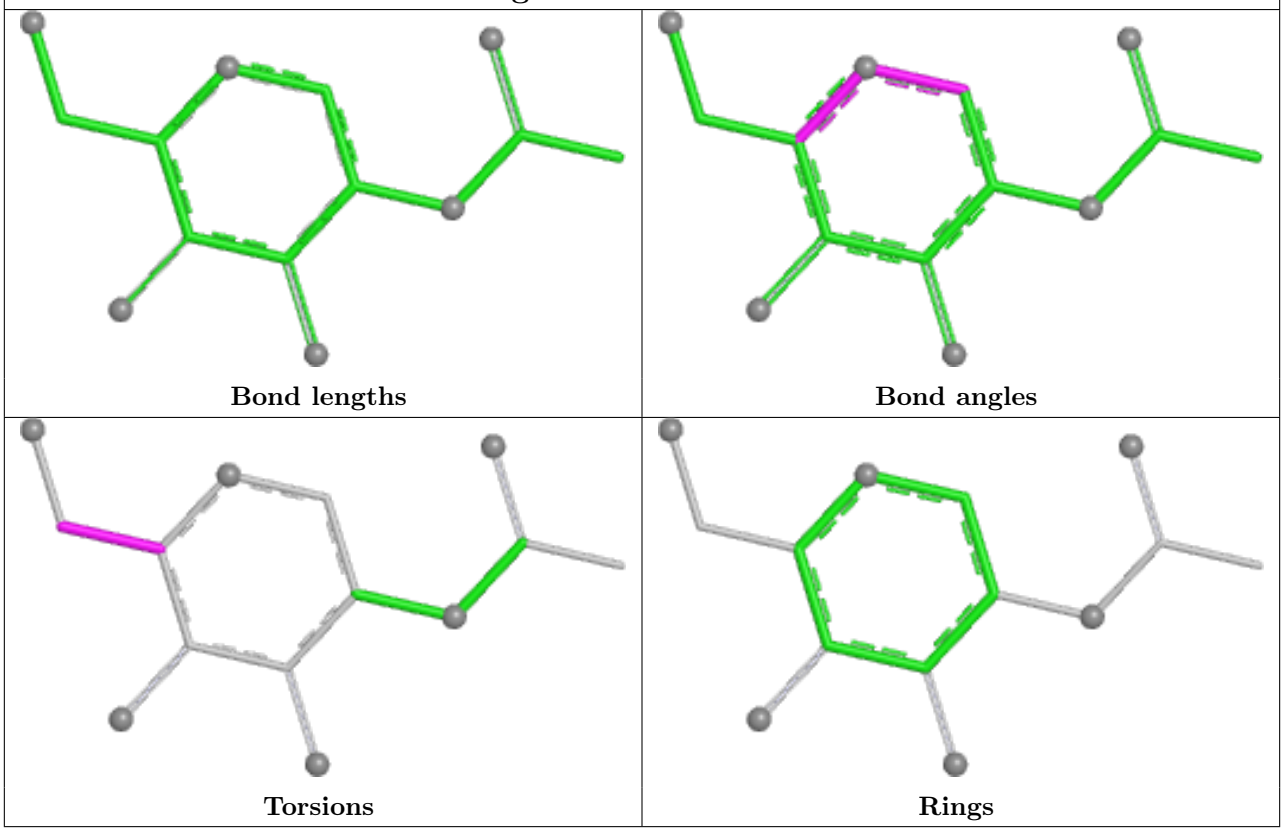
Ligand NAG B 2815



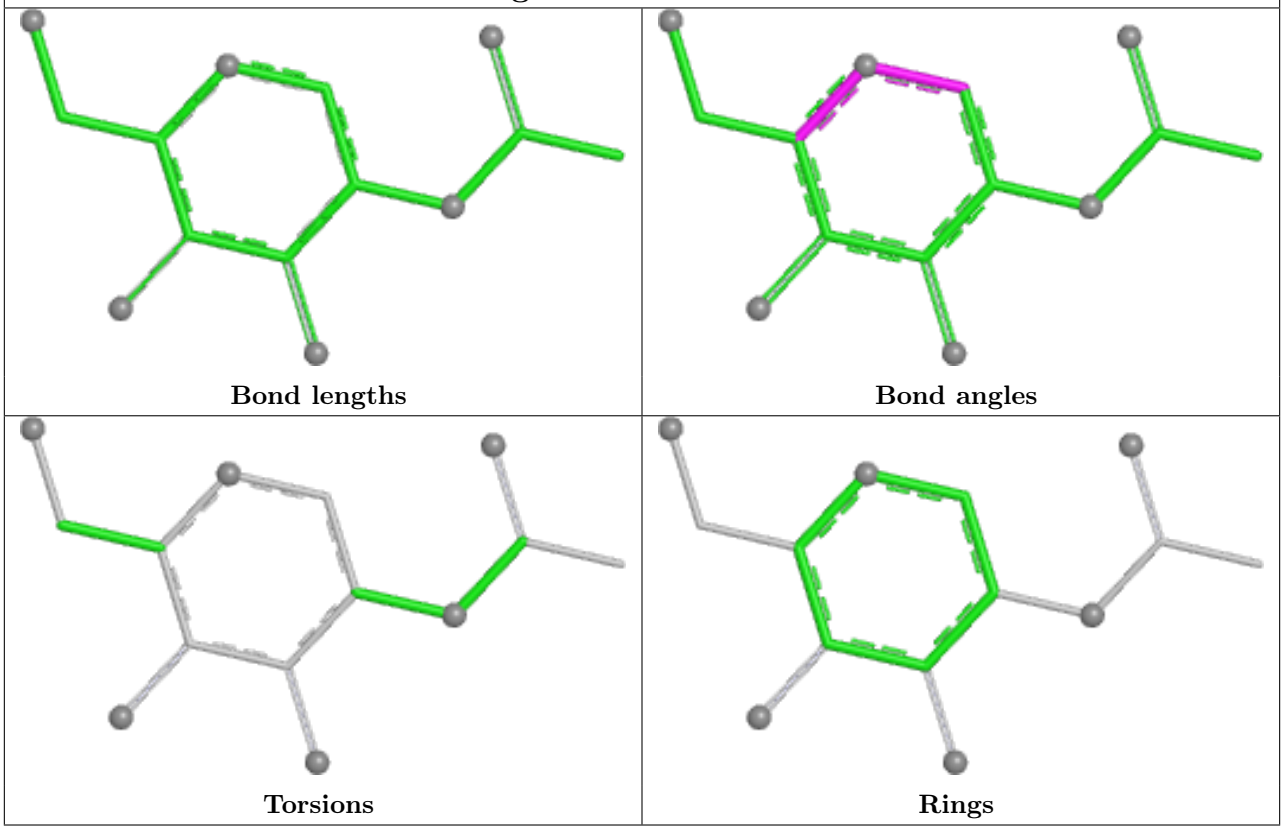
Ligand NAG B 2809



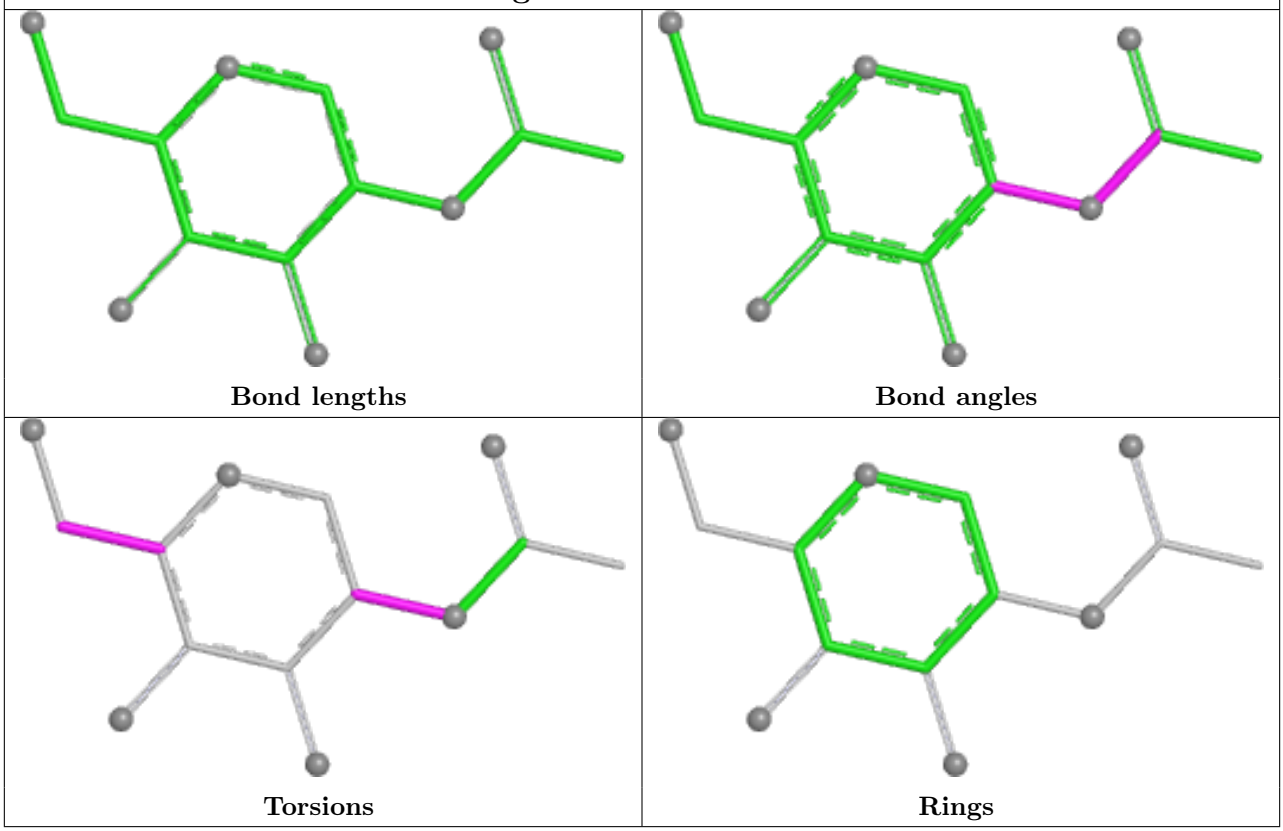
Ligand NAG A 2815



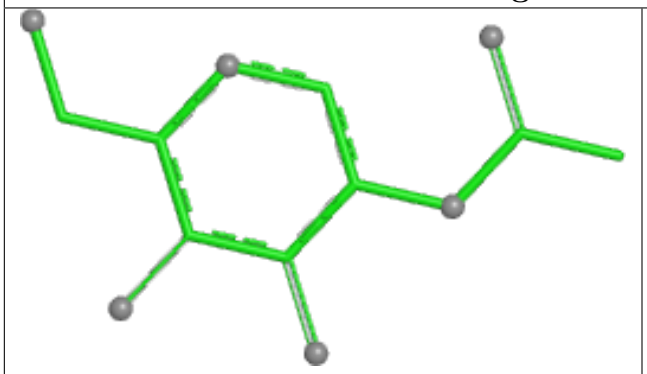
Ligand NAG A 2812



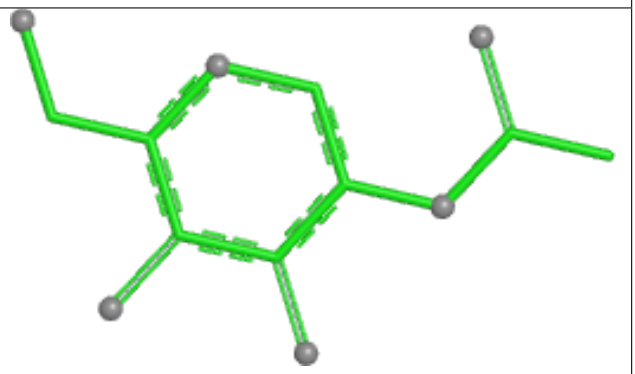
Ligand NAG B 2818



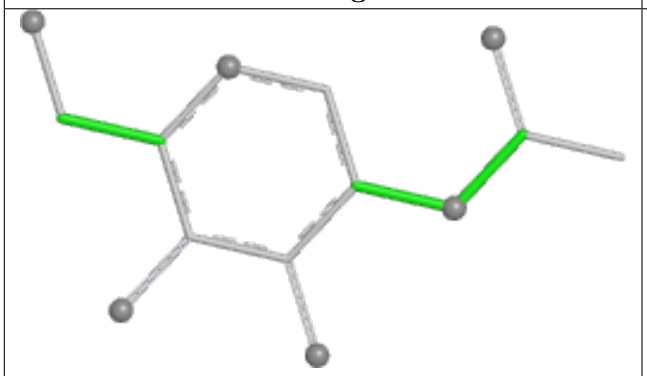
Ligand NAG A 2814



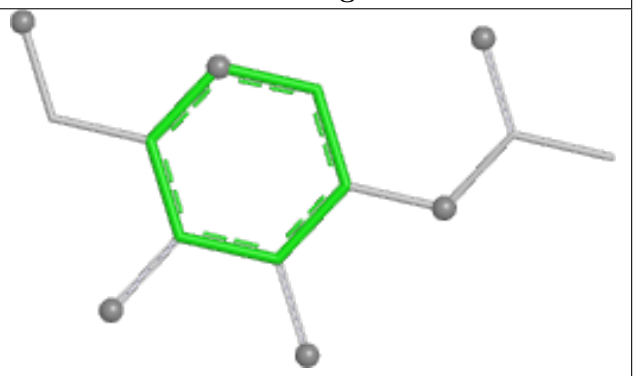
Bond lengths



Bond angles

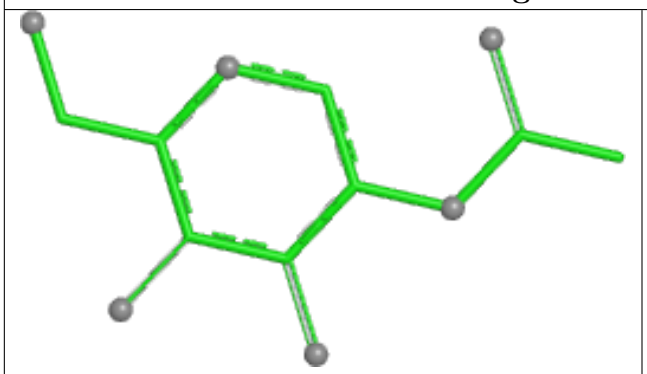


Torsions

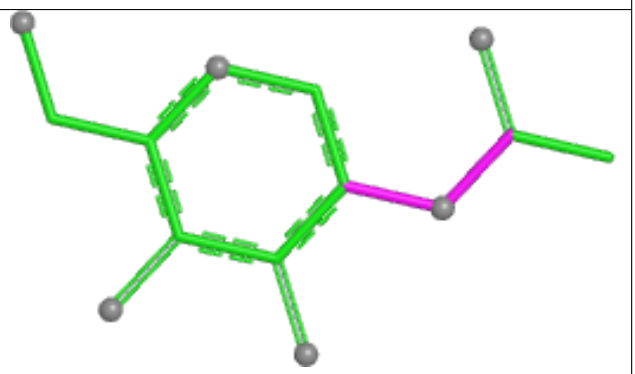


Rings

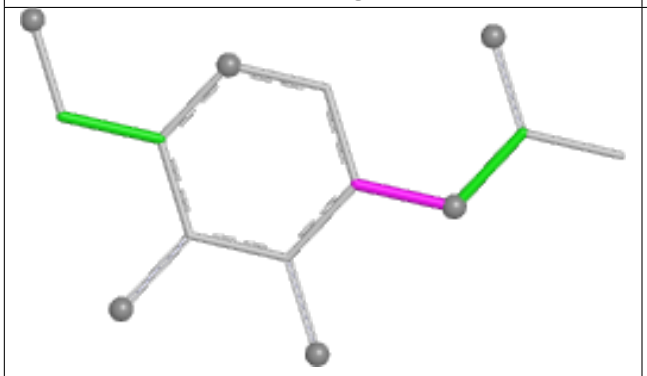
Ligand NAG B 2801



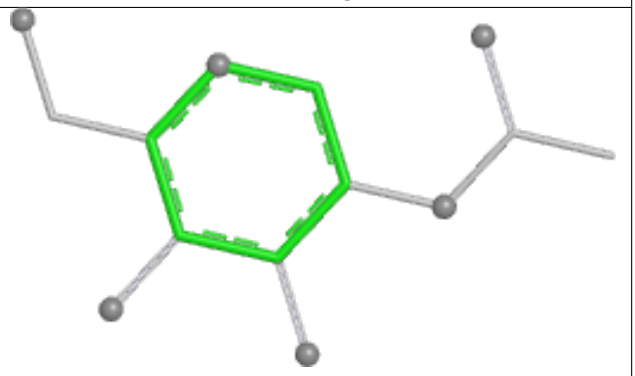
Bond lengths



Bond angles

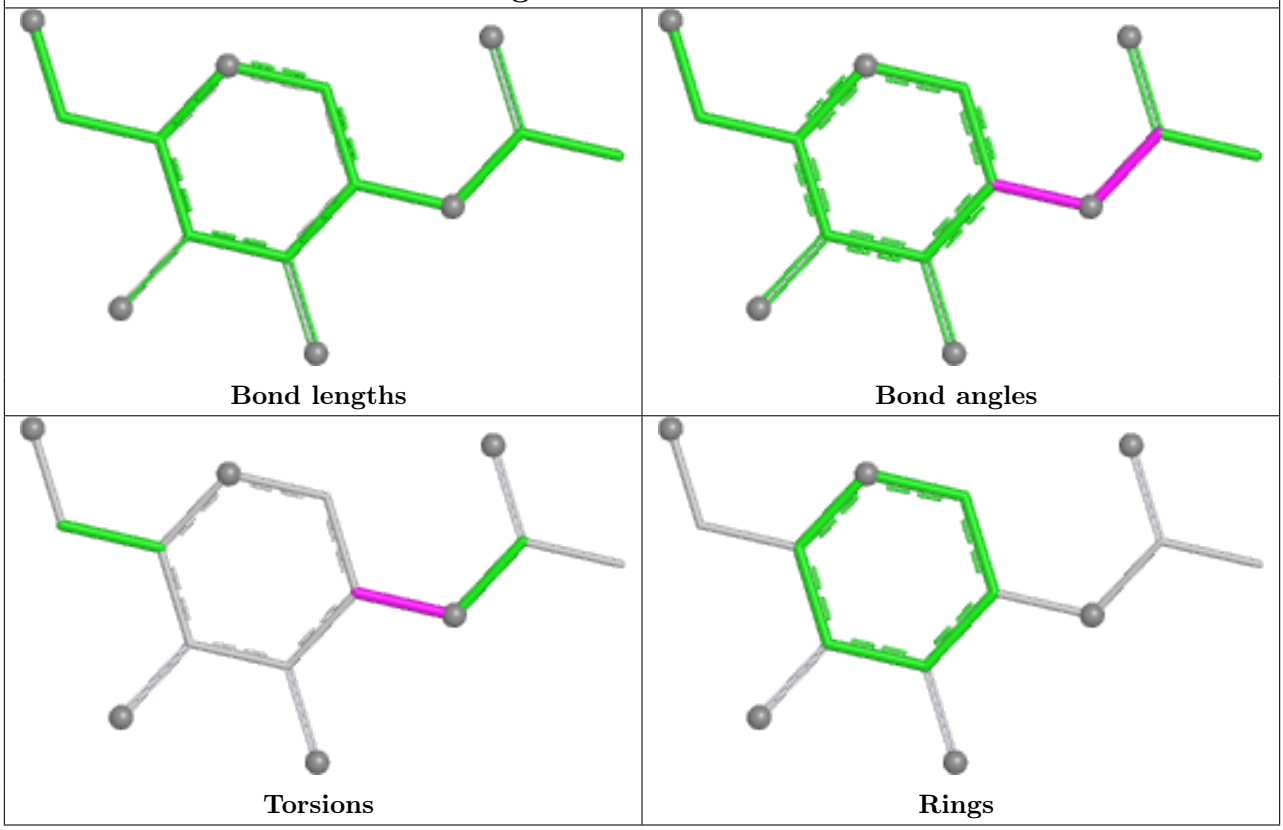


Torsions



Rings

Ligand NAG A 2801



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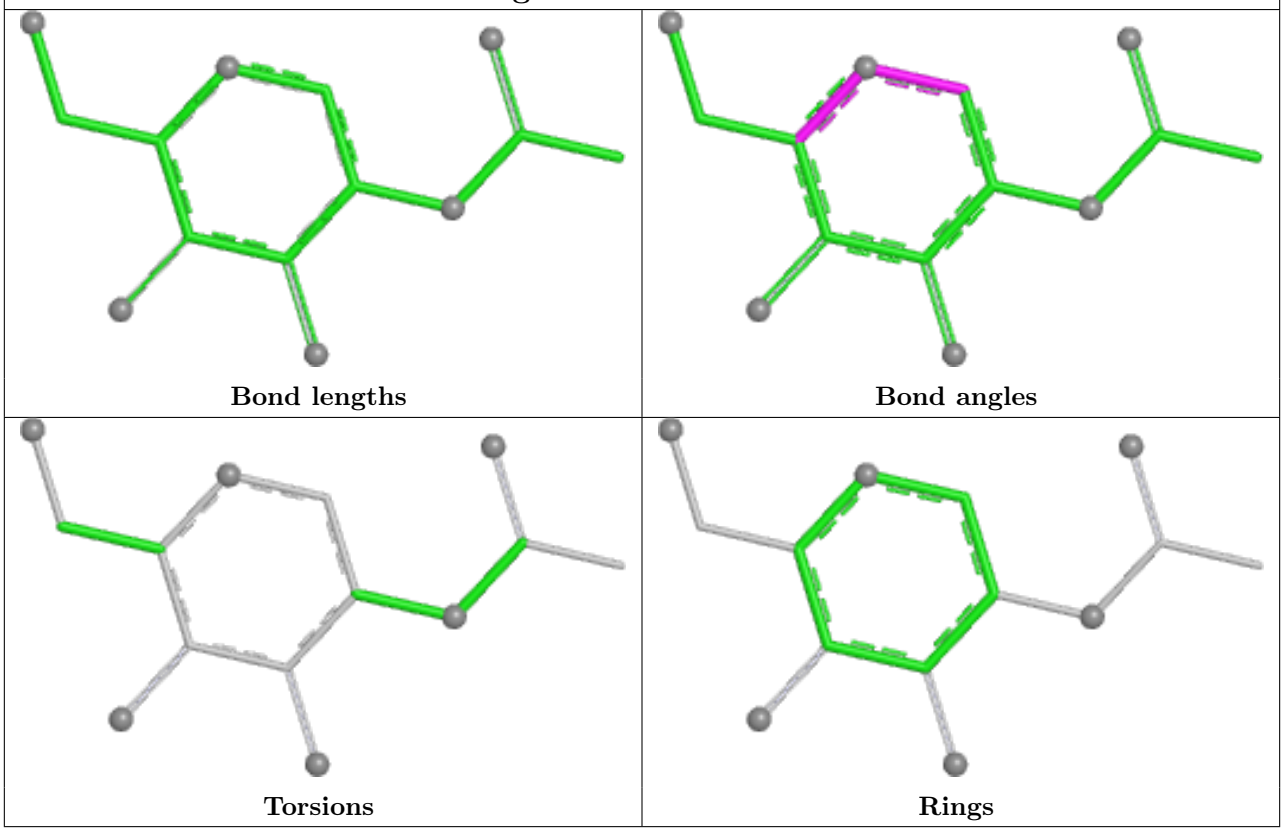
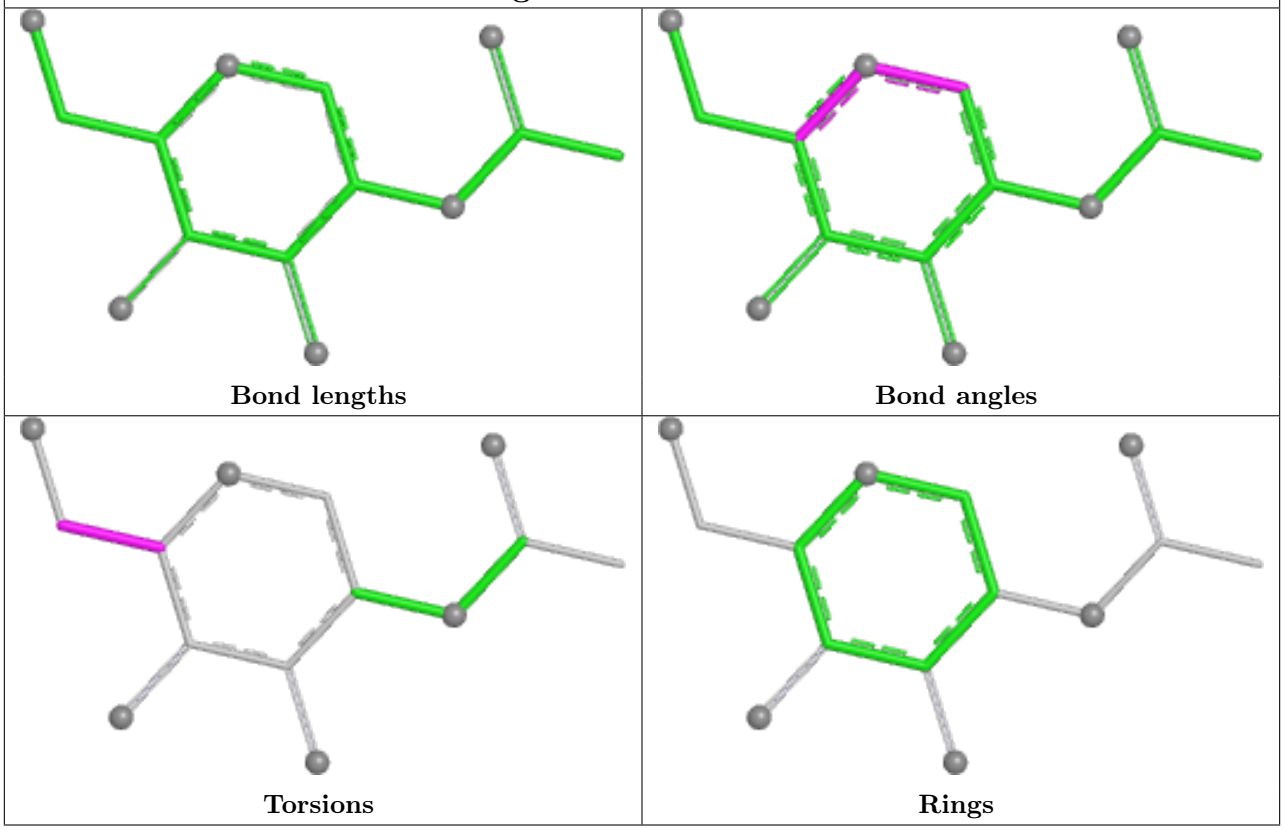
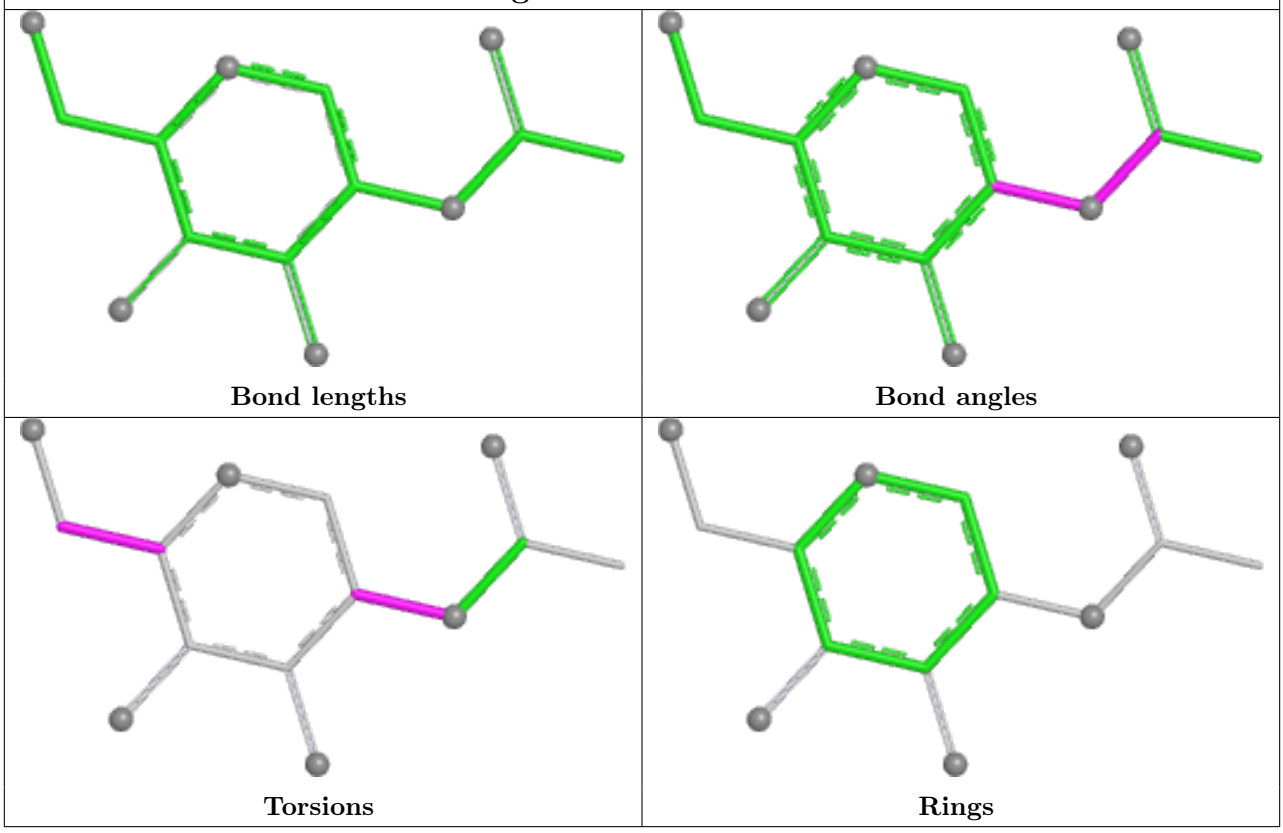


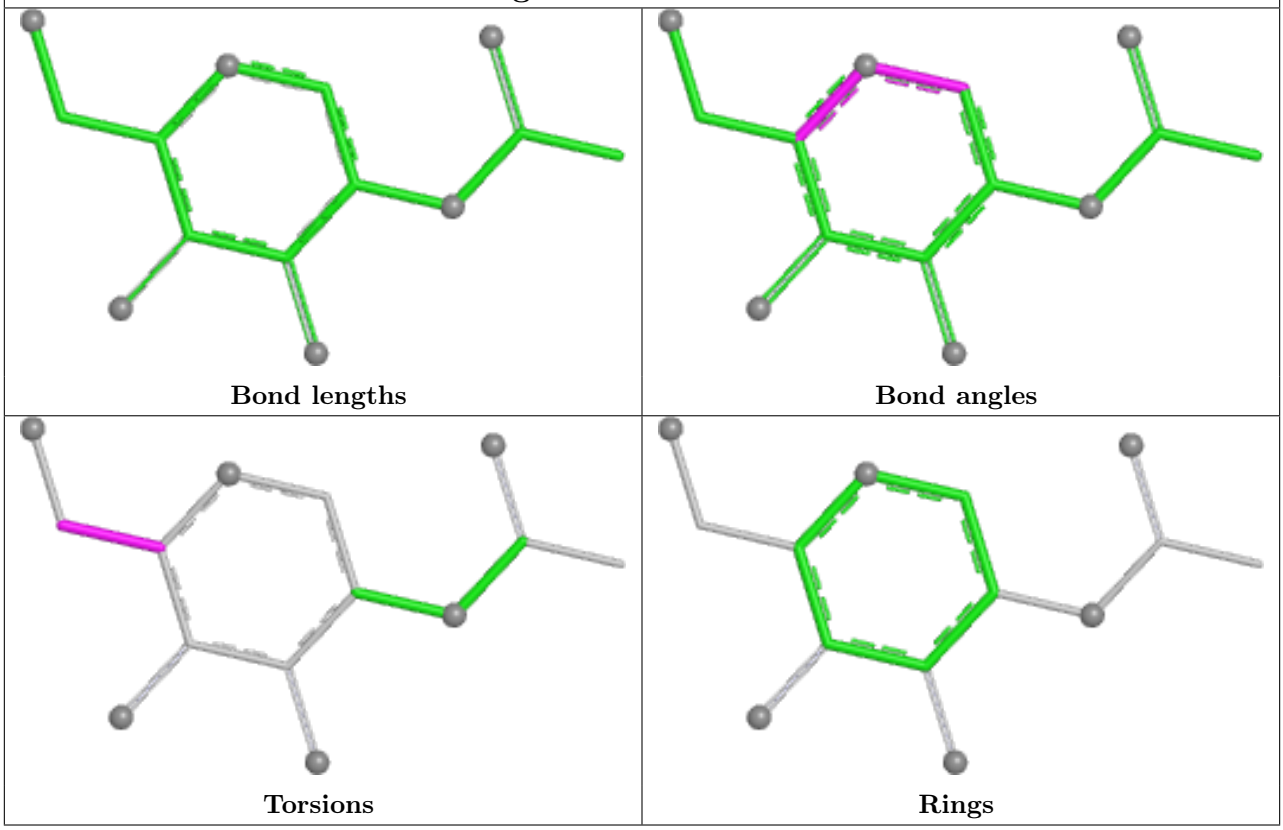
Ligand NAG B 2810



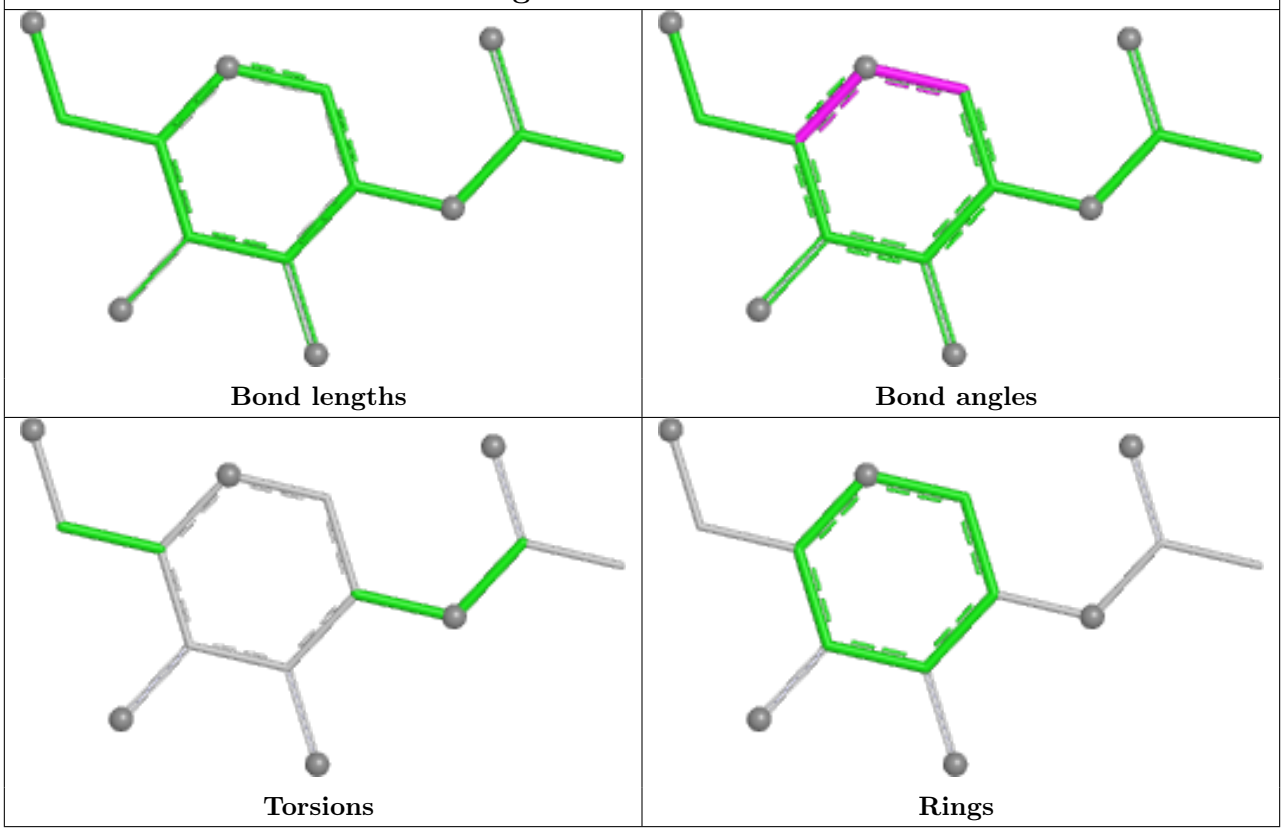
Ligand NAG A 2818



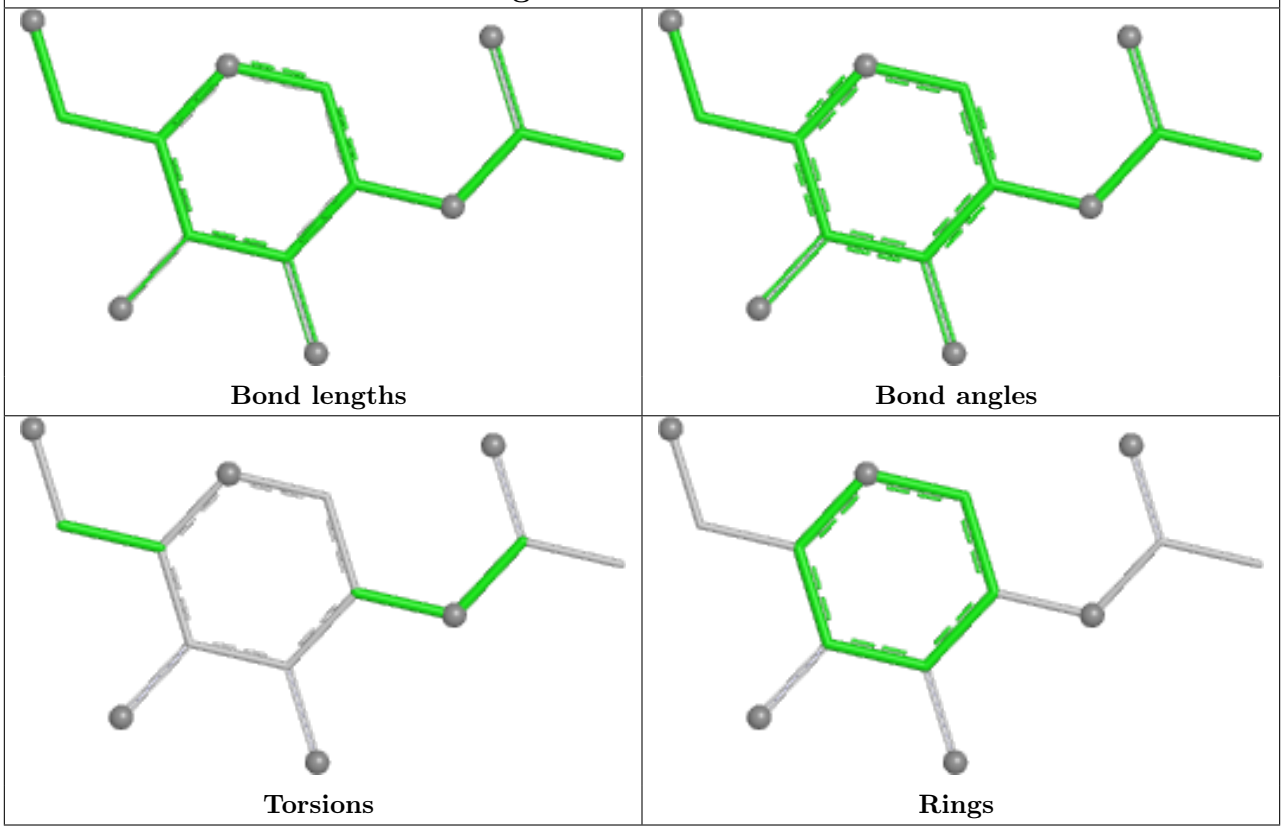
Ligand NAG B 2811



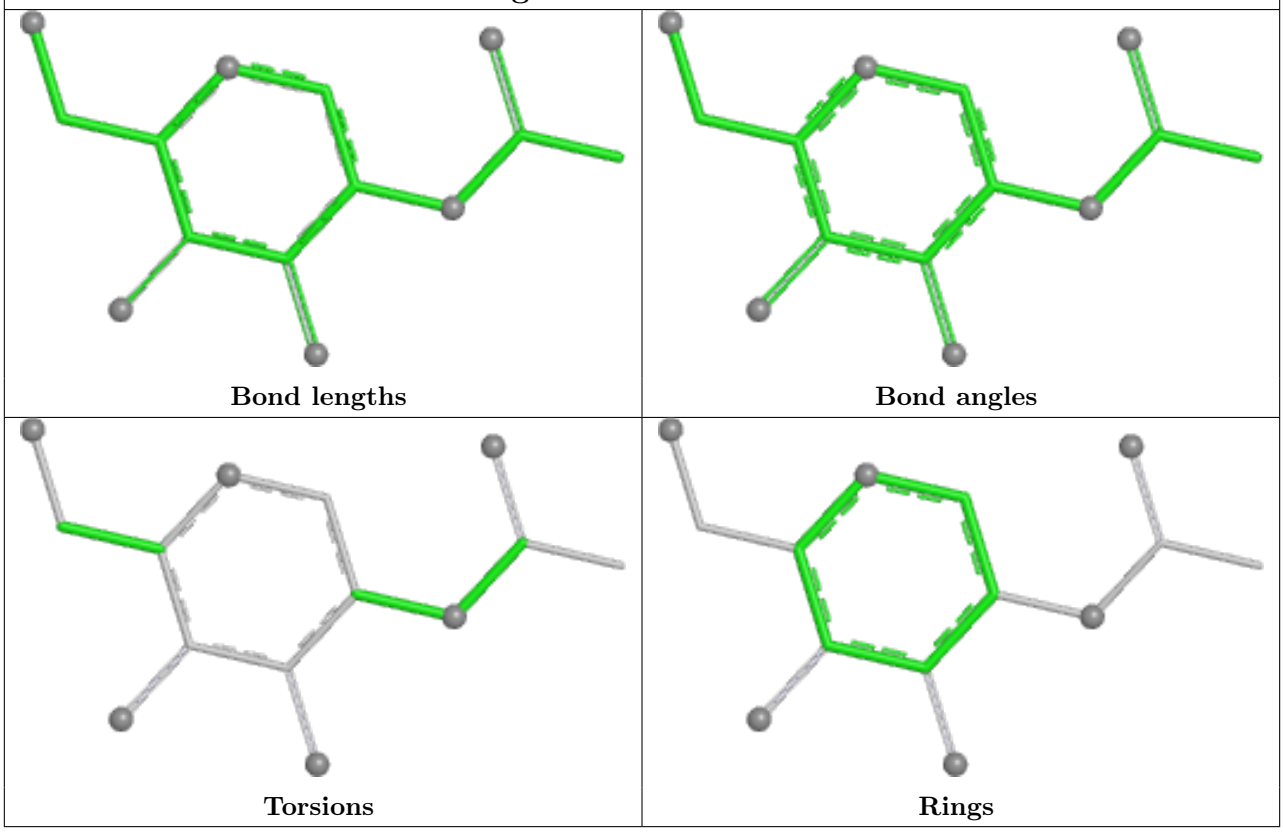
Ligand NAG B 2812



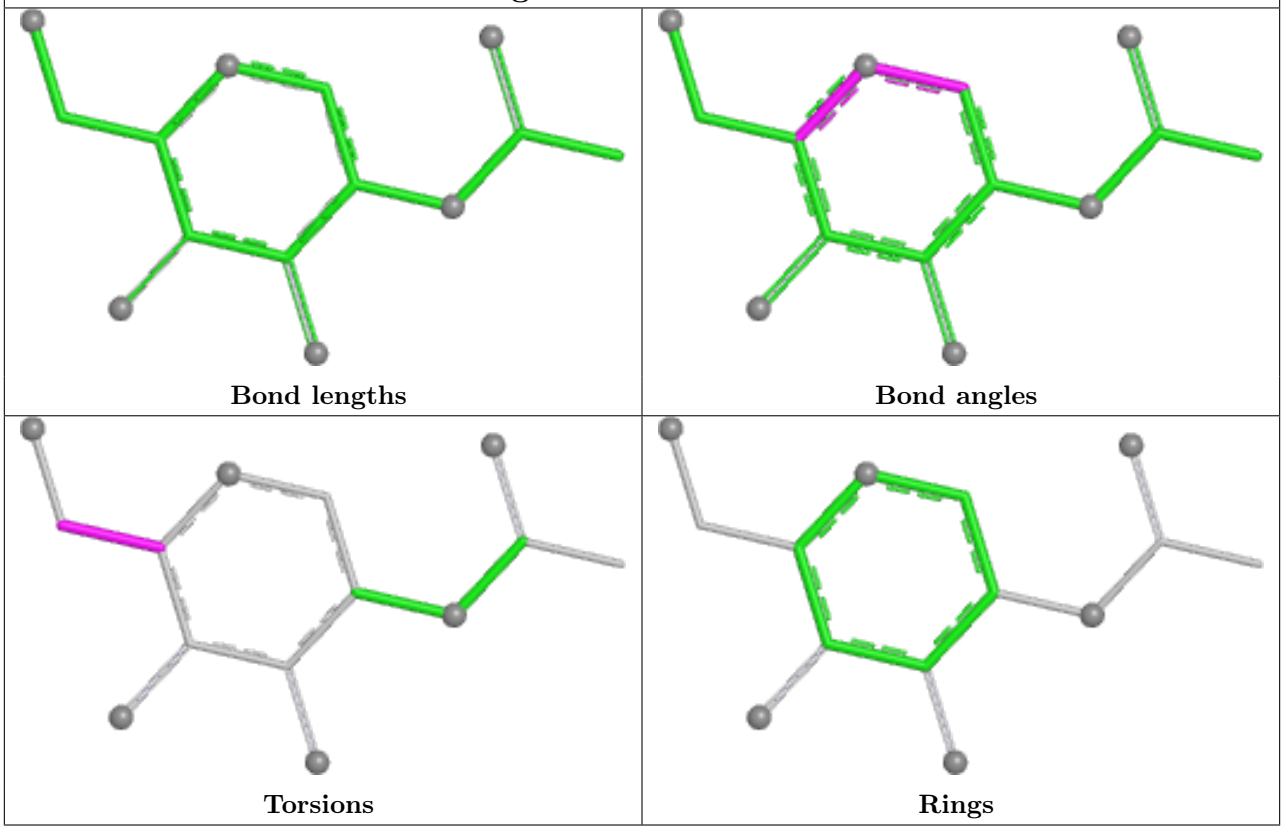
Ligand NAG B 2803



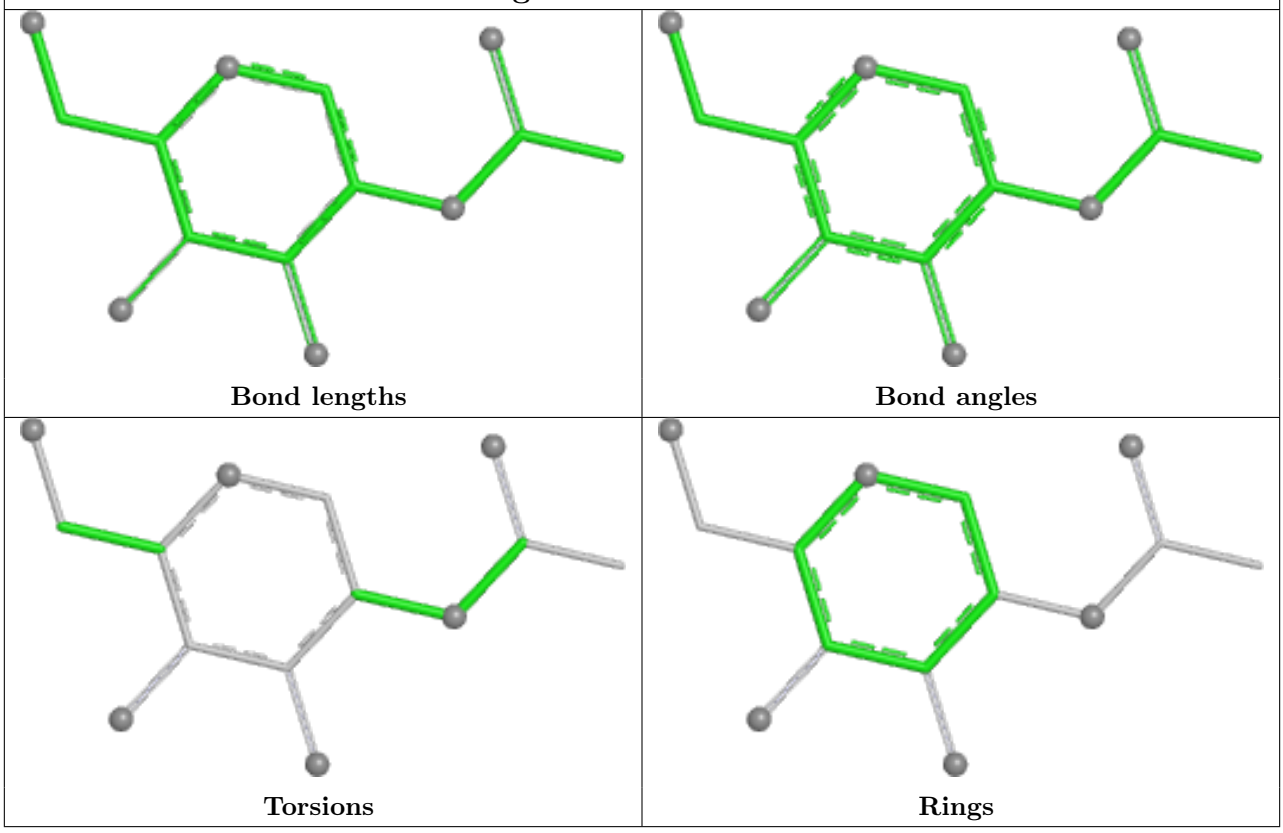
Ligand NAG A 2803



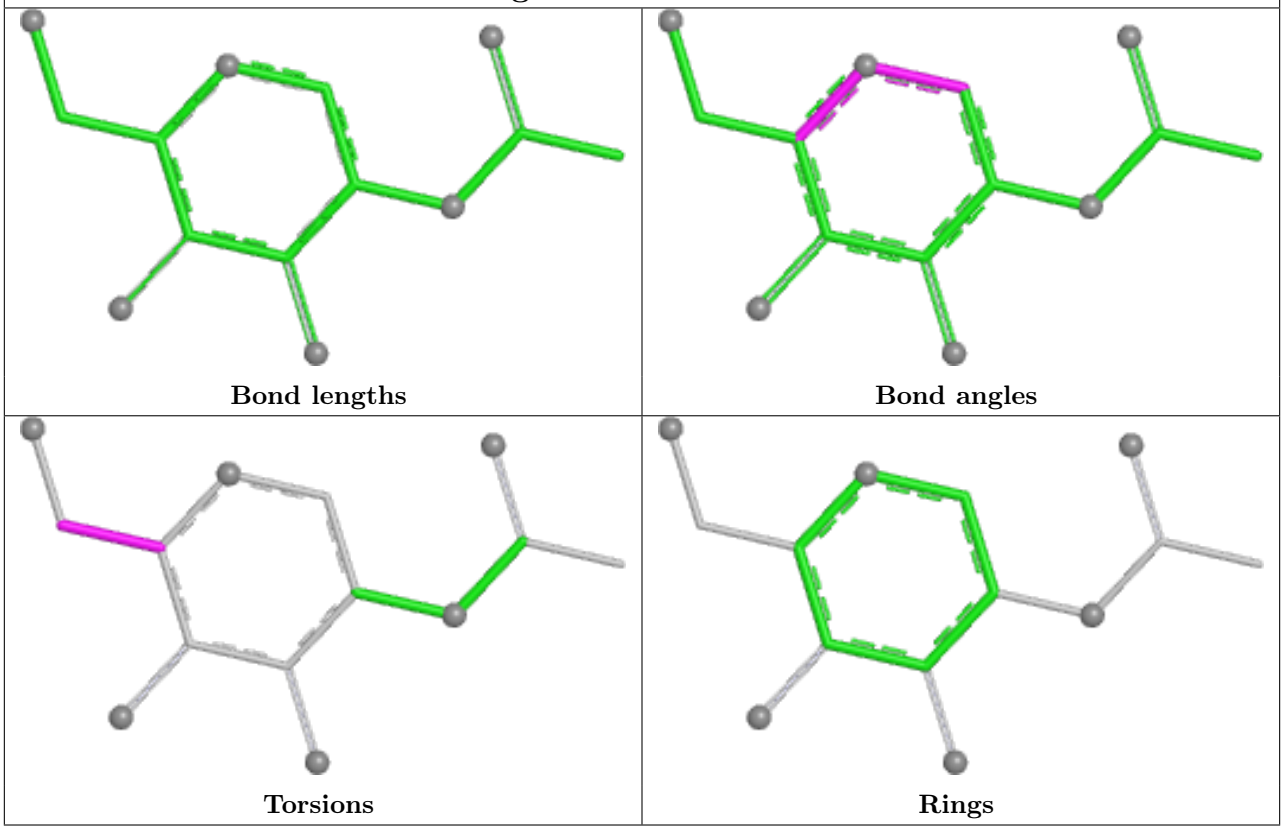
Ligand NAG A 2810



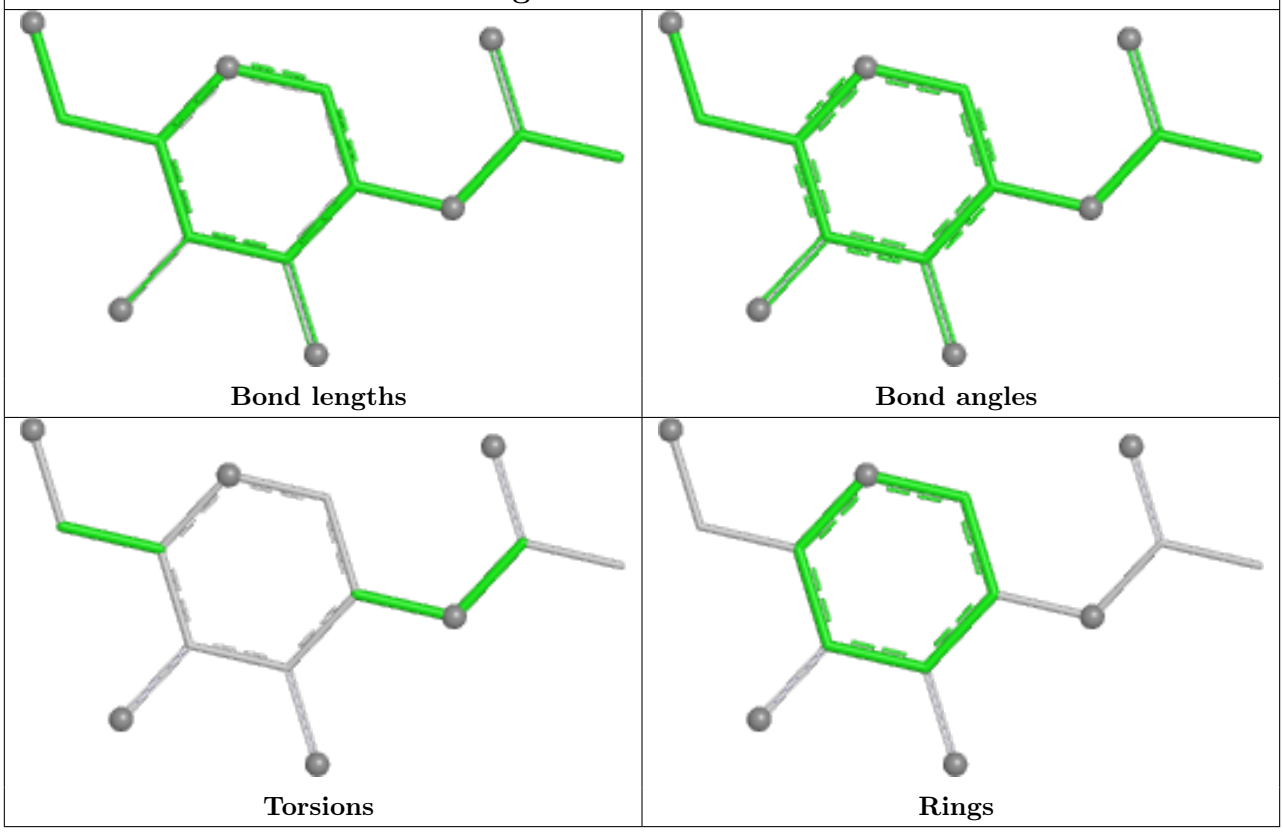
Ligand NAG B 2814

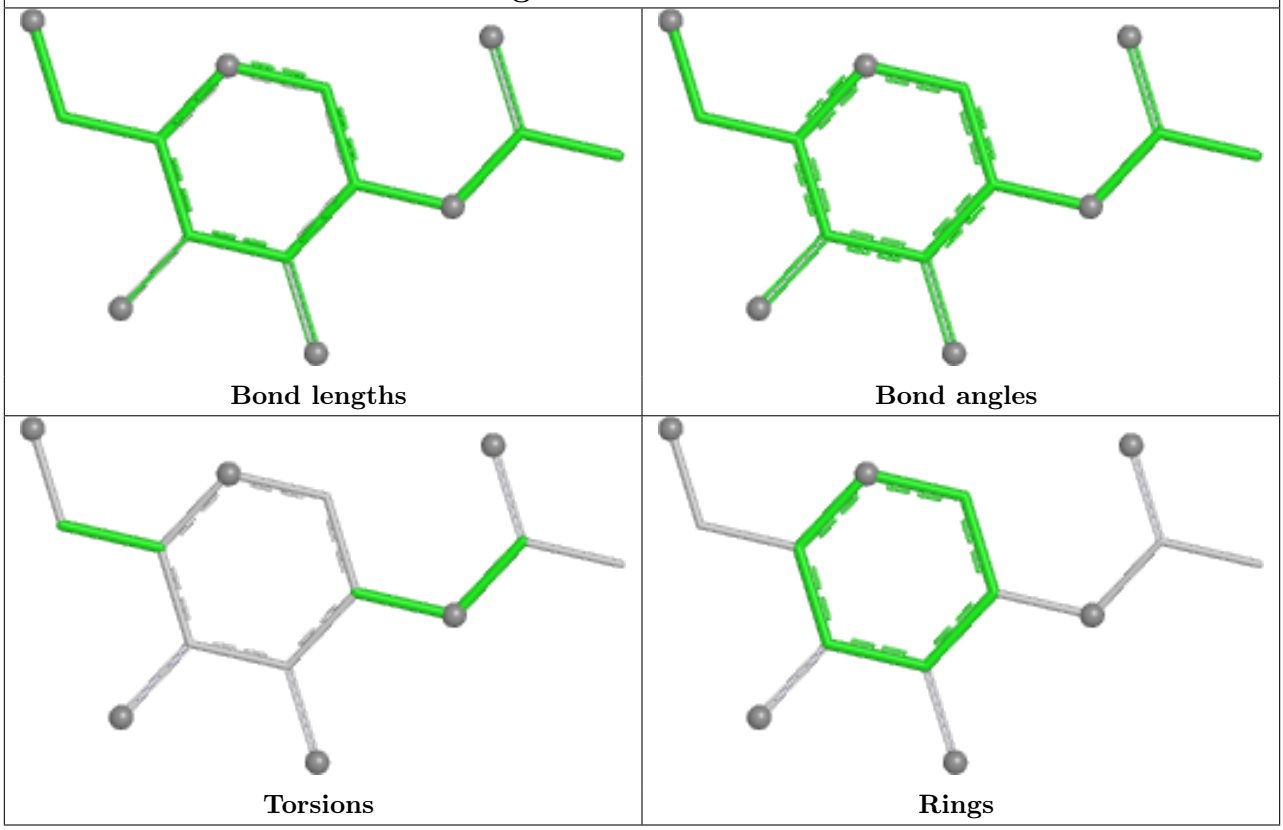


Ligand NAG A 2811



Ligand NAG B 2816



Ligand NAG B 2805	
 Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

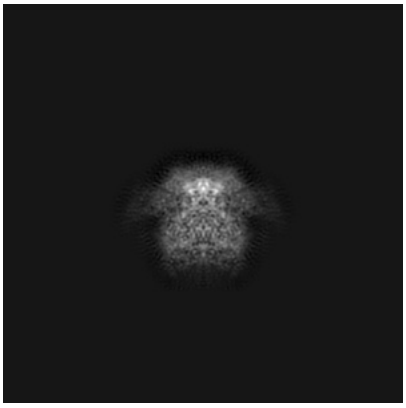
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10141. These allow visual inspection of the internal detail of the map and identification of artifacts.

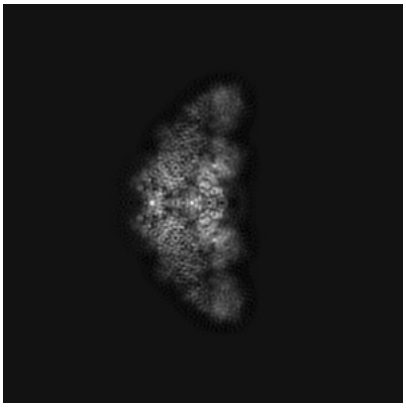
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

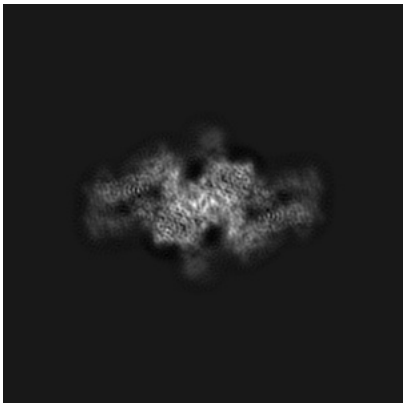
6.1.1 Primary map



X



Y

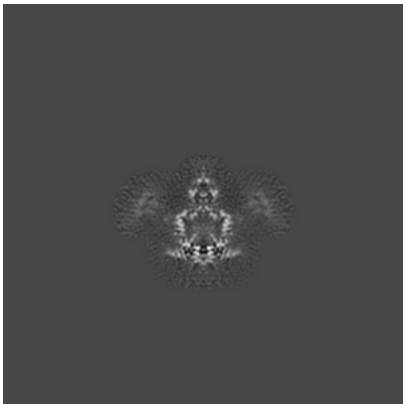


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200

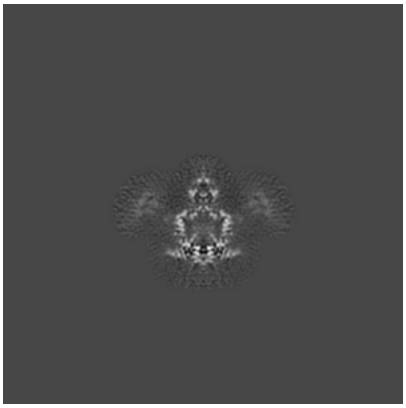
Y Index: 200

Z Index: 200

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

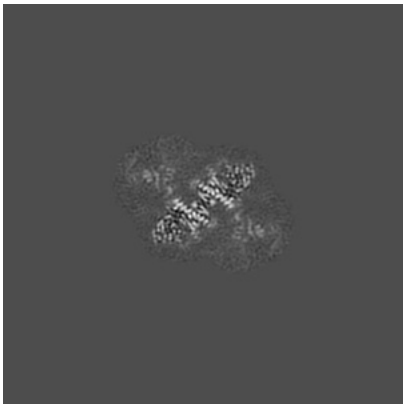
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 200

Y Index: 200

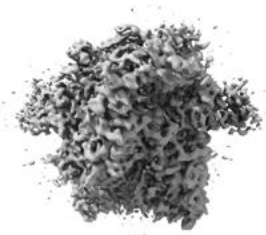


Z Index: 157

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

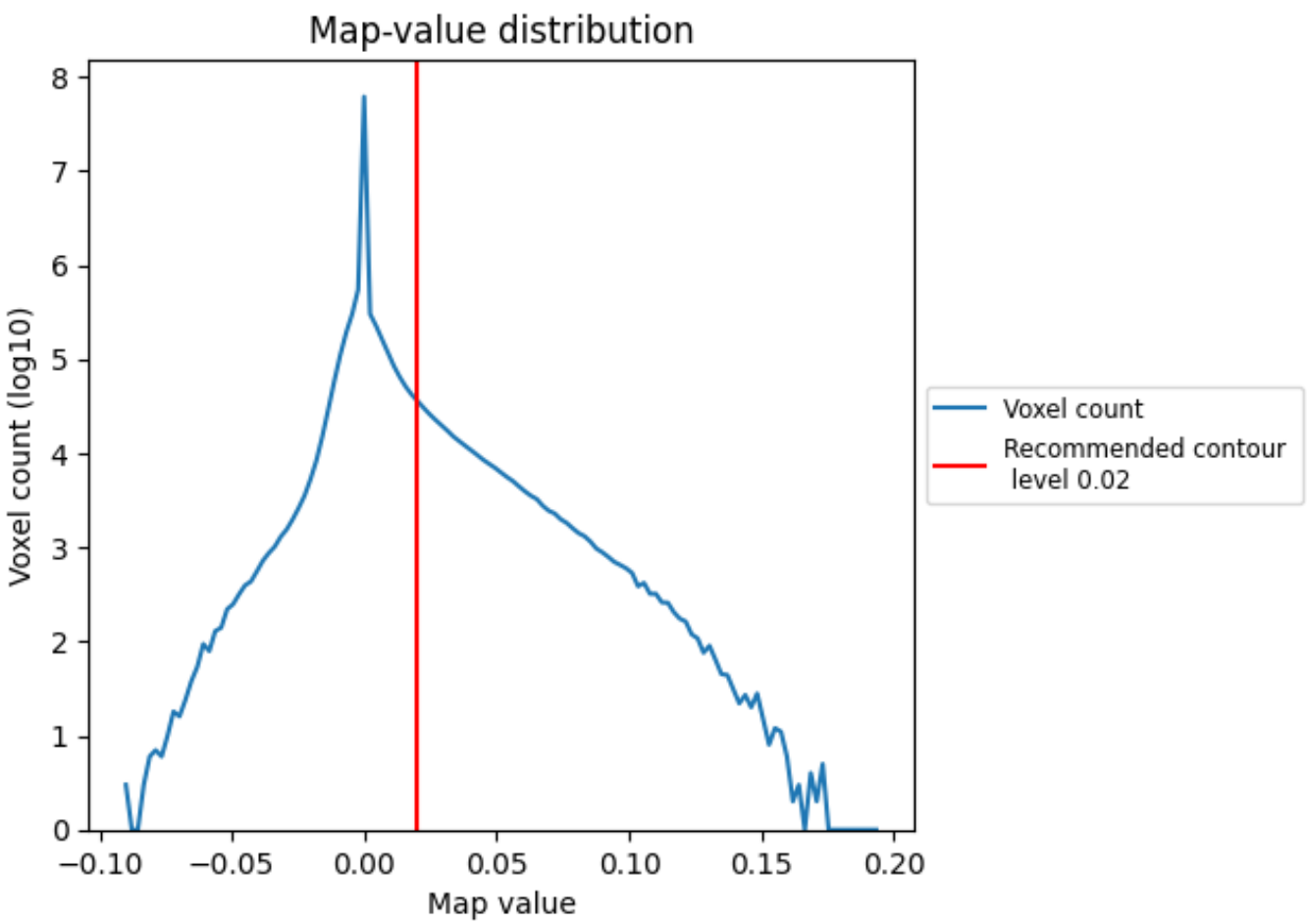
6.5 Mask visualisation (i)

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

7 Map analysis (i)

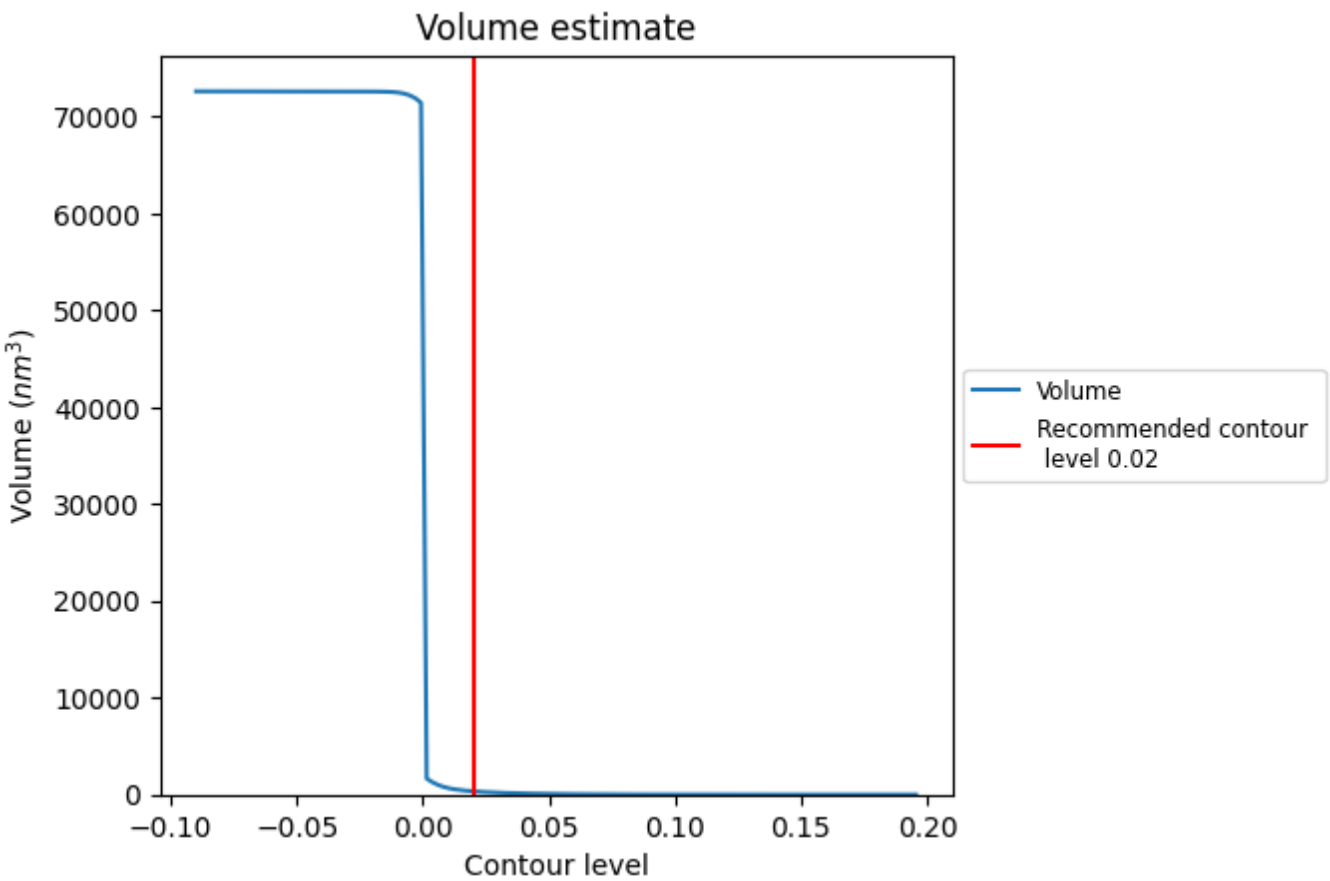
This section contains the results of statistical analysis of the map.

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.

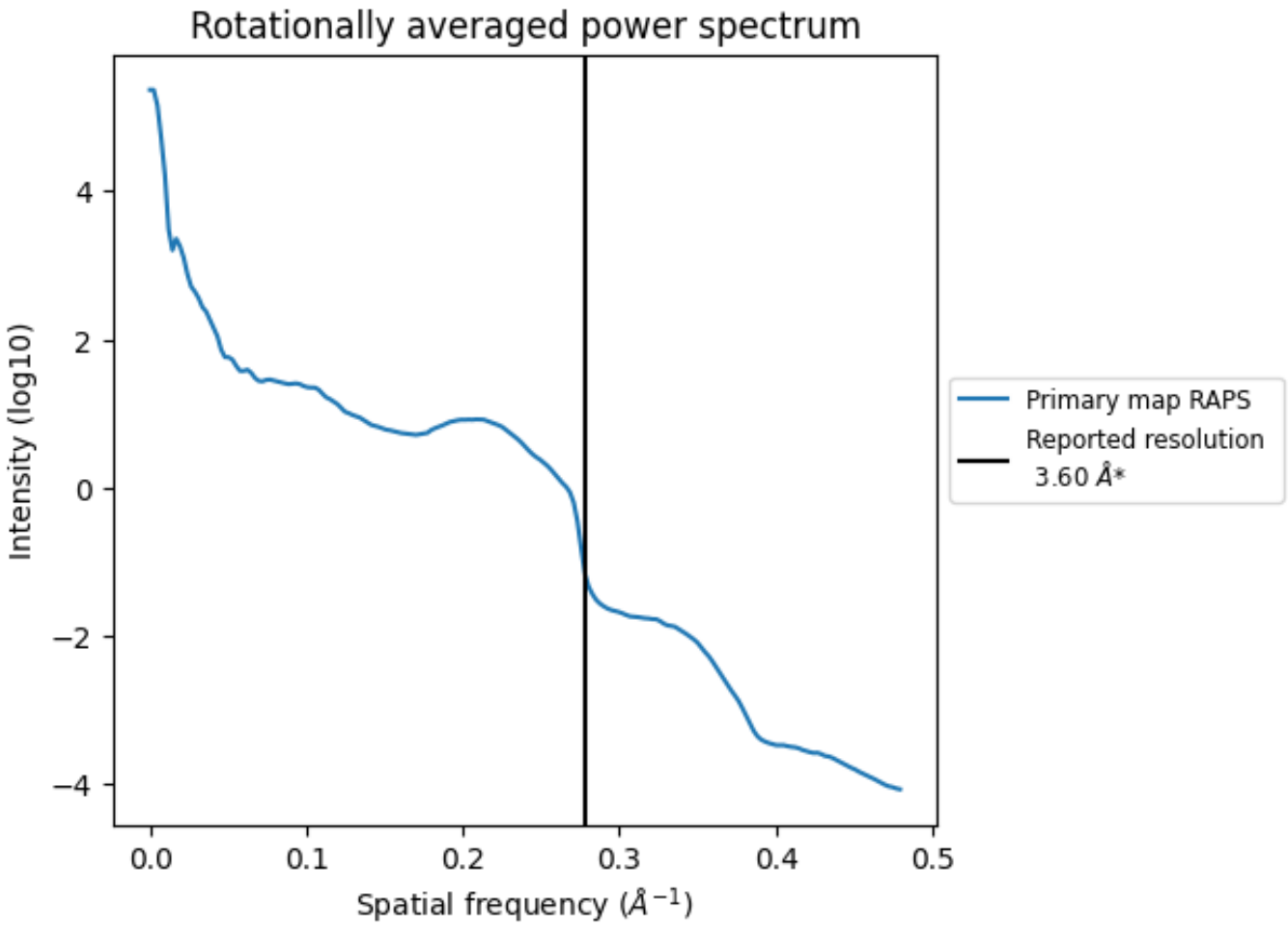
7.2 Volume estimate (i)



The volume at the recommended contour level is 337 nm^3; this corresponds to an approximate mass of 304 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

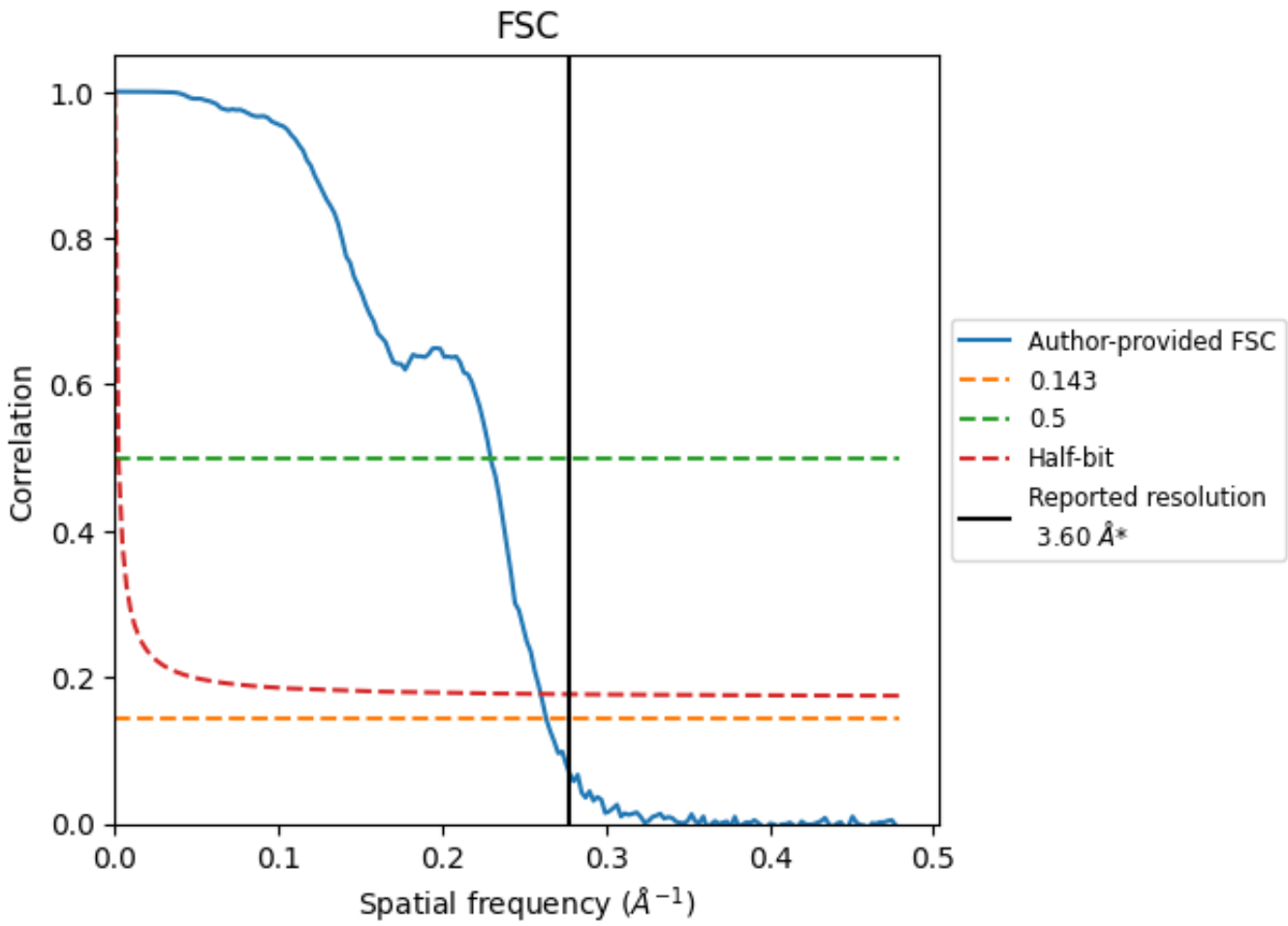


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

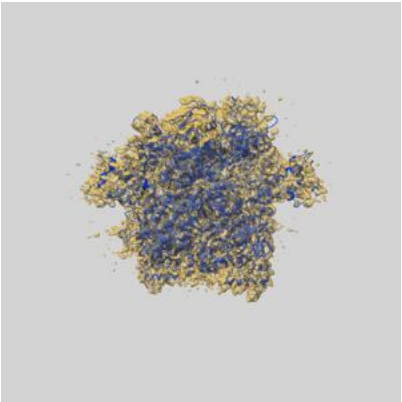
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.80	4.36	3.84
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

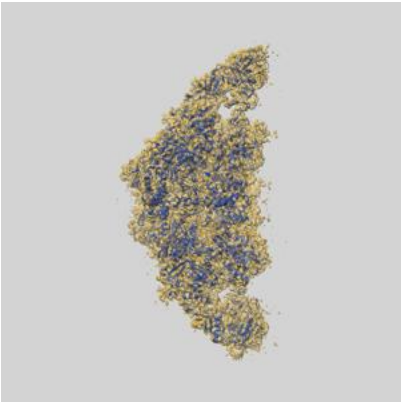
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10141 and PDB model 6SCJ. Per-residue inclusion information can be found in section 3 on page 6.

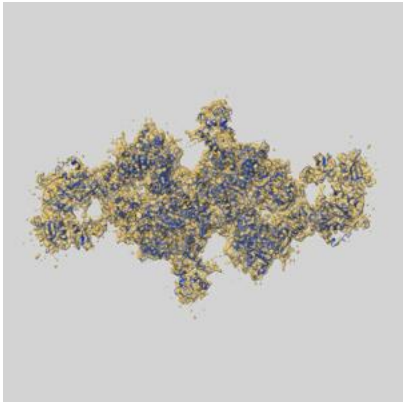
9.1 Map-model overlay (i)



X



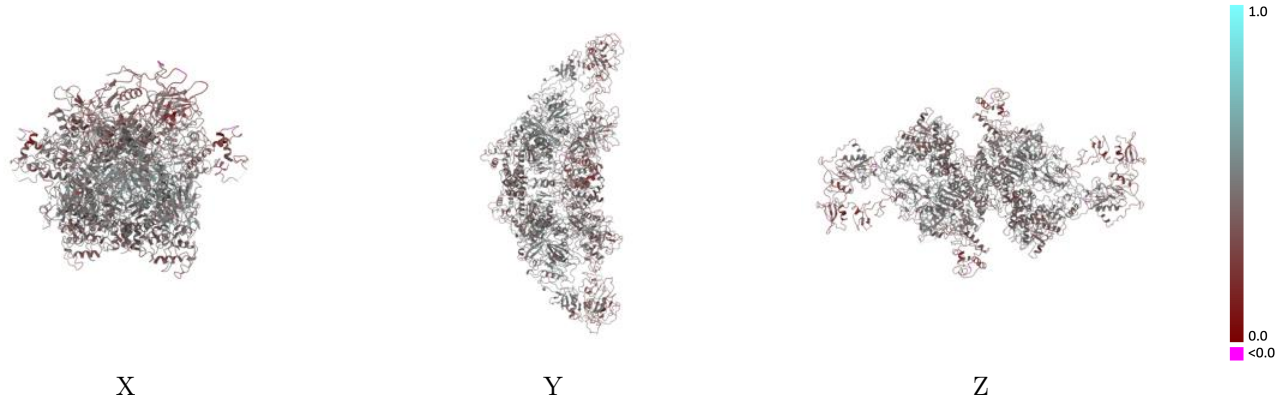
Y



Z

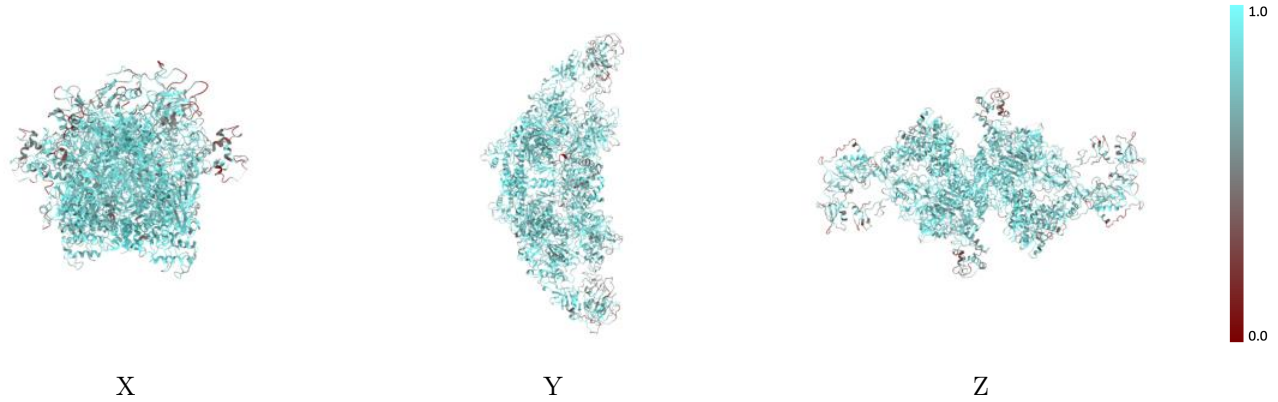
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



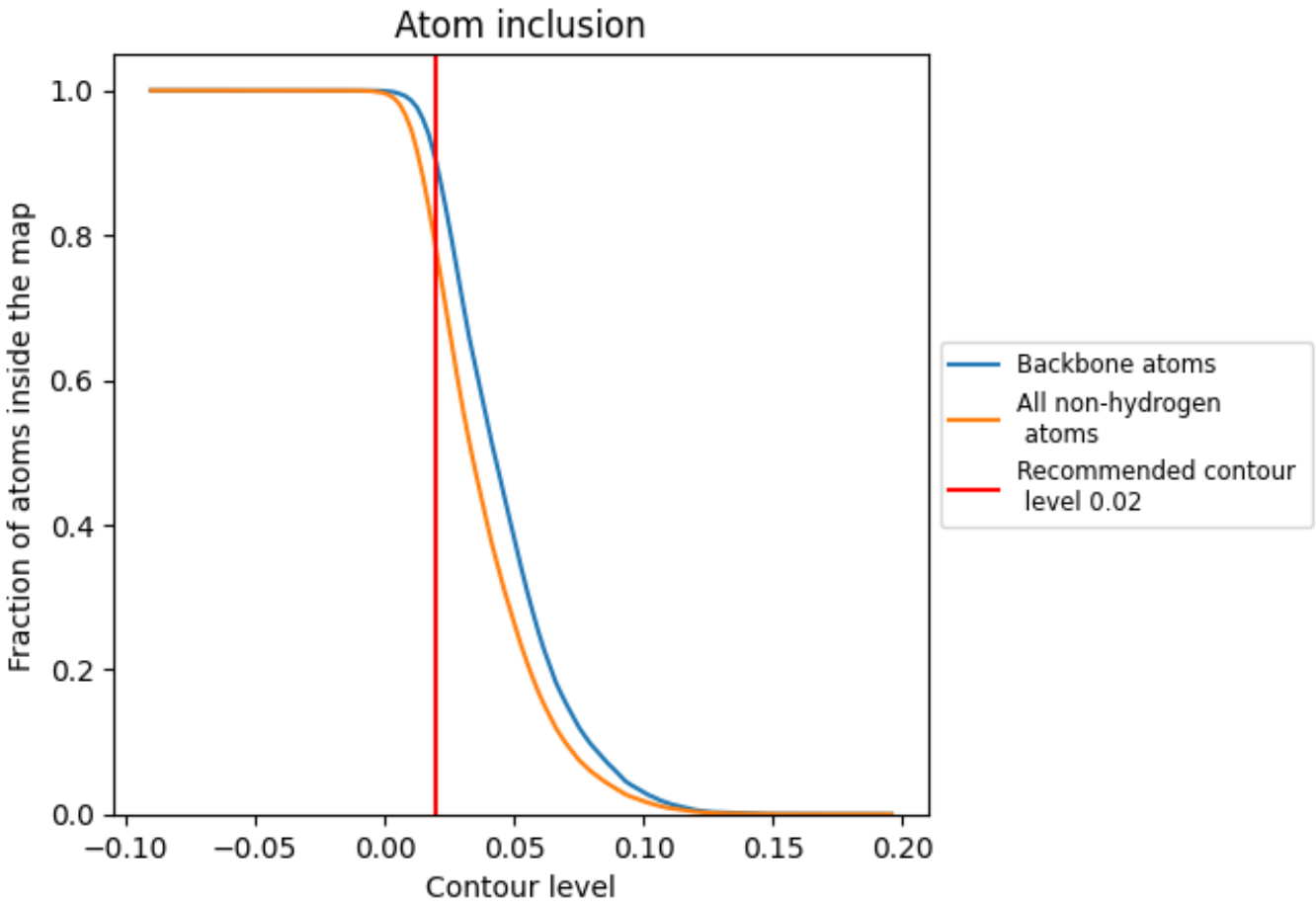
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.4190
A	0.7838	0.4190
B	0.7762	0.4190
C	0.7949	0.4990
D	0.7949	0.4800