



Full wwPDB EM Validation Report ⓘ

Aug 26, 2024 – 11:32 AM EDT

PDB ID : 8VBB
EMDB ID : EMD-43119
Title : The secreted adhesin EtpA of Enterotoxigenic Escherichia coli in complex with the mouse mAb 1G05
Authors : Berndsen, Z.T.; Ward, A.B.
Deposited on : 2023-12-12
Resolution : 3.97 Å(reported)
Based on initial model : .

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.dev112
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

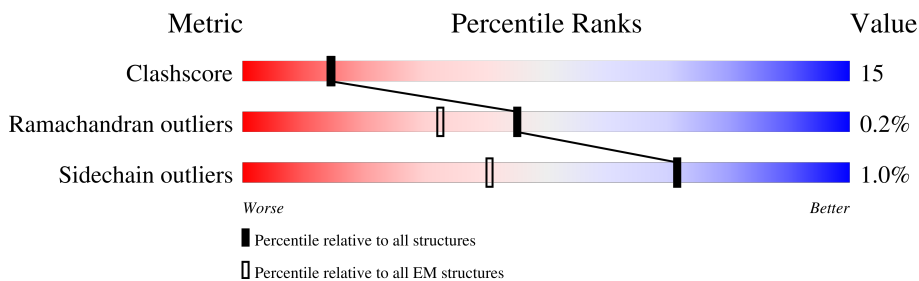
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.97 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1564	
2	H	467	
3	L	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BGC	A	1604	X	-	-	-
4	BGC	A	1614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BGC	A	1620	X	-	-	-
4	BGC	A	1624	X	-	-	-
4	BGC	A	1627	X	-	-	-
4	BGC	A	1630	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9444 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 EtpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1038	7293	4358	1361	1563	11	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	GLY	SER	conflict	UNP Q29XT7
A	534	GLY	SER	conflict	UNP Q29XT7
A	707	HIS	LEU	conflict	UNP Q29XT7
A	1104	ASN	SER	conflict	UNP Q29XT7
A	1476	ALA	THR	conflict	UNP Q29XT7
A	1481	PRO	THR	conflict	UNP Q29XT7
A	1484	ASP	GLY	conflict	UNP Q29XT7
A	1485	ASN	LYS	conflict	UNP Q29XT7
A	1488	TYR	HIS	conflict	UNP Q29XT7
A	1501	SER	ARG	conflict	UNP Q29XT7
A	1509	ASN	HIS	conflict	UNP Q29XT7
A	1512	THR	ALA	conflict	UNP Q29XT7
A	1522	THR	ARG	conflict	UNP Q29XT7
A	1529	THR	ALA	conflict	UNP Q29XT7
A	1535	GLU	-	expression tag	UNP Q29XT7
A	1536	VAL	-	expression tag	UNP Q29XT7
A	1537	TYR	-	expression tag	UNP Q29XT7
A	1538	TRP	-	expression tag	UNP Q29XT7
A	1539	GLN	-	expression tag	UNP Q29XT7
A	1540	LYS	-	expression tag	UNP Q29XT7
A	1541	LEU	-	expression tag	UNP Q29XT7
A	1542	GLY	-	expression tag	UNP Q29XT7
A	1543	PRO	-	expression tag	UNP Q29XT7
A	1544	GLU	-	expression tag	UNP Q29XT7
A	1545	GLN	-	expression tag	UNP Q29XT7
A	1546	LYS	-	expression tag	UNP Q29XT7
A	1547	LEU	-	expression tag	UNP Q29XT7
A	1548	ILE	-	expression tag	UNP Q29XT7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1549	SER	-	expression tag	UNP Q29XT7
A	1550	GLU	-	expression tag	UNP Q29XT7
A	1551	GLU	-	expression tag	UNP Q29XT7
A	1552	ASP	-	expression tag	UNP Q29XT7
A	1553	LEU	-	expression tag	UNP Q29XT7
A	1554	ASN	-	expression tag	UNP Q29XT7
A	1555	SER	-	expression tag	UNP Q29XT7
A	1556	ALA	-	expression tag	UNP Q29XT7
A	1557	VAL	-	expression tag	UNP Q29XT7
A	1558	ASP	-	expression tag	UNP Q29XT7
A	1559	HIS	-	expression tag	UNP Q29XT7
A	1560	HIS	-	expression tag	UNP Q29XT7
A	1561	HIS	-	expression tag	UNP Q29XT7
A	1562	HIS	-	expression tag	UNP Q29XT7
A	1563	HIS	-	expression tag	UNP Q29XT7
A	1564	HIS	-	expression tag	UNP Q29XT7

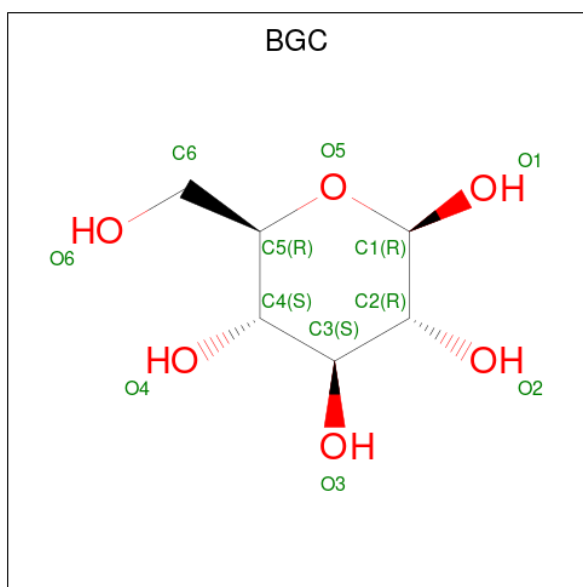
- Molecule 2 is a protein called mouse mAb 1G05 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	116	921	581	154	183	3	0	0

- Molecule 3 is a protein called mouse mAb 1G05 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	106	812	513	131	165	3	0	0

- Molecule 4 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	
4	A	1	Total	C	O	0
			11	6	5	

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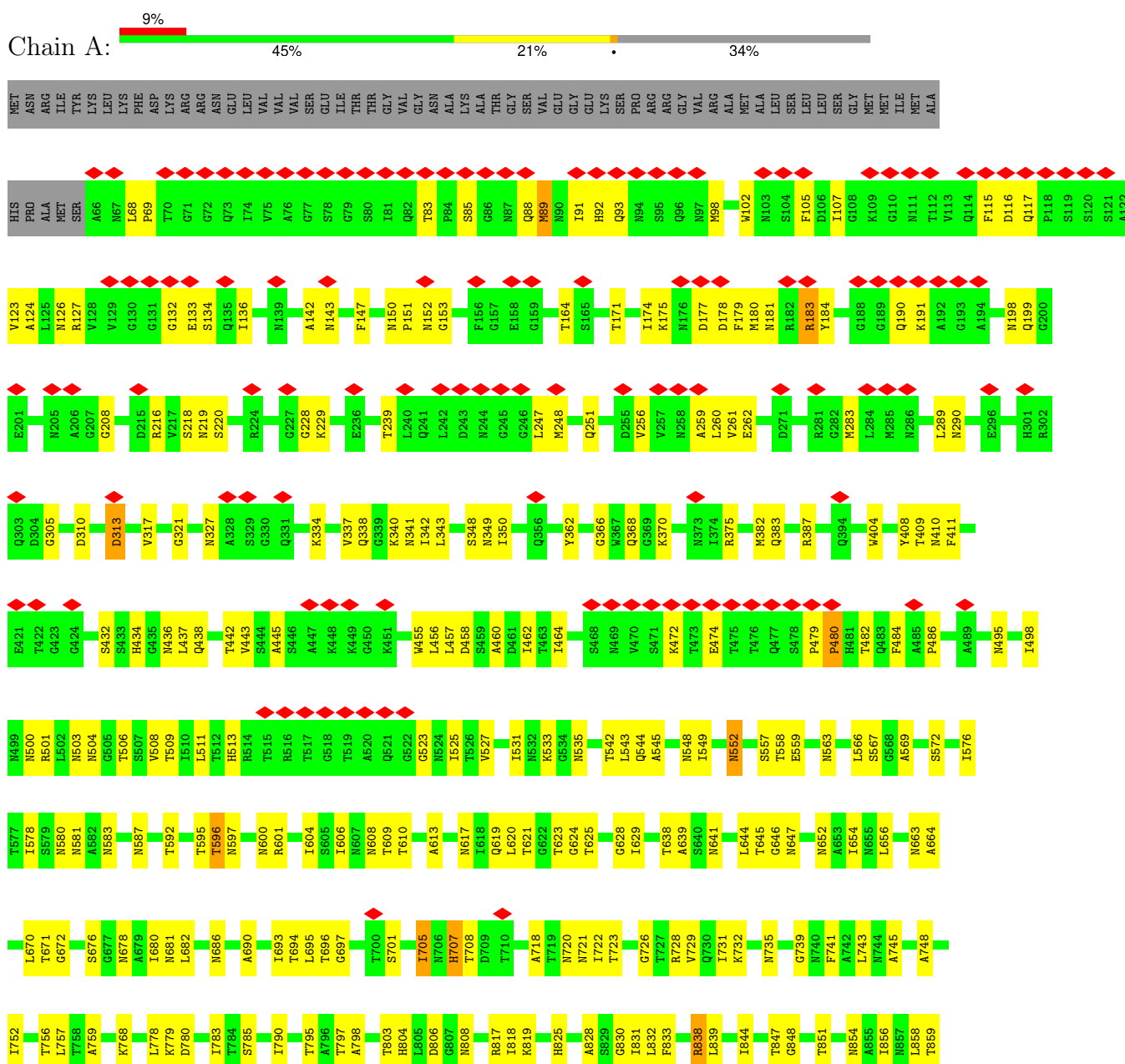
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	A	1	11	6	5	0
4	A	1	11	6	5	0
4	A	1	11	6	5	0

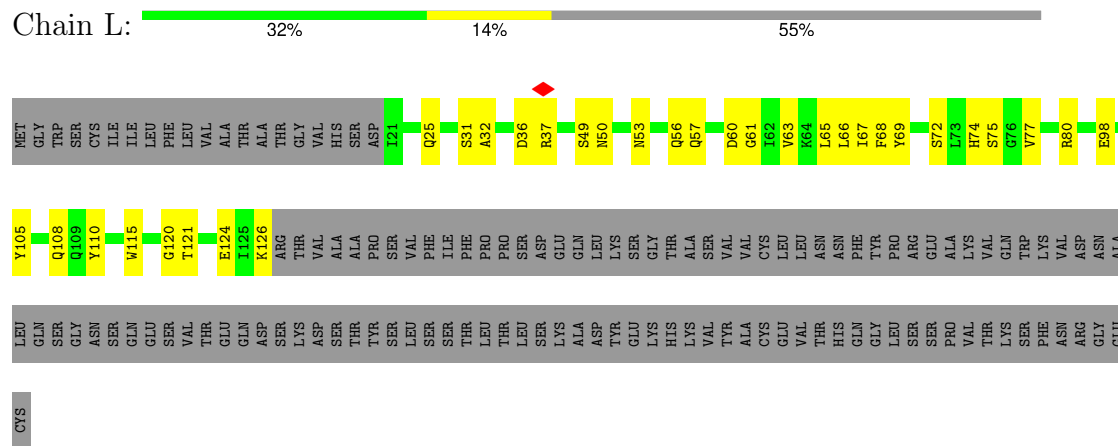
3 Residue-property plots

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

• Molecule 1: EtpA



● Molecule 3: mouse mAb 1G05 Light Chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.318	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0739	Depositor
Map size (Å)	435.0, 435.0, 435.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	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: BGC

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	0.33	0/7344	0.57	2/9993 (0.0%)
2	H	0.26	0/944	0.50	0/1285
3	L	0.28	0/831	0.49	0/1129
All	All	0.31	0/9119	0.56	2/12407 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	PRO	CA-N-CD	-8.13	100.12	111.50
1	A	313	ASP	CB-CG-OD2	6.29	123.96	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	601	ARG	Sidechain

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	7293	0	7132	240	0
2	H	921	0	872	25	0
3	L	812	0	781	18	0
4	A	418	0	379	13	0
All	All	9444	0	9164	280	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 15.

All (280) 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:604:ILE:HG21	1:A:620:LEU:HD23	1.57	0.84
1:A:239:THR:HB	1:A:251:GLN:HB2	1.65	0.79
1:A:656:LEU:HG	1:A:682:LEU:HD22	1.64	0.77
1:A:833:PHE:HB2	1:A:858:LEU:HA	1.65	0.76
1:A:625:THR:H	4:A:1631:BGC:H6C1	1.49	0.75
1:A:583:ASN:ND2	1:A:610:THR:HB	2.01	0.75
1:A:825:HIS:H	1:A:828:ALA:HB3	1.51	0.75
1:A:934:ASN:OD1	1:A:936:THR:HG22	1.89	0.73
1:A:581:ASN:HA	1:A:608:ASN:O	1.90	0.70
1:A:604:ILE:HB	1:A:629:ILE:HG22	1.73	0.70
1:A:935:LEU:HD23	1:A:942:THR:HG21	1.72	0.70
1:A:652:ASN:ND2	4:A:1610:BGC:O2	2.25	0.69
1:A:525:ILE:HG21	1:A:543:LEU:HD23	1.74	0.68
1:A:343:LEU:HD11	1:A:383:GLN:HG3	1.74	0.68
1:A:676:SER:HA	1:A:701:SER:HB2	1.76	0.68
1:A:1033:LEU:HD23	1:A:1037:VAL:HG11	1.74	0.68
1:A:620:LEU:HB2	1:A:644:LEU:HD13	1.75	0.67
1:A:337:VAL:HG12	1:A:342:ILE:HD13	1.76	0.67
1:A:680:ILE:HG21	1:A:695:LEU:HD23	1.78	0.66
1:A:682:LEU:HB3	1:A:686:ASN:HD21	1.62	0.65
1:A:790:ILE:HB	1:A:818:ILE:HD13	1.78	0.65
1:A:436:ASN:OD1	1:A:438:GLN:NE2	2.27	0.64
1:A:936:THR:OG1	1:A:960:LYS:HD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PRO:HD2	1:A:480:PRO:O	1.98	0.62
1:A:768:LYS:HG2	1:A:795:THR:HB	1.80	0.62
1:A:177:ASP:O	1:A:181:ASN:ND2	2.26	0.62
1:A:464:ILE:HG21	1:A:531:ILE:HD11	1.82	0.62
2:H:86:LYS:NZ	2:H:104:SER:O	2.33	0.61
1:A:682:LEU:HB3	1:A:686:ASN:ND2	2.16	0.61
1:A:549:ILE:HB	1:A:576:ILE:HG23	1.83	0.60
1:A:797:THR:HA	1:A:825:HIS:HB2	1.83	0.60
1:A:624:GLY:N	1:A:628:GLY:HA2	2.17	0.60
1:A:305:GLY:HA2	1:A:334:LYS:HB3	1.84	0.60
1:A:944:LEU:HB2	1:A:964:ILE:HG23	1.83	0.60
1:A:623:THR:HG22	1:A:647:ASN:HB2	1.83	0.59
3:L:65:LEU:HD21	3:L:68:PHE:HB3	1.82	0.59
1:A:743:LEU:HD11	1:A:752:ILE:HD11	1.83	0.59
3:L:25:GLN:NE2	3:L:121:THR:OG1	2.35	0.59
1:A:464:ILE:HD12	1:A:527:VAL:HG22	1.85	0.59
3:L:53:ASN:ND2	3:L:108:GLN:OE1	2.30	0.58
3:L:66:LEU:HD22	3:L:77:VAL:HG22	1.86	0.58
1:A:498:ILE:HG13	1:A:508:VAL:HG21	1.85	0.58
1:A:731:ILE:HD11	1:A:743:LEU:HD21	1.86	0.58
1:A:682:LEU:O	1:A:707:HIS:HA	2.04	0.57
1:A:728:ARG:HB2	1:A:748:ALA:HB3	1.85	0.57
1:A:472:LYS:NZ	1:A:474:GLU:OE2	2.36	0.57
1:A:629:ILE:HD11	1:A:654:ILE:HG12	1.87	0.57
1:A:117:GLN:O	1:A:143:ASN:ND2	2.37	0.56
1:A:624:GLY:H	1:A:628:GLY:HA2	1.71	0.56
1:A:578:ILE:HG22	1:A:609:THR:OG1	2.05	0.56
1:A:617:ASN:HD22	1:A:641:ASN:HB2	1.71	0.56
1:A:503:ASN:ND2	1:A:533:LYS:HA	2.21	0.56
1:A:503:ASN:HB3	1:A:535:ASN:HD21	1.71	0.56
1:A:664:ALA:HB3	1:A:690:ALA:HB2	1.87	0.55
2:H:105:LEU:HB3	2:H:135:VAL:HG11	1.88	0.55
2:H:54:HIS:HE1	3:L:115:TRP:CZ3	2.25	0.55
1:A:606:ILE:HG23	1:A:609:THR:HB	1.88	0.55
1:A:987:ALA:HB3	1:A:991:ILE:HG12	1.88	0.55
2:H:21:VAL:HG22	2:H:46:TYR:HB3	1.89	0.55
1:A:368:GLN:OE1	1:A:370:LYS:NZ	2.31	0.55
1:A:198:ASN:ND2	1:A:219:ASN:OD1	2.40	0.54
1:A:69:PRO:HB3	1:A:105:PHE:HA	1.89	0.54
1:A:183:ARG:HH21	1:A:184:TYR:C	2.10	0.54
1:A:617:ASN:ND2	1:A:641:ASN:HD22	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:ASN:OD1	1:A:896:ILE:N	2.40	0.54
1:A:697:GLY:O	1:A:726:GLY:HA2	2.07	0.54
1:A:808:ASN:OD1	1:A:808:ASN:N	2.40	0.54
1:A:134:SER:OG	1:A:150:ASN:ND2	2.37	0.53
1:A:851:THR:HG21	3:L:68:PHE:HZ	1.73	0.53
3:L:110:TYR:HA	3:L:115:TRP:HD1	1.73	0.53
2:H:67:ILE:HG21	2:H:100:MET:HE3	1.91	0.53
1:A:248:MET:SD	1:A:248:MET:N	2.82	0.53
1:A:1061:PHE:HB2	1:A:1086:LEU:HA	1.91	0.53
1:A:1074:LEU:HB2	1:A:1100:LEU:HG	1.90	0.53
4:A:1630:BGC:O6	2:H:50:ASN:O	2.21	0.53
2:H:102:LEU:HB3	2:H:105:LEU:HD21	1.90	0.53
1:A:708:THR:HG23	1:A:732:LYS:HD3	1.90	0.52
1:A:595:THR:HG21	1:A:600:ASN:HD22	1.74	0.52
1:A:349:ASN:OD1	1:A:387:ARG:NH1	2.43	0.52
1:A:434:HIS:CD2	1:A:513:HIS:HE1	2.27	0.52
1:A:563:ASN:ND2	4:A:1632:BGC:O6	2.43	0.52
1:A:971:LEU:HD11	1:A:980:ILE:HD11	1.92	0.52
1:A:180:MET:SD	1:A:180:MET:N	2.83	0.52
1:A:410:ASN:HA	1:A:438:GLN:HB2	1.92	0.52
1:A:525:ILE:HG13	1:A:545:ALA:HB2	1.92	0.52
1:A:646:GLY:O	1:A:672:GLY:HA2	2.10	0.52
2:H:42:LYS:NZ	2:H:95:SER:O	2.32	0.52
1:A:127:ARG:NH2	1:A:174:ILE:O	2.40	0.51
2:H:25:GLN:H	2:H:129:GLN:HE22	1.57	0.51
4:A:1630:BGC:H6C2	2:H:51:TYR:HA	1.92	0.51
1:A:535:ASN:HA	1:A:559:GLU:CD	2.31	0.51
1:A:825:HIS:CD2	2:H:121:VAL:HG23	2.46	0.51
1:A:1039:LEU:HD12	1:A:1067:LEU:HG	1.93	0.51
2:H:47:ILE:HB	2:H:50:ASN:HB2	1.92	0.51
1:A:569:ALA:O	1:A:600:ASN:ND2	2.44	0.51
1:A:735:ASN:ND2	1:A:756:THR:OG1	2.39	0.51
1:A:350:ILE:H	1:A:350:ILE:HD12	1.75	0.51
3:L:36:ASP:OD2	3:L:37:ARG:N	2.43	0.50
1:A:690:ALA:O	1:A:718:ALA:HA	2.12	0.50
2:H:117:ARG:NH2	2:H:125:ASP:OD2	2.44	0.50
1:A:558:THR:O	1:A:587:ASN:ND2	2.45	0.50
1:A:310:ASP:OD1	1:A:375:ARG:NH1	2.45	0.50
1:A:844:ILE:HG21	1:A:864:LEU:HD23	1.93	0.50
3:L:67:ILE:HG23	3:L:72:SER:H	1.77	0.50
1:A:741:PHE:HE2	1:A:743:LEU:HG	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:PHE:HE1	1:A:971:LEU:HG	1.77	0.49
1:A:621:THR:HG23	1:A:645:THR:HB	1.93	0.49
1:A:798:ALA:O	1:A:828:ALA:HB2	2.12	0.49
2:H:27:GLY:O	2:H:131:THR:OG1	2.30	0.49
1:A:933:ILE:HD12	1:A:957:VAL:HG22	1.93	0.49
1:A:623:THR:CG2	1:A:647:ASN:HB2	2.42	0.49
1:A:883:ASN:OD1	1:A:909:ASN:HB3	2.13	0.49
1:A:1045:ARG:HG3	1:A:1071:ASN:HB2	1.95	0.49
1:A:613:ALA:HB3	1:A:639:ALA:HB2	1.94	0.49
1:A:313:ASP:O	1:A:340:LYS:HD2	2.12	0.49
1:A:404:TRP:HE3	1:A:432:SER:HG	1.59	0.49
1:A:549:ILE:HG21	1:A:566:LEU:HB3	1.94	0.49
1:A:880:ASN:OD1	1:A:906:ASN:HB2	2.12	0.48
1:A:92:HIS:HA	1:A:116:ASP:HB3	1.95	0.48
1:A:535:ASN:HA	1:A:559:GLU:OE1	2.13	0.48
1:A:869:ASP:N	1:A:869:ASP:OD1	2.46	0.48
1:A:83:THR:HG22	1:A:89:MET:HG2	1.95	0.48
1:A:678:ASN:ND2	1:A:681:ASN:OD1	2.45	0.48
3:L:32:ALA:O	3:L:126:LYS:N	2.47	0.48
1:A:115:PHE:HB3	1:A:117:GLN:HE21	1.79	0.48
1:A:256:VAL:HG23	1:A:259:ALA:HB2	1.96	0.48
1:A:289:LEU:HB3	1:A:317:VAL:HG22	1.96	0.48
1:A:460:ALA:O	1:A:523:GLY:HA2	2.14	0.48
1:A:123:VAL:HG13	1:A:147:PHE:CE2	2.49	0.47
1:A:445:ALA:H	1:A:506:THR:HG21	1.79	0.47
3:L:57:GLN:HB2	3:L:63:VAL:HG22	1.96	0.47
1:A:93:GLN:HB3	1:A:117:GLN:HA	1.96	0.47
1:A:900:GLY:O	1:A:925:GLY:HA2	2.14	0.47
2:H:23:LEU:HD12	2:H:41:CYS:SG	2.54	0.47
1:A:644:LEU:HB2	1:A:670:LEU:HD22	1.96	0.47
1:A:432:SER:HB2	1:A:458:ASP:HB3	1.96	0.47
3:L:60:ASP:OD1	3:L:61:GLY:N	2.47	0.47
1:A:115:PHE:HZ	1:A:126:ASN:HD21	1.63	0.47
1:A:455:TRP:CE2	1:A:457:LEU:HD11	2.50	0.47
1:A:68:LEU:HD13	1:A:89:MET:HB2	1.96	0.47
1:A:596:THR:HG23	1:A:597:ASN:N	2.30	0.47
1:A:317:VAL:HB	1:A:342:ILE:HG12	1.96	0.46
1:A:341:ASN:HB3	1:A:484:PHE:CE1	2.50	0.46
1:A:229:LYS:HB2	1:A:247:LEU:HD23	1.97	0.46
1:A:970:ALA:HA	1:A:992:ASN:O	2.15	0.46
1:A:911:LYS:HD2	4:A:1638:BGC:O6	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:ARG:HB2	2:H:67:ILE:HD11	1.96	0.46
1:A:580:ASN:HB2	4:A:1614:BGC:O2	2.15	0.46
1:A:693:ILE:HG23	1:A:722:ILE:HG23	1.97	0.46
1:A:362:TYR:CD1	1:A:366:GLY:HA2	2.51	0.46
1:A:705:ILE:HG22	1:A:707:HIS:CE1	2.51	0.46
2:H:124:PHE:CD1	2:H:124:PHE:N	2.83	0.46
1:A:85:SER:HB3	1:A:88:GLN:HB3	1.98	0.46
3:L:56:GLN:NE2	3:L:105:TYR:OH	2.49	0.46
1:A:495:ASN:HA	1:A:498:ILE:HG22	1.97	0.46
1:A:1002:SER:HB2	1:A:1005:TYR:HB2	1.98	0.46
1:A:1053:HIS:H	1:A:1056:ALA:HB3	1.81	0.46
3:L:74:HIS:CG	3:L:75:SER:H	2.34	0.46
1:A:443:VAL:HG21	1:A:455:TRP:CD1	2.51	0.45
1:A:937:ASP:OD2	1:A:940:GLY:N	2.45	0.45
1:A:1014:THR:O	1:A:1043:ASN:ND2	2.47	0.45
1:A:93:GLN:HE22	1:A:124:ALA:HB2	1.80	0.45
1:A:455:TRP:CD2	1:A:457:LEU:HD11	2.51	0.45
1:A:720:ASN:ND2	1:A:721:ASN:OD1	2.50	0.45
1:A:956:ARG:NH1	1:A:976:ALA:O	2.45	0.45
1:A:313:ASP:O	1:A:313:ASP:OD2	2.35	0.45
2:H:79:TYR:OH	2:H:89:LEU:N	2.43	0.45
1:A:694:THR:HG22	1:A:723:THR:HB	1.98	0.45
1:A:1096:ASN:ND2	1:A:1097:ASP:OD1	2.49	0.45
1:A:503:ASN:HB3	1:A:535:ASN:ND2	2.31	0.45
1:A:752:ILE:HB	1:A:778:LEU:HD22	1.98	0.45
1:A:442:THR:HA	1:A:501:ARG:HH12	1.82	0.45
1:A:479:PRO:HD2	1:A:482:THR:HG21	1.99	0.45
1:A:847:THR:HG21	4:A:1630:BGC:H3	1.99	0.45
1:A:918:ALA:O	1:A:946:ALA:HA	2.17	0.45
1:A:443:VAL:H	1:A:501:ARG:CZ	2.30	0.45
1:A:569:ALA:HB3	1:A:572:SER:HB2	1.98	0.44
2:H:60:PRO:O	2:H:61:ILE:HG22	2.18	0.44
2:H:100:MET:HE2	2:H:102:LEU:HD21	1.98	0.44
2:H:105:LEU:HD12	2:H:135:VAL:HG21	1.99	0.44
1:A:69:PRO:HB2	1:A:102:TRP:CE3	2.52	0.44
1:A:408:TYR:CD1	1:A:486:PRO:HB3	2.53	0.44
1:A:720:ASN:HD22	4:A:1612:BGC:H2	1.83	0.44
1:A:955:THR:HB	1:A:975:VAL:HB	1.99	0.44
1:A:1076:GLY:O	1:A:1102:GLY:HA2	2.17	0.44
1:A:1059:ILE:HD11	1:A:1075:THR:O	2.16	0.44
1:A:779:LYS:HA	1:A:806:ASP:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:PHE:CD1	1:A:858:LEU:HG	2.53	0.44
3:L:80:ARG:NH1	3:L:98:GLU:OE2	2.51	0.44
1:A:93:GLN:HG3	1:A:98:MET:CE	2.48	0.44
1:A:229:LYS:HD2	1:A:247:LEU:HG	1.99	0.44
1:A:107:ILE:HD12	1:A:136:ILE:HG23	2.00	0.44
1:A:625:THR:N	4:A:1631:BGC:H6C1	2.24	0.43
2:H:43:ALA:HB1	2:H:46:TYR:CE1	2.53	0.43
1:A:93:GLN:NE2	1:A:124:ALA:HB2	2.34	0.43
1:A:123:VAL:HG12	1:A:179:PHE:CZ	2.53	0.43
1:A:503:ASN:HD21	1:A:533:LYS:HA	1.82	0.43
1:A:720:ASN:O	1:A:739:GLY:HA3	2.19	0.43
1:A:544:GLN:HA	1:A:567:SER:O	2.18	0.43
2:H:55:TRP:CZ3	2:H:115:CYS:HB3	2.53	0.43
1:A:831:ILE:HG22	1:A:856:ILE:HA	2.00	0.43
1:A:729:VAL:HG11	1:A:743:LEU:HD22	2.01	0.43
1:A:98:MET:HE2	1:A:98:MET:HB3	1.93	0.43
1:A:578:ILE:HG21	1:A:609:THR:HG21	2.01	0.43
1:A:638:THR:HA	1:A:663:ASN:O	2.18	0.43
1:A:817:ARG:HH12	1:A:819:LYS:HE3	1.84	0.43
3:L:25:GLN:OE1	3:L:120:GLY:N	2.41	0.43
1:A:500:ASN:O	1:A:504:ASN:ND2	2.49	0.42
1:A:175:LYS:HE3	1:A:175:LYS:HB3	1.66	0.42
1:A:1007:LYS:HA	1:A:1034:ASP:O	2.18	0.42
1:A:613:ALA:HB3	1:A:639:ALA:CB	2.49	0.42
1:A:741:PHE:CE2	1:A:743:LEU:HG	2.54	0.42
1:A:759:ALA:O	1:A:785:SER:HA	2.19	0.42
1:A:178:ASP:HB3	1:A:183:ARG:HG3	2.01	0.42
1:A:462:ILE:HG23	1:A:525:ILE:HG12	2.01	0.42
1:A:509:THR:HG23	1:A:542:THR:OG1	2.20	0.42
1:A:199:GLN:HG2	1:A:220:SER:HB2	2.01	0.42
1:A:409:THR:HB	1:A:437:LEU:HD12	2.01	0.42
1:A:596:THR:HG23	1:A:597:ASN:H	1.85	0.42
1:A:93:GLN:HG3	1:A:98:MET:HE1	2.02	0.42
1:A:604:ILE:HD11	1:A:621:THR:O	2.20	0.42
1:A:956:ARG:HB2	1:A:976:ALA:HB3	2.02	0.42
3:L:31:SER:HA	3:L:124:GLU:O	2.19	0.42
1:A:694:THR:HA	1:A:723:THR:O	2.20	0.42
1:A:132:GLY:HA2	1:A:152:ASN:HD22	1.84	0.42
1:A:142:ALA:HB3	1:A:164:THR:HG22	2.00	0.42
1:A:671:THR:HA	1:A:696:THR:O	2.20	0.42
1:A:868:ASN:O	1:A:894:ASN:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:SER:O	1:A:902:SER:HA	2.20	0.42
1:A:981:SER:HA	1:A:1007:LYS:O	2.20	0.42
1:A:1047:LYS:HA	1:A:1073:ALA:O	2.20	0.42
1:A:892:ALA:O	1:A:918:ALA:HA	2.20	0.41
3:L:49:SER:OG	3:L:50:ASN:N	2.52	0.41
1:A:757:LEU:O	1:A:783:ILE:HA	2.20	0.41
1:A:861:THR:HG22	1:A:887:THR:HB	2.01	0.41
1:A:89:MET:CE	1:A:91:ILE:HG13	2.49	0.41
1:A:177:ASP:OD1	1:A:181:ASN:ND2	2.54	0.41
1:A:208:GLY:O	1:A:228:GLY:HA3	2.19	0.41
1:A:548:ASN:O	1:A:549:ILE:HD13	2.20	0.41
1:A:625:THR:HG23	4:A:1631:BGC:H6C1	2.03	0.41
1:A:151:PRO:O	1:A:191:LYS:HB3	2.20	0.41
1:A:262:GLU:HA	1:A:290:ASN:O	2.19	0.41
1:A:338:GLN:C	1:A:342:ILE:HD11	2.41	0.41
1:A:1027:ASN:HA	1:A:1056:ALA:HB2	2.01	0.41
2:H:124:PHE:N	2:H:124:PHE:HD1	2.17	0.41
1:A:549:ILE:HG22	1:A:549:ILE:O	2.19	0.41
2:H:55:TRP:CE2	2:H:100:MET:HB2	2.55	0.41
1:A:838:ARG:HG3	1:A:863:THR:HB	2.02	0.41
1:A:869:ASP:HB3	1:A:895:ASN:HB3	2.02	0.41
1:A:133:GLU:HG3	1:A:153:GLY:C	2.41	0.41
1:A:948:ASN:OD1	4:A:1624:BGC:O2	2.34	0.41
1:A:171:THR:HG22	1:A:190:GLN:HB2	2.01	0.41
1:A:218:SER:HA	1:A:262:GLU:O	2.21	0.41
1:A:552:ASN:ND2	1:A:580:ASN:HB2	2.35	0.41
1:A:592:THR:HA	1:A:619:GLN:O	2.21	0.41
1:A:726:GLY:O	1:A:745:ALA:HA	2.20	0.41
1:A:654:ILE:HD12	1:A:680:ILE:HG12	2.03	0.41
1:A:729:VAL:HG12	1:A:731:ILE:HG13	2.03	0.41
1:A:804:HIS:CG	1:A:832:LEU:HD23	2.56	0.41
1:A:880:ASN:HA	1:A:906:ASN:O	2.21	0.41
1:A:881:ALA:HB3	1:A:907:ALA:O	2.20	0.41
1:A:321:GLY:O	1:A:348:SER:HA	2.21	0.40
1:A:803:THR:O	1:A:832:LEU:N	2.51	0.40
1:A:830:GLY:N	1:A:854:ASN:O	2.50	0.40
1:A:839:LEU:O	1:A:864:LEU:HA	2.21	0.40
1:A:859:THR:HG23	1:A:885:THR:HG23	2.02	0.40
1:A:216:ARG:HE	1:A:218:SER:HB2	1.87	0.40
1:A:442:THR:HA	1:A:501:ARG:NH1	2.37	0.40
1:A:557:SER:O	1:A:587:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:LEU:HB2	1:A:910:LEU:HD22	2.03	0.40
1:A:933:ILE:HD11	1:A:953:GLN:O	2.21	0.40
1:A:382:MET:HB3	1:A:411:PHE:HA	2.03	0.40
1:A:456:LEU:HD11	1:A:511:LEU:HD13	2.02	0.40
1:A:856:ILE:HG21	1:A:872:LEU:HD23	2.01	0.40
1:A:1059:ILE:HD13	1:A:1074:LEU:HD12	2.03	0.40
1:A:1054:GLY:O	1:A:1079:THR:OG1	2.39	0.40
1:A:260:LEU:HD23	1:A:261:VAL:N	2.36	0.40
1:A:720:ASN:ND2	4:A:1612:BGC:H4	2.36	0.40
1:A:848:GLY:O	1:A:874:GLY:HA2	2.21	0.40
1:A:957:VAL:HG11	1:A:971:LEU:HD22	2.03	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	1036/1564 (66%)	989 (96%)	46 (4%)	1 (0%)	48 81
2	H	114/467 (24%)	108 (95%)	4 (4%)	2 (2%)	7 35
3	L	104/233 (45%)	96 (92%)	8 (8%)	0	100 100
All	All	1254/2264 (55%)	1193 (95%)	58 (5%)	3 (0%)	45 76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	596	THR
2	H	120	ALA
2	H	61	ILE

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	791/1204 (66%)	782 (99%)	9 (1%)	70	80
2	H	103/419 (25%)	103 (100%)	0	100	100
3	L	93/205 (45%)	92 (99%)	1 (1%)	70	80
All	All	987/1828 (54%)	977 (99%)	10 (1%)	71	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	MET
1	A	183	ARG
1	A	283	MET
1	A	327	ASN
1	A	552	ASN
1	A	705	ILE
1	A	707	HIS
1	A	780	ASP
1	A	838	ARG
3	L	69	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	96	GLN
1	A	327	ASN
1	A	331	GLN
1	A	410	ASN
1	A	434	HIS
1	A	503	ASN
1	A	513	HIS
1	A	553	ASN
1	A	563	ASN
1	A	587	ASN

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Mol	Chain	Res	Type
1	A	607	ASN
1	A	617	ASN
1	A	652	ASN
1	A	720	ASN
1	A	825	HIS
1	A	958	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

38 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BGC	A	1606	1	11,11,12	2.51	7 (63%)	15,15,17	1.99	5 (33%)
4	BGC	A	1603	1	11,11,12	2.50	7 (63%)	15,15,17	1.97	6 (40%)
4	BGC	A	1618	1	11,11,12	2.46	6 (54%)	15,15,17	2.00	6 (40%)
4	BGC	A	1638	1	11,11,12	0.20	0	15,15,17	0.44	0
4	BGC	A	1628	1	11,11,12	2.47	6 (54%)	15,15,17	2.18	5 (33%)
4	BGC	A	1626	1	11,11,12	0.17	0	15,15,17	0.47	0
4	BGC	A	1620	1	11,11,12	2.42	7 (63%)	15,15,17	2.03	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BGC	A	1631	1	11,11,12	0.18	0	15,15,17	0.43	0
4	BGC	A	1602	1	11,11,12	2.39	6 (54%)	15,15,17	2.02	7 (46%)
4	BGC	A	1621	1	11,11,12	2.46	6 (54%)	15,15,17	2.07	6 (40%)
4	BGC	A	1635	1	11,11,12	2.46	6 (54%)	15,15,17	1.98	7 (46%)
4	BGC	A	1630	1	11,11,12	2.50	5 (45%)	15,15,17	2.14	6 (40%)
4	BGC	A	1605	1	11,11,12	0.16	0	15,15,17	0.48	0
4	BGC	A	1609	1	11,11,12	0.19	0	15,15,17	0.45	0
4	BGC	A	1607	1	11,11,12	0.20	0	15,15,17	0.41	0
4	BGC	A	1627	1	11,11,12	2.41	7 (63%)	15,15,17	2.01	7 (46%)
4	BGC	A	1637	1	11,11,12	2.46	6 (54%)	15,15,17	1.99	5 (33%)
4	BGC	A	1622	1	11,11,12	2.38	6 (54%)	15,15,17	2.07	6 (40%)
4	BGC	A	1623	1	11,11,12	2.45	6 (54%)	15,15,17	2.04	7 (46%)
4	BGC	A	1625	1	11,11,12	2.48	6 (54%)	15,15,17	1.93	5 (33%)
4	BGC	A	1615	1	11,11,12	2.49	6 (54%)	15,15,17	2.00	6 (40%)
4	BGC	A	1633	1	11,11,12	2.28	7 (63%)	15,15,17	2.21	7 (46%)
4	BGC	A	1636	1	11,11,12	2.43	6 (54%)	15,15,17	1.99	7 (46%)
4	BGC	A	1611	1	11,11,12	0.16	0	15,15,17	0.65	1 (6%)
4	BGC	A	1616	1	11,11,12	2.44	6 (54%)	15,15,17	1.99	7 (46%)
4	BGC	A	1610	1	11,11,12	2.32	6 (54%)	15,15,17	2.16	7 (46%)
4	BGC	A	1617	1	11,11,12	2.37	6 (54%)	15,15,17	2.06	7 (46%)
4	BGC	A	1612	1	11,11,12	0.22	0	15,15,17	0.40	0
4	BGC	A	1632	1	11,11,12	2.53	6 (54%)	15,15,17	1.95	5 (33%)
4	BGC	A	1619	1	11,11,12	2.41	6 (54%)	15,15,17	2.04	7 (46%)
4	BGC	A	1624	1	11,11,12	2.45	6 (54%)	15,15,17	2.01	6 (40%)
4	BGC	A	1629	1	11,11,12	2.46	6 (54%)	15,15,17	2.00	7 (46%)
4	BGC	A	1604	1	11,11,12	2.36	6 (54%)	15,15,17	2.02	7 (46%)
4	BGC	A	1601	1	11,11,12	2.46	6 (54%)	15,15,17	1.99	7 (46%)
4	BGC	A	1614	1	11,11,12	0.24	0	15,15,17	0.65	0
4	BGC	A	1634	1	11,11,12	2.45	6 (54%)	15,15,17	2.04	7 (46%)
4	BGC	A	1608	1	11,11,12	0.18	0	15,15,17	0.40	0
4	BGC	A	1613	1	11,11,12	2.37	6 (54%)	15,15,17	2.12	7 (46%)

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	BGC	A	1606	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1603	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1618	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1638	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1628	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1626	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1620	1	1/1/4/5	2/2/19/22	0/1/1/1
4	BGC	A	1631	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1602	1	-	1/2/19/22	0/1/1/1
4	BGC	A	1621	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1635	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1630	1	1/1/4/5	2/2/19/22	0/1/1/1
4	BGC	A	1605	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1609	1	-	1/2/19/22	0/1/1/1
4	BGC	A	1607	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1627	1	1/1/4/5	1/2/19/22	0/1/1/1
4	BGC	A	1637	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1622	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1623	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1625	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1615	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1633	1	-	1/2/19/22	0/1/1/1
4	BGC	A	1636	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1611	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1616	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1610	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1617	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1612	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1632	1	-	0/2/19/22	0/1/1/1
4	BGC	A	1619	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1624	1	1/1/4/5	1/2/19/22	0/1/1/1
4	BGC	A	1629	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1604	1	1/1/4/5	2/2/19/22	0/1/1/1
4	BGC	A	1614	1	1/1/4/5	0/2/19/22	0/1/1/1
4	BGC	A	1601	1	-	2/2/19/22	0/1/1/1
4	BGC	A	1634	1	-	1/2/19/22	0/1/1/1
4	BGC	A	1608	1	-	1/2/19/22	0/1/1/1
4	BGC	A	1613	1	-	0/2/19/22	0/1/1/1

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1632	BGC	C2-C3	4.80	1.59	1.52
4	A	1606	BGC	C2-C3	4.70	1.59	1.52
4	A	1636	BGC	C2-C3	4.61	1.59	1.52
4	A	1603	BGC	C2-C3	4.58	1.59	1.52
4	A	1615	BGC	C2-C3	4.52	1.59	1.52
4	A	1628	BGC	C2-C3	4.51	1.59	1.52
4	A	1637	BGC	C2-C3	4.50	1.59	1.52
4	A	1618	BGC	C2-C3	4.47	1.59	1.52
4	A	1624	BGC	C2-C3	4.45	1.59	1.52
4	A	1635	BGC	C2-C3	4.42	1.59	1.52
4	A	1621	BGC	C2-C3	4.41	1.59	1.52
4	A	1601	BGC	C2-C3	4.41	1.59	1.52
4	A	1620	BGC	C2-C3	4.38	1.59	1.52
4	A	1625	BGC	C2-C3	4.34	1.59	1.52
4	A	1629	BGC	C2-C3	4.34	1.59	1.52
4	A	1627	BGC	C2-C3	4.31	1.59	1.52
4	A	1616	BGC	C2-C3	4.29	1.59	1.52
4	A	1619	BGC	C2-C3	4.28	1.59	1.52
4	A	1617	BGC	C2-C3	4.28	1.59	1.52
4	A	1602	BGC	C2-C3	4.26	1.59	1.52
4	A	1630	BGC	O5-C1	-4.15	1.36	1.43
4	A	1623	BGC	C2-C3	4.12	1.58	1.52
4	A	1604	BGC	C2-C3	4.11	1.58	1.52
4	A	1634	BGC	C2-C3	4.04	1.58	1.52
4	A	1613	BGC	C2-C3	4.03	1.58	1.52
4	A	1622	BGC	C2-C3	4.03	1.58	1.52
4	A	1610	BGC	C2-C3	3.92	1.58	1.52
4	A	1630	BGC	O5-C5	-3.87	1.35	1.43
4	A	1632	BGC	O5-C5	-3.85	1.35	1.43
4	A	1621	BGC	O5-C5	-3.81	1.36	1.43
4	A	1633	BGC	C2-C3	3.74	1.58	1.52
4	A	1630	BGC	C2-C3	3.73	1.58	1.52
4	A	1623	BGC	O5-C5	-3.69	1.36	1.43
4	A	1625	BGC	O5-C5	-3.69	1.36	1.43
4	A	1616	BGC	O5-C5	-3.68	1.36	1.43
4	A	1606	BGC	O5-C5	-3.66	1.36	1.43
4	A	1603	BGC	O5-C5	-3.64	1.36	1.43
4	A	1634	BGC	O5-C5	-3.64	1.36	1.43
4	A	1624	BGC	O5-C5	-3.63	1.36	1.43
4	A	1628	BGC	O5-C5	-3.63	1.36	1.43
4	A	1615	BGC	O5-C5	-3.59	1.36	1.43
4	A	1634	BGC	O5-C1	-3.56	1.37	1.43
4	A	1637	BGC	O5-C5	-3.55	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1618	BGC	O5-C5	-3.54	1.36	1.43
4	A	1635	BGC	O5-C5	-3.53	1.36	1.43
4	A	1613	BGC	O5-C5	-3.52	1.36	1.43
4	A	1629	BGC	O5-C5	-3.50	1.36	1.43
4	A	1617	BGC	O5-C5	-3.48	1.36	1.43
4	A	1622	BGC	O5-C5	-3.45	1.36	1.43
4	A	1619	BGC	O5-C5	-3.40	1.36	1.43
4	A	1601	BGC	O5-C5	-3.39	1.36	1.43
4	A	1604	BGC	O5-C5	-3.37	1.36	1.43
4	A	1620	BGC	O5-C5	-3.37	1.36	1.43
4	A	1627	BGC	O5-C5	-3.36	1.36	1.43
4	A	1615	BGC	O5-C1	-3.34	1.38	1.43
4	A	1623	BGC	O5-C1	-3.31	1.38	1.43
4	A	1606	BGC	O5-C1	-3.27	1.38	1.43
4	A	1610	BGC	O5-C5	-3.24	1.37	1.43
4	A	1636	BGC	O5-C5	-3.24	1.37	1.43
4	A	1602	BGC	O5-C5	-3.23	1.37	1.43
4	A	1625	BGC	O5-C1	-3.21	1.38	1.43
4	A	1624	BGC	O5-C1	-3.19	1.38	1.43
4	A	1601	BGC	O5-C1	-3.18	1.38	1.43
4	A	1616	BGC	O5-C1	-3.18	1.38	1.43
4	A	1603	BGC	O5-C1	-3.18	1.38	1.43
4	A	1635	BGC	O5-C1	-3.16	1.38	1.43
4	A	1633	BGC	O5-C5	-3.15	1.37	1.43
4	A	1610	BGC	O5-C1	-3.13	1.38	1.43
4	A	1629	BGC	O5-C1	-3.11	1.38	1.43
4	A	1622	BGC	O5-C1	-3.11	1.38	1.43
4	A	1632	BGC	O5-C1	-3.10	1.38	1.43
4	A	1619	BGC	O5-C1	-3.09	1.38	1.43
4	A	1627	BGC	O5-C1	-3.05	1.38	1.43
4	A	1637	BGC	O5-C1	-3.05	1.38	1.43
4	A	1613	BGC	O5-C1	-3.02	1.38	1.43
4	A	1604	BGC	O5-C1	-3.01	1.38	1.43
4	A	1602	BGC	O5-C1	-3.01	1.38	1.43
4	A	1620	BGC	O5-C1	-3.01	1.38	1.43
4	A	1618	BGC	O5-C1	-2.97	1.38	1.43
4	A	1621	BGC	O5-C1	-2.94	1.38	1.43
4	A	1617	BGC	O5-C1	-2.92	1.38	1.43
4	A	1636	BGC	O5-C1	-2.83	1.38	1.43
4	A	1633	BGC	O5-C1	-2.80	1.39	1.43
4	A	1630	BGC	O2-C2	-2.78	1.37	1.43
4	A	1628	BGC	O5-C1	-2.77	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1628	BGC	O2-C2	-2.59	1.37	1.43
4	A	1601	BGC	C4-C3	2.49	1.58	1.52
4	A	1615	BGC	C4-C3	2.46	1.58	1.52
4	A	1619	BGC	C4-C3	2.42	1.58	1.52
4	A	1602	BGC	C4-C3	2.39	1.58	1.52
4	A	1629	BGC	C4-C3	2.37	1.58	1.52
4	A	1635	BGC	C4-C3	2.37	1.58	1.52
4	A	1636	BGC	C4-C3	2.37	1.58	1.52
4	A	1628	BGC	C1-C2	2.35	1.57	1.52
4	A	1610	BGC	O2-C2	-2.34	1.38	1.43
4	A	1621	BGC	O2-C2	-2.33	1.38	1.43
4	A	1625	BGC	O2-C2	-2.33	1.38	1.43
4	A	1618	BGC	C4-C3	2.33	1.58	1.52
4	A	1622	BGC	O2-C2	-2.32	1.38	1.43
4	A	1625	BGC	C4-C3	2.32	1.58	1.52
4	A	1637	BGC	O2-C2	-2.31	1.38	1.43
4	A	1623	BGC	C4-C3	2.31	1.58	1.52
4	A	1613	BGC	O2-C2	-2.31	1.38	1.43
4	A	1634	BGC	C4-C3	2.30	1.58	1.52
4	A	1603	BGC	C4-C3	2.30	1.58	1.52
4	A	1633	BGC	O2-C2	-2.29	1.38	1.43
4	A	1637	BGC	C4-C3	2.28	1.58	1.52
4	A	1616	BGC	C4-C3	2.28	1.58	1.52
4	A	1606	BGC	O2-C2	-2.27	1.38	1.43
4	A	1632	BGC	C4-C3	2.27	1.58	1.52
4	A	1616	BGC	O2-C2	-2.26	1.38	1.43
4	A	1627	BGC	C4-C3	2.25	1.58	1.52
4	A	1604	BGC	C4-C3	2.24	1.58	1.52
4	A	1618	BGC	O2-C2	-2.23	1.38	1.43
4	A	1620	BGC	O2-C2	-2.22	1.38	1.43
4	A	1624	BGC	O2-C2	-2.22	1.38	1.43
4	A	1620	BGC	C4-C3	2.22	1.58	1.52
4	A	1604	BGC	O2-C2	-2.22	1.38	1.43
4	A	1636	BGC	O2-C2	-2.21	1.38	1.43
4	A	1634	BGC	O2-C2	-2.20	1.38	1.43
4	A	1615	BGC	O2-C2	-2.20	1.38	1.43
4	A	1619	BGC	O2-C2	-2.20	1.38	1.43
4	A	1603	BGC	O2-C2	-2.19	1.38	1.43
4	A	1635	BGC	O2-C2	-2.19	1.38	1.43
4	A	1602	BGC	O2-C2	-2.19	1.38	1.43
4	A	1624	BGC	C4-C3	2.18	1.58	1.52
4	A	1617	BGC	O2-C2	-2.18	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1632	BGC	O2-C2	-2.17	1.38	1.43
4	A	1629	BGC	O2-C2	-2.17	1.38	1.43
4	A	1621	BGC	C1-C2	2.16	1.57	1.52
4	A	1613	BGC	C4-C3	2.15	1.57	1.52
4	A	1601	BGC	O2-C2	-2.15	1.38	1.43
4	A	1623	BGC	O2-C2	-2.15	1.38	1.43
4	A	1633	BGC	O3-C3	-2.14	1.37	1.43
4	A	1604	BGC	O3-C3	-2.14	1.37	1.43
4	A	1627	BGC	O2-C2	-2.14	1.38	1.43
4	A	1635	BGC	O3-C3	-2.13	1.37	1.43
4	A	1617	BGC	O3-C3	-2.13	1.37	1.43
4	A	1625	BGC	O3-C3	-2.13	1.37	1.43
4	A	1624	BGC	O3-C3	-2.13	1.37	1.43
4	A	1613	BGC	O3-C3	-2.13	1.37	1.43
4	A	1632	BGC	O3-C3	-2.13	1.37	1.43
4	A	1623	BGC	O3-C3	-2.13	1.37	1.43
4	A	1622	BGC	O3-C3	-2.13	1.37	1.43
4	A	1622	BGC	C4-C3	2.12	1.57	1.52
4	A	1602	BGC	O3-C3	-2.12	1.37	1.43
4	A	1637	BGC	O3-C3	-2.11	1.37	1.43
4	A	1636	BGC	O3-C3	-2.11	1.37	1.43
4	A	1616	BGC	O3-C3	-2.11	1.37	1.43
4	A	1619	BGC	O3-C3	-2.11	1.37	1.43
4	A	1601	BGC	O3-C3	-2.10	1.37	1.43
4	A	1618	BGC	O3-C3	-2.10	1.37	1.43
4	A	1615	BGC	O3-C3	-2.09	1.37	1.43
4	A	1620	BGC	C1-C2	2.09	1.57	1.52
4	A	1627	BGC	O3-C3	-2.09	1.37	1.43
4	A	1620	BGC	O3-C3	-2.09	1.37	1.43
4	A	1630	BGC	O3-C3	-2.09	1.37	1.43
4	A	1606	BGC	C1-C2	2.09	1.57	1.52
4	A	1617	BGC	C4-C3	2.09	1.57	1.52
4	A	1621	BGC	O3-C3	-2.08	1.37	1.43
4	A	1629	BGC	O3-C3	-2.07	1.37	1.43
4	A	1634	BGC	O3-C3	-2.07	1.37	1.43
4	A	1627	BGC	C1-C2	2.06	1.57	1.52
4	A	1610	BGC	C4-C3	2.06	1.57	1.52
4	A	1610	BGC	O3-C3	-2.06	1.37	1.43
4	A	1603	BGC	O3-C3	-2.05	1.37	1.43
4	A	1633	BGC	C1-C2	2.04	1.57	1.52
4	A	1633	BGC	C4-C3	2.04	1.57	1.52
4	A	1606	BGC	O3-C3	-2.03	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1628	BGC	O3-C3	-2.02	1.38	1.43
4	A	1603	BGC	C1-C2	2.02	1.57	1.52
4	A	1606	BGC	C4-C3	2.01	1.57	1.52

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1633	BGC	C1-O5-C5	4.60	118.35	112.19
4	A	1628	BGC	C1-O5-C5	4.47	118.17	112.19
4	A	1630	BGC	C1-O5-C5	4.19	117.80	112.19
4	A	1613	BGC	C1-O5-C5	4.15	117.74	112.19
4	A	1610	BGC	C1-O5-C5	4.12	117.71	112.19
4	A	1623	BGC	C1-O5-C5	4.06	117.63	112.19
4	A	1615	BGC	C1-O5-C5	4.05	117.61	112.19
4	A	1628	BGC	O2-C2-C3	-3.98	101.91	110.15
4	A	1617	BGC	C1-O5-C5	3.96	117.49	112.19
4	A	1629	BGC	C1-O5-C5	3.89	117.40	112.19
4	A	1602	BGC	C1-O5-C5	3.89	117.39	112.19
4	A	1636	BGC	C1-O5-C5	3.89	117.39	112.19
4	A	1601	BGC	C1-O5-C5	3.88	117.39	112.19
4	A	1618	BGC	C1-O5-C5	3.87	117.37	112.19
4	A	1619	BGC	C1-O5-C5	3.83	117.32	112.19
4	A	1620	BGC	C1-O5-C5	3.83	117.32	112.19
4	A	1621	BGC	C1-O5-C5	3.83	117.32	112.19
4	A	1604	BGC	C1-O5-C5	3.80	117.28	112.19
4	A	1622	BGC	C1-O5-C5	3.77	117.24	112.19
4	A	1624	BGC	C1-O5-C5	3.76	117.23	112.19
4	A	1635	BGC	C1-O5-C5	3.66	117.09	112.19
4	A	1634	BGC	C1-O5-C5	3.65	117.07	112.19
4	A	1616	BGC	C1-O5-C5	3.63	117.05	112.19
4	A	1627	BGC	C1-O5-C5	3.62	117.04	112.19
4	A	1603	BGC	C1-O5-C5	3.59	117.00	112.19
4	A	1606	BGC	O2-C2-C3	-3.55	102.79	110.15
4	A	1632	BGC	C1-O5-C5	3.48	116.86	112.19
4	A	1621	BGC	O2-C2-C3	-3.47	102.96	110.15
4	A	1637	BGC	C1-O5-C5	3.47	116.83	112.19
4	A	1606	BGC	C1-O5-C5	3.44	116.80	112.19
4	A	1630	BGC	O2-C2-C3	-3.41	103.10	110.15
4	A	1637	BGC	O2-C2-C3	-3.36	103.19	110.15
4	A	1625	BGC	C1-O5-C5	3.35	116.68	112.19
4	A	1625	BGC	O2-C2-C3	-3.35	103.21	110.15
4	A	1633	BGC	O2-C2-C3	-3.34	103.24	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1610	BGC	O2-C2-C3	-3.33	103.26	110.15
4	A	1624	BGC	O2-C2-C3	-3.25	103.41	110.15
4	A	1627	BGC	O2-C2-C3	-3.25	103.42	110.15
4	A	1622	BGC	O2-C2-C3	-3.23	103.45	110.15
4	A	1603	BGC	O2-C2-C3	-3.21	103.49	110.15
4	A	1632	BGC	O2-C2-C3	-3.19	103.55	110.15
4	A	1618	BGC	O2-C2-C3	-3.18	103.57	110.15
4	A	1613	BGC	O2-C2-C3	-3.14	103.64	110.15
4	A	1634	BGC	O2-C2-C3	-3.13	103.66	110.15
4	A	1617	BGC	O2-C2-C3	-3.12	103.68	110.15
4	A	1620	BGC	O2-C2-C3	-3.10	103.73	110.15
4	A	1619	BGC	O2-C2-C3	-3.09	103.76	110.15
4	A	1629	BGC	O2-C2-C3	-3.07	103.79	110.15
4	A	1604	BGC	O2-C2-C3	-3.06	103.82	110.15
4	A	1616	BGC	O2-C2-C3	-3.05	103.84	110.15
4	A	1635	BGC	O2-C2-C3	-3.02	103.89	110.15
4	A	1634	BGC	O4-C4-C3	-2.99	103.33	110.38
4	A	1623	BGC	O2-C2-C3	-2.98	103.97	110.15
4	A	1601	BGC	O2-C2-C3	-2.97	103.99	110.15
4	A	1615	BGC	O2-C2-C3	-2.95	104.04	110.15
4	A	1636	BGC	O2-C2-C3	-2.95	104.05	110.15
4	A	1602	BGC	O2-C2-C3	-2.94	104.07	110.15
4	A	1637	BGC	O5-C5-C6	2.93	113.38	107.66
4	A	1606	BGC	O4-C4-C3	-2.92	103.49	110.38
4	A	1623	BGC	O4-C4-C3	-2.92	103.50	110.38
4	A	1630	BGC	C2-C3-C4	-2.90	105.75	110.86
4	A	1629	BGC	O4-C4-C3	-2.89	103.57	110.38
4	A	1628	BGC	O4-C4-C3	-2.88	103.58	110.38
4	A	1610	BGC	O4-C4-C3	-2.88	103.60	110.38
4	A	1613	BGC	O4-C4-C3	-2.87	103.61	110.38
4	A	1603	BGC	O4-C4-C3	-2.84	103.69	110.38
4	A	1625	BGC	O4-C4-C3	-2.83	103.70	110.38
4	A	1622	BGC	O5-C5-C6	2.83	113.17	107.66
4	A	1601	BGC	O4-C4-C3	-2.83	103.70	110.38
4	A	1630	BGC	O4-C4-C3	-2.83	103.71	110.38
4	A	1615	BGC	O4-C4-C3	-2.82	103.74	110.38
4	A	1617	BGC	O4-C4-C3	-2.81	103.74	110.38
4	A	1618	BGC	O4-C4-C3	-2.81	103.75	110.38
4	A	1613	BGC	C1-C2-C3	-2.80	105.57	109.64
4	A	1606	BGC	O5-C5-C6	2.79	113.10	107.66
4	A	1602	BGC	O4-C4-C3	-2.79	103.80	110.38
4	A	1621	BGC	O4-C4-C3	-2.79	103.81	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1635	BGC	O4-C4-C3	-2.79	103.81	110.38
4	A	1632	BGC	O4-C4-C3	-2.78	103.82	110.38
4	A	1624	BGC	O4-C4-C3	-2.78	103.83	110.38
4	A	1622	BGC	O4-C4-C3	-2.77	103.84	110.38
4	A	1633	BGC	C2-C3-C4	-2.77	105.99	110.86
4	A	1619	BGC	O4-C4-C3	-2.77	103.85	110.38
4	A	1633	BGC	O4-C4-C3	-2.76	103.88	110.38
4	A	1627	BGC	O4-C4-C3	-2.75	103.91	110.38
4	A	1637	BGC	O4-C4-C3	-2.73	103.95	110.38
4	A	1634	BGC	O3-C3-C2	-2.72	104.50	110.05
4	A	1604	BGC	O4-C4-C3	-2.72	103.97	110.38
4	A	1620	BGC	O4-C4-C3	-2.71	103.98	110.38
4	A	1610	BGC	O5-C5-C6	2.71	112.93	107.66
4	A	1604	BGC	O3-C3-C2	-2.71	104.53	110.05
4	A	1623	BGC	C1-C2-C3	-2.70	105.71	109.64
4	A	1637	BGC	O3-C3-C2	-2.70	104.54	110.05
4	A	1622	BGC	O3-C3-C2	-2.70	104.55	110.05
4	A	1616	BGC	O4-C4-C3	-2.69	104.02	110.38
4	A	1617	BGC	O5-C5-C6	2.69	112.90	107.66
4	A	1636	BGC	O4-C4-C3	-2.69	104.03	110.38
4	A	1610	BGC	O3-C3-C2	-2.69	104.57	110.05
4	A	1628	BGC	O3-C3-C2	-2.69	104.57	110.05
4	A	1627	BGC	O5-C5-C6	2.68	112.88	107.66
4	A	1619	BGC	C1-C2-C3	-2.67	105.76	109.64
4	A	1625	BGC	O3-C3-C2	-2.67	104.61	110.05
4	A	1634	BGC	C1-C2-C3	-2.66	105.77	109.64
4	A	1624	BGC	O5-C5-C6	2.66	112.84	107.66
4	A	1604	BGC	O5-C5-C6	2.66	112.84	107.66
4	A	1628	BGC	O5-C5-C6	2.66	112.84	107.66
4	A	1617	BGC	O3-C3-C2	-2.66	104.63	110.05
4	A	1625	BGC	O5-C5-C6	2.65	112.83	107.66
4	A	1627	BGC	O3-C3-C2	-2.65	104.64	110.05
4	A	1633	BGC	O5-C5-C6	2.65	112.81	107.66
4	A	1606	BGC	O3-C3-C2	-2.64	104.66	110.05
4	A	1603	BGC	O3-C3-C2	-2.64	104.66	110.05
4	A	1610	BGC	C2-C3-C4	-2.64	106.21	110.86
4	A	1633	BGC	O3-C3-C2	-2.64	104.67	110.05
4	A	1635	BGC	O3-C3-C2	-2.64	104.67	110.05
4	A	1601	BGC	O3-C3-C2	-2.64	104.67	110.05
4	A	1630	BGC	C1-C2-C3	-2.64	105.81	109.64
4	A	1618	BGC	O3-C3-C2	-2.63	104.68	110.05
4	A	1623	BGC	O3-C3-C2	-2.63	104.68	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1619	BGC	O3-C3-C2	-2.63	104.69	110.05
4	A	1615	BGC	C1-C2-C3	-2.62	105.82	109.64
4	A	1620	BGC	O3-C3-C2	-2.62	104.70	110.05
4	A	1602	BGC	O5-C5-C6	2.62	112.75	107.66
4	A	1624	BGC	O3-C3-C2	-2.62	104.72	110.05
4	A	1629	BGC	O3-C3-C2	-2.61	104.72	110.05
4	A	1603	BGC	O5-C5-C6	2.61	112.75	107.66
4	A	1632	BGC	O5-C5-C6	2.61	112.74	107.66
4	A	1621	BGC	O5-C5-C6	2.60	112.73	107.66
4	A	1615	BGC	O3-C3-C2	-2.60	104.76	110.05
4	A	1636	BGC	O5-C5-C6	2.59	112.71	107.66
4	A	1616	BGC	O3-C3-C2	-2.59	104.76	110.05
4	A	1602	BGC	O3-C3-C2	-2.59	104.77	110.05
4	A	1613	BGC	O3-C3-C2	-2.58	104.78	110.05
4	A	1621	BGC	O3-C3-C2	-2.58	104.79	110.05
4	A	1632	BGC	O3-C3-C2	-2.57	104.80	110.05
4	A	1619	BGC	O5-C5-C6	2.57	112.66	107.66
4	A	1630	BGC	O3-C3-C2	-2.56	104.84	110.05
4	A	1610	BGC	C1-C2-C3	-2.55	105.93	109.64
4	A	1620	BGC	C2-C3-C4	-2.54	106.39	110.86
4	A	1613	BGC	O5-C5-C6	2.53	112.60	107.66
4	A	1618	BGC	O5-C5-C6	2.53	112.59	107.66
4	A	1620	BGC	O5-C5-C6	2.52	112.56	107.66
4	A	1636	BGC	O3-C3-C2	-2.48	104.98	110.05
4	A	1622	BGC	C2-C3-C4	-2.48	106.49	110.86
4	A	1604	BGC	C2-C3-C4	-2.44	106.56	110.86
4	A	1613	BGC	C2-C3-C4	-2.44	106.56	110.86
4	A	1635	BGC	C1-C2-C3	-2.44	106.08	109.64
4	A	1633	BGC	C1-C2-C3	-2.42	106.12	109.64
4	A	1602	BGC	C1-C2-C3	-2.42	106.13	109.64
4	A	1635	BGC	O5-C5-C6	2.40	112.34	107.66
4	A	1616	BGC	C2-C3-C4	-2.39	106.66	110.86
4	A	1601	BGC	O5-C5-C6	2.38	112.30	107.66
4	A	1634	BGC	O5-C5-C6	2.36	112.26	107.66
4	A	1616	BGC	O5-C5-C6	2.36	112.25	107.66
4	A	1621	BGC	C2-C3-C4	-2.36	106.72	110.86
4	A	1629	BGC	O5-C5-C6	2.35	112.23	107.66
4	A	1601	BGC	C1-C2-C3	-2.34	106.24	109.64
4	A	1617	BGC	C2-C3-C4	-2.33	106.76	110.86
4	A	1602	BGC	C2-C3-C4	-2.31	106.79	110.86
4	A	1629	BGC	C1-C2-C3	-2.28	106.33	109.64
4	A	1627	BGC	C2-C3-C4	-2.24	106.92	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1619	BGC	C2-C3-C4	-2.23	106.93	110.86
4	A	1623	BGC	C2-C3-C4	-2.23	106.94	110.86
4	A	1636	BGC	C2-C3-C4	-2.23	106.94	110.86
4	A	1634	BGC	C2-C3-C4	-2.20	106.99	110.86
4	A	1616	BGC	C1-C2-C3	-2.19	106.46	109.64
4	A	1636	BGC	C1-C2-C3	-2.17	106.49	109.64
4	A	1629	BGC	C2-C3-C4	-2.16	107.06	110.86
4	A	1615	BGC	O5-C5-C6	2.16	111.86	107.66
4	A	1635	BGC	C2-C3-C4	-2.13	107.12	110.86
4	A	1620	BGC	C1-C2-C3	-2.12	106.56	109.64
4	A	1601	BGC	C2-C3-C4	-2.11	107.16	110.86
4	A	1624	BGC	C2-C3-C4	-2.09	107.18	110.86
4	A	1623	BGC	O5-C5-C6	2.08	111.72	107.66
4	A	1604	BGC	C1-C2-C3	-2.07	106.63	109.64
4	A	1618	BGC	C2-C3-C4	-2.06	107.24	110.86
4	A	1611	BGC	C1-C2-C3	2.02	112.58	109.64
4	A	1603	BGC	C2-C3-C4	-2.01	107.32	110.86
4	A	1627	BGC	C1-C2-C3	-2.01	106.72	109.64
4	A	1617	BGC	C1-C2-C3	-2.00	106.73	109.64

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1604	BGC	C1
4	A	1614	BGC	C1
4	A	1620	BGC	C1
4	A	1624	BGC	C1
4	A	1627	BGC	C1
4	A	1630	BGC	C1

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1620	BGC	O5-C5-C6-O6
4	A	1615	BGC	O5-C5-C6-O6
4	A	1618	BGC	O5-C5-C6-O6
4	A	1601	BGC	O5-C5-C6-O6
4	A	1622	BGC	O5-C5-C6-O6
4	A	1615	BGC	C4-C5-C6-O6
4	A	1610	BGC	C4-C5-C6-O6
4	A	1620	BGC	C4-C5-C6-O6
4	A	1610	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1616	BGC	O5-C5-C6-O6
4	A	1617	BGC	O5-C5-C6-O6
4	A	1618	BGC	C4-C5-C6-O6
4	A	1603	BGC	O5-C5-C6-O6
4	A	1604	BGC	O5-C5-C6-O6
4	A	1601	BGC	C4-C5-C6-O6
4	A	1622	BGC	C4-C5-C6-O6
4	A	1629	BGC	O5-C5-C6-O6
4	A	1603	BGC	C4-C5-C6-O6
4	A	1623	BGC	O5-C5-C6-O6
4	A	1604	BGC	C4-C5-C6-O6
4	A	1637	BGC	O5-C5-C6-O6
4	A	1630	BGC	C4-C5-C6-O6
4	A	1621	BGC	C4-C5-C6-O6
4	A	1619	BGC	C4-C5-C6-O6
4	A	1616	BGC	C4-C5-C6-O6
4	A	1619	BGC	O5-C5-C6-O6
4	A	1617	BGC	C4-C5-C6-O6
4	A	1630	BGC	O5-C5-C6-O6
4	A	1633	BGC	O5-C5-C6-O6
4	A	1621	BGC	O5-C5-C6-O6
4	A	1608	BGC	O5-C5-C6-O6
4	A	1609	BGC	O5-C5-C6-O6
4	A	1628	BGC	C4-C5-C6-O6
4	A	1602	BGC	O5-C5-C6-O6
4	A	1629	BGC	C4-C5-C6-O6
4	A	1637	BGC	C4-C5-C6-O6
4	A	1623	BGC	C4-C5-C6-O6
4	A	1624	BGC	C4-C5-C6-O6
4	A	1627	BGC	C4-C5-C6-O6
4	A	1634	BGC	C4-C5-C6-O6
4	A	1628	BGC	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 13 short contacts:

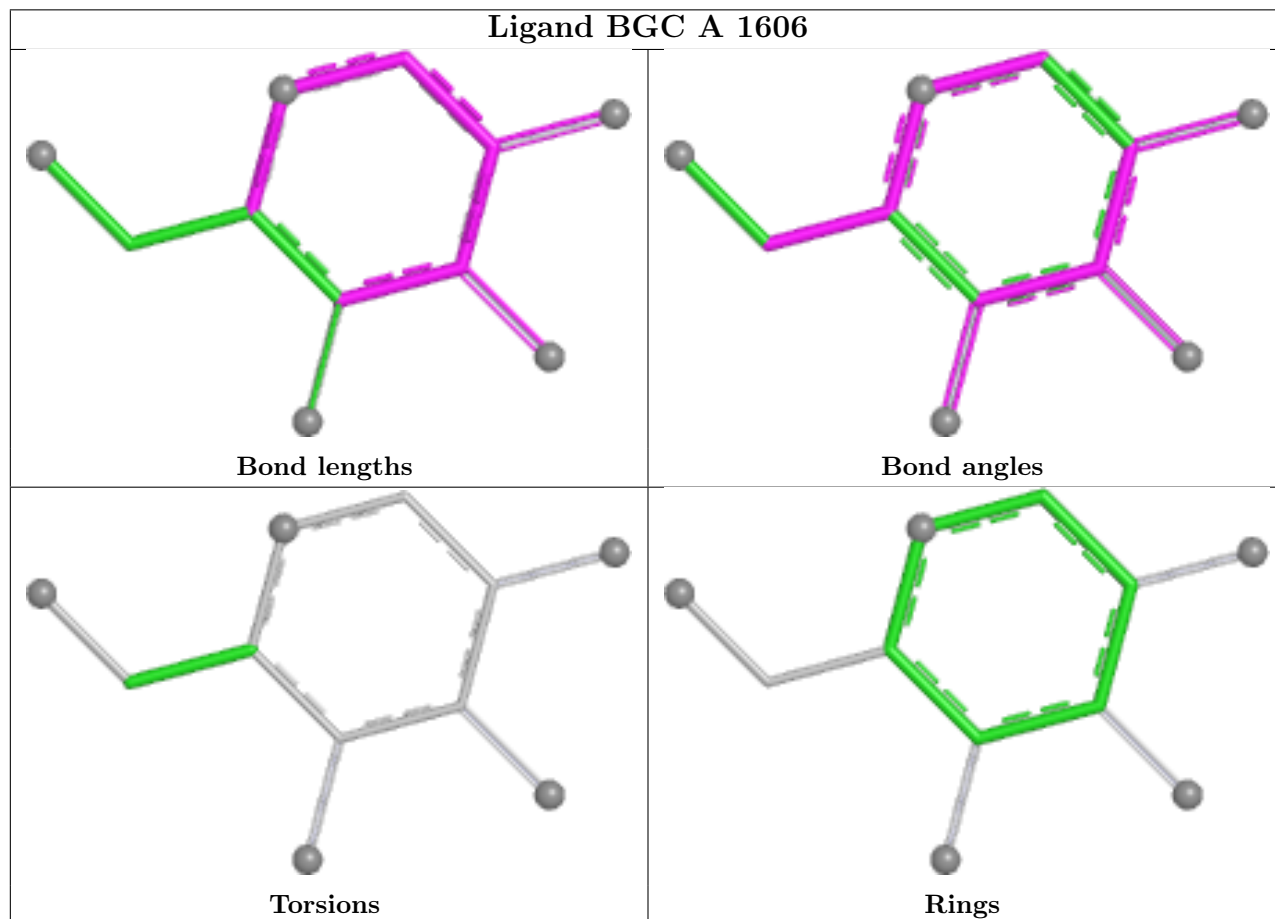
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1638	BGC	1	0
4	A	1631	BGC	3	0
4	A	1630	BGC	3	0
4	A	1610	BGC	1	0
4	A	1612	BGC	2	0

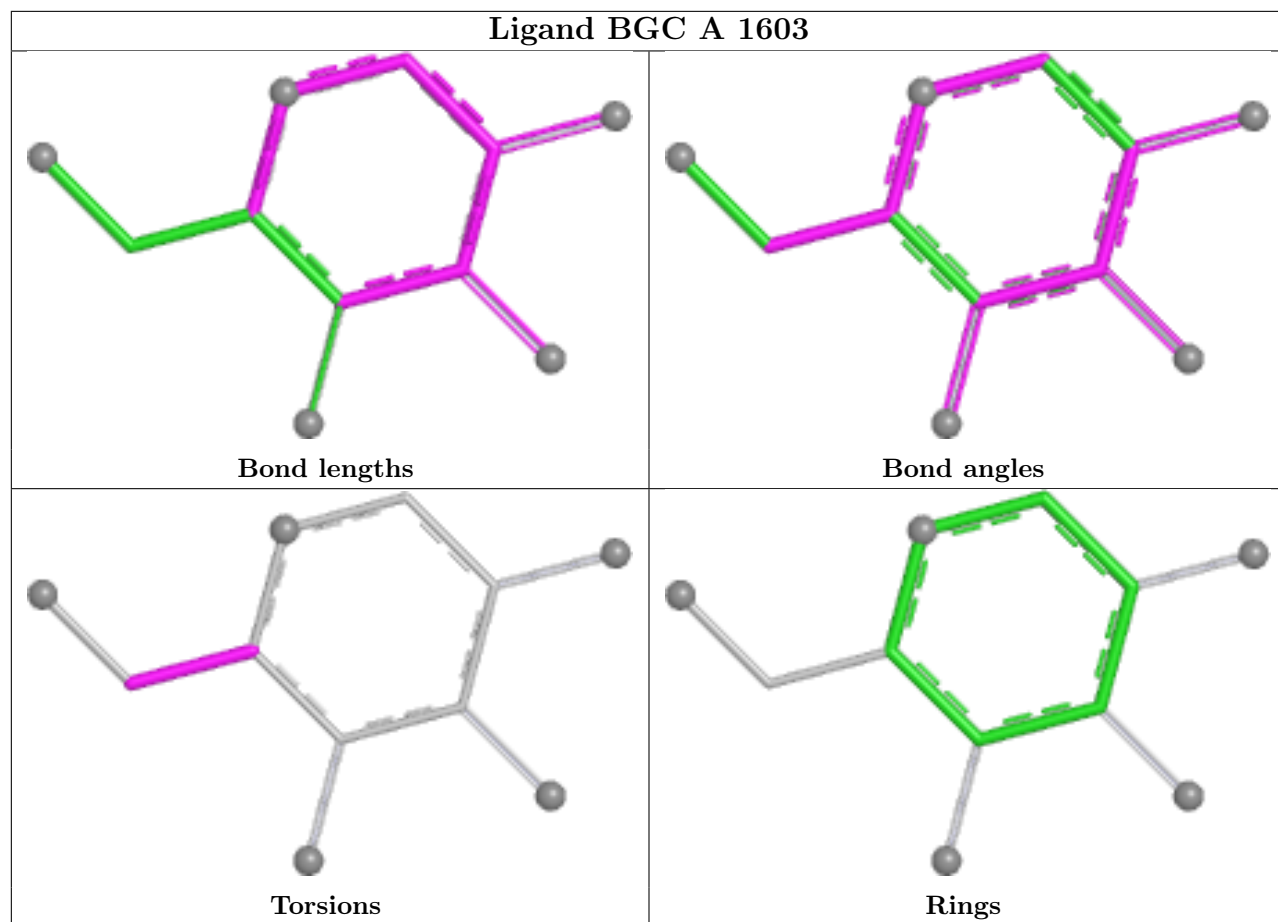
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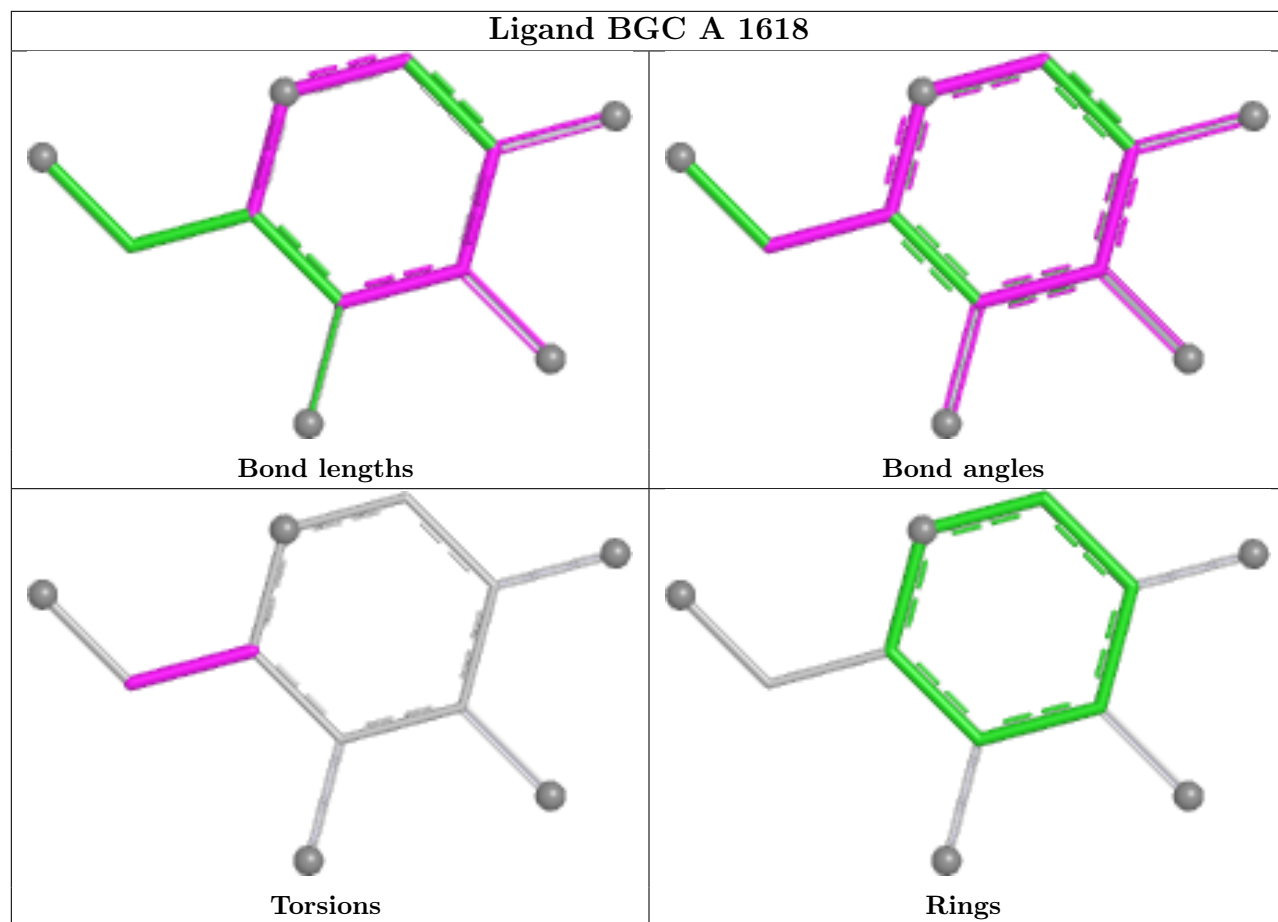
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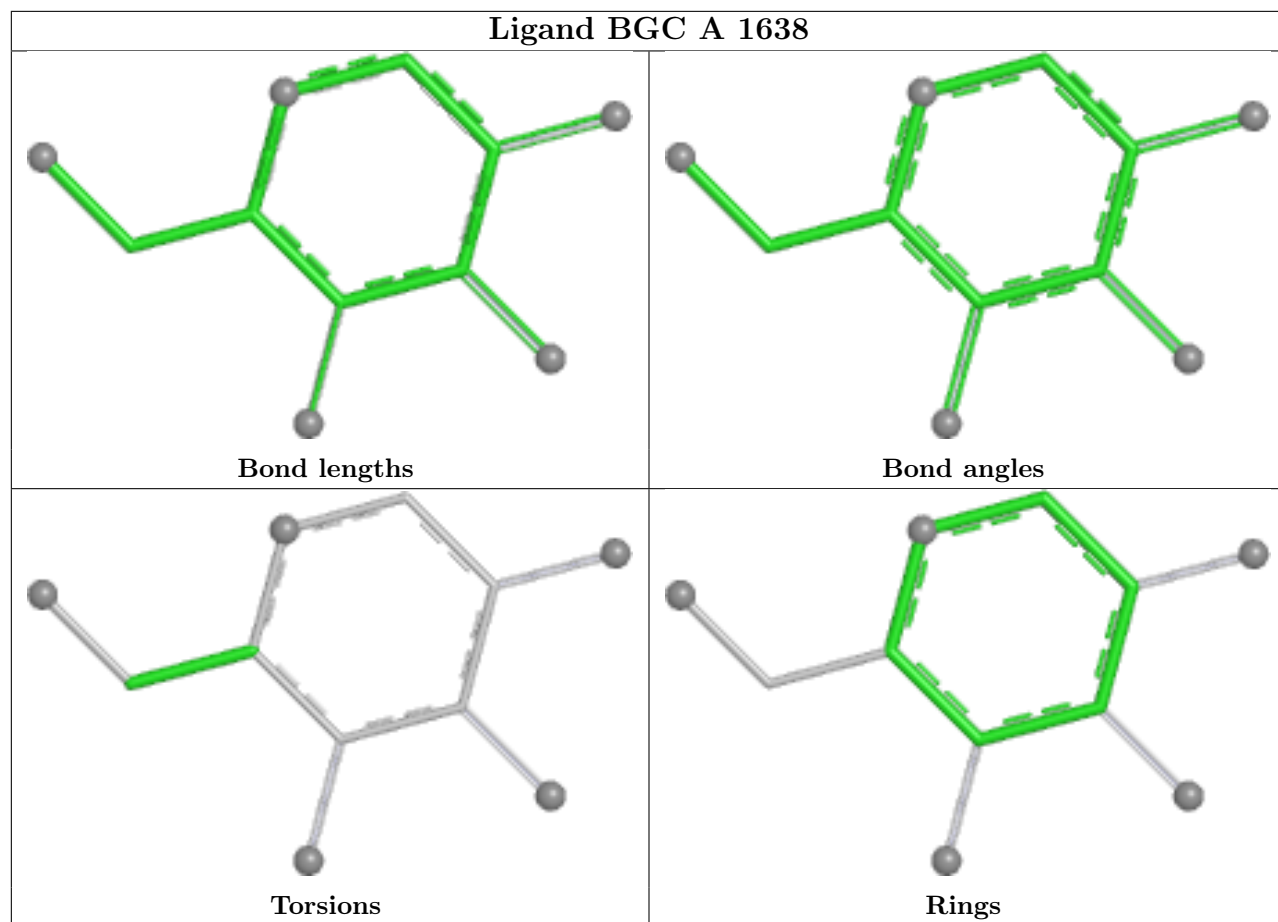
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1632	BGC	1	0
4	A	1624	BGC	1	0
4	A	1614	BGC	1	0

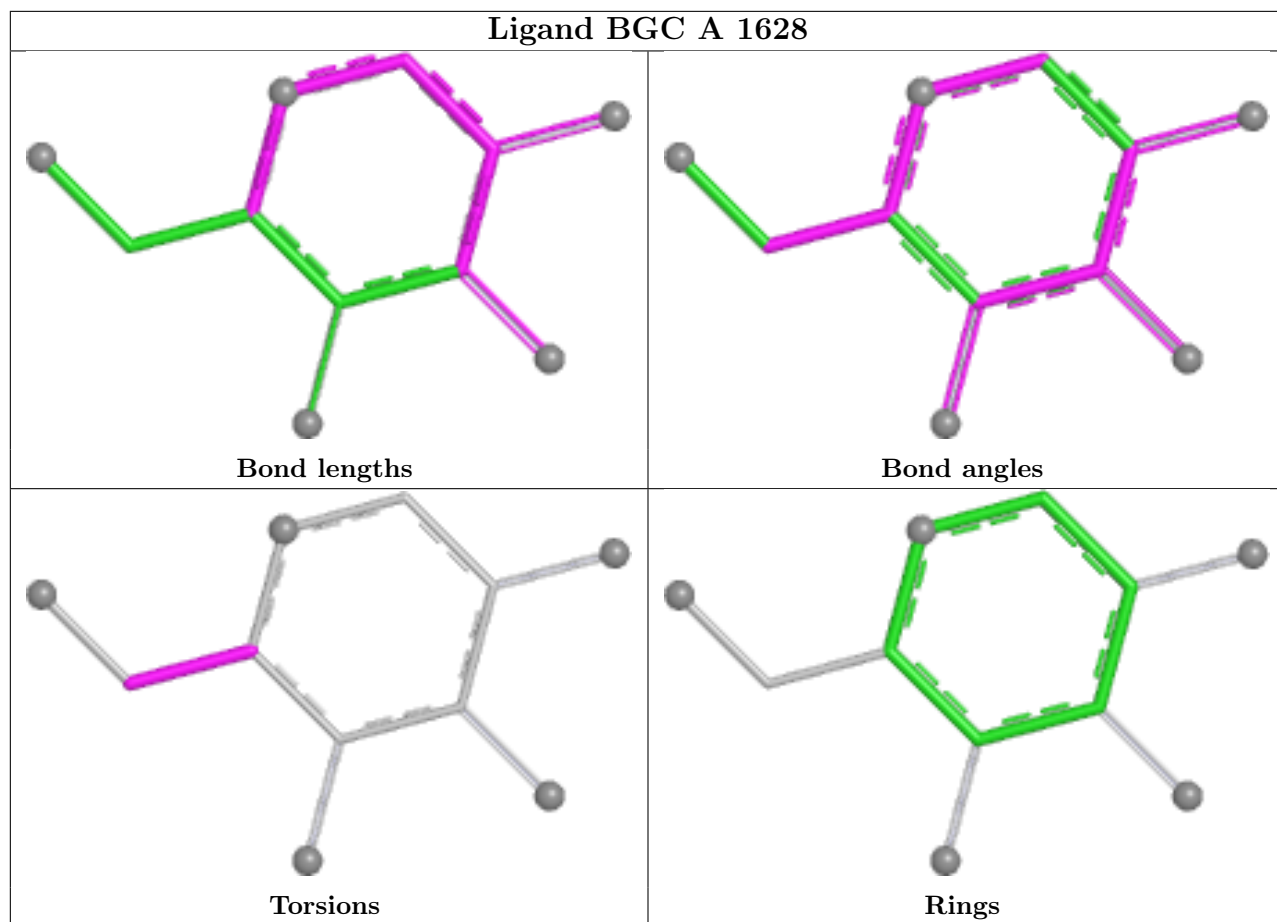
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

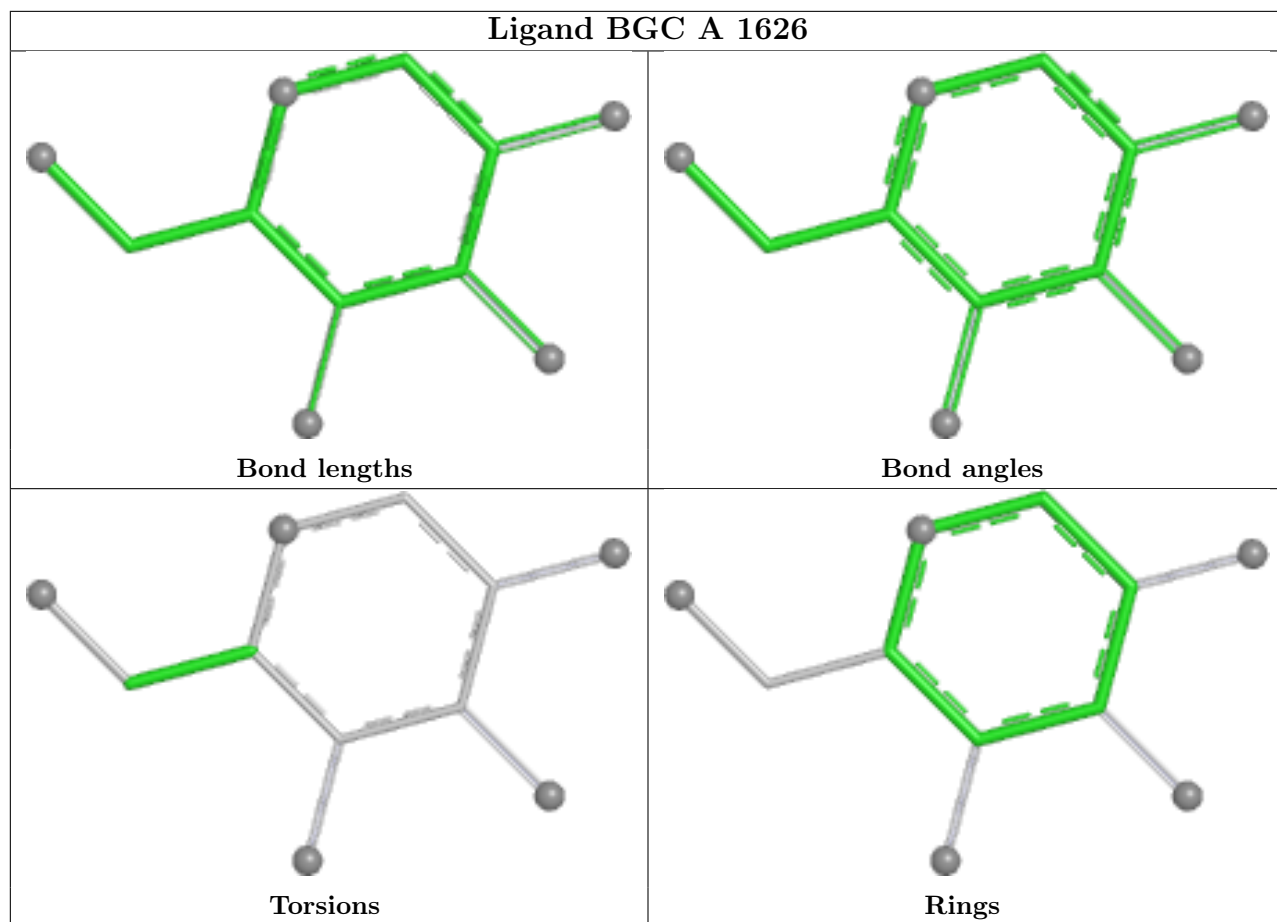


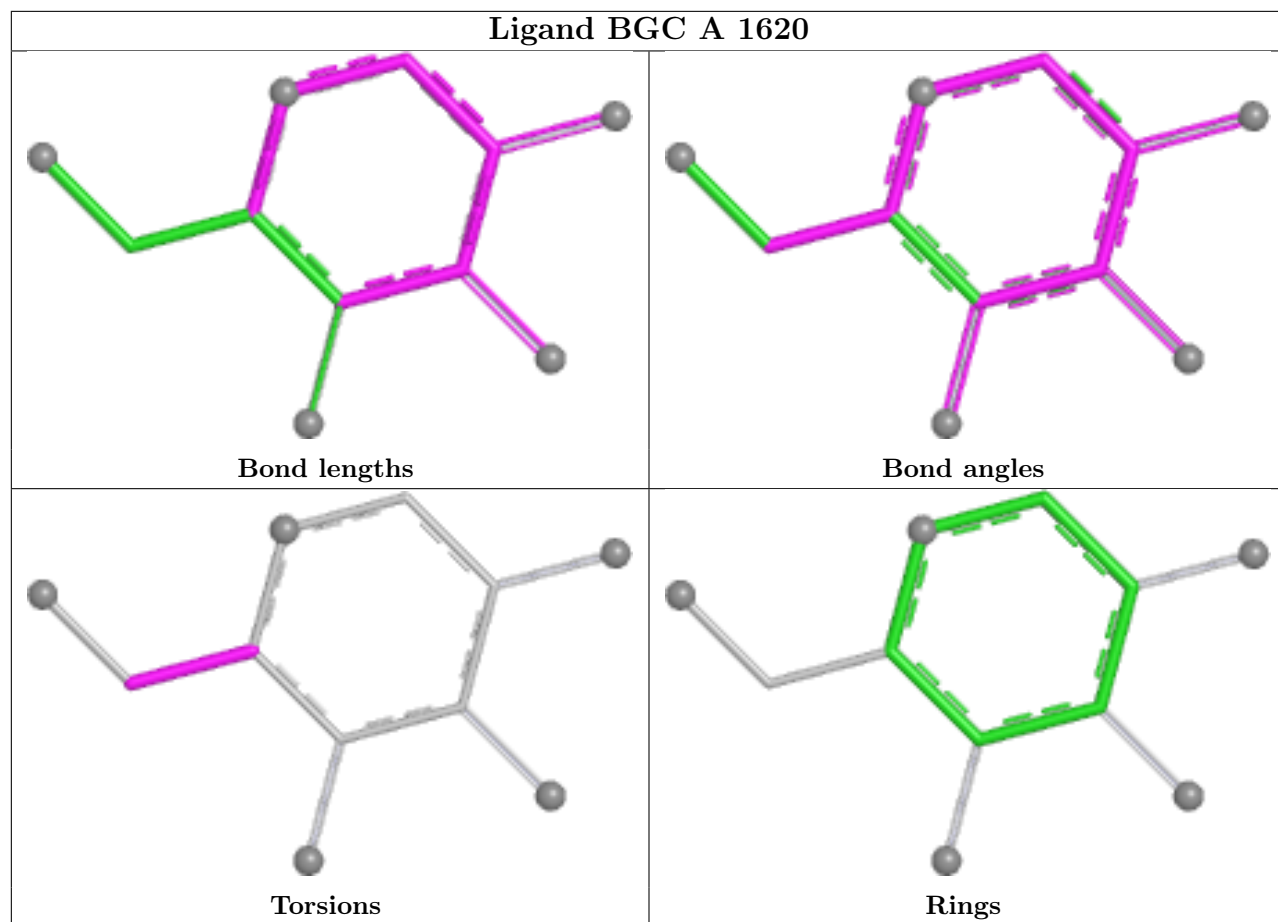


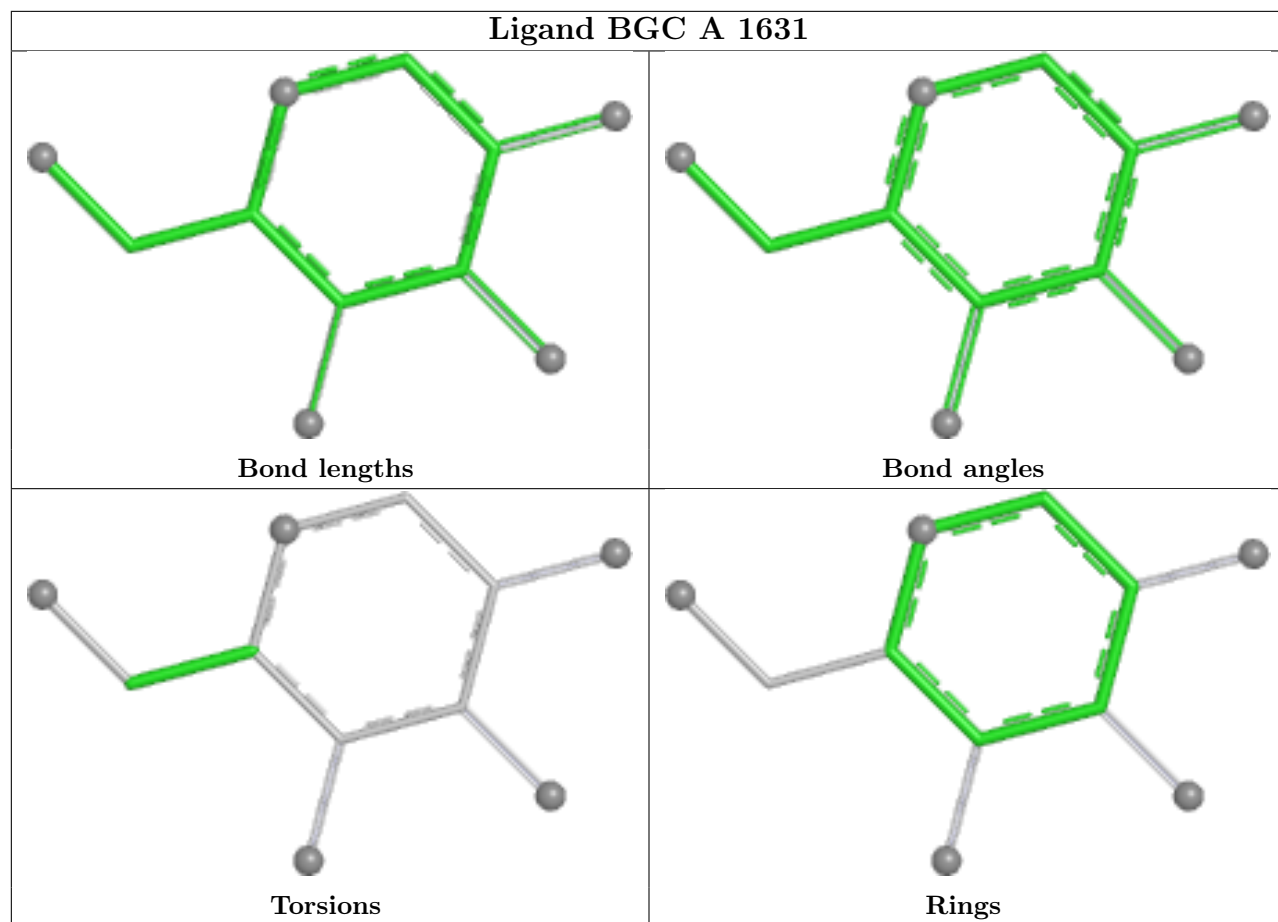


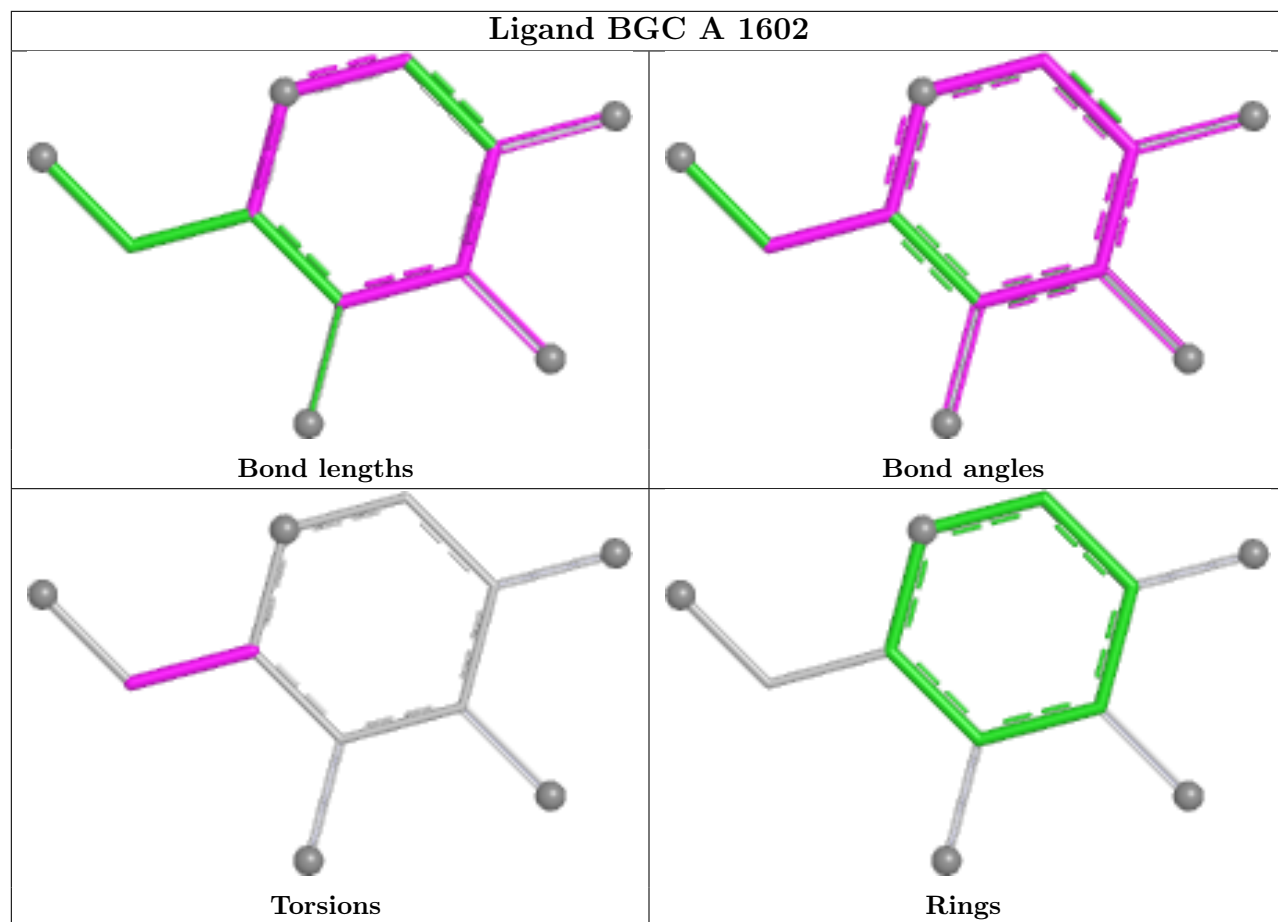


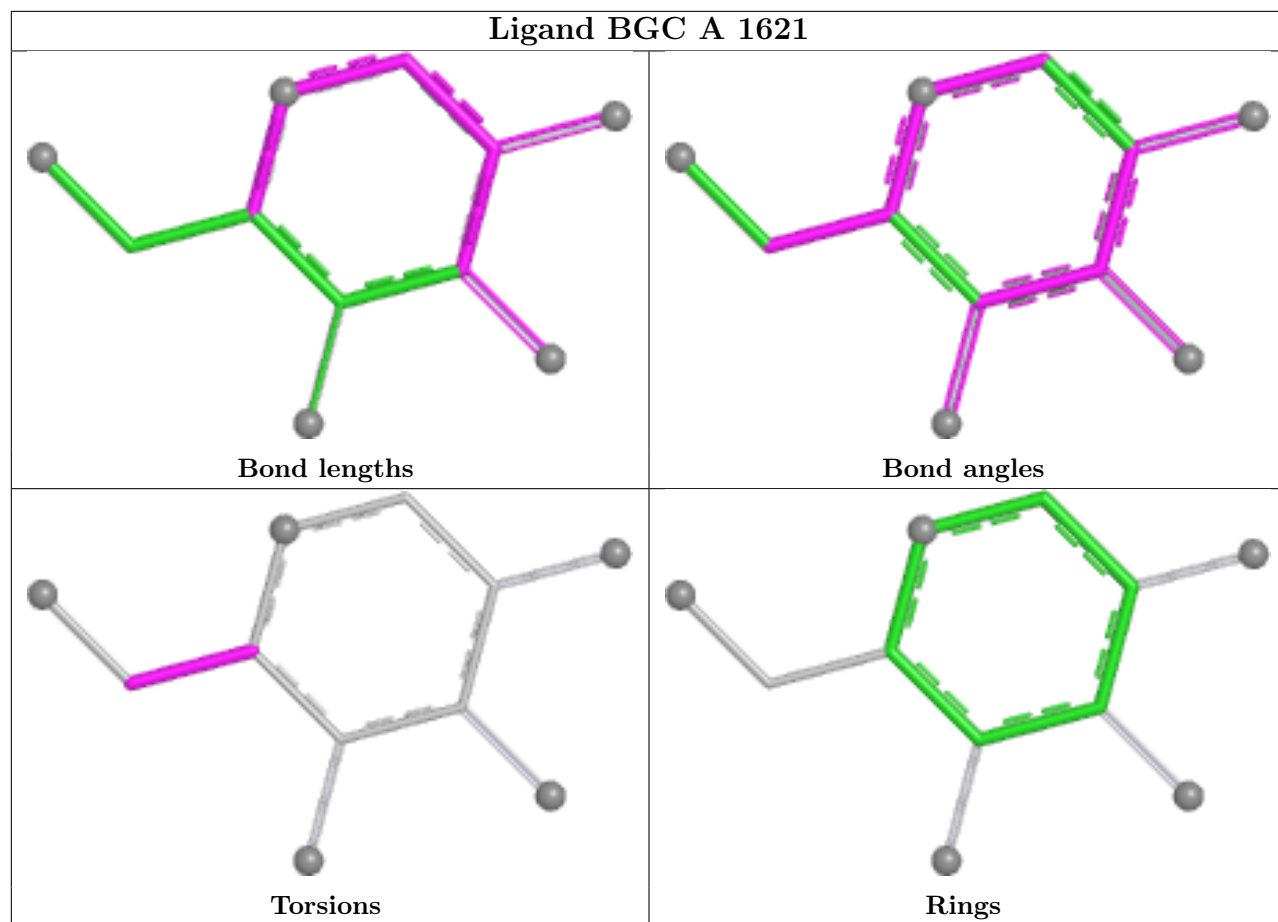


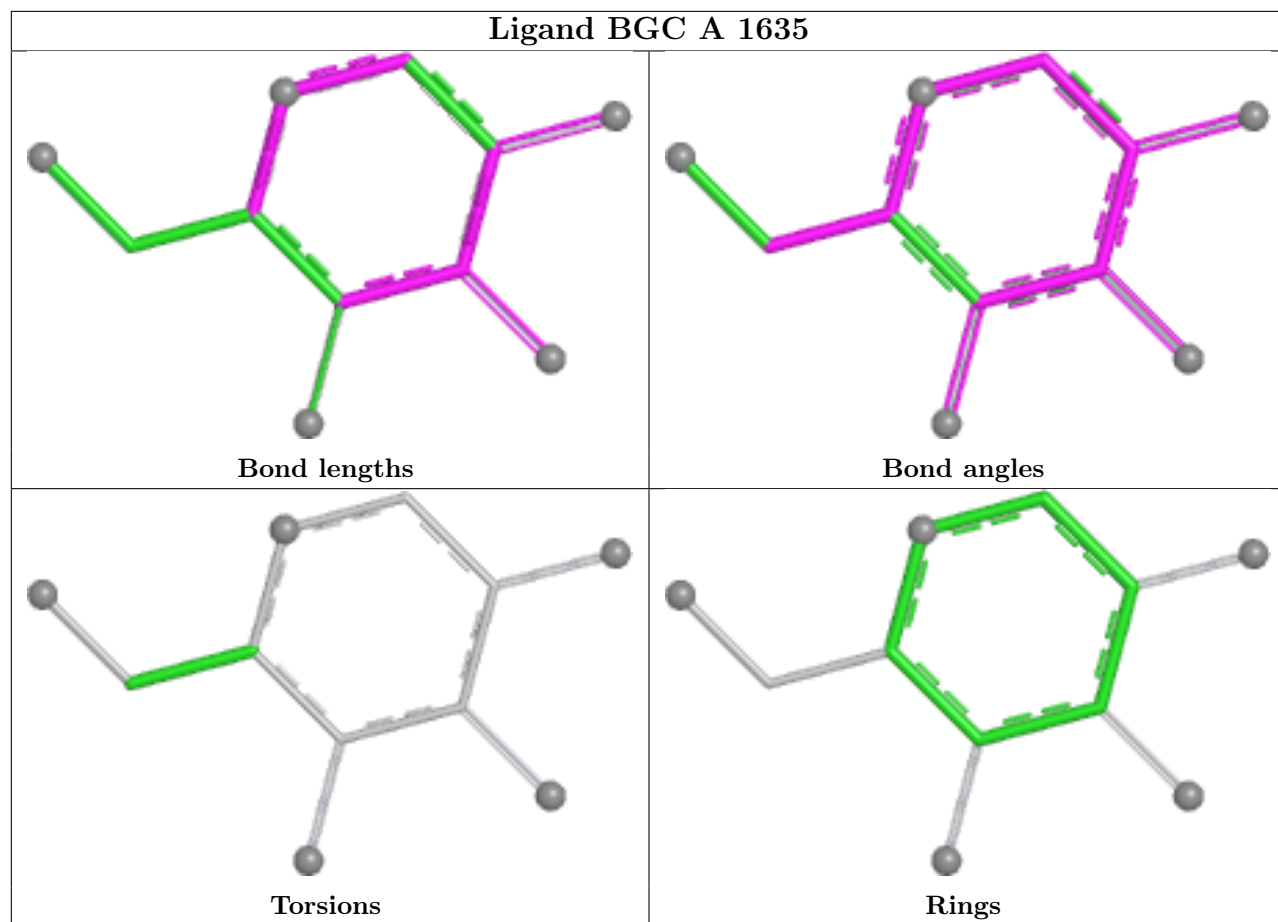


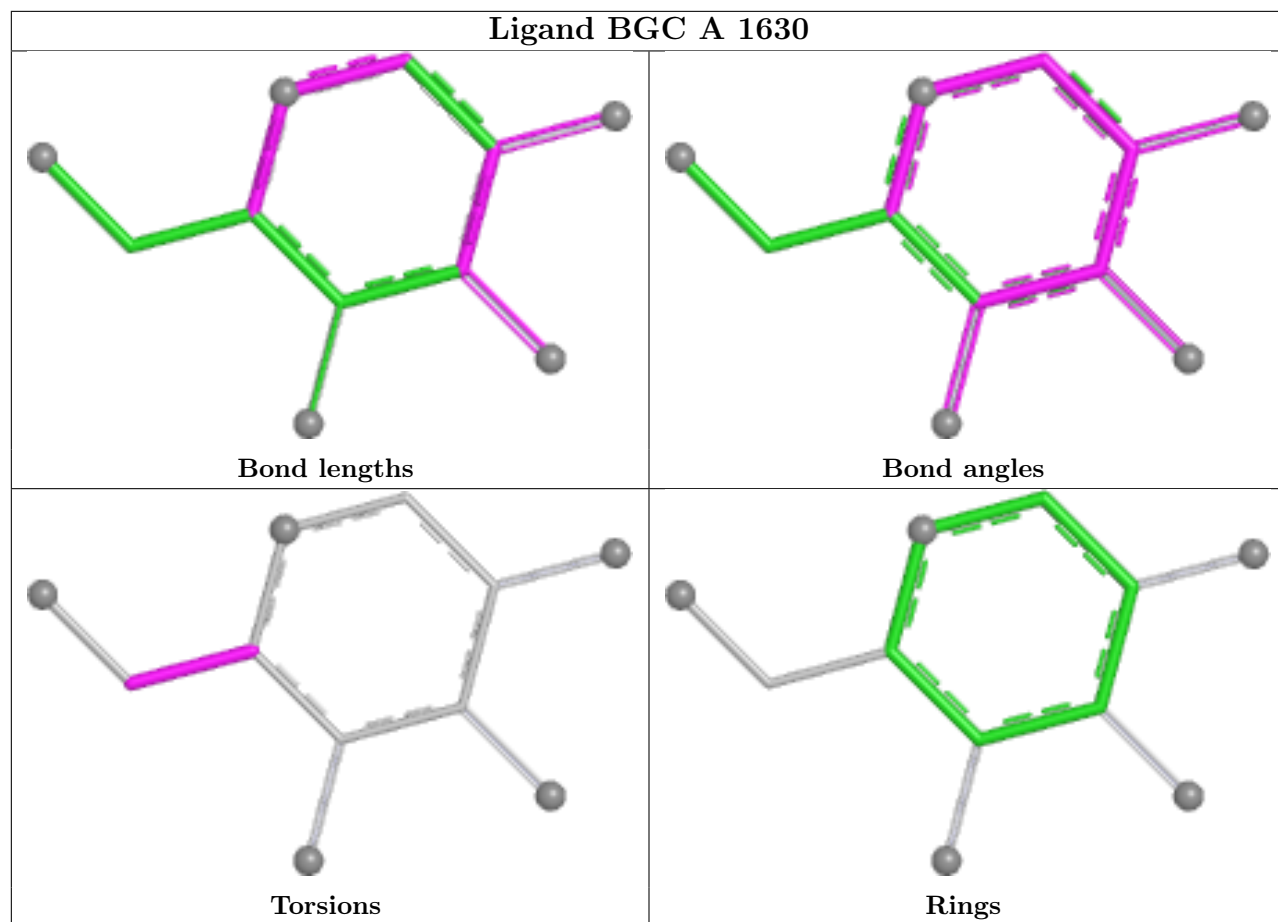


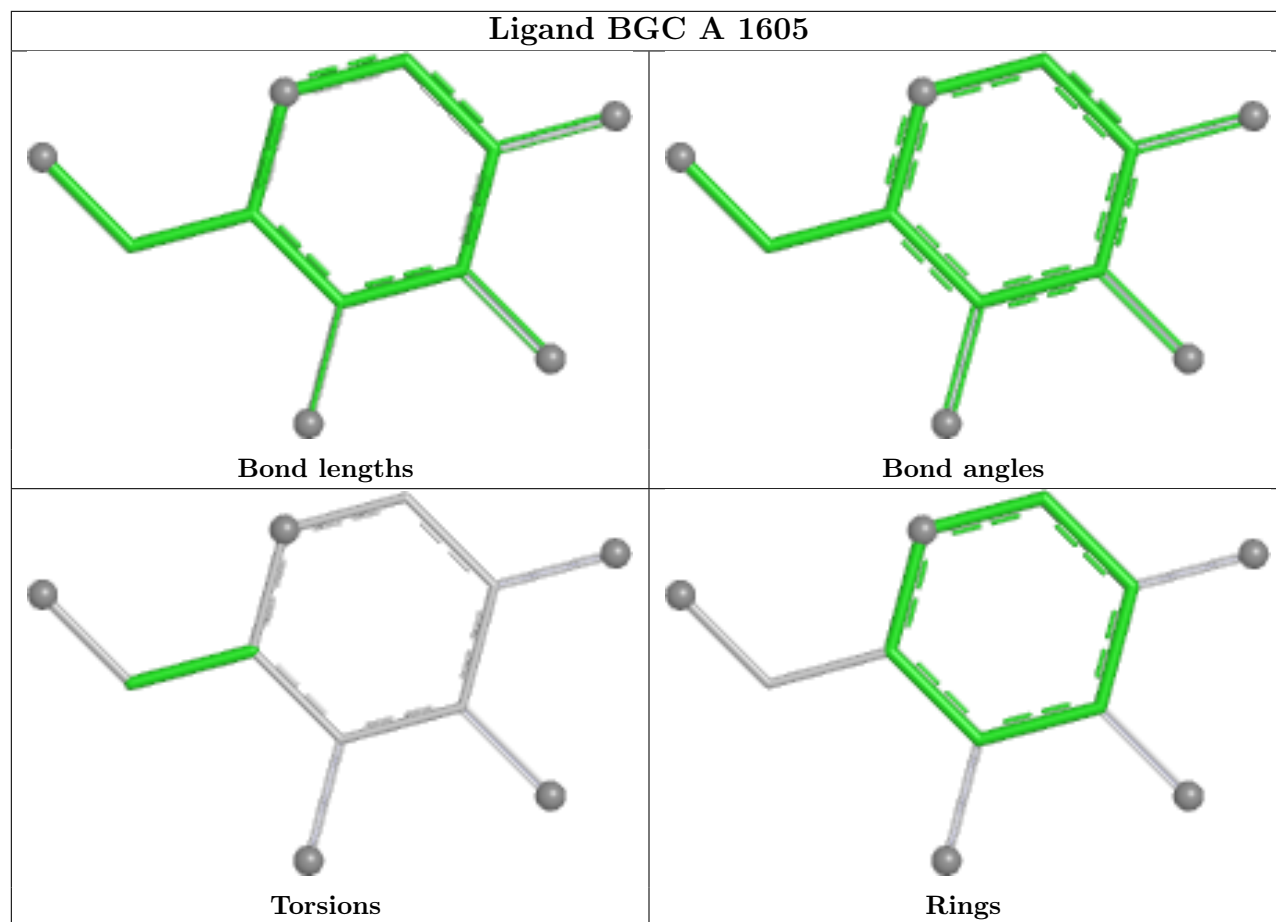


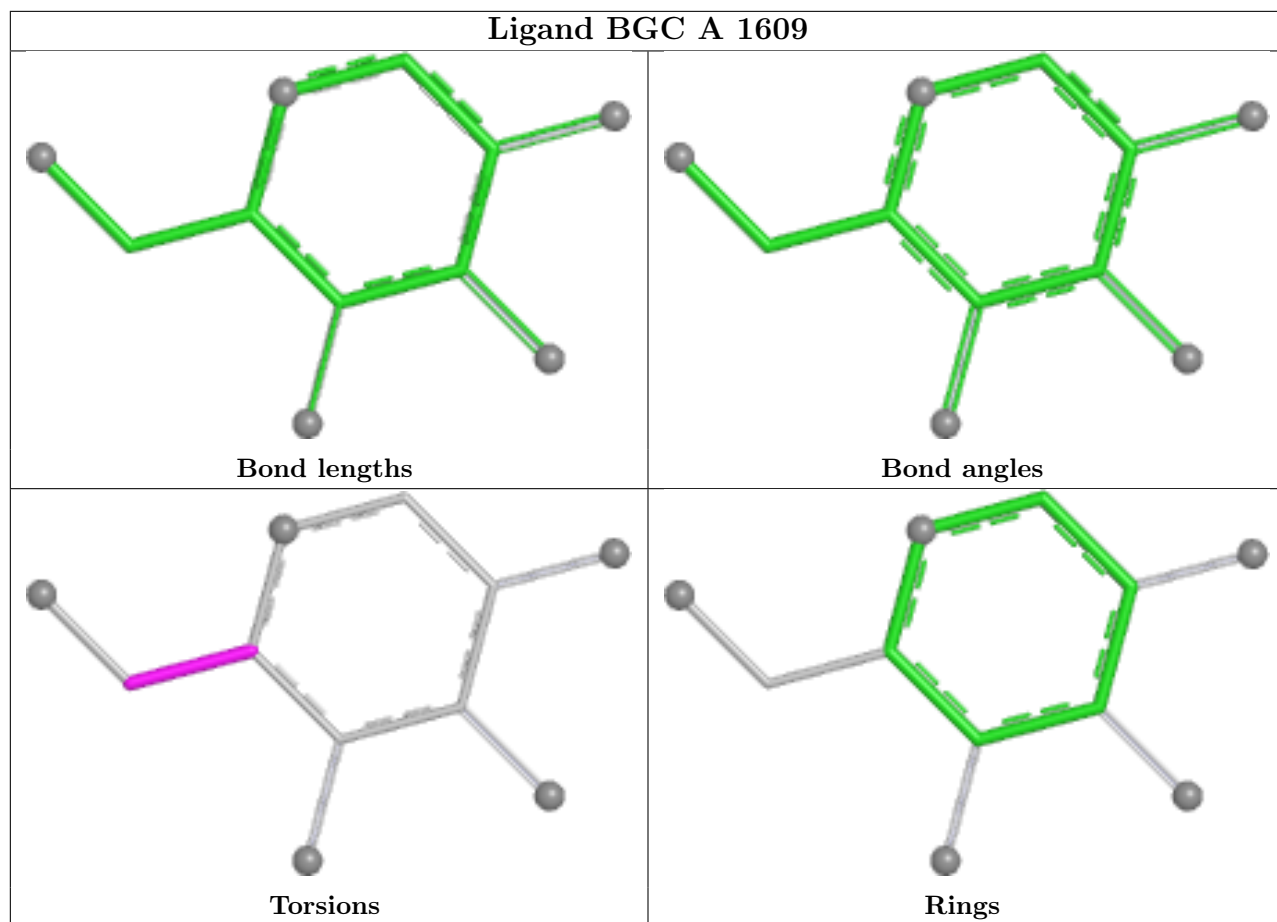


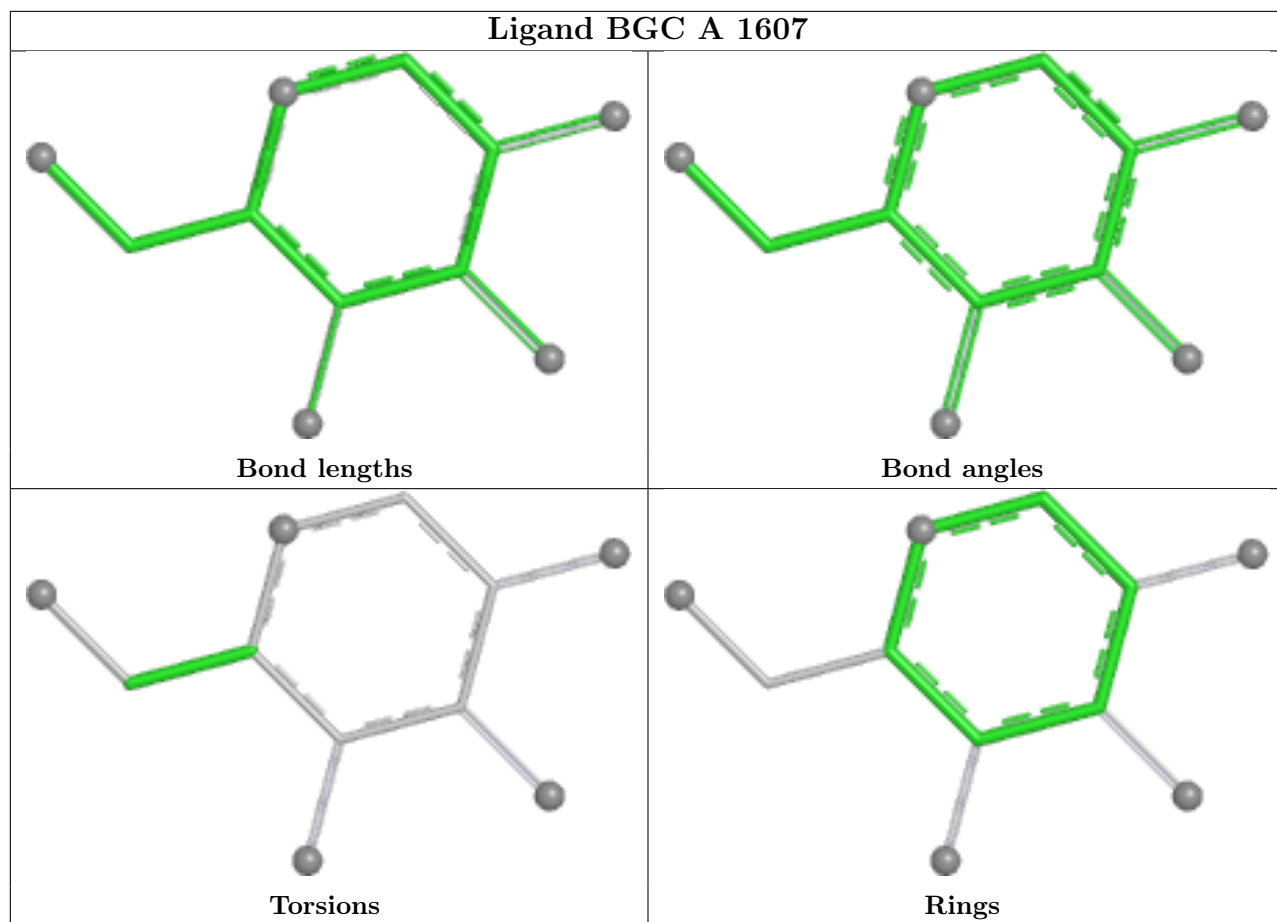


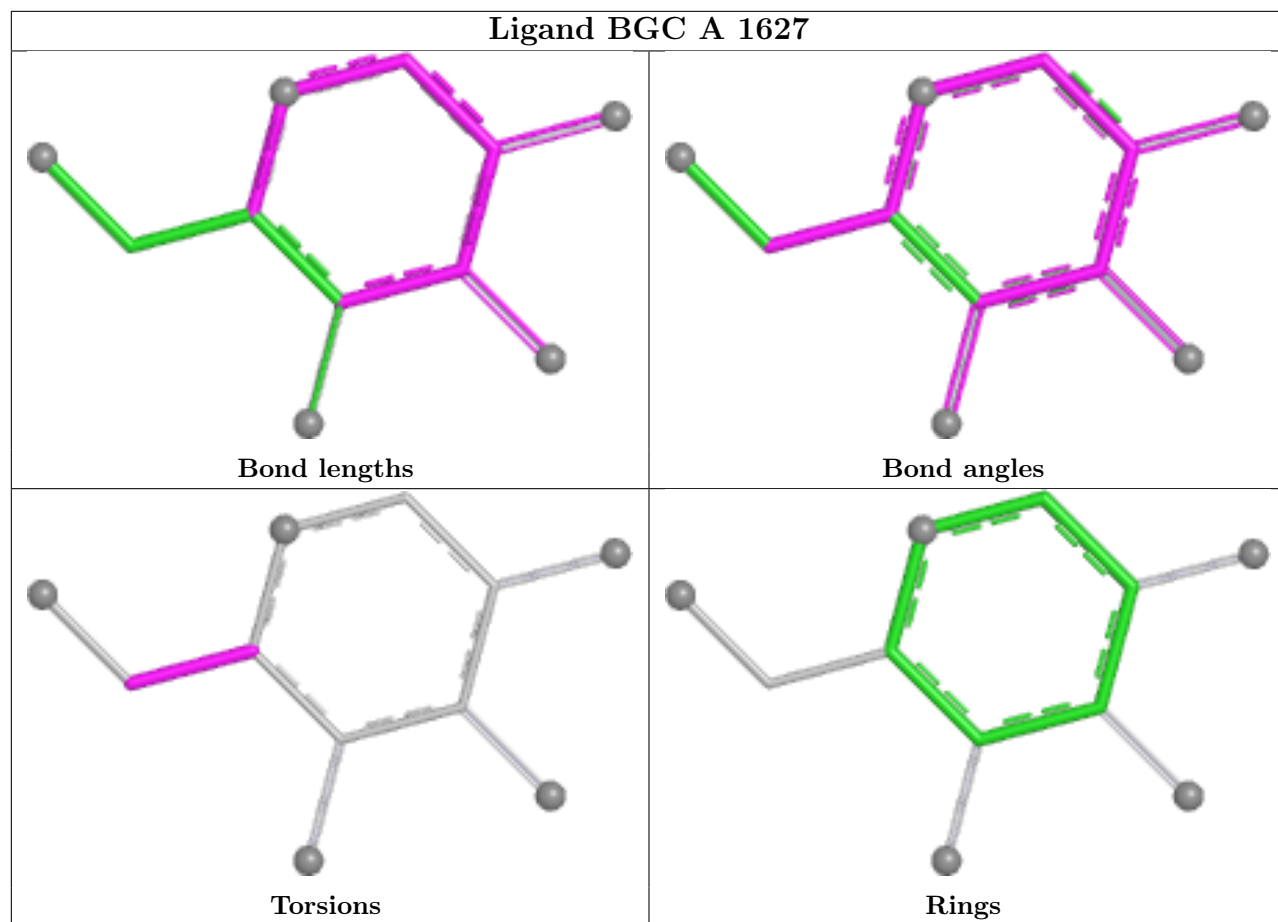


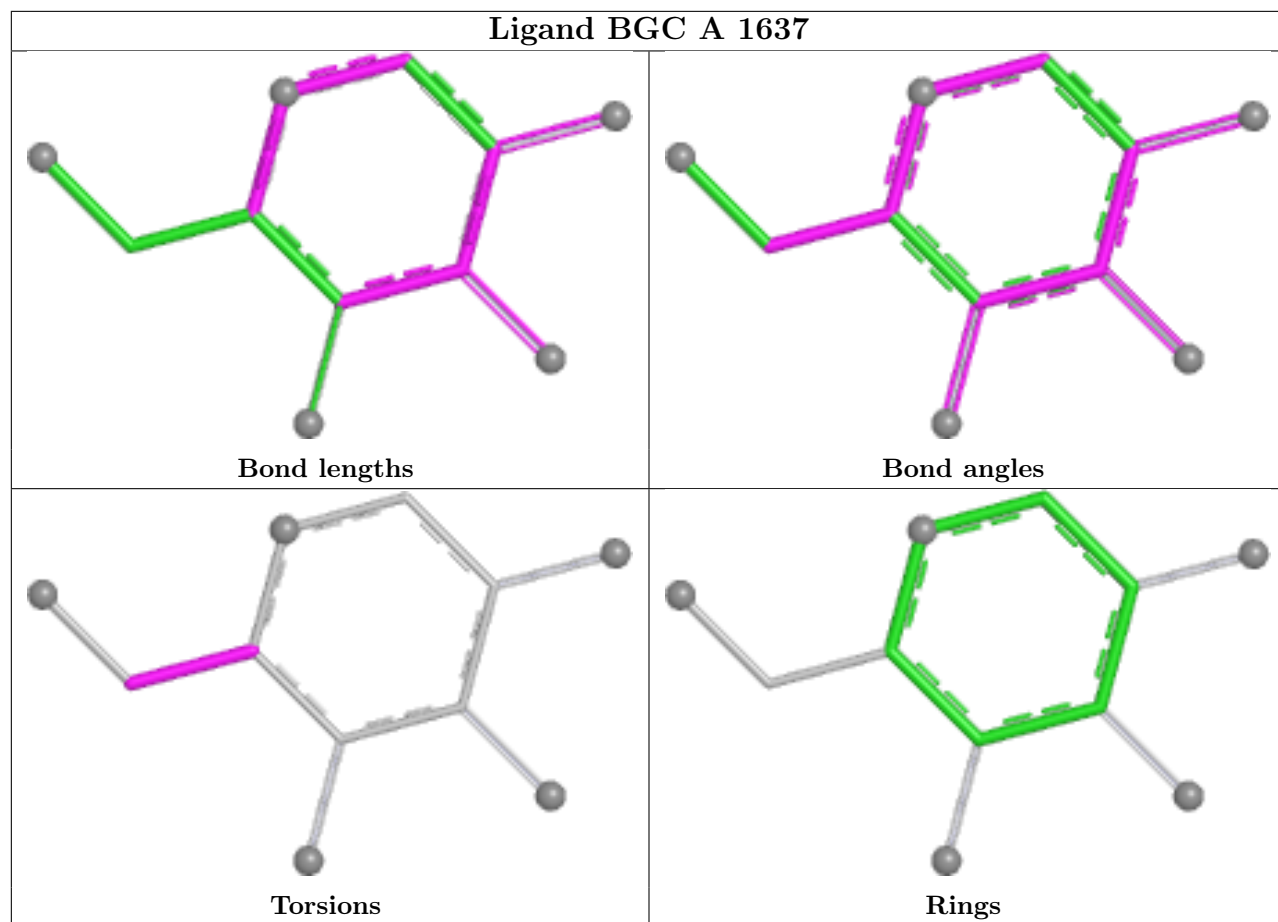


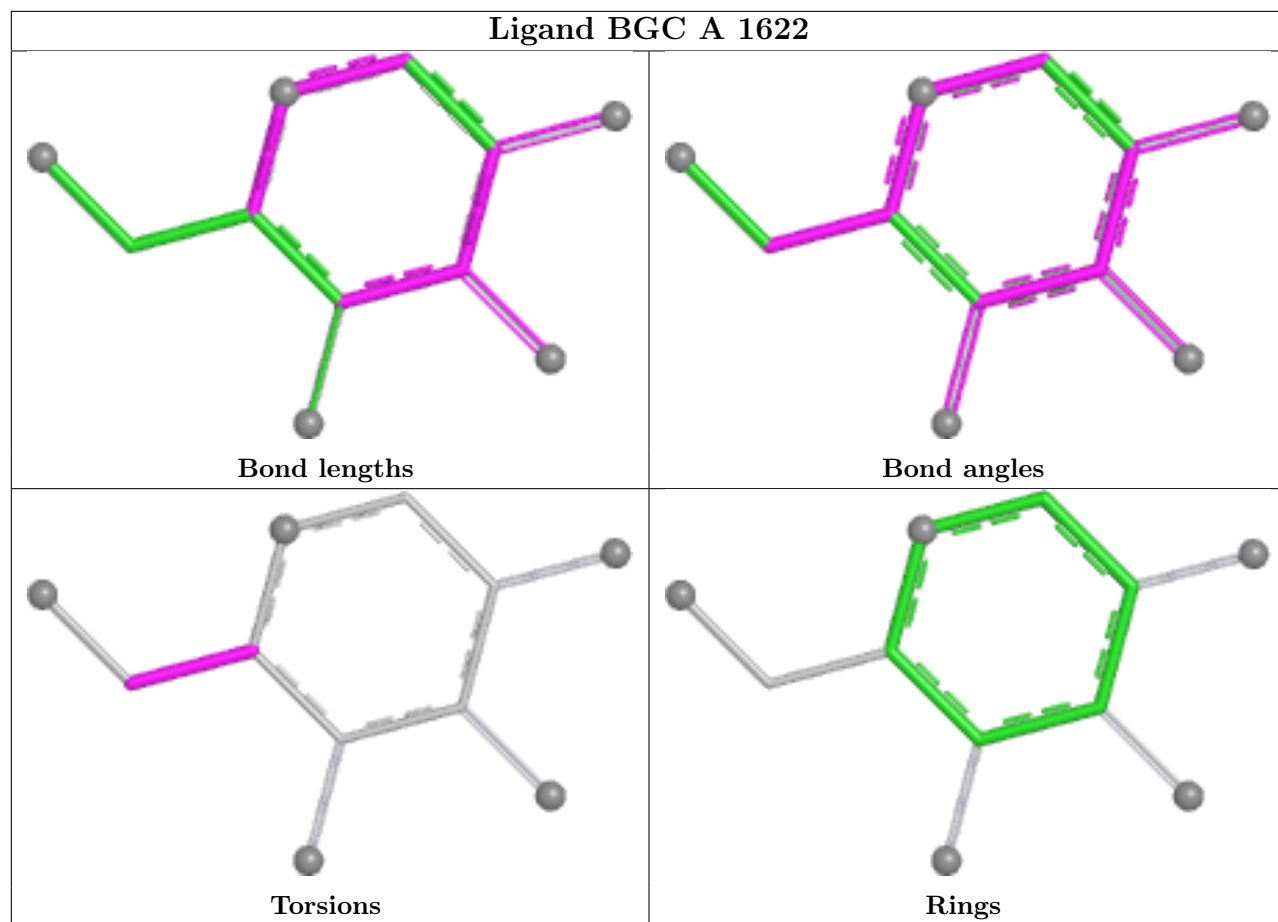


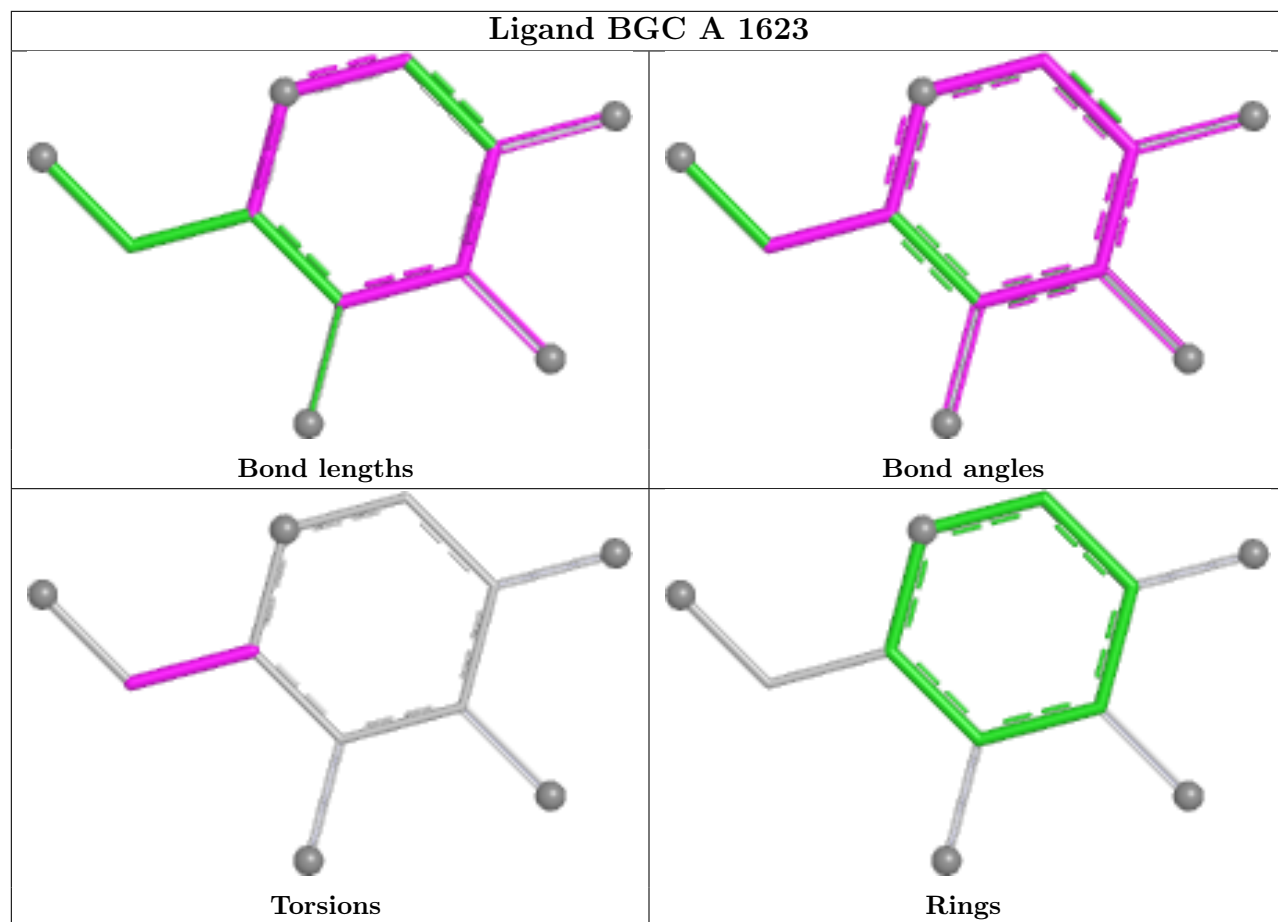


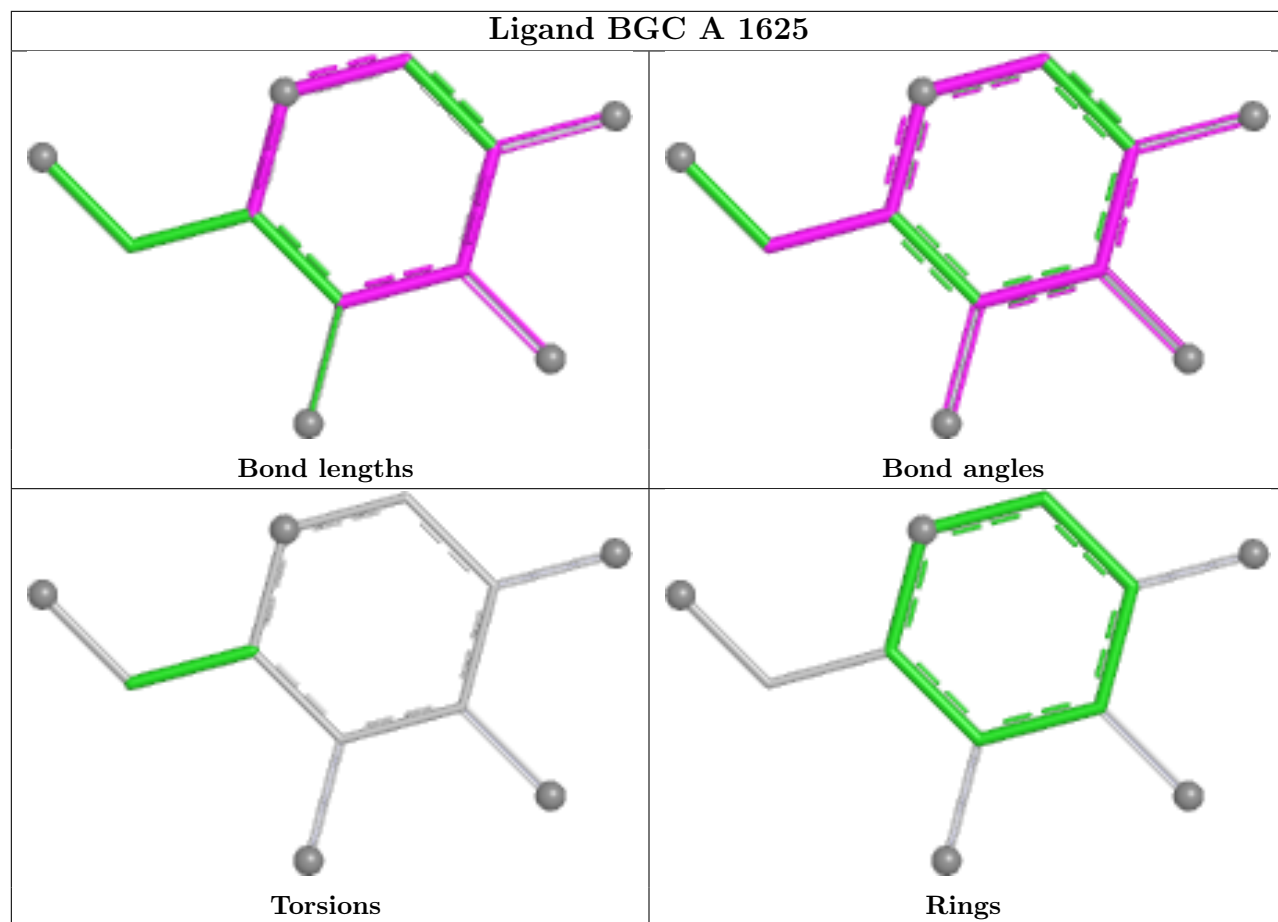


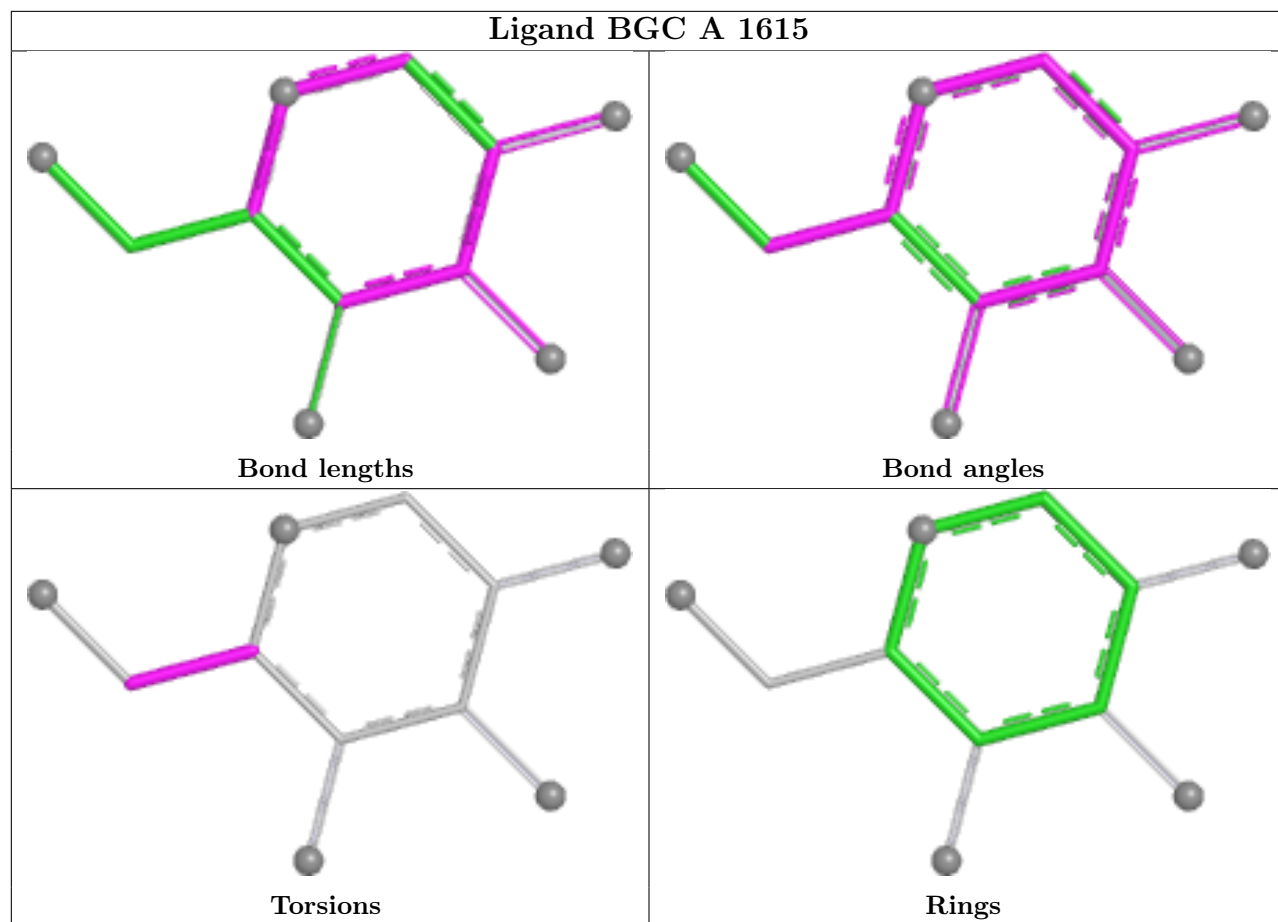


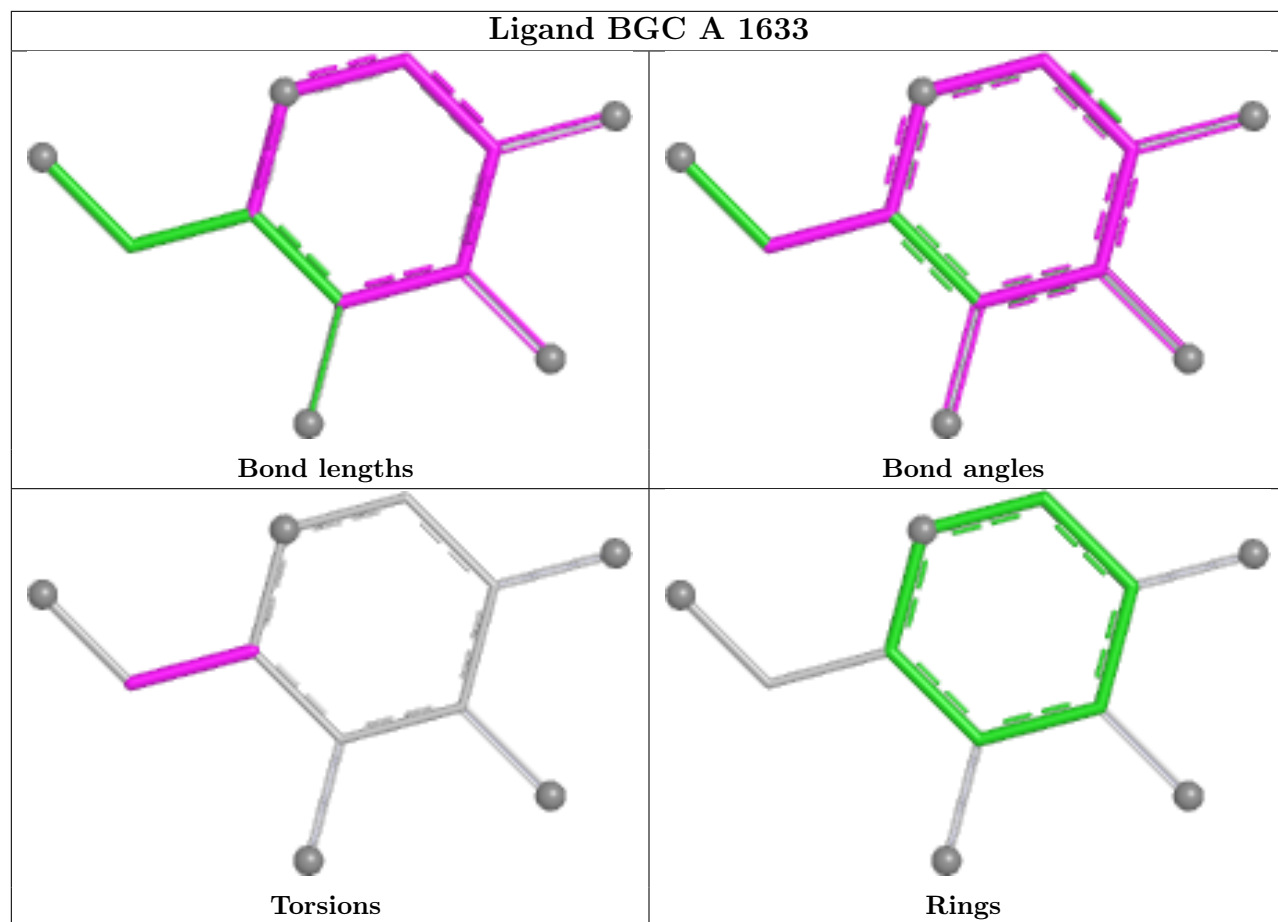


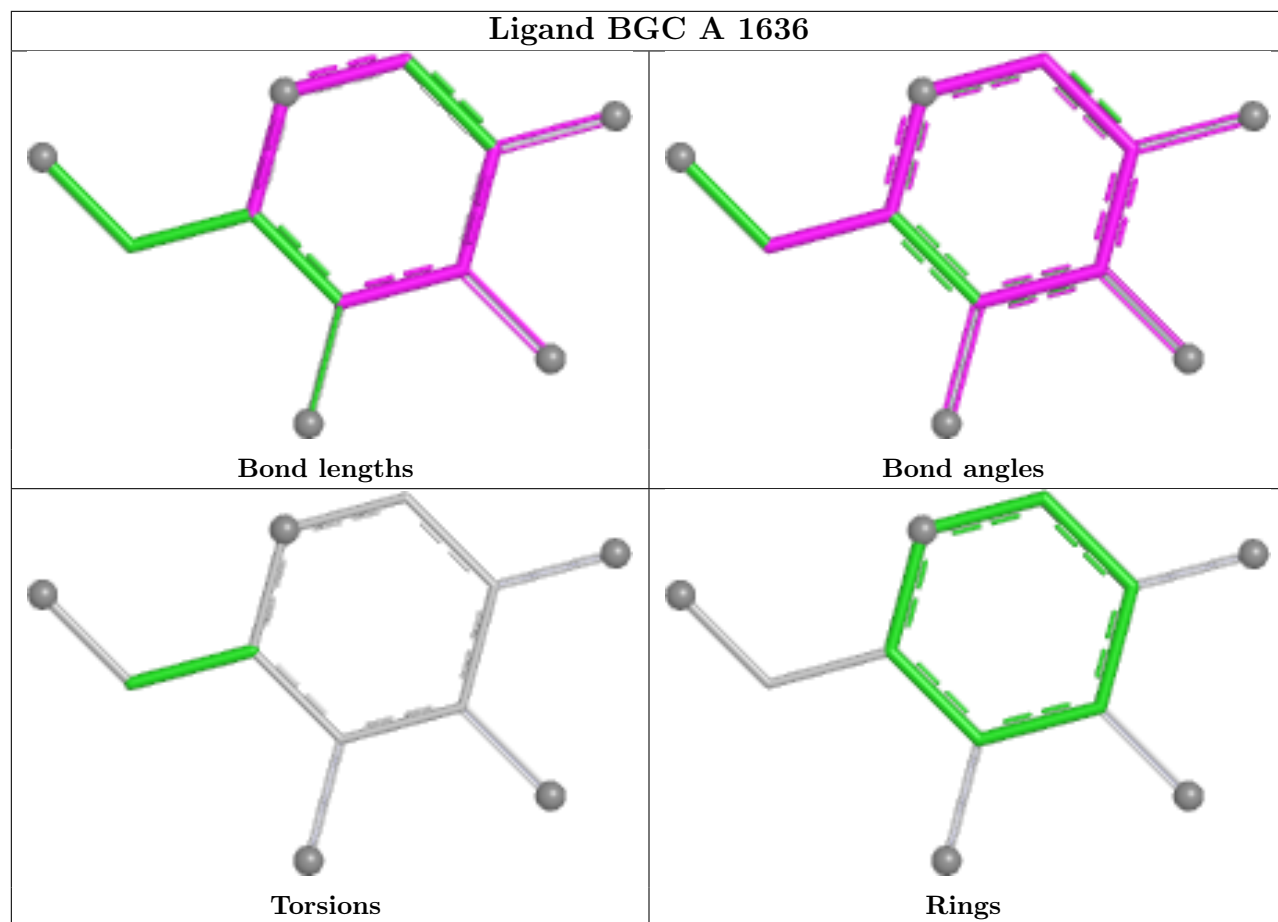


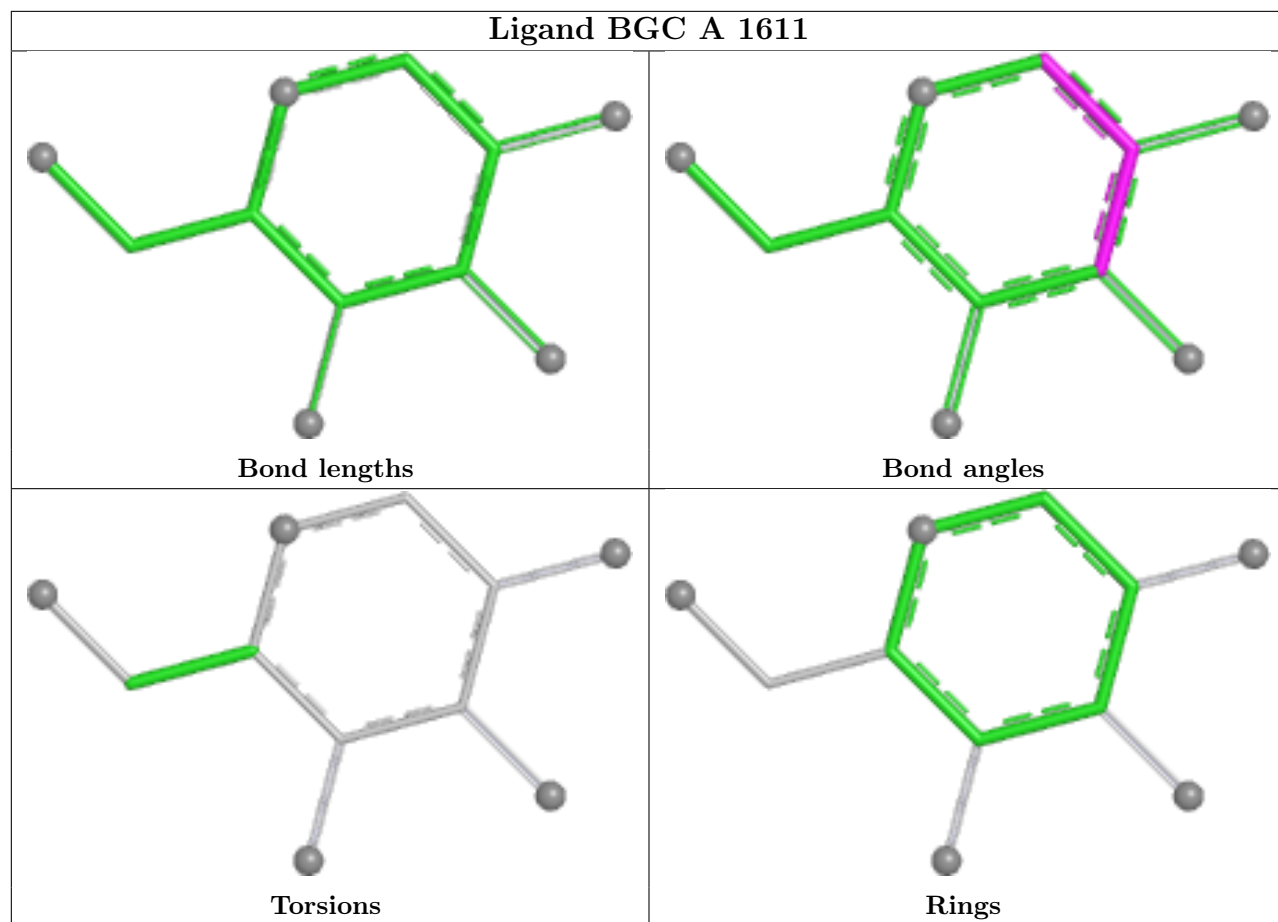


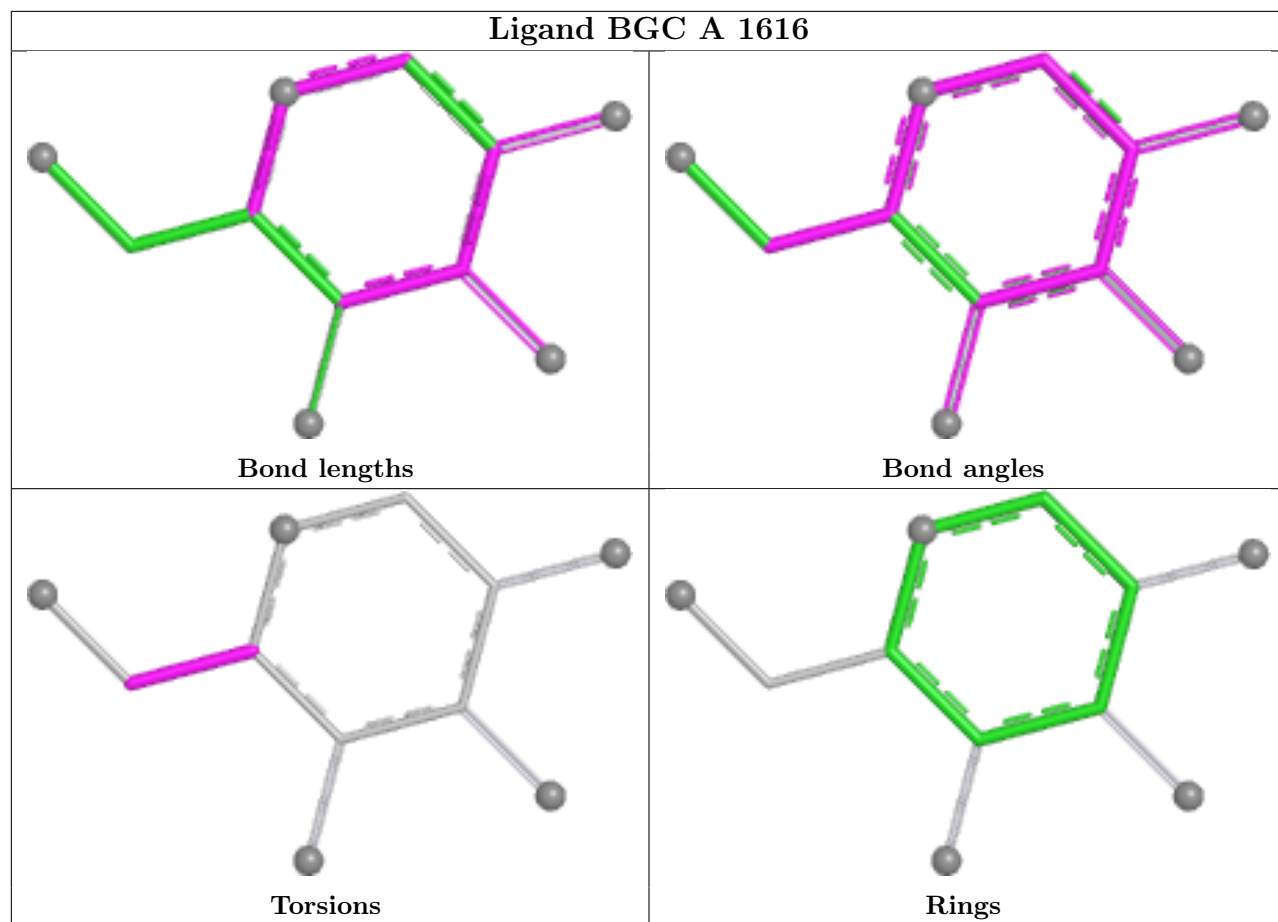


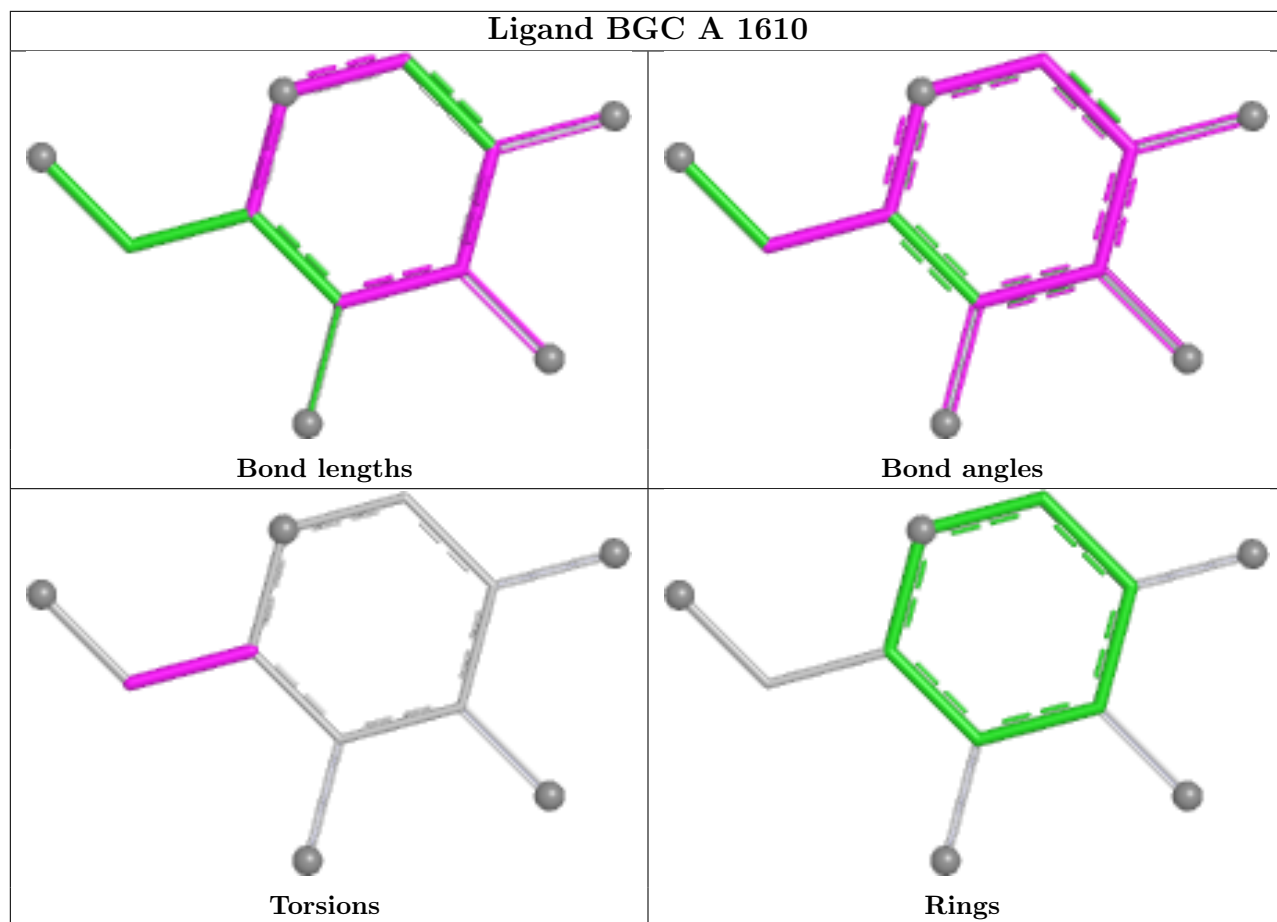


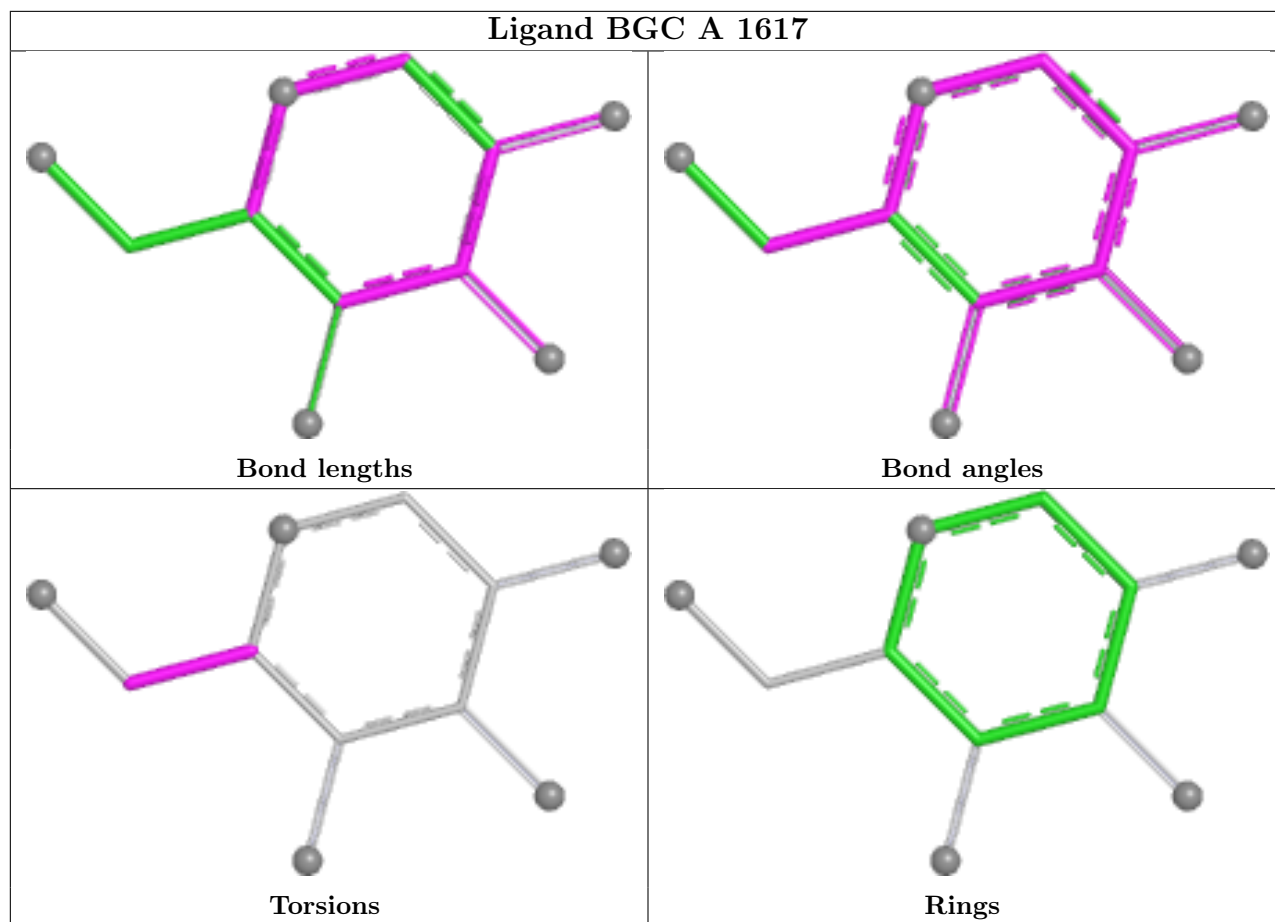


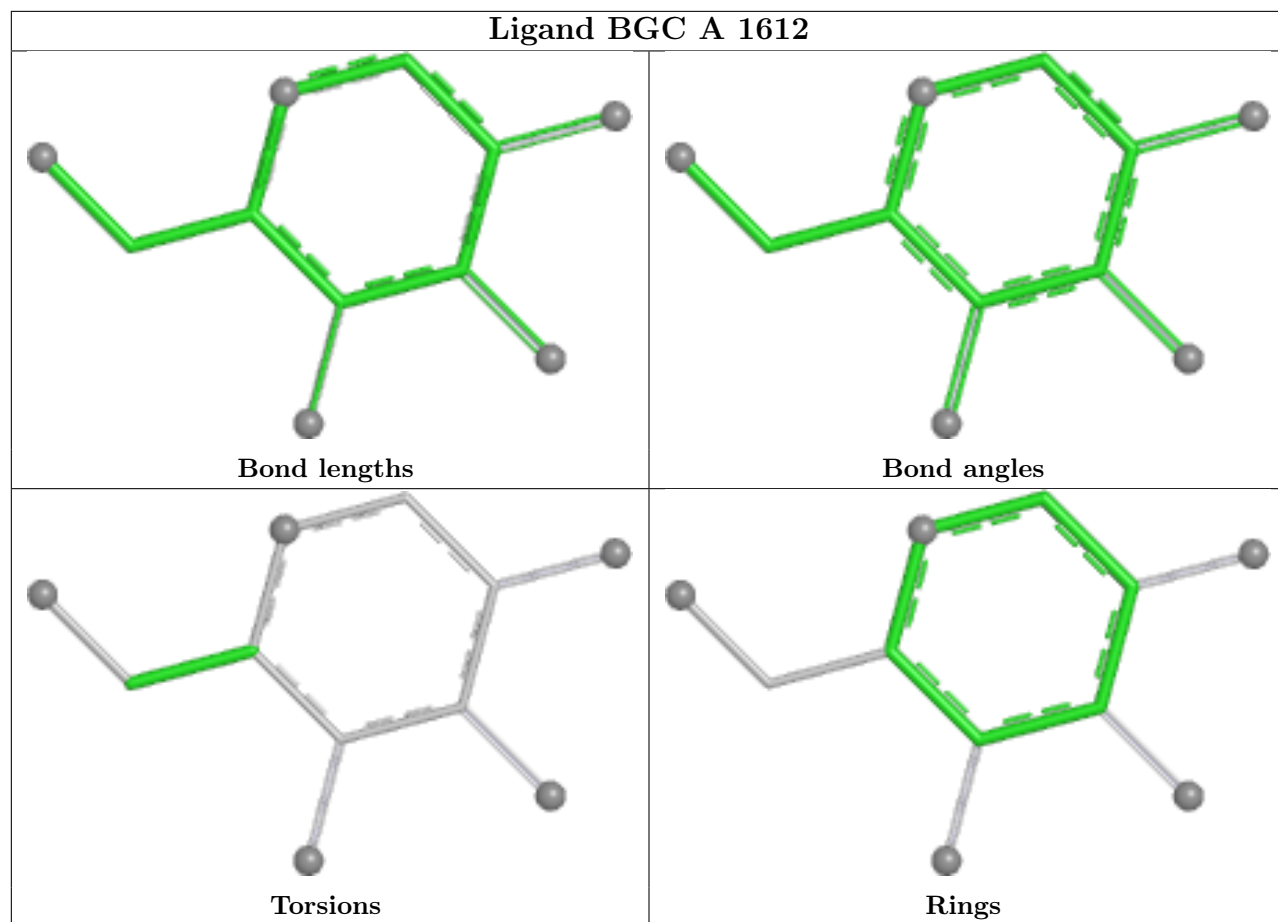


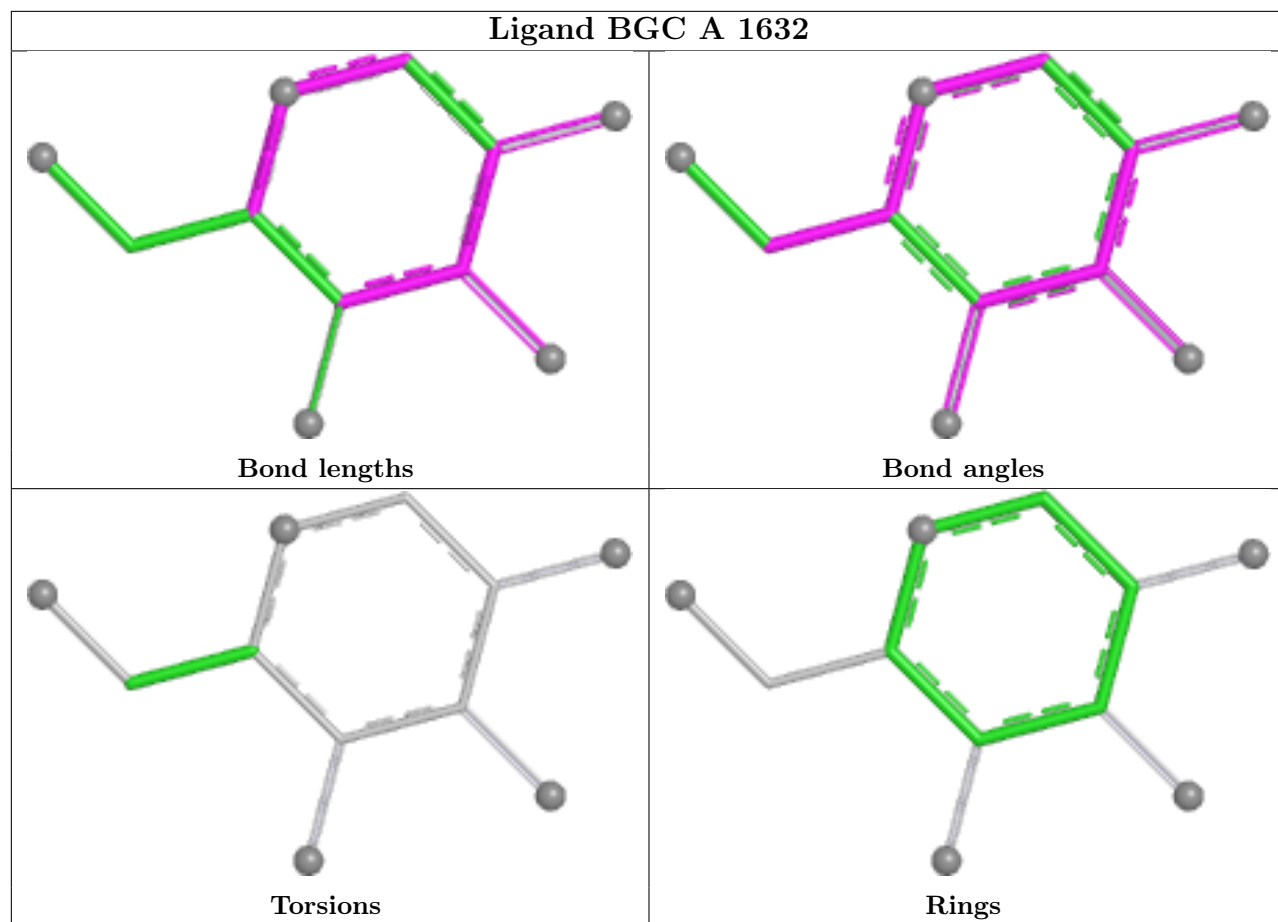


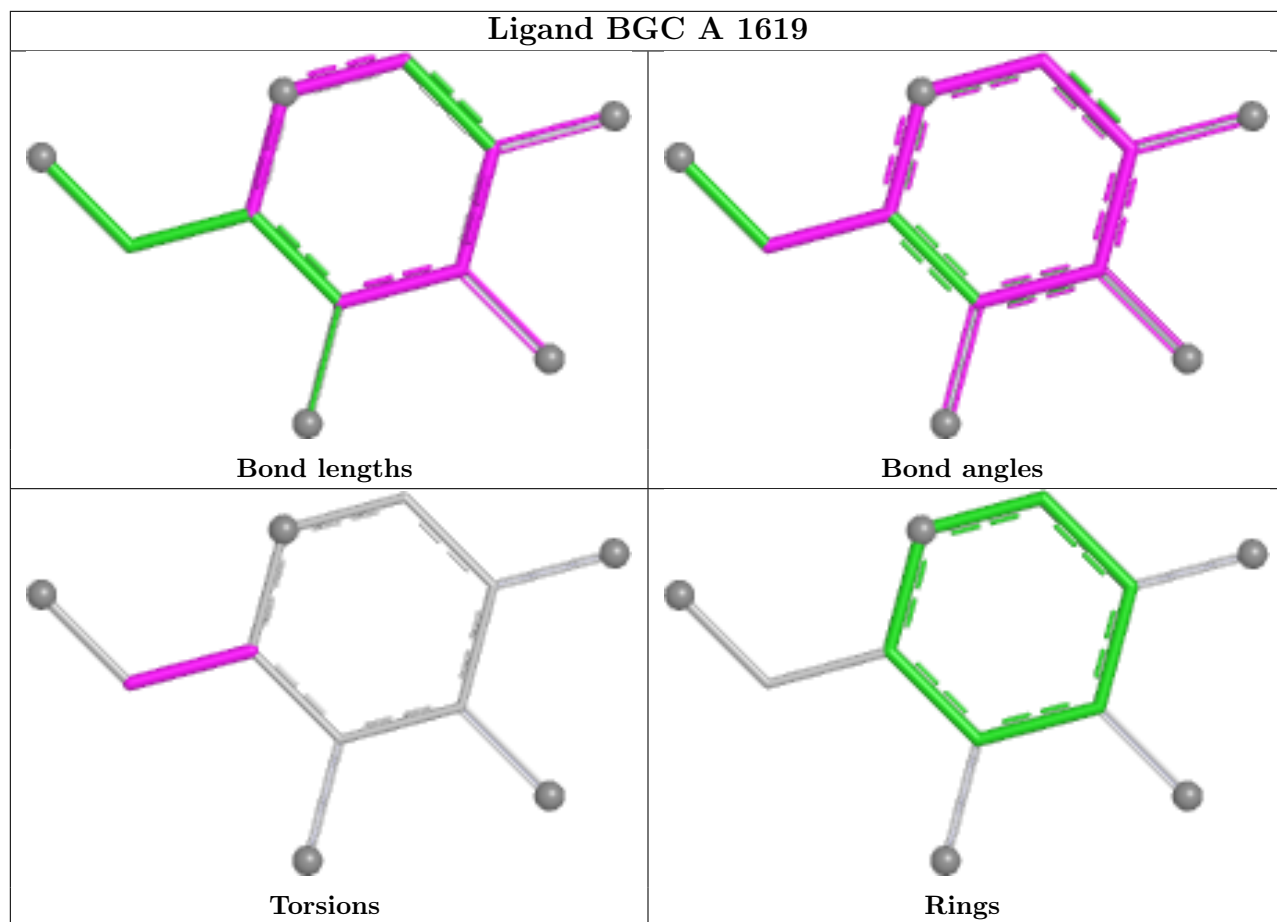


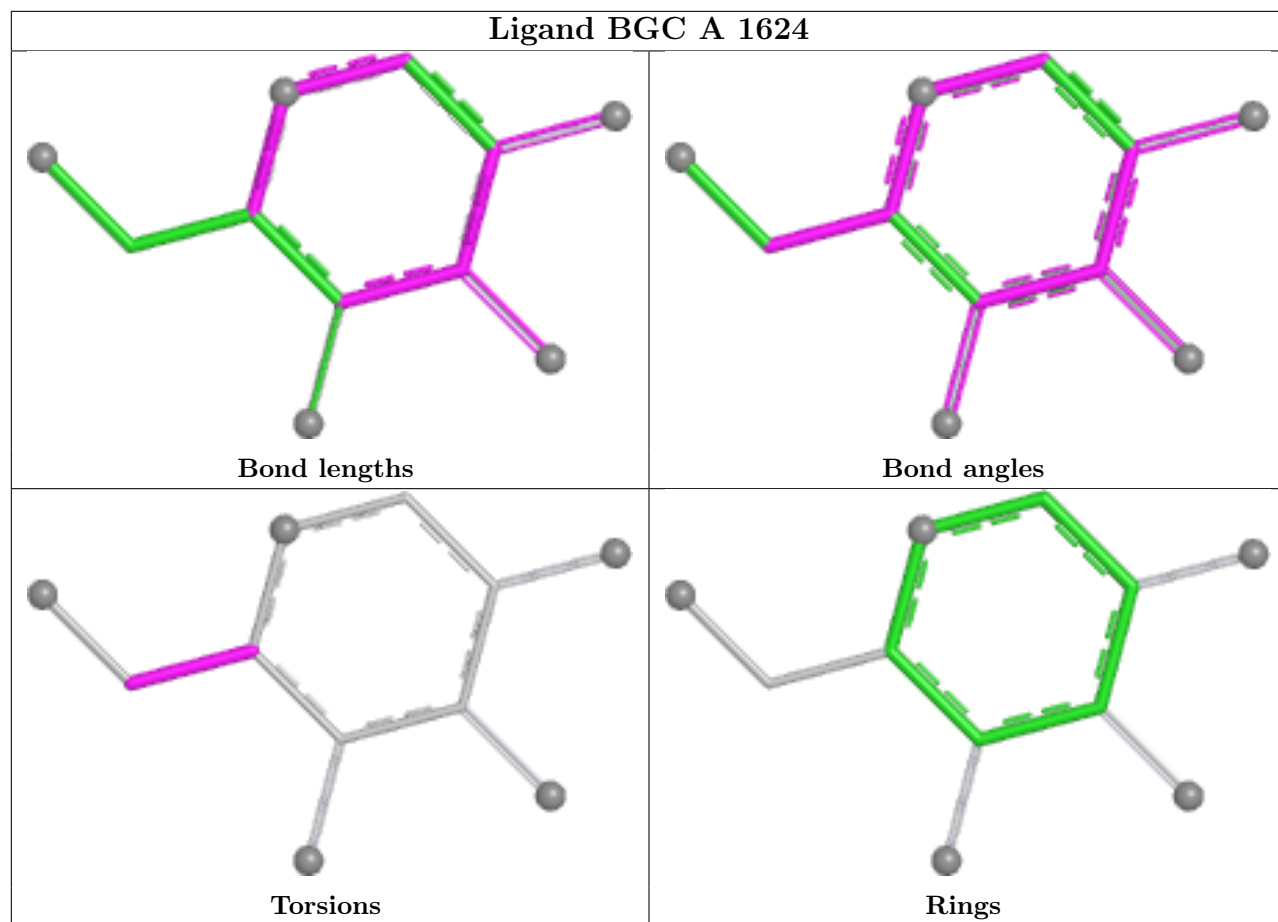


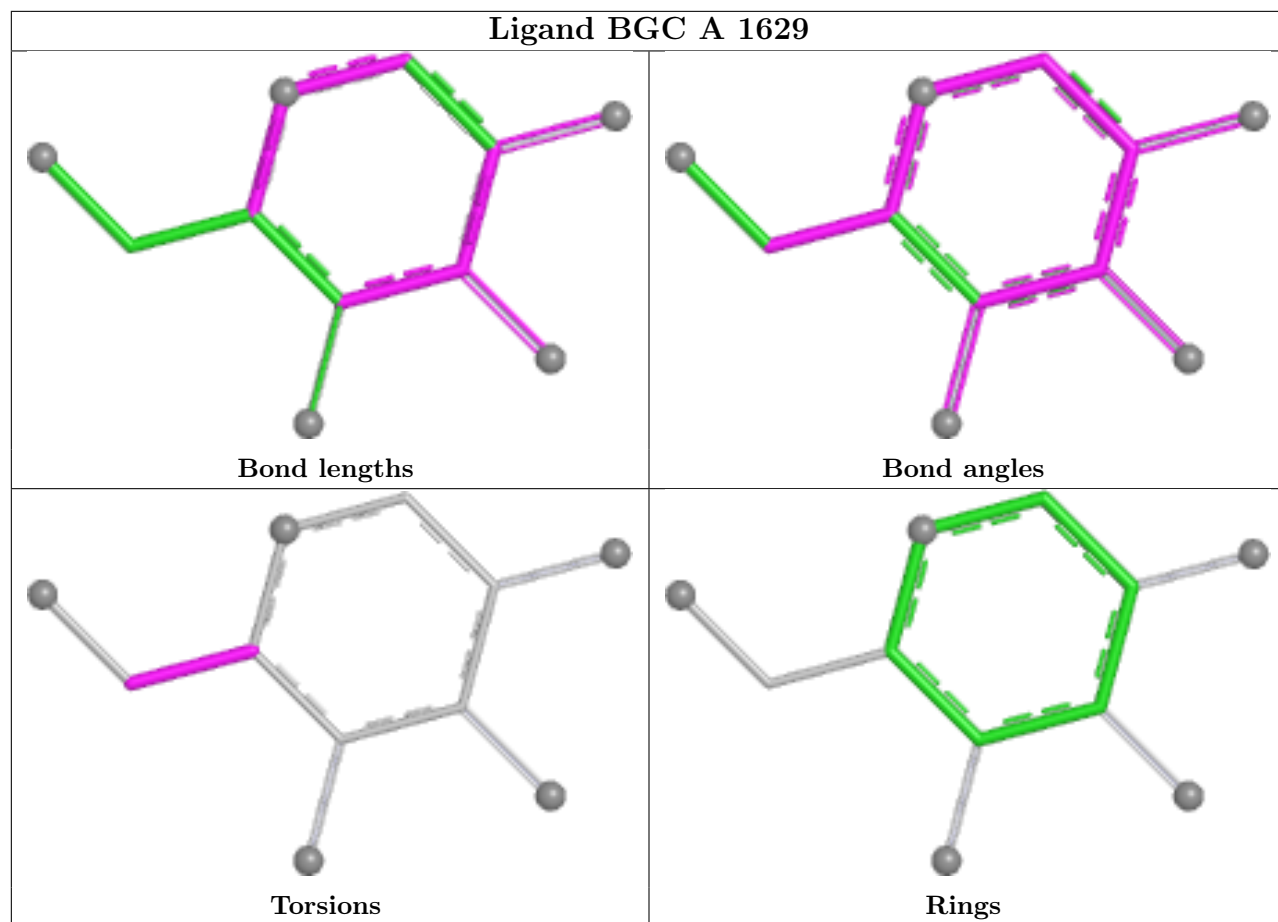


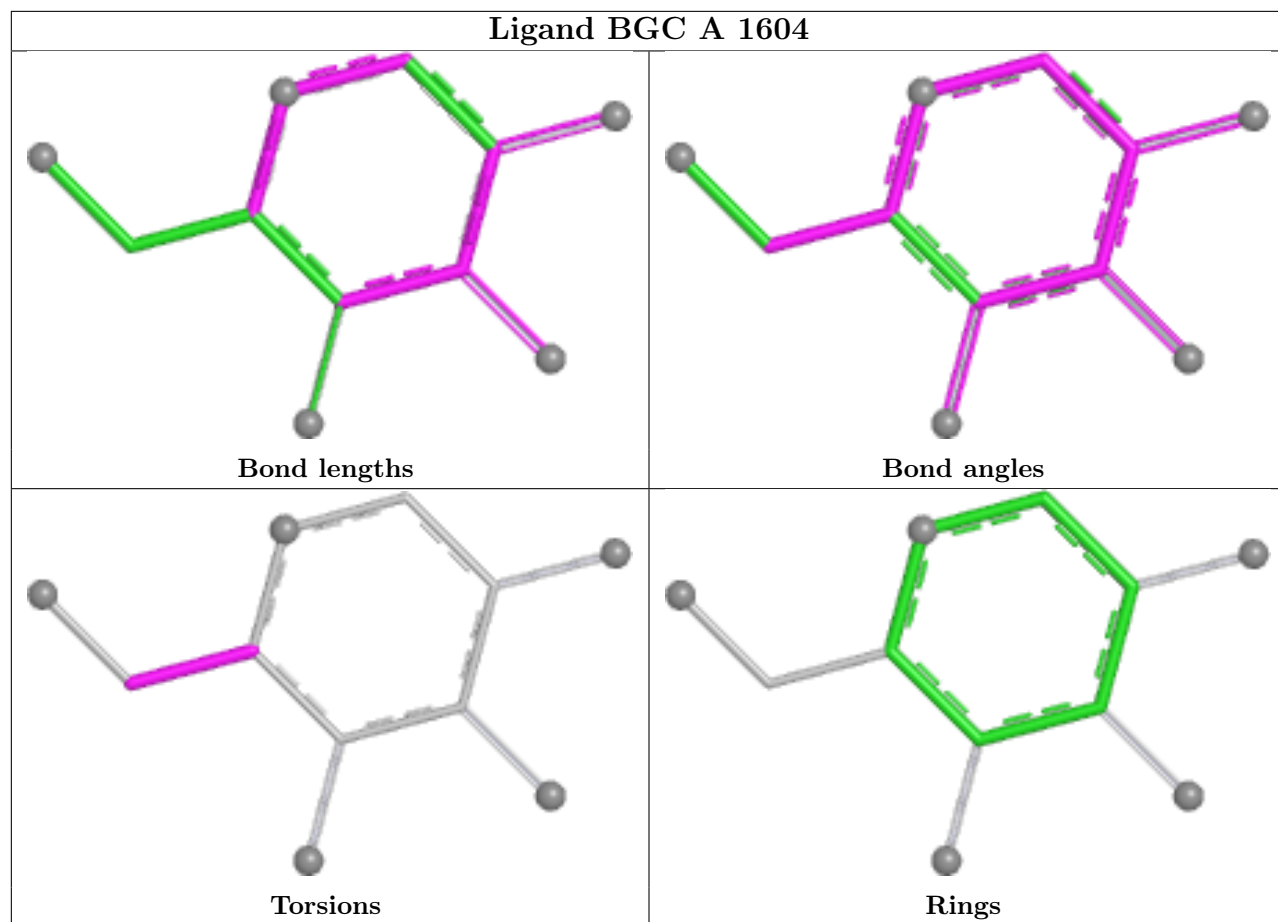


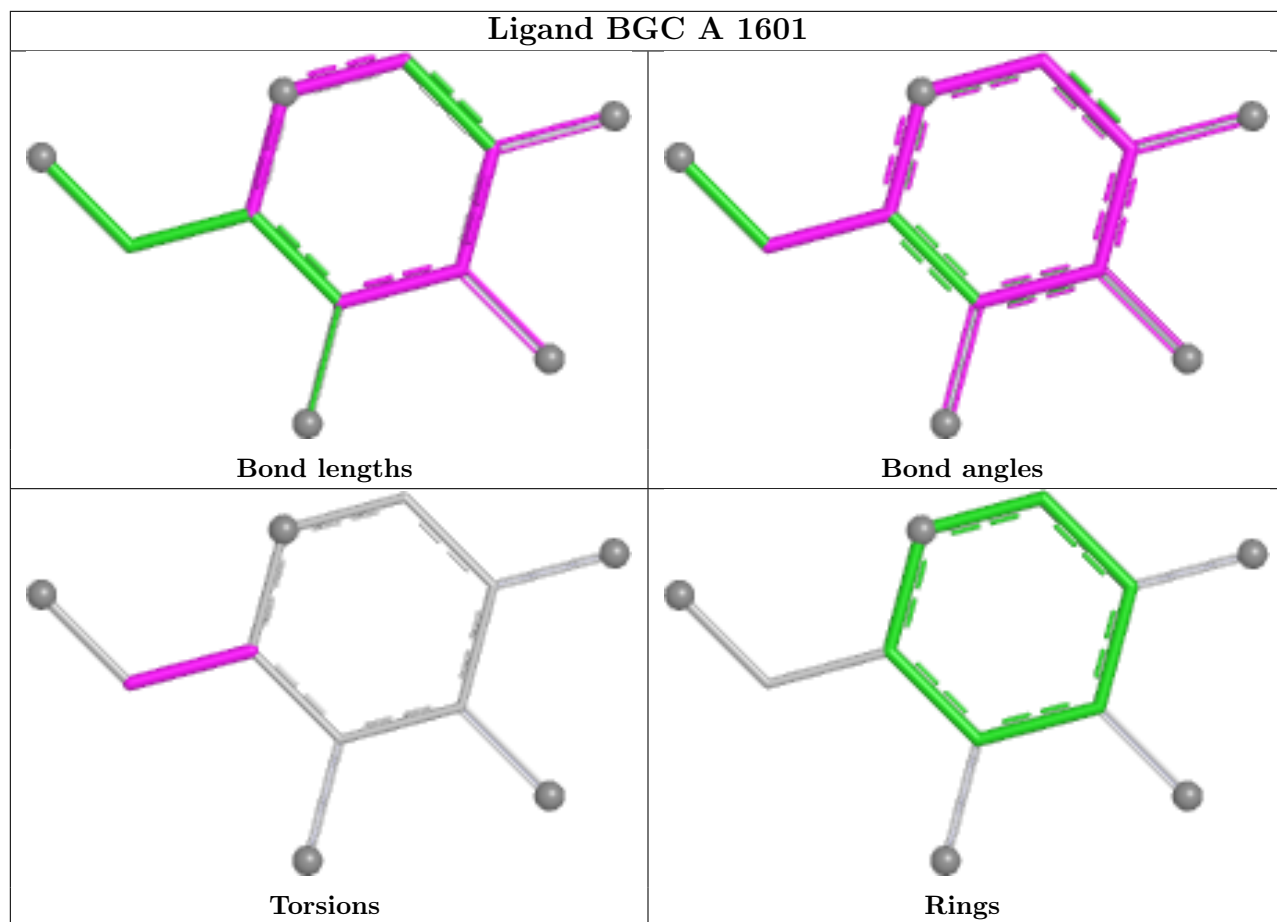


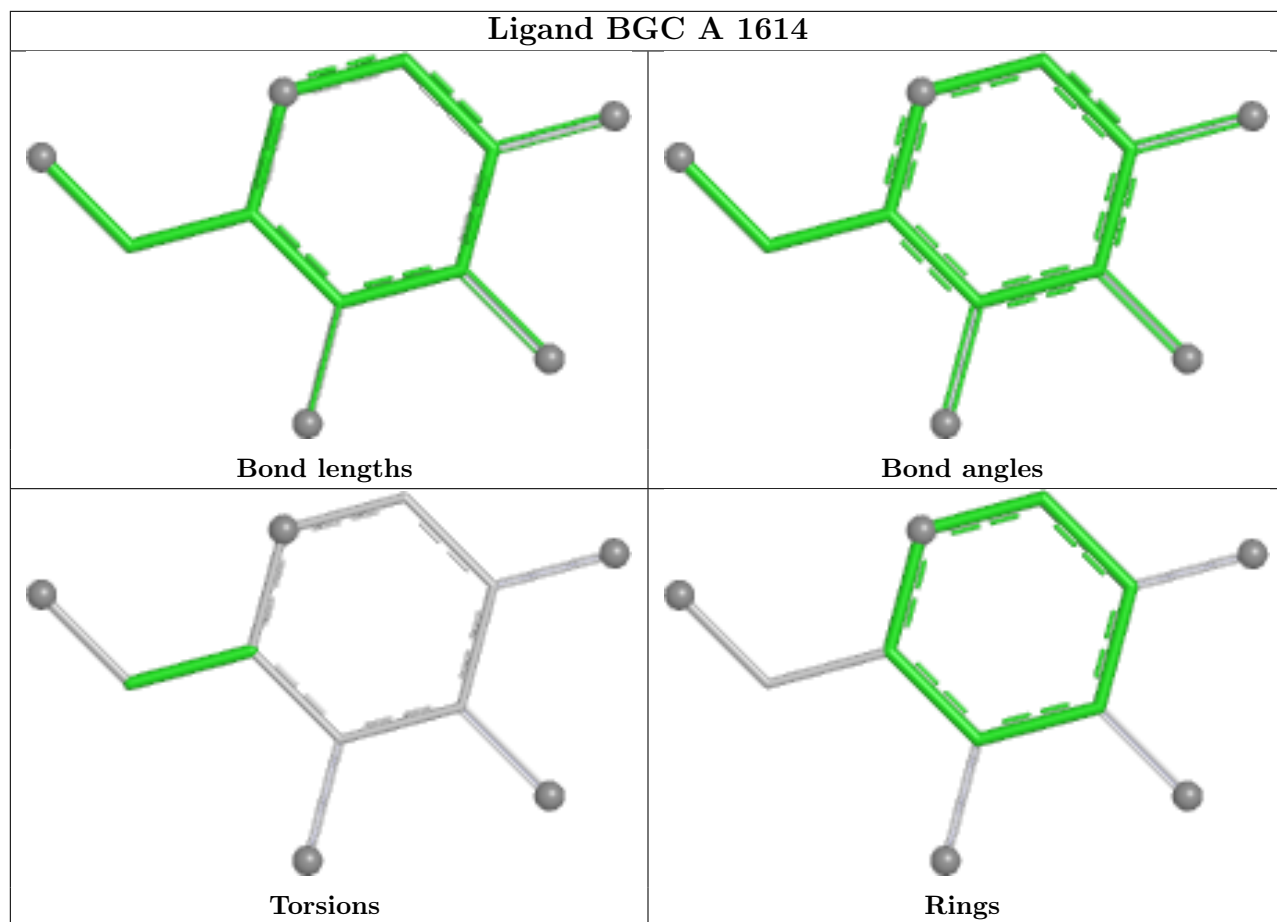


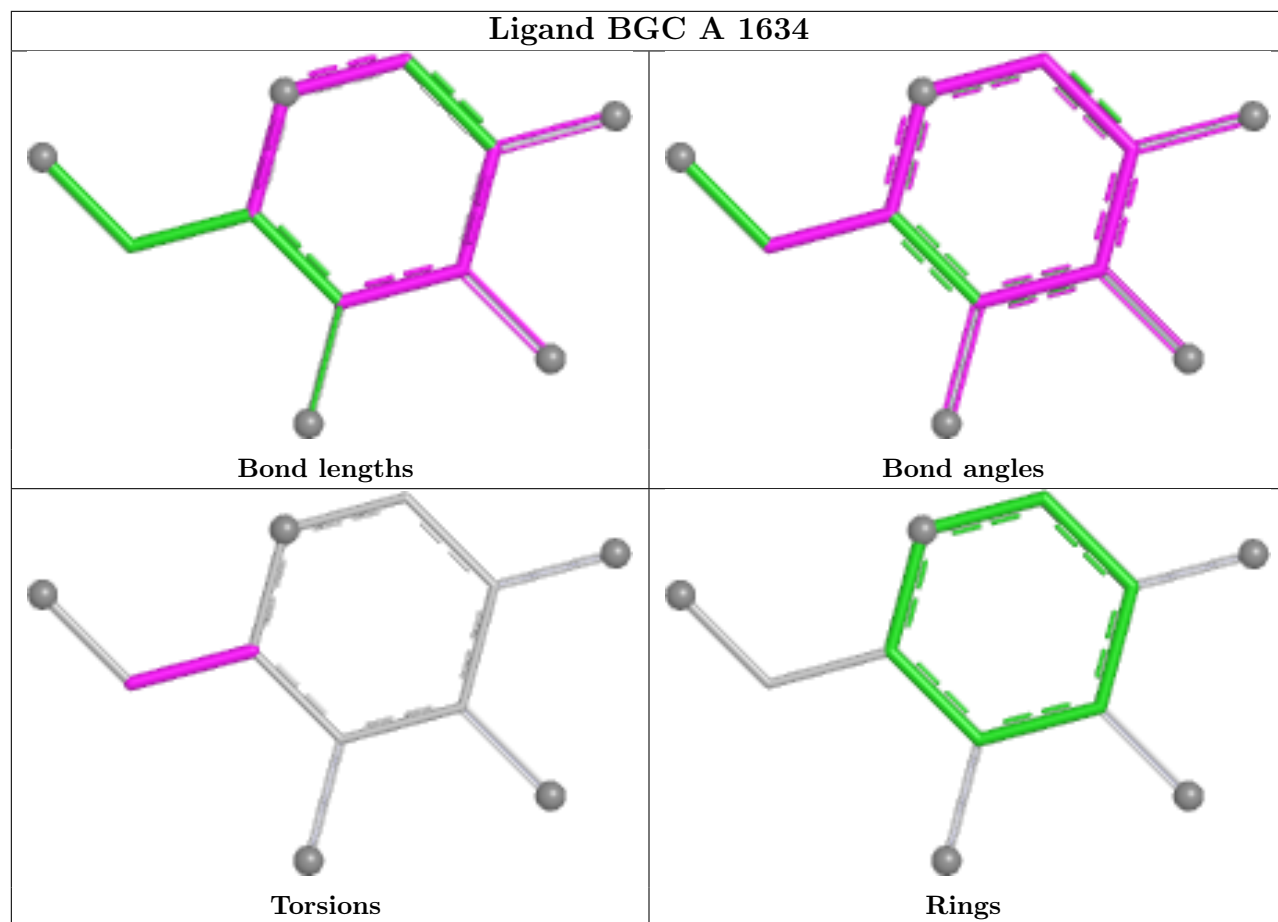


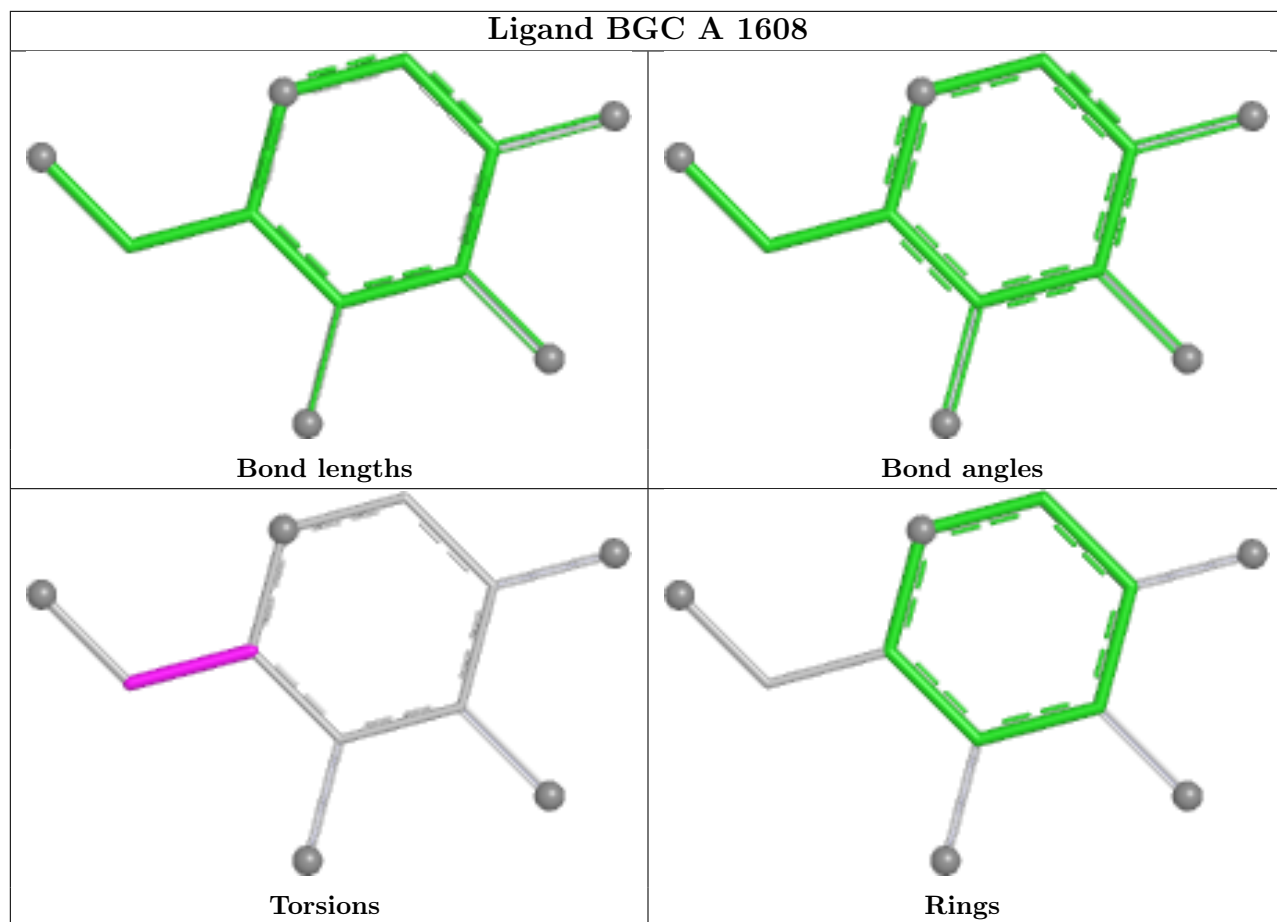


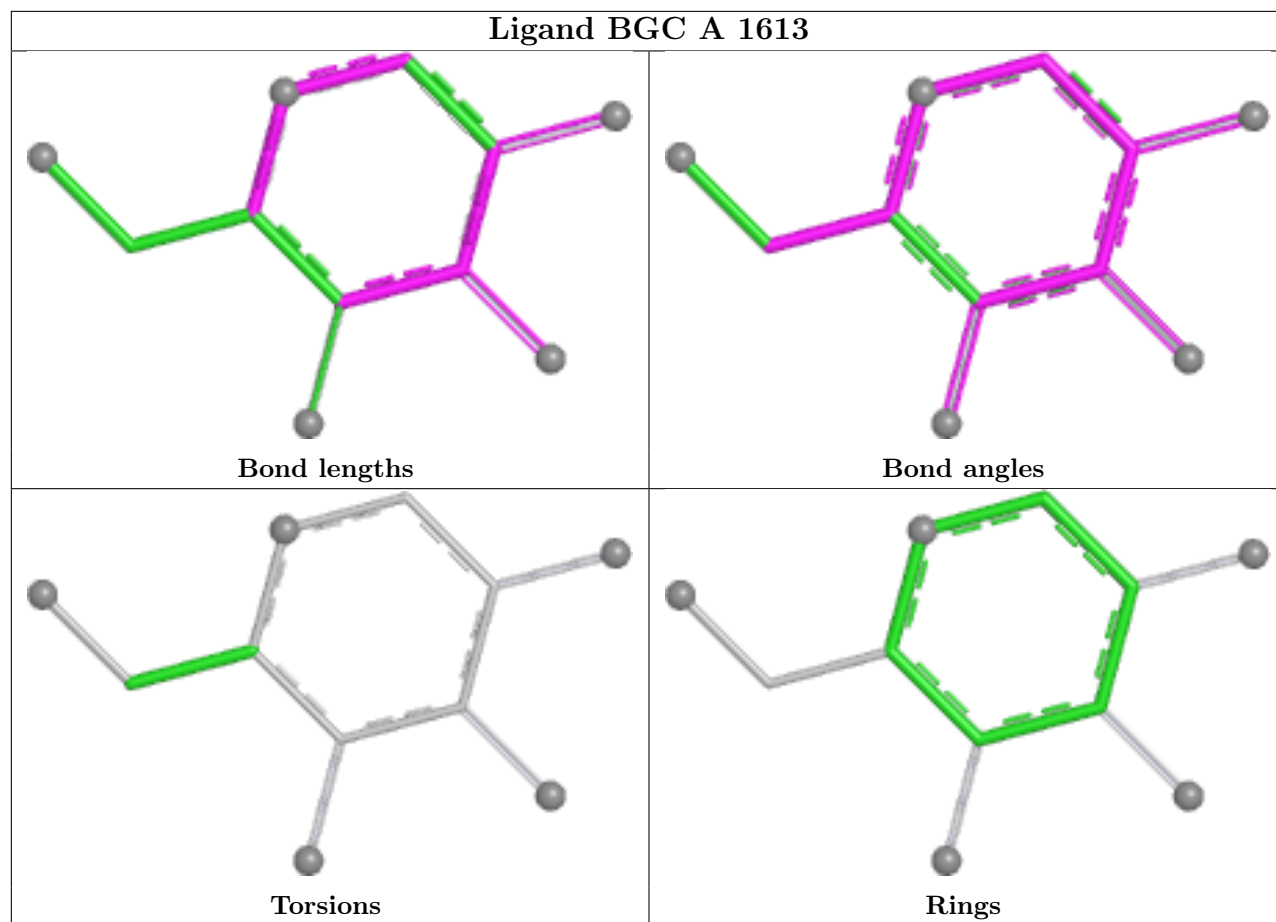












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

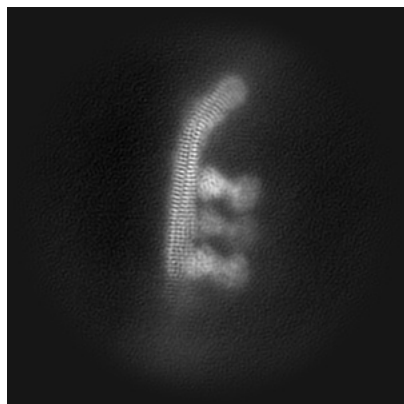
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43119. These allow visual inspection of the internal detail of the map and identification of artifacts.

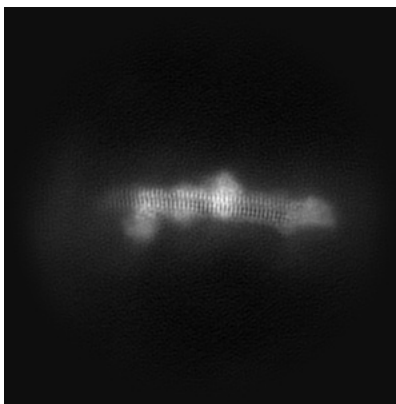
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

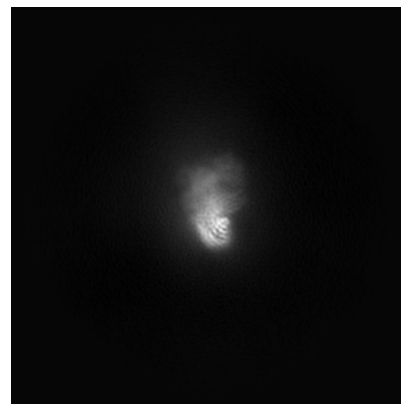
6.1.1 Primary map



X

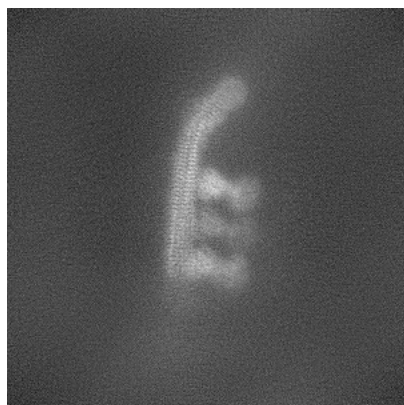


Y

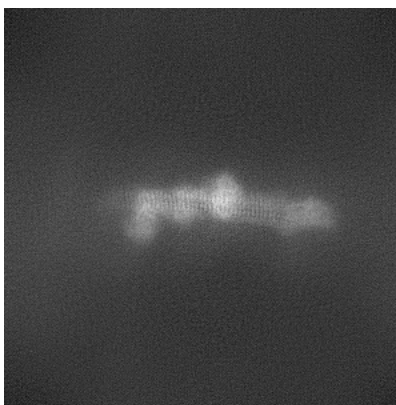


Z

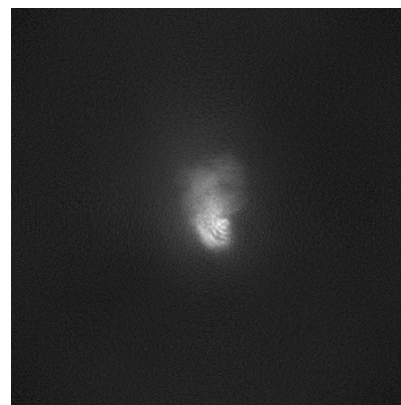
6.1.2 Raw map



X



Y



Z

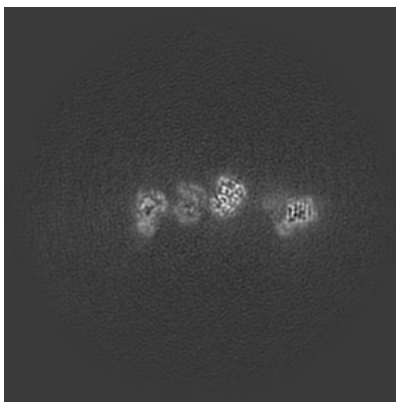
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

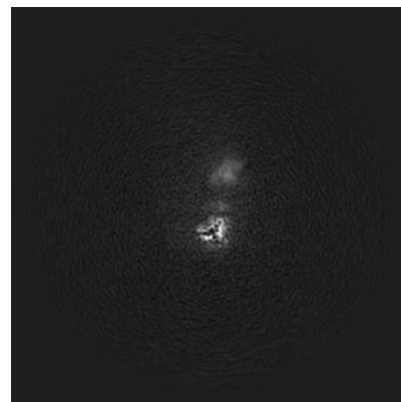
6.2.1 Primary map



X Index: 300

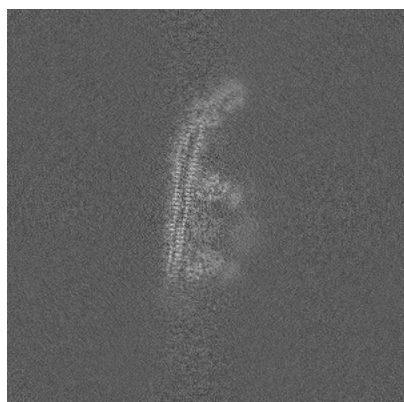


Y Index: 300

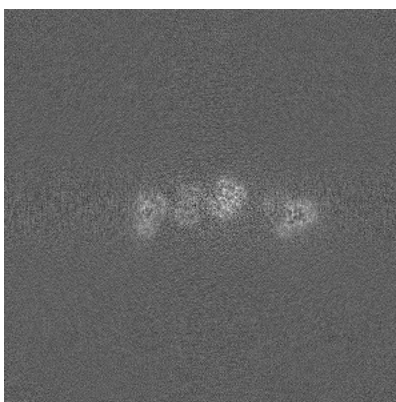


Z Index: 300

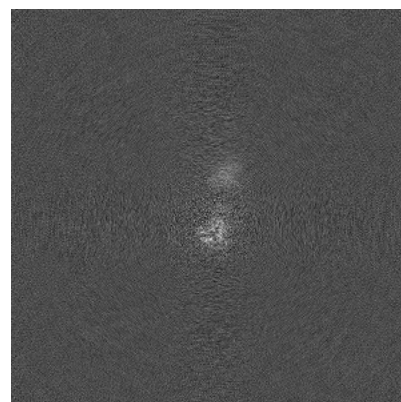
6.2.2 Raw map



X Index: 300



Y Index: 300

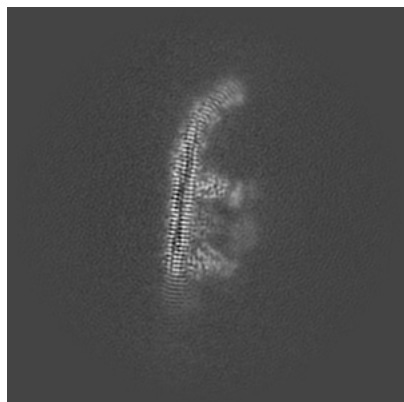


Z Index: 300

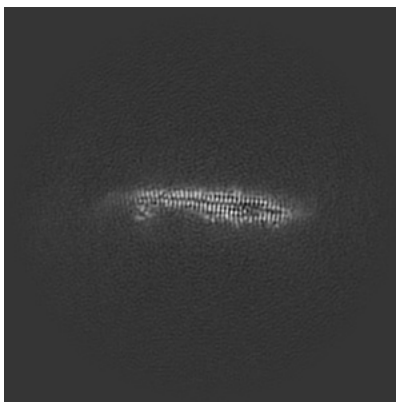
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

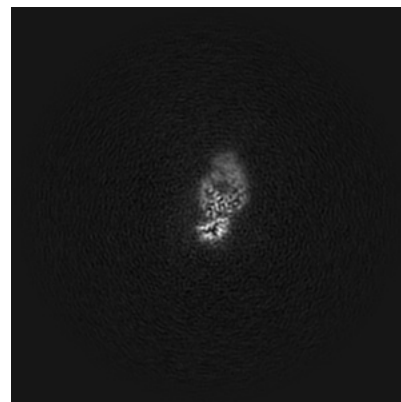
6.3.1 Primary map



X Index: 303

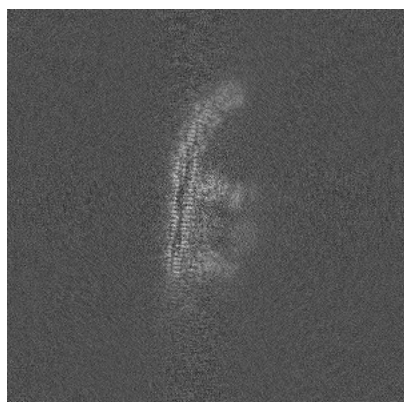


Y Index: 270

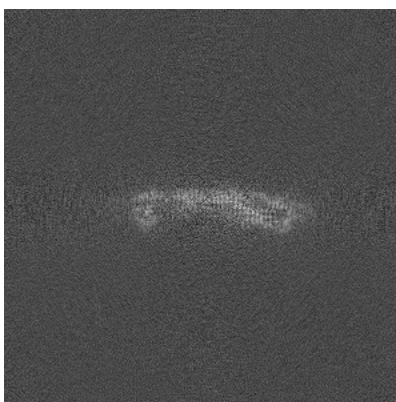


Z Index: 327

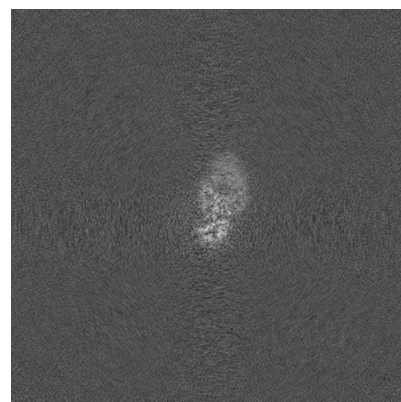
6.3.2 Raw map



X Index: 303



Y Index: 279

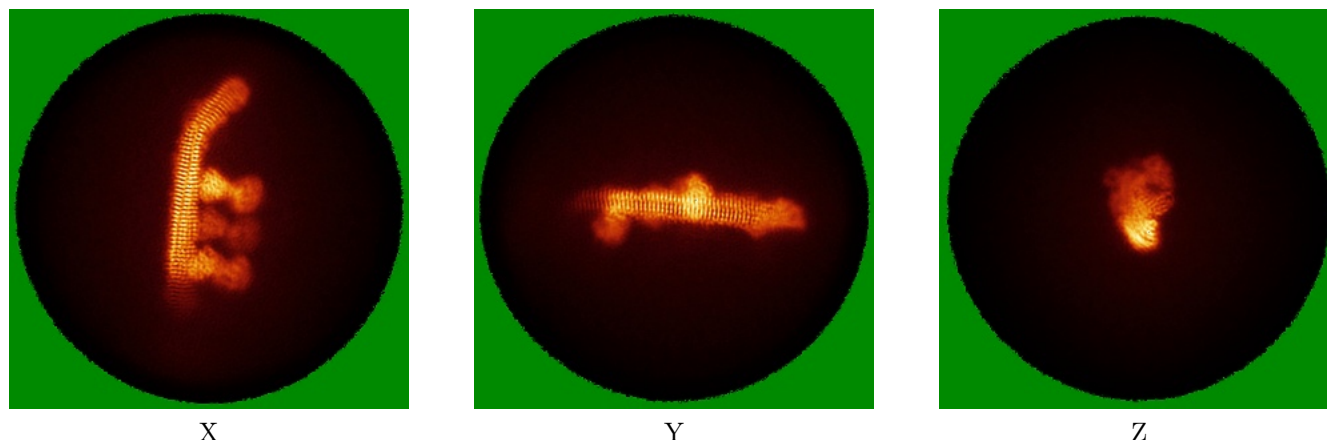


Z Index: 327

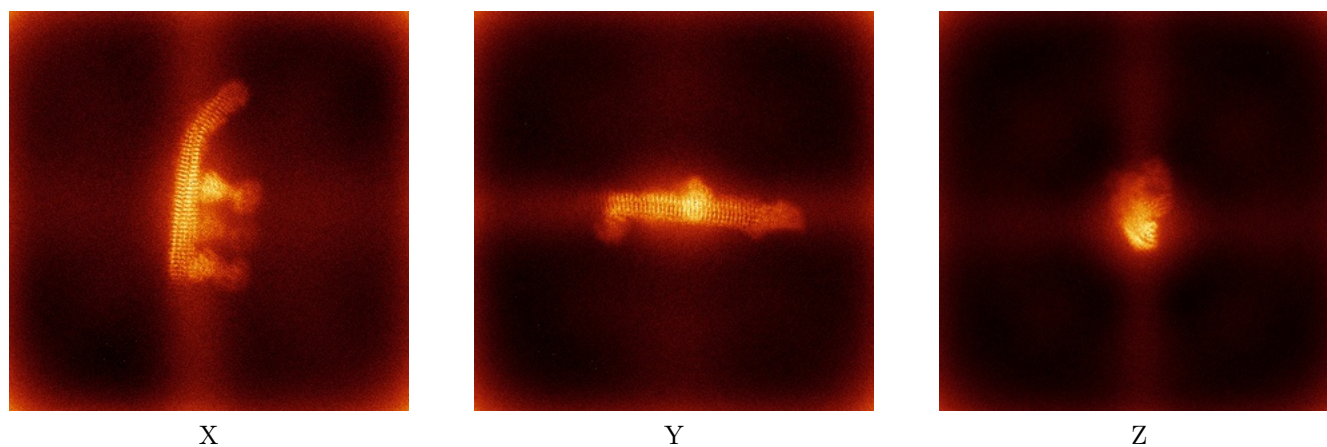
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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 0.0739. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

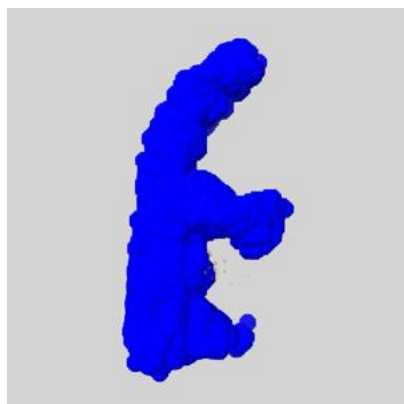
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

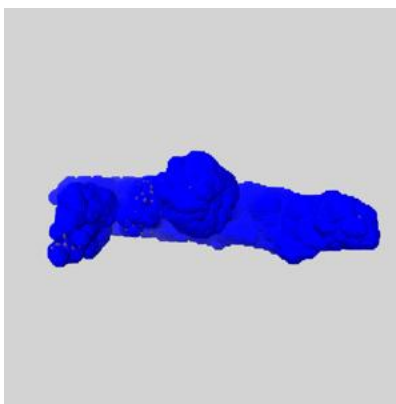
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

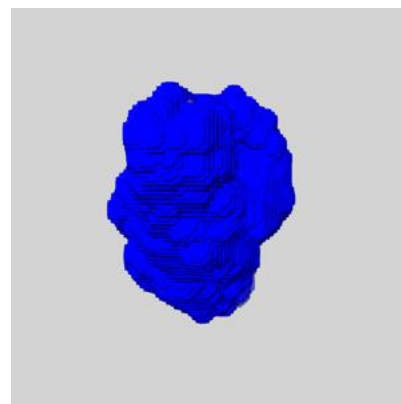
6.6.1 emd_43119_msk_1.map [i](#)



X



Y

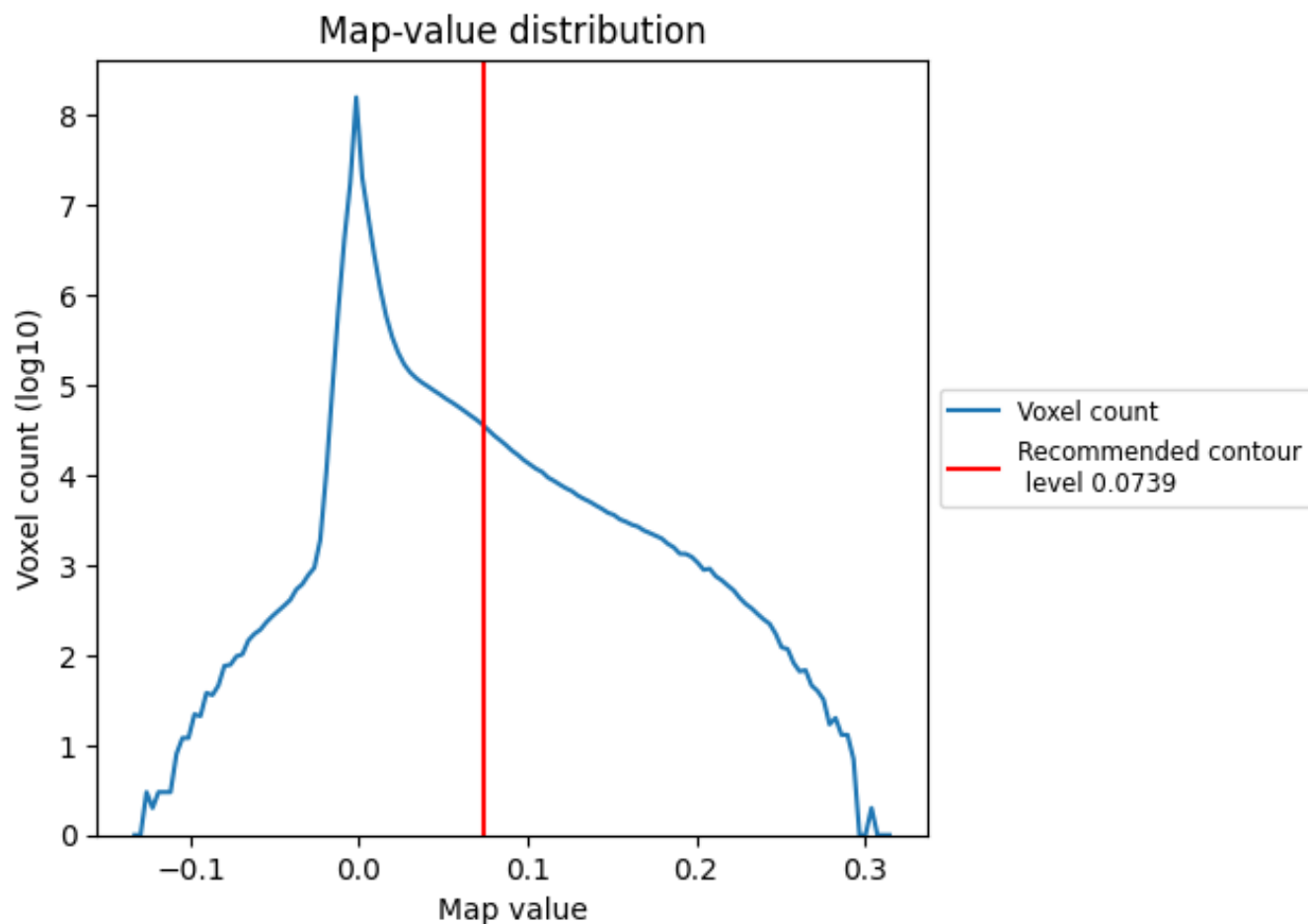


Z

7 Map analysis [i](#)

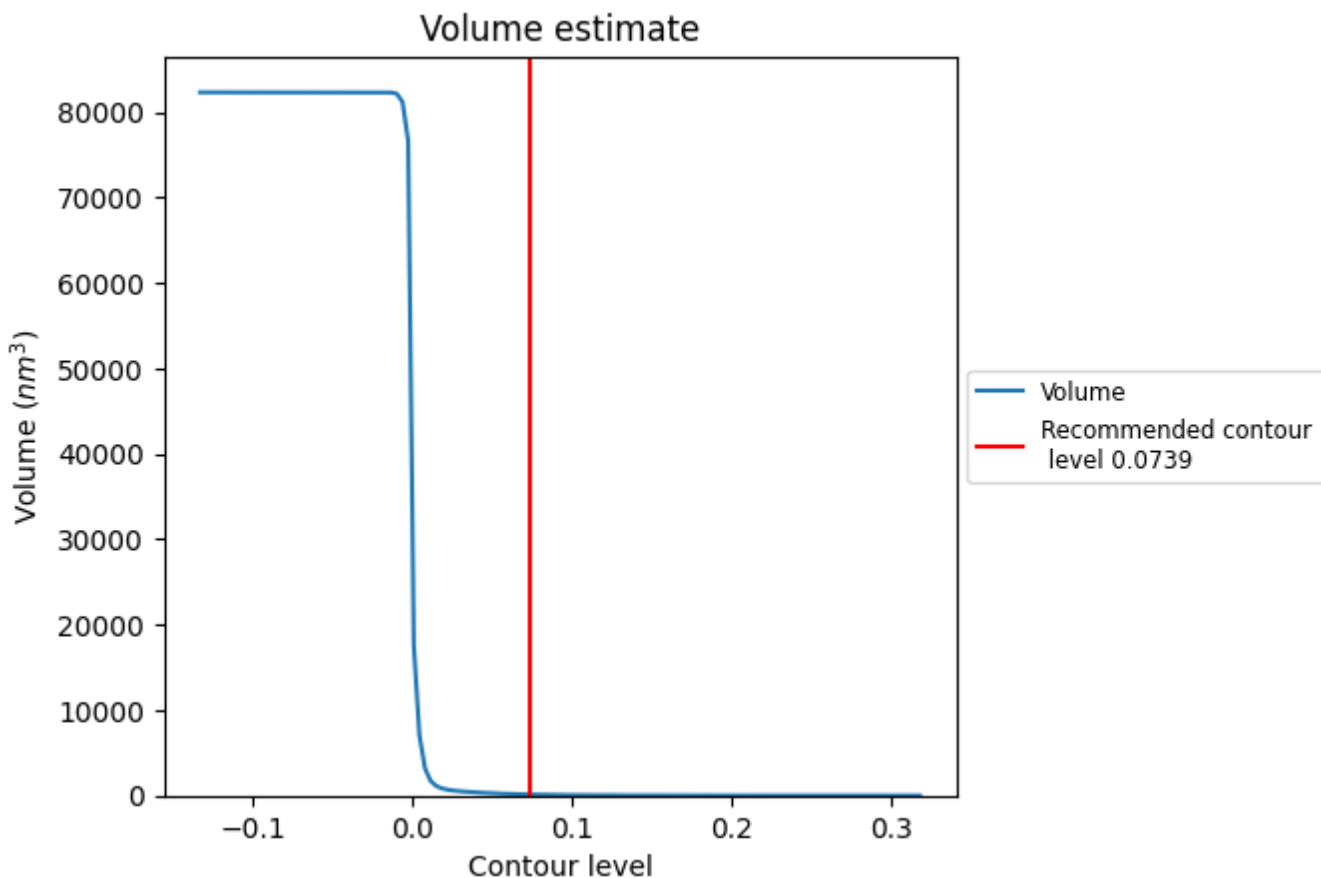
This section contains the results of statistical analysis of the map.

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.

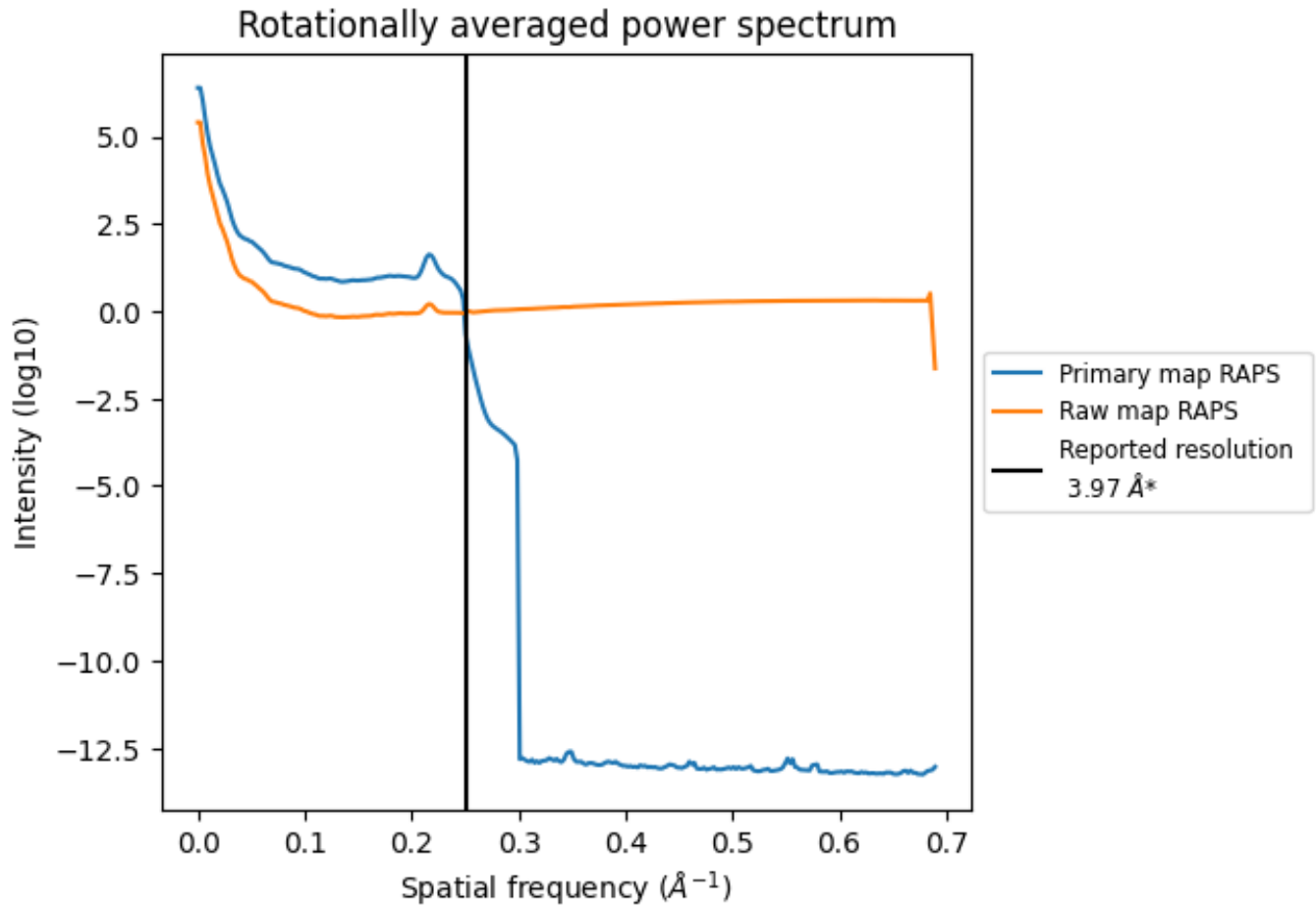
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm³; this corresponds to an approximate mass of 113 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](#)

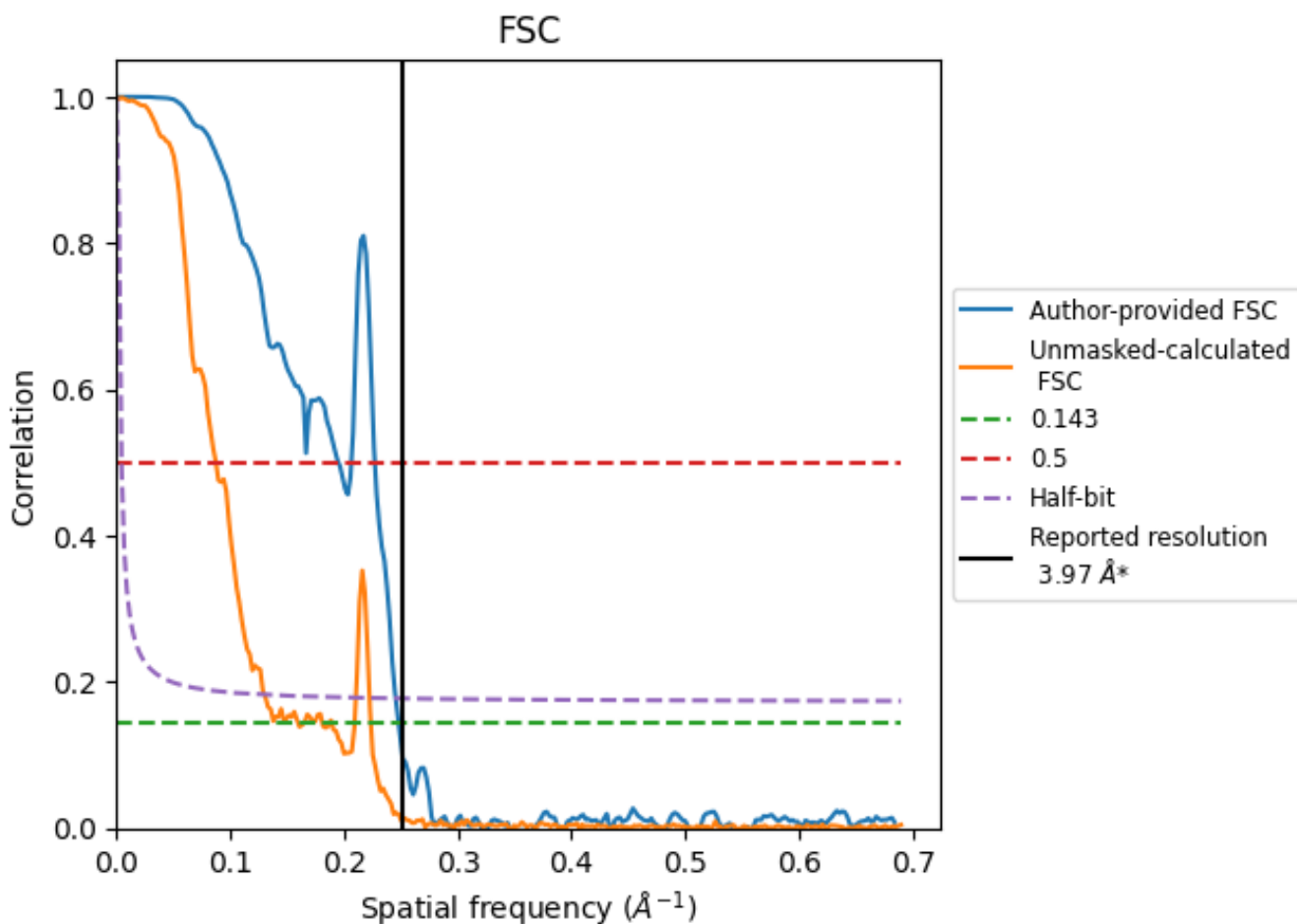


*Reported resolution corresponds to spatial frequency of 0.252 Å⁻¹

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 0.252 Å⁻¹

8.2 Resolution estimates [i](#)

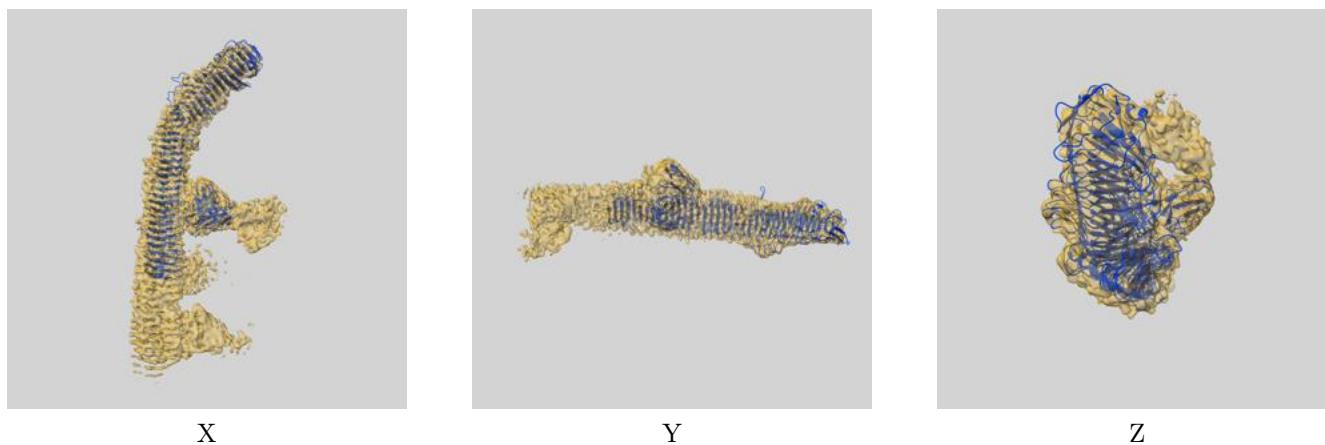
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.97	-	-
Author-provided FSC curve	4.03	5.13	4.07
Unmasked-calculated*	6.26	11.44	7.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.26 differs from the reported value 3.97 by more than 10 %

9 Map-model fit [i](#)

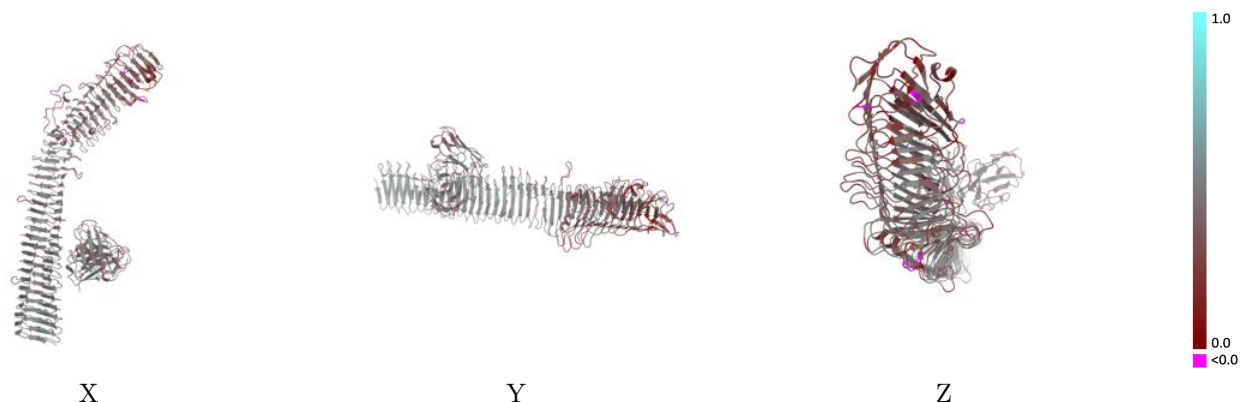
This section contains information regarding the fit between EMDB map EMD-43119 and PDB model 8VBB. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



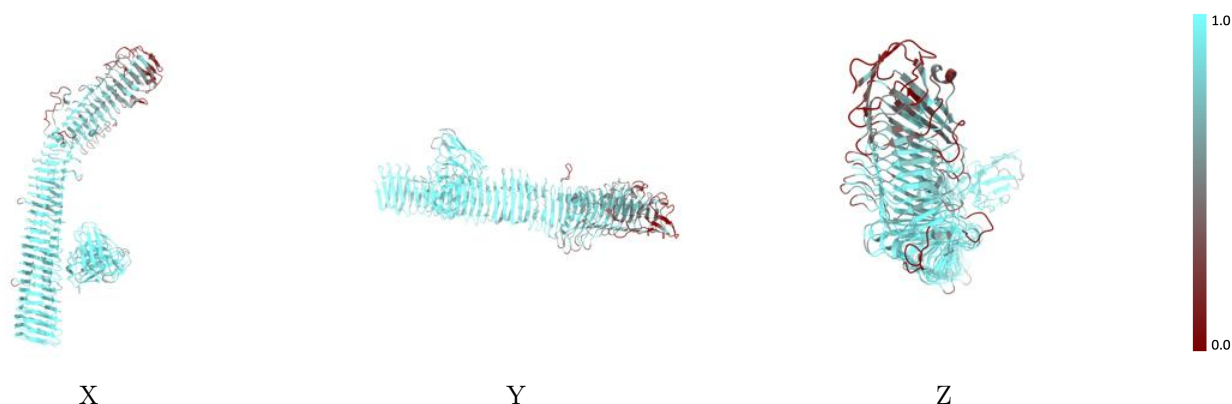
The images above show the 3D surface view of the map at the recommended contour level 0.0739 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



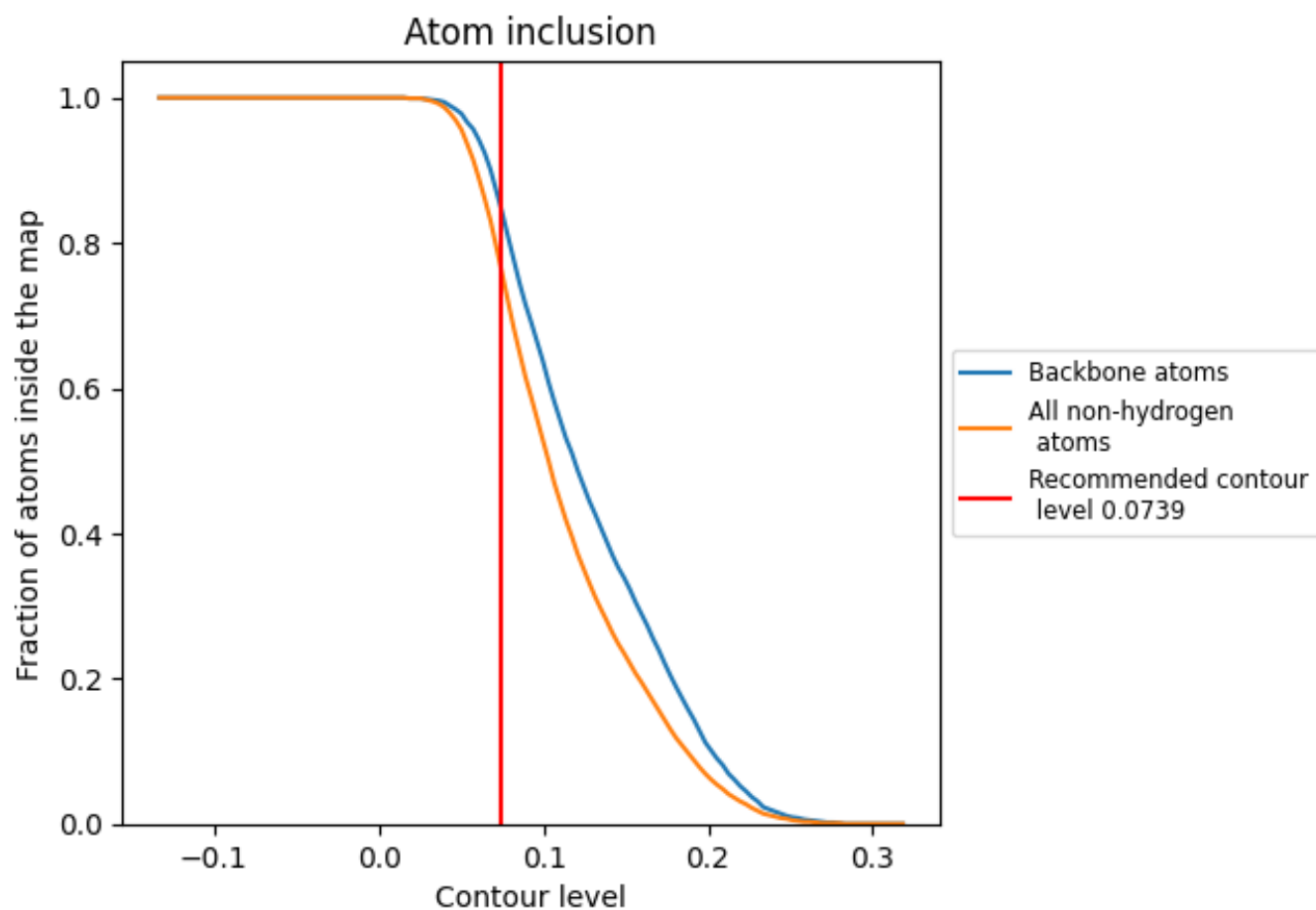
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0739).









9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (0.0739) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.3920
A	 0.7420	 0.3850
H	 0.9010	 0.4280
L	 0.8800	 0.4190

