



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:38 PM UTC

PDB ID : 9TDW / pdb_00009tdw
Title : Structure of D81A-Fructofuranosidase from *Purpureocillum lilacinum* in complex with fructose
Authors : Ruiz-Nunez, M.; Sanz-Aparicio, J.
Deposited on : 2025-11-24
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

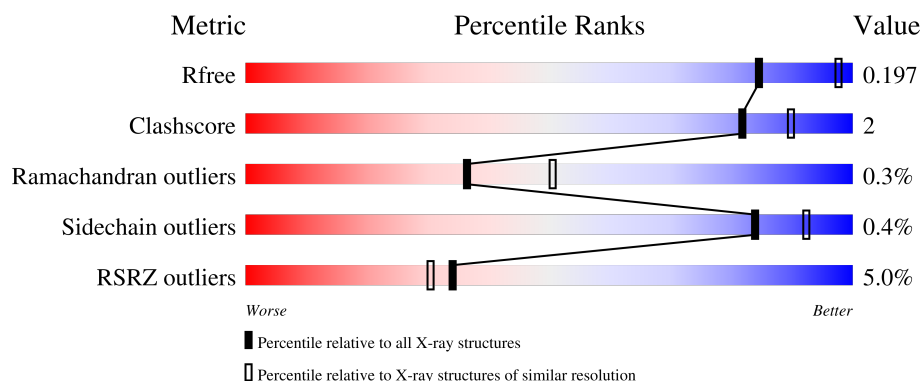
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	4% 86% 6% 7%
1	B	576	5% 87% 6% 7%
1	C	576	5% 86% 7% 7%
1	D	576	5% 88% 5% 7%
2	E	9	44% 56%

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Mol	Chain	Length	Quality of chain
2	F	9	 56% 44%
2	G	9	 78% 22%
2	H	9	 56% 44%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 17695 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

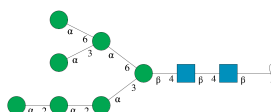
- Molecule 1 is a protein called Invertase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	1	0
			4170	2652	709	795	14			
1	B	536	Total	C	N	O	S	0	0	0
			4153	2643	704	792	14			
1	C	537	Total	C	N	O	S	0	1	0
			4170	2652	709	795	14			
1	D	534	Total	C	N	O	S	0	0	0
			4138	2635	702	787	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ALA	ASP	engineered mutation	UNP A0A179H0Q0
B	81	ALA	ASP	engineered mutation	UNP A0A179H0Q0
C	81	ALA	ASP	engineered mutation	UNP A0A179H0Q0
D	81	ALA	ASP	engineered mutation	UNP A0A179H0Q0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



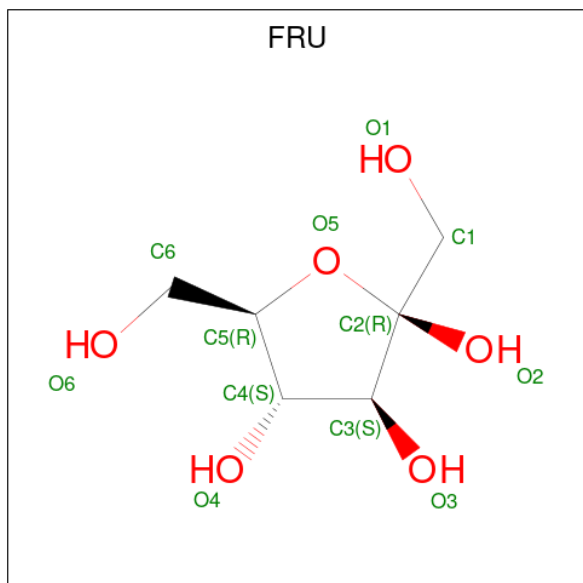
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	F	9	Total	C	N	O	0	0	0
			105	58	2	45			

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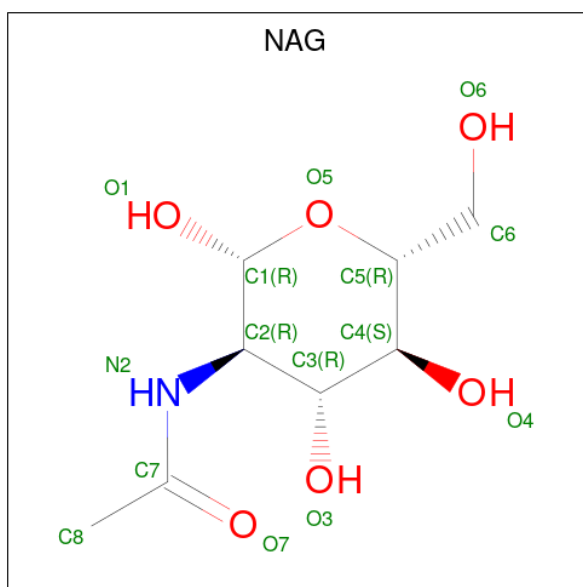
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	H	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 3 is beta-D-fructofuranose (CCD ID: FRU) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



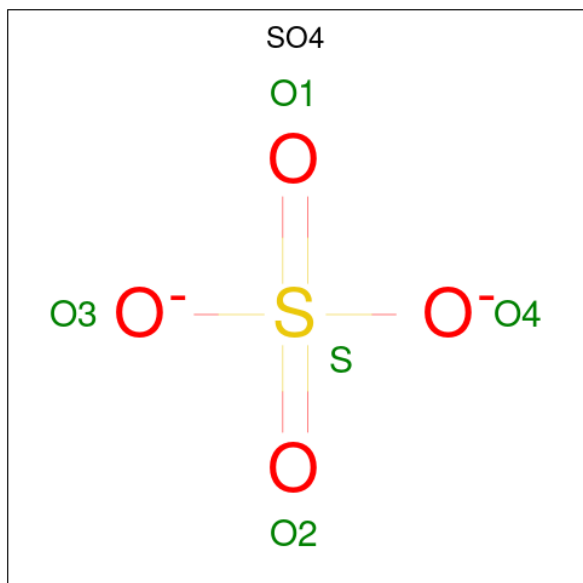
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	108	Total	O	0	0
			108	108		

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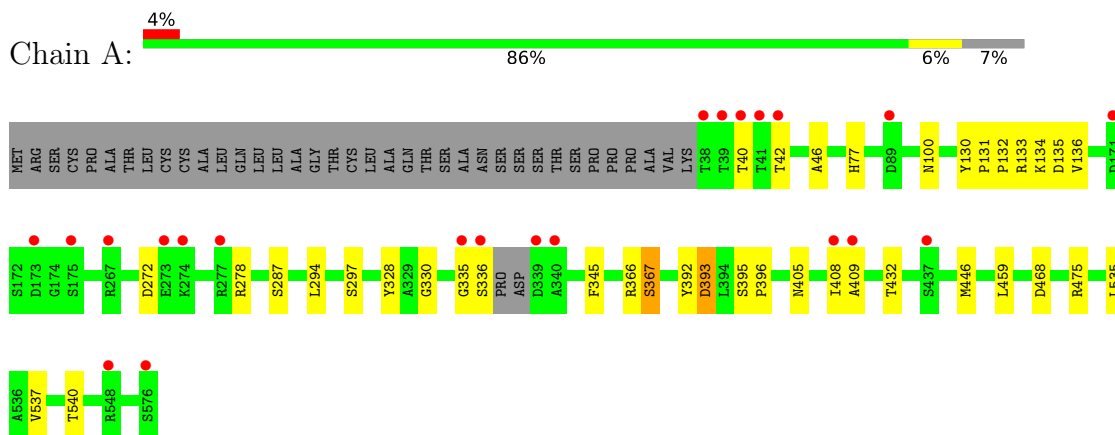
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	69	Total 69	O 69	0	0
6	C	89	Total 89	O 89	0	0
6	D	76	Total 76	O 76	0	0

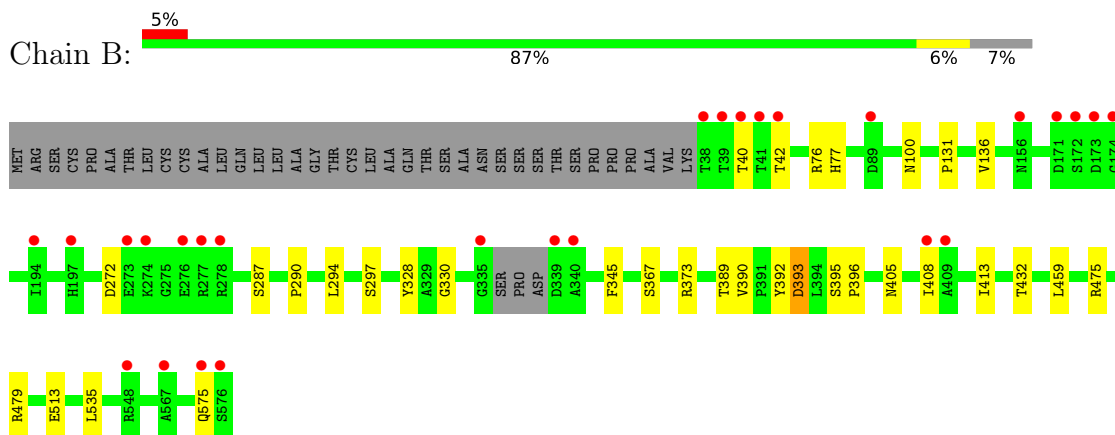
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

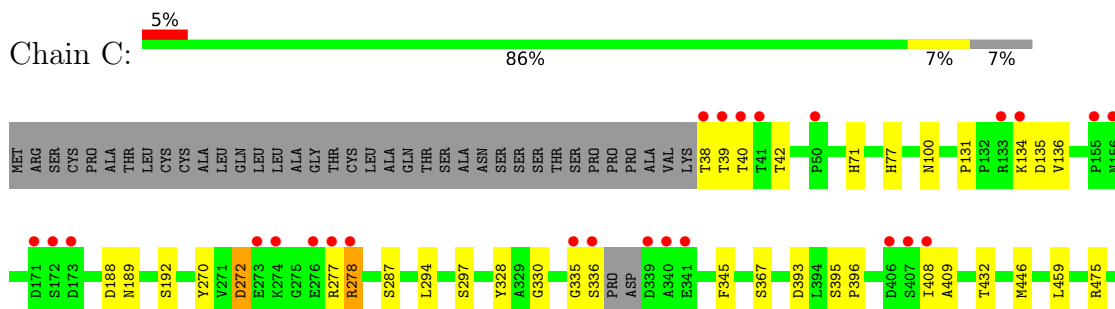
• Molecule 1: Invertase



• Molecule 1: Invertase

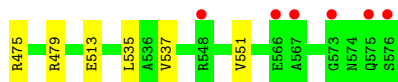
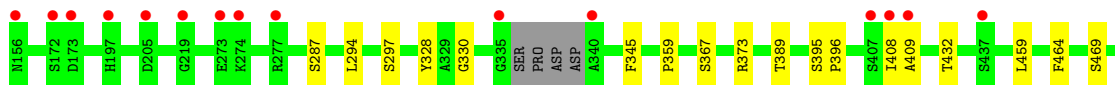
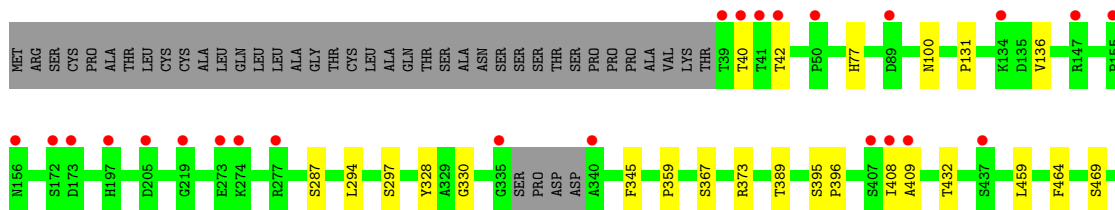
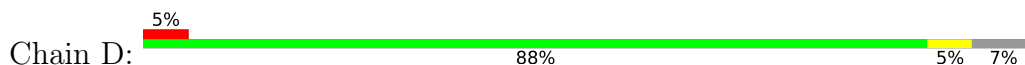


• Molecule 1: Invertase





- Molecule 1: Invertase



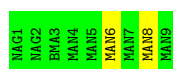
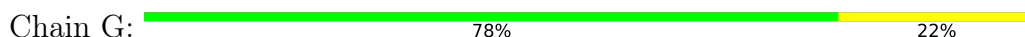
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-

(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  56% 44%

MAG1	MAG2	EMJ3	MAM4	MAM5	MAM6	MAM7	MAM8	MAM9
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.17Å 141.78Å 253.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.40 48.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.80-2.40) 99.7 (48.80-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.199 , 0.229 (Not available) , 0.197	Depositor DCC
R_{free} test set	5644 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17695	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MAN, BMA, NAG, FRU, SO4

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	0.58	0/4310	0.92	1/5902 (0.0%)
1	B	0.57	0/4293	0.93	1/5880 (0.0%)
1	C	0.58	0/4310	0.94	1/5902 (0.0%)
1	D	0.56	0/4278	0.92	1/5859 (0.0%)
All	All	0.57	0/17191	0.93	4/23543 (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
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	359	PRO	N-CA-CB	-6.36	98.59	102.79
1	C	272	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	272	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	272	ASP	CA-CB-CG	5.07	117.67	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	ARG	Sidechain
1	B	479	ARG	Sidechain
1	C	277	ARG	Sidechain
1	C	278	ARG	Sidechain
1	D	479	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	4170	0	3868	24	0
1	B	4153	0	3851	17	0
1	C	4170	0	3868	31	0
1	D	4138	0	3840	18	0
2	E	105	0	88	0	0
2	F	105	0	88	0	0
2	G	105	0	88	0	0
2	H	105	0	88	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
4	A	56	0	52	0	0
4	B	56	0	52	0	0
4	C	56	0	52	1	0
4	D	56	0	52	0	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
5	C	15	0	0	0	0
5	D	5	0	0	0	0
6	A	108	0	0	2	0
6	B	69	0	0	0	0
6	C	89	0	0	0	0
6	D	76	0	0	0	0
All	All	17695	0	16035	83	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 2.

All (83) 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:C:272:ASP:HB2	1:C:278:ARG:NH1	1.72	1.04
1:C:272:ASP:HB3	1:C:278:ARG:NE	1.83	0.93
1:C:272:ASP:CB	1:C:278:ARG:NH1	2.42	0.82
1:C:272:ASP:HB2	1:C:278:ARG:HH11	1.41	0.81
1:B:535:LEU:HD21	1:C:535:LEU:HD21	1.67	0.76
1:C:272:ASP:CB	1:C:278:ARG:HH11	1.99	0.76
1:A:535:LEU:HD21	1:D:535:LEU:HD21	1.75	0.68
1:C:272:ASP:CB	1:C:278:ARG:CZ	2.72	0.67
1:C:272:ASP:HB3	1:C:278:ARG:CZ	2.27	0.64
1:C:272:ASP:CB	1:C:278:ARG:NE	2.60	0.64
1:A:294:LEU:HD23	1:B:294:LEU:HD23	1.82	0.61
1:D:40:THR:HG22	1:D:42:THR:H	1.64	0.61
1:A:335:GLY:O	1:A:336:SER:C	2.44	0.59
1:C:294:LEU:HD23	1:D:294:LEU:HD23	1.83	0.59
1:A:40:THR:HG22	1:A:42:THR:H	1.71	0.56
1:C:287:SER:HB3	1:C:328:TYR:CE1	2.40	0.56
1:D:287:SER:HB3	1:D:328:TYR:CE1	2.41	0.56
1:B:287:SER:HB3	1:B:328:TYR:CE1	2.41	0.56
1:C:39:THR:HG22	1:C:40:THR:H	1.71	0.55
1:C:40:THR:HG22	1:C:42:THR:H	1.72	0.55
1:D:131:PRO:HB3	1:D:136:VAL:O	2.07	0.55
1:C:270:TYR:CE2	1:C:278:ARG:HD2	2.42	0.54
1:A:46:ALA:HB1	1:A:130:TYR:HB2	1.90	0.54
1:A:287:SER:HB3	1:A:328:TYR:CE1	2.43	0.54
1:C:131:PRO:HB3	1:C:136:VAL:O	2.08	0.53
1:A:131:PRO:HB3	1:A:136:VAL:O	2.09	0.53
1:C:272:ASP:CG	1:C:278:ARG:HH11	2.17	0.52
1:C:297:SER:HB2	1:C:328:TYR:CD1	2.45	0.52
1:D:297:SER:HB2	1:D:328:TYR:CD1	2.46	0.51
1:B:40:THR:HG22	1:B:42:THR:H	1.74	0.51
1:B:297:SER:HB2	1:B:328:TYR:CD1	2.46	0.50
1:A:297:SER:HB2	1:A:328:TYR:CD1	2.46	0.50
1:A:535:LEU:HD22	1:D:537:VAL:HG21	1.93	0.50
1:A:77:HIS:HD2	6:A:805:HOH:O	1.94	0.50
1:B:131:PRO:HB3	1:B:136:VAL:O	2.11	0.50
1:A:537:VAL:HG21	1:D:535:LEU:HD22	1.94	0.50
1:C:39:THR:HG23	1:C:192:SER:HB3	1.95	0.49
1:B:395:SER:N	1:B:396:PRO:CD	2.76	0.49
1:C:272:ASP:HB2	1:C:278:ARG:CZ	2.37	0.48
1:C:395:SER:N	1:C:396:PRO:CD	2.77	0.47
1:C:38:THR:HG23	4:C:606:NAG:O5	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ARG:HD3	1:B:389:THR:CG2	2.44	0.47
1:A:395:SER:N	1:A:396:PRO:CD	2.77	0.47
1:A:77:HIS:HE1	6:A:803:HOH:O	1.97	0.46
1:A:468:ASP:HB3	1:B:290:PRO:HG3	1.98	0.46
1:B:373:ARG:NH2	1:B:513:GLU:OE2	2.36	0.46
1:D:459:LEU:HD12	1:D:475:ARG:HA	1.97	0.46
1:A:330:GLY:HA3	1:A:345:PHE:CZ	2.51	0.45
1:D:330:GLY:HA3	1:D:345:PHE:CZ	2.52	0.45
1:D:408:ILE:HD11	1:D:551:VAL:CG1	2.47	0.45
1:D:373:ARG:HD3	1:D:389:THR:CG2	2.47	0.44
1:D:408:ILE:O	1:D:409:ALA:C	2.58	0.44
1:D:373:ARG:NH2	1:D:513:GLU:OE2	2.37	0.44
1:B:77:HIS:HB3	1:B:100:ASN:O	2.18	0.44
1:B:408:ILE:HD12	1:B:413:ILE:CG1	2.48	0.43
1:C:408:ILE:O	1:C:409:ALA:C	2.61	0.43
1:A:392:TYR:O	1:A:393:ASP:C	2.61	0.43
1:B:392:TYR:O	1:B:393:ASP:C	2.61	0.43
1:C:330:GLY:HA3	1:C:345:PHE:CZ	2.54	0.43
1:D:395:SER:N	1:D:396:PRO:CD	2.82	0.43
1:A:408:ILE:O	1:A:409:ALA:C	2.61	0.43
1:B:459:LEU:HD12	1:B:475:ARG:HA	2.01	0.42
1:A:459:LEU:HD12	1:A:475:ARG:HA	2.00	0.42
1:D:395:SER:OG	1:D:396:PRO:HD3	2.19	0.42
1:A:77:HIS:HB3	1:A:100:ASN:O	2.19	0.42
1:A:446:MET:HG3	1:A:540:THR:HG22	2.02	0.42
1:C:272:ASP:HB3	1:C:278:ARG:CD	2.49	0.42
1:D:77:HIS:HB3	1:D:100:ASN:O	2.20	0.42
1:C:459:LEU:HD12	1:C:475:ARG:HA	2.02	0.42
1:B:330:GLY:HA3	1:B:345:PHE:CZ	2.55	0.41
1:A:366:ARG:O	1:A:367:SER:HB2	2.21	0.41
1:C:335:GLY:O	1:C:336:SER:C	2.62	0.41
1:C:77:HIS:HB3	1:C:100:ASN:O	2.20	0.41
1:A:132:PRO:O	1:A:133[B]:ARG:HG3	2.21	0.41
1:C:71:HIS:NE2	1:C:513:GLU:OE1	2.46	0.41
1:B:76:ARG:NH1	5:B:602:SO4:O3	2.53	0.40
1:C:134:LYS:O	1:C:135:ASP:HB2	2.21	0.40
1:C:446:MET:HG3	1:C:540:THR:HG22	2.02	0.40
1:B:405:ASN:HB3	1:B:408:ILE:HD11	2.04	0.40
1:D:464:PHE:O	1:D:469:SER:HA	2.22	0.40
1:A:134:LYS:O	1:A:135:ASP:HB2	2.20	0.40
1:A:405:ASN:HB3	1:A:408:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASP:O	1:C:189:ASN:HB2	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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	534/576 (93%)	512 (96%)	20 (4%)	2 (0%)	30	43
1	B	532/576 (92%)	508 (96%)	22 (4%)	2 (0%)	30	43
1	C	534/576 (93%)	512 (96%)	20 (4%)	2 (0%)	30	43
1	D	530/576 (92%)	506 (96%)	23 (4%)	1 (0%)	43	58
All	All	2130/2304 (92%)	2038 (96%)	85 (4%)	7 (0%)	36	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	SER
1	A	393	ASP
1	B	367	SER
1	B	393	ASP
1	C	367	SER
1	C	393	ASP
1	D	367	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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	443/474 (94%)	442 (100%)	1 (0%)	87	94
1	B	441/474 (93%)	438 (99%)	3 (1%)	76	88
1	C	443/474 (94%)	441 (100%)	2 (0%)	81	91
1	D	427/474 (90%)	426 (100%)	1 (0%)	87	94
All	All	1754/1896 (92%)	1747 (100%)	7 (0%)	84	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	432	THR
1	B	390	VAL
1	B	432	THR
1	B	575	GLN
1	C	432	THR
1	C	575	GLN
1	D	432	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	80	ASN
1	A	83	ASN
1	A	197	HIS
1	A	220	HIS
1	A	259	GLN
1	A	423	ASN
1	B	77	HIS
1	B	80	ASN
1	B	98	GLN
1	B	220	HIS
1	B	259	GLN
1	B	423	ASN
1	C	80	ASN
1	C	98	GLN
1	C	220	HIS
1	C	423	ASN
1	D	80	ASN

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Mol	Chain	Res	Type
1	D	98	GLN
1	D	220	HIS
1	D	259	GLN
1	D	423	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

36 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	E	1	2,1	14,14,15	0.47	0	17,19,21	0.85	0
2	NAG	E	2	2	14,14,15	0.41	0	17,19,21	0.65	0
2	BMA	E	3	2	11,11,12	0.81	1 (9%)	15,15,17	0.59	0
2	MAN	E	4	2	11,11,12	0.73	0	15,15,17	0.75	1 (6%)
2	MAN	E	5	2	11,11,12	0.76	0	15,15,17	0.64	0
2	MAN	E	6	2	11,11,12	0.61	0	15,15,17	0.64	0
2	MAN	E	7	2	11,11,12	0.91	1 (9%)	15,15,17	0.85	0
2	MAN	E	8	2	11,11,12	0.89	1 (9%)	15,15,17	0.82	1 (6%)
2	MAN	E	9	2	11,11,12	0.85	1 (9%)	15,15,17	0.48	0
2	NAG	F	1	2,1	14,14,15	0.32	0	17,19,21	0.65	0
2	NAG	F	2	2	14,14,15	0.37	0	17,19,21	0.56	0
2	BMA	F	3	2	11,11,12	0.85	1 (9%)	15,15,17	0.75	0
2	MAN	F	4	2	11,11,12	0.70	0	15,15,17	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	F	5	2	11,11,12	0.97	1 (9%)	15,15,17	0.85	1 (6%)
2	MAN	F	6	2	11,11,12	0.51	0	15,15,17	0.57	0
2	MAN	F	7	2	11,11,12	0.66	0	15,15,17	0.65	0
2	MAN	F	8	2	11,11,12	0.59	0	15,15,17	1.07	1 (6%)
2	MAN	F	9	2	11,11,12	0.77	1 (9%)	15,15,17	0.50	0
2	NAG	G	1	2,1	14,14,15	0.36	0	17,19,21	0.51	0
2	NAG	G	2	2	14,14,15	0.35	0	17,19,21	0.66	0
2	BMA	G	3	2	11,11,12	0.51	0	15,15,17	0.70	0
2	MAN	G	4	2	11,11,12	0.53	0	15,15,17	0.71	0
2	MAN	G	5	2	11,11,12	0.61	0	15,15,17	0.60	0
2	MAN	G	6	2	11,11,12	0.86	1 (9%)	15,15,17	0.61	0
2	MAN	G	7	2	11,11,12	0.86	0	15,15,17	0.86	0
2	MAN	G	8	2	11,11,12	0.87	1 (9%)	15,15,17	0.79	0
2	MAN	G	9	2	11,11,12	0.65	0	15,15,17	0.72	0
2	NAG	H	1	2,1	14,14,15	0.41	0	17,19,21	0.66	0
2	NAG	H	2	2	14,14,15	0.38	0	17,19,21	0.70	0
2	BMA	H	3	2	11,11,12	0.71	0	15,15,17	0.58	0
2	MAN	H	4	2	11,11,12	0.81	1 (9%)	15,15,17	0.90	1 (6%)
2	MAN	H	5	2	11,11,12	0.66	0	15,15,17	0.80	0
2	MAN	H	6	2	11,11,12	0.87	1 (9%)	15,15,17	0.62	0
2	MAN	H	7	2	11,11,12	0.78	0	15,15,17	0.92	1 (6%)
2	MAN	H	8	2	11,11,12	0.86	0	15,15,17	0.74	0
2	MAN	H	9	2	11,11,12	1.08	1 (9%)	15,15,17	0.77	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	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
2	MAN	E	7	2	-	0/2/19/22	0/1/1/1
2	MAN	E	8	2	-	0/2/19/22	0/1/1/1
2	MAN	E	9	2	-	1/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	2/2/19/22	0/1/1/1
2	MAN	F	6	2	-	0/2/19/22	0/1/1/1
2	MAN	F	7	2	-	0/2/19/22	0/1/1/1
2	MAN	F	8	2	-	0/2/19/22	0/1/1/1
2	MAN	F	9	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	MAN	G	5	2	-	0/2/19/22	0/1/1/1
2	MAN	G	6	2	-	0/2/19/22	0/1/1/1
2	MAN	G	7	2	-	0/2/19/22	0/1/1/1
2	MAN	G	8	2	-	0/2/19/22	0/1/1/1
2	MAN	G	9	2	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	MAN	H	5	2	-	0/2/19/22	0/1/1/1
2	MAN	H	6	2	-	0/2/19/22	0/1/1/1
2	MAN	H	7	2	-	0/2/19/22	0/1/1/1
2	MAN	H	8	2	-	0/2/19/22	0/1/1/1
2	MAN	H	9	2	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	7	MAN	O5-C5	2.53	1.48	1.43
2	H	9	MAN	O5-C5	2.48	1.48	1.43
2	H	6	MAN	C2-C3	-2.44	1.48	1.52
2	E	8	MAN	O5-C5	2.43	1.48	1.43
2	E	9	MAN	O5-C5	2.40	1.48	1.43
2	F	3	BMA	O5-C5	2.38	1.48	1.43
2	G	6	MAN	O5-C5	2.28	1.47	1.43
2	F	5	MAN	O5-C5	2.27	1.47	1.43
2	F	9	MAN	O5-C5	2.22	1.47	1.43
2	H	4	MAN	O5-C5	2.16	1.47	1.43
2	G	8	MAN	O5-C5	2.15	1.47	1.43
2	E	3	BMA	O5-C5	2.08	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	8	MAN	C1-O5-C5	2.78	115.92	112.19
2	H	4	MAN	C1-C2-C3	2.62	113.46	109.64
2	F	5	MAN	C1-O5-C5	2.40	115.40	112.19
2	E	8	MAN	C1-C2-C3	2.30	112.99	109.64
2	H	7	MAN	C1-C2-C3	2.29	112.98	109.64
2	E	4	MAN	C1-C2-C3	2.15	112.78	109.64

There are no chirality outliers.

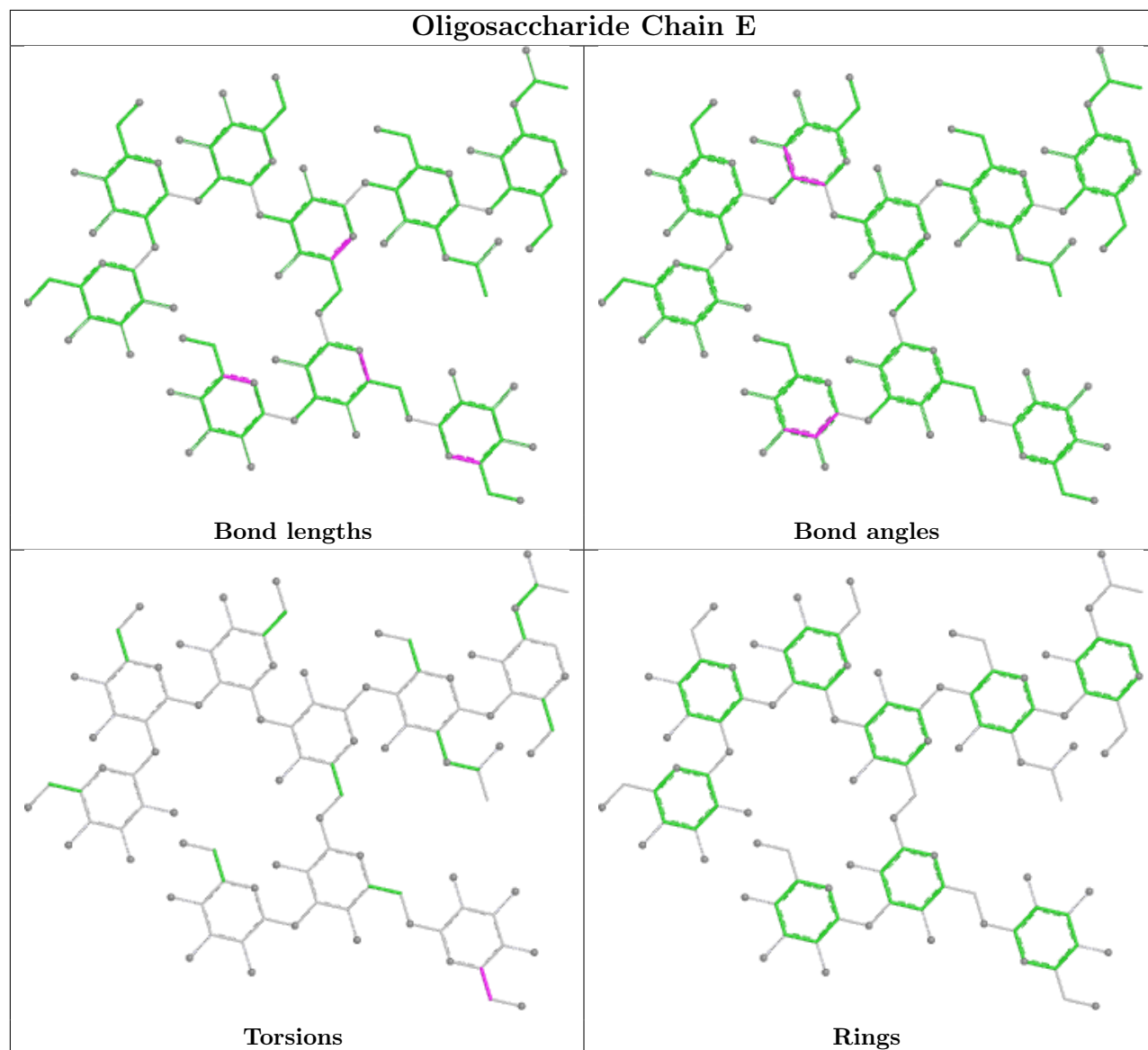
All (6) torsion outliers are listed below:

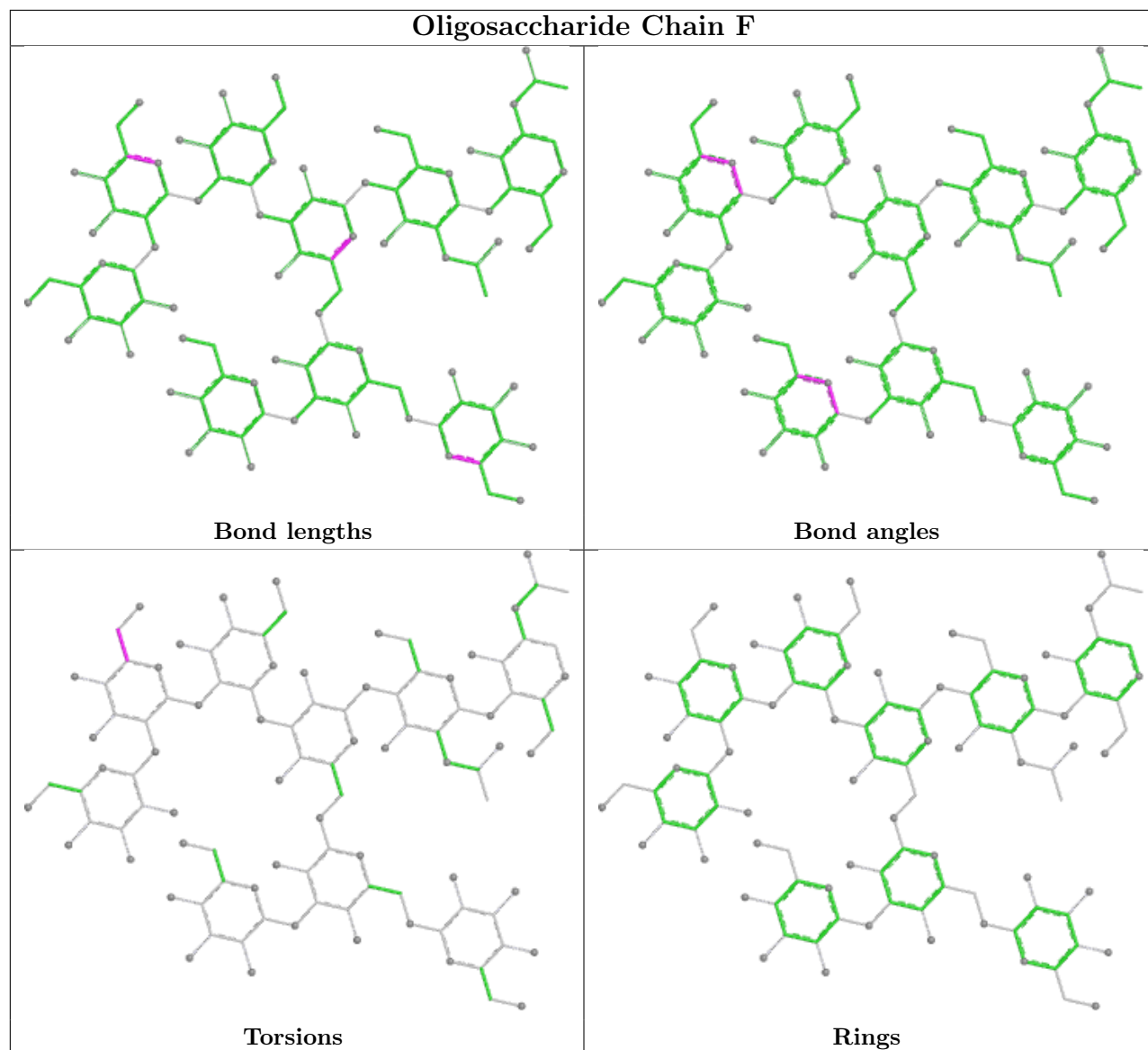
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	E	9	MAN	O5-C5-C6-O6
2	F	5	MAN	O5-C5-C6-O6
2	H	9	MAN	O5-C5-C6-O6
2	F	5	MAN	C4-C5-C6-O6

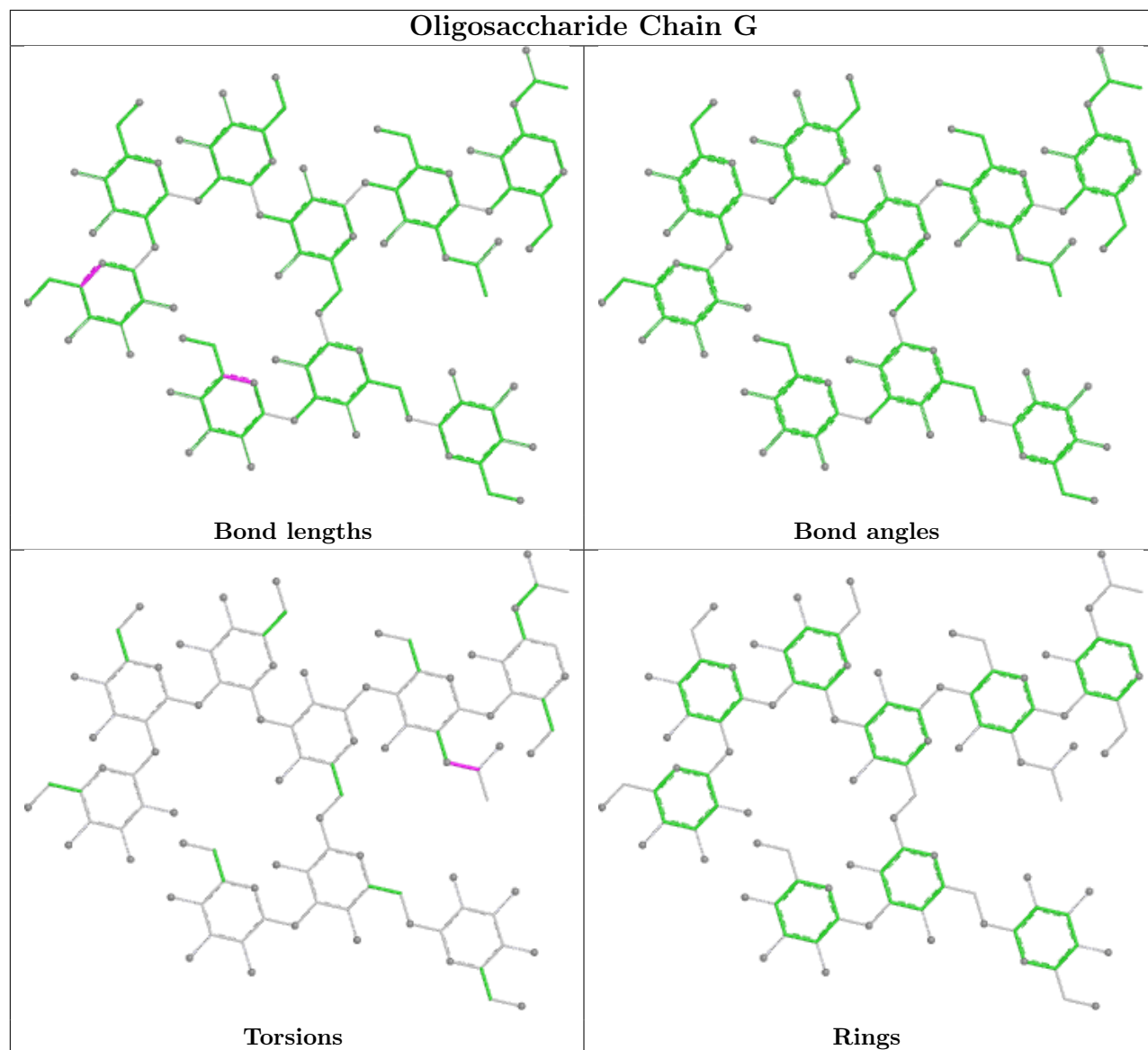
There are no ring outliers.

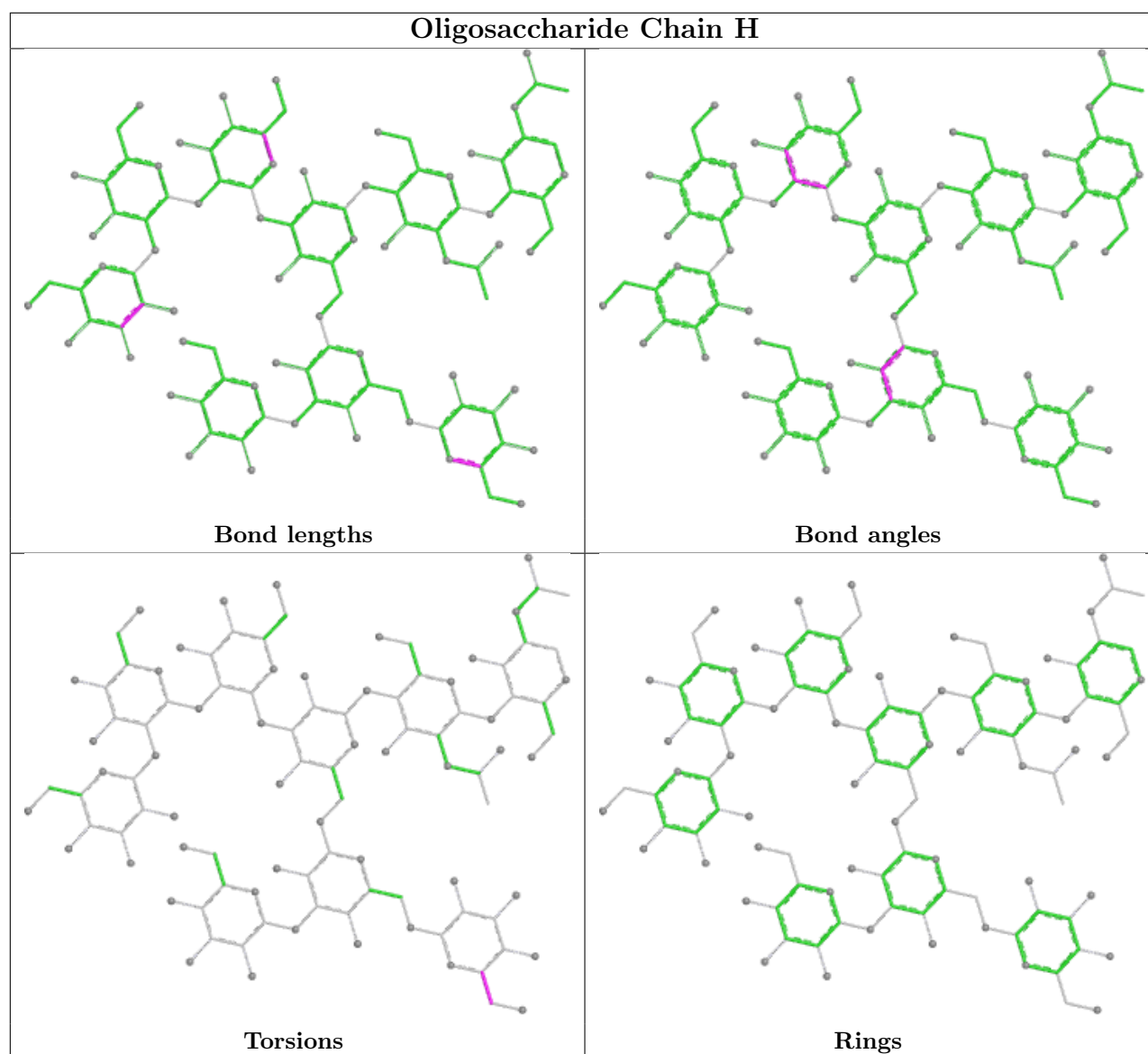
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	C	608	-	4,4,4	0.40	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	605	1	14,14,15	0.25	0	17,19,21	0.53	0
3	FRU	B	601	-	11,12,12	0.48	0	10,18,18	0.79	1 (10%)
4	NAG	D	603	1	14,14,15	0.29	0	17,19,21	0.70	0
4	NAG	B	604	1	14,14,15	0.47	0	17,19,21	0.53	0
5	SO4	C	607	-	4,4,4	0.30	0	6,6,6	0.10	0
5	SO4	D	602	-	4,4,4	0.37	0	6,6,6	0.26	0
4	NAG	B	603	1	14,14,15	0.41	0	17,19,21	0.72	0
3	FRU	C	601	-	11,12,12	0.73	0	10,18,18	0.83	0
4	NAG	C	603	1	14,14,15	0.42	0	17,19,21	0.48	0
5	SO4	B	602	-	4,4,4	0.37	0	6,6,6	0.19	0
3	FRU	A	601	-	11,12,12	0.75	0	10,18,18	0.76	0
4	NAG	D	606	1	14,14,15	0.53	0	17,19,21	0.42	0
4	NAG	B	605	1	14,14,15	0.63	0	17,19,21	0.91	1 (5%)
3	FRU	D	601	-	11,12,12	0.78	0	10,18,18	0.58	0
4	NAG	A	602	1	14,14,15	0.54	0	17,19,21	0.74	0
4	NAG	C	605	1	14,14,15	0.40	0	17,19,21	0.82	0
4	NAG	A	603	1	14,14,15	0.48	0	17,19,21	0.63	0
4	NAG	D	604	1	14,14,15	0.38	0	17,19,21	0.79	0
4	NAG	A	604	1	14,14,15	0.40	0	17,19,21	0.75	0
5	SO4	C	602	-	4,4,4	0.29	0	6,6,6	0.22	0
4	NAG	D	605	1	14,14,15	0.38	0	17,19,21	0.81	1 (5%)
5	SO4	A	606	-	4,4,4	0.29	0	6,6,6	0.17	0
4	NAG	C	606	1	14,14,15	0.45	0	17,19,21	0.77	0
4	NAG	B	606	1	14,14,15	0.55	0	17,19,21	0.64	0
4	NAG	C	604	1	14,14,15	0.44	0	17,19,21	0.69	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
4	NAG	A	605	1	-	0/6/23/26	0/1/1/1
3	FRU	B	601	-	-	0/5/24/24	0/1/1/1
4	NAG	D	603	1	-	0/6/23/26	0/1/1/1
4	NAG	B	604	1	-	0/6/23/26	0/1/1/1
4	NAG	B	603	1	-	2/6/23/26	0/1/1/1
3	FRU	C	601	-	-	1/5/24/24	0/1/1/1
4	NAG	C	603	1	-	0/6/23/26	0/1/1/1
3	FRU	A	601	-	-	2/5/24/24	0/1/1/1
4	NAG	D	606	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	605	1	-	2/6/23/26	0/1/1/1
3	FRU	D	601	-	-	1/5/24/24	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	C	605	1	-	0/6/23/26	0/1/1/1
4	NAG	A	603	1	-	2/6/23/26	0/1/1/1
4	NAG	D	604	1	-	2/6/23/26	0/1/1/1
4	NAG	A	604	1	-	1/6/23/26	0/1/1/1
4	NAG	D	605	1	-	0/6/23/26	0/1/1/1
4	NAG	C	606	1	-	0/6/23/26	0/1/1/1
4	NAG	B	606	1	-	0/6/23/26	0/1/1/1
4	NAG	C	604	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FRU	O1-C1-C2	-2.21	106.79	111.67
4	B	605	NAG	C2-N2-C7	2.17	125.81	122.90
4	D	605	NAG	C2-N2-C7	2.12	125.74	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

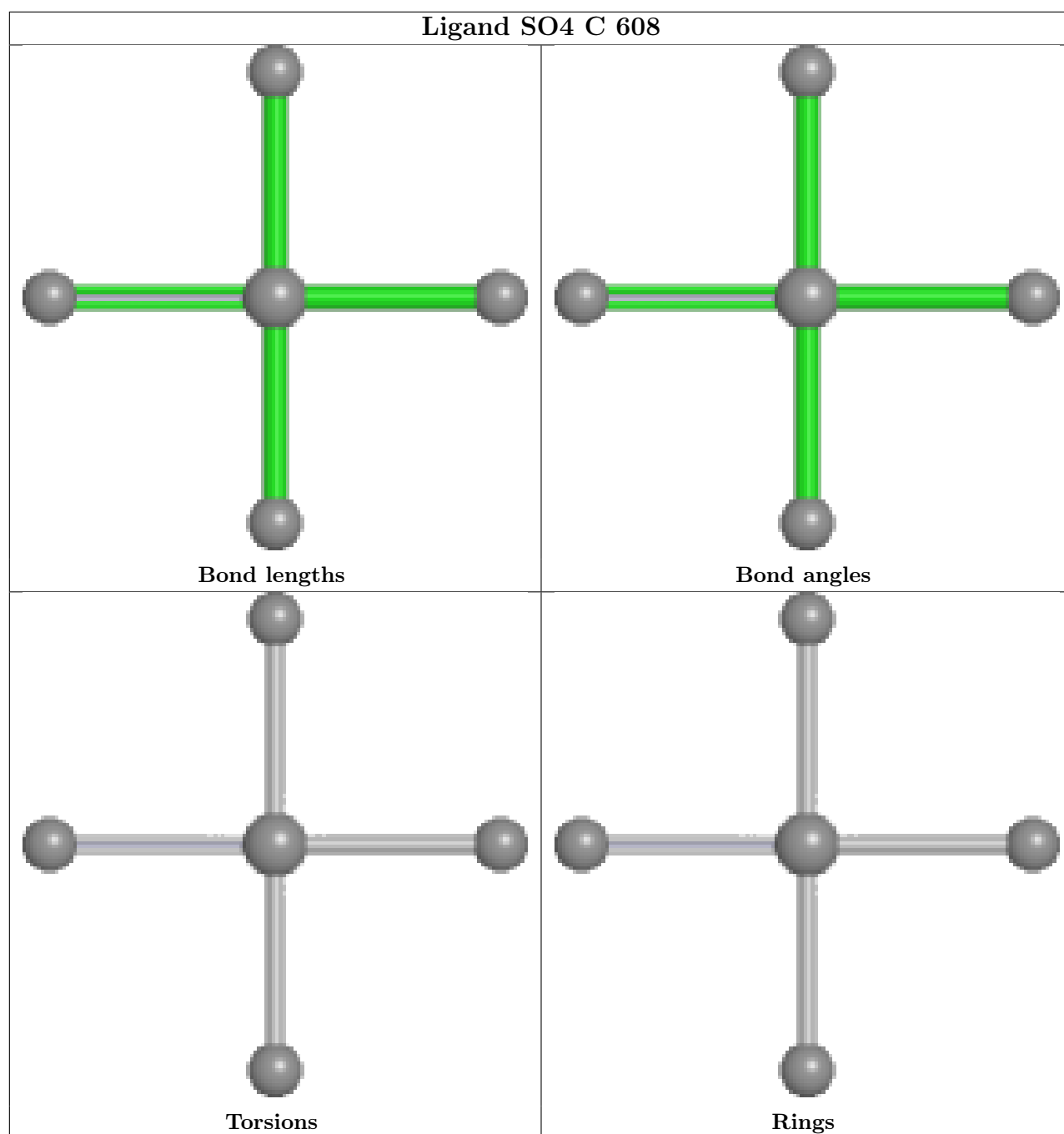
Mol	Chain	Res	Type	Atoms
4	B	603	NAG	O7-C7-N2-C2
4	B	603	NAG	C8-C7-N2-C2
4	D	604	NAG	C8-C7-N2-C2
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	B	605	NAG	C8-C7-N2-C2
4	B	605	NAG	O7-C7-N2-C2
4	D	604	NAG	O7-C7-N2-C2
3	A	601	FRU	O1-C1-C2-O5
3	A	601	FRU	O1-C1-C2-C3
4	A	604	NAG	O5-C5-C6-O6
3	C	601	FRU	O1-C1-C2-C3
3	D	601	FRU	O1-C1-C2-C3

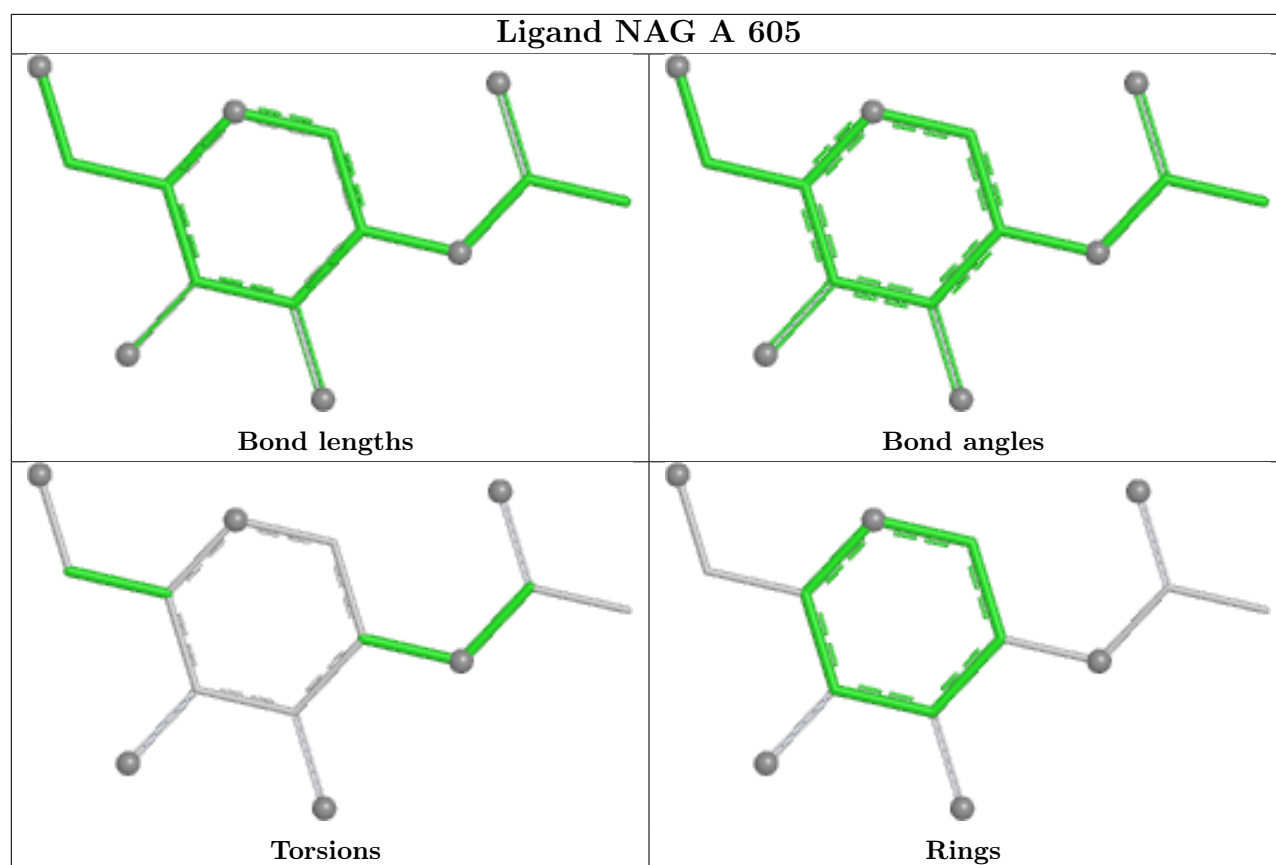
There are no ring outliers.

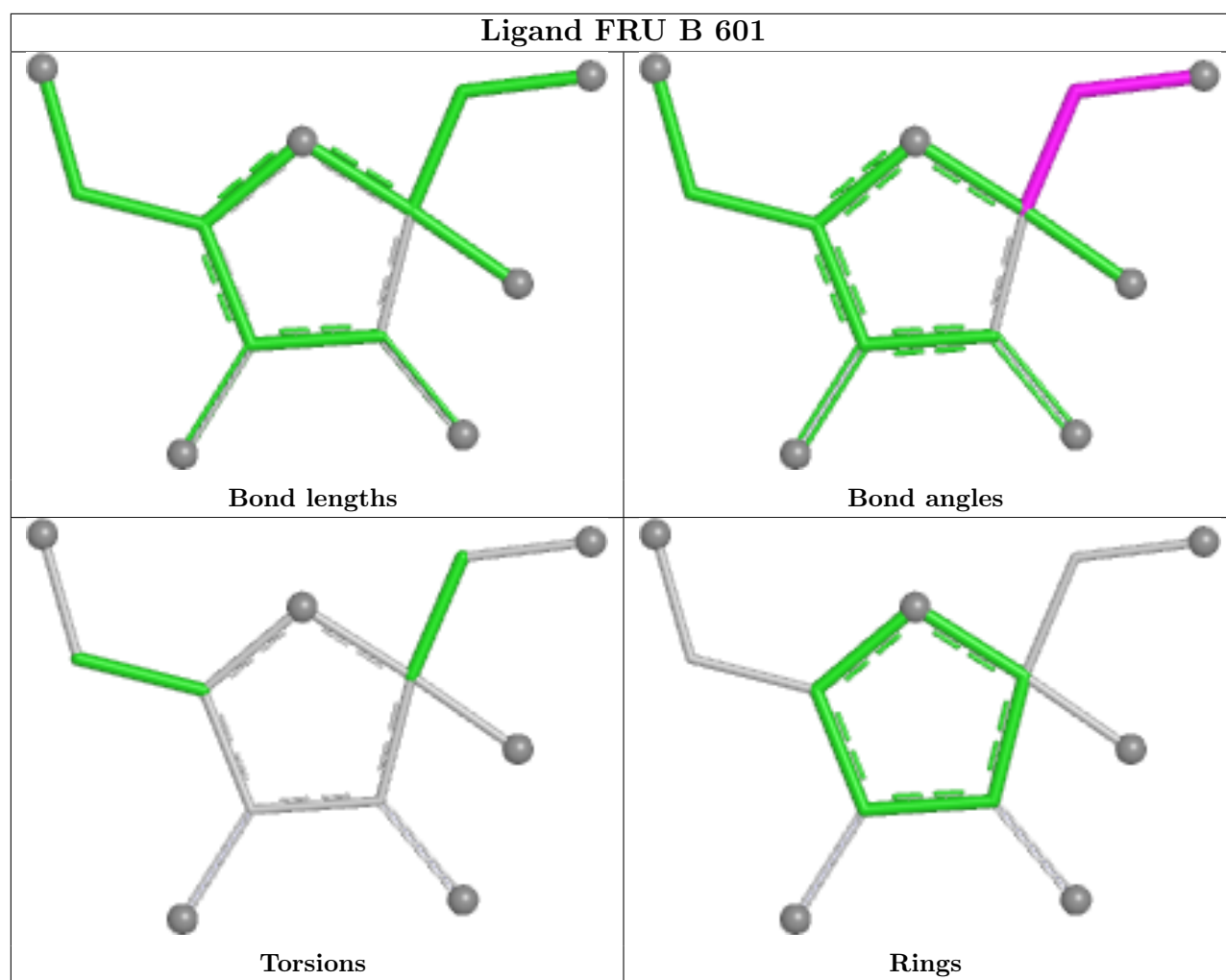
2 monomers are involved in 2 short contacts:

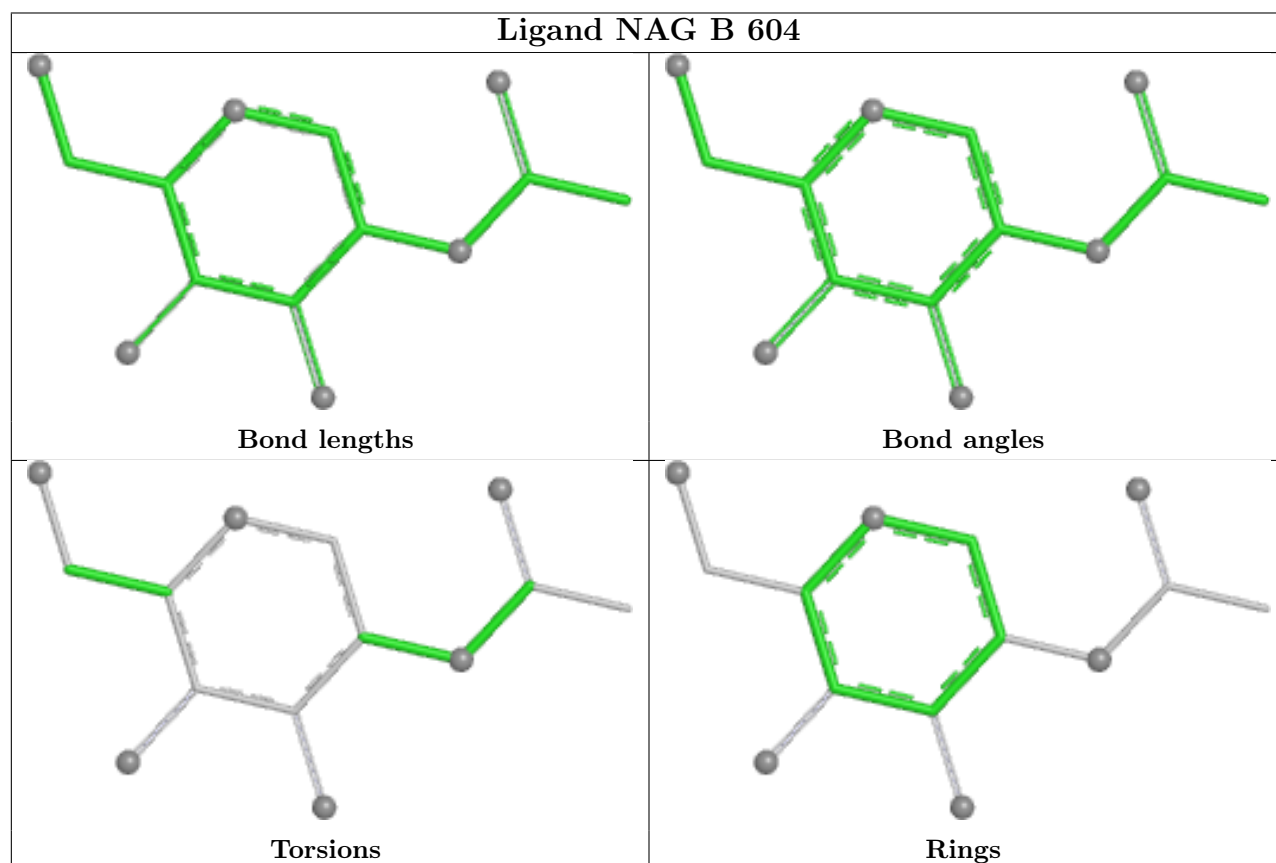
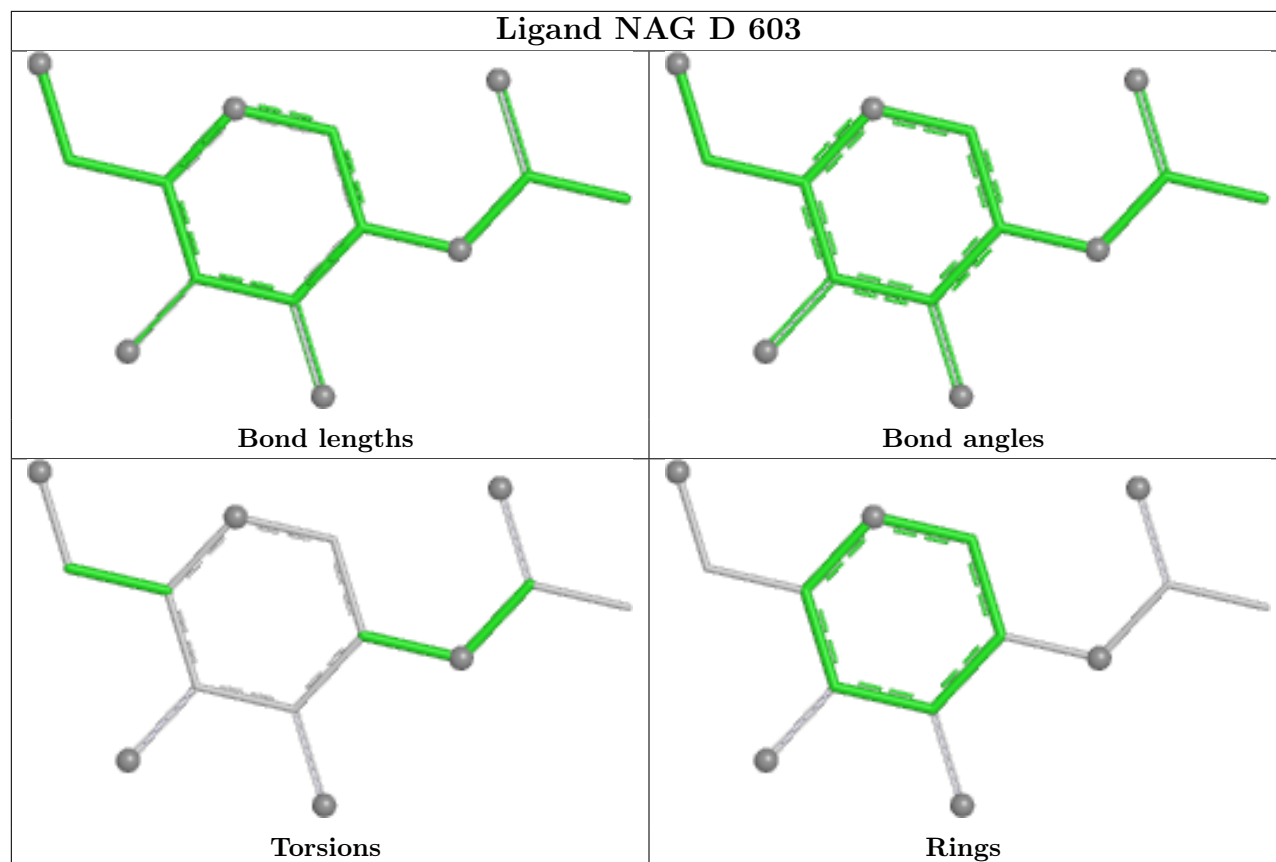
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	SO4	1	0
4	C	606	NAG	1	0

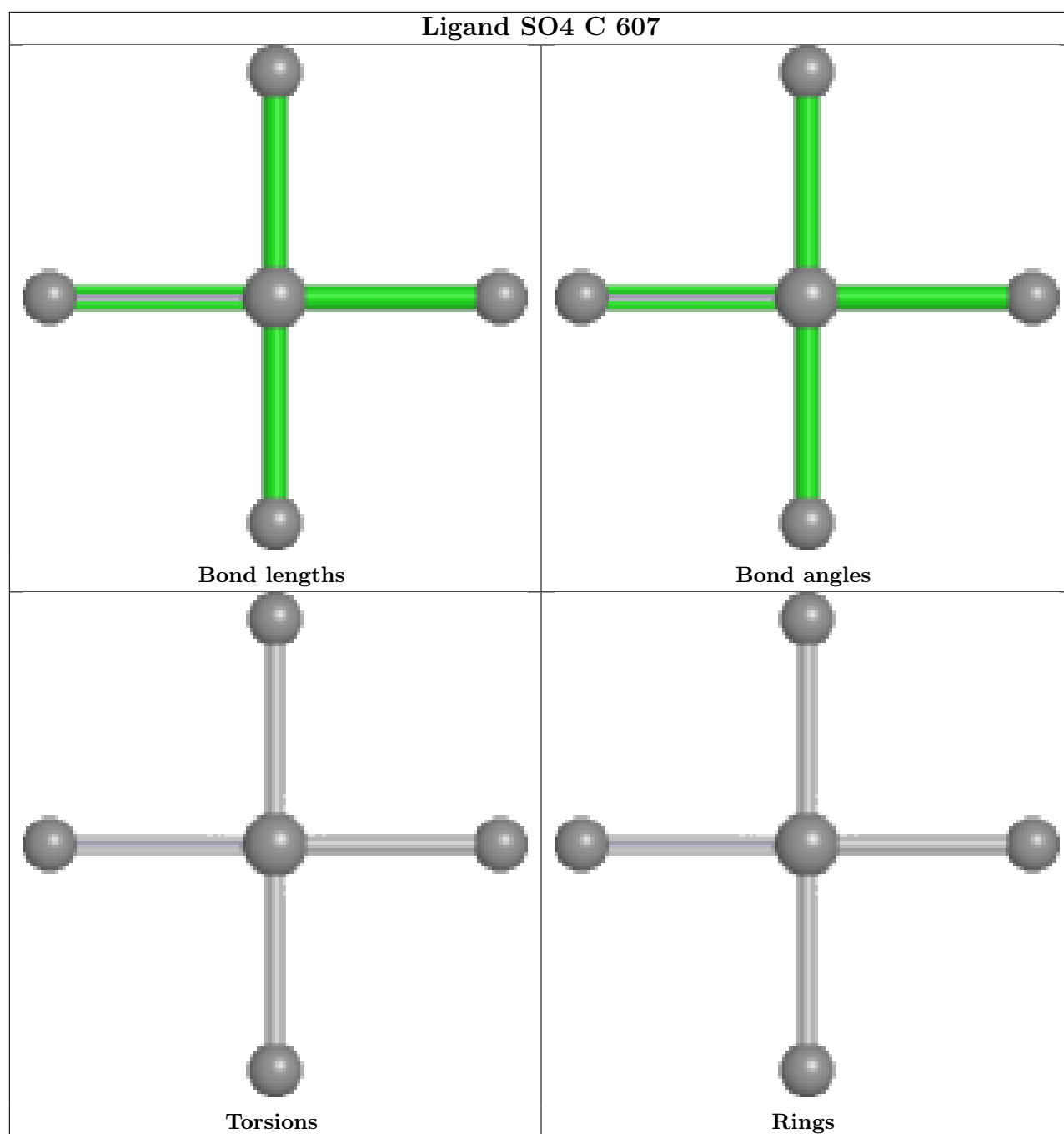
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

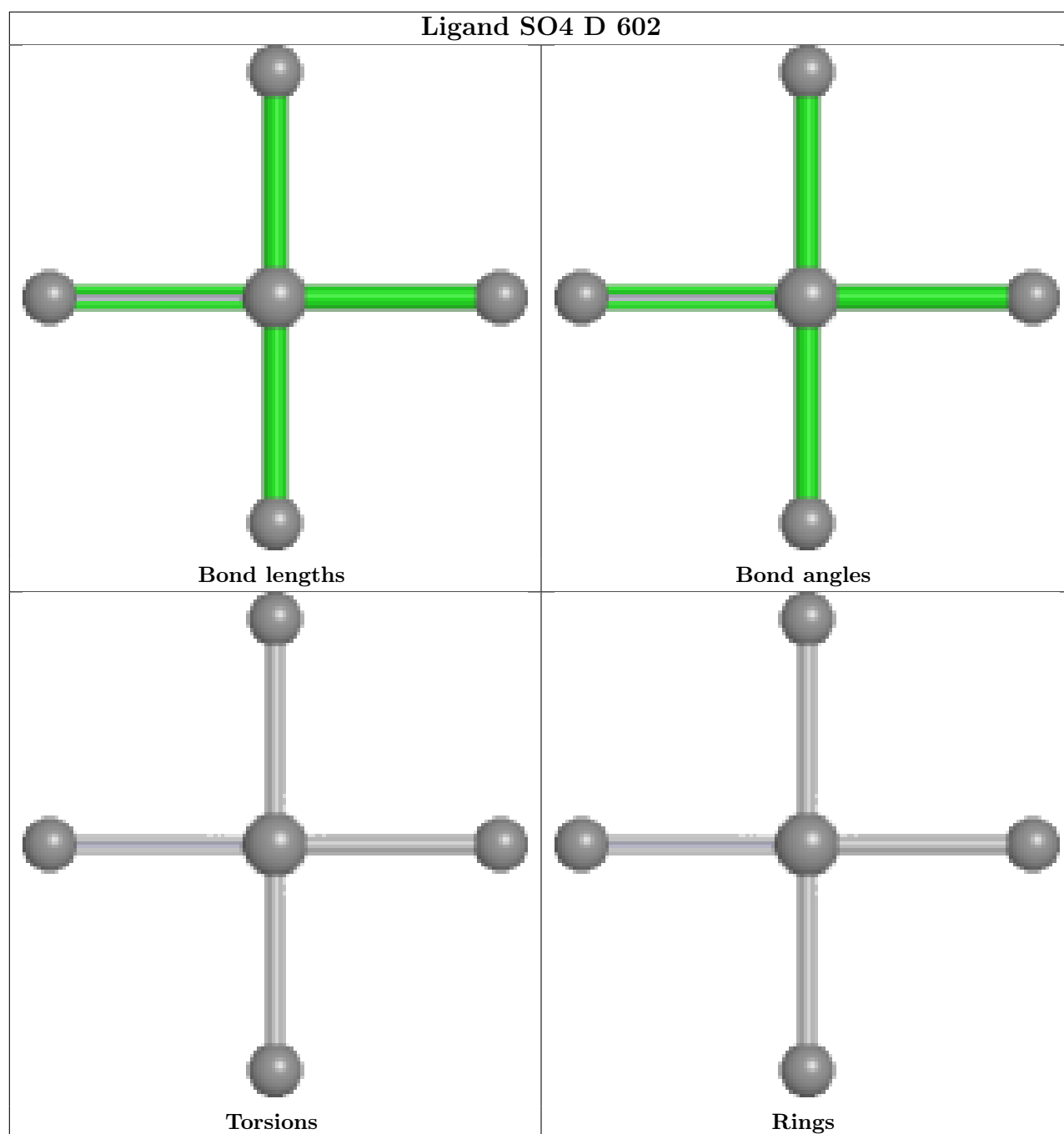


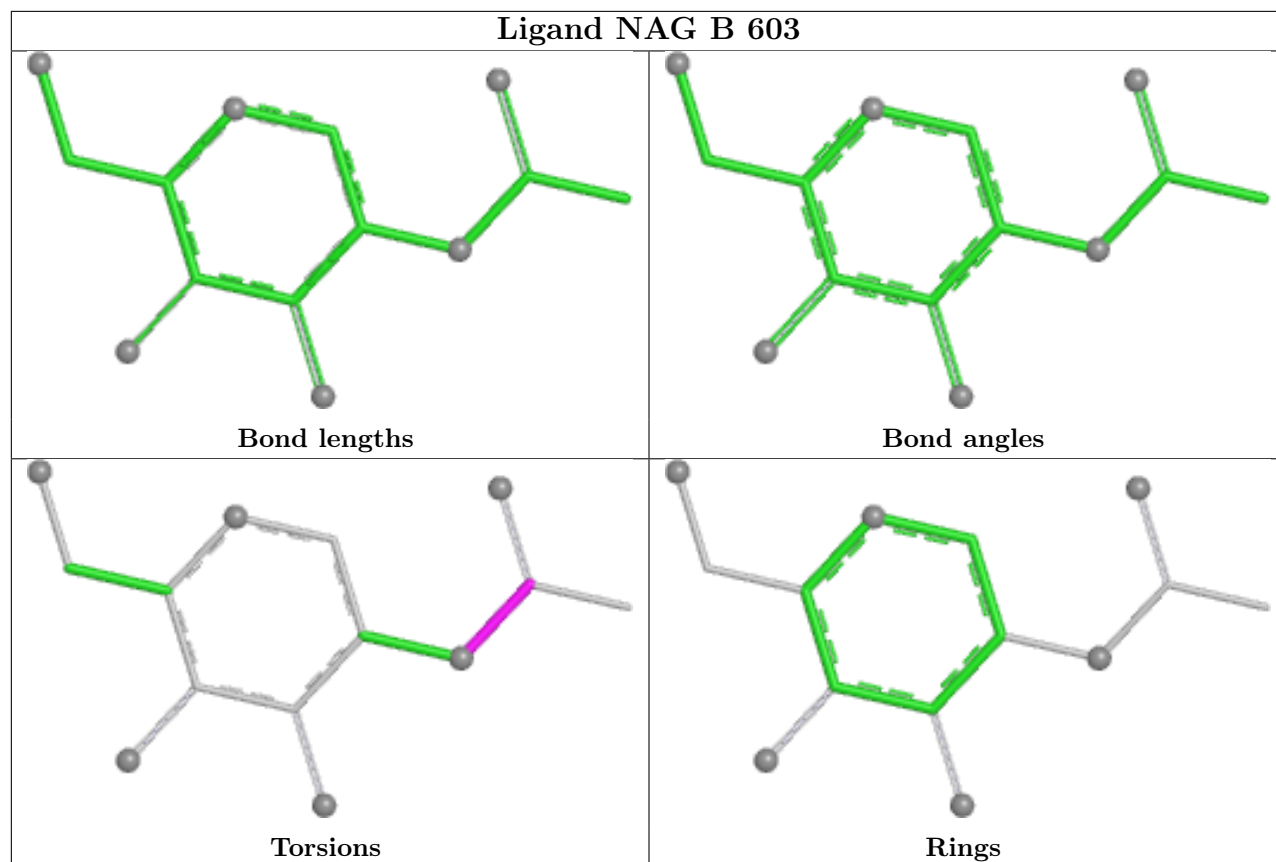


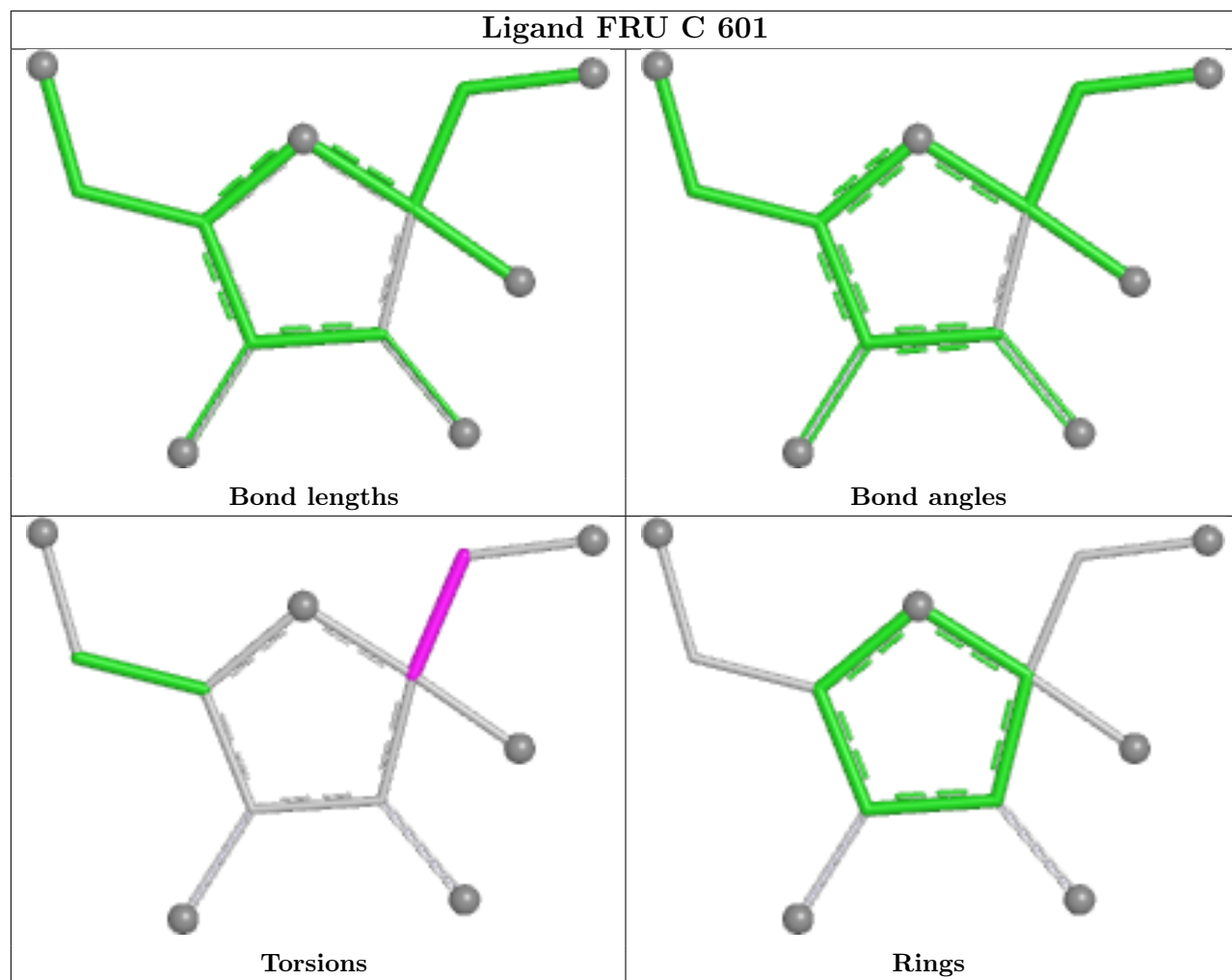


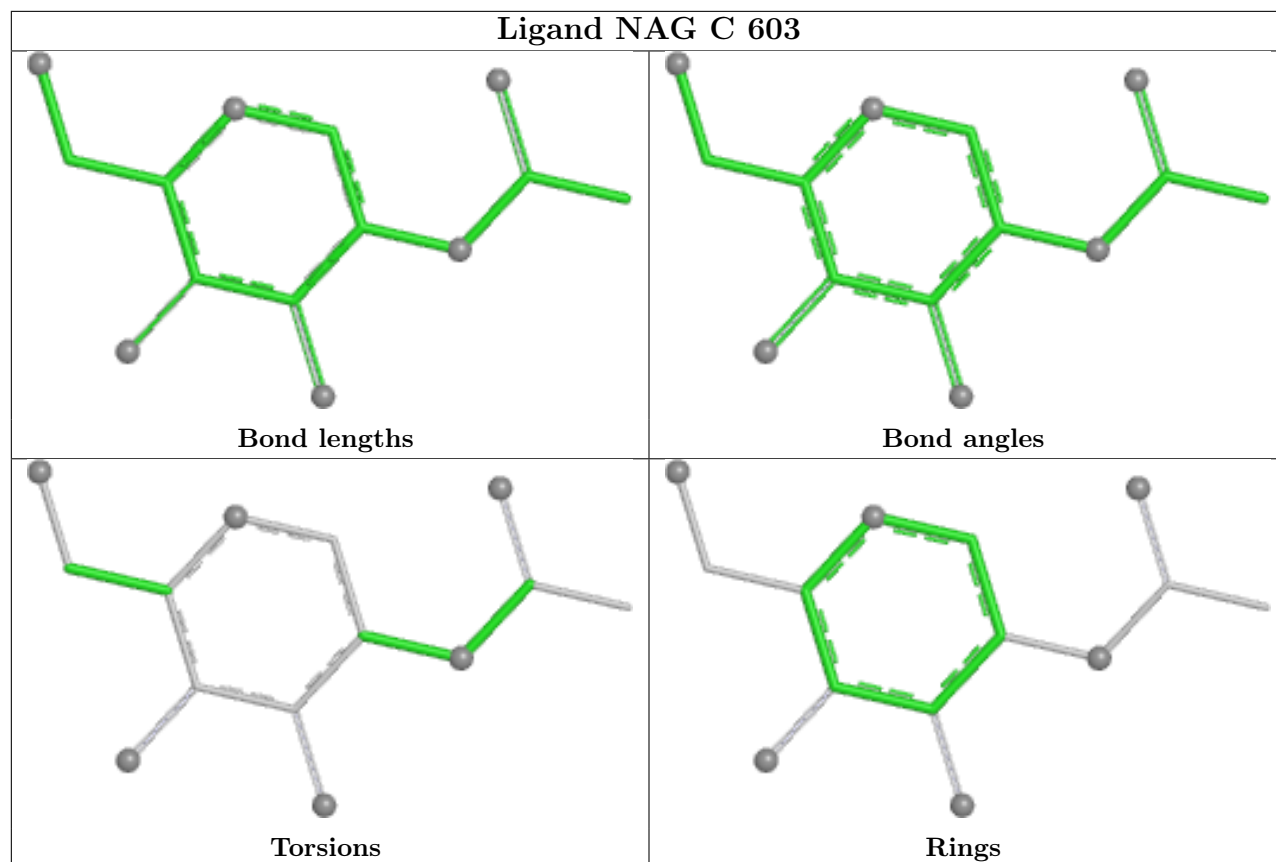


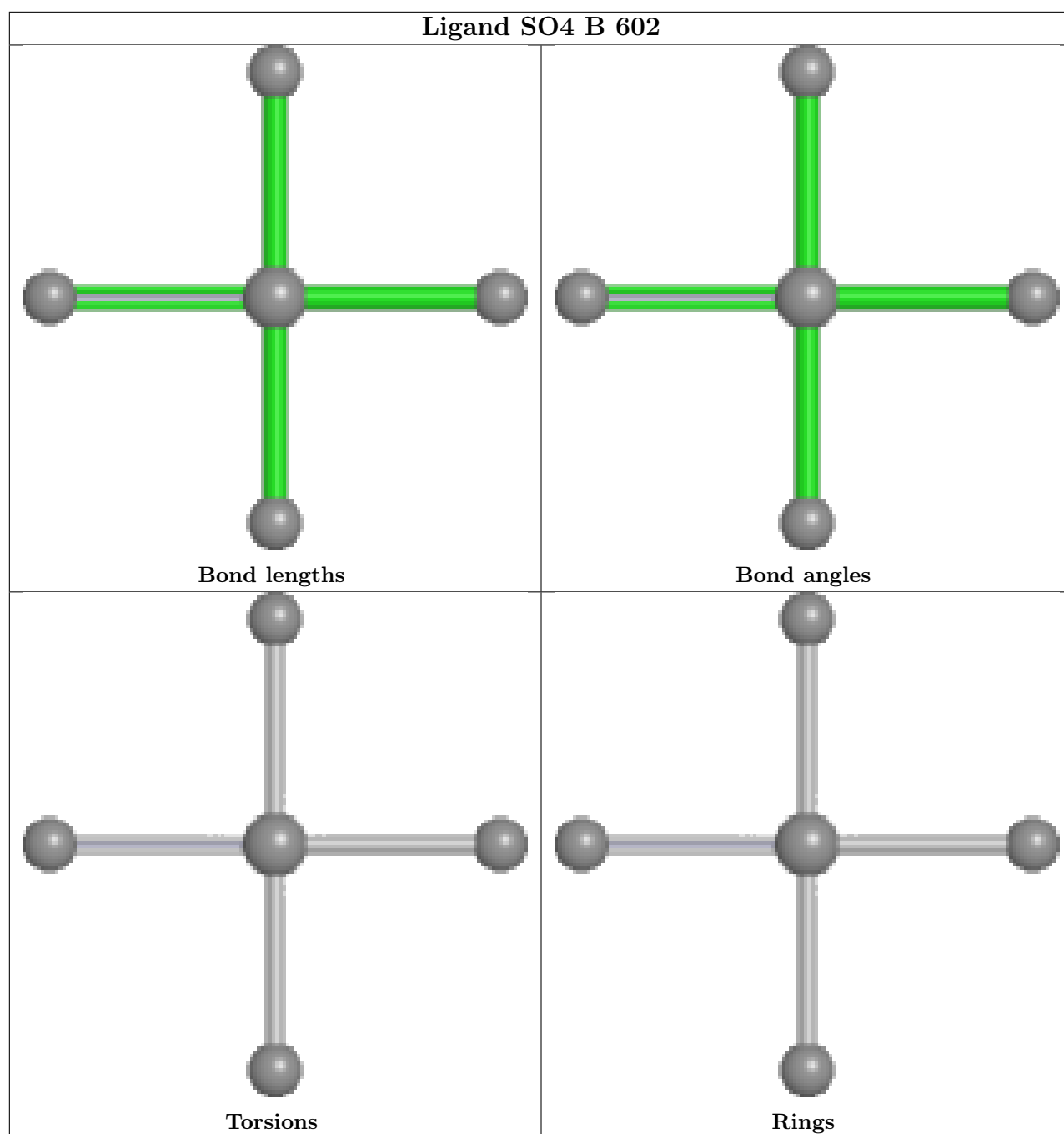


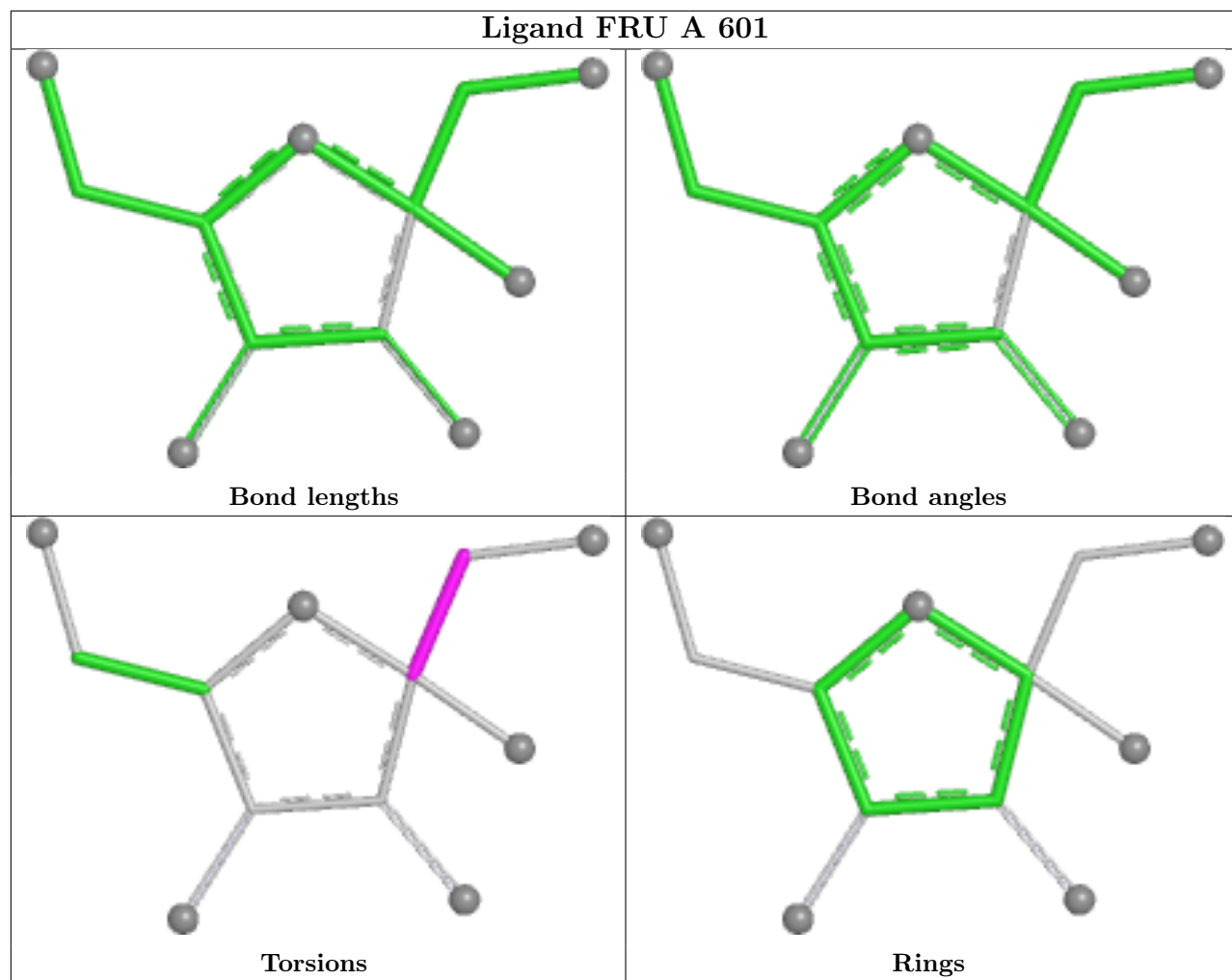


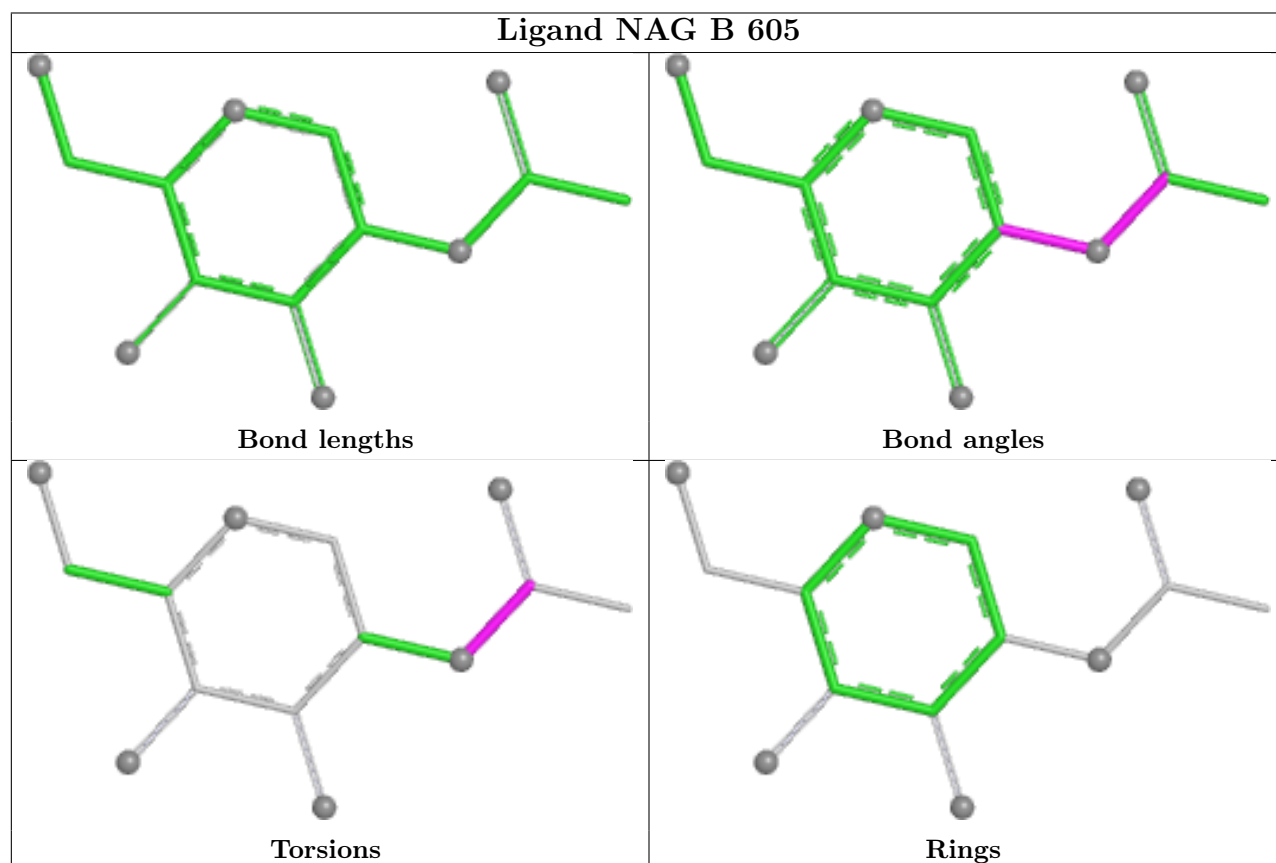
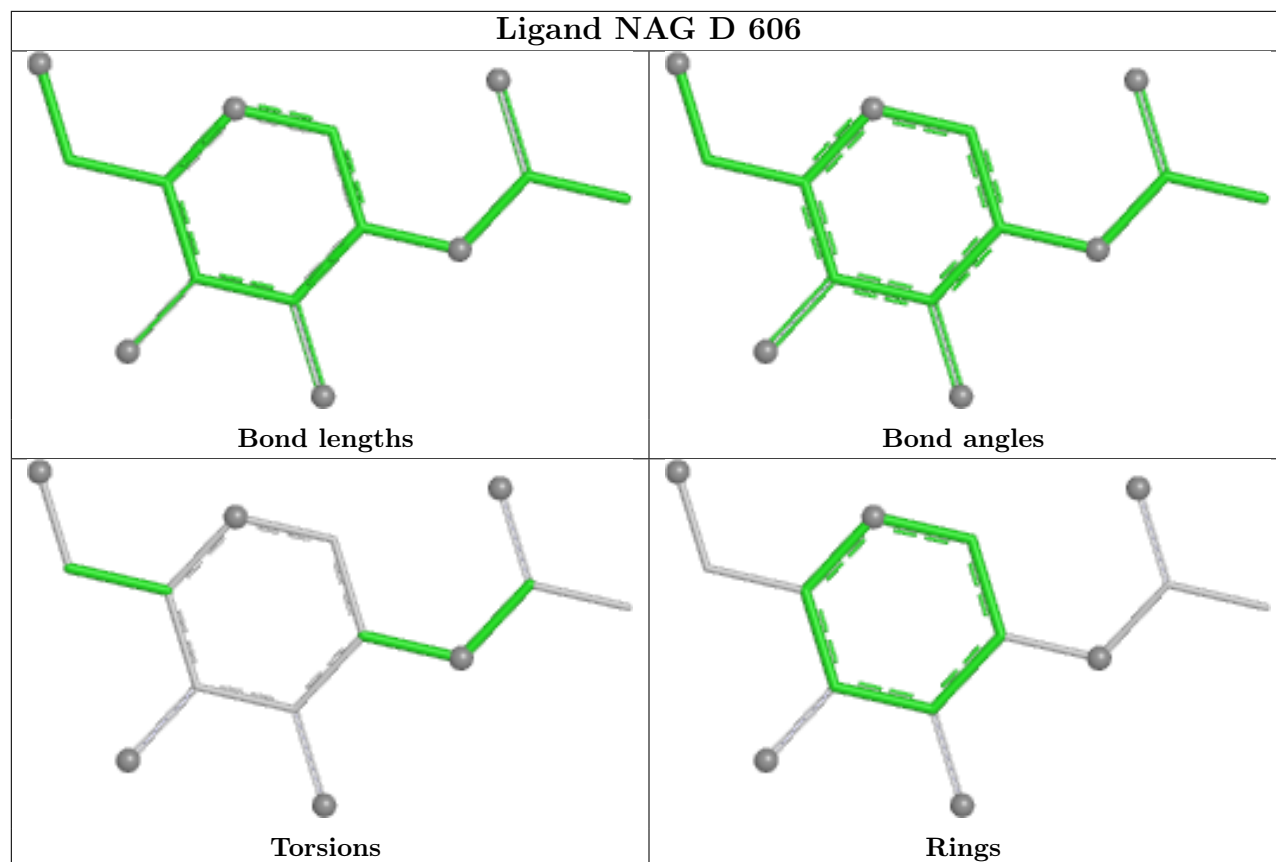


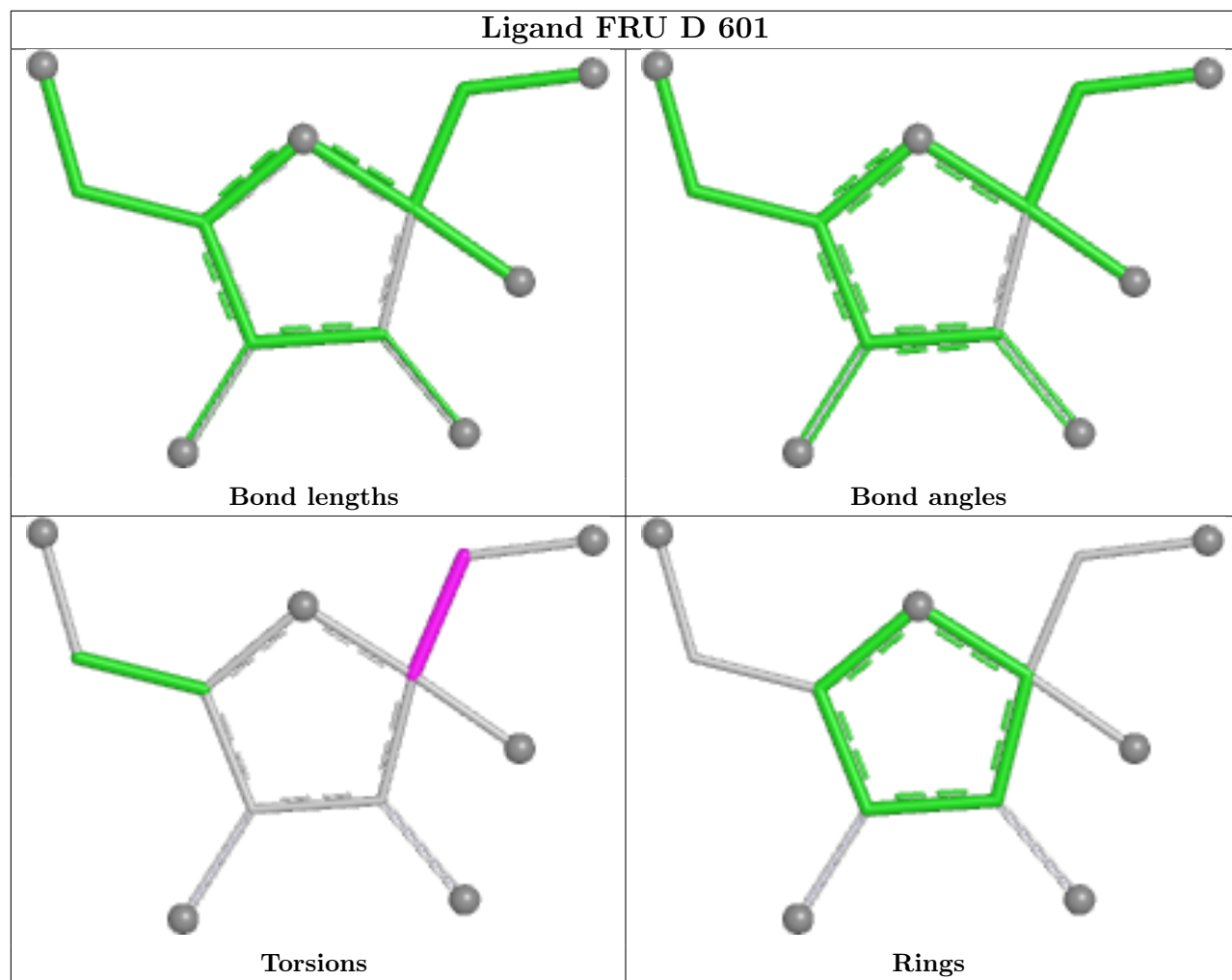


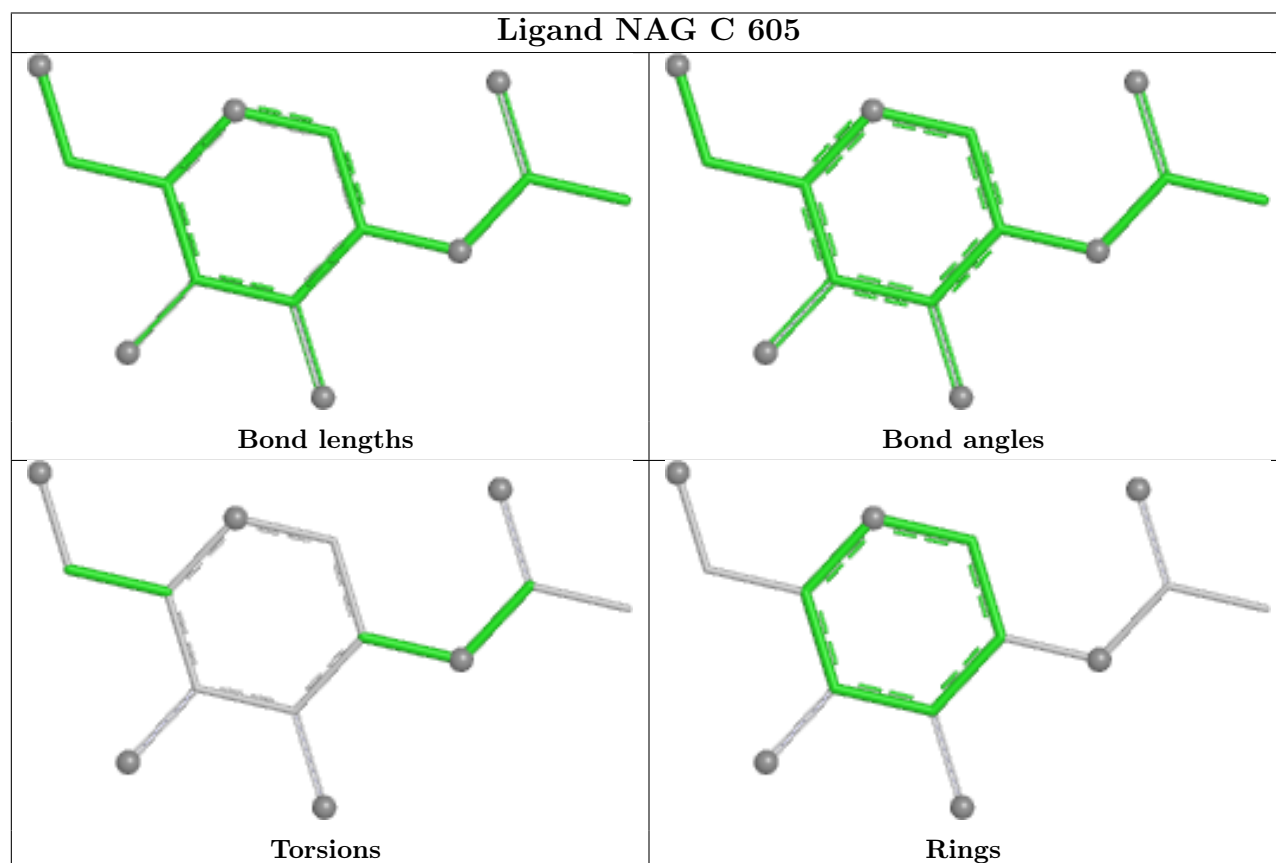
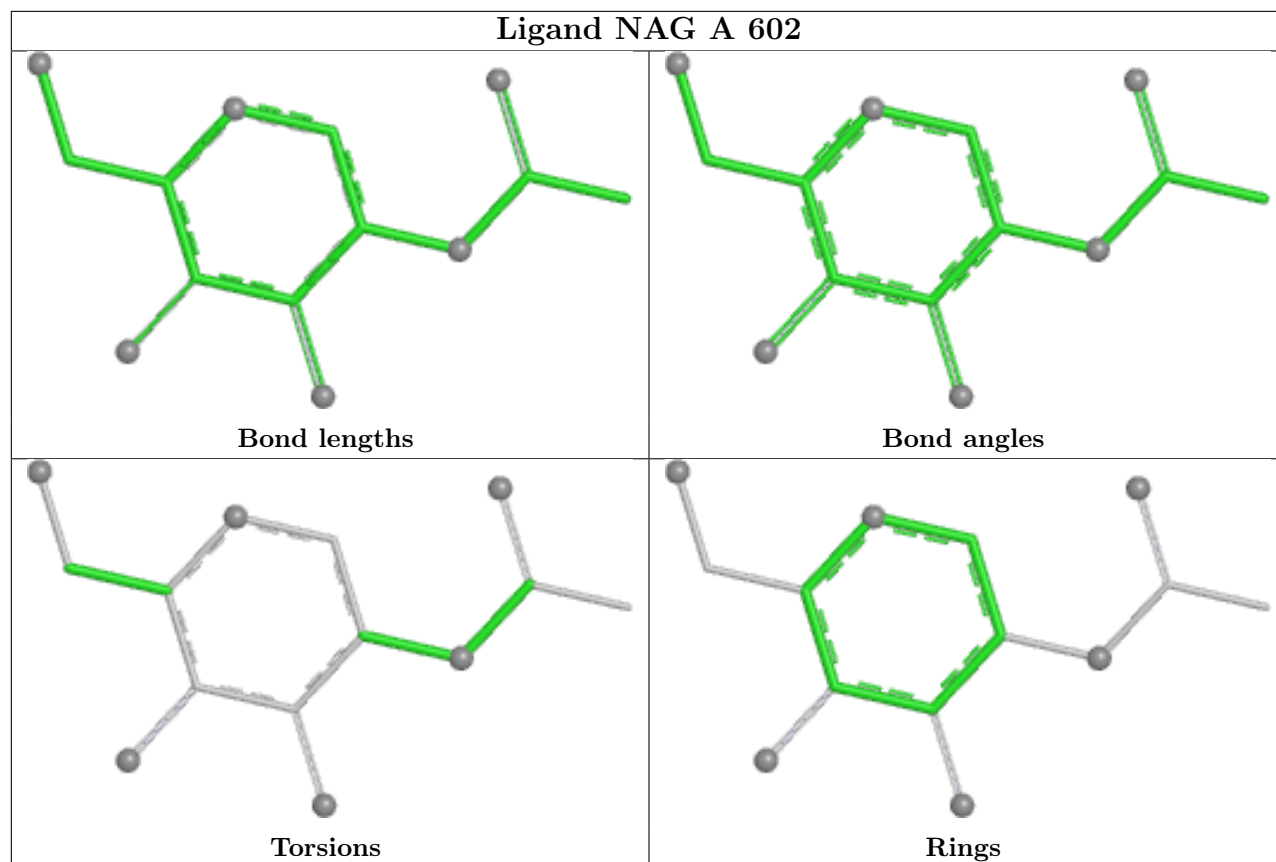


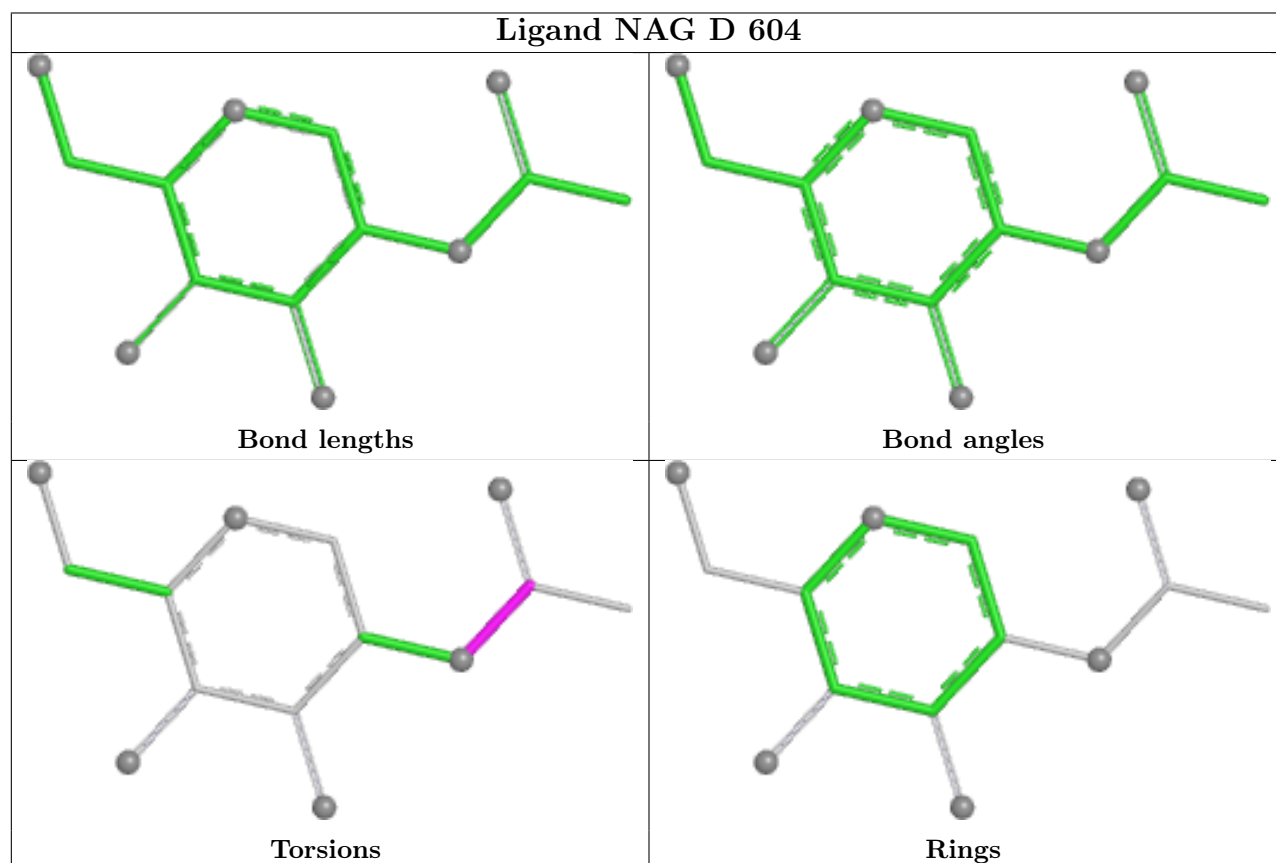
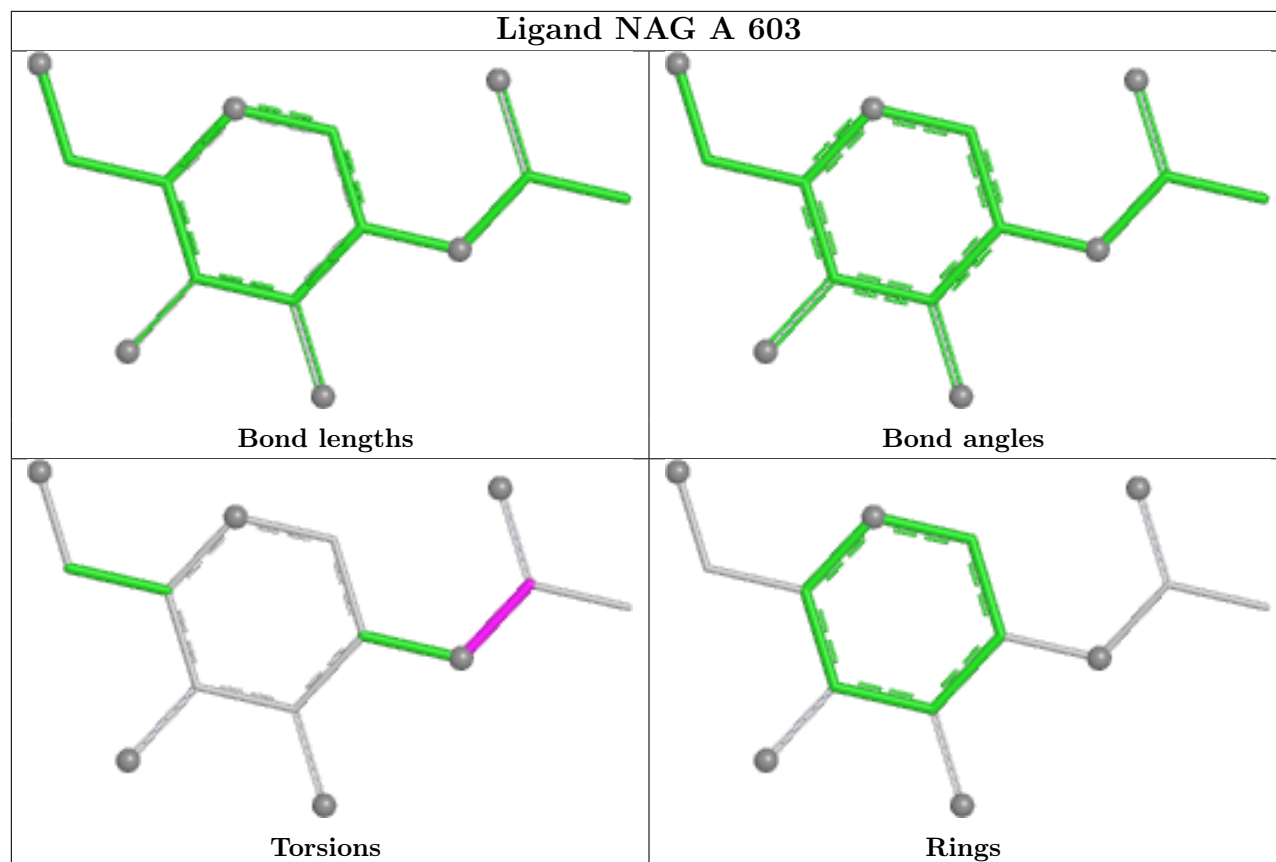


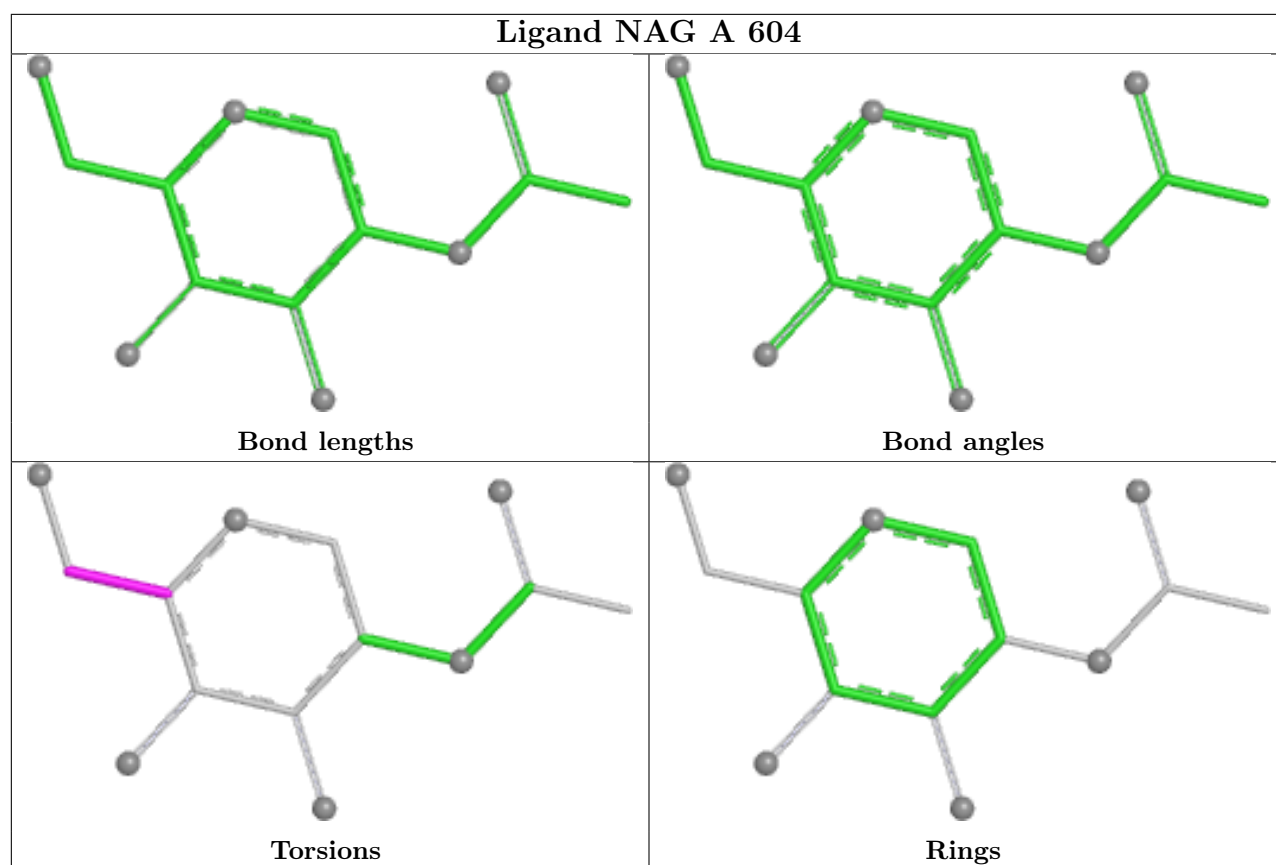


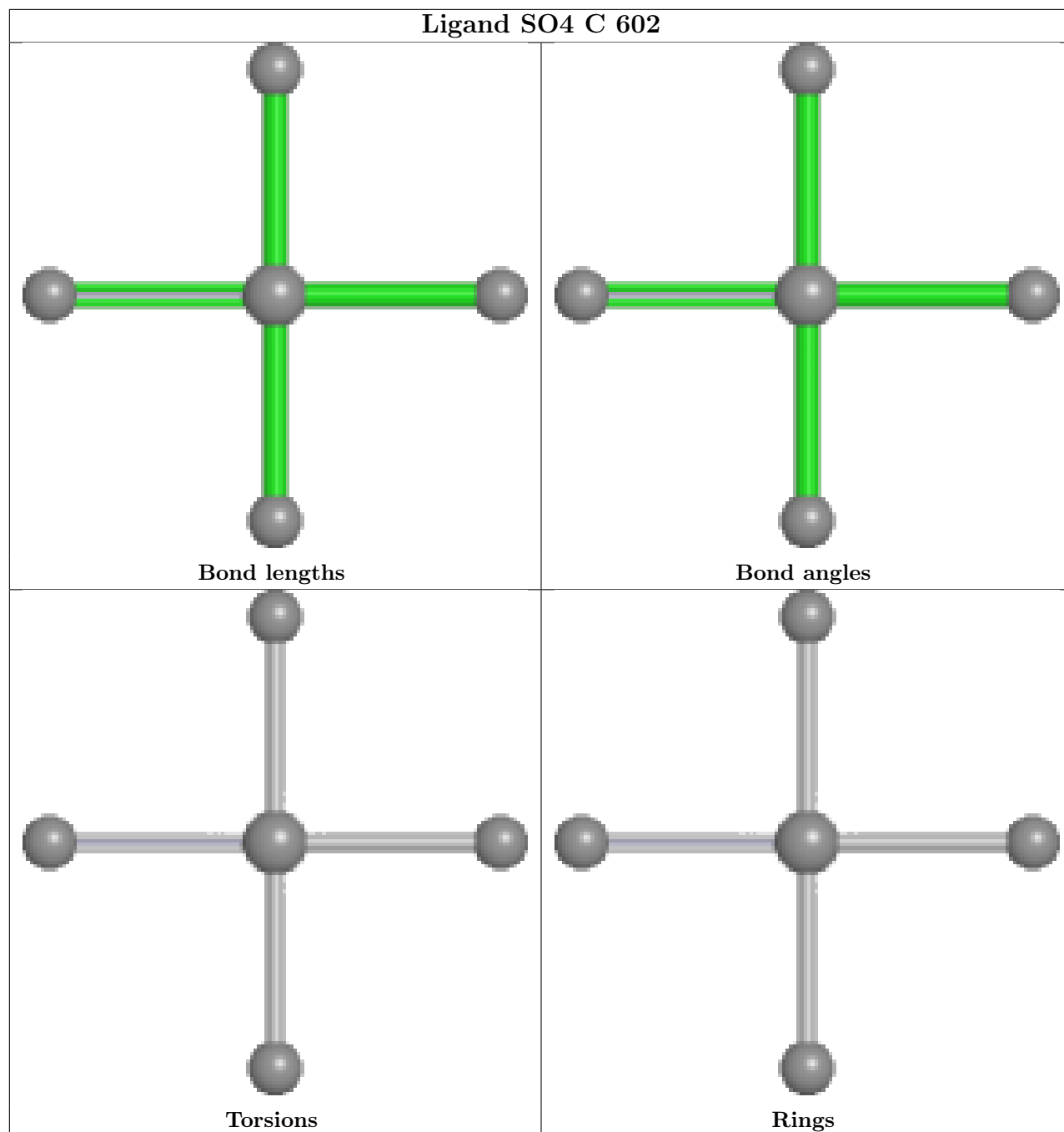


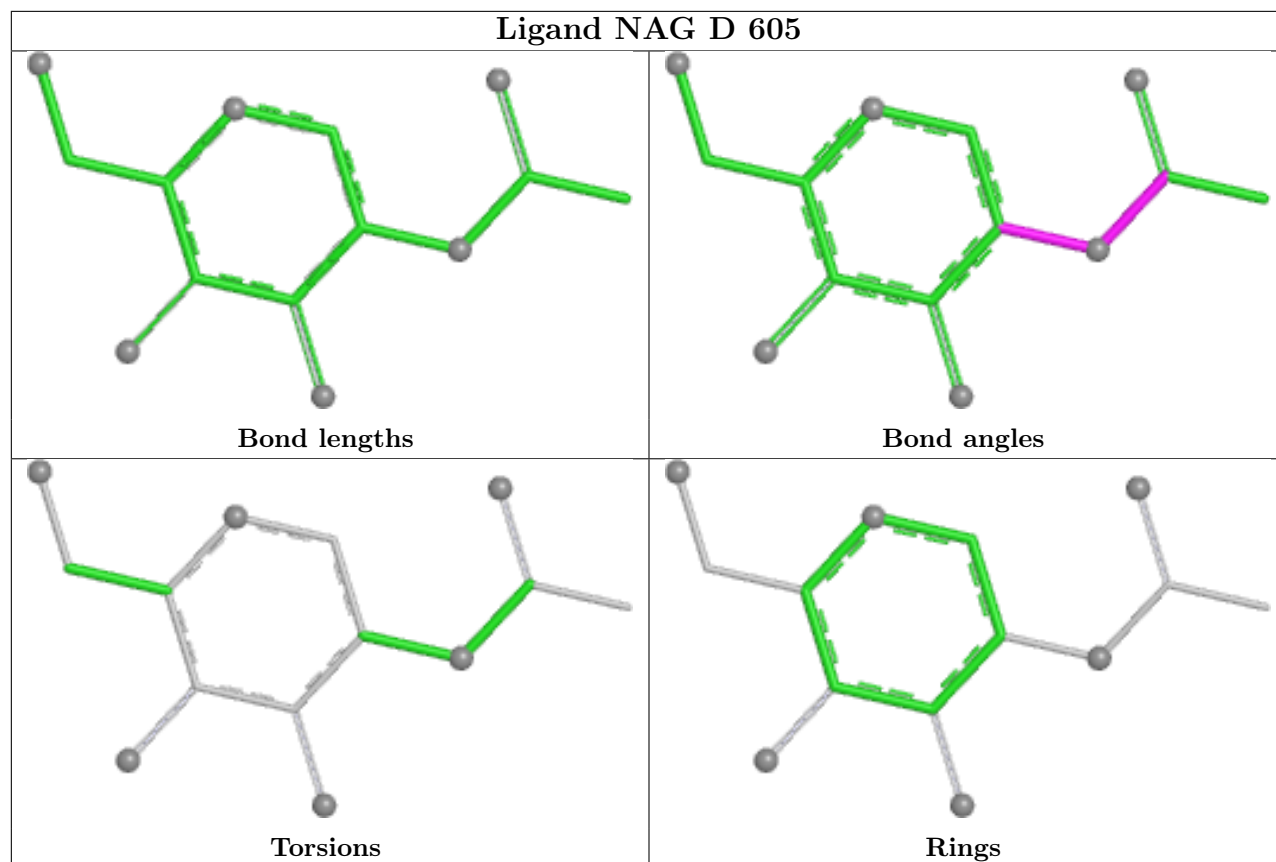


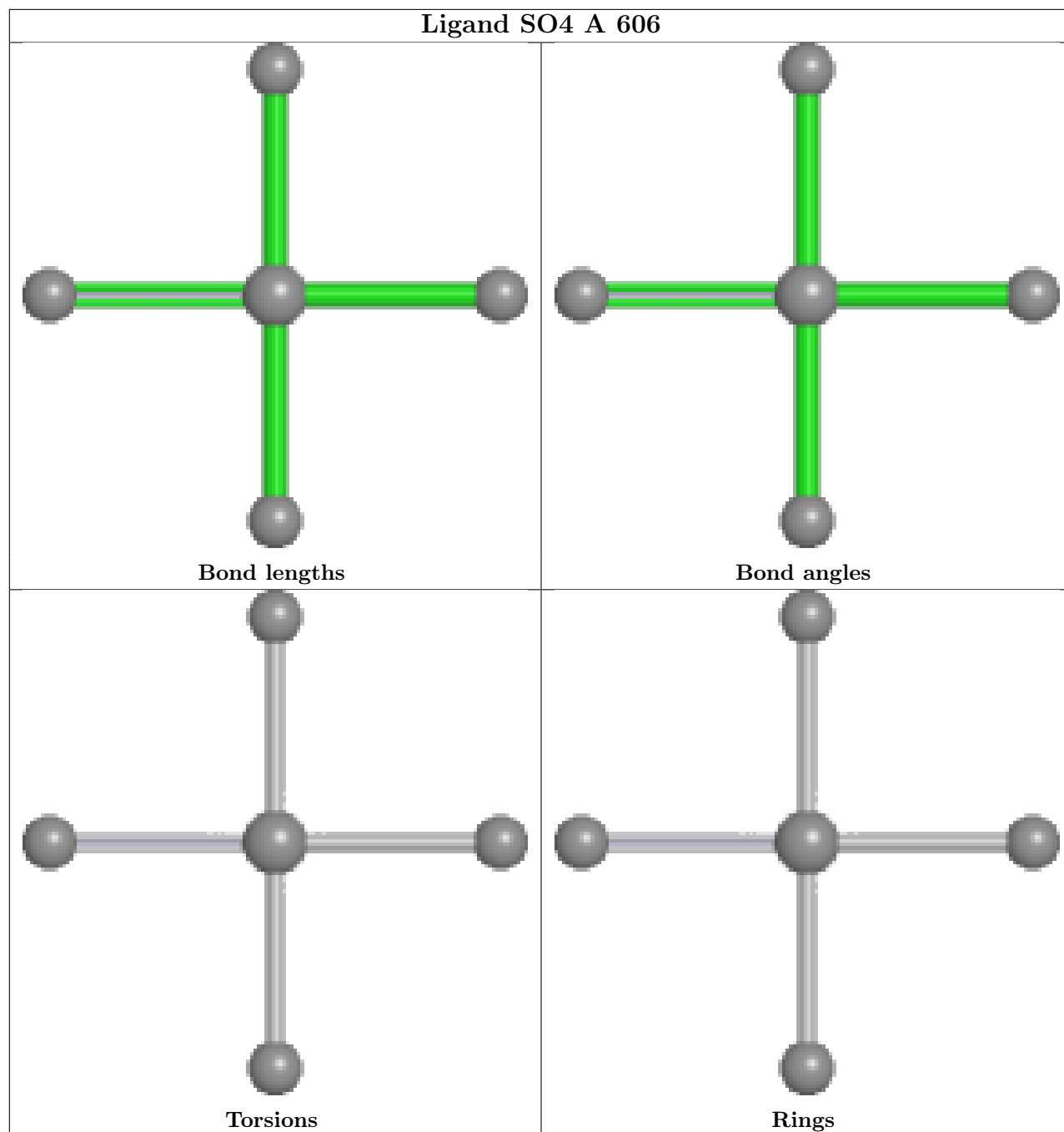


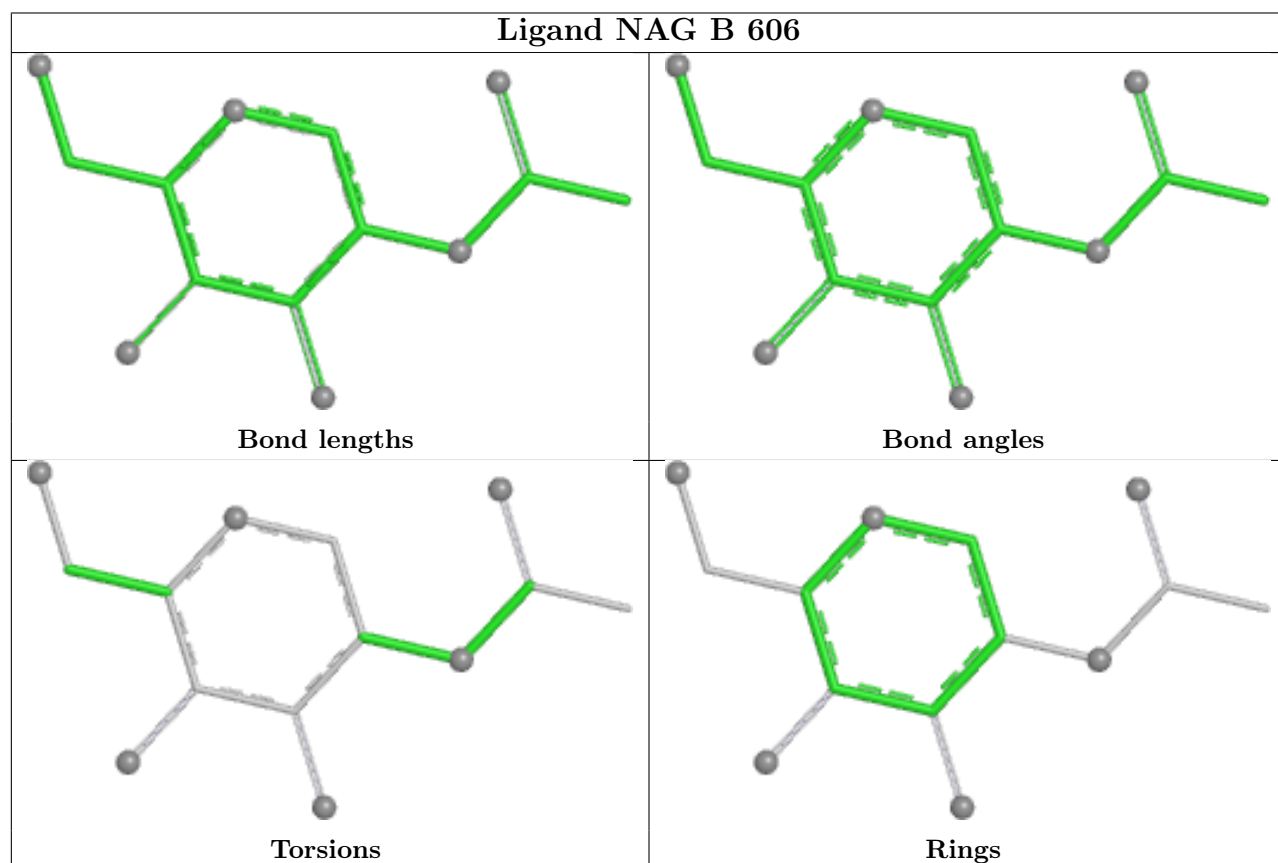
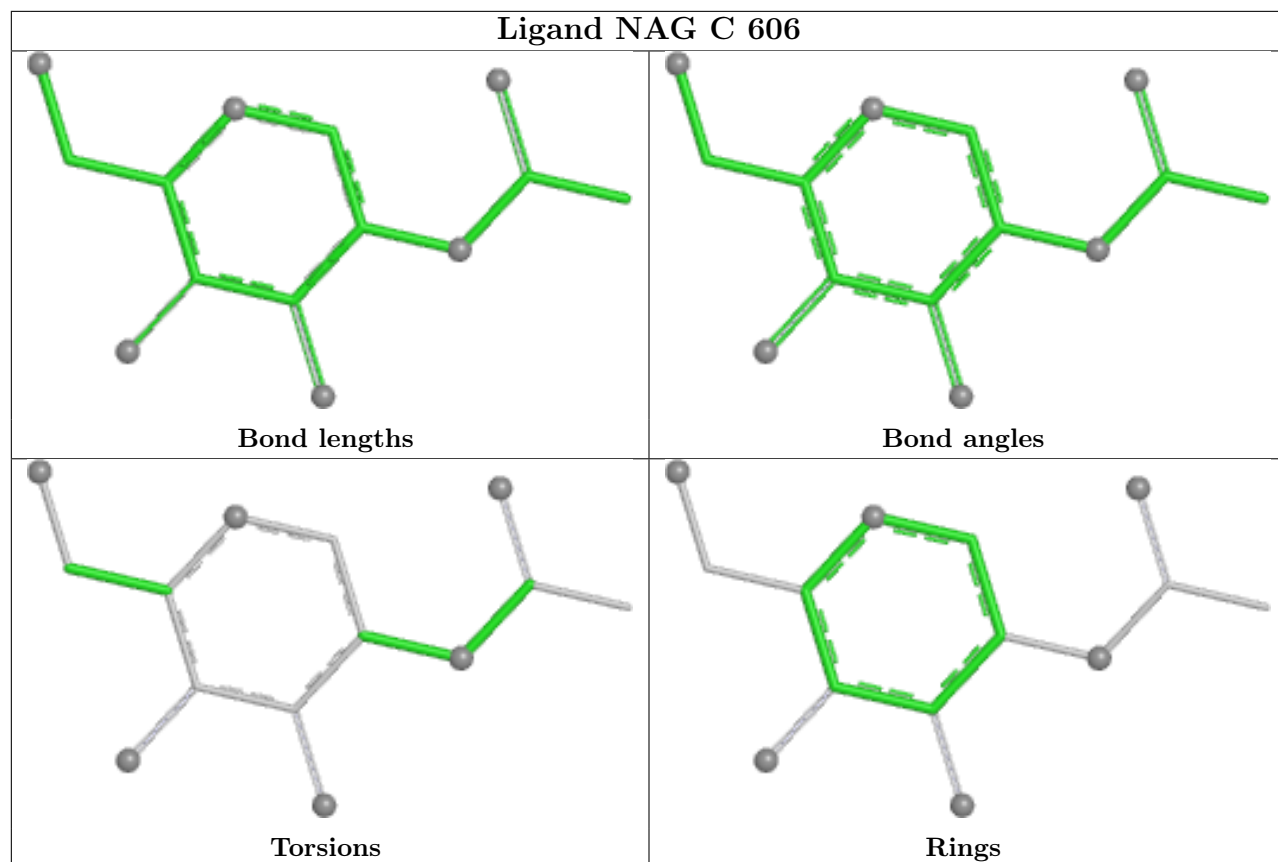


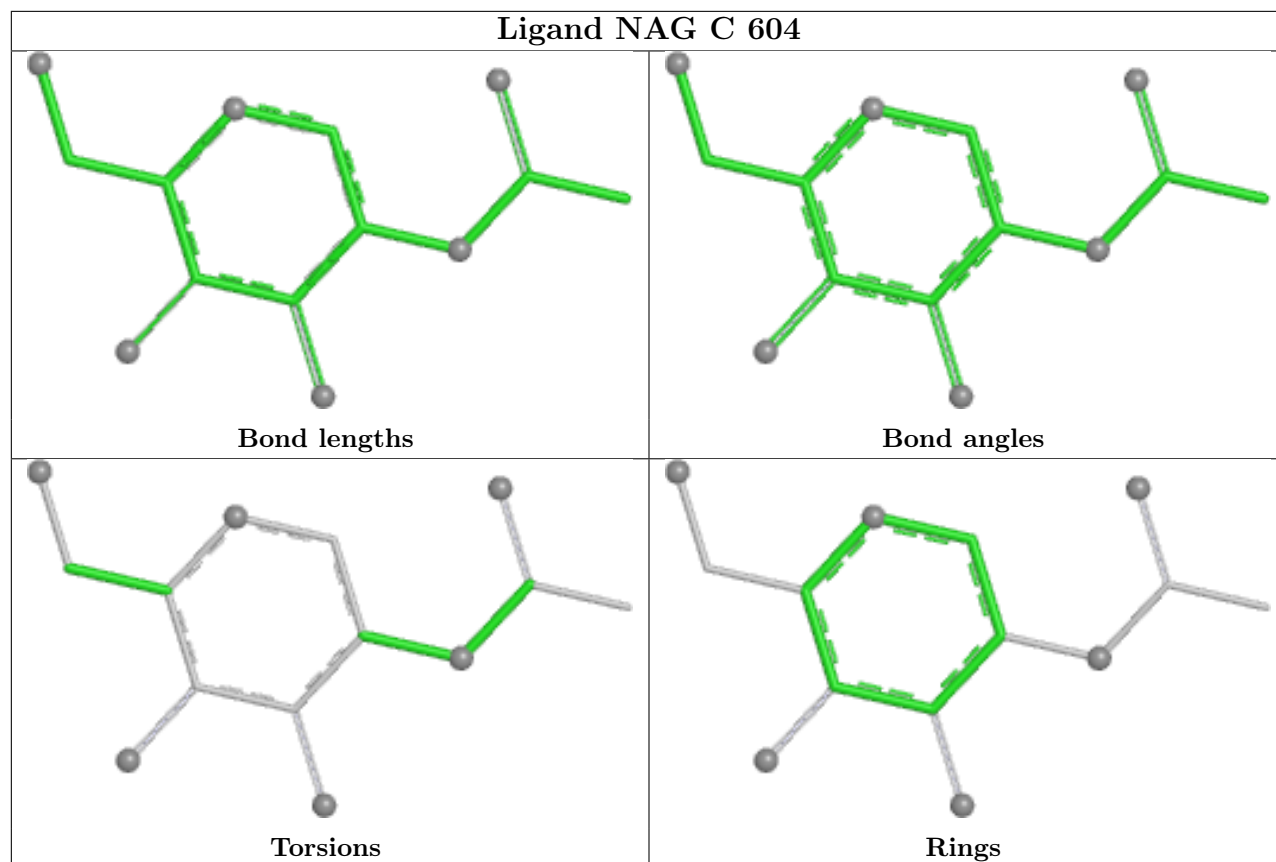












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	537/576 (93%)	0.05	22 (4%)	41	37	21, 37, 77, 114	1 (0%)
1	B	536/576 (93%)	0.29	27 (5%)	34	30	27, 43, 78, 112	0
1	C	537/576 (93%)	0.01	28 (5%)	33	29	24, 36, 73, 111	1 (0%)
1	D	534/576 (92%)	0.30	30 (5%)	30	26	23, 42, 79, 125	0
All	All	2144/2304 (93%)	0.16	107 (4%)	34	30	21, 40, 77, 125	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	340	ALA	6.0
1	D	408	ILE	5.9
1	B	408	ILE	5.5
1	D	40	THR	5.3
1	C	576	SER	5.3
1	B	335	GLY	5.2
1	A	336	SER	5.0
1	A	41	THR	4.9
1	A	39	THR	4.9
1	D	576	SER	4.9
1	B	38	THR	4.7
1	D	41	THR	4.6
1	C	38	THR	4.6
1	C	41	THR	4.6
1	A	335	GLY	4.6
1	B	41	THR	4.4
1	C	340	ALA	4.3
1	A	40	THR	4.2
1	B	576	SER	4.1
1	C	336	SER	4.0
1	A	408	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	38	THR	4.0
1	D	39	THR	4.0
1	C	277	ARG	3.9
1	B	409	ALA	3.9
1	D	274	LYS	3.9
1	C	40	THR	3.9
1	B	340	ALA	3.7
1	A	274	LYS	3.7
1	C	39	THR	3.6
1	D	277	ARG	3.5
1	B	274	LYS	3.5
1	C	339	ASP	3.4
1	D	437	SER	3.4
1	D	548	ARG	3.4
1	B	40	THR	3.4
1	A	339	ASP	3.3
1	C	173	ASP	3.3
1	A	340	ALA	3.3
1	C	575	GLN	3.3
1	D	172	SER	3.2
1	C	156	ASN	3.2
1	D	575	GLN	3.1
1	A	273	GLU	3.1
1	D	197	HIS	3.1
1	A	173	ASP	3.1
1	A	548	ARG	3.1
1	B	278	ARG	3.0
1	C	278	ARG	3.0
1	D	205	ASP	3.0
1	B	156	ASN	2.9
1	C	408	ILE	2.9
1	A	277	ARG	2.9
1	C	155	PRO	2.9
1	B	548	ARG	2.8
1	C	274	LYS	2.8
1	C	335	GLY	2.8
1	B	39	THR	2.8
1	D	567	ALA	2.8
1	D	89	ASP	2.8
1	A	42	THR	2.7
1	A	267	ARG	2.7
1	A	409	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	276	GLU	2.6
1	B	171	ASP	2.6
1	C	134	LYS	2.6
1	B	575	GLN	2.5
1	B	277	ARG	2.5
1	B	89	ASP	2.5
1	D	409	ALA	2.5
1	C	172	SER	2.5
1	B	273	GLU	2.5
1	B	197	HIS	2.4
1	D	42	THR	2.4
1	B	276	GLU	2.4
1	C	341	GLU	2.4
1	A	171	ASP	2.4
1	B	173	ASP	2.4
1	C	171	ASP	2.4
1	B	339	ASP	2.3
1	D	335	GLY	2.3
1	B	567	ALA	2.3
1	C	50	PRO	2.3
1	D	566	GLU	2.3
1	C	133[A]	ARG	2.2
1	D	147	ARG	2.2
1	B	42	THR	2.2
1	A	576	SER	2.2
1	B	194	ILE	2.2
1	C	407	SER	2.2
1	D	173	ASP	2.2
1	D	50	PRO	2.2
1	A	175	SER	2.2
1	D	219	GLY	2.2
1	D	273	GLU	2.2
1	D	155	PRO	2.2
1	D	156	ASN	2.1
1	D	134	LYS	2.1
1	C	273	GLU	2.1
1	C	567	ALA	2.1
1	B	174	GLY	2.1
1	D	573	GLY	2.1
1	B	172	SER	2.1
1	D	407	SER	2.1
1	C	406	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	437	SER	2.1
1	A	89	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

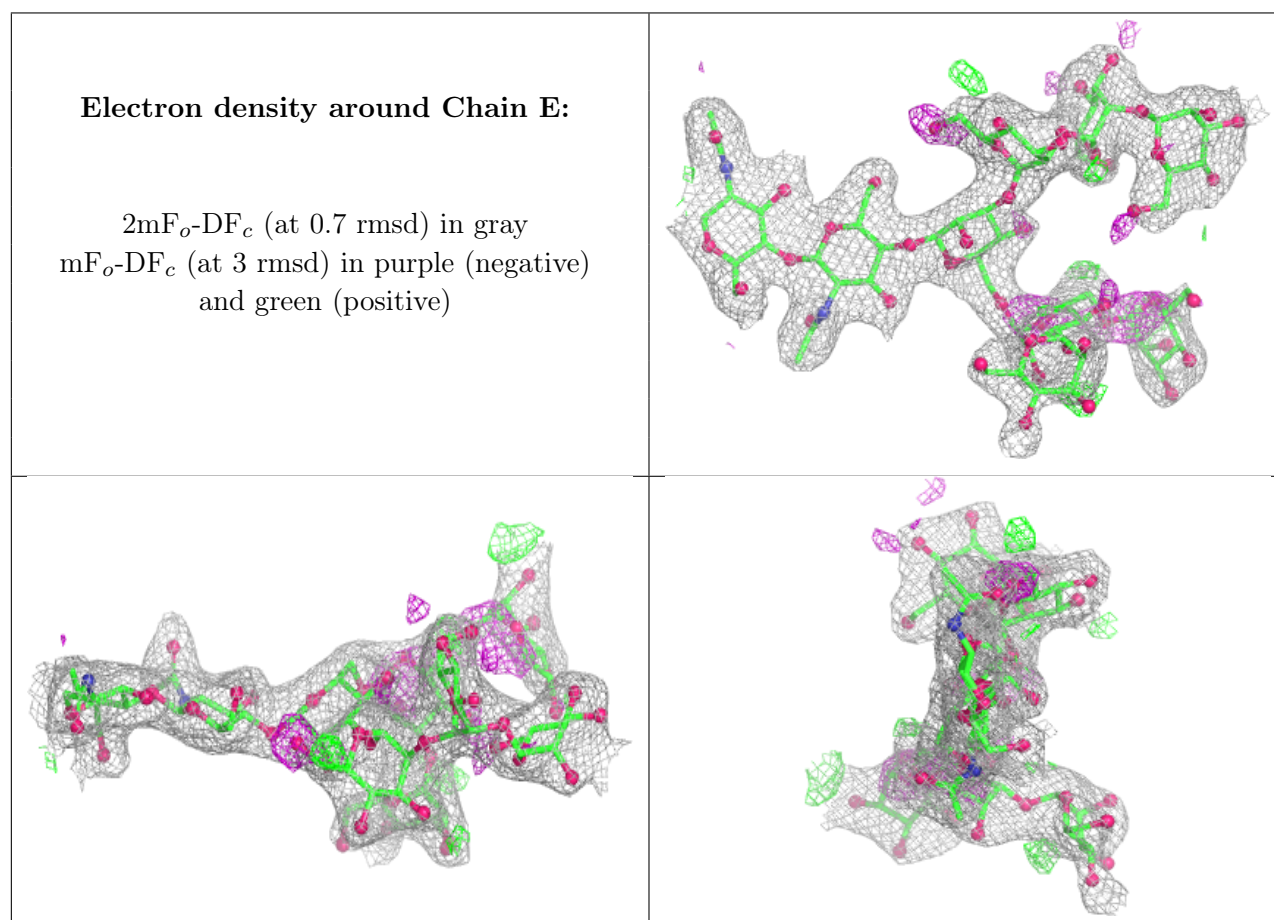
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	G	9	11/12	0.48	0.19	39,41,44,44	11
2	MAN	H	9	11/12	0.48	0.20	39,43,43,43	11
2	MAN	F	9	11/12	0.58	0.18	36,41,42,45	11
2	MAN	E	9	11/12	0.60	0.18	40,42,45,46	11
2	MAN	H	8	11/12	0.61	0.18	38,42,43,44	11
2	MAN	G	8	11/12	0.70	0.17	39,42,44,44	11
2	MAN	E	7	11/12	0.71	0.16	39,40,43,44	0
2	MAN	E	8	11/12	0.72	0.15	40,41,42,43	11
2	MAN	F	8	11/12	0.75	0.15	39,41,42,44	11
2	MAN	H	7	11/12	0.79	0.13	39,40,42,43	0
2	MAN	G	6	11/12	0.81	0.12	36,37,39,41	0
2	MAN	F	7	11/12	0.82	0.12	38,39,42,42	0
2	MAN	G	7	11/12	0.83	0.14	38,41,42,42	0
2	MAN	E	6	11/12	0.84	0.11	37,39,41,42	0
2	BMA	F	3	11/12	0.85	0.10	33,36,39,40	0
2	MAN	G	4	11/12	0.85	0.10	33,37,40,40	0
2	MAN	F	5	11/12	0.85	0.10	35,37,38,42	0
2	MAN	H	6	11/12	0.86	0.11	34,38,41,42	0
2	MAN	E	4	11/12	0.86	0.11	35,37,41,42	0
2	BMA	G	3	11/12	0.88	0.09	33,37,39,40	0
2	MAN	F	6	11/12	0.88	0.10	35,39,41,41	0
2	MAN	F	4	11/12	0.90	0.09	33,35,39,39	0
2	MAN	E	5	11/12	0.90	0.09	35,38,41,41	0
2	BMA	H	3	11/12	0.90	0.09	34,36,39,40	0
2	MAN	H	4	11/12	0.90	0.09	33,35,42,42	0
2	BMA	E	3	11/12	0.91	0.09	34,37,39,40	0

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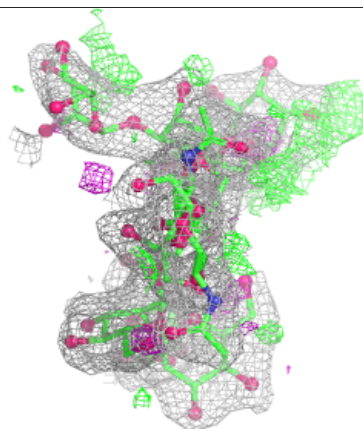
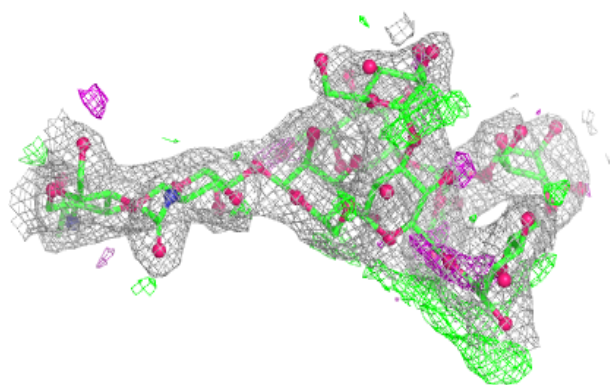
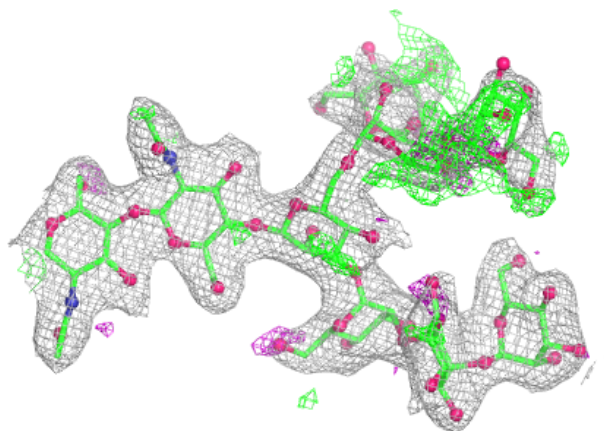
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	G	5	11/12	0.91	0.09	37,37,39,40	0
2	MAN	H	5	11/12	0.92	0.09	35,37,39,40	0
2	NAG	G	2	14/15	0.93	0.07	31,33,34,36	0
2	NAG	F	2	14/15	0.94	0.07	31,34,35,35	0
2	NAG	H	2	14/15	0.95	0.08	29,31,33,34	0
2	NAG	E	2	14/15	0.95	0.08	32,33,36,36	0
2	NAG	E	1	14/15	0.96	0.09	29,31,34,35	0
2	NAG	F	1	14/15	0.96	0.06	30,32,34,36	0
2	NAG	G	1	14/15	0.97	0.07	30,32,33,33	0
2	NAG	H	1	14/15	0.98	0.06	27,30,31,33	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



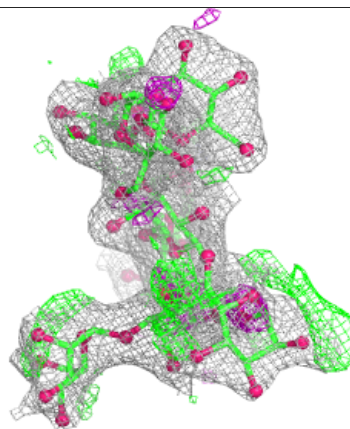
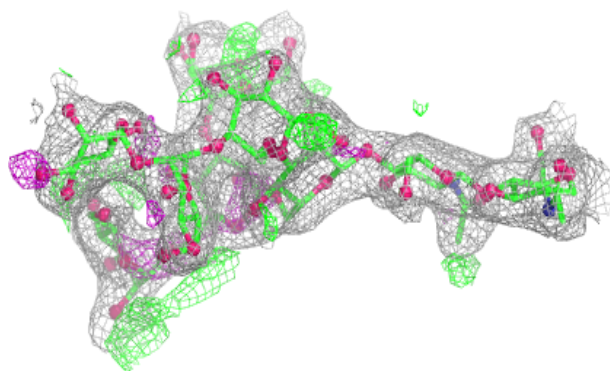
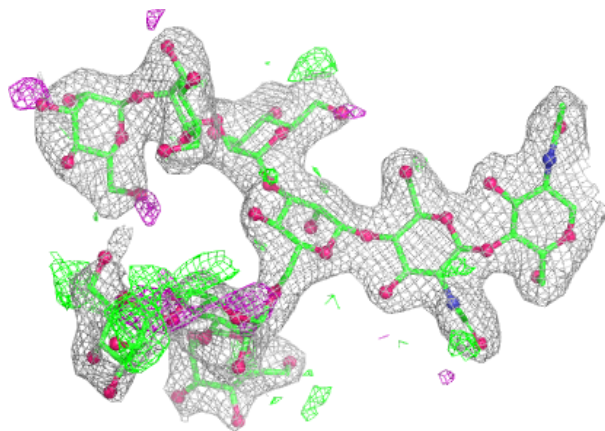
Electron density around Chain F:

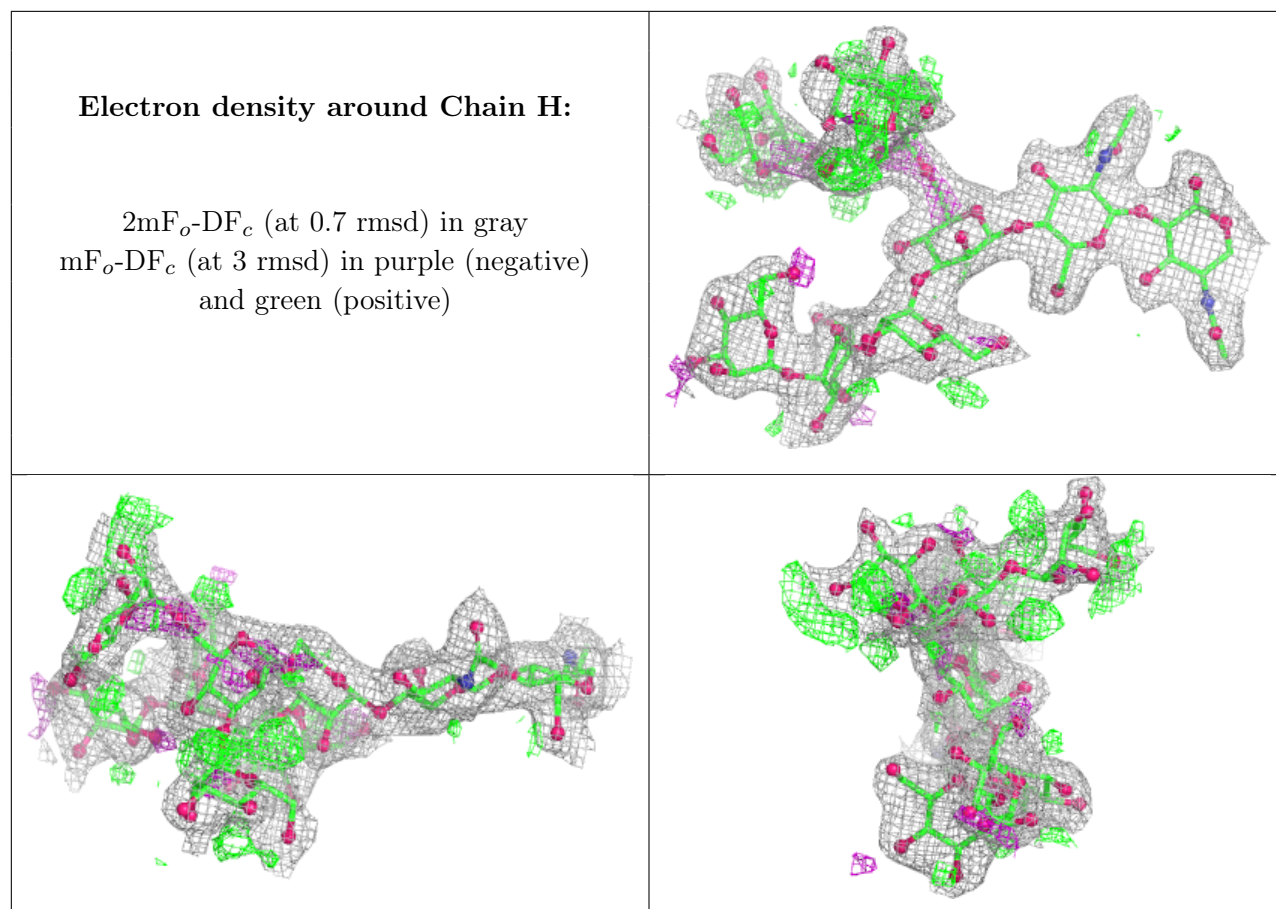
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	604	14/15	0.66	0.14	40,42,44,45	0
4	NAG	A	603	14/15	0.73	0.13	39,41,44,46	0
4	NAG	B	606	14/15	0.74	0.14	39,42,43,44	0
4	NAG	D	606	14/15	0.74	0.14	40,41,44,44	0
4	NAG	B	604	14/15	0.76	0.13	39,41,45,46	0
4	NAG	C	606	14/15	0.78	0.14	38,40,45,47	0
4	NAG	B	605	14/15	0.79	0.13	39,40,44,45	0
4	NAG	C	604	14/15	0.80	0.12	38,40,44,46	0
4	NAG	C	605	14/15	0.83	0.11	39,41,42,43	0
3	FRU	B	601	12/12	0.83	0.20	26,27,30,32	0
4	NAG	A	604	14/15	0.85	0.11	37,39,41,41	0
5	SO4	A	606	5/5	0.85	0.14	27,27,28,30	5
4	NAG	A	605	14/15	0.86	0.10	36,39,41,42	0

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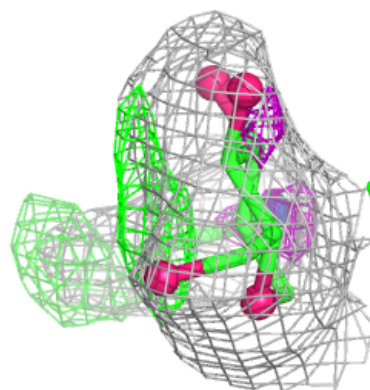
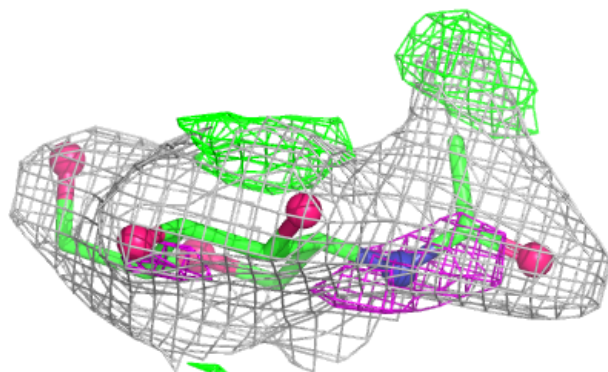
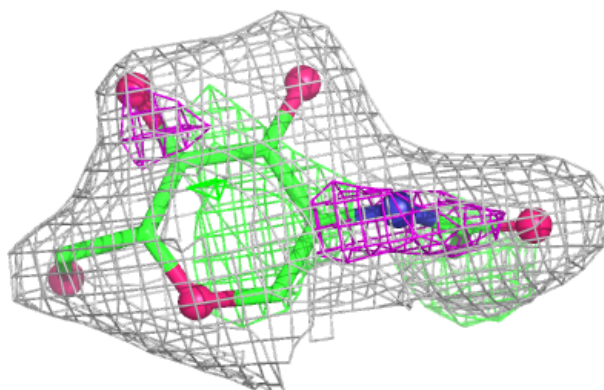
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	D	605	14/15	0.86	0.10	37,40,42,43	0
4	NAG	D	603	14/15	0.87	0.10	36,38,40,42	0
5	SO4	C	607	5/5	0.87	0.13	28,29,30,33	5
5	SO4	C	608	5/5	0.87	0.14	27,28,30,31	5
3	FRU	C	601	12/12	0.88	0.15	25,27,30,34	0
4	NAG	A	602	14/15	0.88	0.10	37,38,41,42	0
3	FRU	D	601	12/12	0.90	0.17	26,28,31,32	0
4	NAG	C	603	14/15	0.90	0.09	33,36,38,40	0
4	NAG	B	603	14/15	0.90	0.09	35,36,43,44	0
3	FRU	A	601	12/12	0.91	0.14	26,27,30,32	0
5	SO4	D	602	5/5	0.94	0.11	23,24,25,26	5
5	SO4	B	602	5/5	0.95	0.14	22,23,25,25	5
5	SO4	C	602	5/5	0.97	0.09	22,23,23,23	5

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

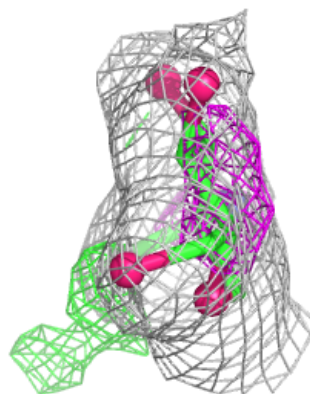
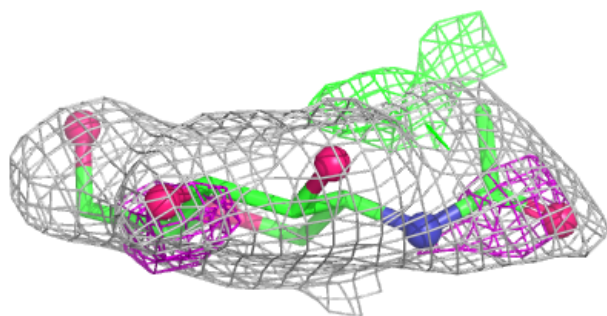
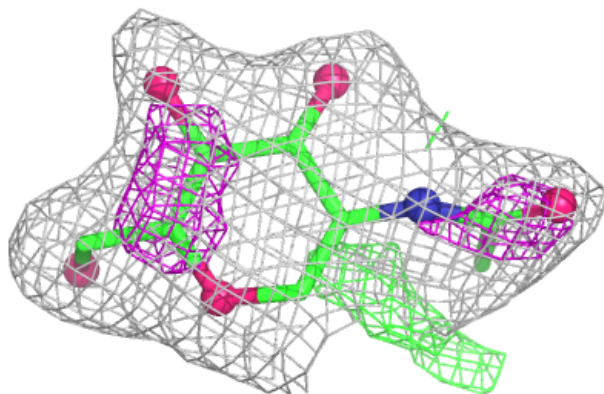
Electron density around NAG D 604:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

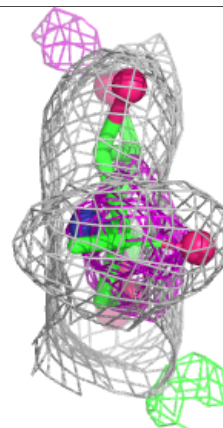
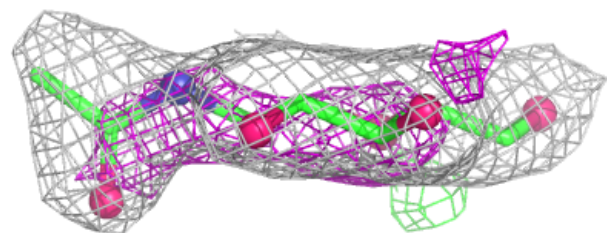
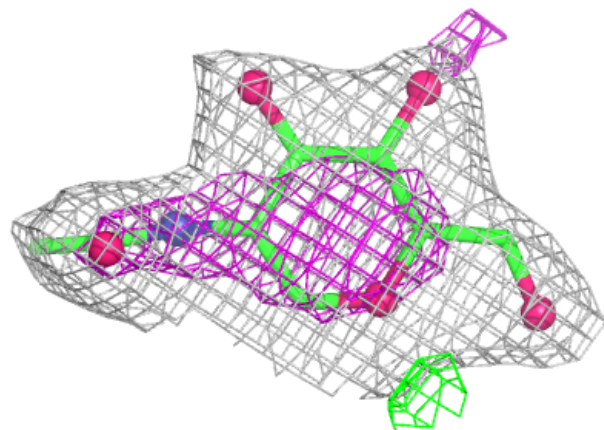


Electron density around NAG A 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

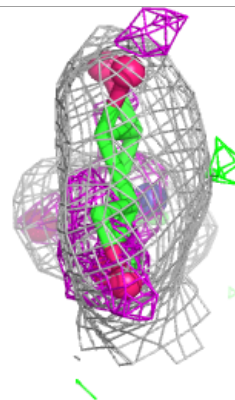
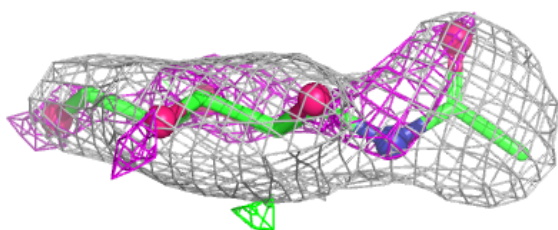
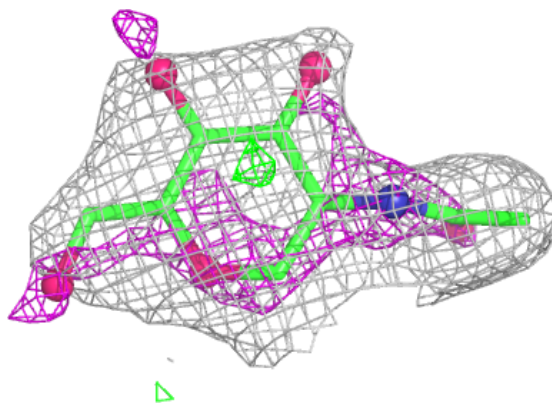
**Electron density around NAG B 606:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

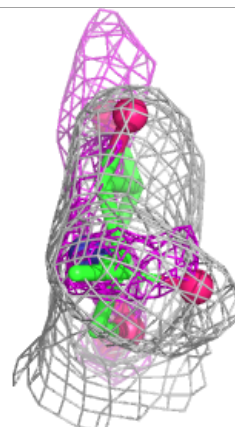
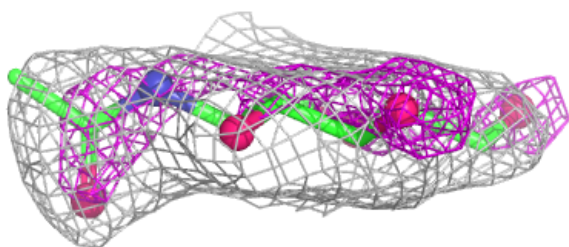
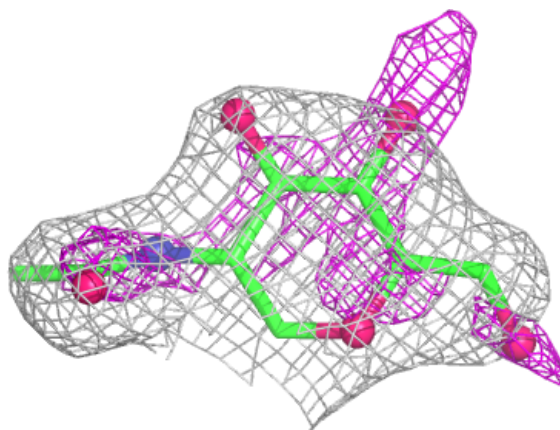


Electron density around NAG D 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

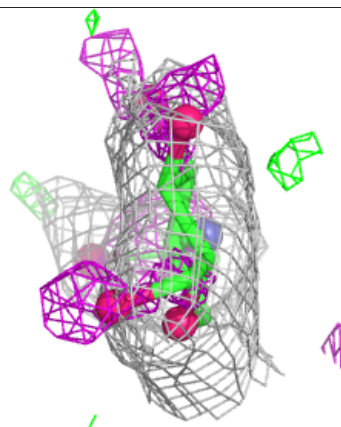
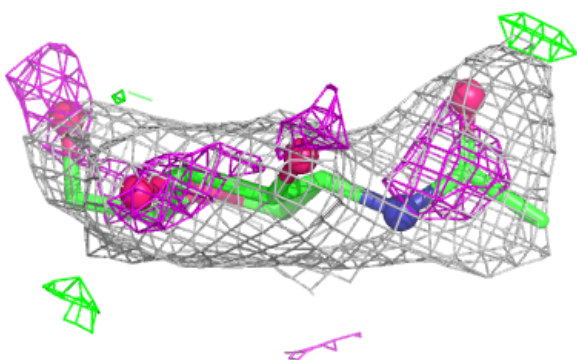
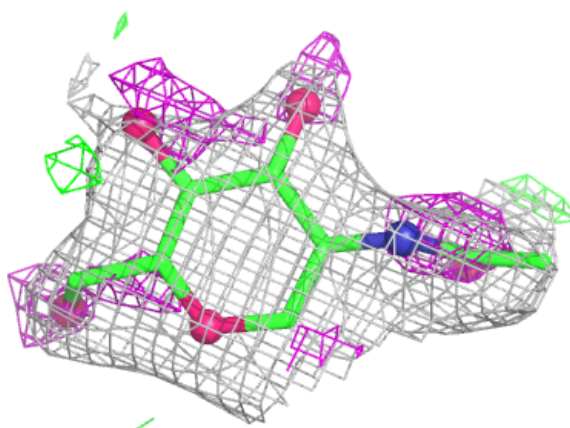
**Electron density around NAG B 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

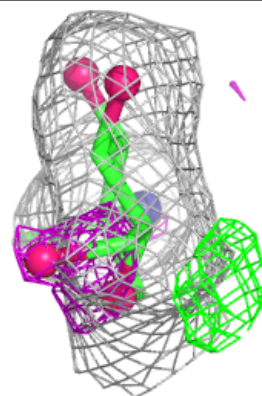
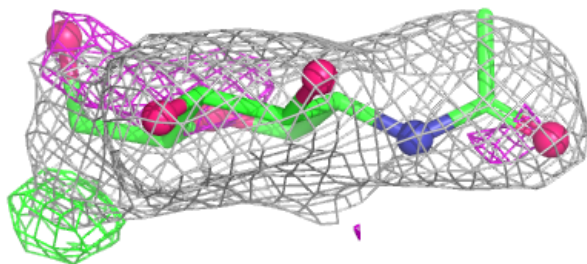
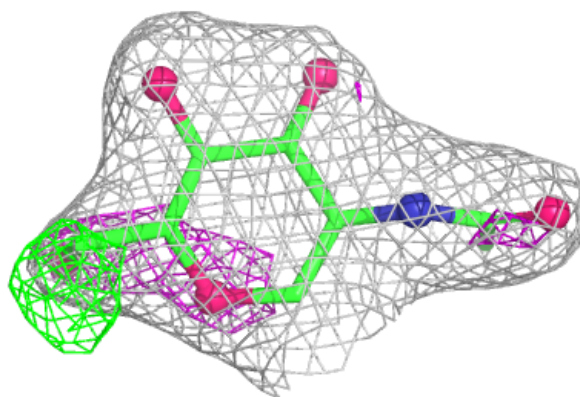


Electron density around NAG C 606:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

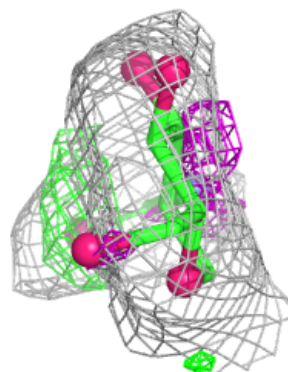
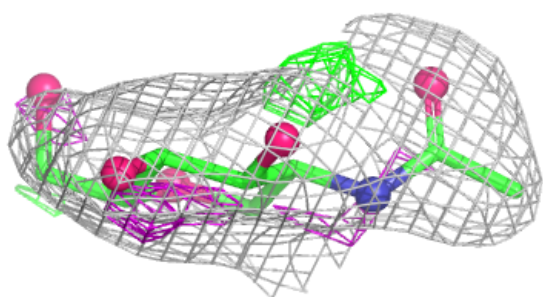
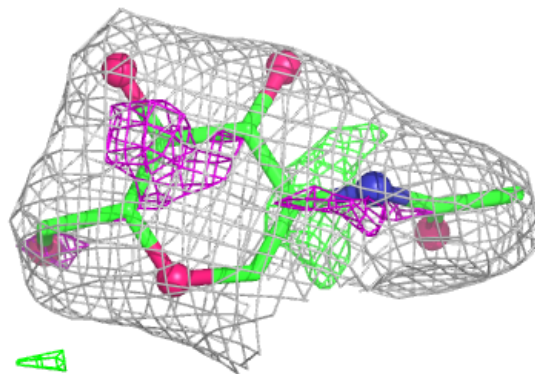
**Electron density around NAG B 605:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

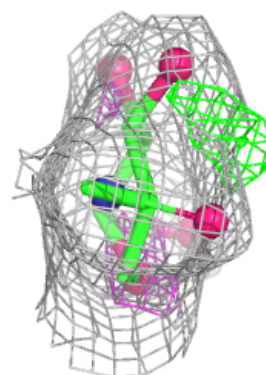
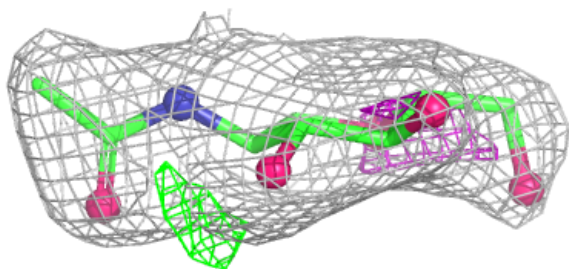
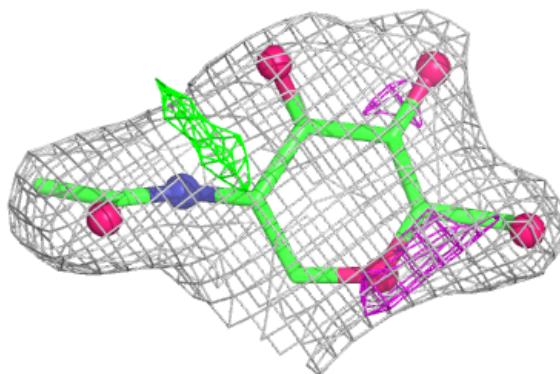


Electron density around NAG C 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

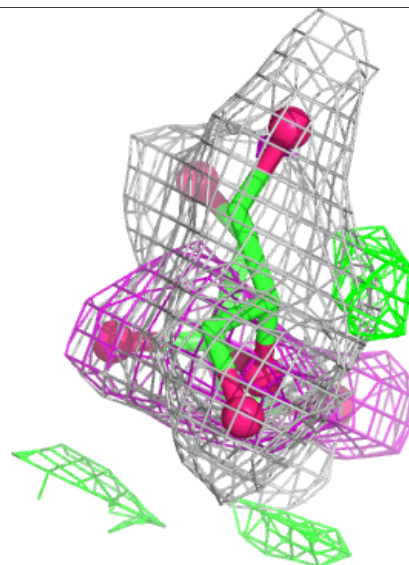
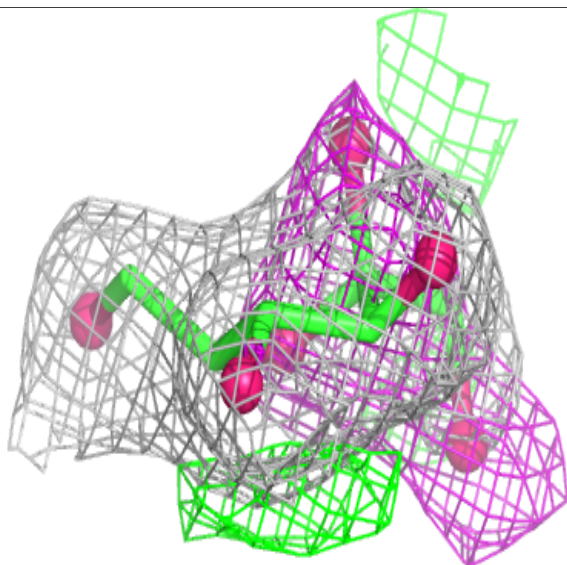
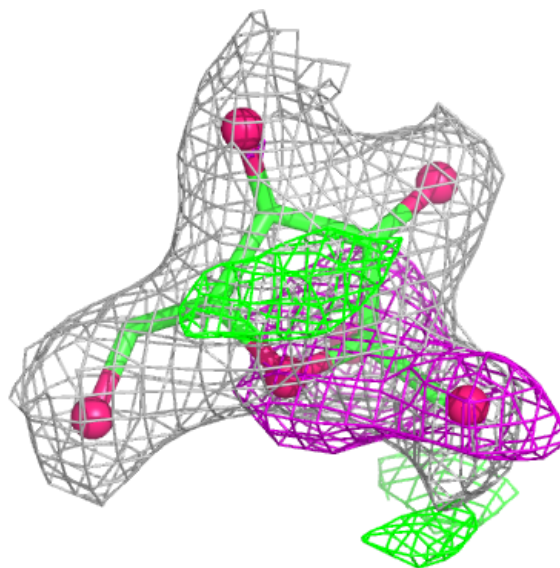
**Electron density around NAG C 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



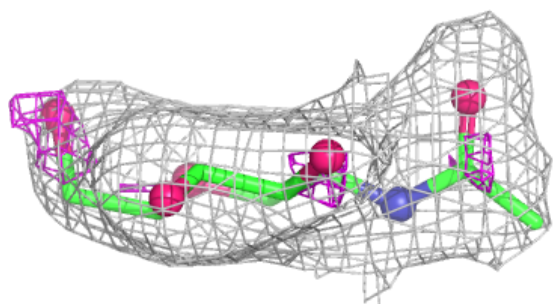
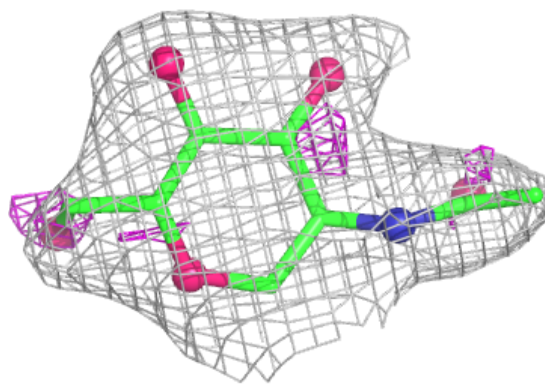
Electron density around FRU B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



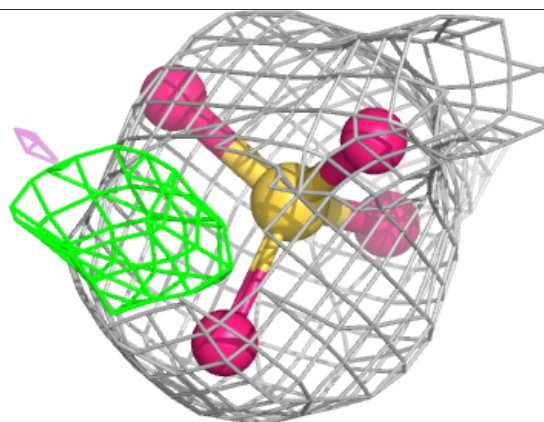
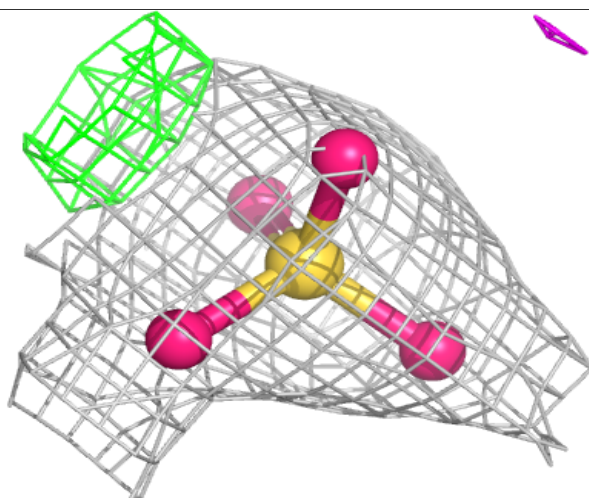
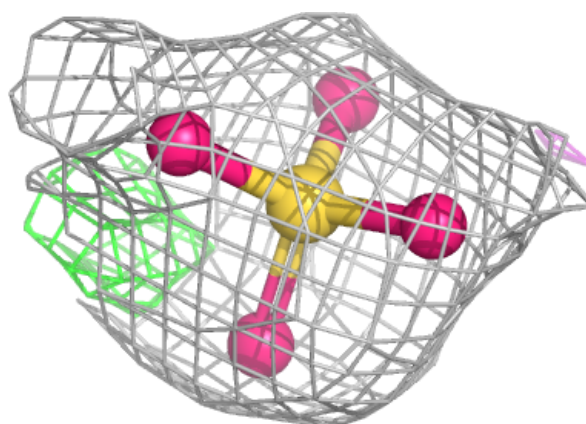
Electron density around NAG A 604:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



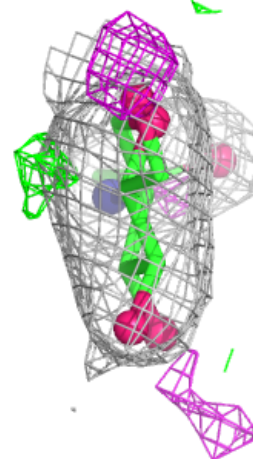
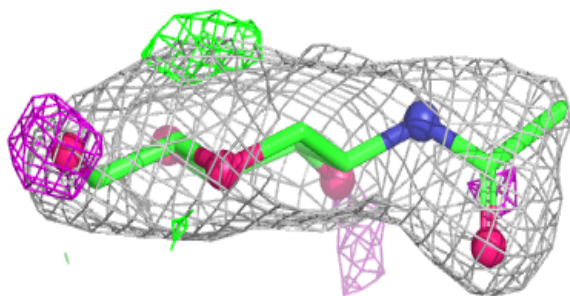
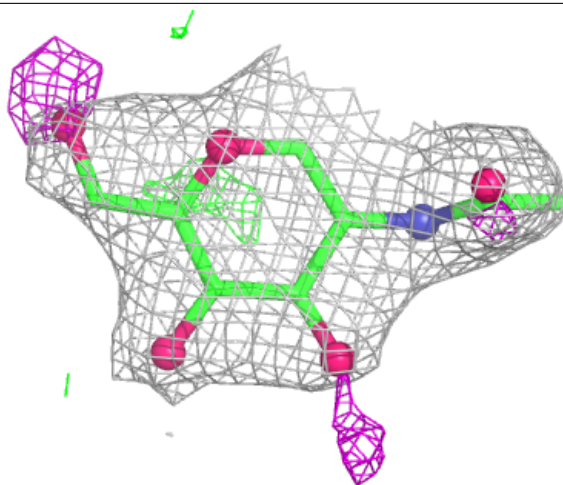
Electron density around SO4 A 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



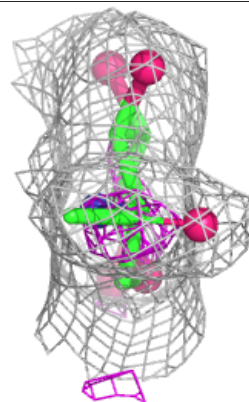
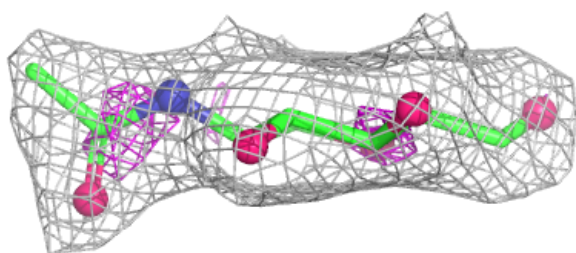
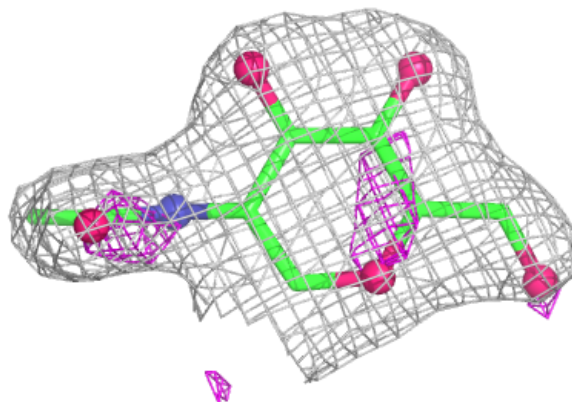
Electron density around NAG A 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)

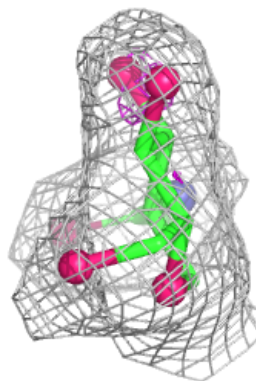
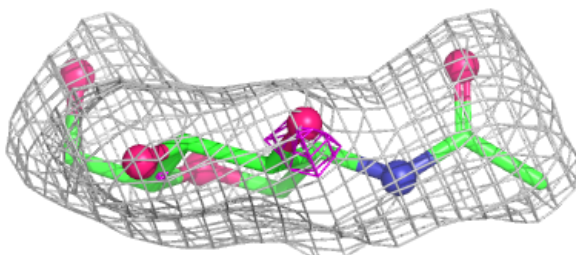
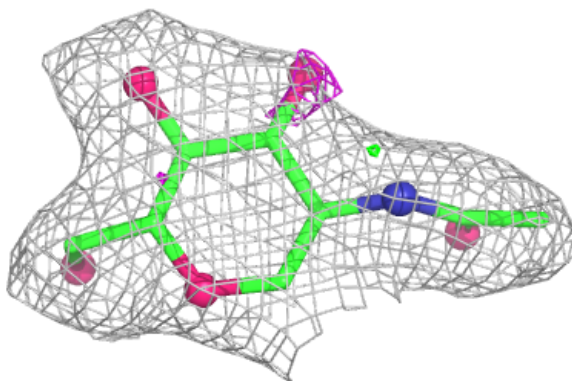


Electron density around NAG D 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

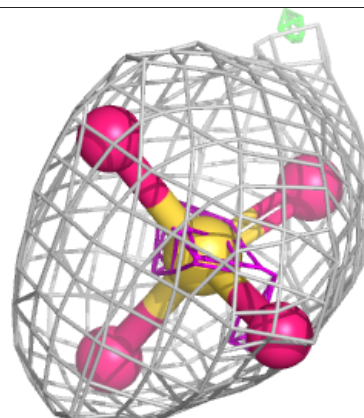
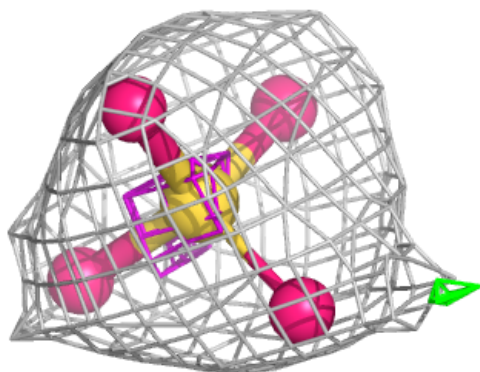
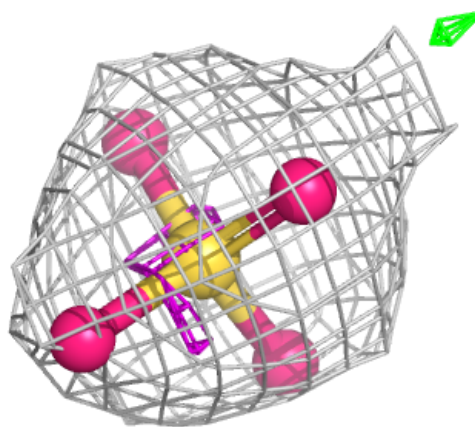
**Electron density around NAG D 603:**

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and green (positive)



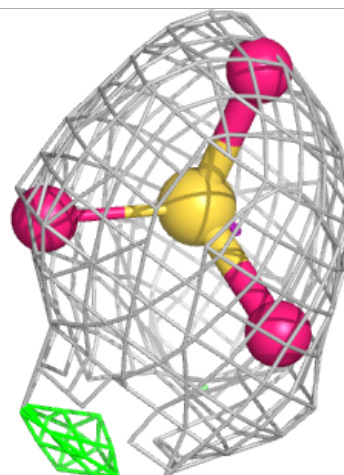
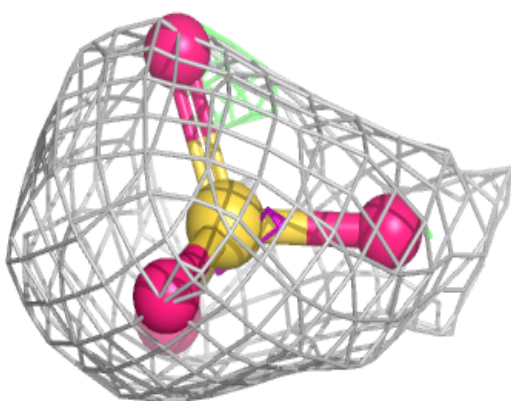
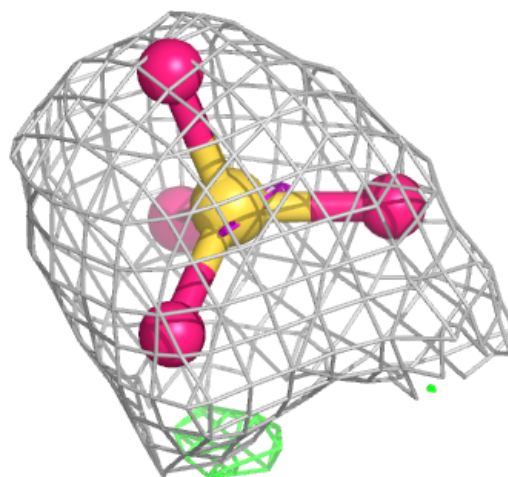
Electron density around SO4 C 607:

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and green (positive)



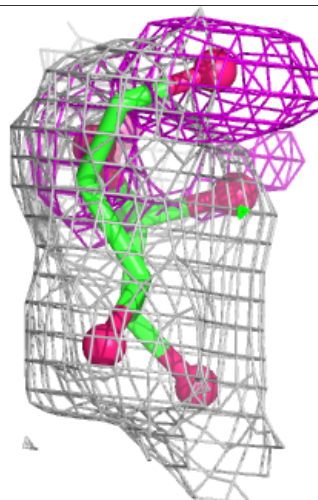
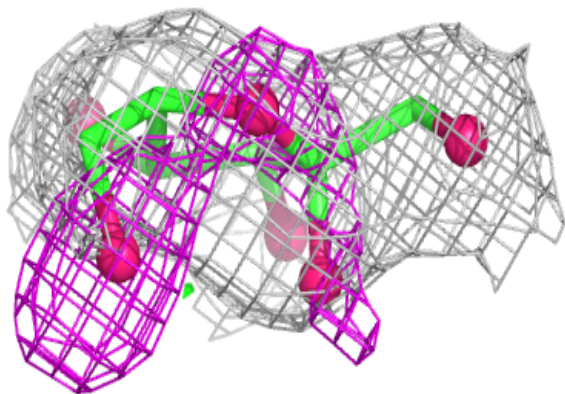
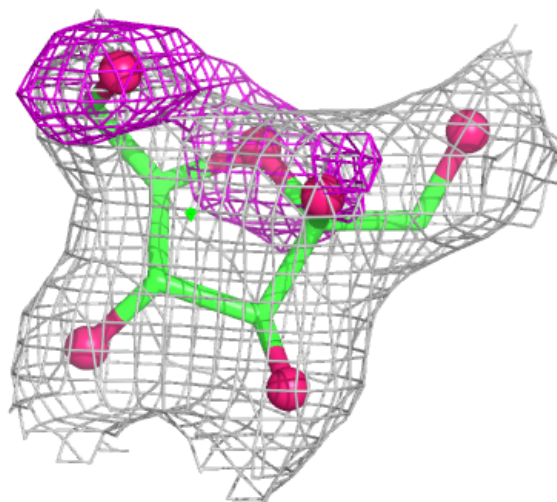
Electron density around SO4 C 608:

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and green (positive)



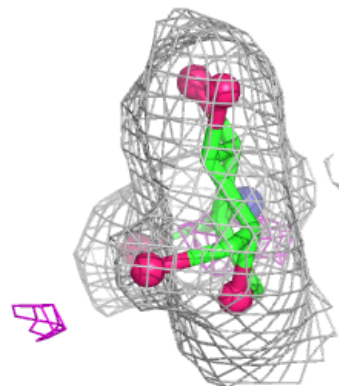
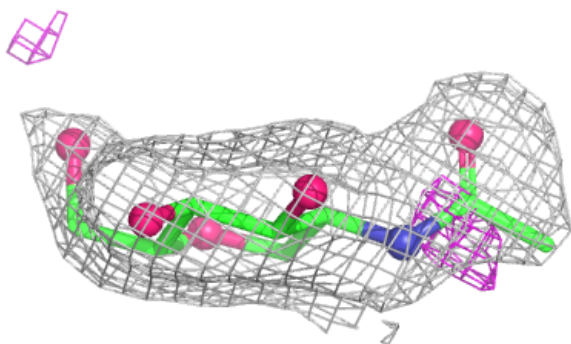
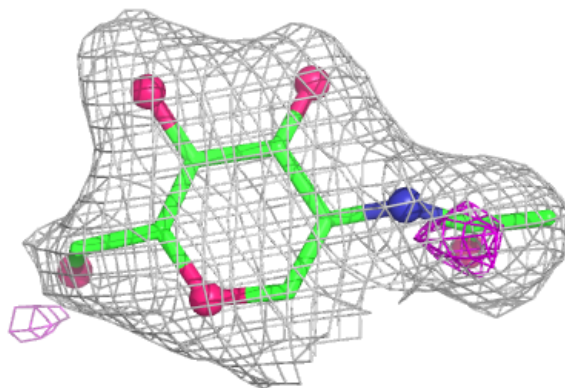
Electron density around FRU C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



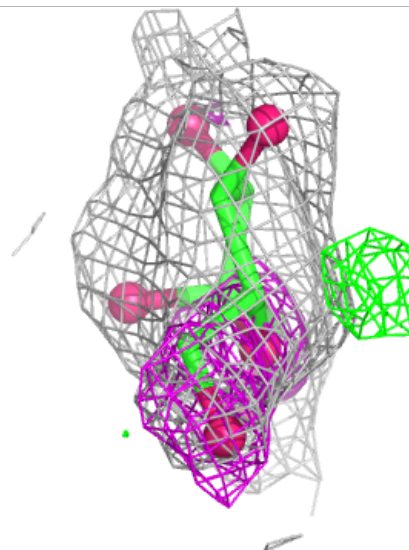
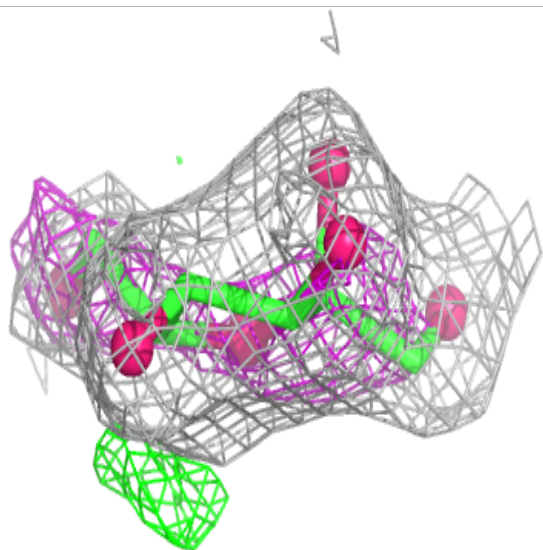
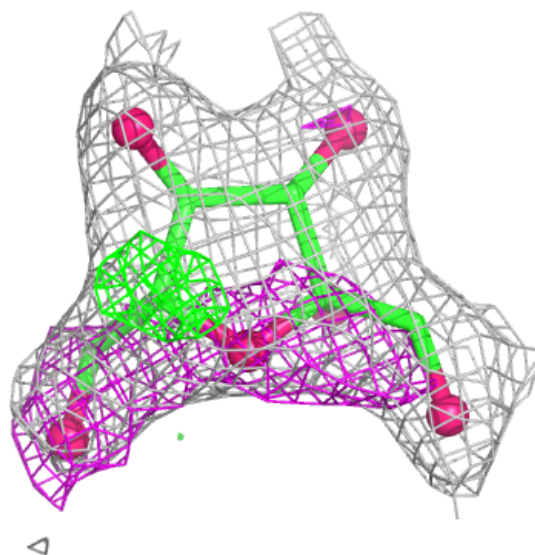
Electron density around NAG A 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



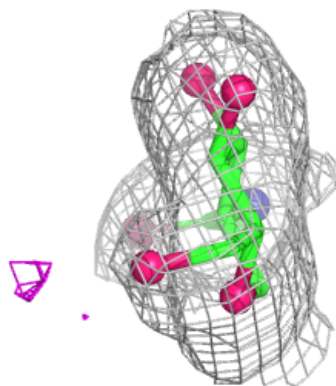
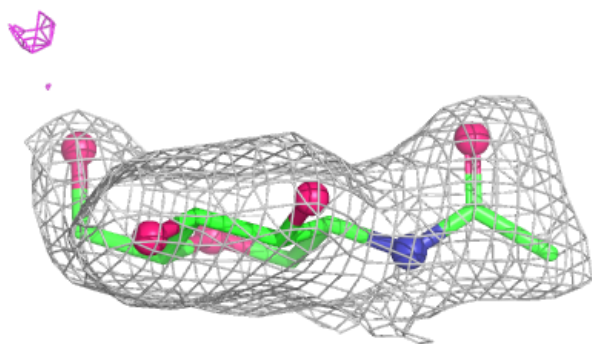
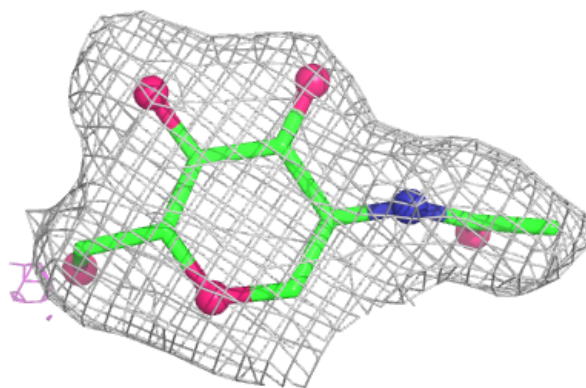
Electron density around FRU D 601:

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and green (positive)

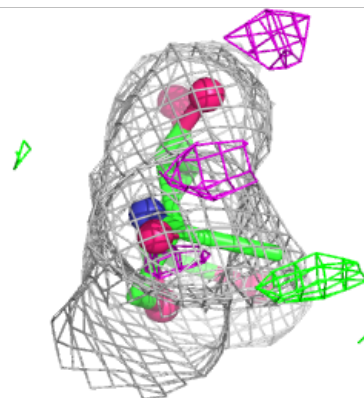
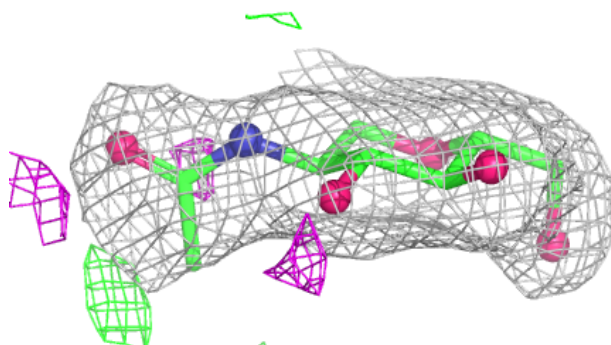
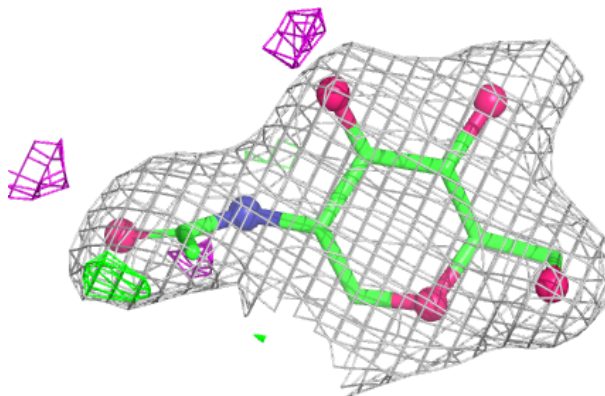


Electron density around NAG C 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

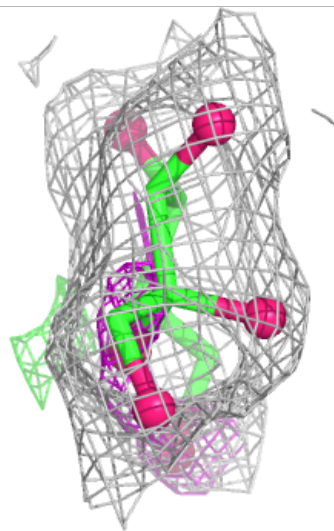
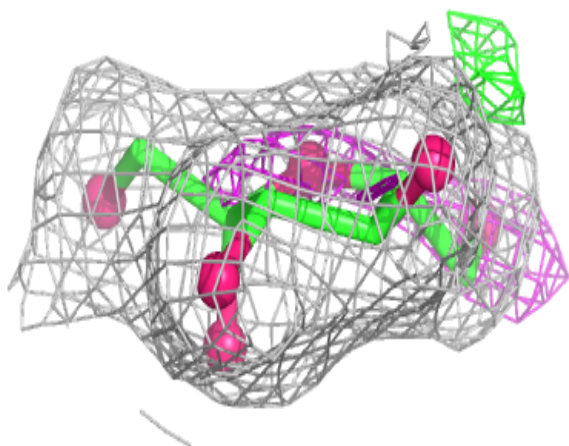
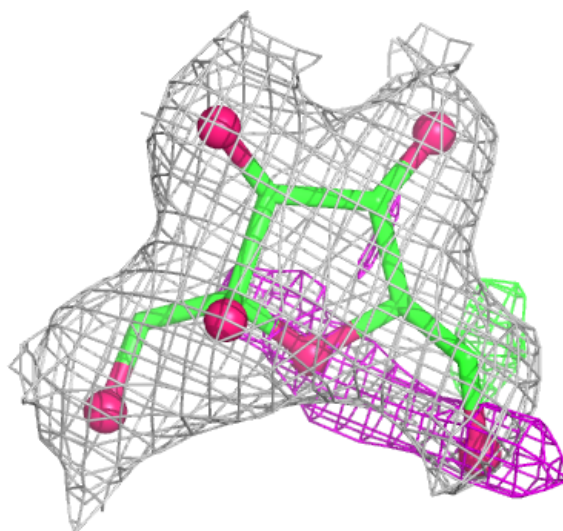
**Electron density around NAG B 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



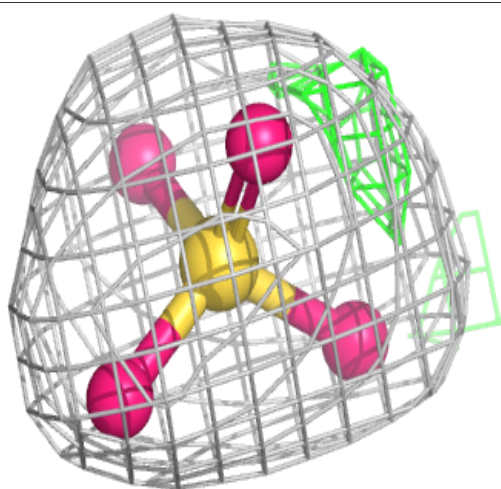
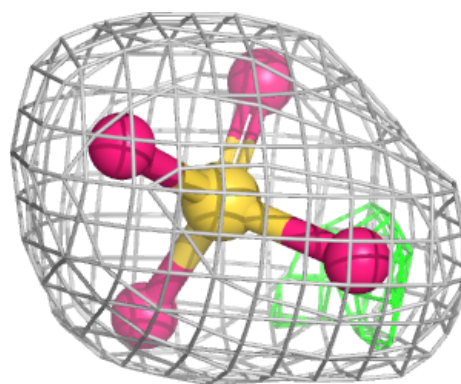
Electron density around FRU A 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



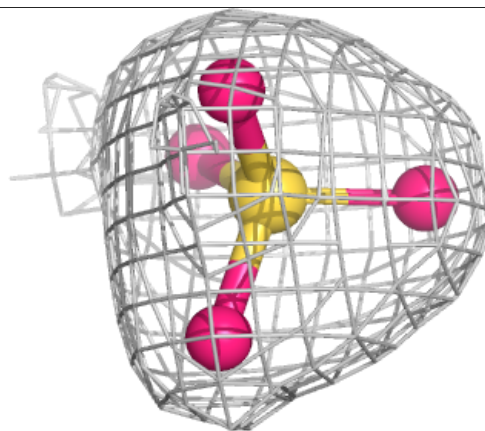
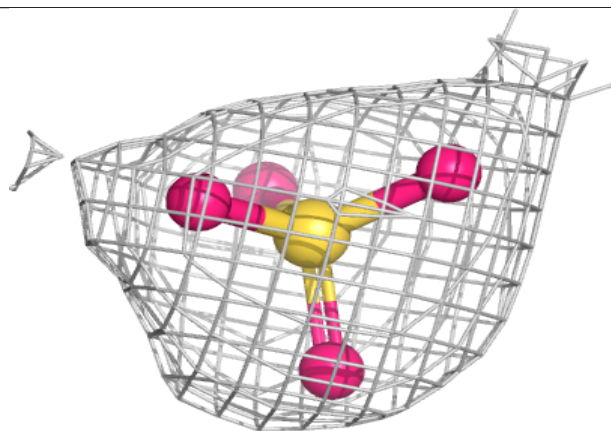
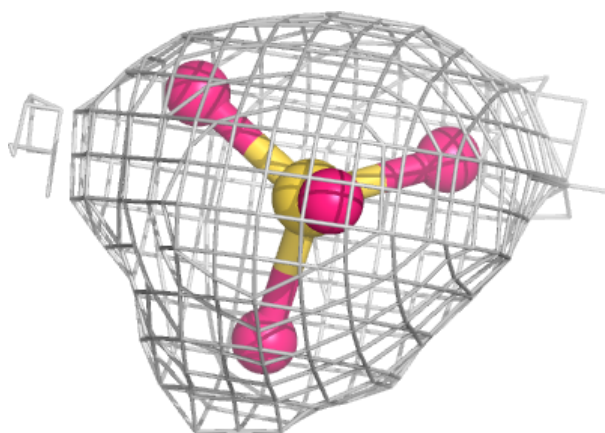
Electron density around SO4 D 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

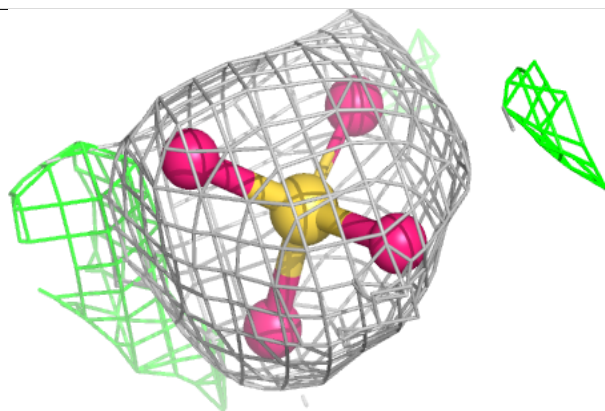
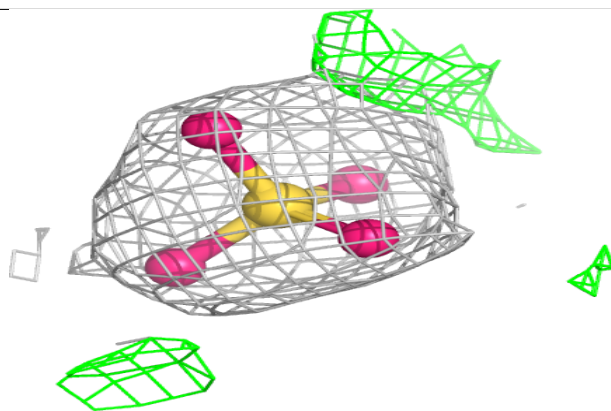
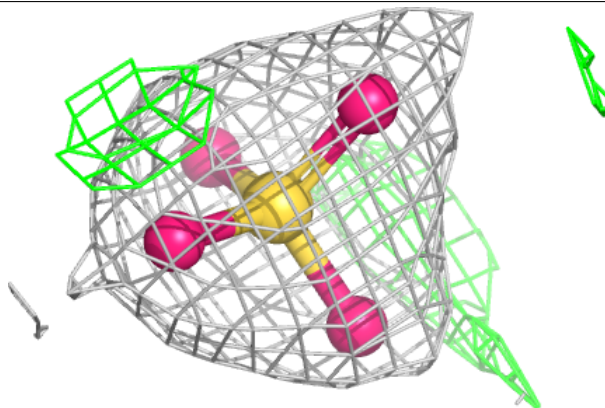


Electron density around SO4 B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SO4 C 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.