



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:59 AM UTC

PDB ID : 7P2Z / pdb_00007p2z
Title : Crystal structure of human lysosomal acid-alpha-glucosidase, GAA, in complex with cyclosulfamidate 4
Authors : Roig-Zamboni, V.; Kok, K.; Overkleeft, H.; Artola, M.; Sulzenbacher, G.
Deposited on : 2021-07-06
Resolution : 1.85 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

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X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
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Percentile relative to all X-ray structures

Percentile relative to X-ray structures of similar resolution

MetricWhole archive
(#Entries)

Similar resolution

 $(\# \text{Entries, resolution range}(\text{\AA}))$ R_{free}

180053

3428 (1.86-1.86)

Clashscore

190562

3579 (1.86-1.86)

Ramachandran outliers

187476

3553 (1.86-1.86)

Sidechain outliers

187428

3553 (1.86-1.86)

RSRZ outliers

180081

3429 (1.86-1.86)

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.

Quality of chain

96%

2%

88%

6%

5%

100

67%

100%

100%

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Mol	Chain	Length	Quality of chain
4	BgB	3	 33% 67%
5	BjB	2	 50% 50%

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
10	YTW	AaA	1002	X	-	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7791 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.

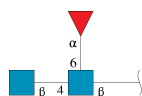
- Molecule 1 is a protein called Lysosomal alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	35	Total	C	N	O	S	0	0	0
			267	161	48	53	5			
1	AaA	816	Total	C	N	O	S	0	10	0
			6481	4168	1083	1201	29			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	199	ARG	HIS	conflict	UNP P10253
AAA	223	HIS	ARG	conflict	UNP P10253
AAA	780	ILE	VAL	conflict	UNP P10253
AaA	199	ARG	HIS	conflict	UNP P10253
AaA	223	HIS	ARG	conflict	UNP P10253
AaA	780	ILE	VAL	conflict	UNP P10253

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



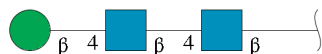
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	BBB	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	BcB	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	BeB	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	BjB	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AaA	1	Total	O	S	0	0
			5	4	1		
6	AaA	1	Total	O	S	0	0
			5	4	1		
6	AaA	1	Total	O	S	0	0
			5	4	1		
6	AaA	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

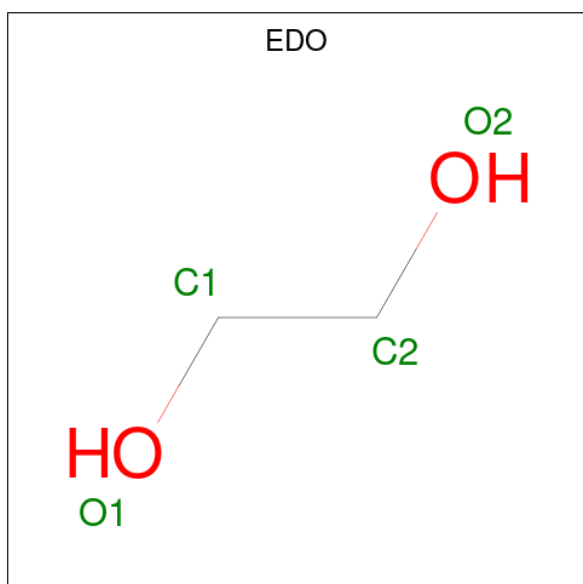
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	2	Total	Cl	0	0
			2	2		
7	AaA	7	Total	Cl	0	0
			7	7		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



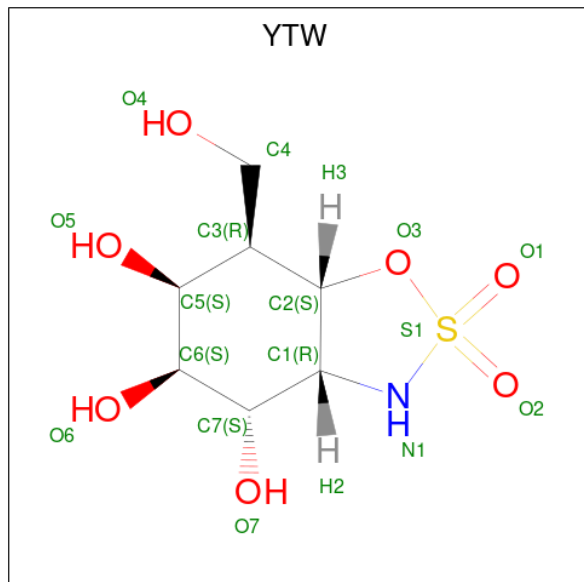
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	C	O	0	0
			6	3	3		
8	AaA	1	Total	C	O	0	0
			6	3	3		
8	AaA	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



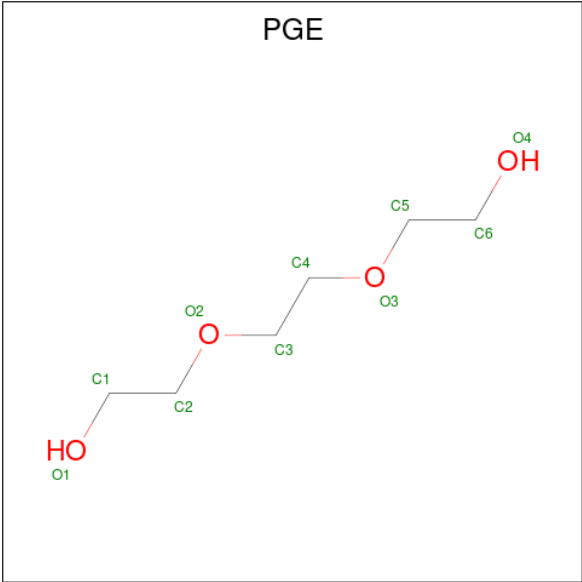
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	1	Total C O 4 2 2	0	0
9	AaA	1	Total C O 4 2 2	0	0
9	AaA	1	Total C O 4 2 2	0	0
9	AaA	1	Total C O 4 2 2	0	0
9	AaA	1	Total C O 4 2 2	0	0

- Molecule 10 is (3 {a} {R},4 {S},5 {S},6 {S},7 {R},7 {a} {S})-7-(hydroxymethyl)-2,2-bis(oxidanylidene)-3 {a},4,5,6,7,7 {a}-hexahydro-3 {H}-benzo[d][1,2,3]oxathiazole-4,5,6-triol (CCD ID: YTW) (formula: C₇H₁₃NO₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AaA	1	Total C N O S 16 7 1 7 1	0	0

- Molecule 11 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄) (labeled as "Ligand of Interest" by depositor).

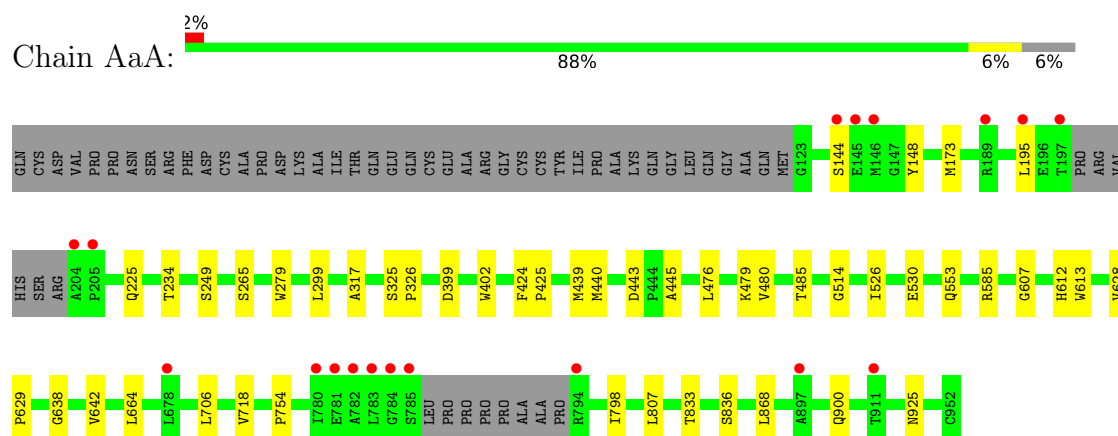


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	AaA	1	Total	C	O	0	0
			10	6	4		
11	AaA	1	Total	C	O	0	0
			10	6	4		

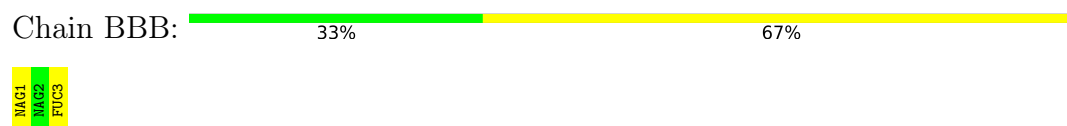
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	AAA	29	Total	O	0	0
			29	29		
12	AaA	749	Total	O	0	0
			749	749		

- Molecule 1: Lysosomal alpha-glucosidase



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



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.16Å 102.54Å 129.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 1.85 47.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.00-1.85) 100.0 (47.00-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.148 , 0.175 0.162 , 0.189	Depositor DCC
R_{free} test set	5503 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.5	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	0.97	EDS
Total number of atoms	7791	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: FUC, EDO, YTW, CL, BMA, PGE, SO4, GOL, NAG, CSO

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	AAA	0.95	0/272	1.22	0/368
1	AaA	0.96	0/6688	1.10	0/9140
All	All	0.96	0/6960	1.11	0/9508

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	267	0	245	0	0
1	AaA	6481	0	6284	30	0
2	BBB	38	0	34	0	0
3	BcB	28	0	25	0	0
3	BeB	28	0	25	0	0
4	BgB	39	0	34	0	0
5	BjB	24	0	22	0	0
6	AAA	5	0	0	0	0
6	AaA	20	0	0	0	0
7	AAA	2	0	0	0	0
7	AaA	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AAA	6	0	8	0	0
8	AaA	12	0	16	0	0
9	AAA	4	0	6	0	0
9	AaA	16	0	24	2	0
10	AaA	16	0	0	0	0
11	AaA	20	0	28	2	0
12	AAA	29	0	0	0	0
12	AaA	749	0	0	4	0
All	All	7791	0	6751	32	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 (32) 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:AaA:148:TYR:CE2	1:AaA:173[B]:MET:CE	2.87	0.57
1:AaA:148:TYR:HE2	1:AaA:173[B]:MET:CE	2.22	0.53
1:AaA:234:THR:HA	1:AaA:249:SER:O	2.10	0.51
1:AaA:628:VAL:HB	1:AaA:629:PRO:HD3	1.92	0.50
1:AaA:526:ILE:C	1:AaA:526:ILE:HD12	2.39	0.48
1:AaA:445:ALA:HB1	1:AaA:485:THR:HB	1.96	0.47
1:AaA:585:ARG:NH2	12:AaA:1122:HOH:O	2.49	0.45
1:AaA:299:LEU:HD23	1:AaA:299:LEU:C	2.41	0.45
1:AaA:925:ASN:HA	12:AaA:1593:HOH:O	2.16	0.45
1:AaA:195:LEU:HD13	11:AaA:1019:PGE:O4	2.17	0.45
1:AaA:607:GLY:HA3	1:AaA:638:GLY:O	2.17	0.44
1:AaA:424:PHE:HB3	1:AaA:425:PRO:HD3	2.00	0.44
1:AaA:325:SER:N	1:AaA:326:PRO:HA	2.33	0.44
1:AaA:718:VAL:HG12	1:AaA:868:LEU:CD1	2.48	0.43
1:AaA:798:ILE:HD11	1:AaA:807:LEU:HD21	2.01	0.43
1:AaA:612:HIS:O	1:AaA:642:VAL:HA	2.18	0.43
1:AaA:148:TYR:CE2	1:AaA:173[B]:MET:HE1	2.54	0.42
1:AaA:476:LEU:C	1:AaA:476:LEU:HD23	2.43	0.42
1:AaA:664:LEU:HD13	1:AaA:754:PRO:HG3	2.00	0.42
11:AaA:1020:PGE:H52	11:AaA:1020:PGE:H32	1.87	0.42
1:AaA:479:LYS:HE2	1:AaA:530:GLU:OE2	2.19	0.42
9:AaA:1017:EDO:H11	12:AaA:1366:HOH:O	2.19	0.42
1:AaA:148:TYR:CE2	1:AaA:173[B]:MET:HE3	2.55	0.41
1:AaA:439[B]:MET:SD	1:AaA:514:GLY:HA3	2.60	0.41
1:AaA:443:ASP:HB3	12:AaA:1653:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AaA:706:LEU:HD23	1:AaA:706:LEU:HA	1.89	0.41
1:AaA:900:GLN:HE22	9:AaA:1018:EDO:H12	1.85	0.41
1:AaA:833:THR:HA	1:AaA:836:SER:OG	2.21	0.41
1:AaA:279:TRP:CE3	1:AaA:317:ALA:HB2	2.57	0.40
1:AaA:798:ILE:HD11	1:AaA:807:LEU:CD2	2.52	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	AAA	33/872 (4%)	33 (100%)	0	0	100	100
1	AaA	819/872 (94%)	795 (97%)	23 (3%)	1 (0%)	48	35
All	All	852/1744 (49%)	828 (97%)	23 (3%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AaA	480	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	30/741 (4%)	30 (100%)	0	100	100
1	AaA	705/741 (95%)	698 (99%)	7 (1%)	68	60
All	All	735/1482 (50%)	728 (99%)	7 (1%)	73	60

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

Mol	Chain	Res	Type
1	AaA	144[A]	SER
1	AaA	144[B]	SER
1	AaA	225	GLN
1	AaA	265	SER
1	AaA	399	ASP
1	AaA	440	MET
1	AaA	613	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSO	AaA	938	1	3,6,7	0.66	0	1,6,8	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
1	CSO	AaA	938	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

12 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	BBB	1	1,2	14,14,15	0.69	0	17,19,21	1.10	1 (5%)
2	NAG	BBB	2	2	14,14,15	0.57	0	17,19,21	0.75	0
2	FUC	BBB	3	2	10,10,11	0.57	0	14,14,16	1.05	1 (7%)
3	NAG	BcB	1	1,3	14,14,15	0.61	0	17,19,21	1.07	1 (5%)
3	NAG	BcB	2	3	14,14,15	0.46	0	17,19,21	1.58	2 (11%)
3	NAG	BeB	1	1,3	14,14,15	0.58	0	17,19,21	1.43	2 (11%)
3	NAG	BeB	2	3	14,14,15	0.44	0	17,19,21	1.61	3 (17%)
4	NAG	BgB	1	1,4	14,14,15	0.65	0	17,19,21	1.22	1 (5%)
4	NAG	BgB	2	4	14,14,15	0.56	0	17,19,21	0.88	0
4	BMA	BgB	3	4	11,11,12	0.49	0	15,15,17	1.13	1 (6%)
5	NAG	BjB	1	1,5	14,14,15	0.74	0	17,19,21	1.02	0
5	FUC	BjB	2	5	10,10,11	0.50	0	14,14,16	1.38	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	BBB	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	BBB	2	2	-	2/6/23/26	0/1/1/1
2	FUC	BBB	3	2	-	-	0/1/1/1
3	NAG	BcB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BcB	2	3	-	0/6/23/26	0/1/1/1
3	NAG	BeB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BeB	2	3	-	0/6/23/26	0/1/1/1
4	NAG	BgB	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	BgB	2	4	-	0/6/23/26	0/1/1/1
4	BMA	BgB	3	4	-	2/2/19/22	0/1/1/1
5	NAG	BjB	1	1,5	-	0/6/23/26	0/1/1/1
5	FUC	BjB	2	5	-	-	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BeB	2	NAG	C1-O5-C5	4.22	117.84	112.19
3	BeB	1	NAG	O5-C1-C2	-3.80	105.41	111.29
2	BBB	1	NAG	O5-C1-C2	-3.61	105.70	111.29
3	BcB	2	NAG	C1-C2-N2	-3.49	104.93	110.43
3	BeB	2	NAG	C1-C2-N2	-3.28	105.26	110.43
4	BgB	1	NAG	O5-C1-C2	-3.10	106.49	111.29
5	BjB	2	FUC	O5-C5-C4	3.10	115.13	109.55
3	BeB	2	NAG	O5-C1-C2	3.07	116.05	111.29
3	BeB	1	NAG	C1-O5-C5	-2.88	108.33	112.19
3	BcB	2	NAG	C3-C4-C5	-2.83	105.09	110.23
4	BgB	3	BMA	O5-C5-C6	2.82	113.15	107.66
2	BBB	3	FUC	C1-O5-C5	2.38	118.58	112.97
5	BjB	2	FUC	C1-O5-C5	2.24	118.24	112.97
3	BcB	1	NAG	C2-N2-C7	-2.10	120.09	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BgB	3	BMA	O5-C5-C6-O6

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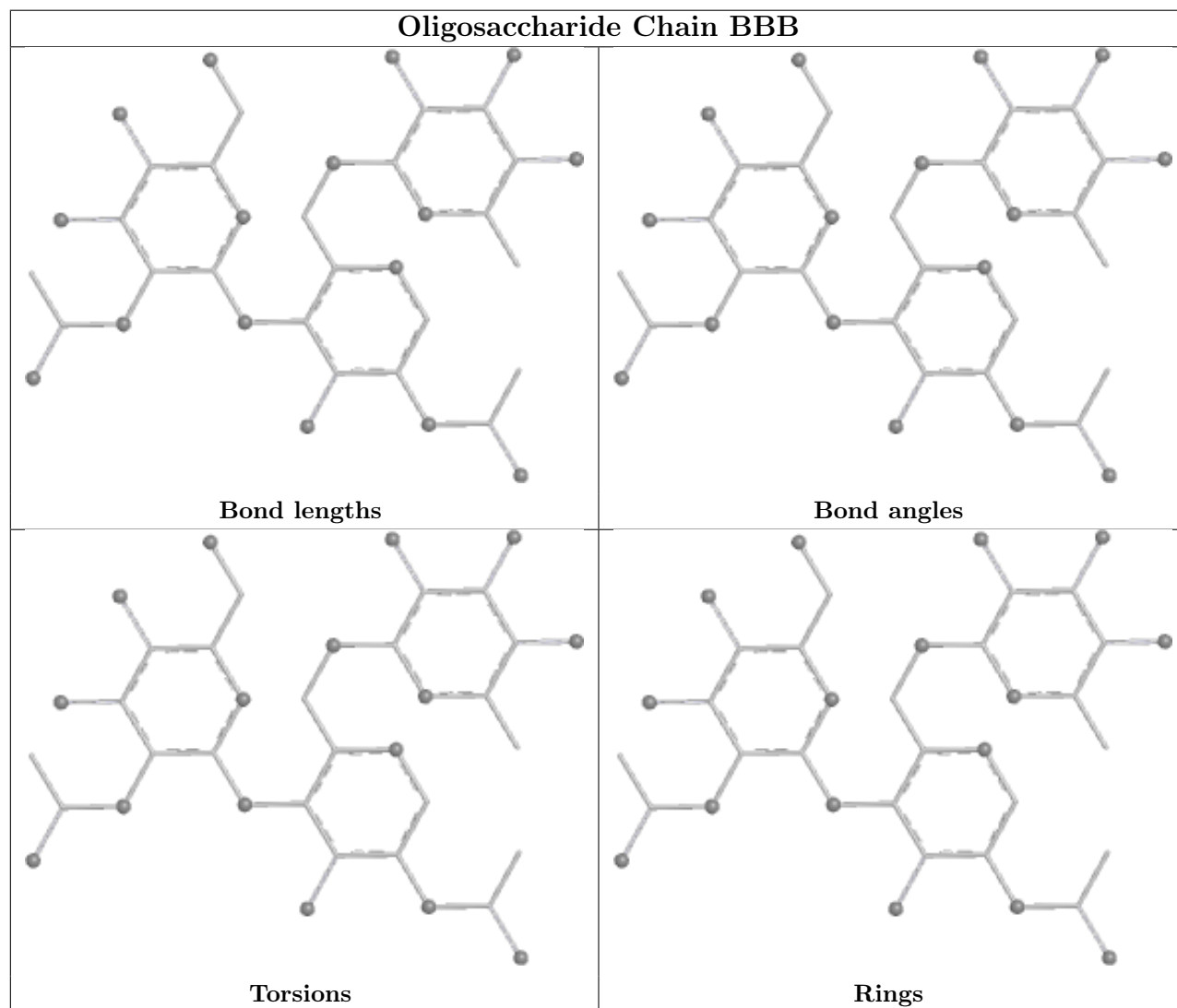
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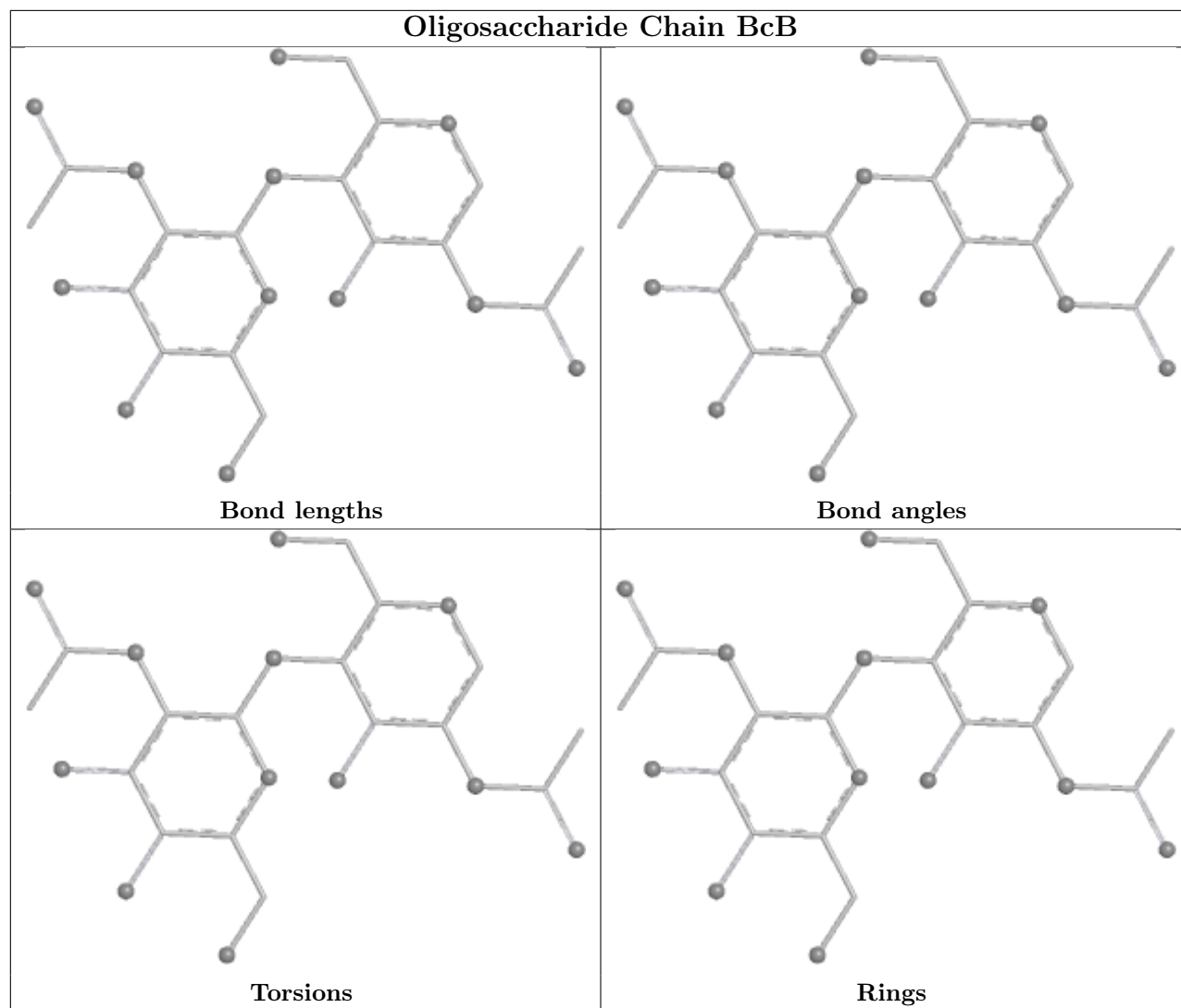
Mol	Chain	Res	Type	Atoms
4	BgB	3	BMA	C4-C5-C6-O6
2	BBB	2	NAG	C4-C5-C6-O6
2	BBB	2	NAG	O5-C5-C6-O6

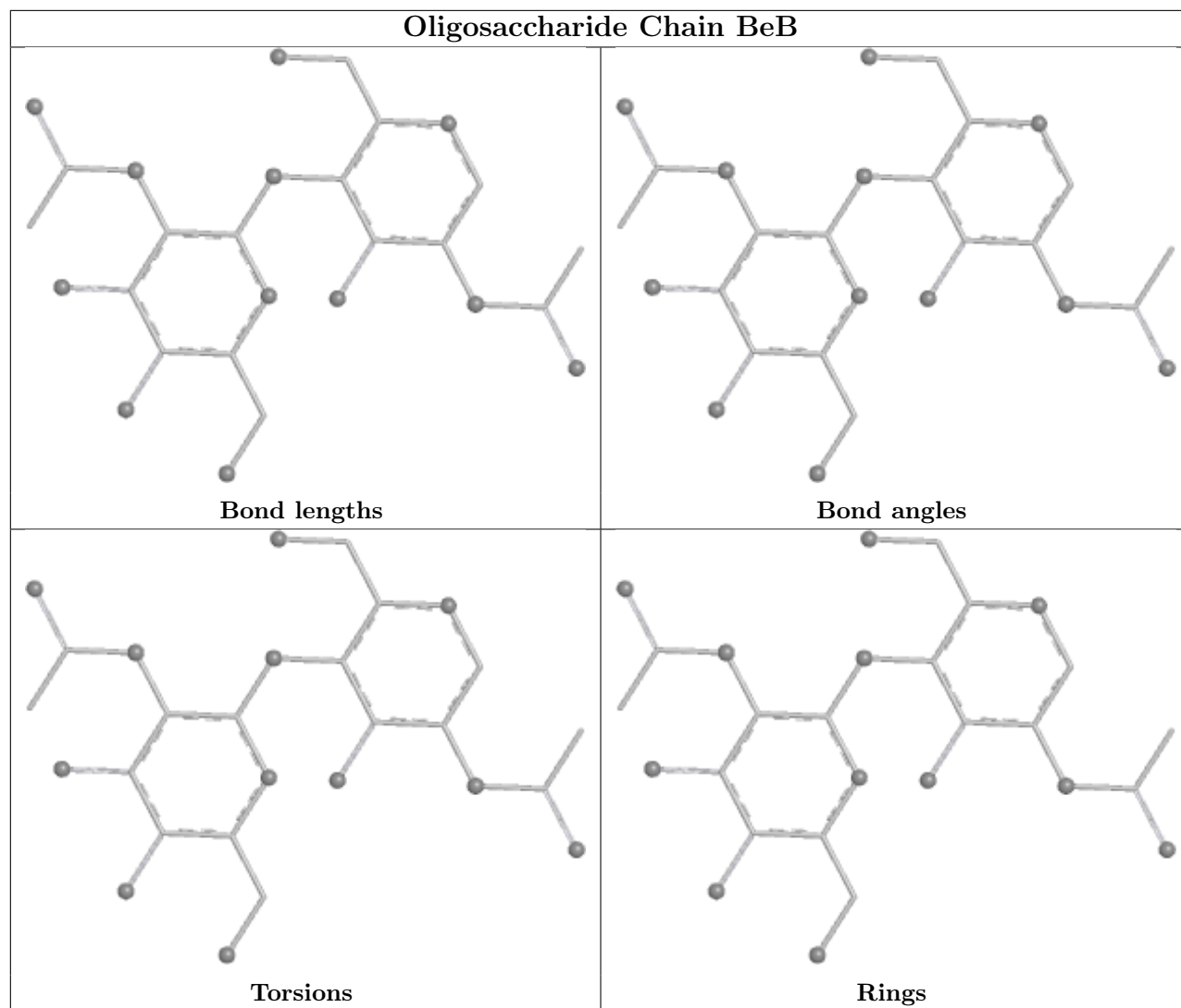
There are no ring outliers.

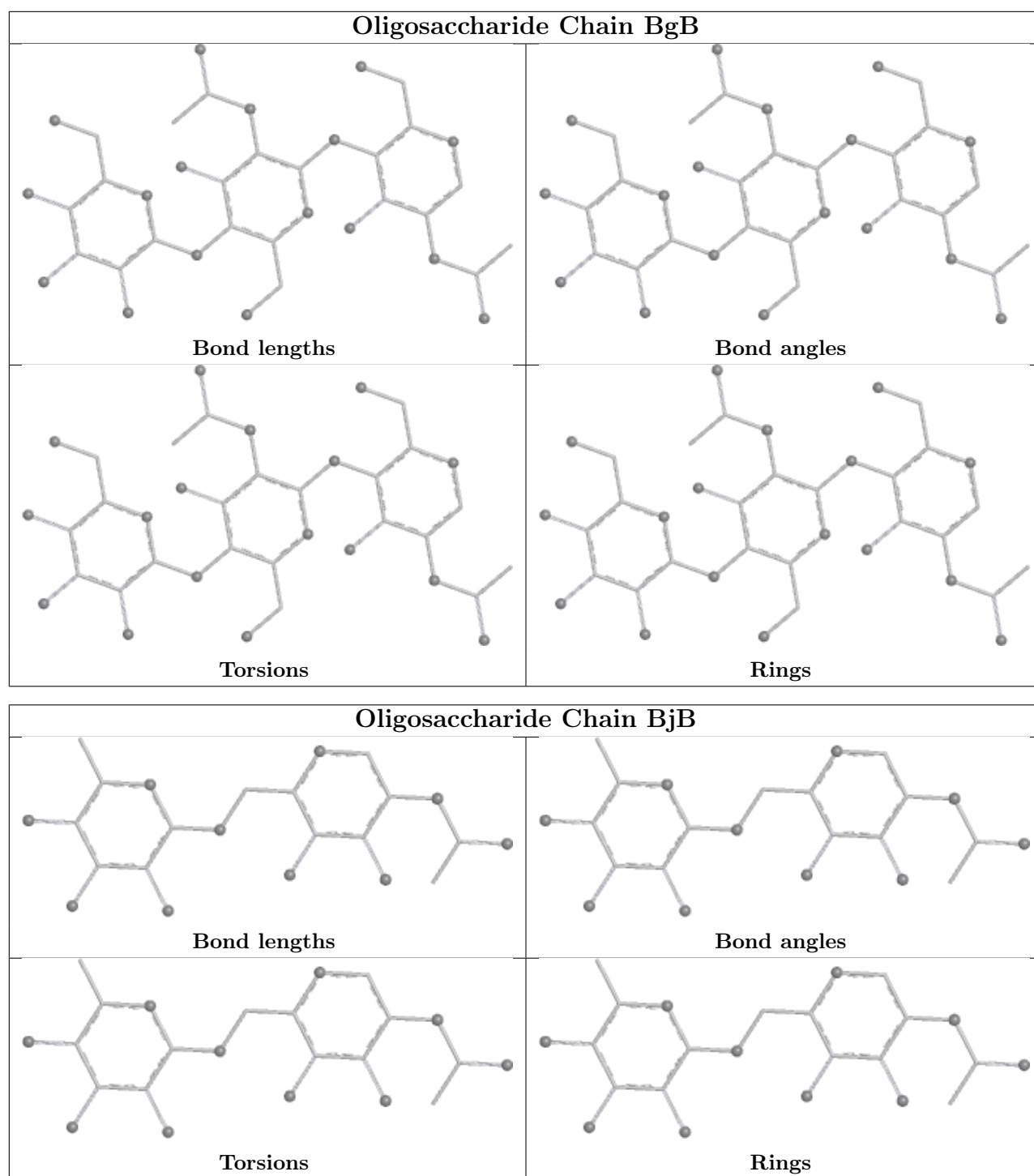
No monomer is involved in short contacts.

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](#)

Of 25 ligands modelled in this entry, 9 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	AAA	1001	-	4,4,4	0.36	0	6,6,6	0.09	0
11	PGE	AaA	1020	-	9,9,9	0.44	0	8,8,8	0.29	0
8	GOL	AaA	1015	-	5,5,5	0.20	0	5,5,5	0.34	0
6	SO4	AaA	1003	-	4,4,4	0.28	0	6,6,6	0.19	0
9	EDO	AAA	1005	-	3,3,3	0.22	0	2,2,2	0.20	0
9	EDO	AaA	1017	-	3,3,3	0.10	0	2,2,2	0.09	0
8	GOL	AAA	1004	-	5,5,5	0.23	0	5,5,5	0.59	0
6	SO4	AaA	1004	-	4,4,4	0.25	0	6,6,6	0.09	0
8	GOL	AaA	1014	-	5,5,5	0.09	0	5,5,5	0.16	0
6	SO4	AaA	1005	-	4,4,4	0.40	0	6,6,6	0.23	0
9	EDO	AaA	1016	-	3,3,3	0.18	0	2,2,2	0.33	0
10	YTW	AaA	1002	-	14,17,17	1.03	2 (14%)	17,27,27	1.45	2 (11%)
11	PGE	AaA	1019	-	9,9,9	0.25	0	8,8,8	0.10	0
9	EDO	AaA	1001	-	3,3,3	0.19	0	2,2,2	0.51	0
6	SO4	AaA	1006	-	4,4,4	0.28	0	6,6,6	0.31	0
9	EDO	AaA	1018	-	3,3,3	0.15	0	2,2,2	0.29	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
11	PGE	AaA	1020	-	-	4/7/7/7	-
8	GOL	AaA	1015	-	-	2/4/4/4	-
9	EDO	AAA	1005	-	-	0/1/1/1	-
9	EDO	AaA	1017	-	-	0/1/1/1	-
8	GOL	AAA	1004	-	-	2/4/4/4	-
8	GOL	AaA	1014	-	-	0/4/4/4	-
9	EDO	AaA	1016	-	-	0/1/1/1	-
10	YTW	AaA	1002	-	1/1/7/8	0/2/36/36	0/2/2/2
11	PGE	AaA	1019	-	-	1/7/7/7	-
9	EDO	AaA	1001	-	-	0/1/1/1	-
9	EDO	AaA	1018	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AaA	1002	YTW	O2-S1	2.31	1.44	1.42
10	AaA	1002	YTW	O1-S1	2.27	1.44	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AaA	1002	YTW	C2-C1-N1	3.02	104.35	100.15
10	AaA	1002	YTW	C7-C6-C5	-2.50	106.45	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	AaA	1002	YTW	C5

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AAA	1004	GOL	O1-C1-C2-C3
8	AAA	1004	GOL	O1-C1-C2-O2
11	AaA	1020	PGE	O2-C3-C4-O3
11	AaA	1020	PGE	O3-C5-C6-O4
8	AaA	1015	GOL	O2-C2-C3-O3
8	AaA	1015	GOL	O1-C1-C2-C3
11	AaA	1020	PGE	C3-C4-O3-C5
11	AaA	1019	PGE	O2-C3-C4-O3
11	AaA	1020	PGE	O1-C1-C2-O2

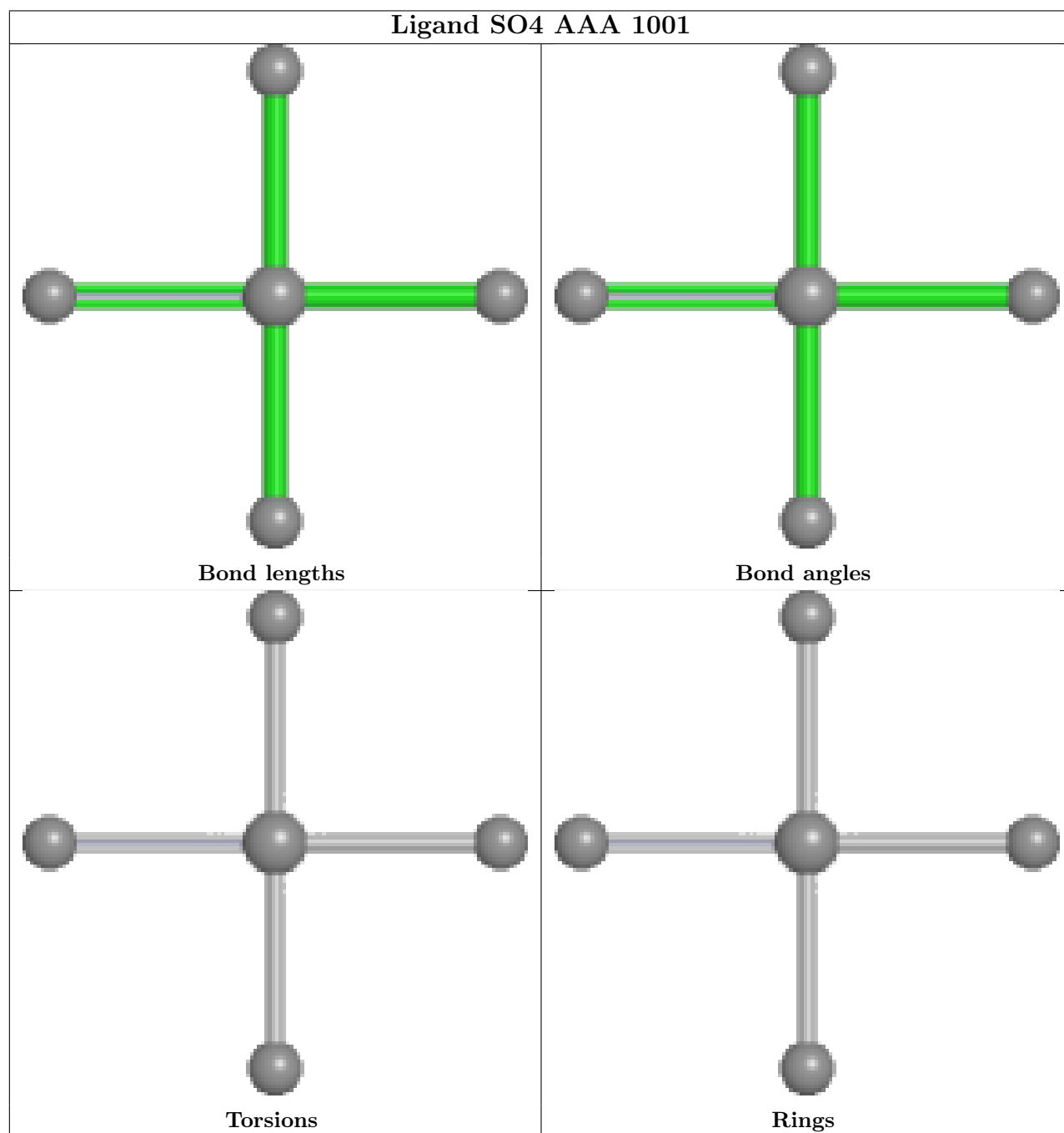
There are no ring outliers.

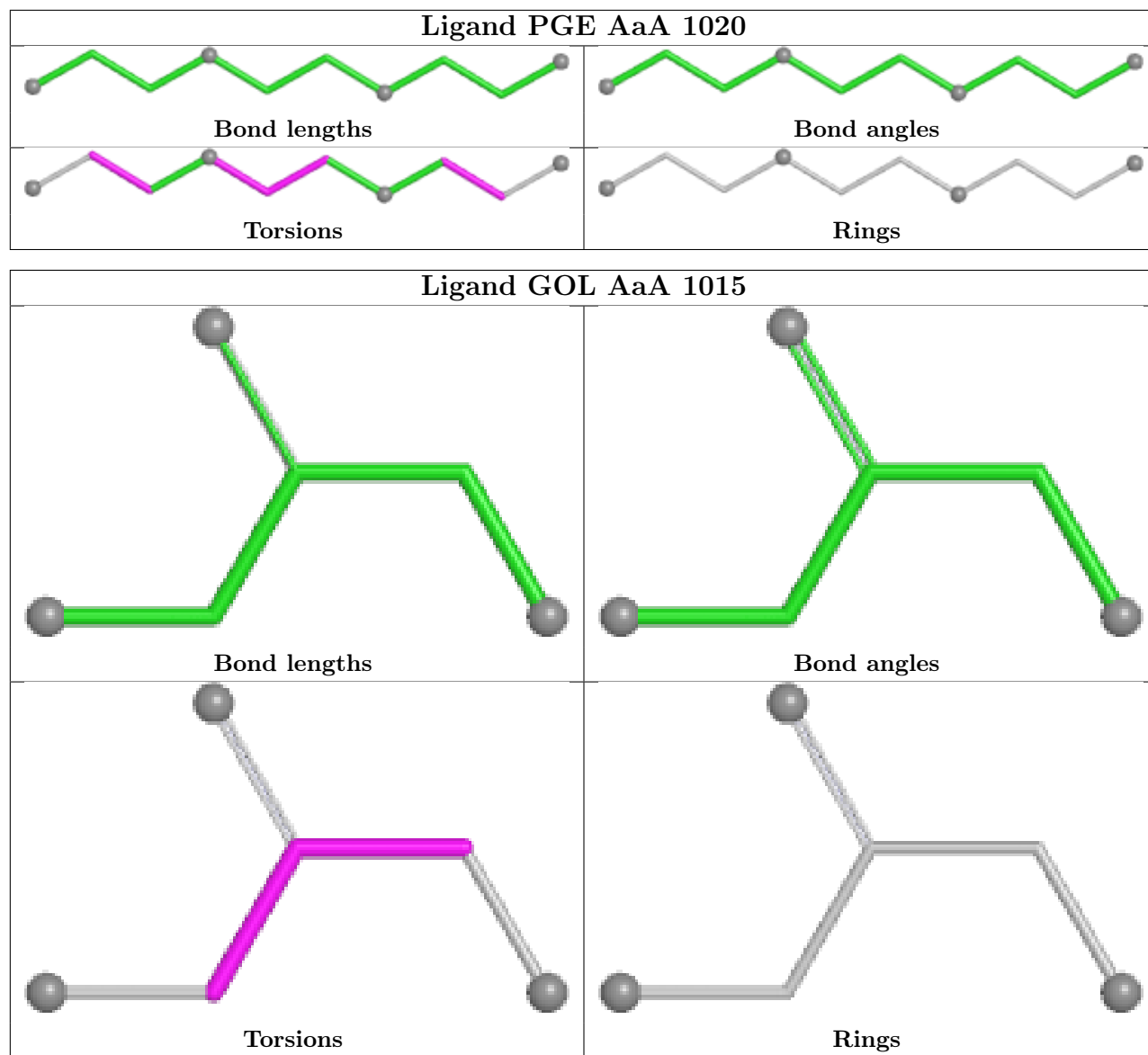
4 monomers are involved in 4 short contacts:

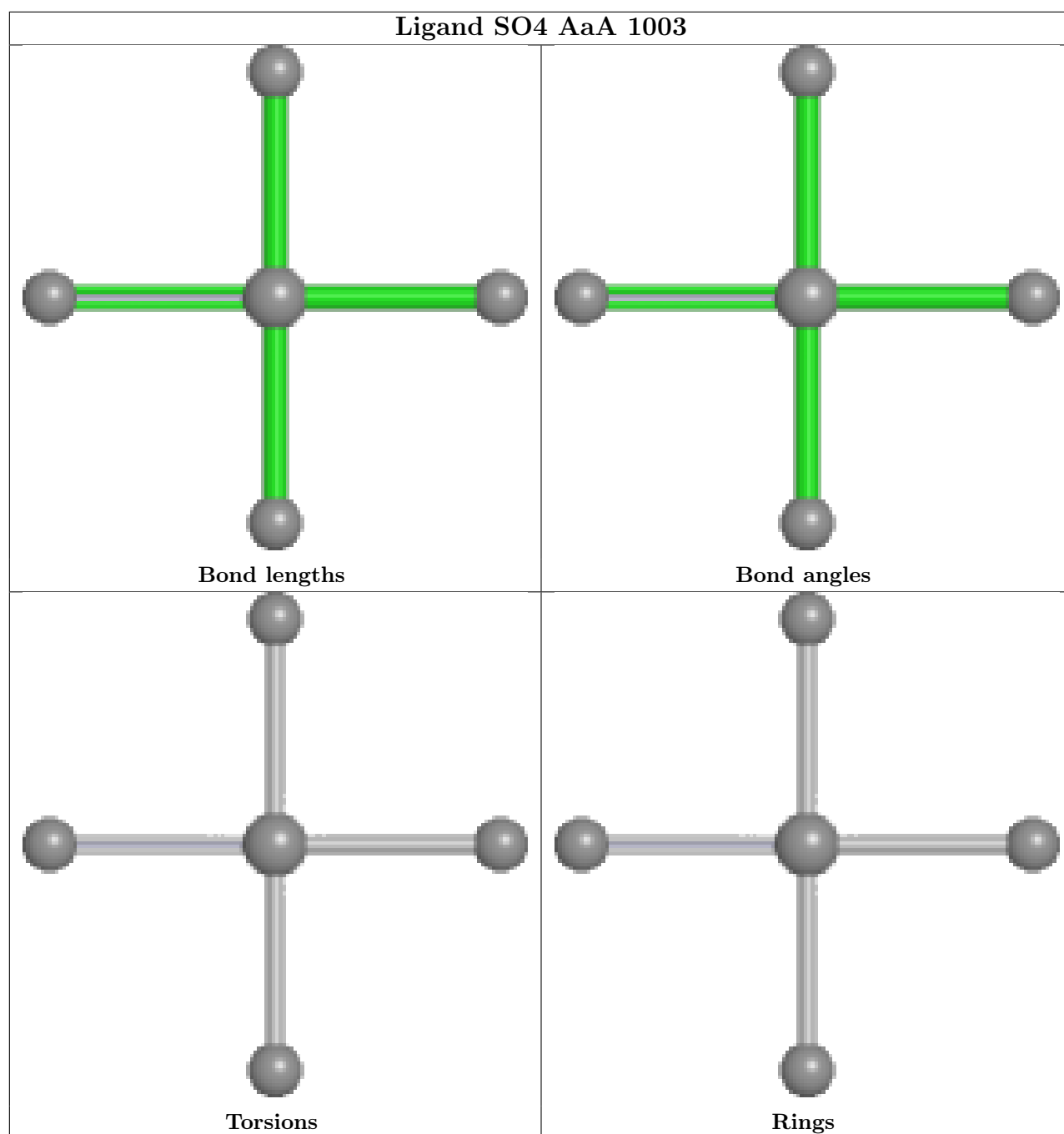
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AaA	1020	PGE	1	0
9	AaA	1017	EDO	1	0
11	AaA	1019	PGE	1	0
9	AaA	1018	EDO	1	0

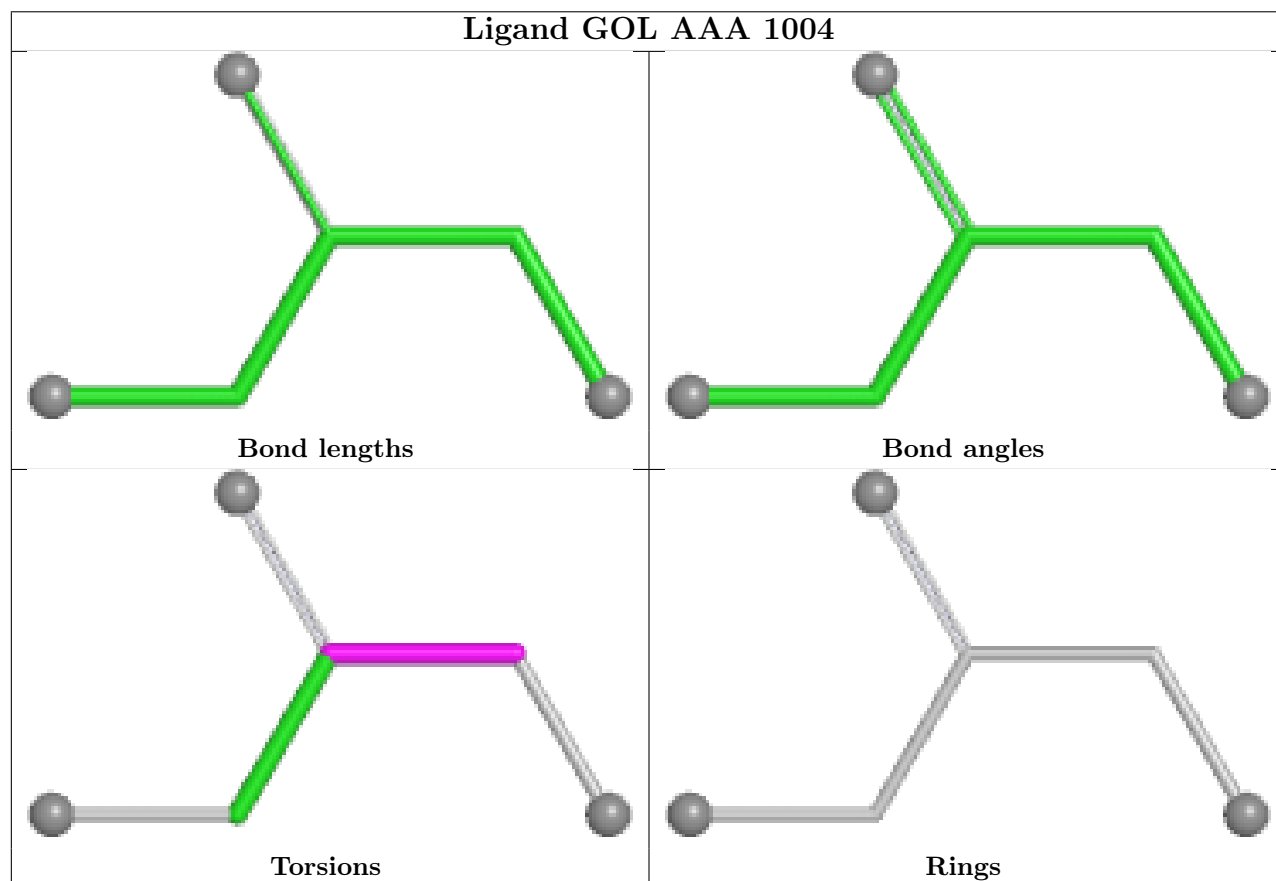
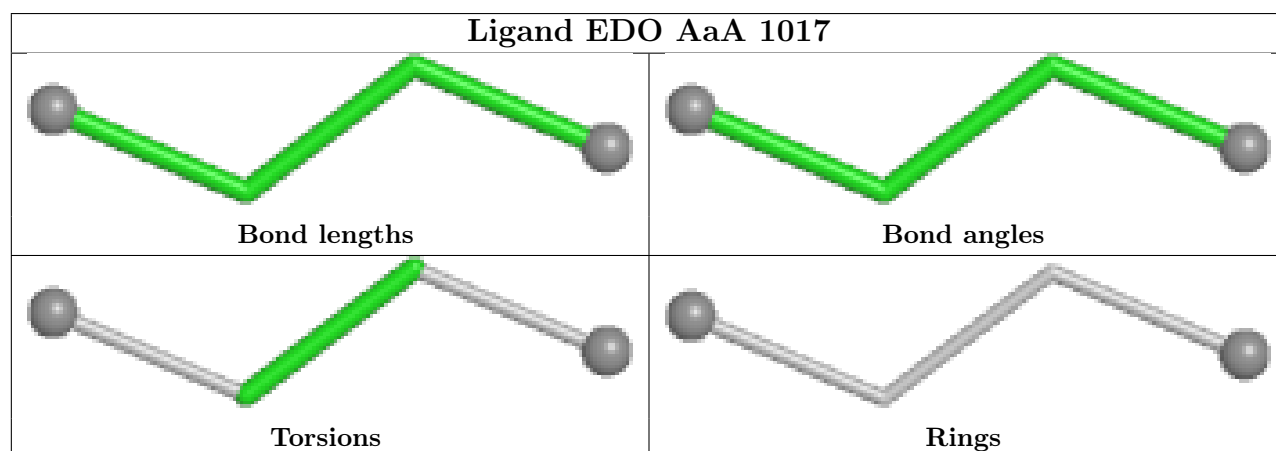
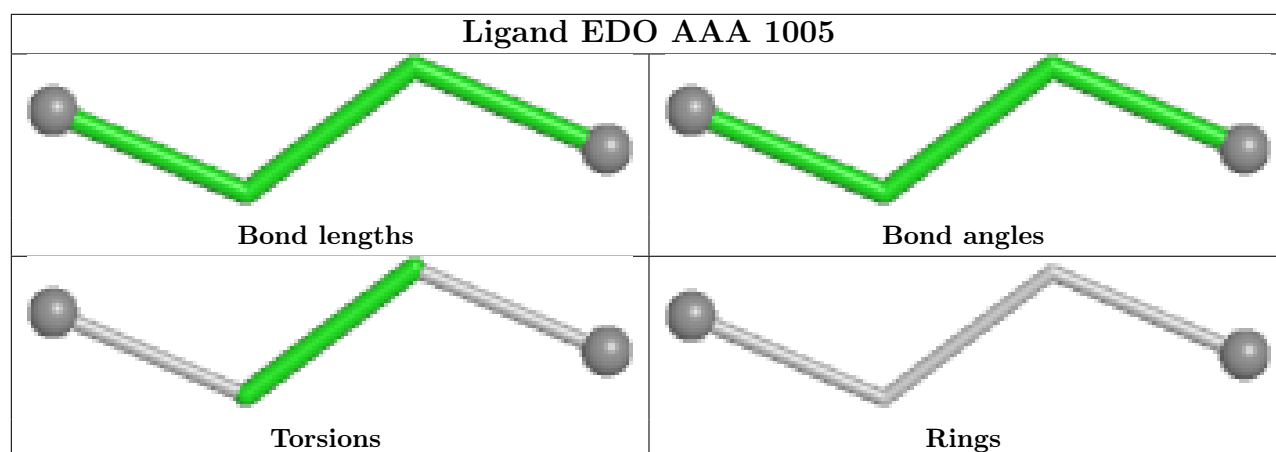
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

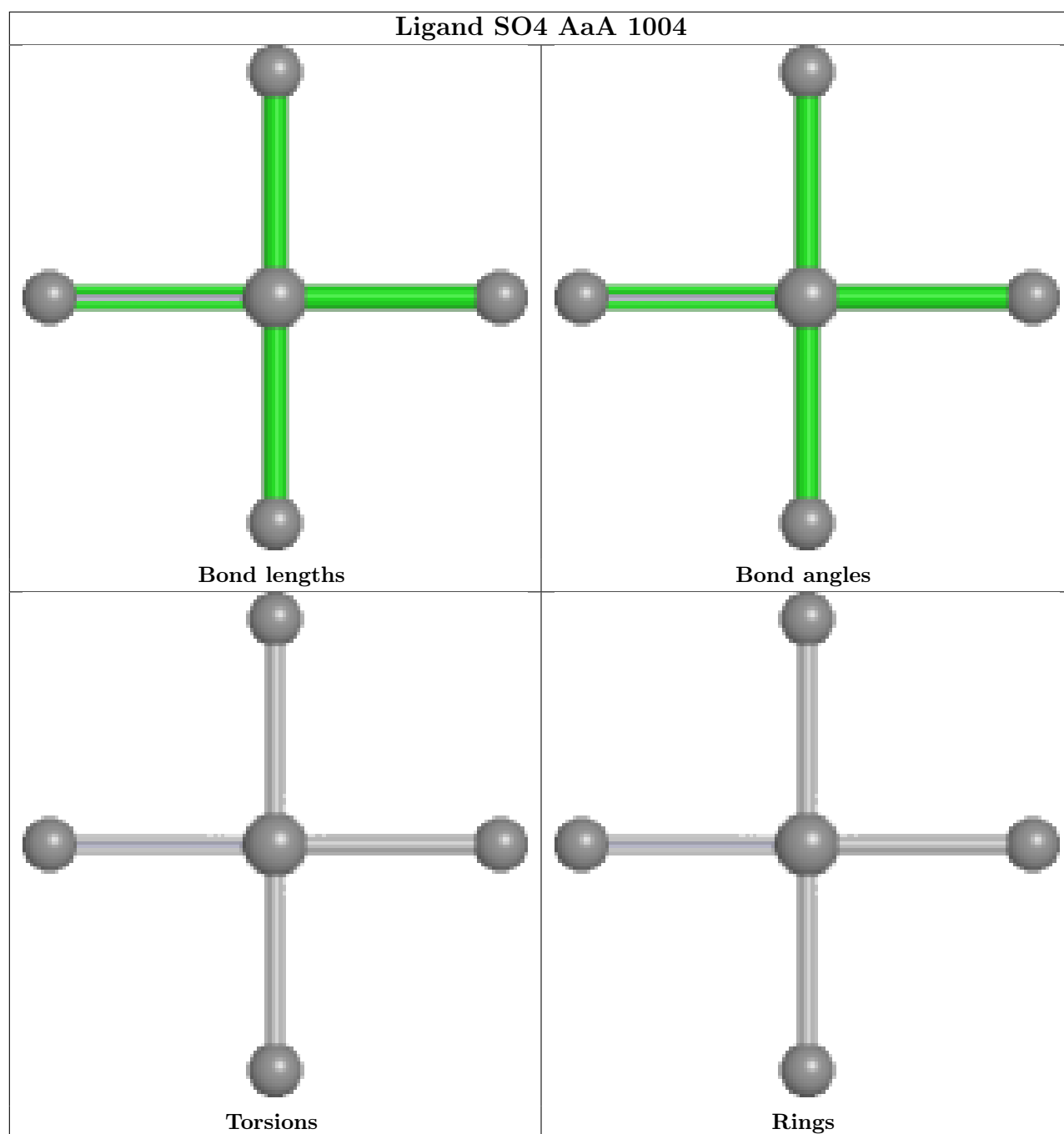
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

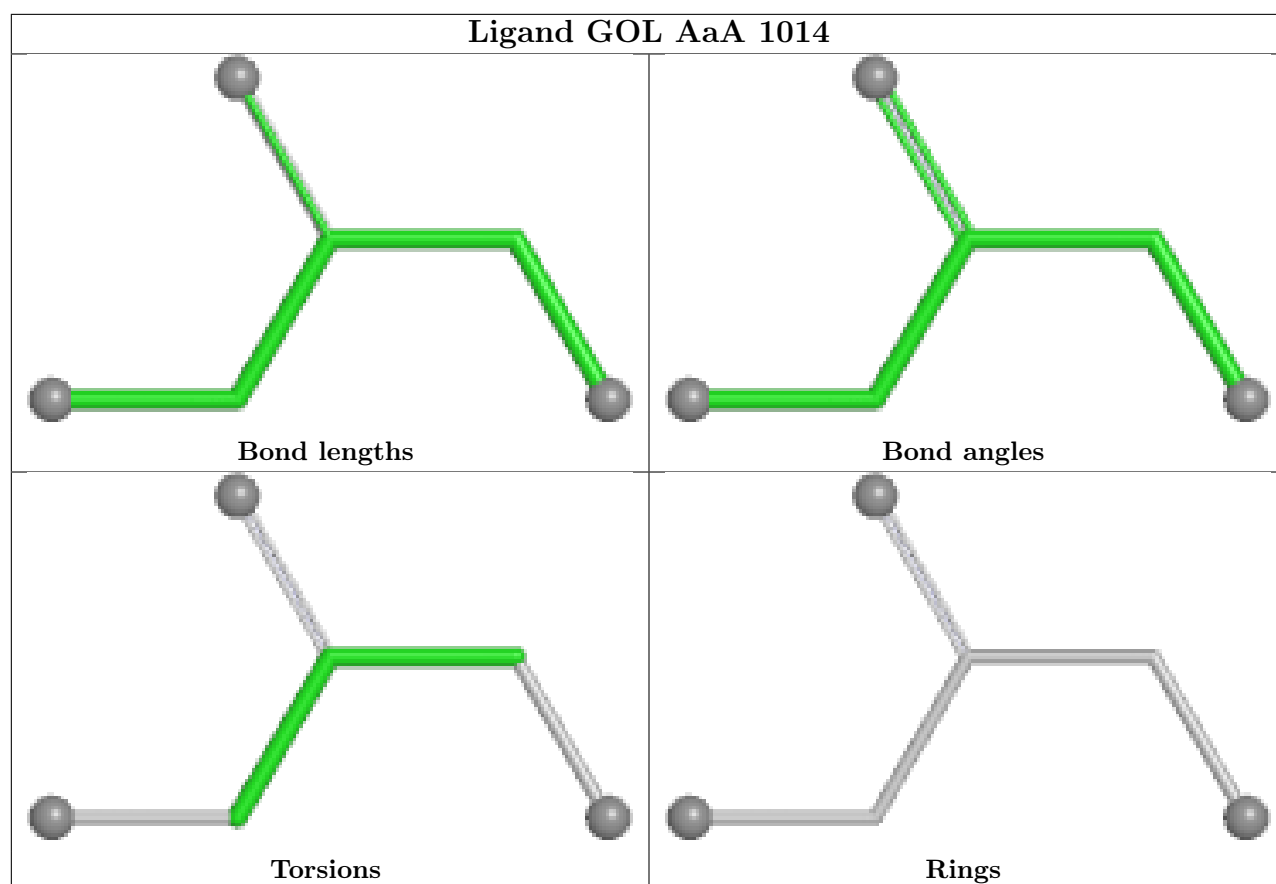


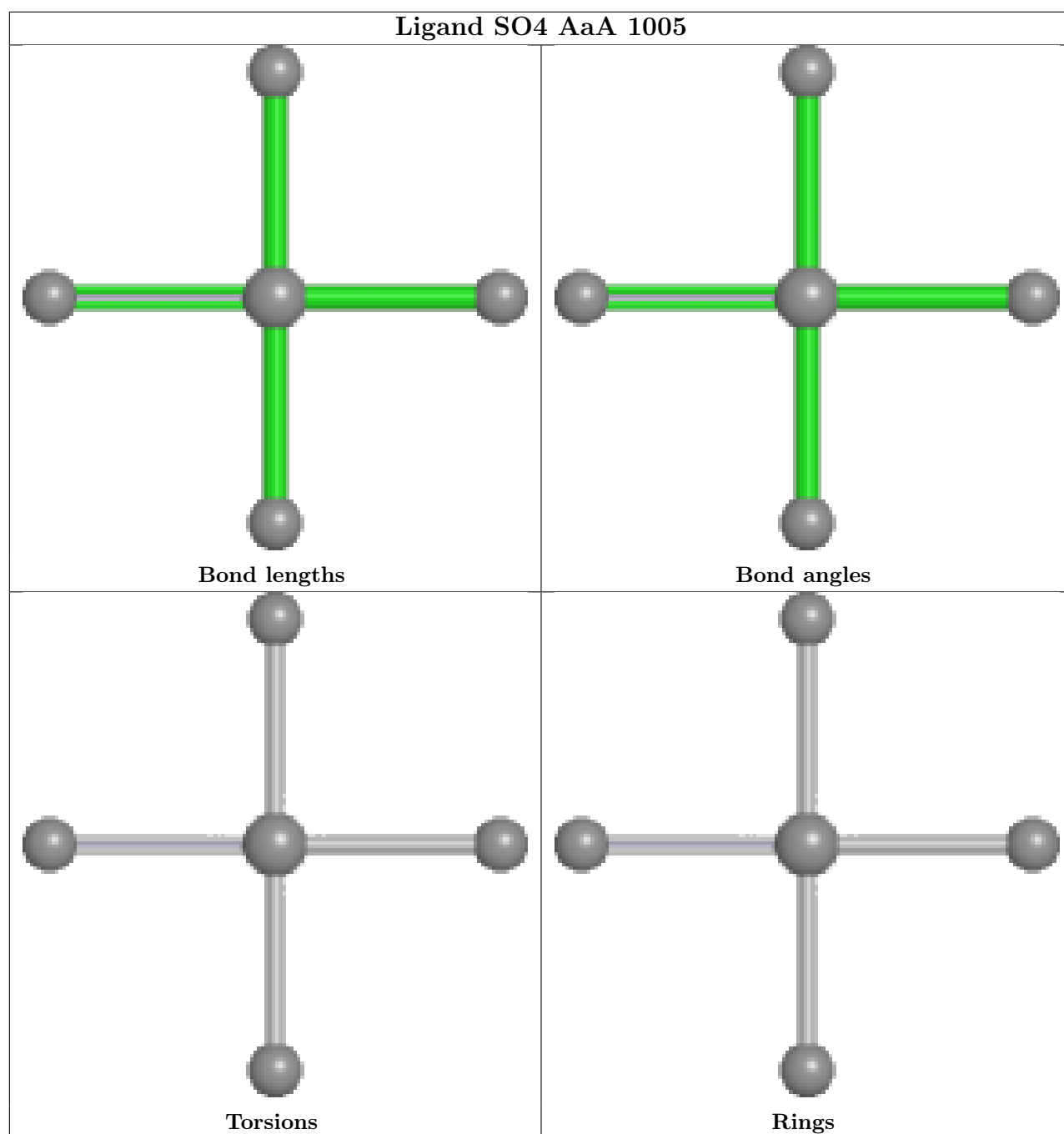




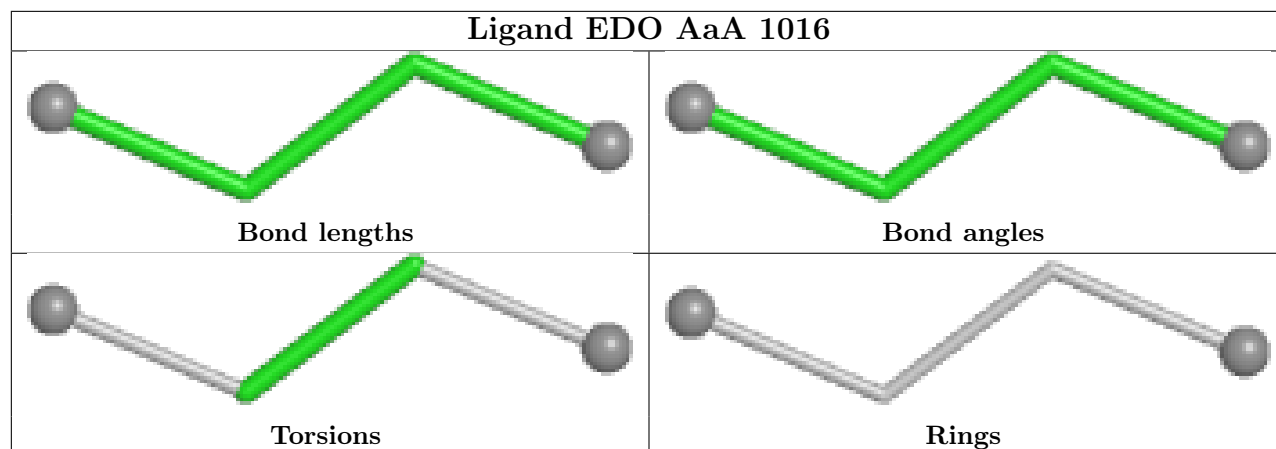




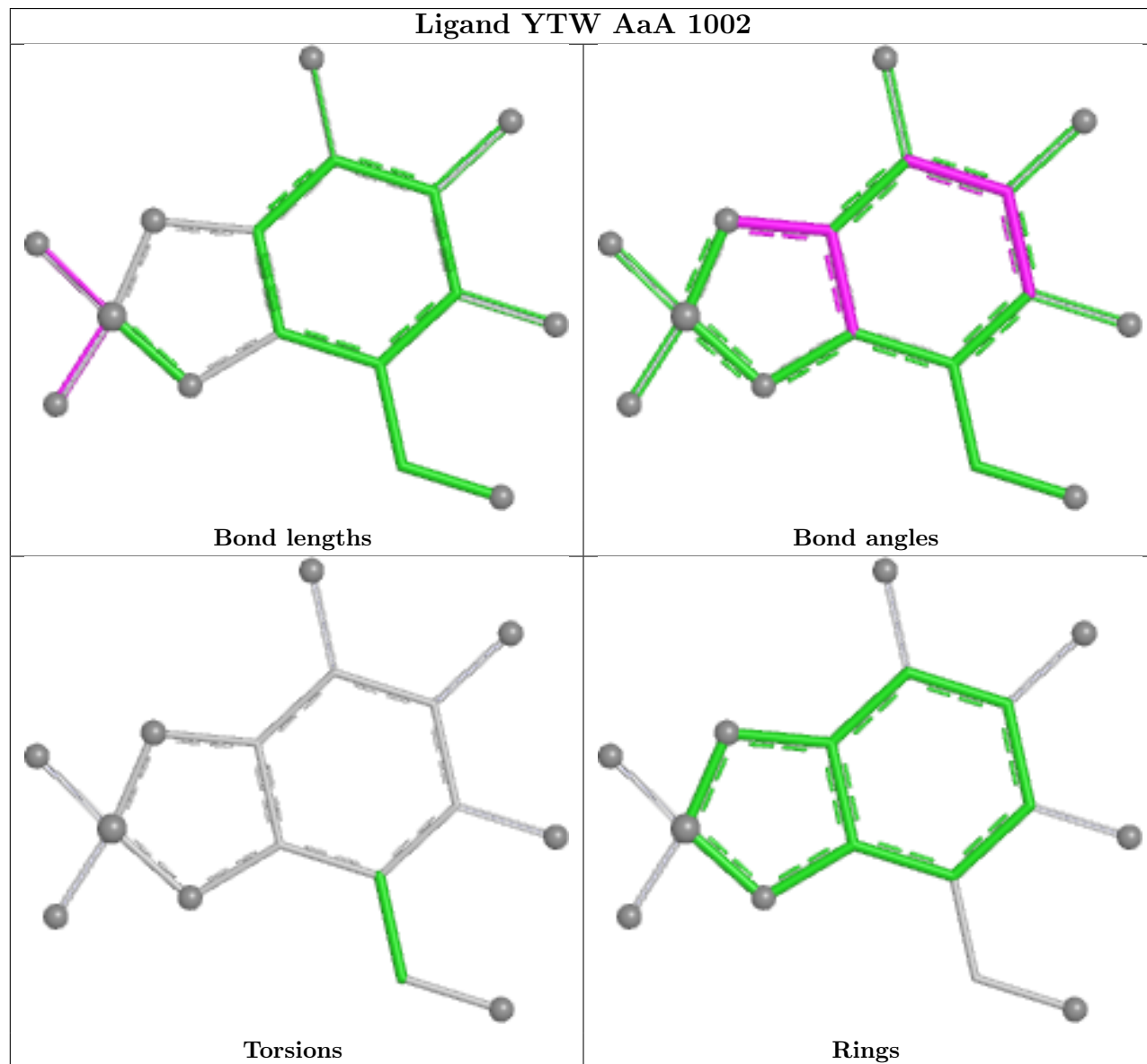


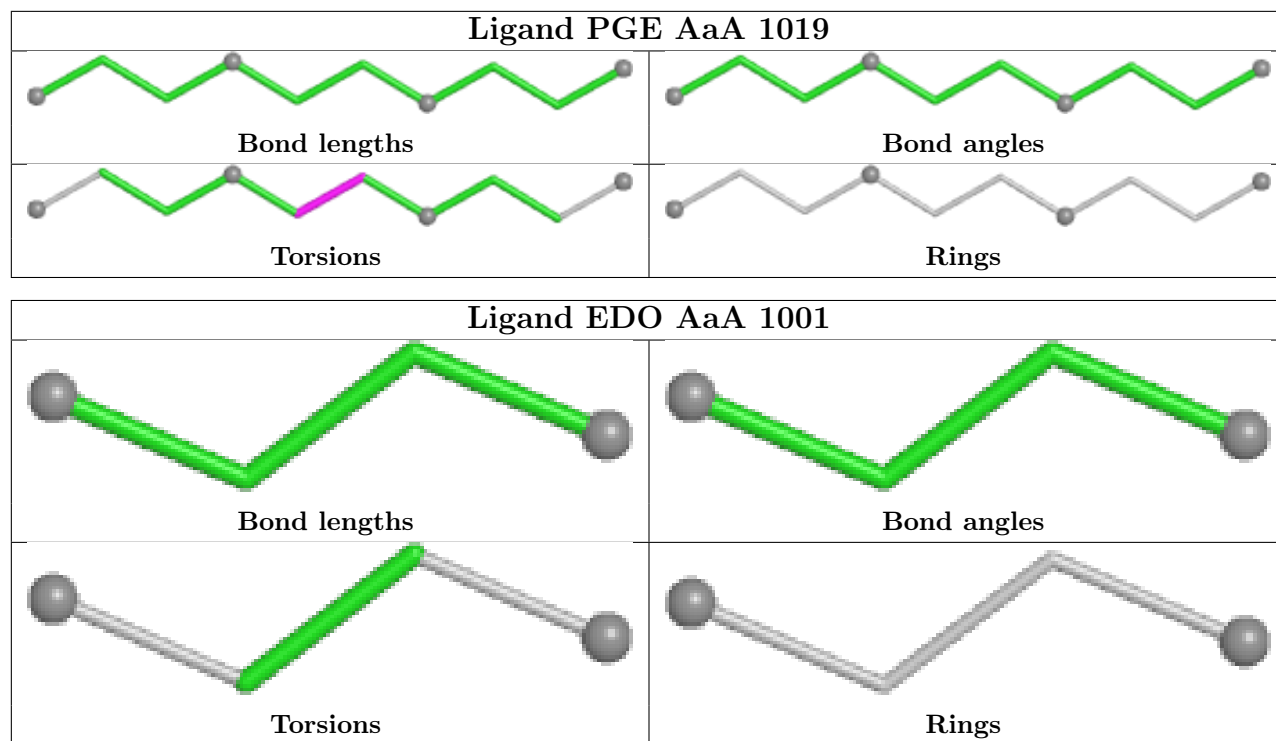


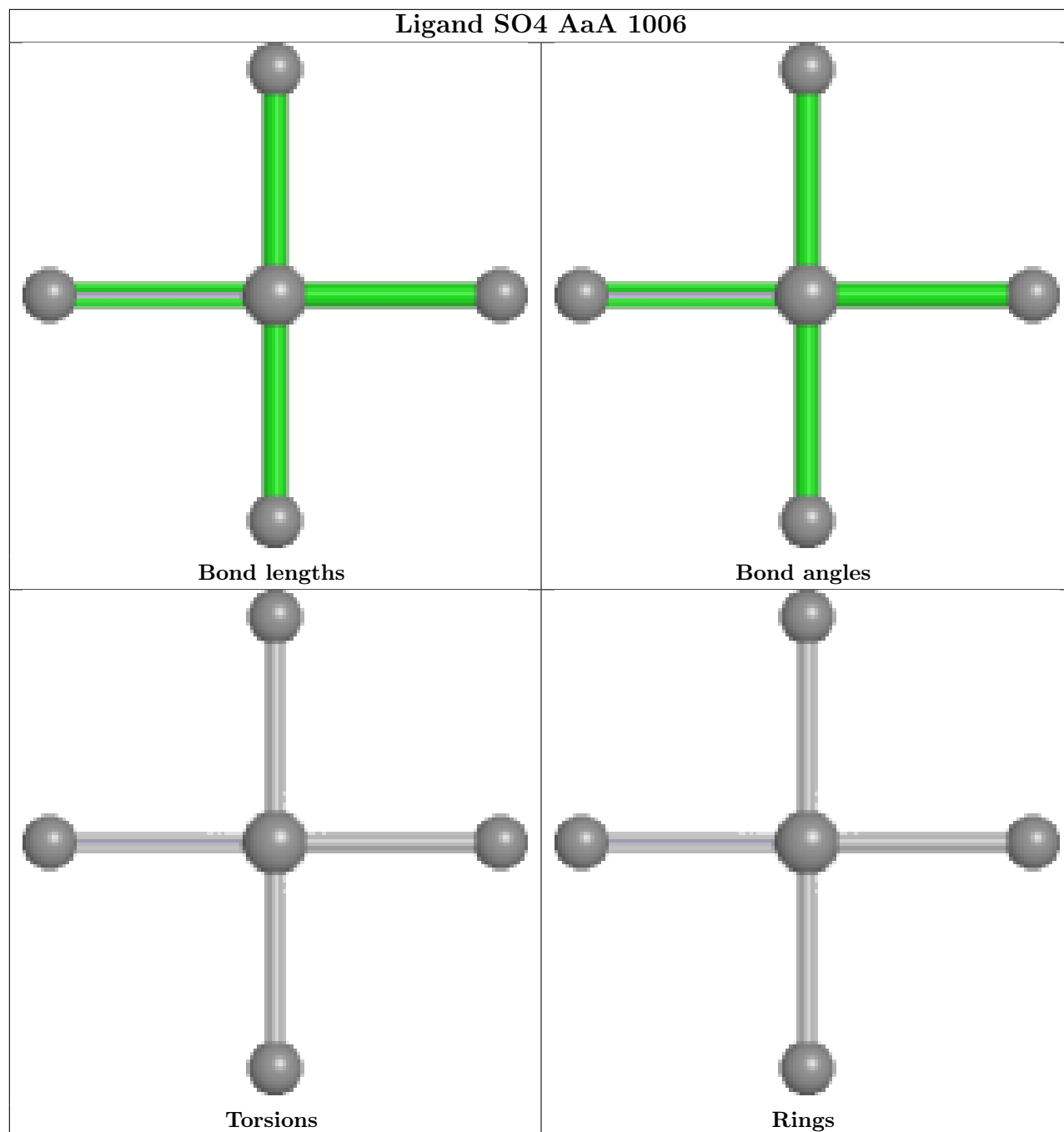
Ligand EDO AaA 1016

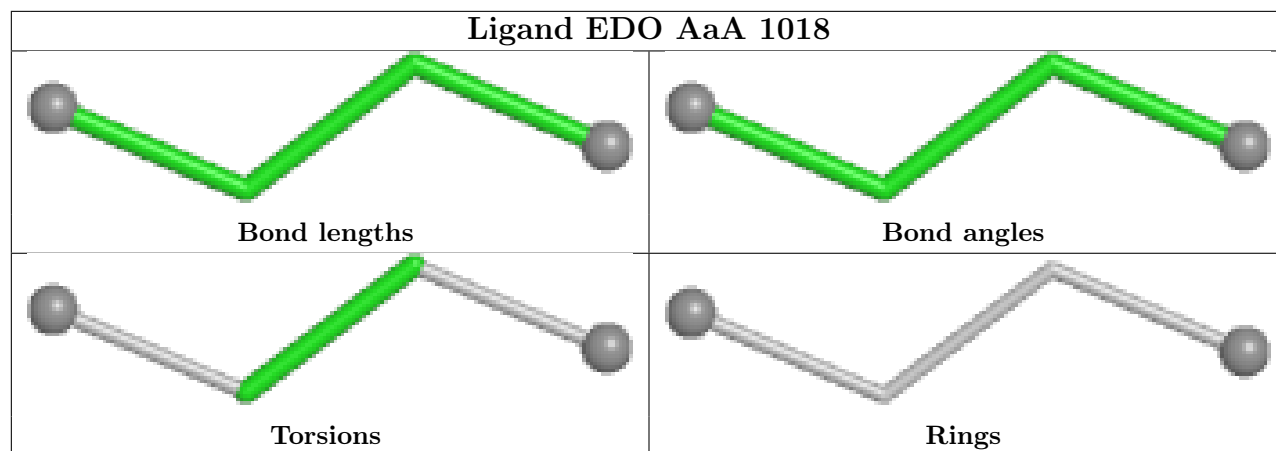


Ligand YTW AaA 1002









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	AAA	35/872 (4%)	0.59	2 (5%)	29	32	24, 34, 63, 79	0
1	AaA	815/872 (93%)	-0.17	18 (2%)	62	66	13, 25, 47, 102	10 (1%)
All	All	850/1744 (48%)	-0.14	20 (2%)	59	63	13, 25, 51, 102	10 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AaA	784	GLY	7.7
1	AaA	783	LEU	6.2
1	AaA	146	MET	5.3
1	AaA	782	ALA	4.7
1	AaA	195	LEU	4.3
1	AaA	897	ALA	4.3
1	AaA	197	THR	3.9
1	AaA	144[A]	SER	3.7
1	AaA	780	ILE	3.7
1	AAA	81	GLN	3.4
1	AaA	204	ALA	3.3
1	AAA	115	GLN	3.2
1	AaA	678	LEU	3.1
1	AaA	785	SER	3.0
1	AaA	205	PRO	2.9
1	AaA	145	GLU	2.9
1	AaA	781	GLU	2.8
1	AaA	911	THR	2.5
1	AaA	189	ARG	2.0
1	AaA	794	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSO	AaA	938	7/8	0.96	0.07	28,33,46,57	0

6.3 Carbohydrates [i](#)

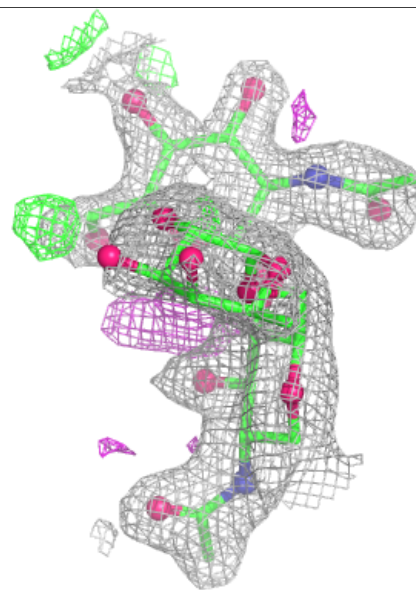
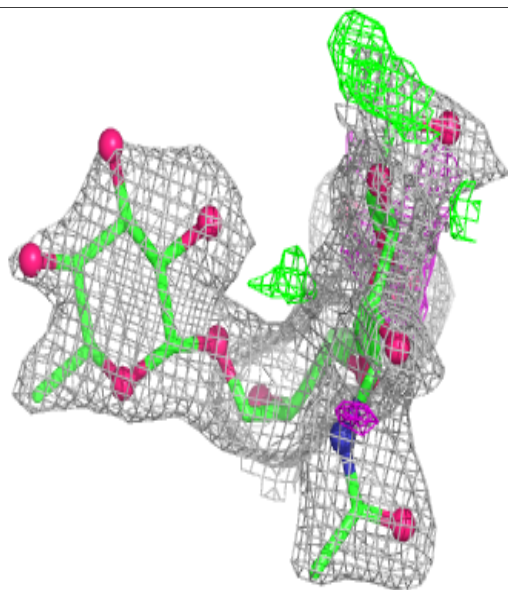
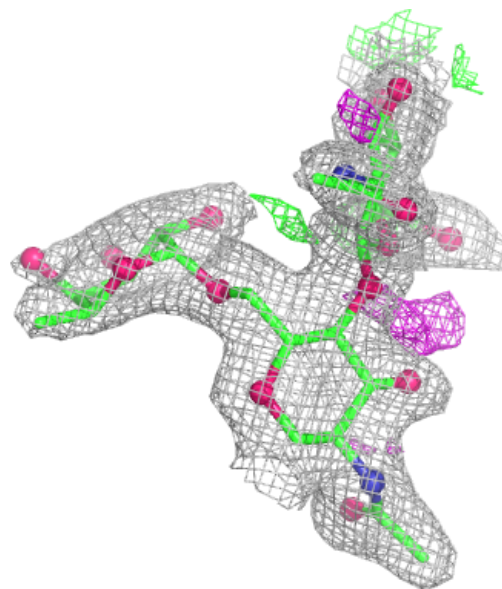
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	BBB	1	14/15	-	-	31,41,51,55	0
2	NAG	BBB	2	14/15	-	-	53,76,137,156	0
2	FUC	BBB	3	10/11	-	-	61,65,97,105	0
3	NAG	BcB	1	14/15	-	-	22,32,40,41	0
3	NAG	BcB	2	14/15	-	-	49,68,94,97	0
3	NAG	BeB	1	14/15	-	-	29,37,62,62	0
3	NAG	BeB	2	14/15	-	-	67,90,124,138	0
4	NAG	BgB	1	14/15	-	-	24,28,34,40	0
4	NAG	BgB	2	14/15	-	-	28,35,52,54	0
4	BMA	BgB	3	11/12	-	-	52,75,103,116	0
5	NAG	BjB	1	14/15	-	-	35,51,66,71	0
5	FUC	BjB	2	10/11	-	-	67,85,124,144	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.

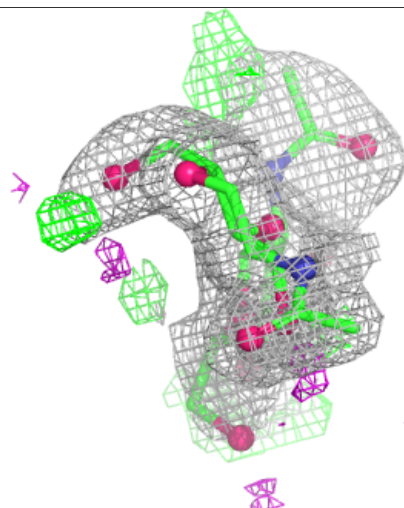
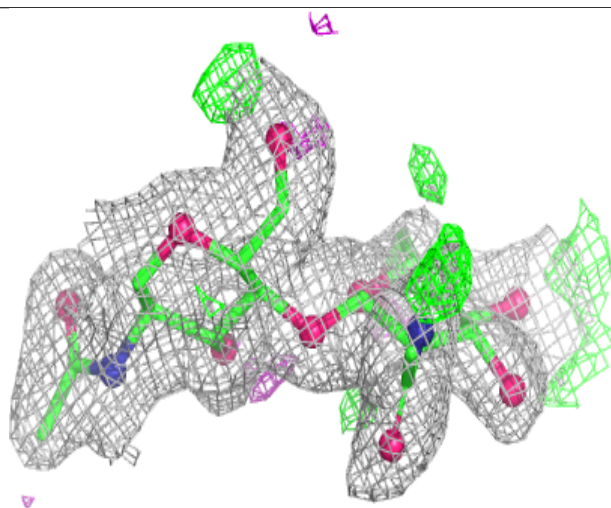
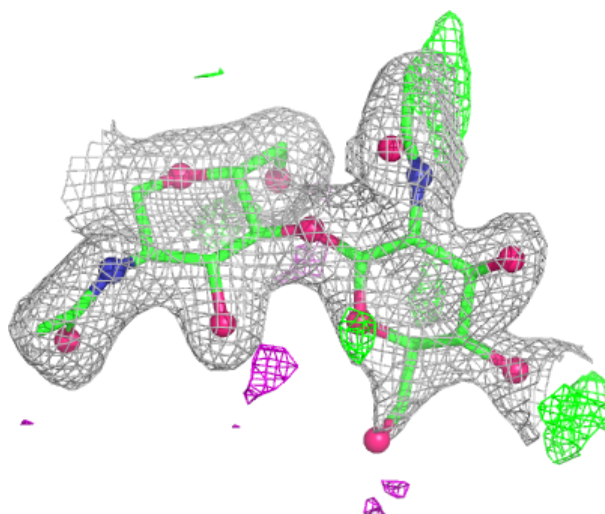
Electron density around Chain BBB:

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



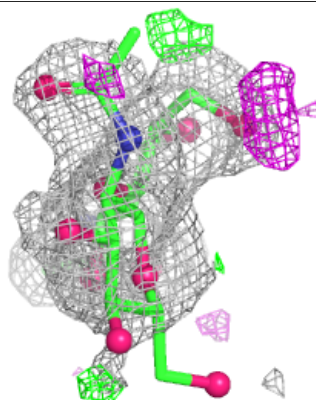
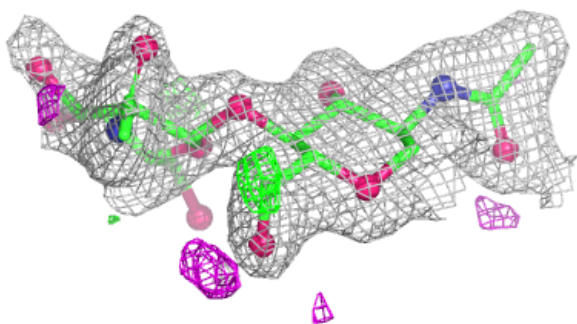
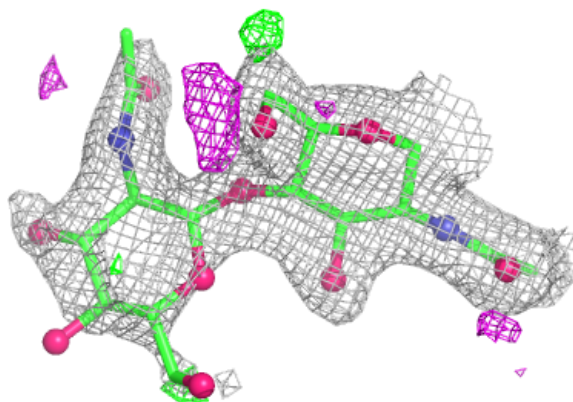
Electron density around Chain BcB:

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

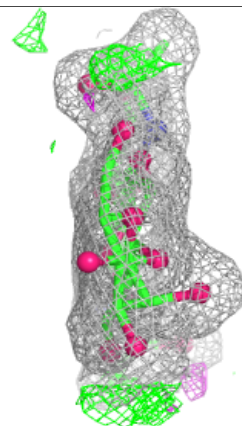
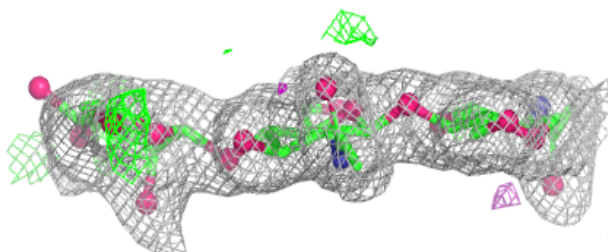
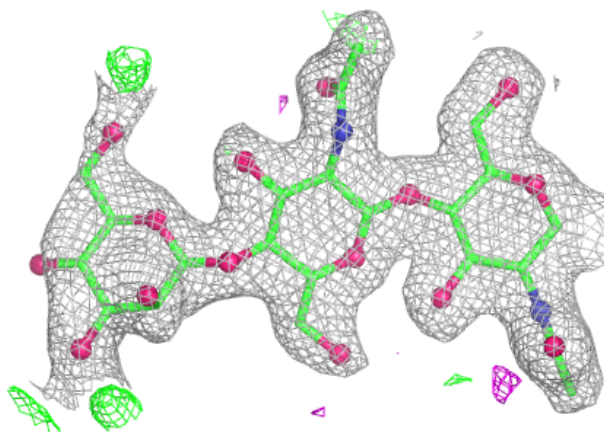


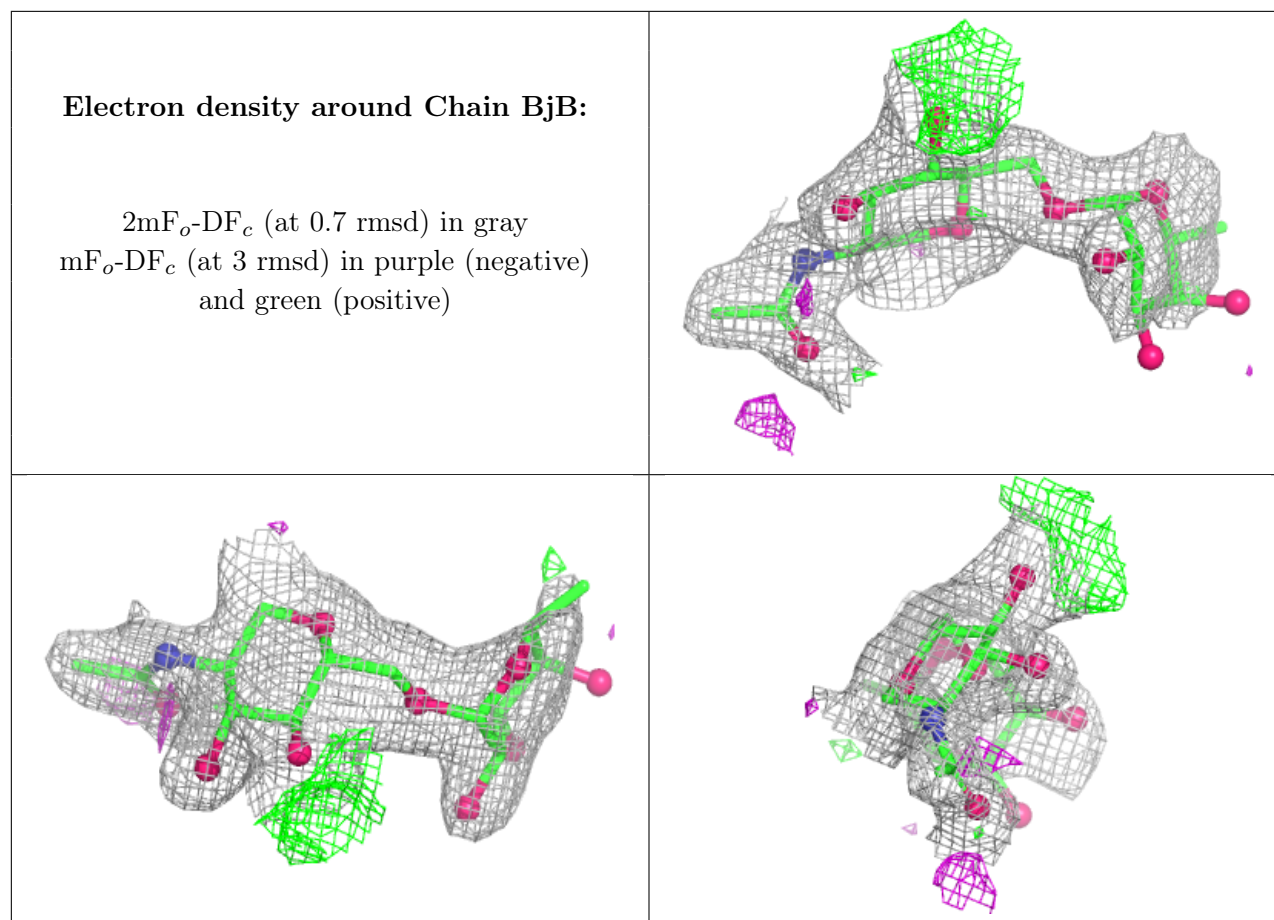
Electron density around Chain BeB:

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

**Electron density around Chain BgB:**

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





6.4 Ligands [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(Å ²)	Q<0.9
6	SO4	AaA	1004	5/5	0.78	0.11	51,64,73,96	0
11	PGE	AaA	1020	10/10	0.79	0.23	60,65,80,91	0
9	EDO	AaA	1016	4/4	0.80	0.20	44,52,63,64	0
11	PGE	AaA	1019	10/10	0.81	0.26	66,71,84,84	0
7	CL	AaA	1013	1/1	0.86	0.17	82,82,82,82	0
9	EDO	AAA	1005	4/4	0.86	0.17	41,53,60,61	0
7	CL	AaA	1010	1/1	0.86	0.15	82,82,82,82	0
7	CL	AaA	1011	1/1	0.86	0.17	73,73,73,73	0
7	CL	AaA	1012	1/1	0.86	0.22	80,80,80,80	0
9	EDO	AaA	1018	4/4	0.87	0.15	54,59,61,62	0
9	EDO	AaA	1017	4/4	0.89	0.18	31,58,59,77	0
7	CL	AaA	1007	1/1	0.89	0.15	65,65,65,65	0

Continued on next page...

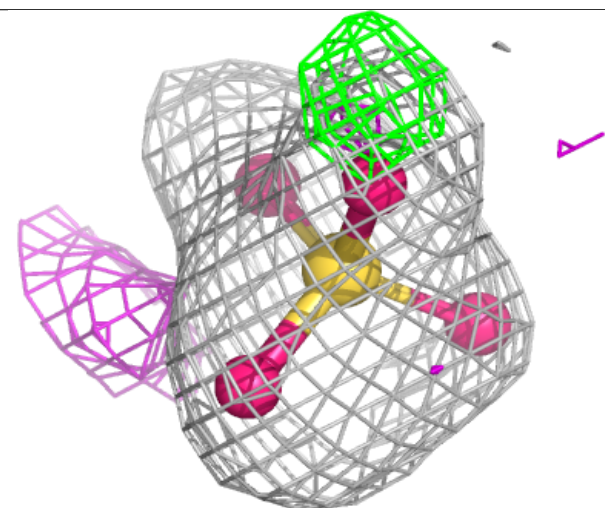
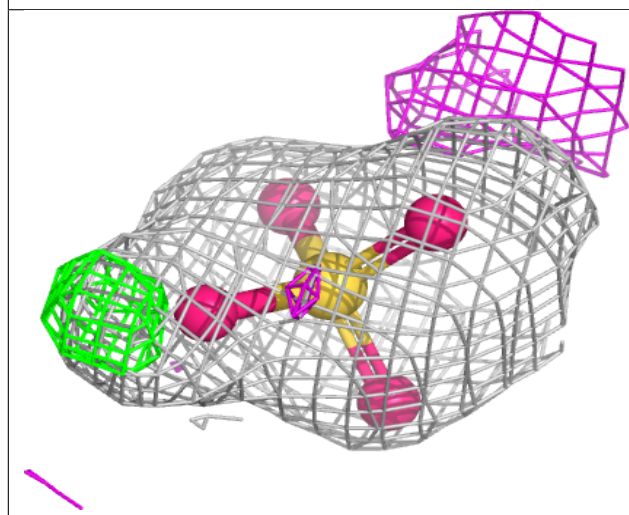
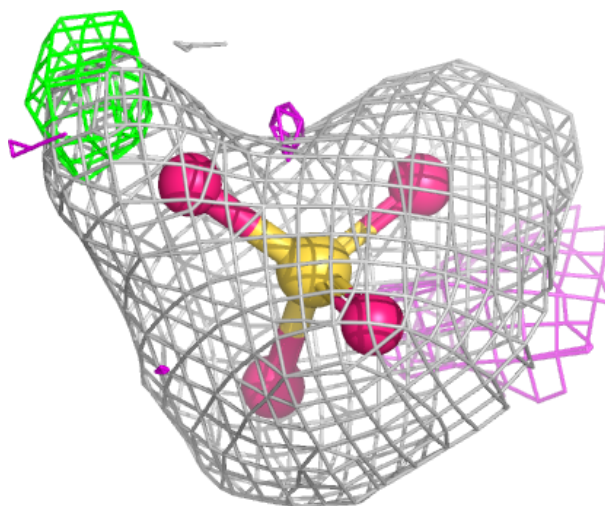
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	EDO	AaA	1001	4/4	0.90	0.12	43,46,48,50	0
7	CL	AAA	1002	1/1	0.90	0.12	64,64,64,64	0
7	CL	AAA	1003	1/1	0.90	0.11	58,58,58,58	0
6	SO4	AAA	1001	5/5	0.91	0.11	39,41,42,46	5
8	GOL	AaA	1015	6/6	0.91	0.12	28,30,35,47	6
6	SO4	AaA	1005	5/5	0.91	0.11	41,41,62,73	5
8	GOL	AaA	1014	6/6	0.92	0.11	32,37,40,54	0
7	CL	AaA	1009	1/1	0.92	0.13	60,60,60,60	0
8	GOL	AAA	1004	6/6	0.92	0.12	31,45,50,56	0
7	CL	AaA	1008	1/1	0.93	0.09	71,71,71,71	0
6	SO4	AaA	1006	5/5	0.96	0.07	23,25,33,43	5
6	SO4	AaA	1003	5/5	0.98	0.10	39,39,41,41	0
10	YTW	AaA	1002	16/16	0.98	0.05	19,22,26,27	0

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.

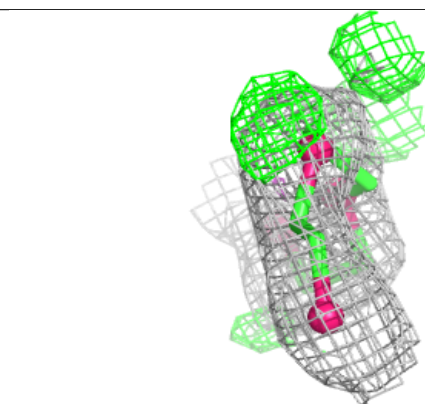
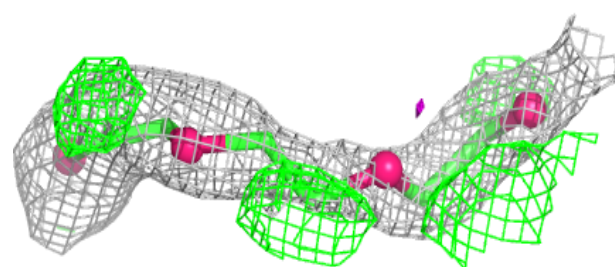
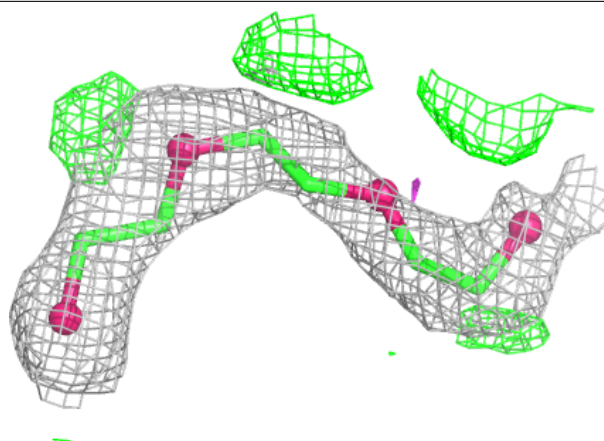
Electron density around SO4 AaA 1004:

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

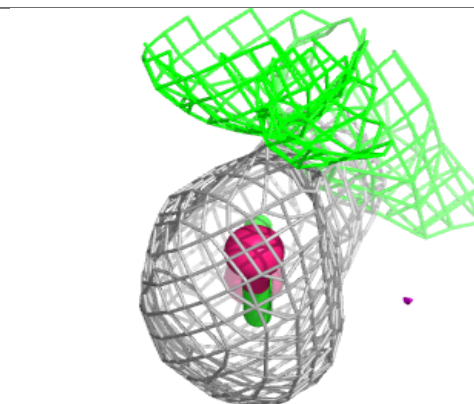
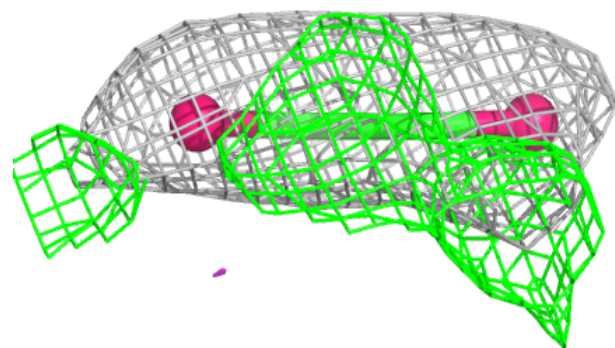
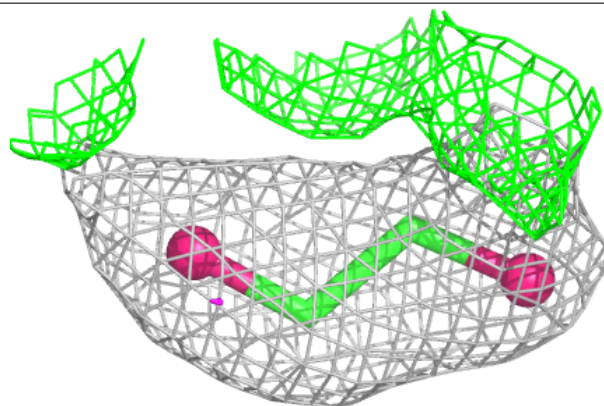


Electron density around PGE AaA 1020:

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

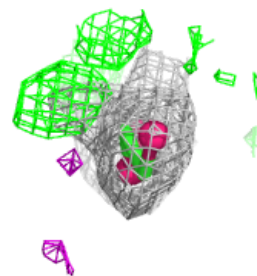
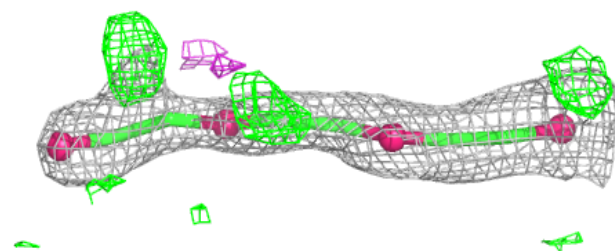
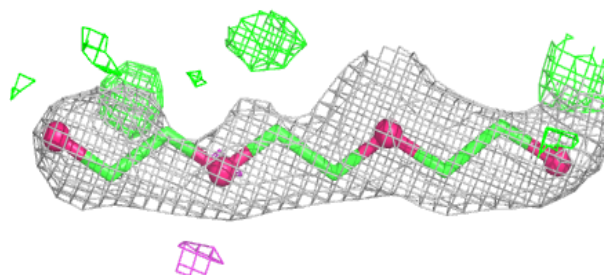
**Electron density around EDO AaA 1016:**

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



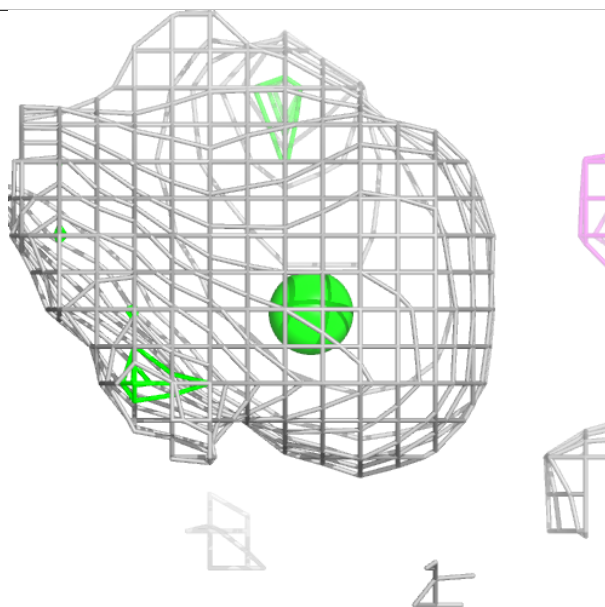
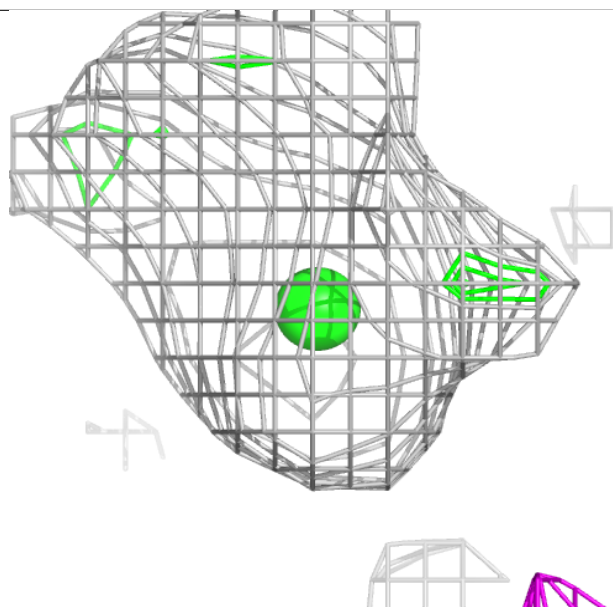
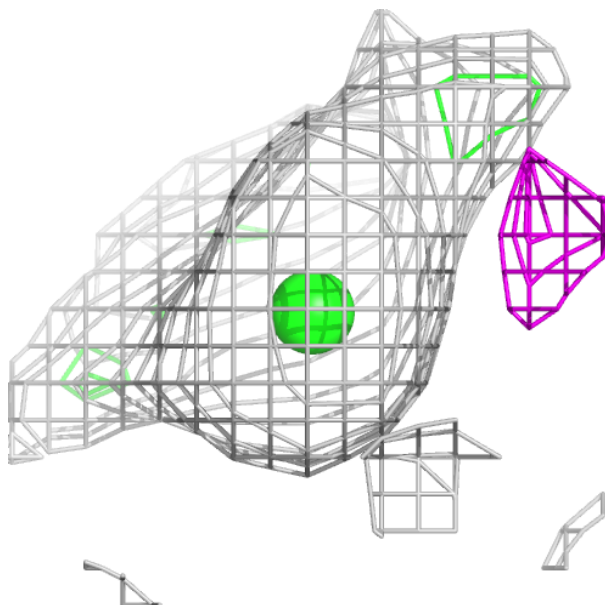
Electron density around PGE AaA 1019:

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



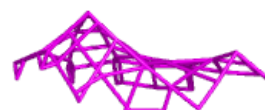
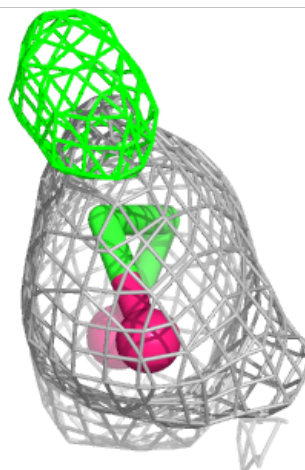
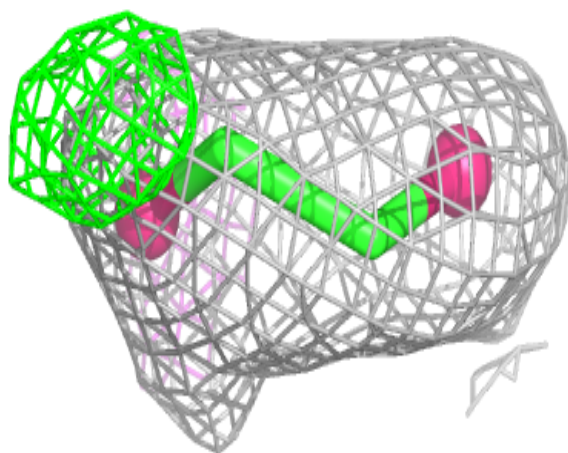
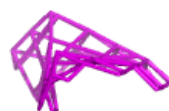
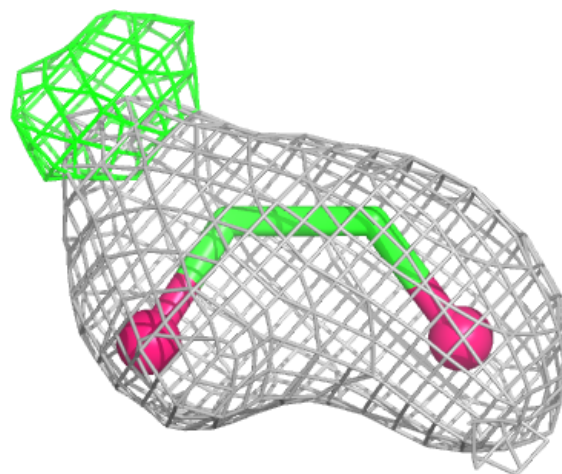
Electron density around CL AaA 1013:

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



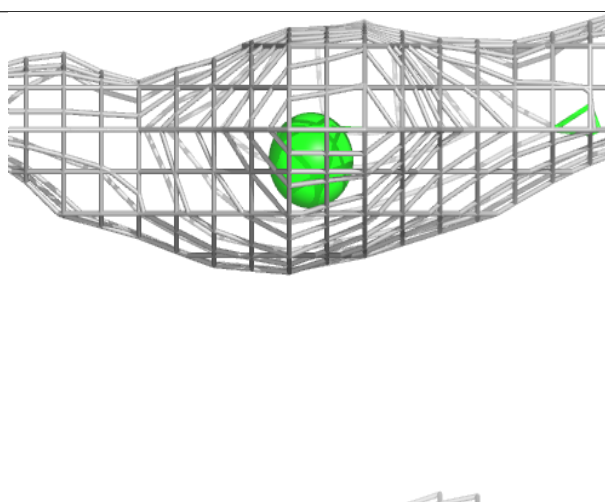
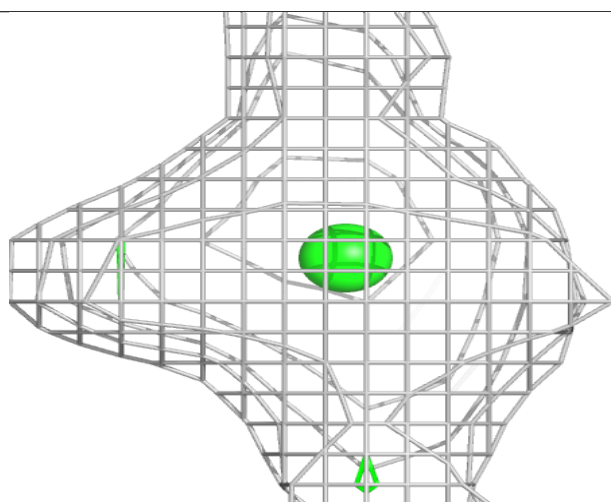
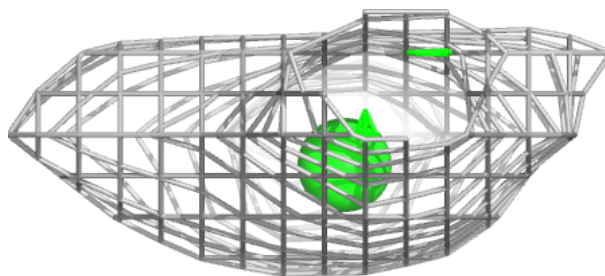
Electron density around EDO AAA 1005:

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



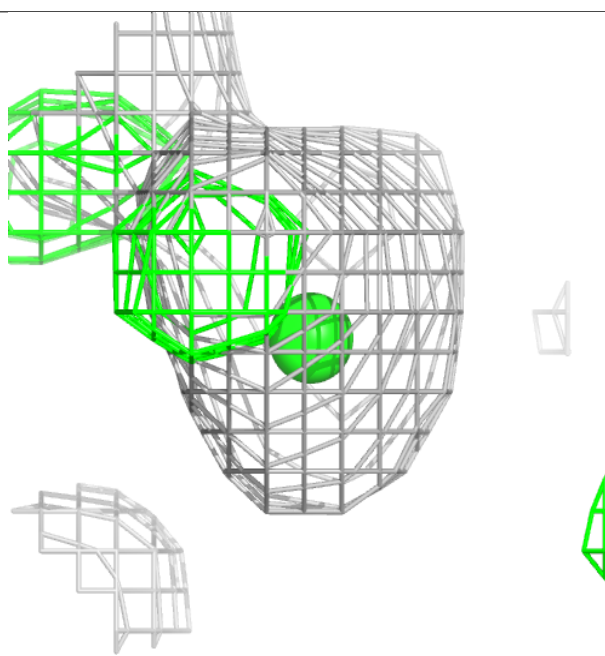
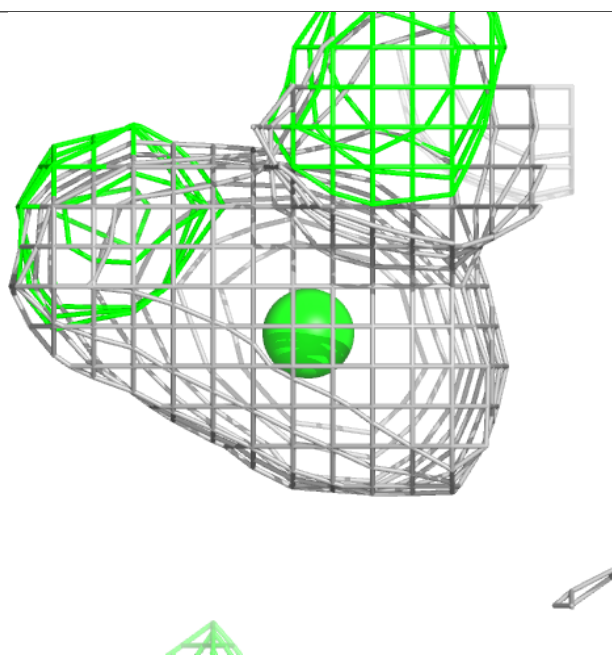
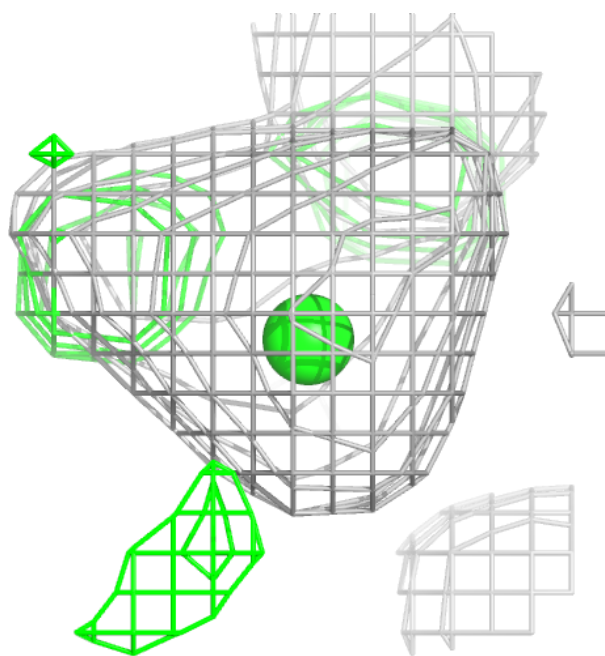
Electron density around CL AaA 1010:

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and green (positive)



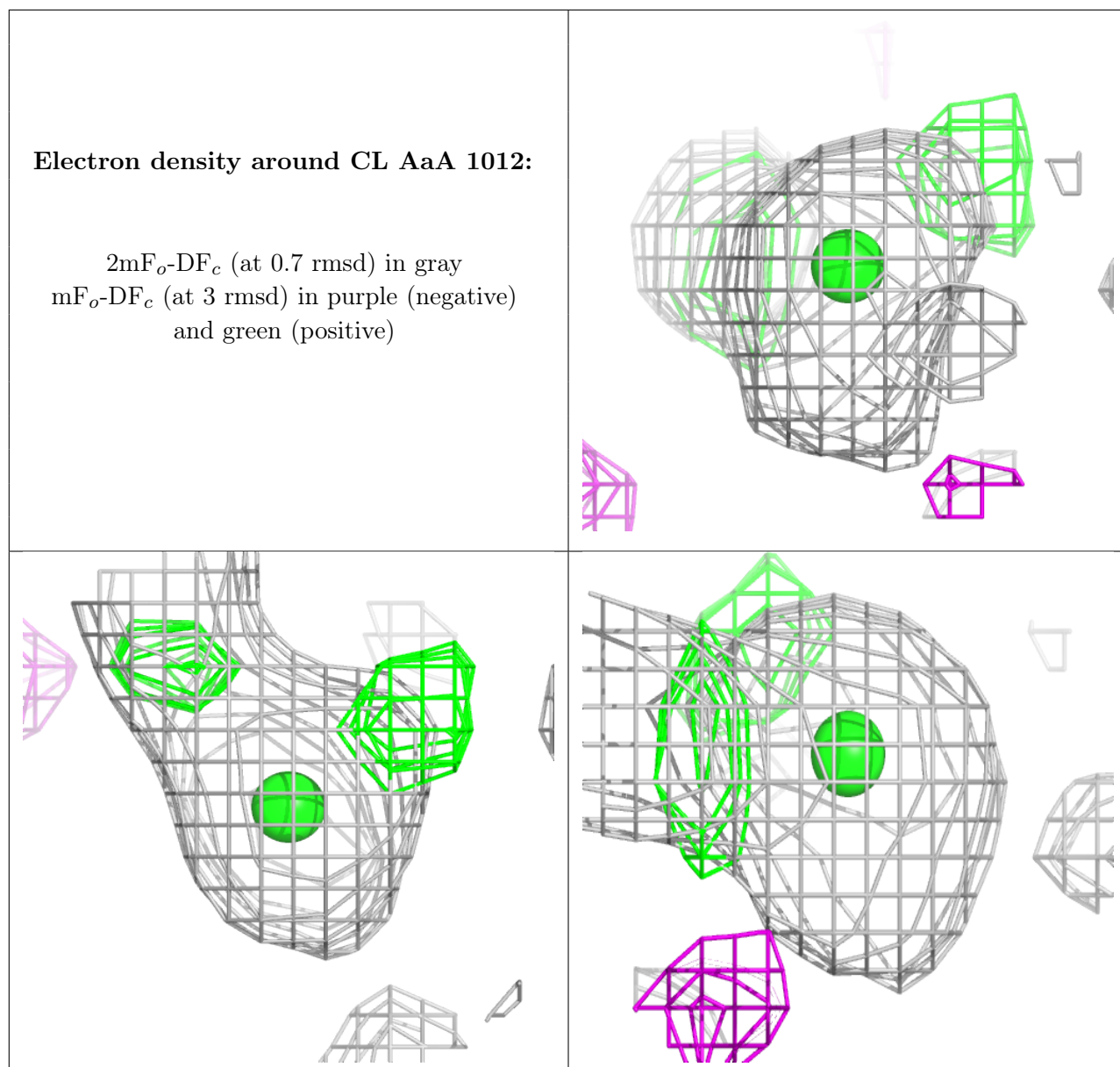
Electron density around CL AaA 1011:

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and green (positive)



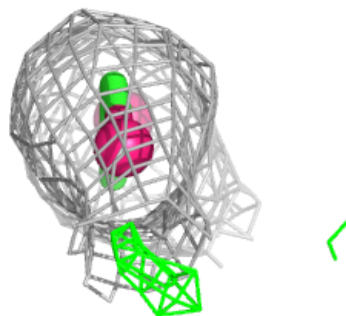
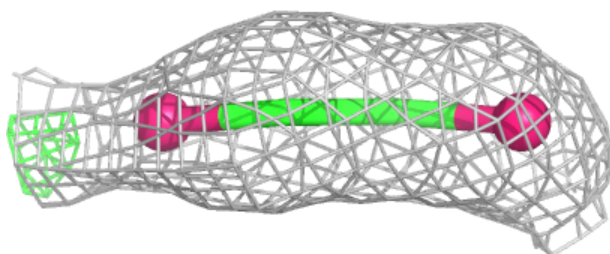
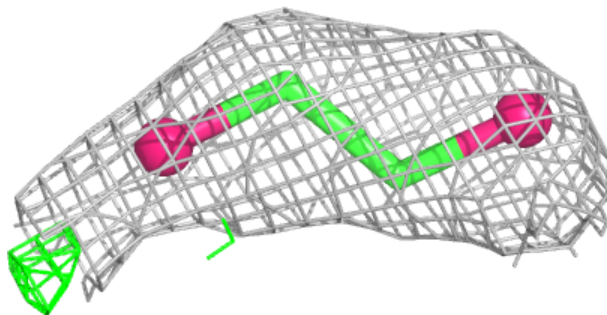
Electron density around CL AaA 1012:

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and green (positive)



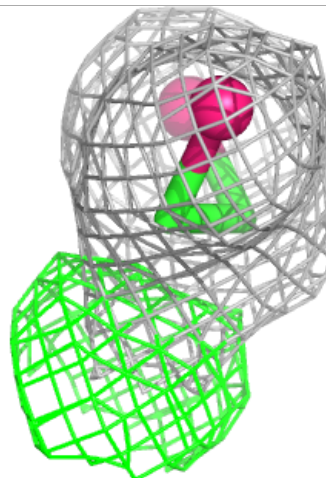
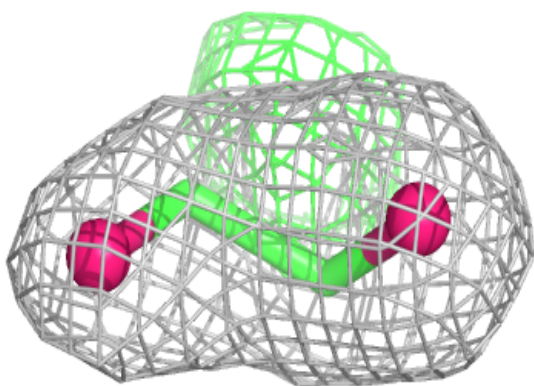
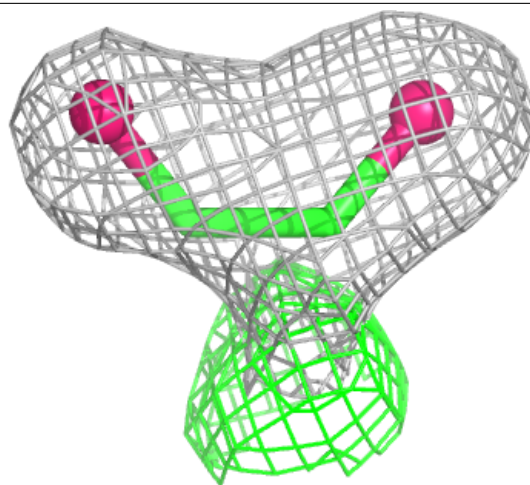
Electron density around EDO AaA 1018:

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and green (positive)



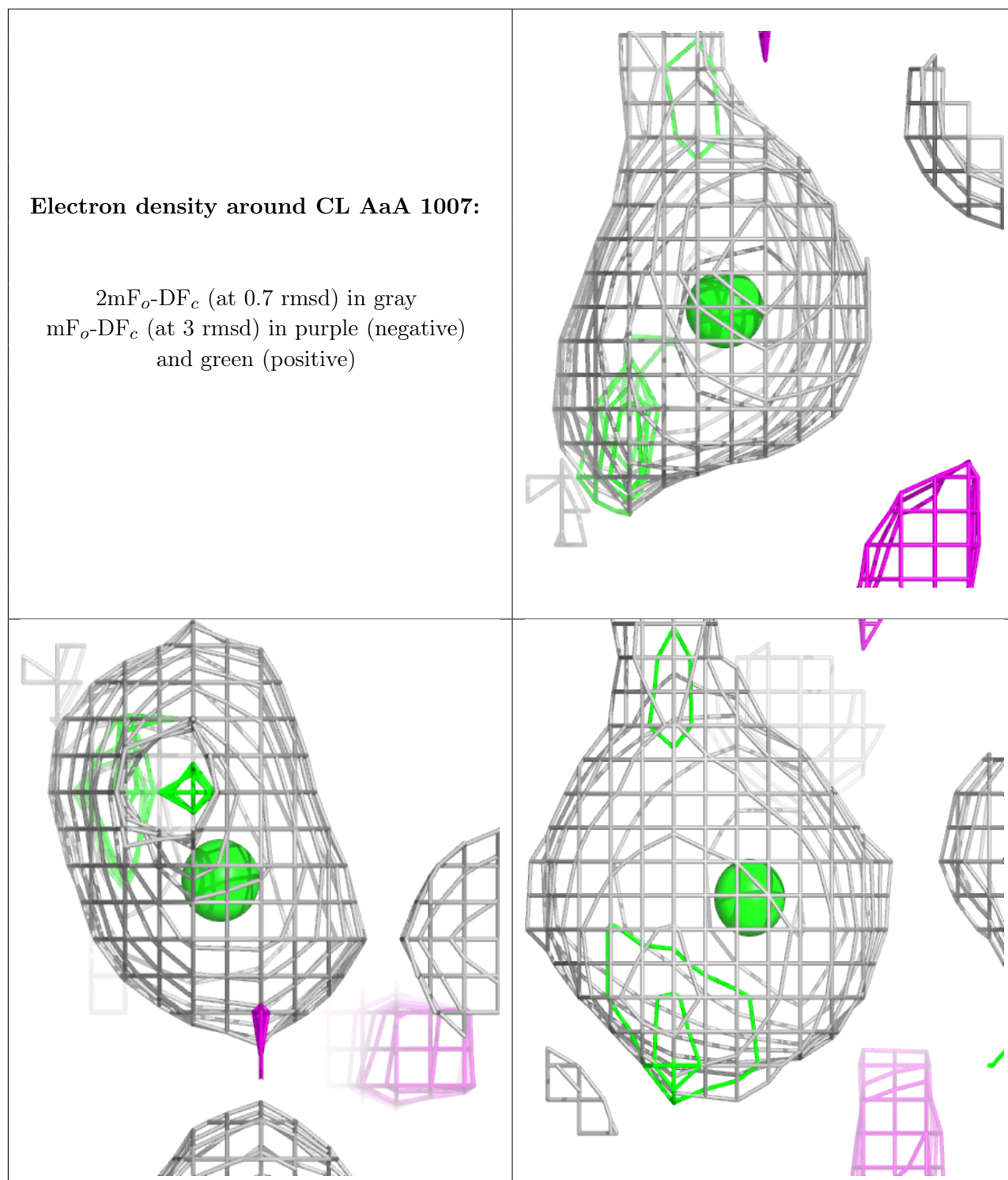
Electron density around EDO AaA 1017:

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and green (positive)



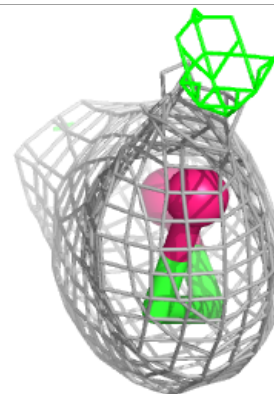
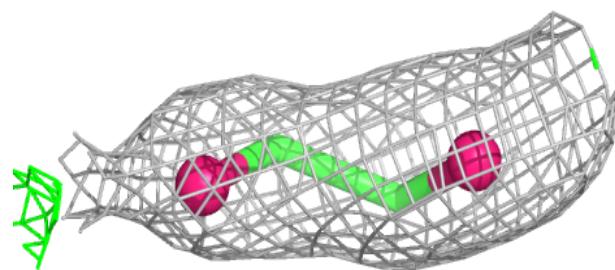
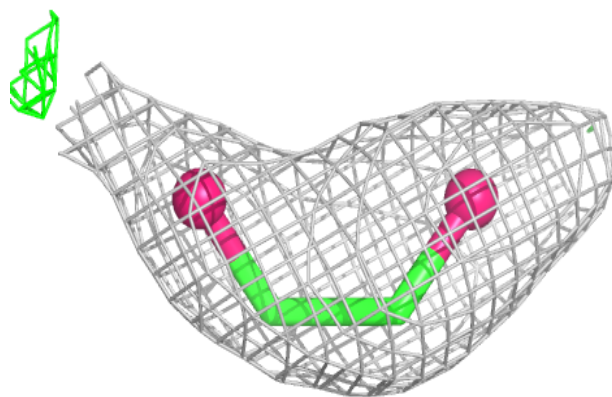
Electron density around CL AaA 1007:

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and green (positive)



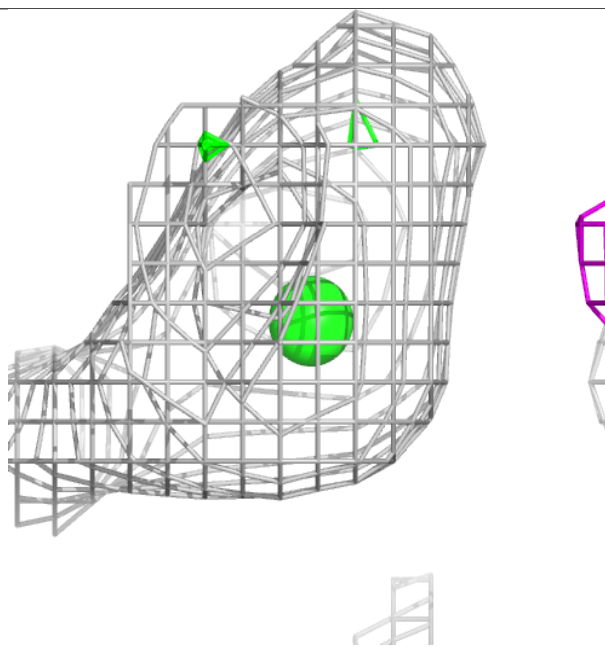
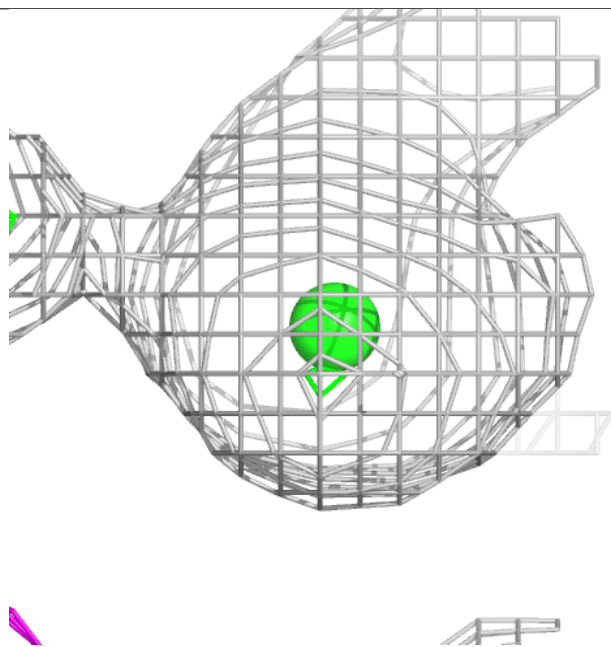
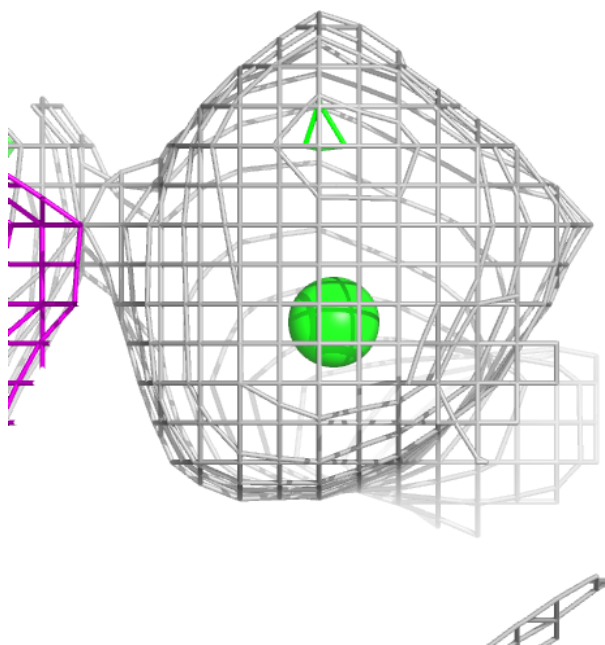
Electron density around EDO AaA 1001:

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



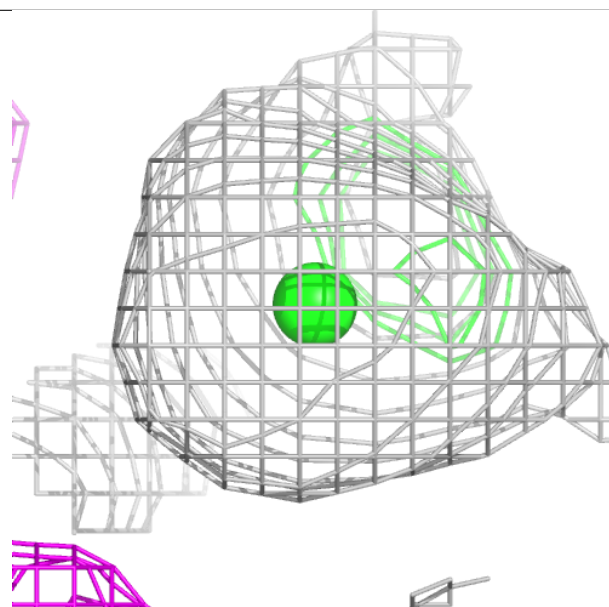
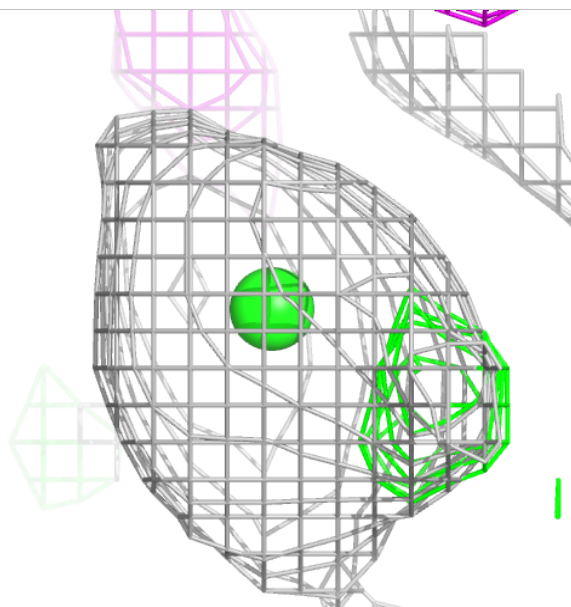
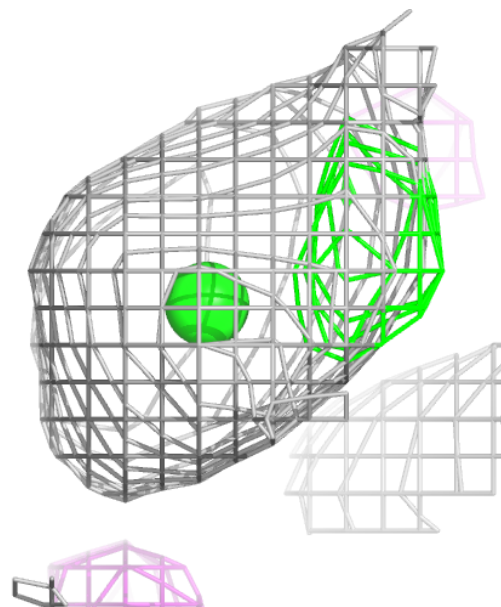
Electron density around CL AAA 1002:

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



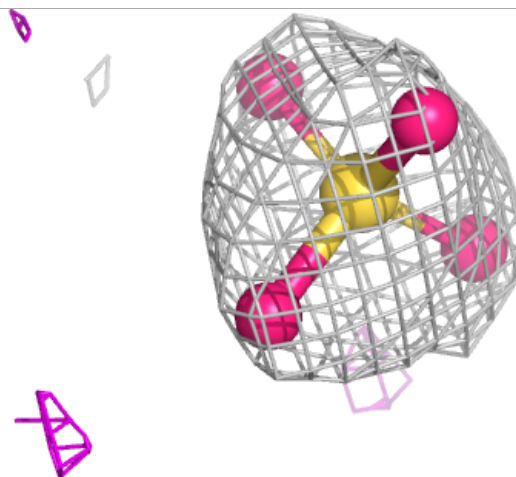
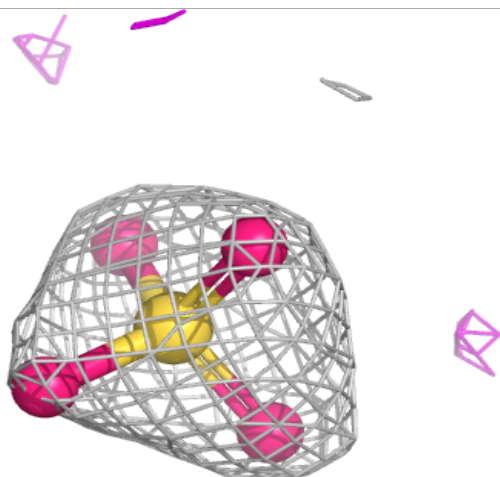
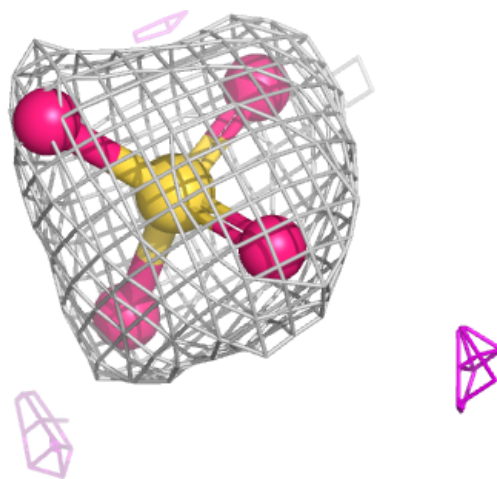
Electron density around CL AAA 1003:

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



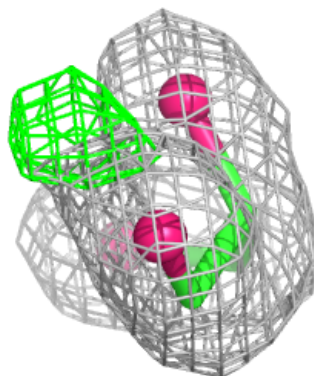
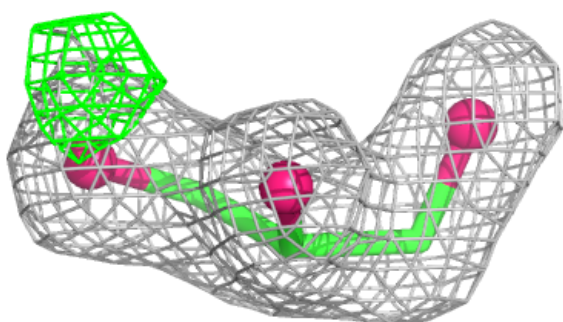
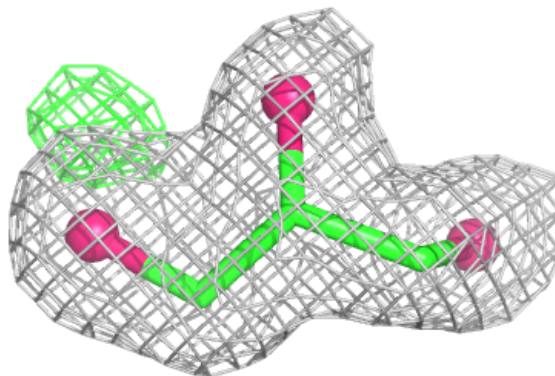
Electron density around SO4 AAA 1001:

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

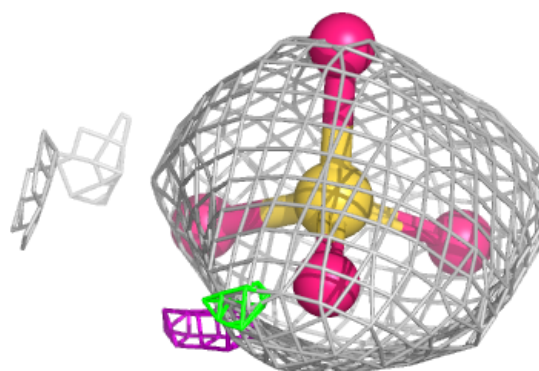
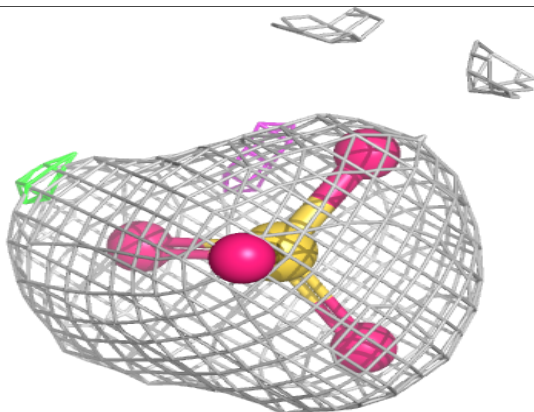
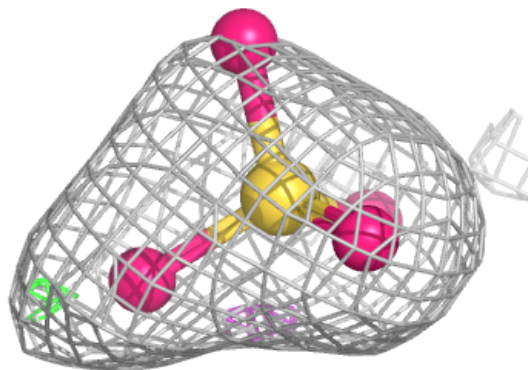


Electron density around GOL AaA 1015:

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

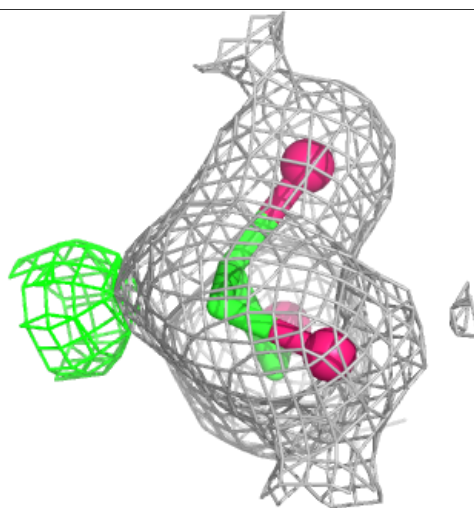
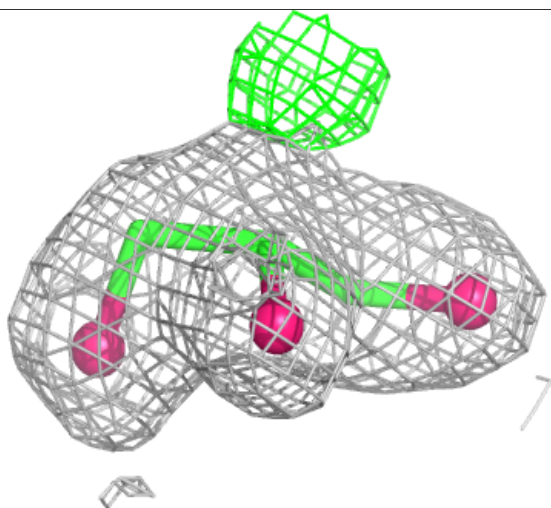
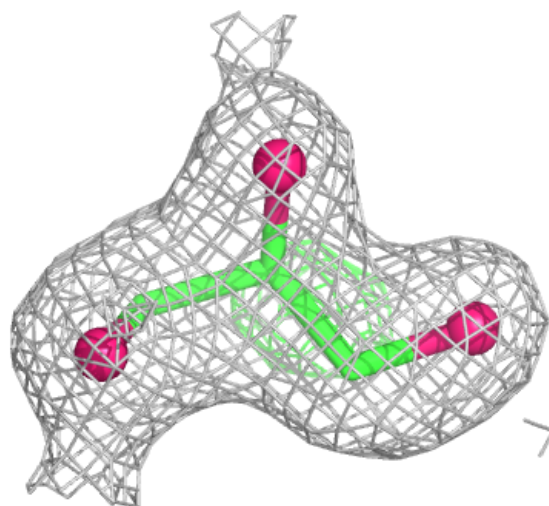
**Electron density around SO4 AaA 1005:**

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and green (positive)



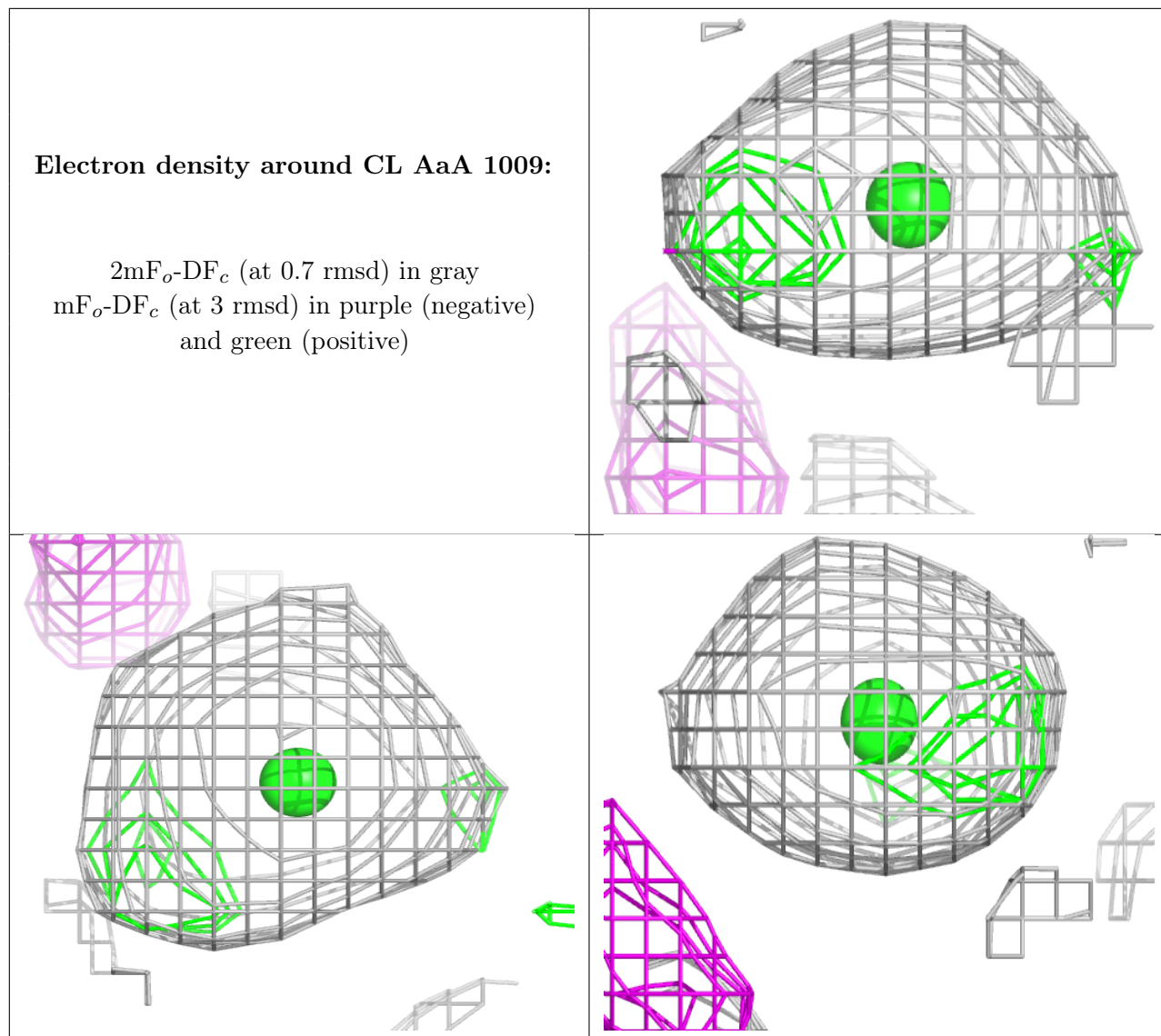
Electron density around GOL AaA 1014:

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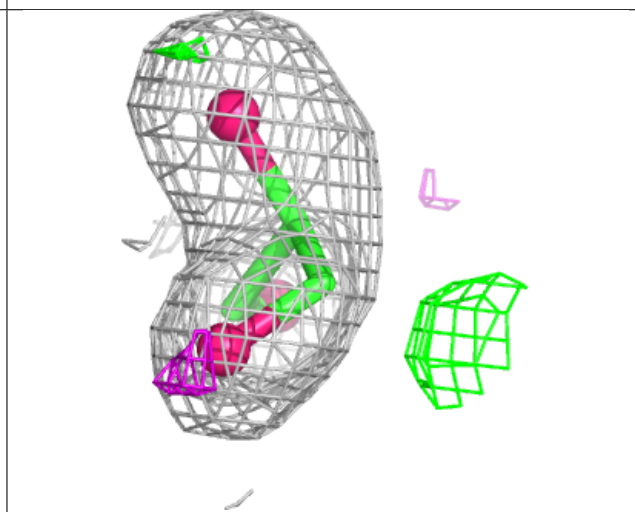
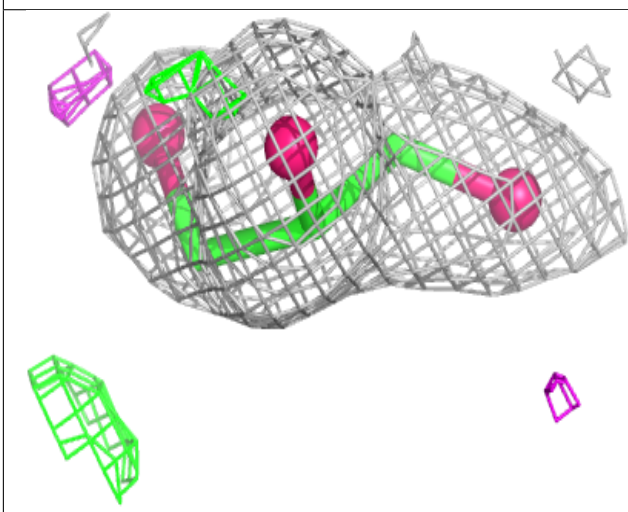
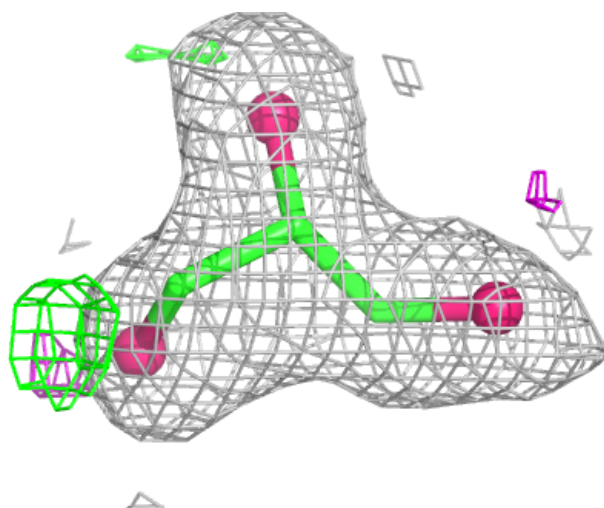
Electron density around CL AaA 1009:

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



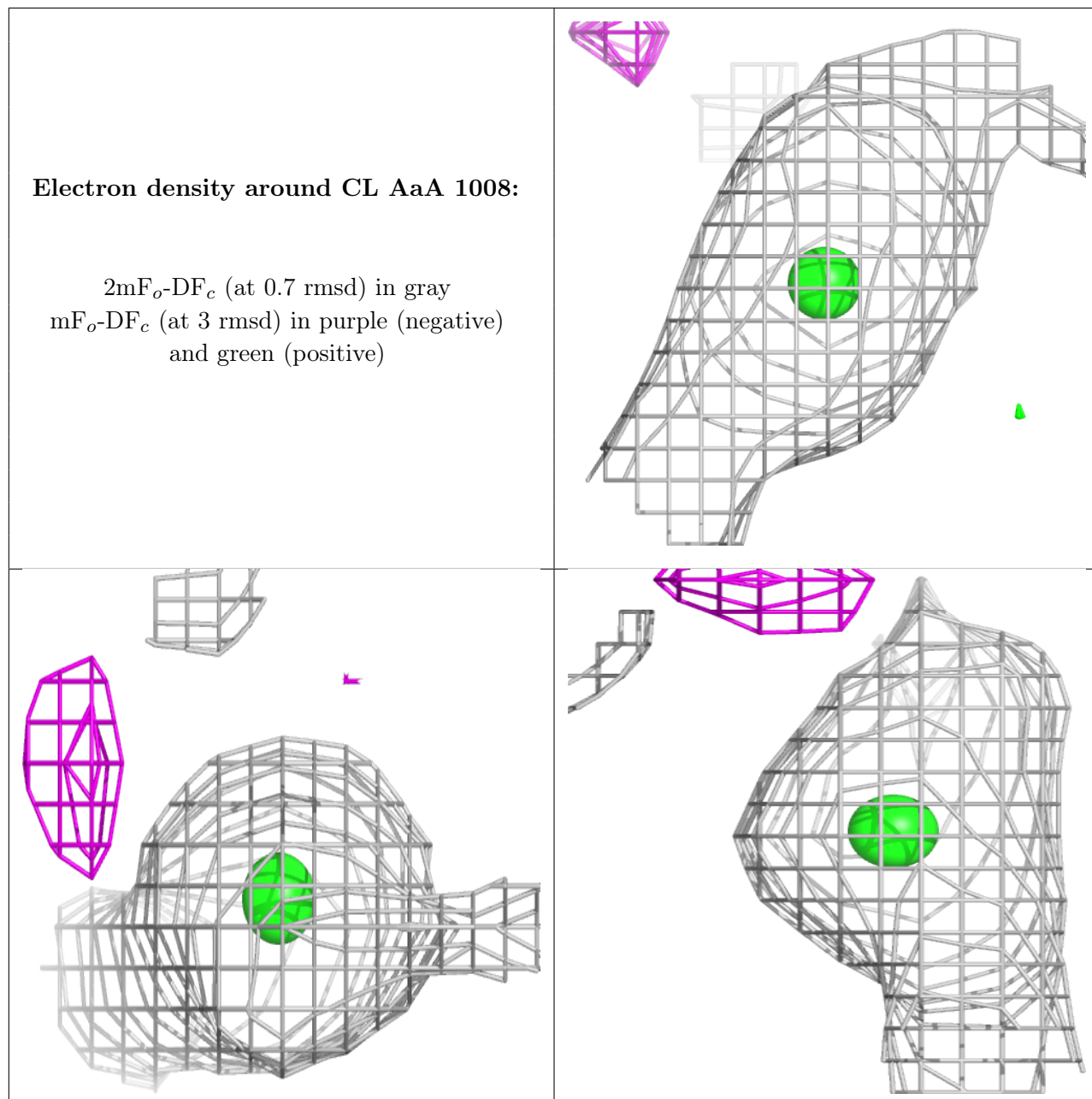
Electron density around GOL AAA 1004:

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and green (positive)



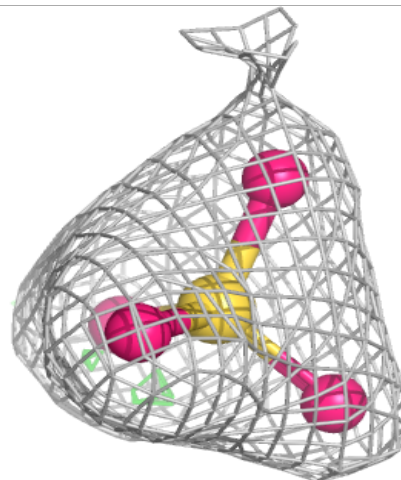
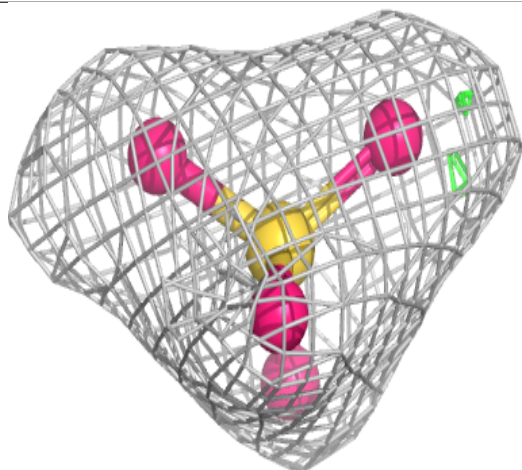
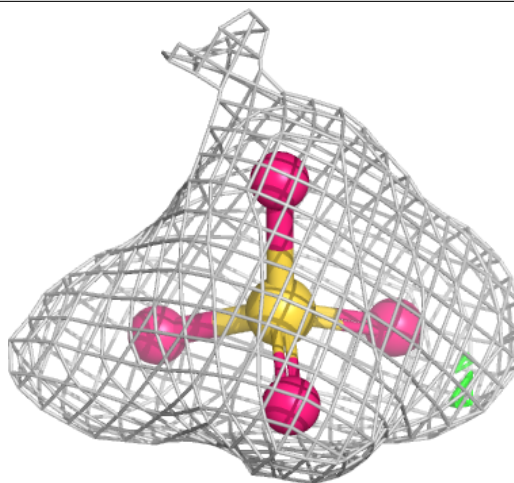
Electron density around CL AaA 1008:

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and green (positive)



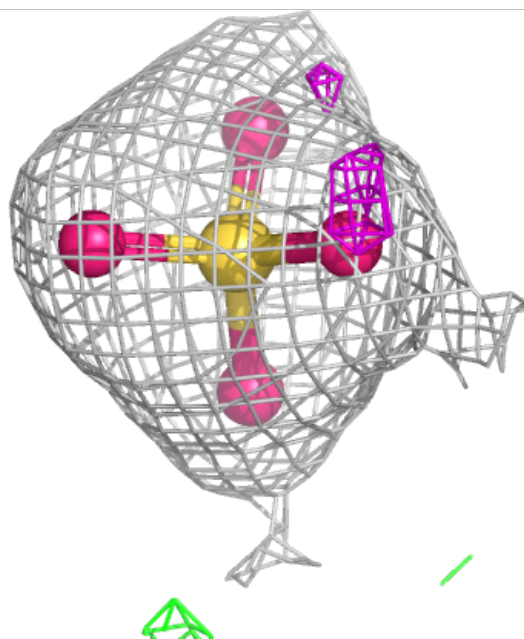
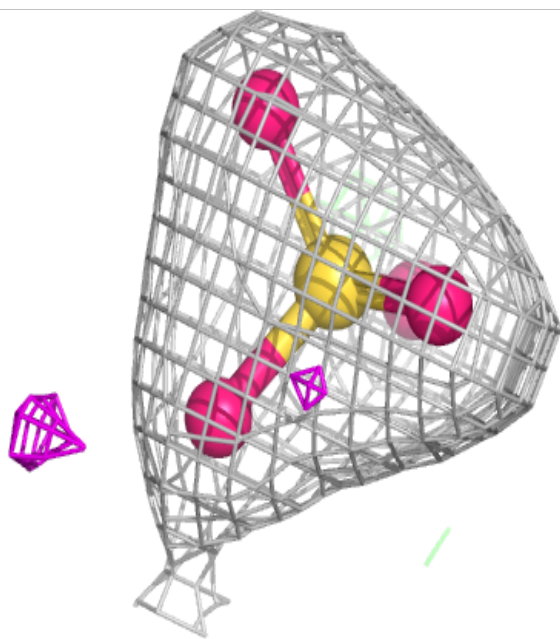
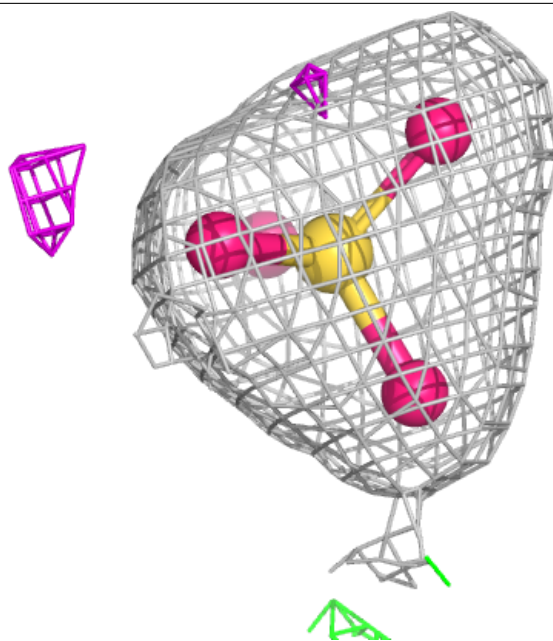
Electron density around SO4 AaA 1006:

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and green (positive)



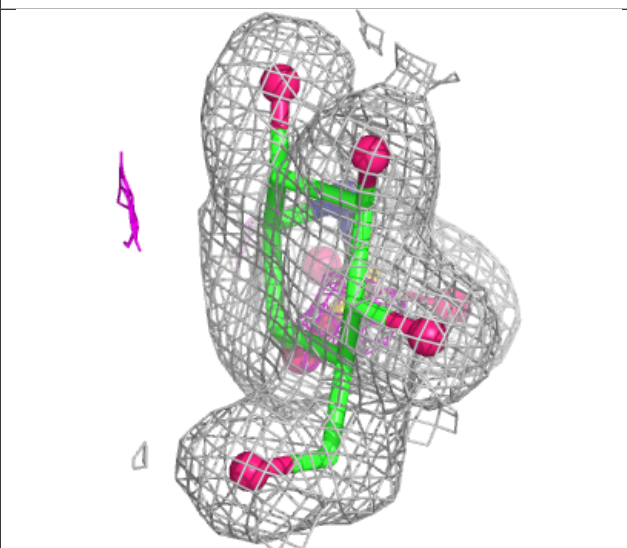
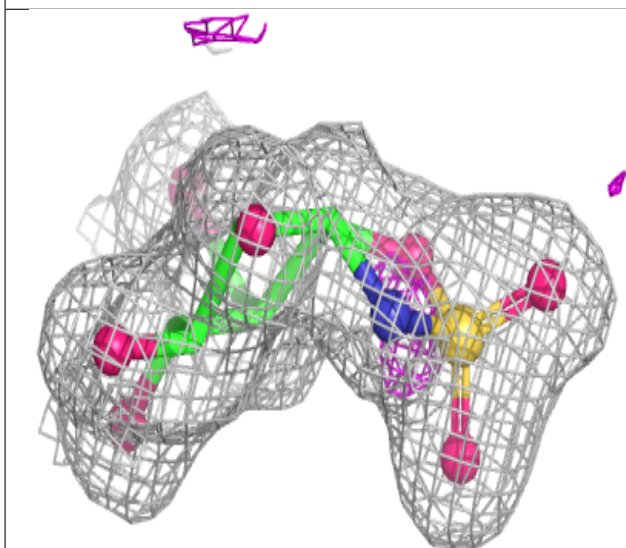
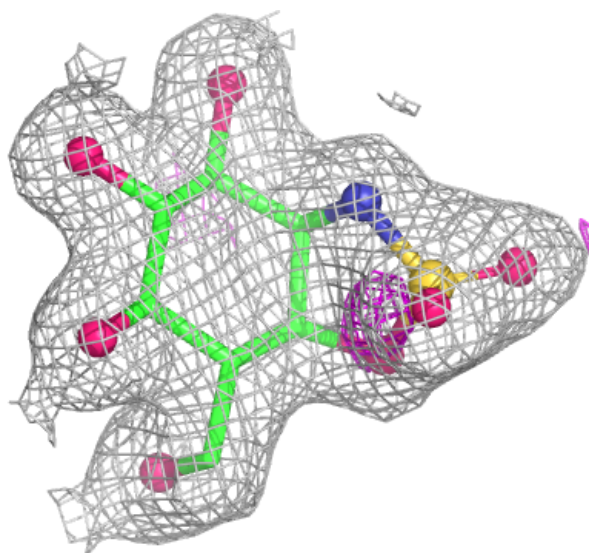
Electron density around SO4 AaA 1003:

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



Electron density around YTW AaA 1002:

$2mF_o-DF_c$ (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.