



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:04 AM UTC

PDB ID : 7Z6T / pdb_00007z6t
Title : Aspergillus clavatus M36 protease without the propeptide
Authors : Wilkens, C.; Qiu, J.; Meyer, A.S.; Morth, J.P.
Deposited on : 2022-03-14
Resolution : 1.51 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

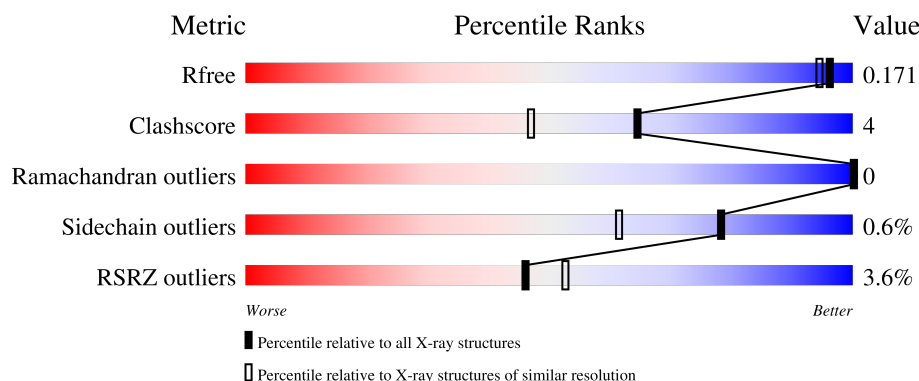
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	AAA	388	4% 93% 7%
2	AaA	7	29% 71%
3	AuA	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
3	DNO	AuA	1	-	X	-	-

2 Entry composition [i](#)

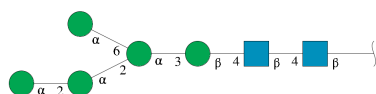
There are 9 unique types of molecules in this entry. The entry contains 3746 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Extracellular metalloproteinase mep.

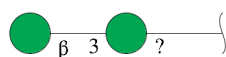
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	388	3110	1938	542	612	18	0	14	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O			
2	AaA	7	83	46	2	35	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-D-mannose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	AuA	2	23	12	11	0	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

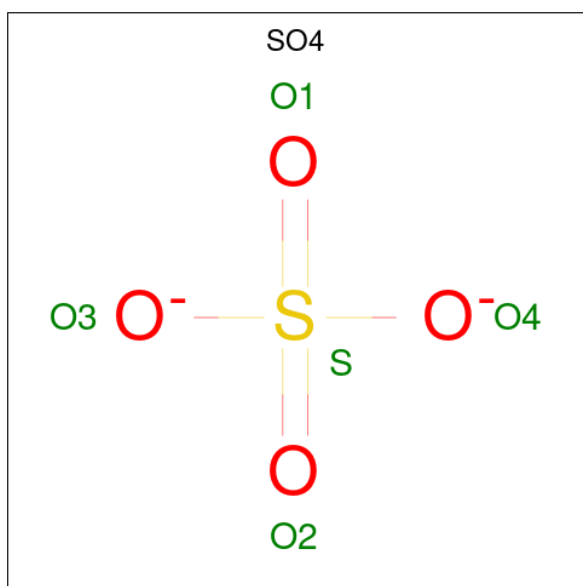
depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	1	Total	Ca	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest"

by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1	Total 1	Na 1	0	0

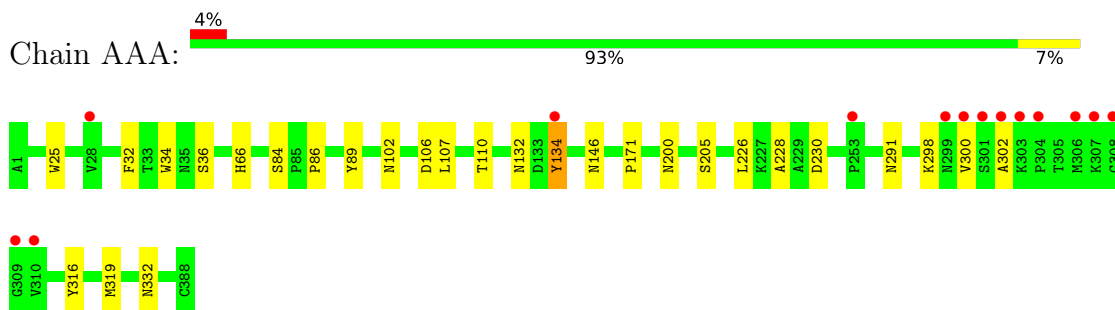
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	449	Total 450	O 450	0	1

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Extracellular metalloproteinase mep



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



- Molecule 3: beta-D-mannopyranose-(1-3)-D-mannose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.83Å 85.04Å 55.32Å 90.00° 111.30° 90.00°	Depositor
Resolution (Å)	45.04 – 1.51 45.04 – 1.51	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.04-1.51) 98.7 (45.04-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 3	Depositor
R, R_{free}	0.177 , 0.196 0.162 , 0.171	Depositor DCC
R_{free} test set	1084 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3746	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: NAG, BMA, MAN, ZN, EDO, DNO, NA, SO4, CA

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	0.62	0/3191	0.95	1/4333 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	332	ASN	CB-CA-C	5.32	115.63	111.00

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	3110	0	2929	24	1
2	AaA	83	0	70	0	0
3	AuA	23	0	21	0	1
4	AAA	52	0	78	4	0
5	AAA	1	0	0	0	0
6	AAA	1	0	0	0	0
7	AAA	25	0	0	0	0
8	AAA	1	0	0	0	0
9	AAA	450	0	0	7	2
All	All	3746	0	3098	25	3

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 4.

All (25) 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:200[B]:ASN:ND2	9:AAA:814[B]:HOH:O	1.84	1.10
1:AAA:134[A]:TYR:OH	9:AAA:501:HOH:O	2.09	0.69
1:AAA:226[B]:LEU:CD2	1:AAA:230:ASP:HB2	2.32	0.59
1:AAA:205:SER:O	4:AAA:411:EDO:H11	2.03	0.57
1:AAA:106:ASP:O	1:AAA:110[B]:THR:HG23	2.06	0.56
1:AAA:110[B]:THR:HG22	9:AAA:725:HOH:O	2.07	0.55
1:AAA:228:ALA:HB2	1:AAA:300:VAL:HG11	1.89	0.55
1:AAA:34:TRP:CE2	1:AAA:102:ASN:HB3	2.43	0.53
1:AAA:66:HIS:HB2	4:AAA:402:EDO:H11	1.90	0.53
1:AAA:132[B]:ASN:ND2	9:AAA:506:HOH:O	2.39	0.53
1:AAA:226[B]:LEU:HD23	1:AAA:230:ASP:OD2	2.11	0.51
1:AAA:84:SER:HB2	1:AAA:171:PRO:HB3	1.93	0.50
1:AAA:316:TYR:CD1	1:AAA:319[B]:MET:CE	2.95	0.49
1:AAA:86:PRO:HA	1:AAA:89:TYR:CZ	2.49	0.48
1:AAA:107:LEU:HD21	1:AAA:319[B]:MET:HE1	1.98	0.46
1:AAA:32:PHE:O	1:AAA:36:SER:HB3	2.18	0.43
1:AAA:316:TYR:CD1	1:AAA:319[B]:MET:HE2	2.53	0.43
1:AAA:316:TYR:HD1	1:AAA:319[B]:MET:CE	2.31	0.43
1:AAA:200[A]:ASN:O	9:AAA:502:HOH:O	2.15	0.43
4:AAA:408:EDO:H22	9:AAA:674:HOH:O	2.16	0.43
1:AAA:291:ASN:OD1	4:AAA:403:EDO:H22	2.18	0.43
1:AAA:134[A]:TYR:C	1:AAA:134[A]:TYR:CD1	2.98	0.42
1:AAA:25:TRP:HB3	1:AAA:34:TRP:CD1	2.55	0.42
1:AAA:134[A]:TYR:C	1:AAA:134[A]:TYR:HD1	2.28	0.41
1:AAA:302:ALA:HB2	9:AAA:926:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AAA:897:HOH:O	9:AAA:912:HOH:O[1_556]	2.10	0.10
9:AAA:516:HOH:O	9:AAA:740:HOH:O[1_554]	2.12	0.08
1:AAA:146:ASN:O	3:AAA:2:BMA:O3[1_655]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	400/388 (103%)	391 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	AAA	331/317 (104%)	328 (99%)	3 (1%)	70	49

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	134[A]	TYR
1	AAA	134[B]	TYR
1	AAA	298	LYS

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 ⓘ

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

5.5 Carbohydrates ⓘ

9 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	AaA	1	2,1	14,14,15	0.57	0	17,19,21	1.53	4 (23%)
2	NAG	AaA	2	2	14,14,15	0.60	0	17,19,21	1.24	1 (5%)
2	BMA	AaA	3	2	11,11,12	0.58	0	15,15,17	1.18	2 (13%)
2	MAN	AaA	4	2	11,11,12	0.97	0	15,15,17	0.96	0
2	MAN	AaA	5	2	11,11,12	0.91	0	15,15,17	1.07	1 (6%)
2	MAN	AaA	6	5,2	11,11,12	0.52	0	15,15,17	1.38	3 (20%)
2	MAN	AaA	7	2	11,11,12	0.69	0	15,15,17	1.05	0
3	DNO	AuA	1	3	10,11,11	1.04	1 (10%)	13,14,14	3.53	8 (61%)
3	BMA	AuA	2	3	11,11,12	0.80	0	15,15,17	2.71	5 (33%)

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	AaA	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	AaA	2	2	-	5/6/23/26	0/1/1/1
2	BMA	AaA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	5	2	-	1/2/19/22	0/1/1/1
2	MAN	AaA	6	5,2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	7	2	-	1/2/19/22	0/1/1/1
3	DNO	AuA	1	3	-	14/15/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	AuA	2	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AuA	1	DNO	O3-C3	2.30	1.48	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AuA	1	DNO	O6-C6-C5	-6.30	97.92	111.16
3	AuA	2	BMA	C1-O5-C5	6.30	120.63	112.19
3	AuA	1	DNO	O3-C3-C2	-5.10	99.66	109.13
3	AuA	1	DNO	O2-C2-C3	5.00	121.17	109.46
3	AuA	2	BMA	C1-C2-C3	4.91	116.79	109.64
3	AuA	1	DNO	O2-C2-C1	-4.29	100.73	110.48
3	AuA	1	DNO	C6-C5-C4	4.19	120.71	112.17
3	AuA	2	BMA	O3-C3-C4	-3.74	101.56	110.38
2	AaA	2	NAG	C2-N2-C7	3.72	127.88	122.90
3	AuA	1	DNO	O5-C5-C6	3.69	117.42	109.03
3	AuA	2	BMA	O5-C5-C6	3.64	114.75	107.66
3	AuA	1	DNO	O3-C3-C4	3.32	117.22	109.46
2	AaA	1	NAG	C2-N2-C7	3.19	127.18	122.90
2	AaA	6	MAN	C1-C2-C3	2.99	114.00	109.64
2	AaA	1	NAG	C1-O5-C5	2.55	115.60	112.19
2	AaA	3	BMA	C1-O5-C5	2.45	115.47	112.19
3	AuA	2	BMA	C6-C5-C4	-2.40	107.13	113.02
2	AaA	1	NAG	C3-C4-C5	2.33	114.46	110.23
2	AaA	5	MAN	O3-C3-C4	2.26	115.69	110.38
3	AuA	1	DNO	C4-C3-C2	2.25	117.44	113.49
2	AaA	6	MAN	O2-C2-C1	-2.13	104.35	109.22
2	AaA	1	NAG	C1-C2-N2	2.13	113.78	110.43
2	AaA	3	BMA	C3-C4-C5	2.08	114.00	110.23
2	AaA	6	MAN	O6-C6-C5	-2.01	104.49	111.33

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AaA	2	NAG	C3-C2-N2-C7
3	AuA	1	DNO	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

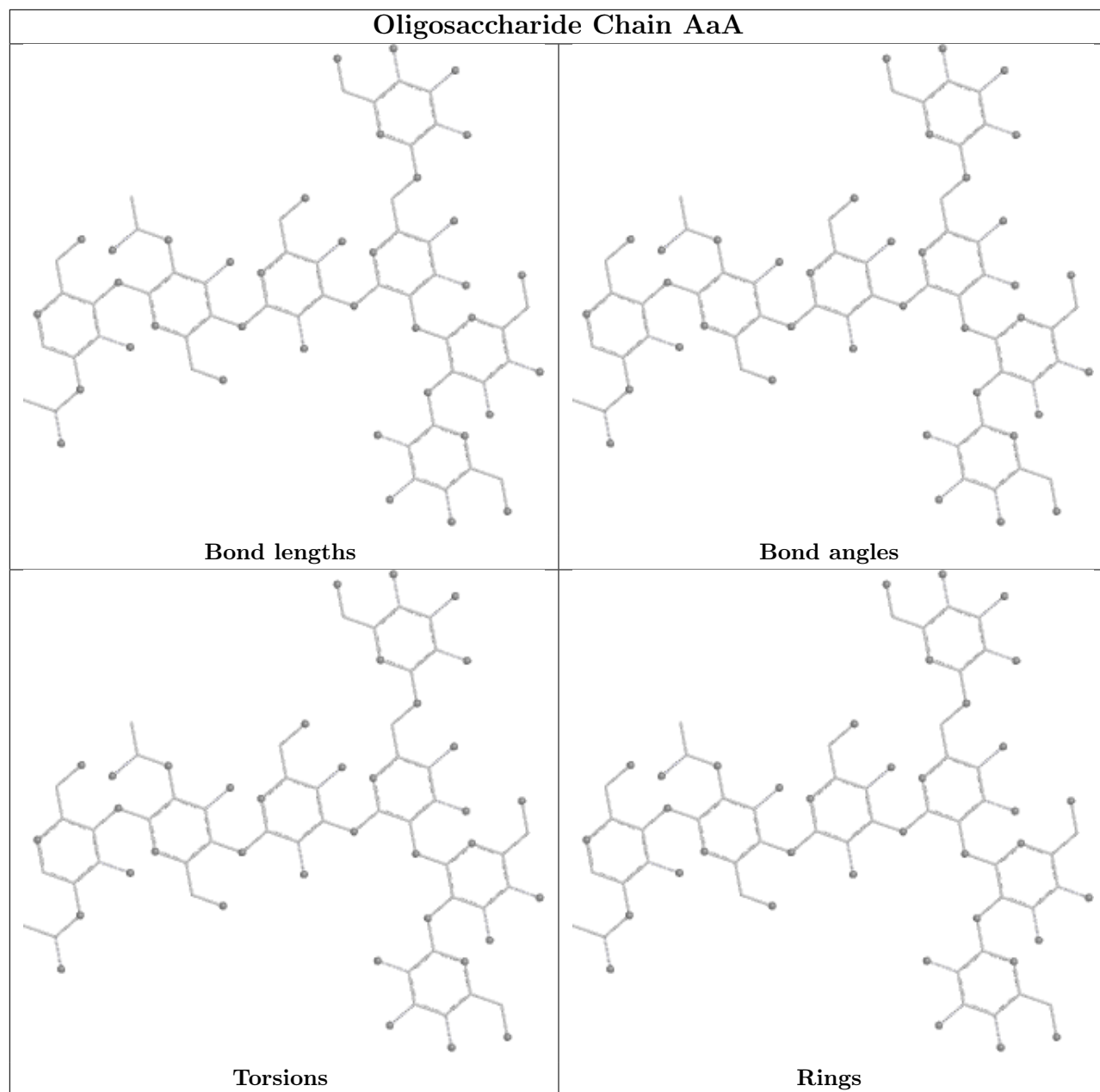
Mol	Chain	Res	Type	Atoms
3	AuA	1	DNO	C1-C2-C3-O3
3	AuA	1	DNO	O2-C2-C3-C4
3	AuA	1	DNO	O2-C2-C3-O3
3	AuA	1	DNO	C2-C3-C4-C5
3	AuA	1	DNO	C2-C3-C4-O4
3	AuA	1	DNO	O3-C3-C4-C5
3	AuA	1	DNO	C3-C4-C5-O5
3	AuA	1	DNO	O4-C4-C5-C6
3	AuA	1	DNO	O4-C4-C5-O5
3	AuA	1	DNO	C4-C5-C6-O6
3	AuA	1	DNO	O5-C5-C6-O6
2	AaA	2	NAG	C8-C7-N2-C2
2	AaA	2	NAG	O7-C7-N2-C2
3	AuA	1	DNO	C3-C4-C5-C6
3	AuA	1	DNO	O3-C3-C4-O4
3	AuA	2	BMA	O5-C5-C6-O6
2	AaA	1	NAG	C4-C5-C6-O6
2	AaA	1	NAG	O5-C5-C6-O6
3	AuA	2	BMA	C4-C5-C6-O6
2	AaA	2	NAG	C4-C5-C6-O6
2	AaA	7	MAN	O5-C5-C6-O6
2	AaA	5	MAN	C4-C5-C6-O6
2	AaA	2	NAG	O5-C5-C6-O6

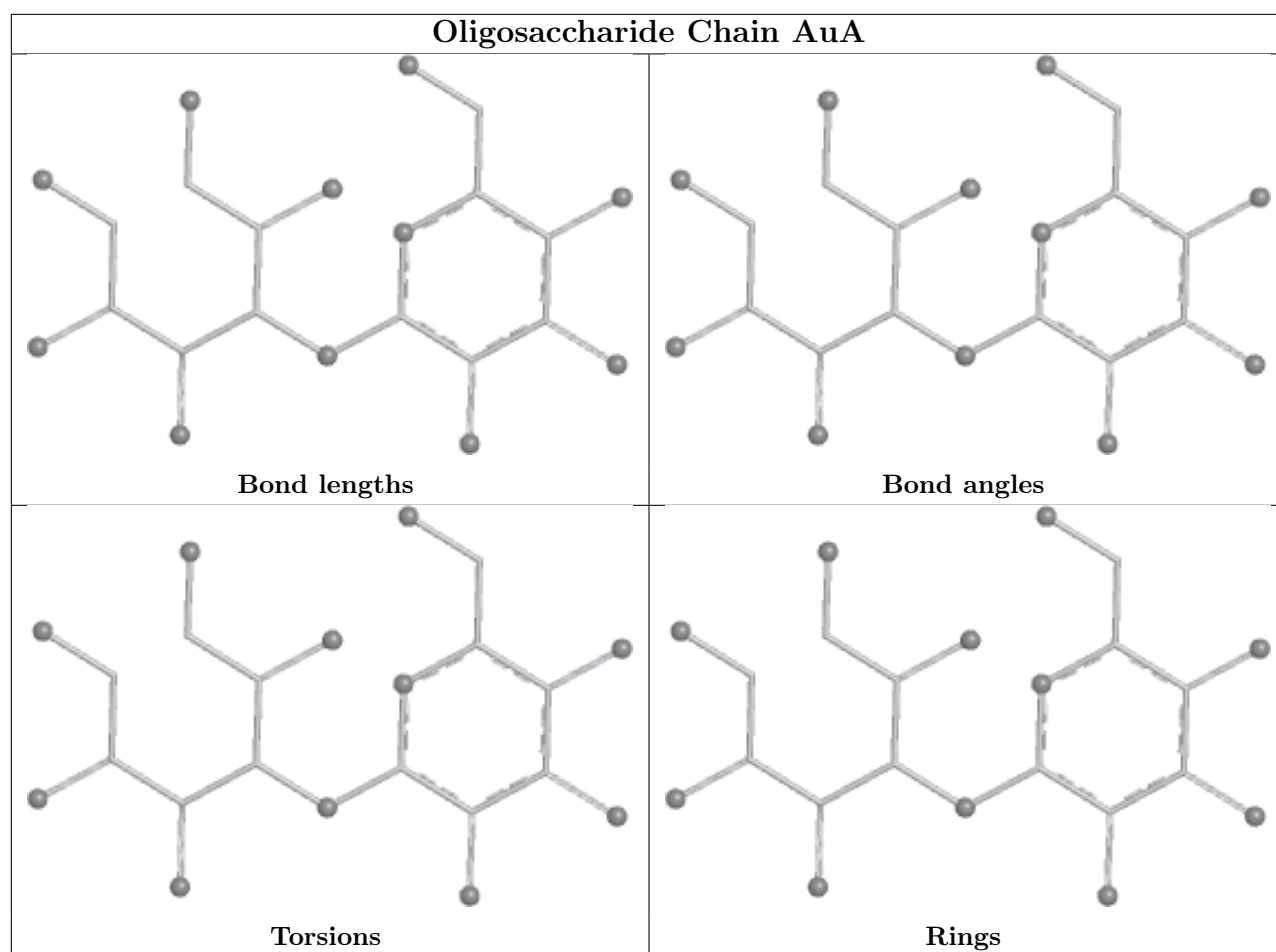
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AuA	2	BMA	0	1

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 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\# Z > 2$
4	EDO	AAA	401	-	3,3,3	0.42	0	2,2,2	0.24	0
7	SO4	AAA	418	-	4,4,4	0.30	0	6,6,6	0.11	0
4	EDO	AAA	404	-	3,3,3	0.35	0	2,2,2	0.78	0
4	EDO	AAA	406	-	3,3,3	0.26	0	2,2,2	0.61	0
7	SO4	AAA	416	-	4,4,4	0.30	0	6,6,6	0.10	0
7	SO4	AAA	417	-	4,4,4	0.32	0	6,6,6	0.11	0
4	EDO	AAA	410	-	3,3,3	0.39	0	2,2,2	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	AAA	412	-	3,3,3	0.15	0	2,2,2	0.30	0
4	EDO	AAA	407	-	3,3,3	0.38	0	2,2,2	0.70	0
4	EDO	AAA	413	-	3,3,3	0.19	0	2,2,2	0.13	0
7	SO4	AAA	420	-	4,4,4	0.28	0	6,6,6	0.12	0
4	EDO	AAA	411	-	3,3,3	0.17	0	2,2,2	0.53	0
4	EDO	AAA	405	-	3,3,3	0.22	0	2,2,2	0.20	0
4	EDO	AAA	408	-	3,3,3	0.18	0	2,2,2	0.60	0
4	EDO	AAA	409	-	3,3,3	0.45	0	2,2,2	0.25	0
7	SO4	AAA	419	-	4,4,4	0.32	0	6,6,6	0.08	0
4	EDO	AAA	403	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	AAA	402	-	3,3,3	0.07	0	2,2,2	0.66	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	EDO	AAA	401	-	-	0/1/1/1	-
4	EDO	AAA	404	-	-	1/1/1/1	-
4	EDO	AAA	406	-	-	1/1/1/1	-
4	EDO	AAA	410	-	-	1/1/1/1	-
4	EDO	AAA	412	-	-	0/1/1/1	-
4	EDO	AAA	407	-	-	1/1/1/1	-
4	EDO	AAA	413	-	-	0/1/1/1	-
4	EDO	AAA	411	-	-	1/1/1/1	-
4	EDO	AAA	405	-	-	0/1/1/1	-
4	EDO	AAA	408	-	-	0/1/1/1	-
4	EDO	AAA	409	-	-	1/1/1/1	-
4	EDO	AAA	403	-	-	1/1/1/1	-
4	EDO	AAA	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	403	EDO	O1-C1-C2-O2
4	AAA	404	EDO	O1-C1-C2-O2
4	AAA	409	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

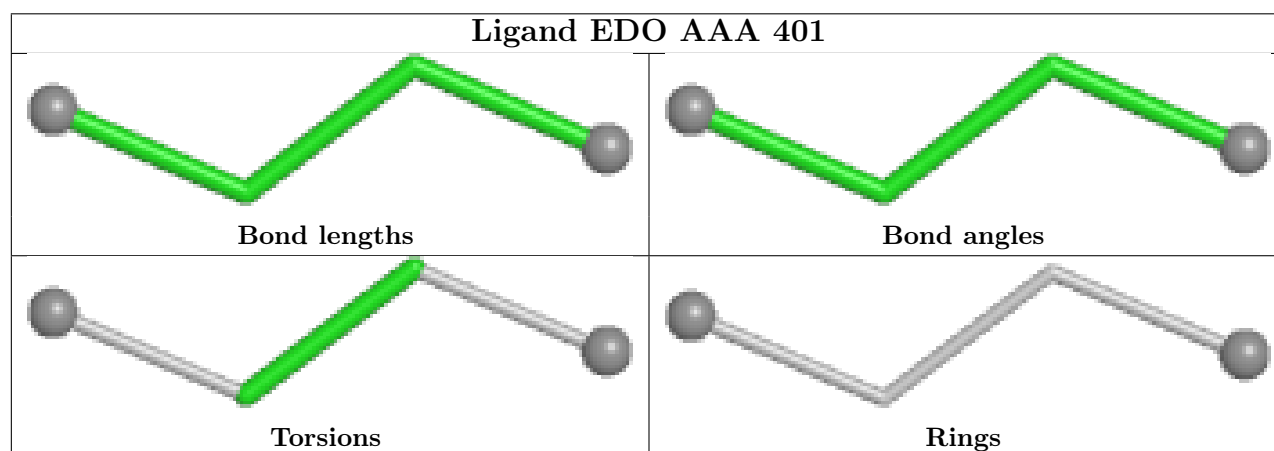
Mol	Chain	Res	Type	Atoms
4	AAA	407	EDO	O1-C1-C2-O2
4	AAA	410	EDO	O1-C1-C2-O2
4	AAA	411	EDO	O1-C1-C2-O2
4	AAA	406	EDO	O1-C1-C2-O2

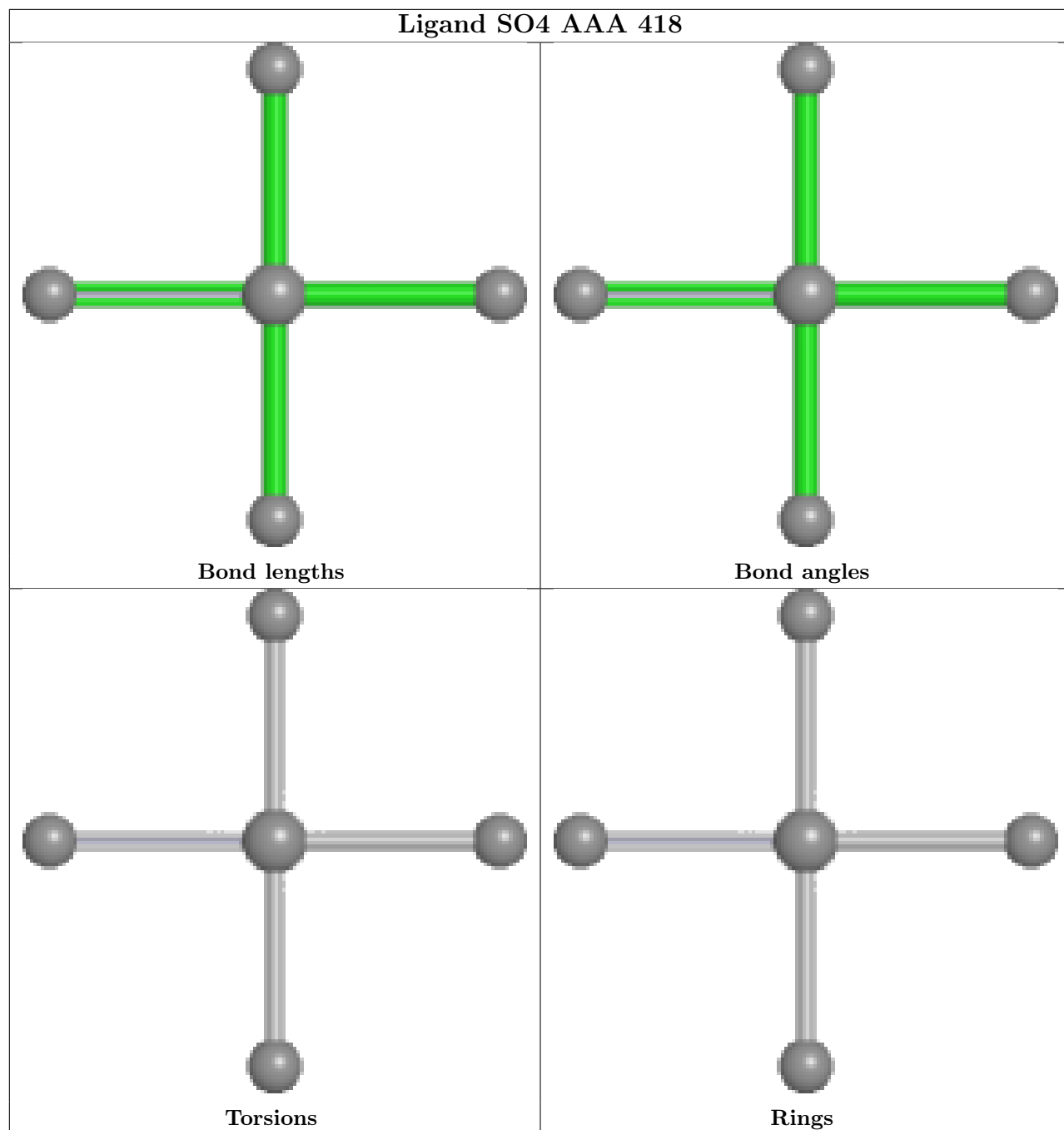
There are no ring outliers.

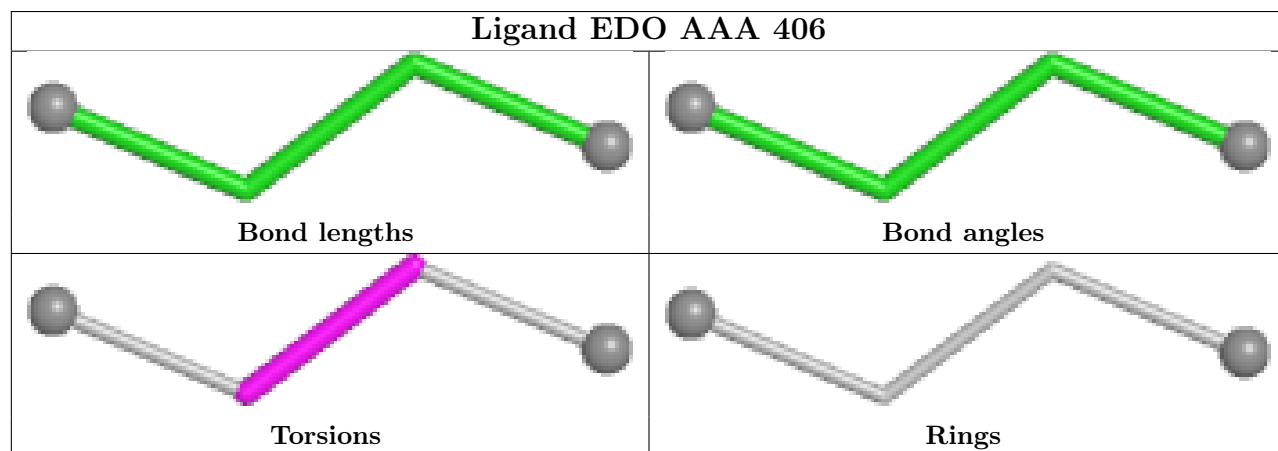
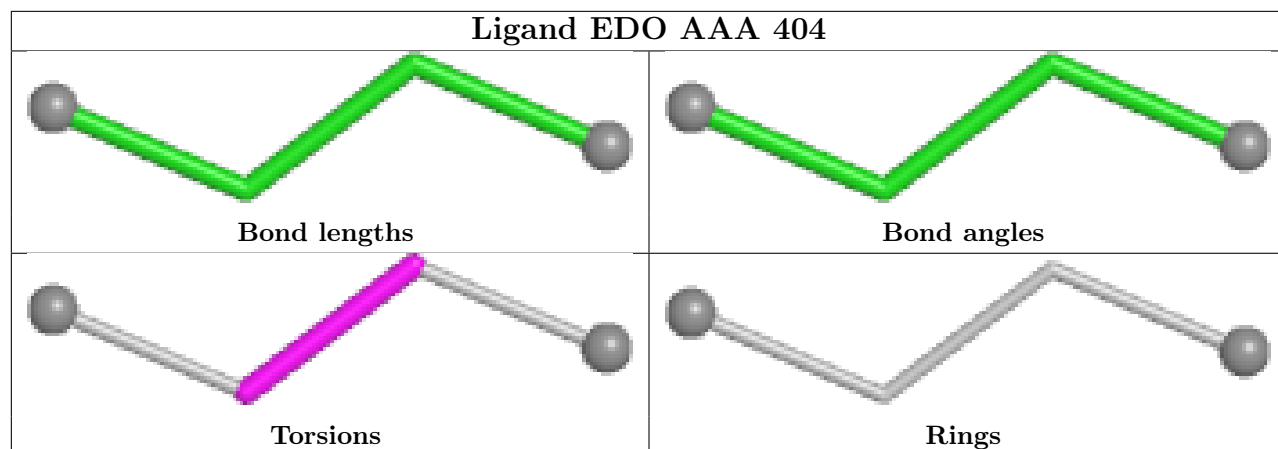
4 monomers are involved in 4 short contacts:

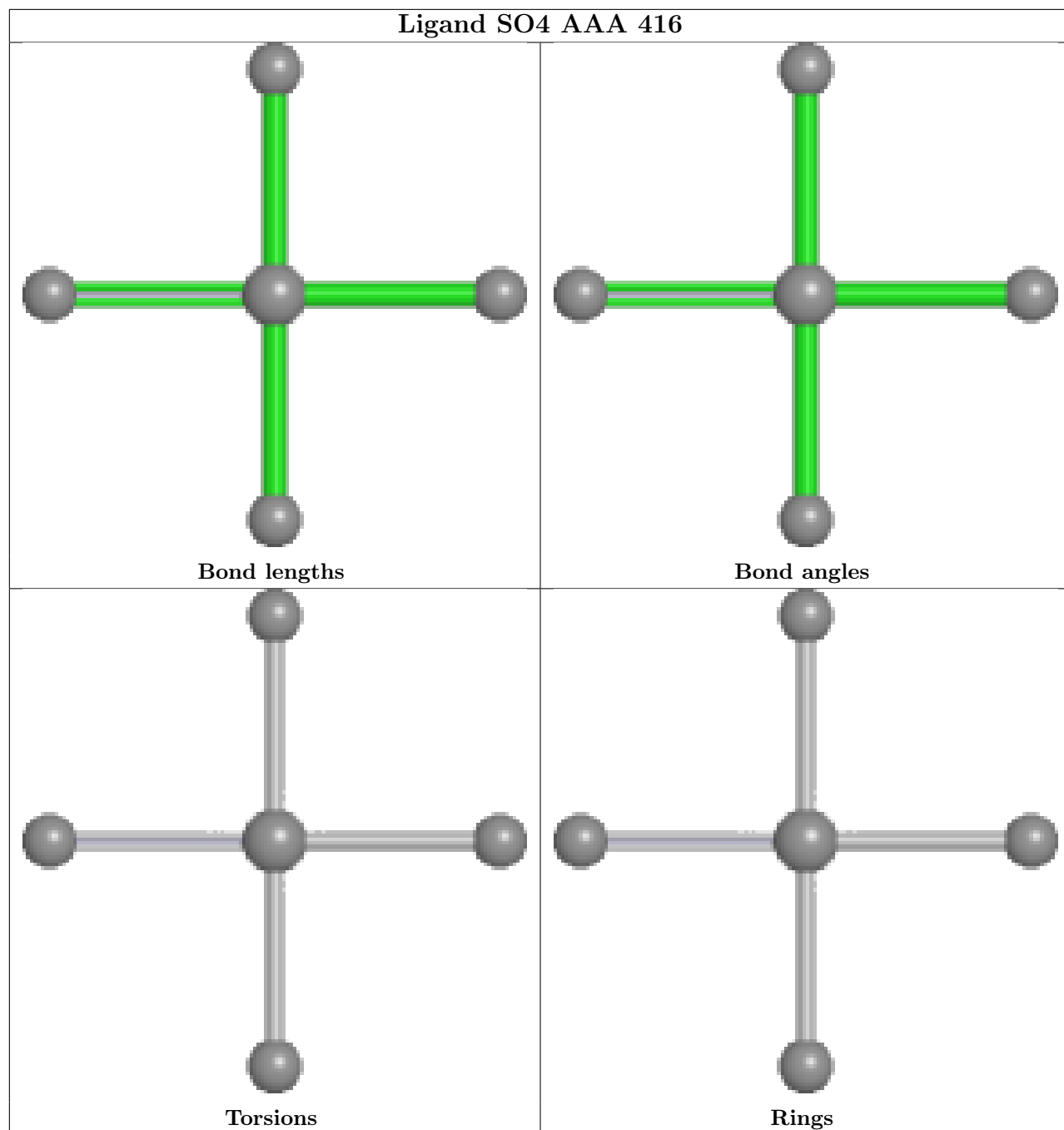
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	411	EDO	1	0
4	AAA	408	EDO	1	0
4	AAA	403	EDO	1	0
4	AAA	402	EDO	1	0

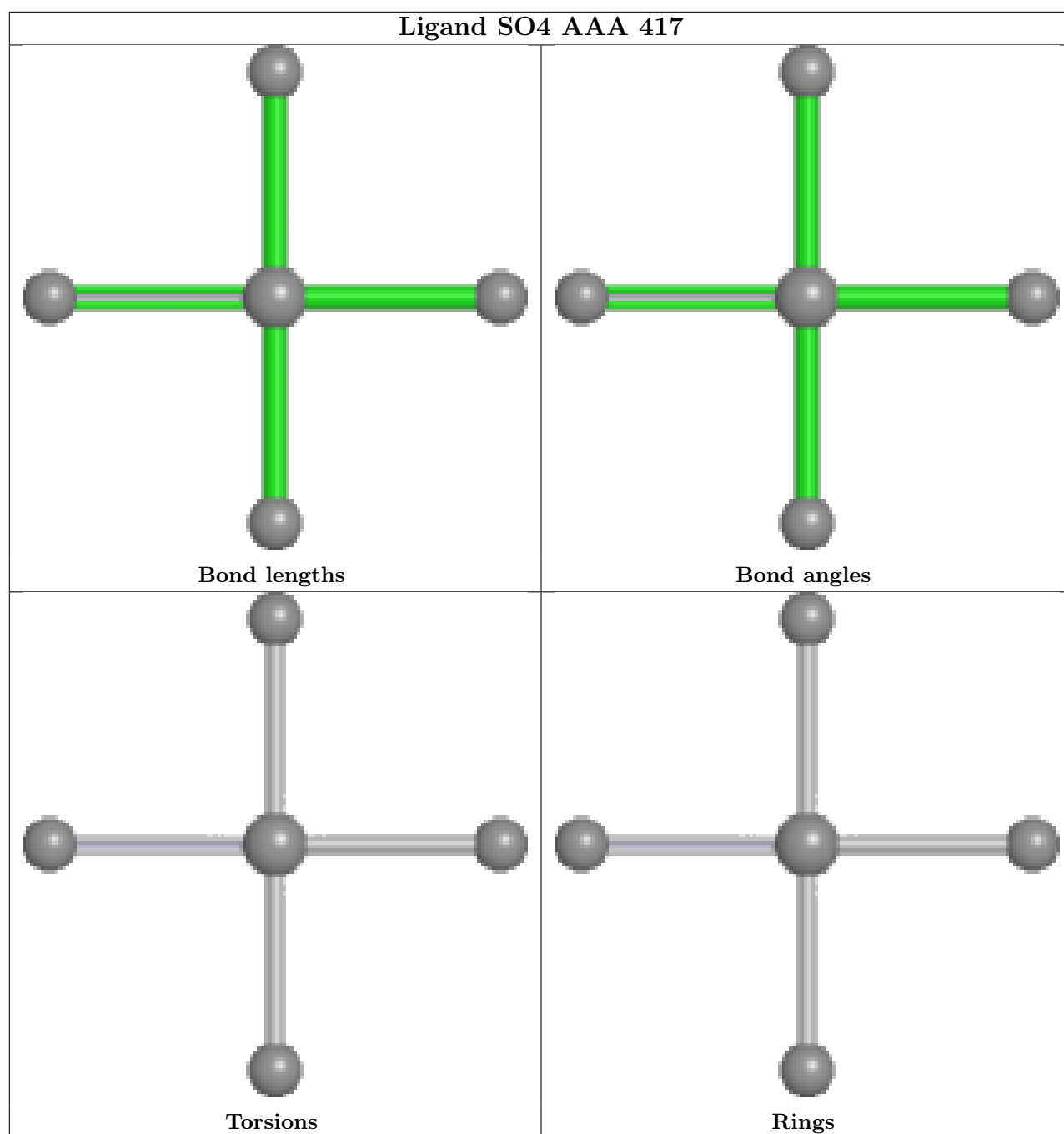
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

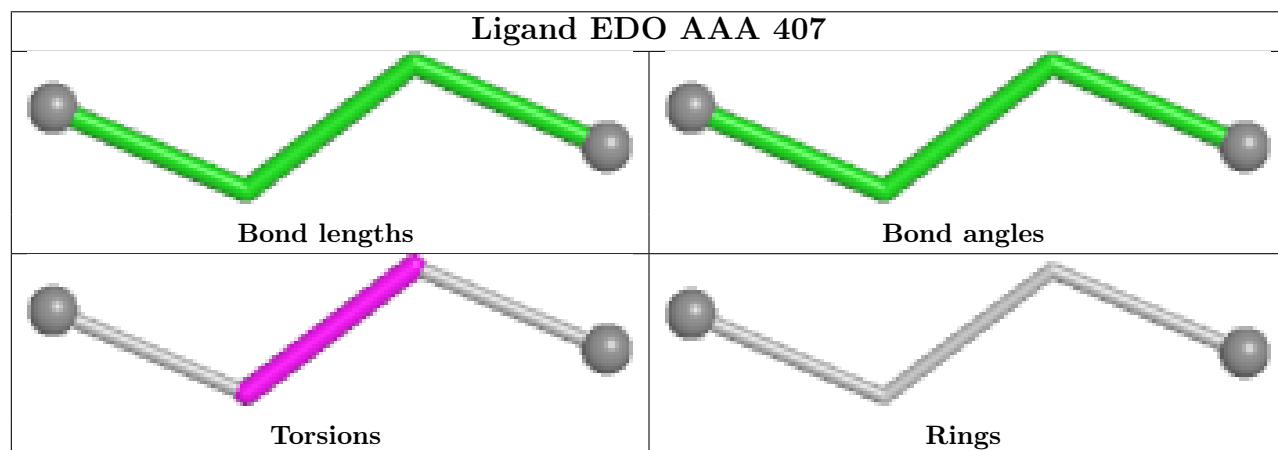
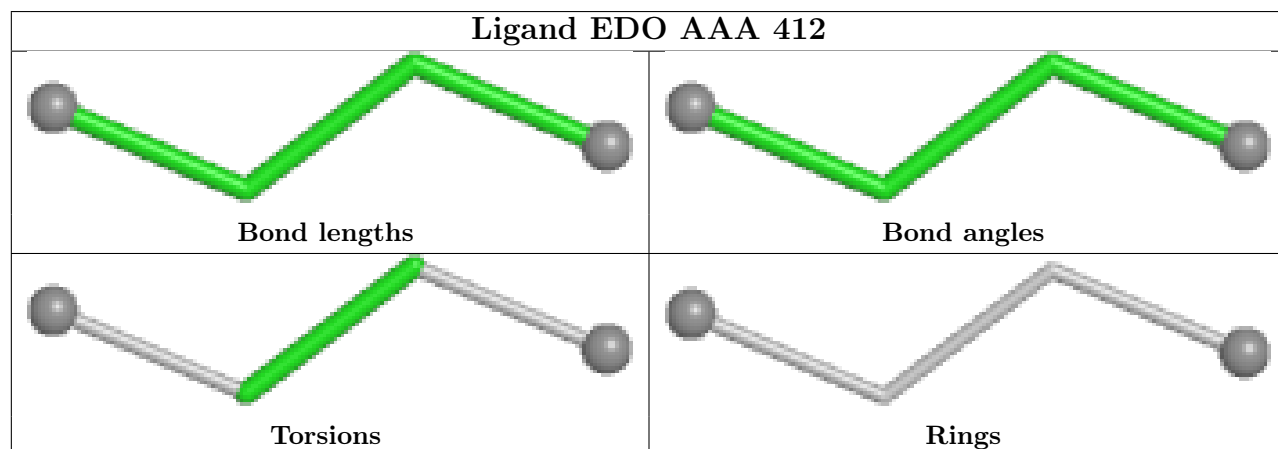
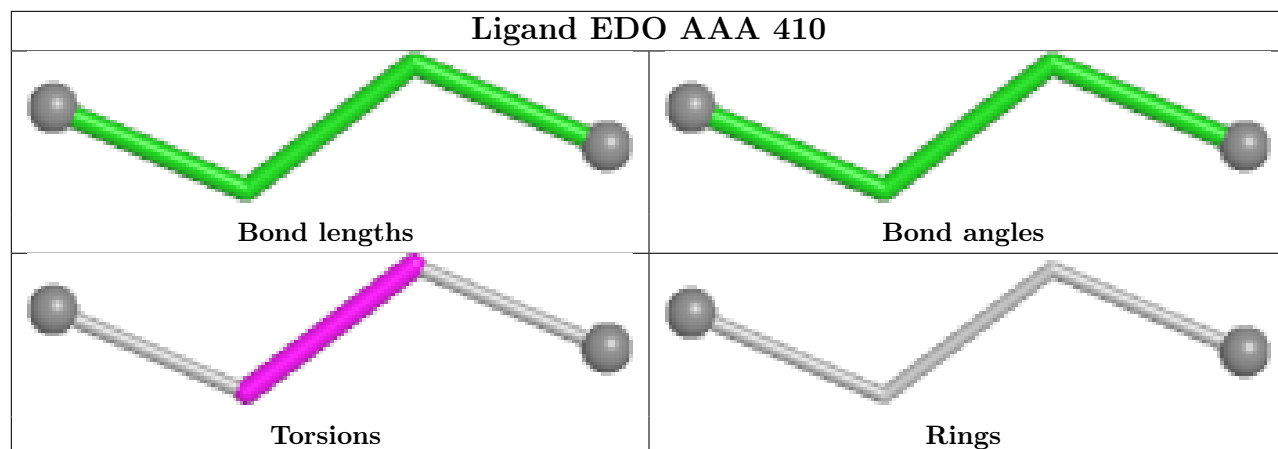


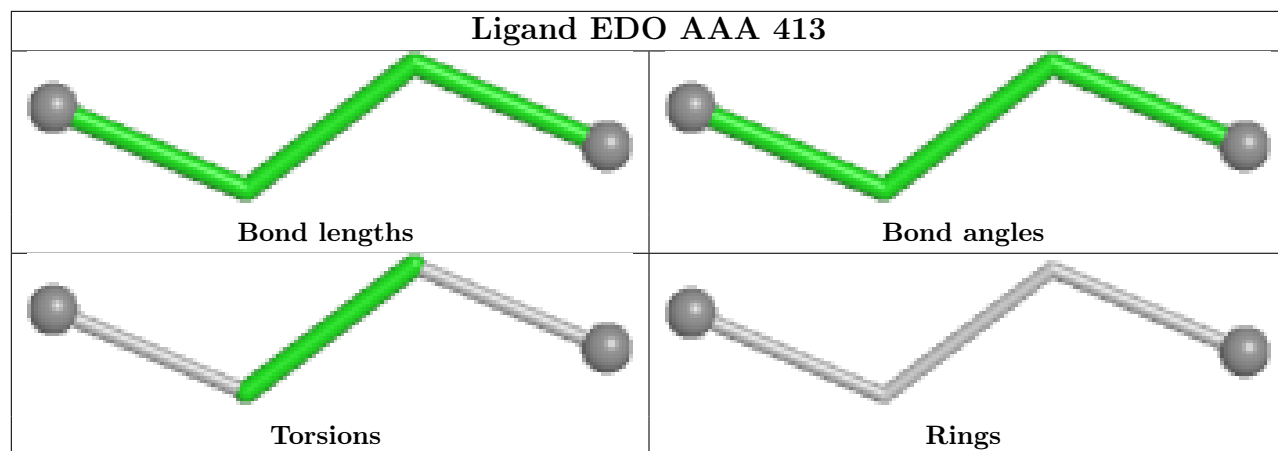


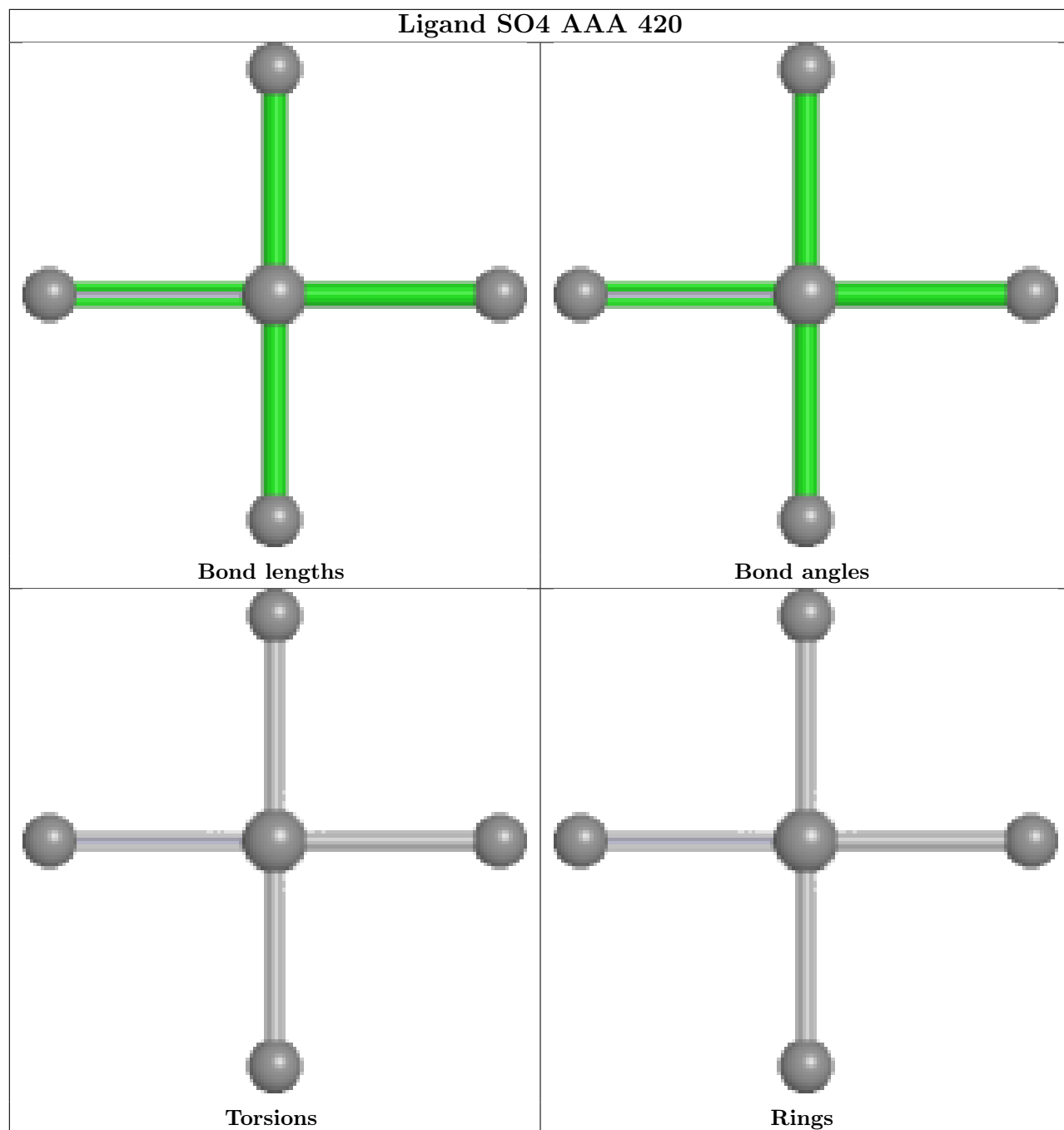


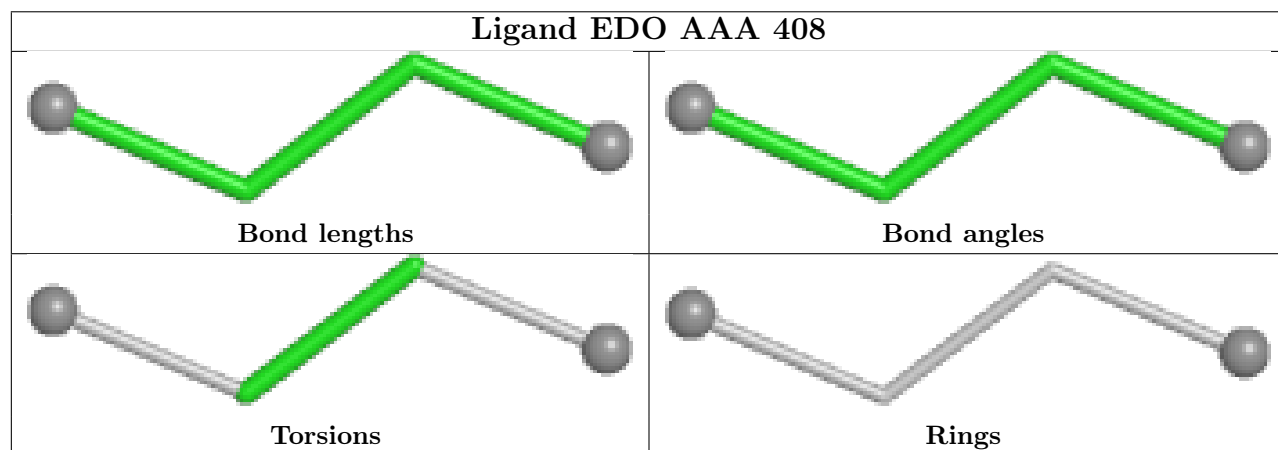
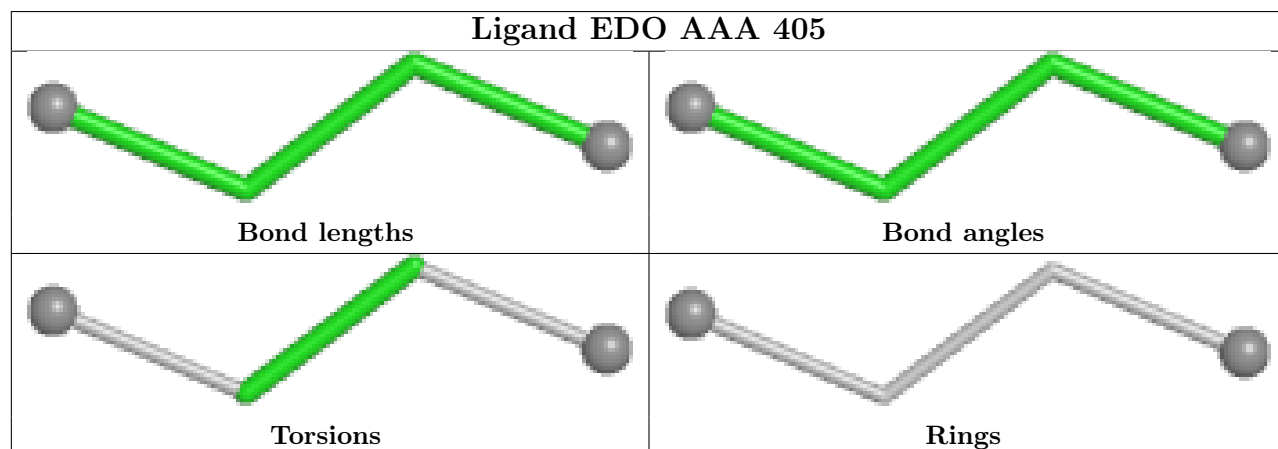
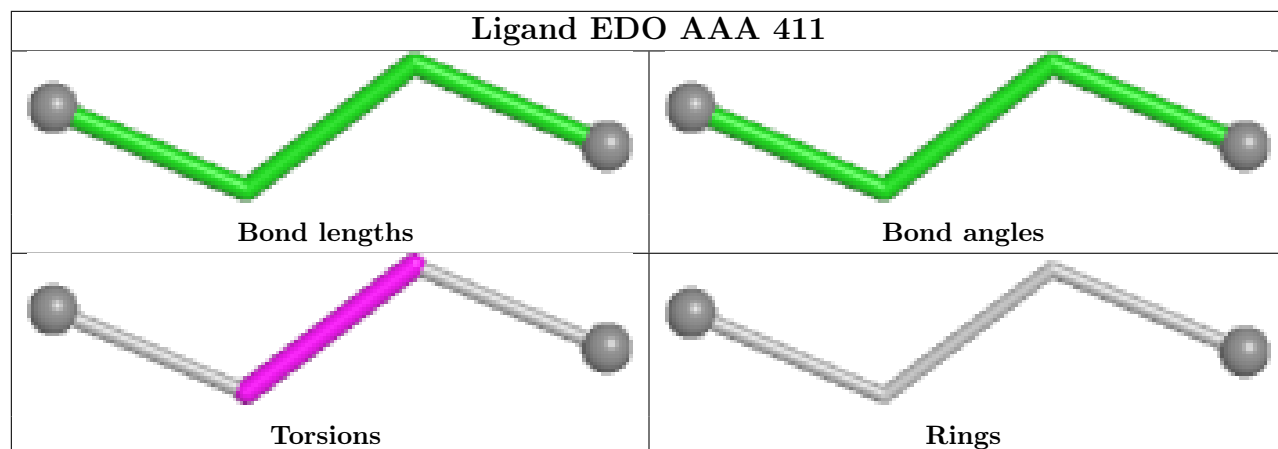


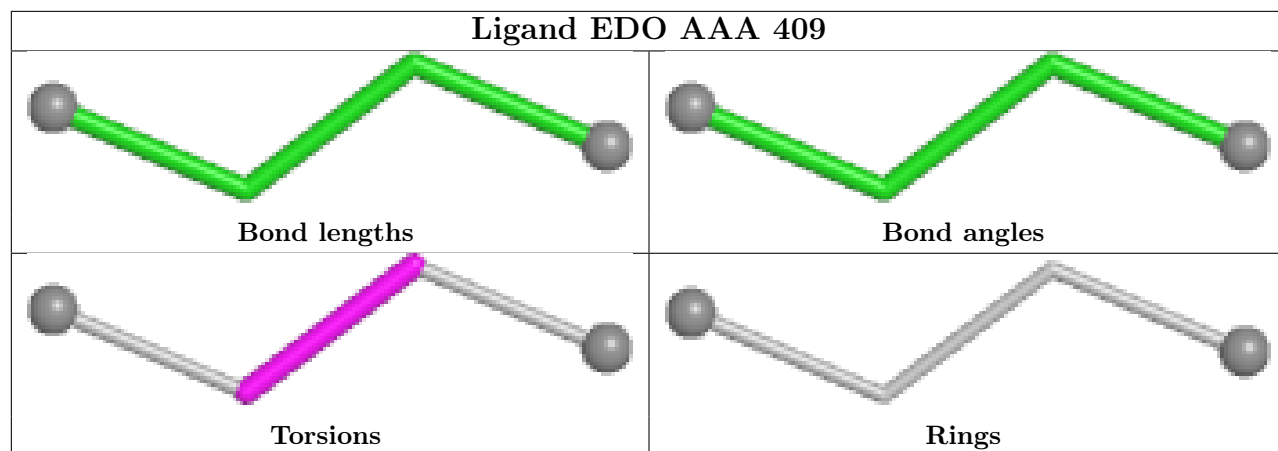


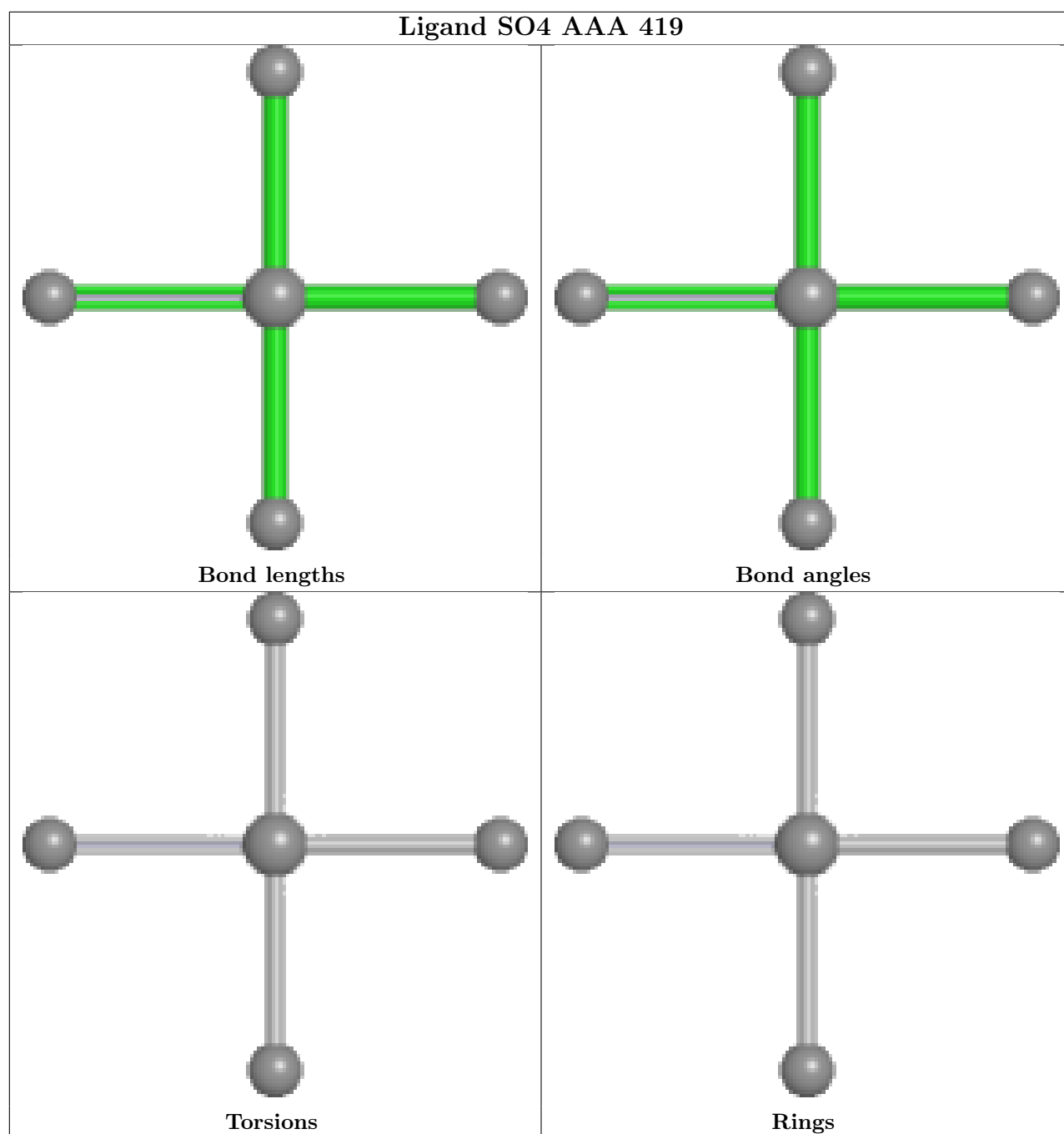


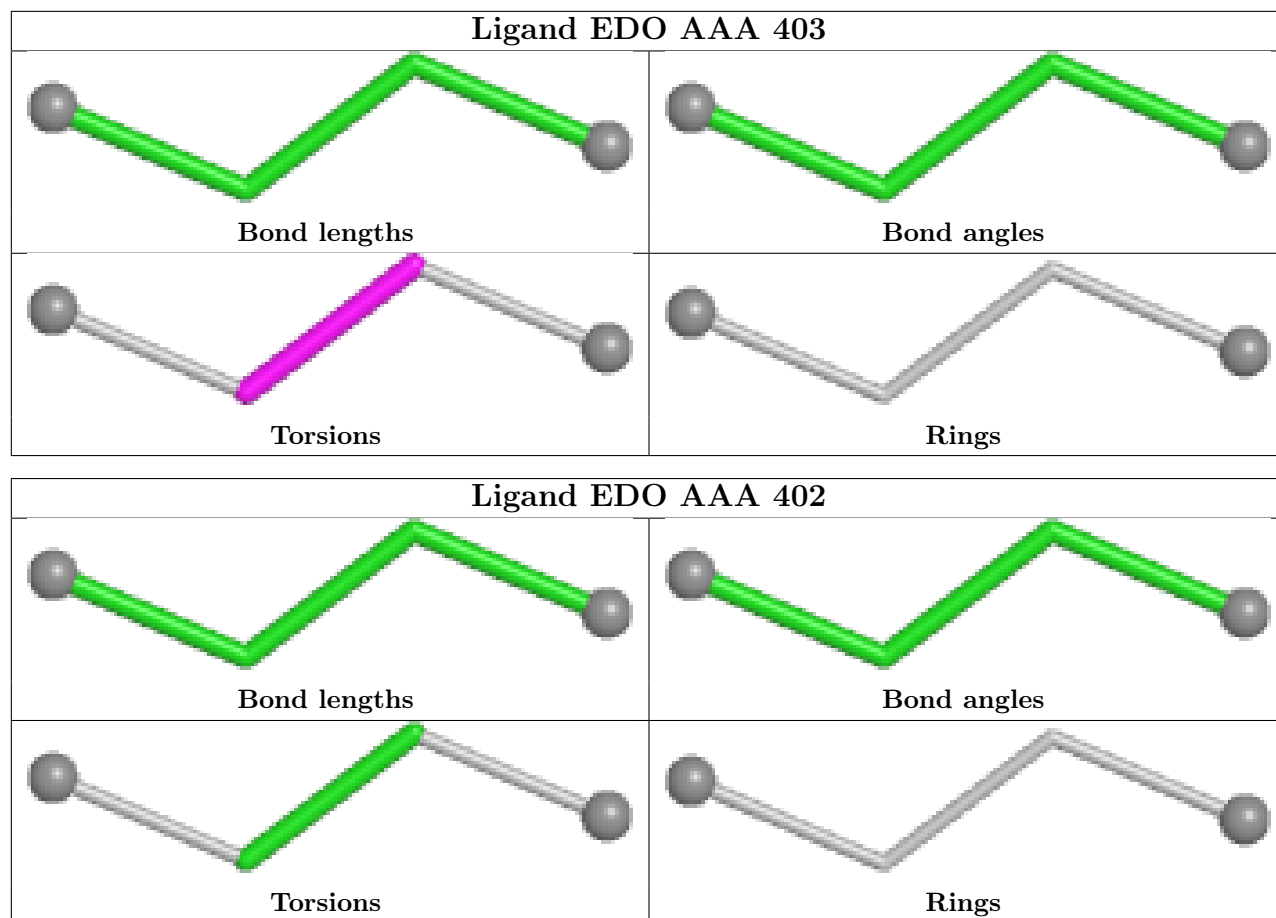












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	388/388 (100%)	-0.18	14 (3%)	46 53	7, 17, 32, 69	14 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	300	VAL	8.4
1	AAA	302	ALA	5.9
1	AAA	308	GLY	3.7
1	AAA	310	VAL	3.5
1	AAA	307	LYS	3.3
1	AAA	301	SER	2.9
1	AAA	303	LYS	2.6
1	AAA	304	PRO	2.6
1	AAA	134[A]	TYR	2.4
1	AAA	299	ASN	2.4
1	AAA	28	VAL	2.3
1	AAA	306	MET	2.2
1	AAA	253[A]	PRO	2.1
1	AAA	309	GLY	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](#)

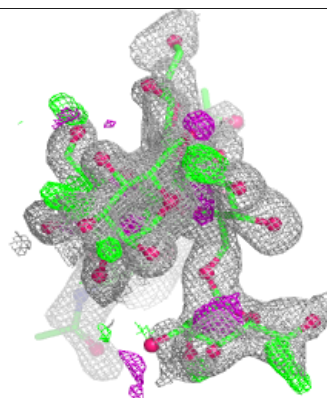
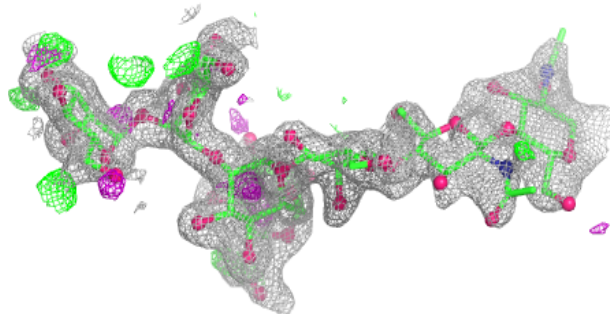
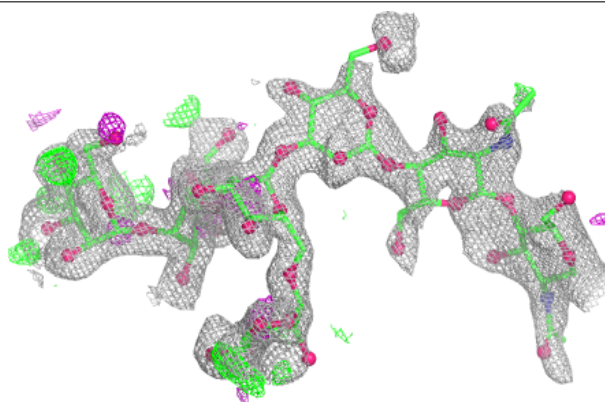
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

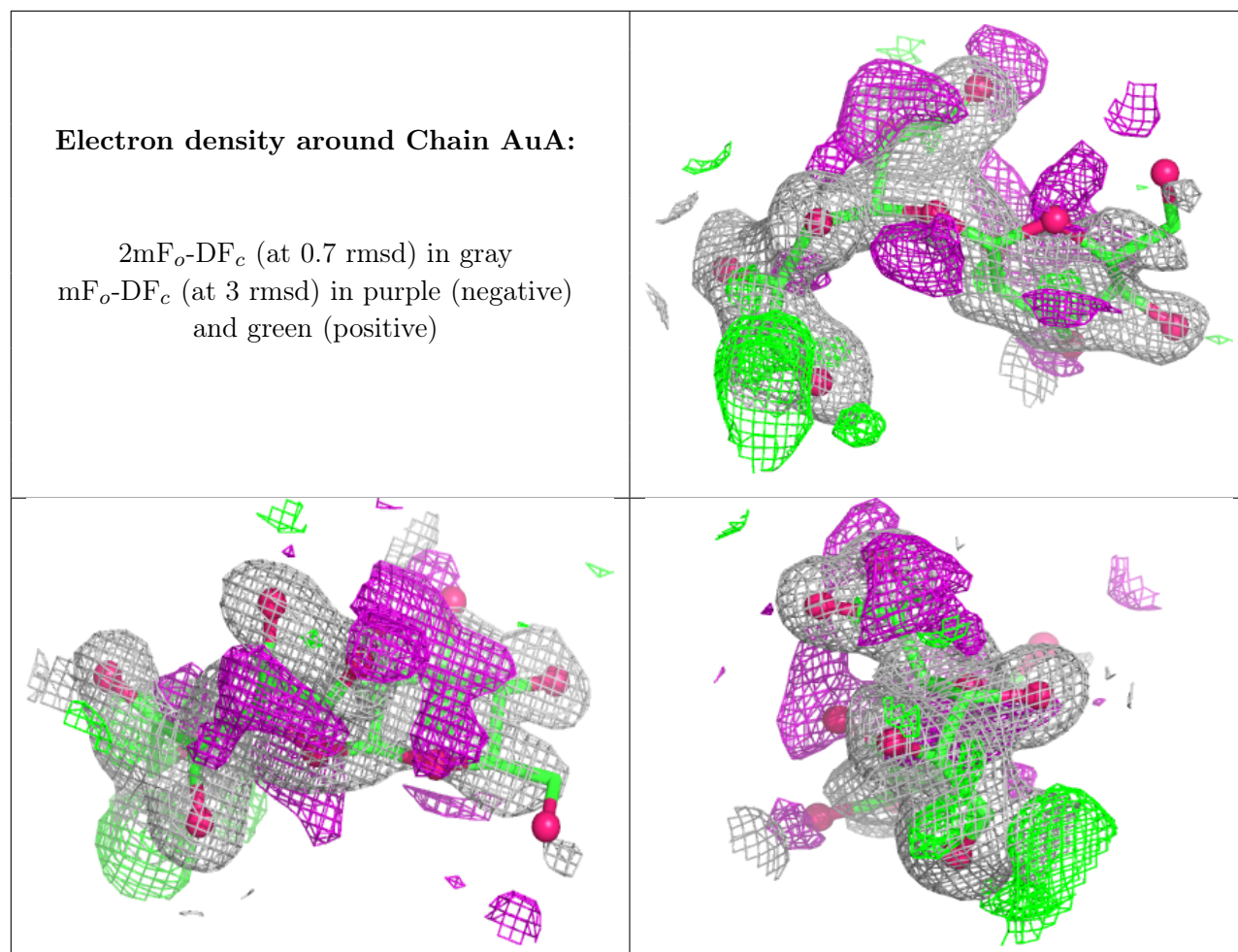
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	AaA	1	14/15	-	-	48,58,67,70	0
2	NAG	AaA	2	14/15	-	-	65,70,73,73	0
2	BMA	AaA	3	11/12	-	-	42,57,64,69	0
2	MAN	AaA	4	11/12	-	-	31,40,44,45	0
2	MAN	AaA	5	11/12	-	-	29,37,44,45	0
2	MAN	AaA	6	11/12	-	-	24,29,38,51	0
2	MAN	AaA	7	11/12	-	-	40,60,65,67	0
3	DNO	AuA	1	12/12	-	-	24,35,41,42	0
3	BMA	AuA	2	11/12	-	-	65,73,85,88	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 AaA:

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($\text{\AA}^2$)	Q<0.9
4	EDO	AAA	409	4/4	0.75	0.19	59,61,63,63	0
4	EDO	AAA	407	4/4	0.76	0.22	53,55,58,61	0
7	SO4	AAA	419	5/5	0.76	0.16	124,125,132,135	0
7	SO4	AAA	418	5/5	0.78	0.15	88,92,100,106	0
7	SO4	AAA	416	5/5	0.79	0.20	109,118,130,130	0
4	EDO	AAA	411	4/4	0.81	0.20	63,64,64,69	0
4	EDO	AAA	408	4/4	0.81	0.17	37,42,46,47	0
7	SO4	AAA	420	5/5	0.81	0.14	71,76,80,82	0
4	EDO	AAA	405	4/4	0.83	0.15	45,47,48,49	0
4	EDO	AAA	404	4/4	0.84	0.19	33,41,44,46	0
7	SO4	AAA	417	5/5	0.85	0.12	58,68,72,76	0

Continued on next page...

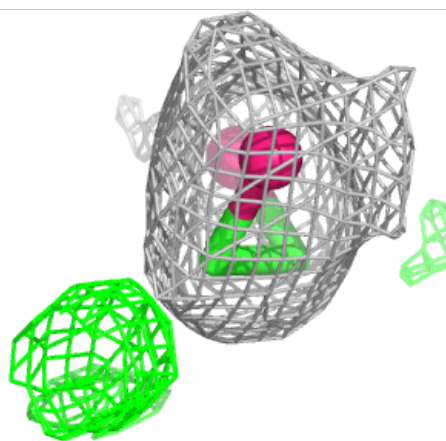
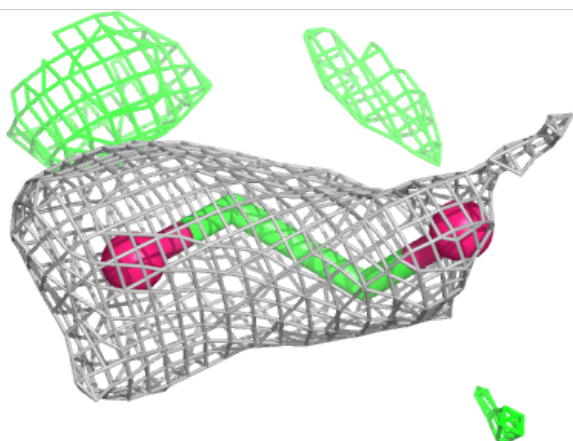
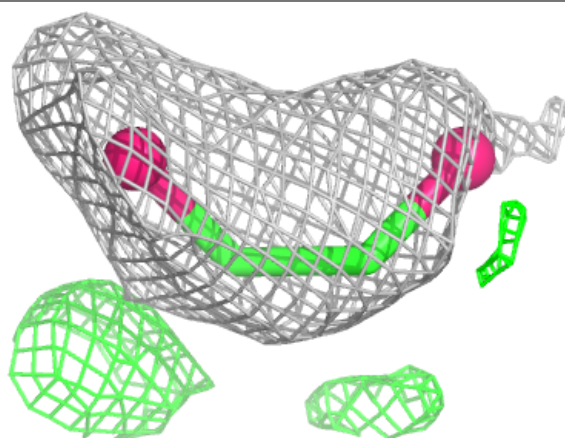
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	AAA	403	4/4	0.89	0.17	18,24,25,41	0
4	EDO	AAA	406	4/4	0.90	0.16	30,39,43,57	0
4	EDO	AAA	402	4/4	0.91	0.12	26,33,36,40	0
4	EDO	AAA	413	4/4	0.92	0.09	33,34,37,38	0
4	EDO	AAA	412	4/4	0.92	0.10	25,29,31,33	0
4	EDO	AAA	401	4/4	0.95	0.10	21,25,27,28	0
4	EDO	AAA	410	4/4	0.95	0.09	20,33,37,42	0
8	NA	AAA	421	1/1	0.98	0.10	21,21,21,21	0
5	ZN	AAA	414	1/1	1.00	0.01	15,15,15,15	0
6	CA	AAA	415	1/1	1.00	0.01	13,13,13,13	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.

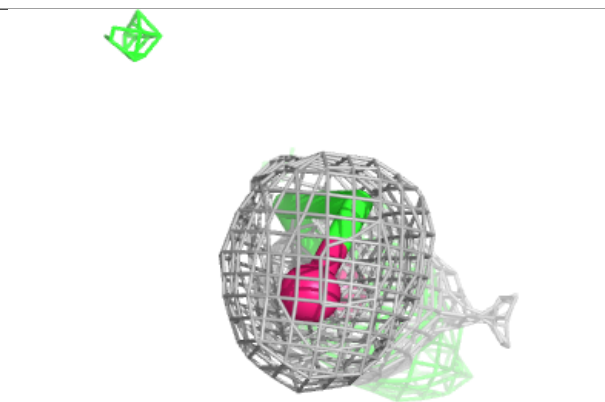
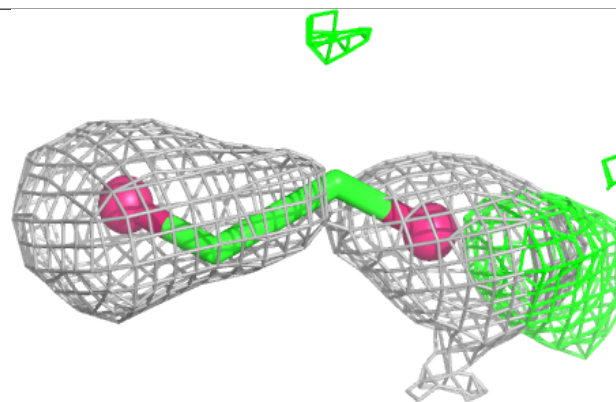
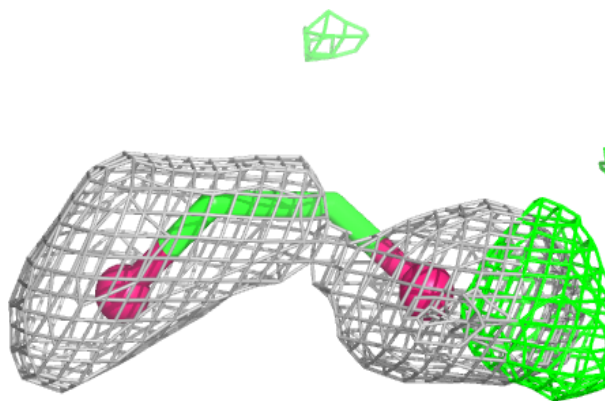
Electron density around EDO AAA 409:

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



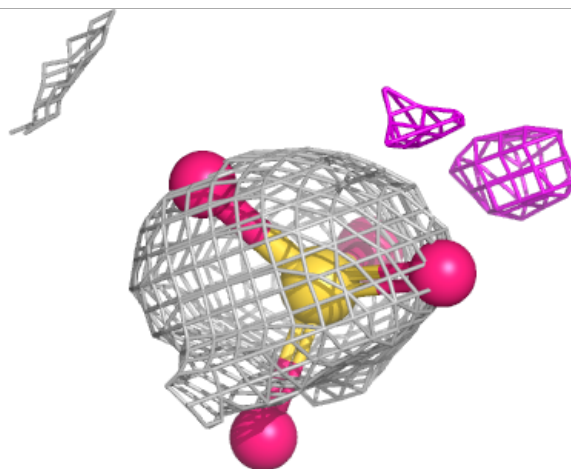
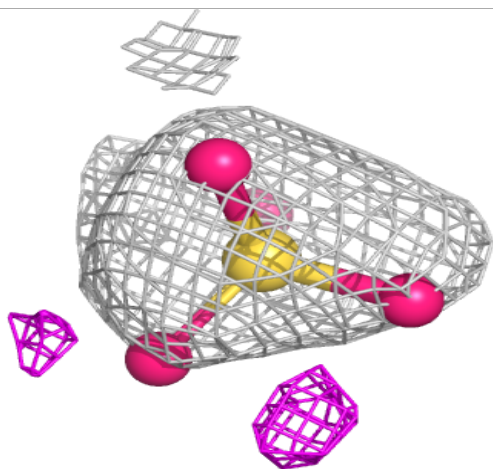
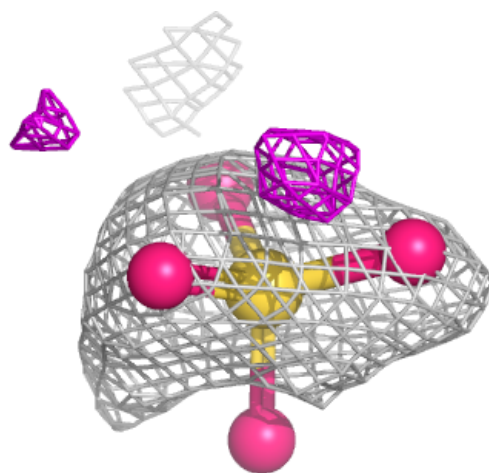
Electron density around EDO AAA 407:

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



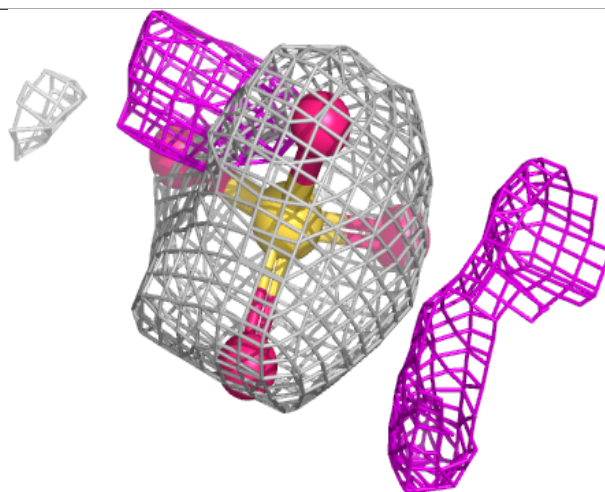
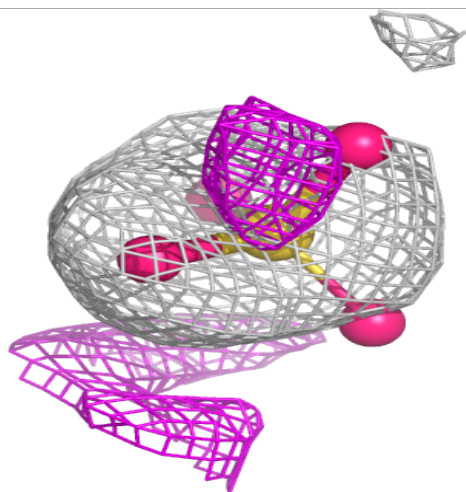
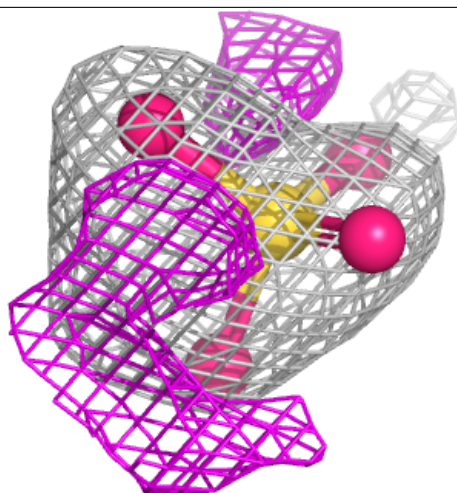
Electron density around SO4 AAA 419:

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



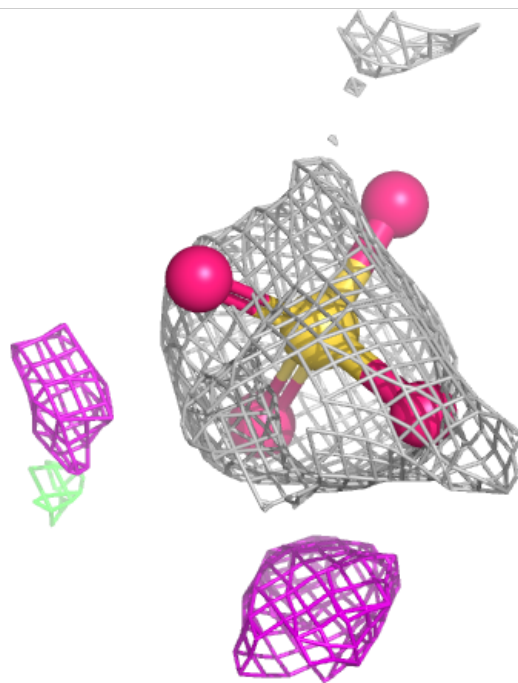
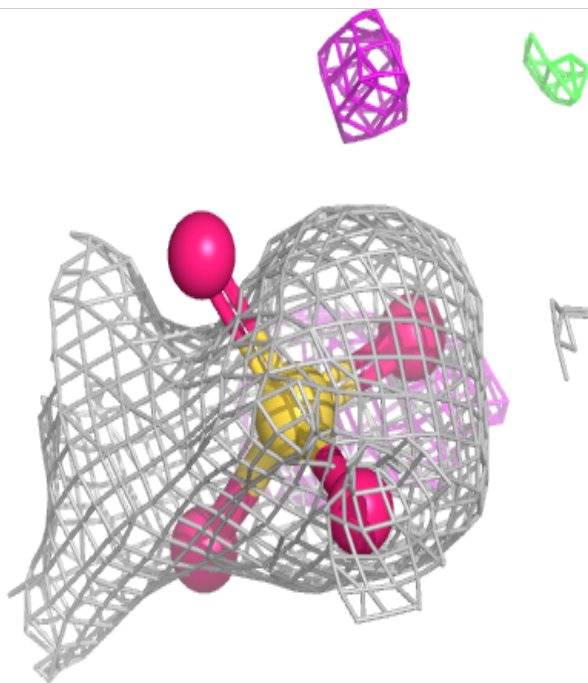
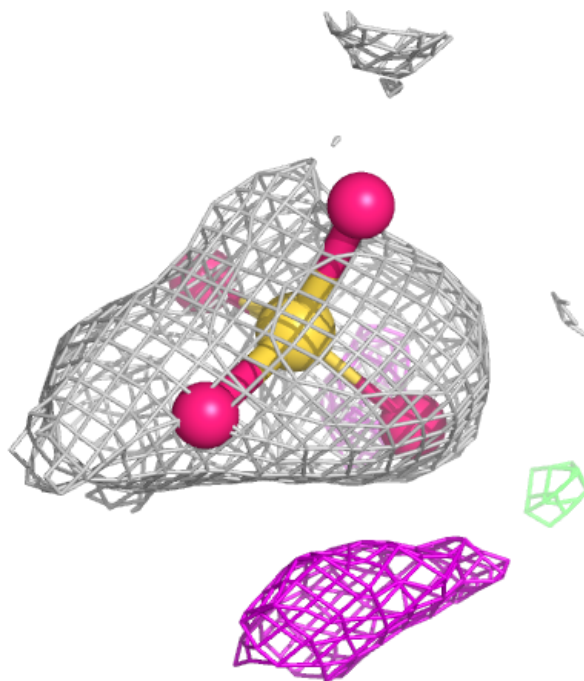
Electron density around SO4 AAA 418:

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



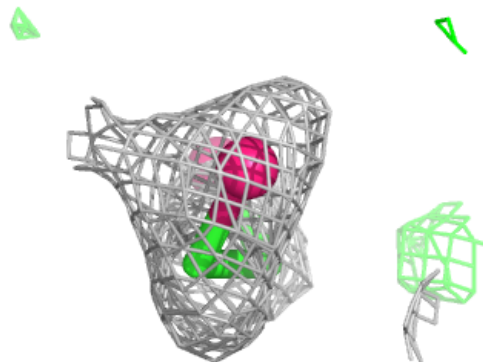
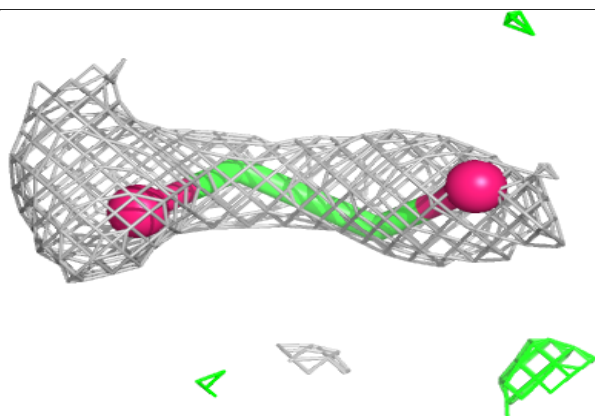
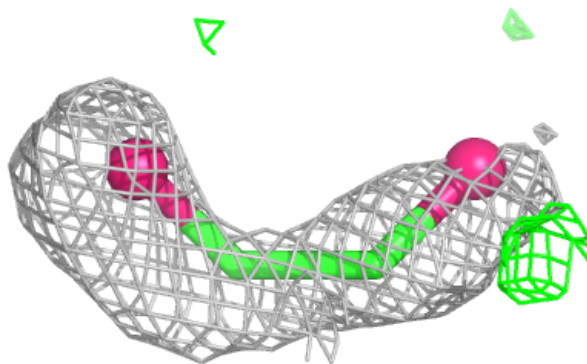
Electron density around SO4 AAA 416:

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

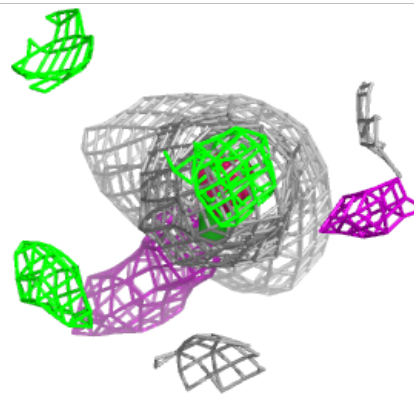
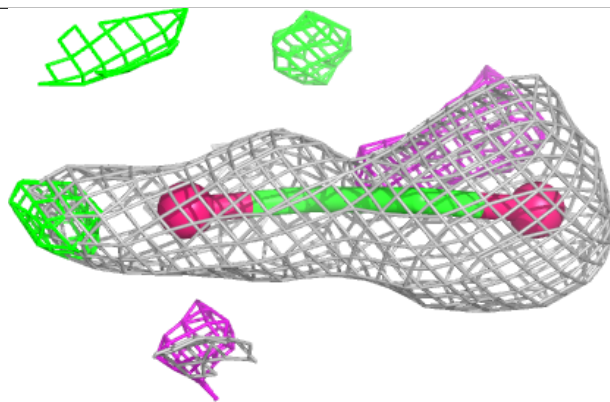
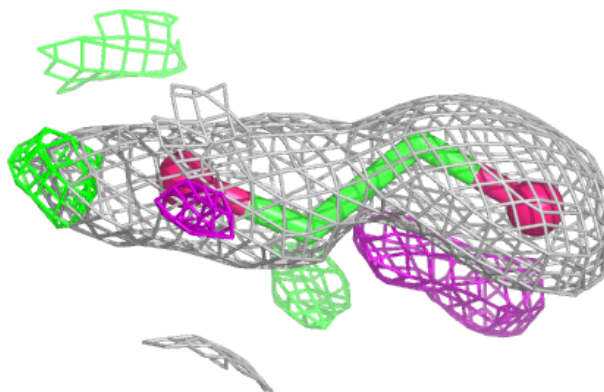


Electron density around EDO AAA 411:

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

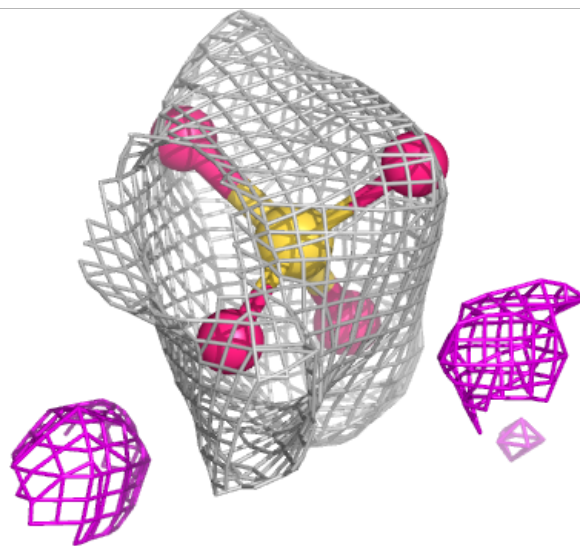
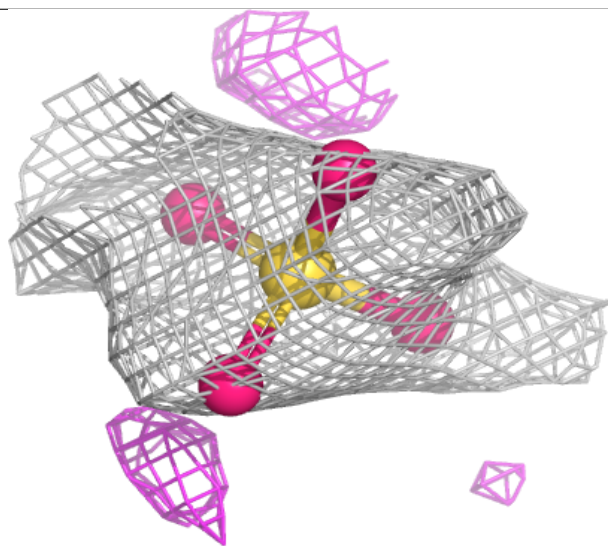
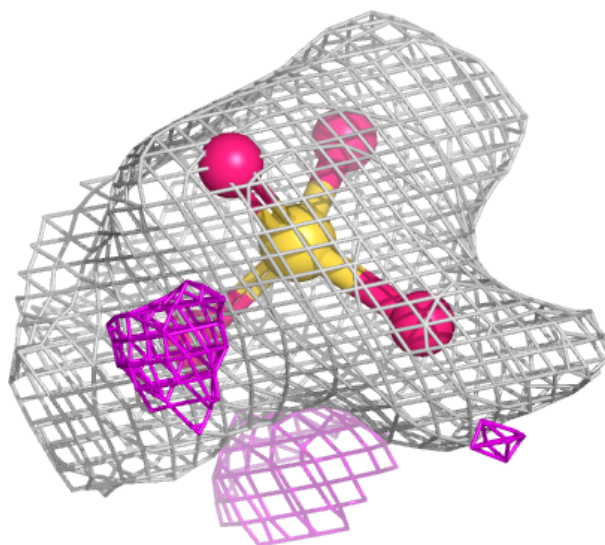
**Electron density around EDO AAA 408:**

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



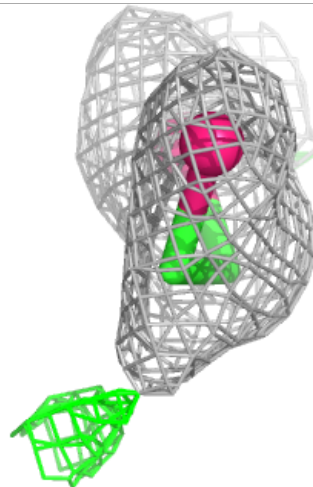
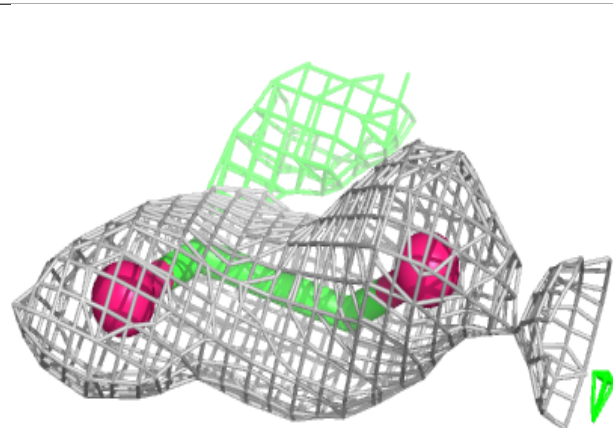
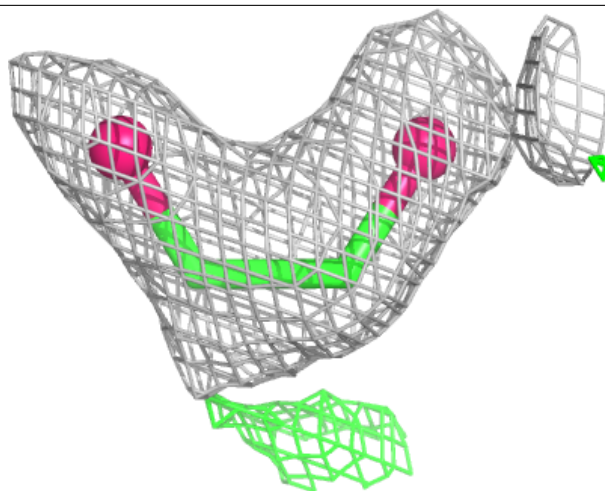
Electron density around SO4 AAA 420:

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



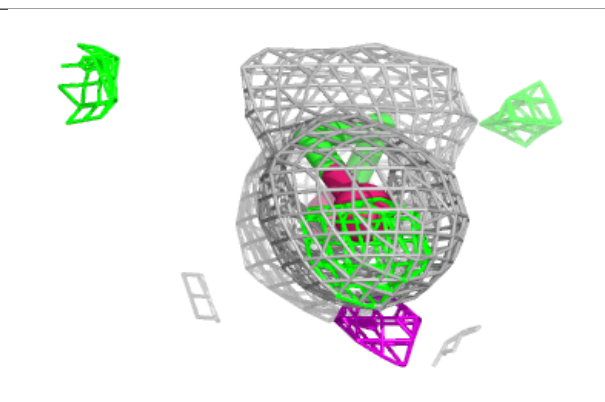
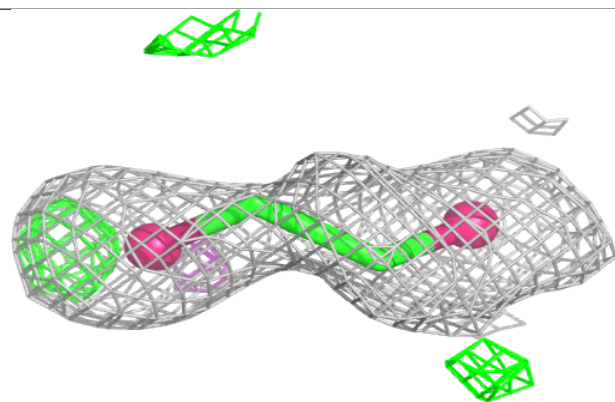
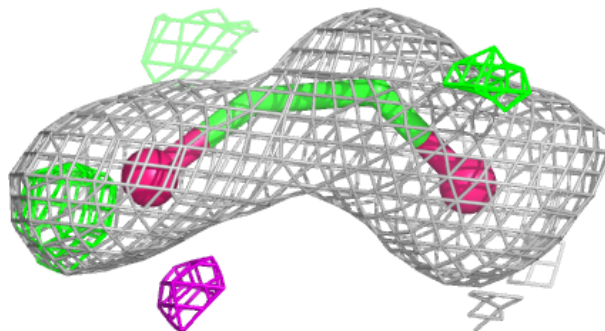
Electron density around EDO AAA 405:

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



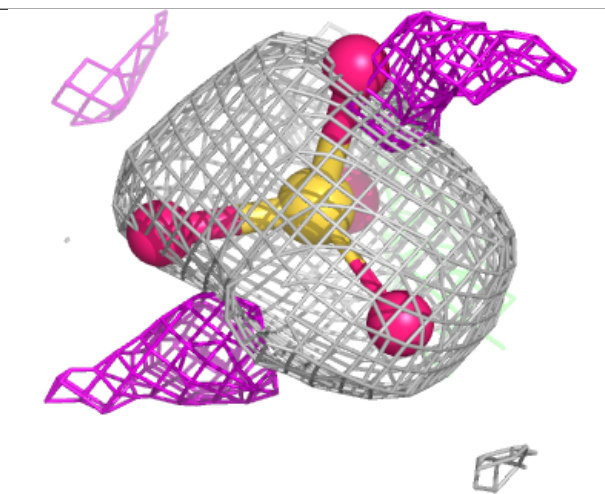
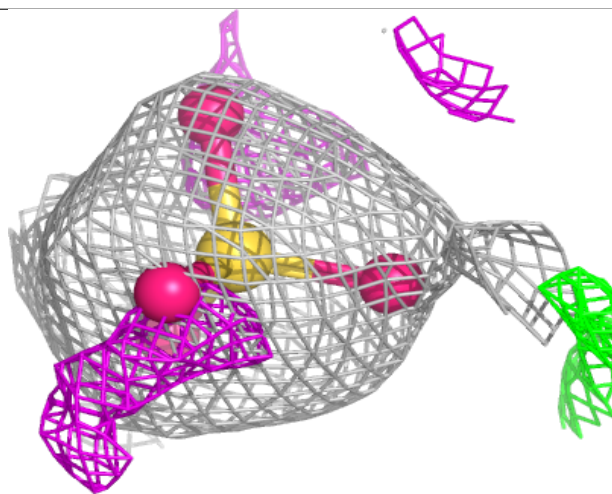
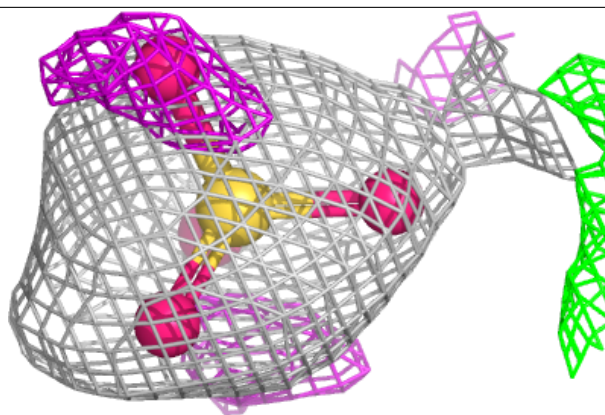
Electron density around EDO AAA 404:

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



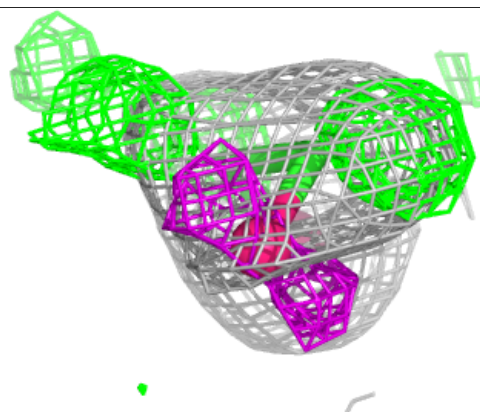
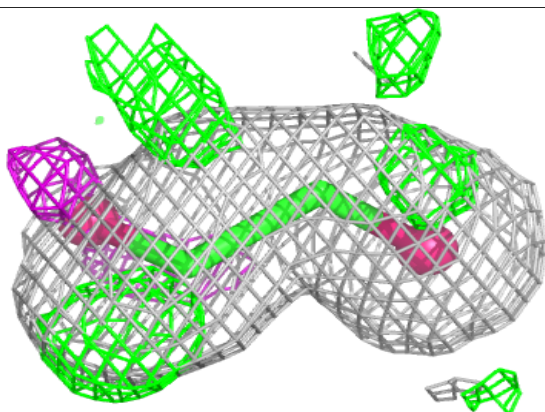
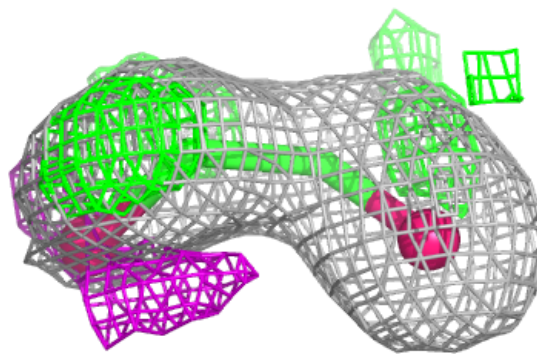
Electron density around SO4 AAA 417:

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



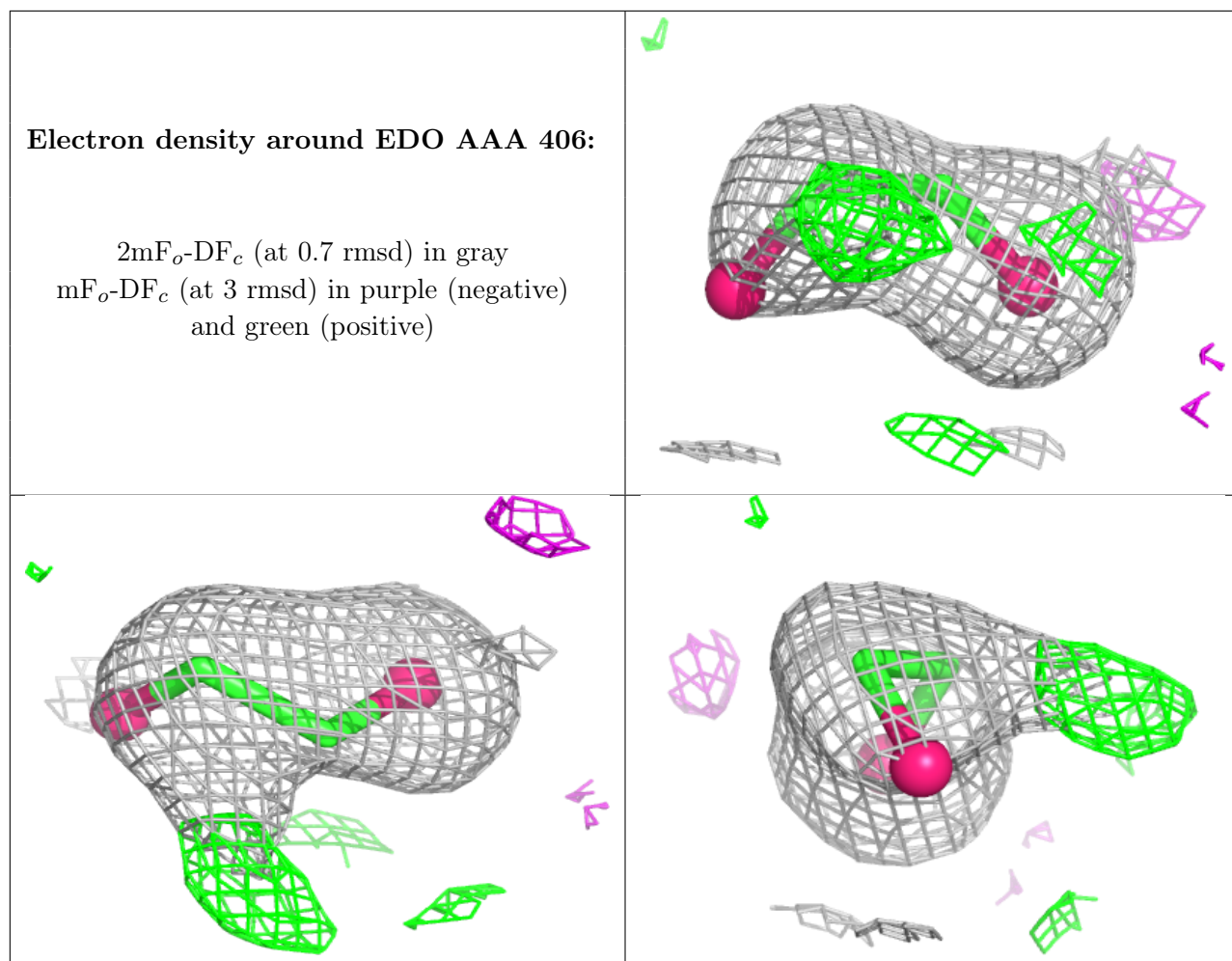
Electron density around EDO AAA 403:

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



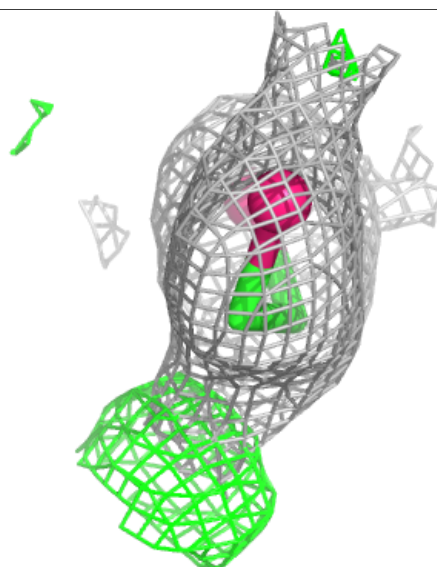
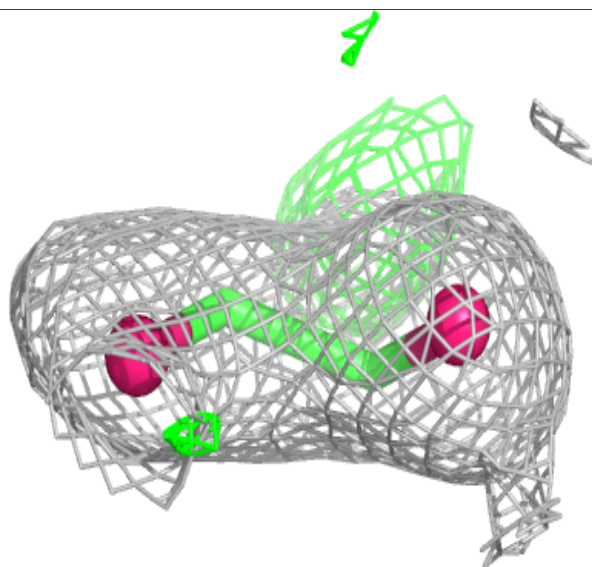
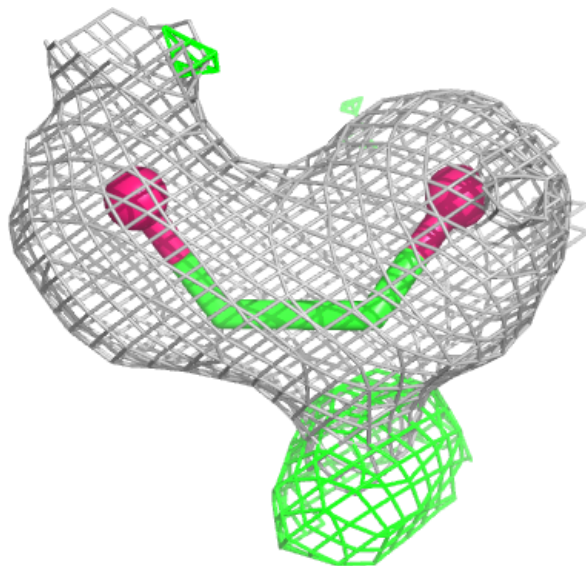
Electron density around EDO AAA 406:

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



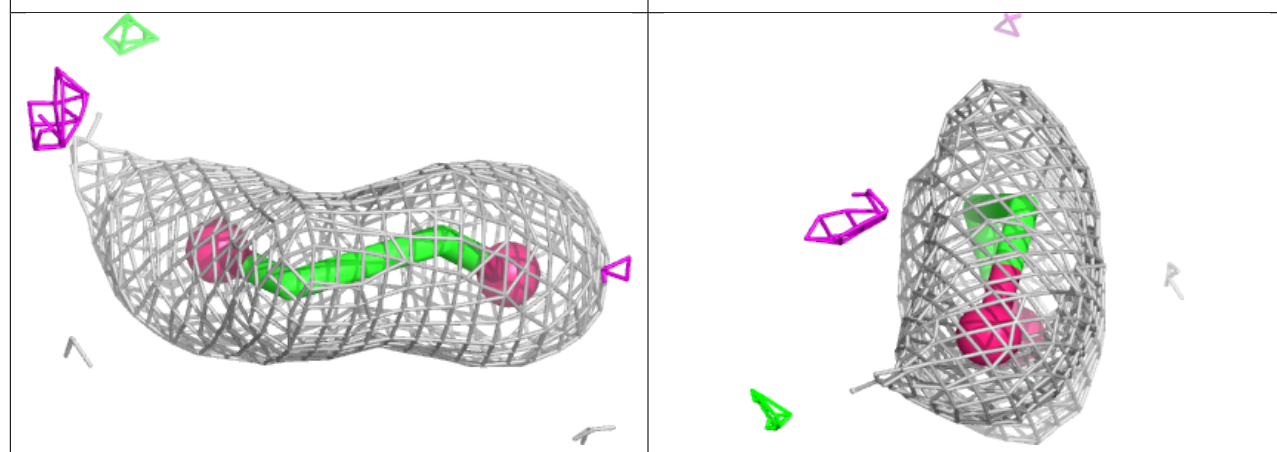
Electron density around EDO AAA 402:

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



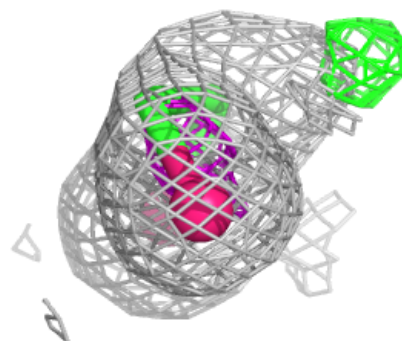
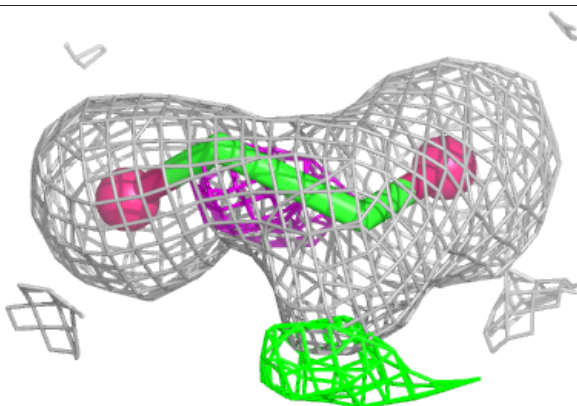
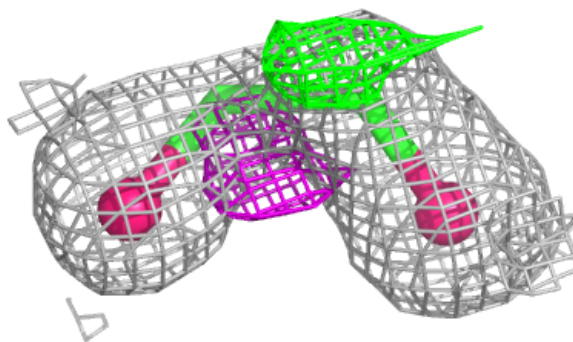
Electron density around EDO AAA 413:

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

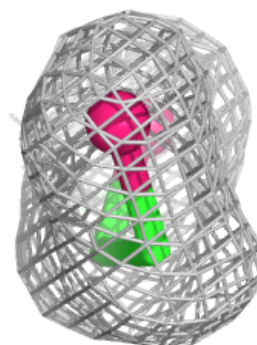
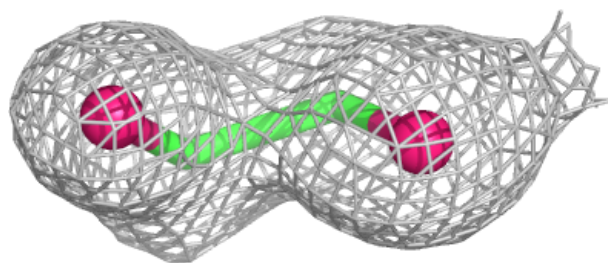
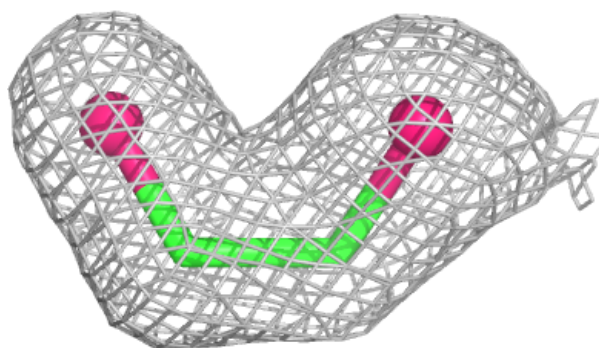


Electron density around EDO AAA 412:

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

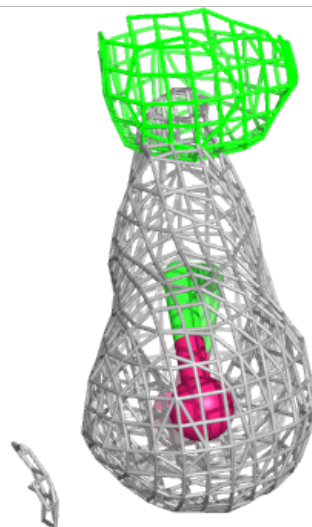
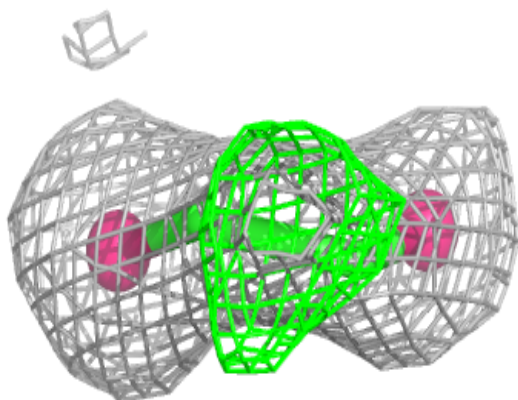
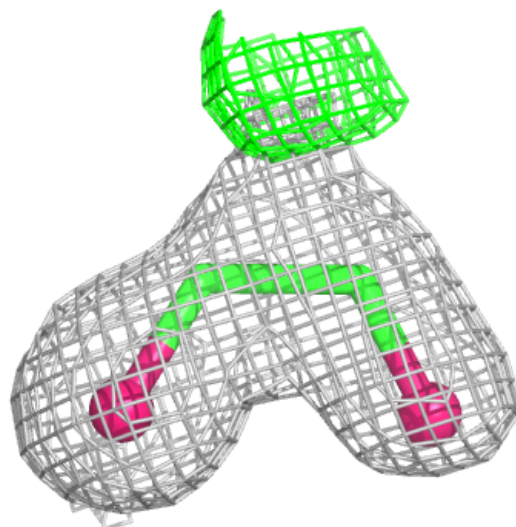
**Electron density around EDO AAA 401:**

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



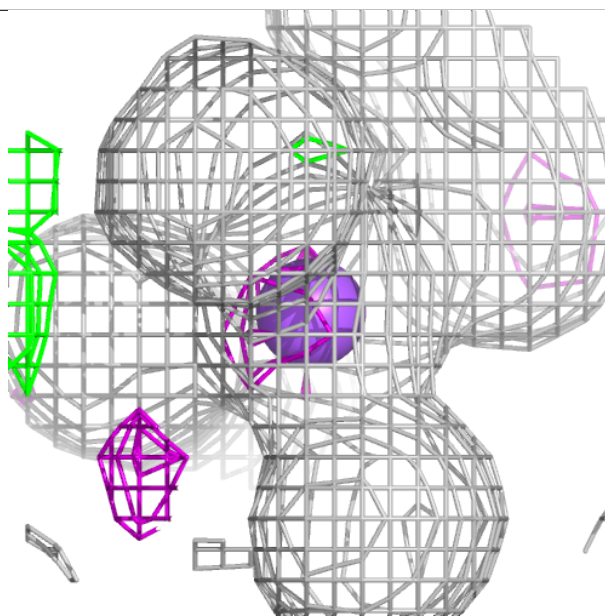
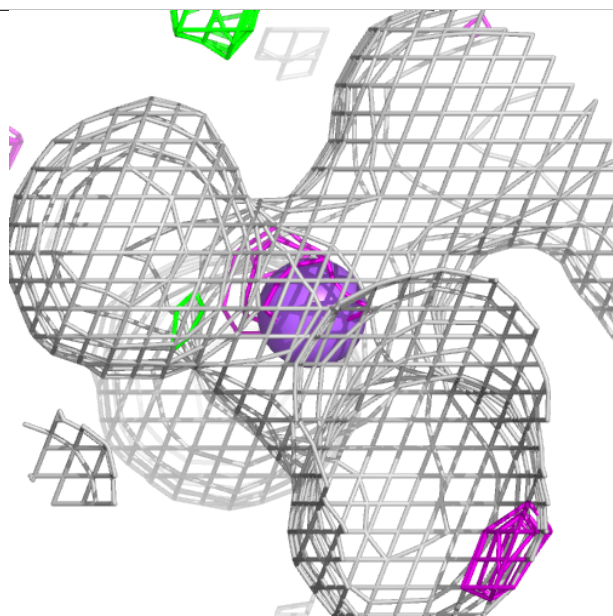
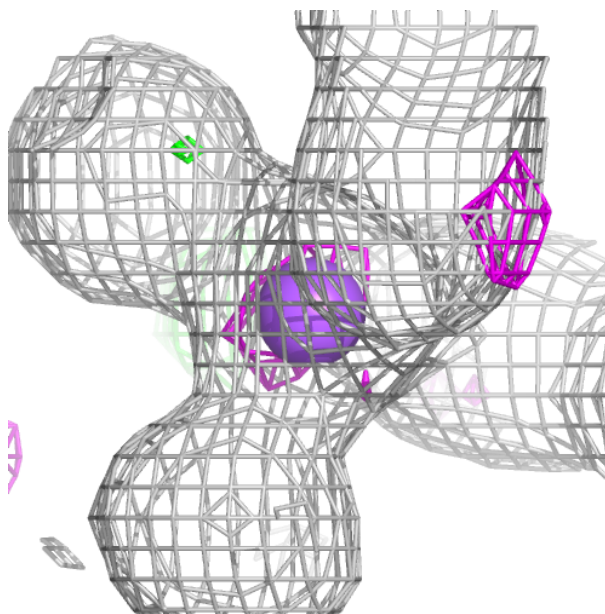
Electron density around EDO AAA 410:

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



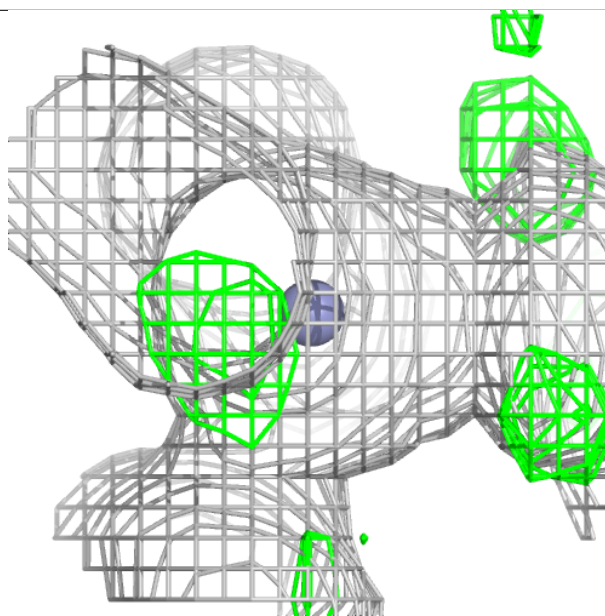
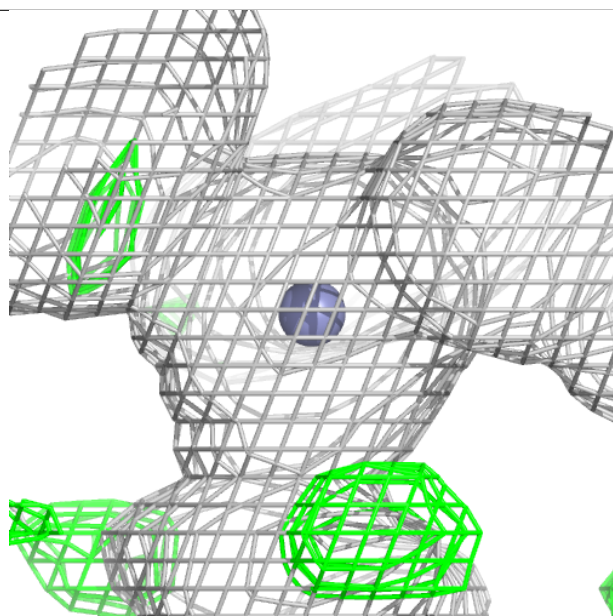
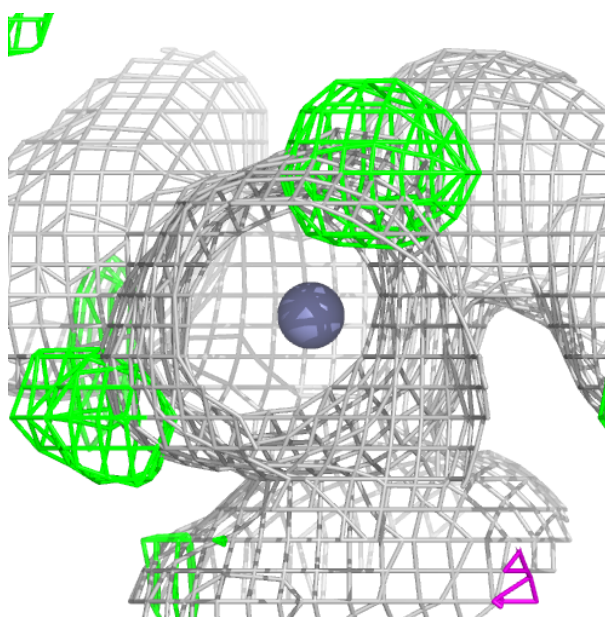
Electron density around NA AAA 421:

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



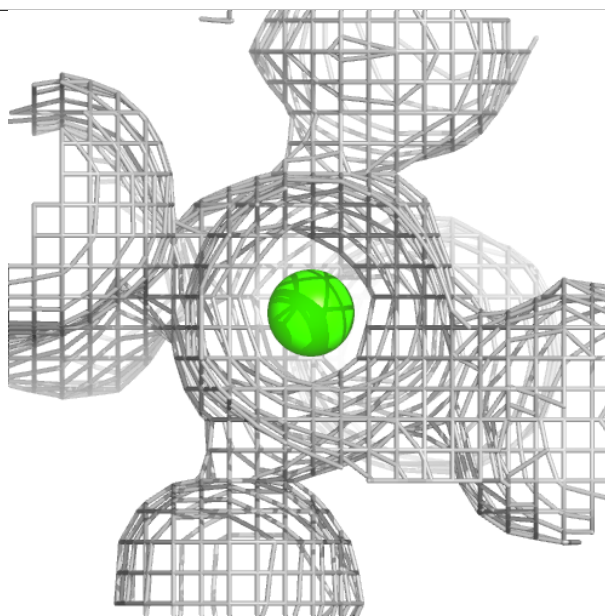
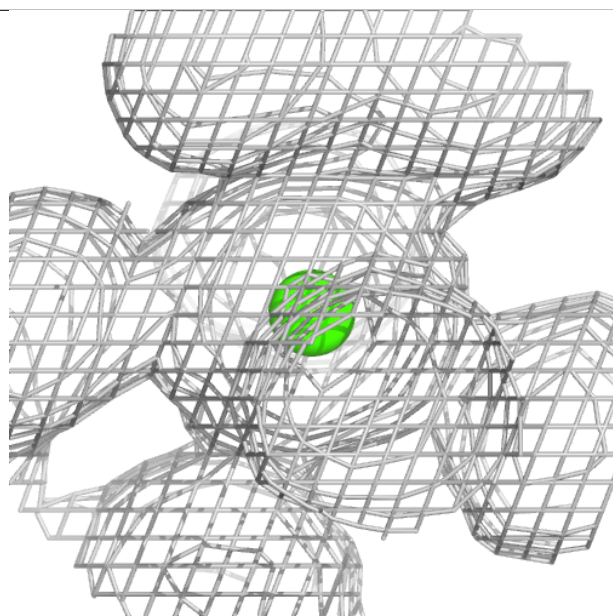
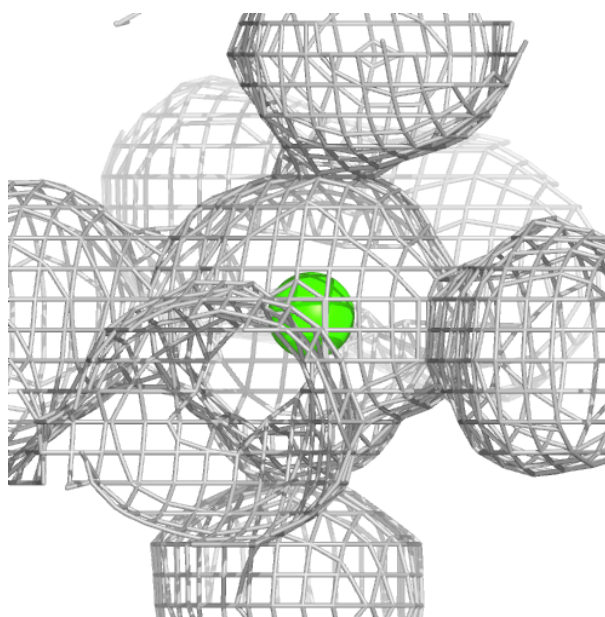
Electron density around ZN AAA 414:

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



Electron density around CA AAA 415:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.