



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2022 – 01:12 am BST

PDB ID : 7OV8  
Title : Crystal structure of pig purple acid phosphatase in complex with 4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid (HEPES) and glycerol  
Authors : Feder, D.; McGeary, R.P.; Guddat, L.W.; Schenk, G.  
Deposited on : 2021-06-14  
Resolution : 2.30 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

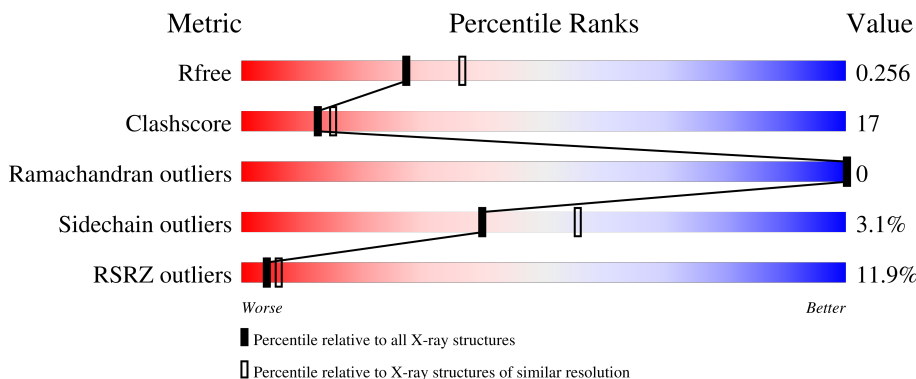
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	
2	C	2	

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
2	NAG	C	2	-	-	-	X
3	EPE	A	702[A]	-	-	-	X
3	EPE	A	702[B]	-	-	-	X
3	EPE	A	703[A]	-	-	-	X
3	EPE	A	703[B]	-	-	-	X
3	EPE	A	712[A]	-	-	-	X
3	EPE	A	712[B]	-	-	-	X
3	EPE	A	712[C]	-	-	-	X
3	EPE	A	725[A]	-	-	-	X
3	EPE	A	725[B]	-	-	-	X
3	EPE	A	728[A]	-	-	-	X
3	EPE	A	728[B]	-	-	-	X
4	GOL	A	705	-	-	-	X
4	GOL	A	706	-	-	-	X
4	GOL	A	720	-	-	-	X
4	GOL	A	721[A]	-	-	-	X
4	GOL	A	721[B]	-	-	-	X
4	GOL	A	724	-	-	X	-
4	GOL	A	726	-	-	-	X
4	GOL	A	727	-	-	-	X
4	GOL	A	729	-	-	-	X
6	PO4	A	715	-	-	X	-
7	EDO	A	716	-	-	X	X
7	EDO	A	717	-	-	-	X
8	PGE	A	730[A]	-	-	-	X
8	PGE	A	730[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3300 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 Tartrate-resistant acid phosphatase type 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	2531	1631	456	437	7	0	16	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	THR	ALA	conflict	UNP P09889

- Molecule 2 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
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
3	A	1	Total	15	8	2	4	1	0	0
3	A	1	Total	30	16	4	8	2	0	1
3	A	1	Total	30	16	4	8	2	0	1
3	A	1	Total	45	24	6	12	3	0	1
3	A	1	Total	30	16	4	8	2	0	1
3	A	1	Total	30	16	4	8	2	0	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

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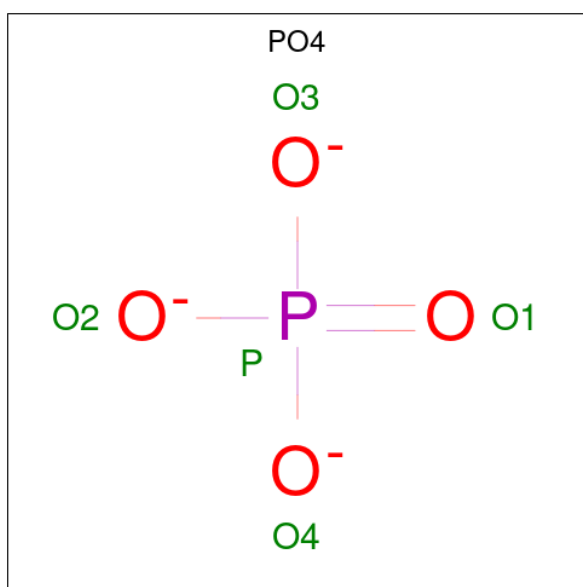
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Fe 2 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



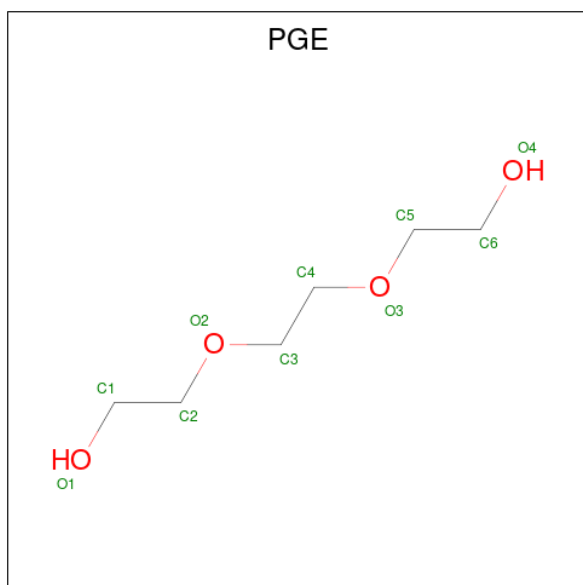
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 14 8 6	0	1

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Na 2 2	0	0

- Molecule 10 is water.

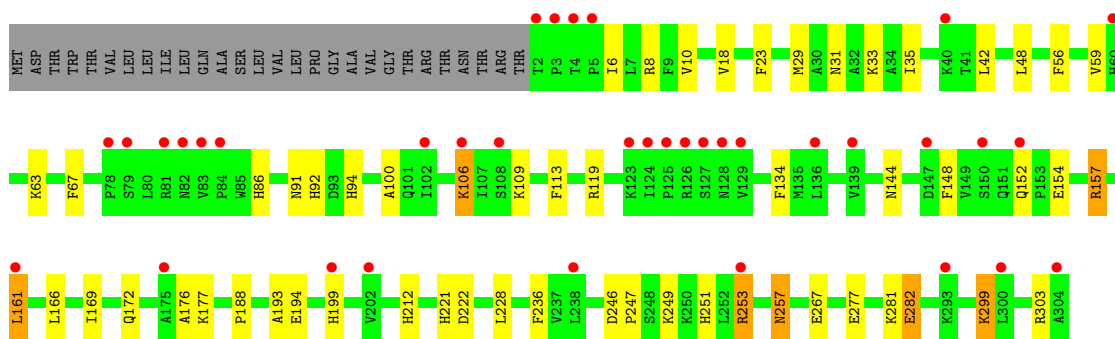
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	418	Total O 420 420	0	2

### 3 Residue-property plots [i](#)

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

- Molecule 1: Tartrate-resistant acid phosphatase type 5

Chain A: 



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

Chain C: 

Chain C: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.38Å 69.77Å 75.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 2.30 39.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.57-2.30) 98.5 (39.57-2.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.162 , 0.256 0.162 , 0.256	Depositor DCC
$R_{free}$ test set	754 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGE, EDO, FE, EPE, NAG, GOL, PO4, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/2637	0.57	0/3574

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	A	2531	0	2538	60	0
2	C	28	0	25	3	0
3	A	180	0	204	30	0
4	A	102	0	135	26	0
5	A	2	0	0	0	0
6	A	5	0	0	2	0
7	A	16	0	24	8	0
8	A	14	0	18	6	0
9	A	2	0	0	0	0
10	A	420	0	0	18	0
All	All	3300	0	2944	97	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 17.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:HA	4:A:711:GOL:H2	1.54	0.87
1:A:176:ALA:O	1:A:303[B]:ARG:NH2	2.09	0.86
1:A:10:VAL:HG11	1:A:35:ILE:HD12	1.62	0.81
3:A:712[C]:EPE:O2S	10:A:801:HOH:O	2.02	0.76
3:A:702[B]:EPE:H91	4:A:722:GOL:H2	1.69	0.74
1:A:246:ASP:HB3	7:A:716:EDO:H21	1.69	0.74
4:A:721[A]:GOL:H12	3:A:725[A]:EPE:H31	1.73	0.70
3:A:725[B]:EPE:H32	3:A:728[B]:EPE:H71	1.74	0.70
1:A:257[A]:ASN:OD1	10:A:804:HOH:O	2.09	0.70
1:A:267:GLU:HG2	4:A:704:GOL:H31	1.73	0.70
1:A:56:PHE:HB3	8:A:730[A]:PGE:H12	1.74	0.68
4:A:704:GOL:O1	4:A:708:GOL:H31	1.96	0.65
3:A:728[A]:EPE:O2S	10:A:805:HOH:O	2.13	0.65
1:A:8[A]:ARG:NH2	1:A:277:GLU:OE2	2.32	0.62
4:A:727:GOL:H31	3:A:728[A]:EPE:H72	1.81	0.62
1:A:31:ASN:O	1:A:35:ILE:HG12	2.00	0.62
1:A:212:HIS:O	1:A:303[B]:ARG:NH1	2.33	0.62
1:A:282[B]:GLU:HG3	1:A:299[B]:LYS:HD2	1.82	0.61
1:A:92:HIS:CE1	8:A:730[B]:PGE:H1	2.36	0.61
1:A:194:GLU:OE2	4:A:709:GOL:H12	2.01	0.61
1:A:251:HIS:NE2	4:A:721[A]:GOL:O2	2.29	0.60
3:A:728[A]:EPE:H92	4:A:729:GOL:O2	2.03	0.59
1:A:63:LYS:HE2	7:A:719:EDO:H22	1.87	0.56
1:A:92:HIS:HE1	8:A:730[B]:PGE:H1	1.69	0.56
1:A:157[B]:ARG:HD2	4:A:724:GOL:H11	1.88	0.56
3:A:725[B]:EPE:H22	4:A:727:GOL:O3	2.05	0.56
1:A:222:ASP:OD1	7:A:716:EDO:H11	2.06	0.55
1:A:92:HIS:CE1	8:A:730[A]:PGE:H4	2.40	0.55
7:A:719:EDO:H11	2:C:2:NAG:H3	1.88	0.54
1:A:228:LEU:HB2	1:A:236:PHE:HB2	1.90	0.53
1:A:29:MET:O	1:A:33:LYS:HG3	2.09	0.53
3:A:712[B]:EPE:H101	10:A:1082:HOH:O	2.09	0.52
1:A:119:ARG:HG3	1:A:134:PHE:CE1	2.43	0.52
1:A:166:LEU:HA	1:A:169:ILE:HD12	1.90	0.52
1:A:247:PRO:HG2	4:A:710:GOL:H11	1.92	0.52
1:A:199[A]:HIS:ND1	10:A:811:HOH:O	2.30	0.51
1:A:157[A]:ARG:HD3	4:A:724:GOL:H11	1.93	0.50
8:A:730[B]:PGE:H12	10:A:848:HOH:O	2.11	0.50
1:A:152[B]:GLN:NE2	10:A:825:HOH:O	2.45	0.50
4:A:723:GOL:H31	10:A:824:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HG2	4:A:708:GOL:H2	1.94	0.49
4:A:706:GOL:H2	4:A:729:GOL:H2	1.94	0.48
3:A:712[A]:EPE:H22	3:A:712[A]:EPE:H101	1.61	0.48
3:A:702[A]:EPE:H51	3:A:702[A]:EPE:H91	1.41	0.48
3:A:702[A]:EPE:O8	10:A:803:HOH:O	2.07	0.48
3:A:702[B]:EPE:H91	3:A:702[B]:EPE:H31	1.64	0.48
3:A:725[B]:EPE:H71	3:A:728[B]:EPE:H31	1.95	0.48
1:A:188:PRO:HD3	1:A:221:HIS:HB3	1.96	0.47
10:A:1198:HOH:O	2:C:2:NAG:H82	2.14	0.47
1:A:92:HIS:HE2	6:A:715:PO4:P	2.37	0.47
1:A:100:ALA:HA	2:C:1:NAG:H62	1.96	0.47
1:A:253[B]:ARG:HA	1:A:253[B]:ARG:HD3	1.81	0.47
1:A:48:LEU:HD12	1:A:86:HIS:HB2	1.97	0.46
1:A:194:GLU:HB3	7:A:716:EDO:C1	2.46	0.46
1:A:106[B]:LYS:HE3	1:A:106[B]:LYS:HB3	1.46	0.46
1:A:91:ASN:ND2	6:A:715:PO4:O4	2.39	0.46
3:A:725[A]:EPE:H61	3:A:728[A]:EPE:N4	2.31	0.46
3:A:728[B]:EPE:H62	3:A:728[B]:EPE:H102	1.48	0.46
1:A:106[B]:LYS:HD2	10:A:884:HOH:O	2.16	0.45
1:A:144:ASN:HB2	3:A:702[B]:EPE:O8	2.16	0.45
1:A:134:PHE:CE1	1:A:172:GLN:HB3	2.52	0.45
3:A:712[C]:EPE:H51	10:A:933:HOH:O	2.17	0.45
1:A:157[B]:ARG:NH2	4:A:724:GOL:O3	2.50	0.44
3:A:703[B]:EPE:H22	10:A:812:HOH:O	2.18	0.44
4:A:706:GOL:H2	4:A:729:GOL:C2	2.47	0.44
1:A:144:ASN:HB2	3:A:702[A]:EPE:C8	2.48	0.44
3:A:701:EPE:H81	3:A:701:EPE:H51	1.70	0.44
1:A:6:ILE:HG12	1:A:8[A]:ARG:HG2	1.99	0.44
1:A:92:HIS:HE1	8:A:730[A]:PGE:H2	1.82	0.43
4:A:704:GOL:H11	10:A:973:HOH:O	2.18	0.43
1:A:94:HIS:O	3:A:702[B]:EPE:H21	2.17	0.43
1:A:193:ALA:HB1	7:A:716:EDO:O2	2.18	0.43
1:A:18:VAL:O	1:A:23:PHE:HA	2.18	0.43
4:A:720:GOL:H2	10:A:894:HOH:O	2.19	0.43
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.92	0.42
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.90	0.42
3:A:703[B]:EPE:H81	3:A:703[B]:EPE:H52	1.71	0.42
3:A:703[A]:EPE:H31	3:A:703[A]:EPE:H81	1.61	0.42
1:A:106[A]:LYS:H	1:A:106[A]:LYS:HG3	1.70	0.42
3:A:725[B]:EPE:H101	10:A:917:HOH:O	2.19	0.42
1:A:177:LYS:HD3	1:A:177:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PHE:CZ	4:A:724:GOL:H12	2.54	0.42
1:A:249:LYS:HE3	10:A:994:HOH:O	2.19	0.42
4:A:709:GOL:H2	4:A:710:GOL:O1	2.20	0.42
3:A:728[A]:EPE:H52	3:A:728[A]:EPE:H82	1.62	0.42
1:A:281[A]:LYS:N	1:A:281[A]:LYS:HD2	2.36	0.41
3:A:725[B]:EPE:H61	3:A:725[B]:EPE:H102	1.52	0.41
4:A:705:GOL:H2	4:A:707:GOL:H2	2.02	0.41
1:A:109:LYS:HE3	1:A:109:LYS:HB3	1.94	0.41
3:A:702[A]:EPE:H22	10:A:986:HOH:O	2.21	0.41
1:A:42:LEU:O	3:A:703[A]:EPE:H72	2.21	0.41
1:A:194:GLU:HB3	7:A:716:EDO:H12	2.03	0.41
3:A:703[B]:EPE:H21	7:A:717:EDO:O1	2.20	0.41
1:A:152[A]:GLN:HG3	4:A:711:GOL:O2	2.20	0.41
1:A:247:PRO:O	4:A:708:GOL:H11	2.21	0.41
1:A:247:PRO:CG	4:A:710:GOL:H11	2.50	0.41
1:A:59:VAL:HG21	1:A:67[B]:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	318/331 (96%)	307 (96%)	11 (4%)	0	<b>100</b> <b>100</b>

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	272/279 (98%)	258 (95%)	14 (5%)	24 33

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106[A]	LYS
1	A	106[B]	LYS
1	A	113	PHE
1	A	157[A]	ARG
1	A	157[B]	ARG
1	A	161	LEU
1	A	253[A]	ARG
1	A	253[B]	ARG
1	A	257[A]	ASN
1	A	257[B]	ASN
1	A	282[A]	GLU
1	A	282[B]	GLU
1	A	299[A]	LYS
1	A	299[B]	LYS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

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



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	1,2	14,14,15	0.79	1 (7%)	17,19,21	0.83	0
2	NAG	C	2	2	14,14,15	1.29	1 (7%)	17,19,21	1.06	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	4.47	1.59	1.52
2	C	1	NAG	O5-C1	-2.85	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C4-C3-C2	2.21	114.25	111.02
2	C	2	NAG	C1-O5-C5	-2.18	109.24	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

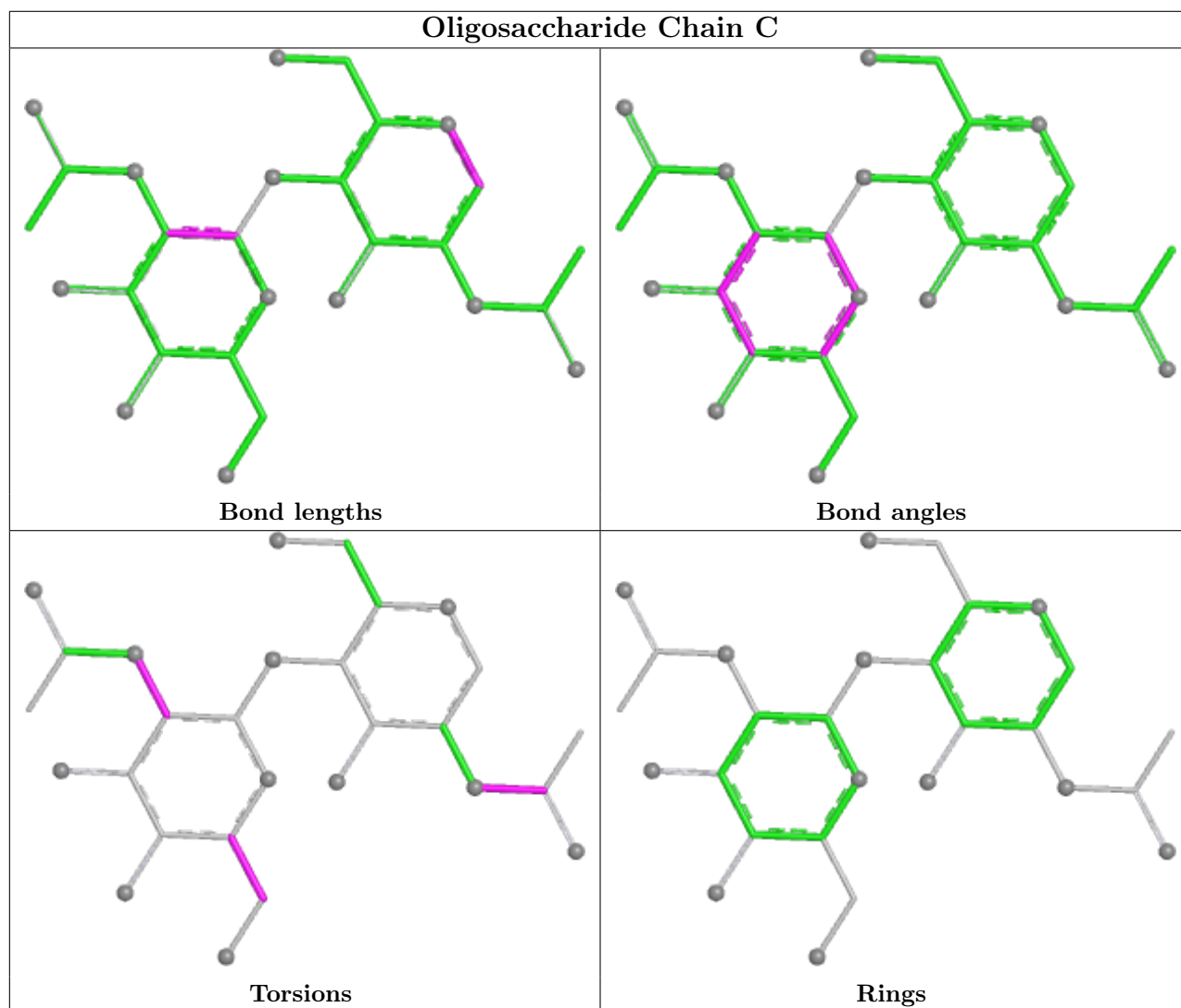
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	C	2	NAG	2	0

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 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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
3	EPE	A	701	-	15,15,15	0.90	1 (6%)	18,20,20	1.82	5 (27%)
3	EPE	A	703[B]	-	15,15,15	0.90	1 (6%)	18,20,20	1.92	4 (22%)
3	EPE	A	728[B]	-	15,15,15	0.90	1 (6%)	18,20,20	1.70	4 (22%)
4	GOL	A	705	-	5,5,5	0.81	0	5,5,5	0.93	0
4	GOL	A	721[B]	-	5,5,5	0.87	0	5,5,5	1.00	0
8	PGE	A	730[A]	-	6,6,9	0.33	0	5,5,8	0.27	0
4	GOL	A	708	-	5,5,5	0.81	0	5,5,5	1.25	1 (20%)
4	GOL	A	710	-	5,5,5	0.93	0	5,5,5	1.06	0
3	EPE	A	703[A]	-	15,15,15	0.94	1 (6%)	18,20,20	1.89	5 (27%)
7	EDO	A	716	-	3,3,3	0.34	0	2,2,2	0.25	0
7	EDO	A	718	-	3,3,3	0.53	0	2,2,2	0.22	0
3	EPE	A	728[A]	-	15,15,15	0.78	1 (6%)	18,20,20	1.82	3 (16%)
4	GOL	A	707	-	5,5,5	1.06	0	5,5,5	1.04	0
4	GOL	A	721[A]	-	5,5,5	0.84	0	5,5,5	0.96	0
4	GOL	A	726	-	5,5,5	0.87	0	5,5,5	1.00	0
4	GOL	A	724	-	5,5,5	0.89	0	5,5,5	1.12	1 (20%)
3	EPE	A	702[B]	-	15,15,15	0.75	1 (6%)	18,20,20	1.93	7 (38%)
6	PO4	A	715	5	4,4,4	0.95	0	6,6,6	0.59	0
4	GOL	A	723	-	5,5,5	0.85	0	5,5,5	1.02	0
3	EPE	A	725[B]	-	15,15,15	0.84	1 (6%)	18,20,20	1.94	5 (27%)
4	GOL	A	709	-	5,5,5	0.92	0	5,5,5	0.88	0
7	EDO	A	717	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EPE	A	702[A]	9	15,15,15	0.70	0	18,20,20	2.04	7 (38%)
3	EPE	A	712[C]	-	15,15,15	0.72	1 (6%)	18,20,20	1.75	5 (27%)
3	EPE	A	712[B]	-	15,15,15	0.84	1 (6%)	18,20,20	1.74	5 (27%)
4	GOL	A	720	-	5,5,5	0.32	0	5,5,5	1.27	1 (20%)
3	EPE	A	725[A]	-	15,15,15	0.92	1 (6%)	18,20,20	1.58	5 (27%)
7	EDO	A	719	-	3,3,3	0.45	0	2,2,2	0.27	0
4	GOL	A	729	-	5,5,5	1.21	1 (20%)	5,5,5	0.94	0
4	GOL	A	706	-	5,5,5	0.98	0	5,5,5	0.97	0
3	EPE	A	712[A]	-	15,15,15	0.80	1 (6%)	18,20,20	1.75	5 (27%)
4	GOL	A	704	-	5,5,5	1.05	0	5,5,5	1.02	0
4	GOL	A	727	-	5,5,5	1.01	0	5,5,5	0.88	0
4	GOL	A	722	-	5,5,5	0.95	0	5,5,5	0.85	0
8	PGE	A	730[B]	-	6,6,9	0.30	0	5,5,8	0.52	0
4	GOL	A	711	-	5,5,5	1.11	0	5,5,5	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	701	-	-	4/9/19/19	0/1/1/1
3	EPE	A	703[B]	-	-	1/9/19/19	0/1/1/1
3	EPE	A	728[B]	-	-	8/9/19/19	0/1/1/1
4	GOL	A	705	-	-	4/4/4/4	-
4	GOL	A	721[B]	-	-	4/4/4/4	-
8	PGE	A	730[A]	-	-	2/4/4/7	-
4	GOL	A	708	-	-	2/4/4/4	-
4	GOL	A	710	-	-	0/4/4/4	-
3	EPE	A	703[A]	-	-	2/9/19/19	0/1/1/1
7	EDO	A	716	-	-	0/1/1/1	-
7	EDO	A	718	-	-	0/1/1/1	-
3	EPE	A	728[A]	-	-	4/9/19/19	0/1/1/1
4	GOL	A	707	-	-	4/4/4/4	-
4	GOL	A	721[A]	-	-	2/4/4/4	-
4	GOL	A	726	-	-	2/4/4/4	-
4	GOL	A	724	-	-	2/4/4/4	-
3	EPE	A	702[B]	-	-	2/9/19/19	0/1/1/1
4	GOL	A	723	-	-	4/4/4/4	-
3	EPE	A	725[B]	-	-	3/9/19/19	0/1/1/1
4	GOL	A	709	-	-	0/4/4/4	-
7	EDO	A	717	-	-	0/1/1/1	-
3	EPE	A	702[A]	9	-	5/9/19/19	0/1/1/1
3	EPE	A	712[C]	-	-	5/9/19/19	0/1/1/1
3	EPE	A	712[B]	-	-	6/9/19/19	0/1/1/1
4	GOL	A	720	-	-	4/4/4/4	-
3	EPE	A	725[A]	-	-	5/9/19/19	0/1/1/1
7	EDO	A	719	-	-	1/1/1/1	-
4	GOL	A	729	-	-	0/4/4/4	-
4	GOL	A	706	-	-	0/4/4/4	-
3	EPE	A	712[A]	-	-	7/9/19/19	0/1/1/1
4	GOL	A	704	-	-	2/4/4/4	-
4	GOL	A	727	-	-	2/4/4/4	-
4	GOL	A	722	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PGE	A	730[B]	-	-	0/4/4/7	-
4	GOL	A	711	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703[A]	EPE	C10-S	3.04	1.81	1.77
3	A	725[A]	EPE	C10-S	3.04	1.81	1.77
3	A	701	EPE	C10-S	3.02	1.81	1.77
3	A	728[B]	EPE	C10-S	3.02	1.81	1.77
3	A	703[B]	EPE	C10-S	3.00	1.81	1.77
3	A	725[B]	EPE	C10-S	2.87	1.81	1.77
3	A	712[B]	EPE	C10-S	2.83	1.81	1.77
3	A	712[A]	EPE	C10-S	2.65	1.81	1.77
3	A	728[A]	EPE	C10-S	2.52	1.81	1.77
3	A	702[B]	EPE	C10-S	2.33	1.80	1.77
3	A	712[C]	EPE	C10-S	2.26	1.80	1.77
4	A	729	GOL	O2-C2	-2.20	1.36	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	725[B]	EPE	C5-N4-C3	4.66	119.32	108.83
3	A	728[A]	EPE	C5-N4-C3	4.28	118.45	108.83
3	A	712[B]	EPE	C5-N4-C3	3.92	117.66	108.83
3	A	701	EPE	C5-N4-C3	3.89	117.59	108.83
3	A	703[B]	EPE	C7-N4-C5	3.84	121.06	111.23
3	A	702[A]	EPE	C9-N1-C6	-3.83	101.45	111.23
3	A	728[A]	EPE	C7-N4-C5	3.79	120.93	111.23
3	A	703[B]	EPE	C7-N4-C3	3.70	120.69	111.23
3	A	703[B]	EPE	C5-N4-C3	3.66	117.06	108.83
3	A	728[B]	EPE	C5-N4-C3	3.61	116.96	108.83
3	A	703[A]	EPE	C7-N4-C5	3.55	120.30	111.23
3	A	725[B]	EPE	C7-N4-C3	3.54	120.30	111.23
3	A	712[A]	EPE	C5-N4-C3	3.43	116.56	108.83
3	A	702[A]	EPE	C5-N4-C3	3.38	116.43	108.83
3	A	725[B]	EPE	C7-N4-C5	3.37	119.85	111.23
3	A	712[C]	EPE	C5-N4-C3	3.36	116.38	108.83
3	A	728[B]	EPE	C7-N4-C5	3.36	119.81	111.23
3	A	703[A]	EPE	C7-N4-C3	3.28	119.62	111.23
3	A	725[A]	EPE	C5-N4-C3	3.28	116.20	108.83
3	A	703[A]	EPE	C5-N4-C3	3.24	116.13	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	712[C]	EPE	C7-N4-C5	3.23	119.50	111.23
3	A	702[B]	EPE	O2S-S-C10	3.22	110.79	106.92
3	A	702[A]	EPE	C5-C6-N1	-3.16	104.15	110.64
3	A	712[C]	EPE	C7-N4-C3	3.16	119.31	111.23
3	A	725[B]	EPE	O3S-S-C10	3.15	110.87	105.77
3	A	701	EPE	O1S-S-C10	3.07	110.61	106.92
3	A	712[B]	EPE	C7-N4-C5	3.06	119.06	111.23
3	A	728[A]	EPE	C7-N4-C3	3.00	118.90	111.23
3	A	701	EPE	O2S-S-C10	2.99	110.52	106.92
3	A	701	EPE	C7-N4-C3	2.95	118.79	111.23
3	A	712[A]	EPE	C7-N4-C3	2.95	118.78	111.23
3	A	712[A]	EPE	C7-N4-C5	2.91	118.69	111.23
3	A	725[A]	EPE	O1S-S-C10	2.90	110.40	106.92
3	A	728[B]	EPE	C7-N4-C3	2.89	118.64	111.23
3	A	701	EPE	C7-N4-C5	2.85	118.52	111.23
3	A	702[A]	EPE	C6-C5-N4	-2.84	104.81	110.64
3	A	712[A]	EPE	O3S-S-C10	2.83	110.35	105.77
3	A	703[B]	EPE	O1S-S-C10	2.75	110.23	106.92
3	A	702[B]	EPE	C3-C2-N1	-2.75	105.00	110.64
3	A	702[B]	EPE	C5-N4-C3	2.72	114.96	108.83
3	A	703[A]	EPE	O3S-S-C10	2.72	110.16	105.77
3	A	712[B]	EPE	O1S-S-C10	2.71	110.18	106.92
3	A	712[C]	EPE	O1S-S-C10	2.68	110.14	106.92
3	A	725[A]	EPE	C7-N4-C3	2.66	118.03	111.23
3	A	712[C]	EPE	O3S-S-C10	2.65	110.05	105.77
3	A	702[A]	EPE	O1S-S-C10	2.54	109.97	106.92
3	A	702[A]	EPE	C7-N4-C3	2.49	117.60	111.23
3	A	702[B]	EPE	C9-N1-C2	-2.45	104.97	111.23
3	A	702[B]	EPE	O3S-S-C10	2.43	109.70	105.77
3	A	712[B]	EPE	C7-N4-C3	2.39	117.36	111.23
4	A	708	GOL	C3-C2-C1	-2.39	102.41	111.70
4	A	720	GOL	C3-C2-C1	-2.36	102.52	111.70
3	A	712[B]	EPE	O3S-S-C10	2.36	109.58	105.77
3	A	725[A]	EPE	C7-N4-C5	2.22	116.92	111.23
3	A	725[A]	EPE	O3S-S-C10	2.19	109.31	105.77
3	A	703[A]	EPE	O2S-S-C10	2.19	109.55	106.92
3	A	702[A]	EPE	O2S-S-C10	2.17	109.53	106.92
3	A	728[B]	EPE	O1S-S-C10	2.16	109.52	106.92
3	A	725[B]	EPE	O2S-S-C10	2.15	109.50	106.92
4	A	724	GOL	C3-C2-C1	-2.12	103.45	111.70
3	A	702[B]	EPE	C7-N4-C5	2.12	116.66	111.23
3	A	702[B]	EPE	C6-N1-C2	2.09	113.53	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	712[A]	EPE	C9-N1-C6	-2.05	106.00	111.23

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	EPE	C8-C7-N4-C5
3	A	702[A]	EPE	C10-C9-N1-C2
3	A	702[A]	EPE	C9-C10-S-O1S
3	A	702[B]	EPE	C8-C7-N4-C3
3	A	702[B]	EPE	S-C10-C9-N1
3	A	703[A]	EPE	C8-C7-N4-C3
3	A	703[B]	EPE	C8-C7-N4-C5
3	A	712[A]	EPE	C10-C9-N1-C2
3	A	712[A]	EPE	S-C10-C9-N1
3	A	712[A]	EPE	C9-C10-S-O2S
3	A	712[A]	EPE	C9-C10-S-O3S
3	A	712[B]	EPE	C10-C9-N1-C2
3	A	712[B]	EPE	C9-C10-S-O1S
3	A	712[B]	EPE	C9-C10-S-O3S
3	A	712[C]	EPE	C8-C7-N4-C5
3	A	725[A]	EPE	S-C10-C9-N1
3	A	725[B]	EPE	C8-C7-N4-C3
3	A	725[B]	EPE	S-C10-C9-N1
3	A	728[A]	EPE	C8-C7-N4-C5
3	A	728[B]	EPE	C10-C9-N1-C6
3	A	728[B]	EPE	C8-C7-N4-C5
3	A	728[B]	EPE	S-C10-C9-N1
3	A	728[B]	EPE	C9-C10-S-O2S
4	A	704	GOL	O1-C1-C2-C3
4	A	705	GOL	O1-C1-C2-C3
4	A	705	GOL	C1-C2-C3-O3
4	A	707	GOL	O1-C1-C2-C3
4	A	707	GOL	C1-C2-C3-O3
4	A	720	GOL	O1-C1-C2-C3
4	A	720	GOL	C1-C2-C3-O3
4	A	721[A]	GOL	C1-C2-C3-O3
4	A	721[B]	GOL	O1-C1-C2-C3
4	A	721[B]	GOL	C1-C2-C3-O3
4	A	723	GOL	O1-C1-C2-C3
4	A	723	GOL	C1-C2-C3-O3
4	A	726	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	712[B]	EPE	N4-C7-C8-O8
3	A	728[A]	EPE	N4-C7-C8-O8
4	A	707	GOL	O2-C2-C3-O3
4	A	720	GOL	O2-C2-C3-O3
3	A	702[A]	EPE	C9-C10-S-O3S
3	A	712[C]	EPE	C9-C10-S-O3S
8	A	730[A]	PGE	O2-C3-C4-O3
4	A	708	GOL	O1-C1-C2-C3
4	A	711	GOL	O1-C1-C2-C3
4	A	722	GOL	C1-C2-C3-O3
4	A	727	GOL	O1-C1-C2-C3
4	A	704	GOL	O1-C1-C2-O2
4	A	705	GOL	O1-C1-C2-O2
4	A	705	GOL	O2-C2-C3-O3
4	A	720	GOL	O1-C1-C2-O2
4	A	721[A]	GOL	O2-C2-C3-O3
4	A	721[B]	GOL	O2-C2-C3-O3
4	A	723	GOL	O2-C2-C3-O3
4	A	726	GOL	O2-C2-C3-O3
3	A	728[B]	EPE	C9-C10-S-O3S
4	A	707	GOL	O1-C1-C2-O2
4	A	723	GOL	O1-C1-C2-O2
3	A	701	EPE	N4-C7-C8-O8
3	A	712[A]	EPE	N4-C7-C8-O8
3	A	702[A]	EPE	S-C10-C9-N1
3	A	701	EPE	C10-C9-N1-C6
3	A	725[A]	EPE	C10-C9-N1-C2
3	A	725[B]	EPE	C10-C9-N1-C6
3	A	728[A]	EPE	C10-C9-N1-C2
3	A	728[A]	EPE	C10-C9-N1-C6
4	A	721[B]	GOL	O1-C1-C2-O2
4	A	727	GOL	O1-C1-C2-O2
4	A	708	GOL	O1-C1-C2-O2
4	A	722	GOL	O2-C2-C3-O3
3	A	702[A]	EPE	C9-C10-S-O2S
3	A	712[A]	EPE	C9-C10-S-O1S
3	A	712[B]	EPE	C9-C10-S-O2S
3	A	712[C]	EPE	C9-C10-S-O1S
3	A	712[C]	EPE	C9-C10-S-O2S
3	A	725[A]	EPE	C9-C10-S-O2S
3	A	728[B]	EPE	C9-C10-S-O1S
3	A	703[A]	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
4	A	724	GOL	C1-C2-C3-O3
3	A	712[B]	EPE	C8-C7-N4-C3
4	A	711	GOL	O1-C1-C2-O2
3	A	728[B]	EPE	N4-C7-C8-O8
8	A	730[A]	PGE	O1-C1-C2-O2
3	A	701	EPE	C10-C9-N1-C2
3	A	725[A]	EPE	C10-C9-N1-C6
3	A	728[B]	EPE	C10-C9-N1-C2
3	A	712[C]	EPE	N4-C7-C8-O8
7	A	719	EDO	O1-C1-C2-O2
4	A	724	GOL	O2-C2-C3-O3
3	A	712[A]	EPE	C8-C7-N4-C3
3	A	725[A]	EPE	C9-C10-S-O1S

There are no ring outliers.

33 monomers are involved in 66 short contacts:

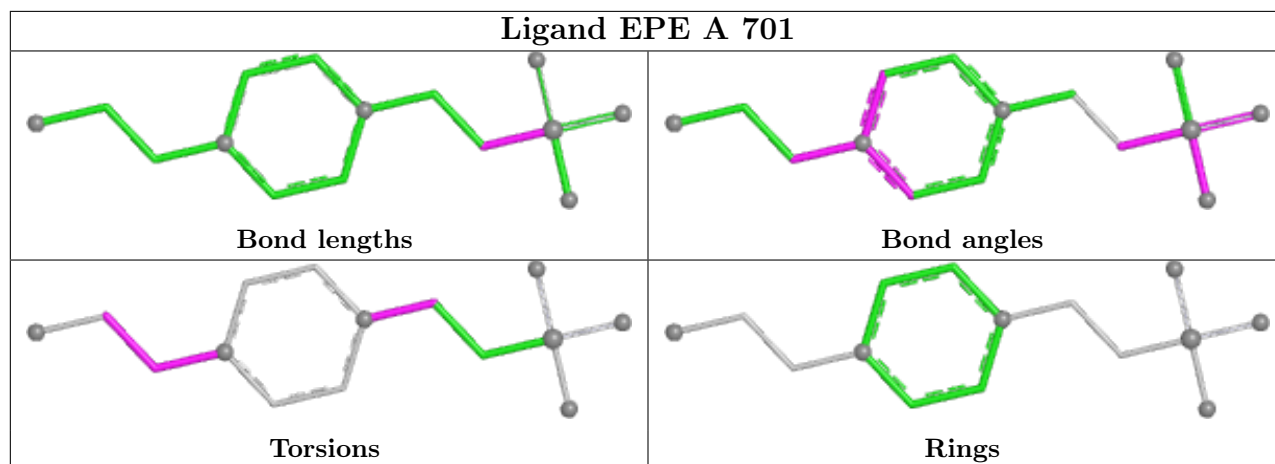
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	EPE	1	0
3	A	703[B]	EPE	3	0
3	A	728[B]	EPE	3	0
4	A	705	GOL	1	0
8	A	730[A]	PGE	3	0
4	A	708	GOL	3	0
4	A	710	GOL	3	0
3	A	703[A]	EPE	2	0
7	A	716	EDO	5	0
3	A	728[A]	EPE	5	0
4	A	707	GOL	1	0
4	A	721[A]	GOL	2	0
4	A	724	GOL	4	0
3	A	702[B]	EPE	4	0
6	A	715	PO4	2	0
4	A	723	GOL	1	0
3	A	725[B]	EPE	5	0
4	A	709	GOL	2	0
7	A	717	EDO	1	0
3	A	702[A]	EPE	4	0
3	A	712[C]	EPE	2	0
3	A	712[B]	EPE	1	0
4	A	720	GOL	1	0
3	A	725[A]	EPE	2	0

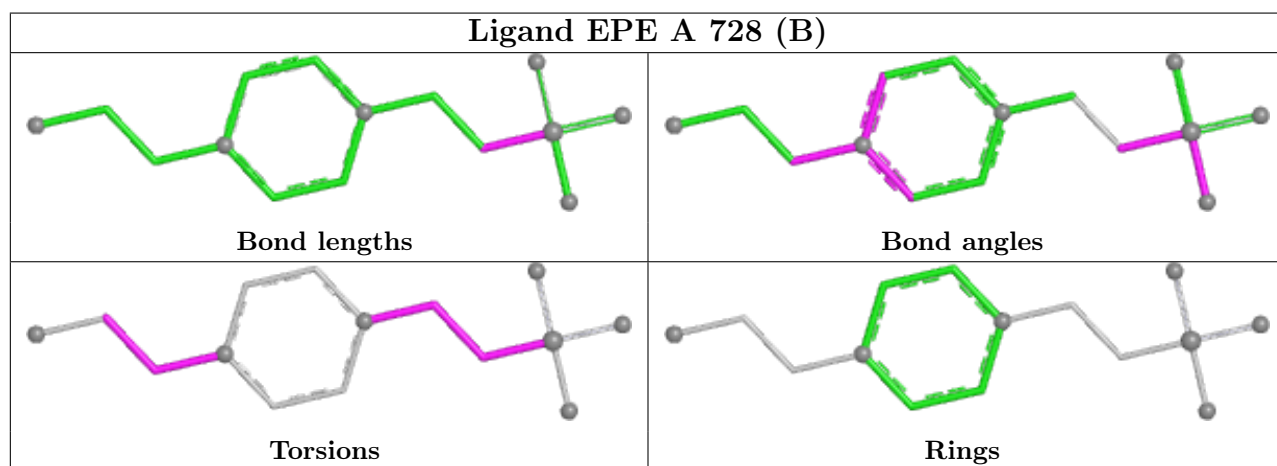
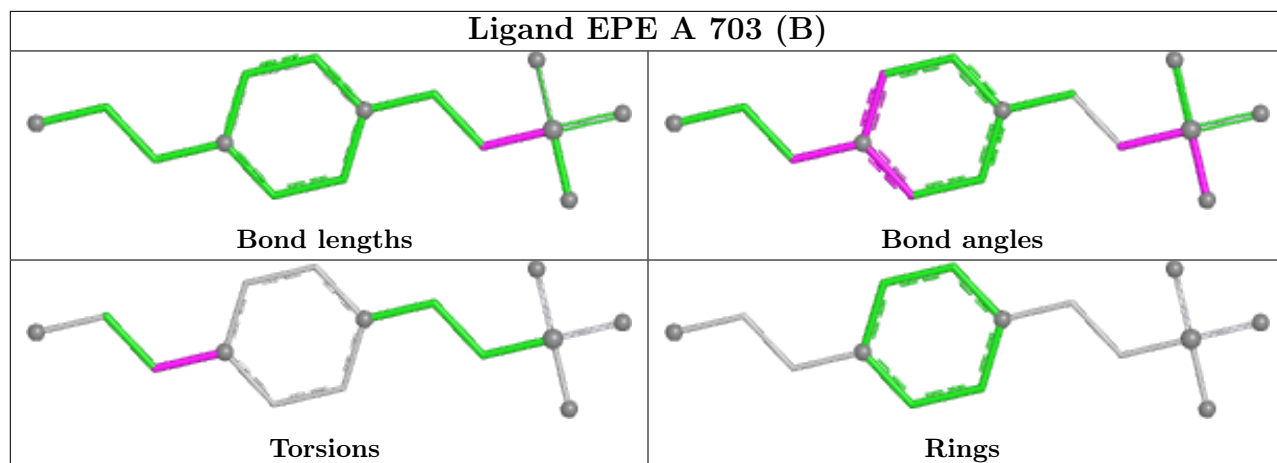
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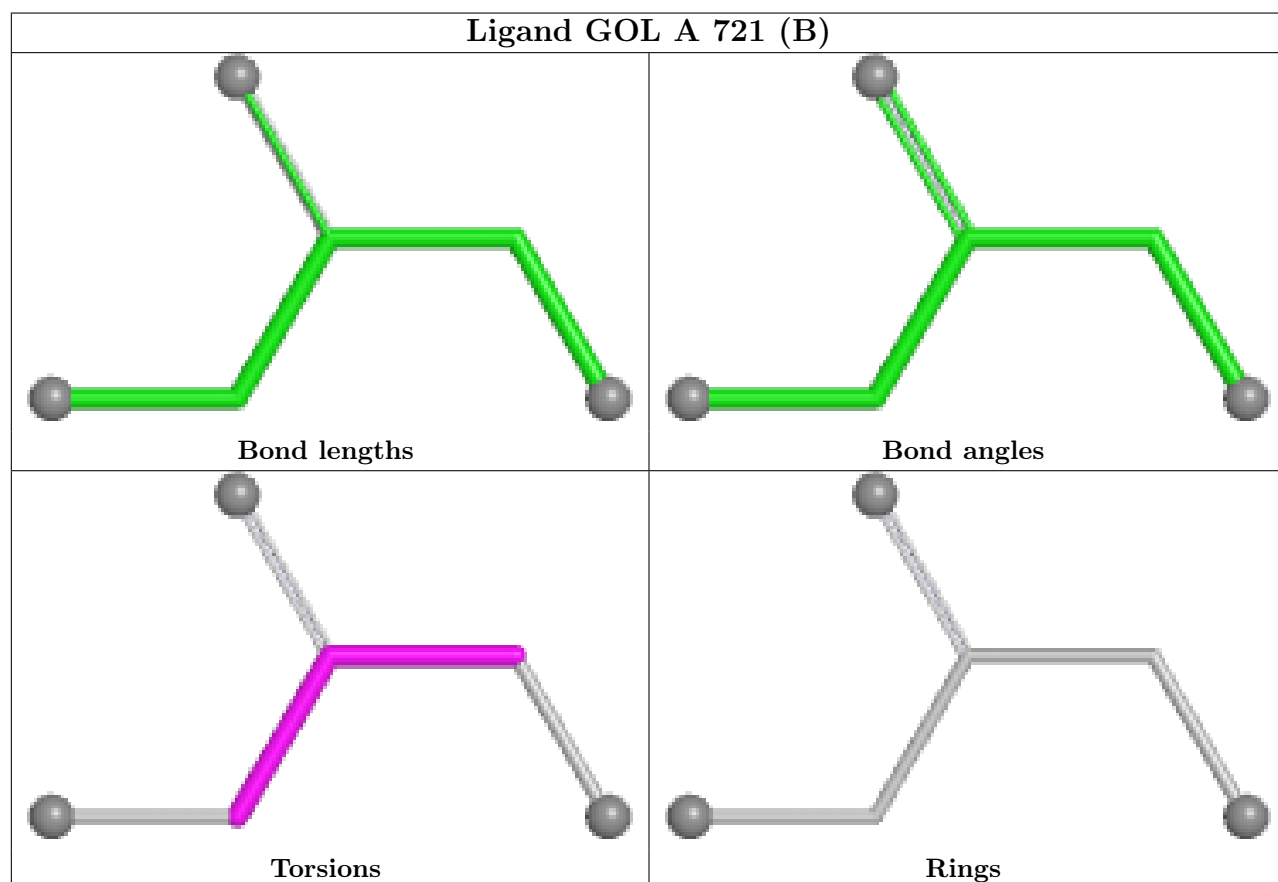
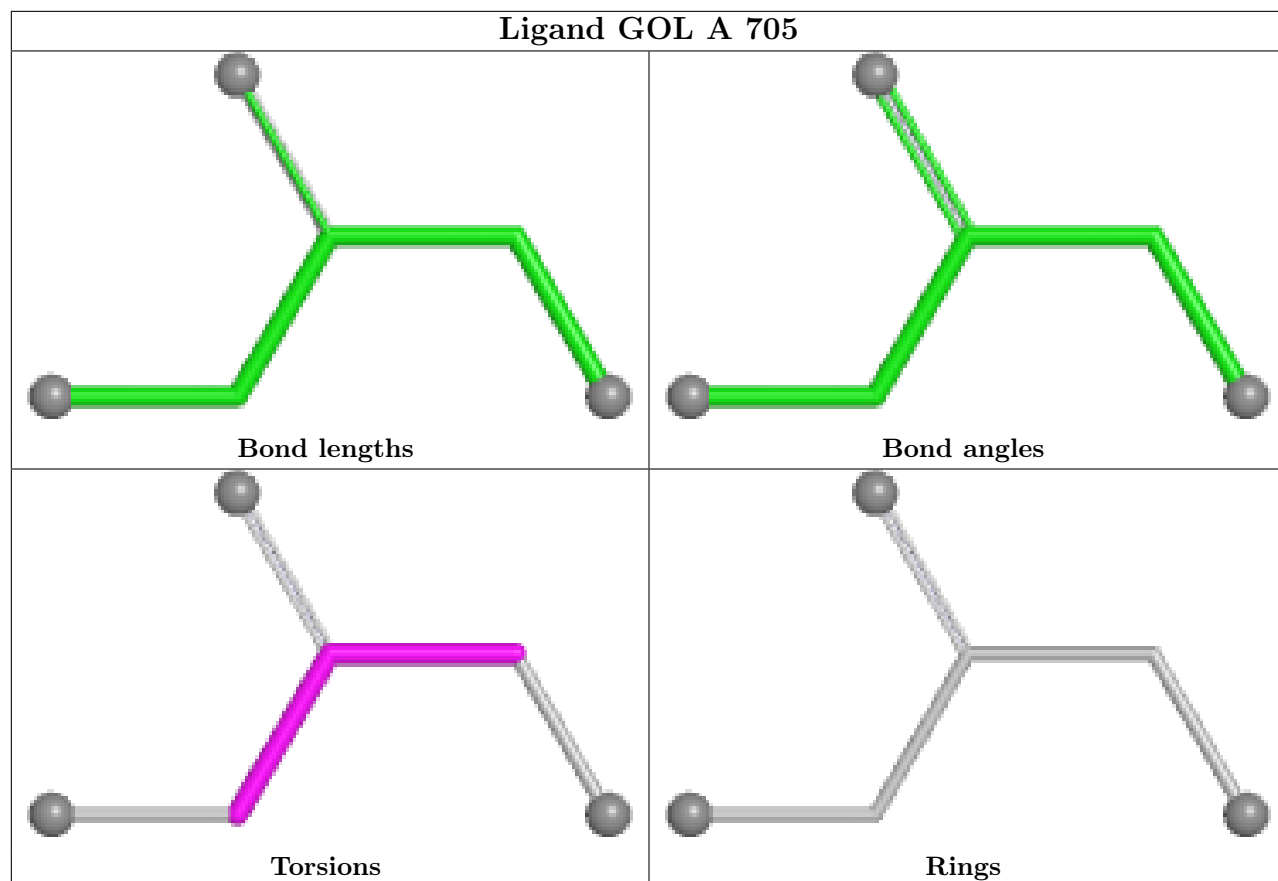
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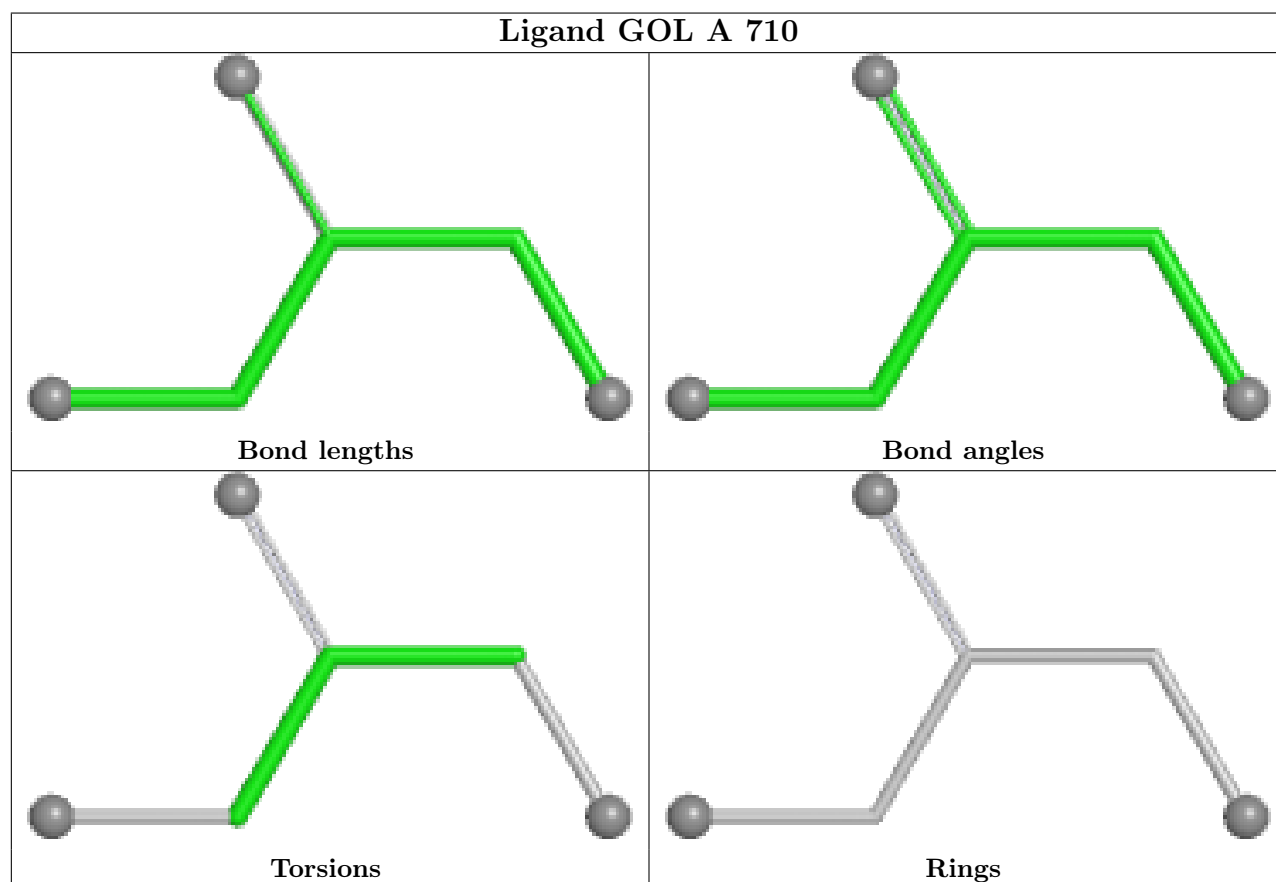
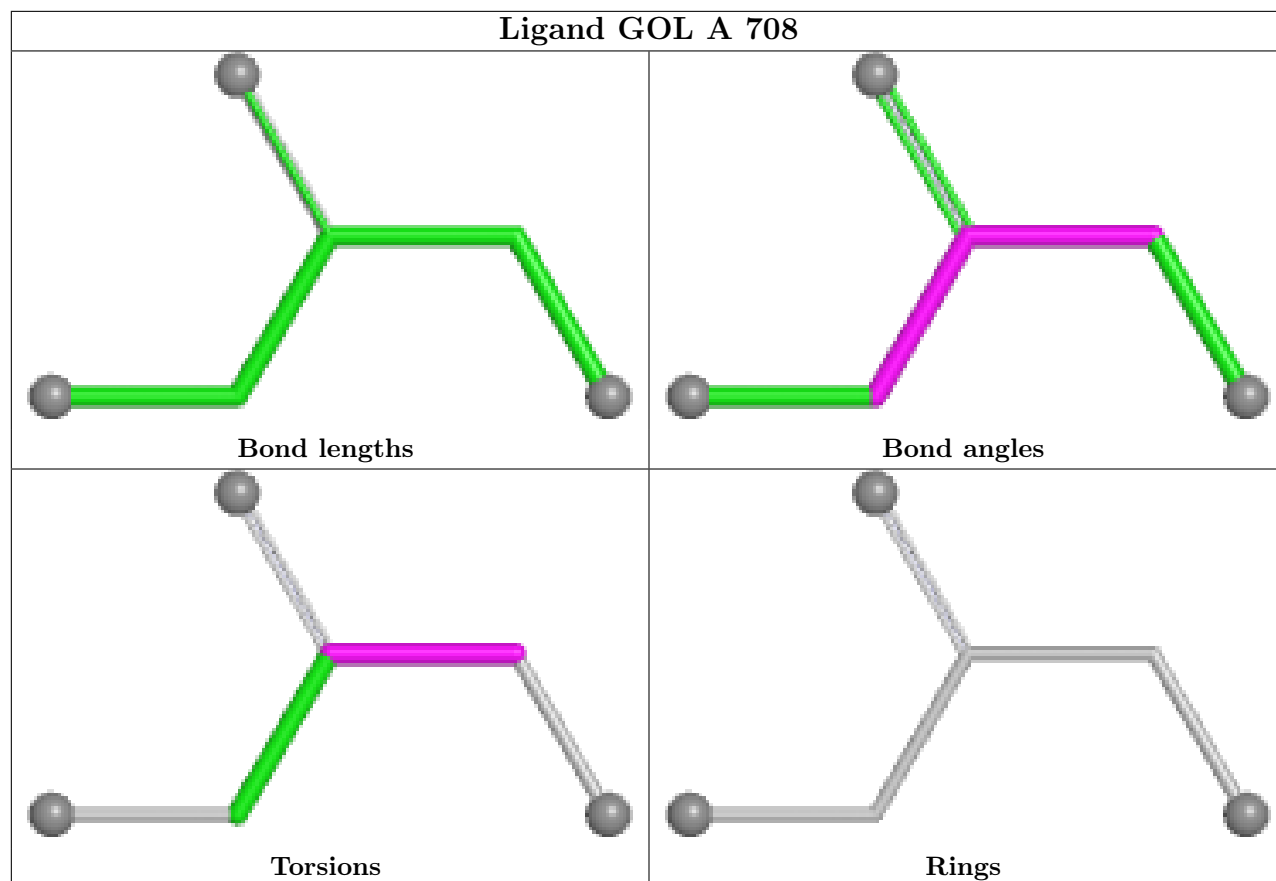
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	719	EDO	2	0
4	A	729	GOL	3	0
4	A	706	GOL	2	0
3	A	712[A]	EPE	1	0
4	A	704	GOL	3	0
4	A	727	GOL	2	0
4	A	722	GOL	1	0
8	A	730[B]	PGE	3	0
4	A	711	GOL	2	0

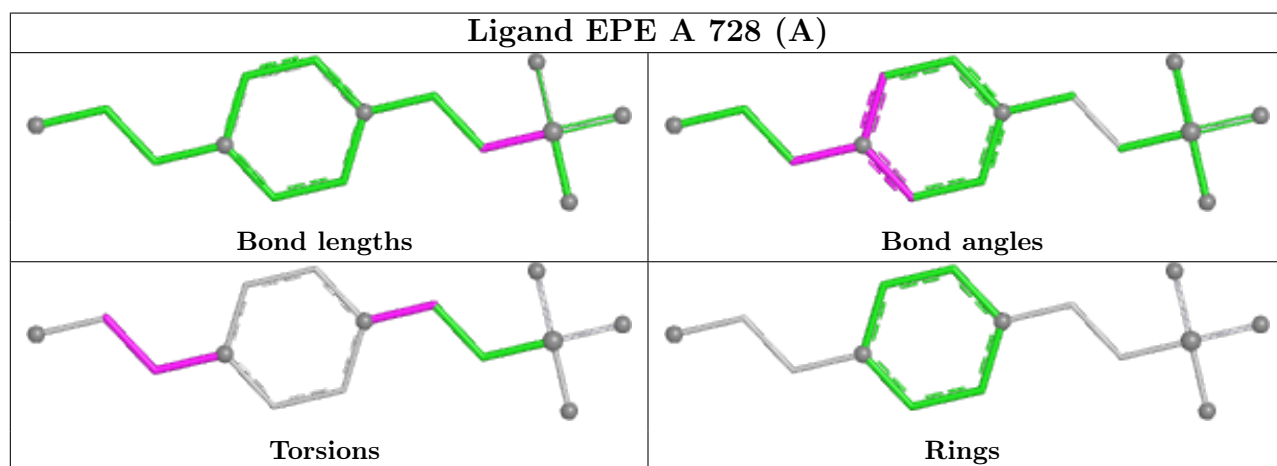
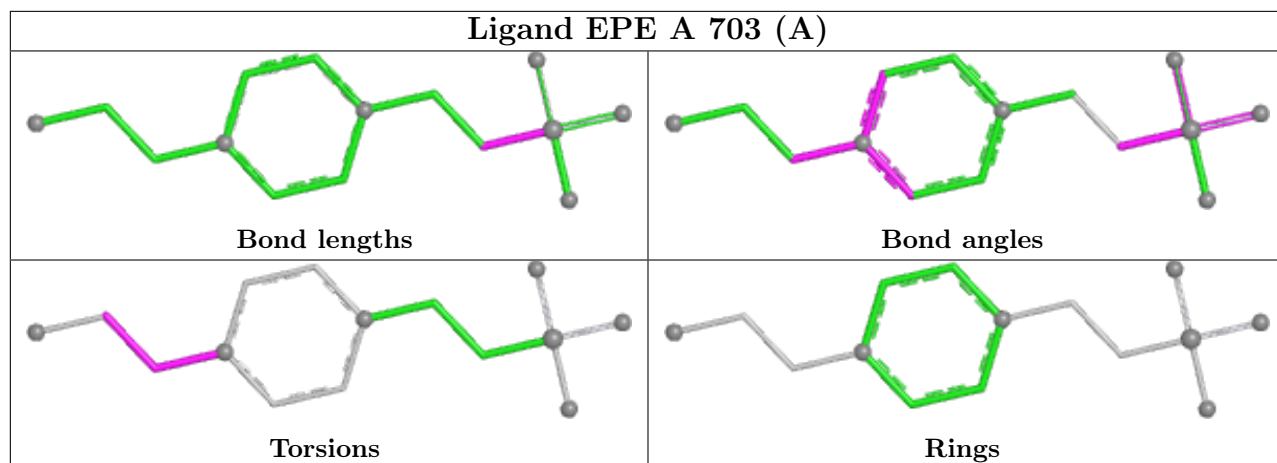
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

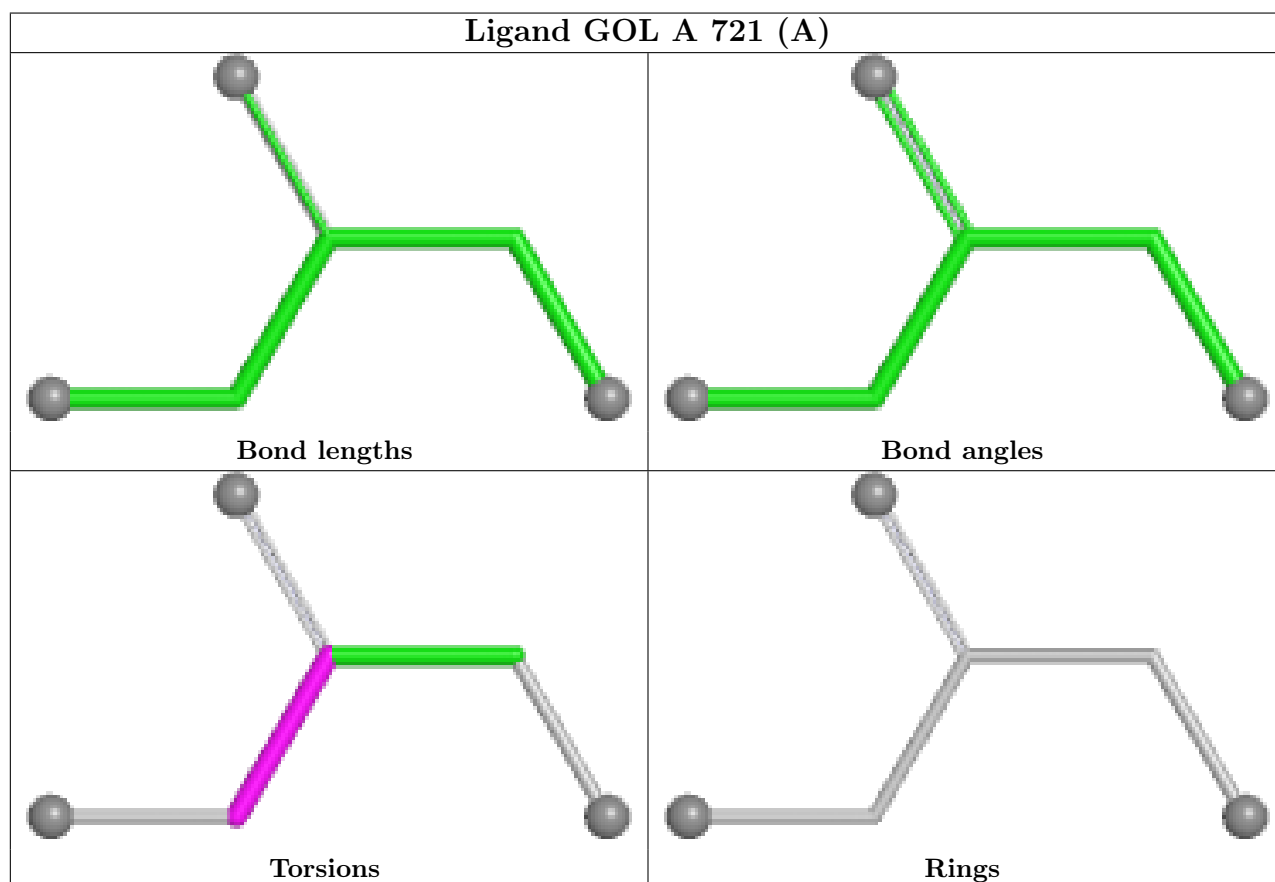
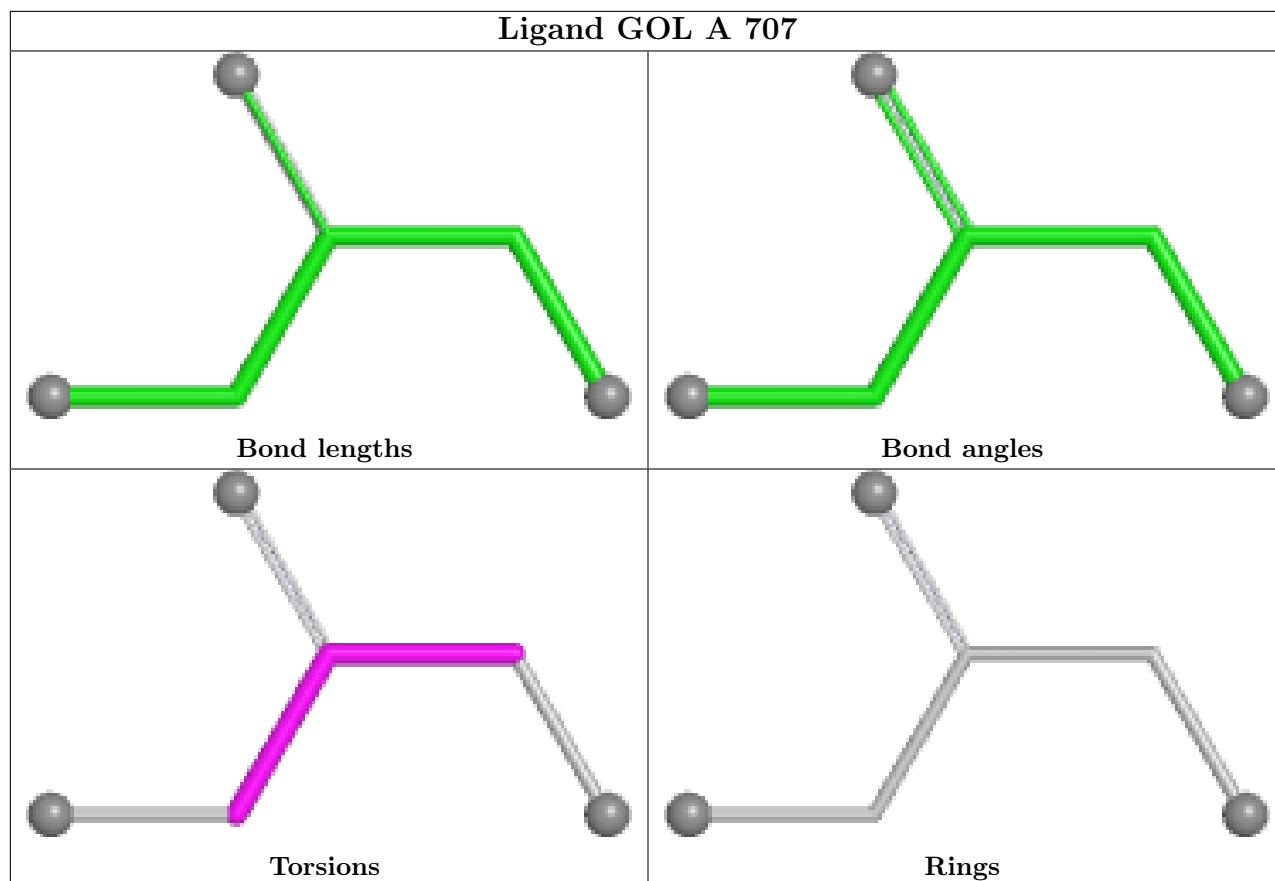


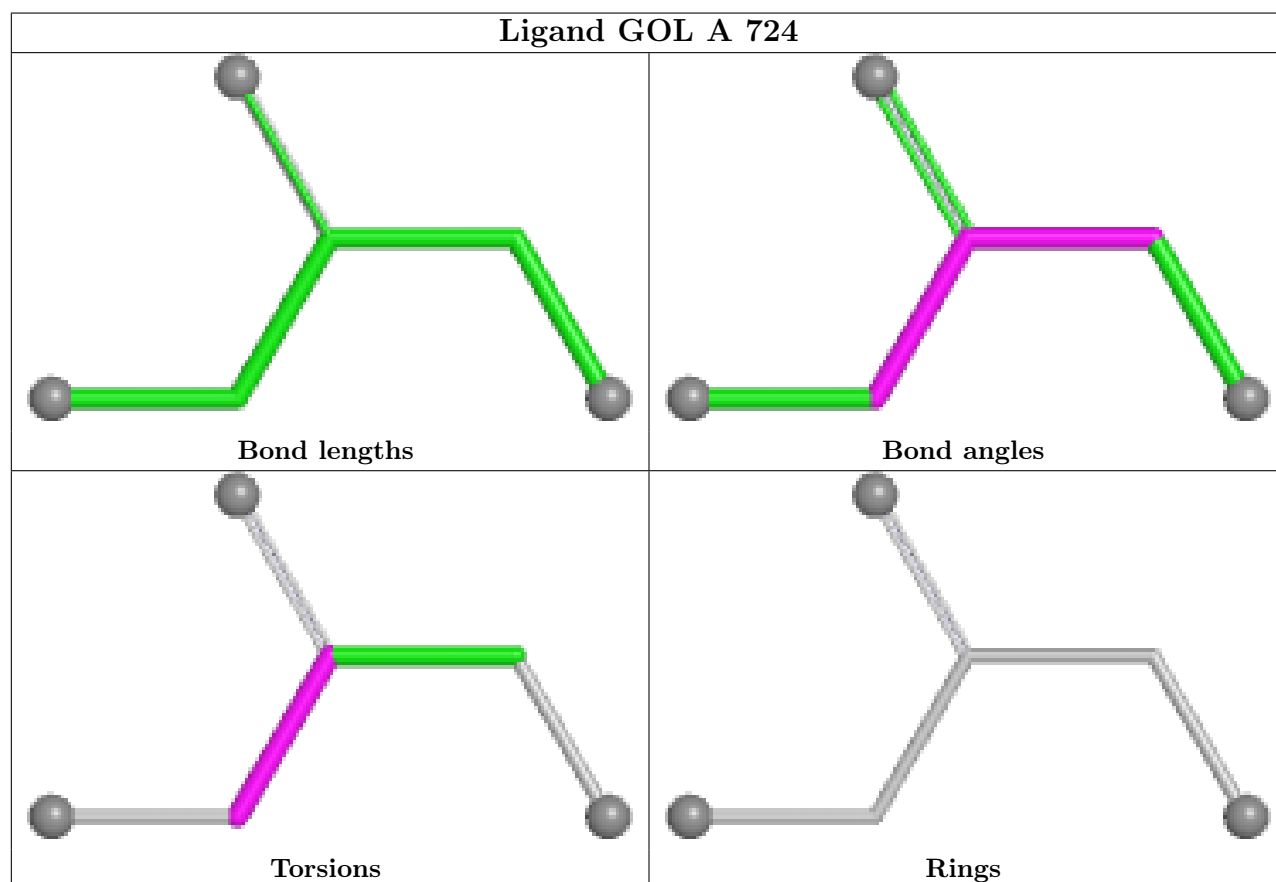
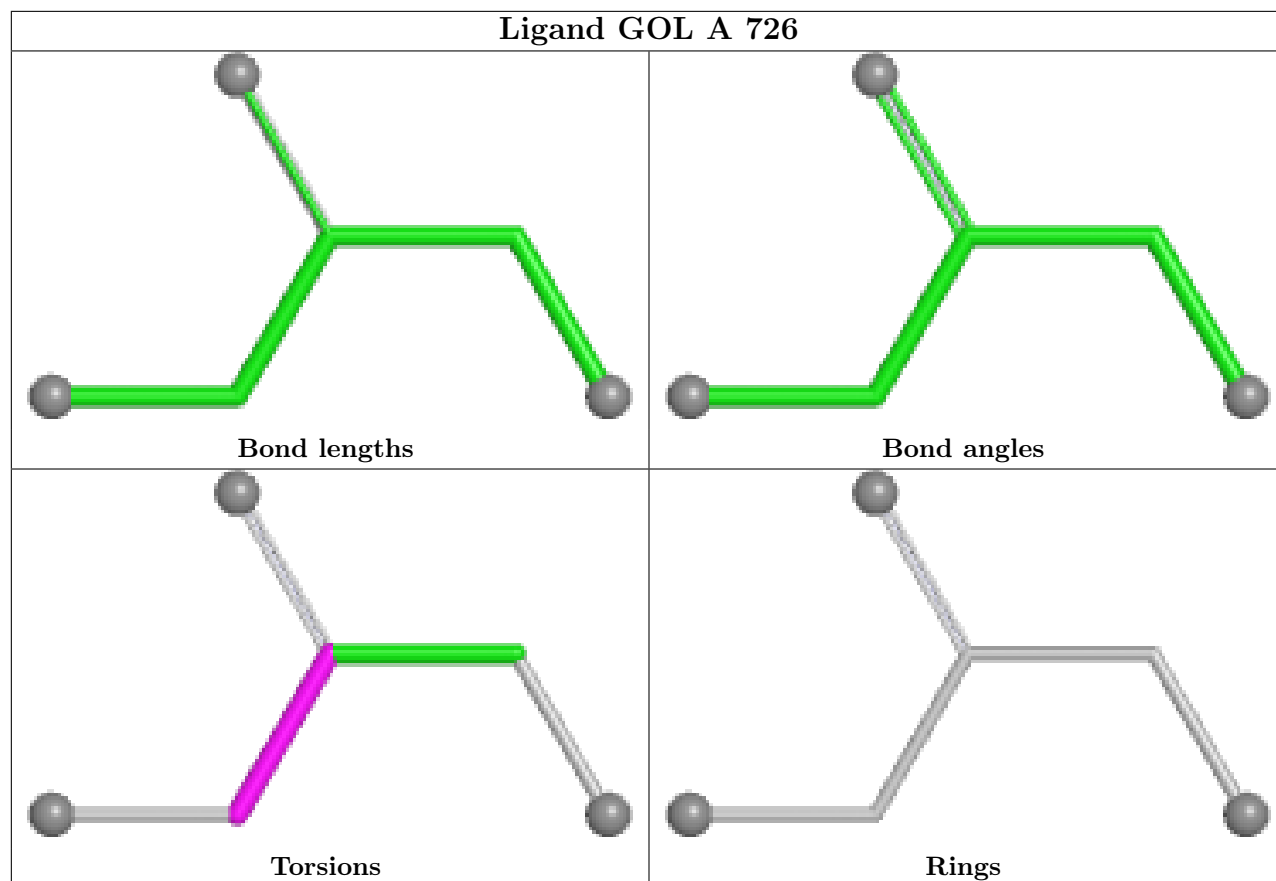




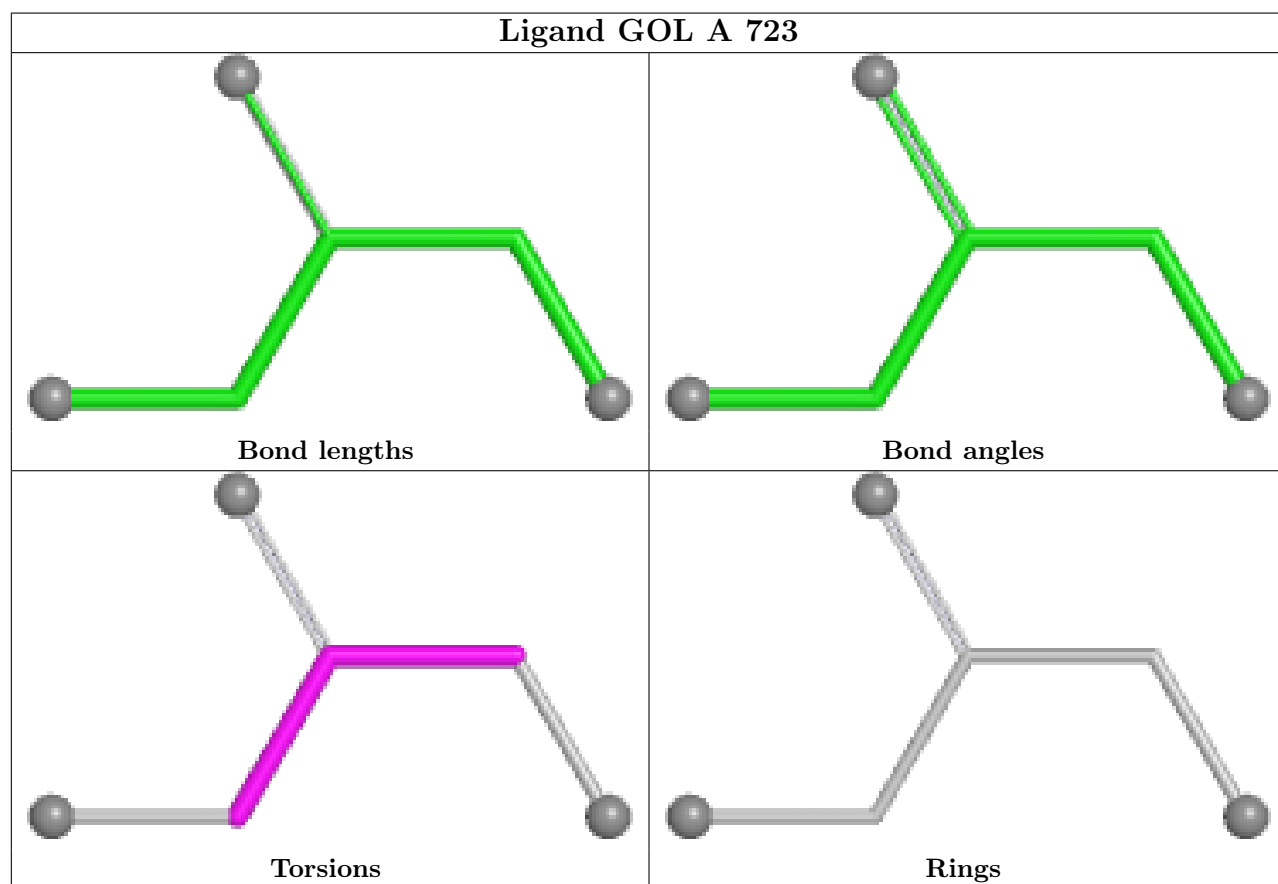
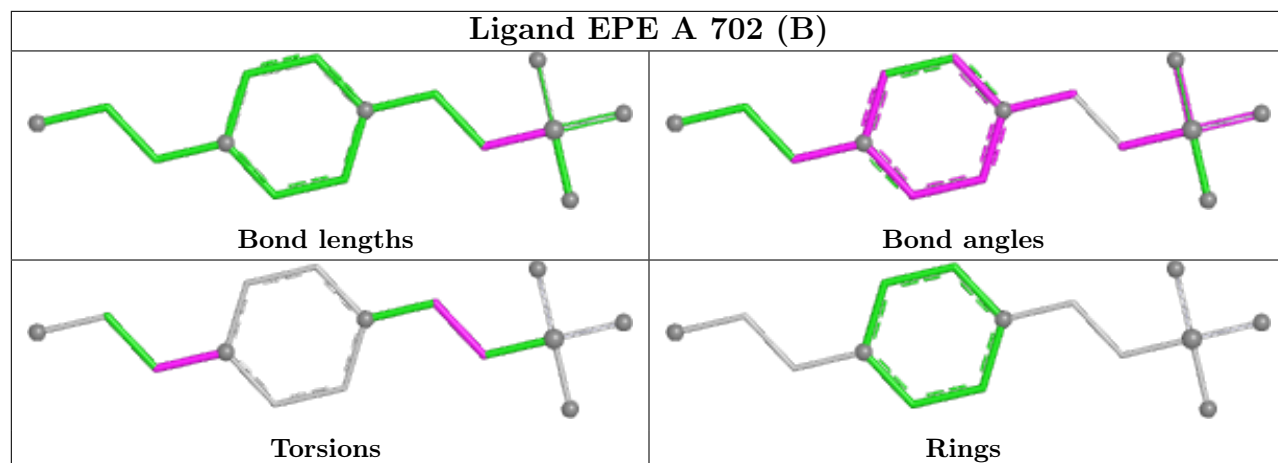


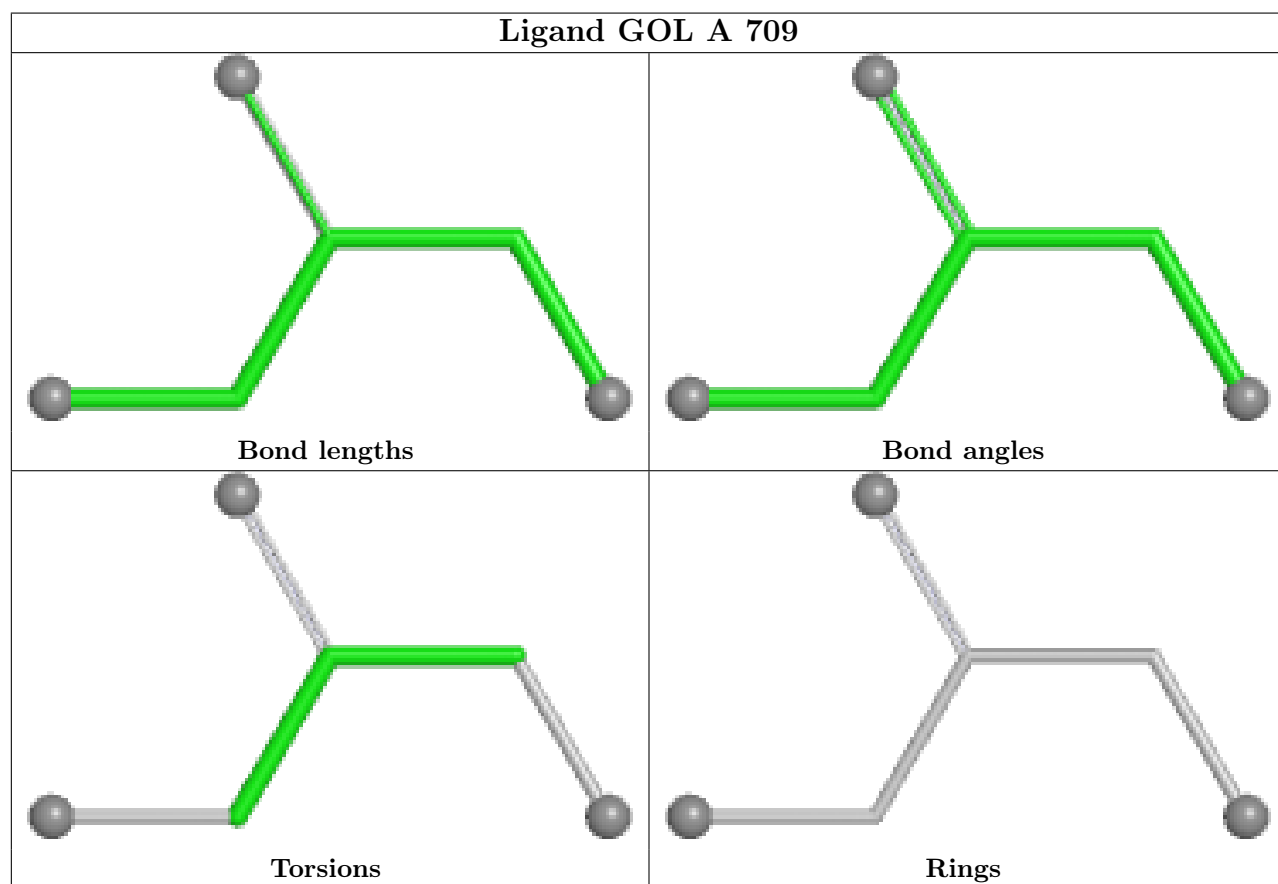
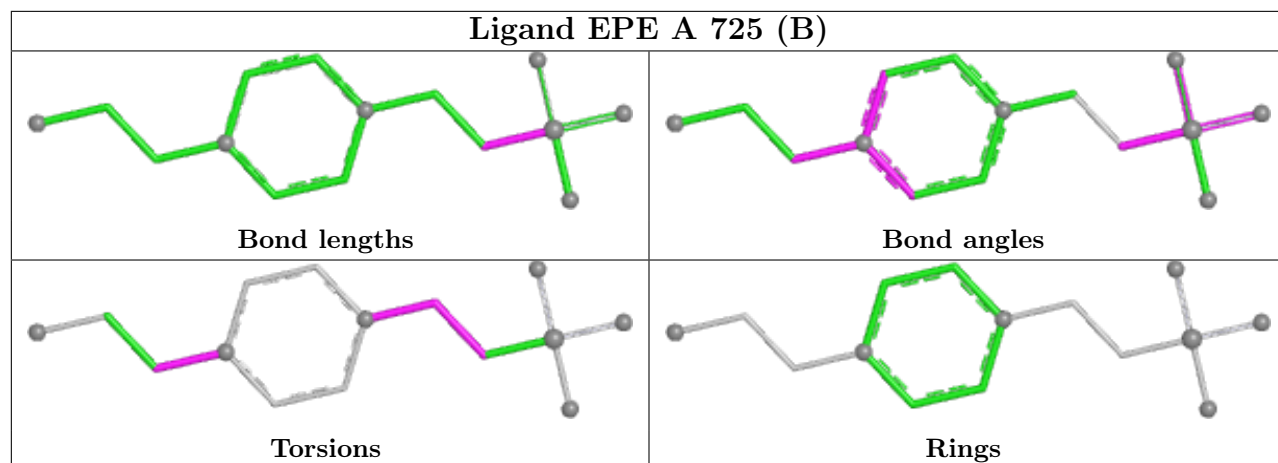


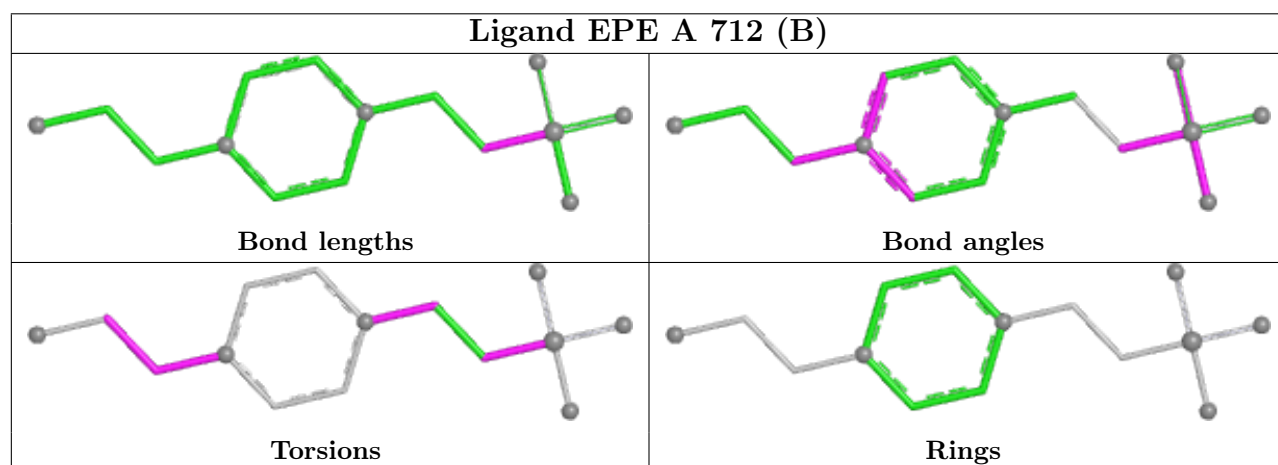
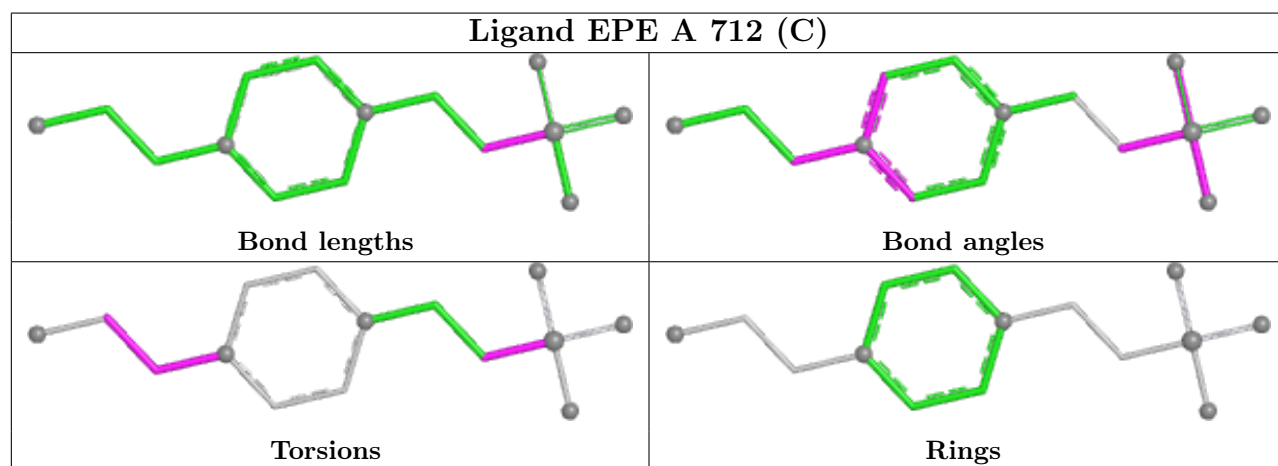
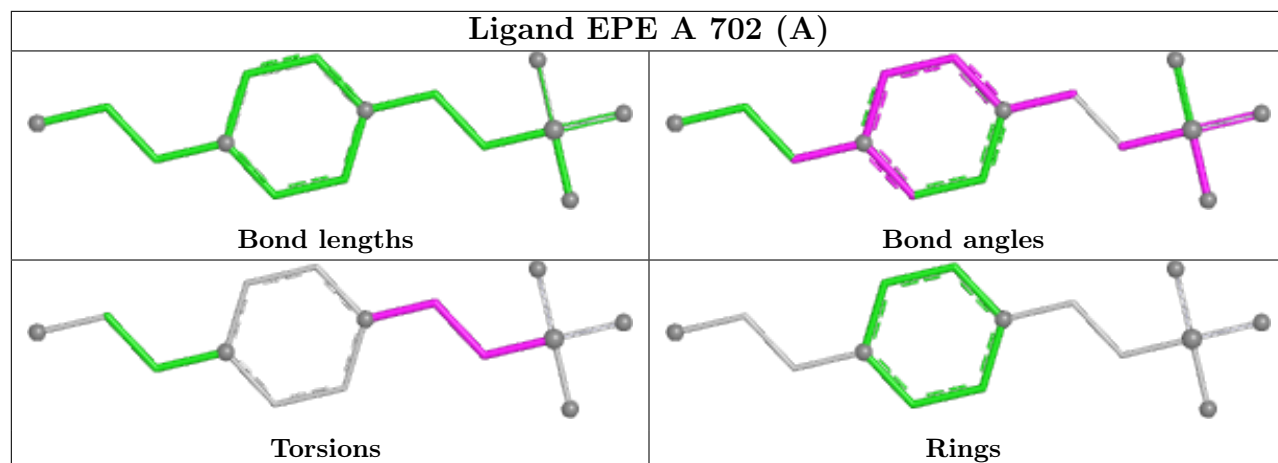


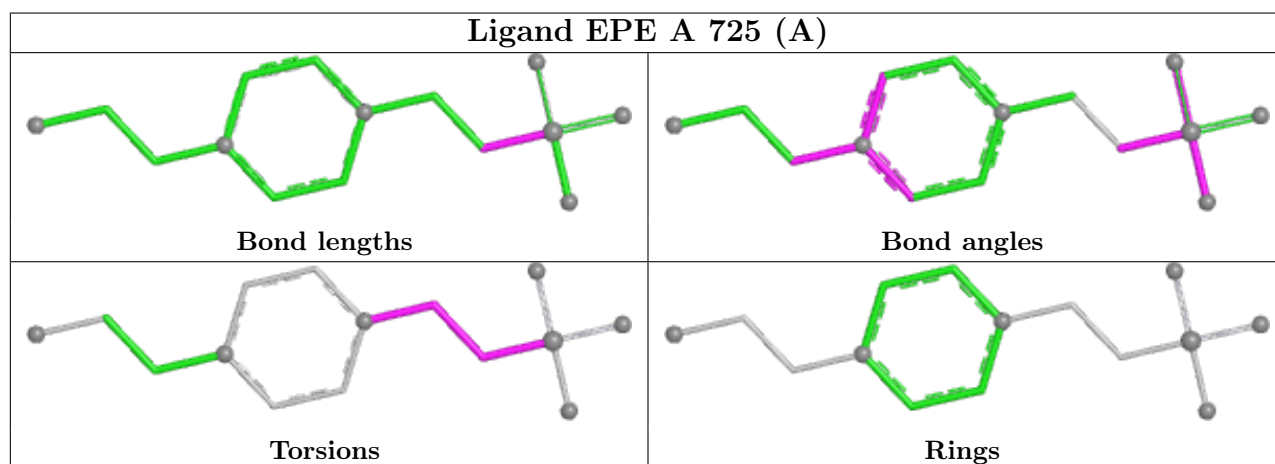
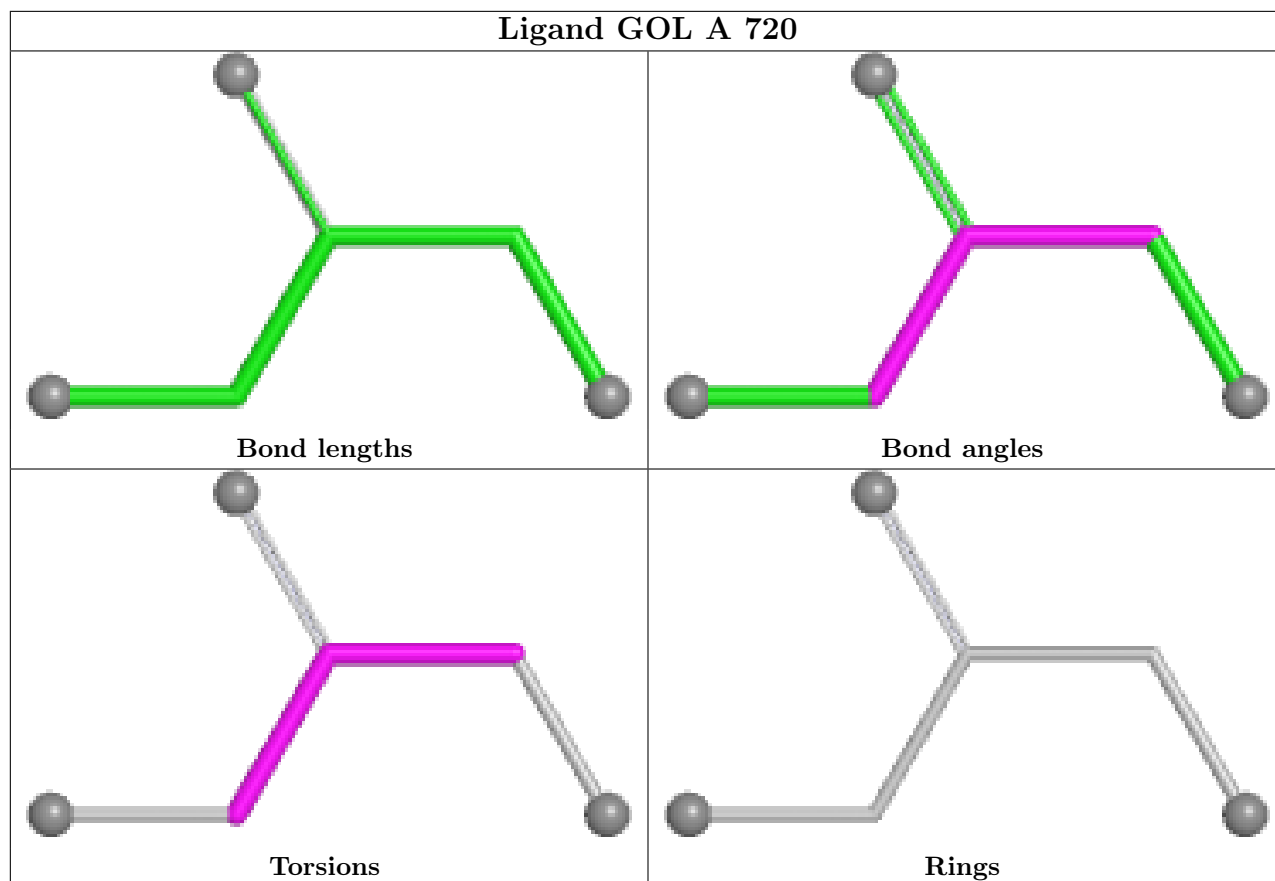


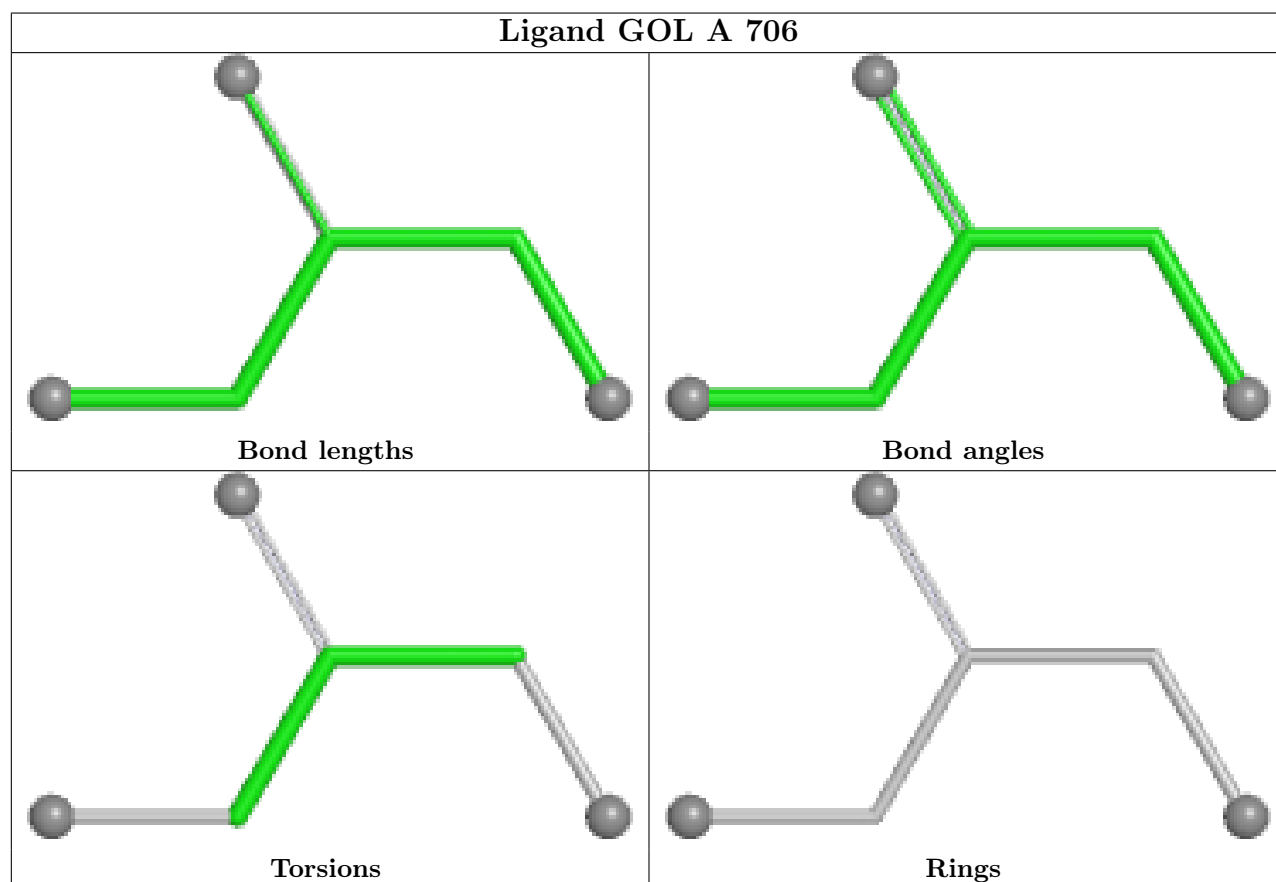
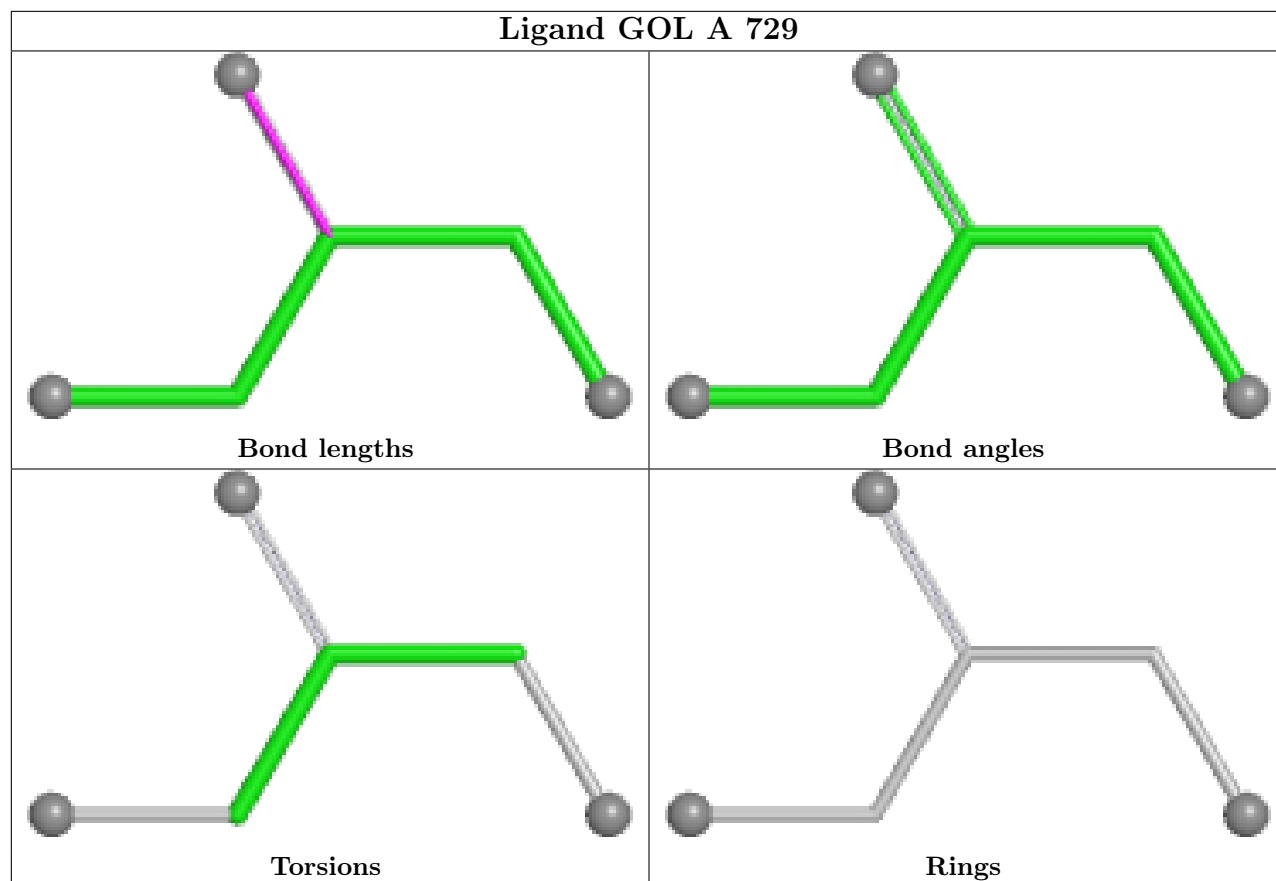


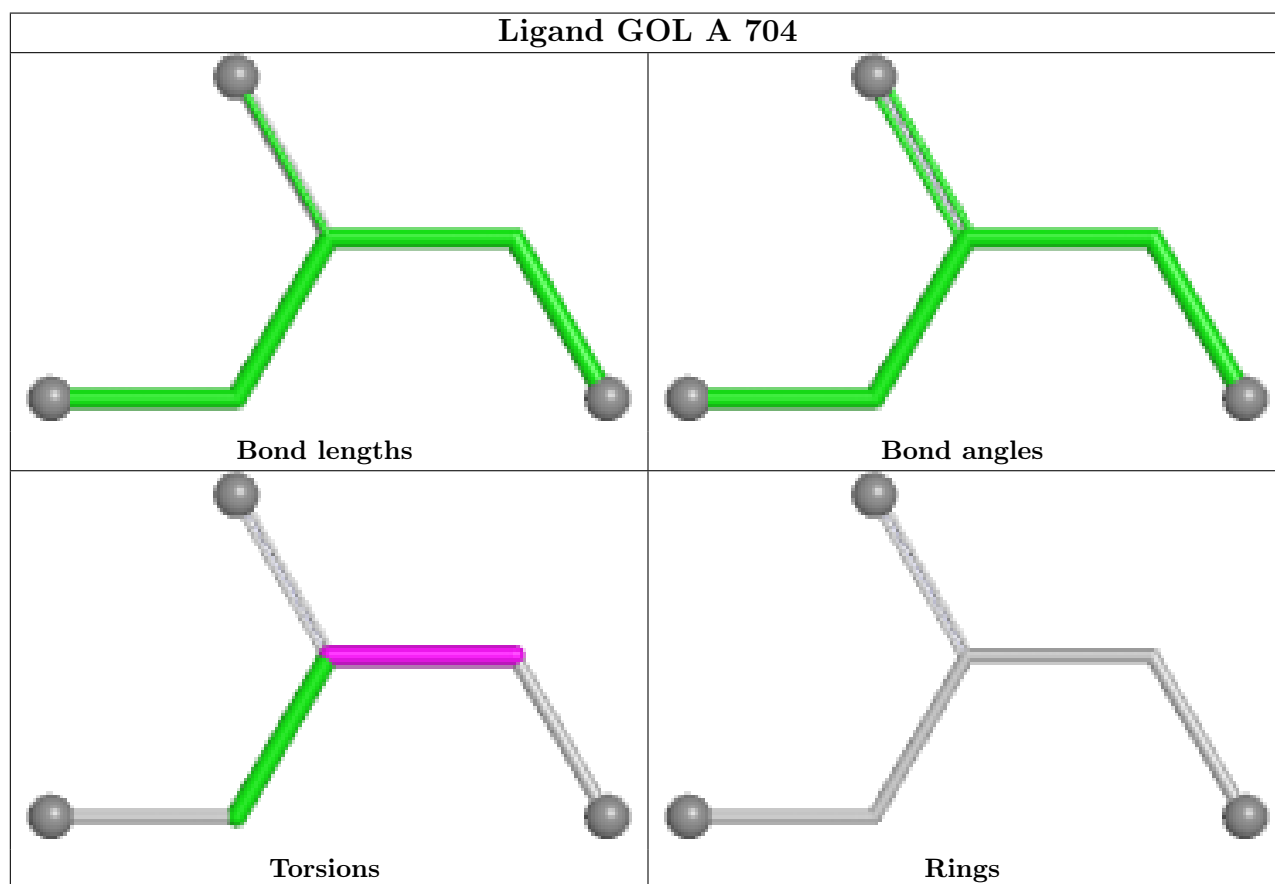
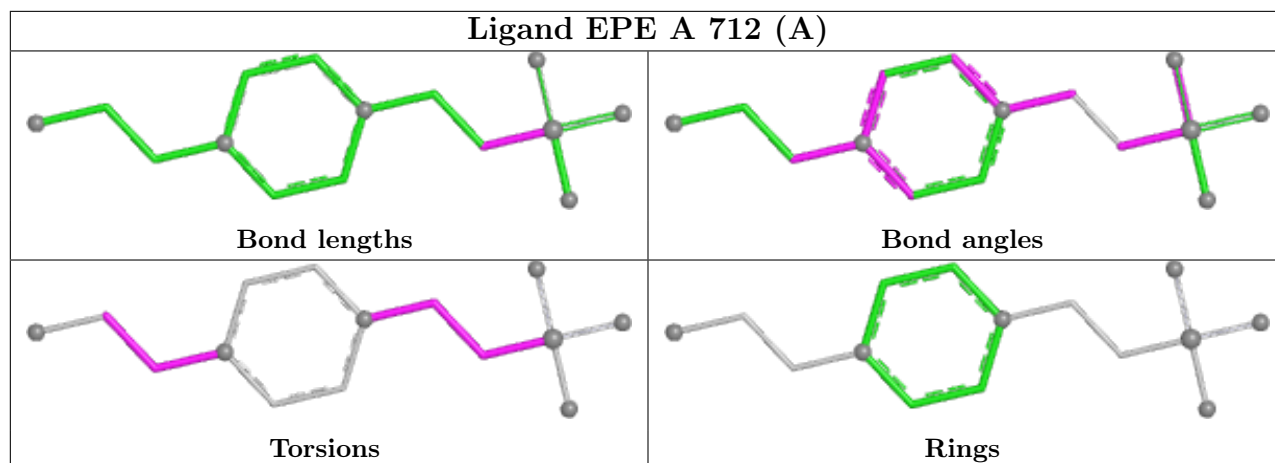


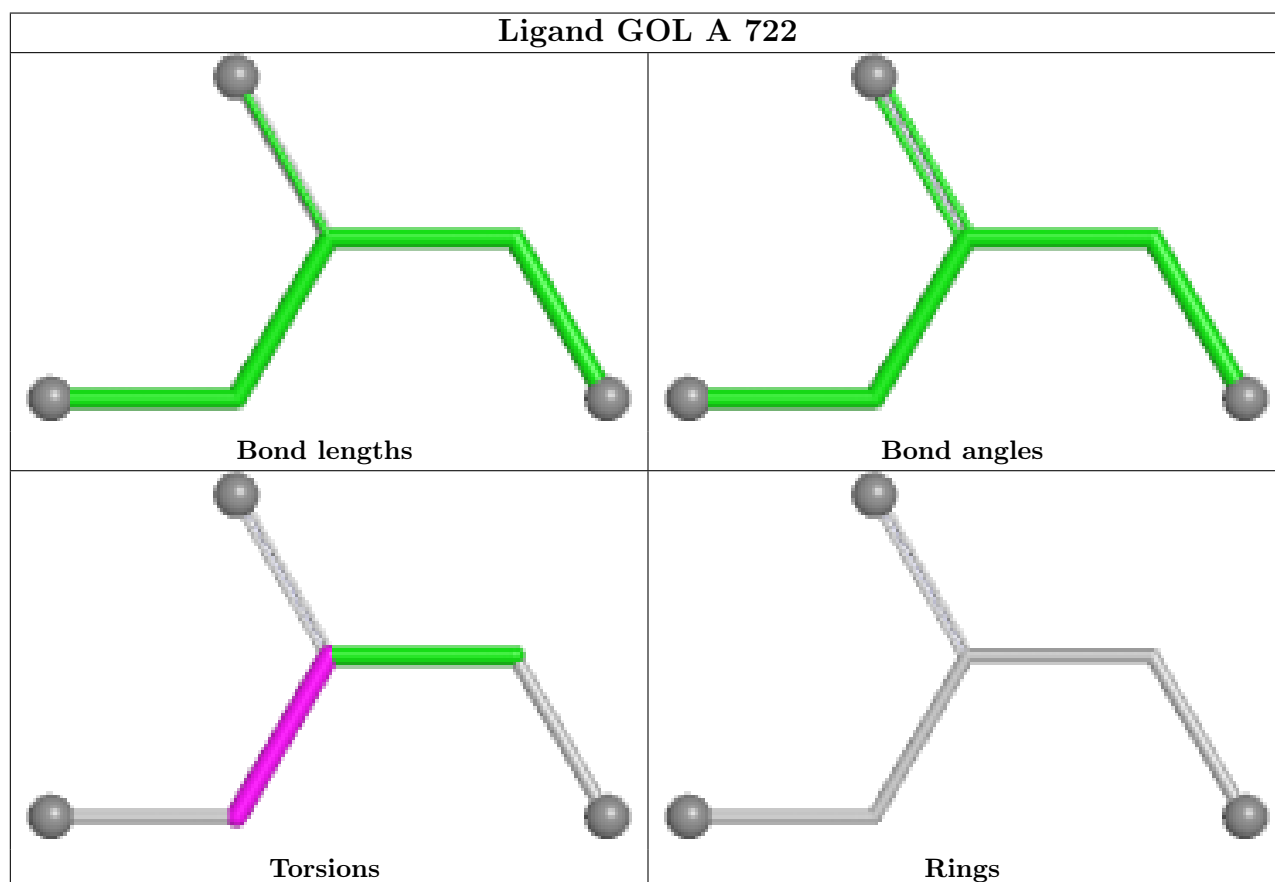
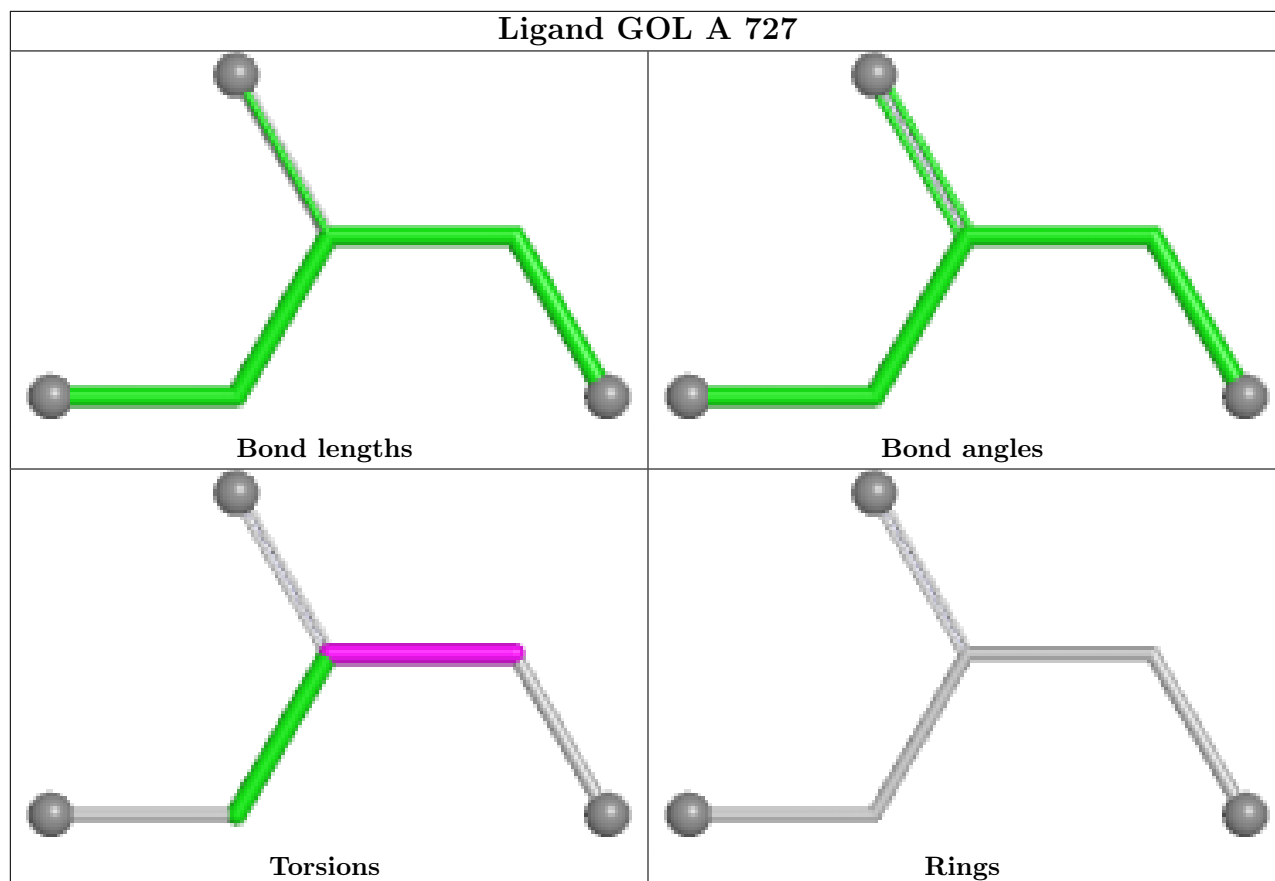


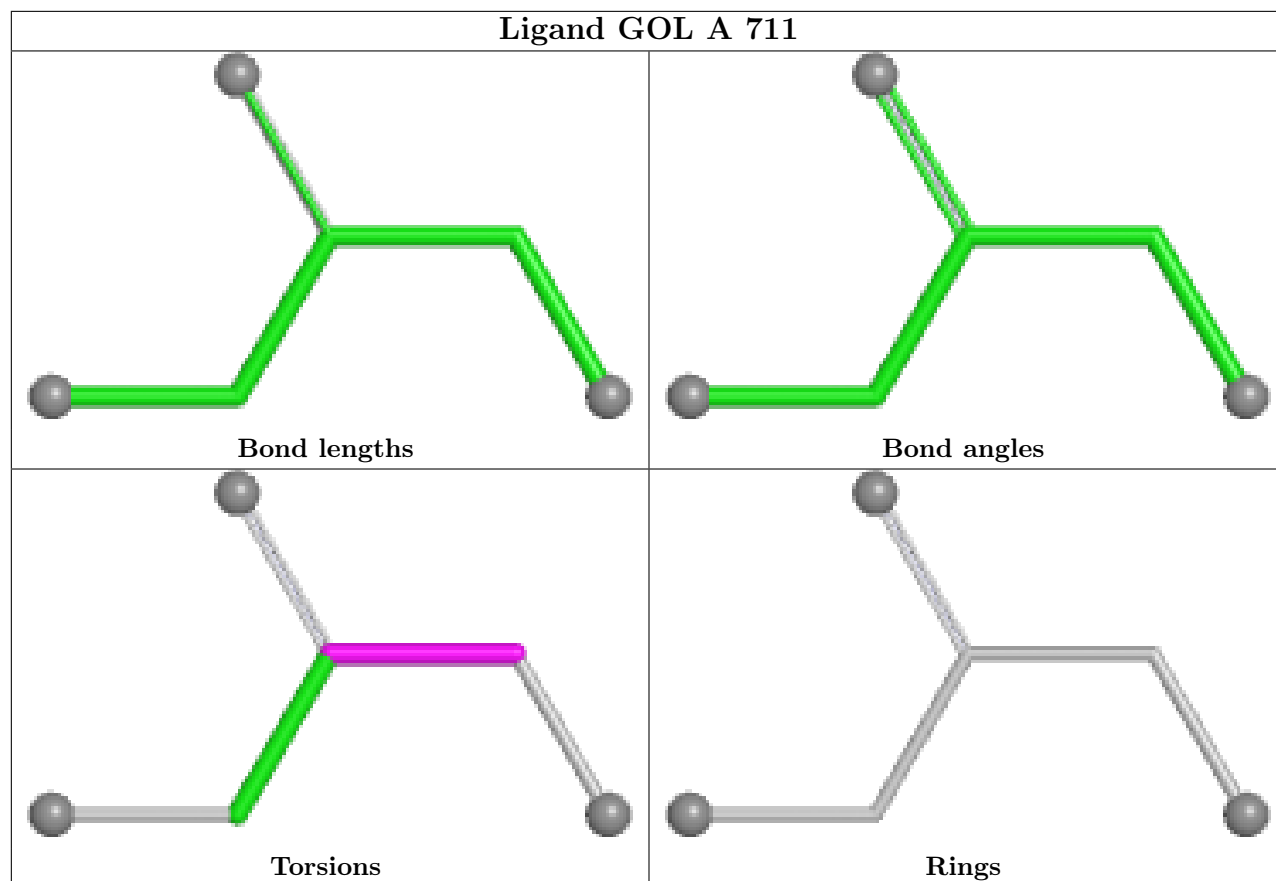












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	303/331 (91%)	0.98	36 (11%) <b>4</b> <b>6</b>	17, 25, 45, 89	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	ASN	6.1
1	A	2	THR	5.7
1	A	3	PRO	5.4
1	A	125	PRO	4.8
1	A	126	ARG	4.5
1	A	127	SER	4.4
1	A	60[A]	HIS	3.9
1	A	150	SER	3.8
1	A	4	THR	3.7
1	A	304	ALA	3.6
1	A	82	ASN	3.6
1	A	84	PRO	3.2
1	A	5	PRO	3.2
1	A	199[A]	HIS	3.1
1	A	253[A]	ARG	3.1
1	A	152[A]	GLN	2.9
1	A	129	VAL	2.7
1	A	106[A]	LYS	2.7
1	A	108	SER	2.6
1	A	81[A]	ARG	2.5
1	A	161	LEU	2.5
1	A	136	LEU	2.4
1	A	124	ILE	2.4
1	A	139	VAL	2.4
1	A	102	ILE	2.4
1	A	147	ASP	2.3
1	A	202	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	40	LYS	2.3
1	A	123	LYS	2.2
1	A	175	ALA	2.2
1	A	238	LEU	2.2
1	A	78	PRO	2.2
1	A	293	LYS	2.1
1	A	79	SER	2.1
1	A	83	VAL	2.1
1	A	300	LEU	2.1

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

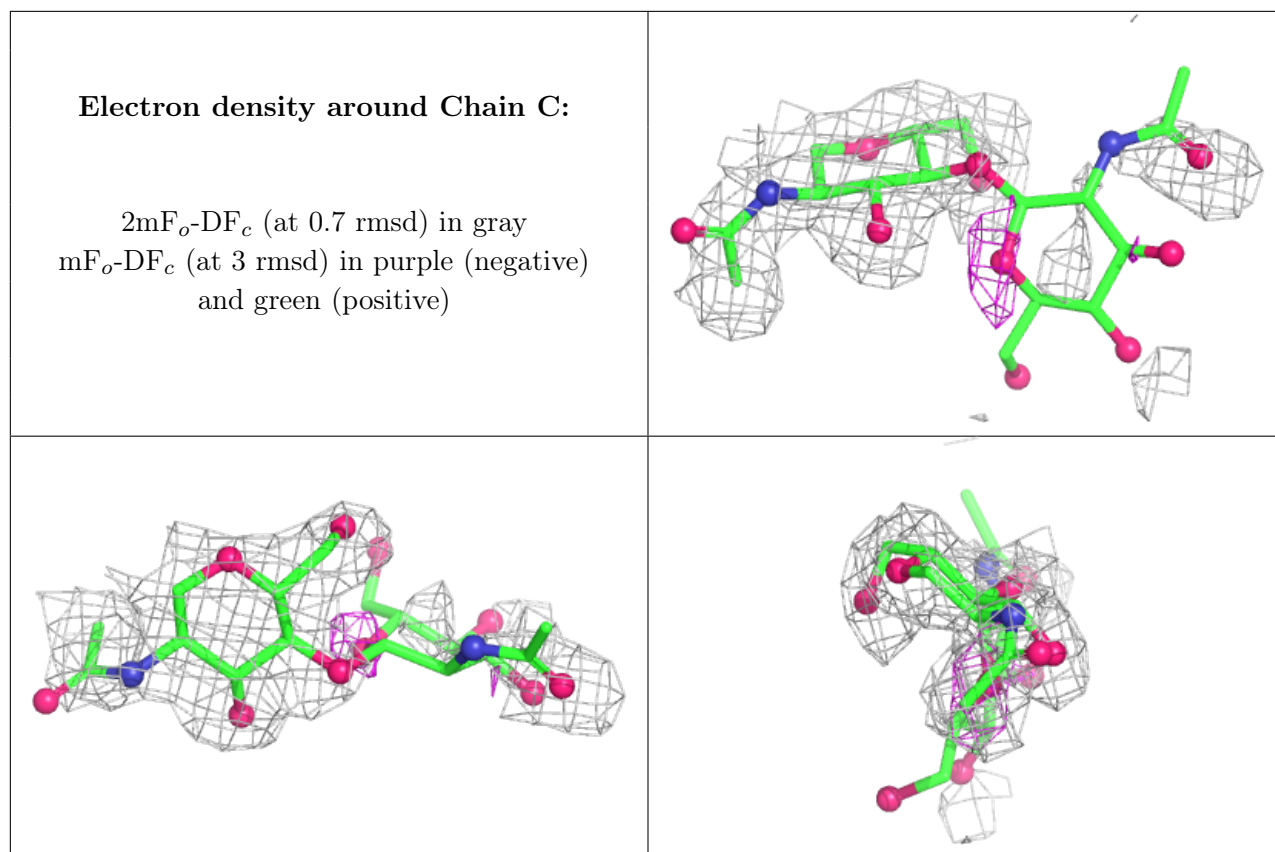
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	C	2	14/15	0.29	0.86	52,63,76,80	14
2	NAG	C	1	14/15	0.78	0.22	28,37,46,59	14

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.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	EDO	A	717	4/4	0.08	0.54	59,64,74,80	4
3	EPE	A	703[B]	15/15	0.32	0.49	58,68,73,74	15
3	EPE	A	703[A]	15/15	0.32	0.49	41,64,82,86	15
4	GOL	A	726	6/6	0.34	0.76	67,77,83,85	6
4	GOL	A	729	6/6	0.36	0.50	63,71,77,78	6
4	GOL	A	727	6/6	0.38	0.69	65,76,83,89	6
3	EPE	A	728[A]	15/15	0.39	0.76	75,82,88,98	15
3	EPE	A	728[B]	15/15	0.39	0.76	70,80,87,88	15
3	EPE	A	725[A]	15/15	0.42	0.69	65,72,79,80	15
3	EPE	A	725[B]	15/15	0.42	0.69	66,73,79,84	15
3	EPE	A	712[C]	15/15	0.48	0.52	47,54,55,56	15
3	EPE	A	712[A]	15/15	0.48	0.52	46,54,56,61	15
3	EPE	A	712[B]	15/15	0.48	0.52	48,54,58,63	15

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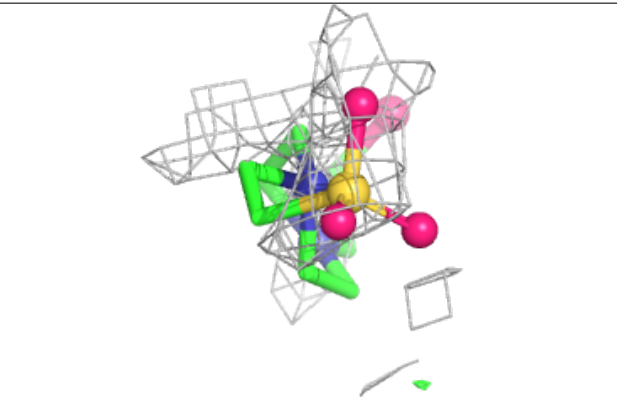
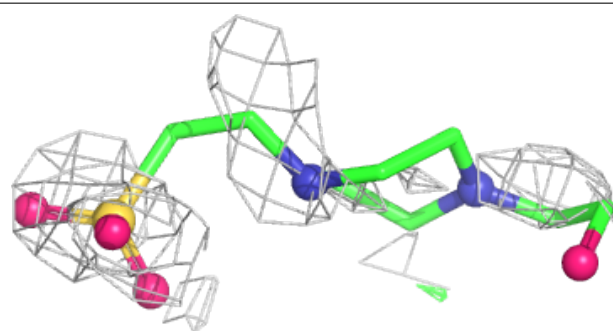
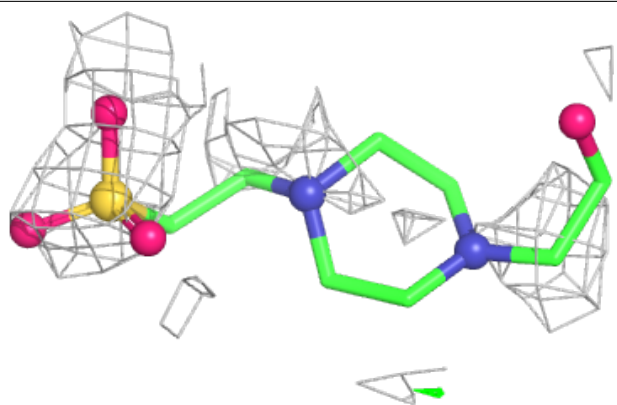
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	720	6/6	0.52	0.47	26,30,33,37	6
3	EPE	A	702[A]	15/15	0.55	0.47	43,59,68,77	15
4	GOL	A	705	6/6	0.55	0.42	34,47,58,61	6
4	GOL	A	708	6/6	0.55	0.40	42,50,52,56	6
3	EPE	A	702[B]	15/15	0.55	0.47	31,50,60,61	15
4	GOL	A	709	6/6	0.64	0.38	36,41,48,50	6
4	GOL	A	721[B]	6/6	0.67	0.40	42,52,53,55	6
4	GOL	A	724	6/6	0.67	0.27	25,42,43,51	6
4	GOL	A	721[A]	6/6	0.67	0.40	42,52,52,53	6
4	GOL	A	706	6/6	0.69	0.43	48,49,57,58	6
4	GOL	A	710	6/6	0.69	0.31	41,51,55,56	6
8	PGE	A	730[A]	7/10	0.71	0.50	20,24,28,28	7
8	PGE	A	730[B]	7/10	0.71	0.50	16,24,28,30	7
4	GOL	A	707	6/6	0.72	0.31	33,49,58,62	0
4	GOL	A	704	6/6	0.73	0.33	35,45,51,54	6
7	EDO	A	716	4/4	0.75	0.50	19,22,31,33	4
7	EDO	A	718	4/4	0.75	0.27	62,65,68,74	4
4	GOL	A	722	6/6	0.76	0.37	42,49,58,60	6
3	EPE	A	701	15/15	0.76	0.29	32,43,61,62	15
4	GOL	A	711	6/6	0.78	0.29	41,53,64,72	6
7	EDO	A	719	4/4	0.81	0.23	48,56,59,60	4
9	NA	A	732	1/1	0.83	0.31	32,32,32,32	1
4	GOL	A	723	6/6	0.85	0.37	29,34,38,39	6
9	NA	A	731	1/1	0.90	0.16	21,21,21,21	0
6	PO4	A	715	5/5	0.90	0.22	21,25,28,32	0
5	FE	A	713	1/1	0.98	0.08	22,22,22,22	0
5	FE	A	714	1/1	1.00	0.09	24,24,24,24	0

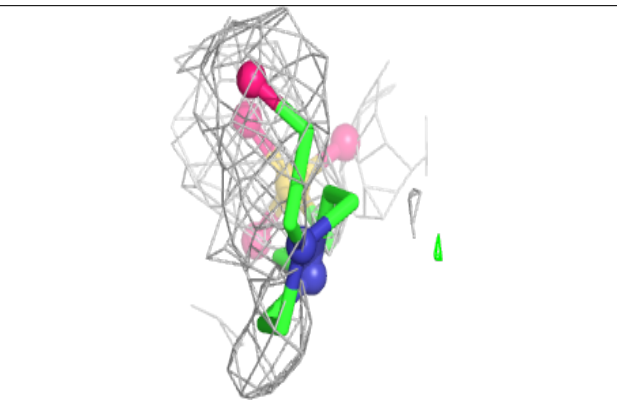
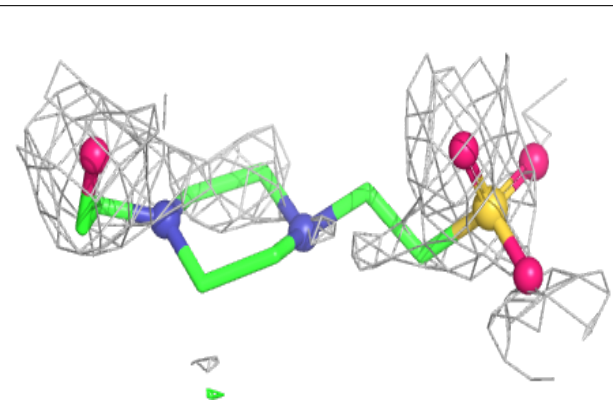
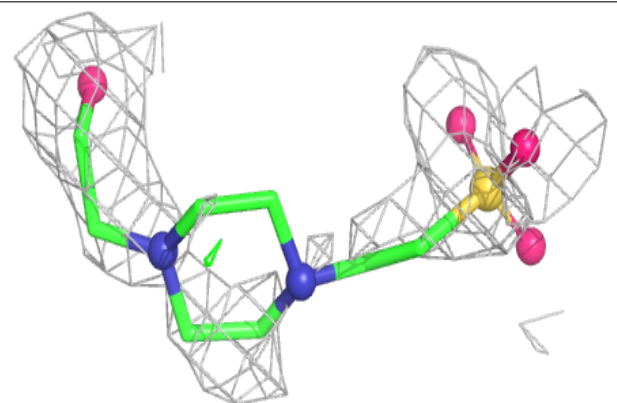
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

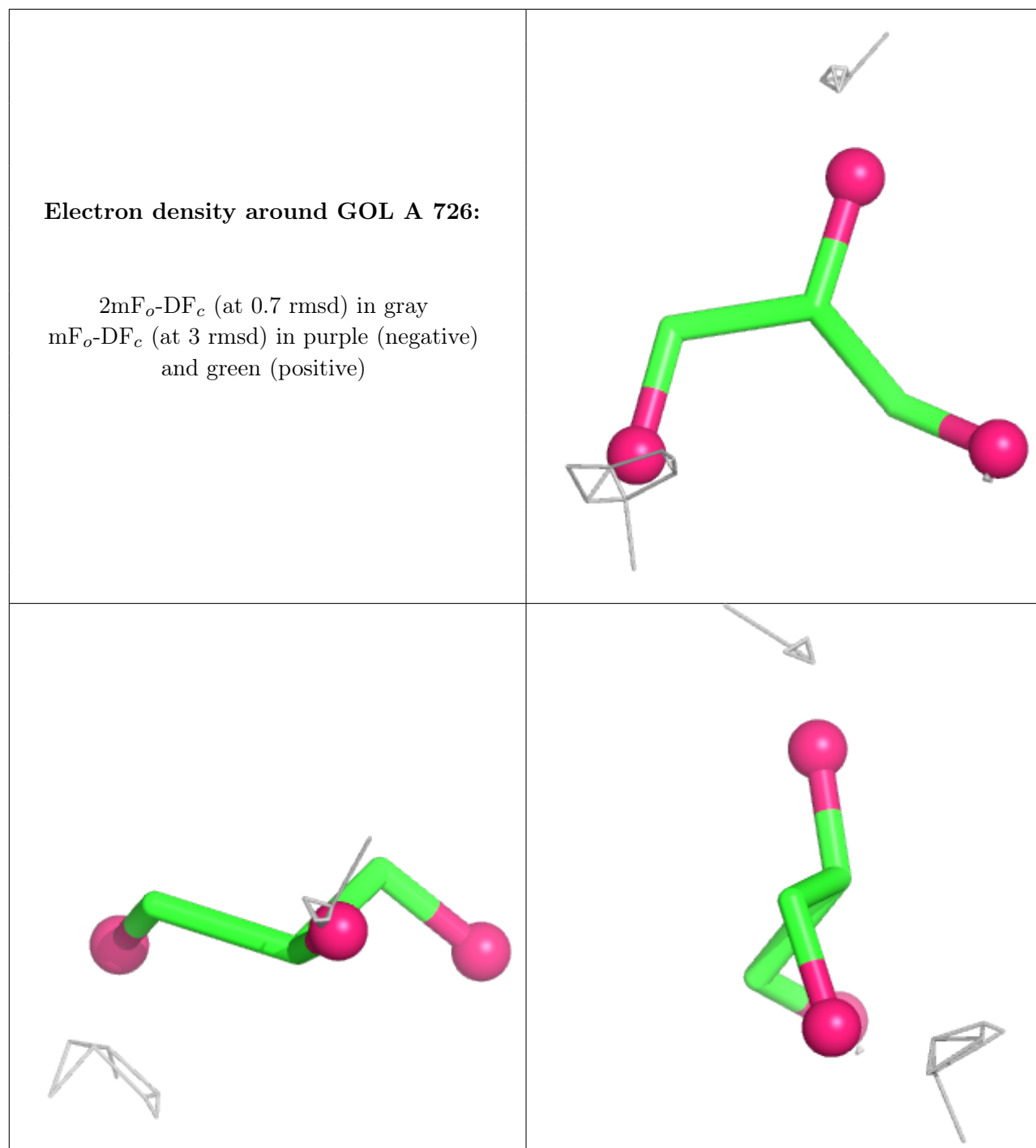
**Electron density around EPE A 703 (B):**

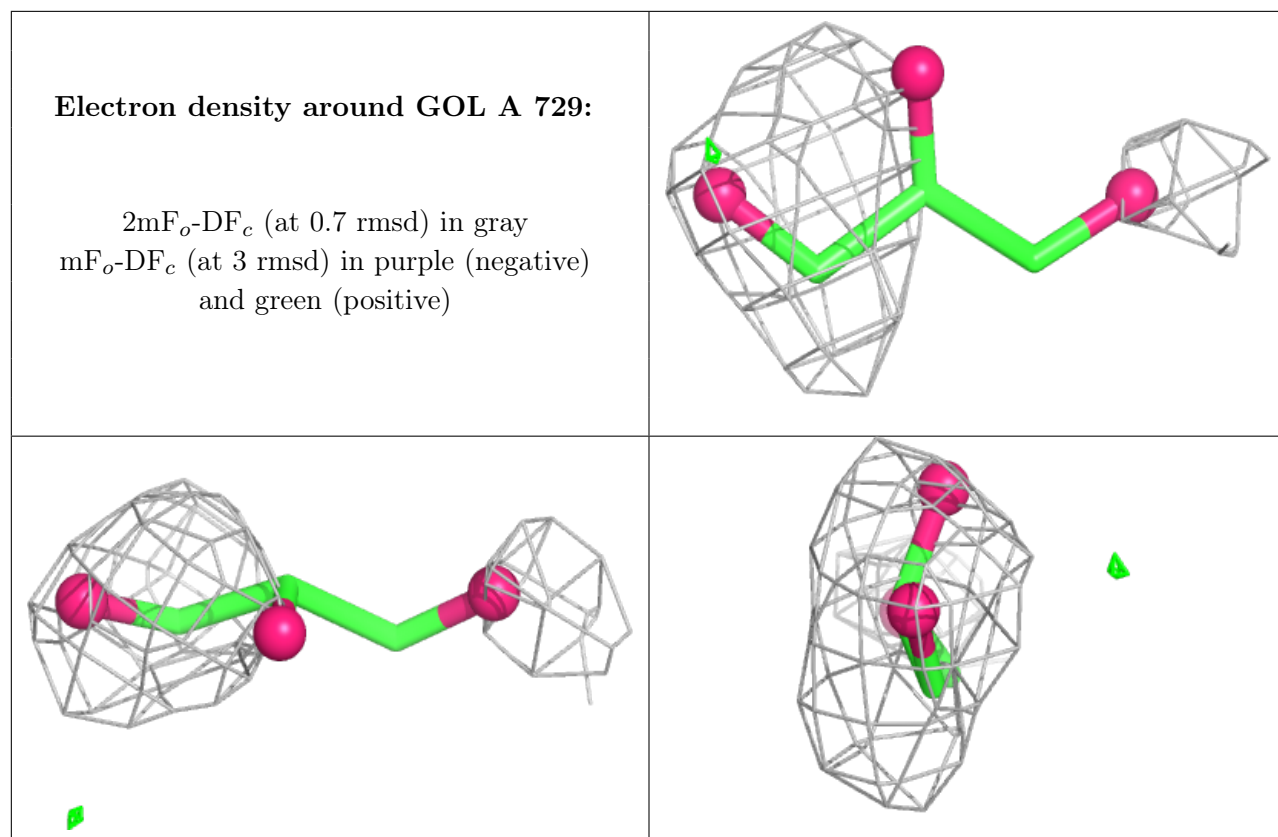
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

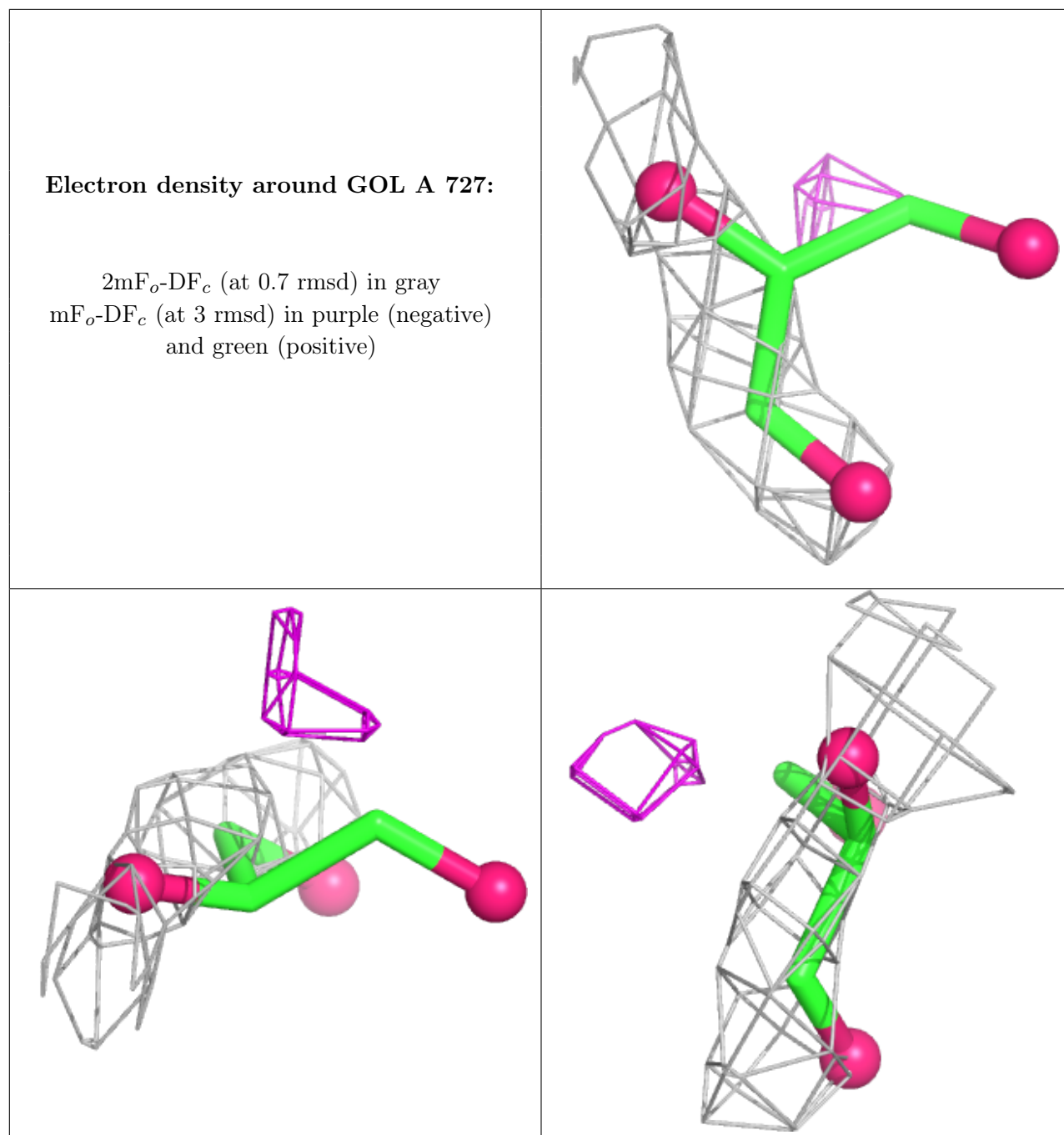
**Electron density around EPE A 703 (A):**

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





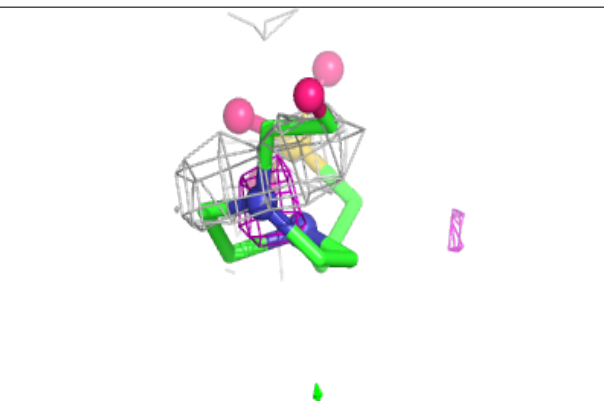
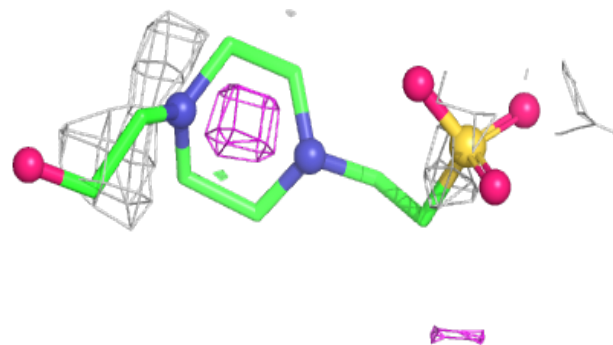
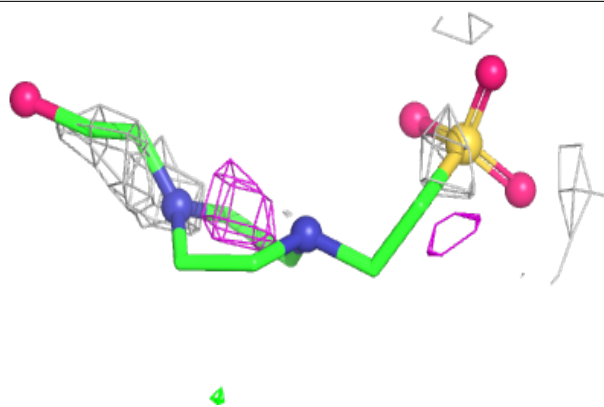




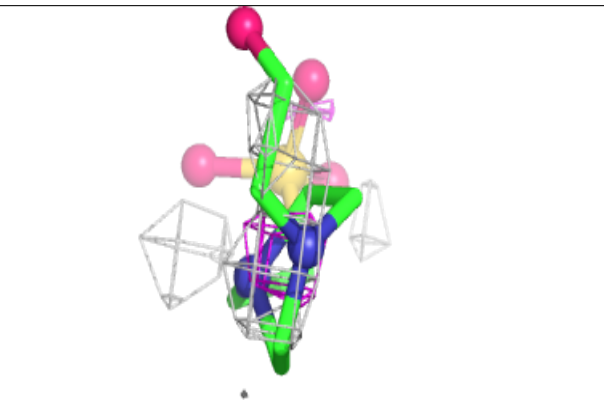
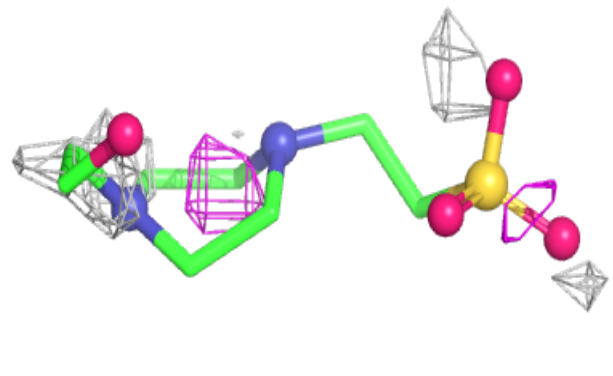
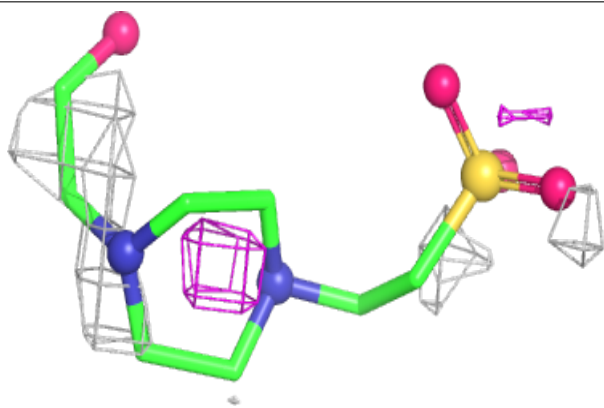


**Electron density around EPE A 728 (A):**

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

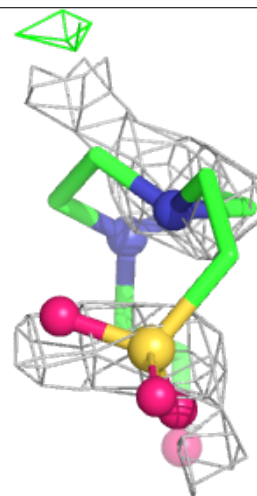
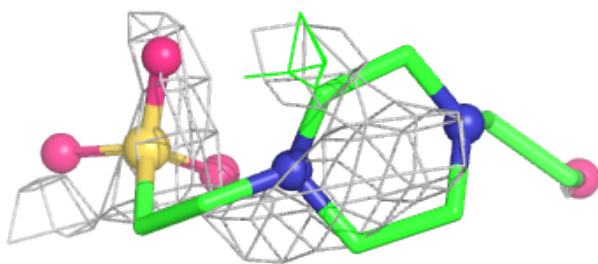
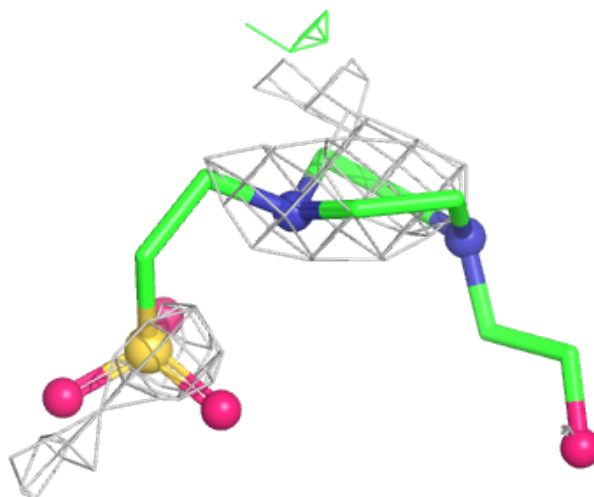
**Electron density around EPE A 728 (B):**

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



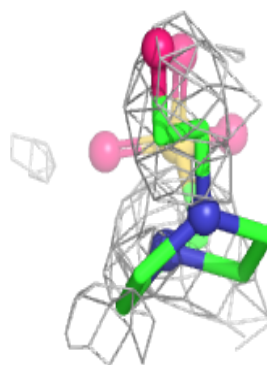
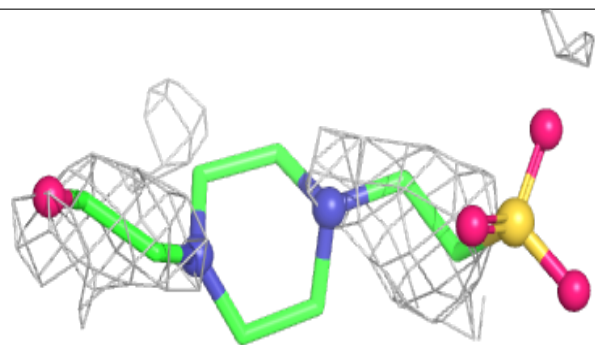
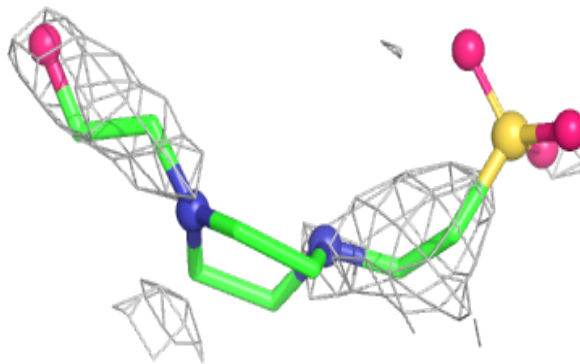
**Electron density around EPE A 725 (A):**

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



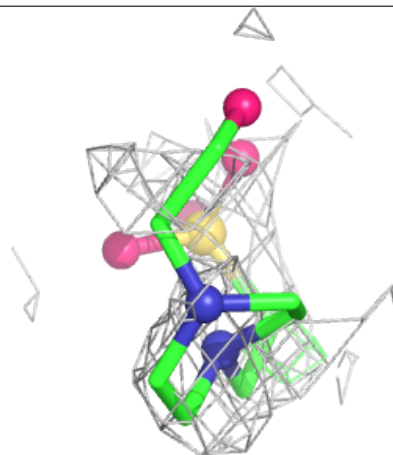
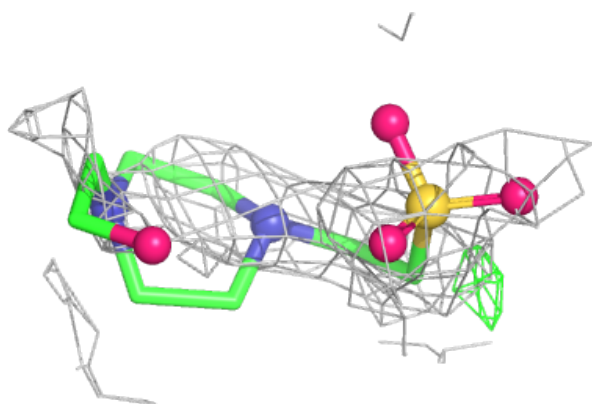
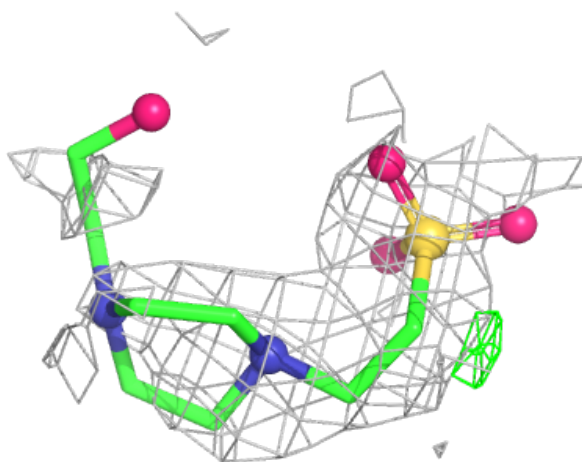
**Electron density around EPE A 725 (B):**

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



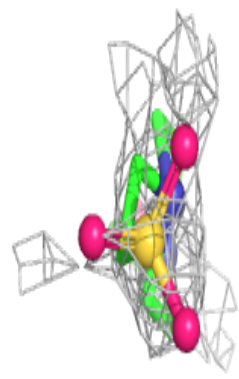
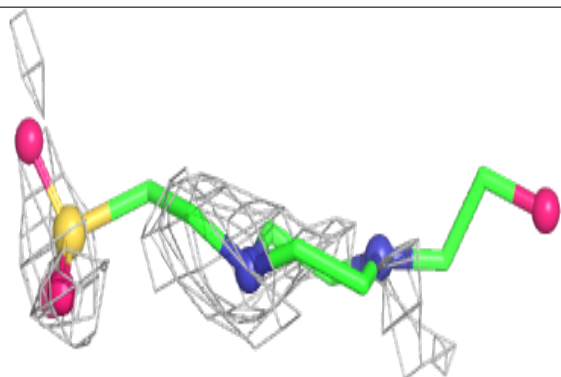
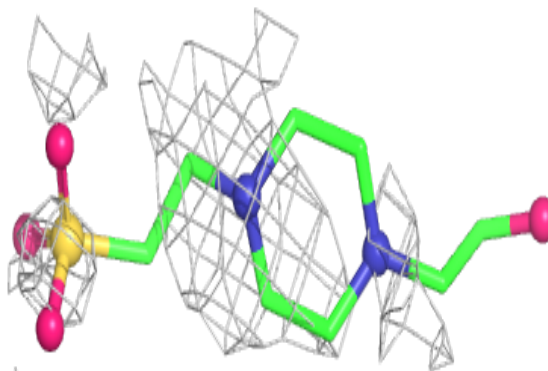
**Electron density around EPE A 712 (C):**

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

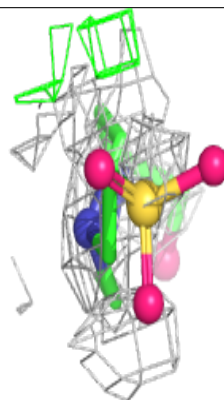
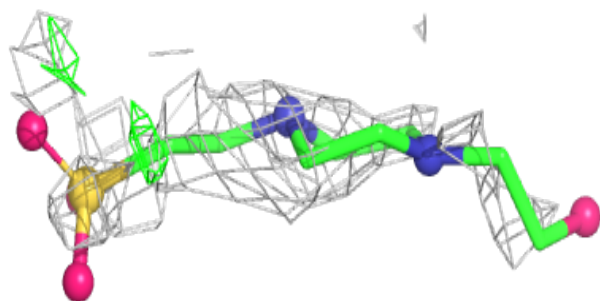
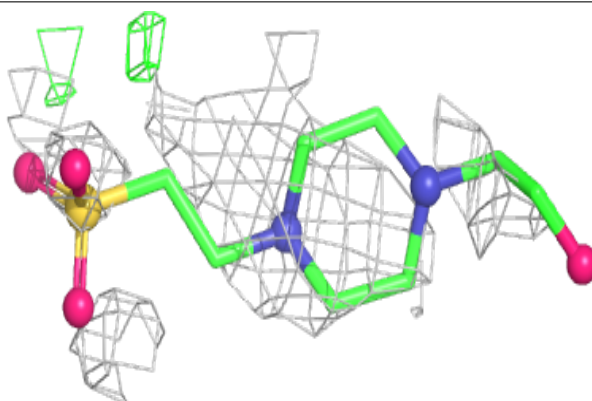


**Electron density around EPE A 712 (A):**

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

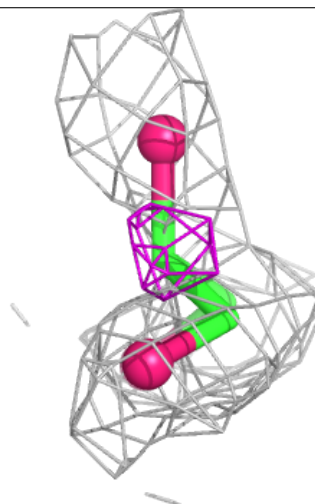
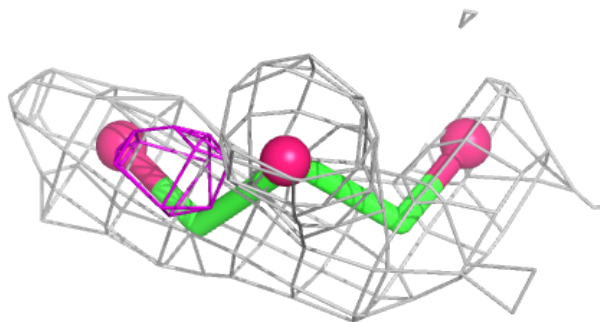
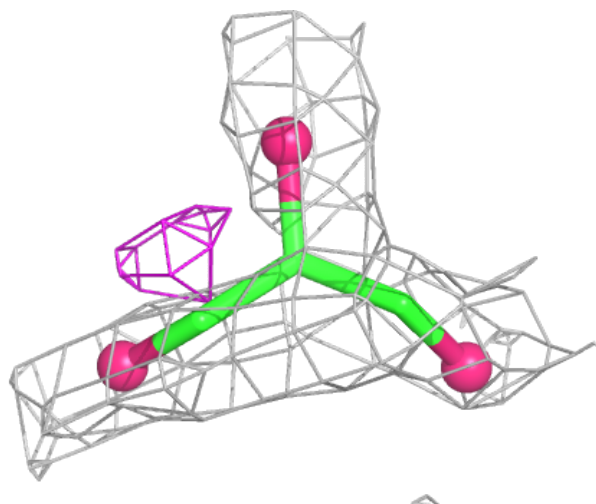
**Electron density around EPE A 712 (B):**

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



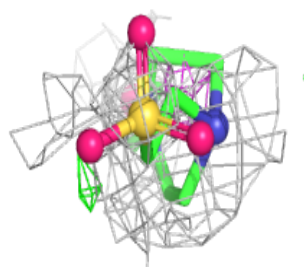
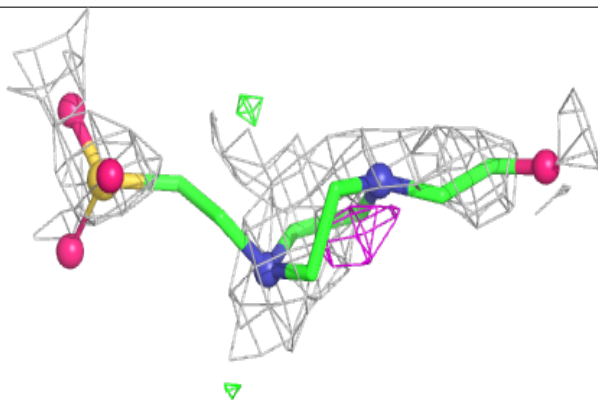
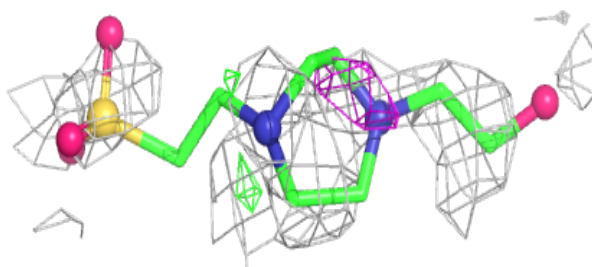
**Electron density around GOL A 720:**

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

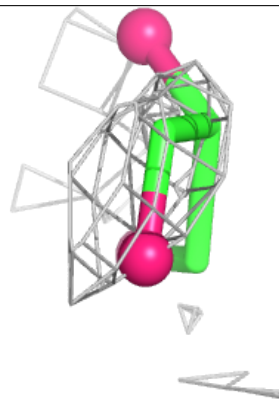
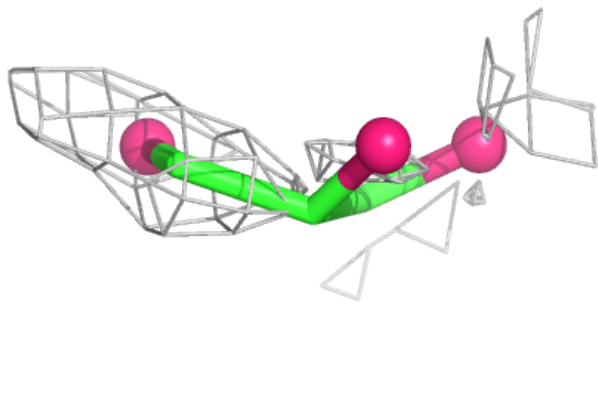
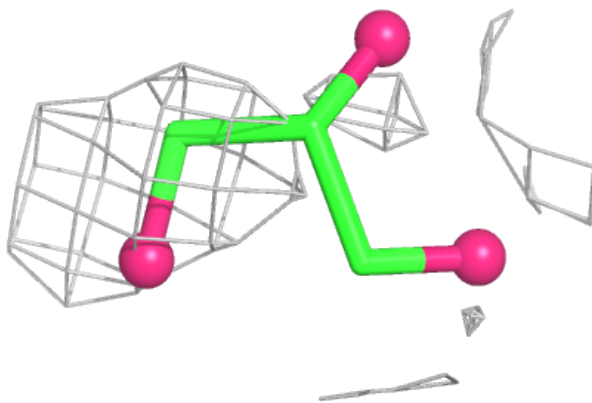


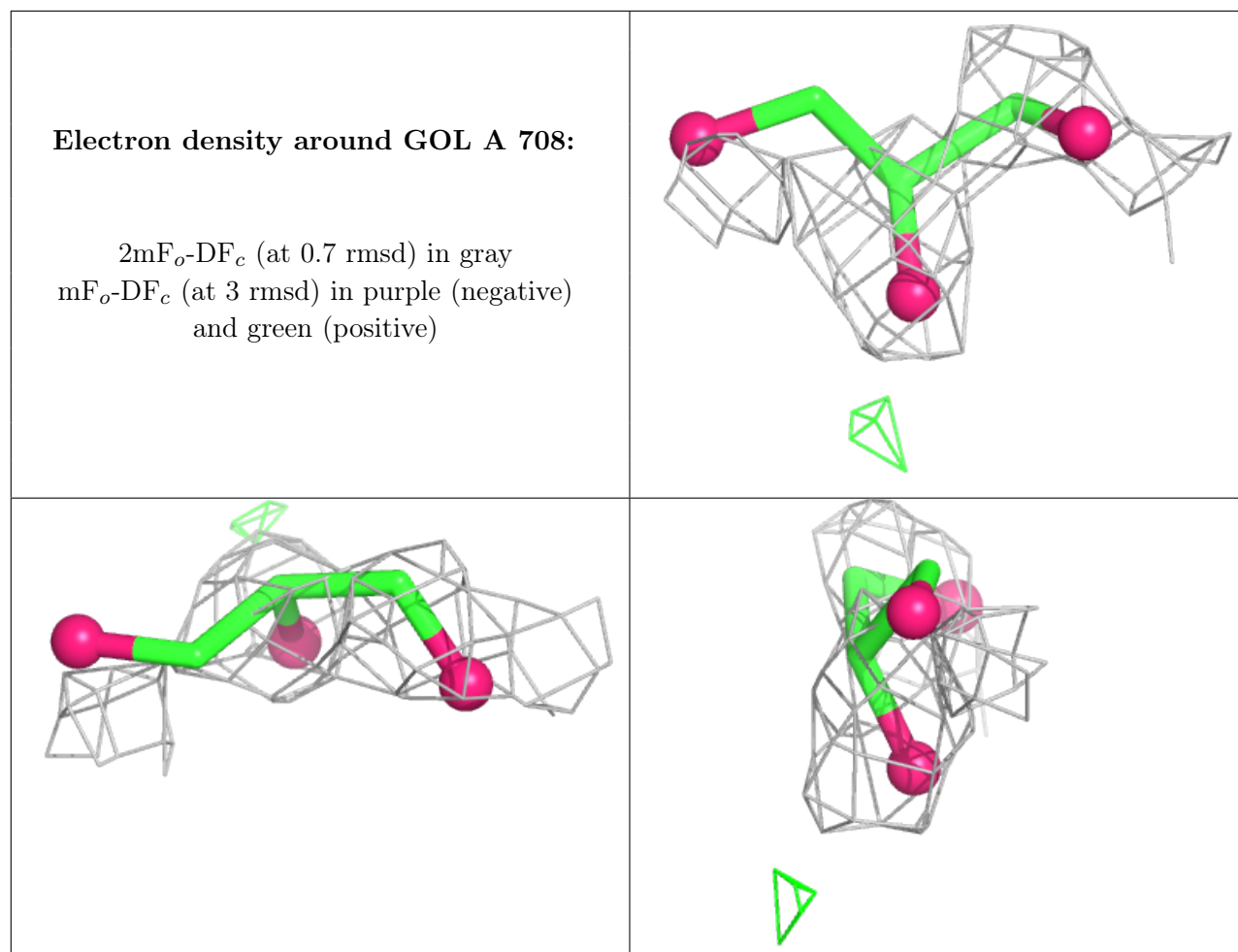
**Electron density around EPE A 702 (A):**

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

**Electron density around GOL A 705:**

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

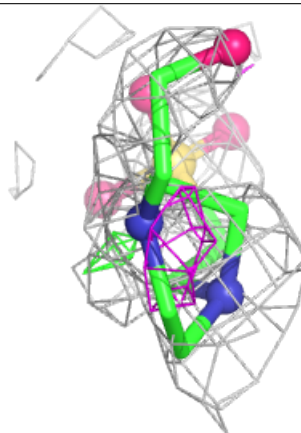
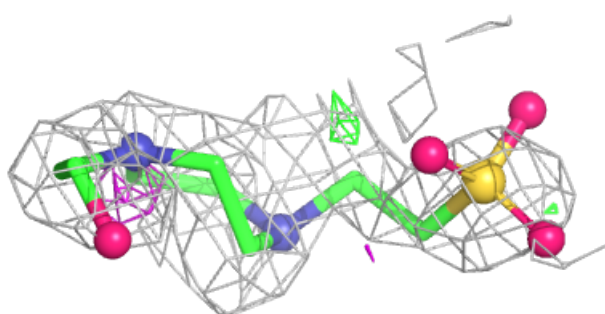
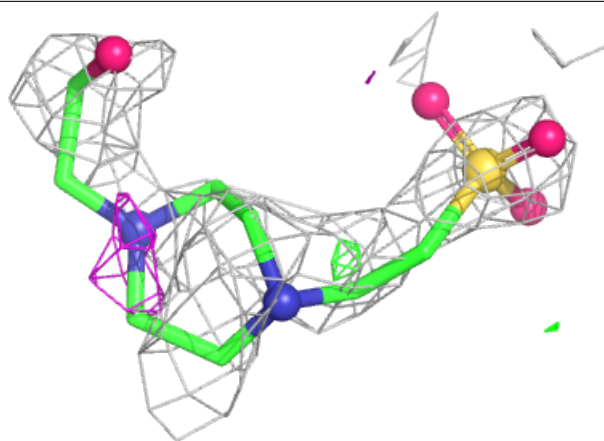


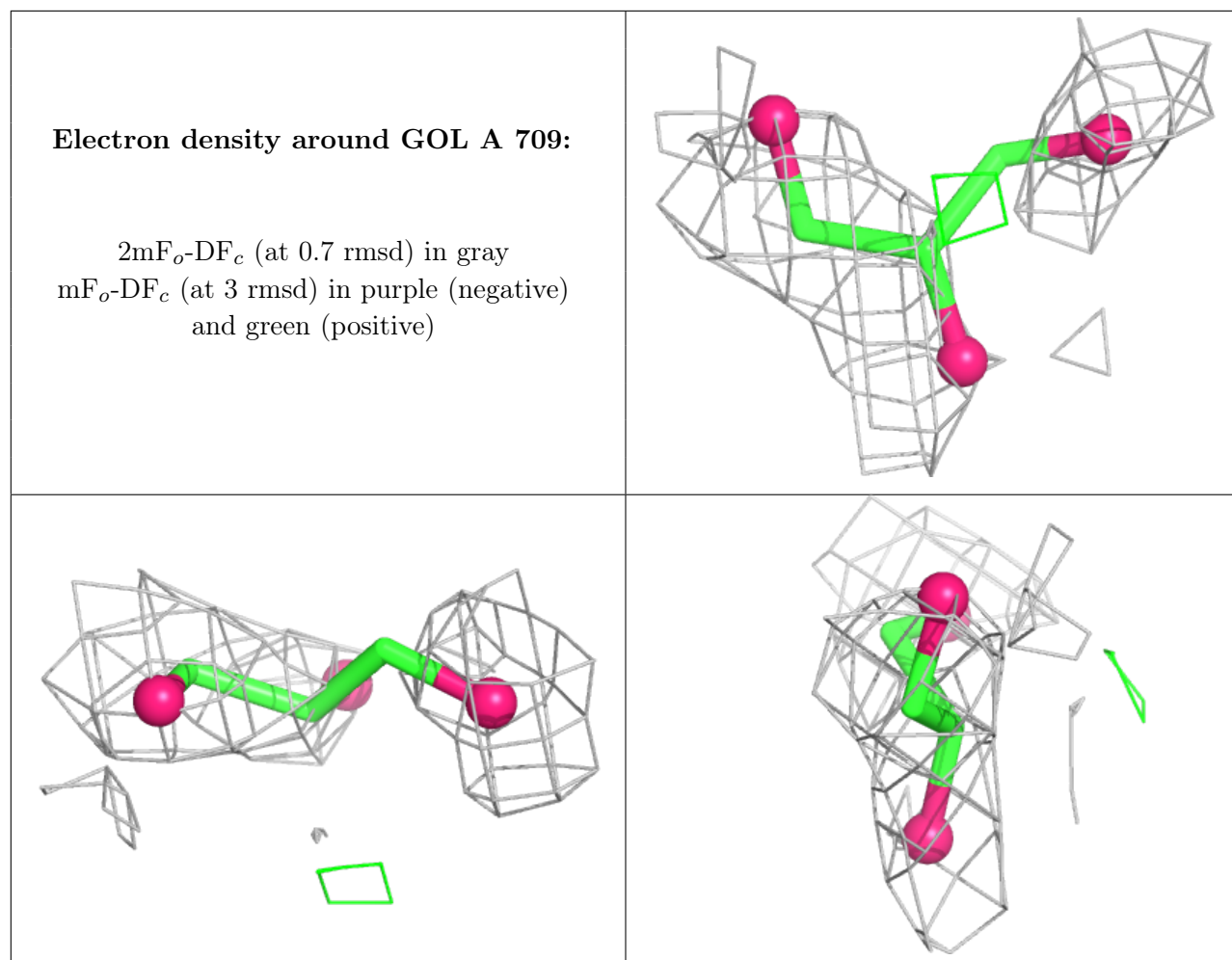




**Electron density around EPE A 702 (B):**

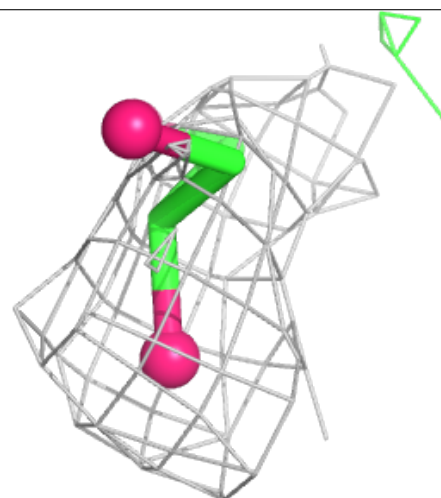
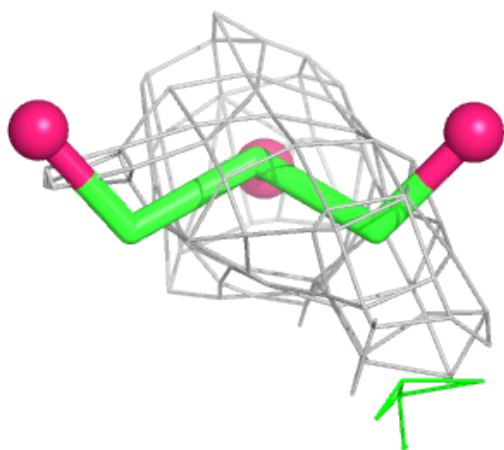
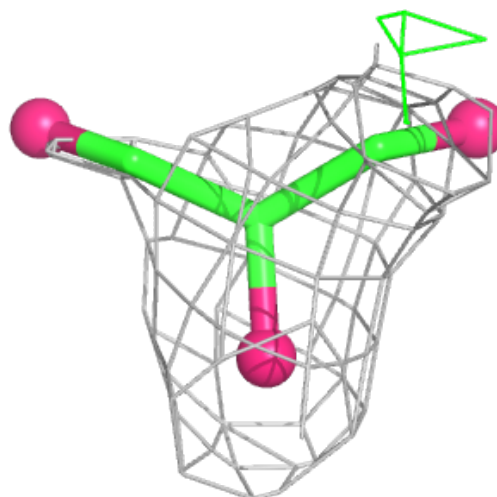
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

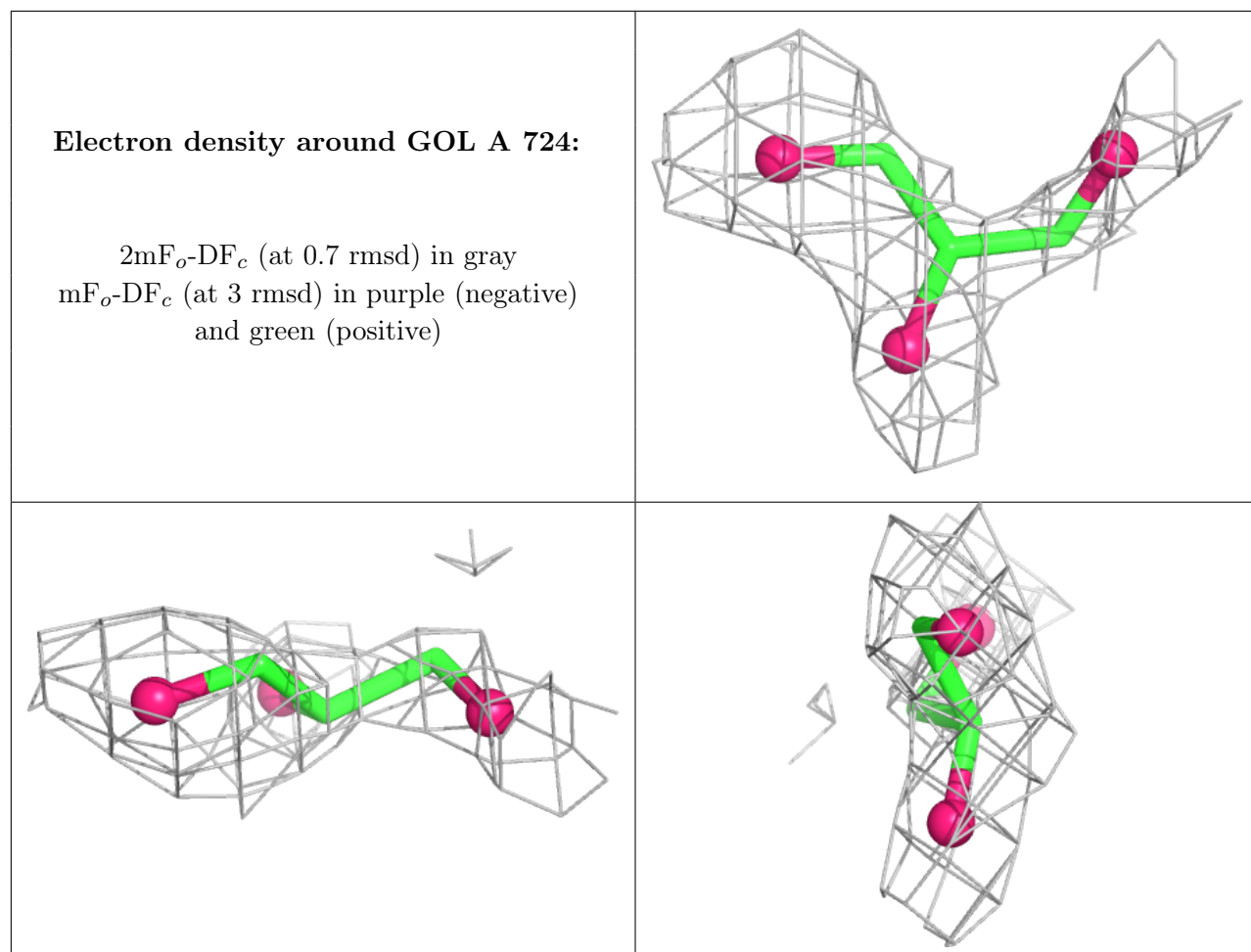




**Electron density around GOL A 721 (B):**

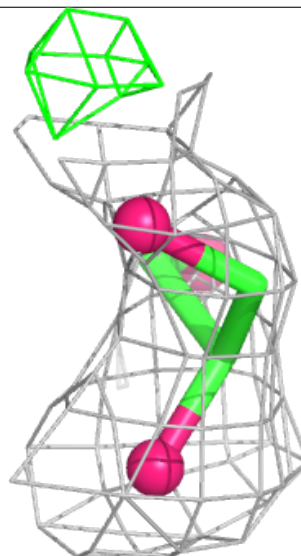
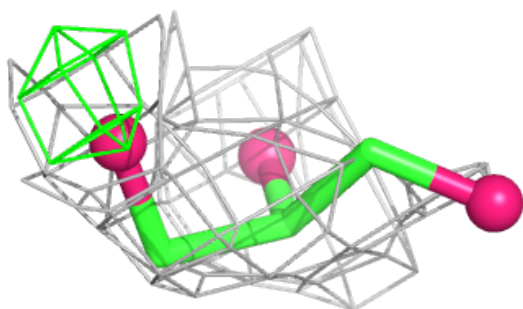
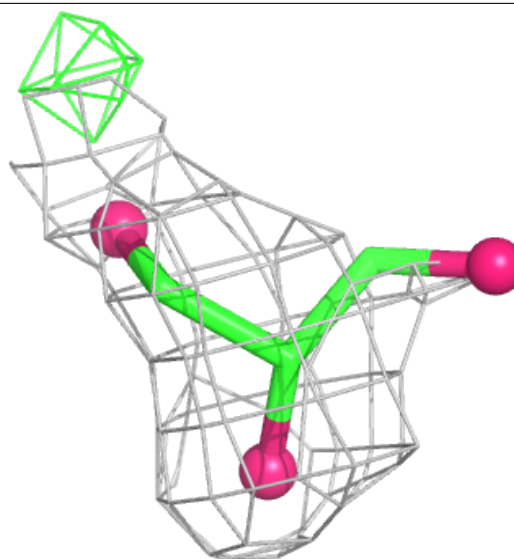
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

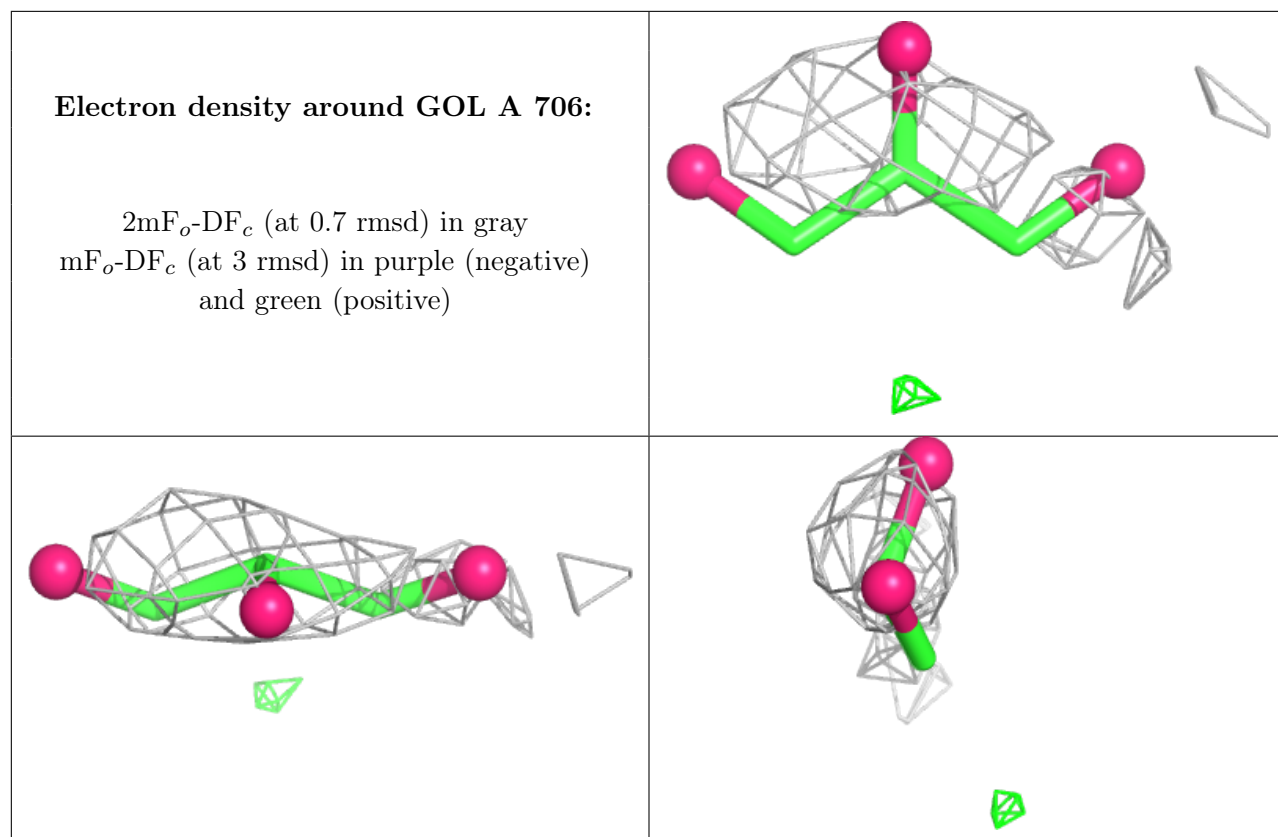


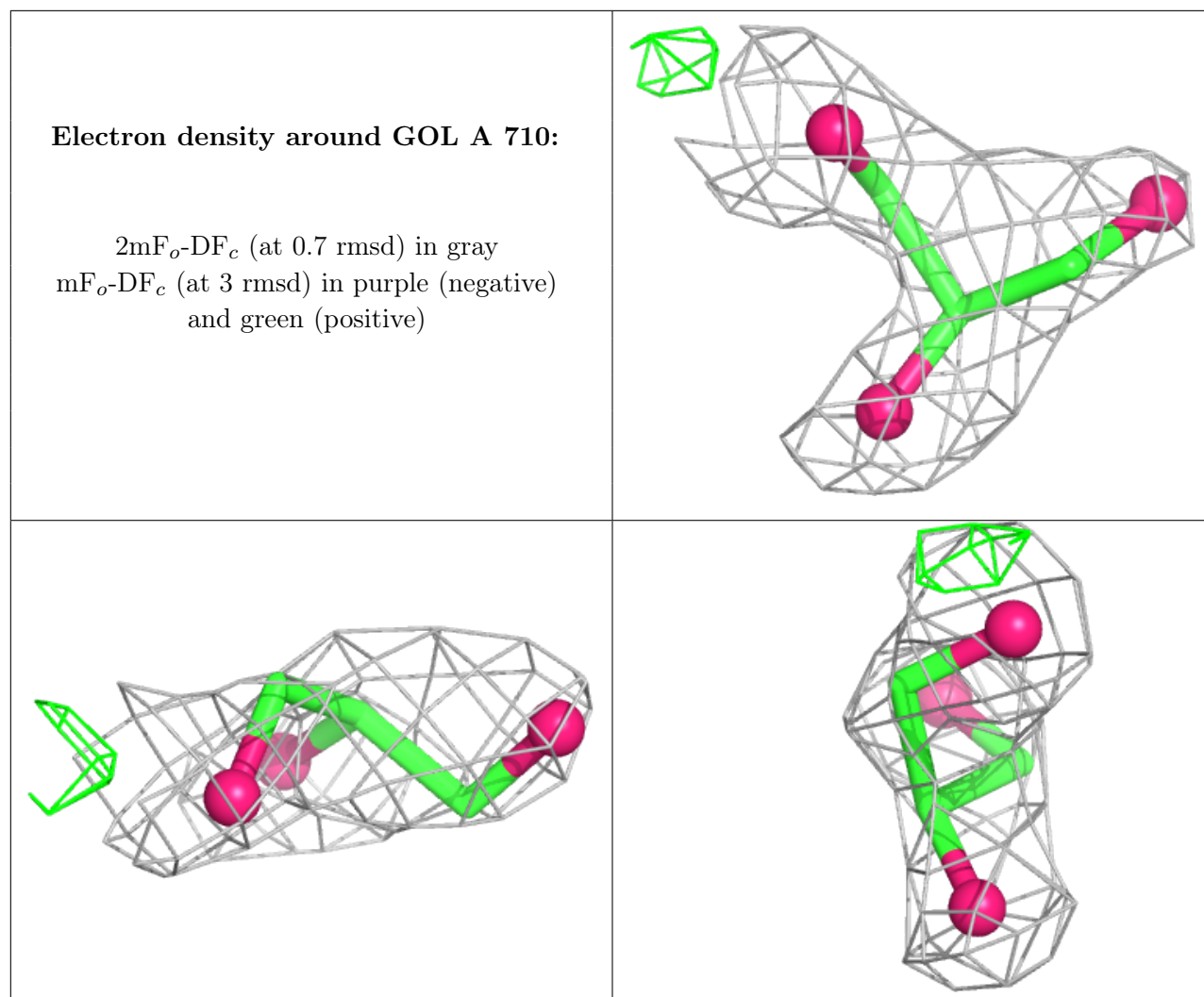


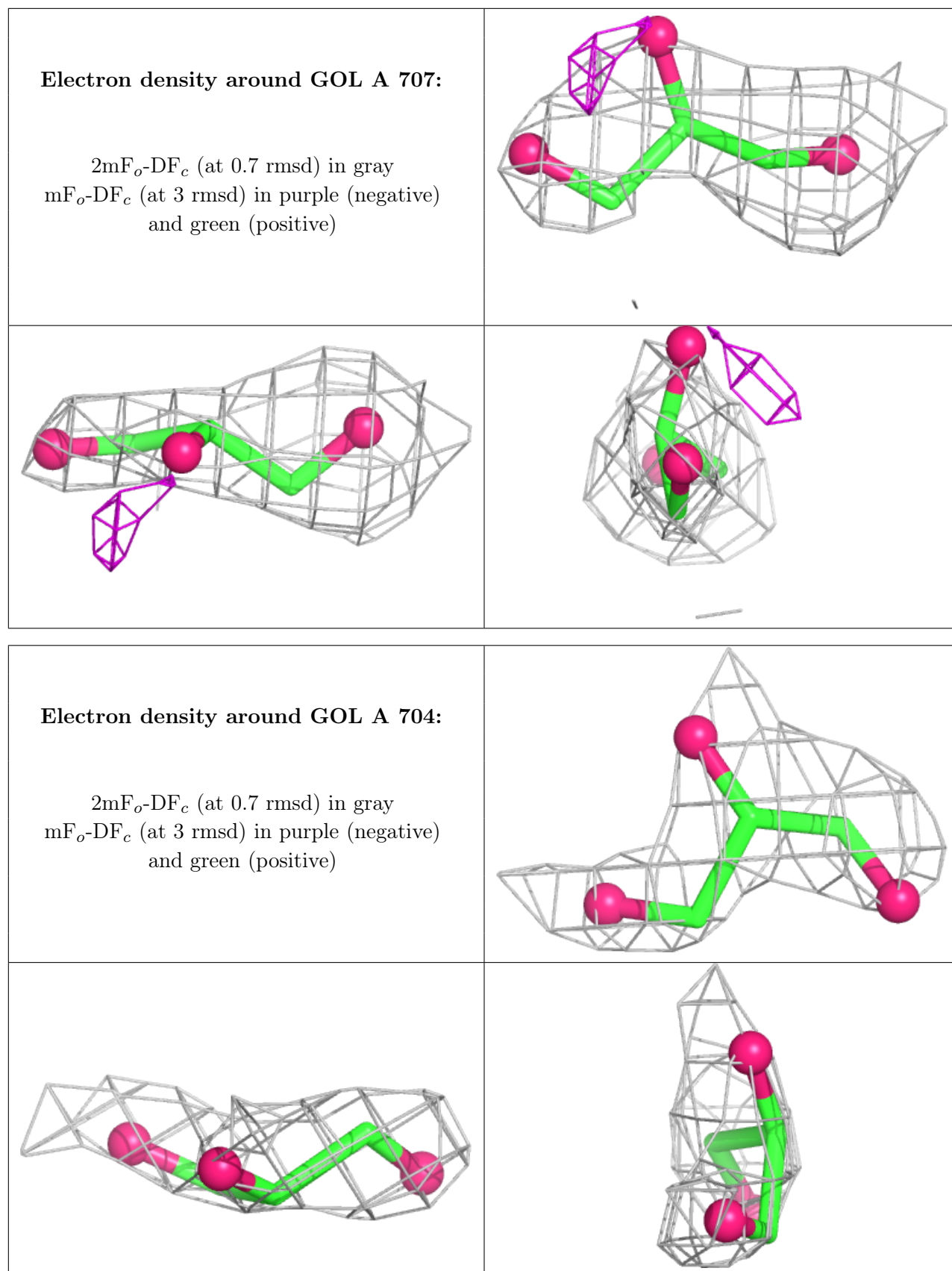
**Electron density around GOL A 721 (A):**

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

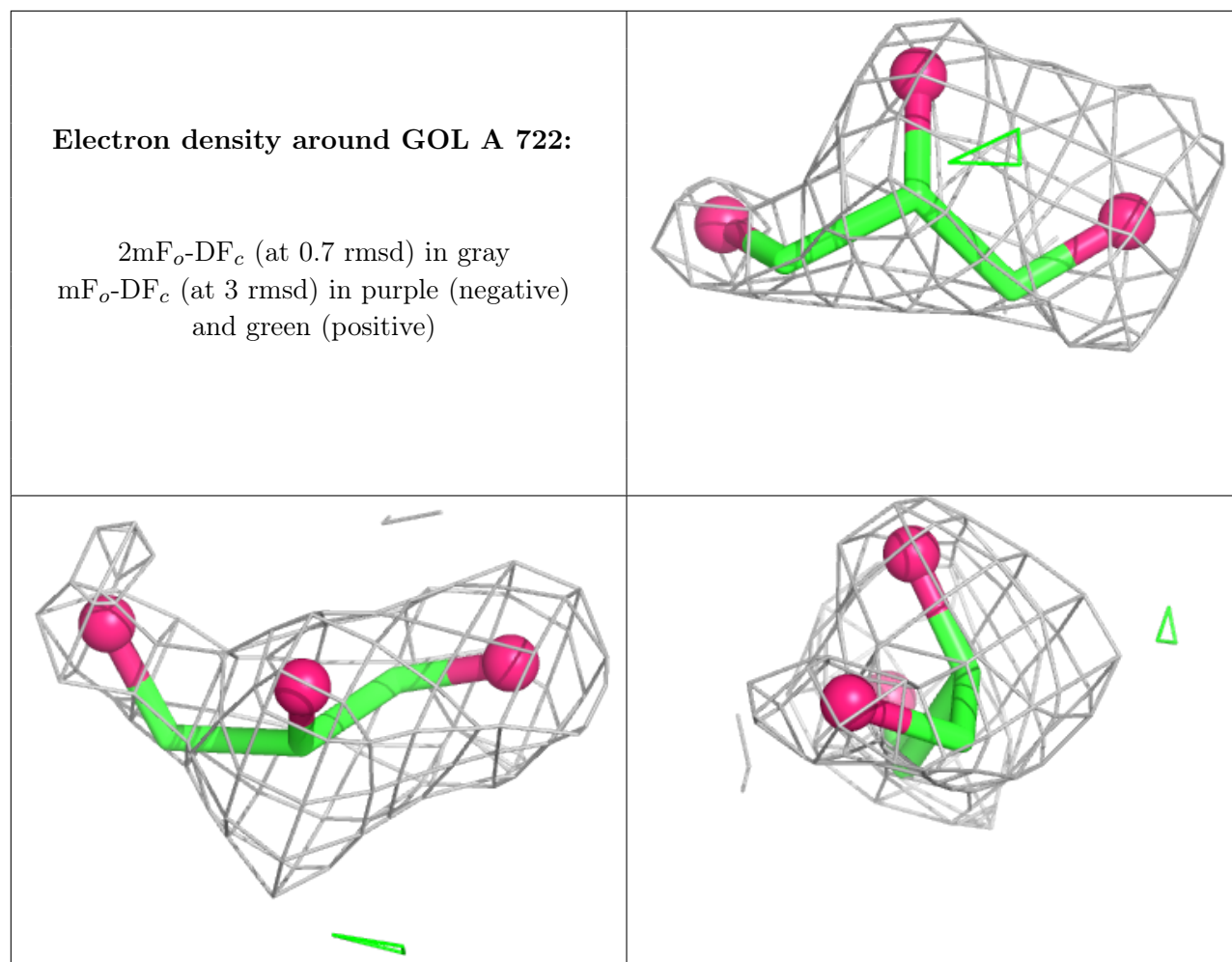






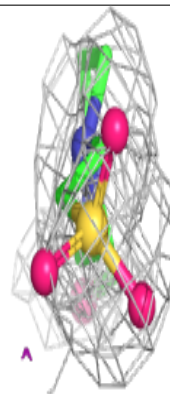
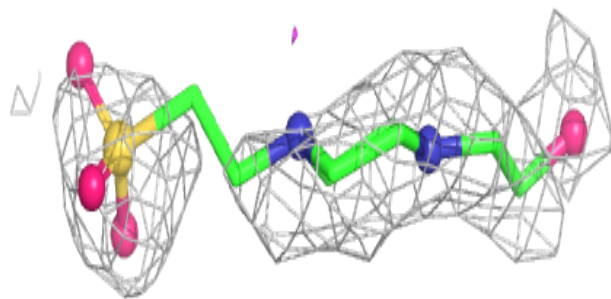
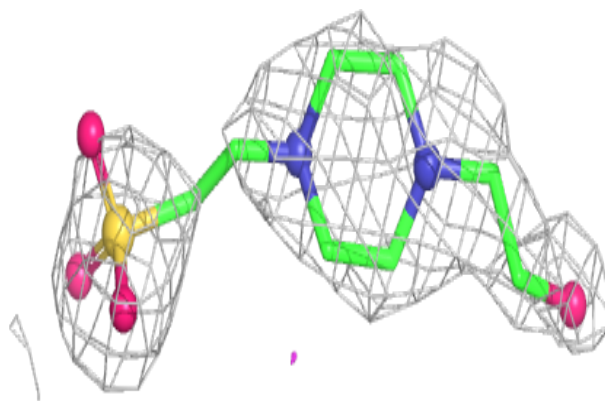


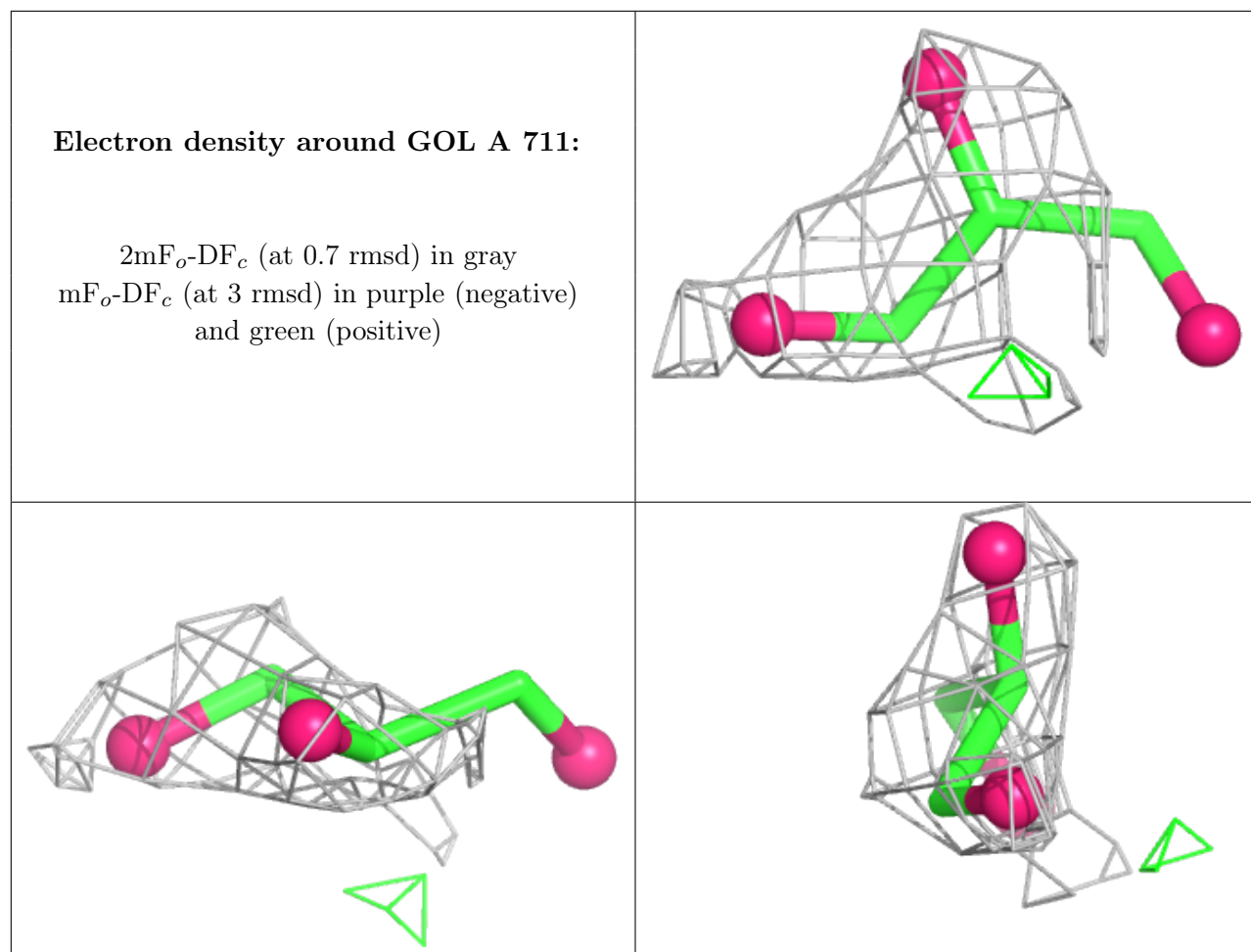


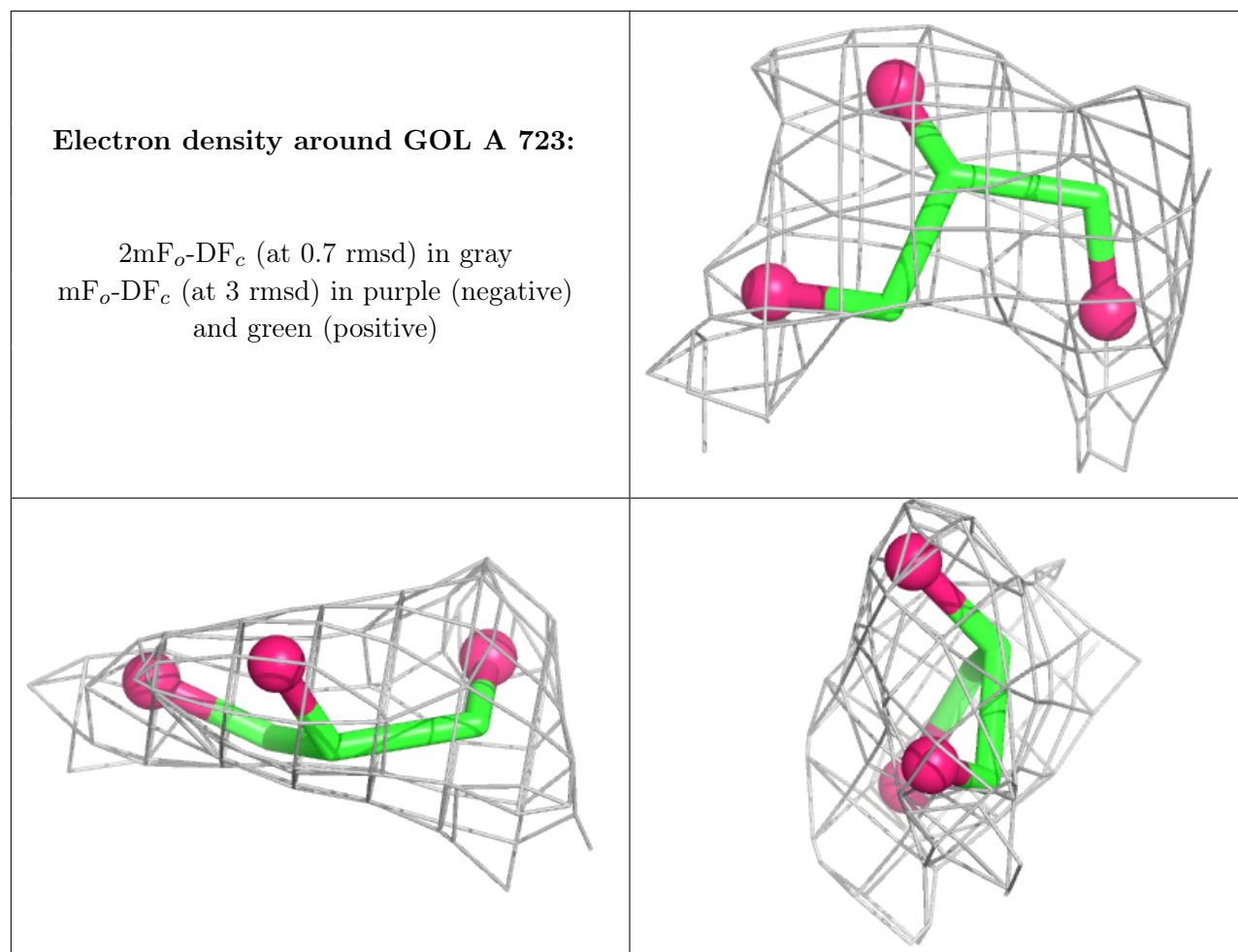


**Electron density around EPE A 701:**

$2mF_o-DF_c$  (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.