



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 02:15 PM JST

PDB ID : 7VTI  
Title : Crystal structure of the Cas13bt3-crRNA binary complex  
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Deposited on : 2021-10-29  
Resolution : 1.89 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.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

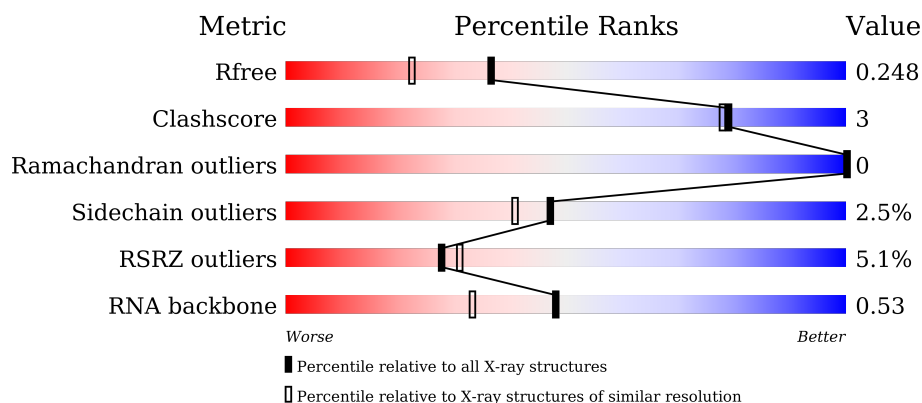
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)
RNA backbone	3102	1013 (2.42-1.38)

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	777	<div> <div>5%</div> <div>86%</div> <div>8%</div> <div>5%</div> </div>
2	B	41	<div> <div>2%</div> <div>54%</div> <div>37%</div> <div>5%</div> <div>••</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7415 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 Cas13bt3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	Se	0	5	0
			6075	3883	1076	1089	16	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A660UUL5
A	0	GLY	-	expression tag	UNP A0A660UUL5
A	84	ALA	ARG	engineered mutation	UNP A0A660UUL5
A	89	ALA	HIS	engineered mutation	UNP A0A660UUL5
A	739	ALA	ARG	engineered mutation	UNP A0A660UUL5
A	744	ALA	HIS	engineered mutation	UNP A0A660UUL5

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	P	0	4	0
			904	402	159	300	43			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Cl	0	0
			5	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Br 1 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total Mg 3 3	0	0

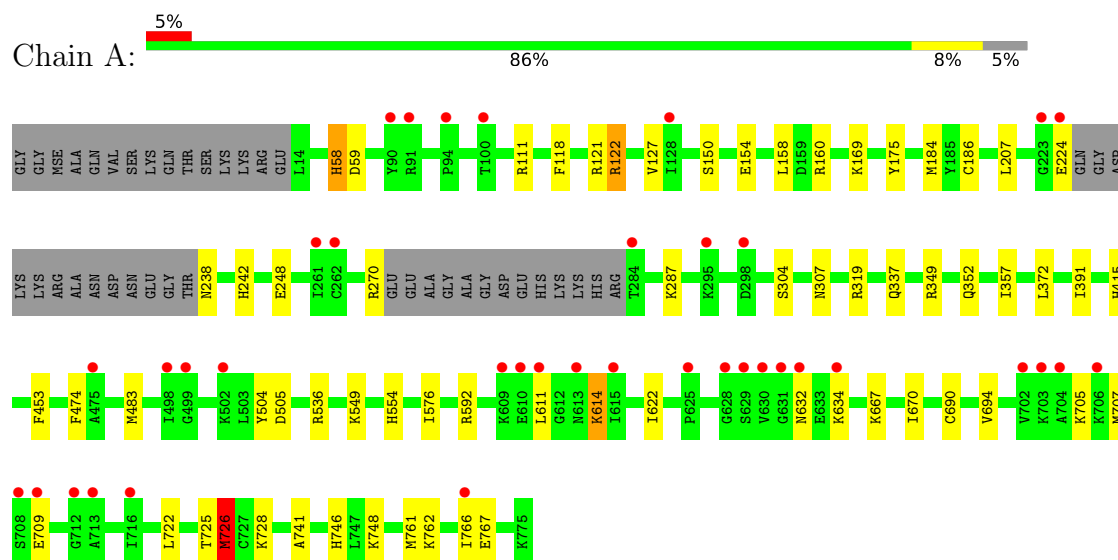
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	248	Total O 248 248	0	0
7	B	91	Total O 91 91	0	1

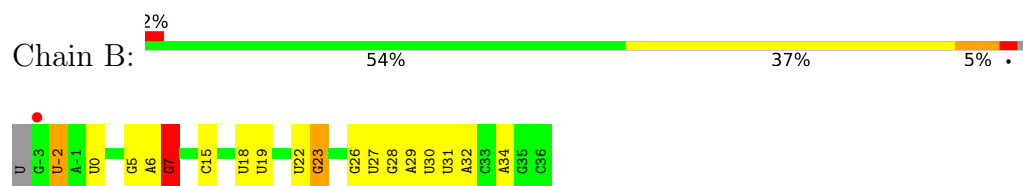
### 3 Residue-property plots

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: Cas13bt3



#### • Molecule 2: crRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.43Å 95.45Å 125.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.99 – 1.89 48.95 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.99-1.89) 99.9 (48.95-1.89)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0291	Depositor
R, $R_{free}$	0.196 , 0.243 0.205 , 0.248	Depositor DCC
$R_{free}$ test set	2287 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, BR, EDO

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	0.74	1/6191 (0.0%)	0.91	5/8292 (0.1%)
2	B	0.93	0/1024	1.64	23/1592 (1.4%)
All	All	0.77	1/7215 (0.0%)	1.06	28/9884 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLU	CD-OE1	6.55	1.32	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	ARG	NE-CZ-NH2	-10.07	115.27	120.30
2	B	26	G	C5-C6-N1	-7.66	107.67	111.50
2	B	7	G	O5'-P-OP2	-7.65	98.82	105.70
1	A	761	MSE	CG-SE-CE	7.54	115.48	98.90
1	A	536	ARG	NE-CZ-NH1	7.27	123.93	120.30
2	B	6	A	OP2-P-O3'	7.18	121.00	105.20
1	A	184	MSE	CG-SE-CE	6.60	113.42	98.90
1	A	726	MSE	CG-SE-CE	6.49	113.17	98.90
2	B	7	G	O3'-P-O5'	-6.27	92.09	104.00
2	B	34	A	O5'-P-OP2	-6.26	100.06	105.70
2	B	22	U	OP1-P-O3'	6.20	118.84	105.20
2	B	22	U	P-O3'-C3'	6.18	127.12	119.70
2	B	15	C	OP2-P-O3'	6.06	118.53	105.20
2	B	5	G	N1-C6-O6	6.02	123.51	119.90
2	B	19	U	O5'-P-OP2	-5.95	100.35	105.70
2	B	26	G	N9-C4-C5	5.87	107.75	105.40
2	B	23	G	O5'-P-OP2	-5.86	100.43	105.70
2	B	26	G	N3-C4-N9	-5.61	122.63	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	G	O4'-C1'-N9	-5.51	103.79	108.20
2	B	26	G	C4-C5-N7	-5.43	108.63	110.80
2	B	31	U	C5-C4-O4	5.39	129.14	125.90
2	B	28	G	O4'-C1'-N9	5.38	112.51	108.20
2	B	23	G	OP1-P-OP2	-5.17	111.84	119.60
2	B	-2[A]	U	OP2-P-O3'	5.17	116.57	105.20
2	B	-2[B]	U	OP2-P-O3'	5.17	116.57	105.20
2	B	19	U	P-O3'-C3'	-5.16	113.51	119.70
2	B	26	G	C6-N1-C2	5.15	128.19	125.10
2	B	32	A	OP2-P-O3'	5.09	116.40	105.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6075	0	6044	38	0
2	B	904	0	449	4	0
3	A	5	0	0	0	0
4	A	76	0	113	7	0
4	B	12	0	18	0	0
5	A	1	0	0	0	0
6	B	3	0	0	0	0
7	A	248	0	0	1	0
7	B	91	0	0	0	0
All	All	7415	0	6624	39	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 3.

All (39) 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:207:LEU:HD13	1:A:622:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:PHE:CD1	1:A:483:MSE:HE2	2.25	0.71
1:A:349:ARG:NH2	4:A:812:EDO:O2	2.24	0.70
1:A:158:LEU:HD22	1:A:186[A]:CYS:SG	2.34	0.67
1:A:121:ARG:NH1	1:A:127:VAL:HG13	2.09	0.67
1:A:319:ARG:HH12	1:A:352:GLN:HE21	1.44	0.65
1:A:122:ARG:NH2	2:B:-2[A]:U:O2	2.30	0.62
1:A:59:ASP:OD1	1:A:270:ARG:NH1	2.34	0.60
1:A:207:LEU:CD1	1:A:622:ILE:HD11	2.32	0.58
1:A:722:LEU:O	1:A:725:THR:OG1	2.18	0.57
1:A:357:ILE:HG22	1:A:372:LEU:HD11	1.87	0.55
1:A:690:CYS:O	1:A:694:VAL:HG23	2.08	0.54
1:A:611:LEU:HD12	1:A:614:LYS:HE2	1.88	0.54
1:A:58:HIS:CE1	2:B:0[B]:U:OP1	2.61	0.53
1:A:726:MSE:O	1:A:726:MSE:HE2	2.08	0.53
1:A:705:LYS:HD3	1:A:707:MSE:HG2	1.93	0.51
1:A:121:ARG:NH1	7:A:905:HOH:O	2.44	0.50
1:A:160:ARG:HE	4:A:820:EDO:H11	1.76	0.50
1:A:58:HIS:NE2	2:B:0[B]:U:OP1	2.44	0.50
1:A:122:ARG:HB2	1:A:415:HIS:HB2	1.95	0.48
1:A:391:ILE:HD13	1:A:504[B]:TYR:CE1	2.49	0.48
1:A:453:PHE:CD2	1:A:483:MSE:HE1	2.49	0.48
1:A:634:LYS:HG2	1:A:670:ILE:HD11	1.98	0.46
1:A:304:SER:O	4:A:821:EDO:H12	2.16	0.45
1:A:632:ASN:HB2	1:A:667:LYS:CB	2.46	0.45
1:A:169:LYS:HG3	1:A:175:TYR:CD1	2.52	0.45
1:A:741:ALA:HA	1:A:746:HIS:CE1	2.51	0.45
1:A:307:ASN:HD22	4:A:821:EDO:H21	1.82	0.44
1:A:242:HIS:HB2	4:A:811:EDO:H12	2.01	0.43
1:A:121:ARG:HH12	1:A:127:VAL:HG13	1.83	0.43
1:A:357:ILE:CG2	1:A:372:LEU:HD11	2.49	0.43
1:A:150:SER:HA	1:A:158:LEU:HD13	2.02	0.42
1:A:746:HIS:CE1	1:A:748:LYS:HB2	2.55	0.42
1:A:337:GLN:HG2	1:A:554:HIS:CE1	2.55	0.41
1:A:307:ASN:HB2	4:A:821:EDO:H12	2.03	0.41
1:A:118:PHE:CE1	1:A:122:ARG:HD2	2.56	0.41
1:A:248:GLU:HG3	4:A:824:EDO:H11	2.01	0.40
1:A:453:PHE:HD2	1:A:483:MSE:HE1	1.86	0.40
2:B:7:G:H2'	2:B:27:U:O4	2.22	0.40

There are no symmetry-related clashes.

## 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	A	735/777 (95%)	715 (97%)	20 (3%)	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	A	637/657 (97%)	621 (98%)	16 (2%)	47	41

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	111	ARG
1	A	122	ARG
1	A	224	GLU
1	A	238	ASN
1	A	287	LYS
1	A	505	ASP
1	A	549	LYS
1	A	576	ILE
1	A	614	LYS
1	A	709	GLU
1	A	726	MSE
1	A	728	LYS

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Mol	Chain	Res	Type
1	A	762	LYS
1	A	766	ILE
1	A	767	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	554	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	36/41 (87%)	5 (13%)	1 (2%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	7	G
2	B	18	U
2	B	23	G
2	B	29	A
2	B	30	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	23	G

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 31 ligands modelled in this entry, 9 are monoatomic - leaving 22 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	A	810	-	3,3,3	0.14	0	2,2,2	0.50	0
4	EDO	A	820	-	3,3,3	0.36	0	2,2,2	0.41	0
4	EDO	A	816	-	3,3,3	0.43	0	2,2,2	0.62	0
4	EDO	A	808	-	3,3,3	0.25	0	2,2,2	0.05	0
4	EDO	A	811	-	3,3,3	0.21	0	2,2,2	0.51	0
4	EDO	A	812	-	3,3,3	0.61	0	2,2,2	0.08	0
4	EDO	A	819	-	3,3,3	0.30	0	2,2,2	0.57	0
4	EDO	B	106	-	3,3,3	0.17	0	2,2,2	0.07	0
4	EDO	A	813	-	3,3,3	0.27	0	2,2,2	0.43	0
4	EDO	A	818	-	3,3,3	0.13	0	2,2,2	0.30	0
4	EDO	B	104	-	3,3,3	0.36	0	2,2,2	0.14	0
4	EDO	A	817	-	3,3,3	0.11	0	2,2,2	0.18	0
4	EDO	A	806	-	3,3,3	0.35	0	2,2,2	0.87	0
4	EDO	A	822	-	3,3,3	0.20	0	2,2,2	0.21	0
4	EDO	A	809	-	3,3,3	0.05	0	2,2,2	0.10	0
4	EDO	B	105	-	3,3,3	0.12	0	2,2,2	0.11	0
4	EDO	A	823	-	3,3,3	0.47	0	2,2,2	0.78	0
4	EDO	A	807	-	3,3,3	0.11	0	2,2,2	0.23	0
4	EDO	A	821	-	3,3,3	0.92	0	2,2,2	0.37	0
4	EDO	A	814	-	3,3,3	0.25	0	2,2,2	0.27	0
4	EDO	A	824	-	3,3,3	0.33	0	2,2,2	0.64	0
4	EDO	A	815	-	3,3,3	0.79	0	2,2,2	0.63	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	A	810	-	-	1/1/1/1	-
4	EDO	A	820	-	-	1/1/1/1	-
4	EDO	A	816	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	808	-	-	1/1/1/1	-
4	EDO	A	811	-	-	0/1/1/1	-
4	EDO	A	812	-	-	1/1/1/1	-
4	EDO	A	819	-	-	0/1/1/1	-
4	EDO	B	106	-	-	1/1/1/1	-
4	EDO	A	813	-	-	0/1/1/1	-
4	EDO	A	818	-	-	1/1/1/1	-
4	EDO	B	104	-	-	1/1/1/1	-
4	EDO	A	817	-	-	1/1/1/1	-
4	EDO	A	806	-	-	1/1/1/1	-
4	EDO	A	822	-	-	0/1/1/1	-
4	EDO	A	809	-	-	0/1/1/1	-
4	EDO	B	105	-	-	0/1/1/1	-
4	EDO	A	823	-	-	1/1/1/1	-
4	EDO	A	807	-	-	1/1/1/1	-
4	EDO	A	821	-	-	0/1/1/1	-
4	EDO	A	814	-	-	1/1/1/1	-
4	EDO	A	824	-	-	1/1/1/1	-
4	EDO	A	815	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

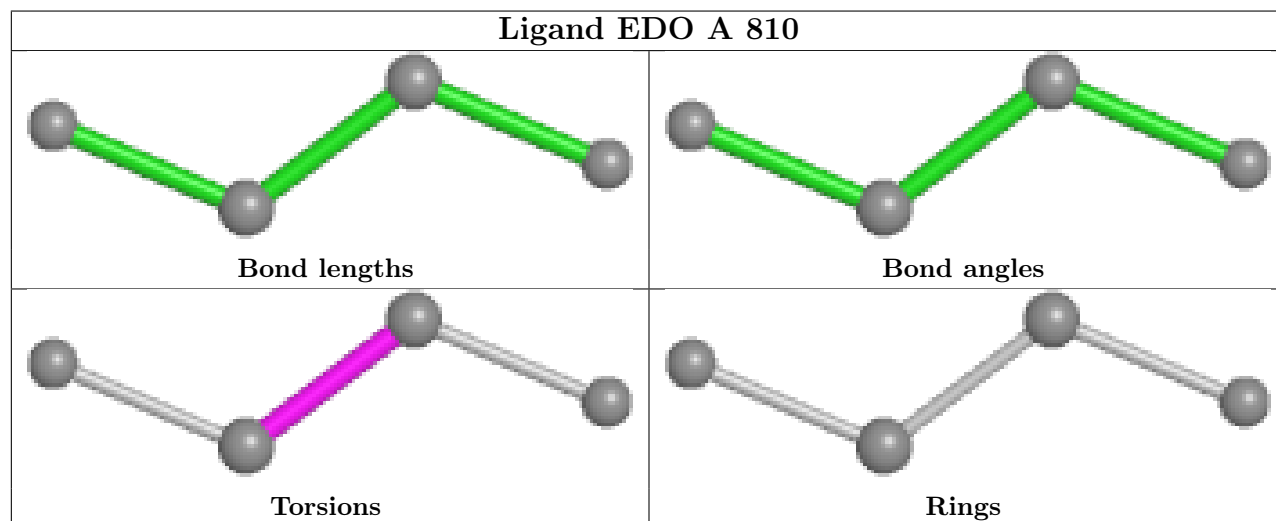
Mol	Chain	Res	Type	Atoms
4	A	812	EDO	O1-C1-C2-O2
4	A	816	EDO	O1-C1-C2-O2
4	A	820	EDO	O1-C1-C2-O2
4	A	824	EDO	O1-C1-C2-O2
4	B	104	EDO	O1-C1-C2-O2
4	A	814	EDO	O1-C1-C2-O2
4	A	815	EDO	O1-C1-C2-O2
4	A	817	EDO	O1-C1-C2-O2
4	A	823	EDO	O1-C1-C2-O2
4	A	808	EDO	O1-C1-C2-O2
4	A	806	EDO	O1-C1-C2-O2
4	A	810	EDO	O1-C1-C2-O2
4	A	818	EDO	O1-C1-C2-O2
4	A	807	EDO	O1-C1-C2-O2
4	B	106	EDO	O1-C1-C2-O2

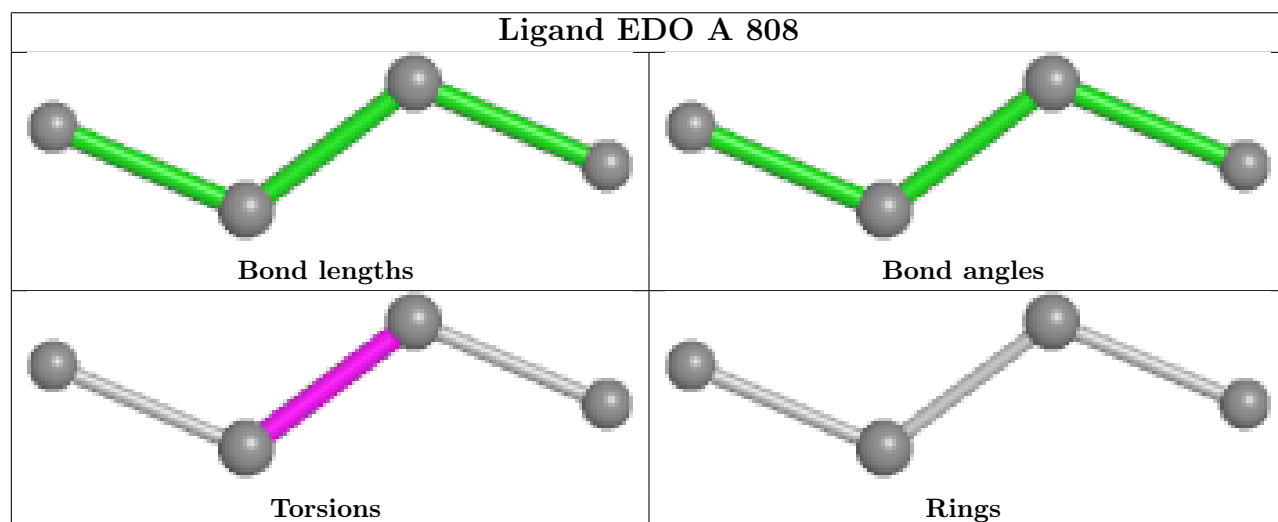
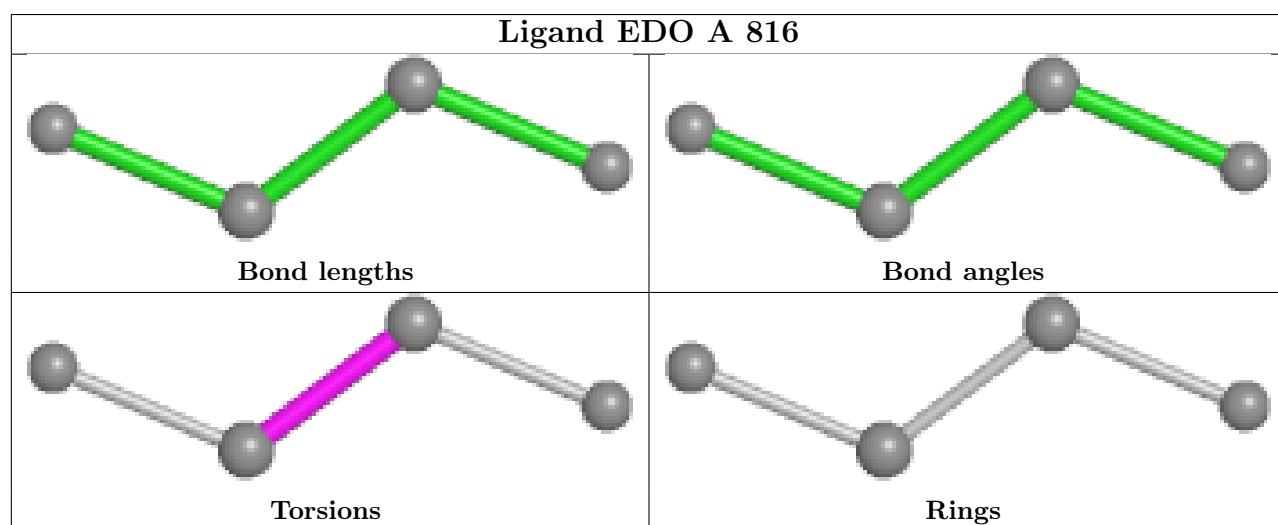
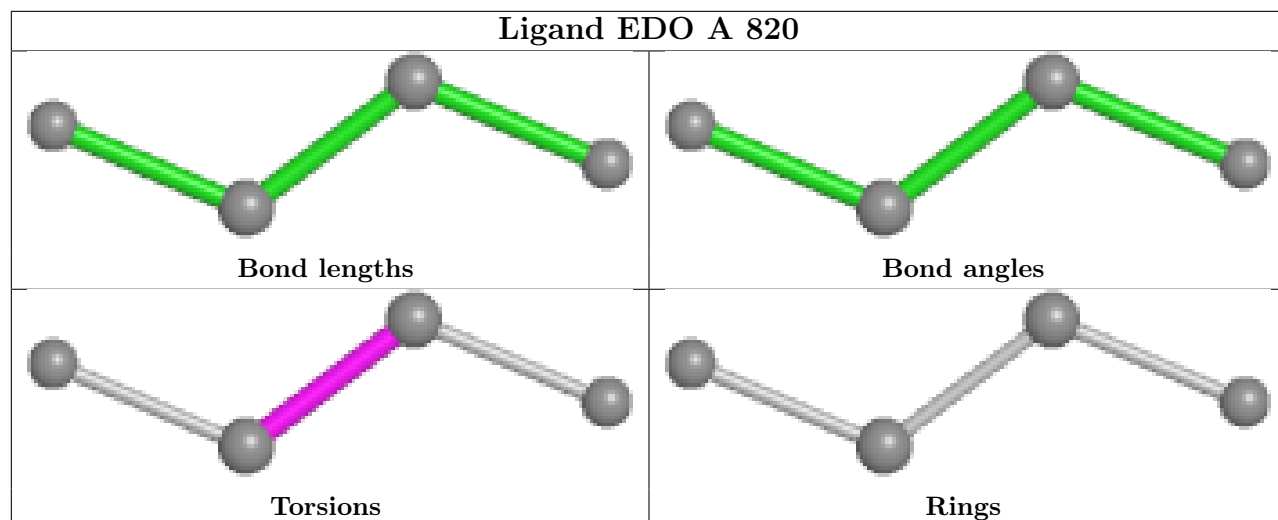
There are no ring outliers.

5 monomers are involved in 7 short contacts:

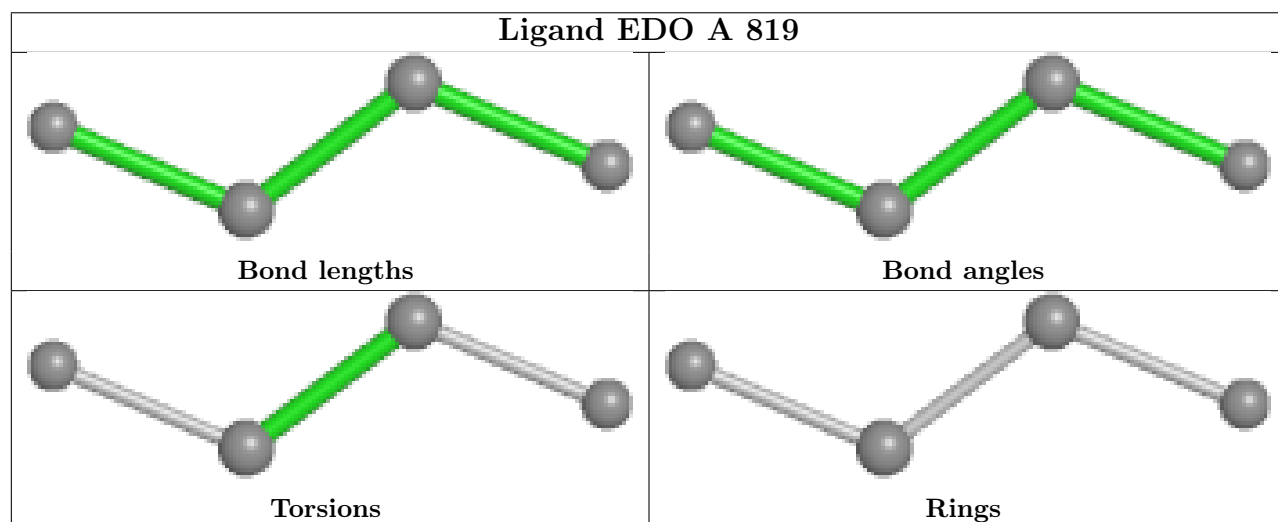
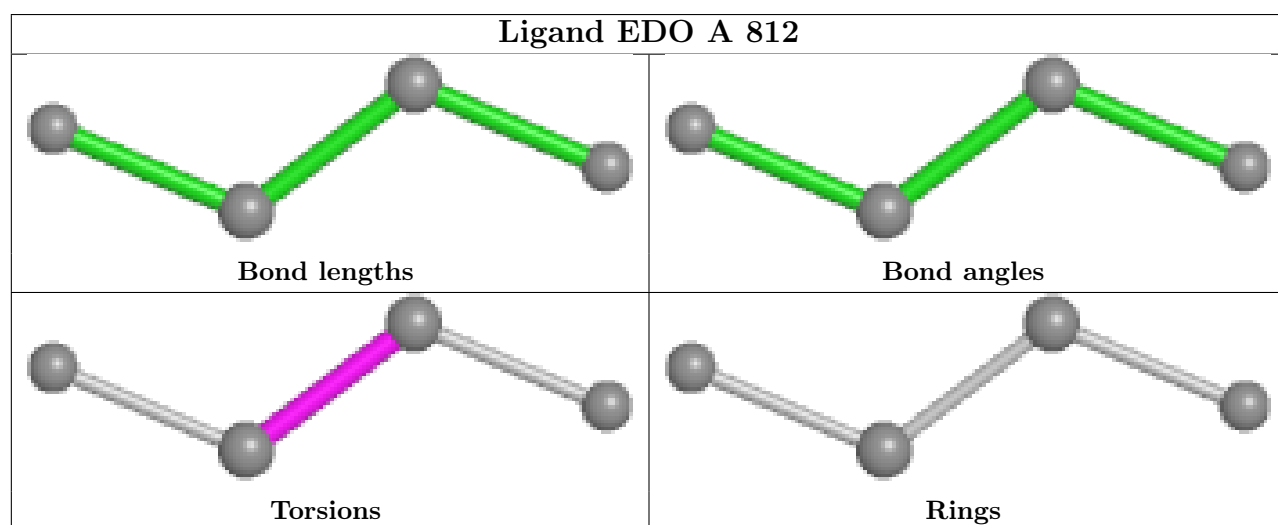
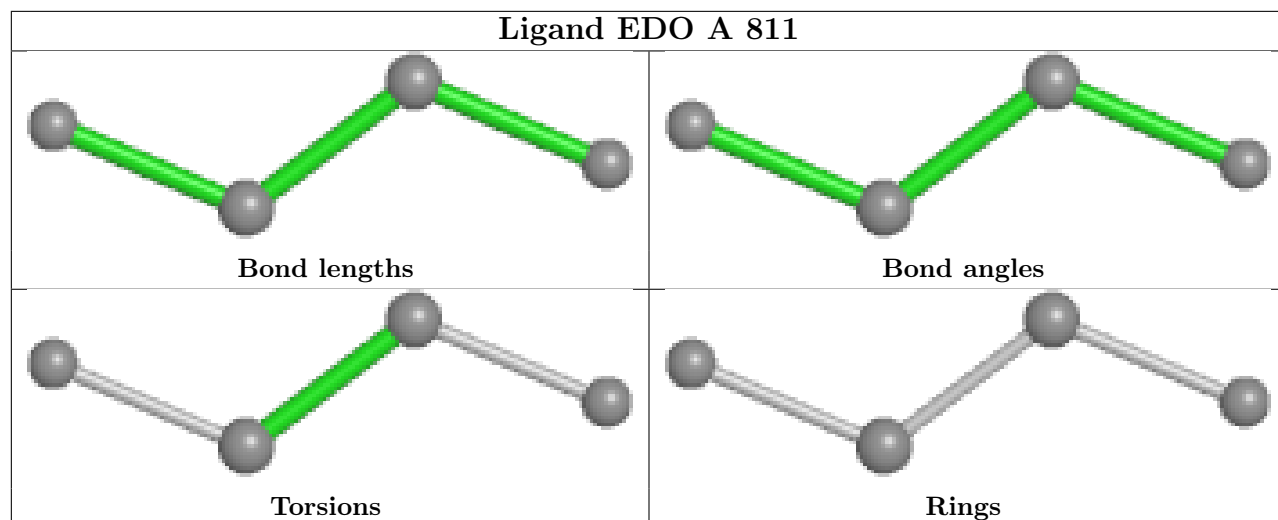
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	820	EDO	1	0
4	A	811	EDO	1	0
4	A	812	EDO	1	0
4	A	821	EDO	3	0
4	A	824	EDO	1	0

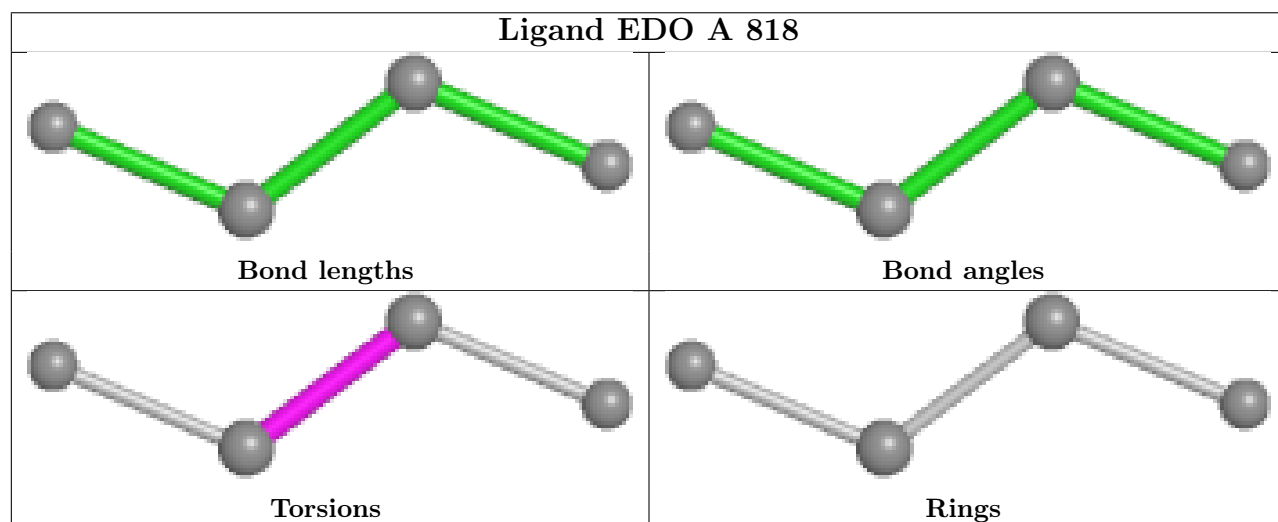
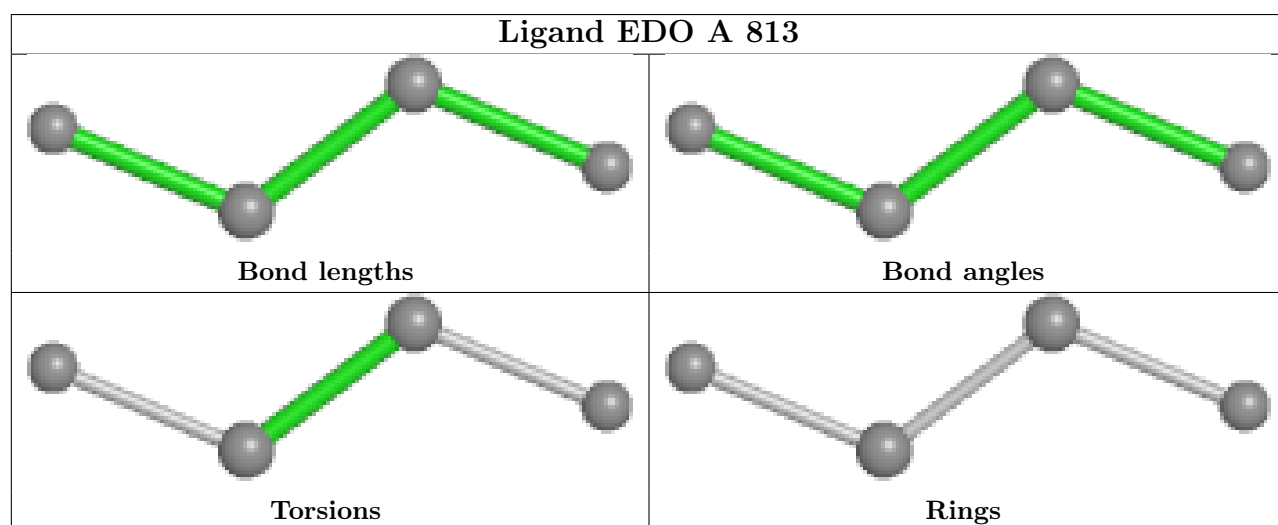
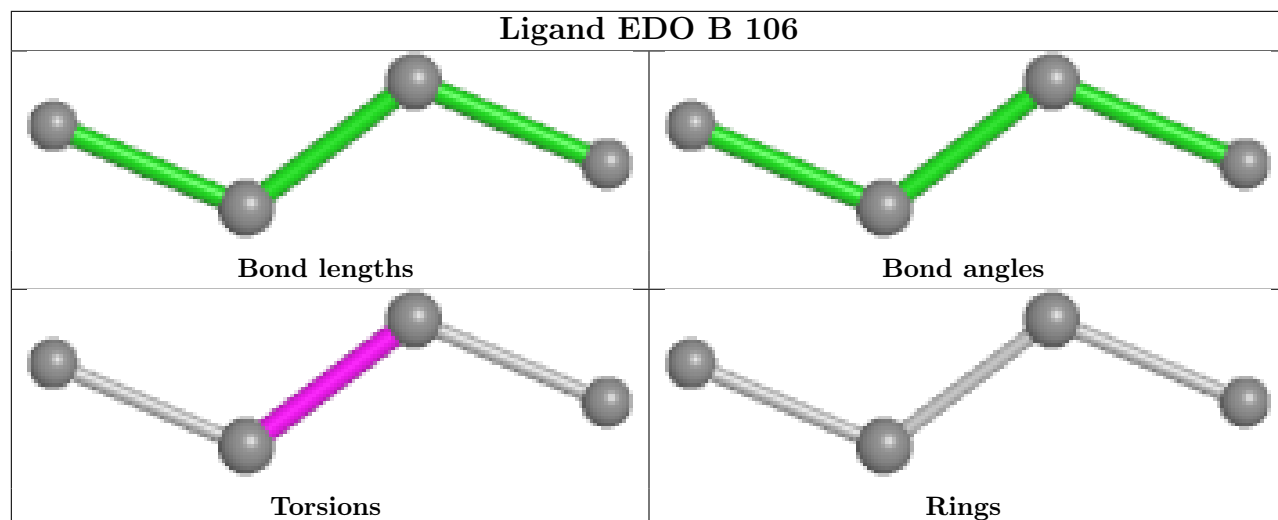
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

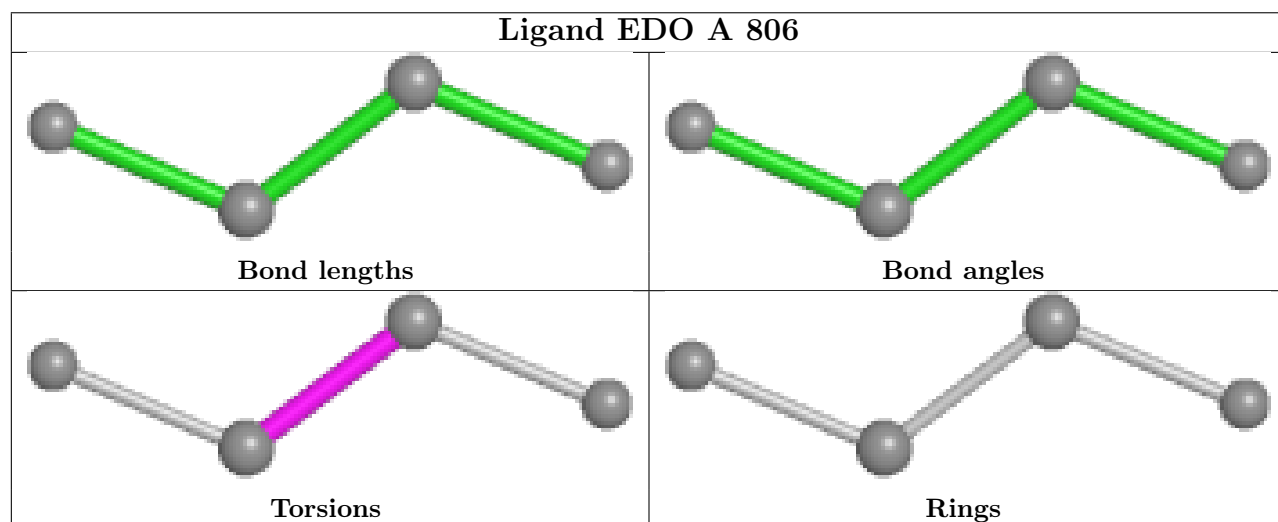
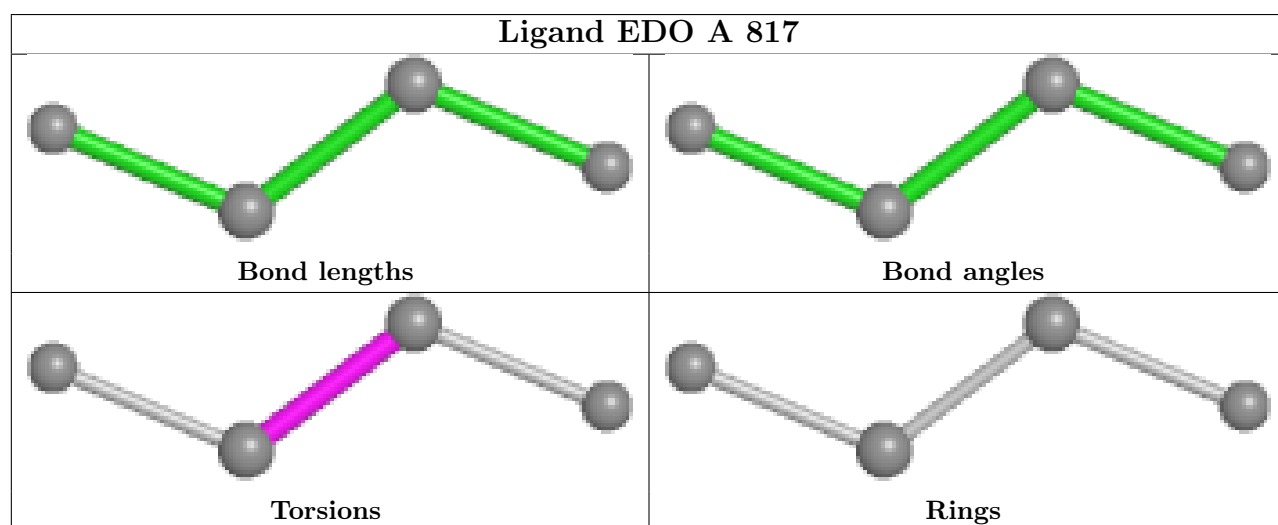
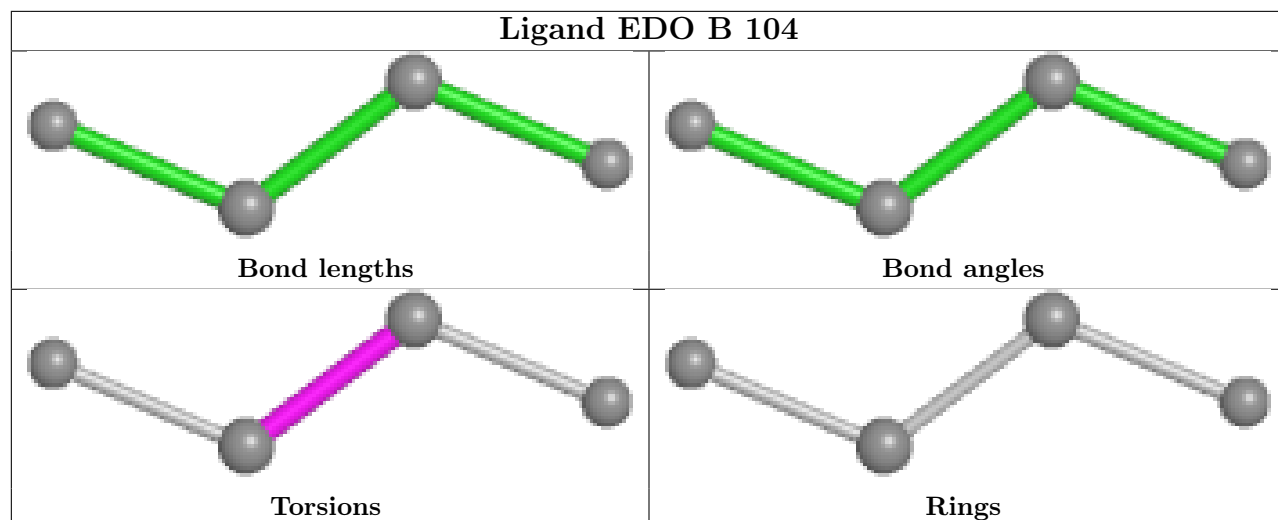


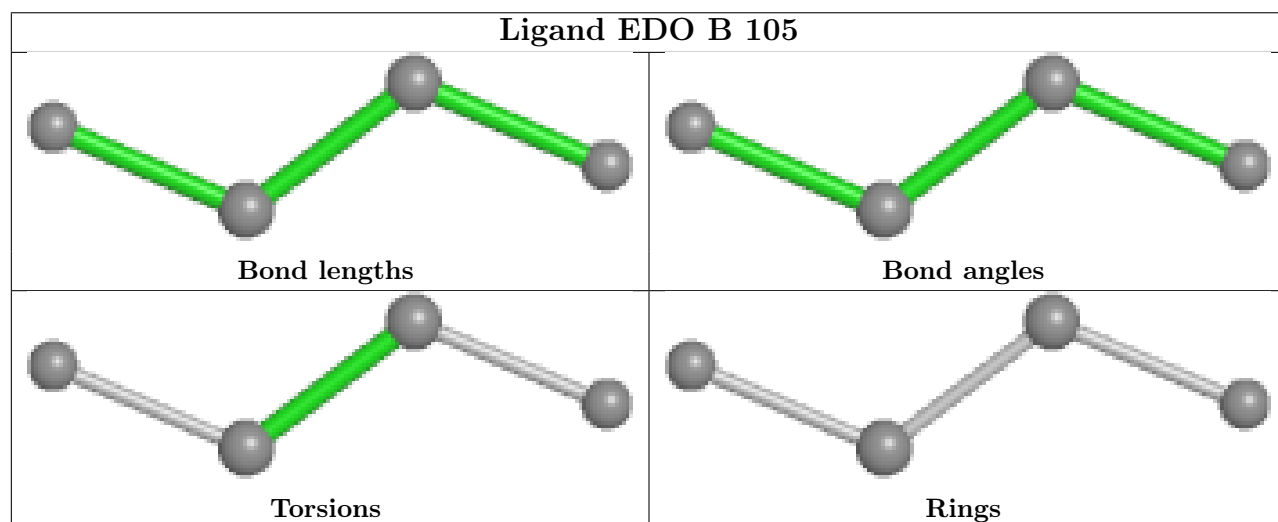
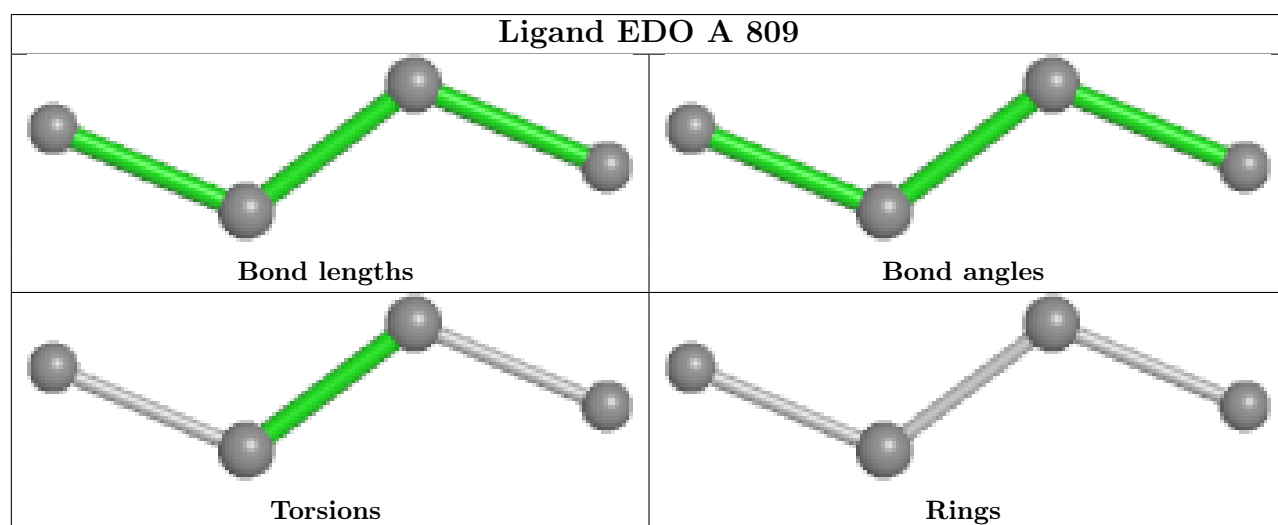
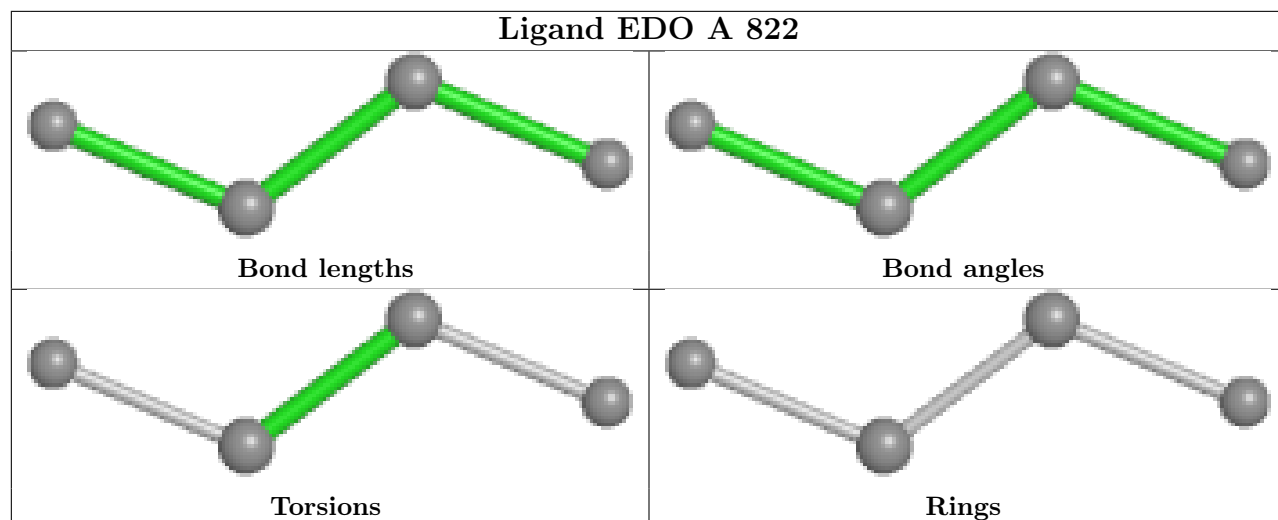


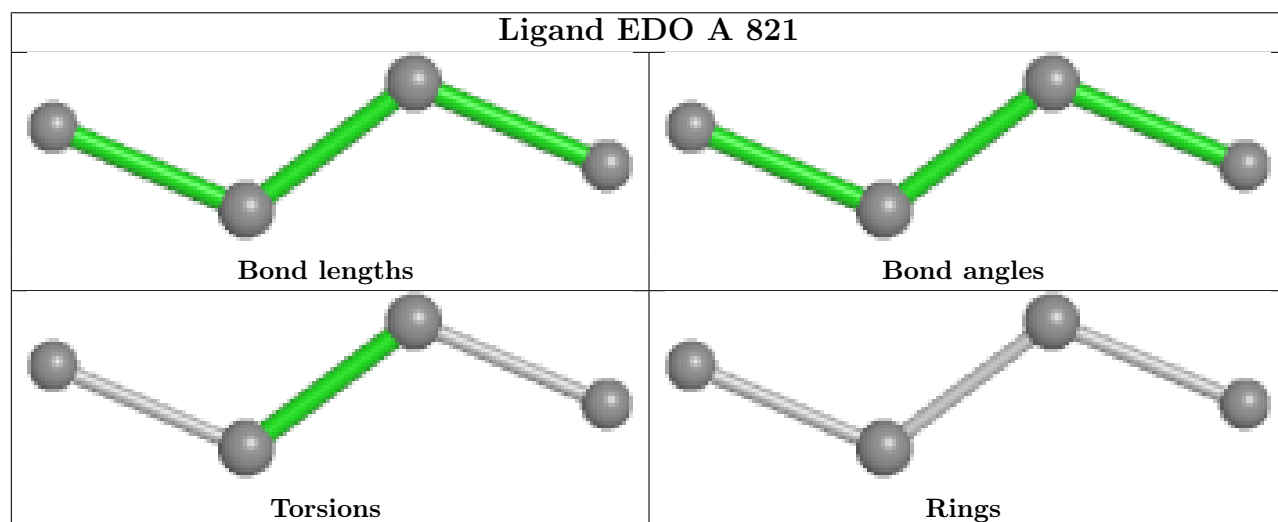
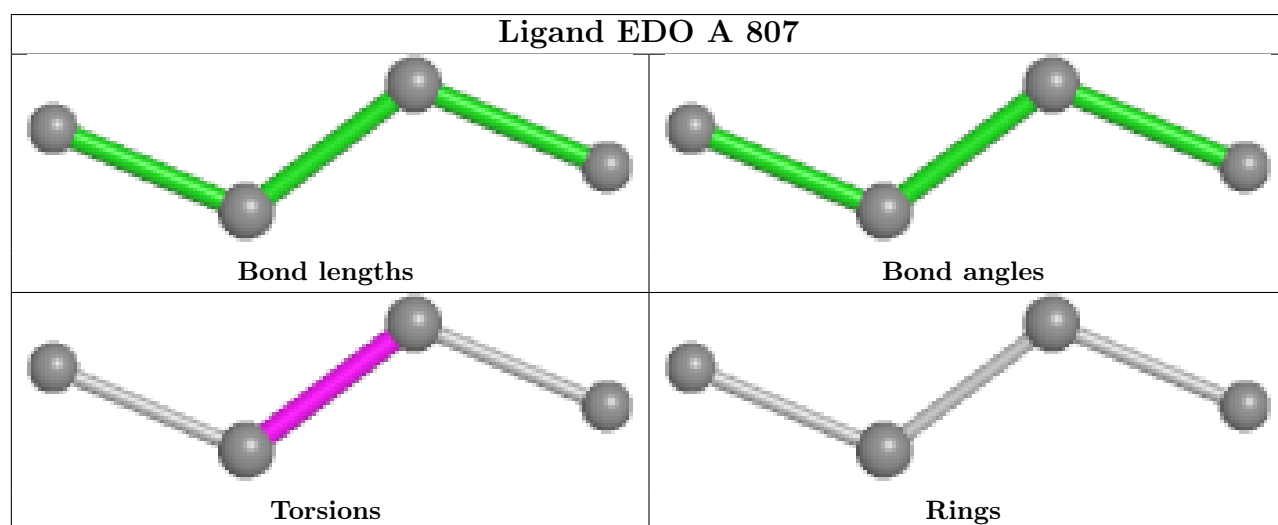
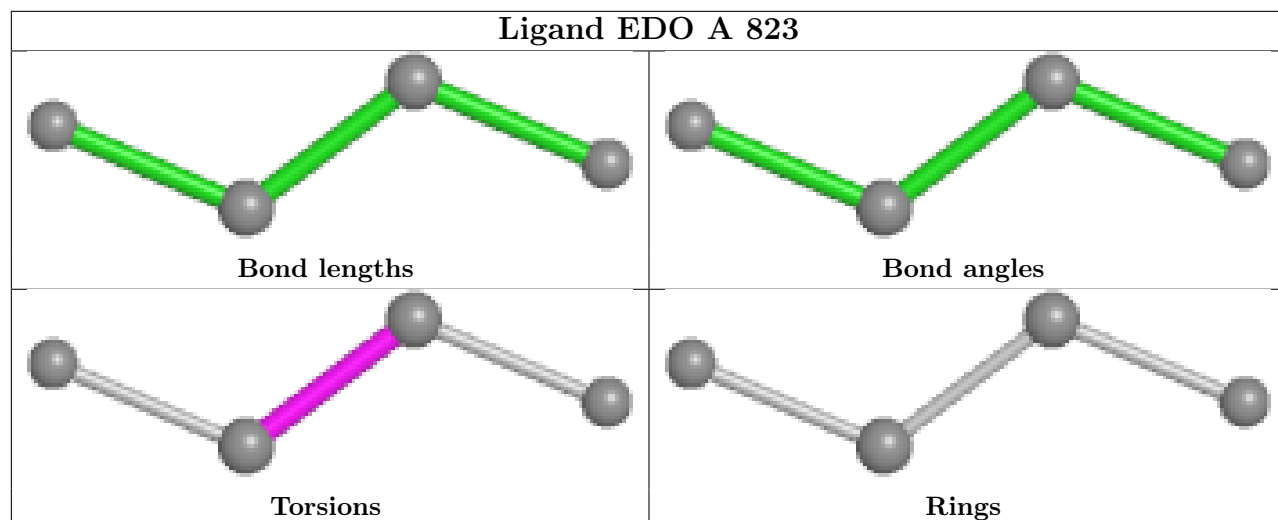


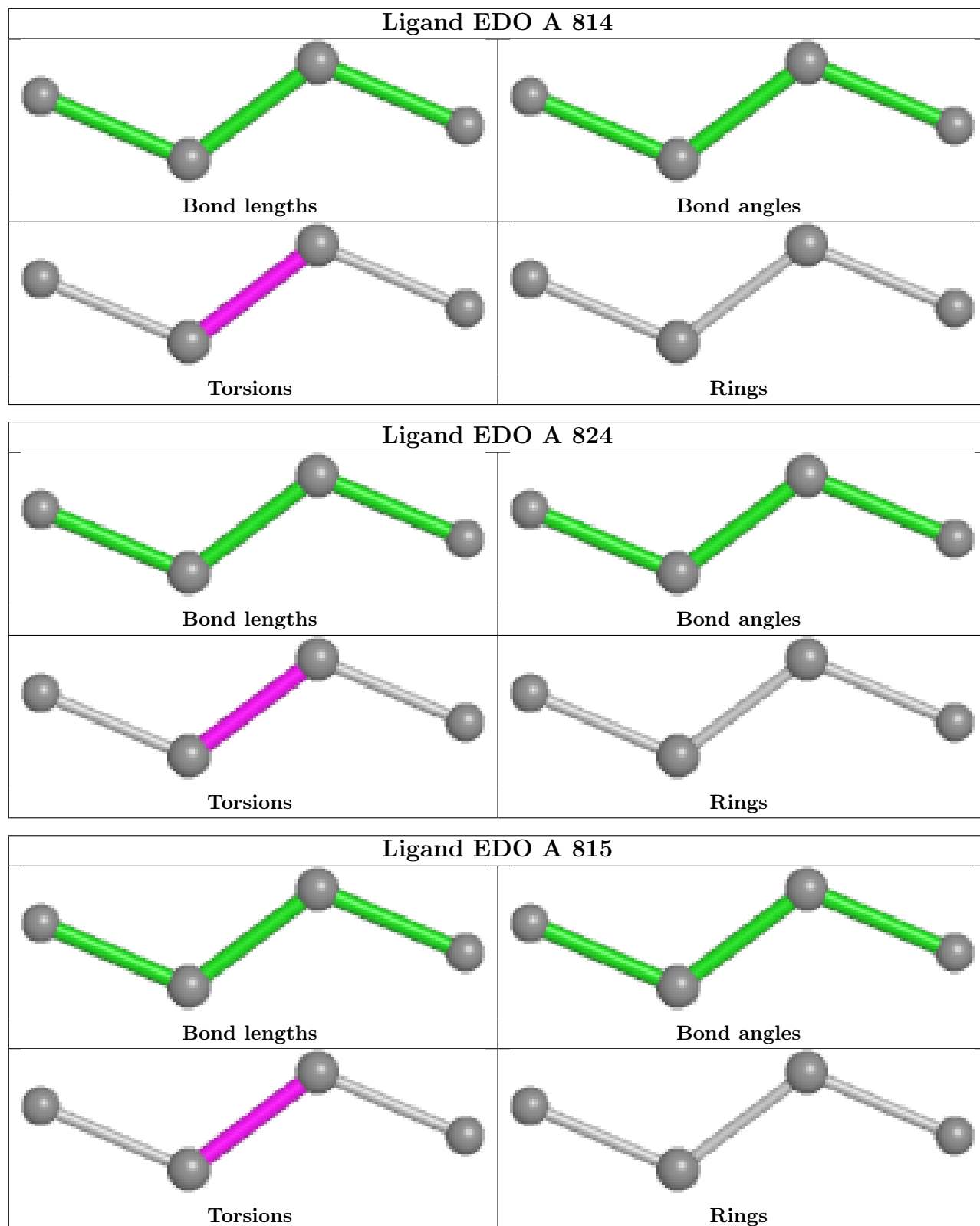












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	725/777 (93%)	0.33	38 (5%) 27 30	27, 46, 86, 126	0
2	B	40/41 (97%)	-0.25	1 (2%) 57 60	29, 38, 64, 71	1 (2%)
All	All	765/818 (93%)	0.30	39 (5%) 28 31	27, 45, 85, 126	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	631	GLY	6.9
1	A	284	THR	6.7
1	A	629	SER	5.7
2	B	-3[B]	G	4.9
1	A	632	ASN	4.9
1	A	706	LYS	4.7
1	A	628	GLY	4.7
1	A	630	VAL	4.5
1	A	610	GLU	4.3
1	A	712	GLY	4.1
1	A	613	ASN	4.0
1	A	611	LEU	4.0
1	A	609	LYS	3.7
1	A	475	ALA	3.4
1	A	298	ASP	3.4
1	A	716	ILE	3.2
1	A	90	TYR	3.0
1	A	128	ILE	3.0
1	A	502	LYS	2.9
1	A	704	ALA	2.8
1	A	498	ILE	2.8
1	A	91	ARG	2.6
1	A	615	ILE	2.6
1	A	766	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	625	PRO	2.4
1	A	261	ILE	2.4
1	A	634	LYS	2.4
1	A	224	GLU	2.4
1	A	708	SER	2.3
1	A	702	VAL	2.3
1	A	295	LYS	2.3
1	A	262	CYS	2.2
1	A	703	LYS	2.2
1	A	223	GLY	2.2
1	A	94	PRO	2.2
1	A	709	GLU	2.1
1	A	713	ALA	2.1
1	A	499	GLY	2.1
1	A	100	THR	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](#)

There are no monosaccharides in this entry.

## 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
4	EDO	A	817	4/4	0.56	0.30	96,103,107,111	0
4	EDO	A	815	4/4	0.64	0.23	45,55,65,65	0
4	EDO	B	105	4/4	0.65	0.30	77,90,91,91	0
4	EDO	A	822	4/4	0.72	0.21	78,86,87,90	0
4	EDO	A	814	4/4	0.73	0.22	62,62,69,70	0
6	MG	B	103	1/1	0.74	0.28	47,47,47,47	0
4	EDO	A	810	4/4	0.78	0.15	76,78,79,80	0
6	MG	B	102	1/1	0.80	0.16	51,51,51,51	0

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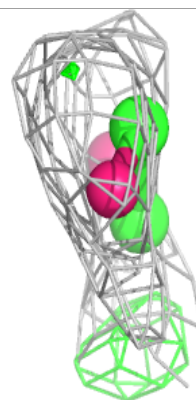
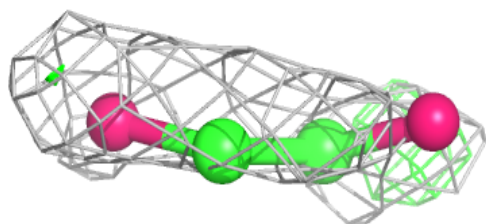
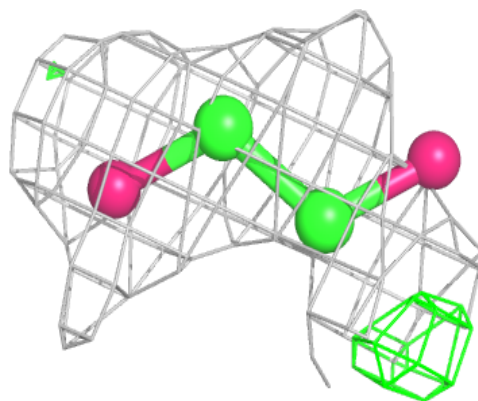
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	819	4/4	0.84	0.35	57,60,72,73	0
4	EDO	A	808	4/4	0.86	0.26	59,59,61,68	0
4	EDO	A	812	4/4	0.86	0.22	41,43,47,51	0
4	EDO	A	816	4/4	0.86	0.24	45,57,63,69	0
4	EDO	A	824	4/4	0.87	0.19	38,46,52,61	0
4	EDO	A	809	4/4	0.87	0.16	45,46,48,54	0
4	EDO	A	818	4/4	0.87	0.37	54,54,65,70	0
4	EDO	A	823	4/4	0.87	0.22	49,57,59,62	0
4	EDO	A	813	4/4	0.88	0.20	42,59,61,67	0
4	EDO	A	811	4/4	0.89	0.20	35,48,55,56	0
4	EDO	A	820	4/4	0.89	0.25	39,54,56,60	0
4	EDO	B	106	4/4	0.93	0.20	65,66,69,71	0
4	EDO	B	104	4/4	0.93	0.22	56,67,70,72	0
3	CL	A	804	1/1	0.93	0.09	56,56,56,56	0
6	MG	B	101	1/1	0.94	0.10	34,34,34,34	0
4	EDO	A	807	4/4	0.95	0.12	44,44,48,49	0
4	EDO	A	821	4/4	0.96	0.34	39,40,48,49	0
4	EDO	A	806	4/4	0.96	0.22	33,42,44,44	0
3	CL	A	805	1/1	0.97	0.13	48,48,48,48	0
3	CL	A	803	1/1	0.97	0.10	49,49,49,49	0
3	CL	A	801	1/1	0.99	0.15	37,37,37,37	0
3	CL	A	802	1/1	0.99	0.15	47,47,47,47	0
5	BR	A	825	1/1	1.00	0.08	40,40,40,40	0

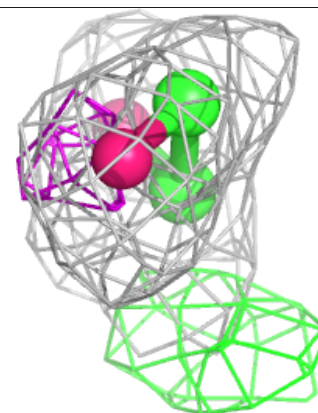
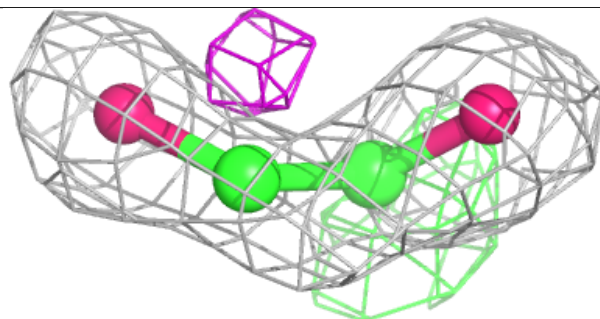
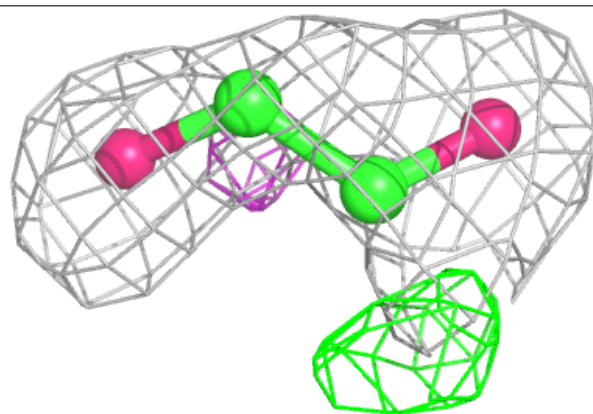
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around EDO A 817:**

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

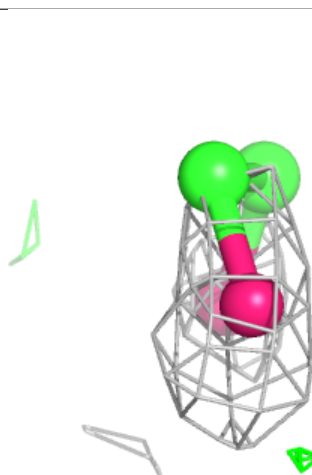
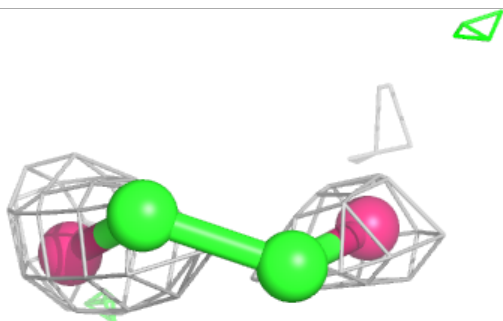
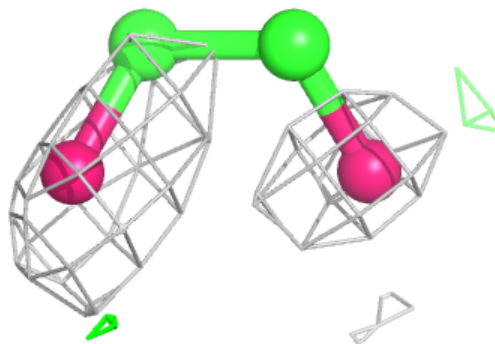
**Electron density around EDO A 815:**

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



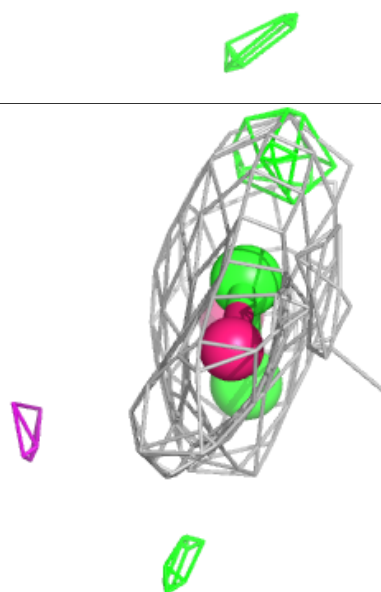
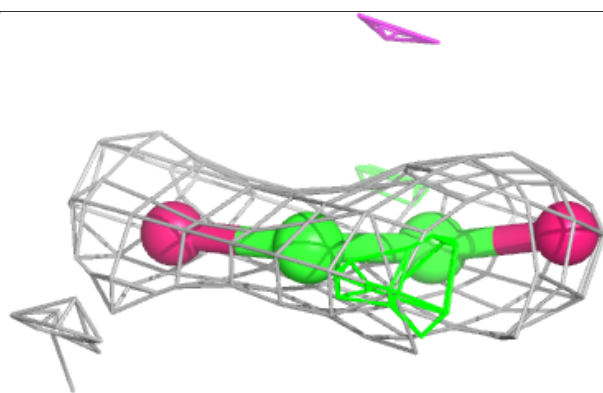
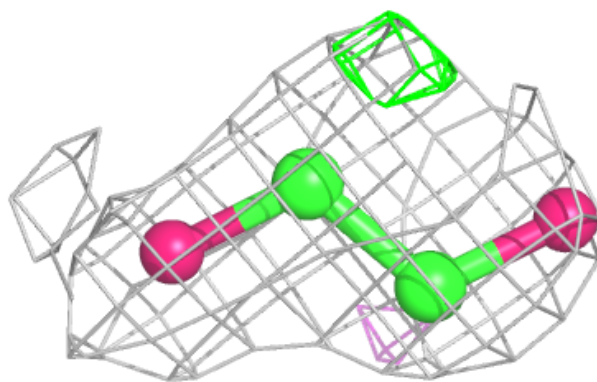
**Electron density around EDO B 105:**

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



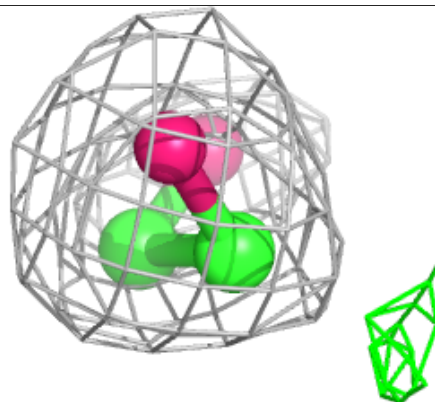
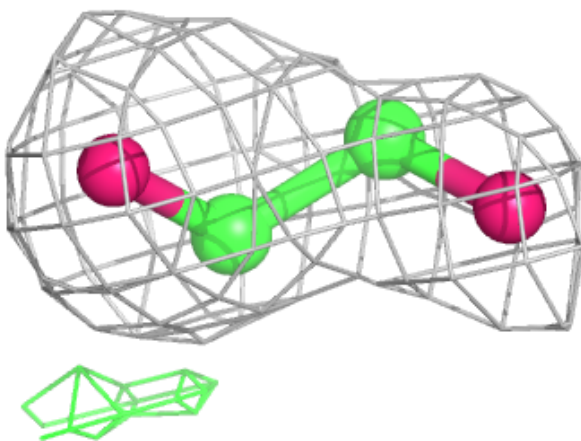
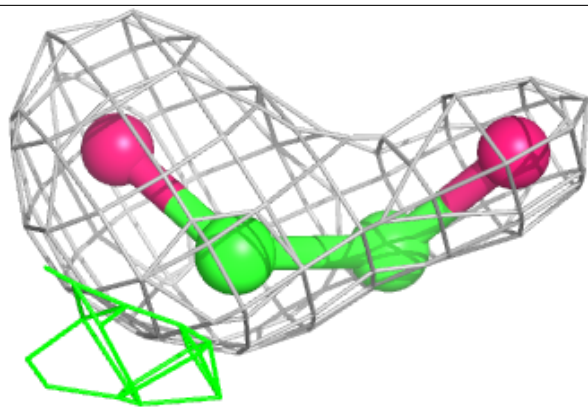
**Electron density around EDO A 822:**

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



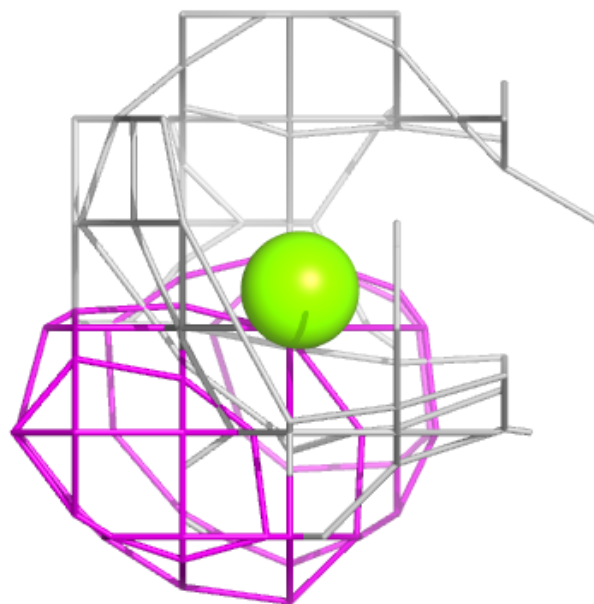
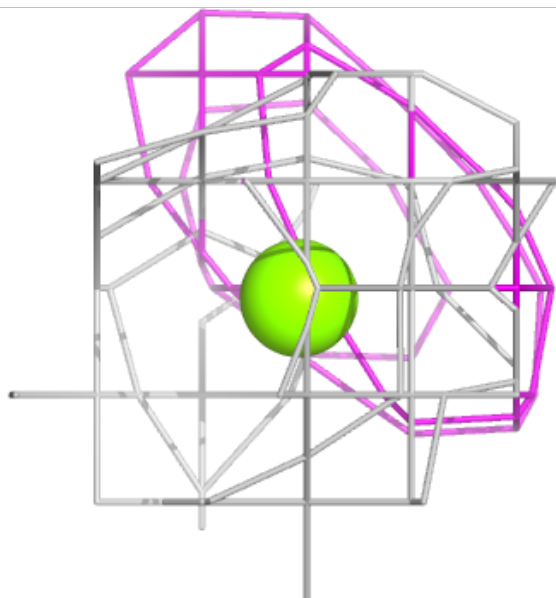
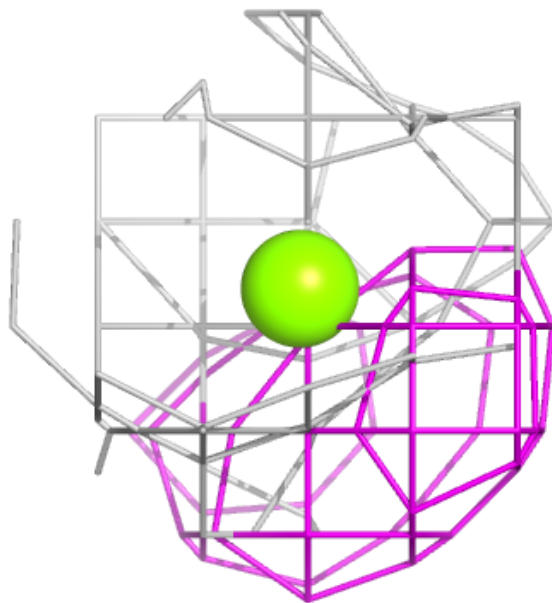
**Electron density around EDO A 814:**

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



**Electron density around MG B 103:**

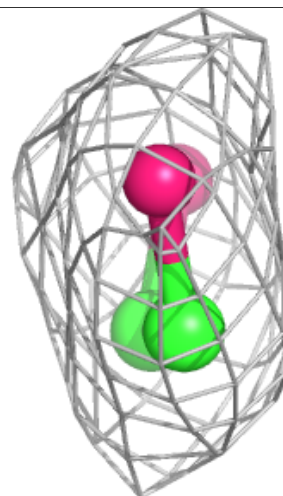
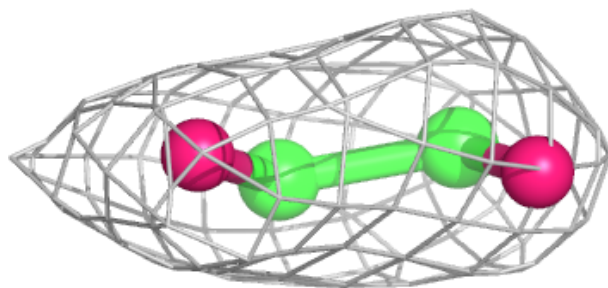
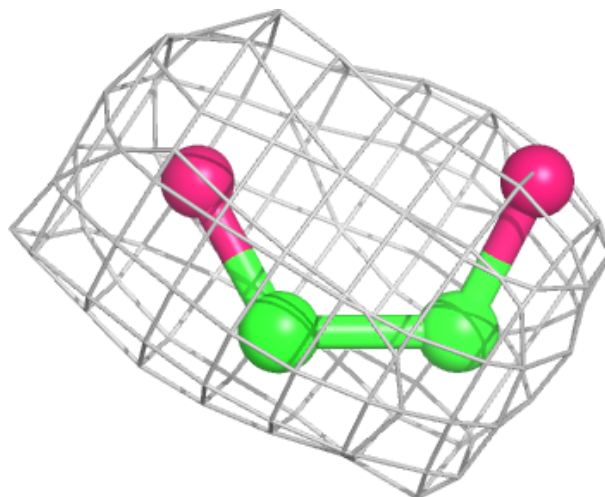
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around EDO A 810:**

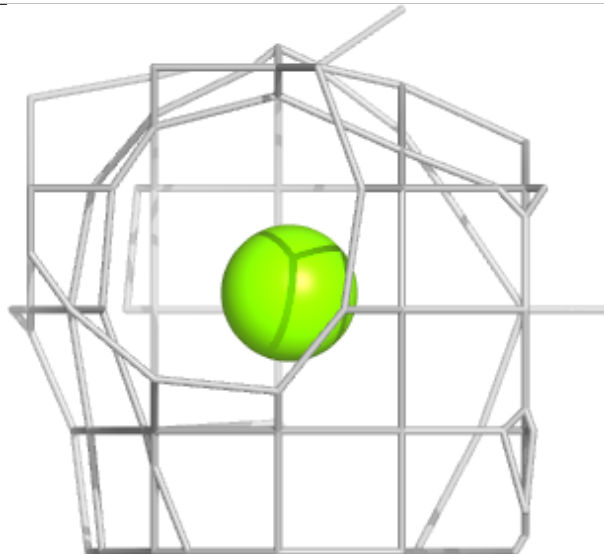
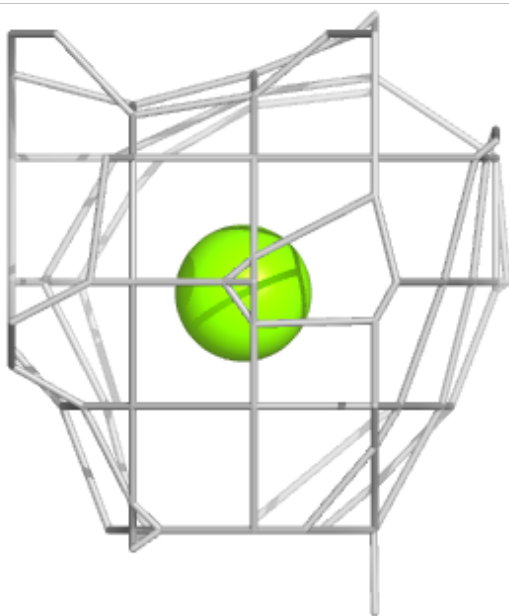
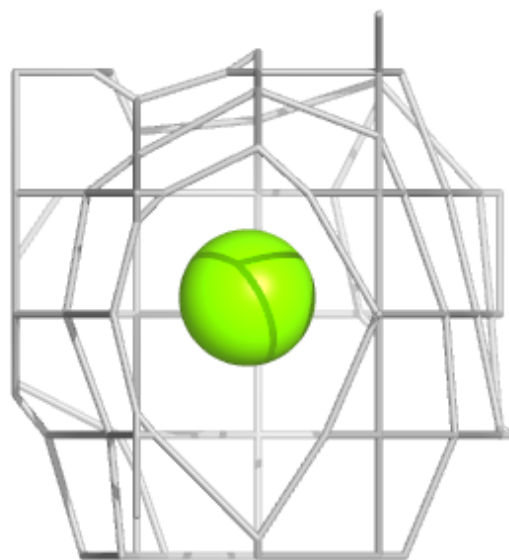
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





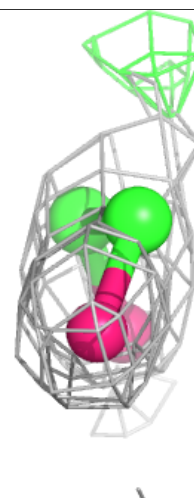
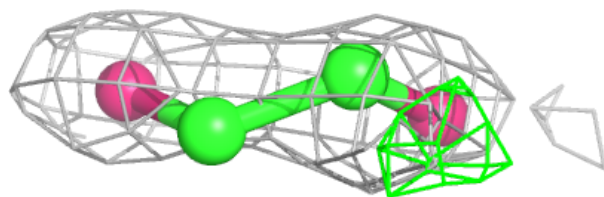
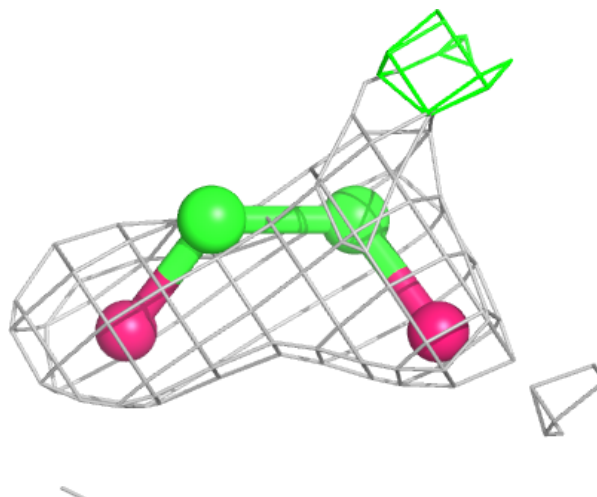
**Electron density around MG B 102:**

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



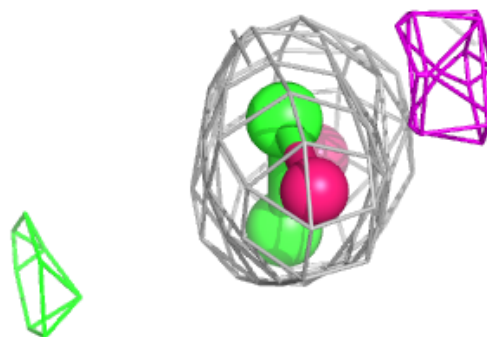
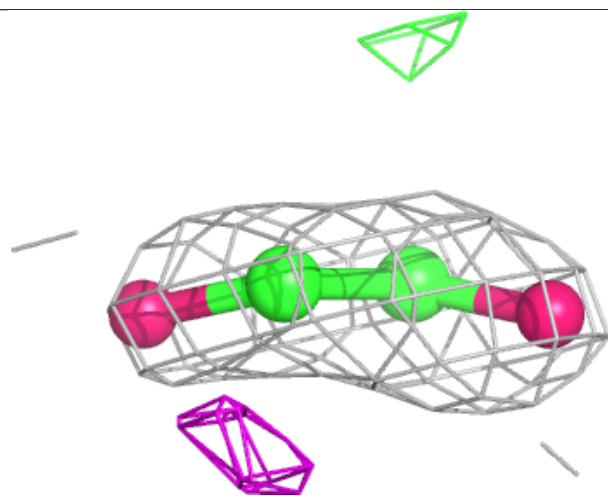
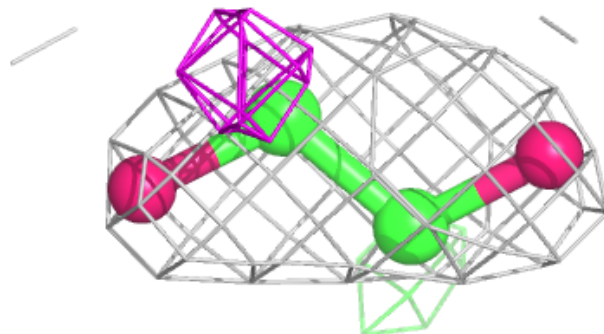
**Electron density around EDO A 819:**

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



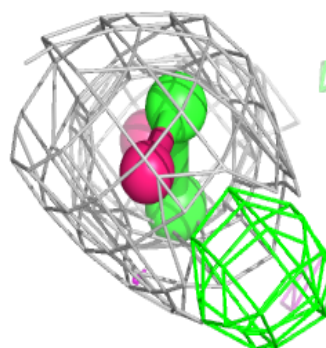
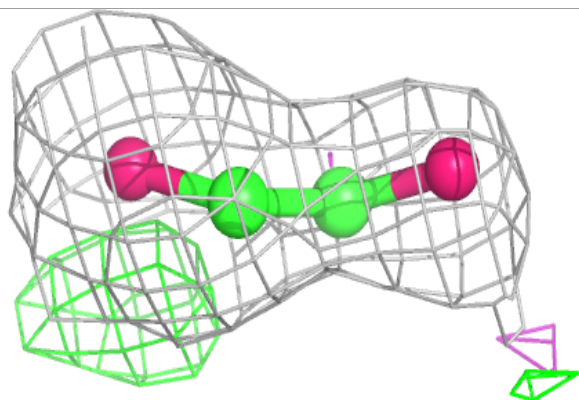
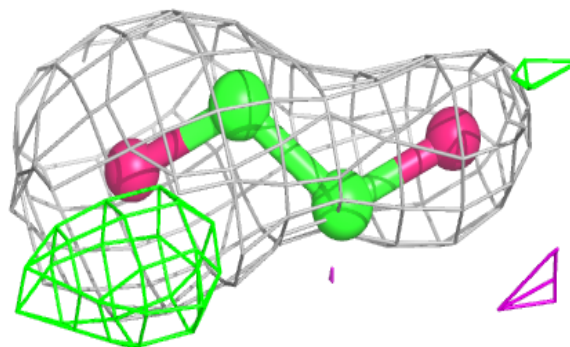
**Electron density around EDO A 808:**

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

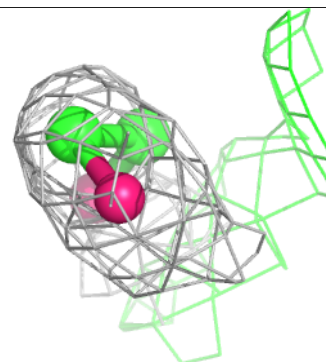
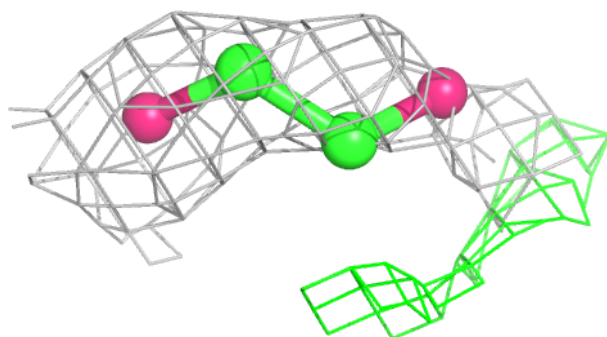
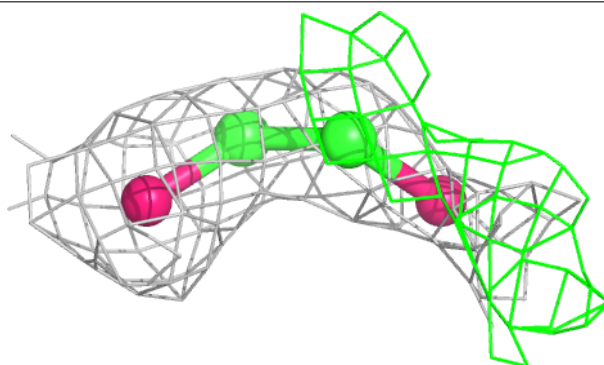


**Electron density around EDO A 812:**

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

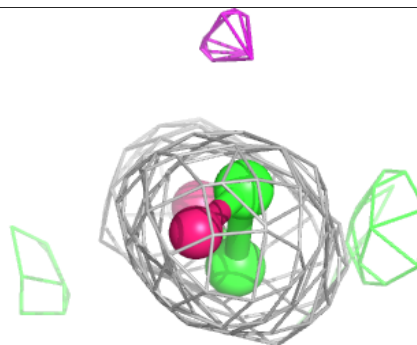
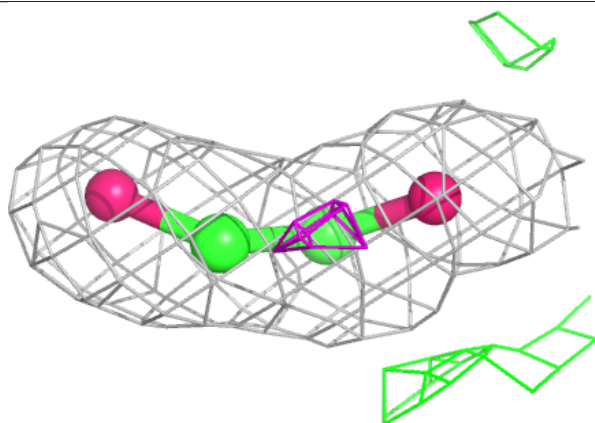
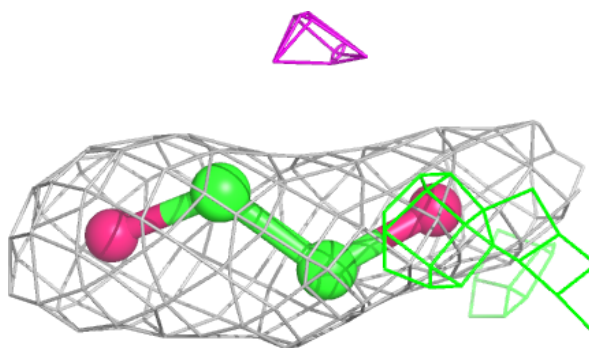
**Electron density around EDO A 816:**

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

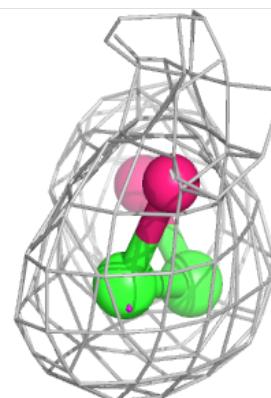
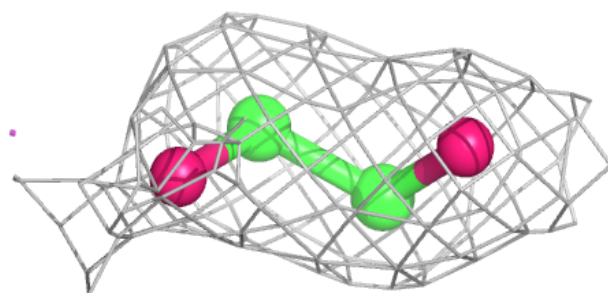
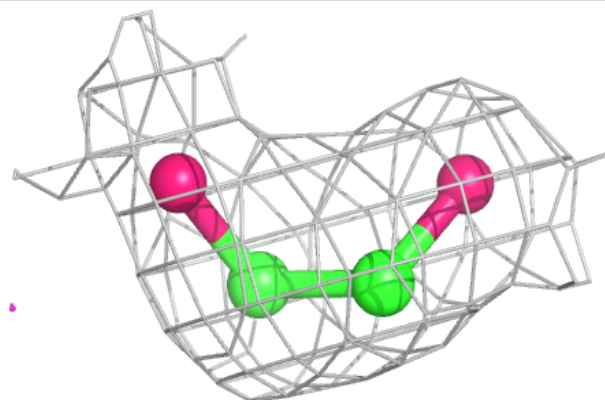


**Electron density around EDO A 824:**

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

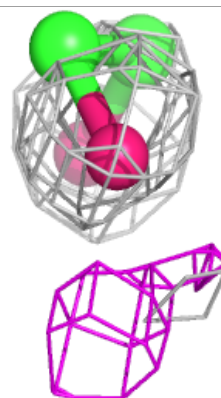
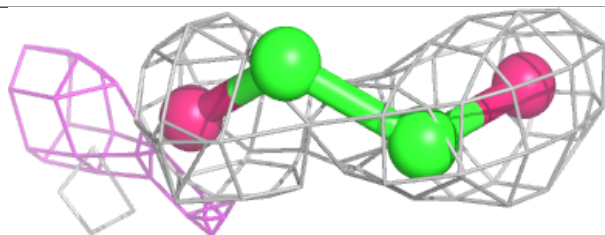
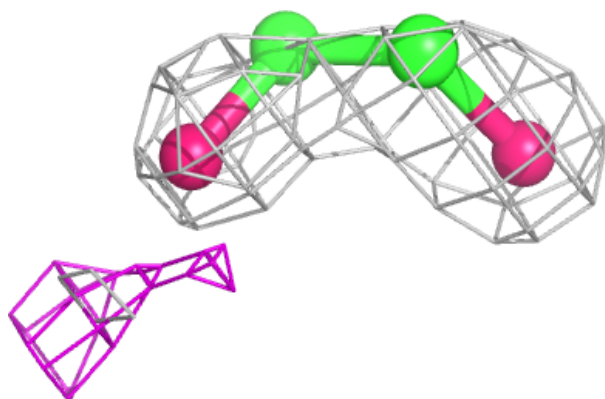
**Electron density around EDO A 809:**

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

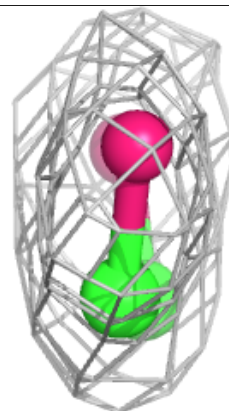
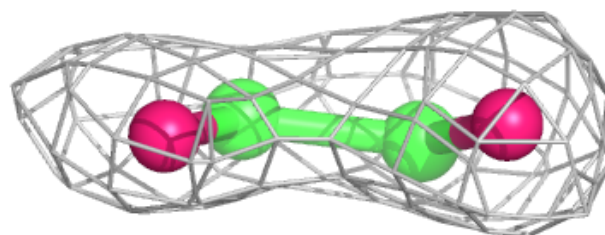
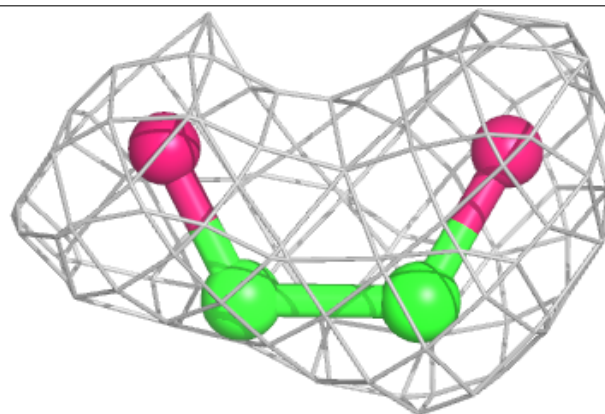


**Electron density around EDO A 818:**

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

**Electron density around EDO A 823:**

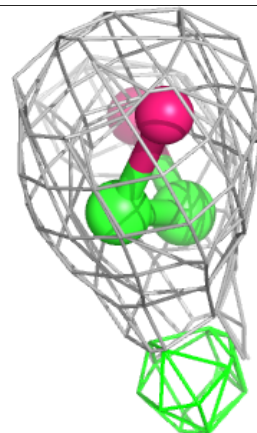
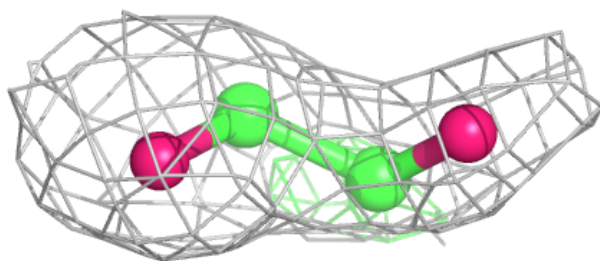
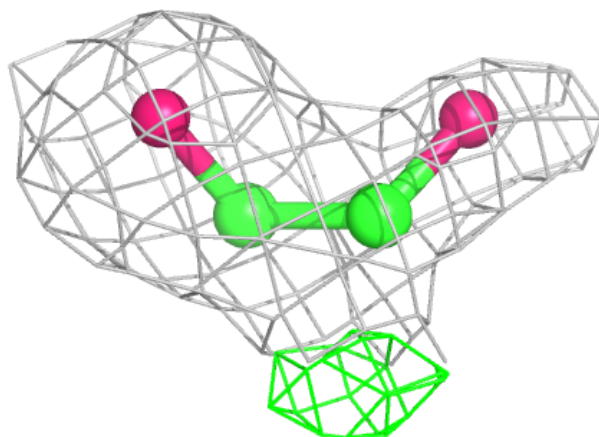
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





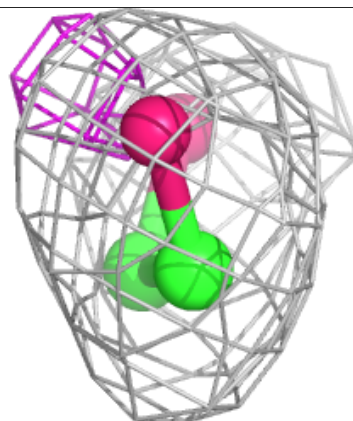
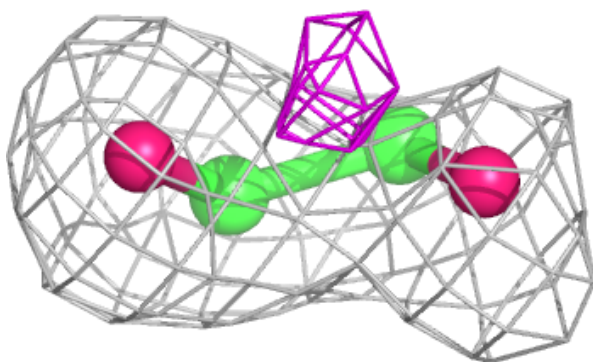
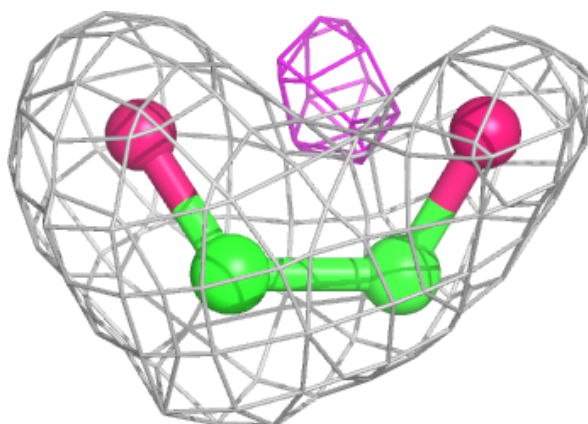
**Electron density around EDO A 813:**

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

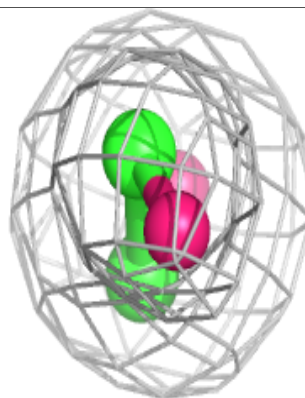
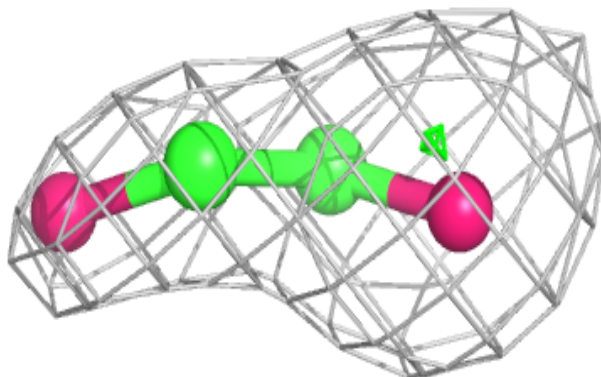
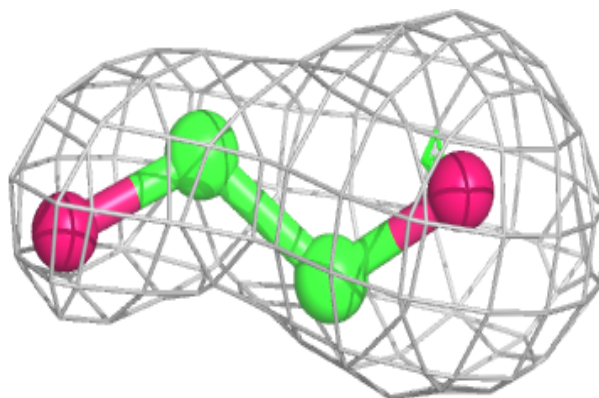


**Electron density around EDO A 811:**

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

**Electron density around EDO A 820:**

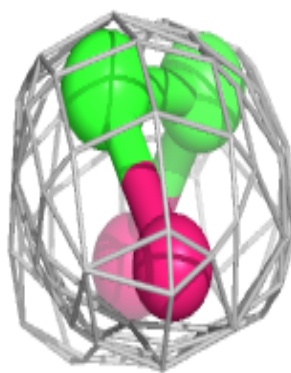
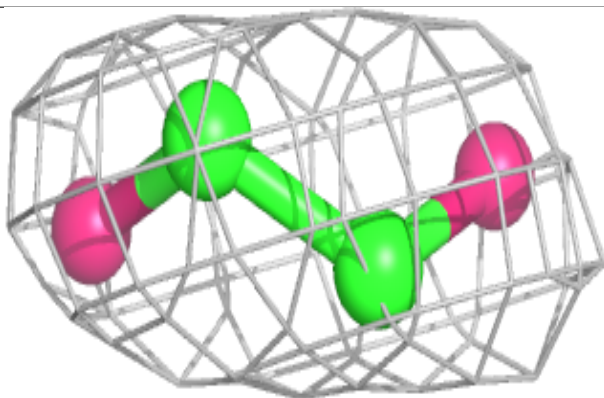
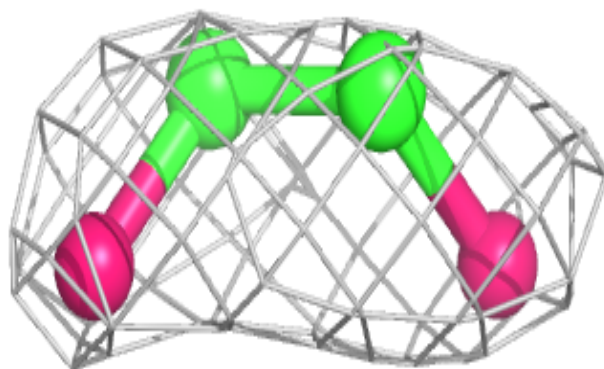
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



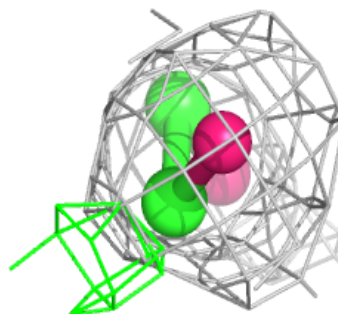
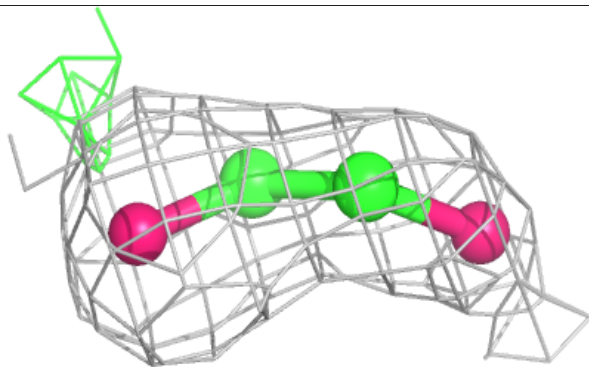
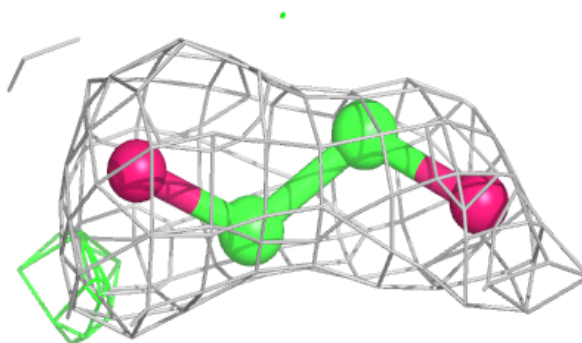


**Electron density around EDO B 106:**

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

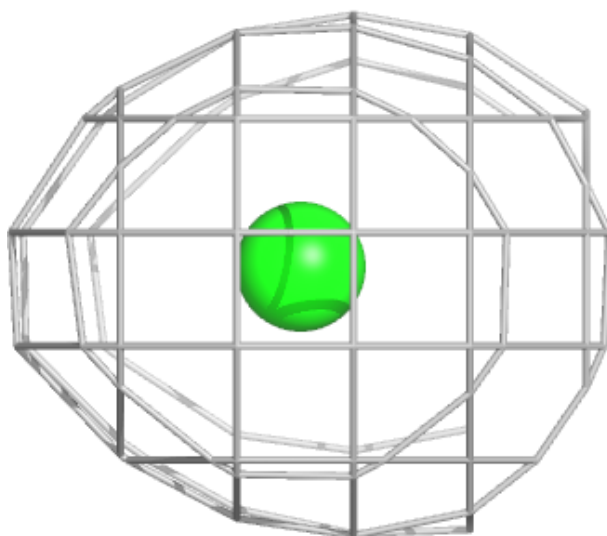
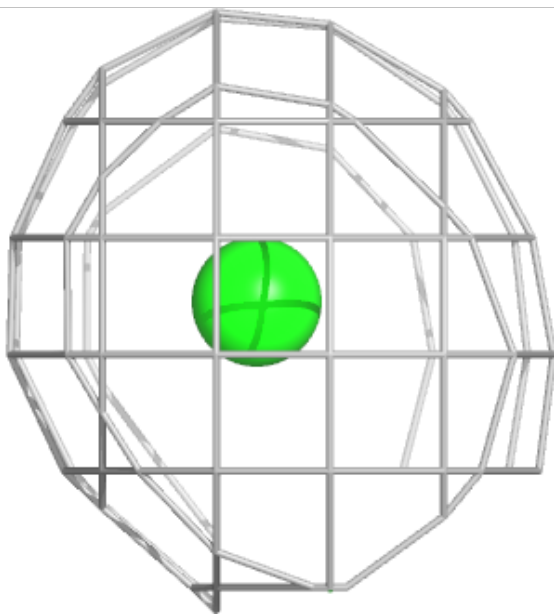
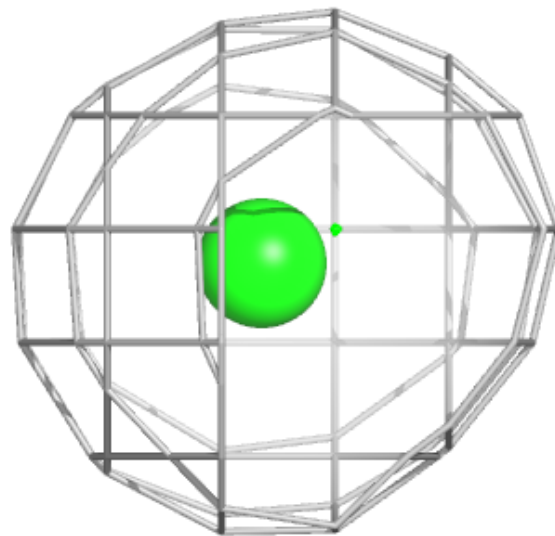
**Electron density around EDO B 104:**

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



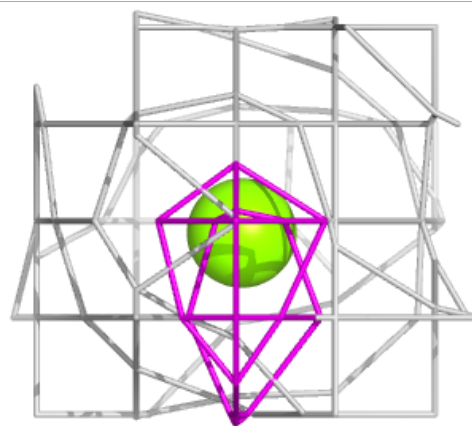
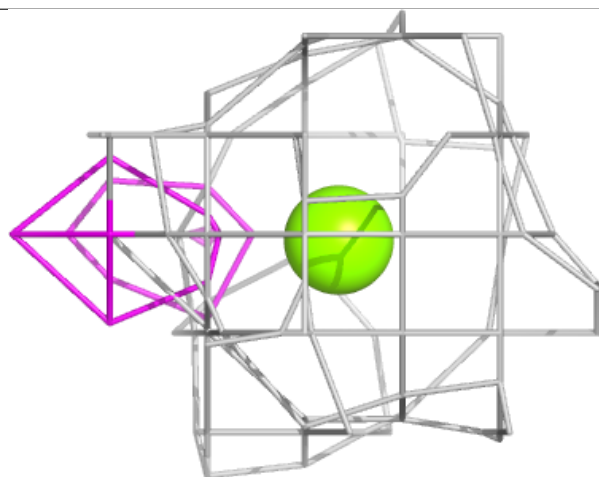
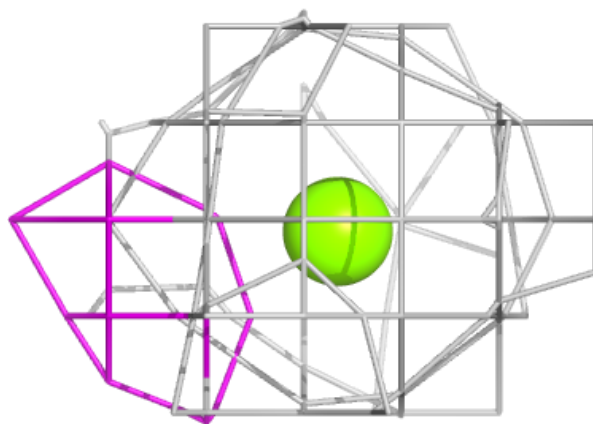
**Electron density around CL A 804:**

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



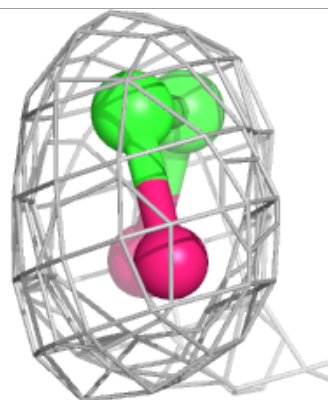
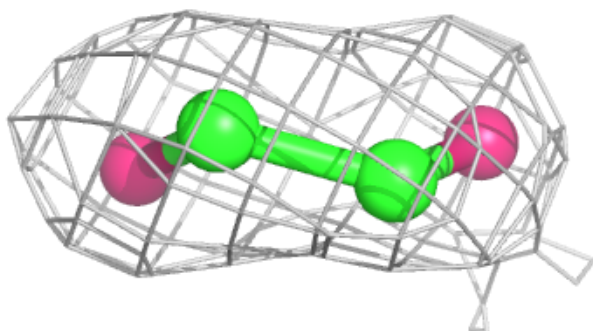
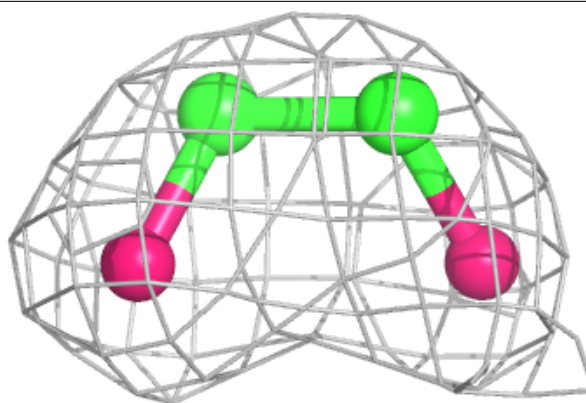
**Electron density around MG B 101:**

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

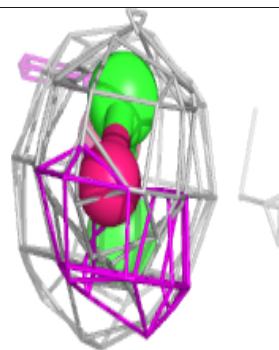
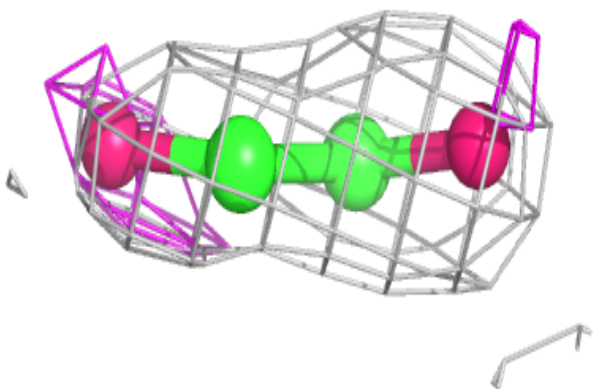
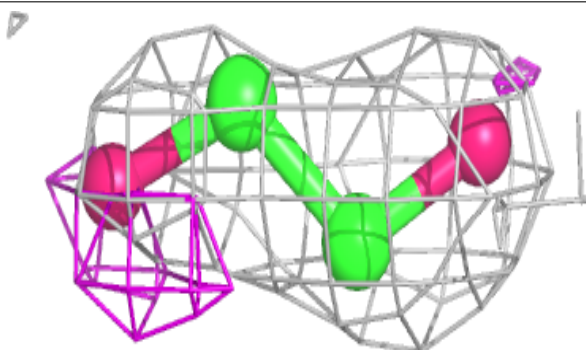


**Electron density around EDO A 807:**

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

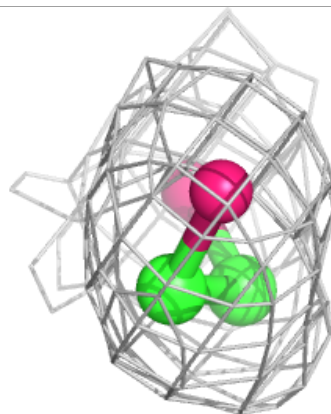
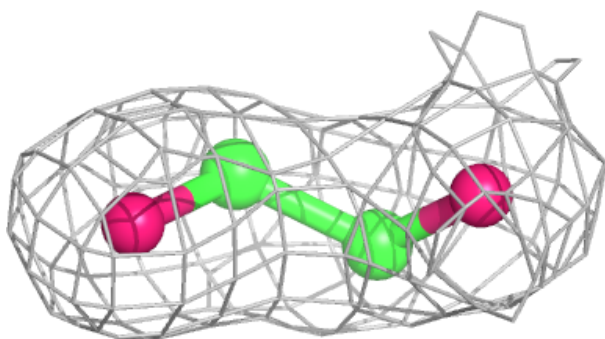
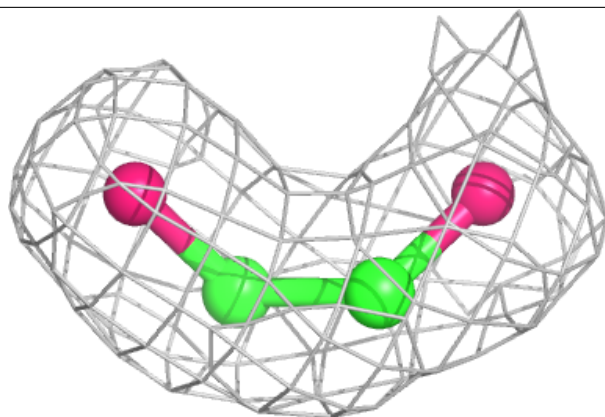
**Electron density around EDO A 821:**

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



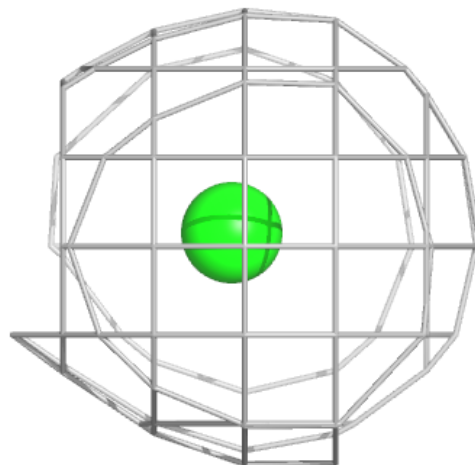
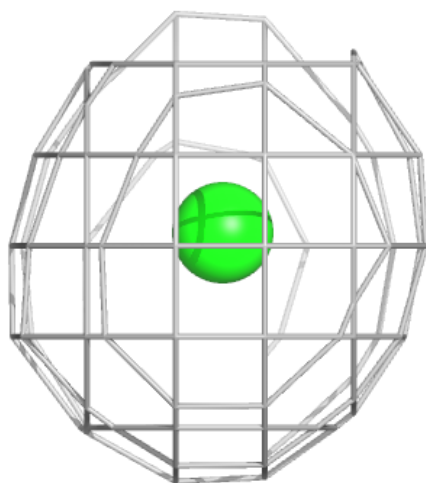
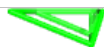
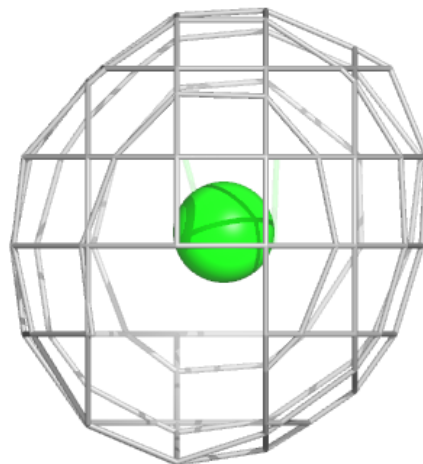
**Electron density around EDO A 806:**

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



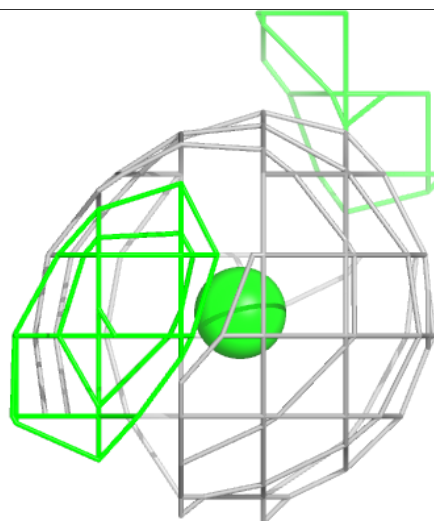
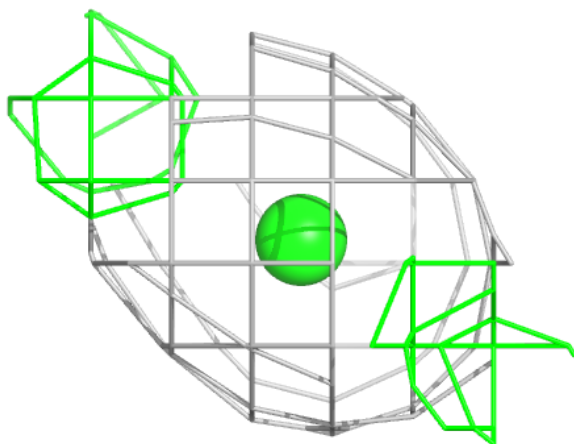
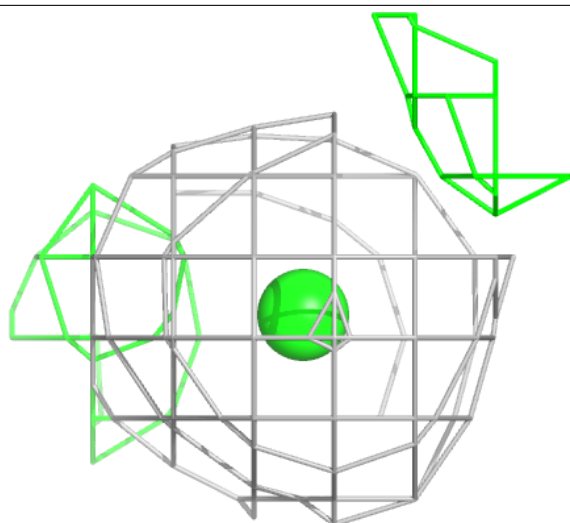
**Electron density around CL A 805:**

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



**Electron density around CL A 803:**

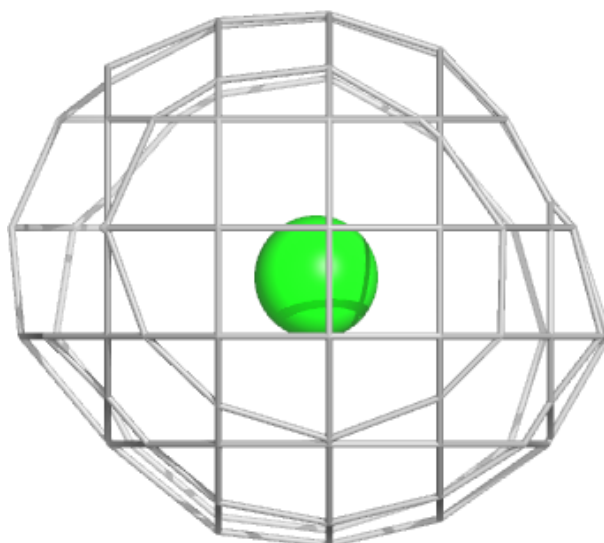
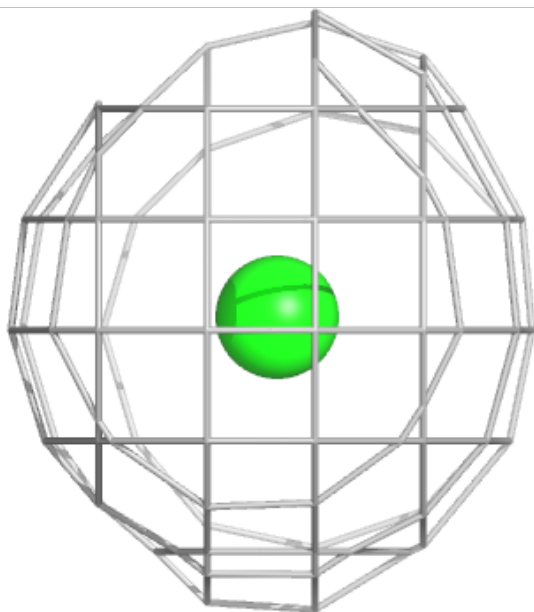
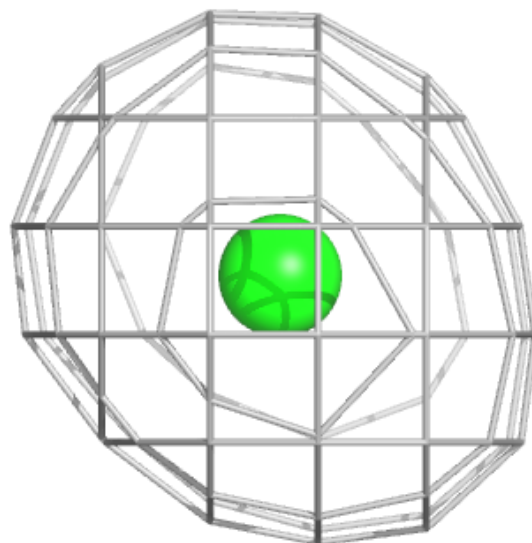
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CL A 801:**

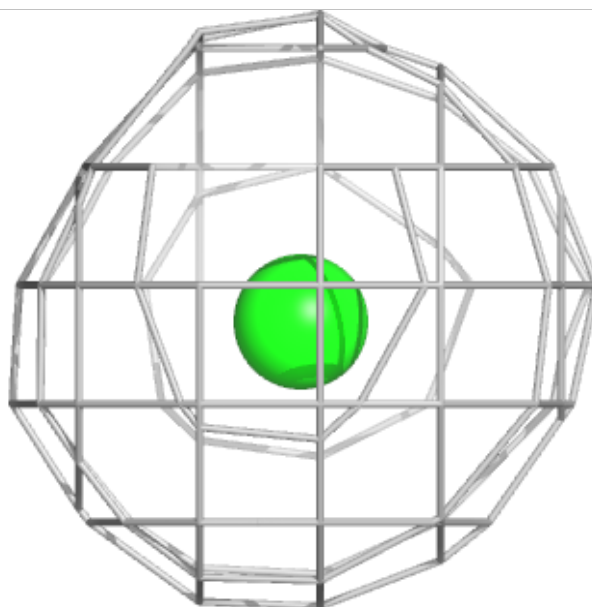
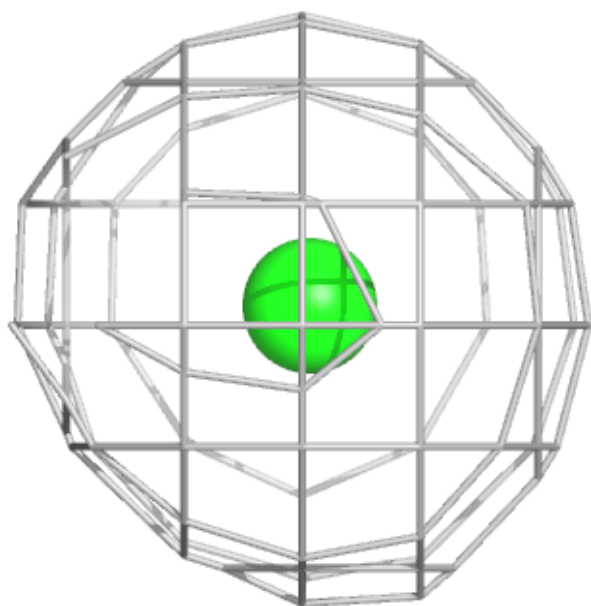
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





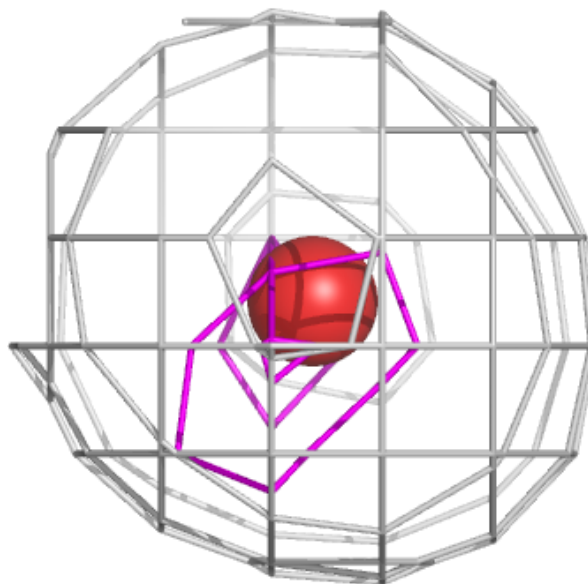
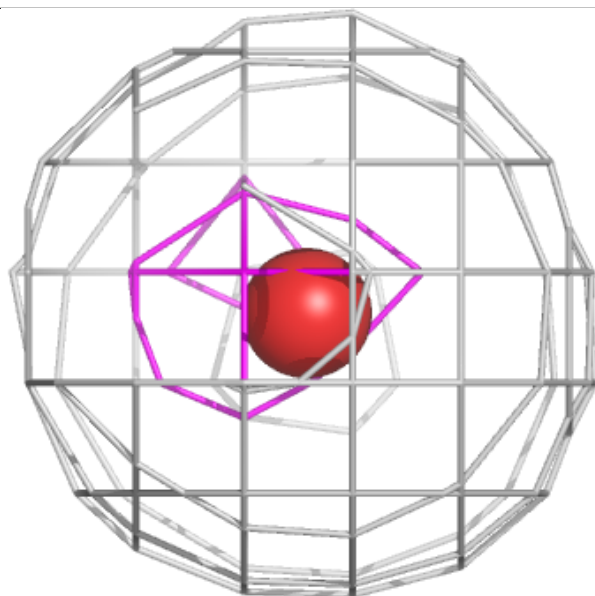
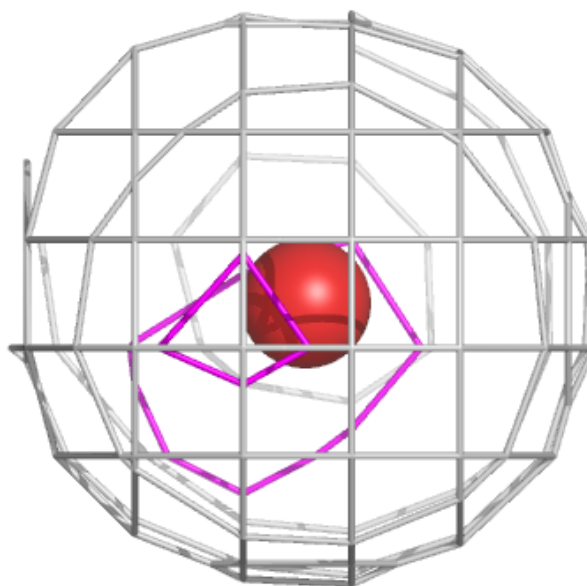
**Electron density around CL A 802:**

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



**Electron density around BR A 825:**

$2mF_o-DF_c$  (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.