wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2022 – 07:24 pm BST

PDB ID	:	7R0P
Title	:	CRYSTAL STRUCTURE OF E.coli ALCOHOL DEHYDROGENASE - FucO MUTANT F254I COMPLEXED WITH FE, NAD+, AND ETHYLENE GLYCOL
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Deposited on	:	2022-02-02
Resolution	:	1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

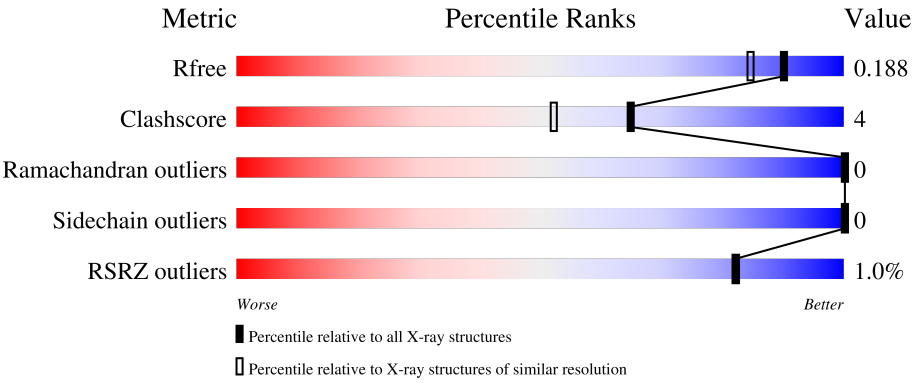
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	390	2% 89% 9%
1	BBB	390	% 94% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12487 atoms, of which 5984 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.

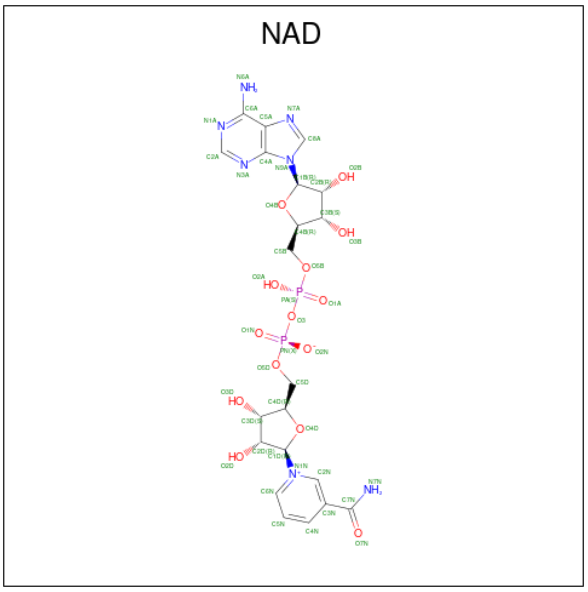
- Molecule 1 is a protein called Lactaldehyde reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	384	Total	C	H	N	O	S	70	8	0
			5841	1834	2934	509	548	16			
1	BBB	384	Total	C	H	N	O	S	69	4	0
			5779	1817	2896	503	547	16			

There are 18 discrepancies between the modelled and reference sequences:

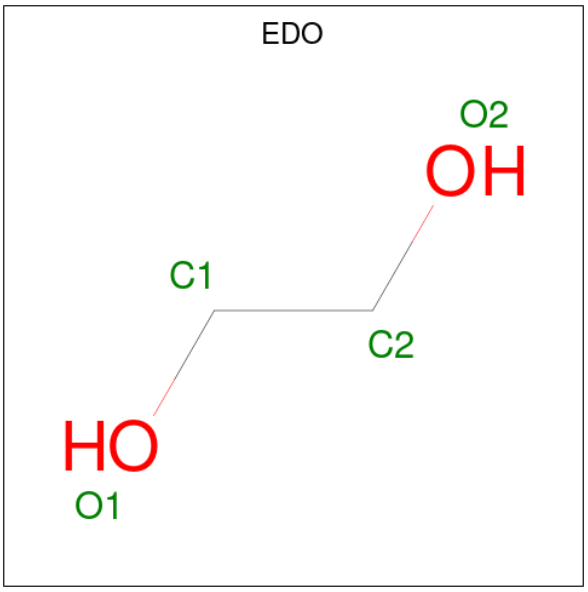
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP P0A9S2
AAA	254	ILE	PHE	engineered mutation	UNP P0A9S2
AAA	384	THR	-	expression tag	UNP P0A9S2
AAA	385	SER	-	expression tag	UNP P0A9S2
AAA	386	HIS	-	expression tag	UNP P0A9S2
AAA	387	HIS	-	expression tag	UNP P0A9S2
AAA	388	HIS	-	expression tag	UNP P0A9S2
AAA	389	HIS	-	expression tag	UNP P0A9S2
AAA	390	HIS	-	expression tag	UNP P0A9S2
BBB	1	MET	-	initiating methionine	UNP P0A9S2
BBB	254	ILE	PHE	engineered mutation	UNP P0A9S2
BBB	384	THR	-	expression tag	UNP P0A9S2
BBB	385	SER	-	expression tag	UNP P0A9S2
BBB	386	HIS	-	expression tag	UNP P0A9S2
BBB	387	HIS	-	expression tag	UNP P0A9S2
BBB	388	HIS	-	expression tag	UNP P0A9S2
BBB	389	HIS	-	expression tag	UNP P0A9S2
BBB	390	HIS	-	expression tag	UNP P0A9S2

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	P	6	0
			70	21	26	7	14	2		
2	BBB	1	Total	C	H	N	O	P	6	0
			70	21	26	7	14	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	AAA	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0
3	BBB	1	Total C H O 10 2 6 2	1	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Fe 1 1	0	0
4	BBB	1	Total Fe 1 1	0	0

- Molecule 5 is water.

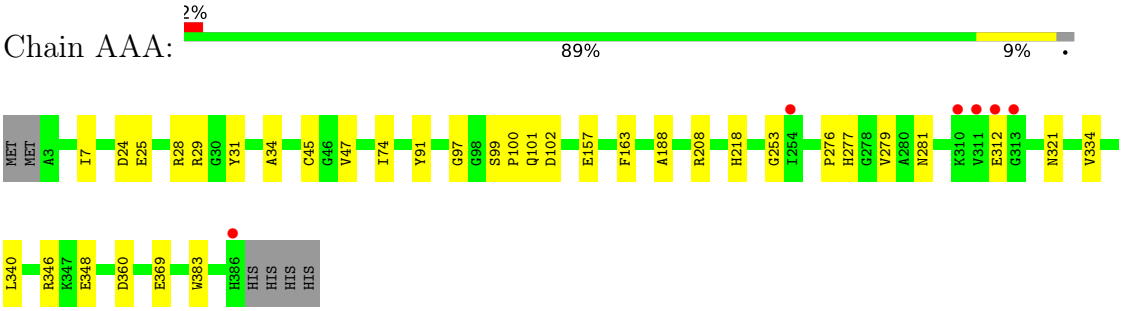
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	259	Total O 259 259	0	0
5	BBB	296	Total O 296 296	0	0

3 Residue-property plots (i)

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

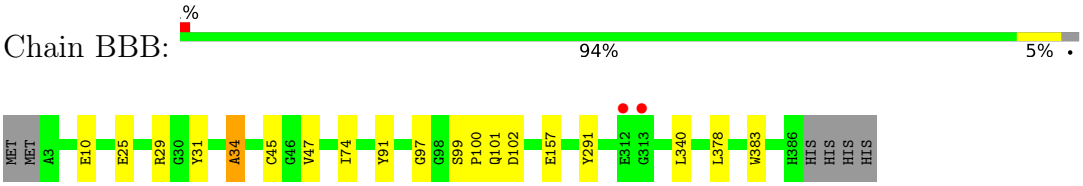
• Molecule 1: Lactaldehyde reductase

Chain AAA:



• Molecule 1: Lactaldehyde reductase

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.98Å 86.16Å 147.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.77 – 1.60 42.74 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.77-1.60) 100.0 (42.74-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.156 , 0.177 0.169 , 0.188	Depositor DCC
R_{free} test set	4792 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12487	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAD, FE, 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	AAA	0.65	0/2979	0.72	0/4053
1	BBB	0.65	0/2943	0.72	0/4006
All	All	0.65	0/5922	0.72	0/8059

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BBB	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	34	ALA	Peptide

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	AAA	2907	2934	2927	27	0
1	BBB	2883	2896	2885	13	0
2	AAA	44	26	26	7	0
2	BBB	44	26	26	5	0
3	AAA	32	48	48	8	0
3	BBB	36	54	54	2	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	259	0	0	6	0
5	BBB	296	0	0	4	0
All	All	6503	5984	5966	49	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 4.

The worst 5 of 49 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)
2:AAA:501:NAD:H5N	5:AAA:606:HOH:O	1.37	1.21
2:AAA:501:NAD:C5N	5:AAA:606:HOH:O	1.87	1.13
2:BBB:501:NAD:C5N	5:BBB:606:HOH:O	2.19	0.90
2:AAA:501:NAD:C5N	5:AAA:805:HOH:O	2.20	0.88
2:AAA:501:NAD:C6N	5:AAA:606:HOH:O	2.18	0.75

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	390/390 (100%)	385 (99%)	5 (1%)	0	100	100
1	BBB	386/390 (99%)	381 (99%)	5 (1%)	0	100	100
All	All	776/780 (100%)	766 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	301/299 (101%)	301 (100%)	0	100	100
1	BBB	297/299 (99%)	297 (100%)	0	100	100
All	All	598/598 (100%)	598 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	EDO	BBB	510	-	3,3,3	0.08	0	2,2,2	0.35	0
3	EDO	AAA	504	-	3,3,3	0.26	0	2,2,2	0.33	0
3	EDO	BBB	506	-	3,3,3	0.18	0	2,2,2	0.03	0
3	EDO	AAA	506	-	3,3,3	0.26	0	2,2,2	0.22	0
3	EDO	BBB	505	-	3,3,3	0.30	0	2,2,2	0.25	0
3	EDO	BBB	502	-	3,3,3	0.15	0	2,2,2	0.16	0
3	EDO	BBB	507	-	3,3,3	0.34	0	2,2,2	0.43	0
3	EDO	BBB	503	-	3,3,3	0.41	0	2,2,2	0.32	0
3	EDO	AAA	509	-	3,3,3	0.08	0	2,2,2	0.24	0
3	EDO	AAA	508	-	3,3,3	0.13	0	2,2,2	0.25	0
3	EDO	AAA	507	-	3,3,3	0.61	0	2,2,2	0.69	0
3	EDO	BBB	509	-	3,3,3	0.30	0	2,2,2	0.18	0
3	EDO	AAA	510	-	3,3,3	0.17	0	2,2,2	0.44	0
3	EDO	BBB	511	-	3,3,3	0.09	0	2,2,2	0.20	0
3	EDO	AAA	502	-	3,3,3	0.30	0	2,2,2	0.40	0
2	NAD	BBB	501	-	42,48,48	1.21	1 (2%)	50,73,73	0.90	3 (6%)
2	NAD	AAA	501	-	42,48,48	1.47	2 (4%)	50,73,73	0.98	4 (8%)
3	EDO	AAA	503	-	3,3,3	0.12	0	2,2,2	0.16	0
3	EDO	BBB	504	-	3,3,3	0.32	0	2,2,2	0.09	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	EDO	BBB	510	-	-	1/1/1/1	-
3	EDO	AAA	504	-	-	1/1/1/1	-
3	EDO	BBB	506	-	-	1/1/1/1	-
3	EDO	AAA	506	-	-	0/1/1/1	-
3	EDO	BBB	505	-	-	0/1/1/1	-
3	EDO	BBB	502	-	-	0/1/1/1	-
3	EDO	BBB	507	-	-	1/1/1/1	-
3	EDO	BBB	503	-	-	0/1/1/1	-
3	EDO	AAA	509	-	-	1/1/1/1	-
3	EDO	AAA	508	-	-	1/1/1/1	-
3	EDO	AAA	507	-	-	1/1/1/1	-
3	EDO	BBB	509	-	-	1/1/1/1	-
3	EDO	AAA	510	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	BBB	511	-	-	1/1/1/1	-
3	EDO	AAA	502	-	-	0/1/1/1	-
2	NAD	BBB	501	-	-	5/26/62/62	0/5/5/5
2	NAD	AAA	501	-	-	5/26/62/62	0/5/5/5
3	EDO	AAA	503	-	-	0/1/1/1	-
3	EDO	BBB	504	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	501	NAD	C2N-N1N	8.74	1.45	1.35
2	BBB	501	NAD	C2N-N1N	6.79	1.43	1.35
2	AAA	501	NAD	C6N-N1N	-2.17	1.30	1.35

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	501	NAD	O4D-C1D-C2D	-3.35	102.04	106.93
2	AAA	501	NAD	C6N-N1N-C2N	-3.34	118.93	121.97
2	BBB	501	NAD	C6N-N1N-C2N	-2.89	119.34	121.97
2	AAA	501	NAD	C5A-C6A-N6A	2.33	123.89	120.35
2	AAA	501	NAD	O4D-C1D-C2D	-2.29	103.57	106.93

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	NAD	O4D-C1D-N1N-C2N
2	AAA	501	NAD	O4D-C1D-N1N-C6N
2	AAA	501	NAD	C2D-C1D-N1N-C2N
2	BBB	501	NAD	O4D-C1D-N1N-C2N
2	BBB	501	NAD	O4D-C1D-N1N-C6N

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	504	EDO	2	0
3	BBB	507	EDO	2	0
3	AAA	509	EDO	1	0

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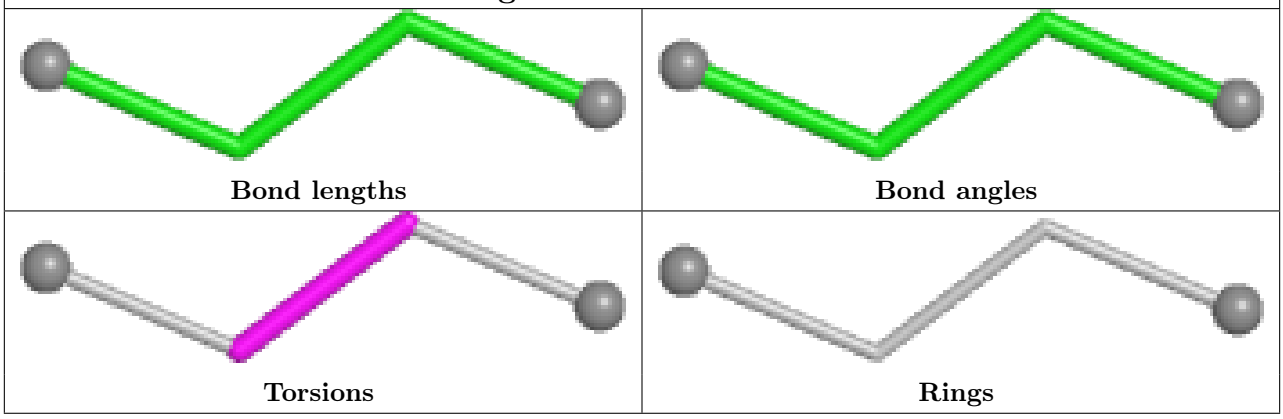
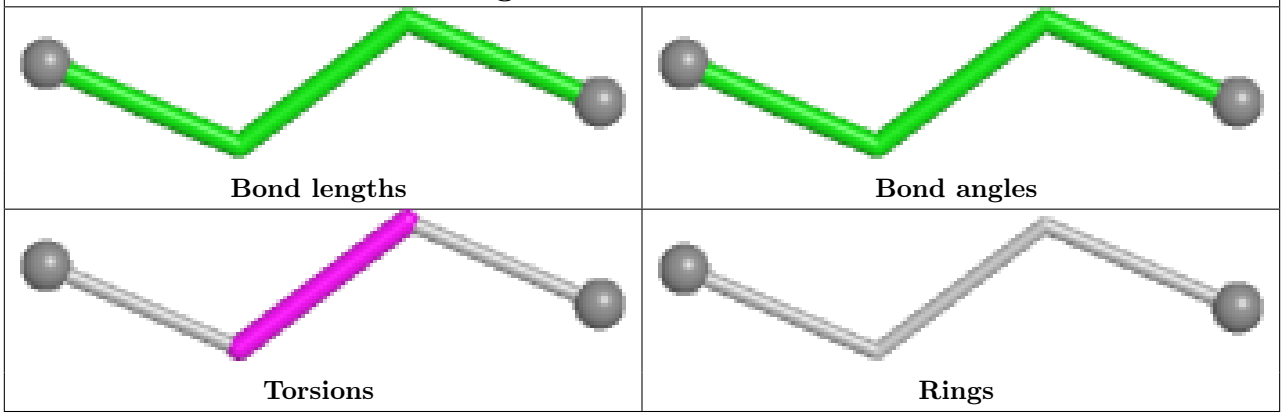
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	508	EDO	1	0
3	AAA	507	EDO	2	0
3	AAA	510	EDO	2	0
2	BBB	501	NAD	5	0
2	AAA	501	NAD	7	0

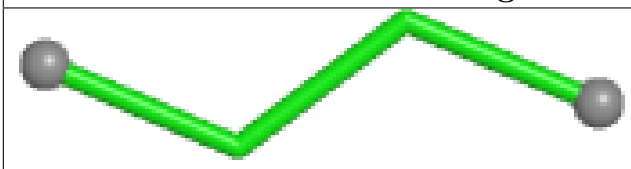
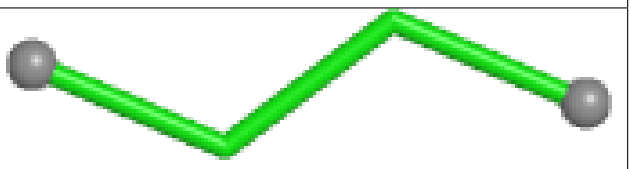
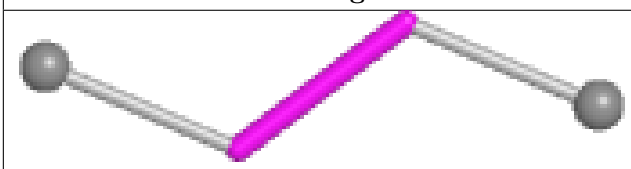
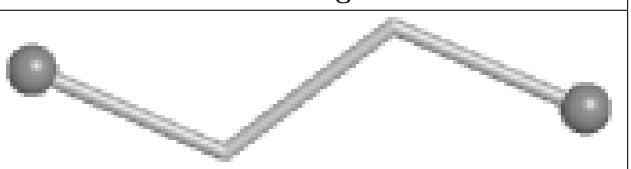
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand EDO BBB 510



Ligand EDO AAA 504



Ligand EDO BBB 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

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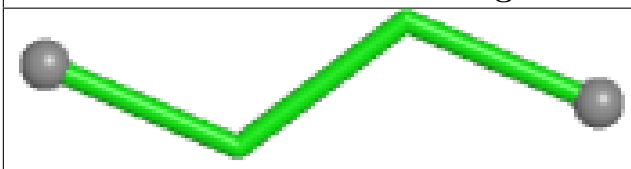
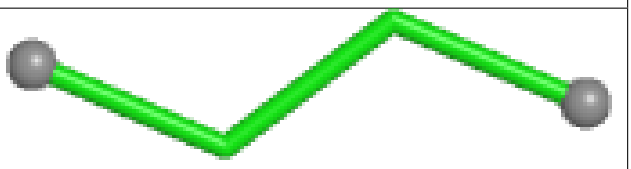
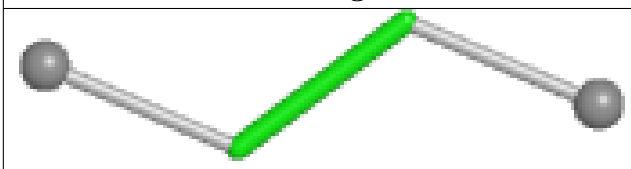
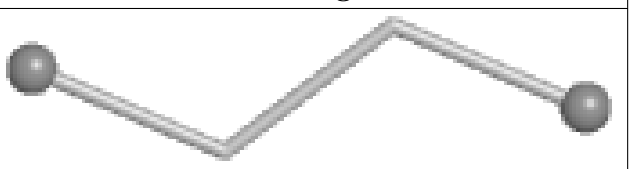
 Bond lengths	 Bond angles
 Torsions	 Rings

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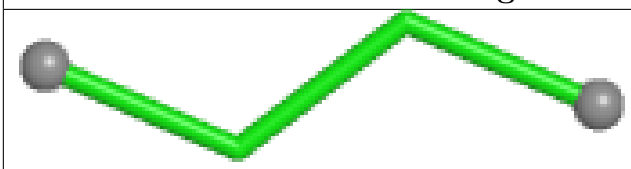
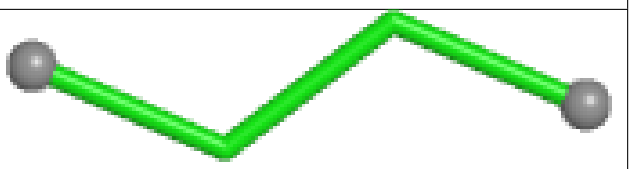
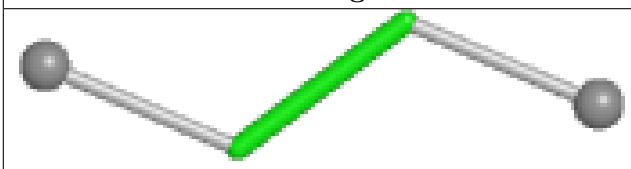
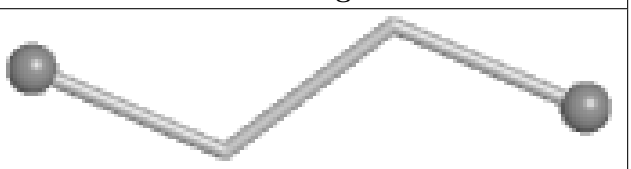
 Bond lengths	 Bond angles
 Torsions	 Rings

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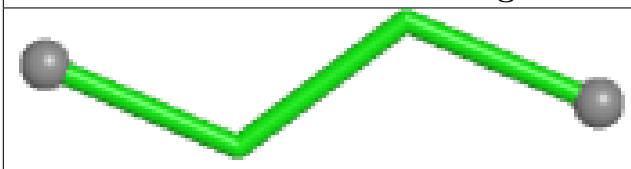
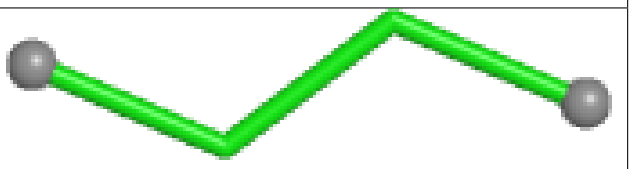
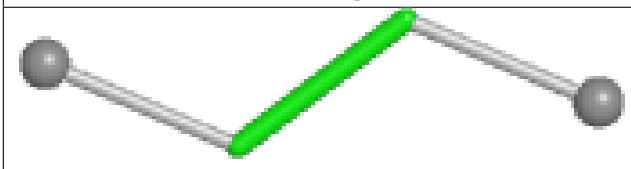
 Bond lengths	 Bond angles
 Torsions	 Rings

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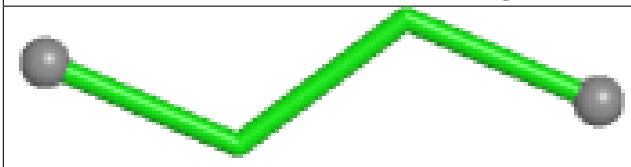
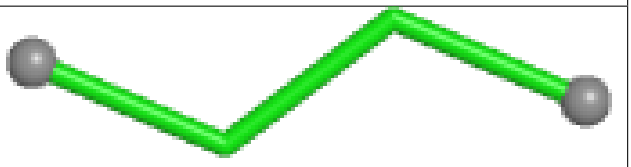
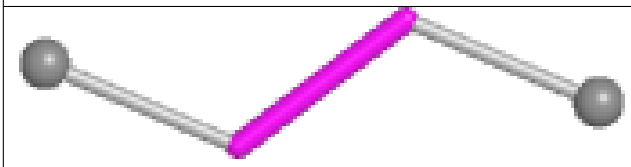
 Bond lengths	 Bond angles
 Torsions	 Rings

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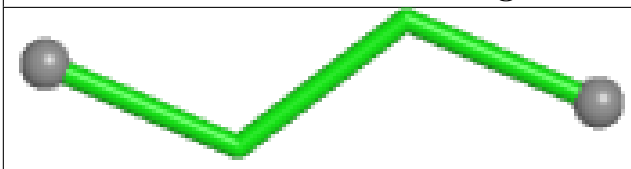
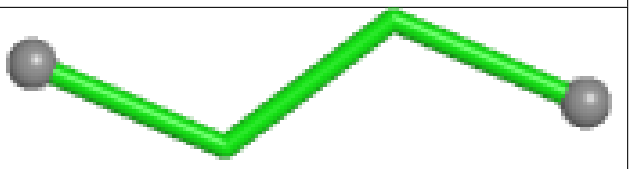
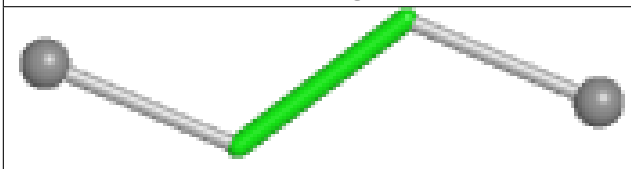
 Bond lengths	 Bond angles
 Torsions	 Rings

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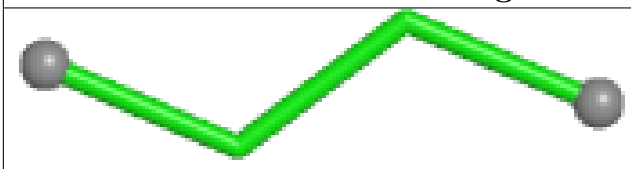
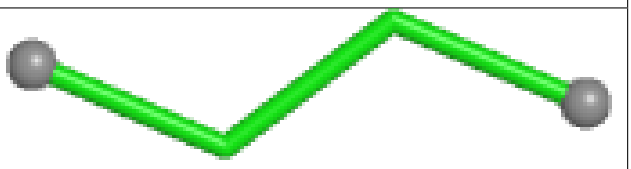
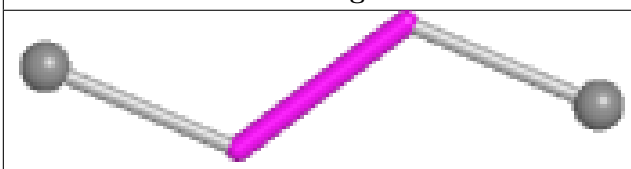
 Bond lengths	 Bond angles
 Torsions	 Rings

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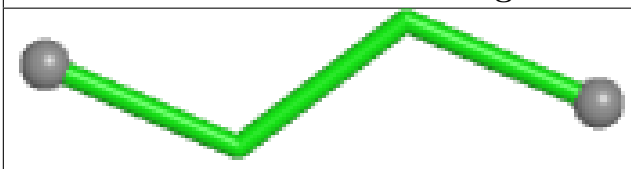
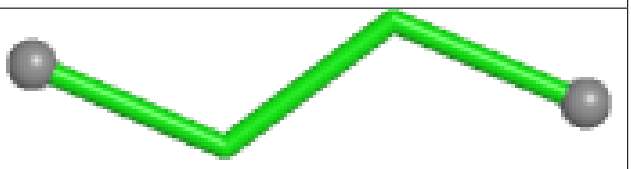
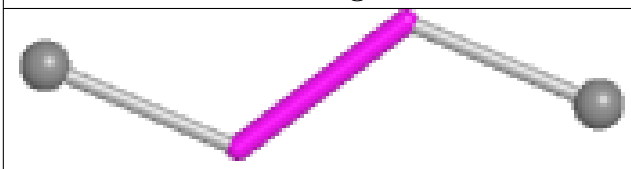
 Bond lengths	 Bond angles
 Torsions	 Rings

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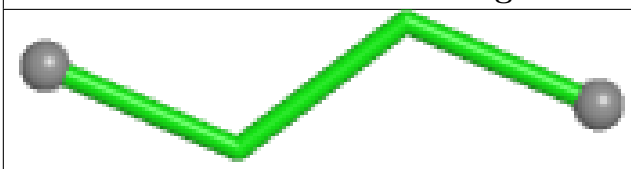
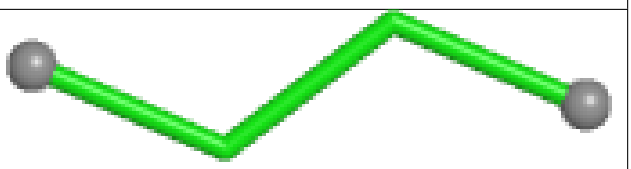
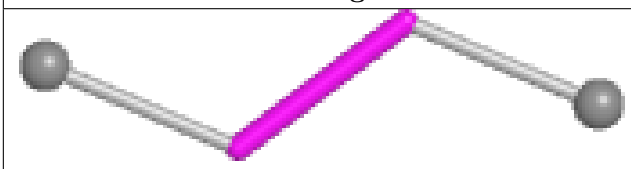
 Bond lengths	 Bond angles
 Torsions	 Rings

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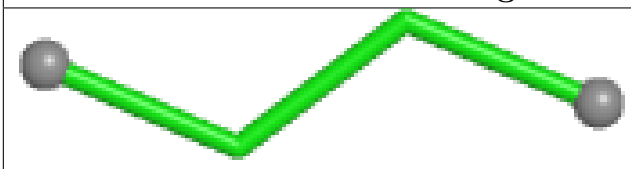
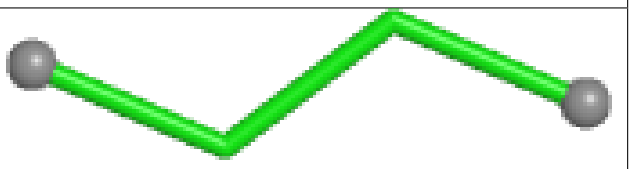
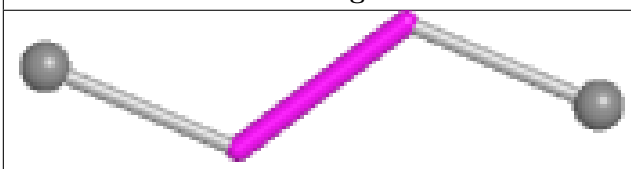
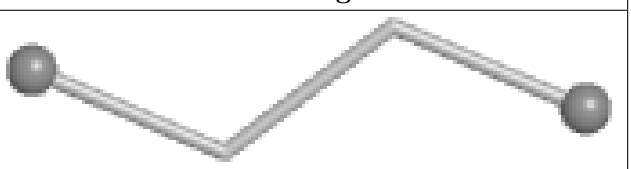
 Bond lengths	 Bond angles
 Torsions	 Rings

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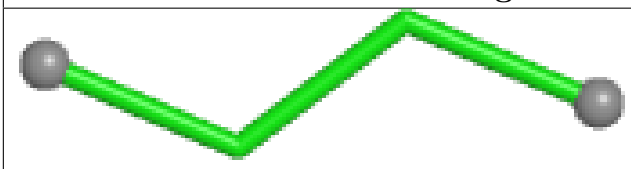
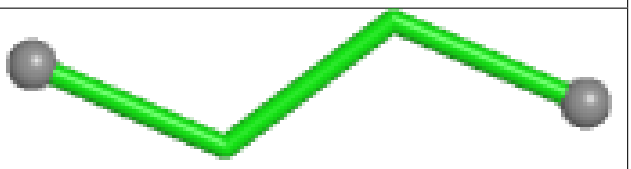
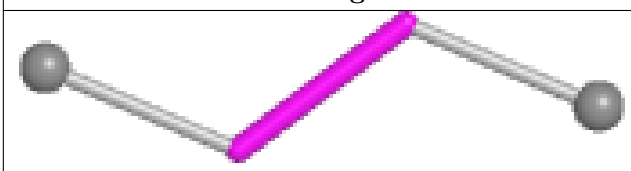
 Bond lengths	 Bond angles
 Torsions	 Rings

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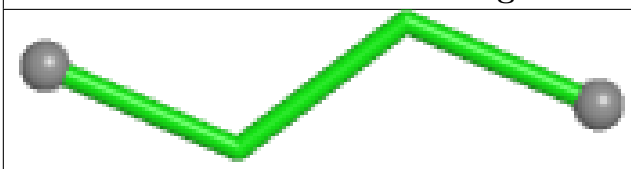
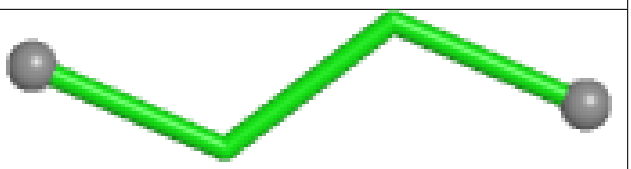
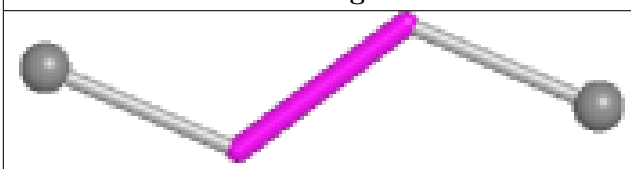
 Bond lengths	 Bond angles
 Torsions	 Rings

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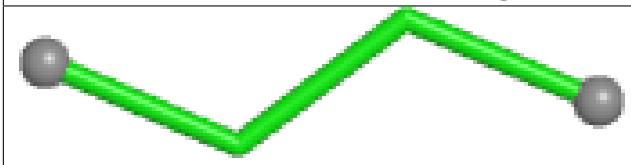
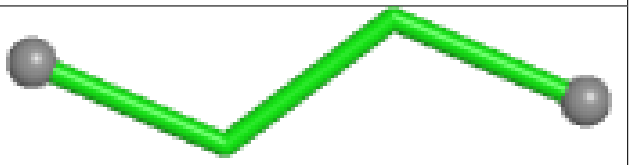
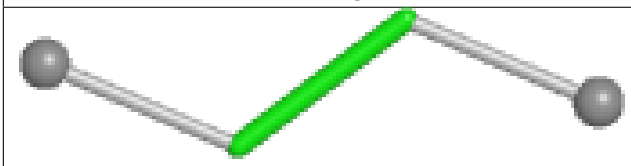
 Bond lengths	 Bond angles
 Torsions	 Rings

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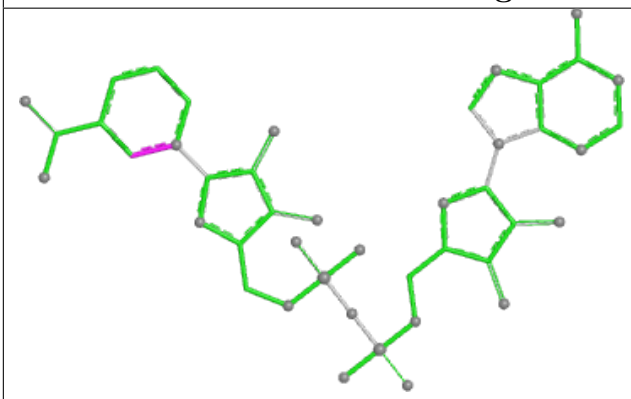
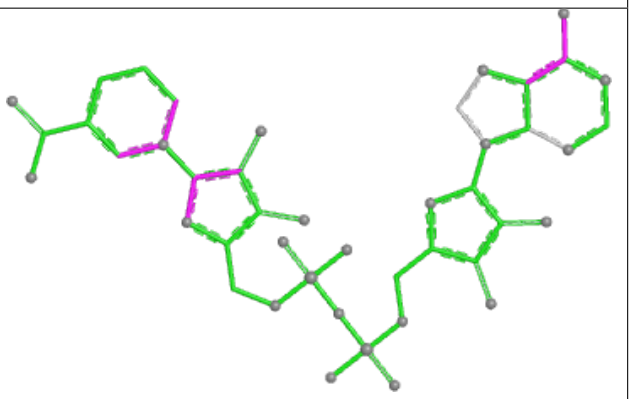
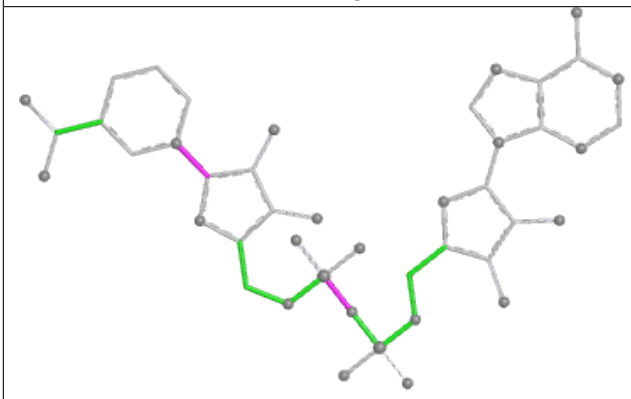
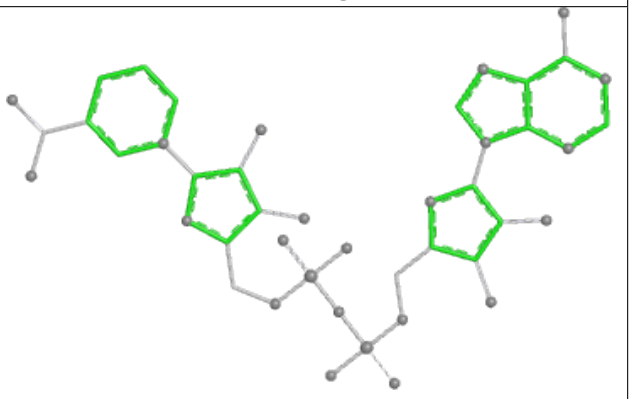
 Bond lengths	 Bond angles
 Torsions	 Rings

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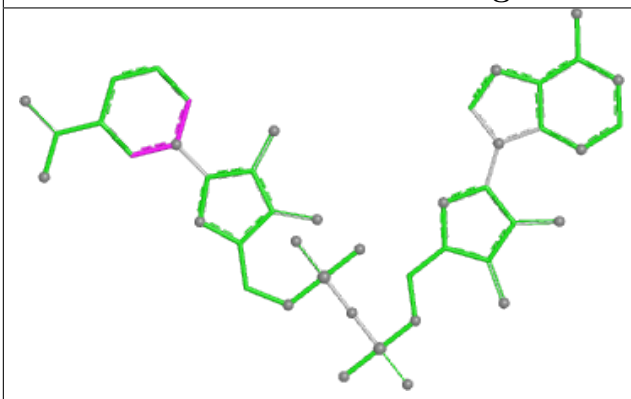

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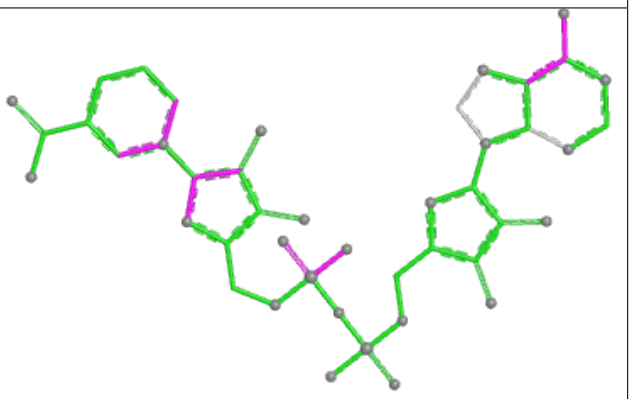

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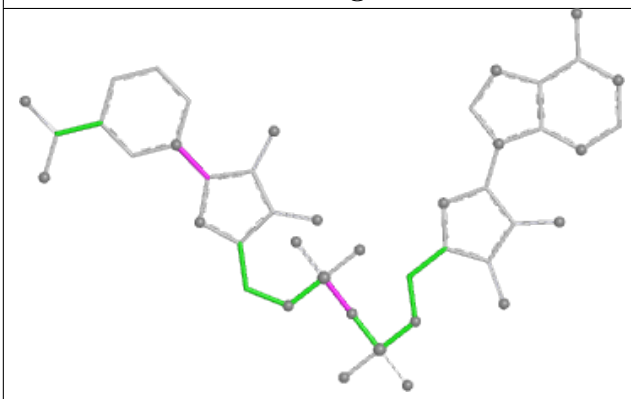

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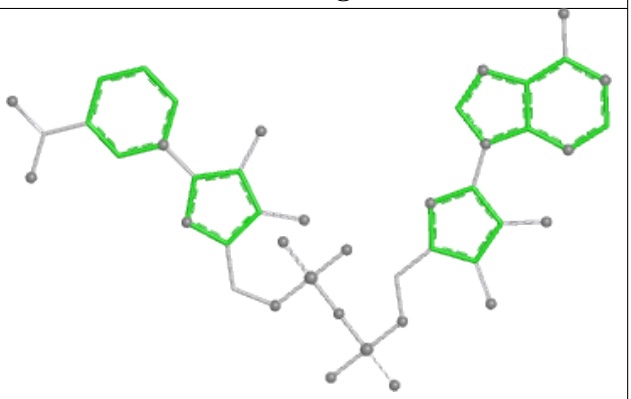
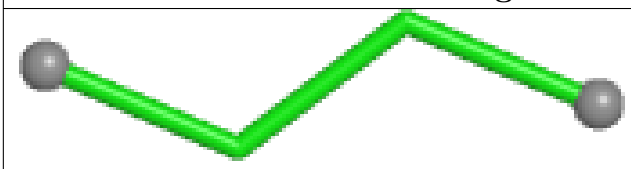


Rings

Ligand EDO AAA 503



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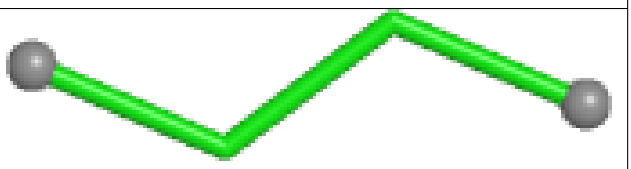

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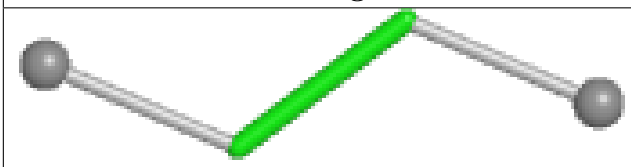
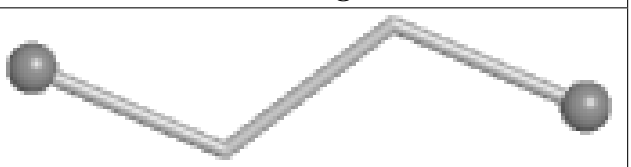
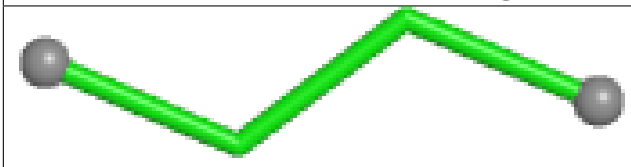
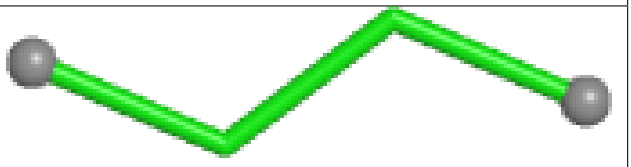
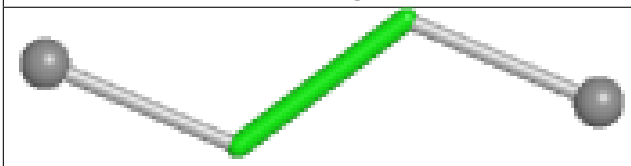


Torsions



Rings

Ligand EDO BBB 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	AAA	384/390 (98%)	-0.30	6 (1%)	72 71	11, 16, 27, 60	0
1	BBB	384/390 (98%)	-0.41	2 (0%)	91 90	10, 16, 27, 44	0
All	All	768/780 (98%)	-0.36	8 (1%)	82 82	10, 16, 27, 60	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	312	GLU	3.1
1	AAA	386	HIS	2.9
1	BBB	312	GLU	2.8
1	BBB	313	GLY	2.8
1	AAA	313	GLY	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

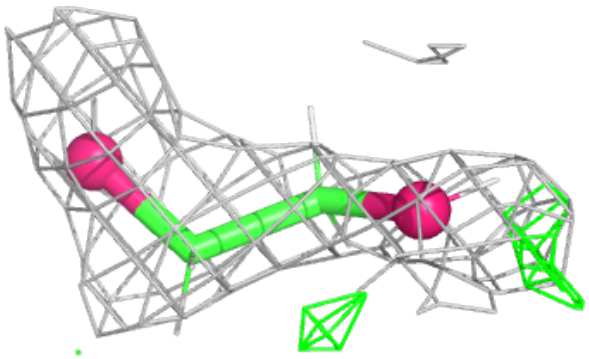
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

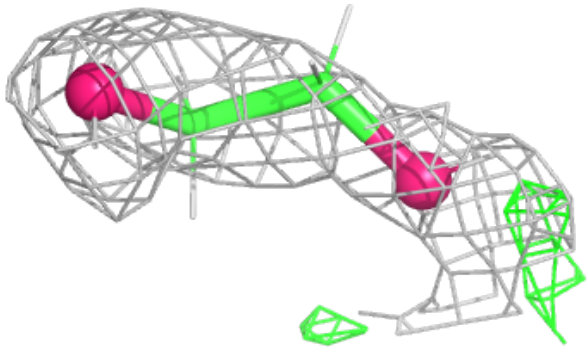
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	AAA	510	4/4	0.57	0.20	42,45,49,50	1
3	EDO	BBB	503	4/4	0.69	0.20	27,27,33,33	1
3	EDO	BBB	509	4/4	0.72	0.20	33,35,38,39	1
3	EDO	BBB	507	4/4	0.74	0.20	28,30,31,32	1
3	EDO	AAA	507	4/4	0.75	0.20	25,26,27,28	1
3	EDO	AAA	509	4/4	0.77	0.30	42,43,45,45	1
3	EDO	BBB	506	4/4	0.79	0.18	40,42,43,44	1
3	EDO	AAA	508	4/4	0.81	0.14	48,48,49,50	1
3	EDO	BBB	511	4/4	0.83	0.17	20,42,44,45	1
3	EDO	AAA	503	4/4	0.87	0.14	31,33,38,39	1
3	EDO	BBB	510	4/4	0.87	0.09	27,29,36,36	1
3	EDO	AAA	502	4/4	0.87	0.15	20,21,22,22	1
3	EDO	AAA	504	4/4	0.90	0.18	29,31,35,35	1
3	EDO	AAA	506	4/4	0.90	0.21	35,37,38,38	1
3	EDO	BBB	504	4/4	0.91	0.18	24,31,36,36	1
3	EDO	BBB	505	4/4	0.92	0.16	18,21,24,24	1
2	NAD	AAA	501	44/44	0.97	0.08	12,14,23,27	6
3	EDO	BBB	502	4/4	0.97	0.09	16,17,18,18	1
2	NAD	BBB	501	44/44	0.98	0.06	12,14,18,21	6
4	FE	AAA	505	1/1	0.98	0.06	18,18,18,18	0
4	FE	BBB	508	1/1	0.99	0.04	21,21,21,21	0

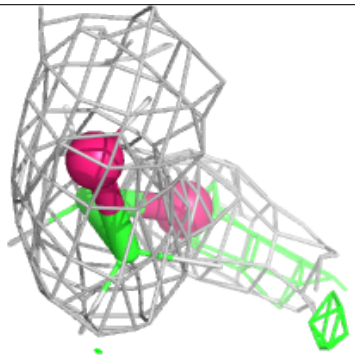
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDO AAA 510:

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

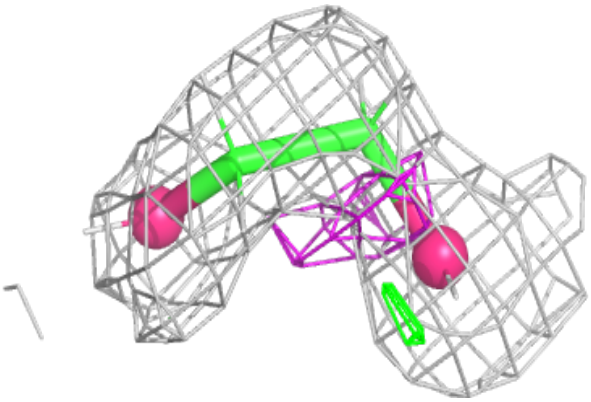


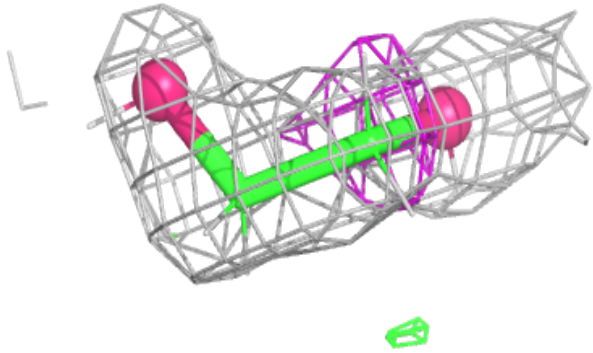


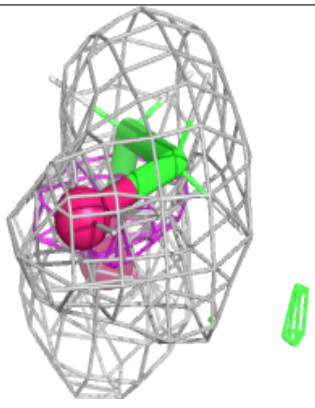


Electron density around EDO BBB 503:

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

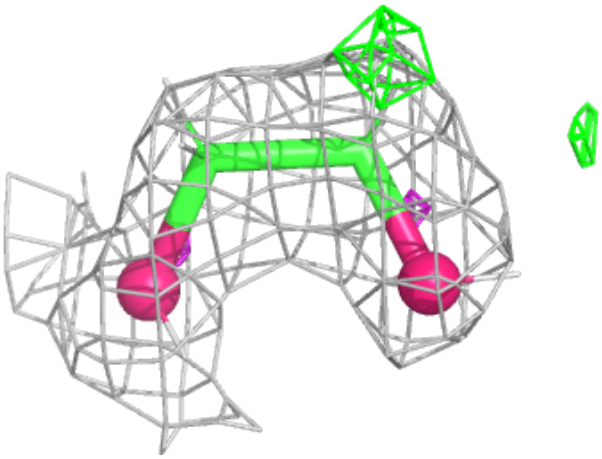


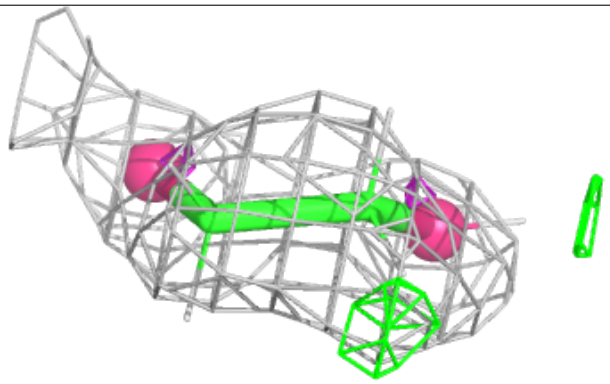


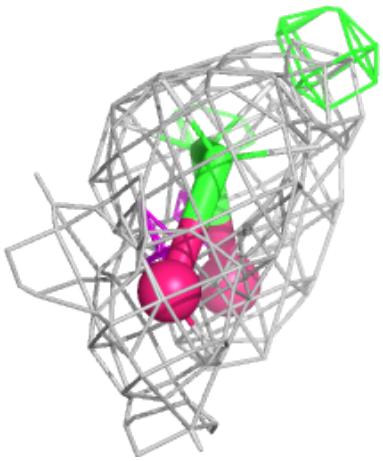


Electron density around EDO BBB 509:

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

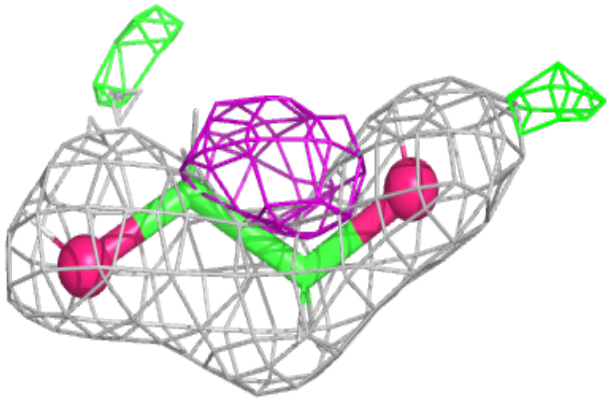


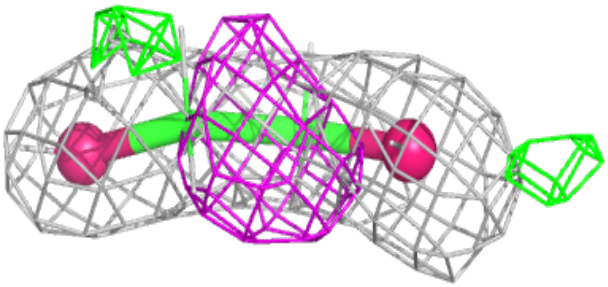


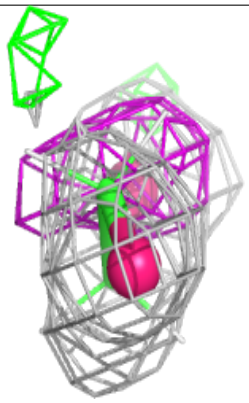


Electron density around EDO BBB 507:

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

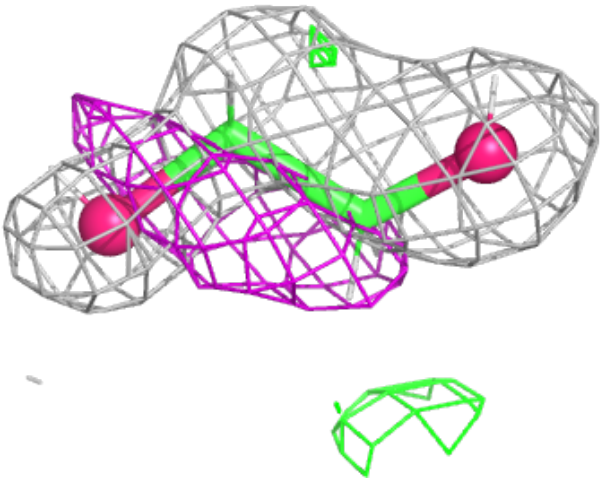


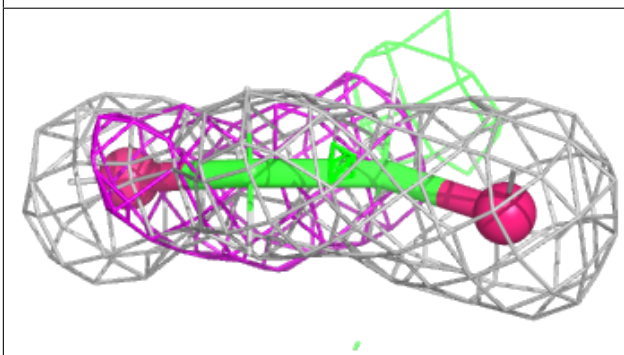


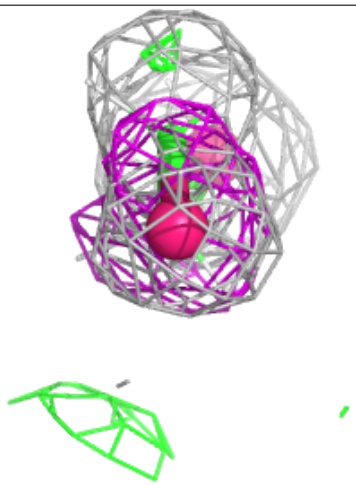


Electron density around EDO AAA 507:

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

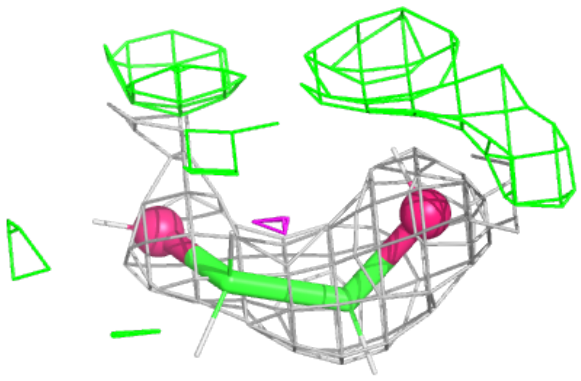


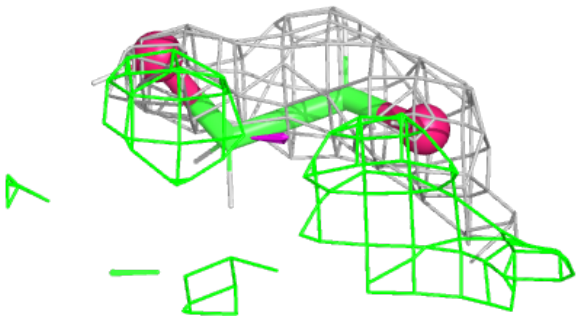


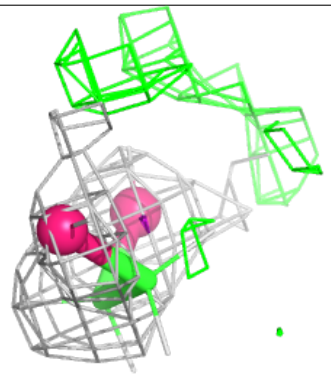


Electron density around EDO AAA 509:

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

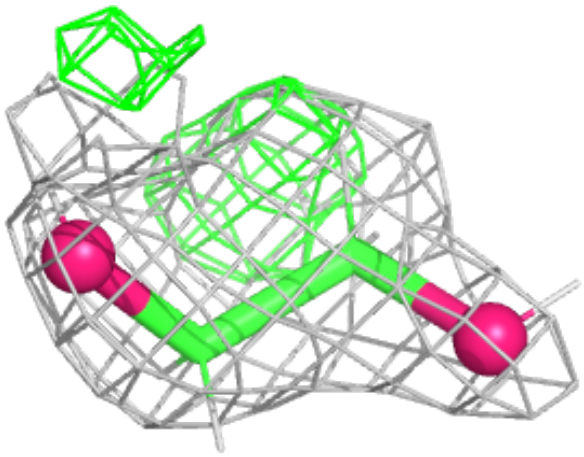


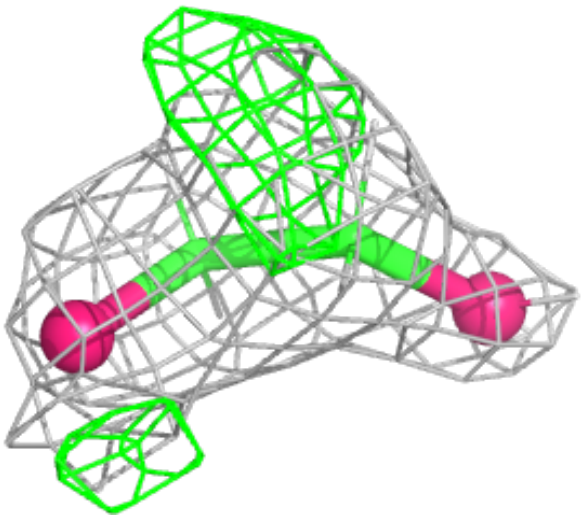


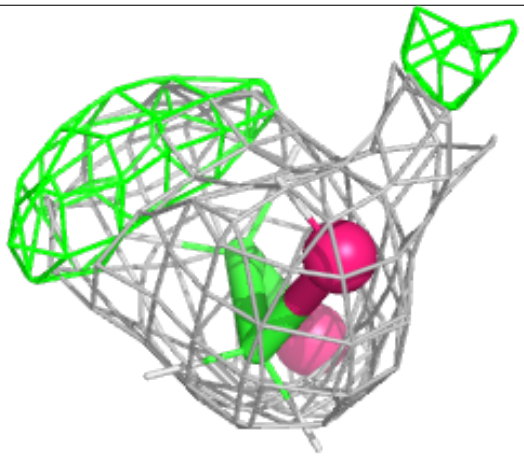


Electron density around EDO BBB 506:

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

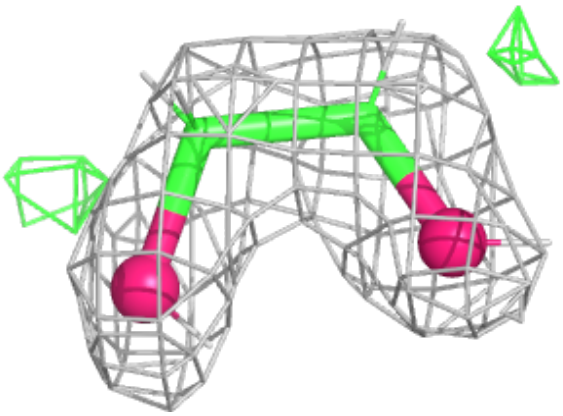


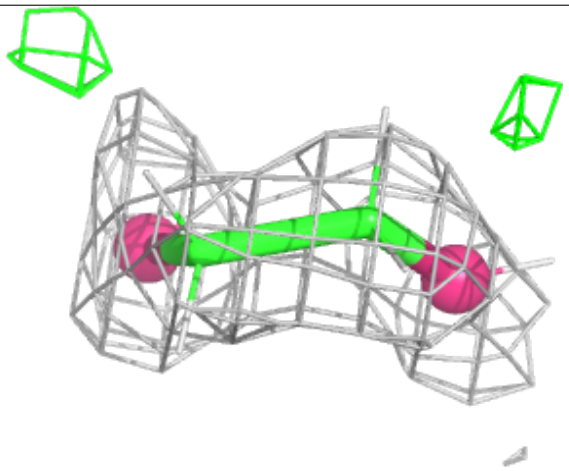


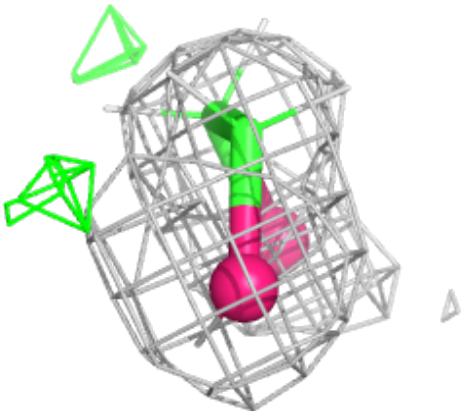


Electron density around EDO AAA 508:

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

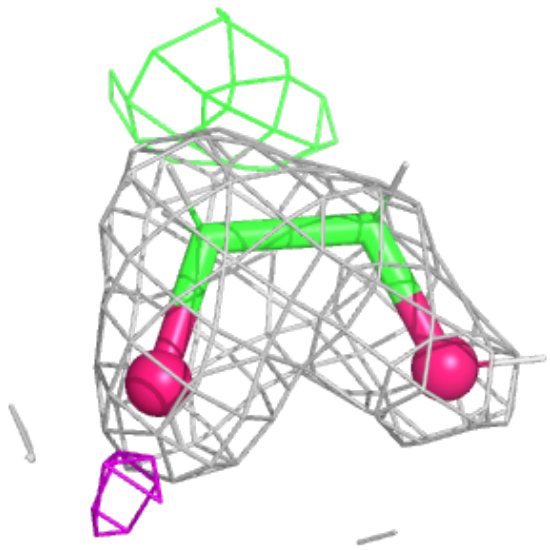


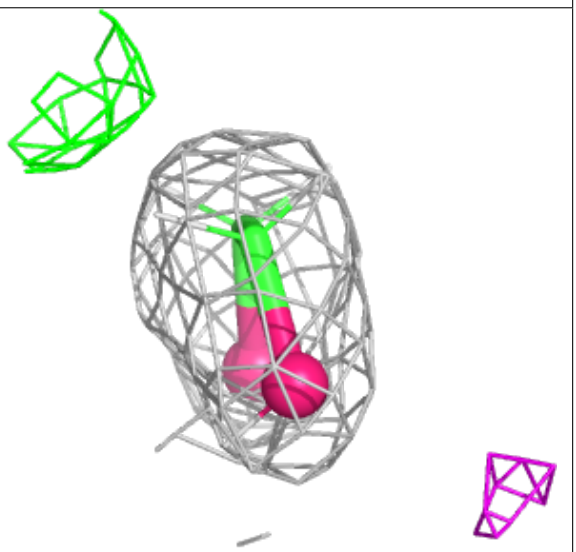




Electron density around EDO BBB 511:

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





Electron density around EDO AAA 503:

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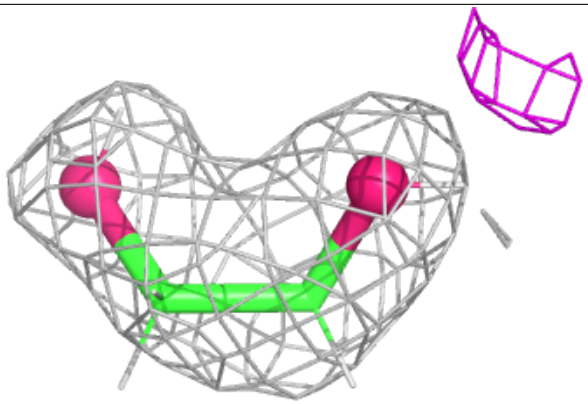
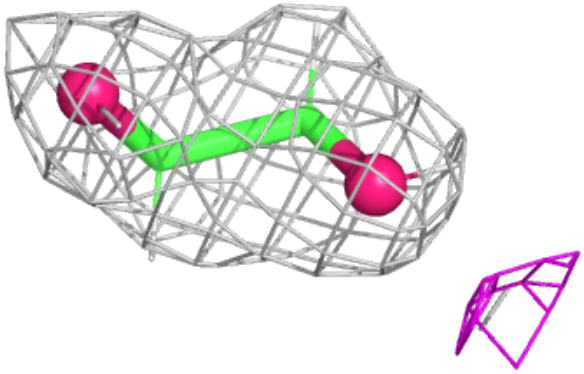
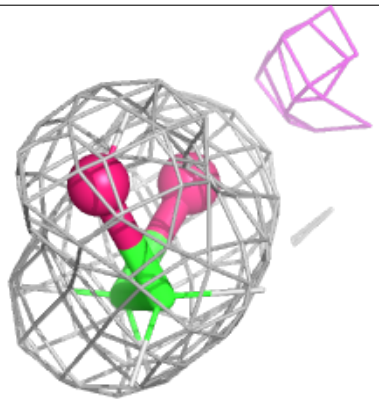
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

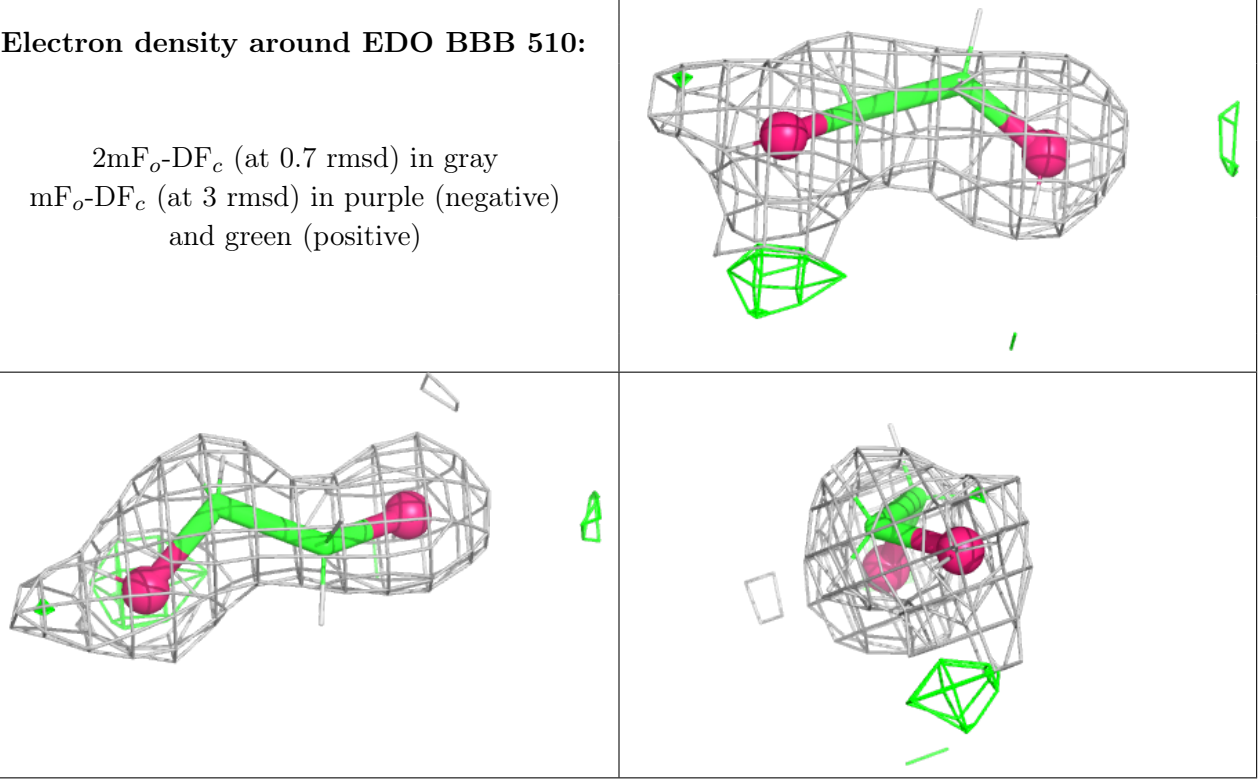






Electron density around EDO BBB 510:

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



Electron density around EDO AAA 502:

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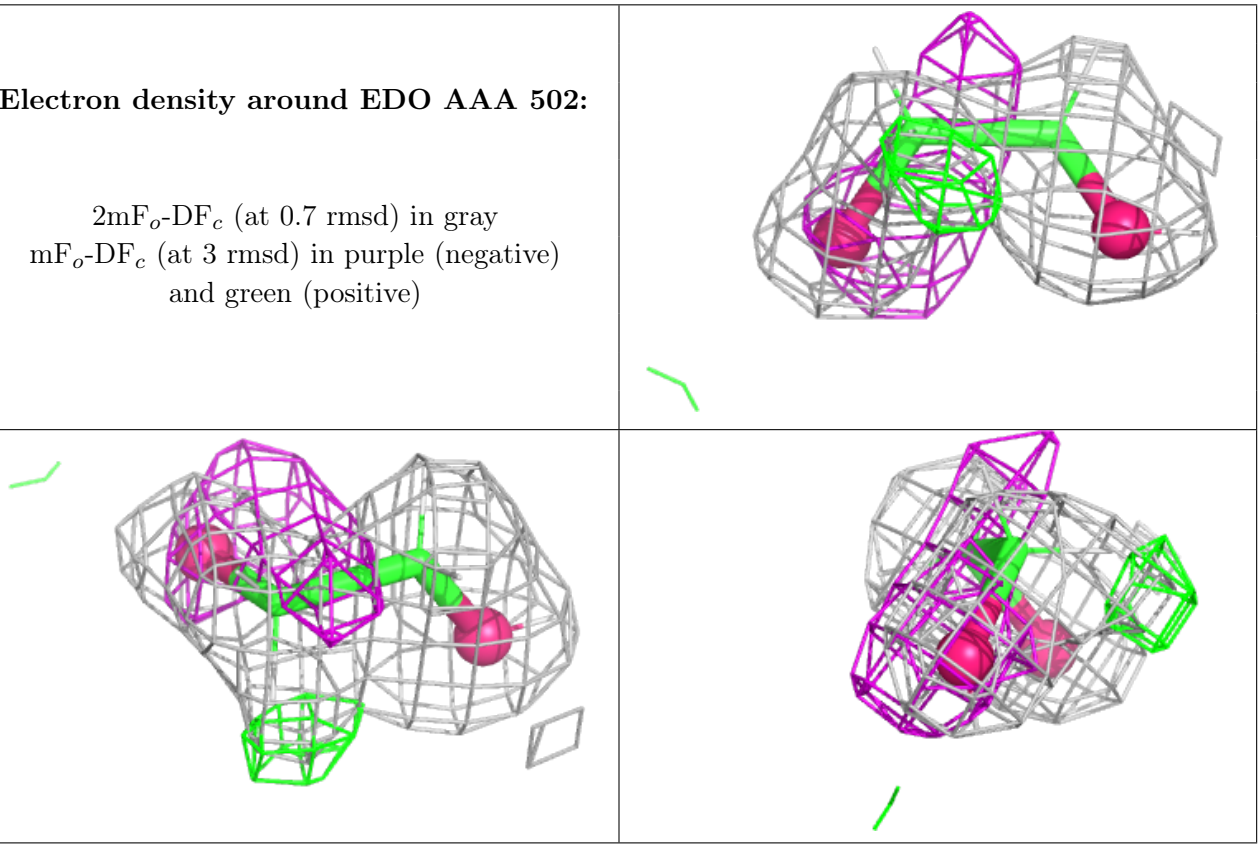
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EDO AAA 504:

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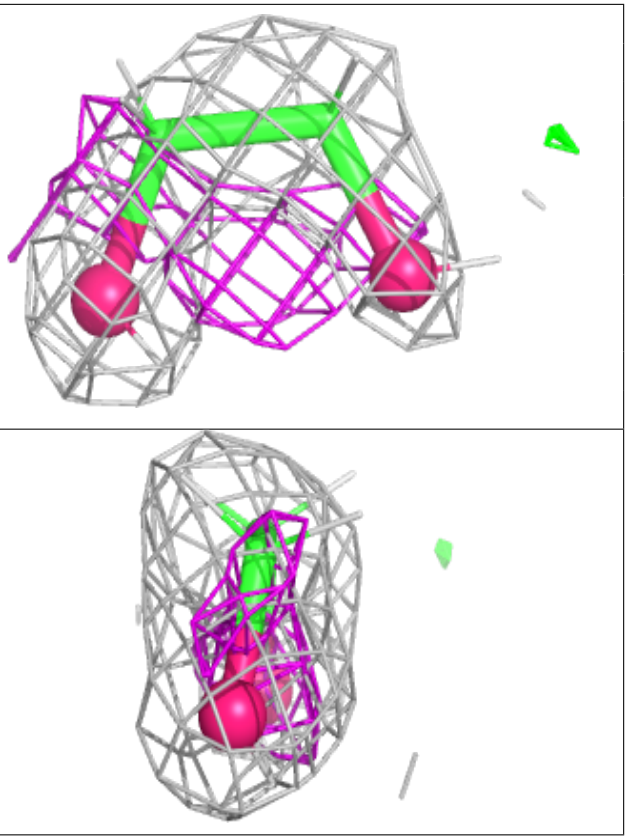
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EDO AAA 506:

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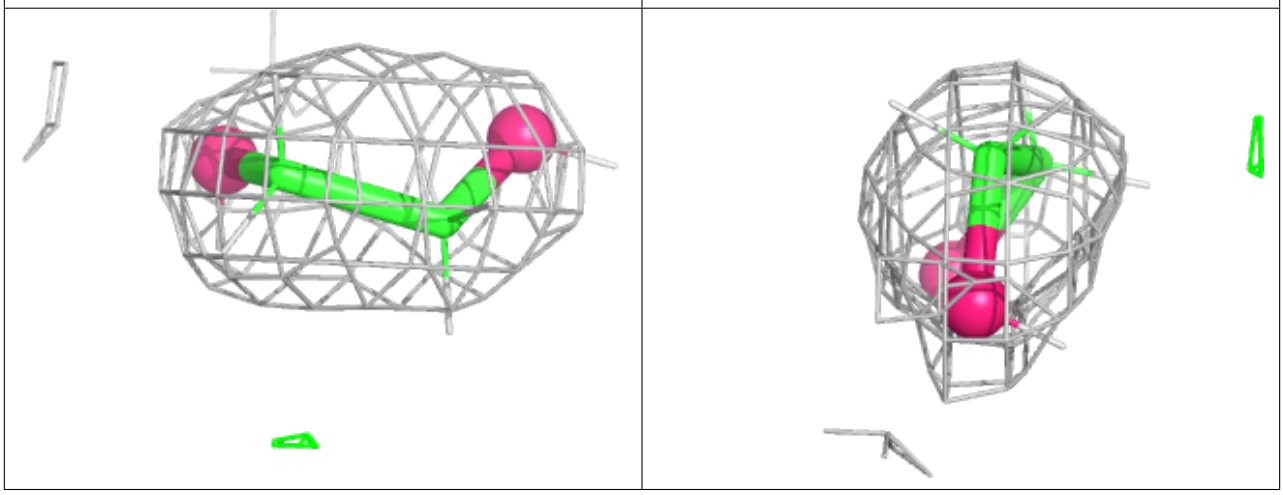
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EDO BBB 504:

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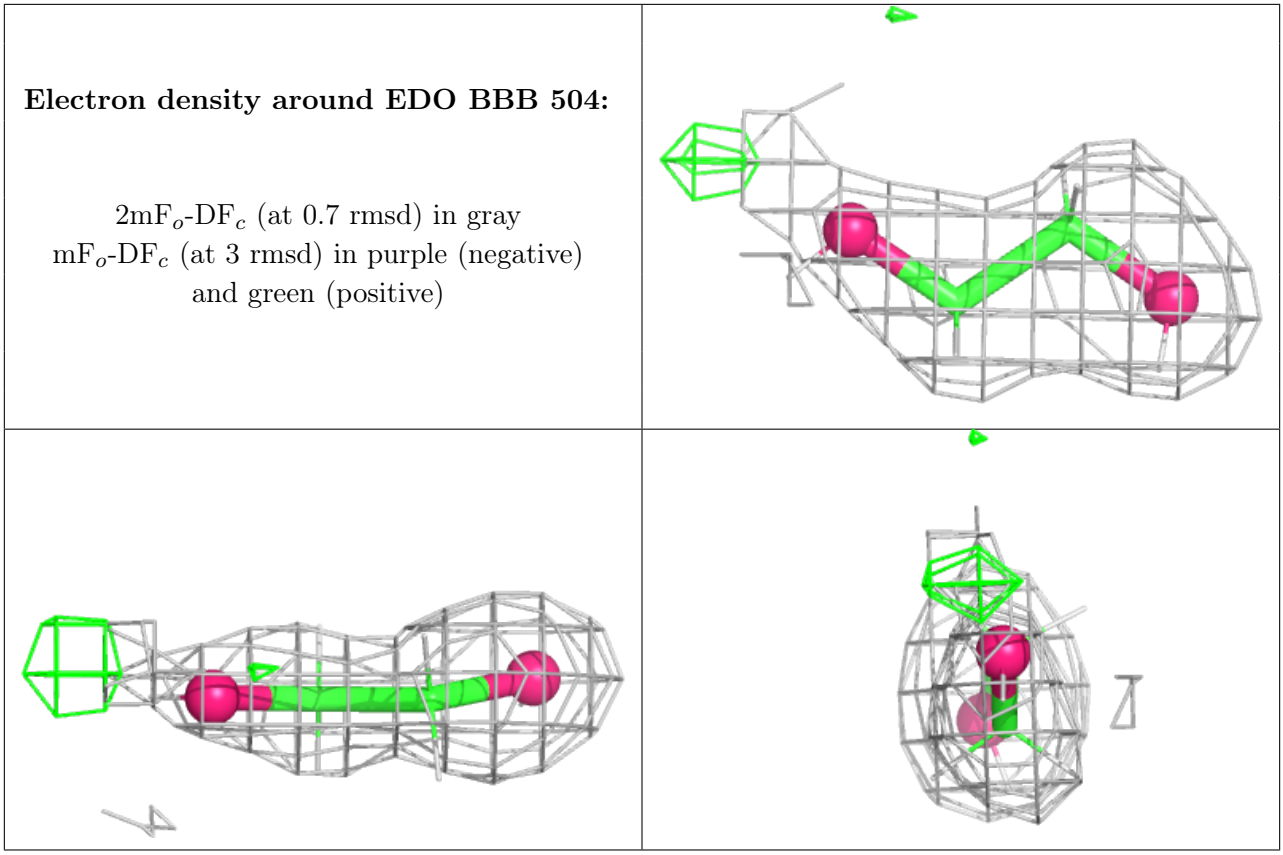
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EDO BBB 505:

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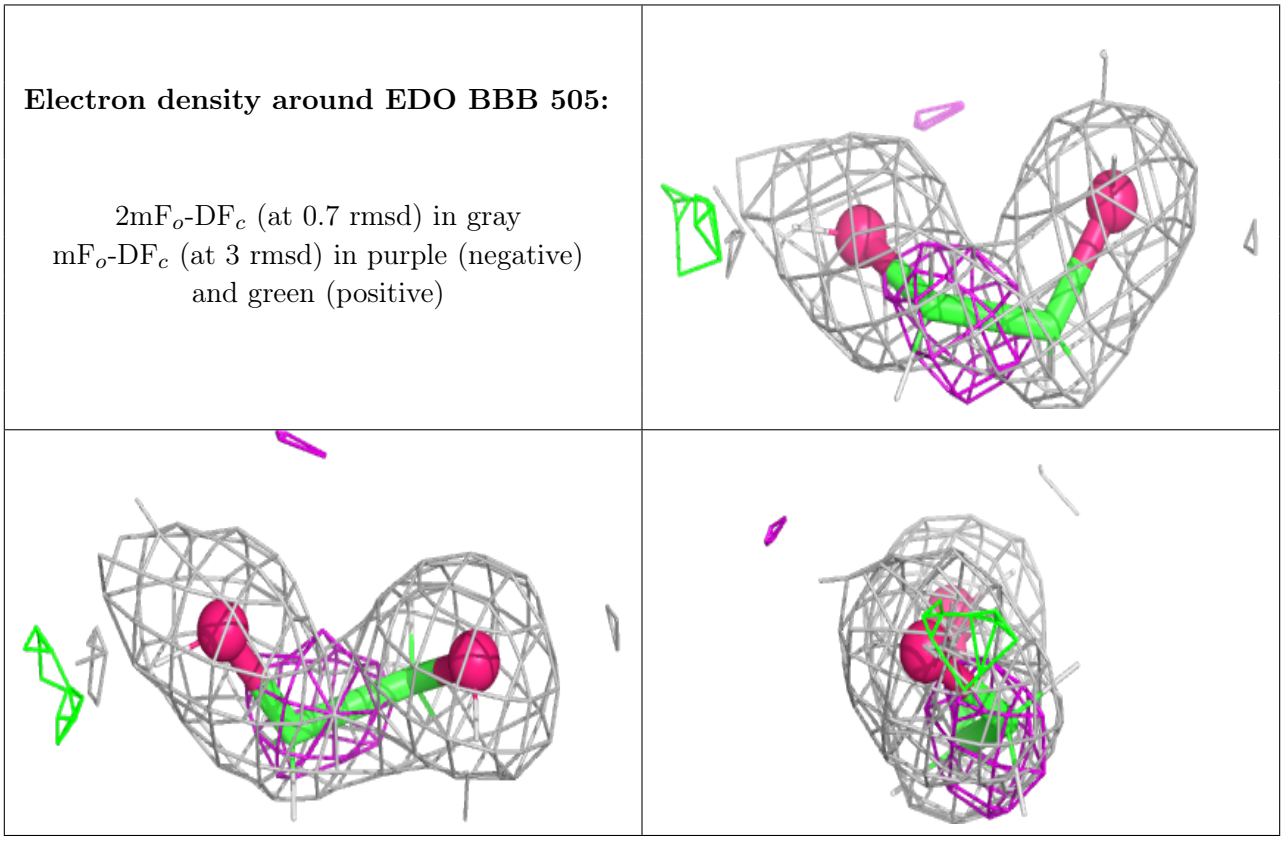
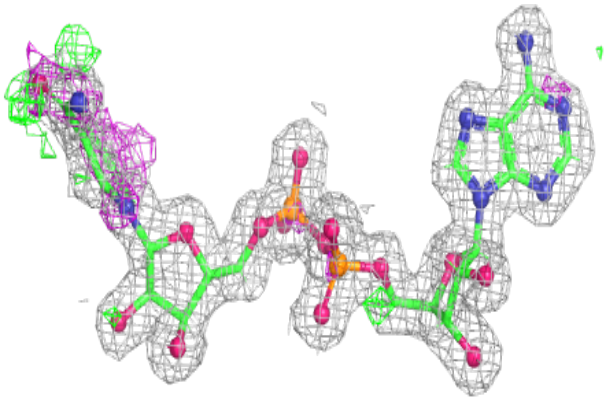
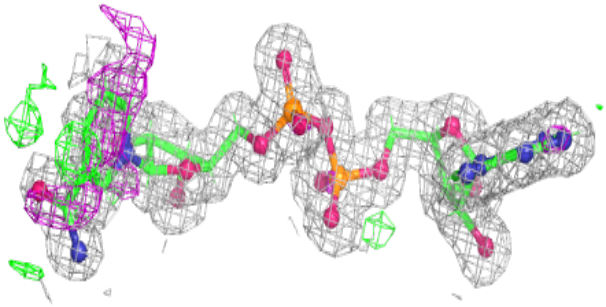
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

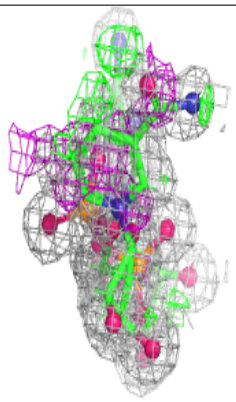


Electron density around NAD AAA 501:

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

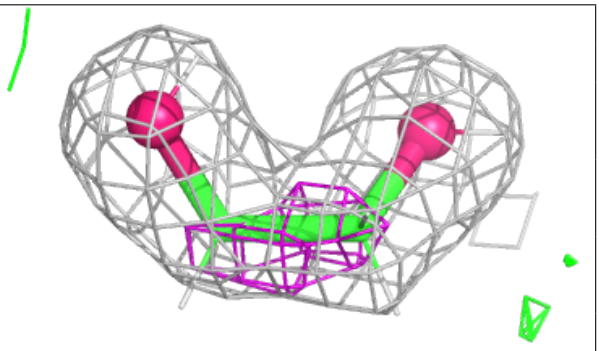


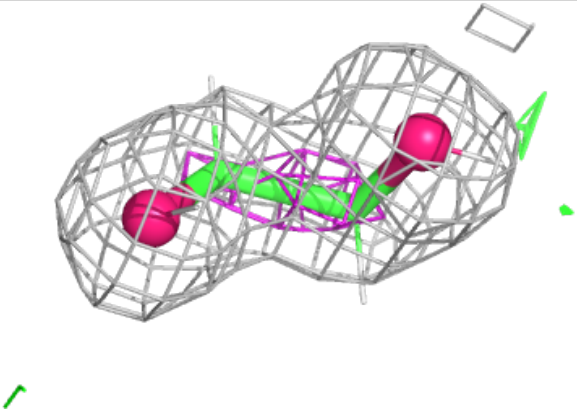


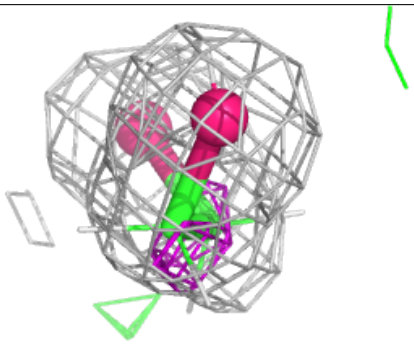


Electron density around EDO BBB 502:

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

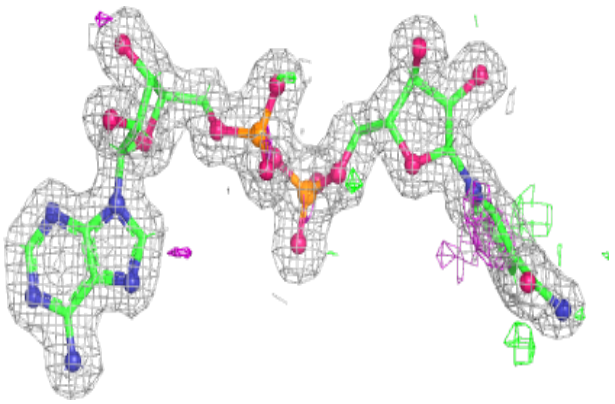


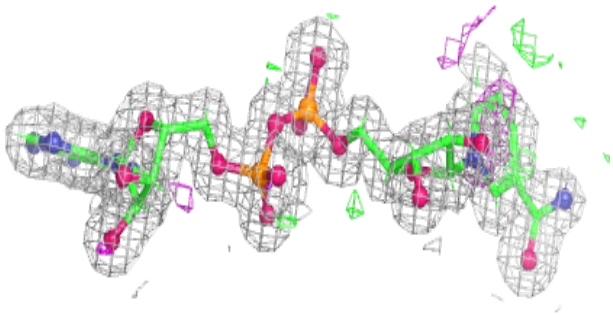


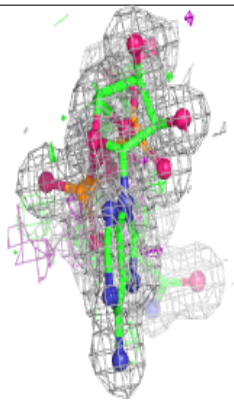


Electron density around NAD BBB 501:

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

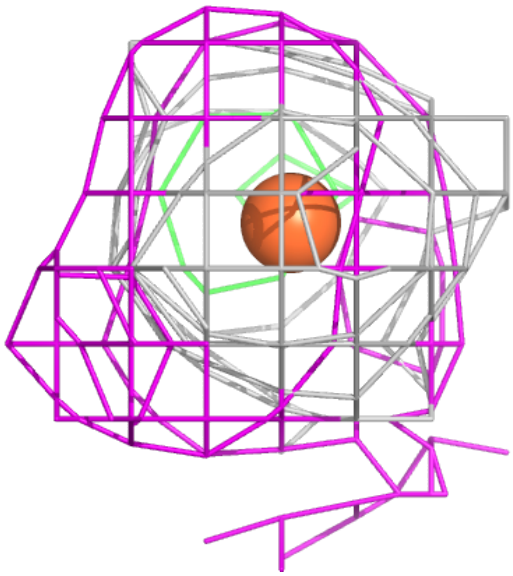


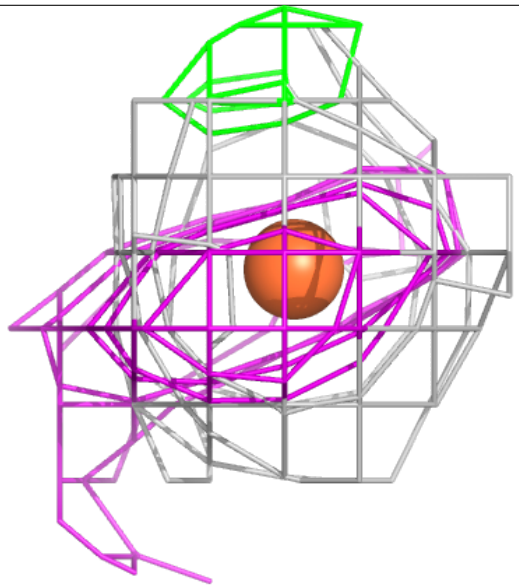


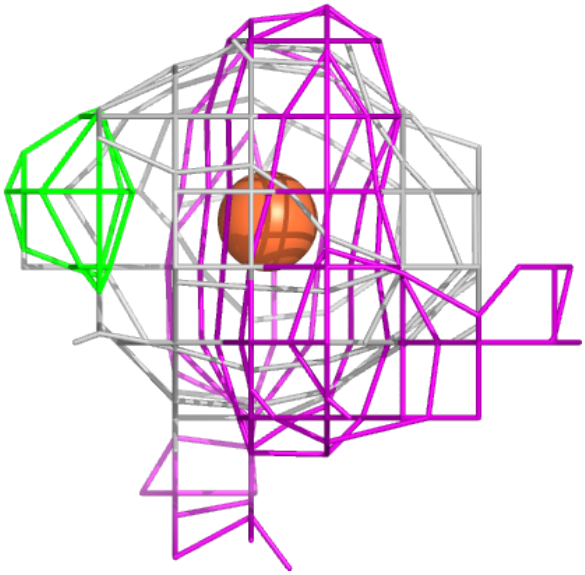


Electron density around FE AAA 505:

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

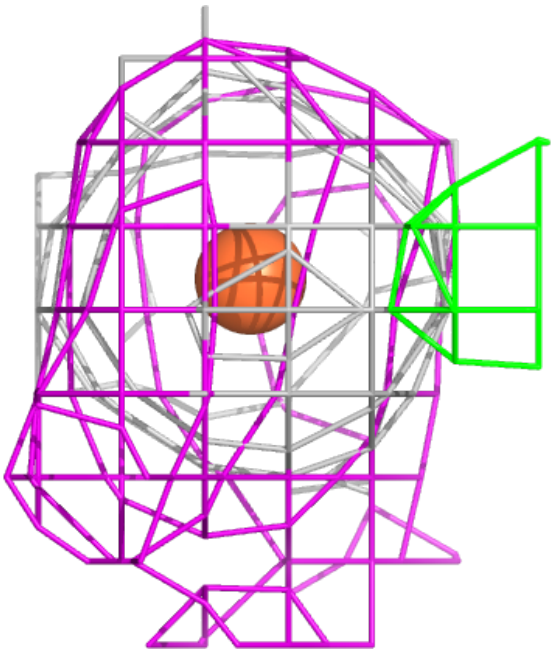


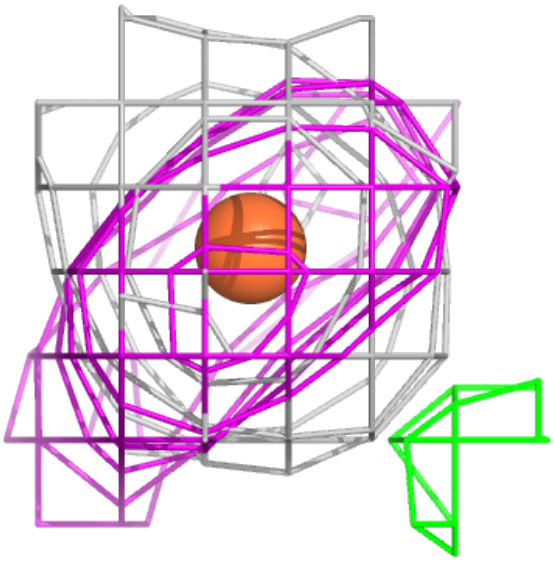


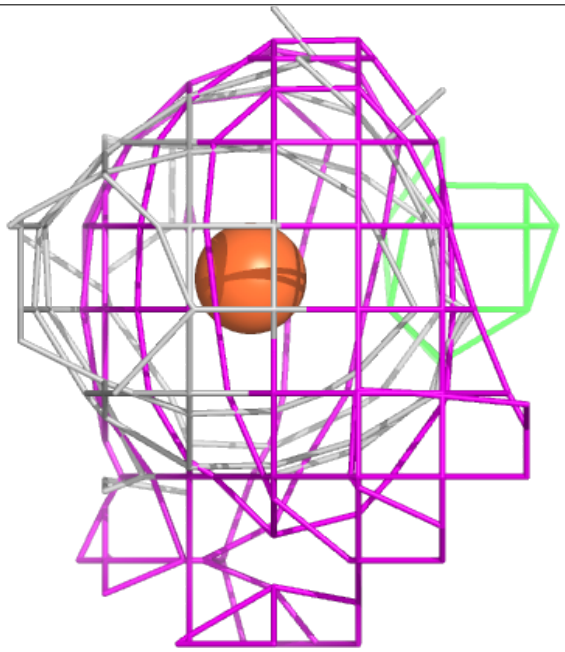


Electron density around FE BBB 508:

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







6.5 Other polymers

There are no such residues in this entry.