



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:13 AM UTC

PDB ID : 8UX6 / pdb_00008ux6
Title : Structure of Fab201 with a T. parva sporozoite neutralizing B cell epitope of p67
Authors : Singer, A.U.; Gopalsamy, A.; Fellouse, F.A.; Miersch, S.; Sidhu, S.S.
Deposited on : 2023-11-08
Resolution : 2.00 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

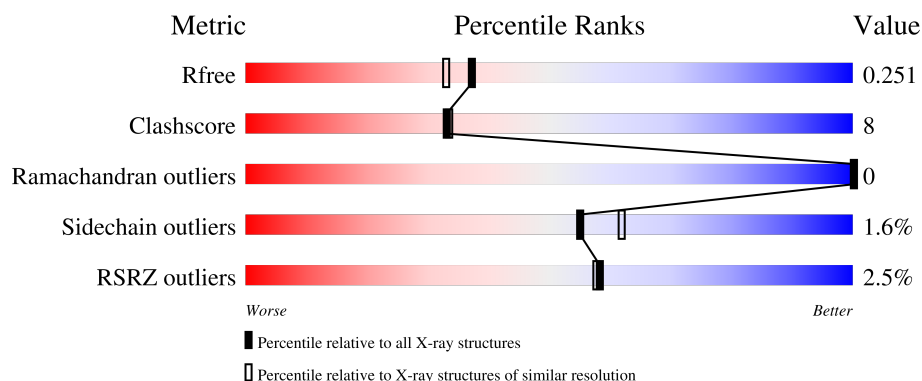
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	216	5% 79% 18% ..
1	C	216	2% 82% 17% .
2	B	221	2% 82% 12% 5%
2	D	221	% 84% 11% 5%
3	E	41	2% 46% 51% .

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Mol	Chain	Length	Quality of chain
3	F	41	 A horizontal bar chart showing the quality of chain F. The bar is divided into two segments: a green segment on the left representing 46% and a grey segment on the right representing 51%. A small yellow dot is located at the boundary between the two segments, slightly to the right of the 46% mark. 46% . 51%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7202 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 Fab201 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	213	Total	C	N	O	S	0	3	0
			1624	1018	267	334	5			
1	A	211	Total	C	N	O	S	0	3	0
			1556	980	255	316	5			

- Molecule 2 is a protein called Fab201 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	2	0
			1550	976	257	311	6			
2	D	211	Total	C	N	O	S	0	1	0
			1545	975	255	309	6			

- Molecule 3 is a protein called p67 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	0	0	0
			138	87	20	31			
3	F	20	Total	C	N	O	0	0	0
			143	91	21	31			

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



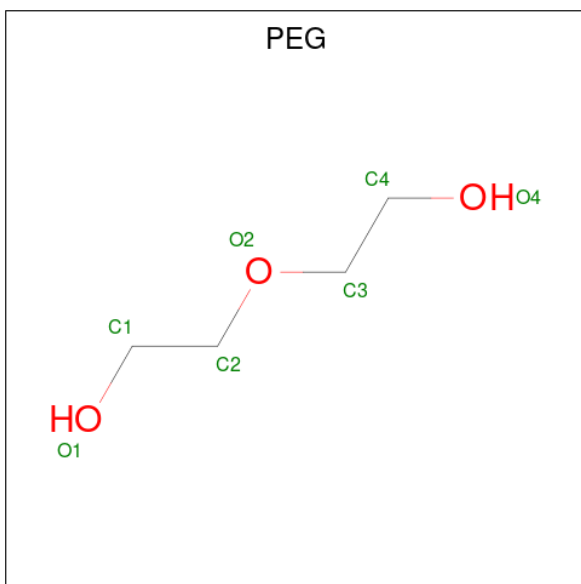
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	1
			8	4	4		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 14 8 6	0	1
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Na 1 1	0	0
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	D	3	Total Na 3 3	0	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	2	Total Ca 2 2	0	0
8	A	1	Total Ca 1 1	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0

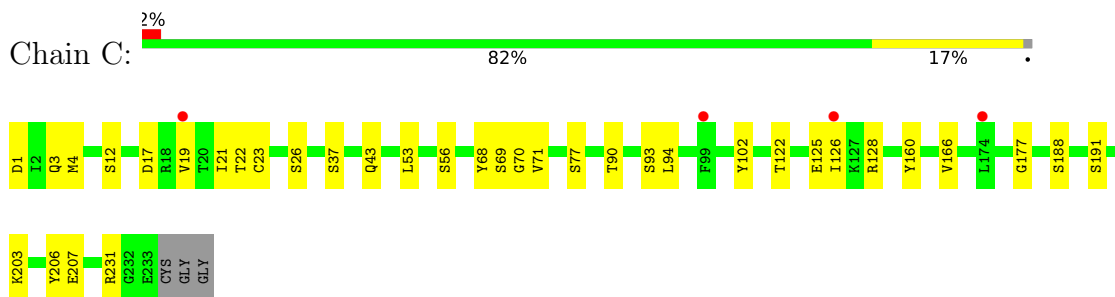
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	110	Total 113	O 113	0	3
10	A	75	Total 77	O 77	0	2
10	B	135	Total 137	O 137	0	2
10	D	139	Total 142	O 142	0	3
10	E	11	Total 11	O 11	0	0
10	F	17	Total 18	O 18	0	1

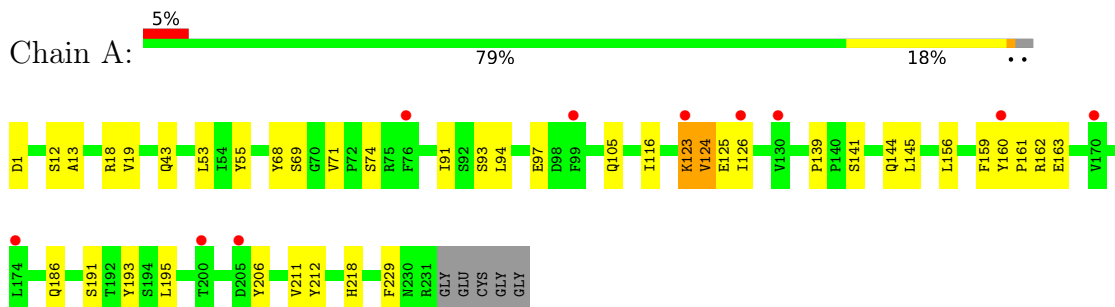
3 Residue-property plots [i](#)

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.

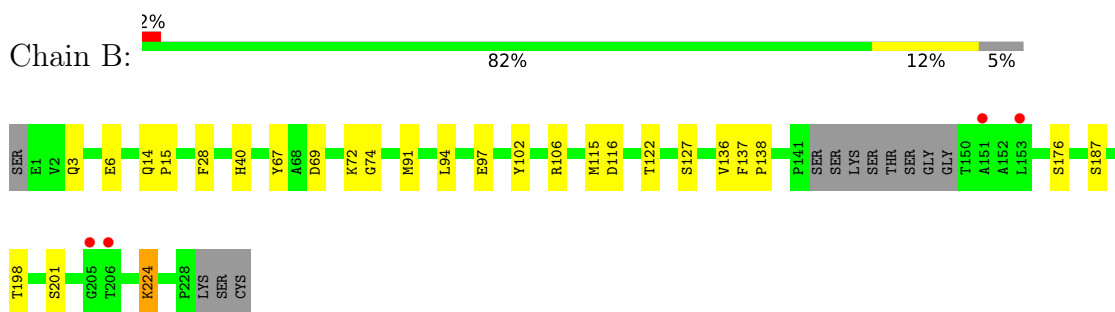
- Molecule 1: Fab201 light chain



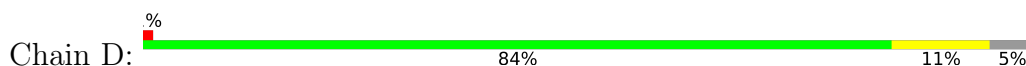
- Molecule 1: Fab201 light chain

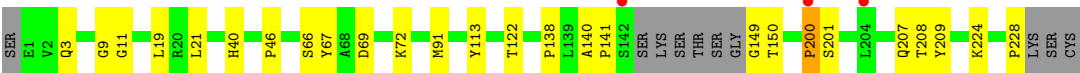


- Molecule 2: Fab201 heavy chain



- Molecule 2: Fab201 heavy chain





• Molecule 3: p67 protein



• Molecule 3: p67 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.01Å 75.56Å 90.59Å 69.26° 77.60° 76.08°	Depositor
Resolution (Å)	19.52 – 2.00 19.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.3 (19.52-2.00) 87.2 (19.52-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.204 , 0.251 0.204 , 0.251	Depositor DCC
R_{free} test set	2012 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7202	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9148e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EPE, CL, PEG, EDO, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/1590	0.49	0/2174
1	C	0.33	0/1660	0.54	0/2260
2	B	0.36	0/1588	0.50	0/2172
2	D	0.42	0/1583	0.61	1/2167 (0.0%)
3	E	0.30	0/137	0.44	0/186
3	F	0.31	0/142	0.51	0/191
All	All	0.35	0/6700	0.53	1/9150 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	200	PRO	N-CD-CG	-9.10	89.54	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1556	0	1424	33	0
1	C	1624	0	1530	29	0
2	B	1550	0	1484	18	0
2	D	1545	0	1467	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	138	0	120	1	0
3	F	143	0	136	3	0
4	A	12	0	18	0	0
4	B	8	0	12	3	0
4	C	20	0	30	1	0
4	D	12	0	18	0	0
5	A	15	0	17	2	0
5	C	15	0	17	2	0
6	A	7	0	10	0	0
6	B	14	0	18	0	0
6	C	7	0	10	0	0
6	D	28	0	40	7	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	3	0	0	0	0
8	A	1	0	0	0	0
8	C	2	0	0	0	0
9	B	1	0	0	0	0
10	A	77	0	0	3	0
10	B	137	0	0	4	0
10	C	113	0	0	8	0
10	D	142	0	0	3	0
10	E	11	0	0	0	0
10	F	18	0	0	2	0
All	All	7202	0	6351	102	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 8.

The worst 5 of 102 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:D:69[B]:ASP:HA	2:D:72:LYS:HD2	1.41	1.03
2:D:69[A]:ASP:HA	2:D:72:LYS:HD2	1.53	0.89
2:B:69:ASP:HA	2:B:72:LYS:HE3	1.56	0.85
1:C:1:ASP:HB2	5:C:302:EPE:H92	1.62	0.80
2:B:3:GLN:HG2	10:B:485:HOH:O	1.86	0.76

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	212/216 (98%)	207 (98%)	5 (2%)	0	100	100
1	C	214/216 (99%)	206 (96%)	8 (4%)	0	100	100
2	B	207/221 (94%)	202 (98%)	5 (2%)	0	100	100
2	D	208/221 (94%)	204 (98%)	4 (2%)	0	100	100
3	E	18/41 (44%)	18 (100%)	0	0	100	100
3	F	18/41 (44%)	18 (100%)	0	0	100	100
All	All	877/956 (92%)	855 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/188 (85%)	155 (97%)	5 (3%)	35	37
1	C	179/188 (95%)	178 (99%)	1 (1%)	78	85
2	B	171/183 (93%)	166 (97%)	5 (3%)	37	40
2	D	167/183 (91%)	166 (99%)	1 (1%)	78	85
3	E	13/33 (39%)	13 (100%)	0	100	100
3	F	14/33 (42%)	14 (100%)	0	100	100
All	All	704/808 (87%)	692 (98%)	12 (2%)	55	60

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	187	SER
2	B	198	THR
2	D	208	THR
2	B	201	SER
1	A	123[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	29	ASN
2	B	207	GLN
2	D	179	HIS
2	D	44	GLN
1	A	186	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 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	C	307	-	3,3,3	0.47	0	2,2,2	0.43	0
4	EDO	D	309	-	3,3,3	0.45	0	2,2,2	0.32	0
4	EDO	A	307	-	3,3,3	0.07	0	2,2,2	0.17	0
4	EDO	C	309	-	3,3,3	0.51	0	2,2,2	0.21	0
4	EDO	C	301	-	3,3,3	0.60	0	2,2,2	0.16	0
6	PEG	C	303	-	6,6,6	0.22	0	5,5,5	0.06	0
6	PEG	A	301	-	6,6,6	0.18	0	5,5,5	0.05	0
4	EDO	B	303	-	3,3,3	0.49	0	2,2,2	0.35	0
6	PEG	D	302	-	6,6,6	0.17	0	5,5,5	0.09	0
6	PEG	D	303	-	6,6,6	0.11	0	5,5,5	0.13	0
4	EDO	A	303	-	3,3,3	0.52	0	2,2,2	0.33	0
4	EDO	A	306	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	D	308[B]	-	3,3,3	0.46	0	2,2,2	0.32	0
6	PEG	D	301	-	6,6,6	0.17	0	5,5,5	0.14	0
6	PEG	B	304[B]	-	6,6,6	0.16	0	5,5,5	0.04	0
4	EDO	B	301	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EPE	A	302	-	15,15,15	0.90	1 (6%)	19,20,20	1.88	5 (26%)
4	EDO	D	308[A]	-	3,3,3	0.46	0	2,2,2	0.43	0
6	PEG	B	304[A]	-	6,6,6	0.15	0	5,5,5	0.22	0
6	PEG	D	304	-	6,6,6	0.10	0	5,5,5	0.17	0
4	EDO	C	310	-	3,3,3	0.47	0	2,2,2	0.38	0
5	EPE	C	302	-	15,15,15	0.83	1 (6%)	19,20,20	1.67	3 (15%)
4	EDO	C	308	-	3,3,3	0.50	0	2,2,2	0.33	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	C	307	-	-	1/1/1/1	-
4	EDO	D	309	-	-	0/1/1/1	-
4	EDO	A	307	-	-	1/1/1/1	-
4	EDO	C	309	-	-	1/1/1/1	-
4	EDO	C	301	-	-	1/1/1/1	-
6	PEG	C	303	-	-	2/4/4/4	-
6	PEG	A	301	-	-	2/4/4/4	-
4	EDO	B	303	-	-	1/1/1/1	-
6	PEG	D	302	-	-	2/4/4/4	-
6	PEG	D	303	-	-	3/4/4/4	-
4	EDO	A	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	306	-	-	1/1/1/1	-
4	EDO	D	308[B]	-	-	0/1/1/1	-
6	PEG	D	301	-	-	1/4/4/4	-
6	PEG	B	304[B]	-	-	3/4/4/4	-
4	EDO	B	301	-	-	0/1/1/1	-
5	EPE	A	302	-	-	4/9/19/19	0/1/1/1
4	EDO	D	308[A]	-	-	0/1/1/1	-
6	PEG	B	304[A]	-	-	2/4/4/4	-
6	PEG	D	304	-	-	3/4/4/4	-
4	EDO	C	310	-	-	0/1/1/1	-
5	EPE	C	302	-	-	6/9/19/19	0/1/1/1
4	EDO	C	308	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	302	EPE	C10-S	3.03	1.81	1.77
5	C	302	EPE	C10-S	2.80	1.81	1.77

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	302	EPE	C5-N4-C3	4.91	119.42	108.84
5	C	302	EPE	C5-N4-C3	4.54	118.63	108.84
5	A	302	EPE	C2-C3-N4	2.99	116.68	110.65
5	C	302	EPE	O3S-S-C10	2.96	111.80	106.00
5	A	302	EPE	O2S-S-C10	2.67	110.76	106.73

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

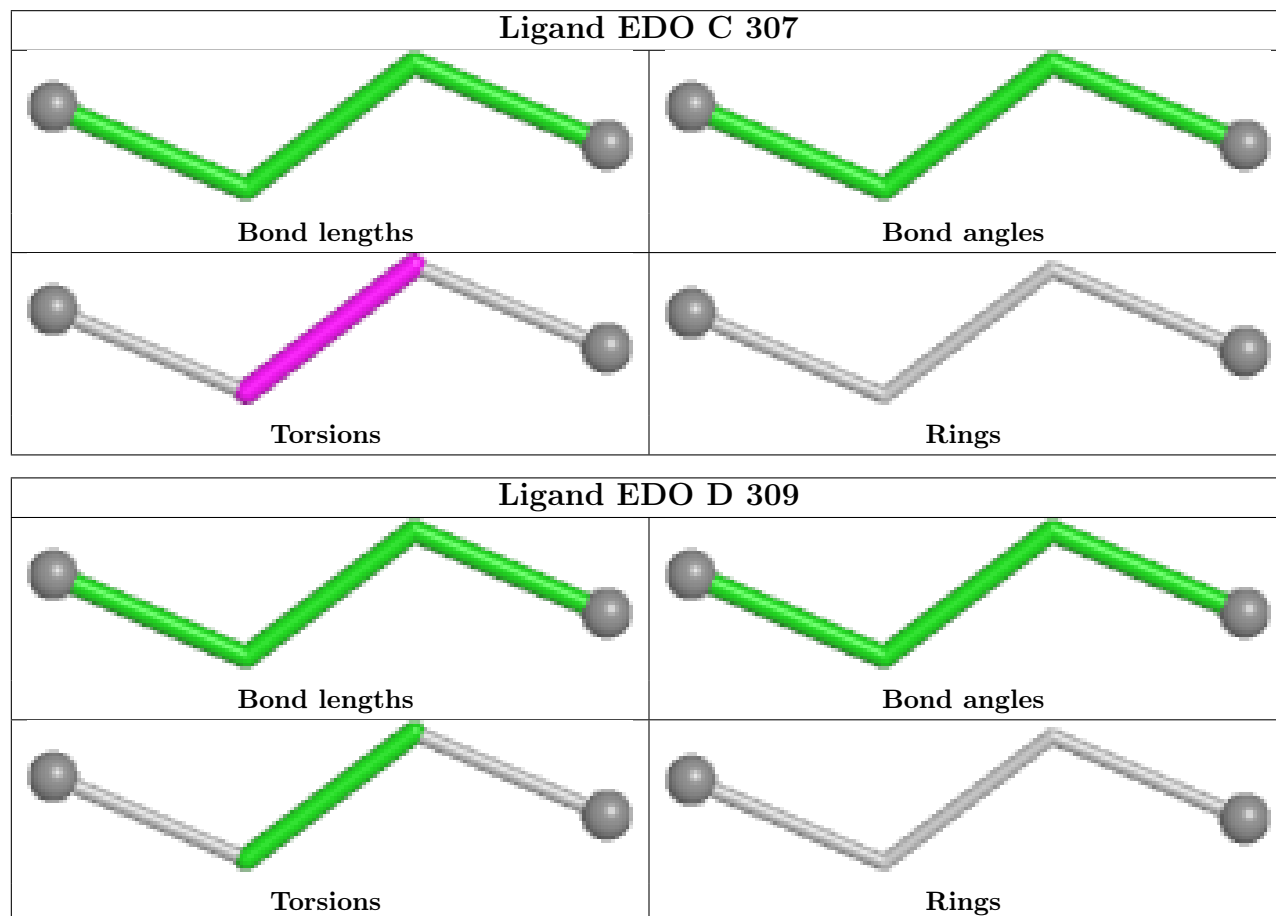
Mol	Chain	Res	Type	Atoms
5	A	302	EPE	C8-C7-N4-C5
6	D	301	PEG	C1-C2-O2-C3
6	D	303	PEG	O2-C3-C4-O4
5	C	302	EPE	C9-C10-S-O3S
6	B	304[A]	PEG	O1-C1-C2-O2

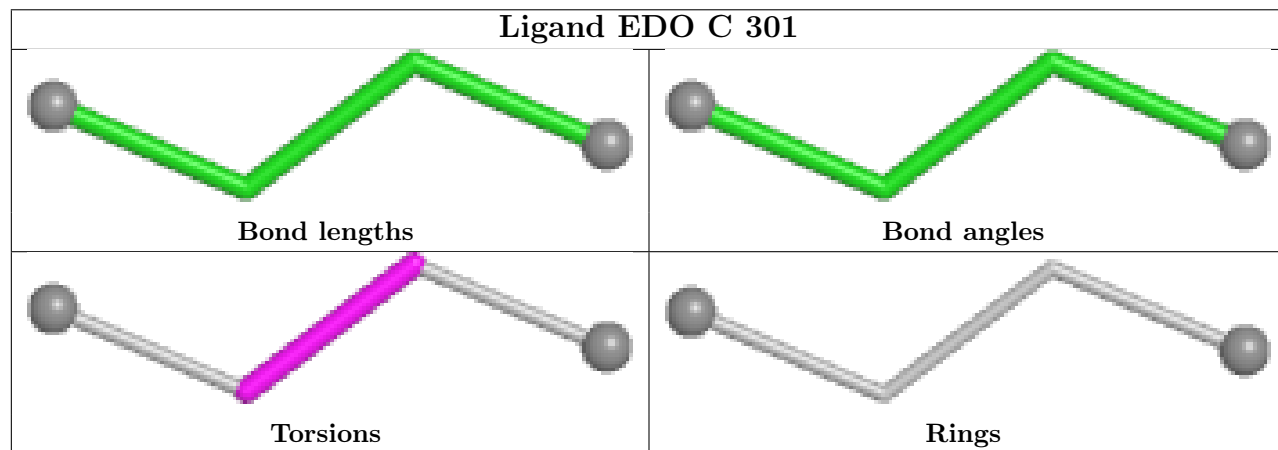
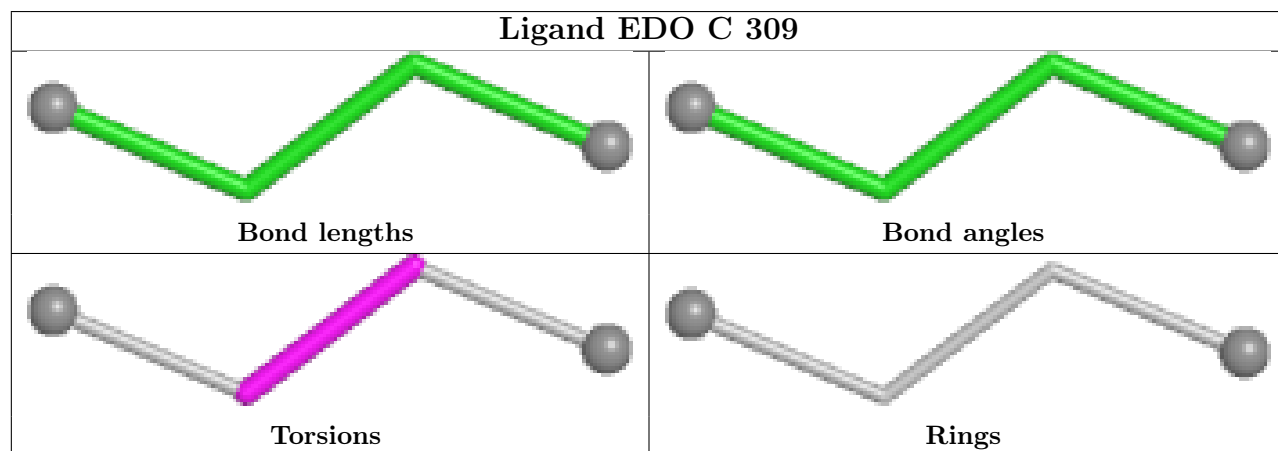
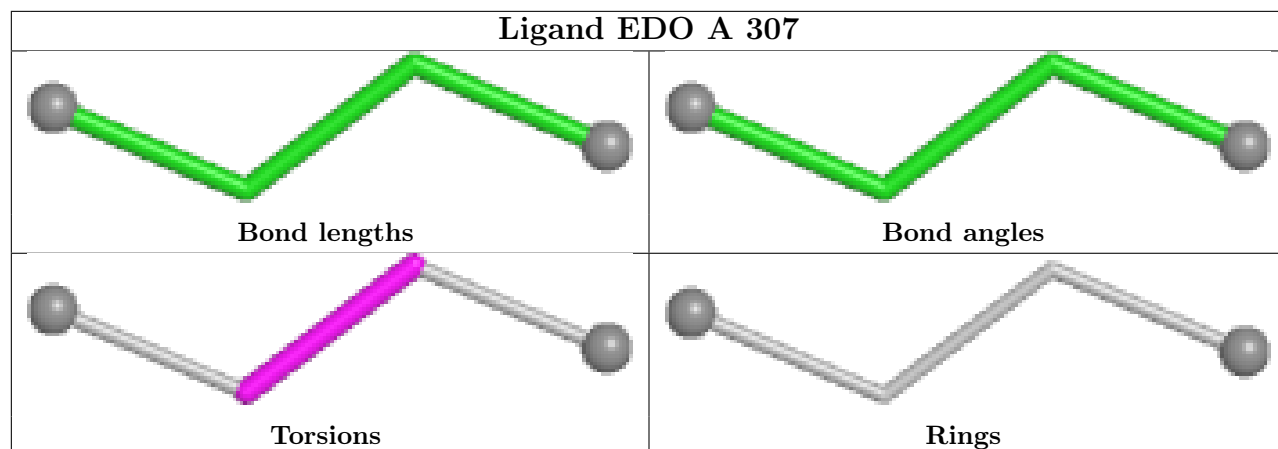
There are no ring outliers.

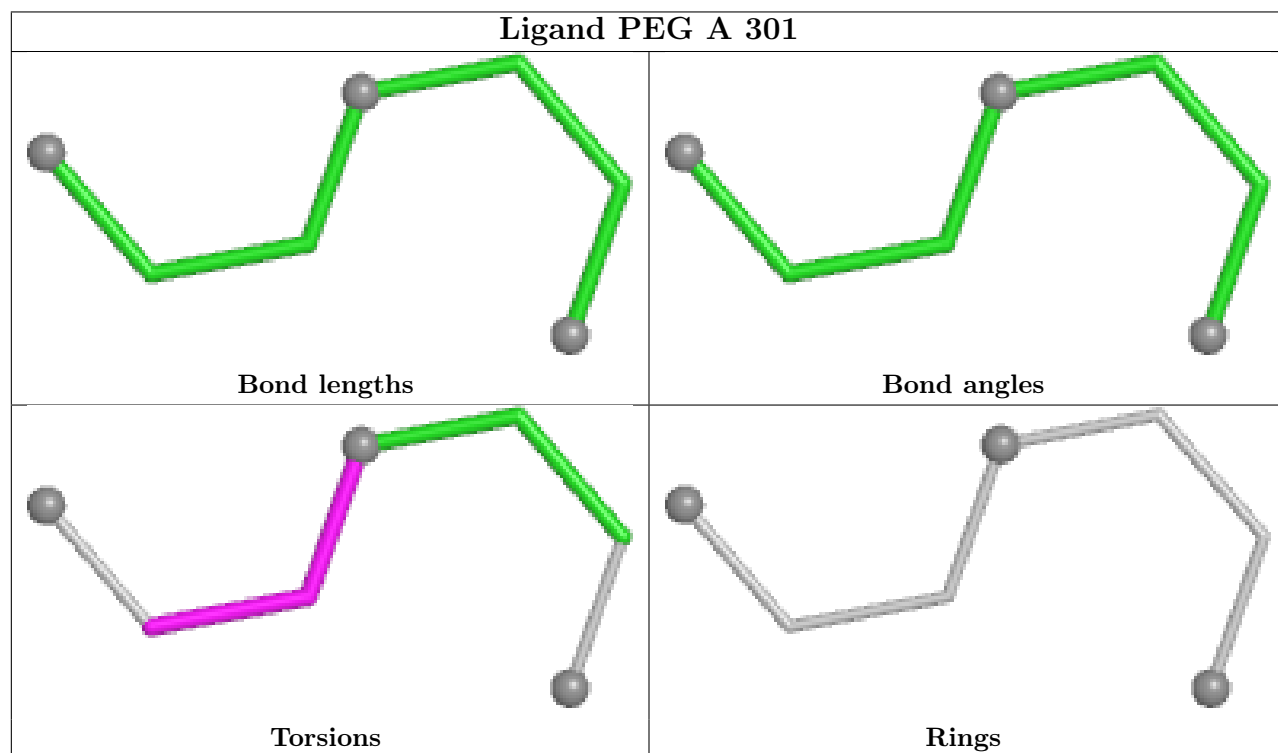
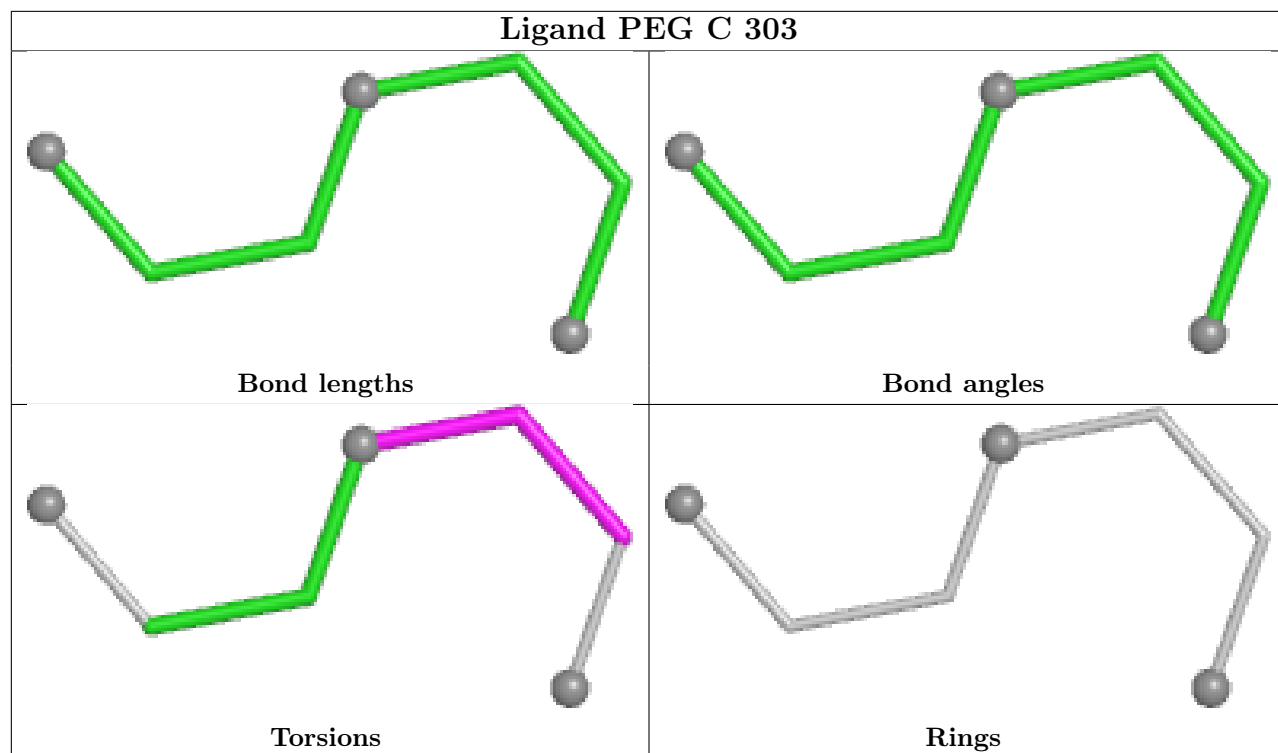
7 monomers are involved in 15 short contacts:

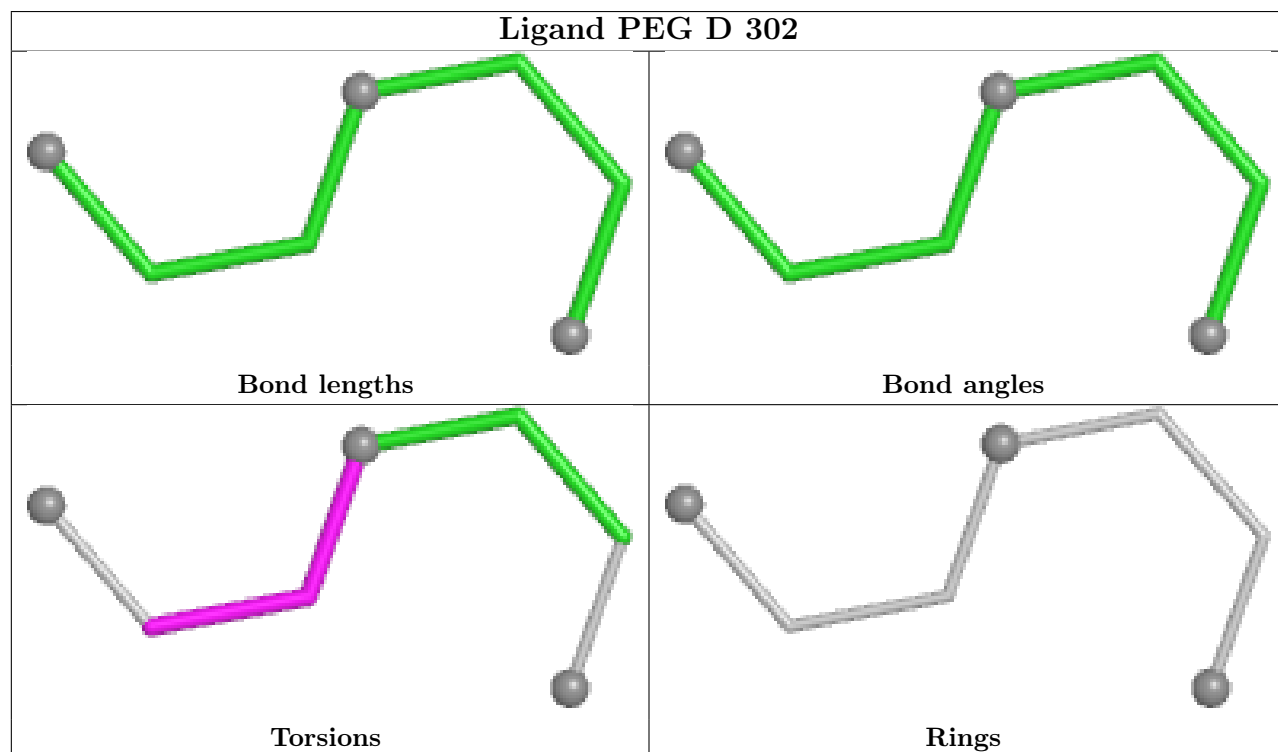
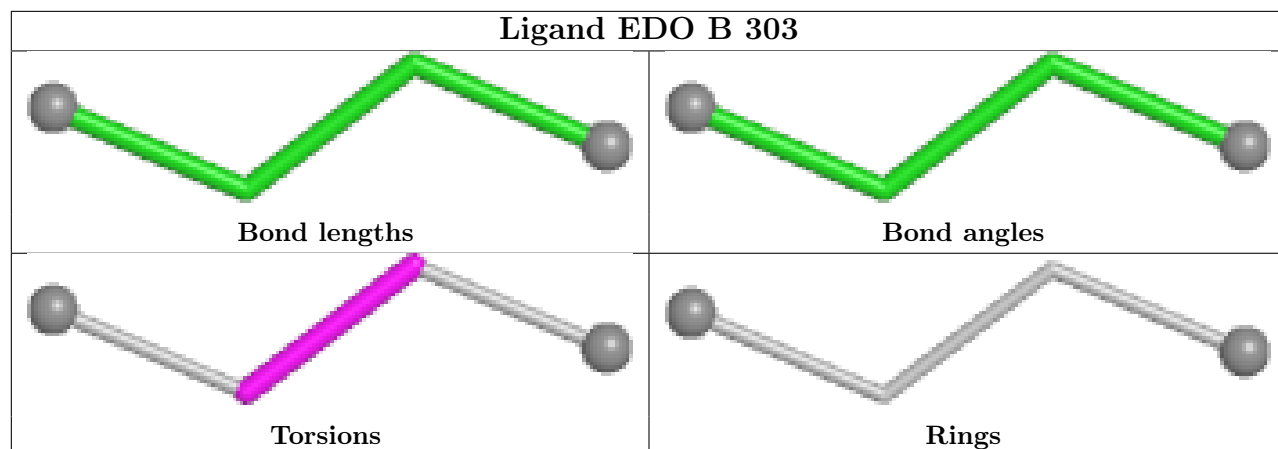
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	303	PEG	1	0
6	D	301	PEG	3	0
4	B	301	EDO	3	0
5	A	302	EPE	2	0
6	D	304	PEG	3	0
5	C	302	EPE	2	0
4	C	308	EDO	1	0

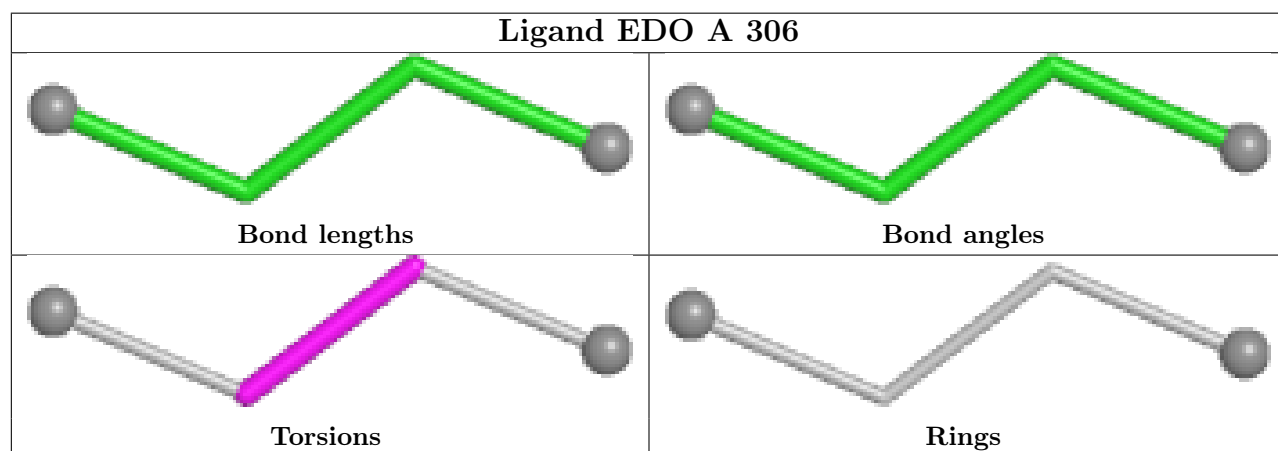
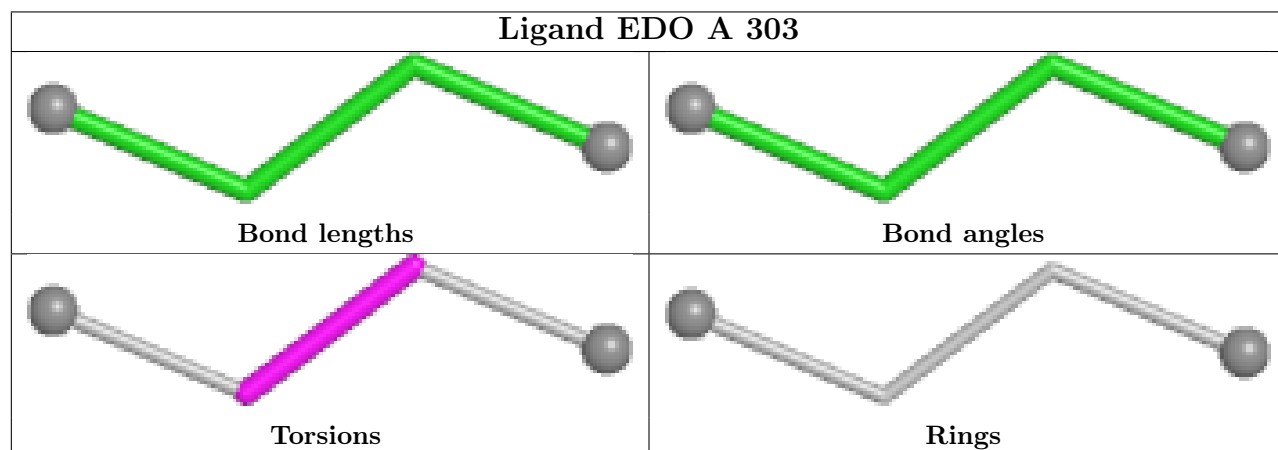
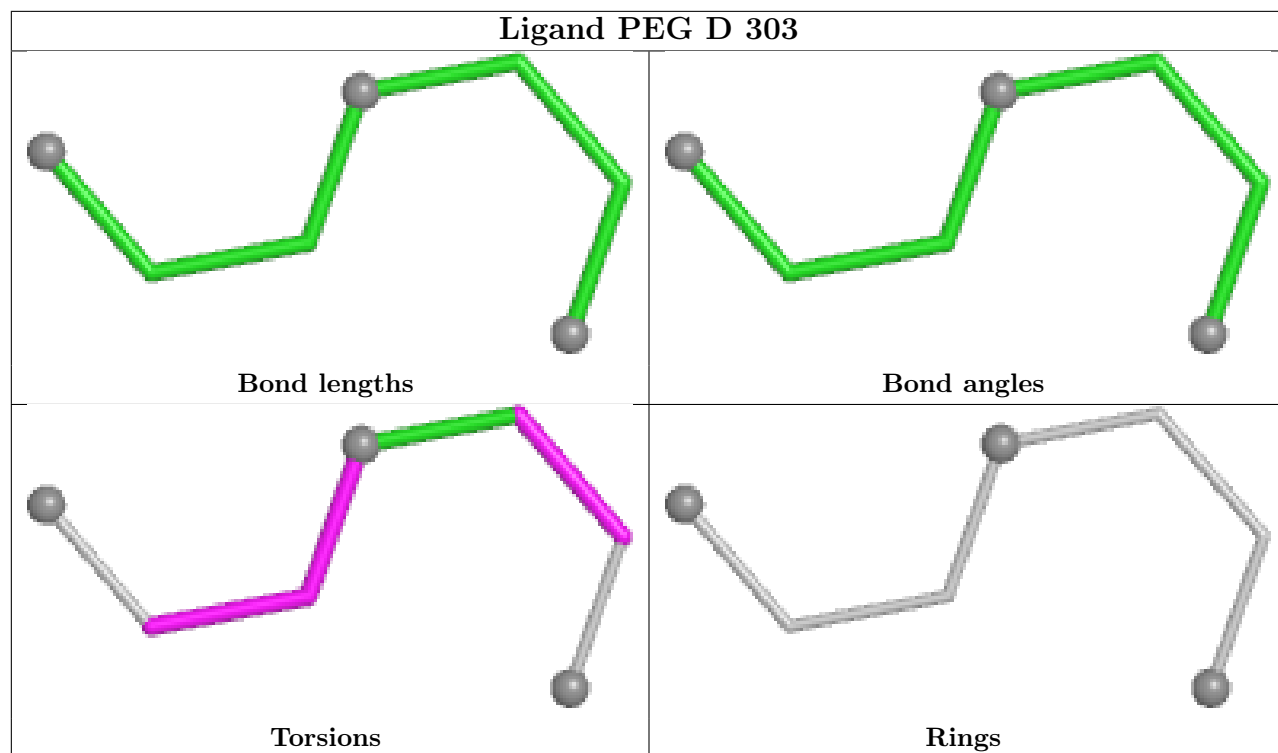
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

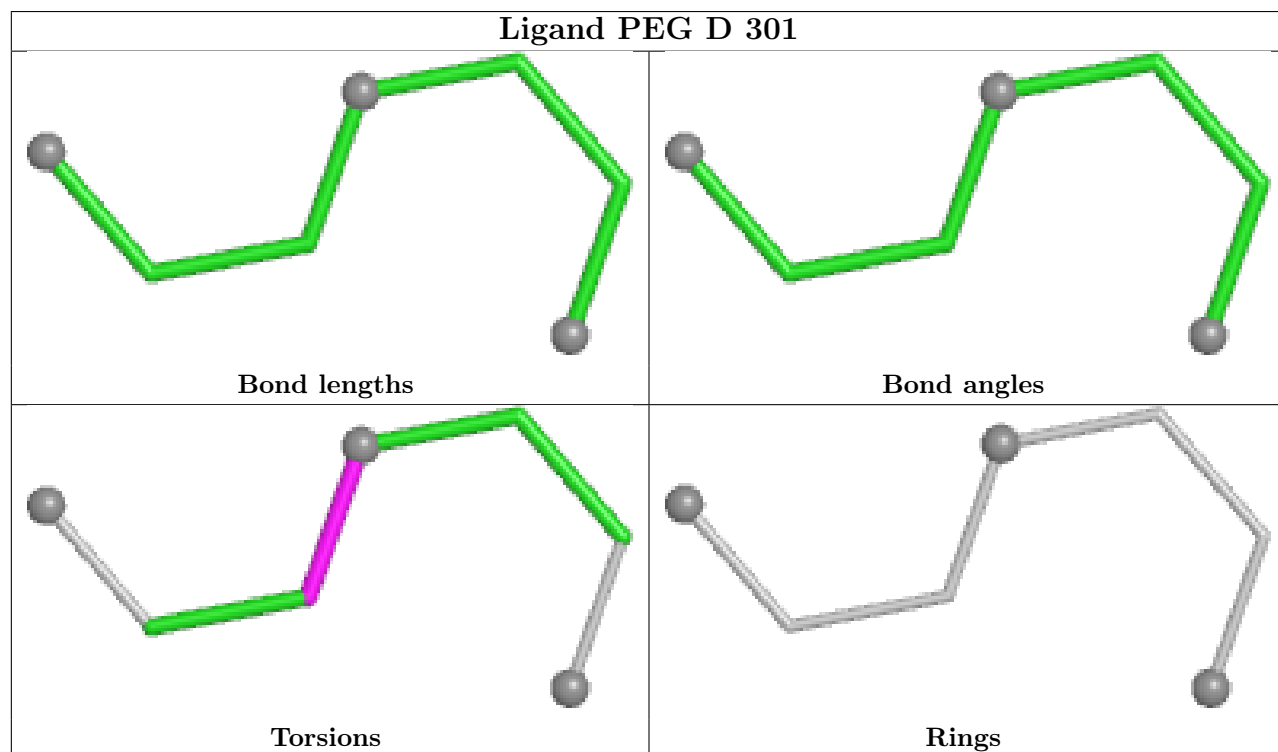
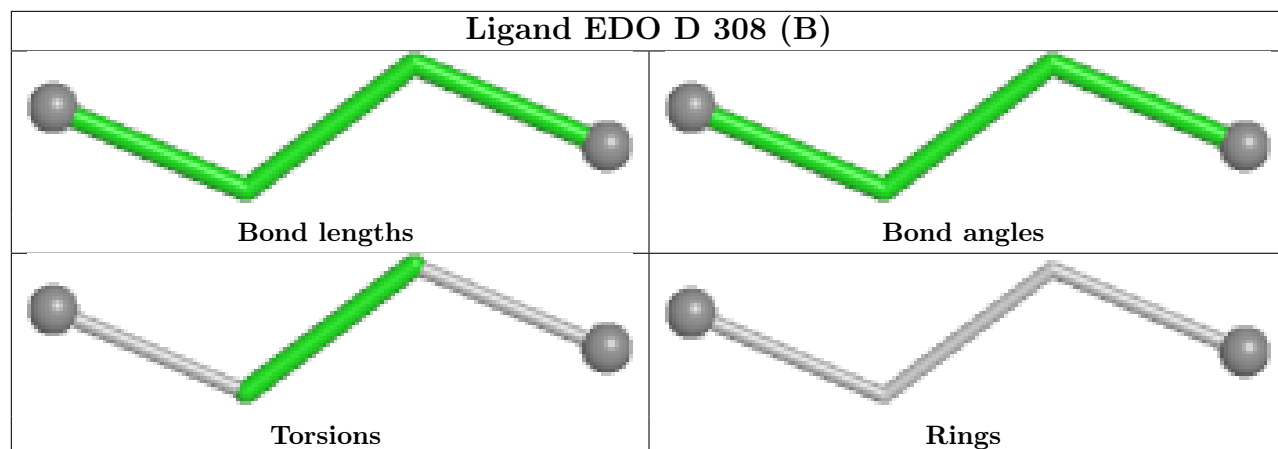


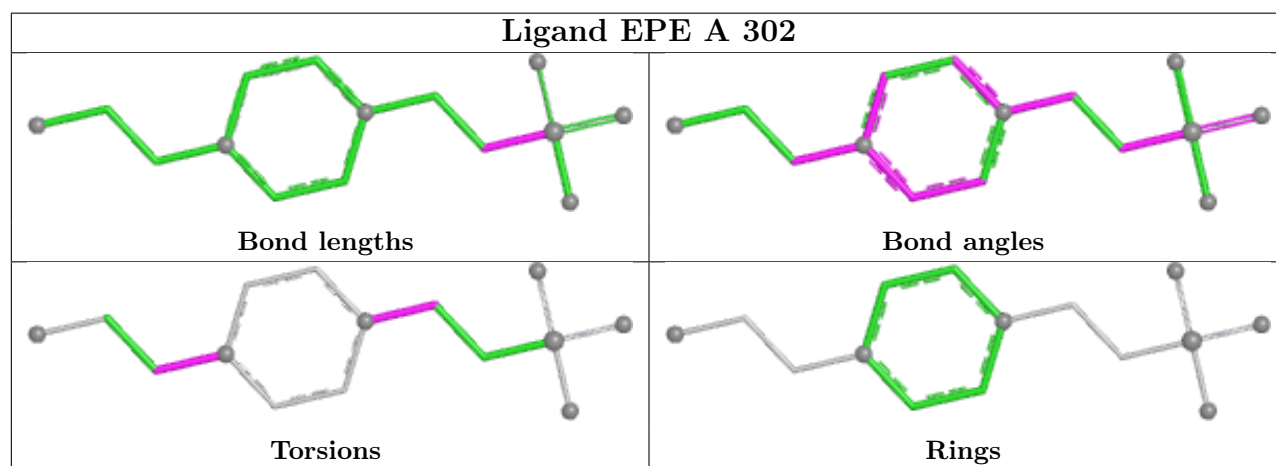
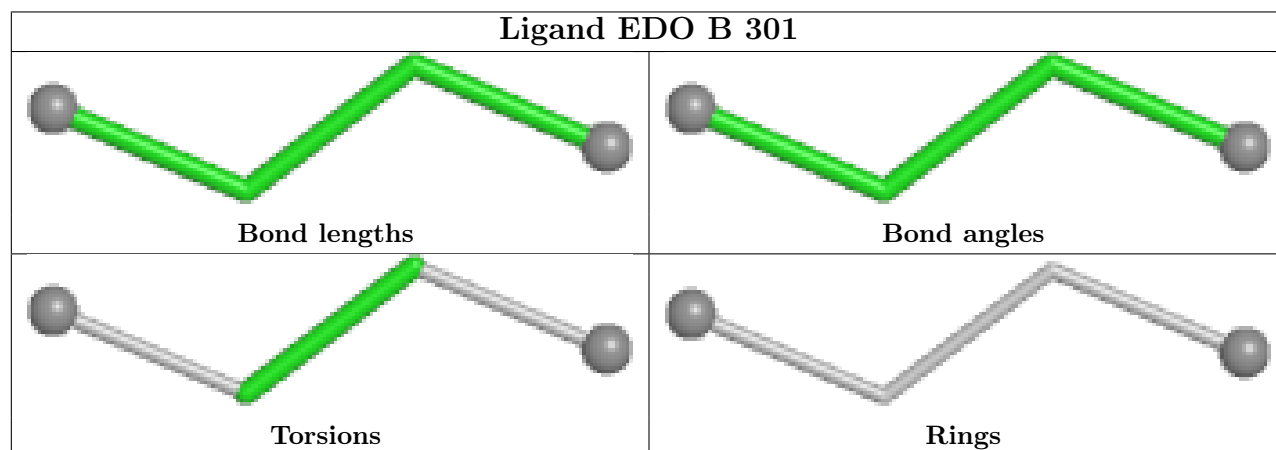
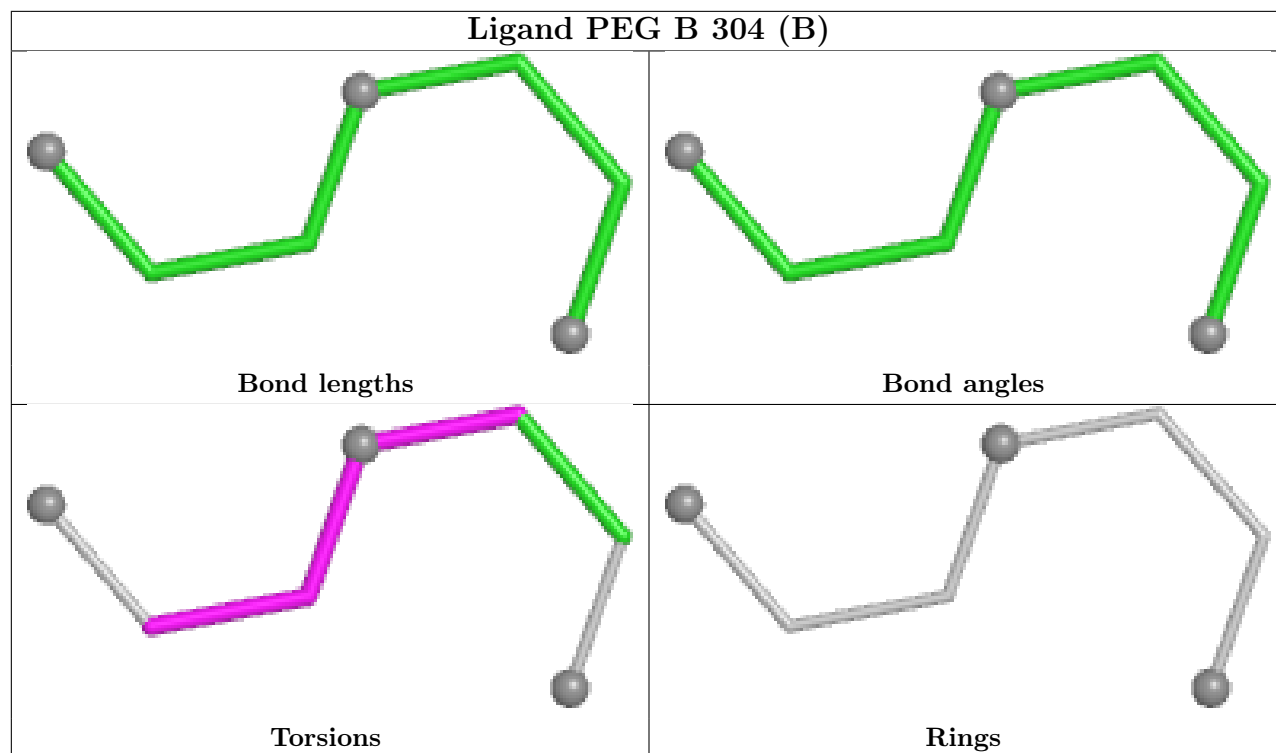


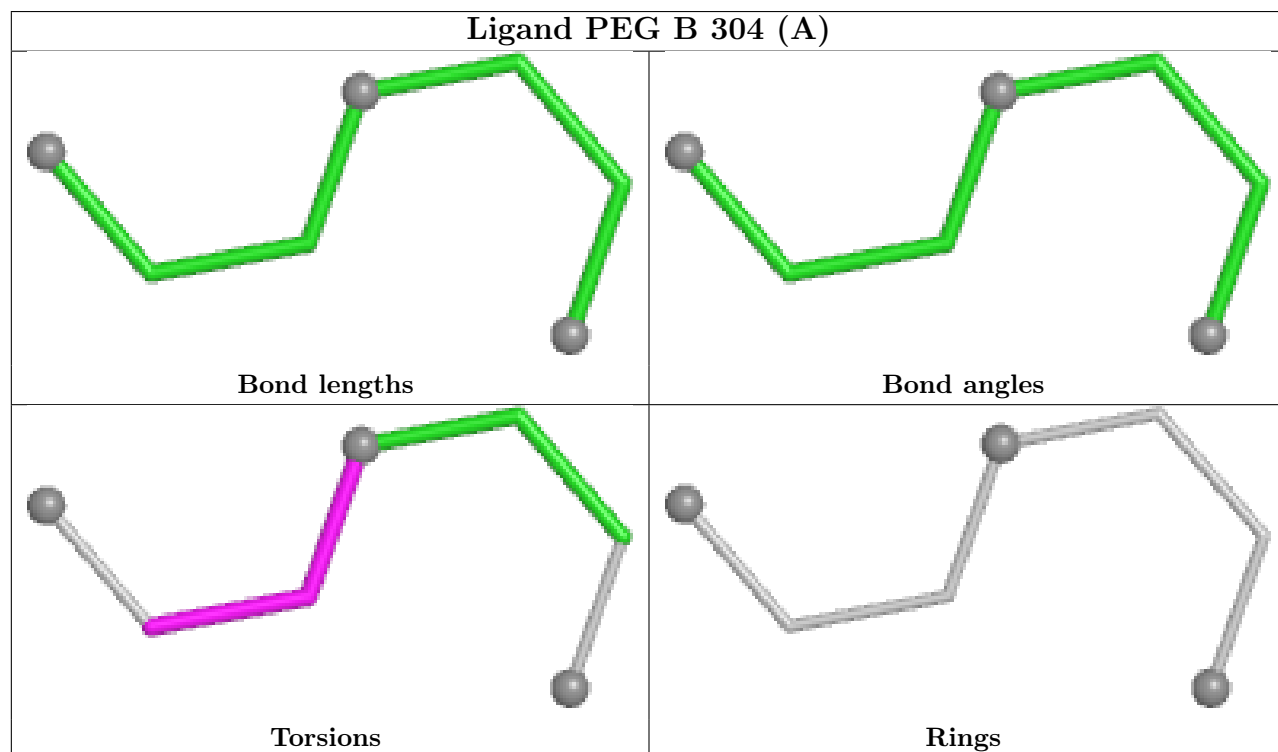
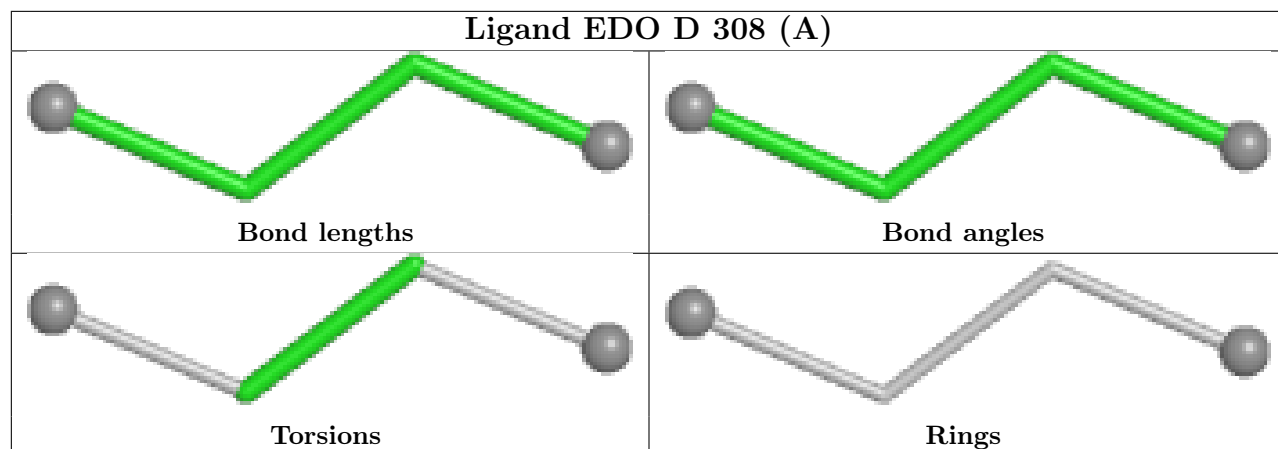


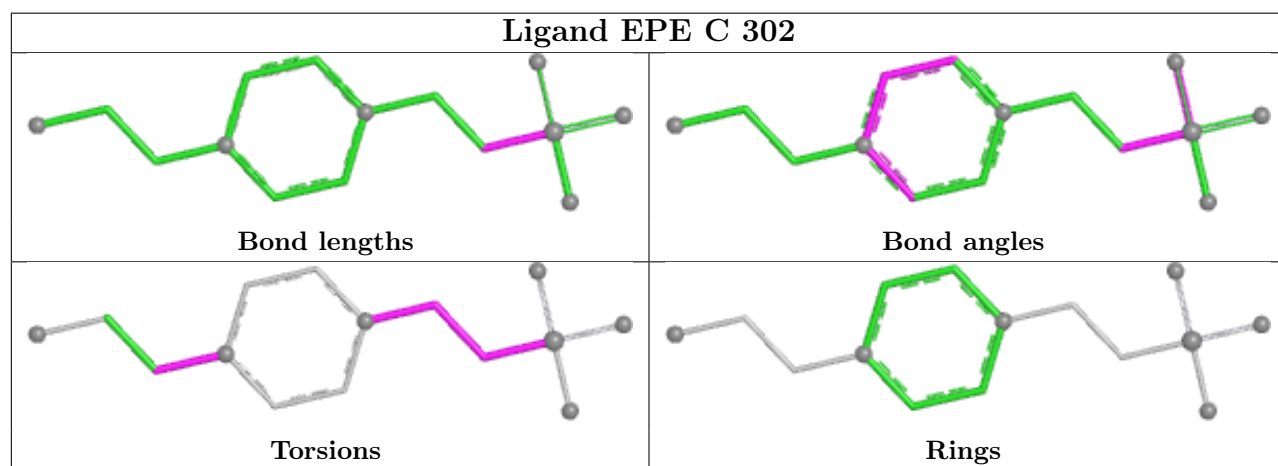
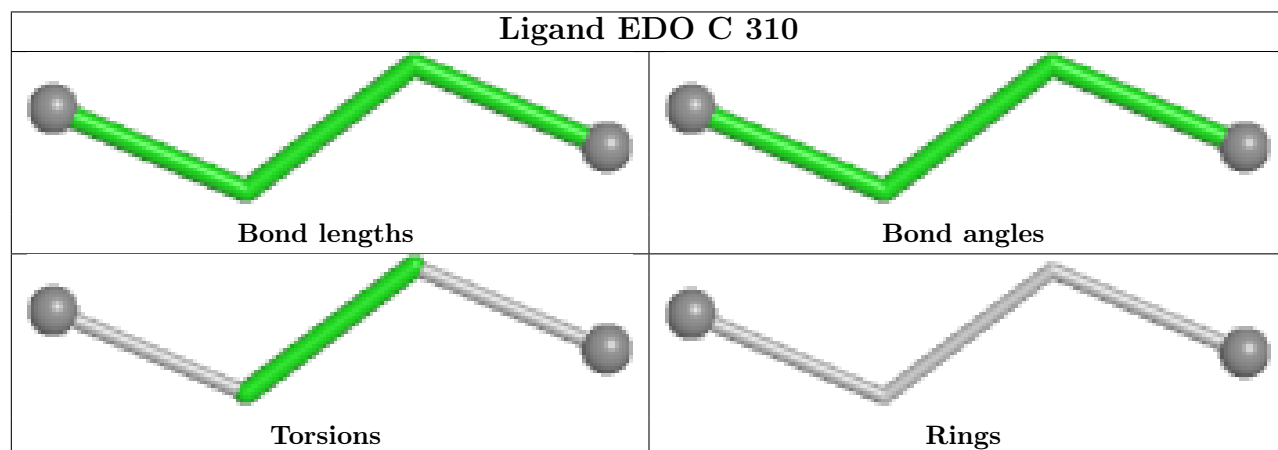
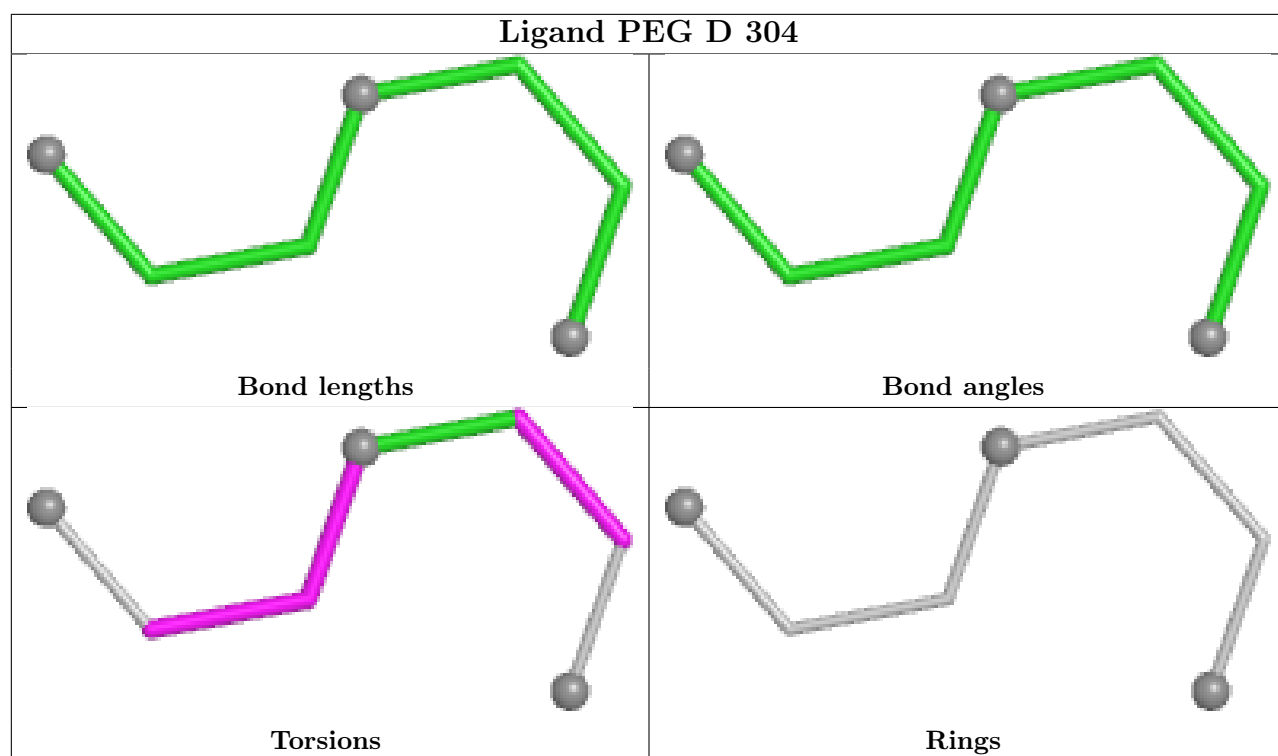


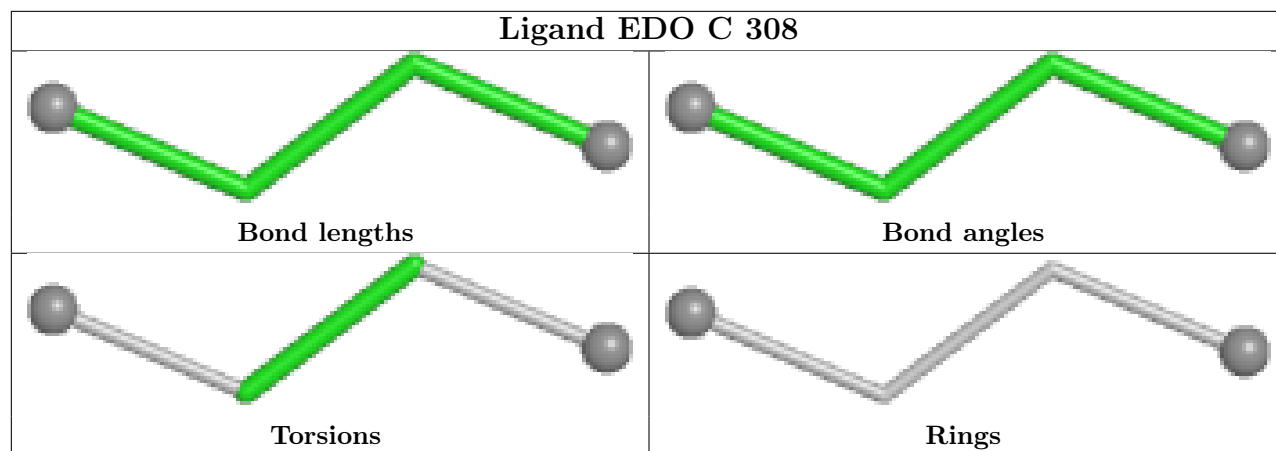












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	211/216 (97%)	0.75	10 (4%) 36 35	15, 55, 87, 98	3 (1%)
1	C	213/216 (98%)	0.45	4 (1%) 66 66	20, 43, 62, 79	3 (1%)
2	B	209/221 (94%)	0.08	4 (1%) 66 66	13, 32, 72, 88	2 (0%)
2	D	211/221 (95%)	-0.08	3 (1%) 73 73	16, 30, 56, 73	1 (0%)
3	E	20/41 (48%)	0.60	1 (5%) 34 33	34, 47, 67, 68	0
3	F	20/41 (48%)	0.37	0 100 100	32, 44, 67, 70	0
All	All	884/956 (92%)	0.31	22 (2%) 58 58	13, 40, 75, 98	9 (1%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	2	ARG	5.0
1	A	99	PHE	3.1
2	D	200	PRO	3.0
2	B	153	LEU	3.0
1	C	99	PHE	3.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

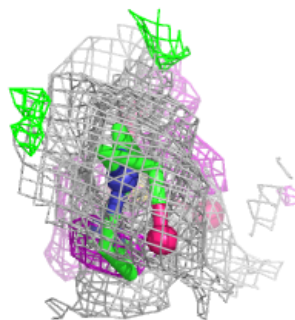
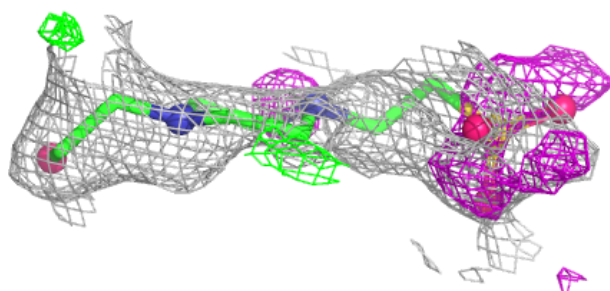
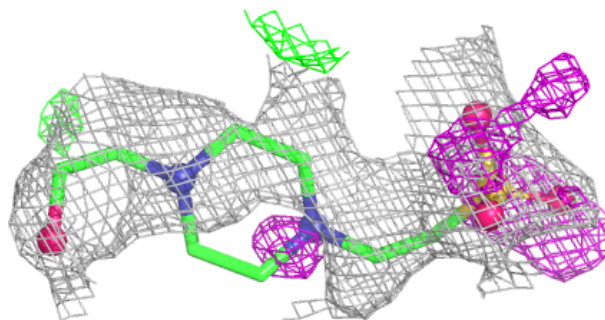
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EPE	C	302	15/15	0.57	0.17	54,60,81,82	0
5	EPE	A	302	15/15	0.67	0.17	50,58,91,93	0
6	PEG	C	303	7/7	0.68	0.15	42,51,55,60	0
4	EDO	D	308[B]	4/4	0.73	0.15	41,41,41,45	4
4	EDO	D	308[A]	4/4	0.73	0.15	40,42,45,45	4
4	EDO	A	307	4/4	0.78	0.13	53,57,57,58	0
4	EDO	B	303	4/4	0.80	0.10	44,46,51,51	0
6	PEG	B	304[A]	7/7	0.81	0.11	32,43,50,52	7
6	PEG	B	304[B]	7/7	0.81	0.11	46,48,51,53	7
6	PEG	D	301	7/7	0.81	0.22	38,40,45,46	0
8	CA	C	306	1/1	0.81	0.11	80,80,80,80	0
4	EDO	C	308	4/4	0.82	0.13	48,49,52,53	0
6	PEG	A	301	7/7	0.82	0.12	44,50,51,55	0
4	EDO	A	303	4/4	0.82	0.14	40,51,54,62	0
4	EDO	D	309	4/4	0.83	0.12	56,58,64,66	0
4	EDO	C	301	4/4	0.84	0.15	40,41,43,52	0
4	EDO	C	307	4/4	0.85	0.10	41,44,53,57	0
7	NA	D	305	1/1	0.86	0.11	44,44,44,44	0
8	CA	A	305	1/1	0.87	0.11	82,82,82,82	0
6	PEG	D	303	7/7	0.88	0.17	26,33,41,52	0
7	NA	C	304	1/1	0.88	0.11	58,58,58,58	0
7	NA	B	302	1/1	0.88	0.13	68,68,68,68	0
4	EDO	C	310	4/4	0.88	0.08	48,51,52,54	0
7	NA	D	307	1/1	0.88	0.10	57,57,57,57	0
4	EDO	A	306	4/4	0.88	0.08	53,55,58,65	0
6	PEG	D	302	7/7	0.88	0.10	33,43,56,60	0
4	EDO	C	309	4/4	0.90	0.11	42,44,54,54	0
6	PEG	D	304	7/7	0.91	0.11	31,38,44,47	0
4	EDO	B	301	4/4	0.91	0.10	21,40,40,42	0
7	NA	D	306	1/1	0.91	0.08	44,44,44,44	0
9	CL	B	305	1/1	0.91	0.13	78,78,78,78	0
8	CA	C	305	1/1	0.94	0.12	49,49,49,49	0
7	NA	A	304	1/1	0.99	0.06	23,23,23,23	0

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

orientation to approximate a three-dimensional view.

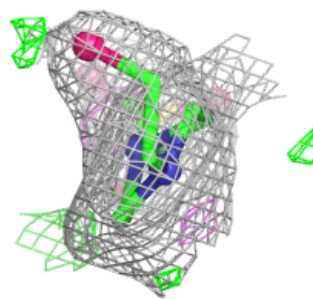
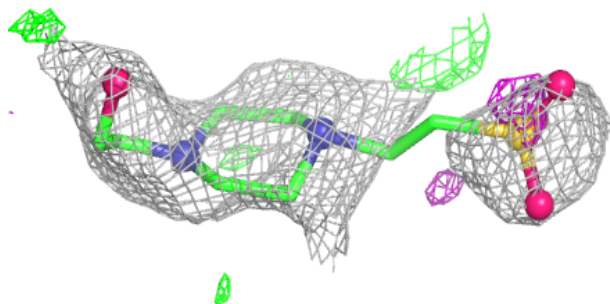
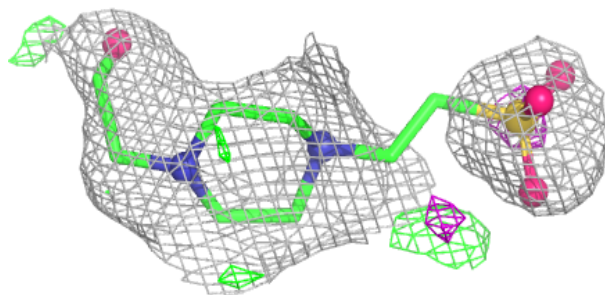
Electron density around EPE C 302:

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



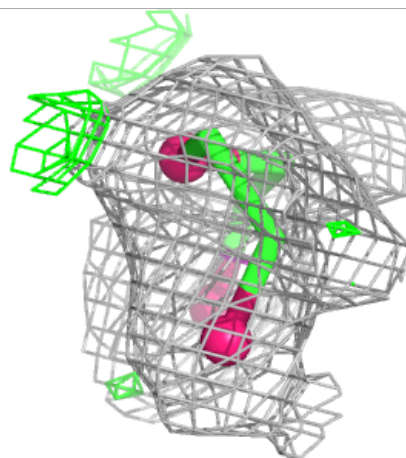
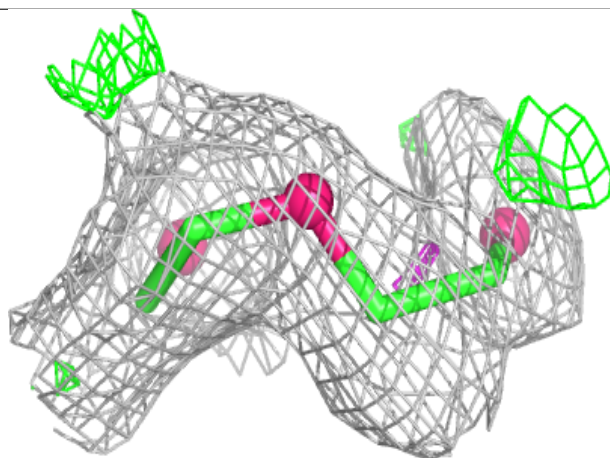
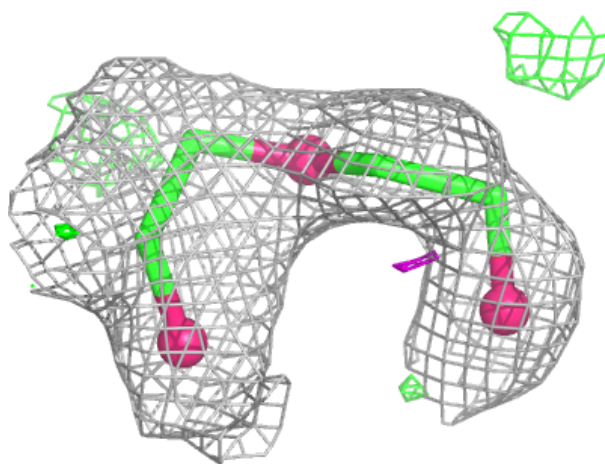
Electron density around EPE A 302:

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



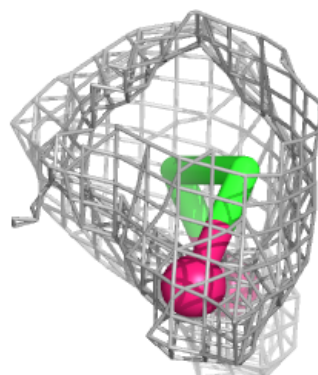
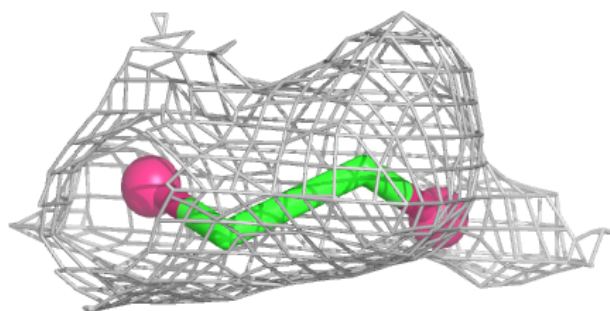
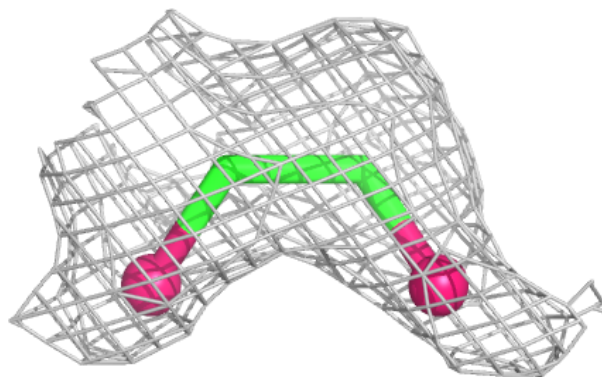
Electron density around PEG C 303:

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

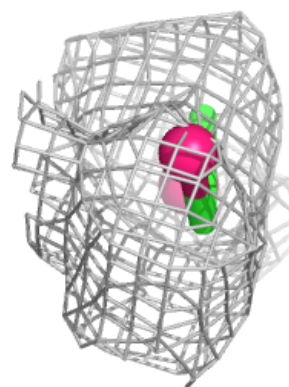
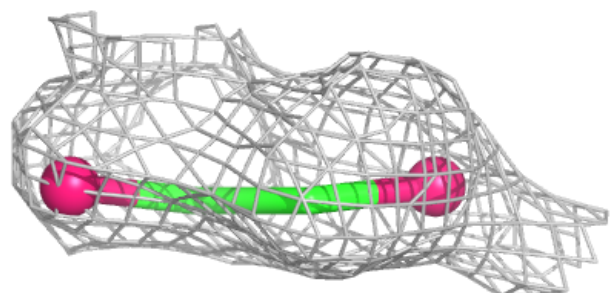
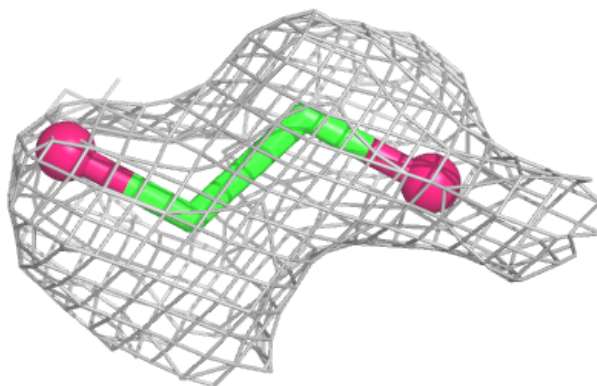


Electron density around EDO D 308 (B):

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

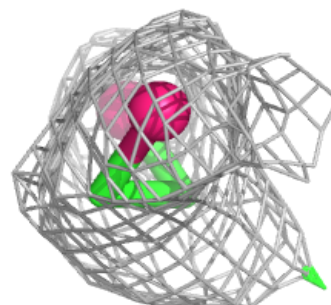
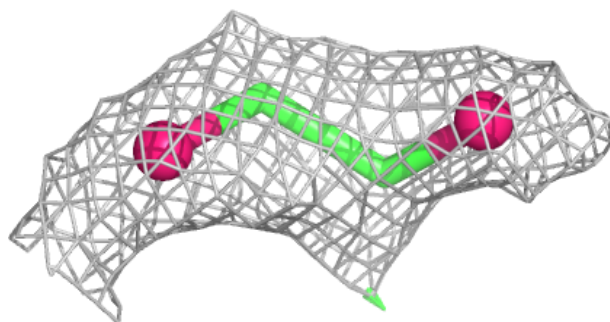
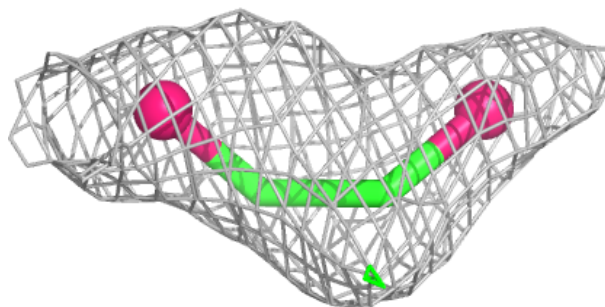
**Electron density around EDO D 308 (A):**

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

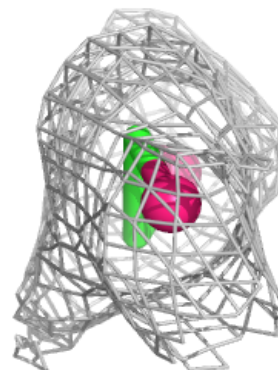
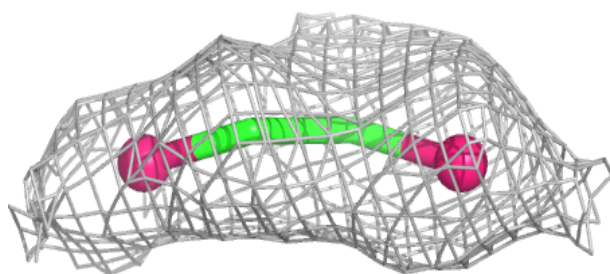
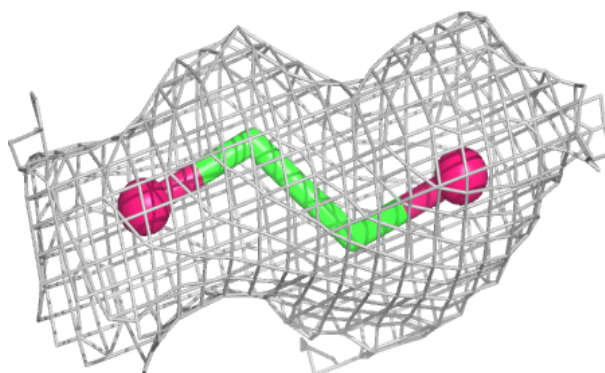


Electron density around EDO A 307:

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

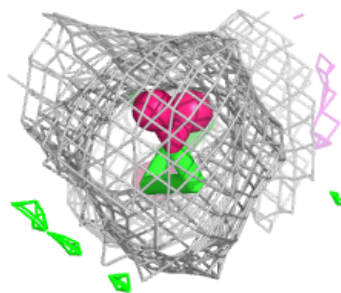
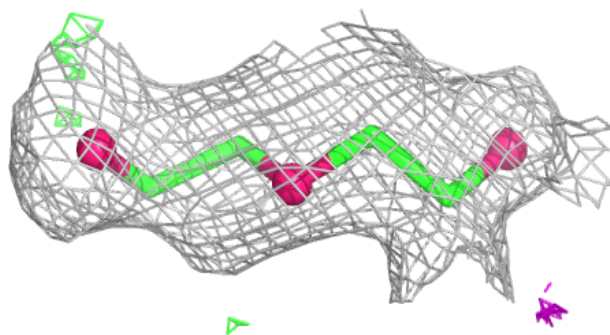
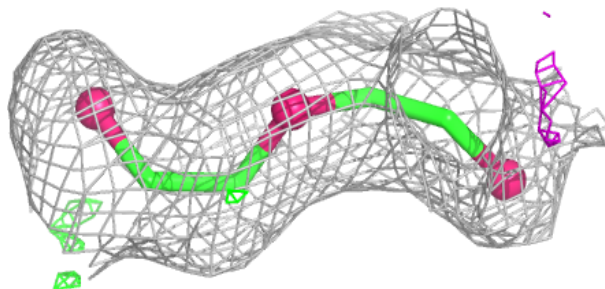
**Electron density around EDO B 303:**

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

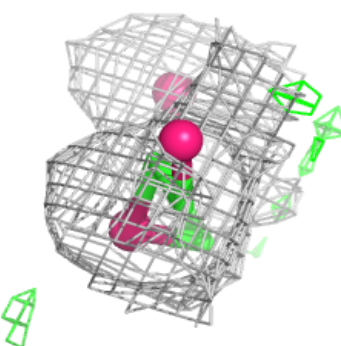
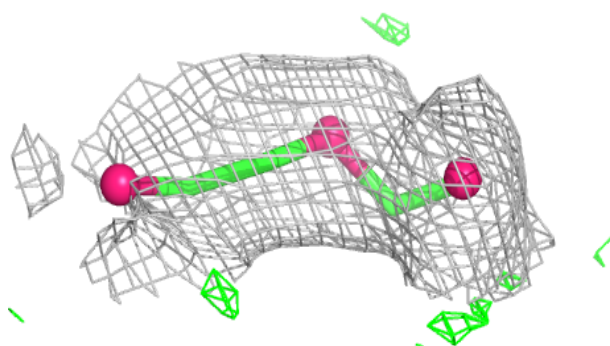
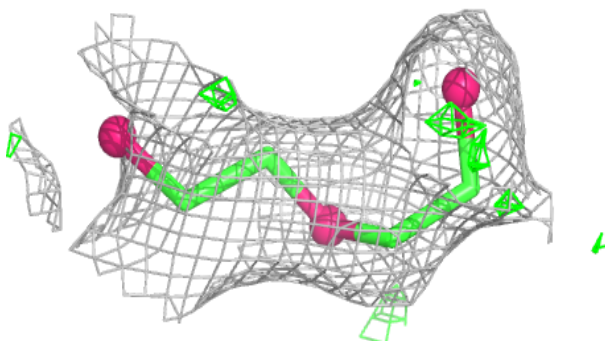


Electron density around PEG B 304 (A):

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

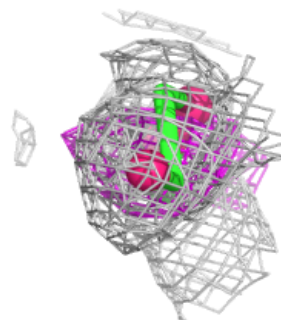
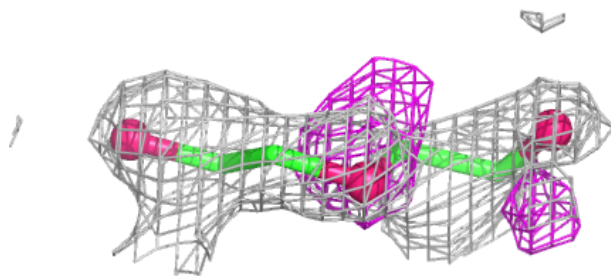
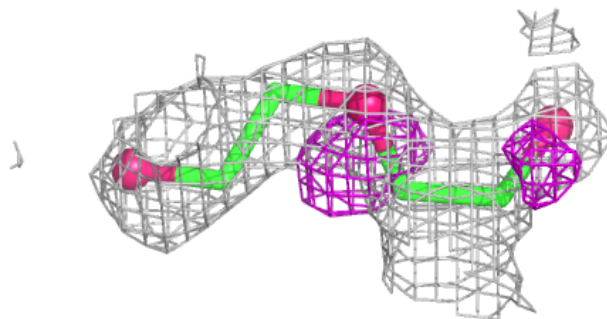
**Electron density around PEG B 304 (B):**

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



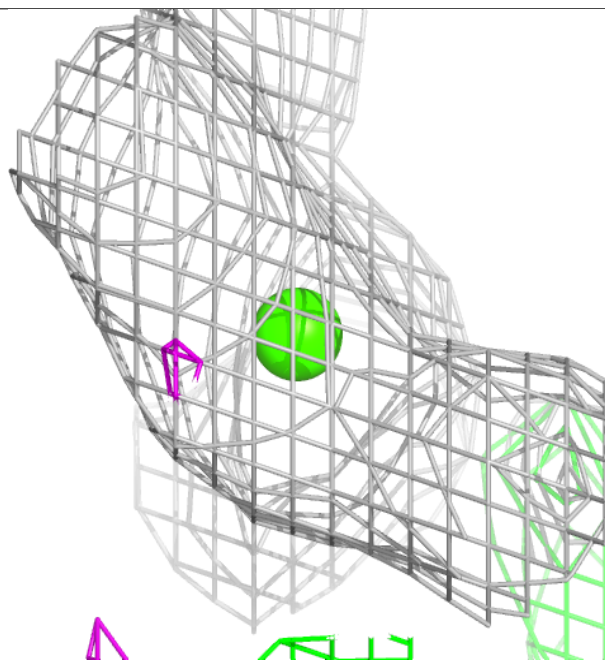
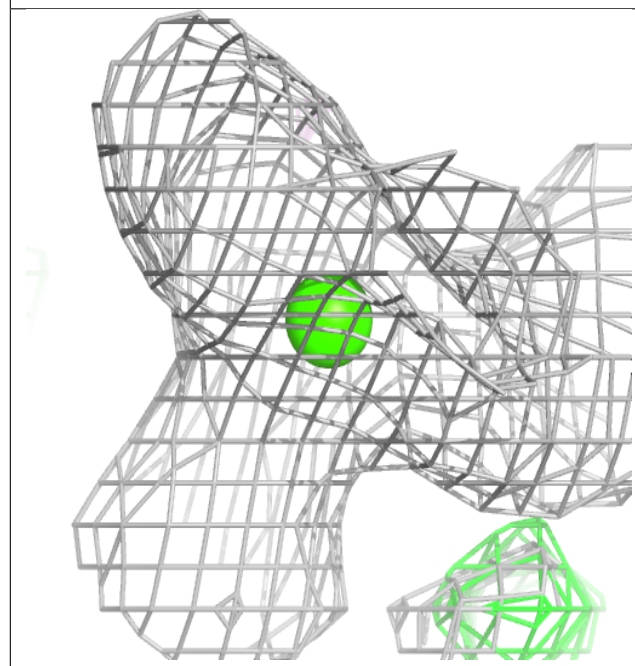
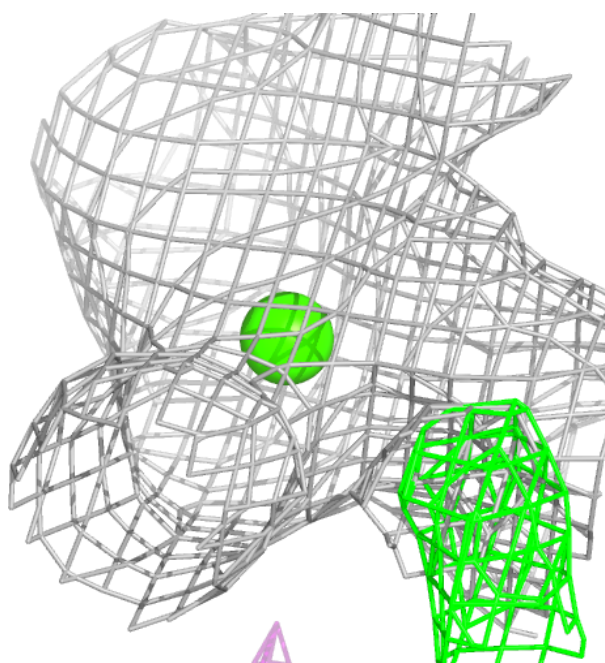
Electron density around PEG D 301:

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



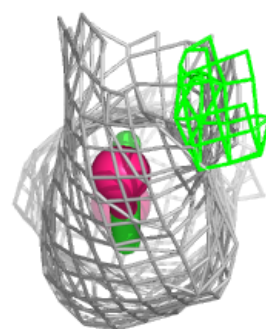
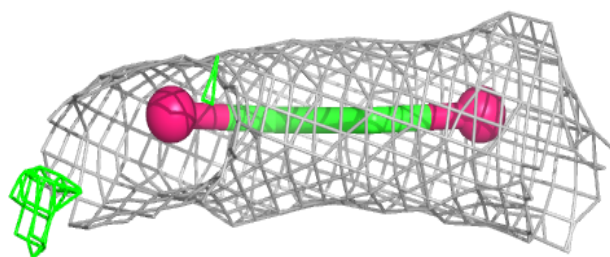
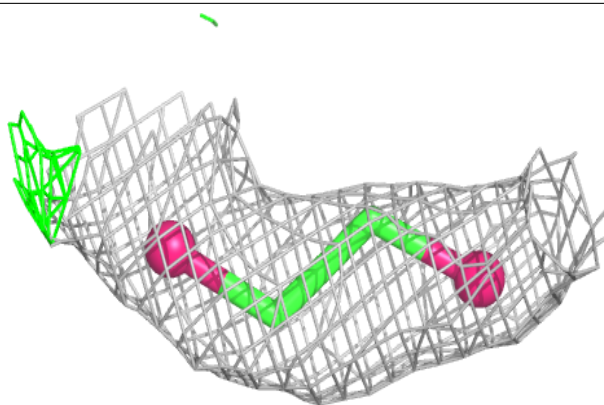
Electron density around CA C 306:

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

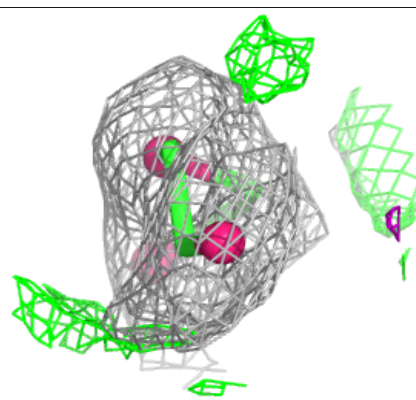
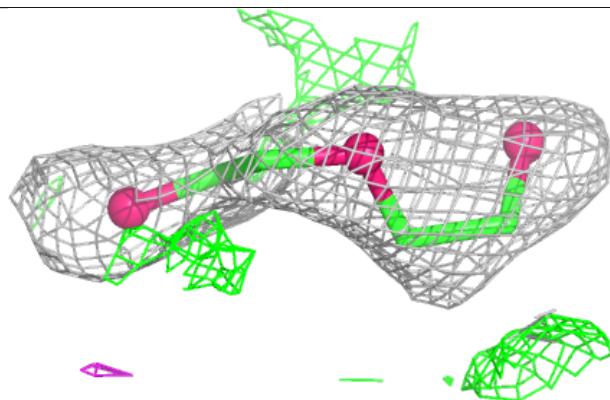
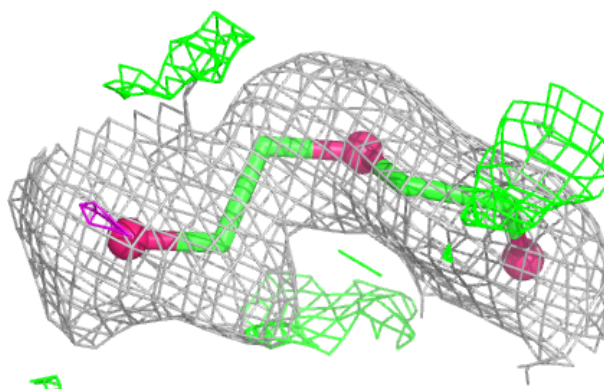


Electron density around EDO C 308:

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

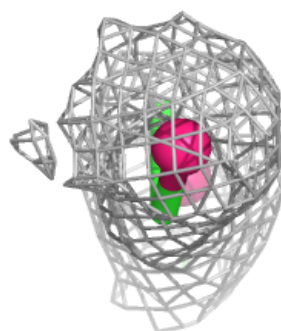
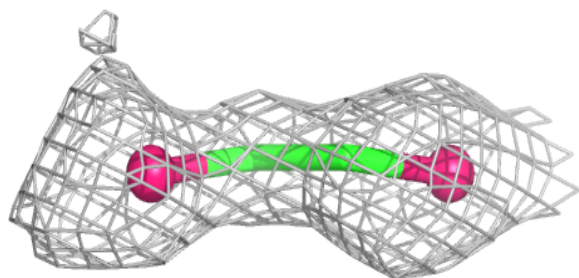
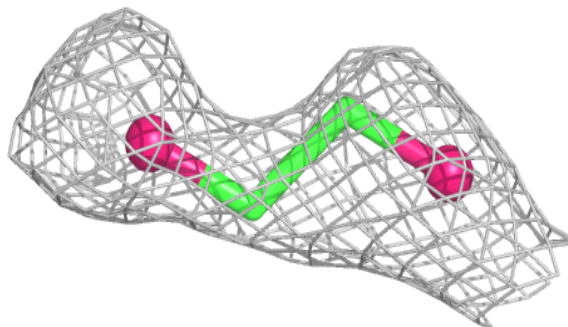
**Electron density around PEG A 301:**

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

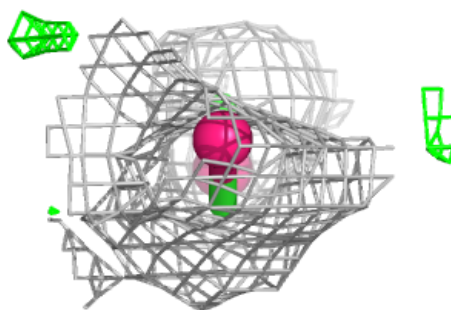
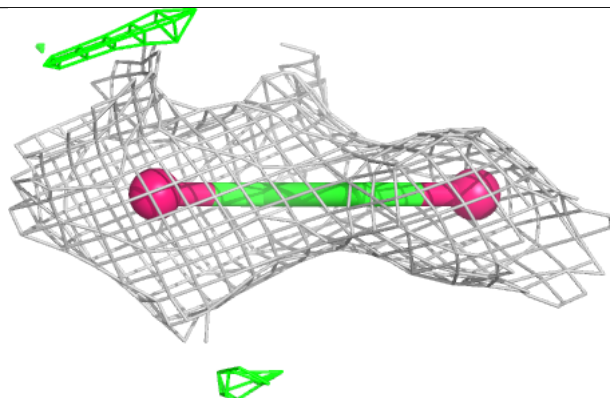
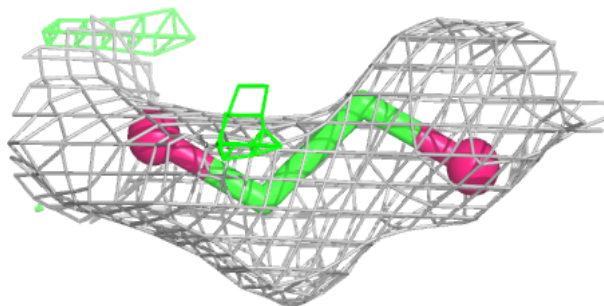


Electron density around EDO A 303:

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

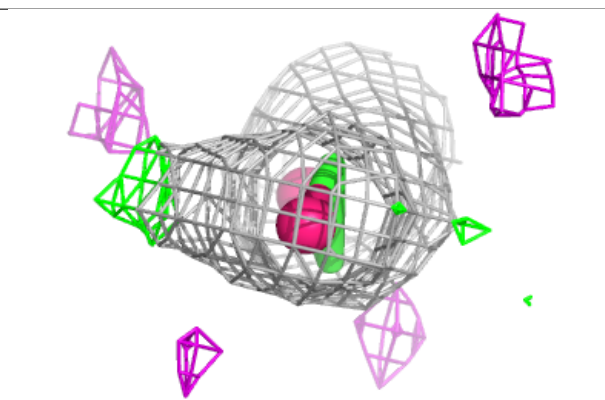
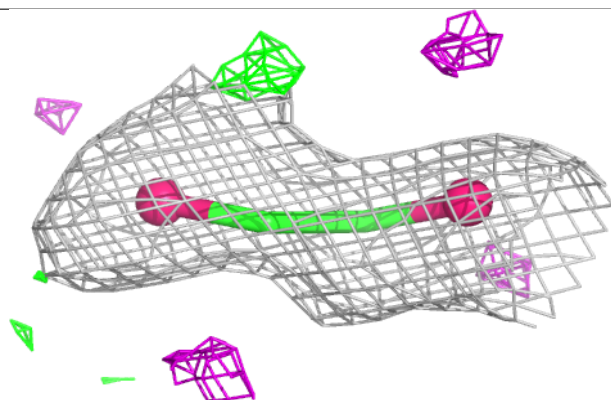
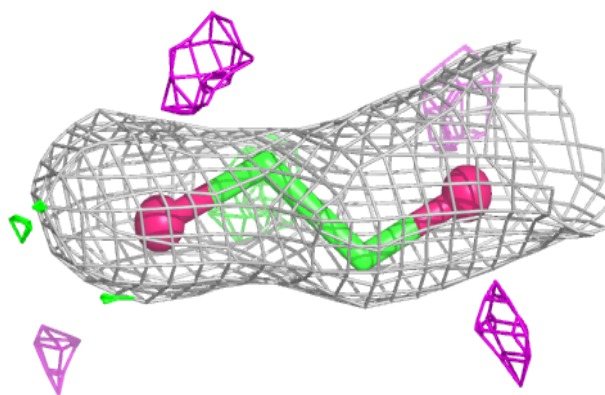
**Electron density around EDO D 309:**

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

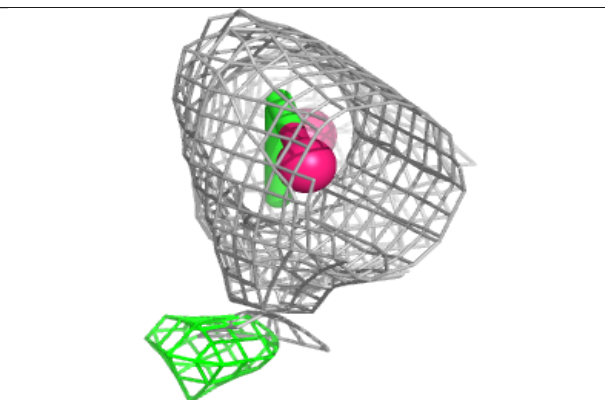
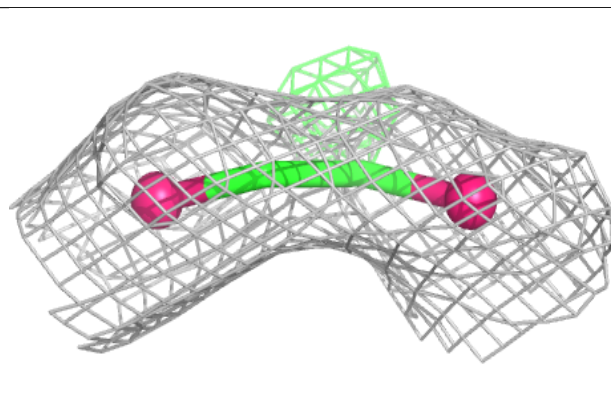
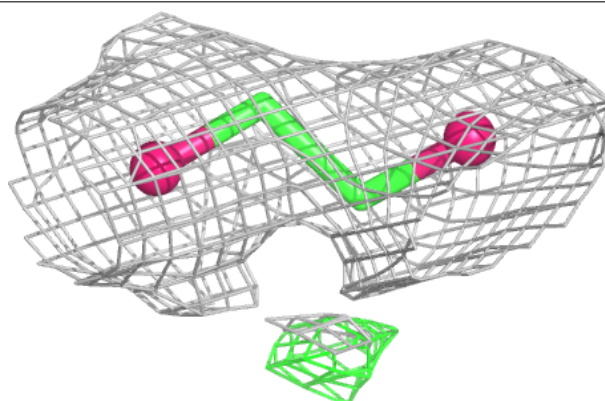


Electron density around EDO C 301:

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

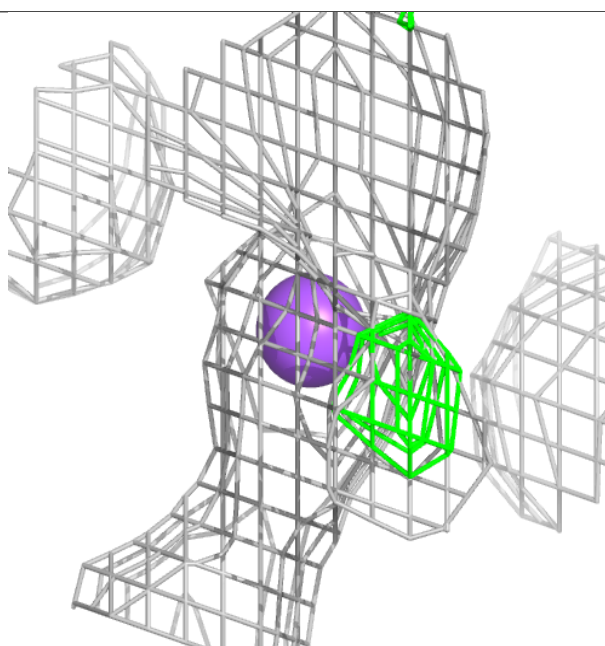
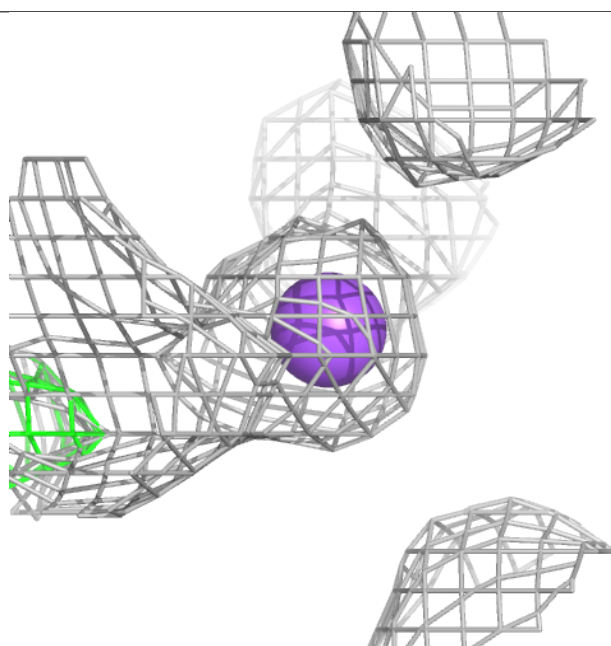
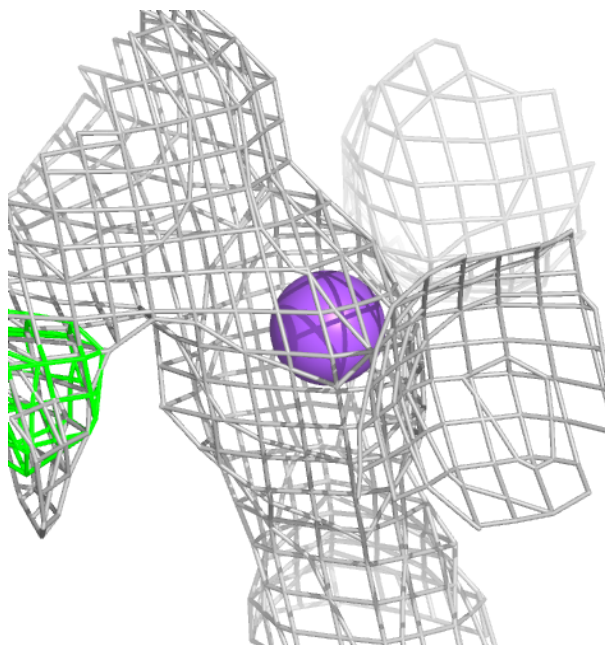
**Electron density around EDO C 307:**

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



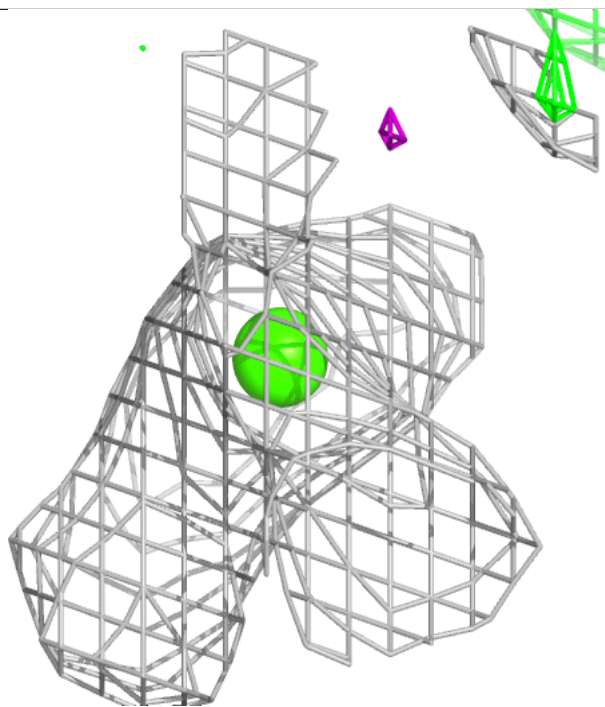
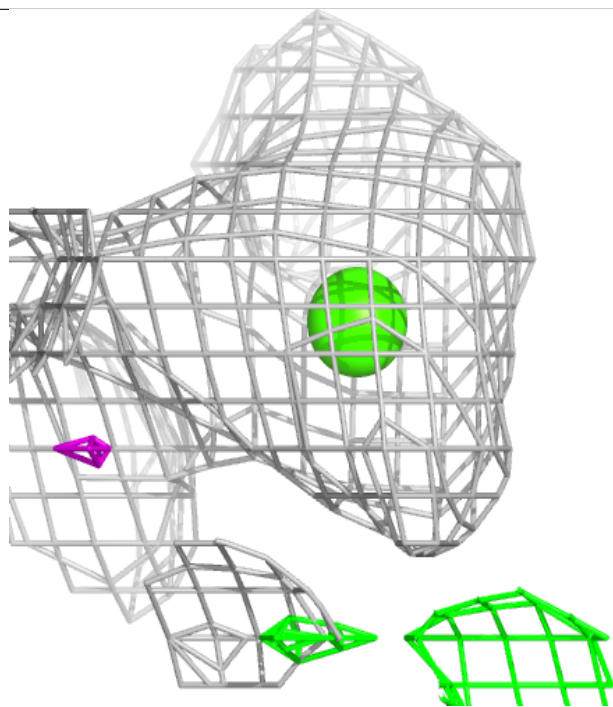
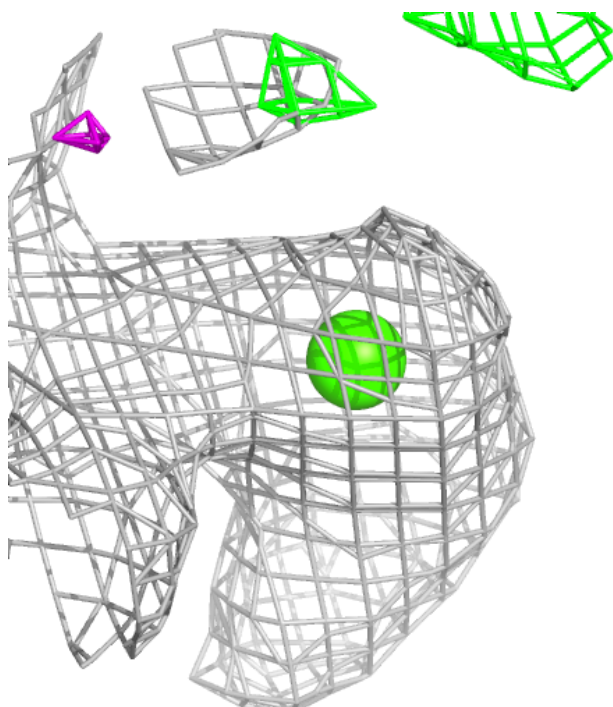
Electron density around NA D 305:

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



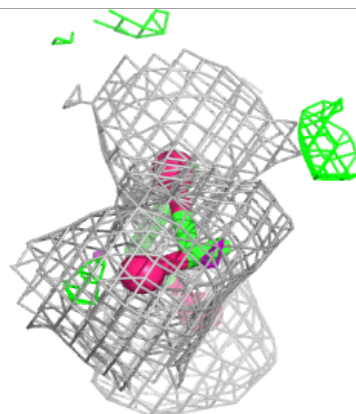
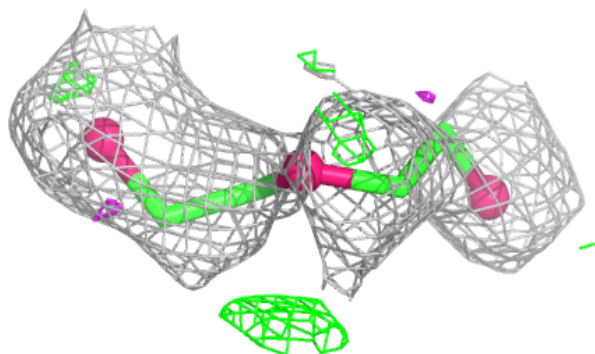
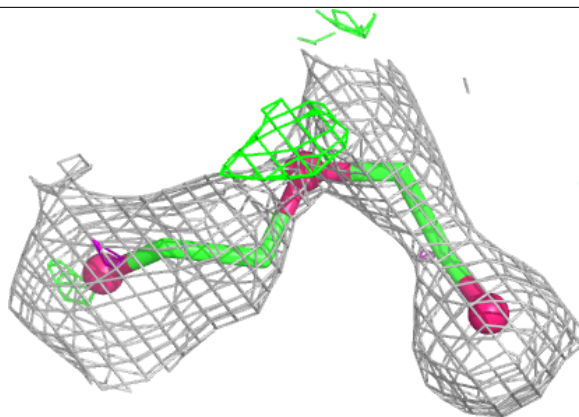
Electron density around CA A 305:

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



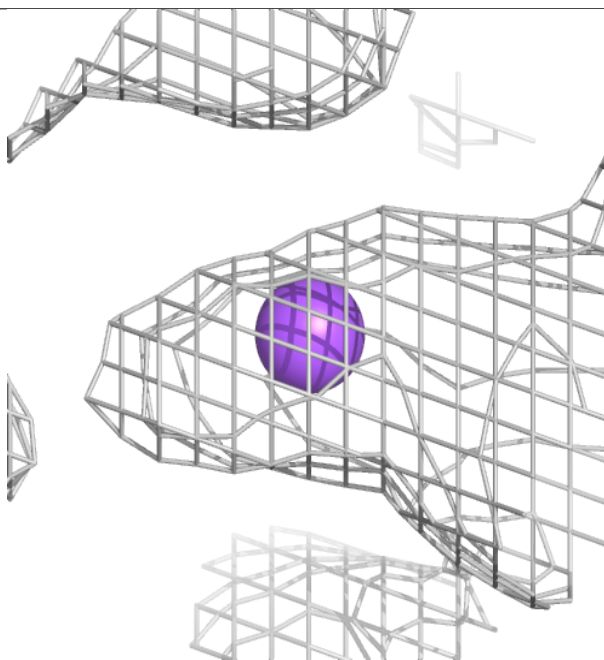
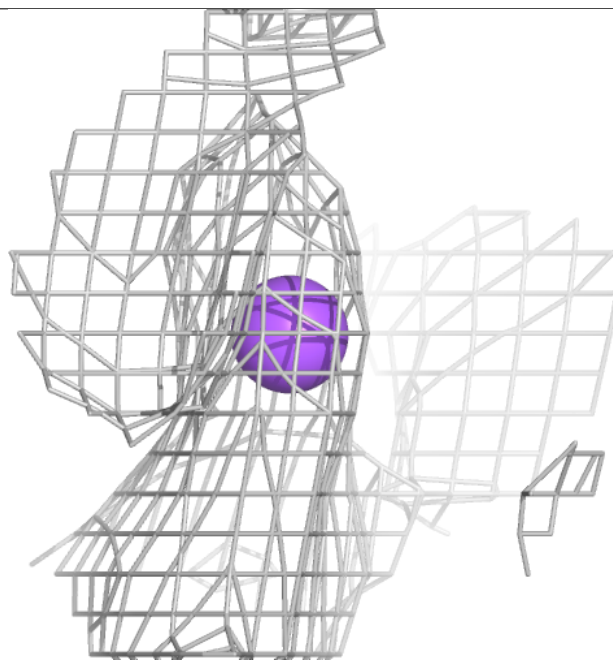
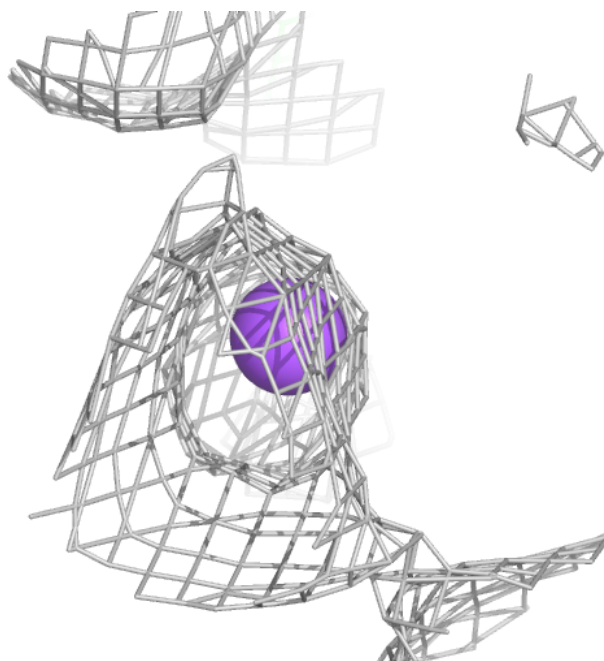
Electron density around PEG D 303:

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



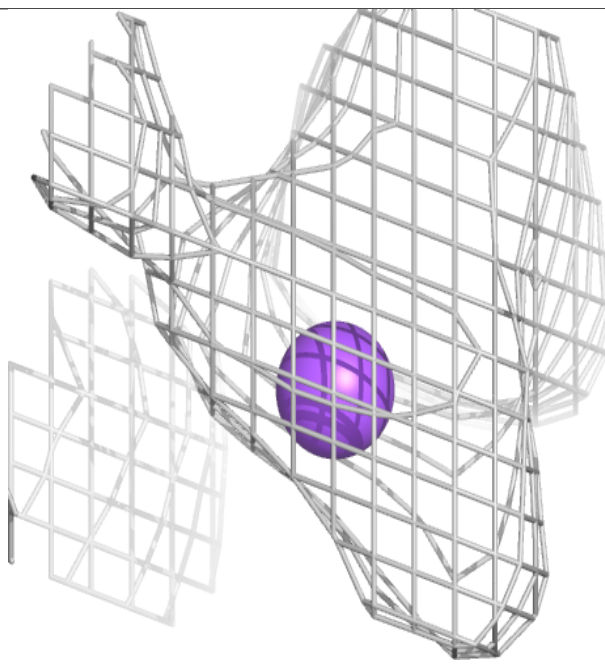
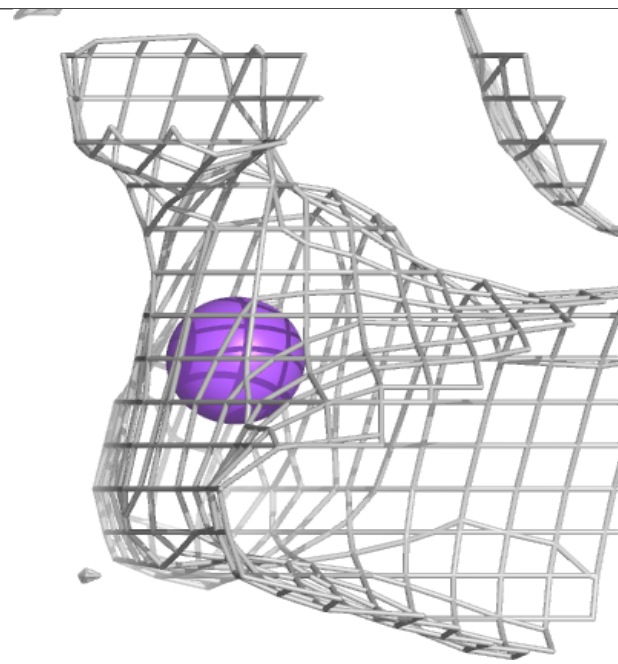
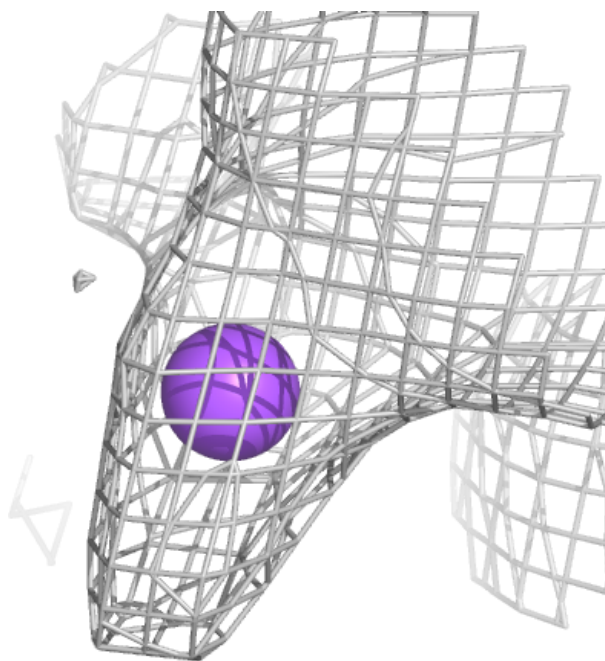
Electron density around NA C 304:

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



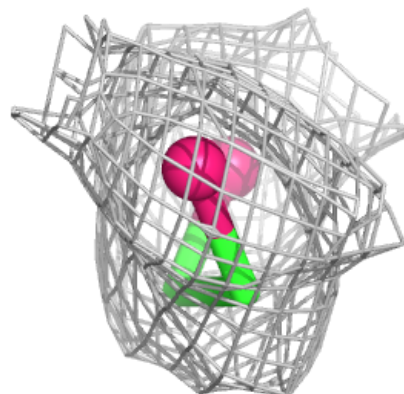
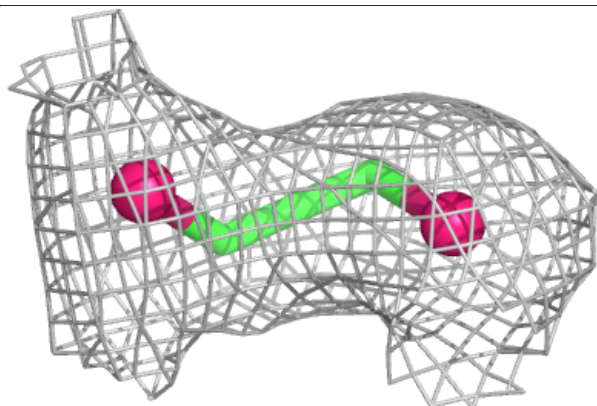
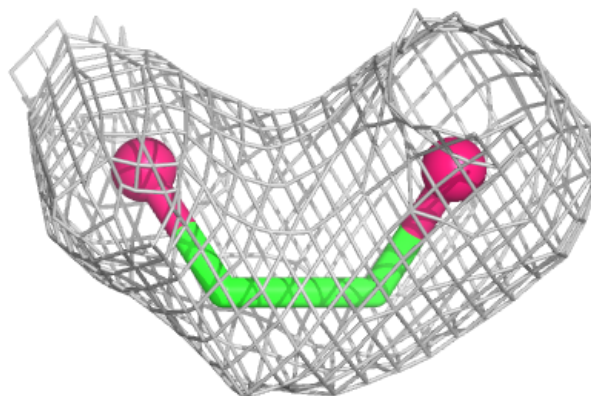
Electron density around NA B 302:

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



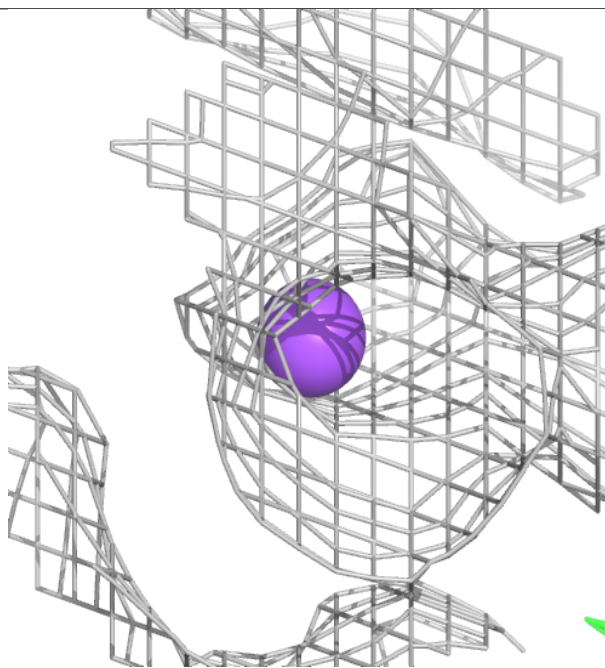
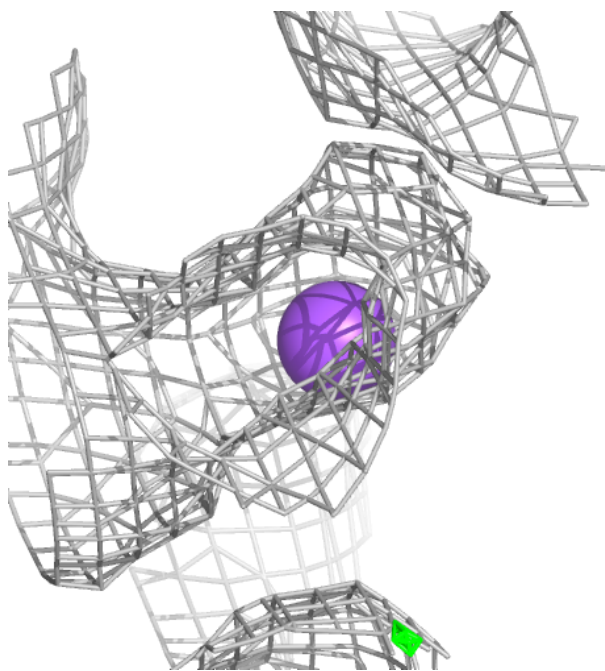
Electron density around EDO C 310:

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



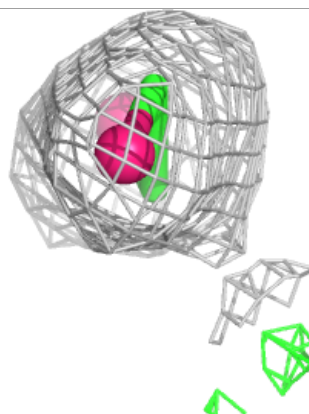
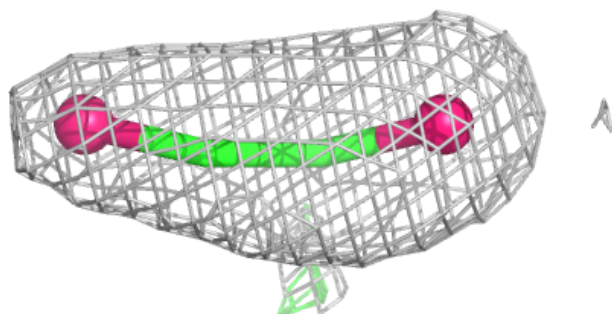
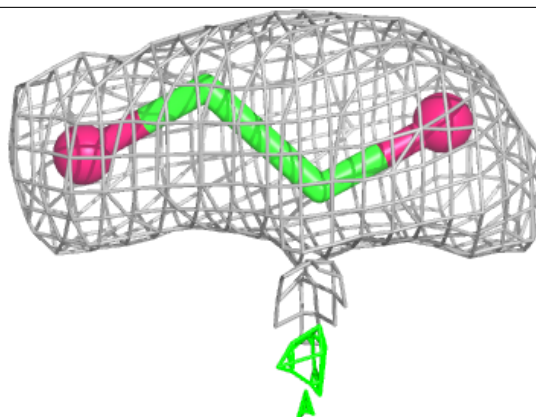
Electron density around NA D 307:

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

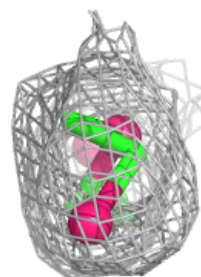
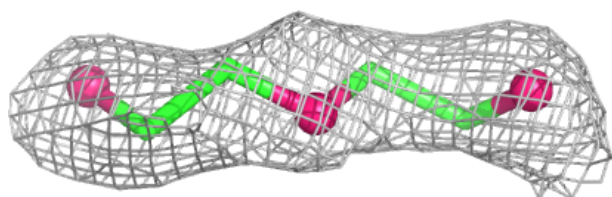
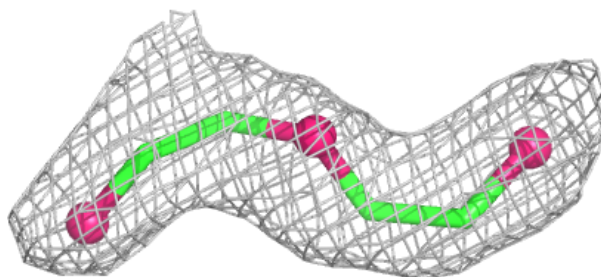


Electron density around EDO A 306:

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

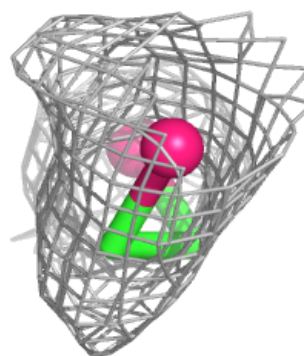
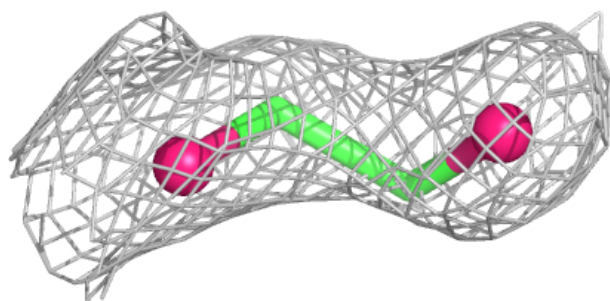
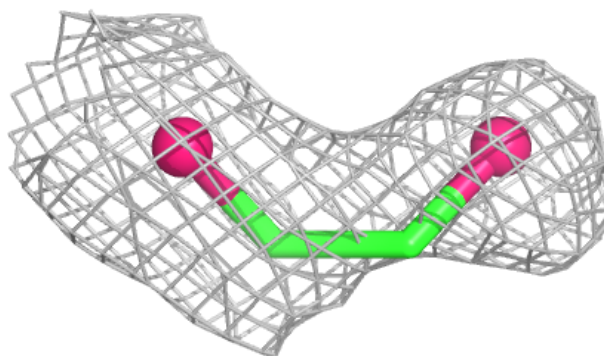
**Electron density around PEG D 302:**

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

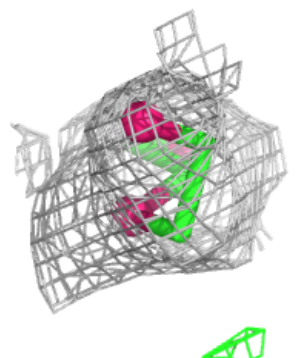
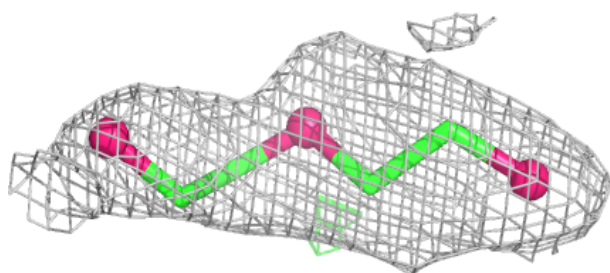
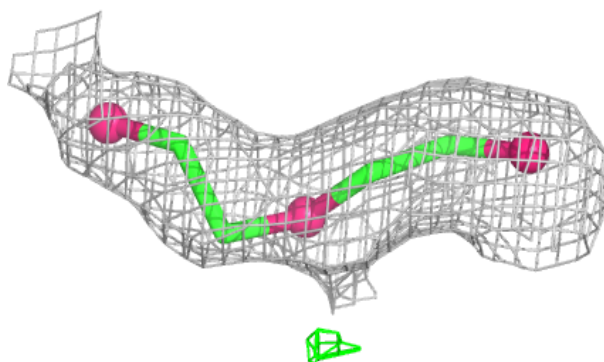


Electron density around EDO C 309:

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

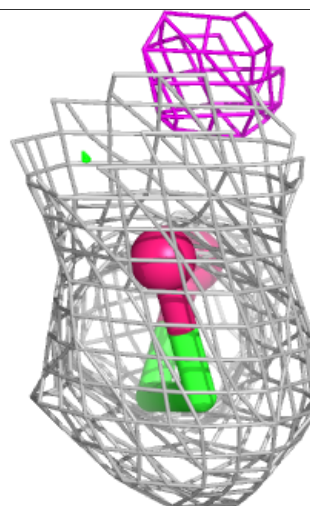
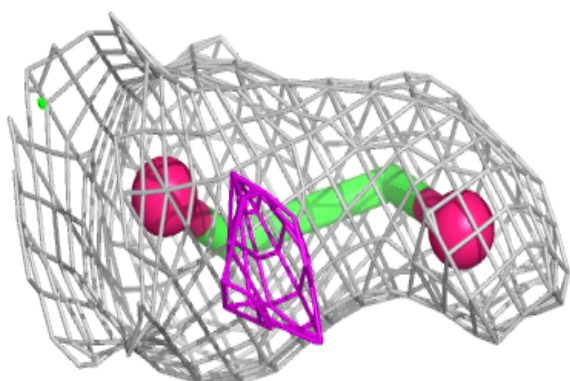
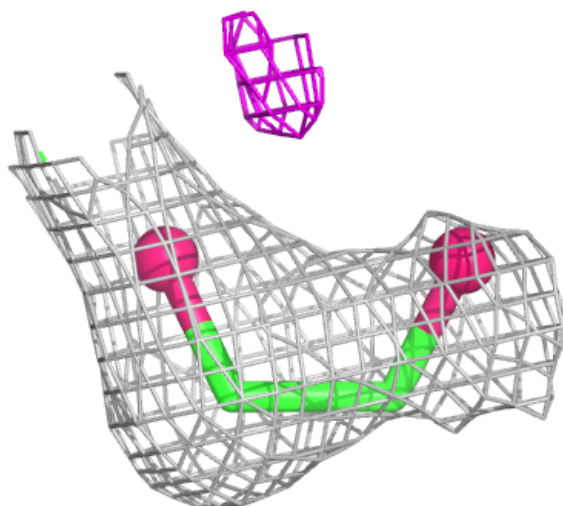
**Electron density around PEG D 304:**

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



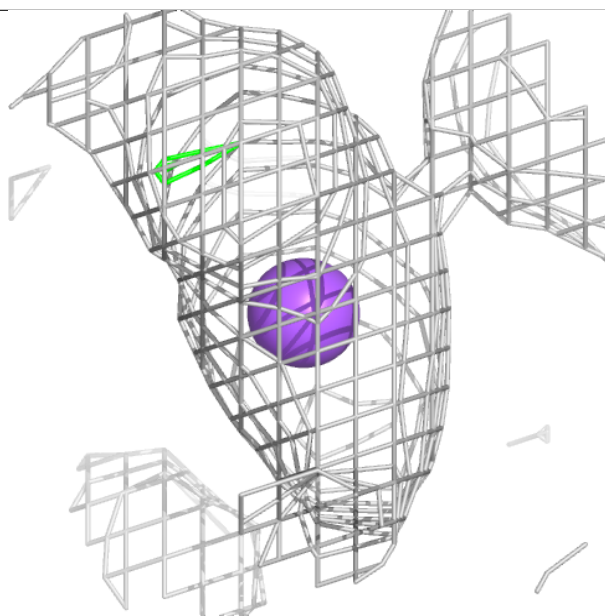
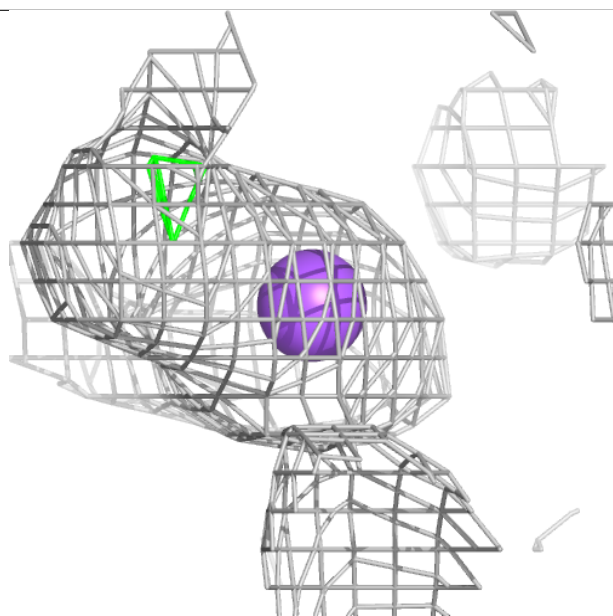
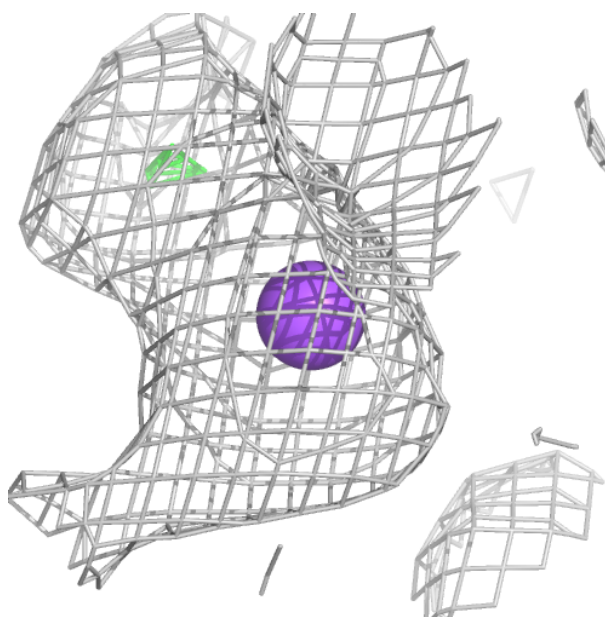
Electron density around EDO B 301:

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



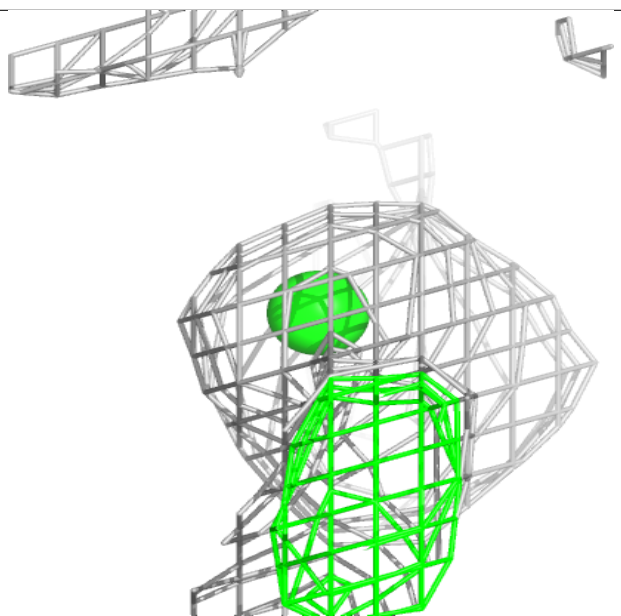
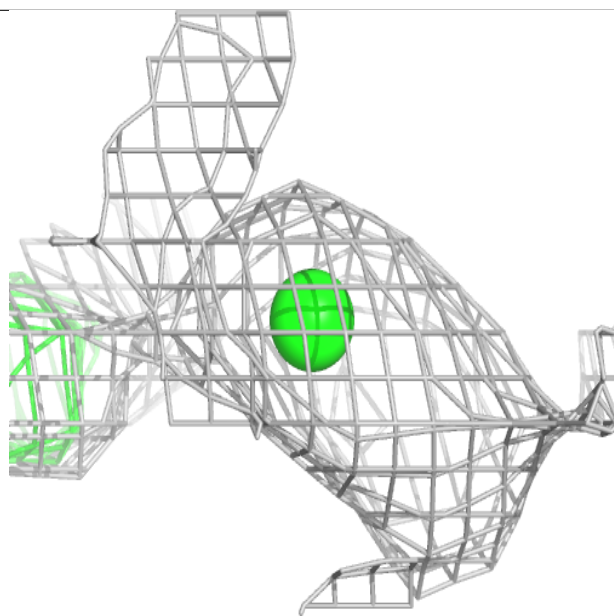
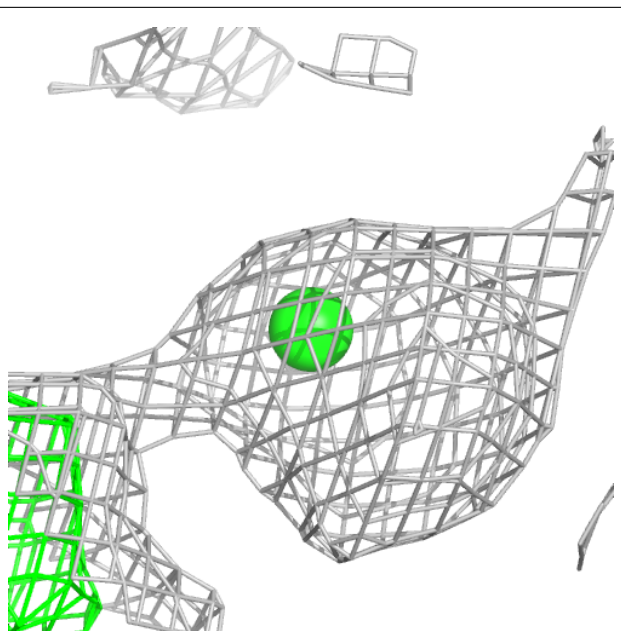
Electron density around NA D 306:

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



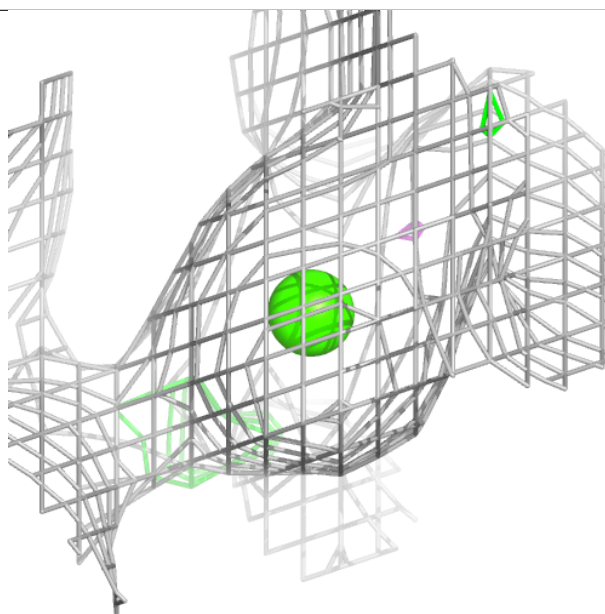
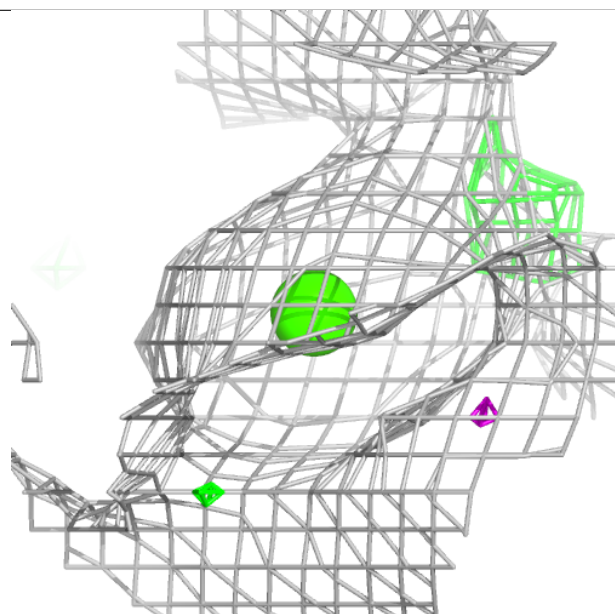
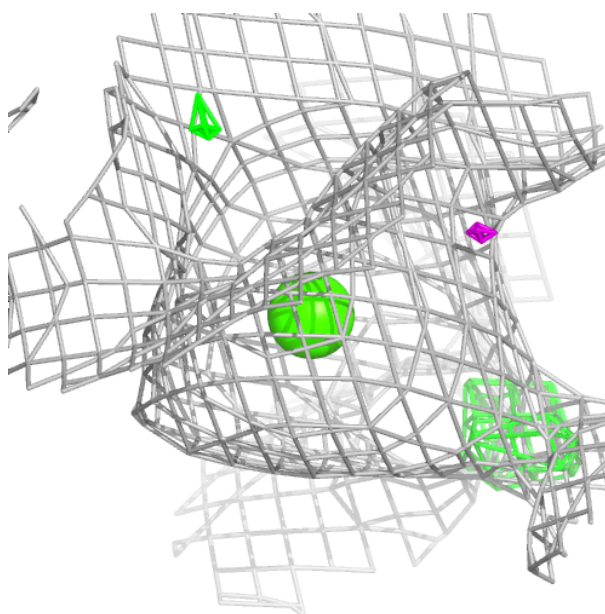
Electron density around CL B 305:

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



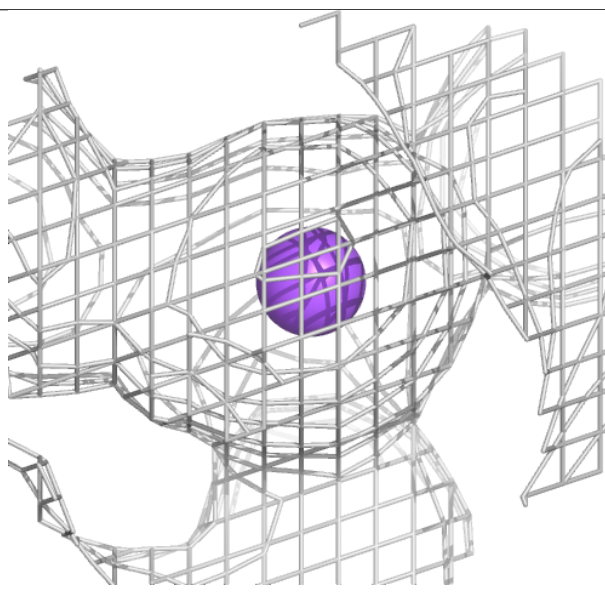
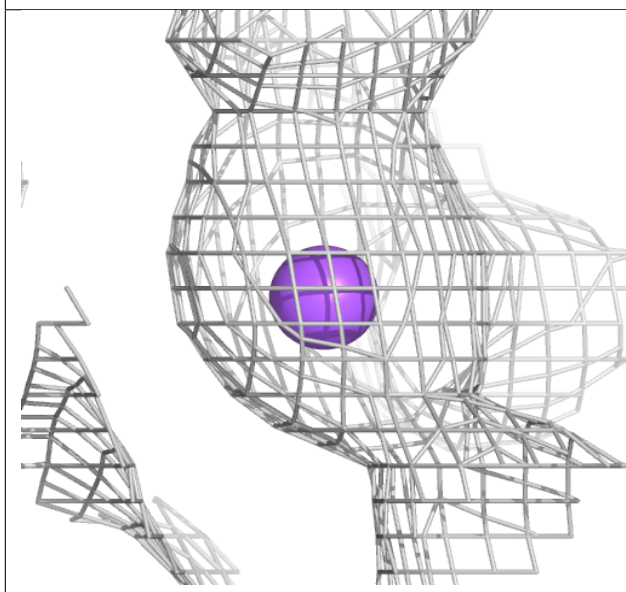
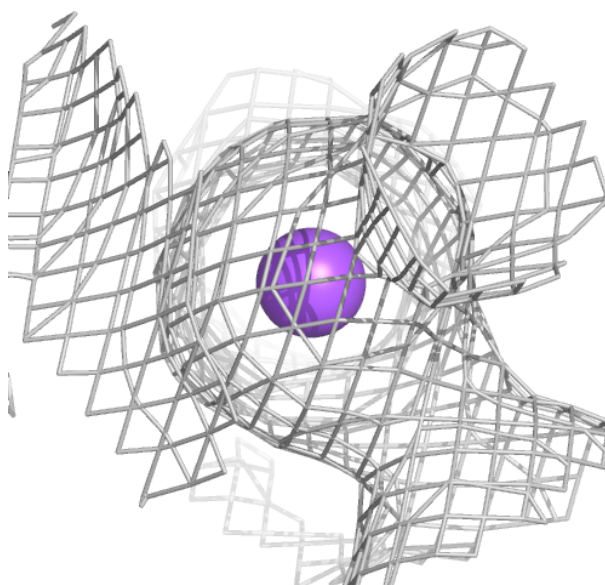
Electron density around CA C 305:

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



Electron density around NA A 304:

$2mF_o-DF_c$ (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.