



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:21 AM UTC

PDB ID : 8ZN4 / pdb_00008zn4
Title : Crystal structure of Poly(ethylene glycol) stabilized erythrose-4-phosphate dehydrogenase from *Acinetobacter baumannii* at 2.30 Å resolution
Authors : Viswanathan, V.; Kumari, A.; Singh, A.; Kumar, A.; Sharma, P.; Chopra, S.; Sharma, S.; Raje, C.I.; Singh, T.P.
Deposited on : 2024-05-25
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

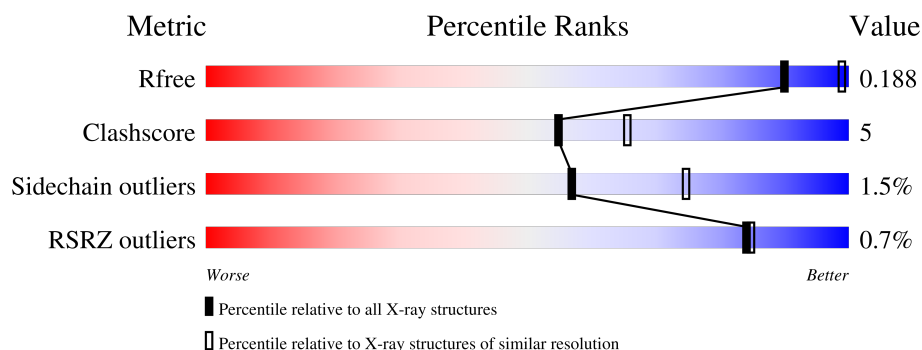
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	341	% 87% 12% .
1	B	341	% 90% 10%
1	C	341	% 89% 9% .
1	D	341	% 89% 11% .

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 11897 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	1	0
			2690	1707	474	500	9			
1	B	341	Total	C	N	O	S	0	1	0
			2690	1707	474	500	9			
1	C	341	Total	C	N	O	S	0	1	0
			2690	1707	474	500	9			
1	D	341	Total	C	N	O	S	0	2	0
			2698	1713	475	501	9			

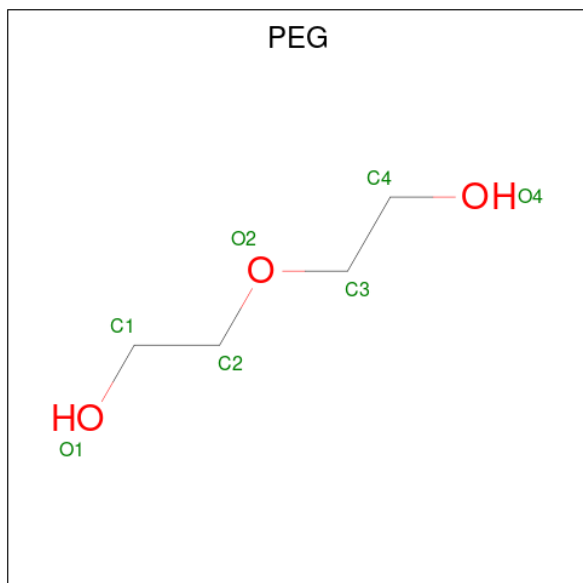
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



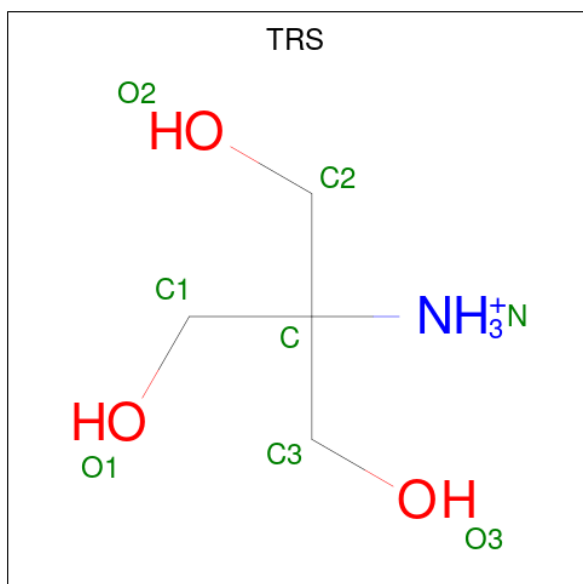
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃) (labeled as "Ligand of Interest" by depositor).



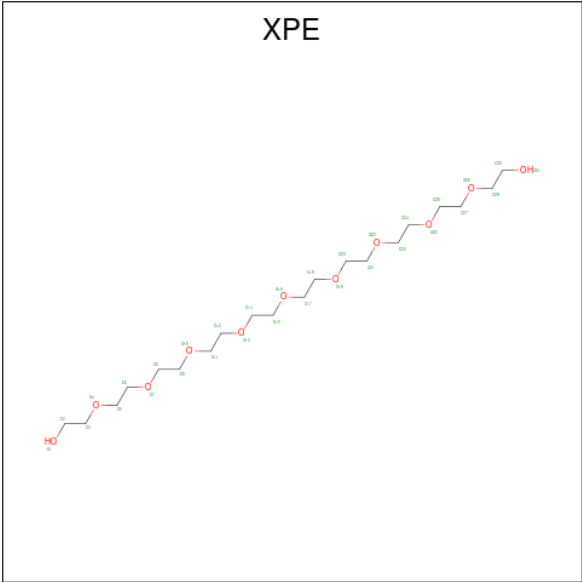
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



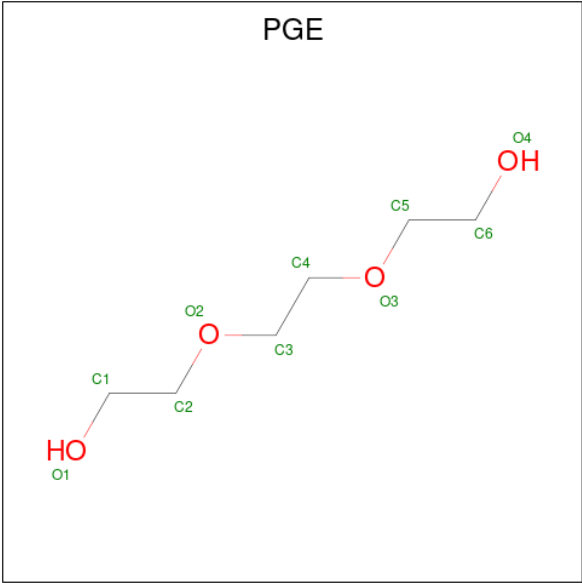
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (CCD ID: XPE) (formula: C₂₀H₄₂O₁₁) (labeled as "Ligand of Interest" by depositor).



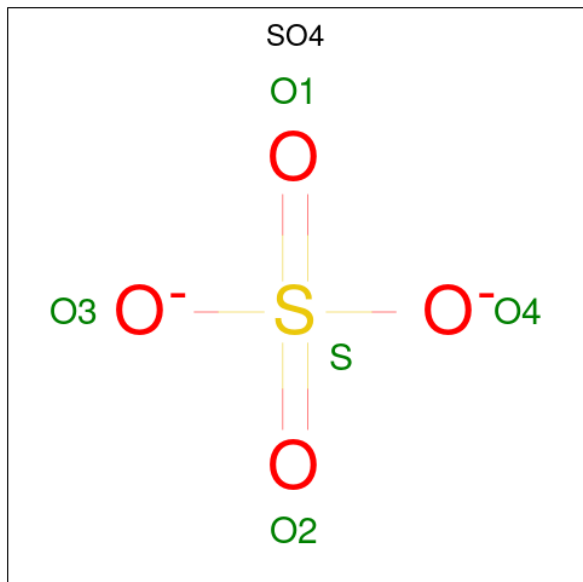
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			31	20	11		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		
9	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Mg	0	0
			1	1		

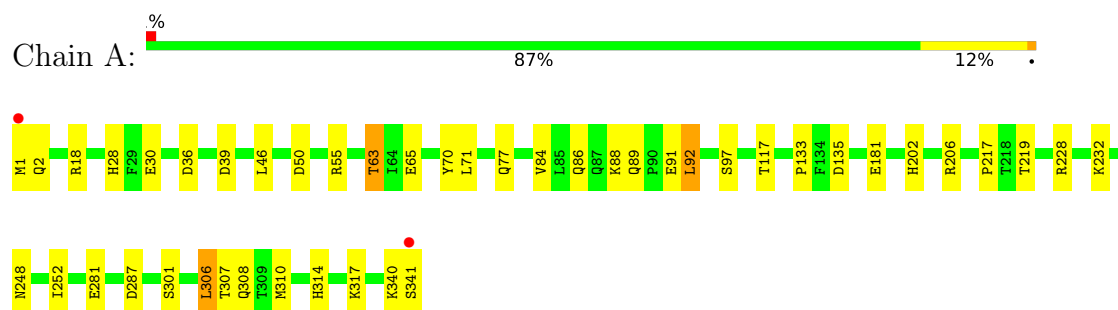
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	178	Total	O	0	0
			178	178		
12	B	153	Total	O	0	0
			153	153		
12	C	164	Total	O	0	0
			164	164		
12	D	146	Total	O	0	0
			146	146		

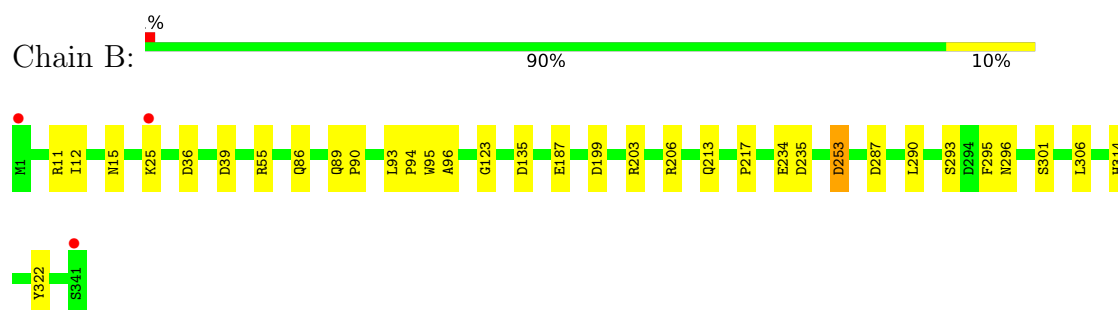
3 Residue-property plots [i](#)

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.

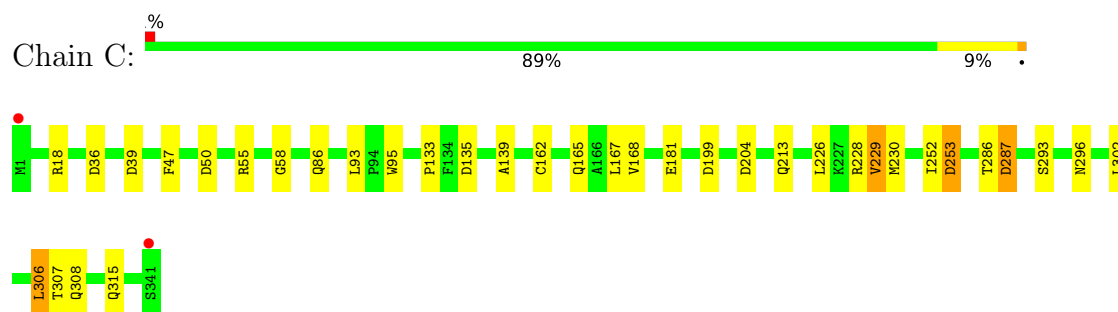
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



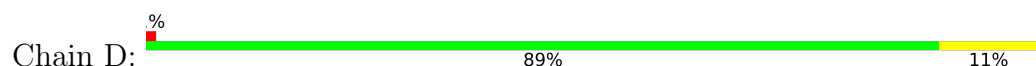
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

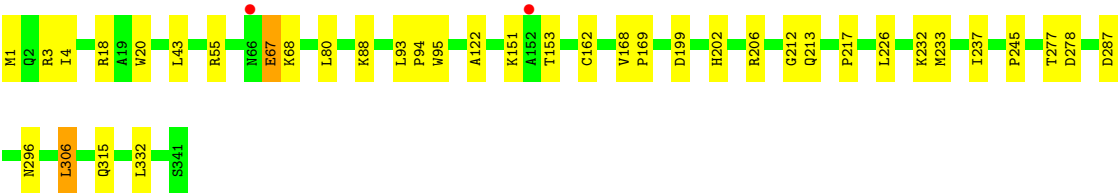


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	145.78Å 167.13Å 150.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.30 46.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.70-2.30) 100.0 (46.70-2.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.152 , 0.201 (Not available) , 0.188	Depositor DCC
R_{free} test set	2400 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11897	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XPE, NAD, GOL, PGE, SO4, PG4, EDO, MG, TRS, PEG

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	0.59	0/2744	1.06	7/3730 (0.2%)
1	B	0.59	0/2744	1.04	5/3730 (0.1%)
1	C	0.60	0/2744	1.05	9/3730 (0.2%)
1	D	0.59	0/2752	1.09	9/3741 (0.2%)
All	All	0.59	0/10984	1.06	30/14931 (0.2%)

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	B	0	1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ASP	CA-CB-CG	7.29	119.89	112.60
1	D	199	ASP	CA-CB-CG	7.09	119.69	112.60
1	C	213	GLN	N-CA-CB	-6.75	101.93	110.90
1	A	2	GLN	CB-CA-C	6.52	121.30	109.62
1	B	94	PRO	N-CA-CB	-6.41	98.51	102.81
1	A	202	HIS	CA-CB-CG	6.26	120.06	113.80
1	A	219	THR	CA-CB-OG1	-6.12	100.41	109.60
1	C	204	ASP	CA-CB-CG	6.11	118.71	112.60
1	D	278	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	50	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	18	ARG	CB-CA-C	-5.78	101.19	110.79
1	A	135	ASP	CA-CB-CG	5.78	118.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ASP	CA-CB-CG	5.70	118.30	112.60
1	C	199	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	67	GLU	CB-CG-CD	5.65	122.21	112.60
1	D	18	ARG	CB-CA-C	-5.62	101.46	110.79
1	B	295	PHE	CA-CB-CG	-5.55	108.25	113.80
1	D	94	PRO	N-CA-CB	-5.52	99.11	102.81
1	C	135	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	253	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	202	HIS	CA-CB-CG	5.39	119.19	113.80
1	C	181	GLU	CB-CA-C	5.37	119.28	110.95
1	D	18	ARG	N-CA-CB	5.29	117.90	110.12
1	A	117	THR	CA-CB-OG1	-5.23	101.75	109.60
1	B	199	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	286	THR	CA-CB-OG1	-5.21	101.79	109.60
1	C	287	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	245	PRO	N-CA-C	5.15	119.44	112.48
1	D	277	THR	O-C-N	5.11	124.61	120.83
1	C	50	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	203	ARG	Sidechain

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	2690	0	2696	30	0
1	B	2690	0	2696	26	0
1	C	2690	0	2696	23	0
1	D	2698	0	2706	27	0
2	A	44	0	26	0	0
2	B	44	0	26	3	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	20	1	0
3	B	21	0	30	1	0
3	C	7	0	10	1	0
3	D	7	0	10	2	0
4	A	13	0	18	3	0
4	B	26	0	36	5	0
4	C	26	0	36	3	0
4	D	13	0	18	2	0
5	A	28	0	42	1	0
5	B	12	0	18	0	0
5	C	8	0	12	0	0
5	D	24	0	36	1	0
6	A	8	0	12	4	0
6	B	8	0	12	1	0
7	A	6	0	8	1	0
7	B	12	0	16	2	0
7	C	6	0	8	3	0
7	D	6	0	8	1	0
8	A	31	0	40	2	0
9	A	10	0	14	3	0
9	C	10	0	14	1	0
10	A	5	0	0	0	0
10	C	5	0	0	0	0
10	D	5	0	0	0	0
11	B	1	0	0	0	0
12	A	178	0	0	6	0
12	B	153	0	0	2	0
12	C	164	0	0	1	0
12	D	146	0	0	7	0
All	All	11897	0	11316	108	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 5.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HG2	12:D:612:HOH:O	1.88	0.71
1:C:58:GLY:HA2	4:C:406:PG4:H61	1.73	0.71
1:D:68:LYS:HE3	12:D:611:HOH:O	1.90	0.71
1:C:165:GLN:HB2	7:C:408:GOL:H32	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:HB3	1:B:306:LEU:HD21	1.75	0.68
1:A:63:THR:HG22	1:A:70:TYR:HB2	1.78	0.66
5:D:404:EDO:O2	12:D:501:HOH:O	2.15	0.64
1:A:287:ASP:HB3	1:A:306:LEU:HD21	1.80	0.64
1:B:293:SER:HA	4:B:409:PG4:H12	1.80	0.64
1:B:12:ILE:HG12	12:B:620:HOH:O	1.98	0.64
1:C:229:VAL:HG23	1:C:230:MET:HG3	1.82	0.61
1:A:232:LYS:HG2	12:A:634:HOH:O	2.01	0.61
6:A:407:TRS:H21	12:A:645:HOH:O	2.01	0.60
1:A:306:LEU:HD12	1:A:306:LEU:C	2.27	0.60
1:A:1:MET:SD	1:A:30:GLU:HG3	2.43	0.59
1:C:306:LEU:C	1:C:306:LEU:HD12	2.28	0.58
8:A:414:XPE:H31A	12:B:503:HOH:O	2.03	0.58
1:D:287:ASP:HB3	1:D:306:LEU:HD21	1.85	0.58
1:D:233:MET:HE2	1:D:237[B]:ILE:HD11	1.86	0.57
1:C:287:ASP:HB3	1:C:306:LEU:HD21	1.86	0.57
1:A:307:THR:OG1	1:B:206[A]:ARG:NH1	2.38	0.56
1:A:287:ASP:HA	1:A:306:LEU:HG	1.87	0.56
1:B:11:ARG:O	1:B:15:ASN:ND2	2.39	0.54
1:A:248:ASN:O	4:A:403:PG4:H82	2.08	0.54
1:D:213:GLN:O	1:D:213:GLN:HG3	2.08	0.54
1:A:281:GLU:OE1	6:A:407:TRS:H11	2.08	0.54
1:C:93:LEU:HD13	1:C:95:TRP:CZ2	2.42	0.54
1:A:55:ARG:HH22	9:A:415:PGE:C6	2.21	0.53
1:C:55:ARG:HH22	9:C:401:PGE:H3	1.73	0.53
1:B:93:LEU:HD13	1:B:95:TRP:CZ2	2.44	0.52
1:A:36:ASP:O	1:A:86:GLN:HA	2.09	0.52
1:A:314:HIS:CD2	3:A:402:PEG:H32	2.46	0.51
1:D:67:GLU:HG2	1:D:68:LYS:HG3	1.91	0.51
1:C:139:ALA:HA	3:C:405:PEG:H22	1.91	0.51
1:C:293:SER:HA	4:C:403:PG4:H71	1.92	0.51
1:A:55:ARG:HH22	9:A:415:PGE:H62	1.76	0.50
1:D:226:LEU:HD22	1:D:237[A]:ILE:HG21	1.92	0.50
1:C:36:ASP:O	1:C:86:GLN:HA	2.10	0.50
1:A:55:ARG:HH12	9:A:415:PGE:H62	1.77	0.50
1:B:12:ILE:CD1	2:B:402:NAD:O4D	2.60	0.49
1:C:308:GLN:HE21	1:D:206[B]:ARG:NH2	2.11	0.49
1:D:55:ARG:HH12	3:D:401:PEG:H12	1.77	0.49
1:D:306:LEU:C	1:D:306:LEU:HD12	2.37	0.49
1:A:28:HIS:HB2	1:A:341:SER:OG	2.13	0.48
1:A:91:GLU:HG2	1:A:92:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:OE1	1:B:206[A]:ARG:NH1	2.46	0.48
1:C:162:CYS:HB2	7:C:408:GOL:H11	1.96	0.48
1:D:93:LEU:HD13	1:D:95:TRP:CZ2	2.48	0.48
1:B:36:ASP:O	1:B:86:GLN:HA	2.13	0.48
1:A:206[B]:ARG:HD3	1:A:217:PRO:O	2.14	0.48
1:D:232:LYS:HG2	12:D:607:HOH:O	2.14	0.48
1:B:287:ASP:HB3	1:B:306:LEU:CD2	2.44	0.47
1:C:133:PRO:HG2	1:C:228:ARG:HD3	1.94	0.47
1:B:206[B]:ARG:HD2	1:B:217:PRO:O	2.14	0.47
6:A:407:TRS:C2	12:A:645:HOH:O	2.61	0.47
1:A:281:GLU:OE1	6:A:407:TRS:C1	2.64	0.46
1:D:67:GLU:H	1:D:67:GLU:CD	2.24	0.46
1:A:301:SER:HA	7:A:413:GOL:H12	1.97	0.46
1:D:296:ASN:CB	4:D:407:PG4:H31	2.45	0.46
1:A:181:GLU:OE2	6:B:401:TRS:O3	2.33	0.46
1:A:340:LYS:HA	12:A:639:HOH:O	2.16	0.46
1:B:213:GLN:HG3	1:B:213:GLN:O	2.15	0.46
1:D:151:LYS:HB3	1:D:153:THR:HG22	1.98	0.46
1:D:168:VAL:HB	1:D:169:PRO:HD3	1.97	0.45
1:B:301:SER:O	7:B:411:GOL:O2	2.35	0.45
1:B:301:SER:HA	7:B:411:GOL:H12	1.98	0.45
1:A:77:GLN:HB2	5:A:404:EDO:H21	1.99	0.45
1:C:18:ARG:HG3	1:C:47:PHE:CE1	2.51	0.45
1:C:165:GLN:CB	7:C:408:GOL:H32	2.44	0.45
1:C:226:LEU:C	1:C:226:LEU:HD23	2.43	0.44
1:C:168:VAL:HG21	1:C:229:VAL:HG21	1.99	0.44
8:A:414:XPE:H172	1:D:212:GLY:CA	2.47	0.44
1:C:307:THR:OG1	1:D:206[B]:ARG:NH2	2.51	0.44
1:A:206[A]:ARG:NH2	1:B:290:LEU:O	2.48	0.44
1:B:234:GLU:O	1:B:235:ASP:HB2	2.17	0.44
1:C:315:GLN:HE21	1:D:315:GLN:HE21	1.66	0.43
4:A:403:PG4:H61	12:A:587:HOH:O	2.18	0.43
1:B:12:ILE:HD11	2:B:402:NAD:N1N	2.33	0.43
1:B:293:SER:CA	4:B:409:PG4:H12	2.48	0.43
1:B:306:LEU:C	1:B:306:LEU:HD12	2.43	0.43
1:C:296:ASN:HB2	4:C:403:PG4:H61	2.00	0.43
1:A:46:LEU:HD23	12:A:617:HOH:O	2.18	0.43
1:C:167:LEU:HD13	1:C:252:ILE:HD11	2.00	0.43
1:C:162:CYS:H	2:C:402:NAD:H5N	1.84	0.43
1:A:310:MET:HE2	1:A:317:LYS:HD2	2.01	0.43
1:D:206[A]:ARG:HD3	1:D:217:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLU:OE2	1:B:322:TYR:OH	2.28	0.43
1:D:162:CYS:HB2	7:D:410:GOL:H12	2.01	0.43
1:A:71:LEU:HG	1:A:84:VAL:CG2	2.48	0.43
1:D:20:TRP:CH2	1:D:80:LEU:HD21	2.53	0.43
1:D:93:LEU:O	1:D:122:ALA:HB1	2.19	0.43
1:B:96:ALA:HB2	1:B:123:GLY:HA3	2.01	0.42
1:C:302:LEU:N	1:C:302:LEU:HD23	2.34	0.42
1:A:88:LYS:HG3	1:A:89:GLN:HG3	2.01	0.42
1:D:296:ASN:HB3	4:D:407:PG4:H31	2.00	0.42
1:B:314:HIS:HD2	3:B:406:PEG:H42	1.85	0.42
1:D:332:LEU:HD23	1:D:332:LEU:HA	1.91	0.42
4:A:403:PG4:H21	12:C:604:HOH:O	2.19	0.42
1:A:63:THR:HG23	1:A:65:GLU:HG3	2.03	0.41
1:B:296:ASN:HB3	4:B:409:PG4:H61	2.01	0.41
1:B:55:ARG:HH22	4:B:413:PG4:H51	1.85	0.41
3:D:401:PEG:C1	12:D:570:HOH:O	2.69	0.41
1:D:3:ARG:HD2	12:D:578:HOH:O	2.20	0.41
1:D:237[A]:ILE:O	1:D:237[A]:ILE:HG23	2.20	0.41
1:B:89:GLN:HA	1:B:90:PRO:HD3	1.95	0.41
1:B:12:ILE:HD11	2:B:402:NAD:O4D	2.21	0.40
1:A:133:PRO:HG2	1:A:228:ARG:HD3	2.03	0.40
4:B:413:PG4:H61	12:D:590:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/292 (100%)	287 (98%)	6 (2%)	48	67
1	B	293/292 (100%)	290 (99%)	3 (1%)	68	82
1	C	293/292 (100%)	289 (99%)	4 (1%)	59	76
1	D	294/292 (101%)	290 (99%)	4 (1%)	59	76
All	All	1173/1168 (100%)	1156 (99%)	17 (1%)	57	76

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	63	THR
1	A	92	LEU
1	A	97	SER
1	A	252	ILE
1	A	306	LEU
1	B	25	LYS
1	B	39	ASP
1	B	253	ASP
1	C	39	ASP
1	C	229	VAL
1	C	253	ASP
1	C	306	LEU
1	D	4	ILE
1	D	43	LEU
1	D	88	LYS
1	D	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	113	HIS
1	A	155	GLN
1	A	200	HIS
1	A	276	GLN
1	A	315	GLN
1	B	113	HIS
1	B	248	ASN
1	C	2	GLN
1	C	113	HIS

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Mol	Chain	Res	Type
1	C	248	ASN
1	C	308	GLN
1	D	2	GLN
1	D	28	HIS
1	D	74	GLN
1	D	248	ASN
1	D	315	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 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	$\# Z > 2$
5	EDO	B	408	-	3,3,3	0.10	0	2,2,2	0.14	0
3	PEG	B	406	-	6,6,6	0.32	0	5,5,5	0.22	0
3	PEG	B	410	-	6,6,6	0.24	0	5,5,5	0.15	0
2	NAD	A	401	-	46,48,48	0.81	2 (4%)	64,73,73	0.73	0
7	GOL	D	410	-	5,5,5	0.21	0	5,5,5	0.60	0
10	SO4	D	408	-	4,4,4	0.33	0	6,6,6	0.05	0
6	TRS	B	401	-	7,7,7	0.28	0	9,9,9	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PGE	C	401	-	9,9,9	0.31	0	8,8,8	0.27	0
2	NAD	C	402	-	46,48,48	0.89	2 (4%)	64,73,73	0.74	1 (1%)
3	PEG	A	402	-	6,6,6	0.39	0	5,5,5	0.49	0
5	EDO	A	405	-	3,3,3	0.14	0	2,2,2	0.23	0
10	SO4	C	409	-	4,4,4	0.27	0	6,6,6	0.13	0
4	PG4	B	409	-	12,12,12	0.25	0	11,11,11	0.28	0
3	PEG	B	405	-	6,6,6	0.37	0	5,5,5	0.35	0
5	EDO	D	406	-	3,3,3	0.15	0	2,2,2	0.27	0
4	PG4	D	407	-	12,12,12	0.33	0	11,11,11	0.25	0
5	EDO	A	410	-	3,3,3	0.38	0	2,2,2	0.44	0
4	PG4	B	413	-	12,12,12	0.22	0	11,11,11	0.23	0
9	PGE	A	415	-	9,9,9	0.26	0	8,8,8	0.19	0
5	EDO	A	409	-	3,3,3	0.21	0	2,2,2	0.40	0
5	EDO	A	412	-	3,3,3	0.14	0	2,2,2	0.17	0
8	XPE	A	414	11	30,30,30	0.32	0	29,29,29	0.28	0
10	SO4	A	416	-	4,4,4	0.30	0	6,6,6	0.13	0
5	EDO	D	409	-	3,3,3	0.17	0	2,2,2	0.26	0
6	TRS	A	407	-	7,7,7	0.23	0	9,9,9	0.54	0
5	EDO	A	411	-	3,3,3	0.13	0	2,2,2	0.24	0
5	EDO	D	405	-	3,3,3	0.28	0	2,2,2	0.24	0
7	GOL	B	411	-	5,5,5	0.28	0	5,5,5	0.76	0
3	PEG	C	405	-	6,6,6	0.38	0	5,5,5	0.22	0
2	NAD	D	402	-	46,48,48	0.81	2 (4%)	64,73,73	0.70	1 (1%)
4	PG4	C	403	-	12,12,12	0.55	0	11,11,11	0.37	0
7	GOL	A	413	-	5,5,5	0.19	0	5,5,5	0.60	0
5	EDO	A	404	-	3,3,3	0.28	0	2,2,2	0.48	0
4	PG4	A	403	-	12,12,12	0.41	0	11,11,11	0.24	0
5	EDO	D	404	-	3,3,3	0.10	0	2,2,2	0.33	0
5	EDO	C	407	-	3,3,3	0.14	0	2,2,2	0.23	0
5	EDO	C	404	-	3,3,3	0.20	0	2,2,2	0.34	0
3	PEG	A	408	-	6,6,6	0.21	0	5,5,5	0.19	0
7	GOL	C	408	-	5,5,5	0.12	0	5,5,5	0.32	0
5	EDO	D	411	-	3,3,3	0.14	0	2,2,2	0.16	0
3	PEG	D	401	-	6,6,6	0.20	0	5,5,5	0.23	0
5	EDO	B	404	-	3,3,3	0.09	0	2,2,2	0.19	0
5	EDO	B	412	-	3,3,3	0.09	0	2,2,2	0.25	0
5	EDO	D	403	-	3,3,3	0.22	0	2,2,2	0.41	0
2	NAD	B	402	-	46,48,48	1.05	4 (8%)	64,73,73	0.71	1 (1%)
7	GOL	B	407	-	5,5,5	0.10	0	5,5,5	0.26	0
4	PG4	C	406	-	12,12,12	0.26	0	11,11,11	0.31	0
5	EDO	A	406	-	3,3,3	0.10	0	2,2,2	0.13	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
5	EDO	B	408	-	-	1/1/1/1	-
3	PEG	B	406	-	-	1/4/4/4	-
3	PEG	B	410	-	-	2/4/4/4	-
2	NAD	A	401	-	-	8/30/62/62	0/5/5/5
7	GOL	D	410	-	-	4/4/4/4	-
6	TRS	B	401	-	-	3/9/9/9	-
9	PGE	C	401	-	-	2/7/7/7	-
2	NAD	C	402	-	-	10/30/62/62	0/5/5/5
3	PEG	A	402	-	-	3/4/4/4	-
5	EDO	A	405	-	-	1/1/1/1	-
4	PG4	B	409	-	-	7/10/10/10	-
3	PEG	B	405	-	-	1/4/4/4	-
5	EDO	D	406	-	-	1/1/1/1	-
4	PG4	D	407	-	-	5/10/10/10	-
5	EDO	A	410	-	-	1/1/1/1	-
4	PG4	B	413	-	-	6/10/10/10	-
9	PGE	A	415	-	-	5/7/7/7	-
5	EDO	A	409	-	-	1/1/1/1	-
5	EDO	A	412	-	-	1/1/1/1	-
8	XPE	A	414	11	-	11/28/28/28	-
5	EDO	D	409	-	-	1/1/1/1	-
6	TRS	A	407	-	-	3/9/9/9	-
5	EDO	A	411	-	-	0/1/1/1	-
5	EDO	D	405	-	-	1/1/1/1	-
7	GOL	B	411	-	-	2/4/4/4	-
3	PEG	C	405	-	-	1/4/4/4	-
2	NAD	D	402	-	-	10/30/62/62	0/5/5/5
4	PG4	C	403	-	-	7/10/10/10	-
7	GOL	A	413	-	-	2/4/4/4	-
5	EDO	A	404	-	-	0/1/1/1	-
4	PG4	A	403	-	-	6/10/10/10	-
5	EDO	D	404	-	-	1/1/1/1	-
5	EDO	C	407	-	-	1/1/1/1	-
5	EDO	C	404	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	408	-	-	2/4/4/4	-
7	GOL	C	408	-	-	2/4/4/4	-
5	EDO	D	411	-	-	1/1/1/1	-
3	PEG	D	401	-	-	3/4/4/4	-
5	EDO	B	404	-	-	0/1/1/1	-
5	EDO	B	412	-	-	1/1/1/1	-
5	EDO	D	403	-	-	1/1/1/1	-
2	NAD	B	402	-	-	6/30/62/62	0/5/5/5
7	GOL	B	407	-	-	2/4/4/4	-
4	PG4	C	406	-	-	6/10/10/10	-
5	EDO	A	406	-	-	1/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	NAD	C2N-N1N	3.93	1.39	1.35
2	C	402	NAD	C2N-N1N	3.72	1.39	1.35
2	A	401	NAD	C2N-N1N	3.56	1.38	1.35
2	B	402	NAD	PN-O3	3.53	1.63	1.59
2	D	402	NAD	C2N-N1N	3.06	1.38	1.35
2	C	402	NAD	O4D-C1D	2.91	1.44	1.40
2	D	402	NAD	O4D-C1D	2.90	1.44	1.40
2	A	401	NAD	O4D-C1D	2.76	1.44	1.40
2	B	402	NAD	O4D-C1D	2.68	1.44	1.40
2	B	402	NAD	PA-O3	2.56	1.62	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	NAD	C6N-N1N-C2N	-3.47	118.92	121.88
2	C	402	NAD	C6N-N1N-C2N	-3.36	119.02	121.88
2	D	402	NAD	C6N-N1N-C2N	-2.38	119.85	121.88

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	C5D-O5D-PN-O2N
2	A	401	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	402	NAD	O4D-C1D-N1N-C2N
2	B	402	NAD	O4D-C1D-N1N-C6N
2	B	402	NAD	C2D-C1D-N1N-C2N
2	B	402	NAD	C2D-C1D-N1N-C6N
2	C	402	NAD	C5B-O5B-PA-O1A
2	C	402	NAD	C5B-O5B-PA-O3
2	C	402	NAD	O4D-C1D-N1N-C2N
2	C	402	NAD	O4D-C1D-N1N-C6N
2	D	402	NAD	C5B-O5B-PA-O1A
2	D	402	NAD	C5B-O5B-PA-O3
2	D	402	NAD	O4D-C1D-N1N-C2N
2	D	402	NAD	O4D-C1D-N1N-C6N
7	A	413	GOL	O1-C1-C2-C3
7	B	411	GOL	O1-C1-C2-C3
7	C	408	GOL	C1-C2-C3-O3
4	A	403	PG4	O2-C3-C4-O3
4	A	403	PG4	O3-C5-C6-O4
4	B	409	PG4	O3-C5-C6-O4
7	D	410	GOL	O1-C1-C2-O2
4	C	406	PG4	O2-C3-C4-O3
4	B	409	PG4	O1-C1-C2-O2
9	A	415	PGE	O1-C1-C2-O2
9	C	401	PGE	O3-C5-C6-O4
8	A	414	XPE	O4-C5-C6-O7
4	C	403	PG4	O2-C3-C4-O3
3	A	402	PEG	O2-C3-C4-O4
3	A	408	PEG	O1-C1-C2-O2
3	B	410	PEG	O1-C1-C2-O2
4	B	413	PG4	O1-C1-C2-O2
4	C	406	PG4	O4-C7-C8-O5
4	D	407	PG4	O4-C7-C8-O5
8	A	414	XPE	O1-C2-C3-O4
3	A	402	PEG	C1-C2-O2-C3
4	B	413	PG4	O2-C3-C4-O3
7	B	407	GOL	C1-C2-C3-O3
7	D	410	GOL	O1-C1-C2-C3
7	D	410	GOL	C1-C2-C3-O3
3	D	401	PEG	O2-C3-C4-O4
4	B	413	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
4	C	403	PG4	O1-C1-C2-O2
4	C	403	PG4	O4-C7-C8-O5
8	A	414	XPE	O28-C29-C30-O31
8	A	414	XPE	O7-C8-C9-O10
7	A	413	GOL	O1-C1-C2-O2
7	B	411	GOL	O1-C1-C2-O2
7	C	408	GOL	O2-C2-C3-O3
7	D	410	GOL	O2-C2-C3-O3
4	D	407	PG4	O1-C1-C2-O2
4	B	413	PG4	O3-C5-C6-O4
3	B	405	PEG	O2-C3-C4-O4
3	D	401	PEG	O1-C1-C2-O2
4	A	403	PG4	O4-C7-C8-O5
8	A	414	XPE	O13-C14-C15-O16
2	C	402	NAD	O4B-C4B-C5B-O5B
5	A	405	EDO	O1-C1-C2-O2
5	C	407	EDO	O1-C1-C2-O2
5	D	404	EDO	O1-C1-C2-O2
5	D	409	EDO	O1-C1-C2-O2
2	C	402	NAD	C3B-C4B-C5B-O5B
6	A	407	TRS	N-C-C1-O1
6	B	401	TRS	C2-C-C3-O3
6	B	401	TRS	N-C-C3-O3
5	B	412	EDO	O1-C1-C2-O2
5	C	404	EDO	O1-C1-C2-O2
3	C	405	PEG	O1-C1-C2-O2
9	A	415	PGE	C6-C5-O3-C4
4	A	403	PG4	C5-C6-O4-C7
8	A	414	XPE	C30-C29-O28-C27
9	A	415	PGE	C4-C3-O2-C2
4	C	406	PG4	C8-C7-O4-C6
8	A	414	XPE	C11-C12-O13-C14
4	B	409	PG4	C1-C2-O2-C3
4	B	409	PG4	O4-C7-C8-O5
4	D	407	PG4	C3-C4-O3-C5
4	C	406	PG4	C1-C2-O2-C3
4	B	413	PG4	C8-C7-O4-C6
3	B	406	PEG	C4-C3-O2-C2
8	A	414	XPE	C20-C21-O22-C23
6	A	407	TRS	C2-C-C1-O1
6	A	407	TRS	C3-C-C1-O1
6	B	401	TRS	C1-C-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	409	PG4	C8-C7-O4-C6
2	D	402	NAD	O4B-C4B-C5B-O5B
2	C	402	NAD	C5B-O5B-PA-O2A
2	D	402	NAD	C5B-O5B-PA-O2A
2	B	402	NAD	C4N-C3N-C7N-N7N
4	C	406	PG4	C4-C3-O2-C2
4	D	407	PG4	C8-C7-O4-C6
4	A	403	PG4	C6-C5-O3-C4
5	A	406	EDO	O1-C1-C2-O2
2	C	402	NAD	C2D-C1D-N1N-C2N
2	C	402	NAD	C2D-C1D-N1N-C6N
2	D	402	NAD	C2D-C1D-N1N-C2N
2	D	402	NAD	C2D-C1D-N1N-C6N
4	C	403	PG4	C6-C5-O3-C4
4	B	409	PG4	O2-C3-C4-O3
4	A	403	PG4	C1-C2-O2-C3
5	A	409	EDO	O1-C1-C2-O2
3	A	408	PEG	C1-C2-O2-C3
2	A	401	NAD	O4B-C4B-C5B-O5B
3	B	410	PEG	C4-C3-O2-C2
4	B	413	PG4	C4-C3-O2-C2
5	A	410	EDO	O1-C1-C2-O2
5	A	412	EDO	O1-C1-C2-O2
5	B	408	EDO	O1-C1-C2-O2
5	D	406	EDO	O1-C1-C2-O2
9	C	401	PGE	C6-C5-O3-C4
9	A	415	PGE	O3-C5-C6-O4
4	C	406	PG4	O3-C5-C6-O4
2	B	402	NAD	O4B-C4B-C5B-O5B
4	C	403	PG4	C5-C6-O4-C7
4	B	409	PG4	C6-C5-O3-C4
2	D	402	NAD	C2B-C1B-N9A-C8A
5	D	403	EDO	O1-C1-C2-O2
5	D	405	EDO	O1-C1-C2-O2
5	D	411	EDO	O1-C1-C2-O2
4	C	403	PG4	C3-C4-O3-C5
2	A	401	NAD	C2B-C1B-N9A-C8A
4	D	407	PG4	C5-C6-O4-C7
8	A	414	XPE	C23-C24-O25-C26
8	A	414	XPE	C14-C15-O16-C17
2	C	402	NAD	C4N-C3N-C7N-N7N
3	A	402	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	D	401	PEG	C4-C3-O2-C2
9	A	415	PGE	O2-C3-C4-O3
7	B	407	GOL	O2-C2-C3-O3
8	A	414	XPE	O10-C11-C12-O13
4	C	403	PG4	O3-C5-C6-O4
2	D	402	NAD	C3B-C4B-C5B-O5B

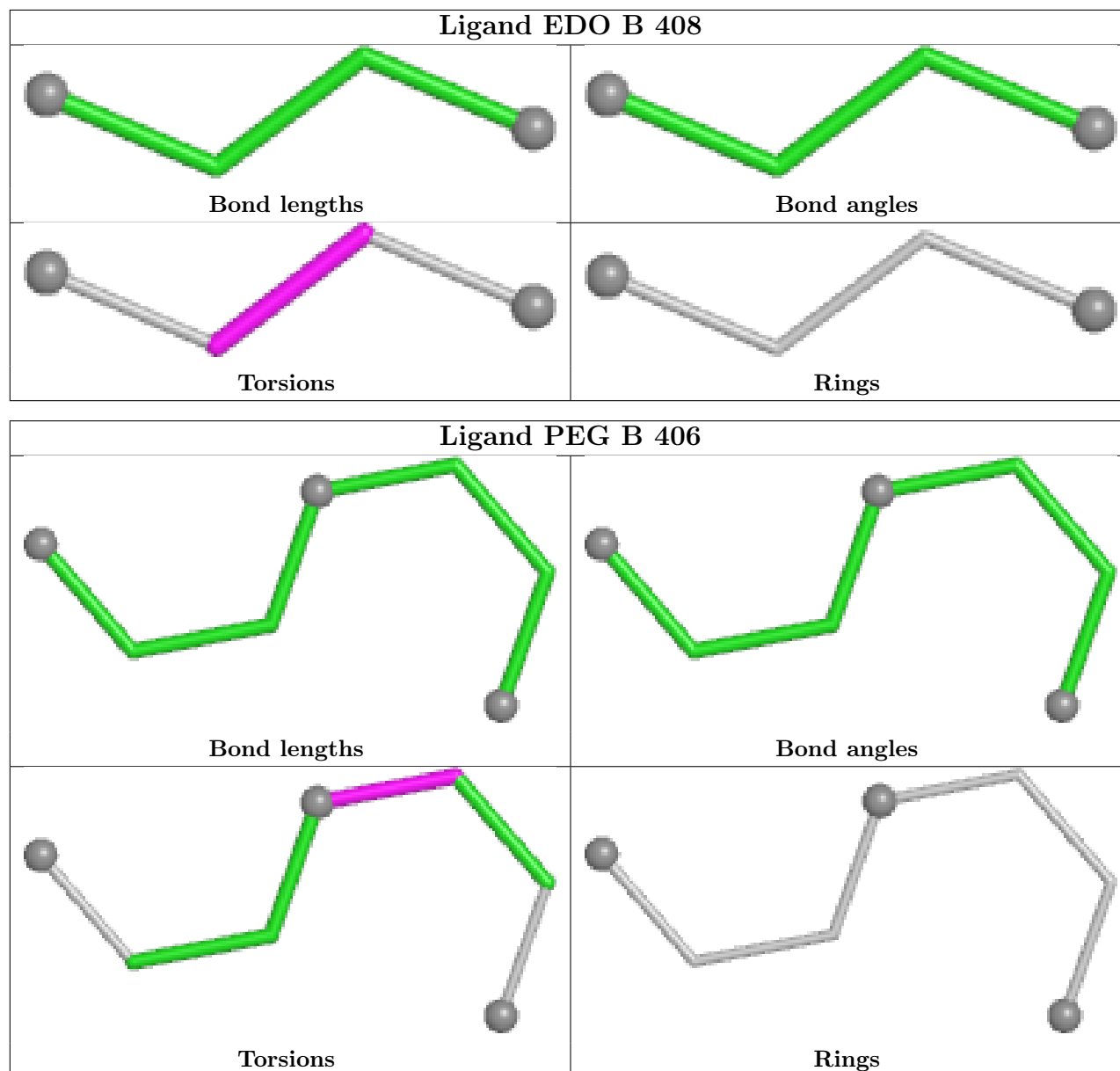
There are no ring outliers.

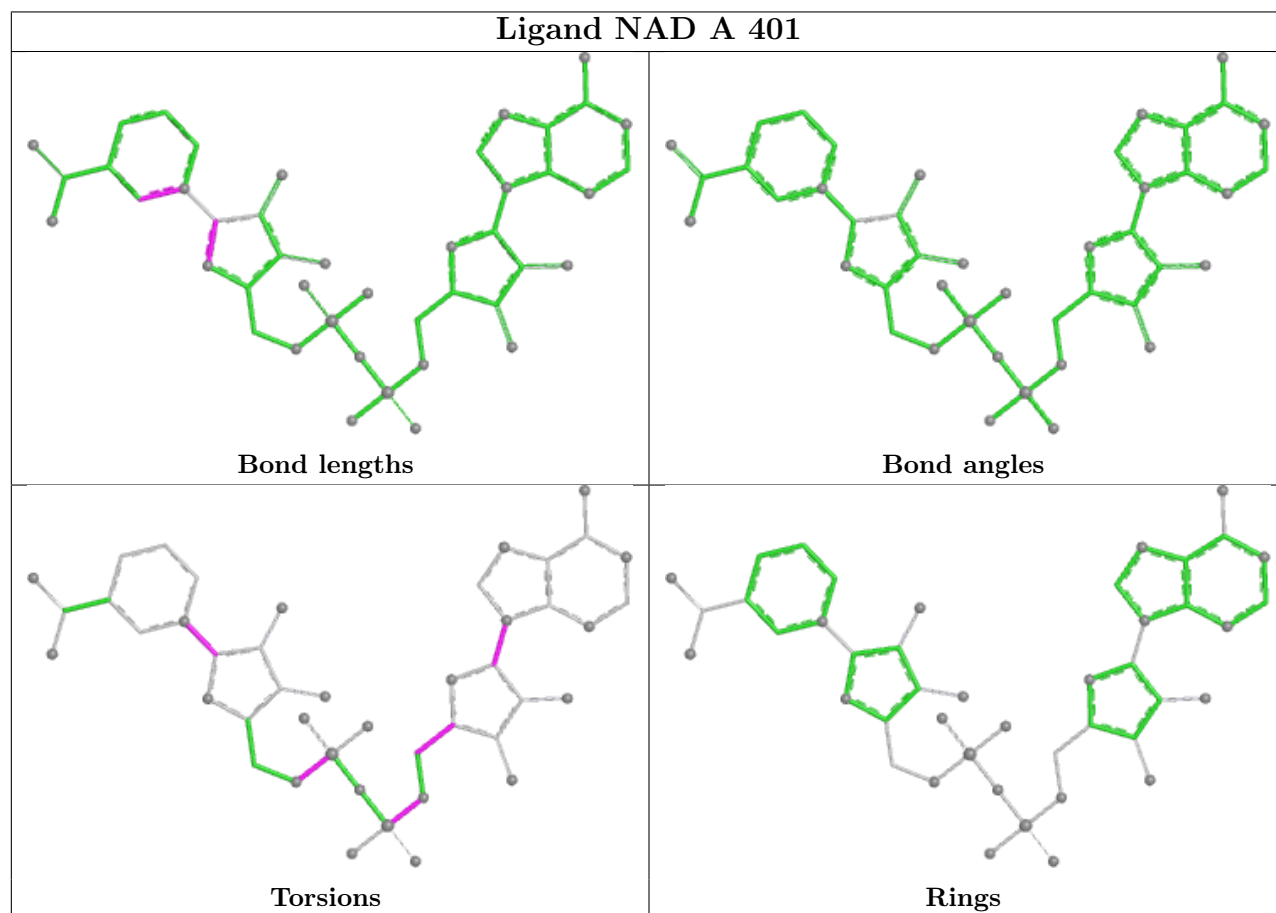
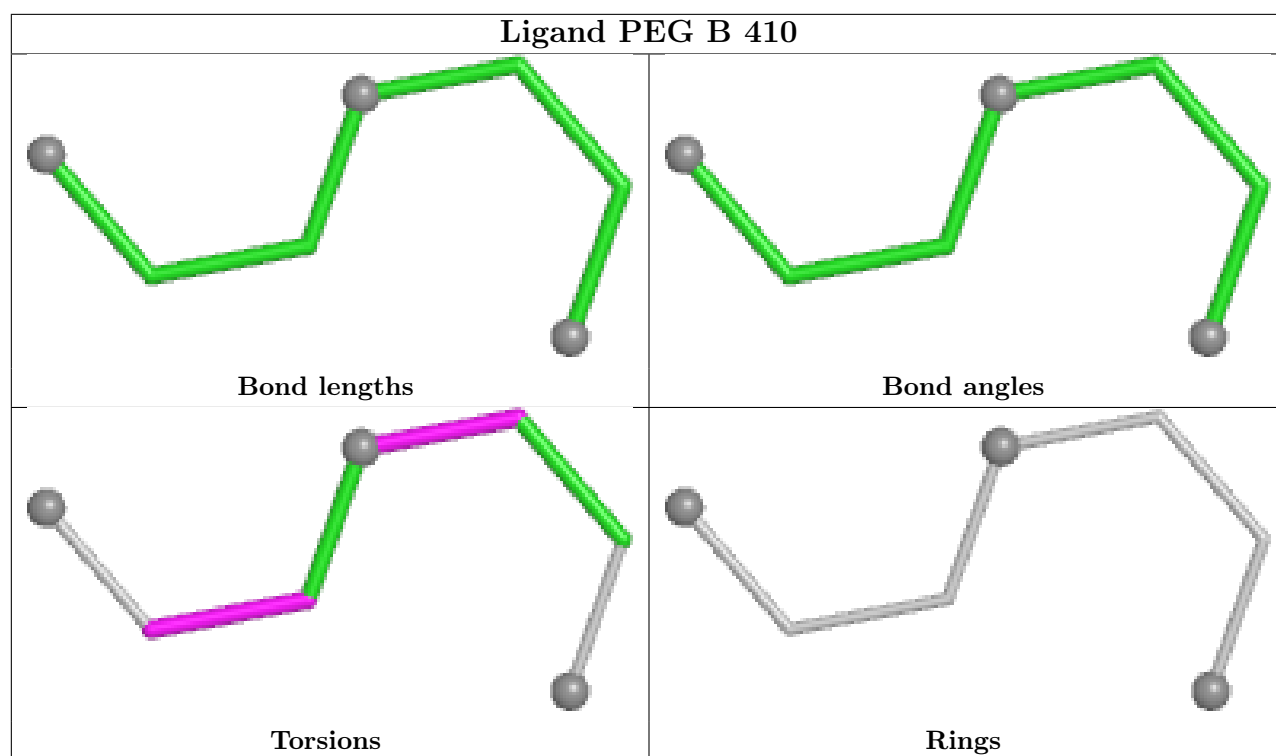
23 monomers are involved in 42 short contacts:

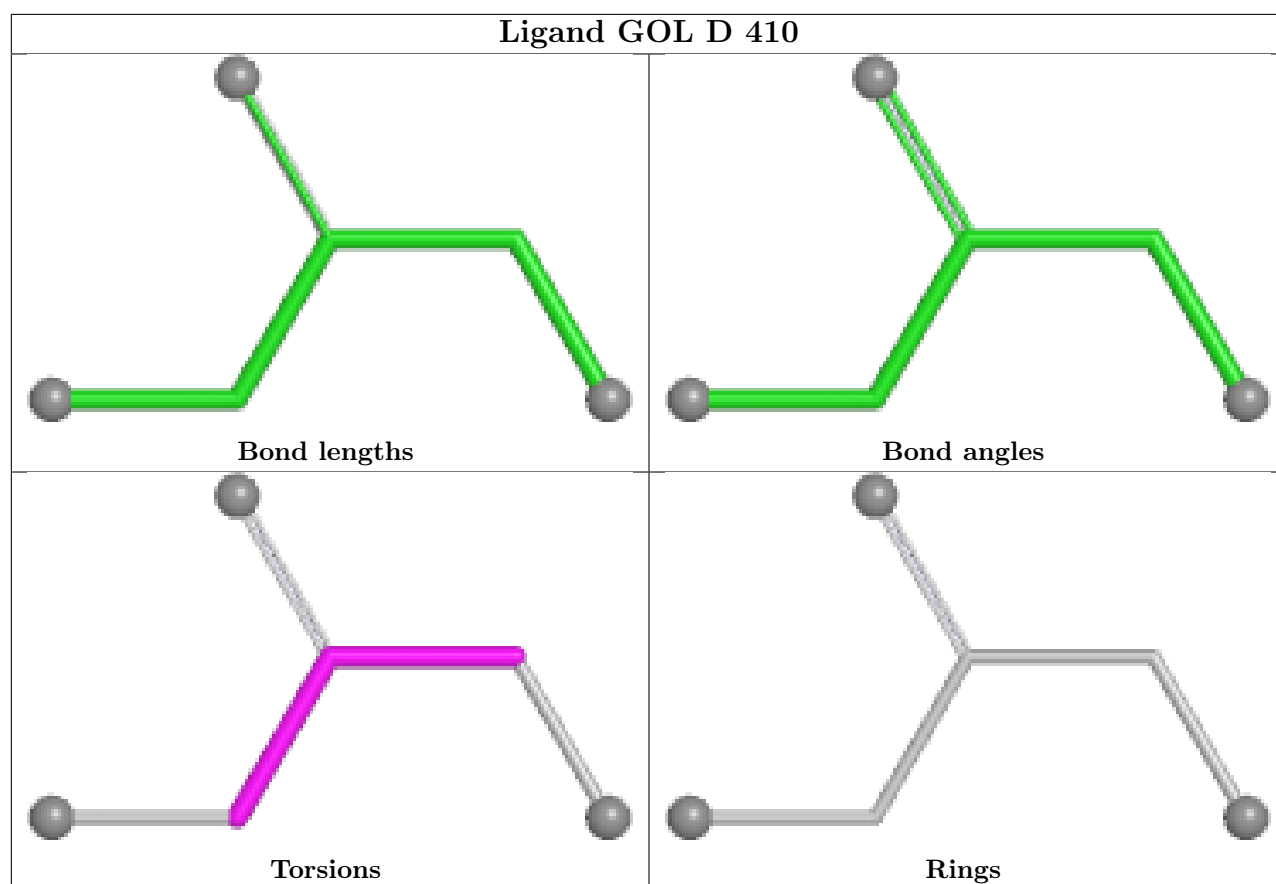
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	PEG	1	0
7	D	410	GOL	1	0
6	B	401	TRS	1	0
9	C	401	PGE	1	0
2	C	402	NAD	1	0
3	A	402	PEG	1	0
4	B	409	PG4	3	0
4	D	407	PG4	2	0
4	B	413	PG4	2	0
9	A	415	PGE	3	0
8	A	414	XPE	2	0
6	A	407	TRS	4	0
7	B	411	GOL	2	0
3	C	405	PEG	1	0
4	C	403	PG4	2	0
7	A	413	GOL	1	0
5	A	404	EDO	1	0
4	A	403	PG4	3	0
5	D	404	EDO	1	0
7	C	408	GOL	3	0
3	D	401	PEG	2	0
2	B	402	NAD	3	0
4	C	406	PG4	1	0

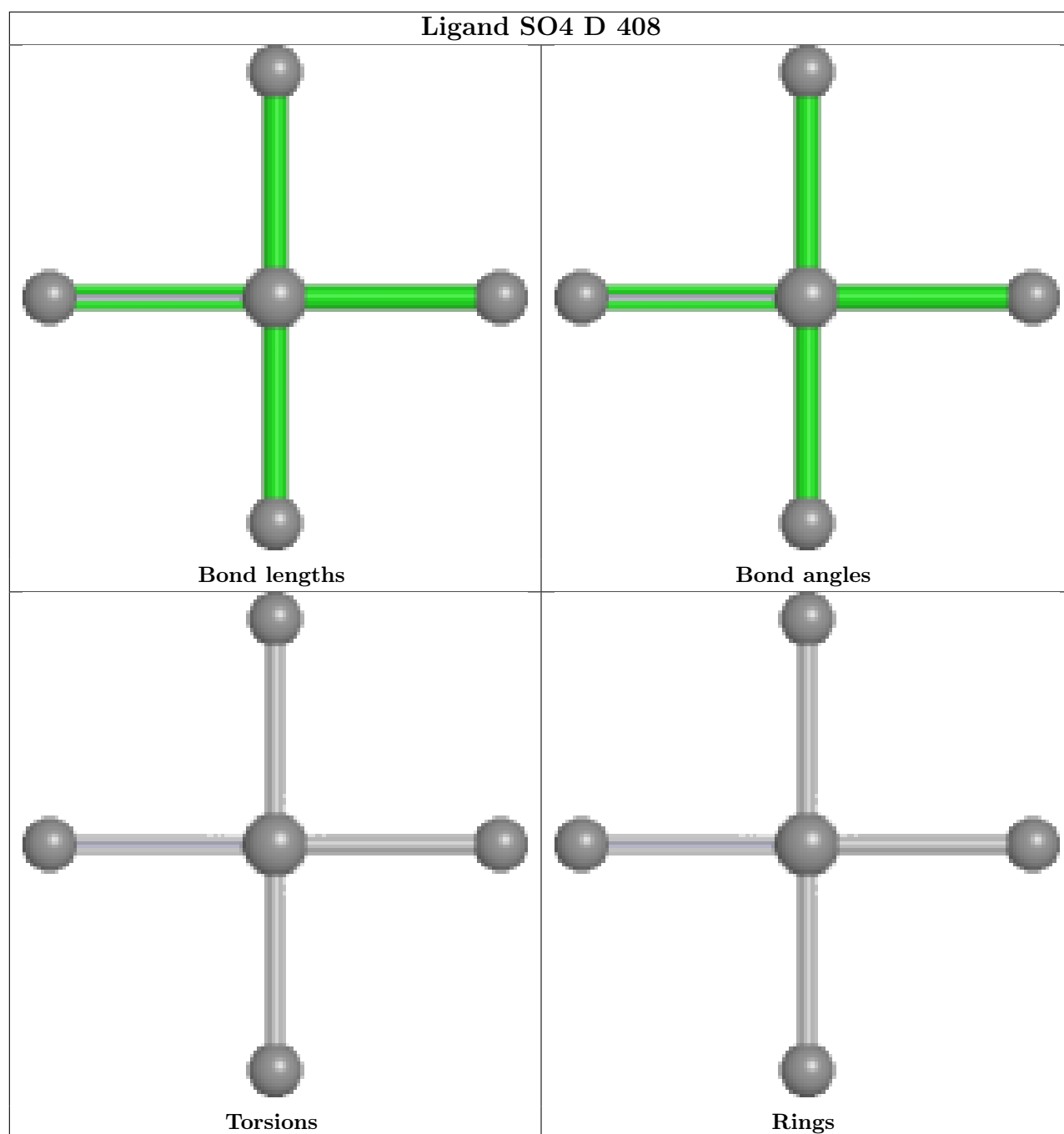
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

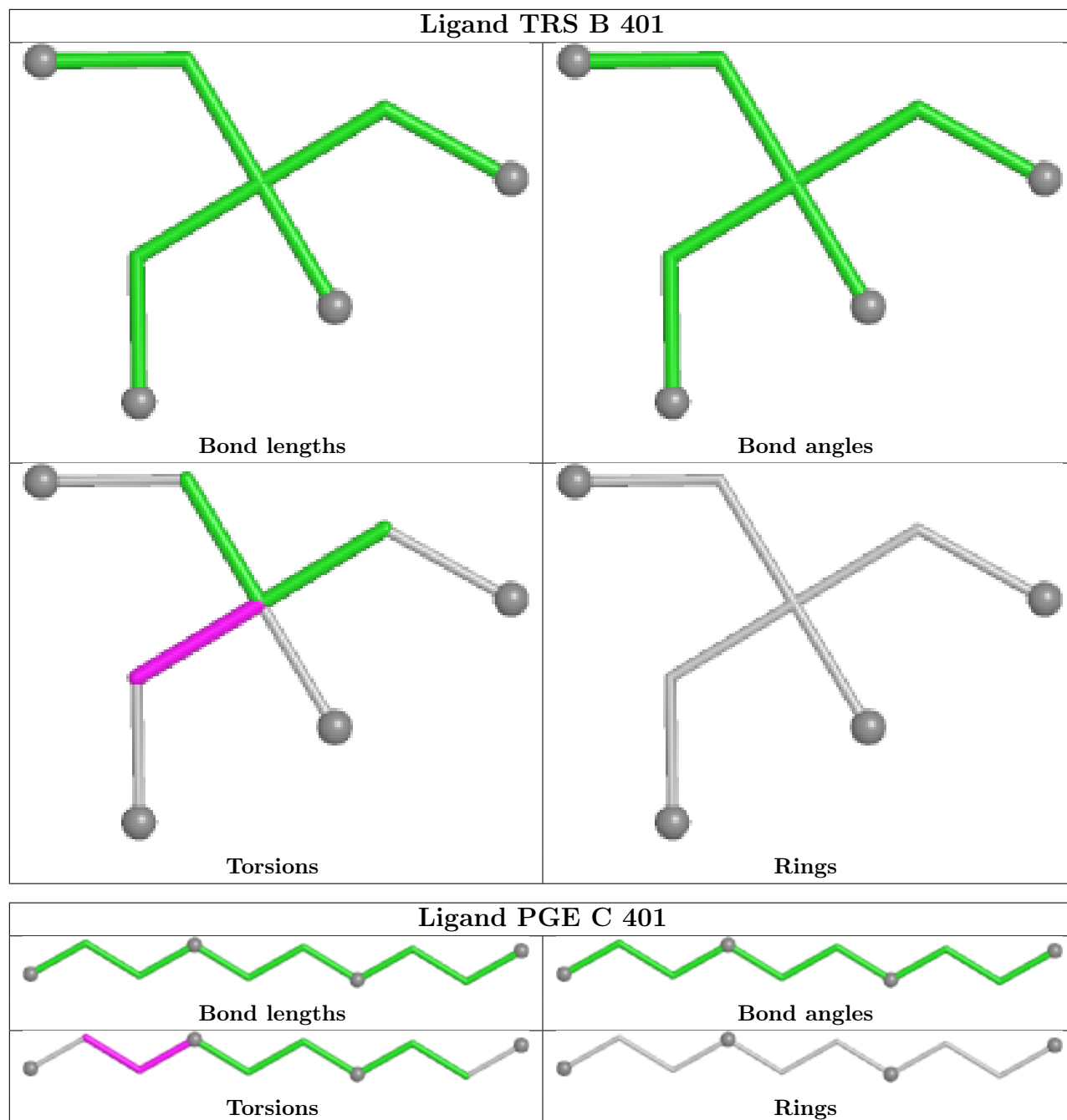
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

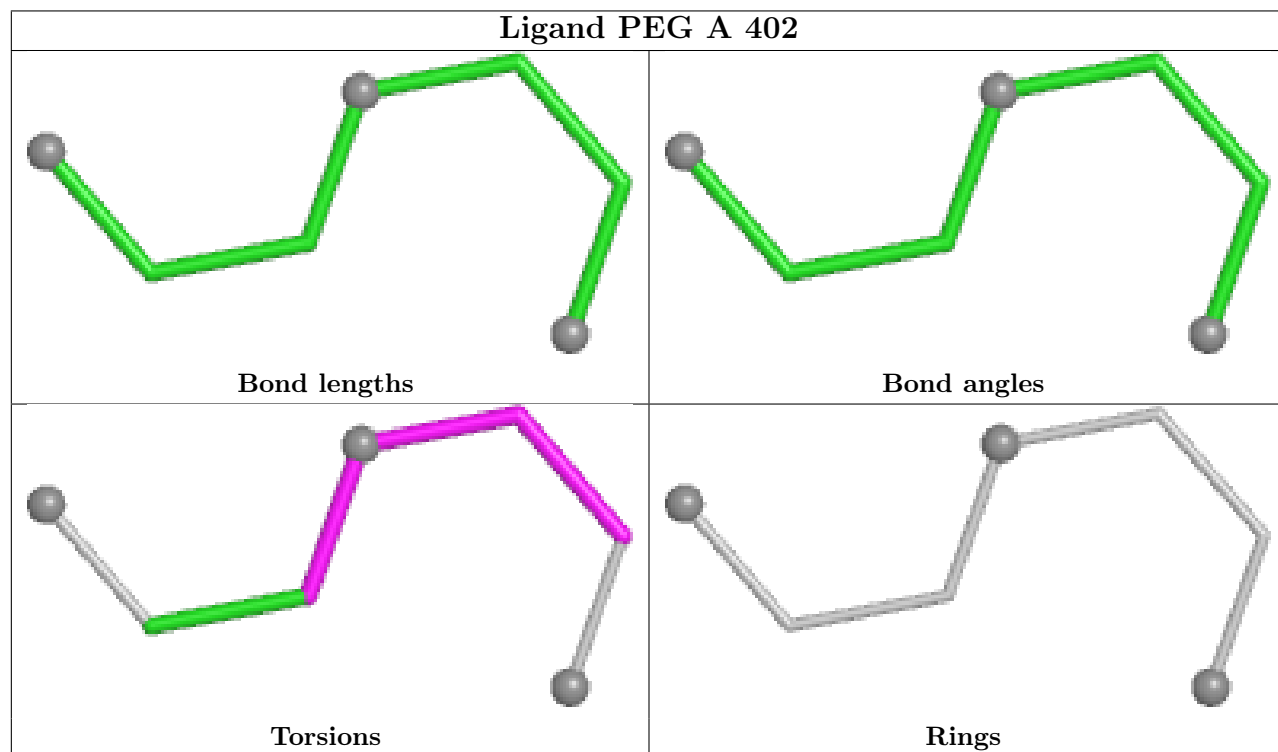
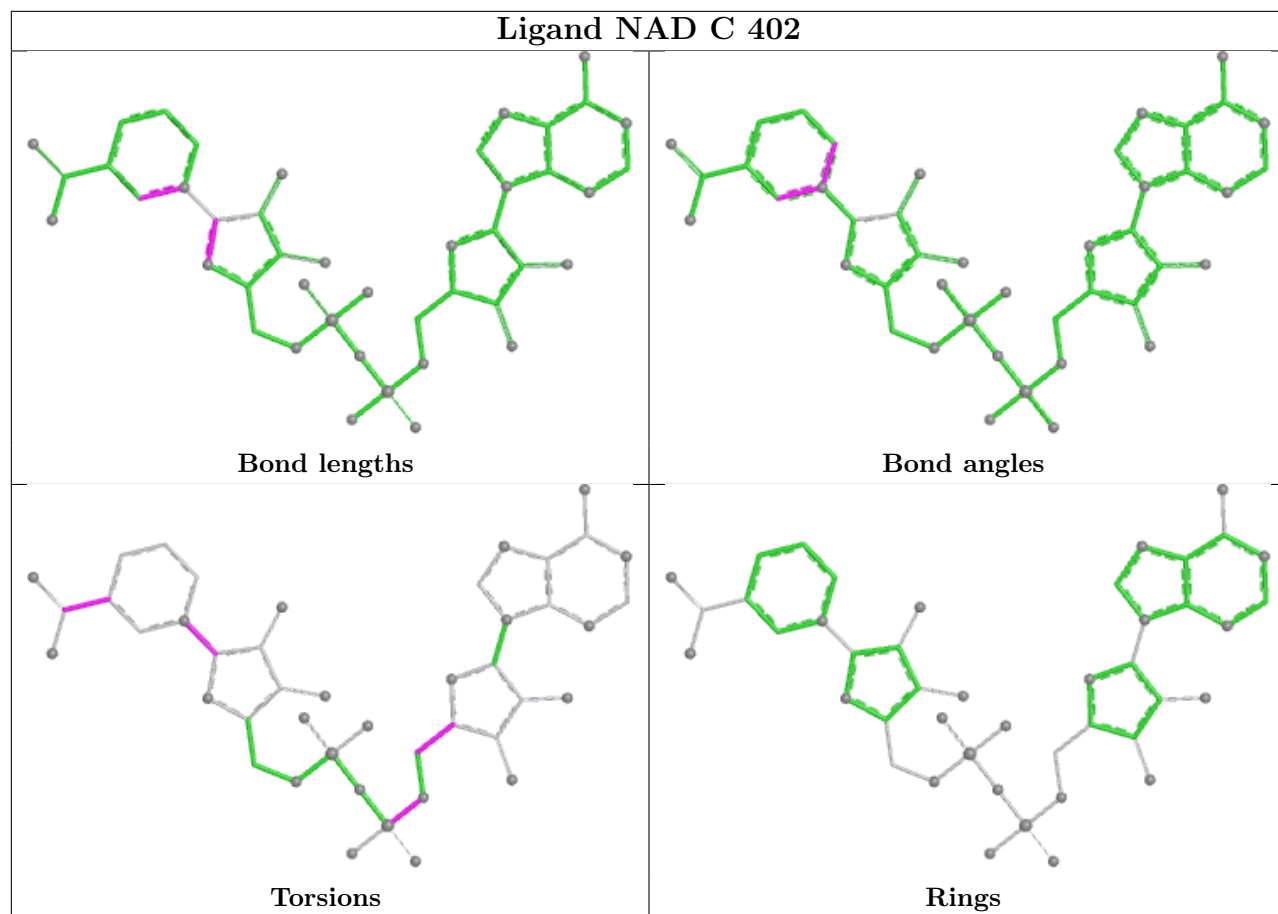


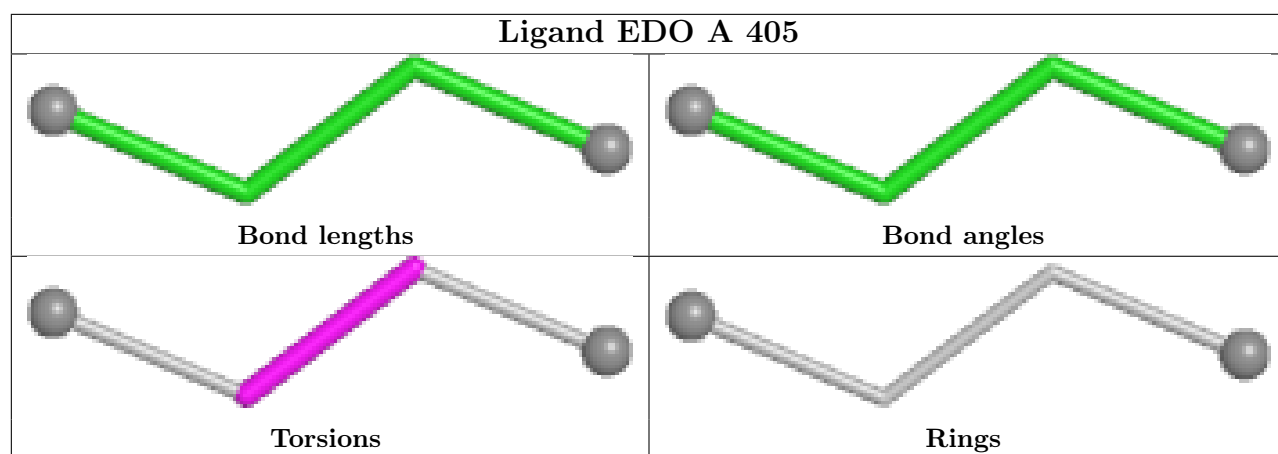


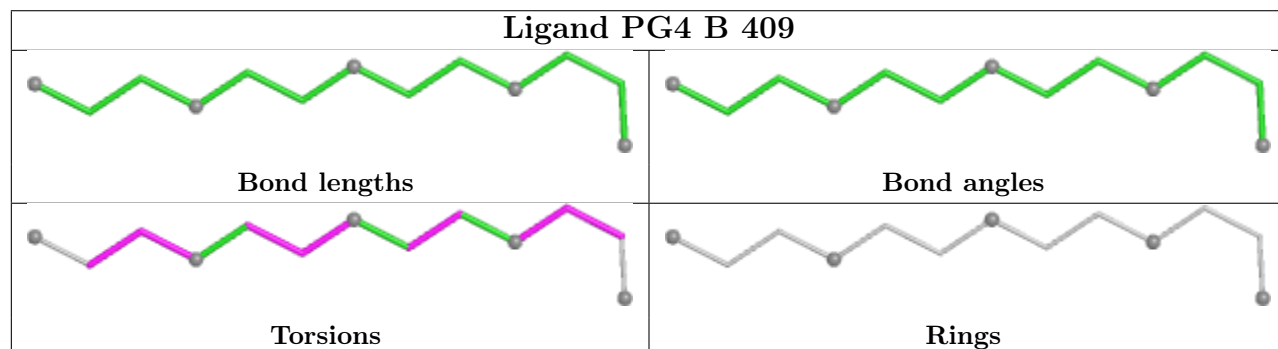
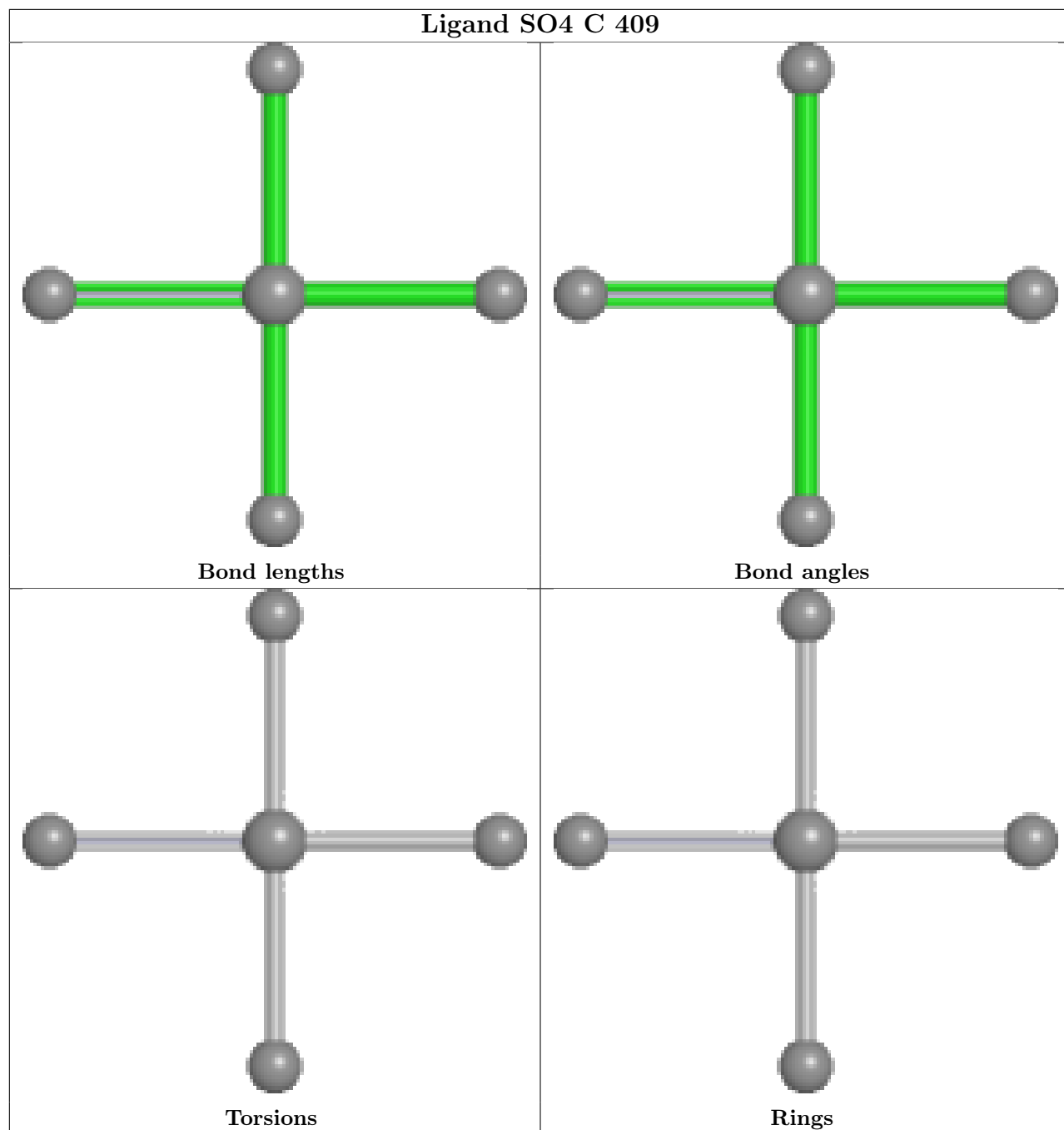


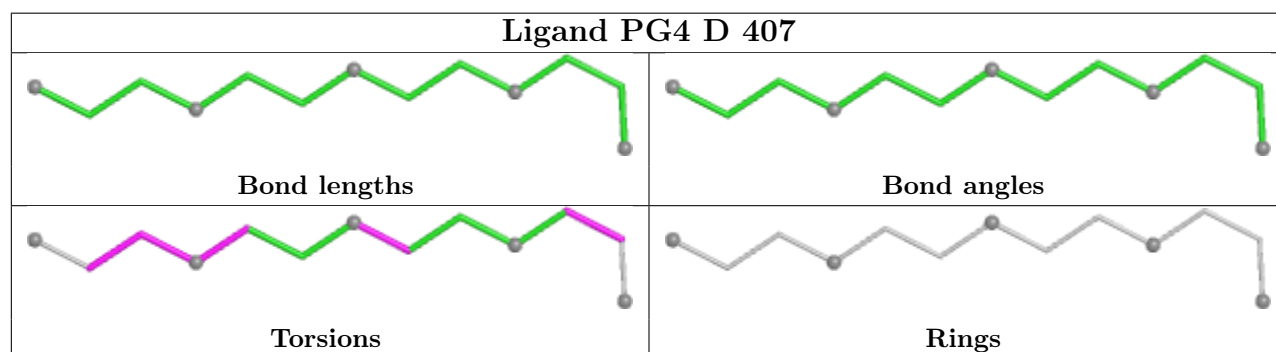
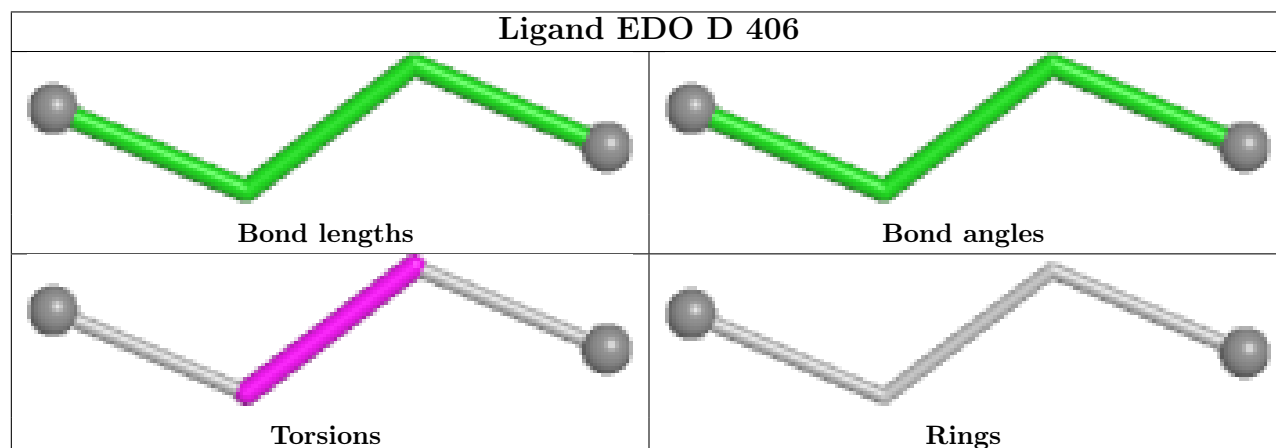
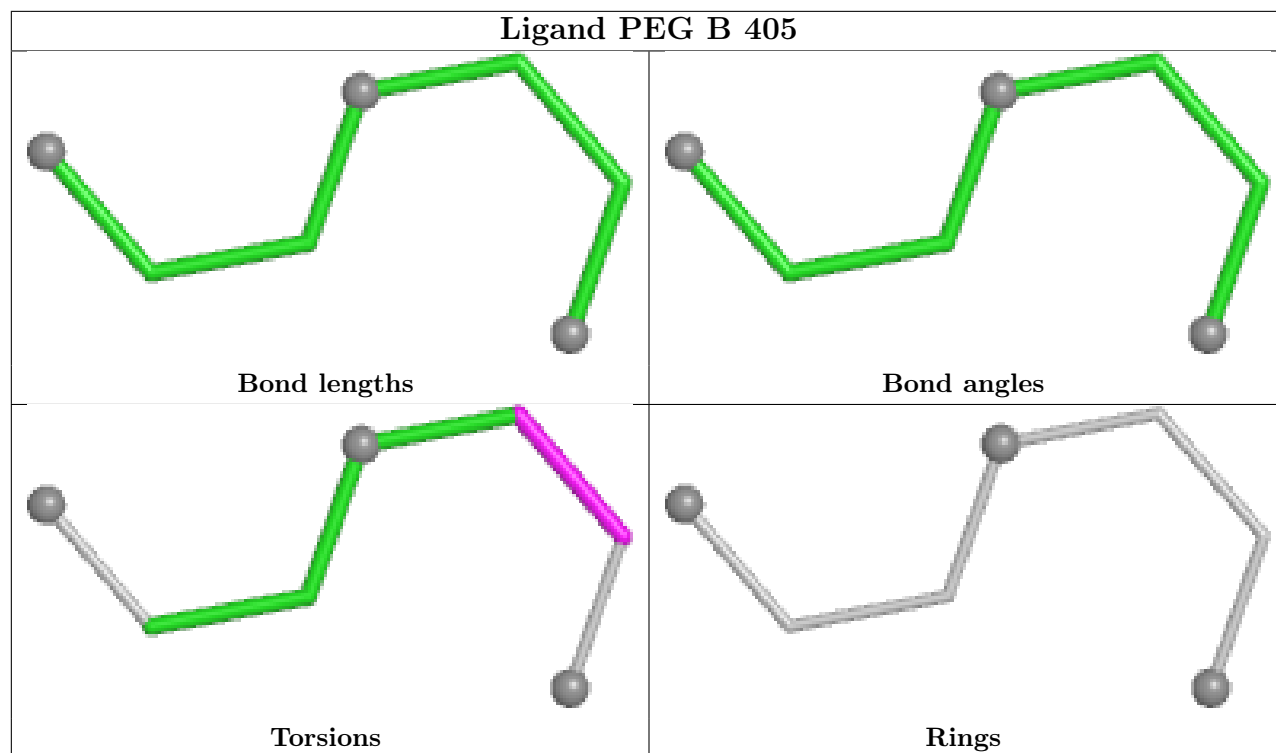


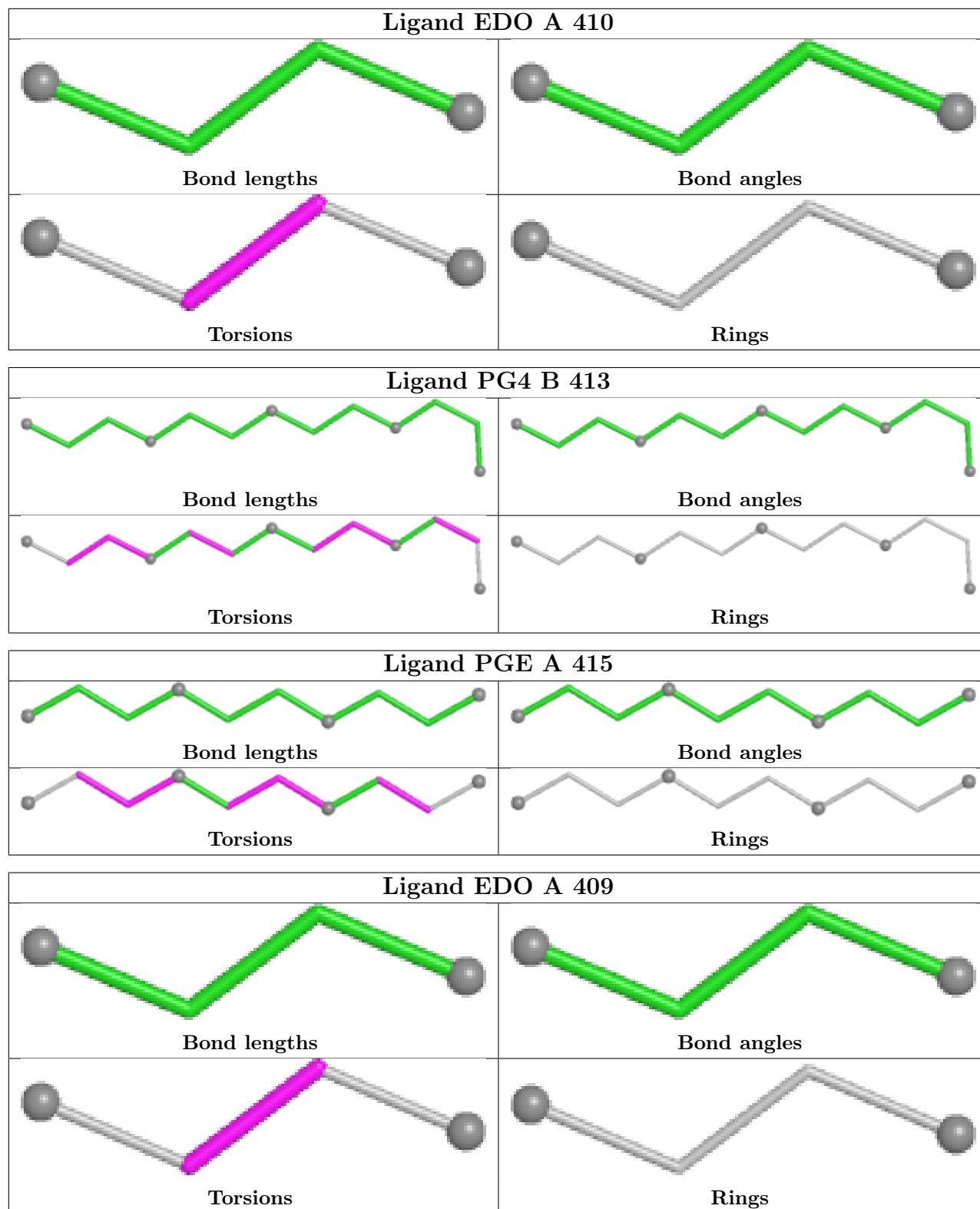


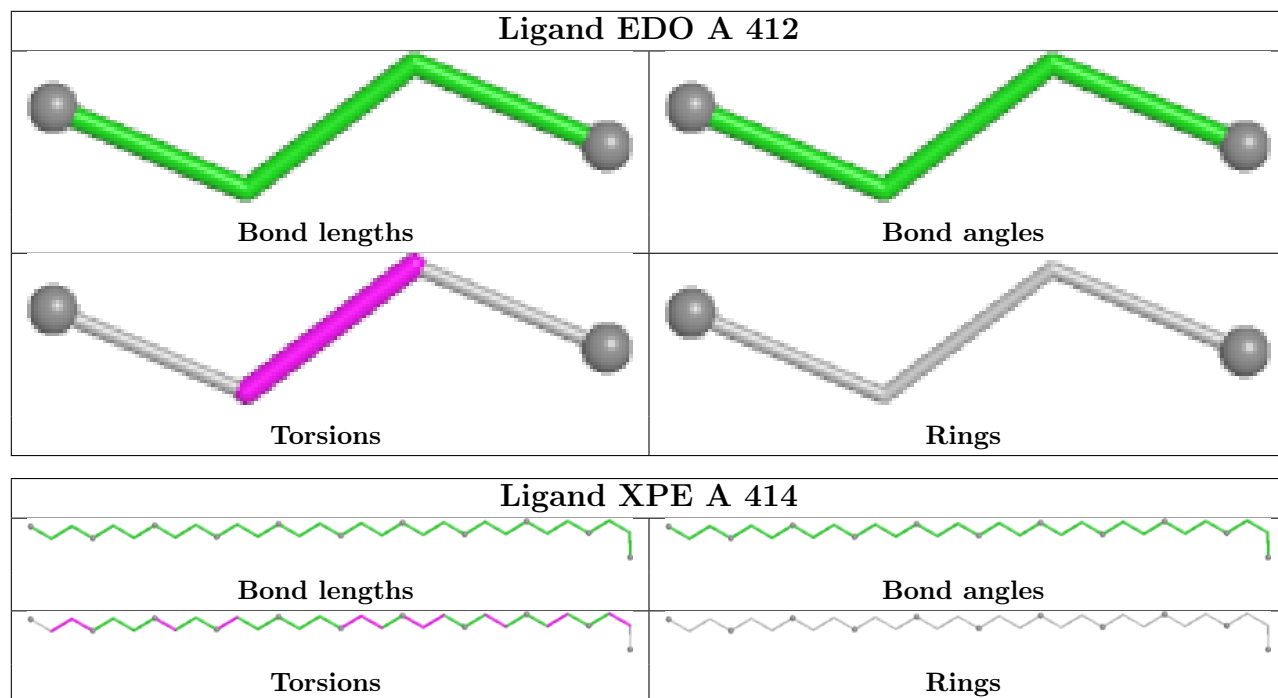


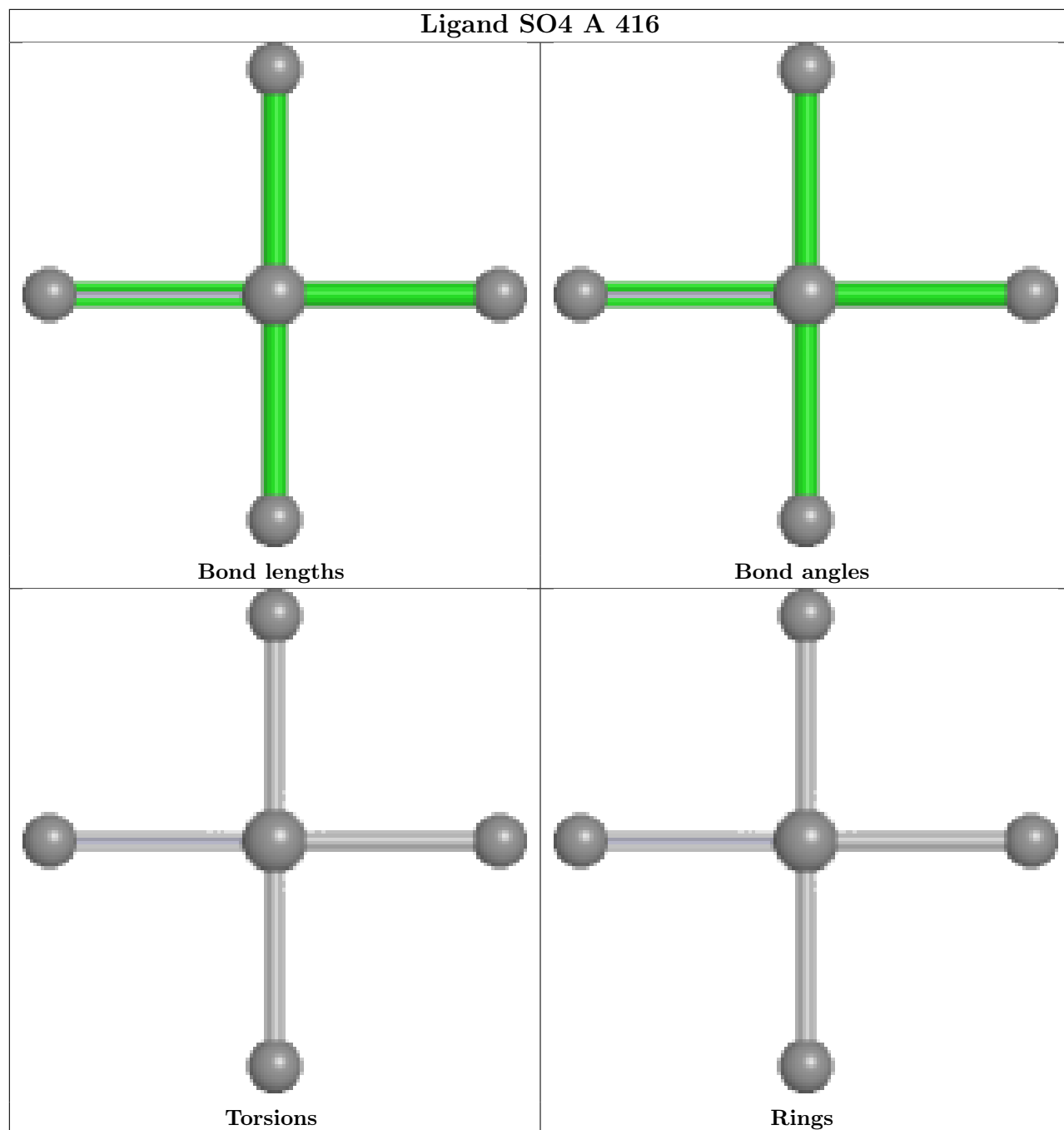


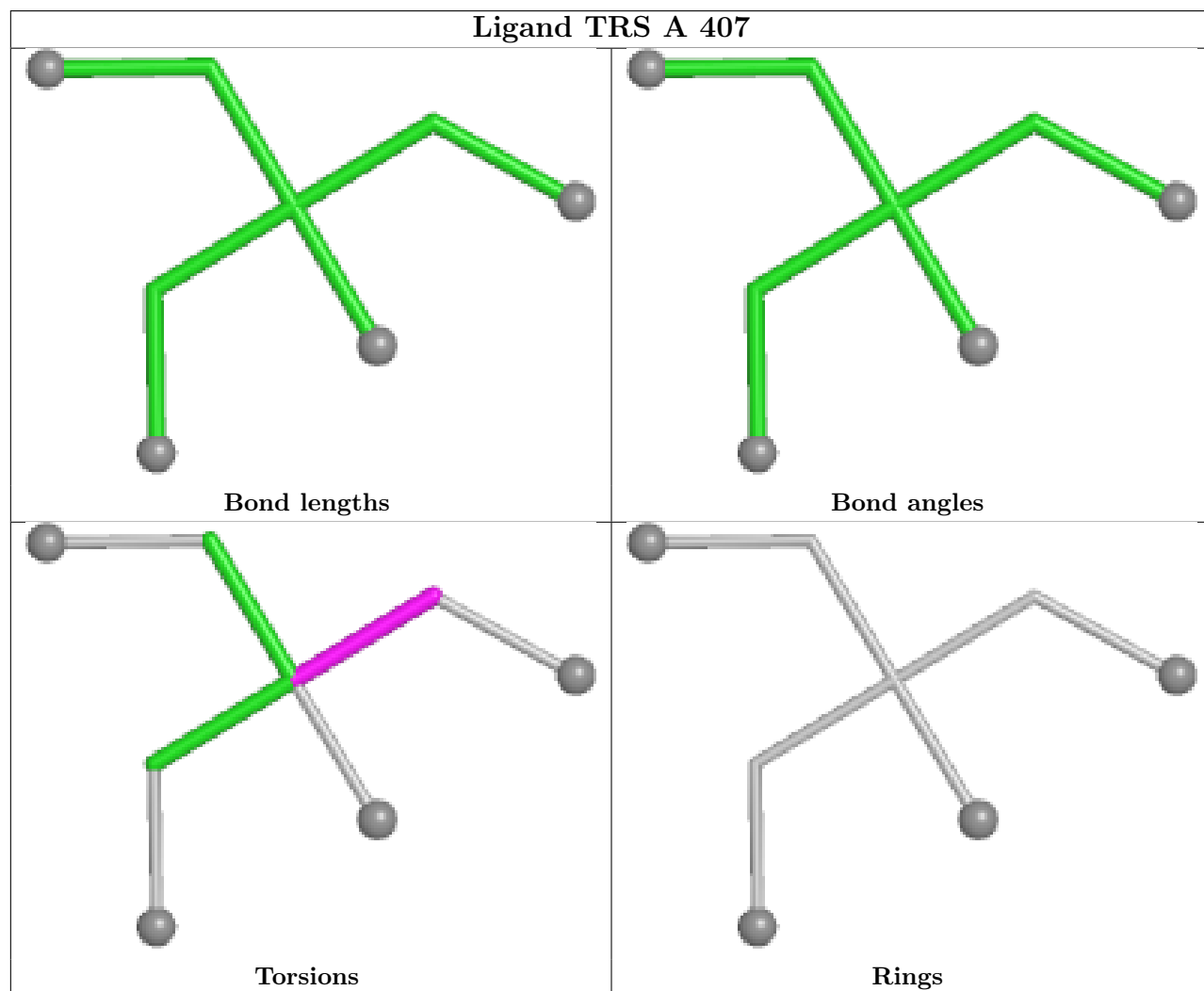
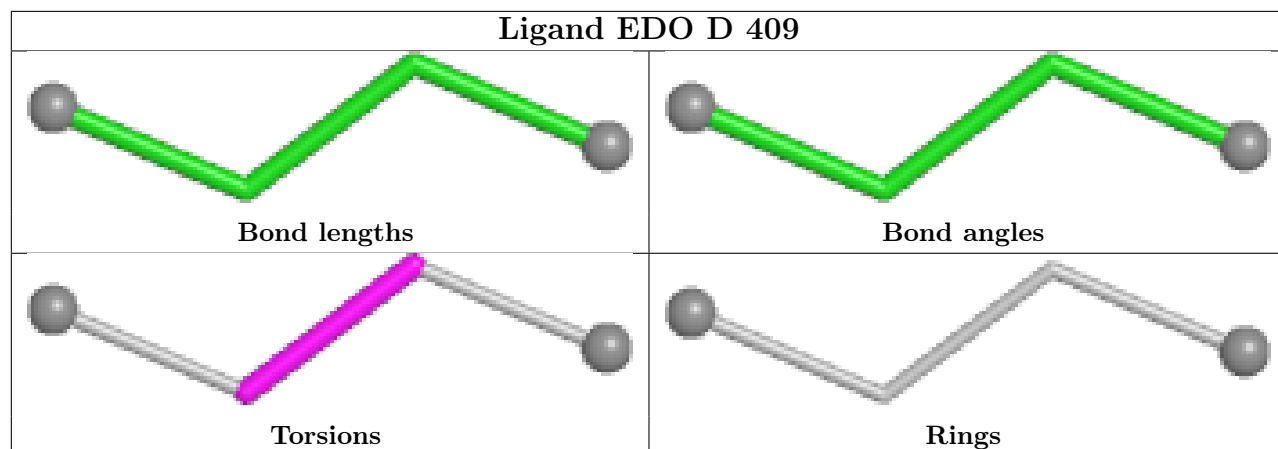


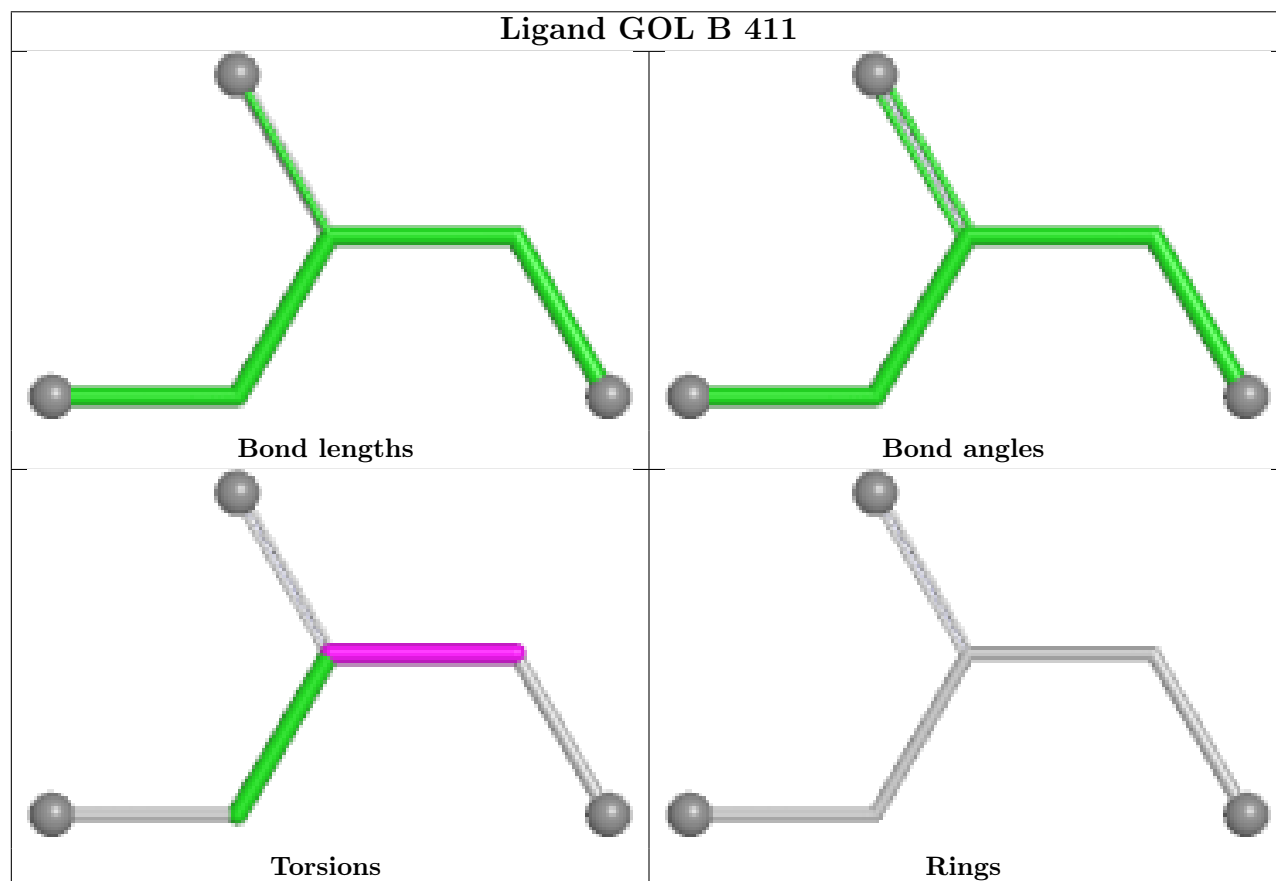
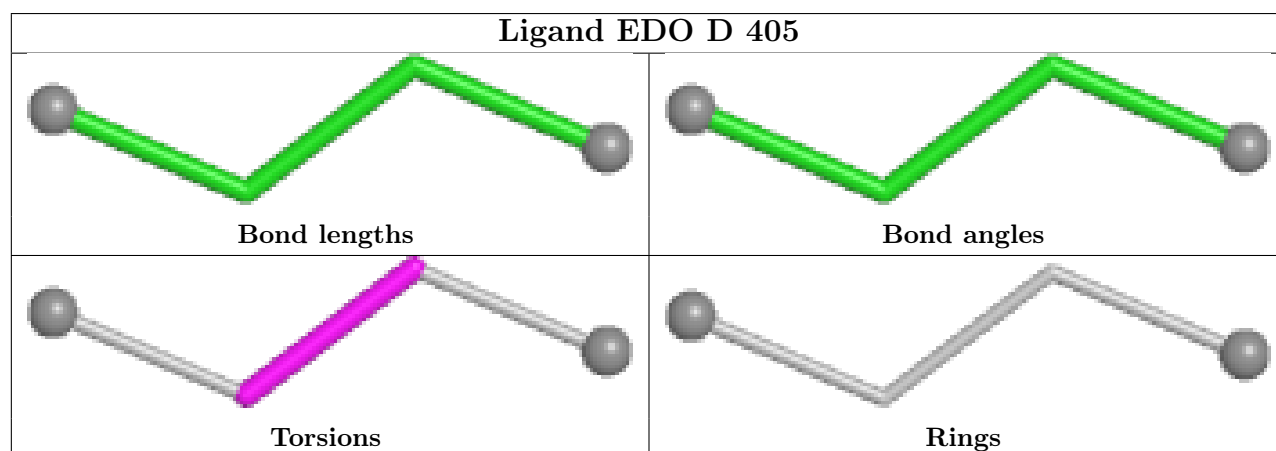
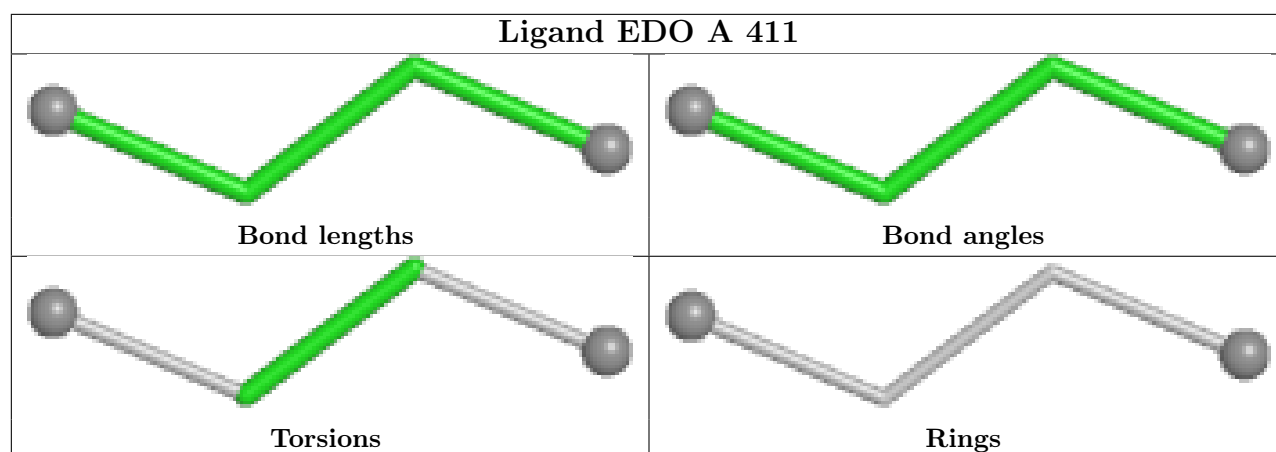


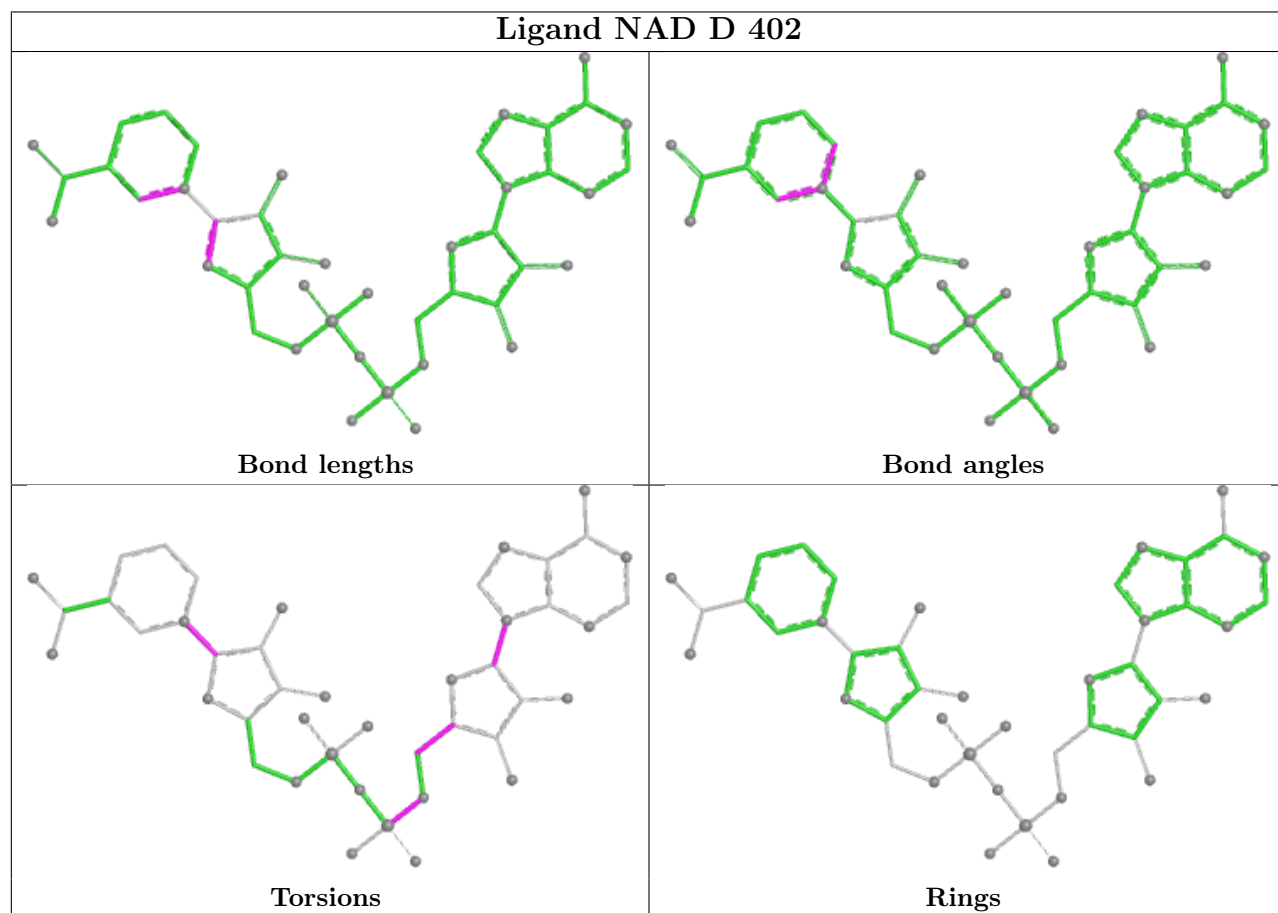
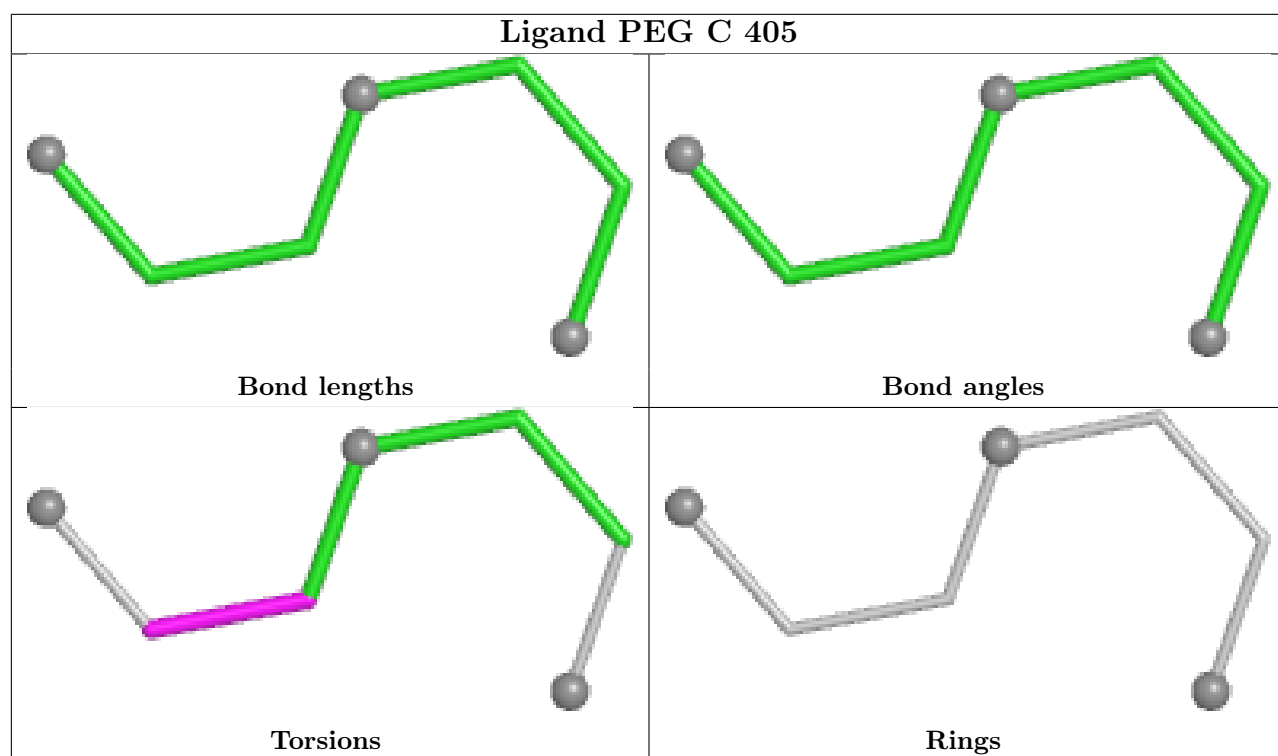


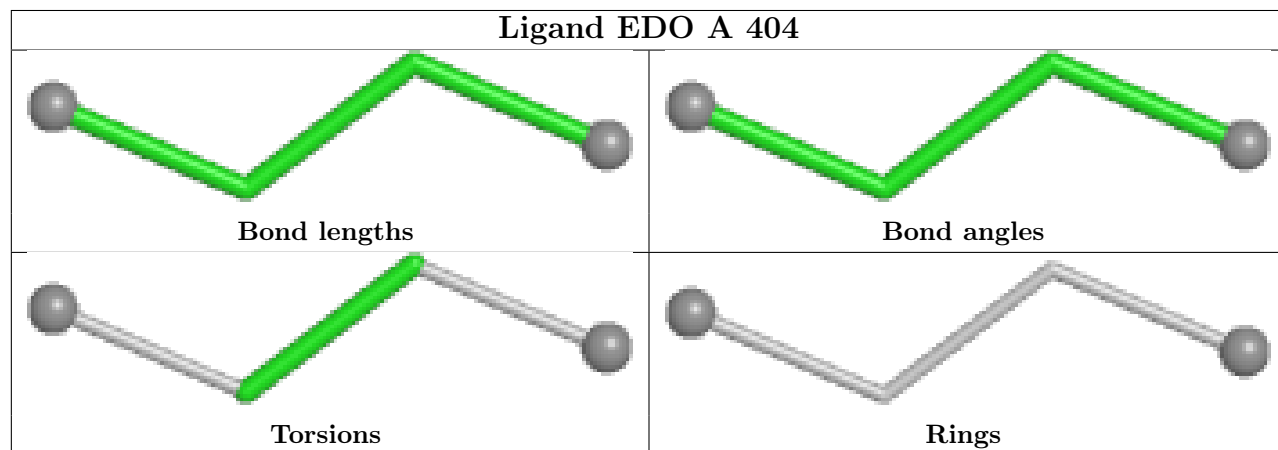
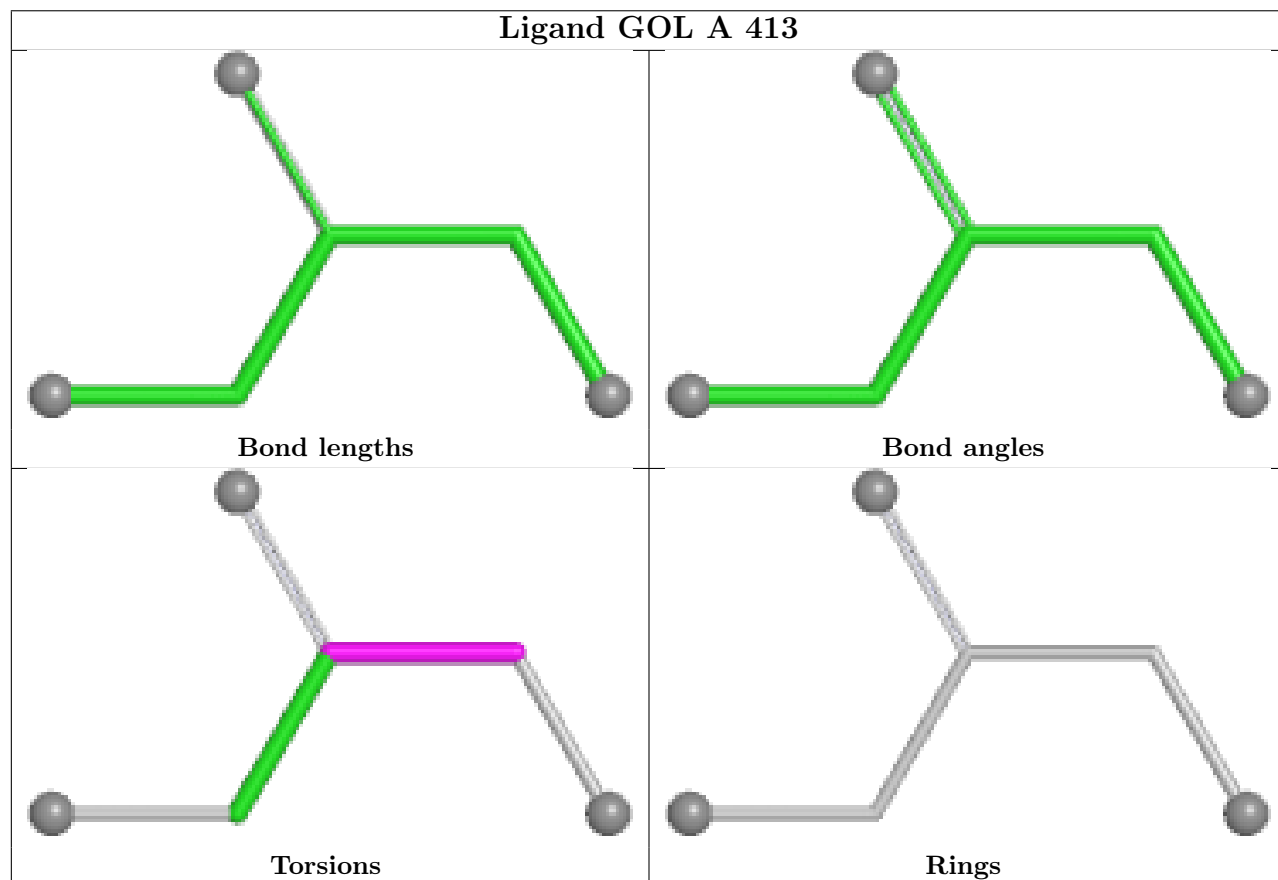
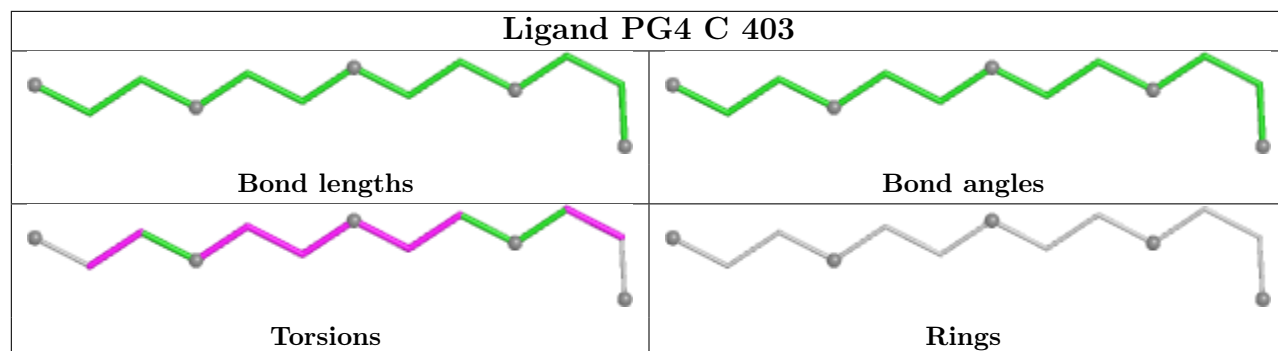


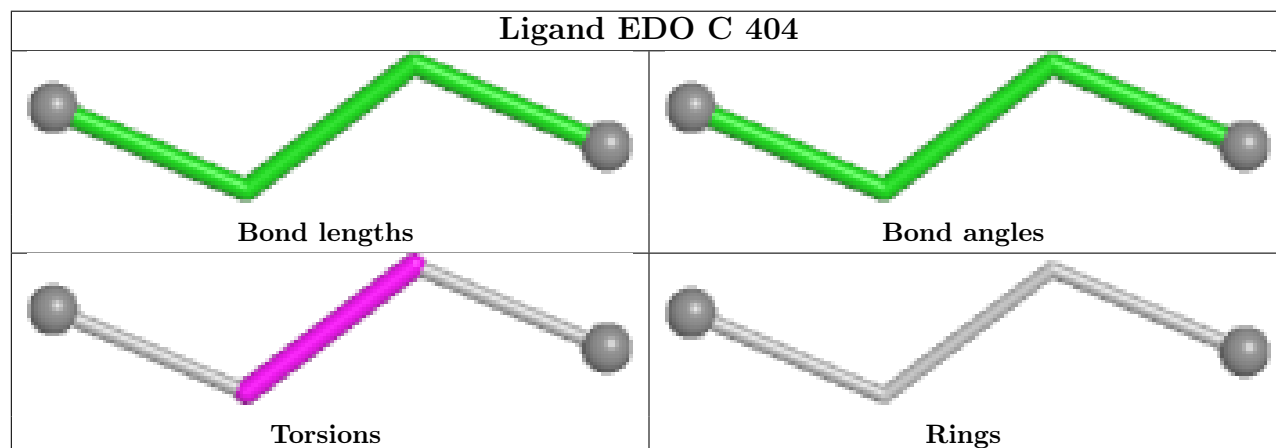
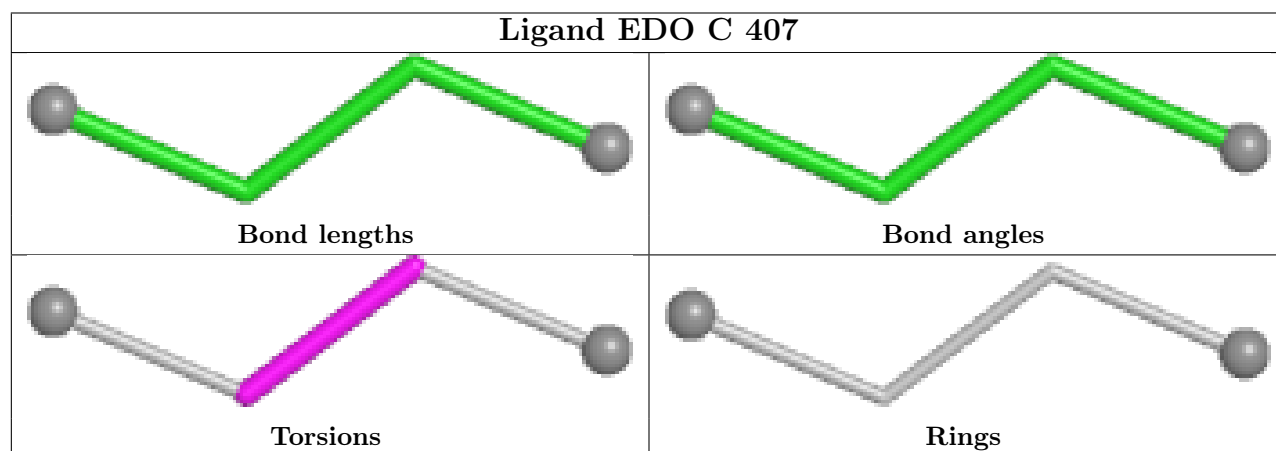
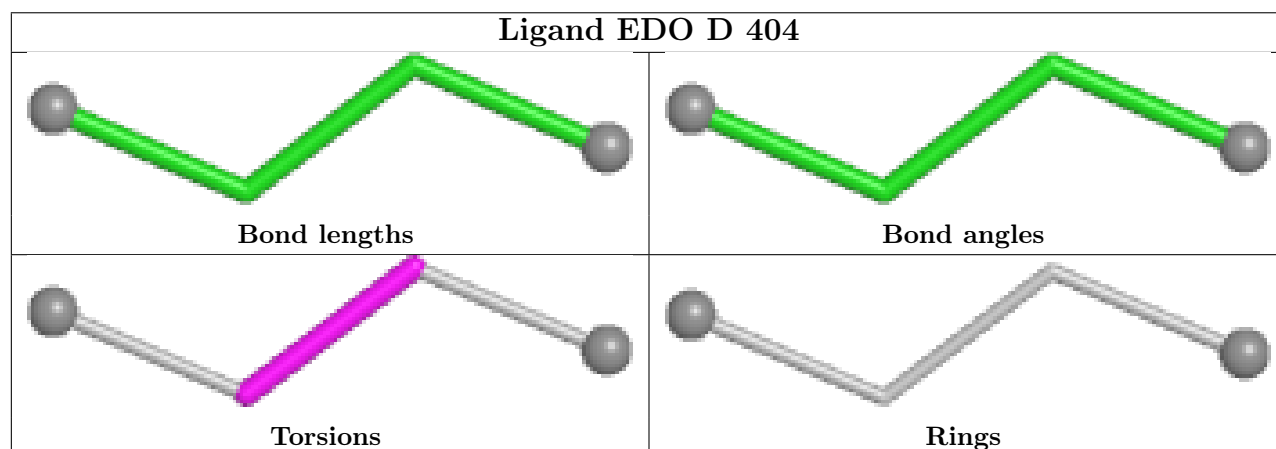
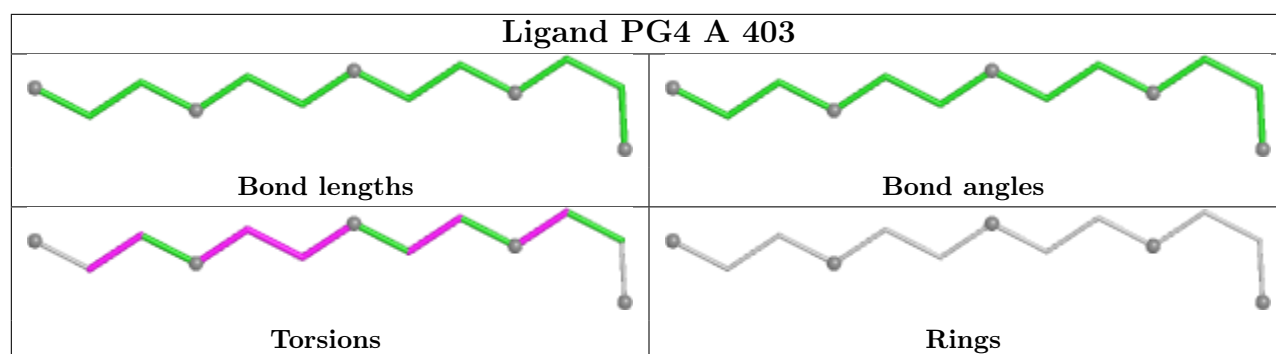


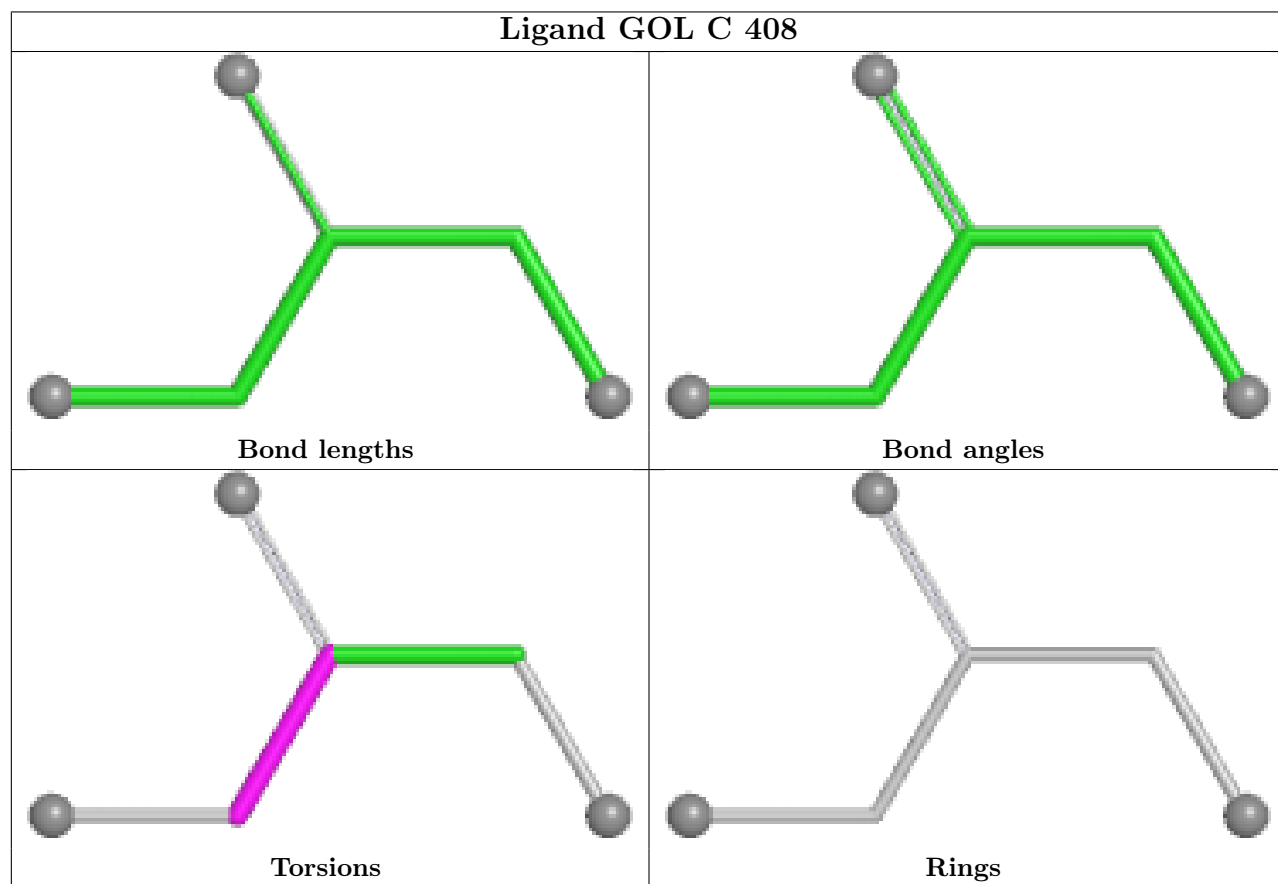
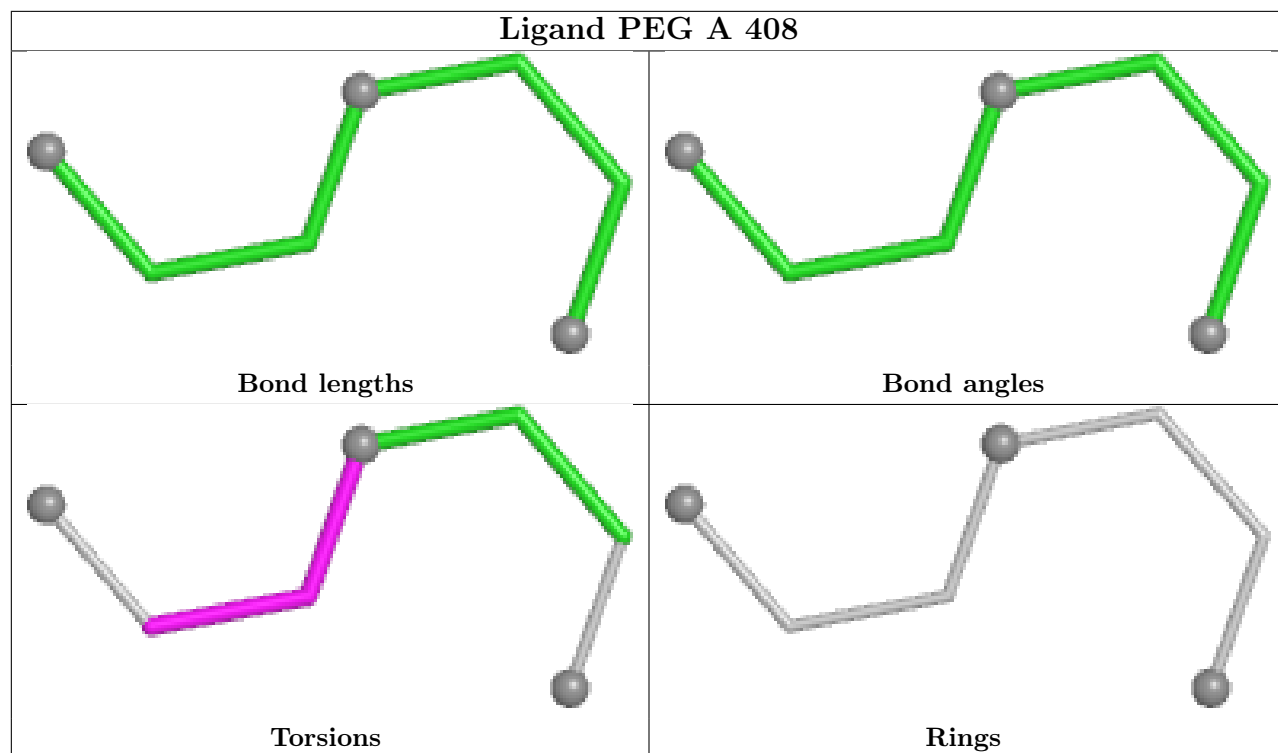


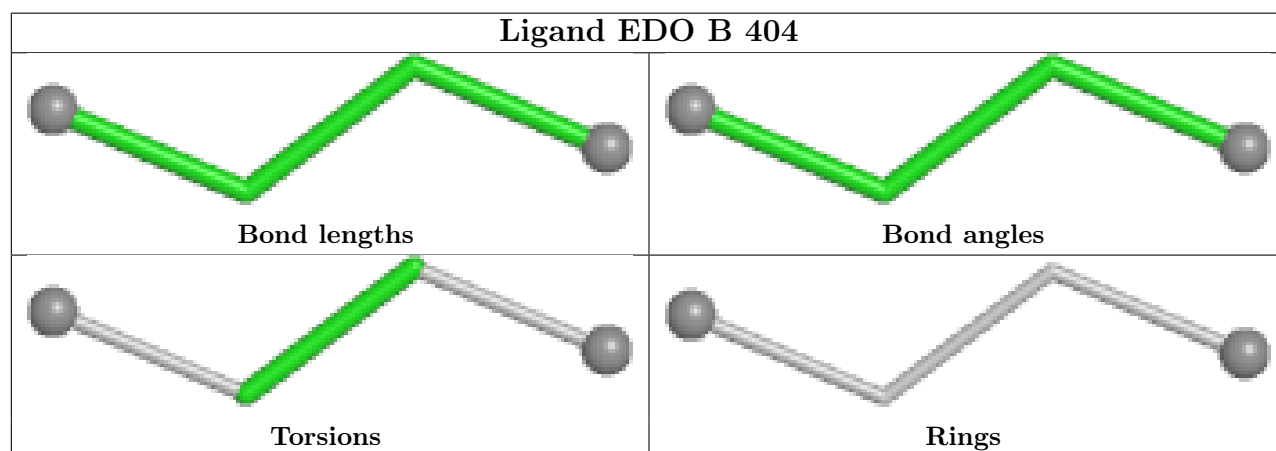
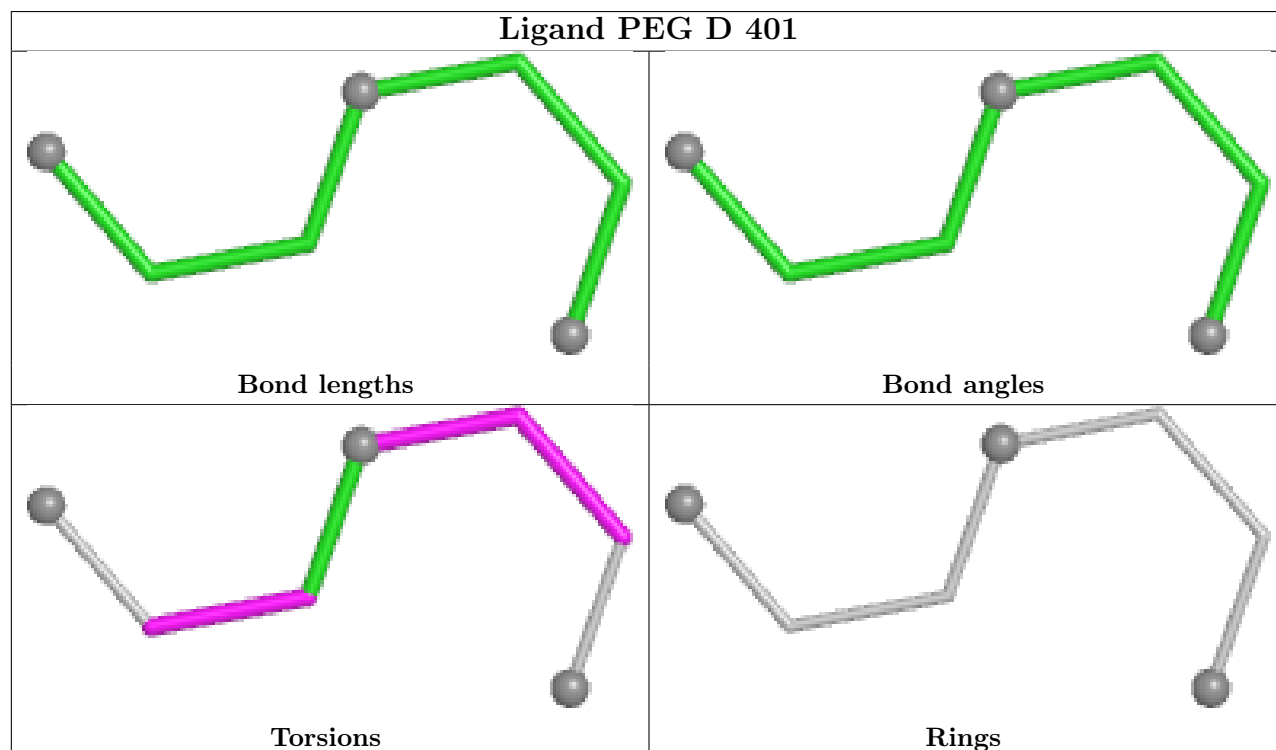
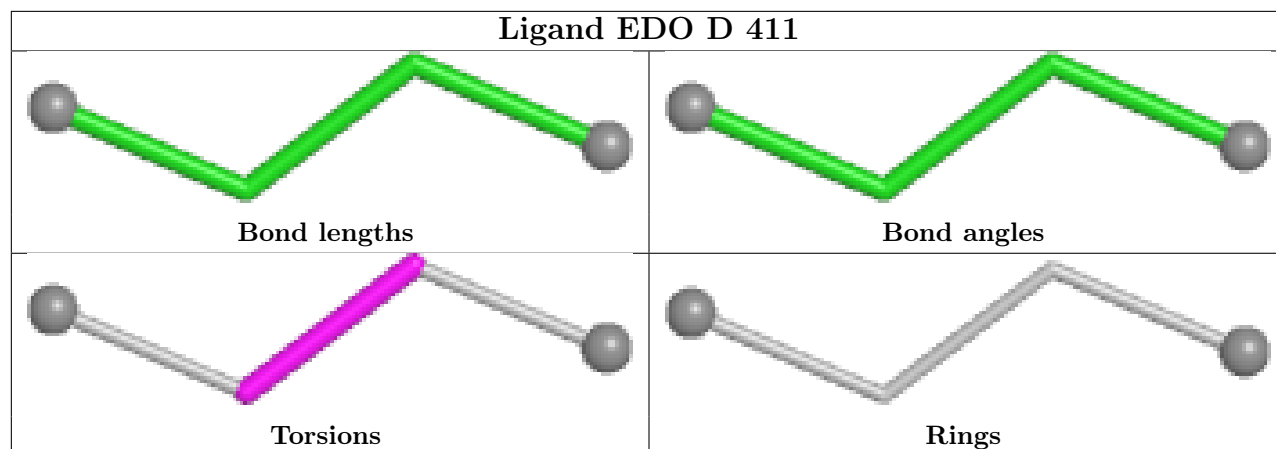


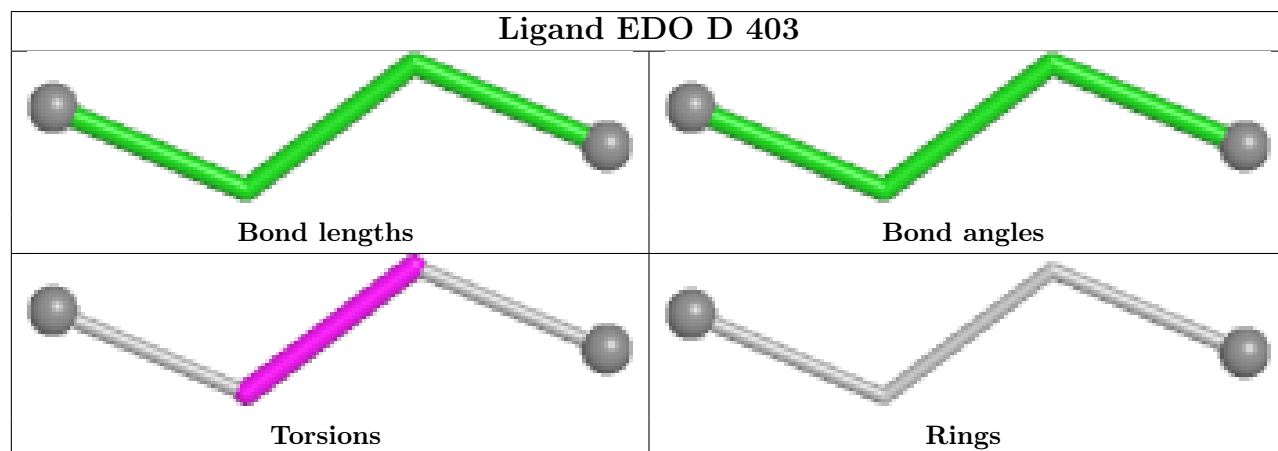
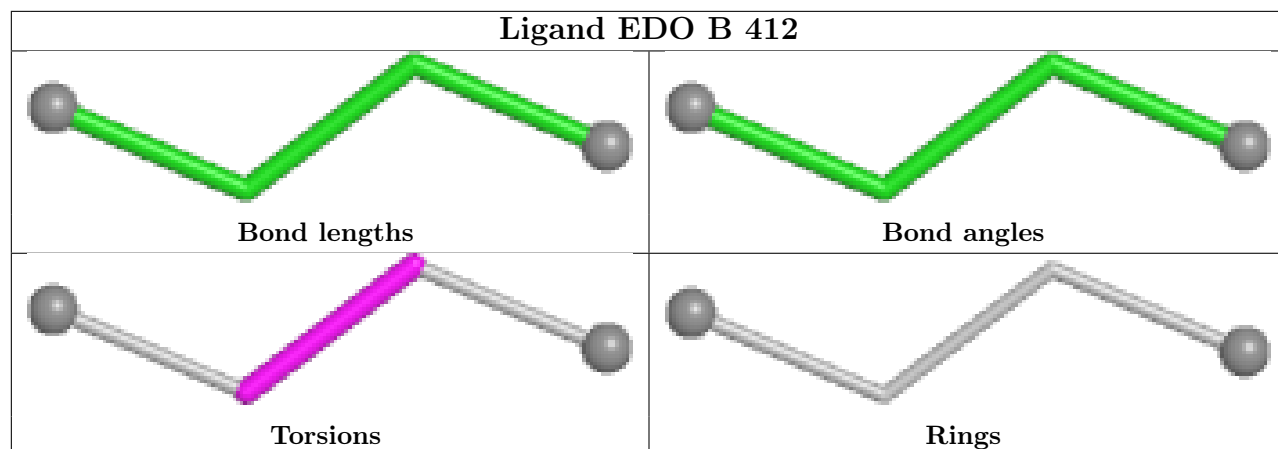


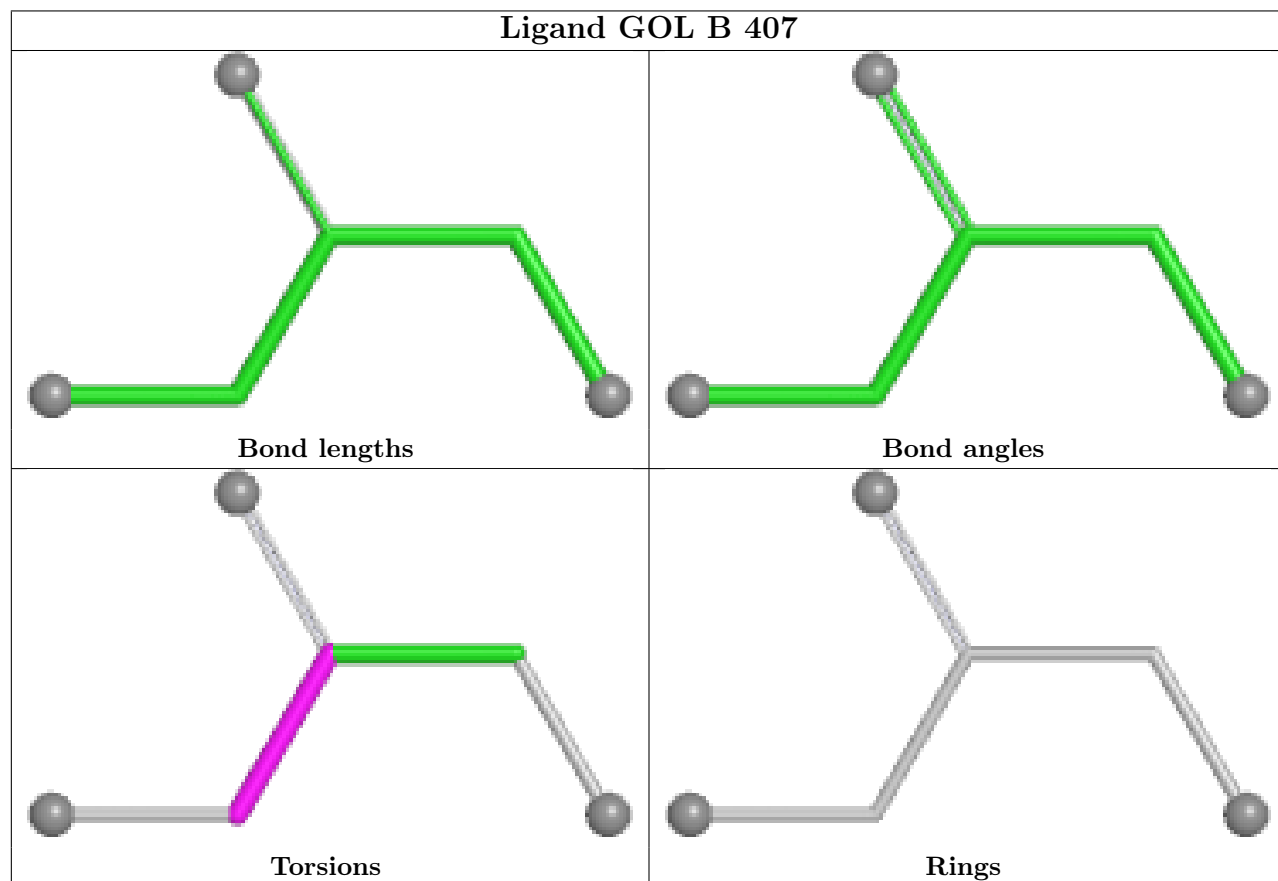
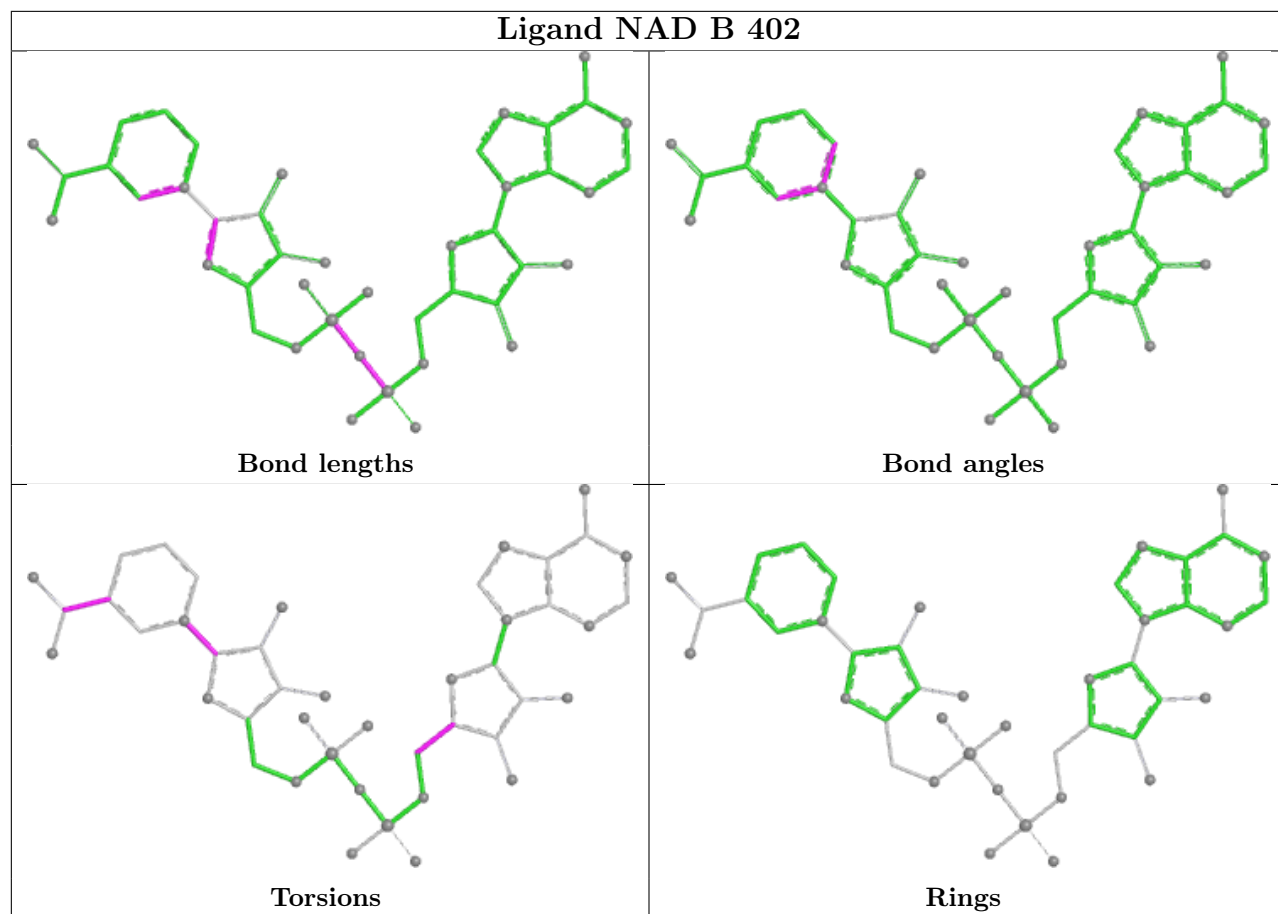


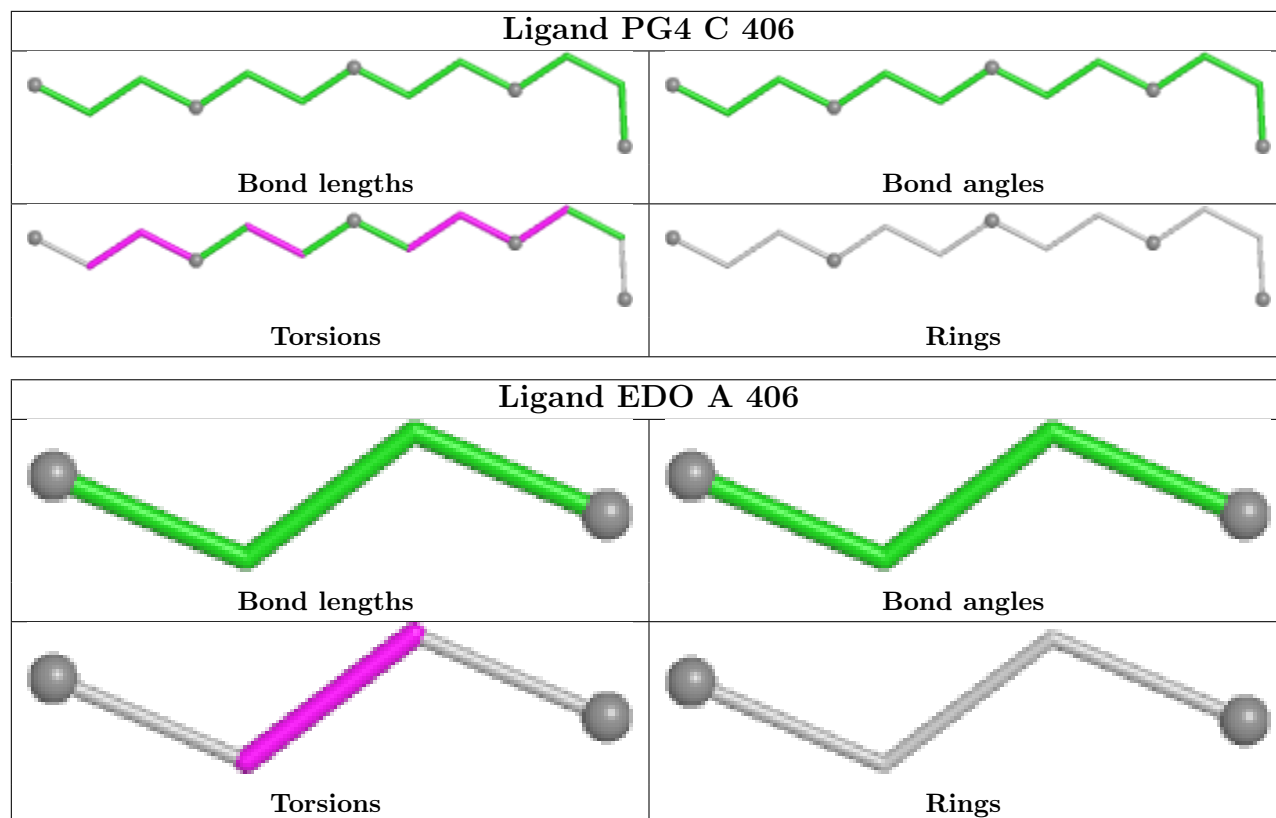












5.7 Other polymers [i](#)

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

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, 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	341/341 (100%)	-0.38	2 (0%) 85 86	16, 41, 65, 116	1 (0%)
1	B	341/341 (100%)	-0.30	3 (0%) 81 82	18, 42, 78, 129	1 (0%)
1	C	341/341 (100%)	-0.37	2 (0%) 85 86	17, 41, 67, 129	1 (0%)
1	D	341/341 (100%)	-0.15	2 (0%) 85 86	17, 45, 73, 113	2 (0%)
All	All	1364/1364 (100%)	-0.30	9 (0%) 84 85	16, 42, 72, 129	5 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	SER	4.2
1	D	152	ALA	3.8
1	A	1	MET	3.6
1	D	66	ASN	2.5
1	B	1	MET	2.3
1	B	25	LYS	2.3
1	C	1	MET	2.3
1	C	341	SER	2.2
1	B	341	SER	2.1

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 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	EDO	A	410	4/4	0.71	0.24	59,66,72,74	0
5	EDO	B	404	4/4	0.73	0.22	78,84,85,86	0
5	EDO	D	405	4/4	0.74	0.22	70,75,81,83	0
10	SO4	D	408	5/5	0.78	0.12	68,70,70,82	5
3	PEG	B	405	7/7	0.80	0.19	68,77,82,84	0
5	EDO	A	406	4/4	0.81	0.24	58,82,87,89	0
5	EDO	D	409	4/4	0.82	0.18	67,67,70,70	0
6	TRS	B	401	8/8	0.82	0.15	61,71,79,84	0
7	GOL	B	407	6/6	0.82	0.15	80,83,90,90	0
10	SO4	C	409	5/5	0.82	0.13	76,77,80,95	5
5	EDO	C	407	4/4	0.82	0.21	72,80,82,84	0
10	SO4	A	416	5/5	0.83	0.10	78,81,83,95	5
5	EDO	A	405	4/4	0.85	0.19	72,72,73,75	0
5	EDO	D	403	4/4	0.85	0.14	64,68,68,69	0
5	EDO	A	404	4/4	0.85	0.17	69,72,75,78	0
5	EDO	D	404	4/4	0.86	0.21	73,74,75,80	0
3	PEG	A	402	7/7	0.86	0.14	59,73,85,86	0
3	PEG	B	410	7/7	0.86	0.15	80,83,90,95	0
5	EDO	A	411	4/4	0.86	0.19	76,77,80,81	0
7	GOL	D	410	6/6	0.87	0.24	53,55,56,58	0
5	EDO	A	412	4/4	0.87	0.18	71,73,76,77	0
5	EDO	B	412	4/4	0.87	0.16	56,62,73,84	0
5	EDO	D	406	4/4	0.87	0.18	48,59,68,81	0
6	TRS	A	407	8/8	0.88	0.11	59,75,78,83	0
7	GOL	B	411	6/6	0.88	0.28	44,47,50,53	0
5	EDO	A	409	4/4	0.88	0.14	67,69,70,70	0
5	EDO	B	408	4/4	0.89	0.15	82,88,93,95	0
4	PG4	C	403	13/13	0.89	0.16	46,57,72,74	0
3	PEG	C	405	7/7	0.89	0.14	57,65,69,69	0
4	PG4	A	403	13/13	0.89	0.15	45,59,68,68	0
9	PGE	A	415	10/10	0.90	0.14	60,65,80,83	0
9	PGE	C	401	10/10	0.90	0.13	58,67,76,78	0
3	PEG	B	406	7/7	0.90	0.13	61,73,83,84	0
4	PG4	B	413	13/13	0.90	0.12	55,65,83,84	0
3	PEG	D	401	7/7	0.90	0.13	54,57,67,70	0
4	PG4	B	409	13/13	0.91	0.14	39,54,63,71	0
5	EDO	D	411	4/4	0.91	0.12	73,74,77,79	0

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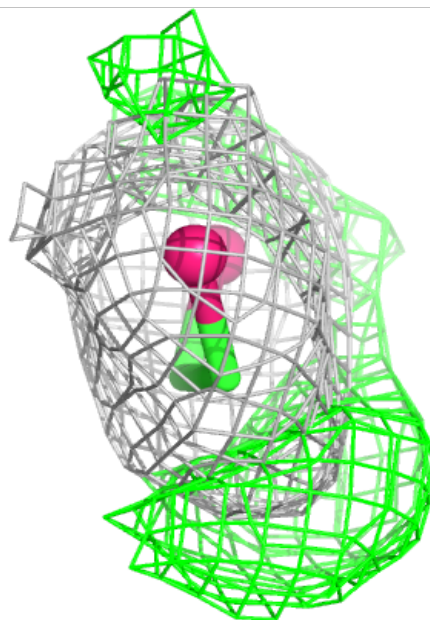
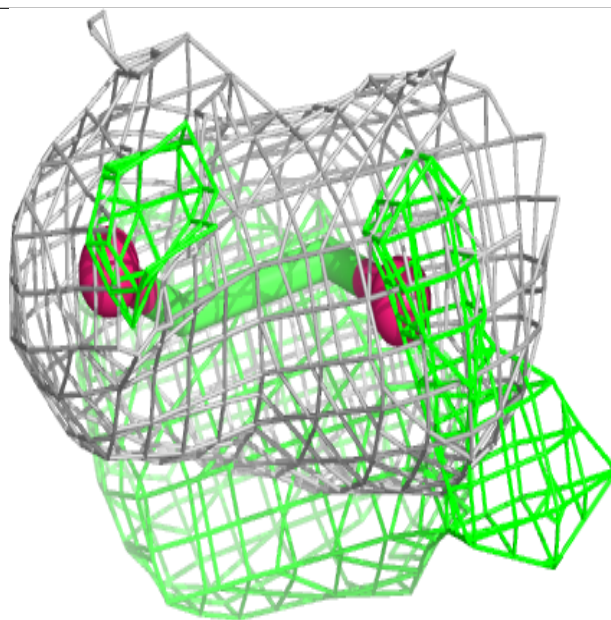
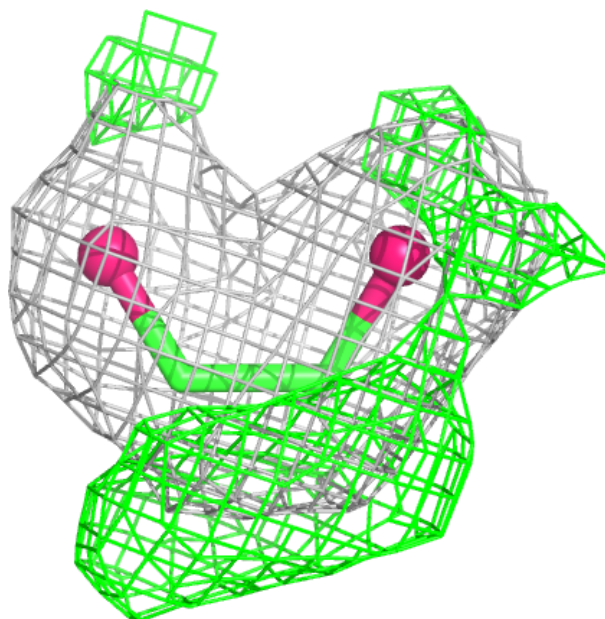
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	D	407	13/13	0.92	0.13	56,62,71,72	0
7	GOL	C	408	6/6	0.92	0.30	47,54,59,61	0
5	EDO	C	404	4/4	0.92	0.14	67,69,69,75	0
2	NAD	C	402	44/44	0.92	0.11	43,56,79,89	0
2	NAD	B	402	44/44	0.92	0.11	48,58,92,102	0
3	PEG	A	408	7/7	0.92	0.12	67,80,94,97	0
7	GOL	A	413	6/6	0.92	0.15	45,50,53,58	0
4	PG4	C	406	13/13	0.92	0.11	53,60,71,71	0
8	XPE	A	414	31/31	0.95	0.11	32,42,64,70	0
2	NAD	A	401	44/44	0.95	0.08	38,50,66,71	0
2	NAD	D	402	44/44	0.96	0.07	35,52,60,66	0
11	MG	B	403	1/1	0.99	0.04	50,50,50,50	0

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

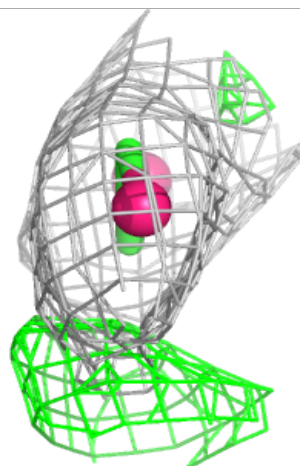
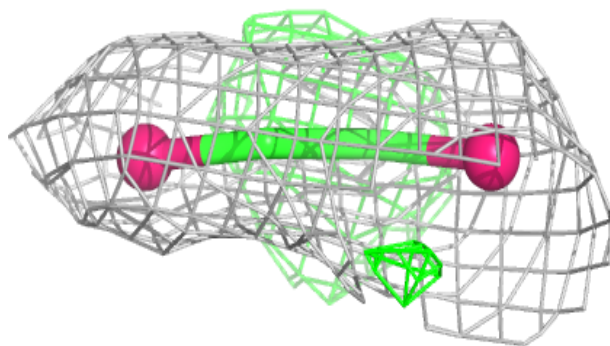
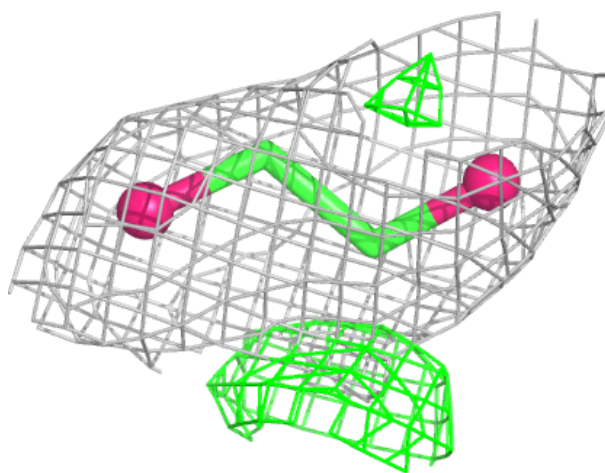
Electron density around EDO A 410:

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



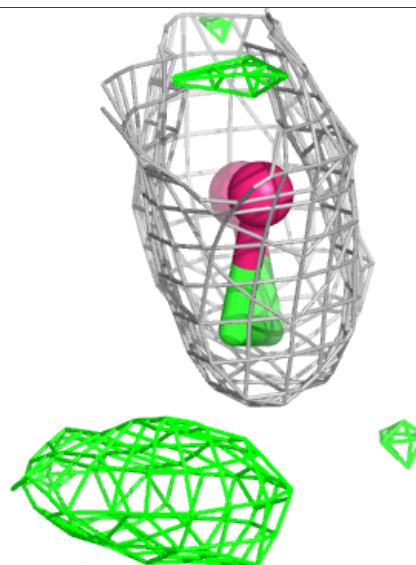
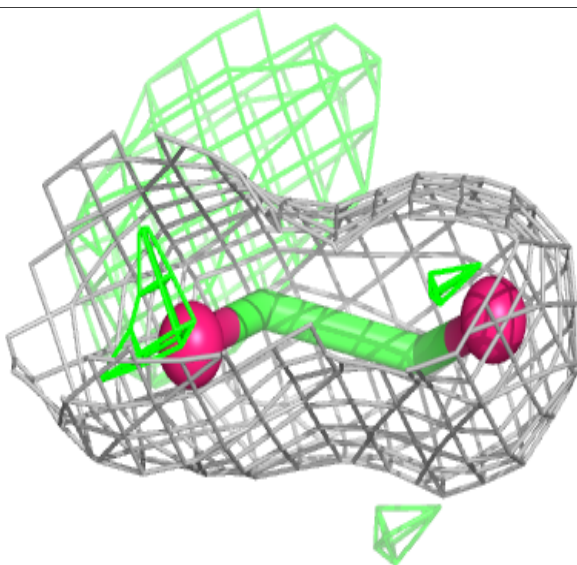
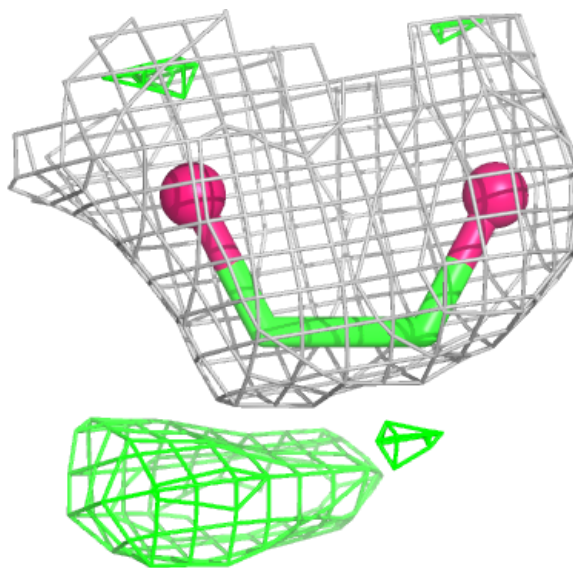
Electron density around EDO B 404:

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



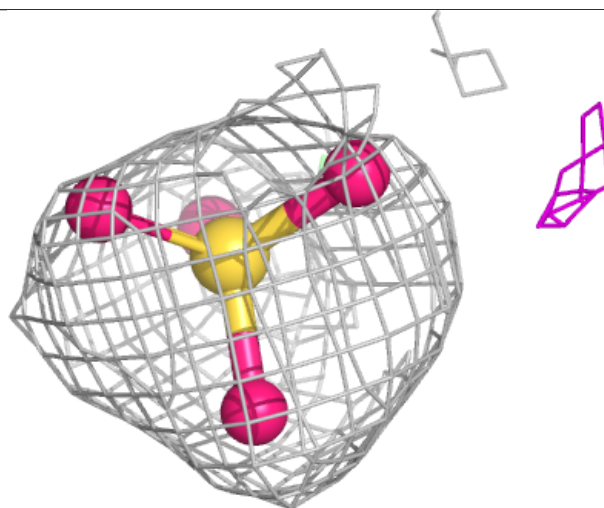
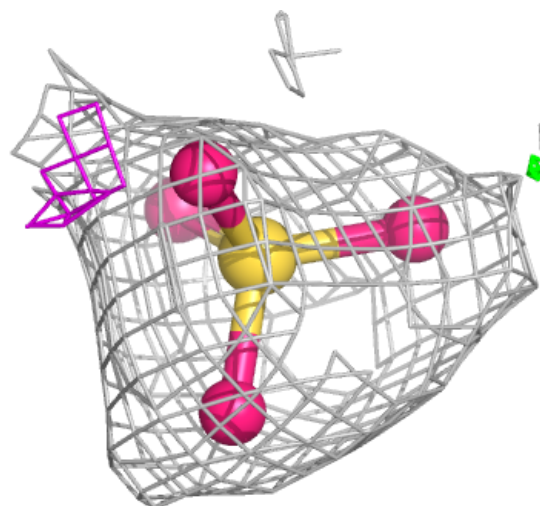
Electron density around EDO D 405:

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



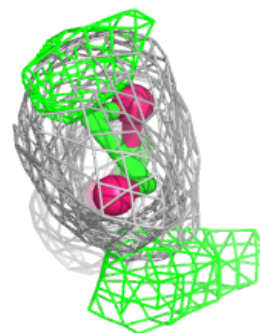
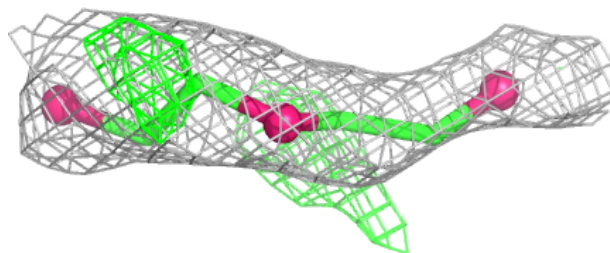
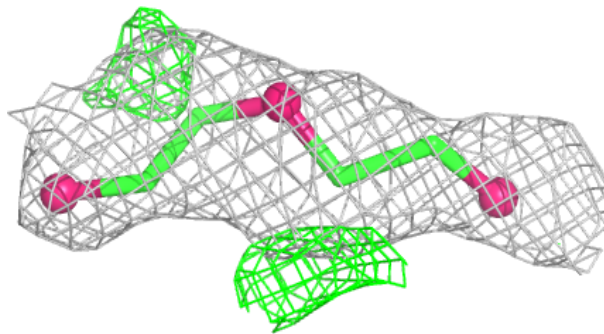
Electron density around SO4 D 408:

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



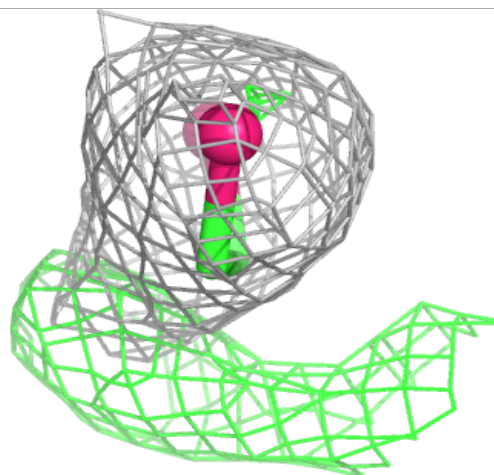
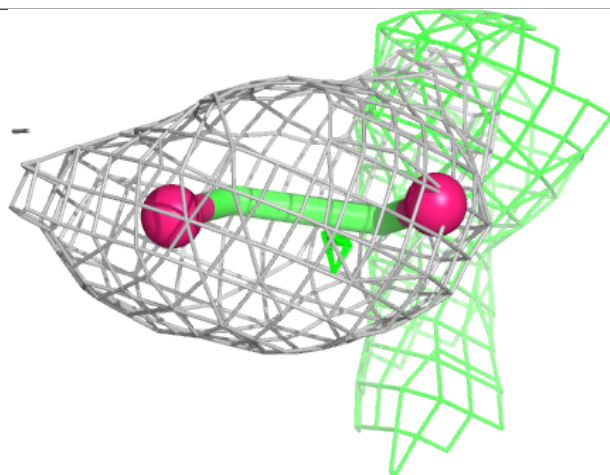
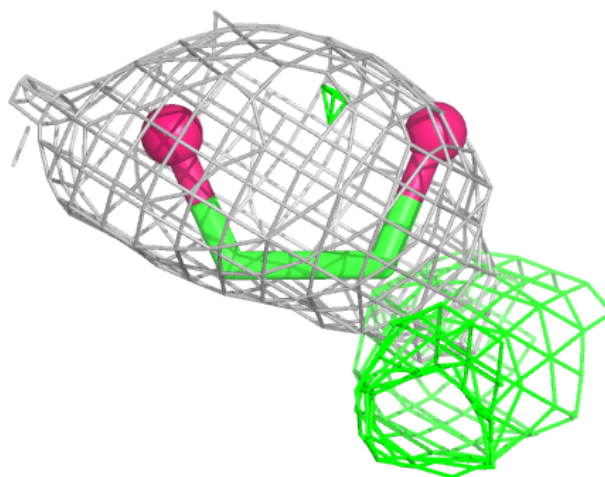
Electron density around PEG B 405:

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



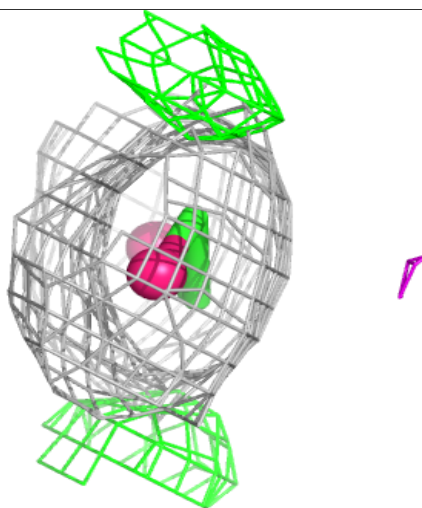
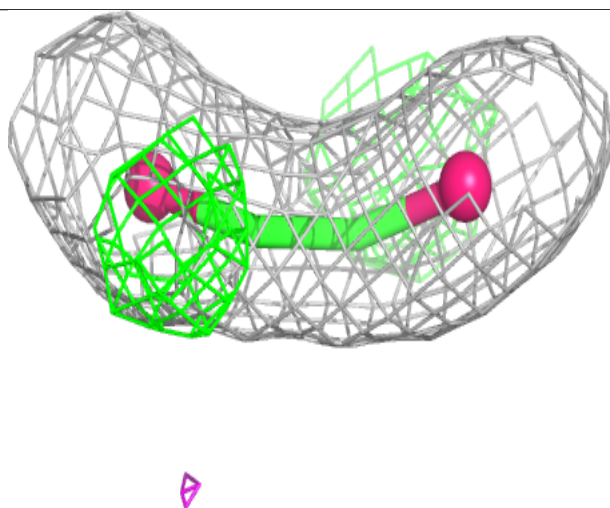
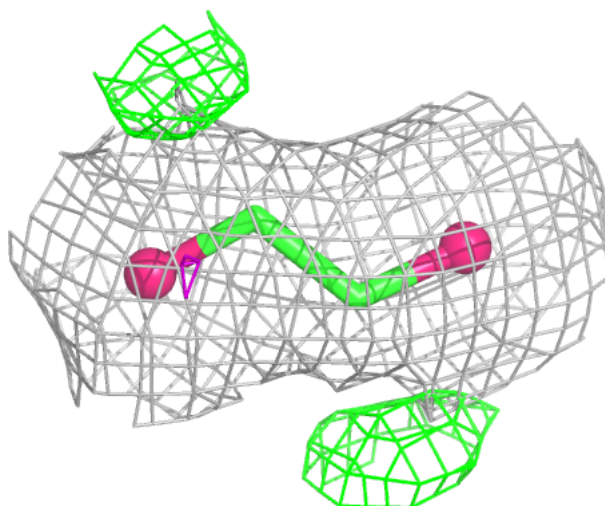
Electron density around EDO A 406:

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



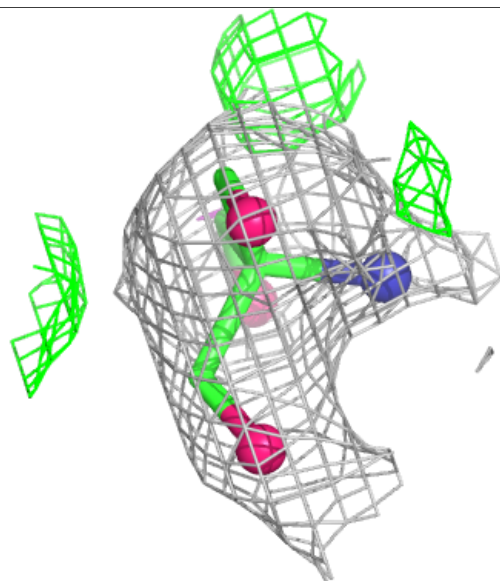
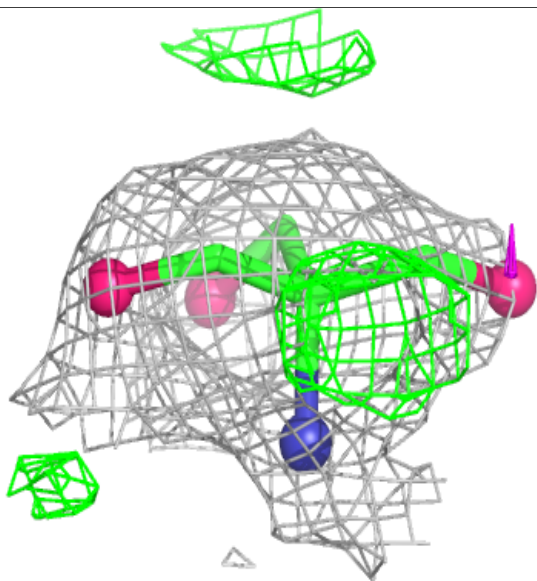
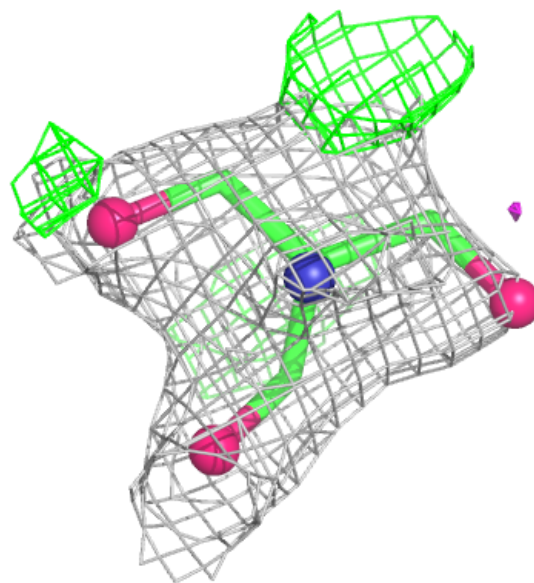
Electron density around EDO D 409:

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



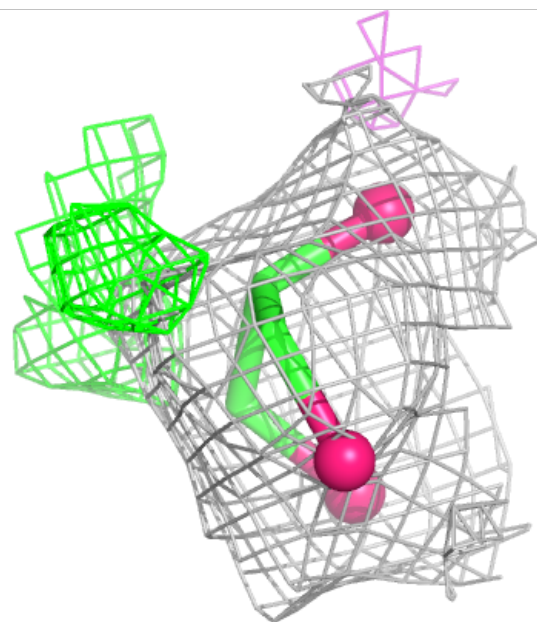
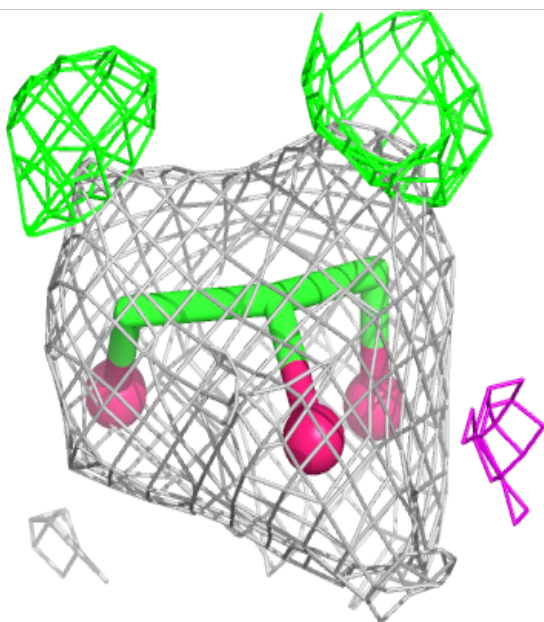
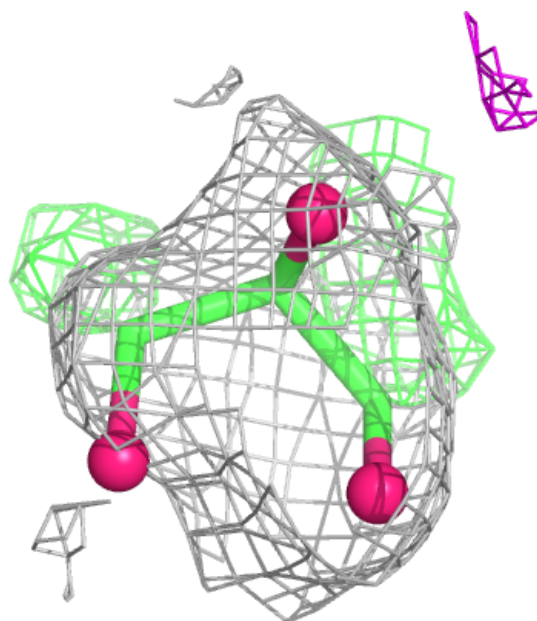
Electron density around TRS B 401:

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



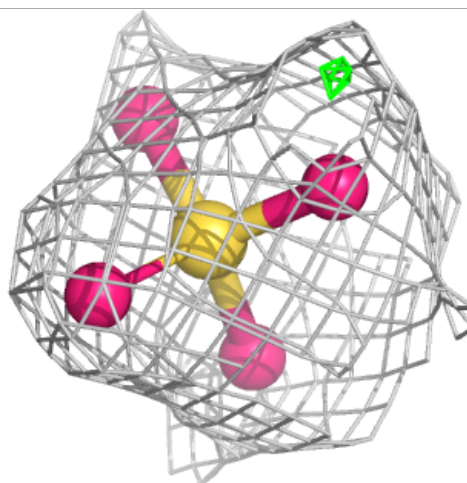
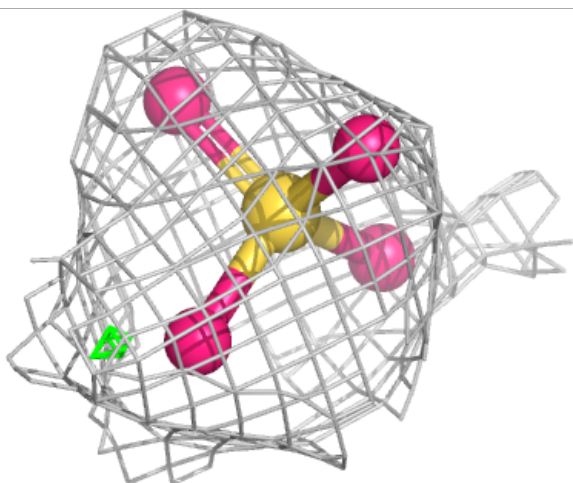
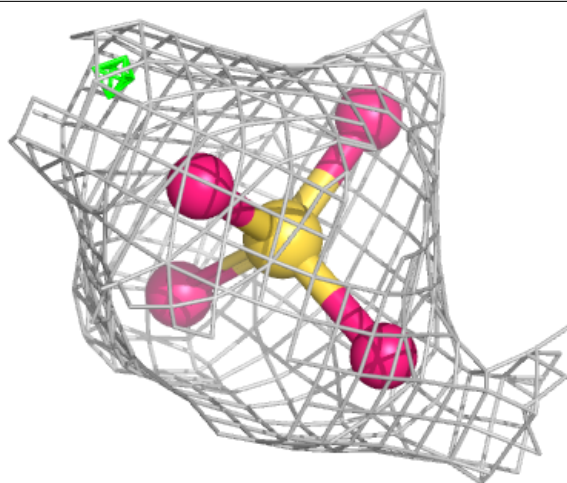
Electron density around GOL B 407:

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



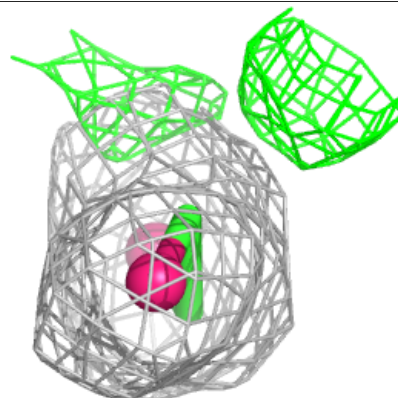
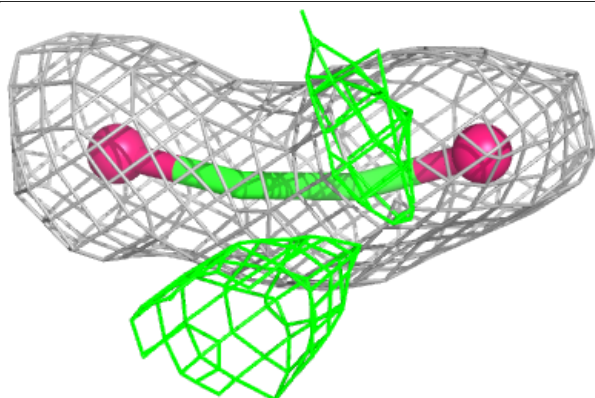
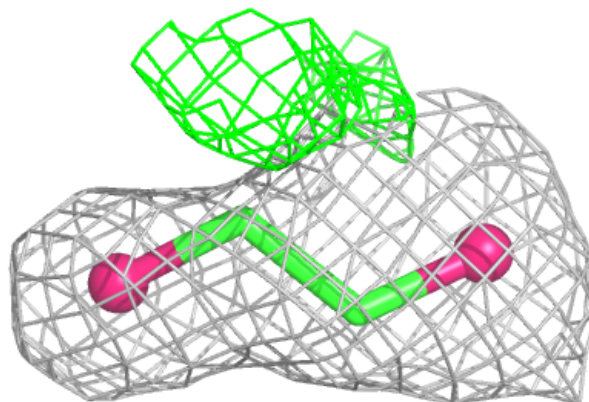
Electron density around SO4 C 409:

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



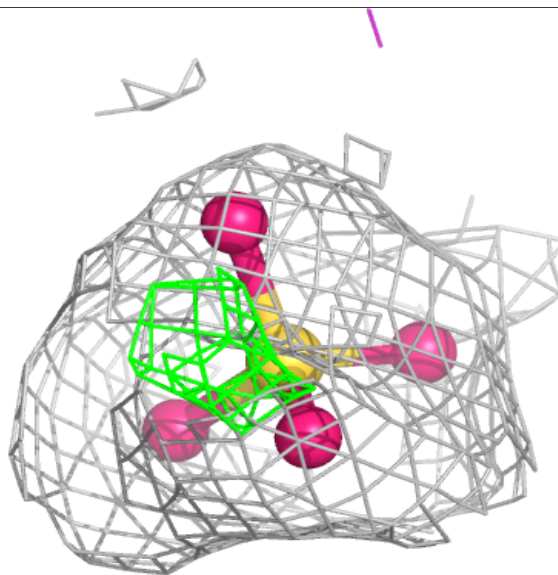
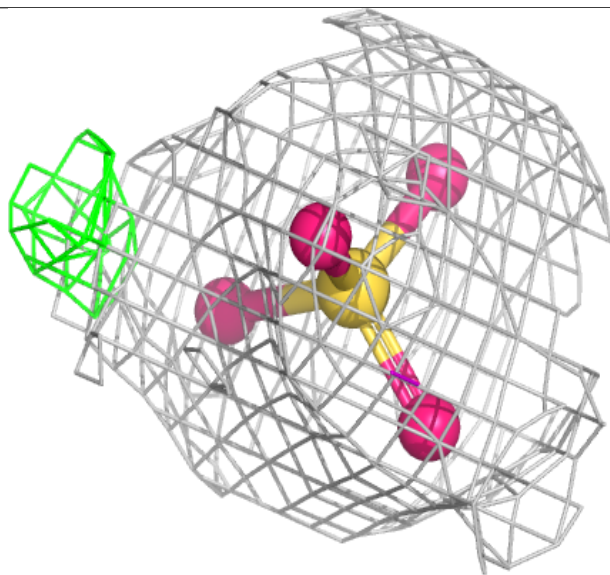
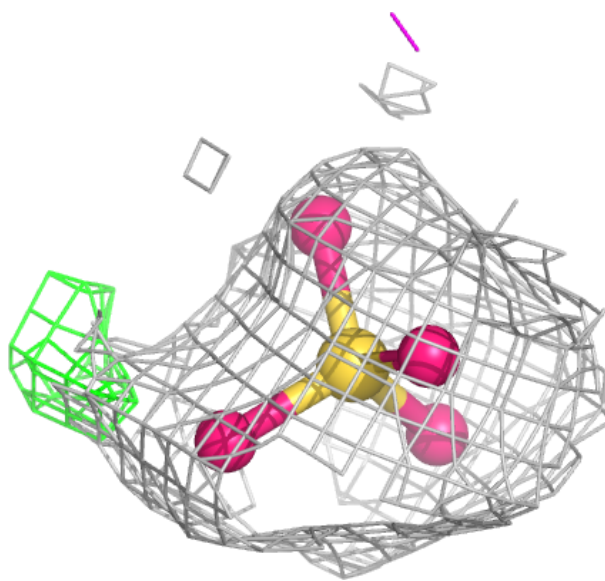
Electron density around EDO C 407:

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



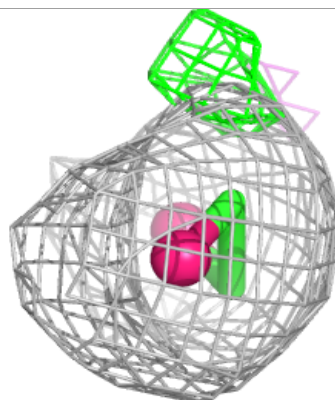
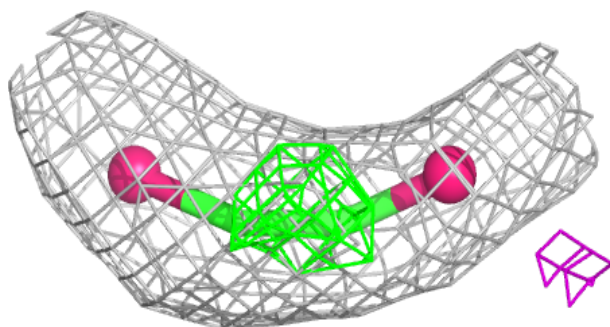
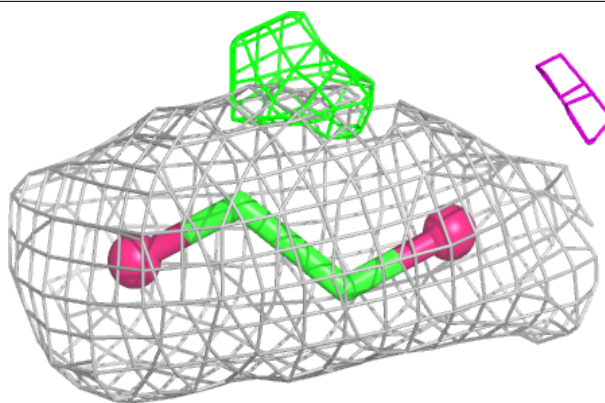
Electron density around SO4 A 416:

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

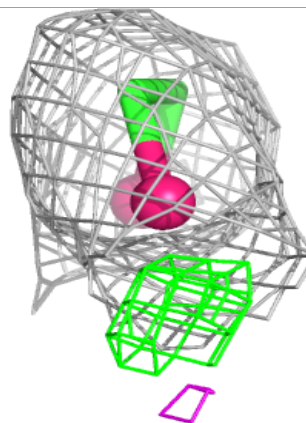
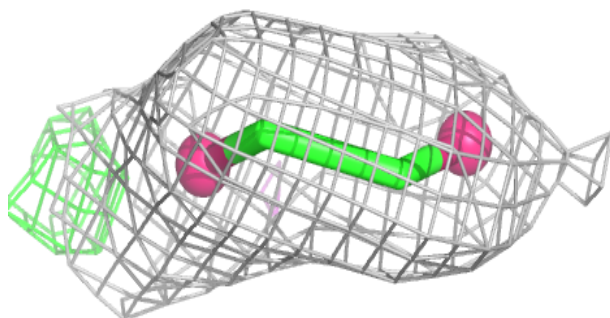
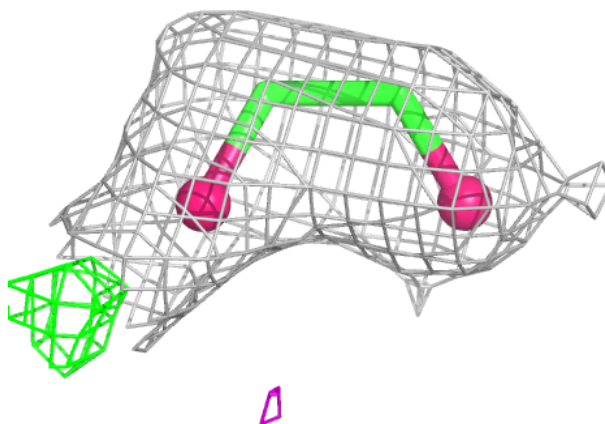


Electron density around EDO A 405:

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

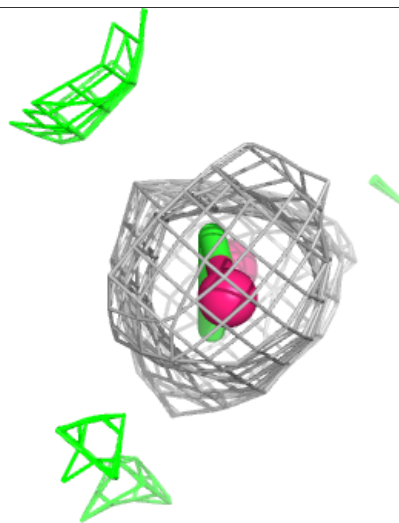
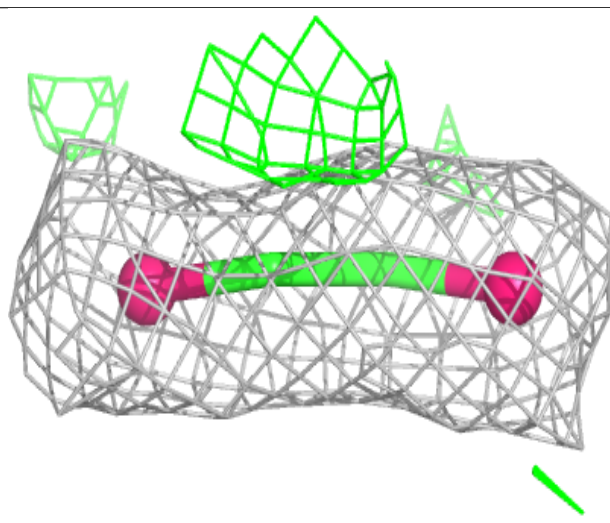
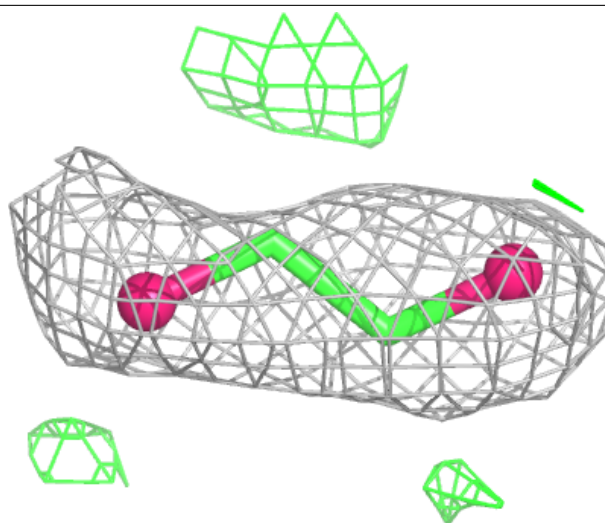
**Electron density around EDO D 403:**

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



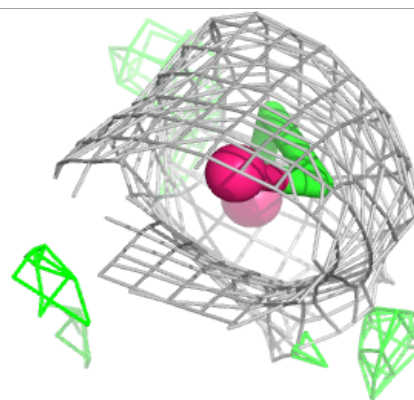
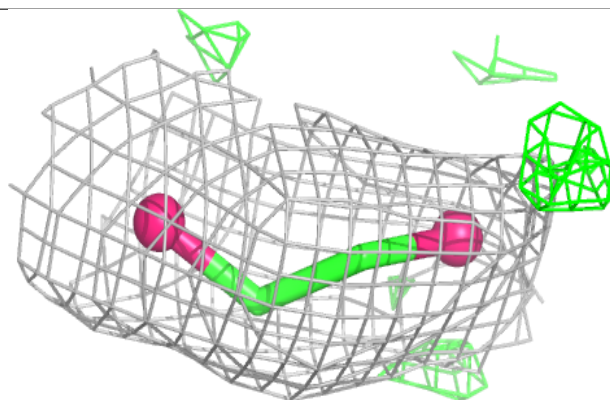
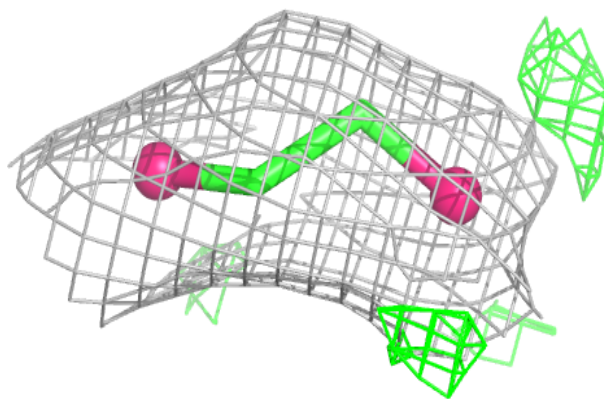
Electron density around EDO A 404:

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

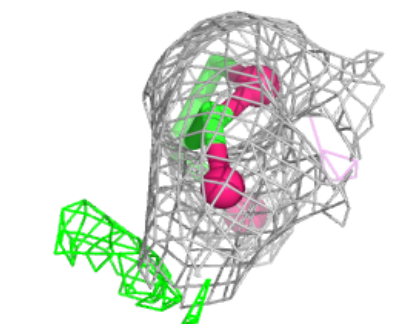
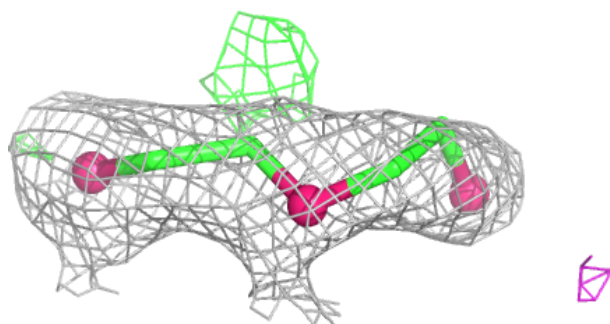
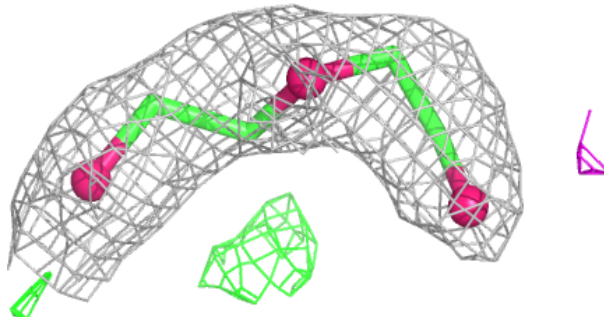


Electron density around EDO D 404:

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

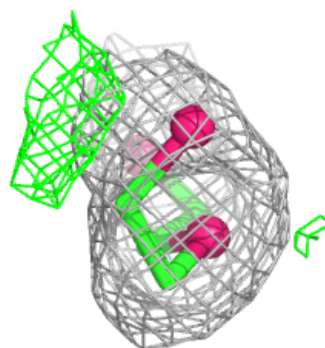
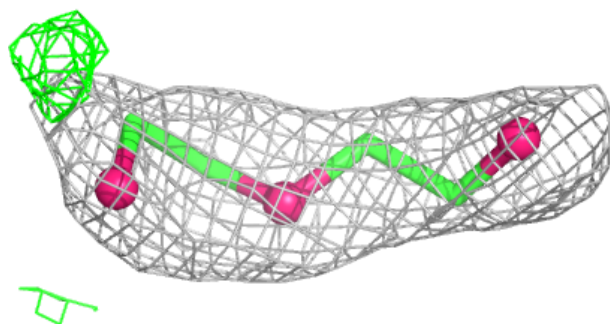
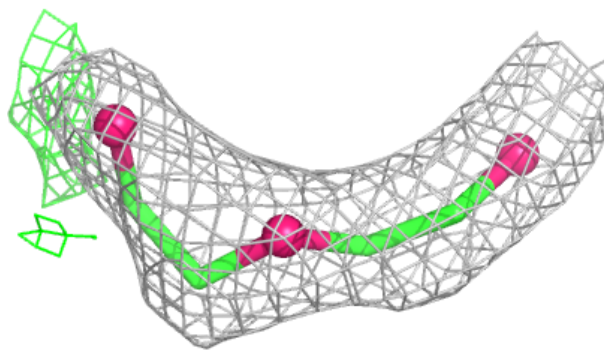
**Electron density around PEG A 402:**

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



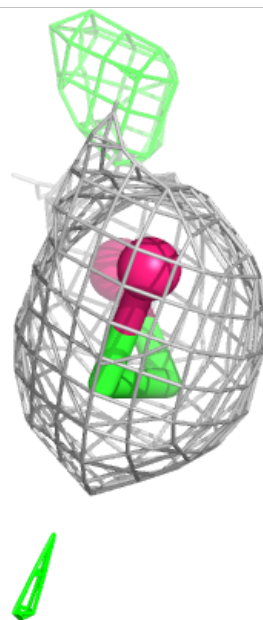
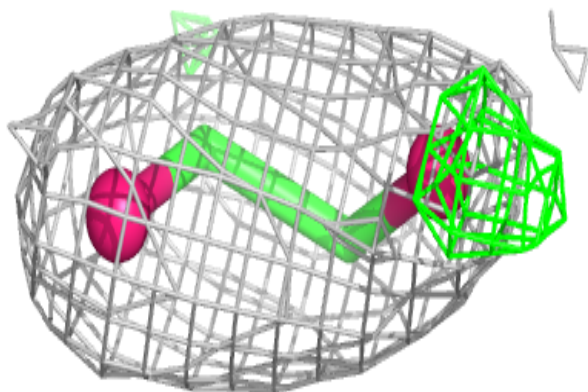
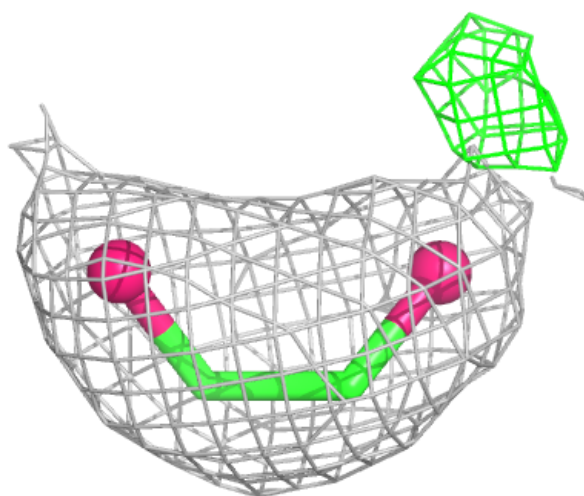
Electron density around PEG B 410:

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



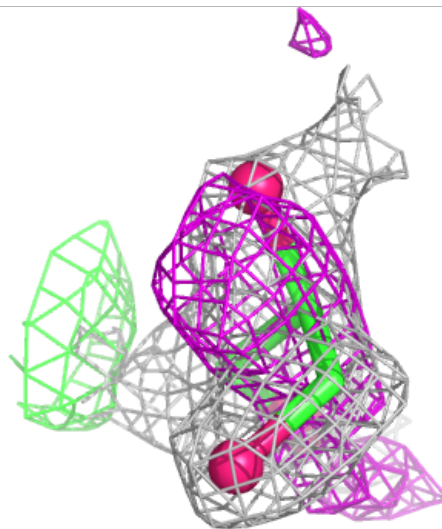
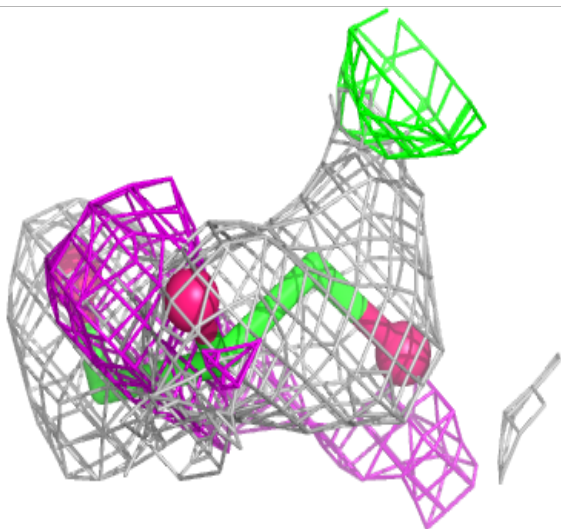
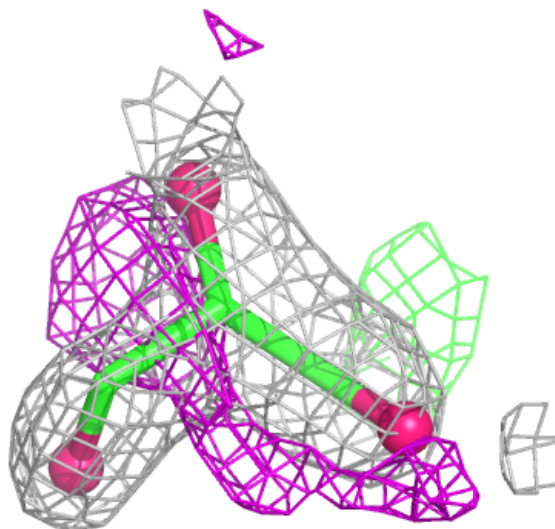
Electron density around EDO A 411:

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



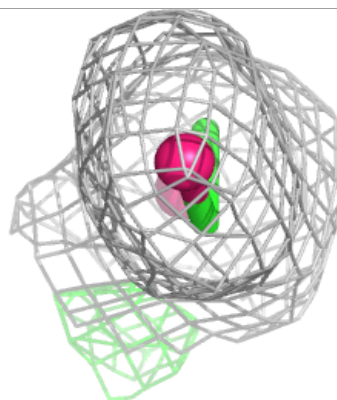
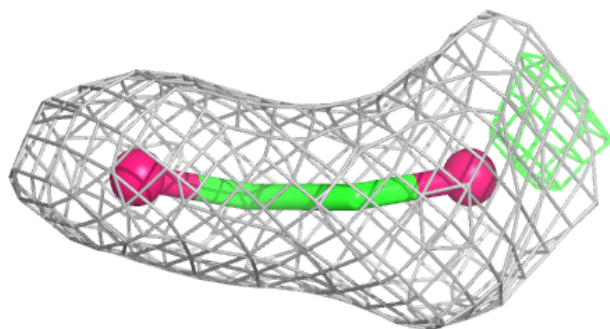
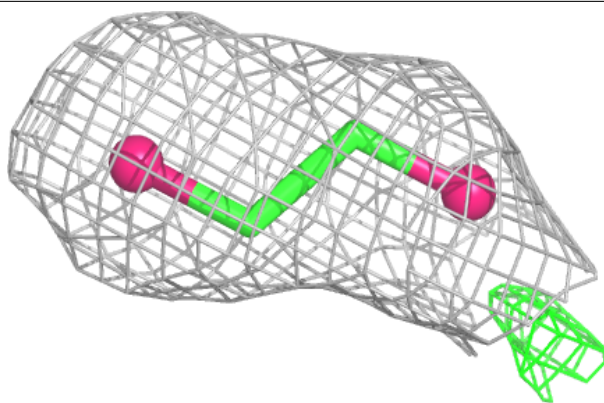
Electron density around GOL D 410:

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



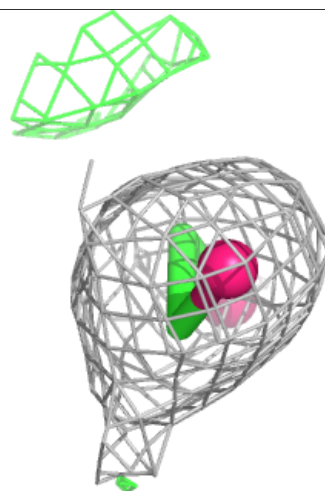
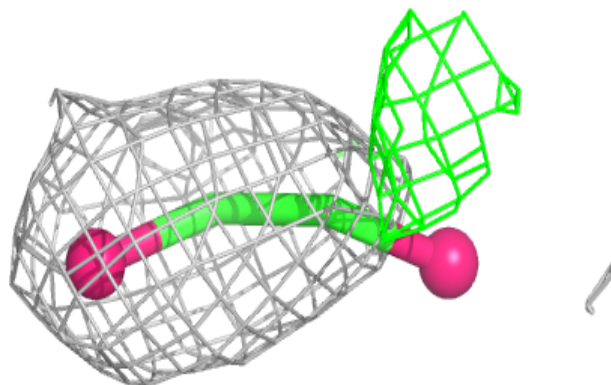
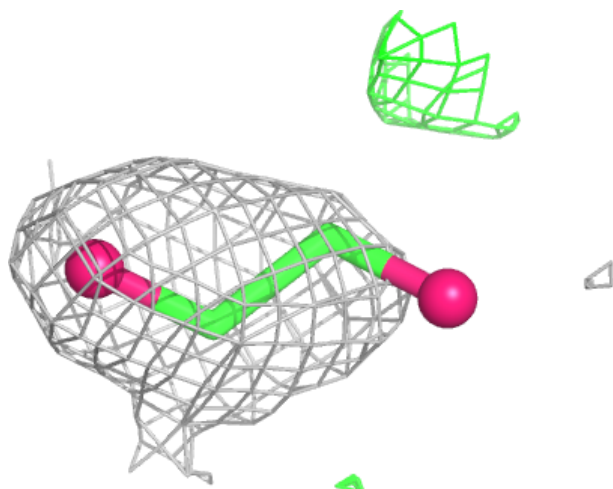
Electron density around EDO A 412:

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



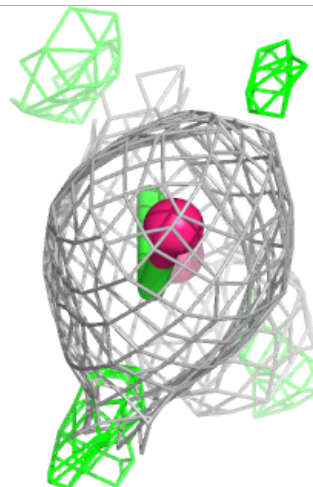
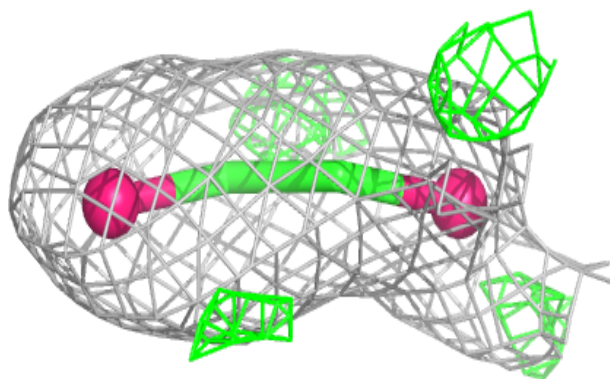
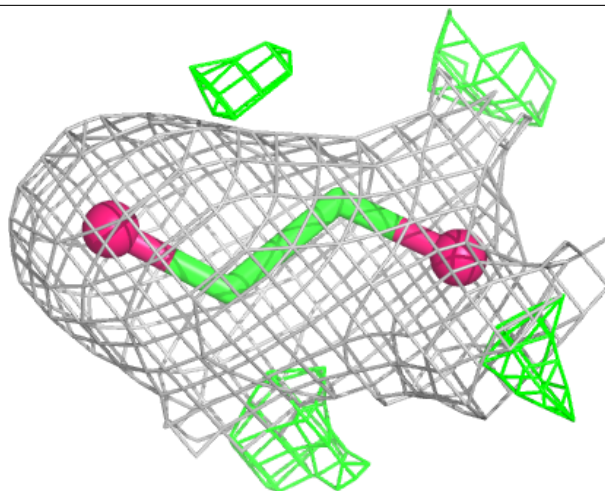
Electron density around EDO B 412:

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and green (positive)



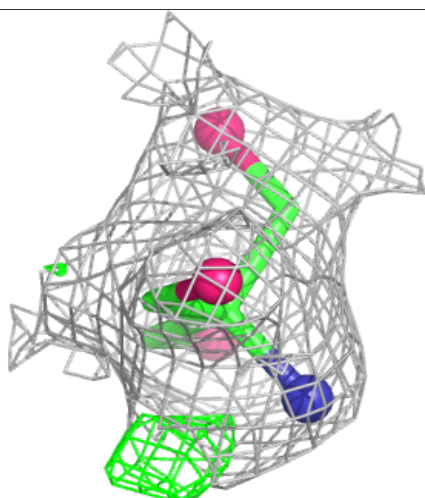
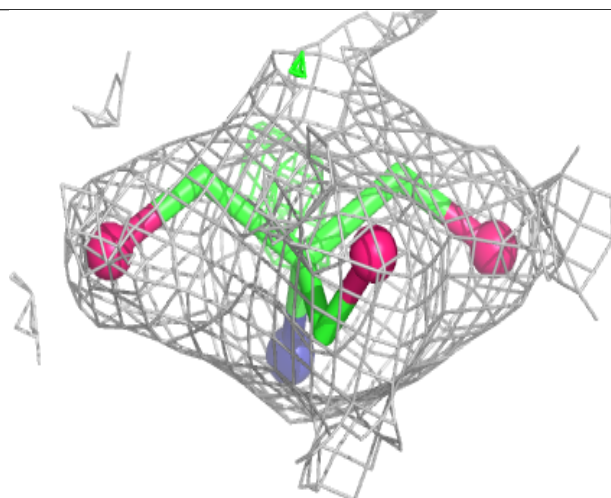
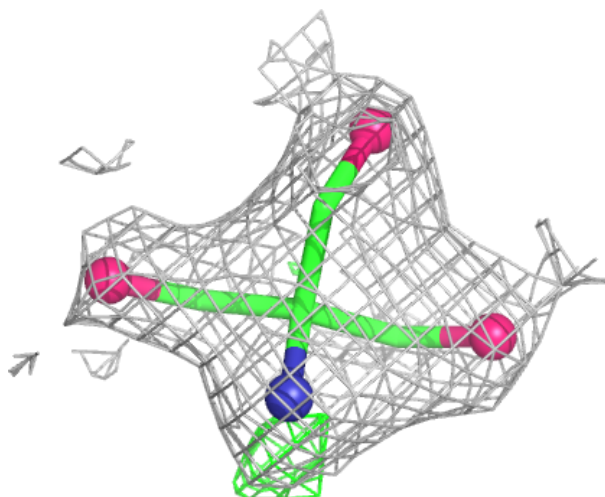
Electron density around EDO D 406:

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



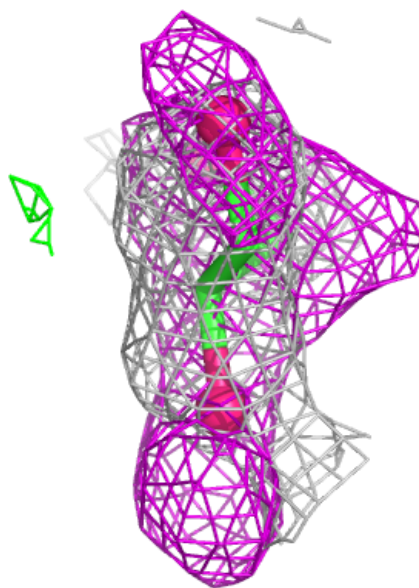
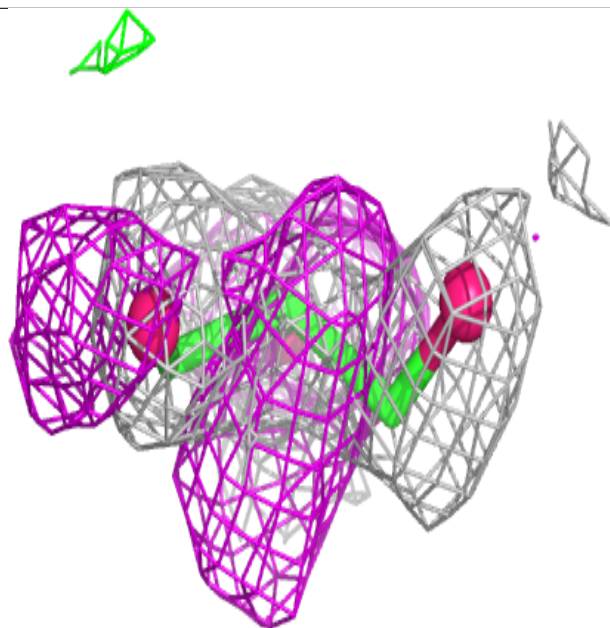
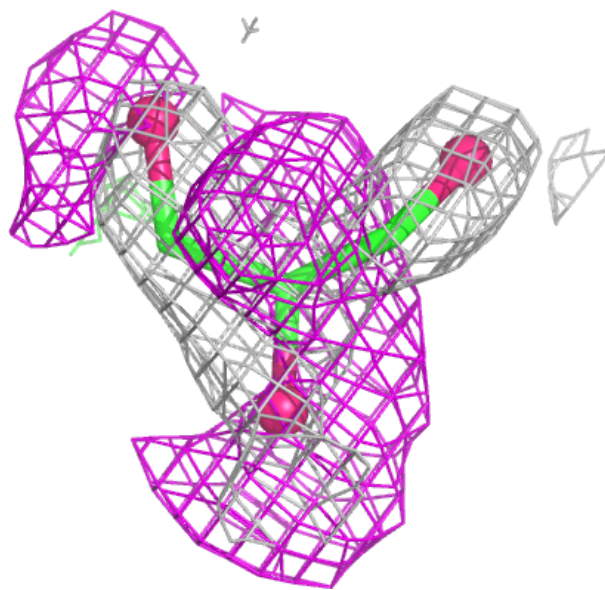
Electron density around TRS A 407:

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



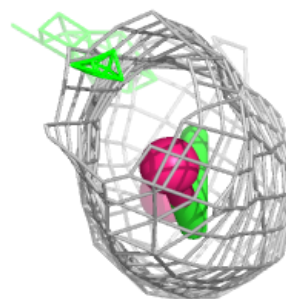
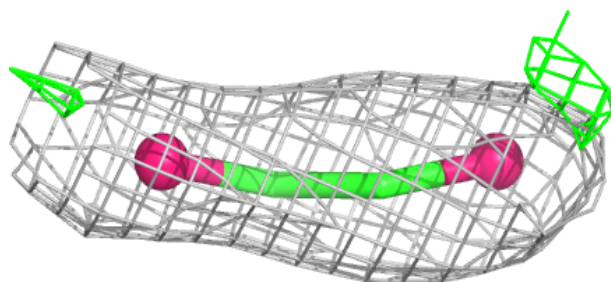
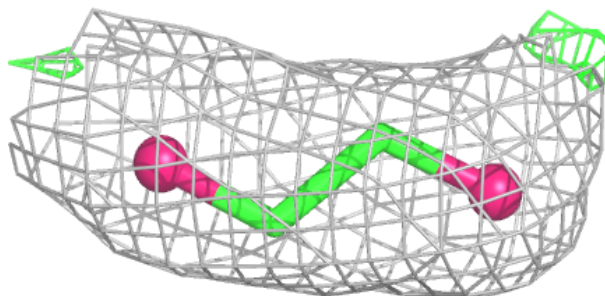
Electron density around GOL B 411:

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



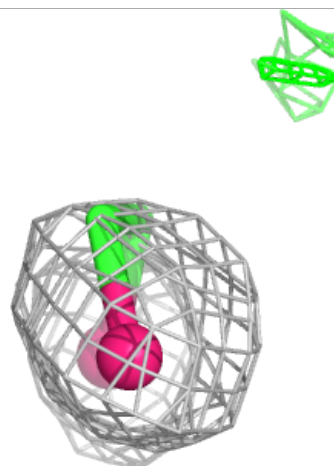
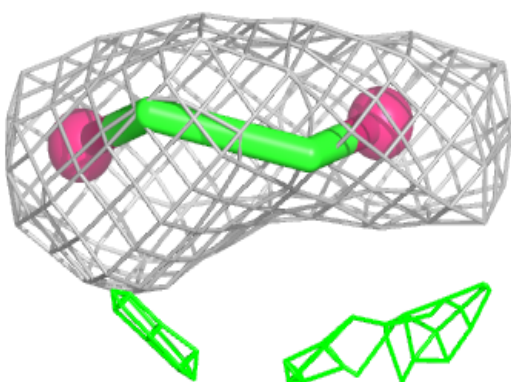
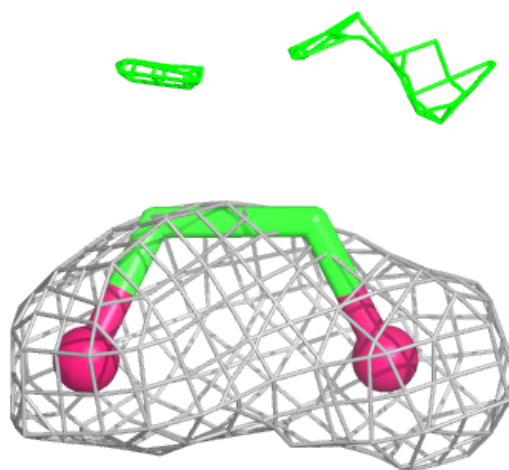
Electron density around EDO A 409:

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



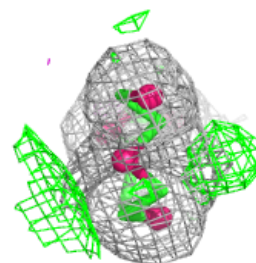
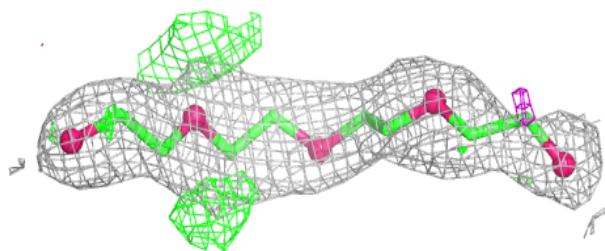
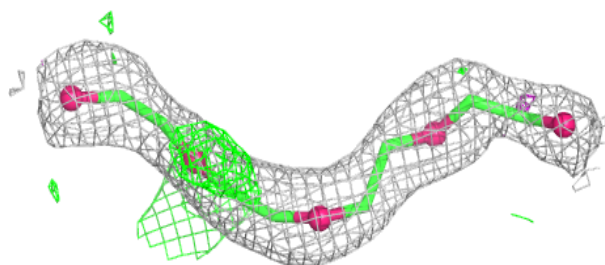
Electron density around EDO B 408:

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

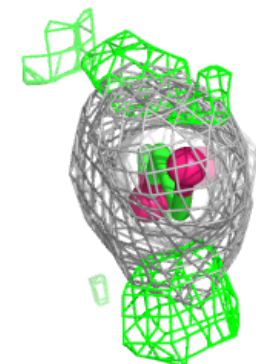
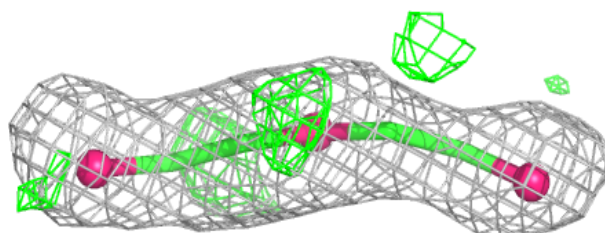
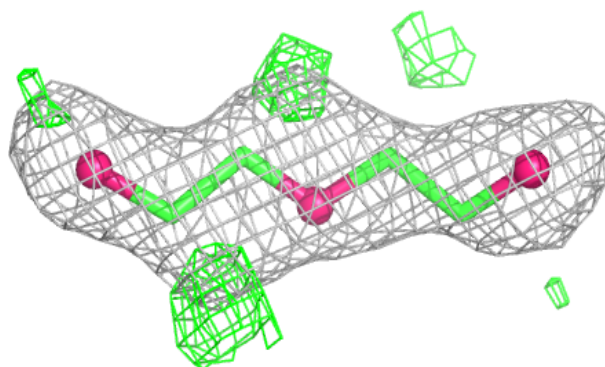


Electron density around PG4 C 403:

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

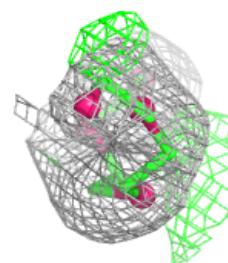
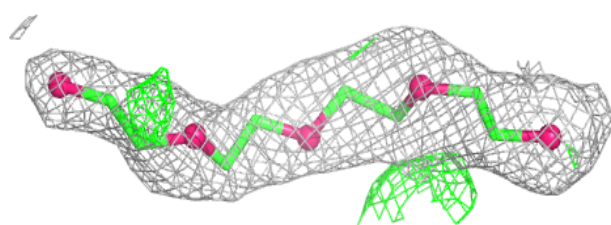
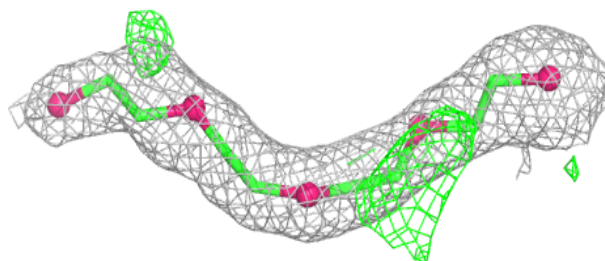
**Electron density around PEG C 405:**

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

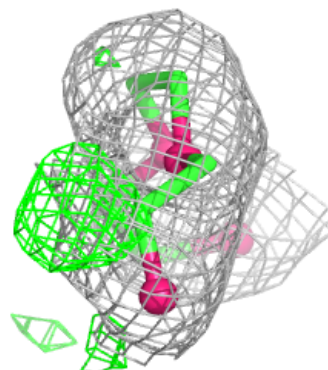
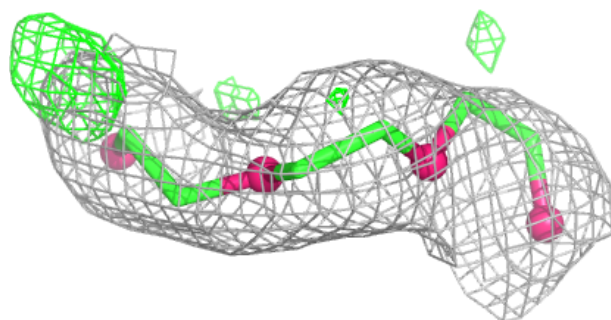
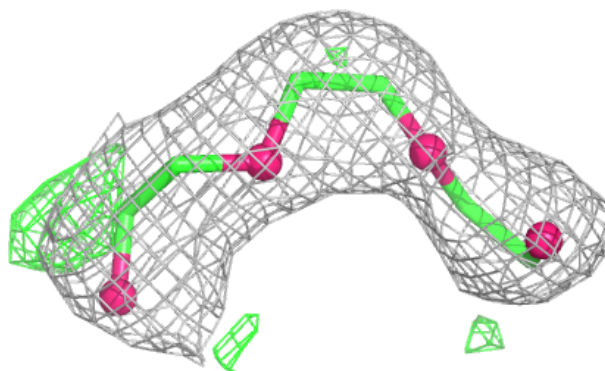


Electron density around PG4 A 403:

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

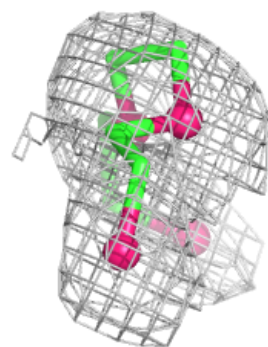
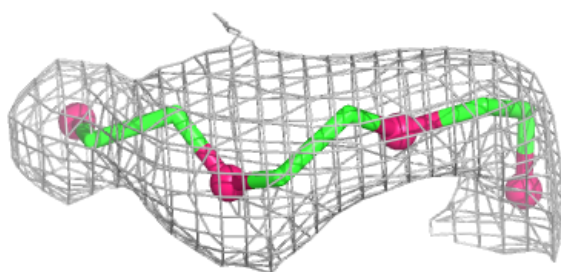
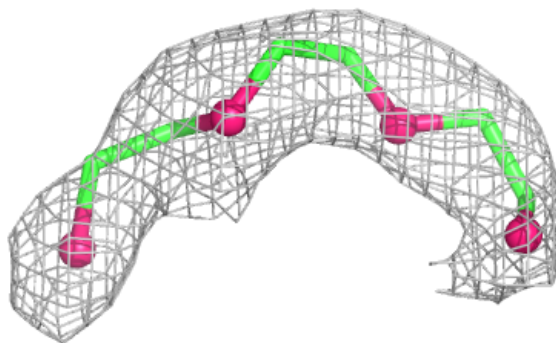
**Electron density around PGE A 415:**

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

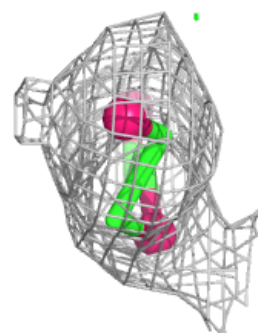
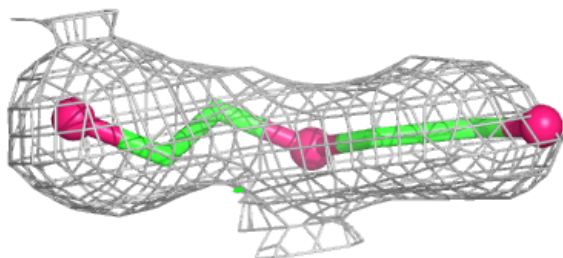
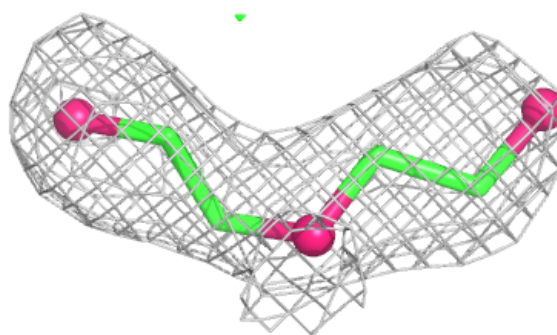


Electron density around PGE C 401:

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

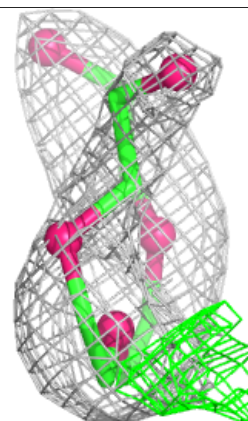
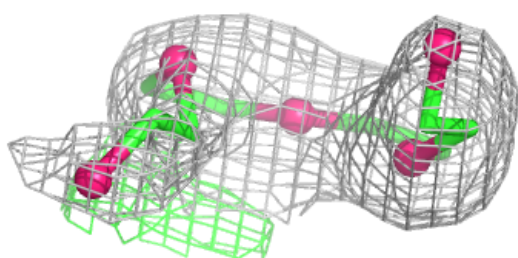
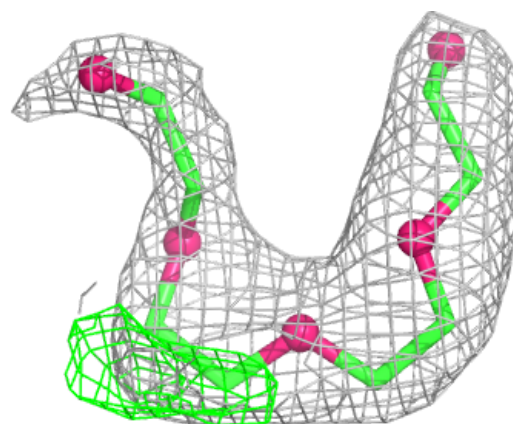
**Electron density around PEG B 406:**

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

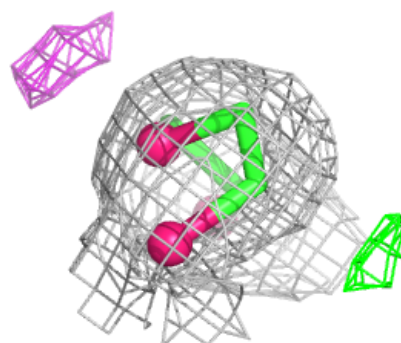
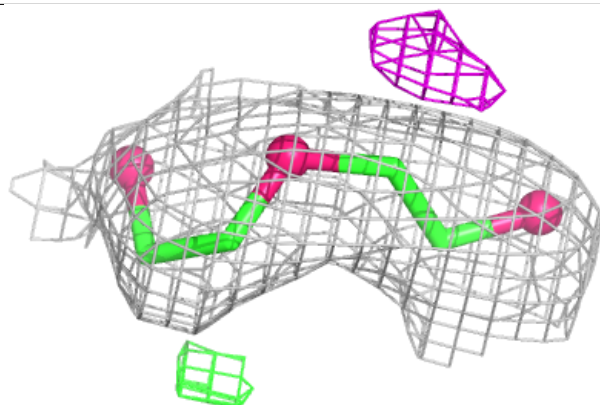
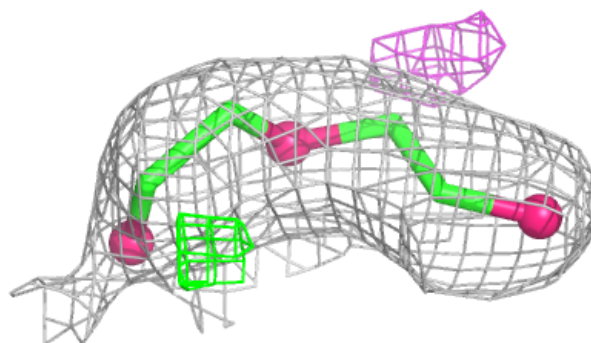


Electron density around PG4 B 413:

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

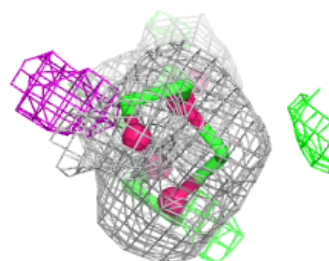
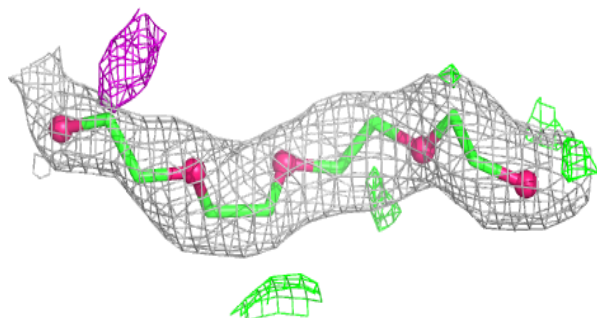
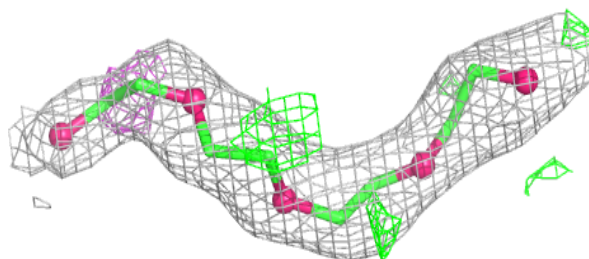
**Electron density around PEG D 401:**

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

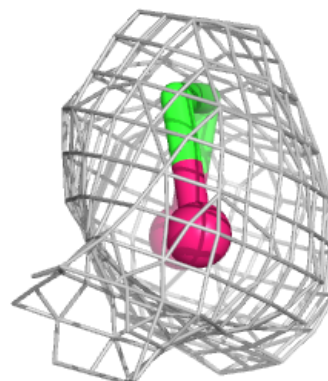
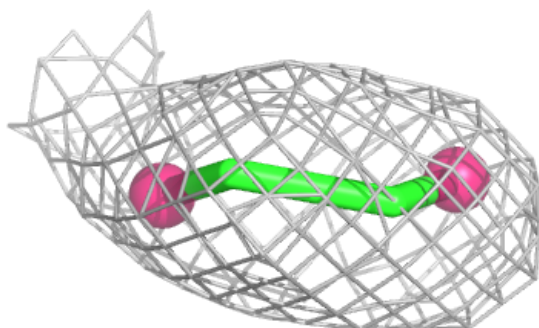
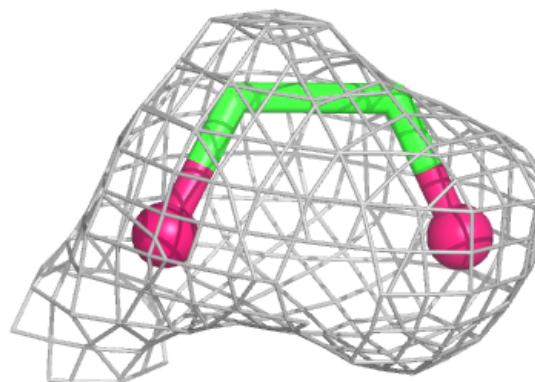


Electron density around PG4 B 409:

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

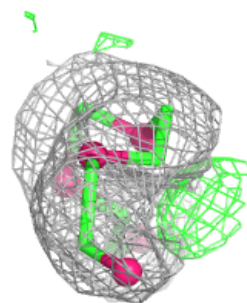
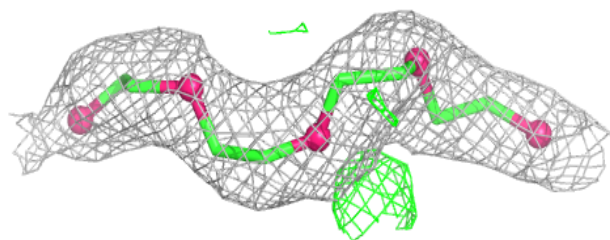
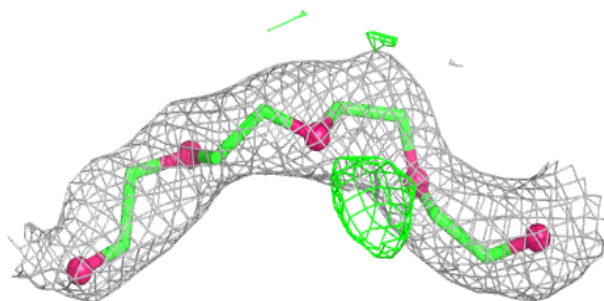
**Electron density around EDO D 411:**

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



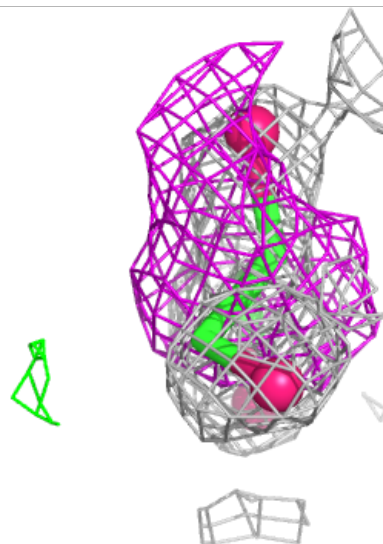
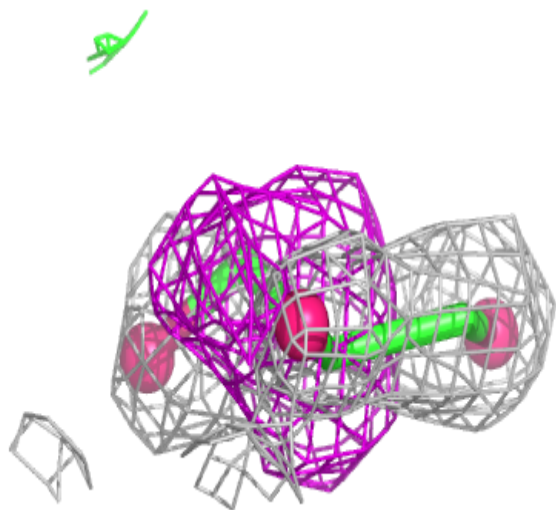
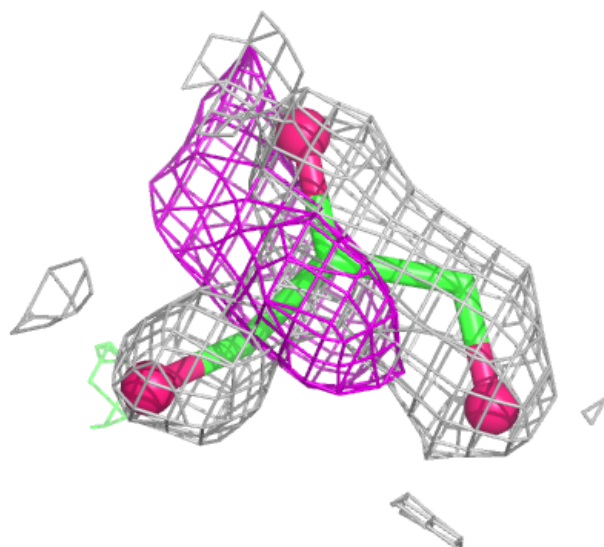
Electron density around PG4 D 407:

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



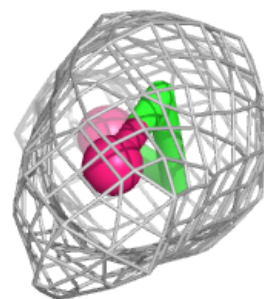
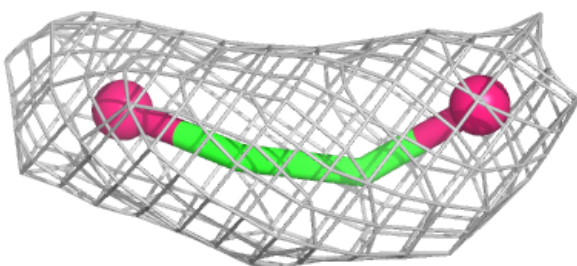
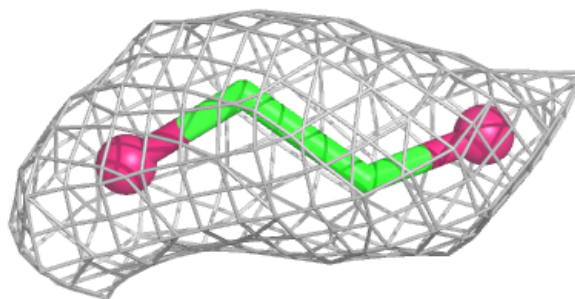
Electron density around GOL C 408:

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

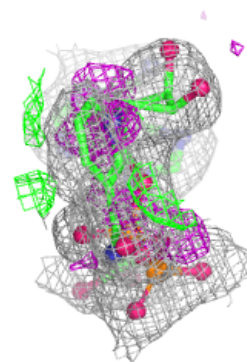
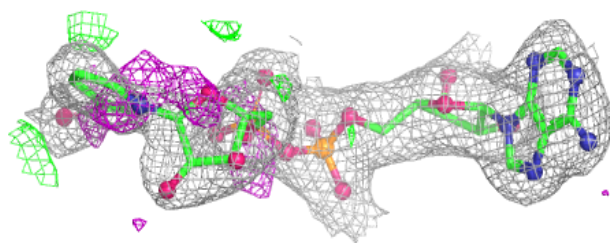
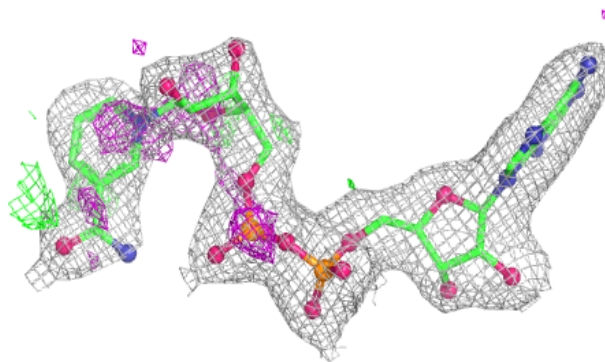


Electron density around EDO C 404:

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

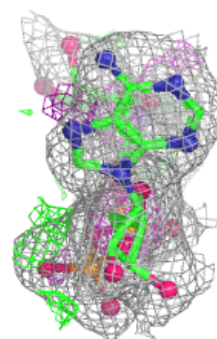
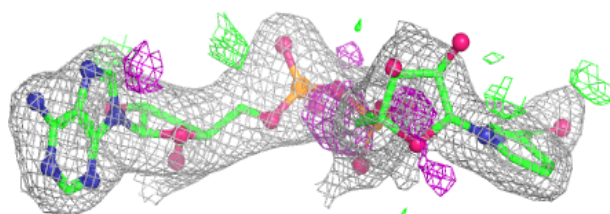
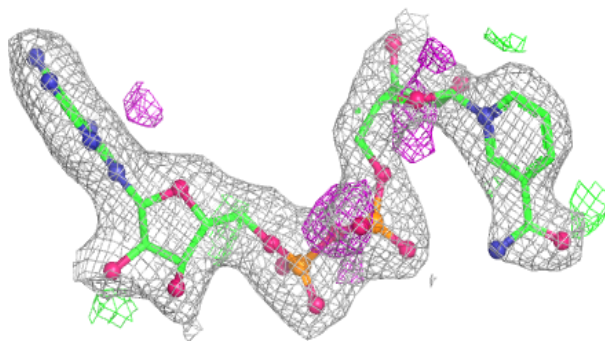
**Electron density around NAD C 402:**

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

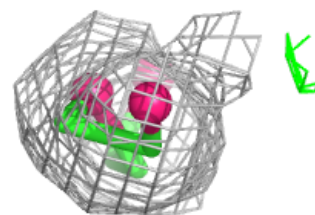
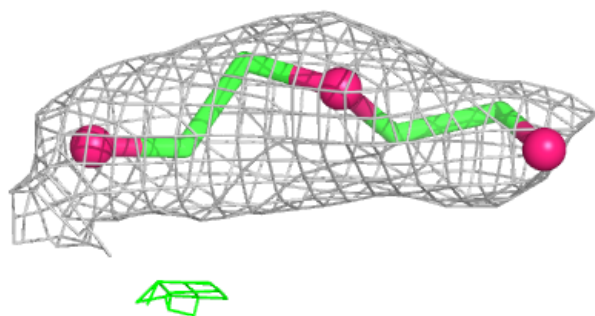
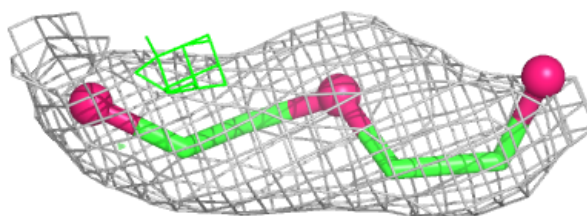


Electron density around NAD B 402:

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

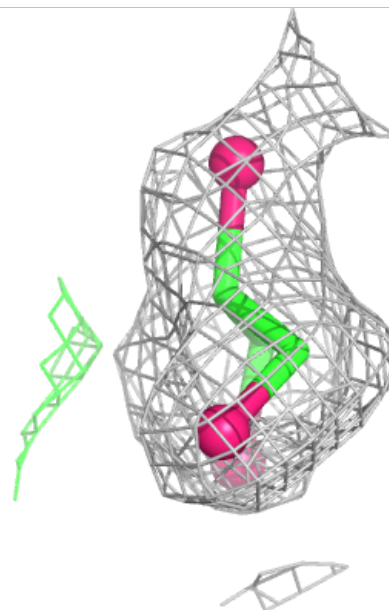
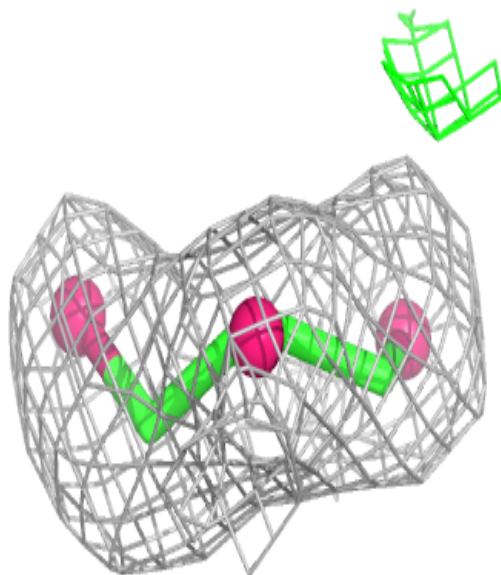
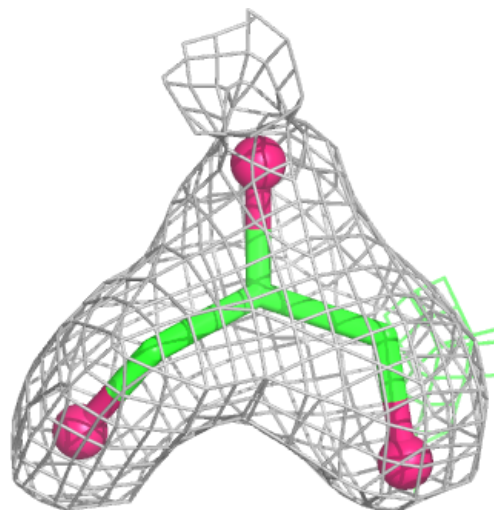
**Electron density around PEG A 408:**

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



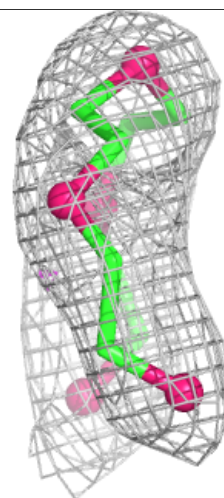
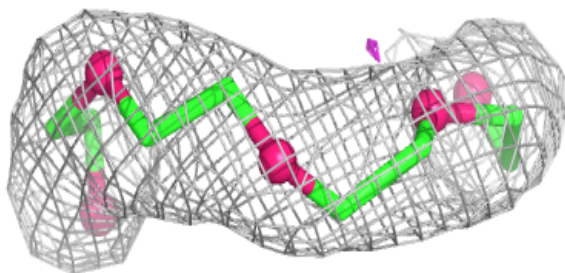
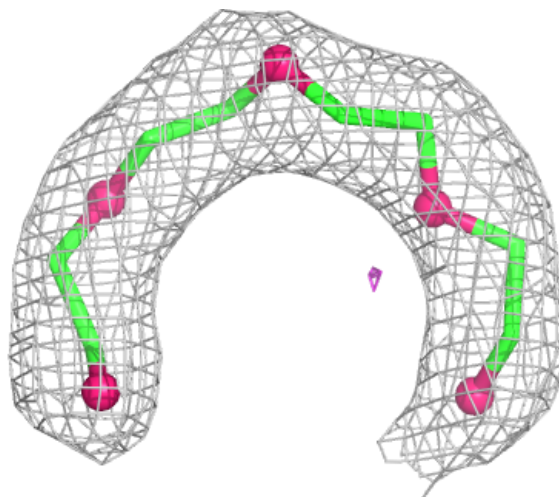
Electron density around GOL A 413:

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



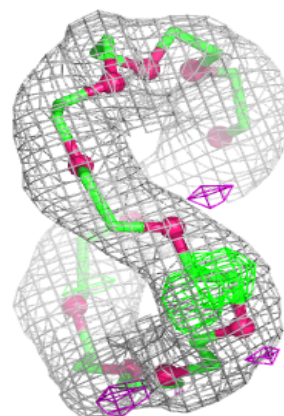
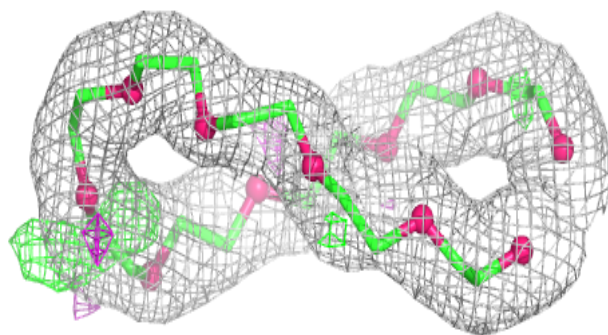
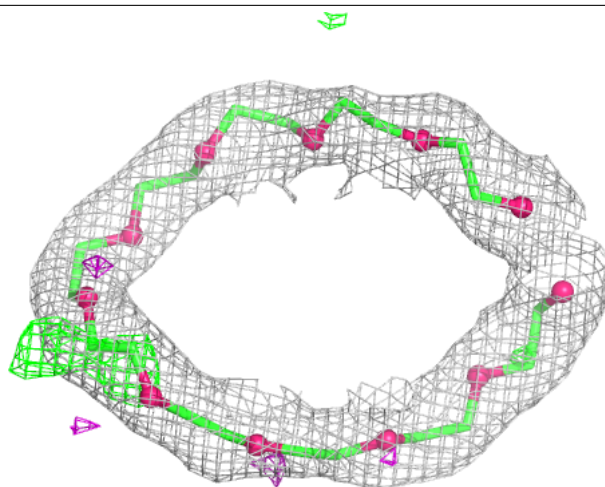
Electron density around PG4 C 406:

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



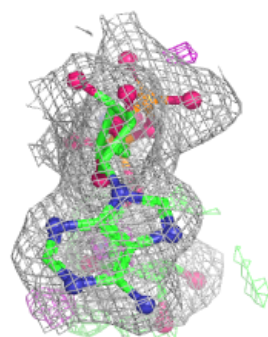
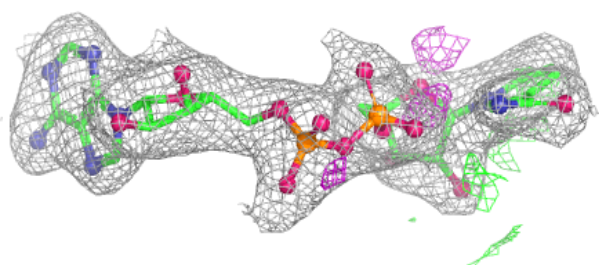
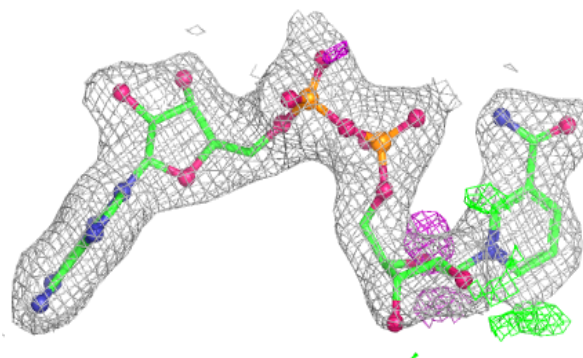
Electron density around XPE A 414:

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

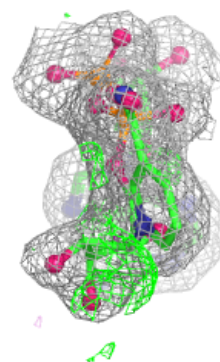
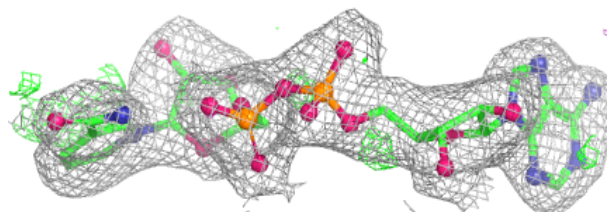
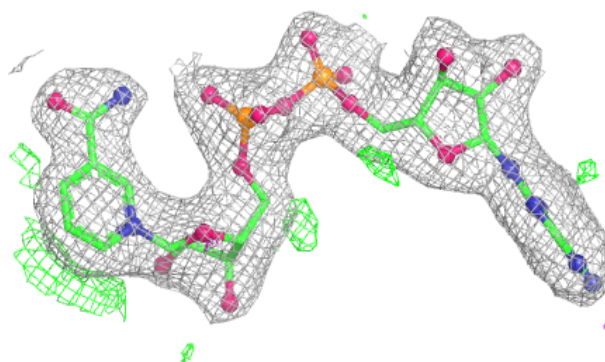


Electron density around NAD A 401:

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

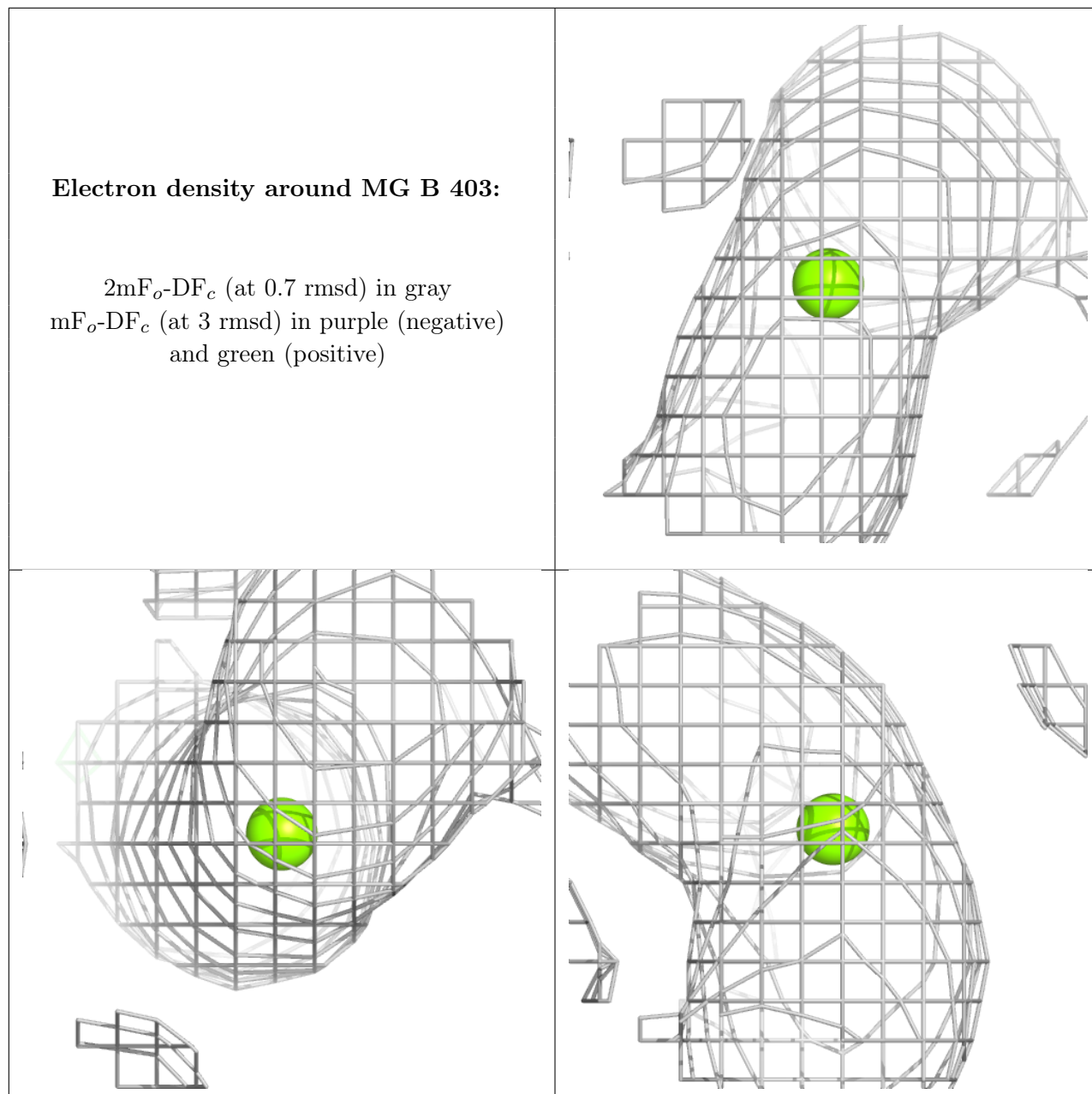
**Electron density around NAD D 402:**

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



Electron density around MG B 403:

$2mF_o-DF_c$ (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.