



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:56 PM UTC

PDB ID : 6YN7 / pdb_00006yn7
Title : Crystal Structure of AHE enzyme from Alicyclobacillus herbarius
Authors : Gourlay, L.J.; Di Pisa, F.
Deposited on : 2020-04-11
Resolution : 1.98 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

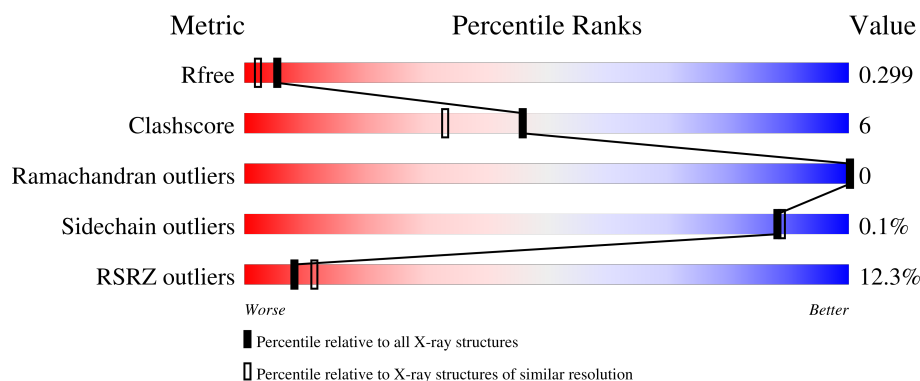
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	452	8% 83% 15% .
1	B	452	6% 86% 13% .
1	C	452	21% 86% 12% .
1	D	452	13% 83% 15% .

2 Entry composition [i](#)

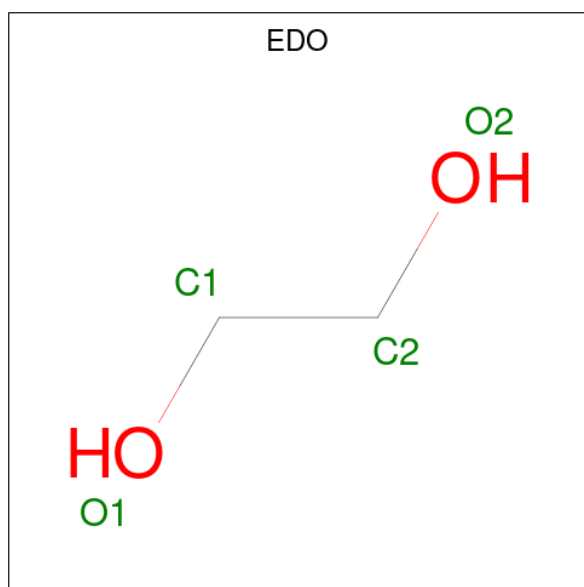
There are 6 unique types of molecules in this entry. The entry contains 14649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AHE, beta-glucosidase enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	1	0
			3557	2285	621	644	7			
1	B	447	Total	C	N	O	S	0	0	0
			3597	2307	635	648	7			
1	C	440	Total	C	N	O	S	0	0	0
			3515	2258	617	633	7			
1	D	440	Total	C	N	O	S	0	2	0
			3574	2289	627	650	8			

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



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

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

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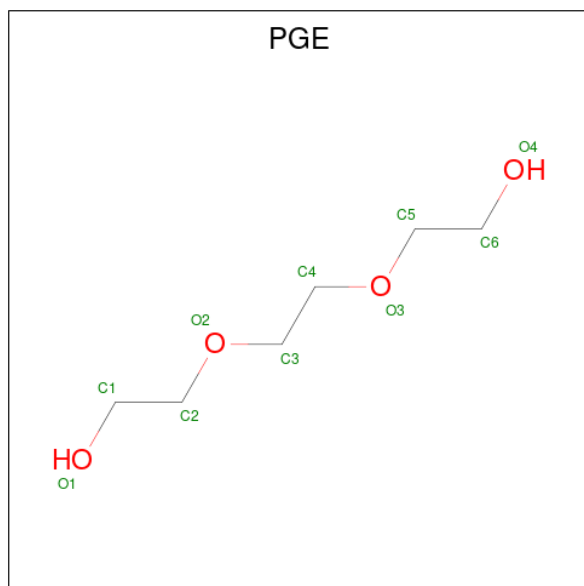
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



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

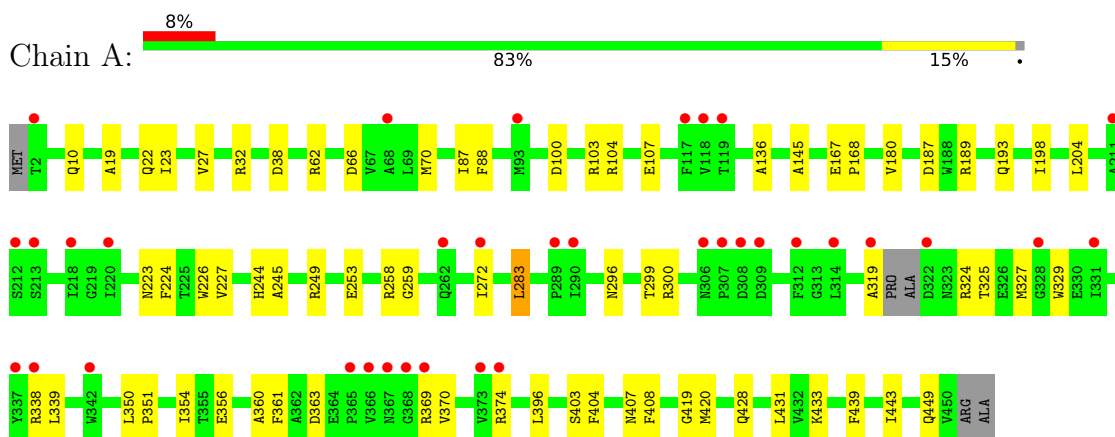
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total	O	0	0
			76	76		
6	B	62	Total	O	0	0
			62	62		
6	C	54	Total	O	0	0
			54	54		
6	D	81	Total	O	0	0
			81	81		

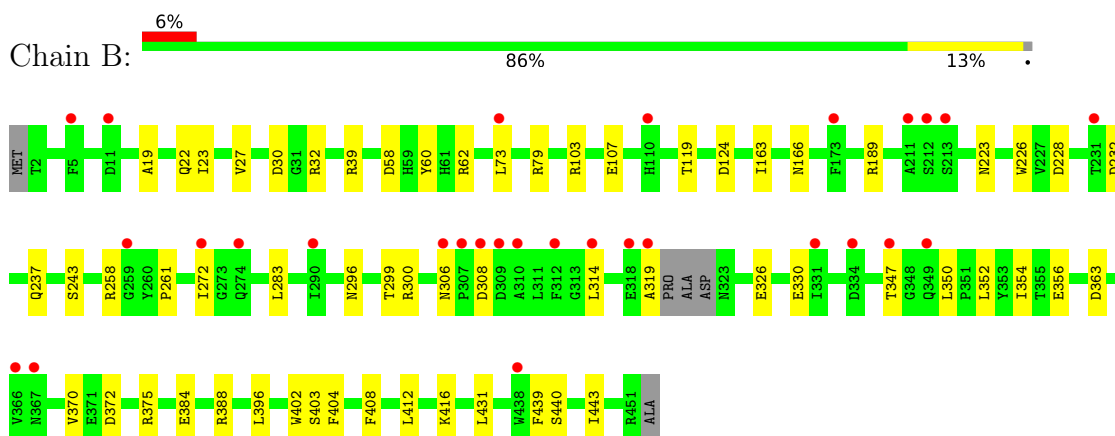
3 Residue-property plots [i](#)

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.

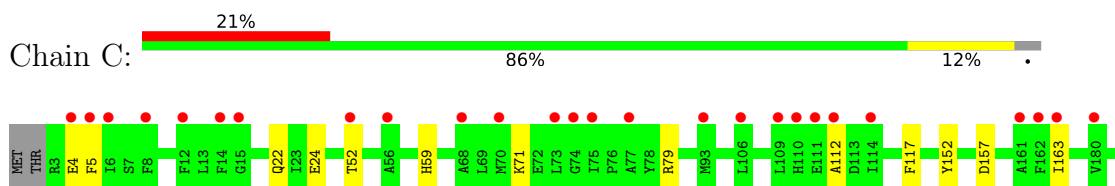
- Molecule 1: AHE, beta-glucosidase enzyme

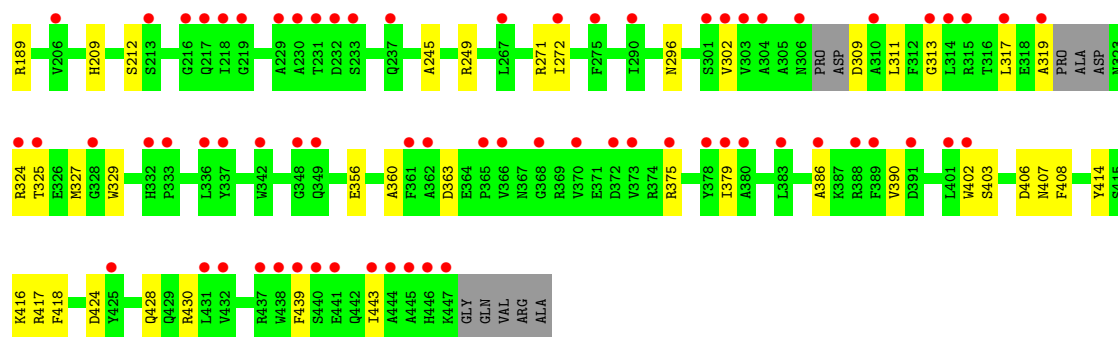


- Molecule 1: AHE, beta-glucosidase enzyme

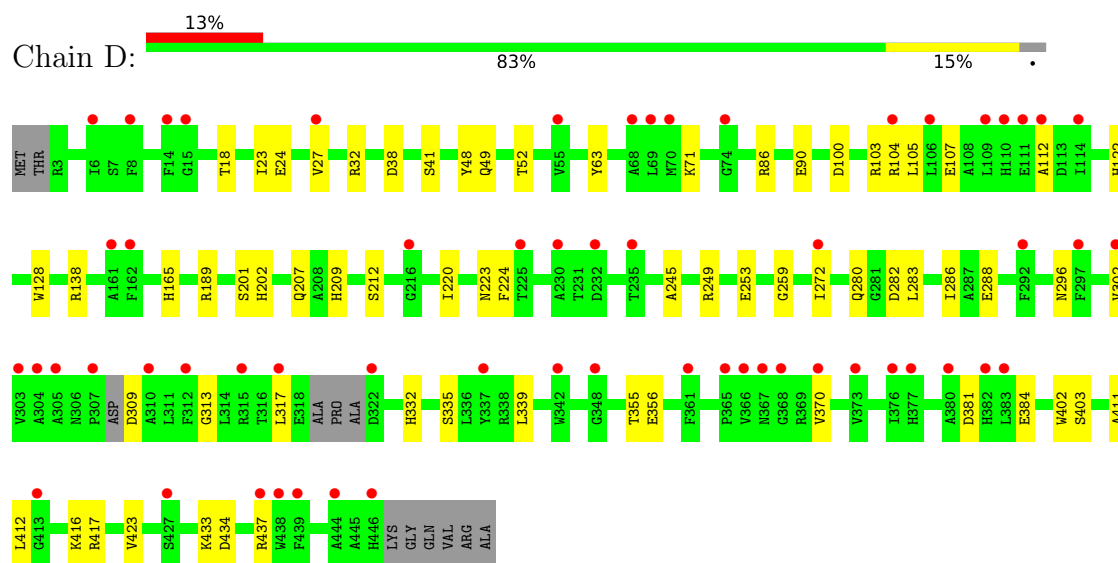


- Molecule 1: AHE, beta-glucosidase enzyme





- Molecule 1: AHE, beta-glucosidase enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.05Å 93.35Å 106.38Å 90.00° 98.69° 90.00°	Depositor
Resolution (Å)	98.90 – 1.98 98.90 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.5 (98.90-1.98) 43.5 (98.90-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.247 , 0.298 0.247 , 0.299	Depositor DCC
R_{free} test set	1997 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14649	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 62.71 % 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 1.0810e-05. 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: PEG, NI, PGE, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.10	0/3673	0.28	0/5000
1	B	0.11	0/3710	0.29	0/5042
1	C	0.10	0/3626	0.31	0/4930
1	D	0.11	0/3689	0.31	0/5013
All	All	0.11	0/14698	0.29	0/19985

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3557	0	3274	47	0
1	B	3597	0	3351	40	0
1	C	3515	0	3244	31	0
1	D	3574	0	3315	41	0
2	A	32	0	48	3	0
2	B	12	0	18	0	0
2	C	20	0	30	0	0
2	D	40	0	60	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	10	0	14	3	0
4	B	10	0	14	0	0
5	B	7	0	10	3	0
6	A	76	0	0	0	0
6	B	62	0	0	1	0
6	C	54	0	0	0	0
6	D	81	0	0	2	0
All	All	14649	0	13378	160	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 6.

All (160) 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:C:325:THR:HG22	1:C:327:MET:H	1.42	0.81
1:A:325:THR:HG23	1:A:327:MET:H	1.46	0.80
1:B:261:PRO:HA	5:B:506:PEG:H12	1.67	0.74
1:D:434:ASP:HA	1:D:437:ARG:HD3	1.70	0.72
1:A:369:ARG:HA	1:A:431:LEU:HD21	1.74	0.69
1:D:27:VAL:HG23	1:D:32:ARG:HH21	1.60	0.67
1:A:32:ARG:NH2	1:A:38:ASP:OD2	2.28	0.66
1:A:10:GLN:HA	2:A:501:EDO:H22	1.75	0.66
1:A:100:ASP:OD1	1:A:104:ARG:NH1	2.29	0.65
1:D:32:ARG:NH2	1:D:38:ASP:OD2	2.31	0.64
1:B:306:ASN:OD1	1:B:308:ASP:N	2.30	0.63
1:D:259:GLY:HA2	1:D:283:LEU:HD22	1.80	0.63
1:D:18:THR:HB	1:D:23:ILE:HG21	1.81	0.62
1:B:232:ASP:HA	1:B:237:GLN:HE22	1.65	0.61
1:C:406:ASP:OD2	1:C:417:ARG:NH1	2.33	0.61
1:D:71:LYS:NZ	6:D:603:HOH:O	2.33	0.60
1:D:245:ALA:HA	1:D:249:ARG:HB2	1.85	0.58
1:D:417:ARG:NH1	1:D:423:VAL:O	2.37	0.57
1:A:258:ARG:HD3	2:A:507:EDO:H11	1.87	0.57
1:C:327:MET:SD	1:C:416:LYS:HG2	2.43	0.57
1:D:302:VAL:HG23	1:D:317:LEU:HB2	1.87	0.57
1:A:319:ALA:HB3	1:A:324:ARG:HD2	1.87	0.57
1:A:361:PHE:CZ	1:A:374:ARG:HG2	2.39	0.57
1:B:354:ILE:HG13	1:B:396:LEU:HD11	1.85	0.57
1:A:180:VAL:HG11	4:A:510:PGE:H1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ALA:HB3	1:C:324:ARG:HD2	1.87	0.55
1:C:428:GLN:NE2	1:C:430:ARG:HH12	2.04	0.55
1:B:243:SER:HB2	1:B:314:LEU:HD13	1.90	0.54
1:A:245:ALA:HA	1:A:249:ARG:HB2	1.89	0.54
1:C:245:ALA:HA	1:C:249:ARG:HB2	1.89	0.53
1:A:449:GLN:HB3	2:A:501:EDO:H11	1.91	0.53
1:C:325:THR:HG23	1:C:360:ALA:H	1.73	0.53
1:C:71:LYS:HB2	1:C:112:ALA:HB1	1.91	0.52
1:D:71:LYS:HB2	1:D:112:ALA:HB1	1.91	0.52
1:C:79:ARG:HE	1:C:163:ILE:HD13	1.75	0.52
1:C:24:GLU:HA	1:C:59:HIS:HB3	1.92	0.52
4:A:510:PGE:H2	4:A:510:PGE:H52	1.90	0.52
1:A:226:TRP:CD1	1:A:338:ARG:HH21	2.27	0.51
1:A:259:GLY:HA2	1:A:283:LEU:HD11	1.93	0.51
1:B:258:ARG:HH11	5:B:506:PEG:H41	1.75	0.51
1:D:41:SER:HB3	1:D:52:THR:HG22	1.93	0.51
1:D:282:ASP:O	1:D:286:ILE:HG13	2.11	0.51
1:B:79:ARG:NH2	1:B:166:ASN:OD1	2.38	0.50
1:D:103:ARG:O	1:D:107:GLU:HG3	2.10	0.50
1:D:412:LEU:HD13	1:D:416:LYS:HE3	1.92	0.50
1:A:325:THR:HG22	1:A:329:TRP:H	1.77	0.50
1:A:361:PHE:CE1	1:A:374:ARG:CZ	2.95	0.50
1:A:187:ASP:OD2	1:B:39:ARG:NE	2.41	0.49
1:B:258:ARG:HD3	5:B:506:PEG:H41	1.93	0.49
1:C:189:ARG:HH11	1:C:272:ILE:HG22	1.77	0.49
1:C:302:VAL:HG23	1:C:317:LEU:HD13	1.94	0.49
1:A:145:ALA:HB2	1:A:204:LEU:HB3	1.92	0.49
1:D:223:ASN:HA	1:D:296:ASN:HB2	1.94	0.49
1:D:381:ASP:O	1:D:384:GLU:HG2	2.12	0.49
1:A:223:ASN:HA	1:A:296:ASN:HB2	1.94	0.49
1:A:168:PRO:HB3	1:A:198:ILE:HG21	1.95	0.48
1:B:27:VAL:HB	1:B:32:ARG:NH1	2.29	0.48
1:B:372:ASP:OD2	1:B:375:ARG:NH1	2.43	0.48
1:A:363:ASP:HB3	1:A:370:VAL:HG11	1.94	0.48
1:B:319:ALA:CB	1:B:330:GLU:HB2	2.43	0.48
1:C:424:ASP:O	1:C:428:GLN:N	2.44	0.48
1:A:22:GLN:NE2	1:A:407:ASN:OD1	2.47	0.48
1:C:79:ARG:HA	1:C:117:PHE:O	2.14	0.48
1:B:402:TRP:HA	1:B:403:SER:HA	1.53	0.48
1:C:439:PHE:O	1:C:443:ILE:HG12	2.13	0.48
1:D:370:VAL:HG12	1:D:433:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:NE	1:A:253:GLU:OE2	2.44	0.48
1:D:309:ASP:HB3	1:D:313:GLY:HA2	1.95	0.48
1:B:232:ASP:CA	1:B:237:GLN:HE22	2.27	0.47
1:D:23:ILE:HG13	1:D:24:GLU:N	2.28	0.47
1:A:296:ASN:CG	1:A:356:GLU:HB2	2.39	0.47
1:D:209:HIS:HA	1:D:212:SER:HB3	1.96	0.47
1:A:439:PHE:O	1:A:443:ILE:HG12	2.14	0.47
1:B:439:PHE:O	1:B:443:ILE:HG12	2.15	0.47
1:B:363:ASP:HB3	1:B:370:VAL:HG11	1.96	0.47
1:C:375:ARG:O	1:C:379:ILE:HG12	2.15	0.47
1:B:412:LEU:HD13	1:B:416:LYS:HE3	1.97	0.46
1:C:22:GLN:NE2	1:C:408:PHE:O	2.29	0.46
1:A:27:VAL:HA	1:A:32:ARG:HE	1.80	0.46
1:B:19:ALA:O	1:B:23:ILE:HG12	2.15	0.46
1:B:30:ASP:OD2	1:B:60:TYR:OH	2.29	0.46
1:A:324:ARG:O	1:A:374:ARG:NH2	2.28	0.46
1:A:62:ARG:HH21	1:A:428:GLN:HG3	1.81	0.46
1:B:189:ARG:HB2	1:B:272:ILE:HG21	1.98	0.46
1:A:22:GLN:NE2	1:A:408:PHE:O	2.44	0.46
1:C:402:TRP:HA	1:C:403:SER:HA	1.55	0.46
1:A:167:GLU:HG2	1:A:223:ASN:HB3	1.98	0.45
1:D:122:HIS:NE2	6:D:604:HOH:O	2.34	0.45
1:D:48:TYR:CZ	1:D:49:GLN:HG3	2.52	0.45
1:D:296:ASN:CG	1:D:356:GLU:HB2	2.42	0.45
1:D:332:HIS:CE1	1:D:335:SER:HG	2.34	0.45
1:A:189:ARG:HH11	1:A:272:ILE:HG22	1.82	0.45
1:C:22:GLN:O	1:C:407:ASN:HB2	2.17	0.45
1:D:411:ALA:HB3	2:D:510:EDO:H22	1.99	0.45
1:B:296:ASN:CG	1:B:356:GLU:HB2	2.42	0.45
1:B:58:ASP:O	1:B:62:ARG:HG3	2.17	0.44
1:C:296:ASN:CG	1:C:356:GLU:HB2	2.41	0.44
1:C:363:ASP:OD2	1:C:375:ARG:NH2	2.50	0.44
1:A:103:ARG:NE	1:A:107:GLU:OE1	2.46	0.44
1:B:226:TRP:NE1	1:B:228:ASP:OD1	2.49	0.44
1:B:299:THR:OG1	1:B:300:ARG:N	2.50	0.44
1:B:103:ARG:O	1:B:107:GLU:HG3	2.17	0.44
1:D:32:ARG:HG3	1:D:86:ARG:HG2	1.99	0.44
1:D:249:ARG:NE	1:D:253:GLU:OE2	2.48	0.44
1:A:420:MET:O	1:A:433:LYS:HG3	2.18	0.43
1:B:27:VAL:HA	1:B:32:ARG:HD3	2.00	0.43
1:B:403:SER:OG	1:B:404:PHE:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ASP:HB3	1:C:313:GLY:HA2	2.00	0.43
1:D:224:PHE:HB2	1:D:339:LEU:HD21	2.00	0.43
1:B:73:LEU:O	1:B:440:SER:OG	2.33	0.43
1:A:420:MET:C	1:A:433:LYS:HG3	2.43	0.43
1:B:319:ALA:HB1	1:B:330:GLU:HB2	2.00	0.43
1:B:370:VAL:HG23	1:B:431:LEU:HD23	2.01	0.43
1:C:52:THR:O	1:C:414:TYR:OH	2.33	0.43
1:A:19:ALA:O	1:A:23:ILE:HG12	2.18	0.43
1:D:202:HIS:CE1	1:D:220:ILE:HB	2.54	0.43
1:A:350:LEU:HD12	1:A:351:PRO:HD2	1.99	0.43
1:A:100:ASP:O	1:A:104:ARG:HG3	2.19	0.42
1:B:326:GLU:O	1:B:416:LYS:NZ	2.41	0.42
1:D:165:HIS:NE2	1:D:201:SER:OG	2.50	0.42
1:A:66:ASP:O	1:A:70:MET:HG3	2.19	0.42
1:A:224:PHE:HB2	1:A:339:LEU:HD21	2.02	0.42
1:A:325:THR:OG1	1:A:360:ALA:O	2.37	0.42
1:D:90:GLU:HA	1:D:128:TRP:CD1	2.54	0.42
1:D:402:TRP:HA	1:D:403:SER:HA	1.52	0.42
1:A:299:THR:OG1	1:A:300:ARG:N	2.52	0.42
1:C:152:TYR:HB3	1:C:212:SER:HB2	2.01	0.42
1:B:347:THR:HG21	1:B:352:LEU:HD21	2.01	0.42
1:C:271:ARG:HD3	1:C:311:LEU:O	2.20	0.42
1:C:360:ALA:HB2	1:C:418:PHE:CE1	2.54	0.42
1:C:386:ALA:O	1:C:390:VAL:HG23	2.19	0.42
1:B:189:ARG:HH11	1:B:272:ILE:HG22	1.85	0.42
1:C:209:HIS:HA	1:C:212:SER:HB3	2.01	0.42
1:D:207:GLN:HG3	1:D:288:GLU:HG3	2.01	0.42
1:C:327:MET:HE2	1:C:329:TRP:CZ2	2.55	0.42
1:B:223:ASN:HA	1:B:296:ASN:HB2	2.01	0.42
1:A:403:SER:OG	1:A:404:PHE:N	2.52	0.41
1:B:22:GLN:NE2	1:B:408:PHE:O	2.39	0.41
1:D:370:VAL:HG11	1:D:433:LYS:HG2	2.02	0.41
1:A:325:THR:HG23	1:A:327:MET:N	2.26	0.41
1:B:232:ASP:C	1:B:237:GLN:HE22	2.28	0.41
1:D:27:VAL:HG23	1:D:32:ARG:HE	1.85	0.41
1:D:280:GLN:H	1:D:280:GLN:HG2	1.62	0.41
1:B:350:LEU:O	6:B:601:HOH:O	2.22	0.41
1:B:124:ASP:OD1	1:B:124:ASP:N	2.48	0.41
1:D:63:TYR:HB2	1:D:105:LEU:HD13	2.03	0.41
1:A:419:GLY:O	1:A:433:LYS:NZ	2.40	0.41
4:A:510:PGE:H2	4:A:510:PGE:H4	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ASP:OD2	1:C:157:ASP:N	2.54	0.41
1:D:138:ARG:NH2	1:D:282:ASP:OD2	2.54	0.41
1:D:189:ARG:HB2	1:D:272:ILE:HG21	2.03	0.41
1:D:296:ASN:OD1	1:D:355:THR:OG1	2.28	0.41
1:B:119:THR:HA	1:B:163:ILE:O	2.21	0.41
1:A:136:ALA:O	1:A:193:GLN:NE2	2.54	0.40
1:B:384:GLU:O	1:B:388:ARG:HG3	2.21	0.40
1:D:100:ASP:O	1:D:104[A]:ARG:HG3	2.21	0.40
1:A:227:VAL:HG21	1:A:244:HIS:HB2	2.04	0.40
1:C:4:GLU:HG3	1:C:5:PHE:O	2.21	0.40
1:A:354:ILE:HG13	1:A:396:LEU:HD11	2.04	0.40
1:A:87:ILE:HG22	1:A:88:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/452 (98%)	428 (96%)	16 (4%)	0	100	100
1	B	443/452 (98%)	425 (96%)	18 (4%)	0	100	100
1	C	434/452 (96%)	418 (96%)	16 (4%)	0	100	100
1	D	436/452 (96%)	417 (96%)	19 (4%)	0	100	100
All	All	1757/1808 (97%)	1688 (96%)	69 (4%)	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	344/364 (94%)	343 (100%)	1 (0%)	86	86
1	B	353/364 (97%)	352 (100%)	1 (0%)	86	86
1	C	340/364 (93%)	340 (100%)	0	100	100
1	D	354/364 (97%)	354 (100%)	0	100	100
All	All	1391/1456 (96%)	1389 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	LEU
1	B	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	266	GLN
1	B	28	HIS
1	B	217	GLN
1	B	237	GLN
1	C	217	GLN
1	C	266	GLN
1	C	428	GLN
1	D	28	HIS
1	D	248	ASN
1	D	367	ASN

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 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	$\# Z > 2$
2	EDO	C	505	-	3,3,3	0.42	0	2,2,2	0.42	0
2	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	D	507	-	3,3,3	0.42	0	2,2,2	0.37	0
2	EDO	A	503	-	3,3,3	0.43	0	2,2,2	0.41	0
2	EDO	C	503	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	C	501	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	A	504	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	A	506	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	D	501	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	A	508	-	3,3,3	0.44	0	2,2,2	0.35	0
2	EDO	D	505	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	D	508	-	3,3,3	0.41	0	2,2,2	0.43	0
2	EDO	B	503	-	3,3,3	0.42	0	2,2,2	0.39	0
2	EDO	A	502	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	A	501	-	3,3,3	0.41	0	2,2,2	0.42	0
2	EDO	D	506	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.36	0
4	PGE	B	505	-	9,9,9	0.32	0	8,8,8	0.28	0
2	EDO	A	505	-	3,3,3	0.43	0	2,2,2	0.37	0
4	PGE	A	510	-	9,9,9	0.32	0	8,8,8	0.32	0
2	EDO	D	510	-	3,3,3	0.42	0	2,2,2	0.39	0
5	PEG	B	506	-	6,6,6	0.51	0	5,5,5	0.21	0
2	EDO	B	501	-	3,3,3	0.42	0	2,2,2	0.40	0
2	EDO	A	507	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	D	502	-	3,3,3	0.39	0	2,2,2	0.61	0
2	EDO	D	504	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	C	504	-	3,3,3	0.43	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	503	-	3,3,3	0.42	0	2,2,2	0.39	0
2	EDO	D	509	-	3,3,3	0.43	0	2,2,2	0.38	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
2	EDO	C	505	-	-	0/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	D	507	-	-	0/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	C	503	-	-	0/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	A	504	-	-	0/1/1/1	-
2	EDO	A	506	-	-	0/1/1/1	-
2	EDO	D	501	-	-	0/1/1/1	-
2	EDO	A	508	-	-	0/1/1/1	-
2	EDO	D	505	-	-	0/1/1/1	-
2	EDO	D	508	-	-	0/1/1/1	-
2	EDO	B	503	-	-	0/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	D	506	-	-	0/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
4	PGE	B	505	-	-	5/7/7/7	-
2	EDO	A	505	-	-	0/1/1/1	-
4	PGE	A	510	-	-	6/7/7/7	-
2	EDO	D	510	-	-	0/1/1/1	-
5	PEG	B	506	-	-	3/4/4/4	-
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	A	507	-	-	0/1/1/1	-
2	EDO	D	502	-	-	0/1/1/1	-
2	EDO	D	504	-	-	0/1/1/1	-
2	EDO	C	504	-	-	0/1/1/1	-
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	D	509	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

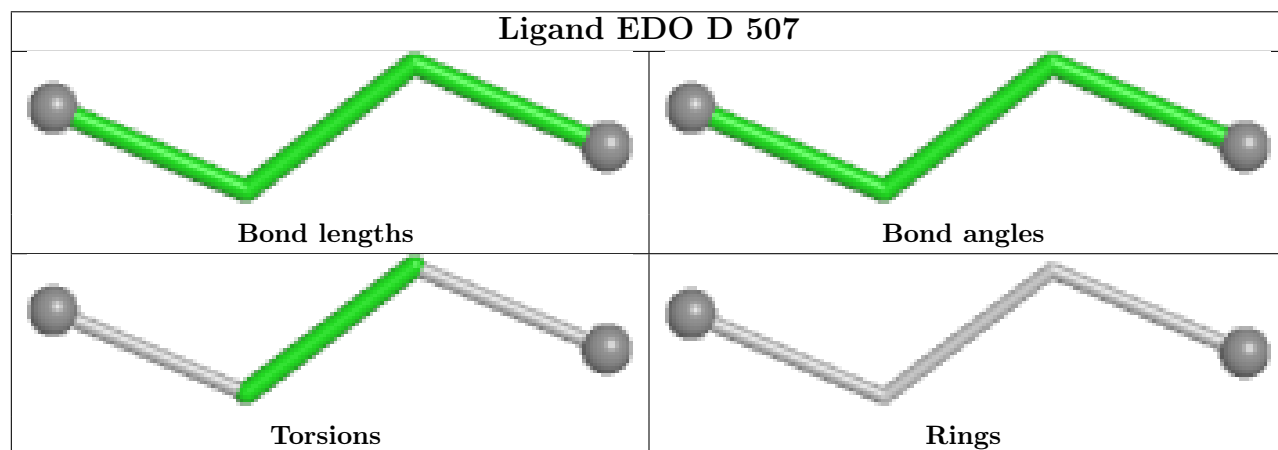
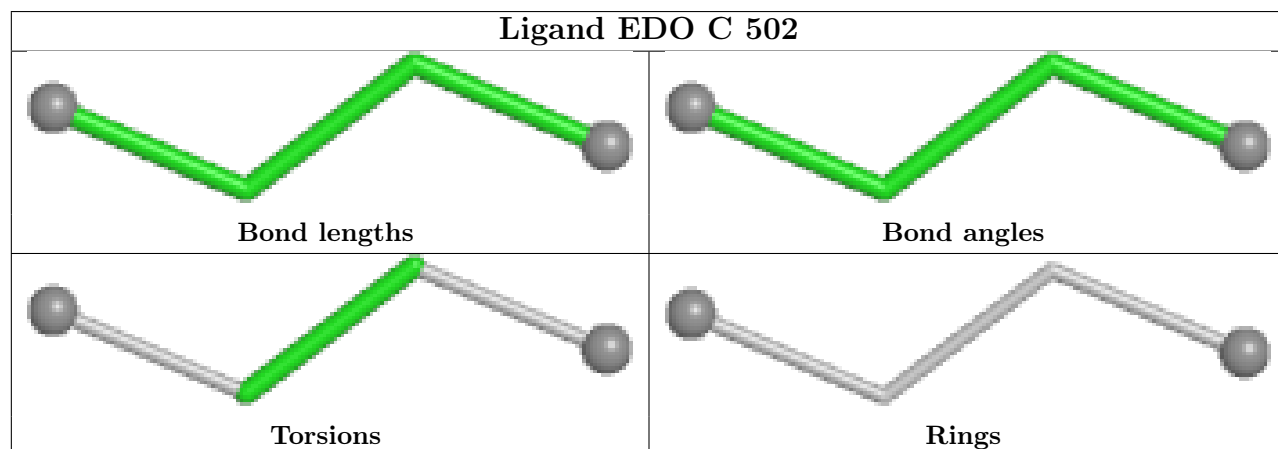
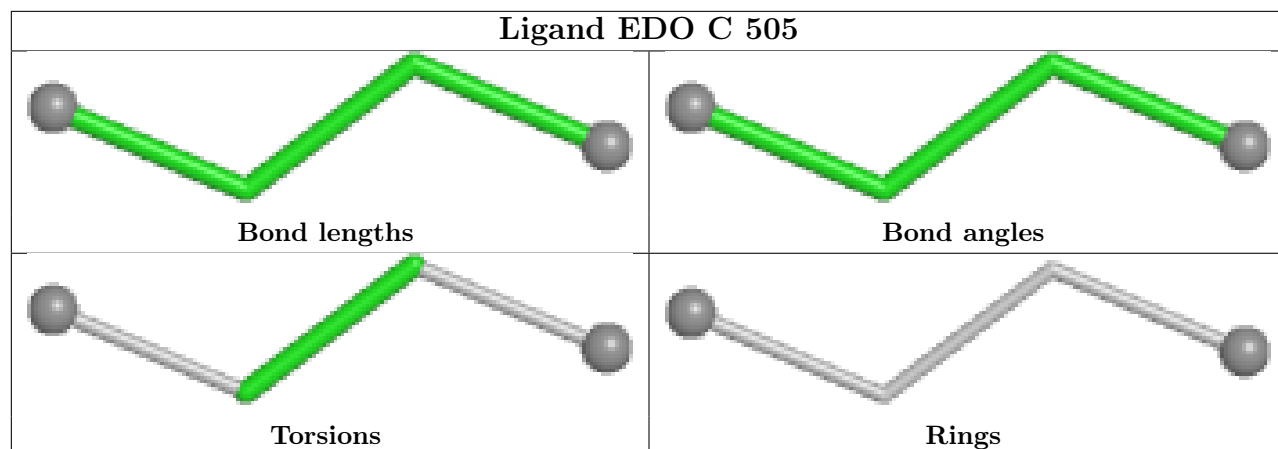
Mol	Chain	Res	Type	Atoms
4	B	505	PGE	C4-C3-O2-C2
4	A	510	PGE	O2-C3-C4-O3
4	B	505	PGE	O2-C3-C4-O3
5	B	506	PEG	O1-C1-C2-O2
4	A	510	PGE	C4-C3-O2-C2
4	A	510	PGE	O1-C1-C2-O2
4	B	505	PGE	O3-C5-C6-O4
4	B	505	PGE	O1-C1-C2-O2
4	A	510	PGE	C6-C5-O3-C4
4	A	510	PGE	C1-C2-O2-C3
4	B	505	PGE	C3-C4-O3-C5
5	B	506	PEG	C4-C3-O2-C2
5	B	506	PEG	C1-C2-O2-C3
4	A	510	PGE	O3-C5-C6-O4

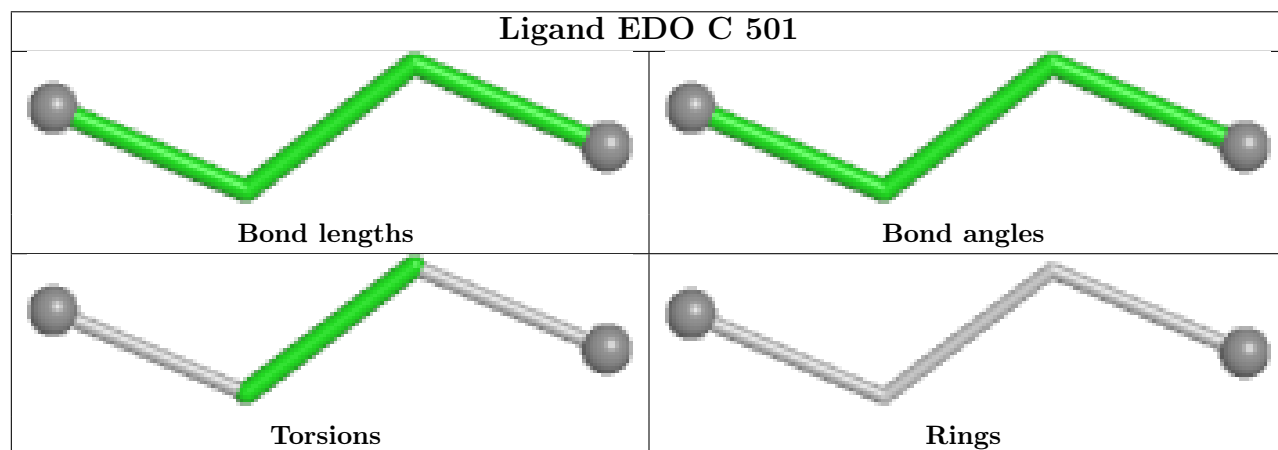
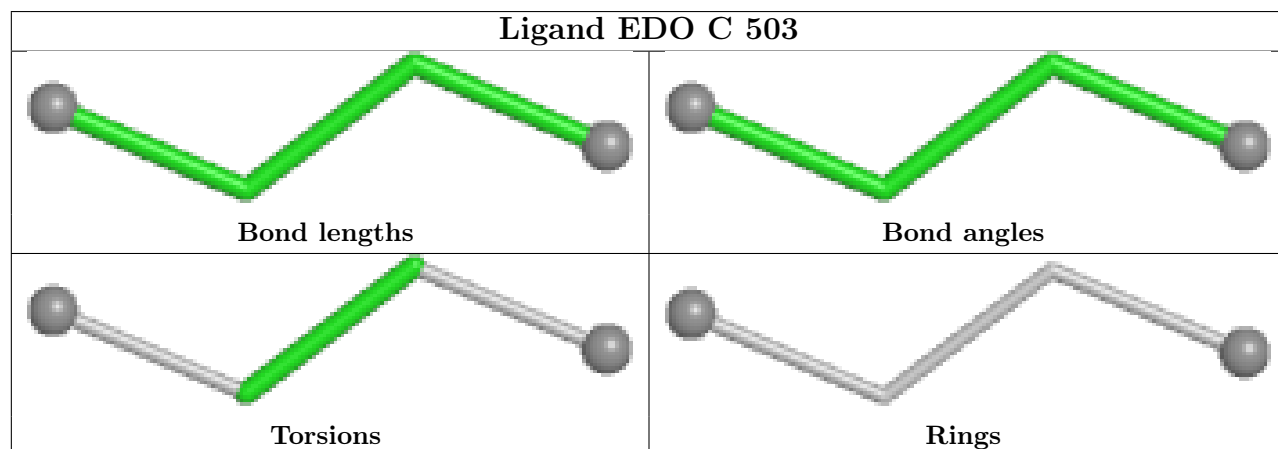
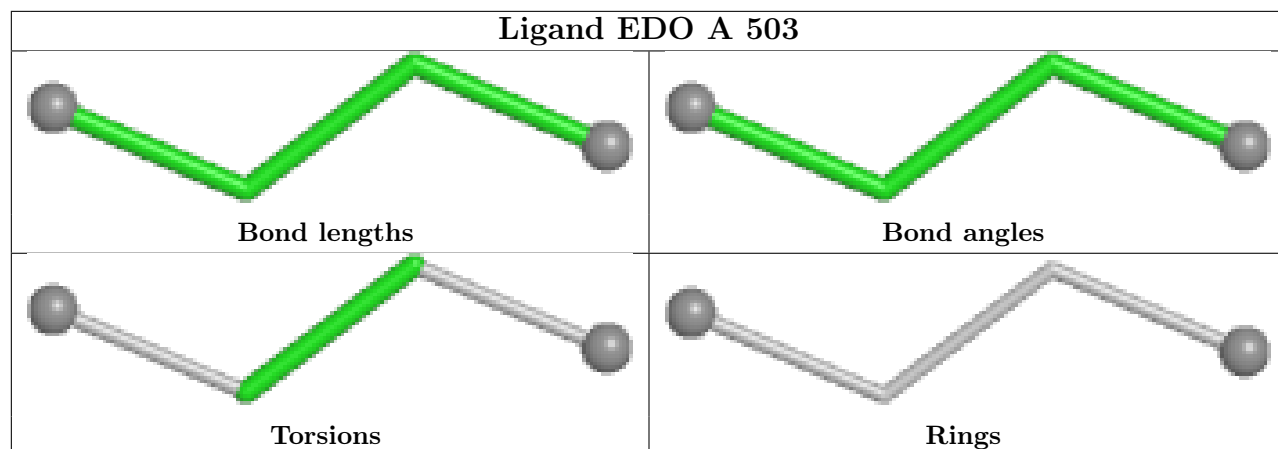
There are no ring outliers.

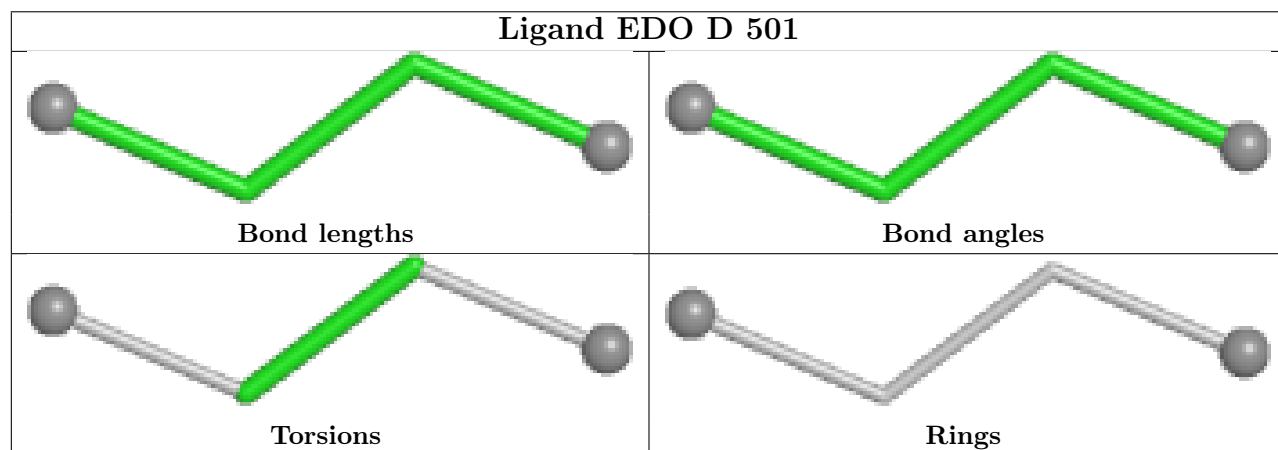
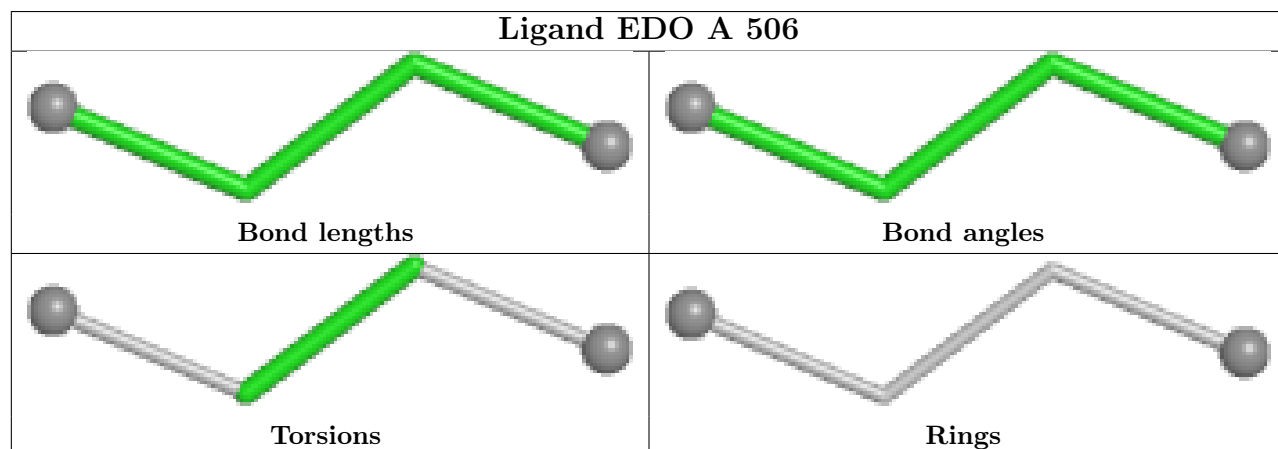
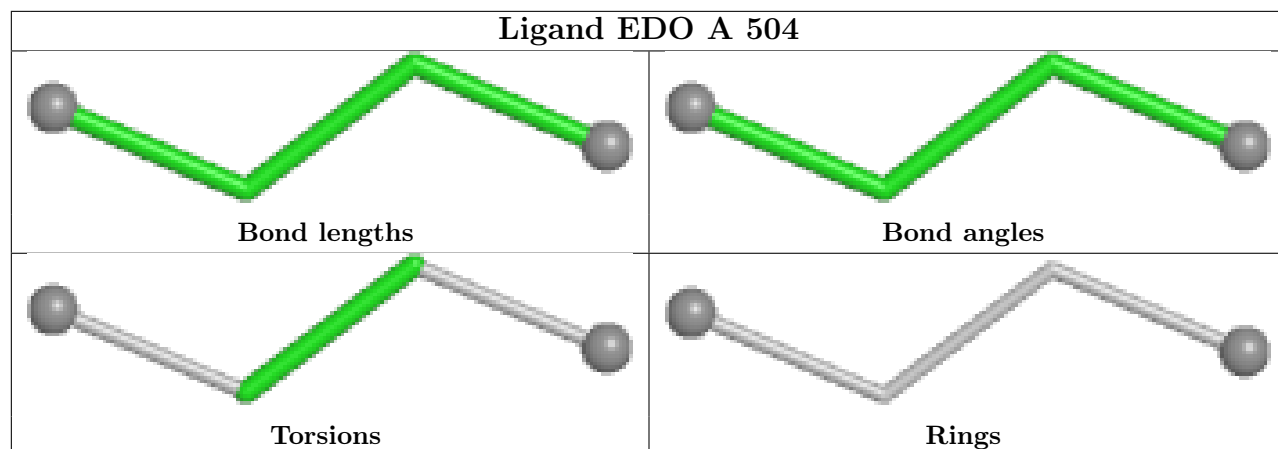
5 monomers are involved in 10 short contacts:

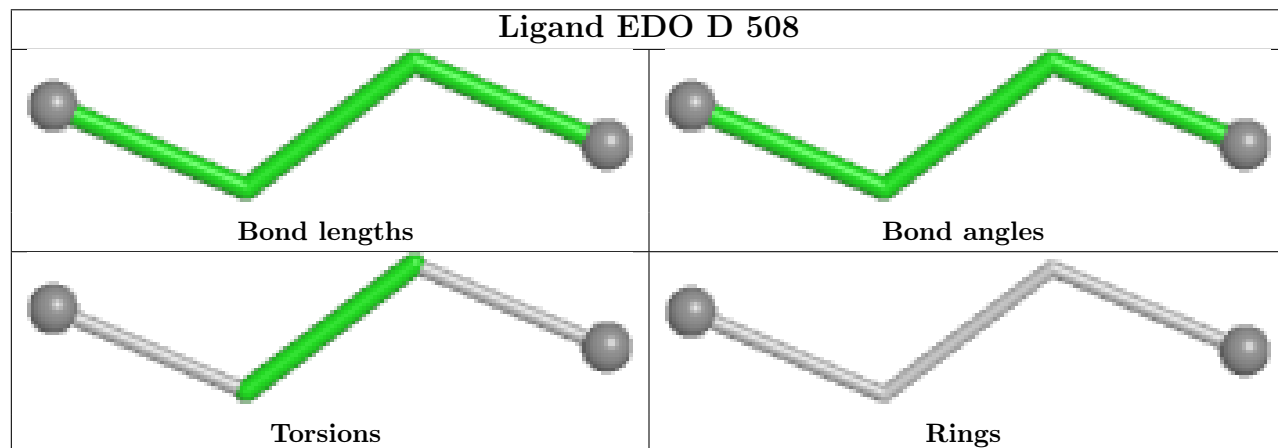
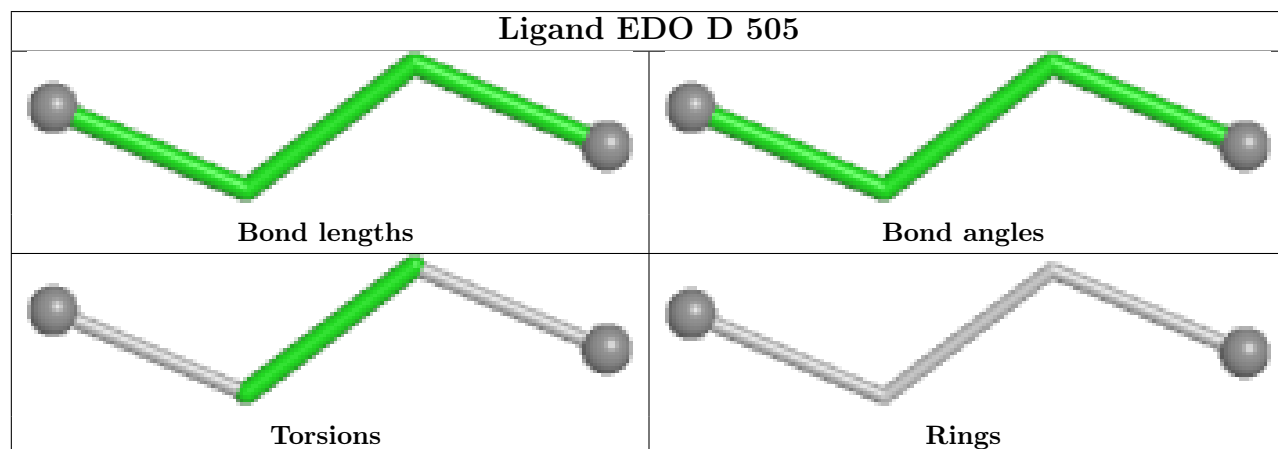
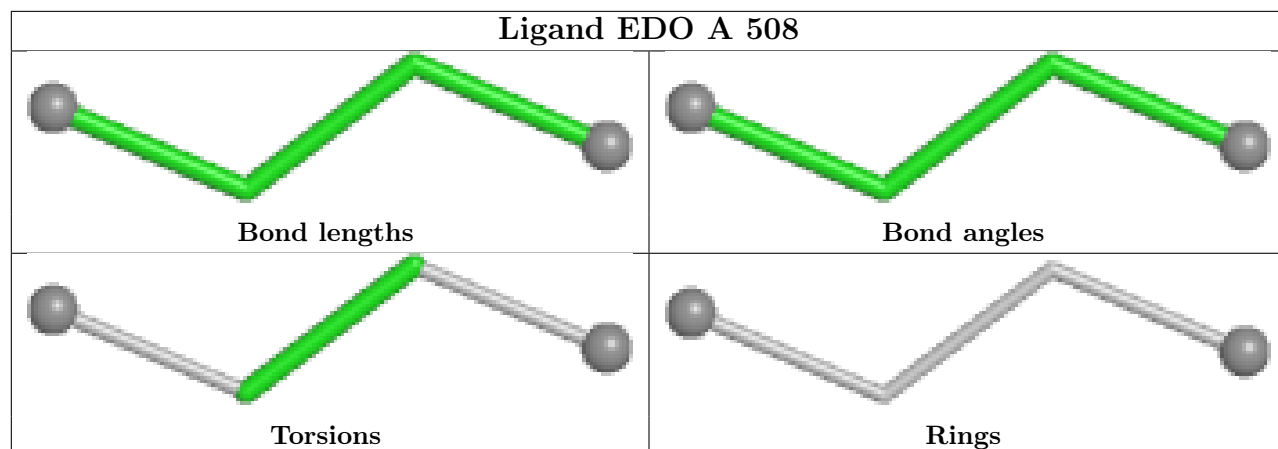
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	EDO	2	0
4	A	510	PGE	3	0
2	D	510	EDO	1	0
5	B	506	PEG	3	0
2	A	507	EDO	1	0

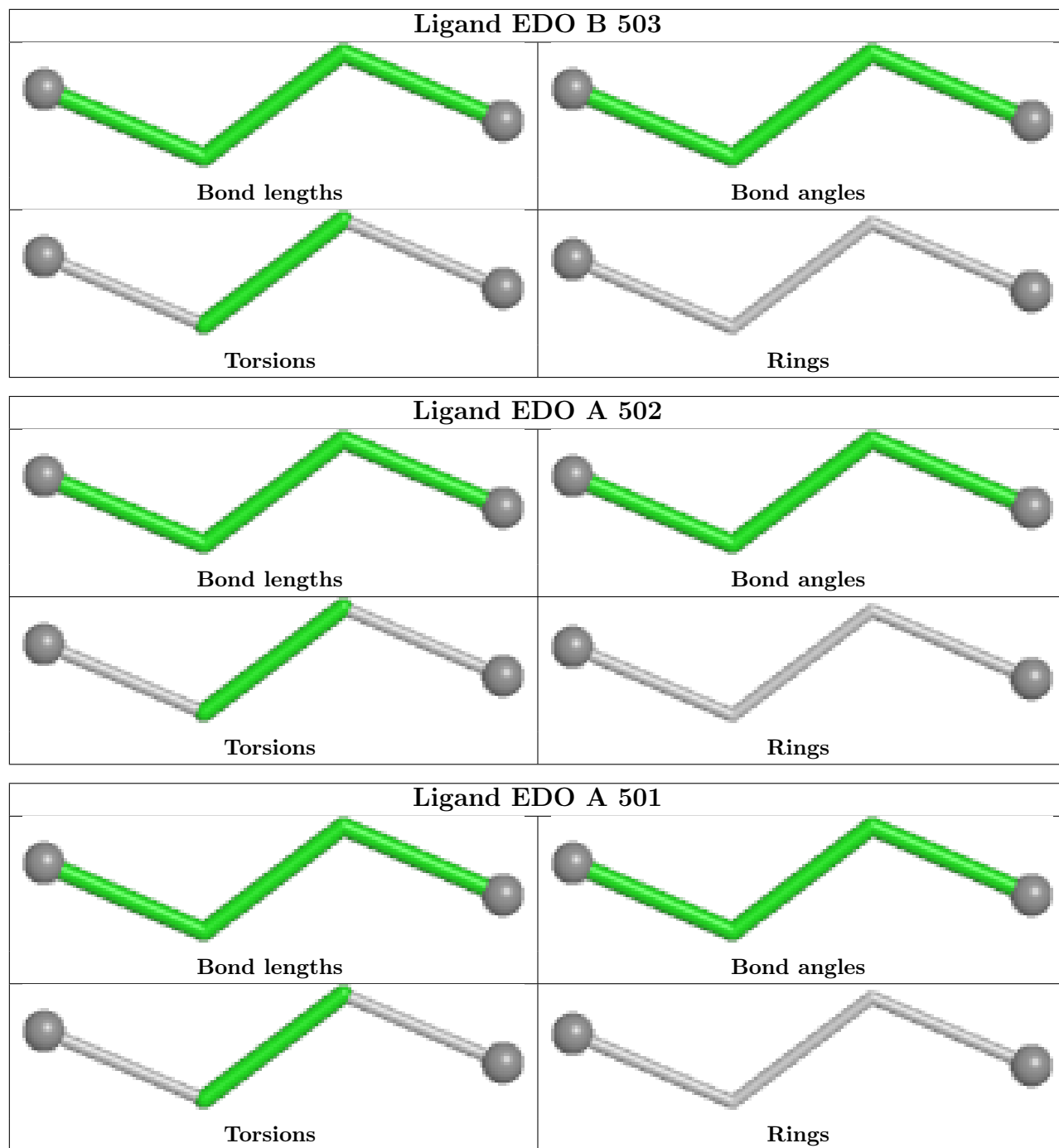
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

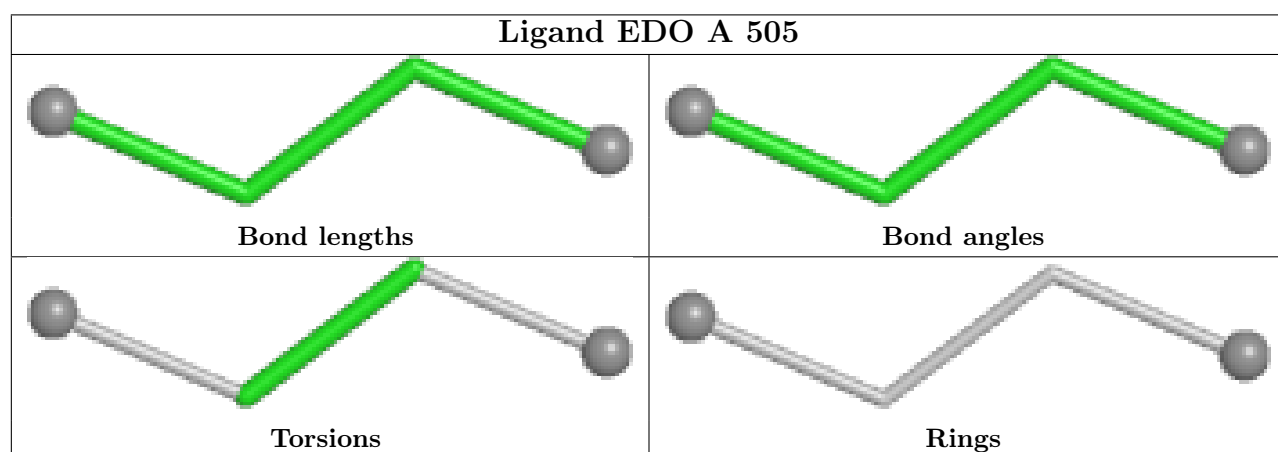
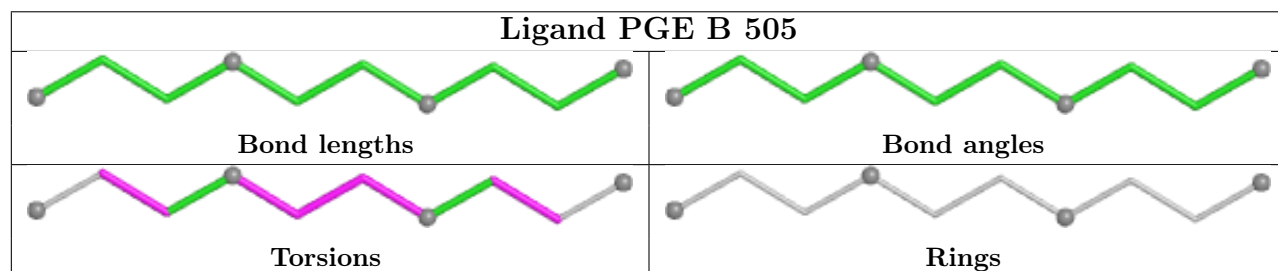
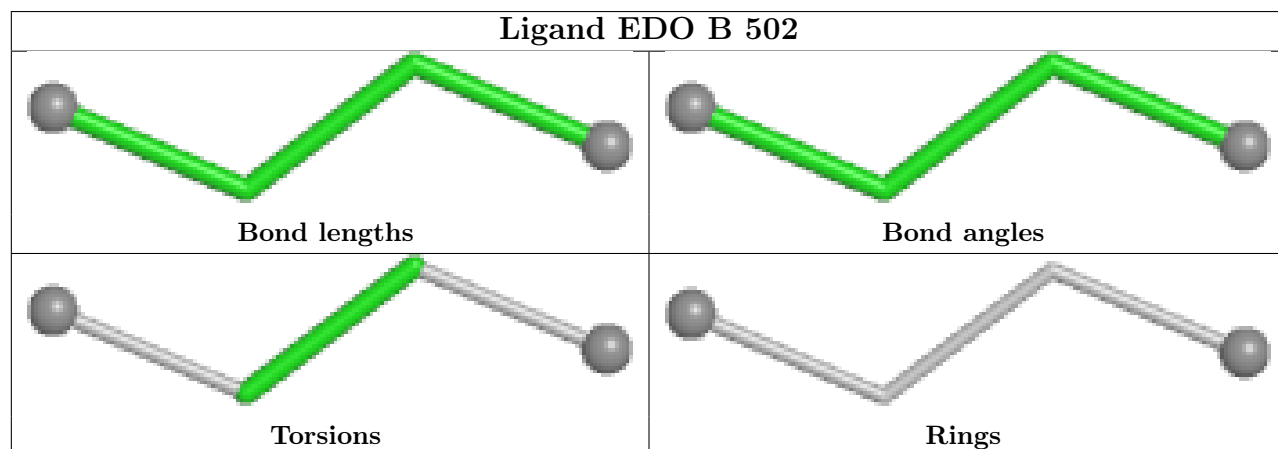
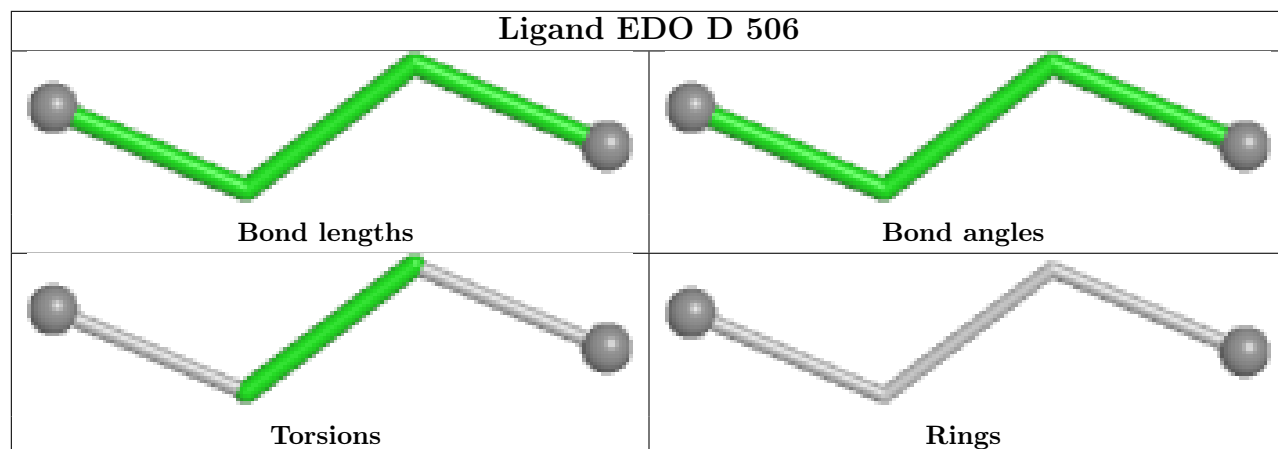


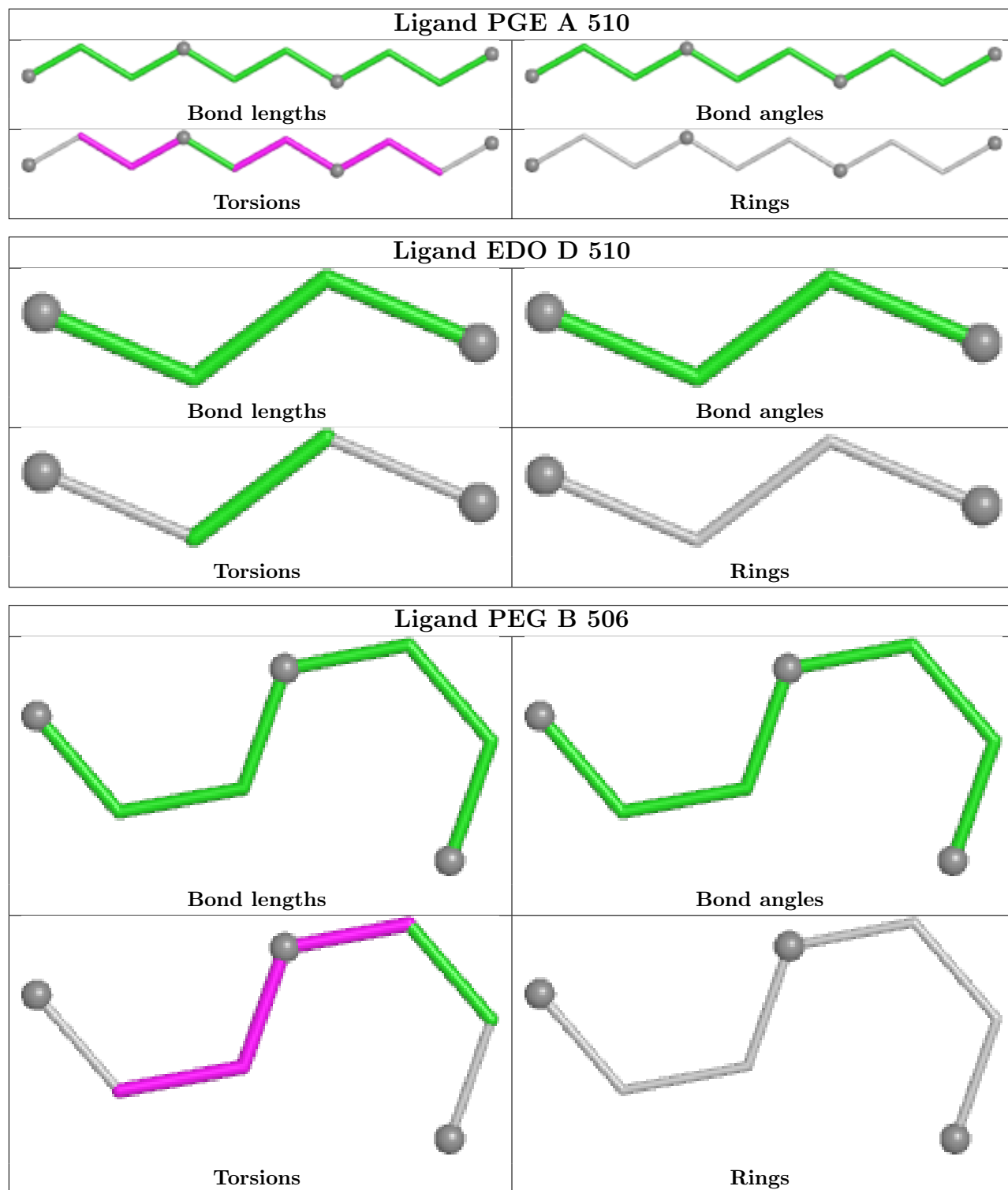


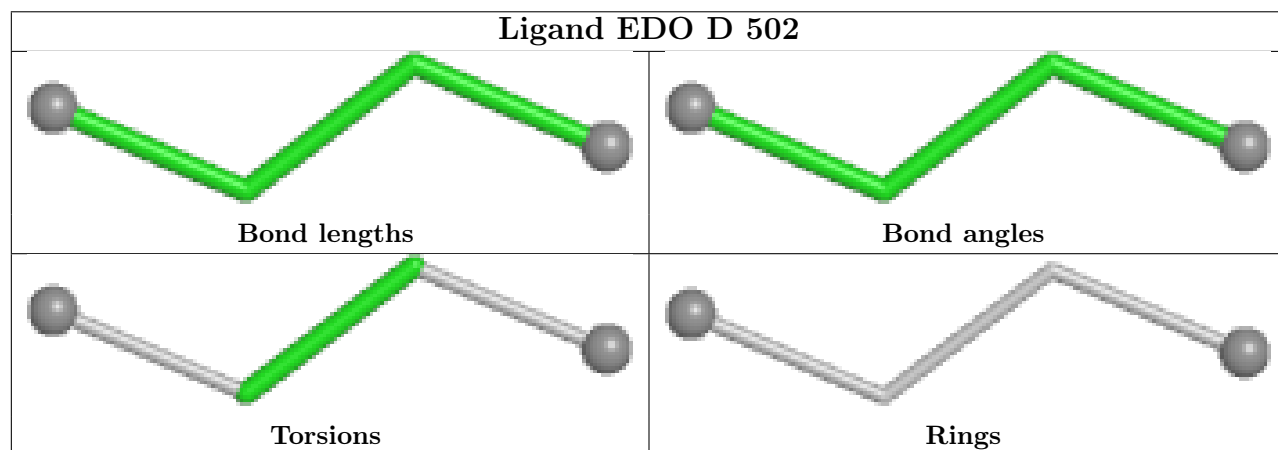
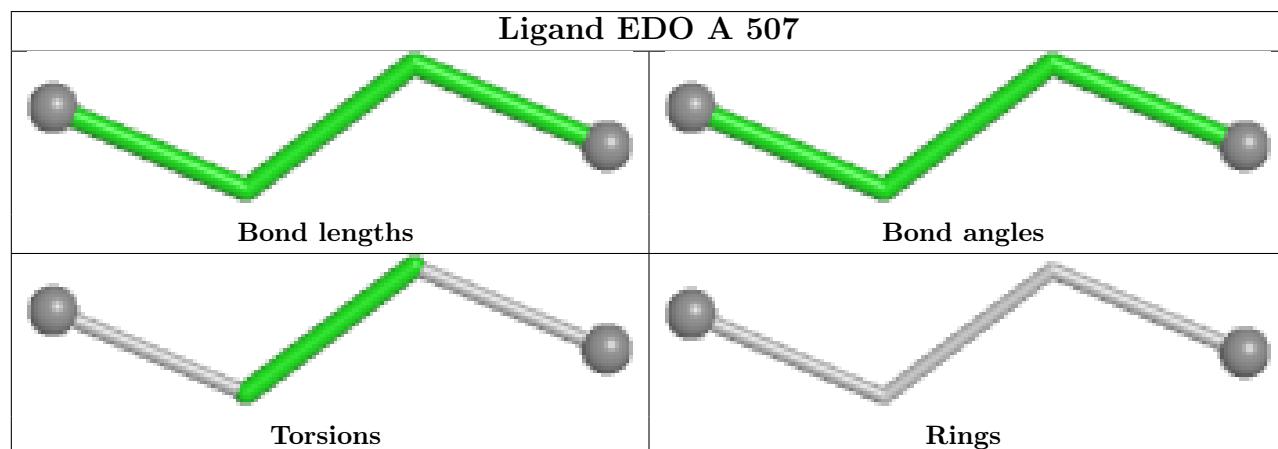
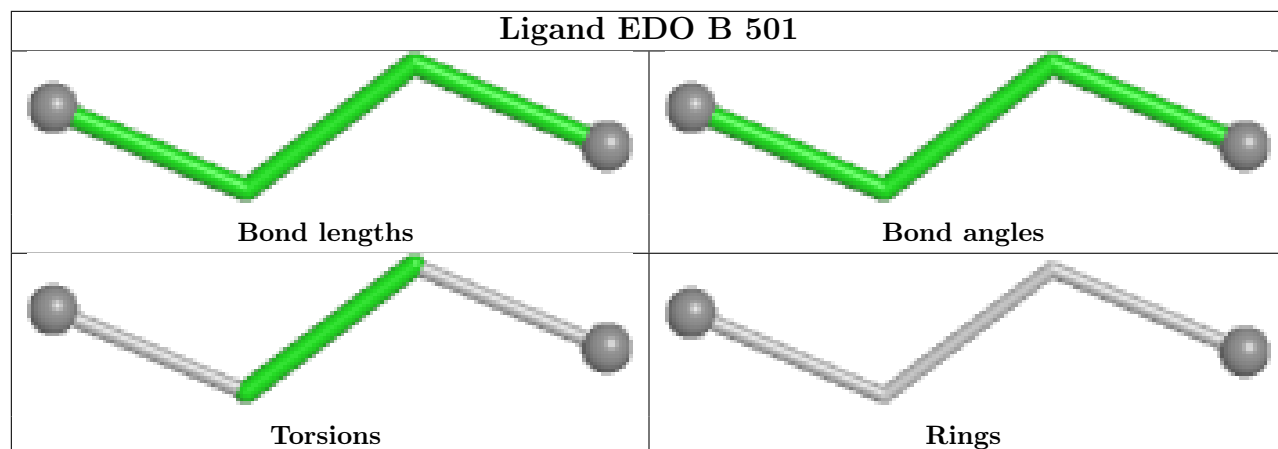


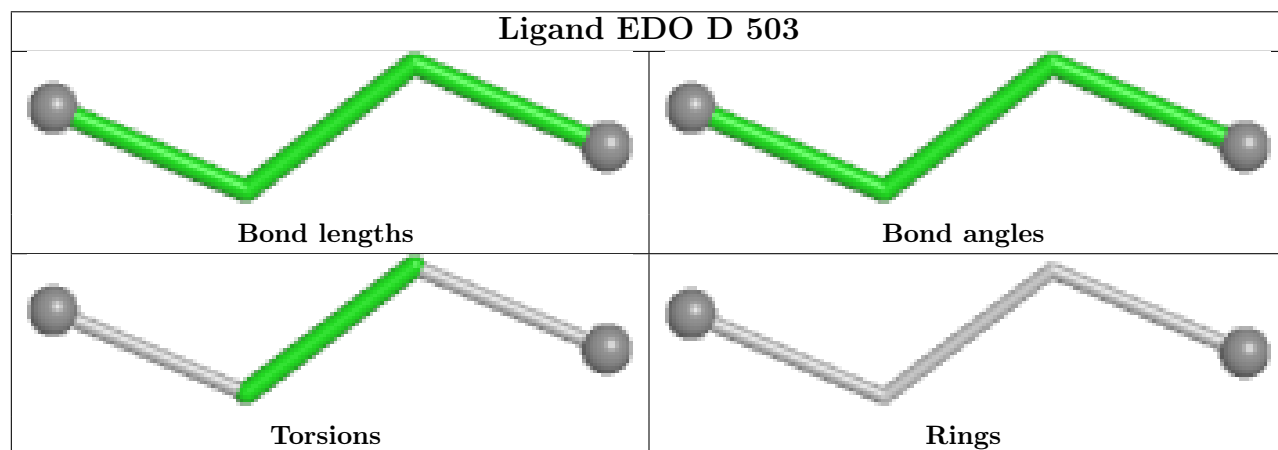
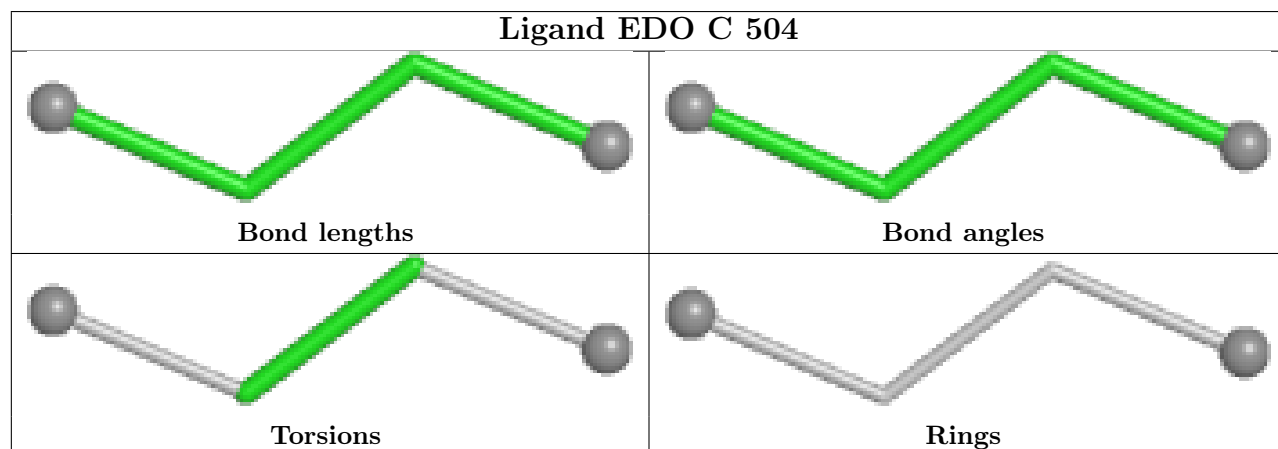
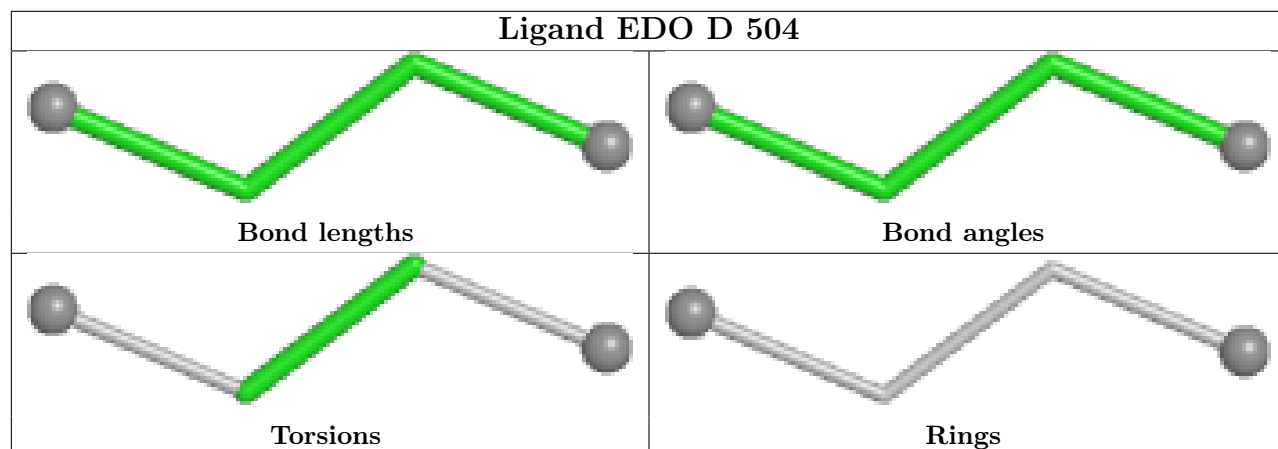


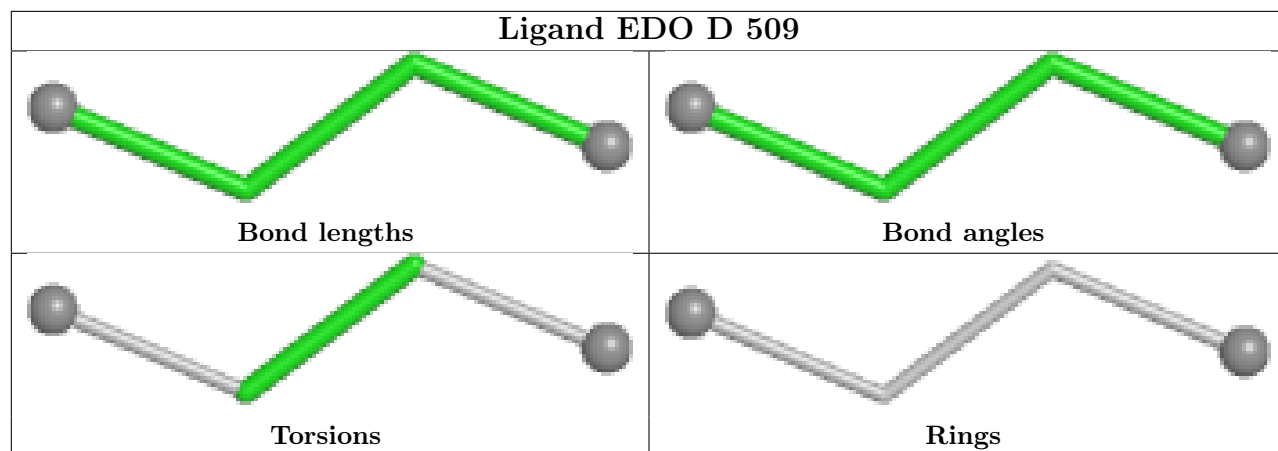












5.7 Other polymers [i](#)

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 ⓘ

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	447/452 (98%)	0.78	35 (7%)	19 25	12, 22, 41, 55	1 (0%)
1	B	447/452 (98%)	0.70	29 (6%)	25 33	11, 21, 40, 58	0
1	C	440/452 (97%)	1.24	95 (21%)	2 2	13, 30, 50, 59	0
1	D	440/452 (97%)	1.06	59 (13%)	7 10	13, 27, 47, 65	2 (0%)
All	All	1774/1808 (98%)	0.94	218 (12%)	8 11	11, 25, 46, 65	3 (0%)

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	373	VAL	6.1
1	C	439	PHE	4.9
1	C	319	ALA	4.8
1	A	322	ASP	4.3
1	C	290	ILE	4.2
1	D	162	PHE	4.1
1	D	370	VAL	4.1
1	C	5	PHE	4.1
1	A	2	THR	4.0
1	C	342	TRP	3.9
1	B	272	ILE	3.9
1	D	310	ALA	3.8
1	C	370	VAL	3.8
1	C	75	ILE	3.8
1	C	304	ALA	3.8
1	D	114	ILE	3.8
1	C	114	ILE	3.7
1	C	74	GLY	3.7
1	A	272	ILE	3.7
1	D	439	PHE	3.7
1	C	272	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	366	VAL	3.6
1	D	110	HIS	3.6
1	D	380	ALA	3.5
1	D	272	ILE	3.5
1	D	302	VAL	3.5
1	C	362	ALA	3.5
1	D	68	ALA	3.5
1	B	319	ALA	3.4
1	C	444	ALA	3.4
1	C	447	LYS	3.4
1	C	302	VAL	3.4
1	C	303	VAL	3.4
1	B	314	LEU	3.3
1	B	308	ASP	3.3
1	A	312	PHE	3.3
1	D	376	ILE	3.3
1	C	109	LEU	3.3
1	D	317	LEU	3.3
1	D	342	TRP	3.3
1	C	219	GLY	3.2
1	D	367	ASN	3.2
1	A	220	ILE	3.2
1	C	380	ALA	3.2
1	D	111	GLU	3.2
1	A	93	MET	3.1
1	C	438	TRP	3.1
1	A	314	LEU	3.1
1	B	318	GLU	3.1
1	A	117	PHE	3.1
1	C	73	LEU	3.1
1	C	230	ALA	3.1
1	A	309	ASP	3.0
1	C	106	LEU	3.0
1	C	110	HIS	3.0
1	D	438	TRP	3.0
1	C	161	ALA	3.0
1	C	217	GLN	3.0
1	D	437	ARG	3.0
1	A	308	ASP	2.9
1	B	312	PHE	2.9
1	C	68	ALA	2.9
1	D	69	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	373	VAL	2.9
1	C	365	PRO	2.9
1	D	8	PHE	2.9
1	D	304	ALA	2.9
1	C	379	ILE	2.9
1	D	106	LEU	2.9
1	C	328	GLY	2.8
1	D	303	VAL	2.8
1	C	378	TYR	2.8
1	C	218	ILE	2.8
1	C	231	THR	2.8
1	C	443	ILE	2.8
1	B	367	ASN	2.7
1	C	14	PHE	2.7
1	D	307	PRO	2.7
1	A	374	ARG	2.7
1	C	315	ARG	2.7
1	A	367	ASN	2.7
1	A	342	TRP	2.7
1	D	161	ALA	2.7
1	C	337	TYR	2.7
1	C	8	PHE	2.7
1	D	322	ASP	2.7
1	B	213	SER	2.7
1	B	307	PRO	2.7
1	D	383	LEU	2.7
1	C	111	GLU	2.7
1	A	373	VAL	2.7
1	C	313	GLY	2.6
1	D	14	PHE	2.6
1	D	427	SER	2.6
1	D	446	HIS	2.6
1	C	77	ALA	2.6
1	C	391	ASP	2.6
1	B	349	GLN	2.6
1	C	301	SER	2.6
1	C	306	ASN	2.6
1	C	389	PHE	2.6
1	C	401	LEU	2.6
1	D	112	ALA	2.6
1	D	305	ALA	2.6
1	C	431	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	290	ILE	2.6
1	D	6	ILE	2.6
1	B	259	GLY	2.6
1	D	216	GLY	2.6
1	D	368	GLY	2.6
1	C	366	VAL	2.6
1	B	274	GLN	2.5
1	B	11	ASP	2.5
1	D	74	GLY	2.5
1	A	306	ASN	2.5
1	D	377	HIS	2.5
1	C	267	LEU	2.5
1	C	317	LEU	2.5
1	A	218	ILE	2.5
1	C	229	ALA	2.5
1	B	212	SER	2.5
1	C	445	ALA	2.5
1	C	383	LEU	2.4
1	B	309	ASP	2.4
1	C	446	HIS	2.4
1	A	212	SER	2.4
1	A	213	SER	2.4
1	C	233	SER	2.4
1	D	312	PHE	2.4
1	C	232	ASP	2.4
1	C	372	ASP	2.4
1	D	225	THR	2.4
1	A	365	PRO	2.4
1	C	349	GLN	2.4
1	B	110	HIS	2.4
1	C	12	PHE	2.4
1	A	319	ALA	2.4
1	A	307	PRO	2.4
1	C	70	MET	2.4
1	C	213	SER	2.4
1	D	104[A]	ARG	2.3
1	C	237	GLN	2.3
1	B	290	ILE	2.3
1	B	310	ALA	2.3
1	D	444	ALA	2.3
1	B	306	ASN	2.3
1	C	15	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	216	GLY	2.3
1	C	206	VAL	2.3
1	D	292	PHE	2.3
1	A	369	ARG	2.3
1	D	27	VAL	2.3
1	D	232	ASP	2.3
1	D	109	LEU	2.3
1	C	112	ALA	2.3
1	C	310	ALA	2.3
1	C	6	ILE	2.3
1	C	440	SER	2.3
1	A	366	VAL	2.3
1	C	432	VAL	2.3
1	D	55	VAL	2.3
1	C	336	LEU	2.3
1	C	437	ARG	2.2
1	B	5	PHE	2.2
1	B	211	ALA	2.2
1	C	56	ALA	2.2
1	D	15	GLY	2.2
1	B	331	ILE	2.2
1	C	325	THR	2.2
1	A	328	GLY	2.2
1	C	348	GLY	2.2
1	B	438	TRP	2.2
1	A	119	THR	2.2
1	B	73	LEU	2.2
1	D	348	GLY	2.2
1	D	413	GLY	2.2
1	D	297	PHE	2.2
1	C	52	THR	2.2
1	D	365	PRO	2.2
1	C	324	ARG	2.2
1	C	375	ARG	2.2
1	D	315	ARG	2.2
1	A	337	TYR	2.1
1	C	425	TYR	2.1
1	C	402	TRP	2.1
1	B	231	THR	2.1
1	B	334	ASP	2.1
1	A	289	PRO	2.1
1	C	314	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	333	PRO	2.1
1	C	93	MET	2.1
1	C	162	PHE	2.1
1	D	361	PHE	2.1
1	D	337	TYR	2.1
1	A	338	ARG	2.1
1	B	366	VAL	2.1
1	C	180	VAL	2.1
1	D	382	HIS	2.1
1	D	230	ALA	2.1
1	B	173	PHE	2.1
1	C	275	PHE	2.1
1	C	368	GLY	2.1
1	A	262	GLN	2.1
1	A	68	ALA	2.1
1	C	4	GLU	2.0
1	C	163	ILE	2.0
1	C	361	PHE	2.0
1	C	441	GLU	2.0
1	A	368	GLY	2.0
1	C	332	HIS	2.0
1	A	118	VAL	2.0
1	A	211	ALA	2.0
1	C	386	ALA	2.0
1	D	70[A]	MET	2.0
1	A	331	ILE	2.0
1	B	347	THR	2.0
1	D	235	THR	2.0
1	C	388	ARG	2.0

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 ⓘ

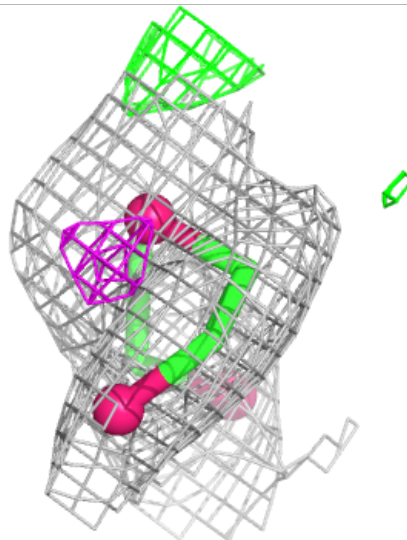
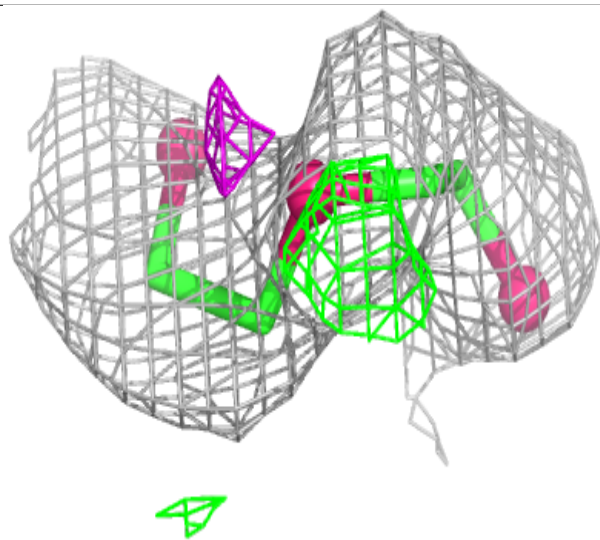
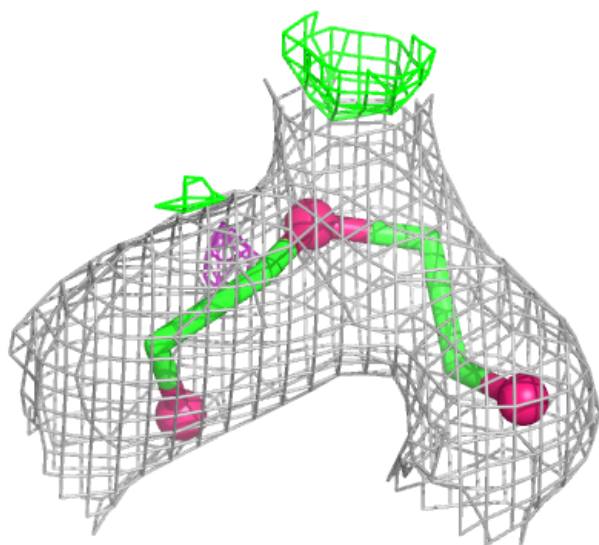
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEG	B	506	7/7	0.62	0.19	32,33,36,37	0
2	EDO	A	504	4/4	0.64	0.20	31,34,38,46	0
2	EDO	A	503	4/4	0.64	0.12	28,28,29,30	0
4	PGE	B	505	10/10	0.69	0.16	32,36,48,50	0
2	EDO	B	501	4/4	0.70	0.14	24,25,32,39	0
2	EDO	D	506	4/4	0.70	0.16	42,42,42,44	0
2	EDO	C	503	4/4	0.74	0.14	34,36,36,44	0
2	EDO	D	509	4/4	0.74	0.14	26,26,35,41	0
4	PGE	A	510	10/10	0.75	0.15	28,38,47,49	0
2	EDO	D	503	4/4	0.76	0.15	28,29,31,43	0
2	EDO	A	507	4/4	0.77	0.12	33,33,38,41	0
2	EDO	D	510	4/4	0.78	0.13	14,28,30,30	0
2	EDO	A	508	4/4	0.80	0.13	21,24,26,29	0
2	EDO	D	504	4/4	0.81	0.13	23,32,32,34	0
2	EDO	D	501	4/4	0.82	0.12	28,32,32,34	0
2	EDO	C	505	4/4	0.83	0.13	22,23,26,38	0
2	EDO	A	502	4/4	0.84	0.12	29,31,34,36	0
2	EDO	C	504	4/4	0.85	0.13	24,27,28,36	0
2	EDO	D	502	4/4	0.85	0.12	23,25,30,36	0
2	EDO	C	501	4/4	0.87	0.12	24,25,32,37	0
2	EDO	D	507	4/4	0.88	0.14	24,24,32,34	0
2	EDO	B	503	4/4	0.88	0.12	28,31,31,37	0
2	EDO	D	505	4/4	0.89	0.09	28,33,34,34	0
2	EDO	C	502	4/4	0.89	0.10	24,27,28,30	0
2	EDO	A	501	4/4	0.90	0.11	19,19,21,26	0
2	EDO	B	502	4/4	0.90	0.10	20,27,29,31	0
2	EDO	D	508	4/4	0.92	0.09	22,23,24,24	0
2	EDO	A	506	4/4	0.93	0.10	17,20,38,47	0
2	EDO	A	505	4/4	0.95	0.08	14,15,16,20	0
3	NI	B	504	1/1	0.99	0.01	15,15,15,15	0
3	NI	A	509	1/1	1.00	0.01	14,14,14,14	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.

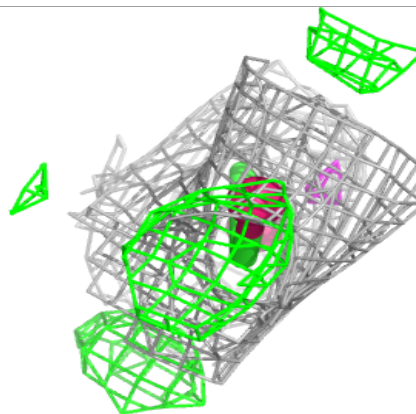
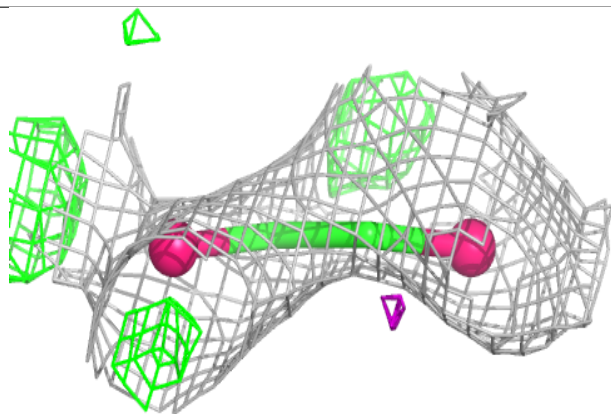
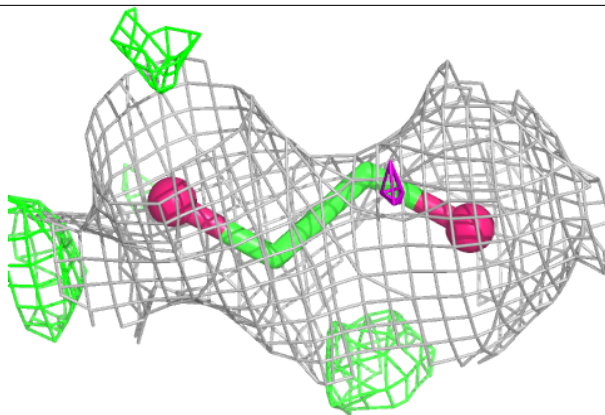
Electron density around PEG B 506:

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

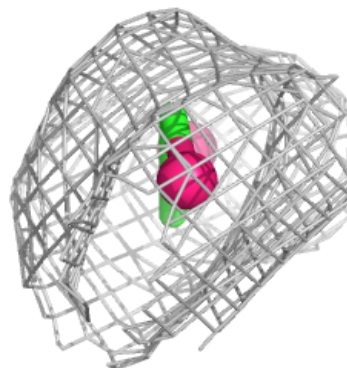
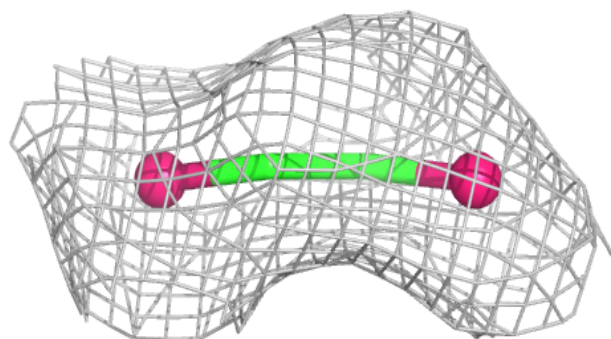
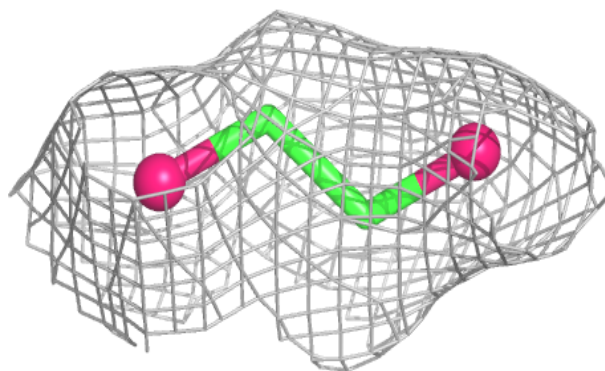


Electron density around EDO A 504:

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

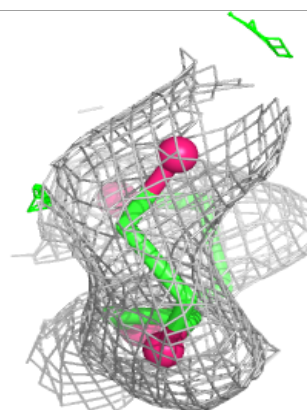
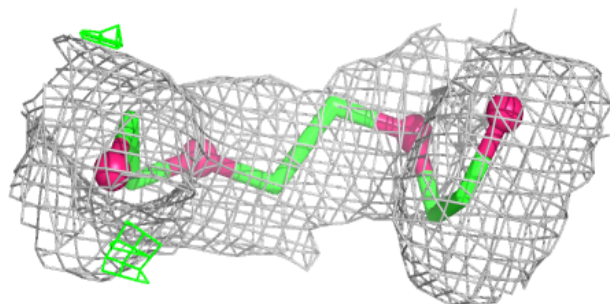
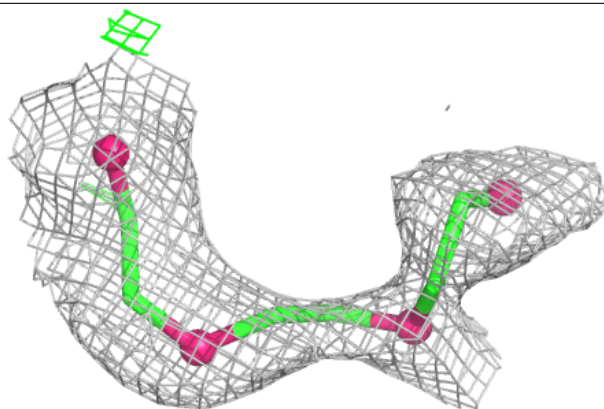
**Electron density around EDO A 503:**

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



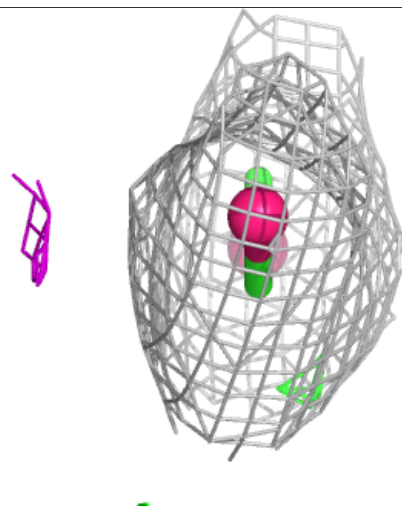
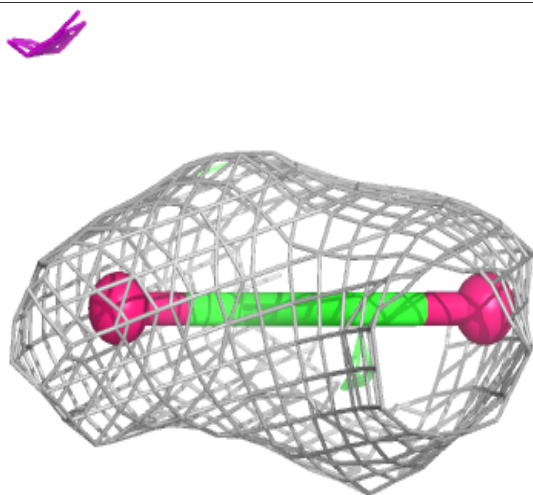
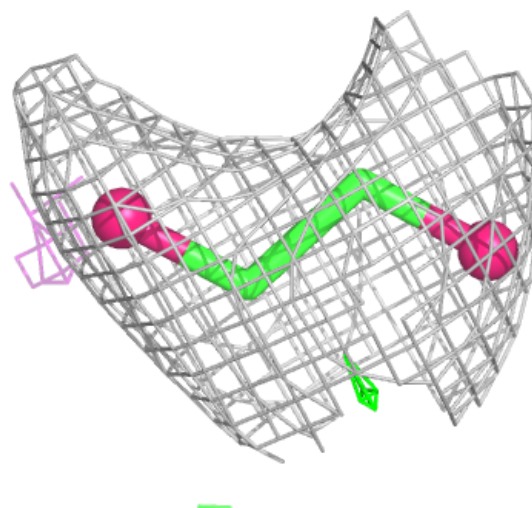
Electron density around PGE B 505:

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



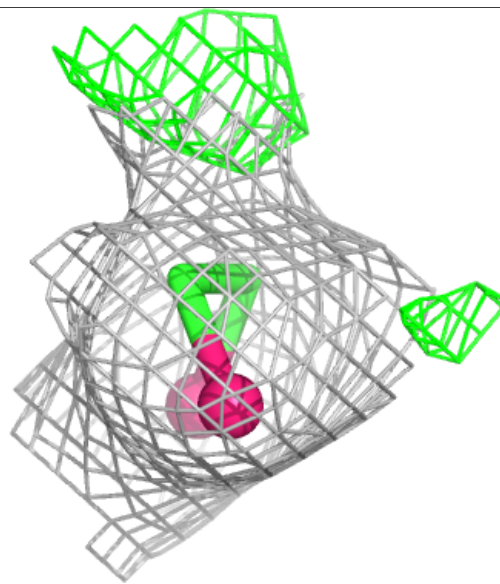
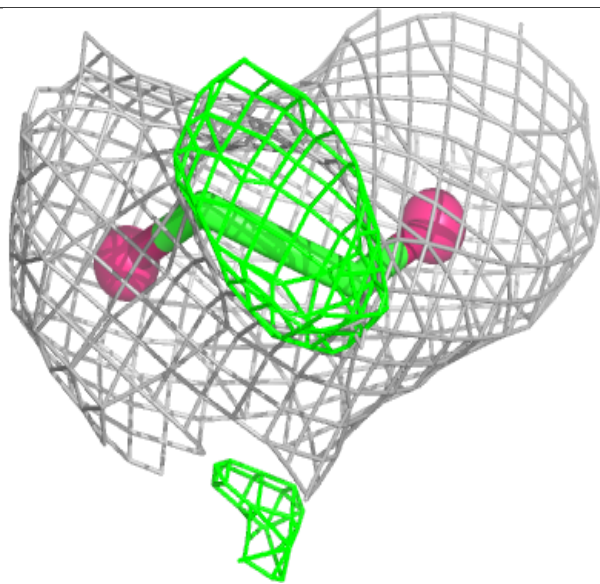
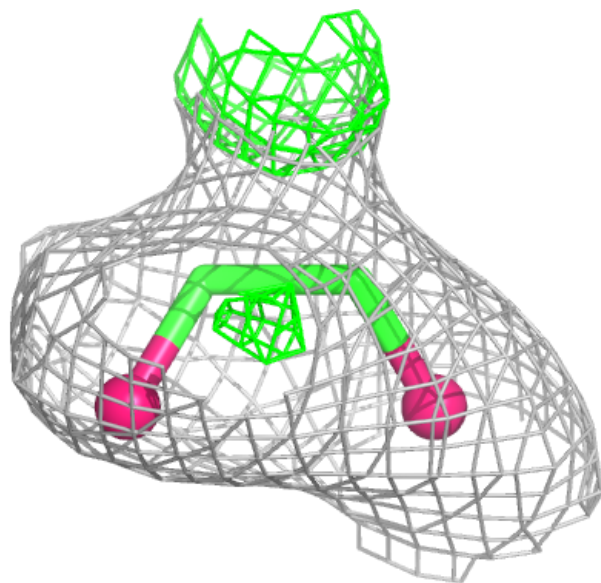
Electron density around EDO B 501:

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



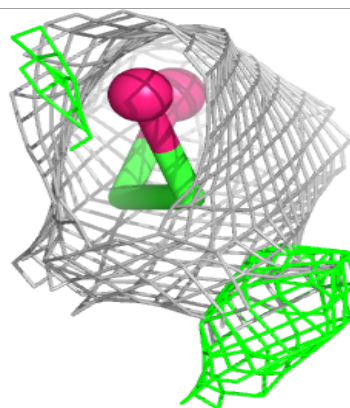
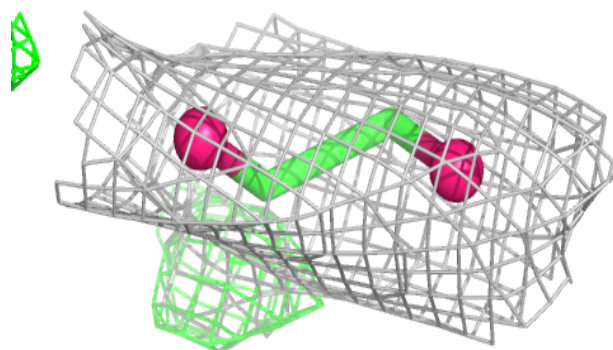
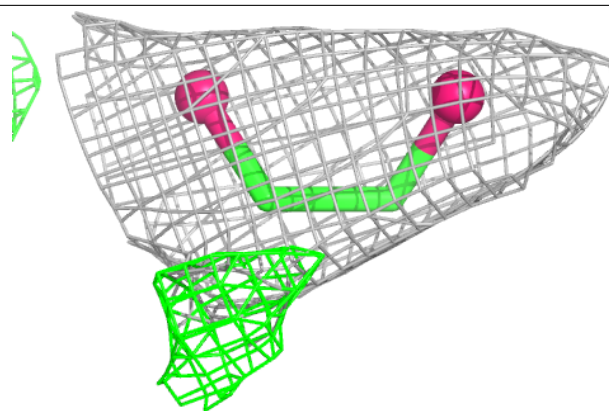
Electron density around EDO D 506:

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

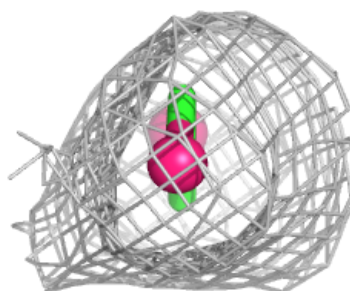
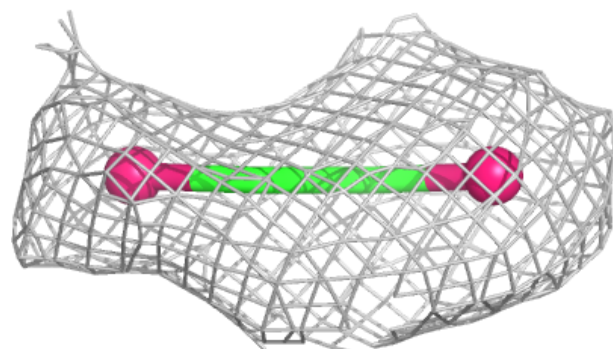
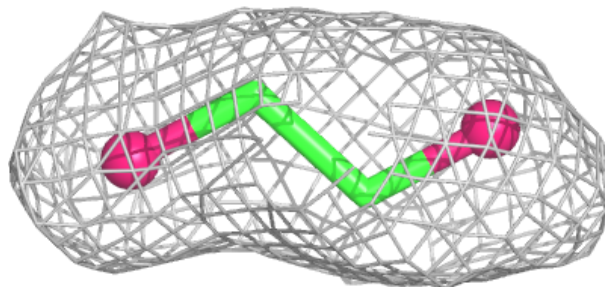


Electron density around EDO C 503:

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

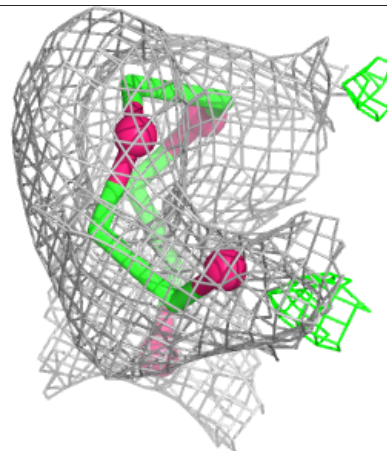
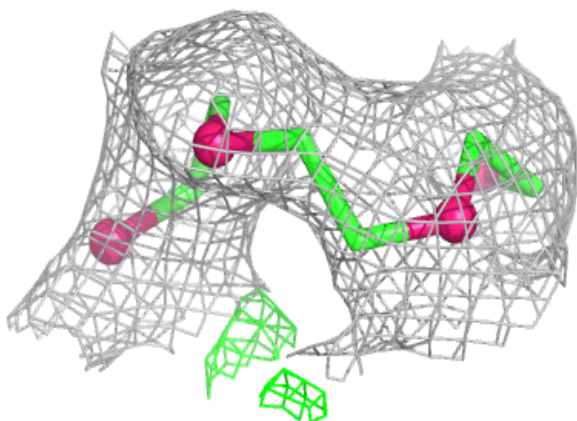
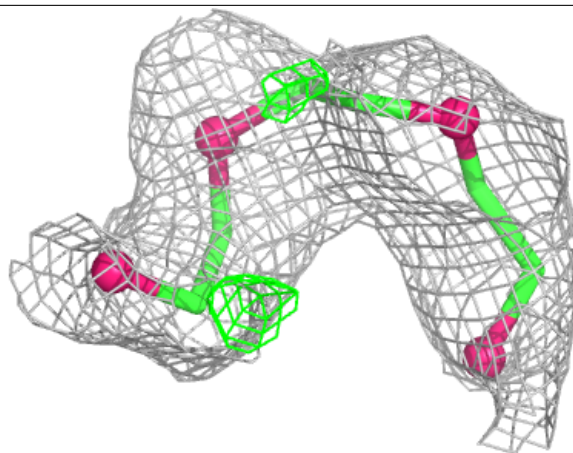
**Electron density around EDO D 509:**

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



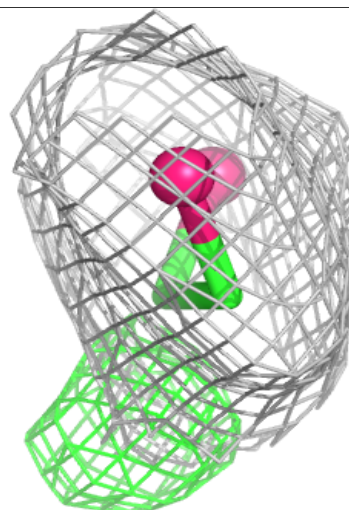
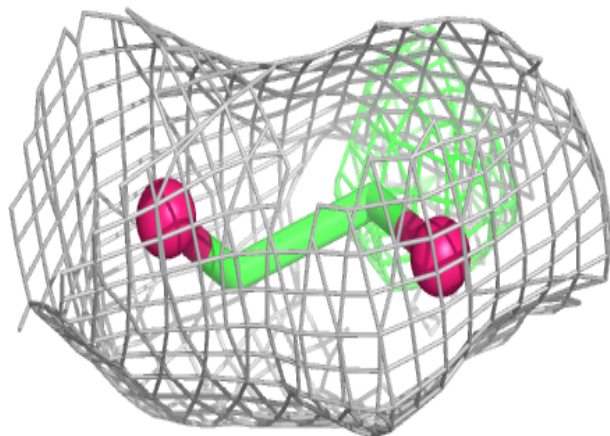
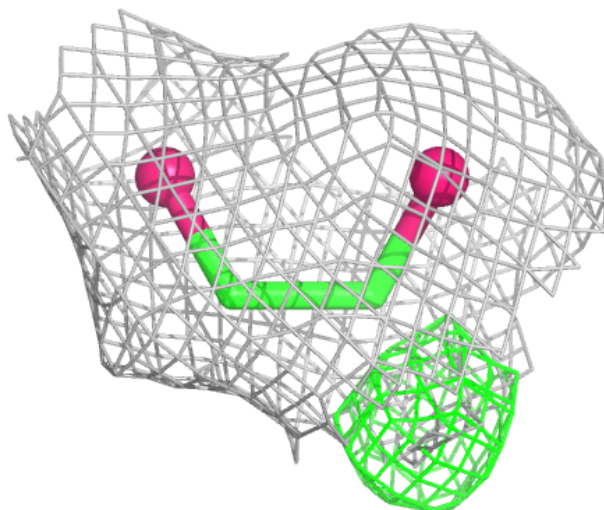
Electron density around PGE A 510:

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



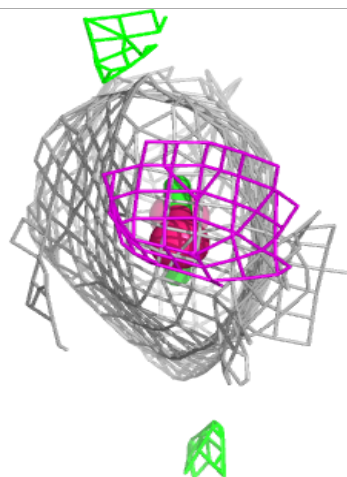
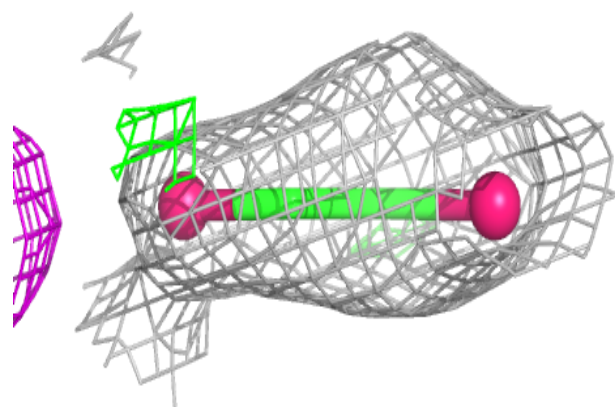
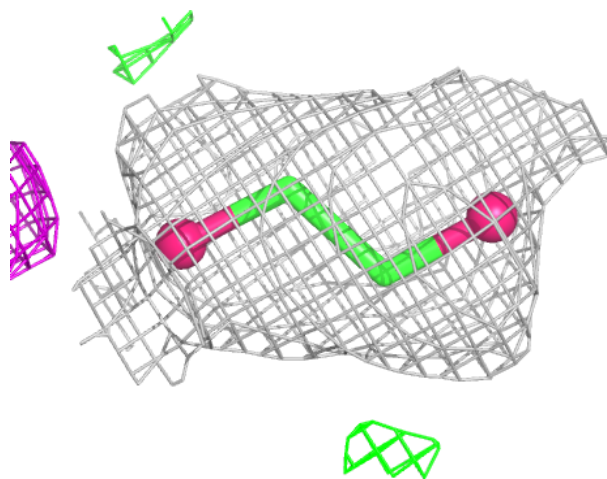
Electron density around EDO D 503:

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



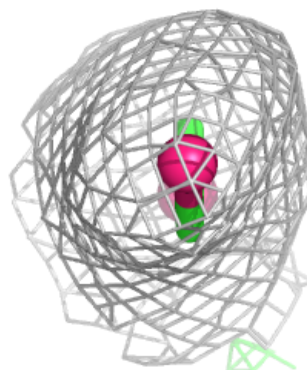
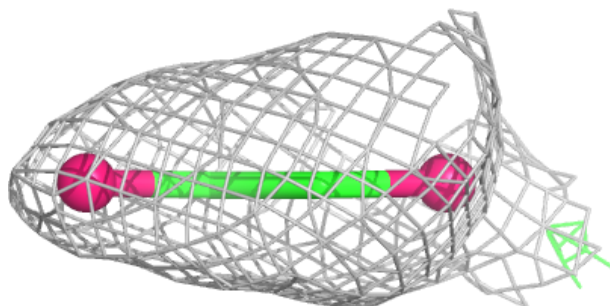
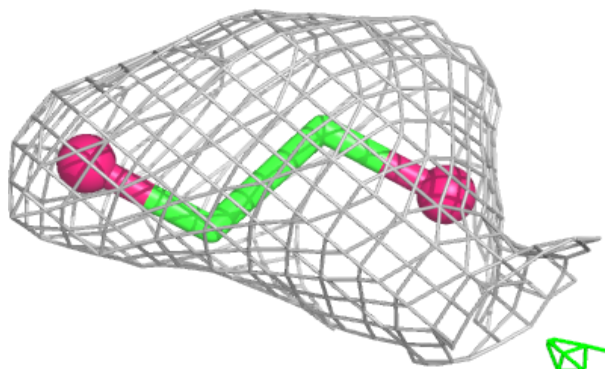
Electron density around EDO A 507:

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and green (positive)

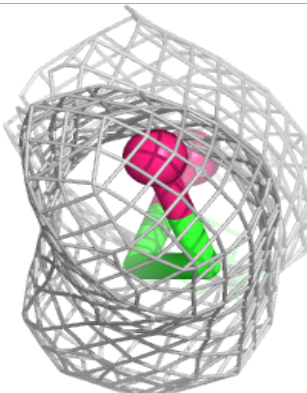
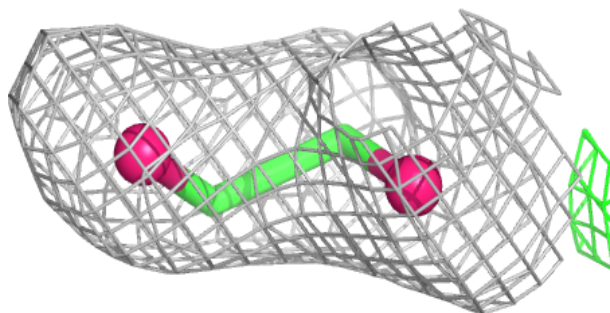
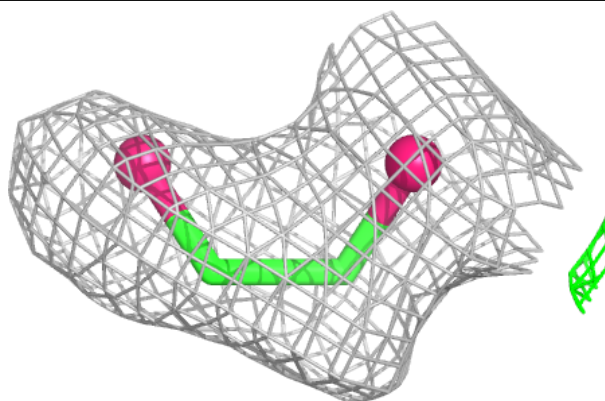


Electron density around EDO D 510:

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

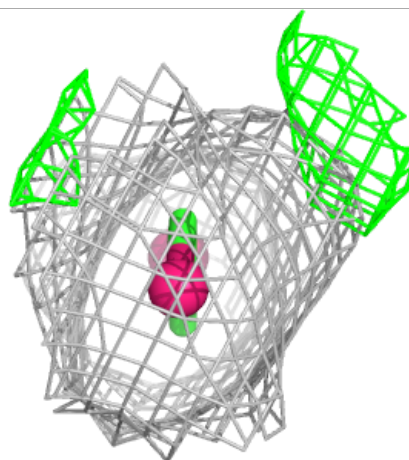
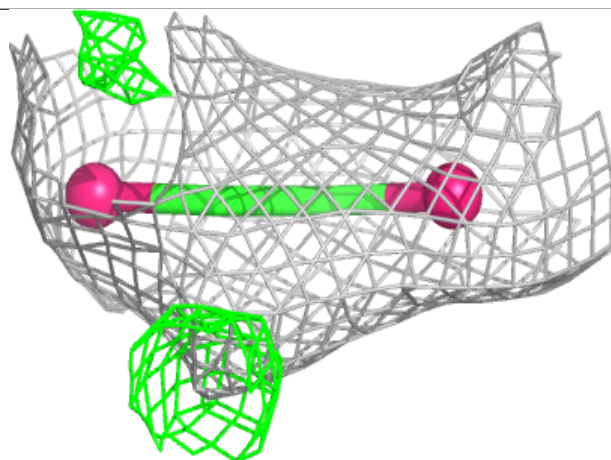
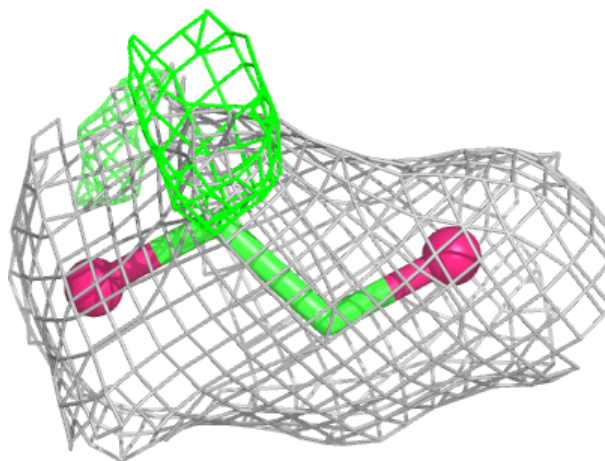
**Electron density around EDO A 508:**

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



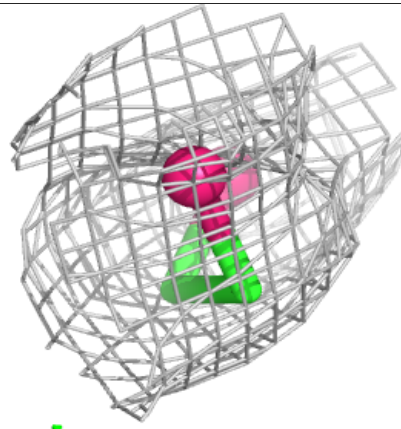
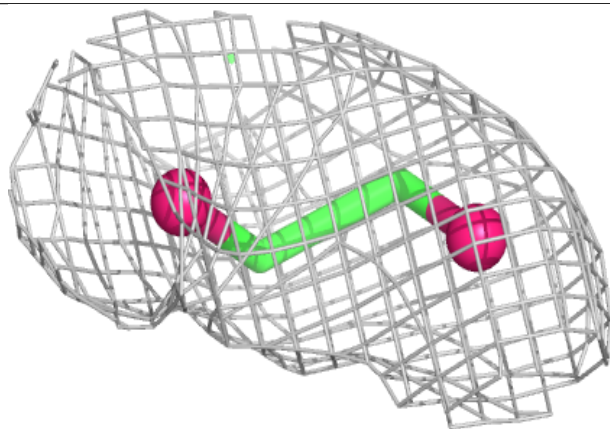
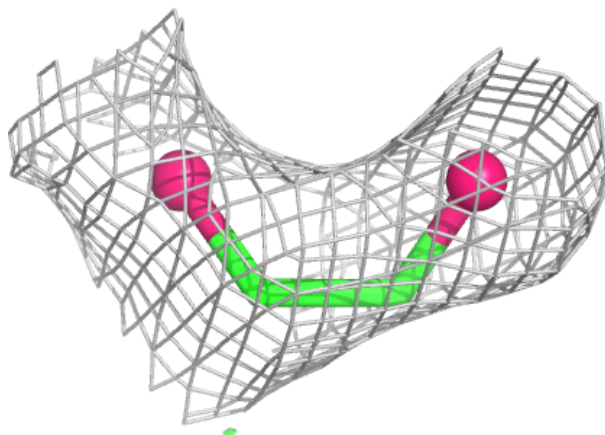
Electron density around EDO D 504:

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



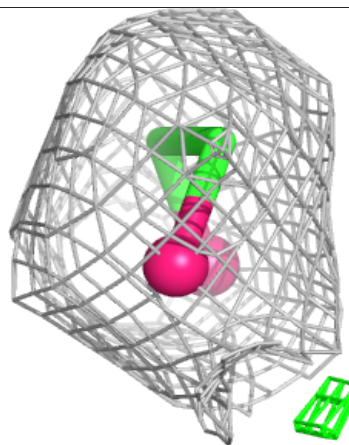
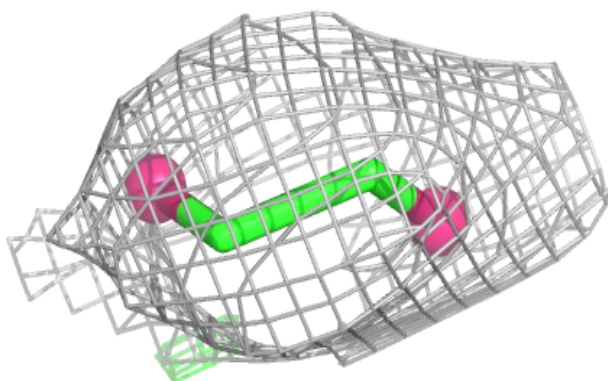
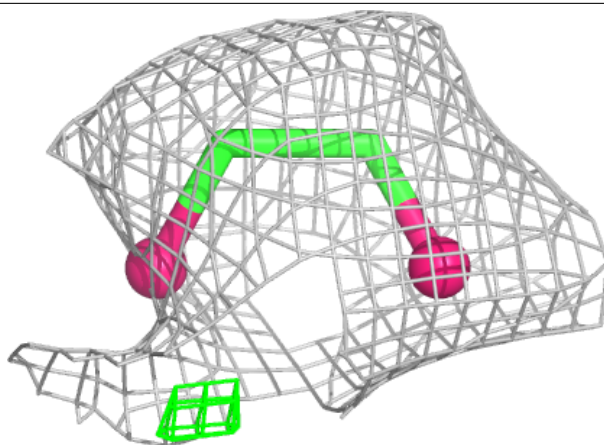
Electron density around EDO D 501:

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

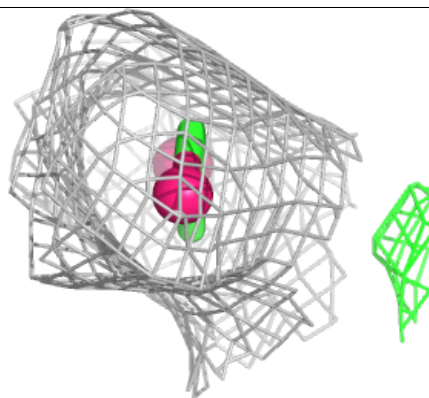
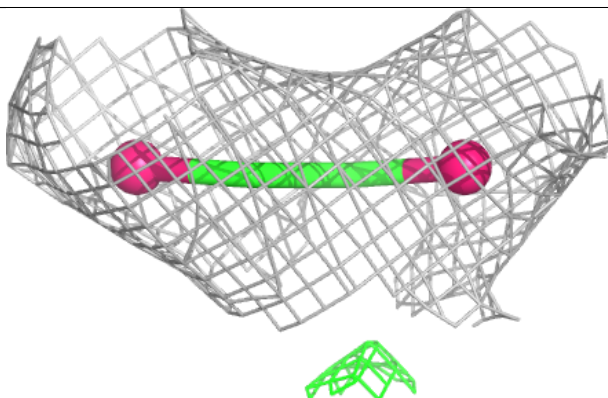
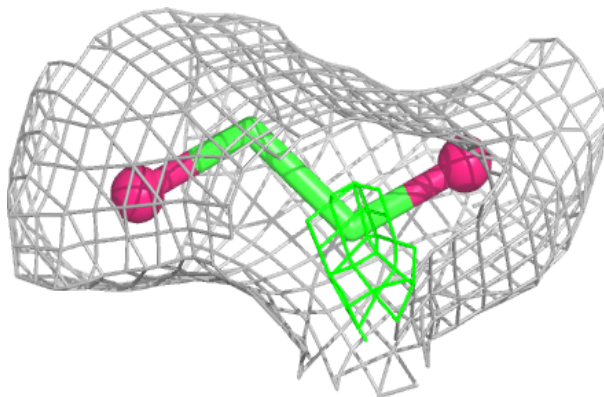


Electron density around EDO C 505:

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

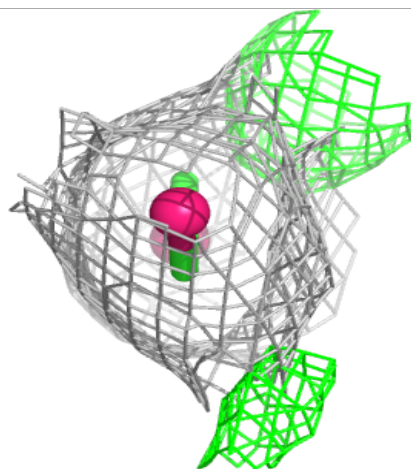
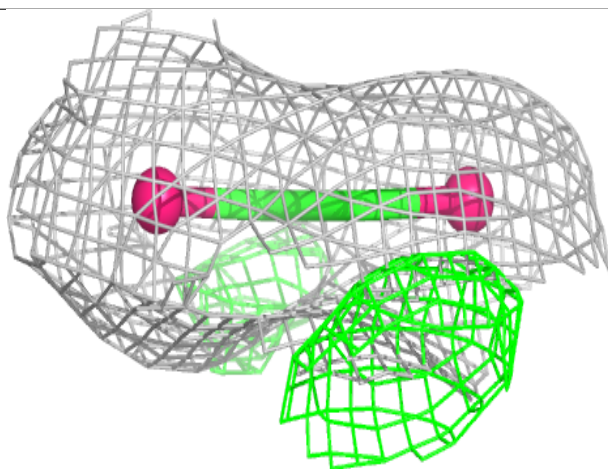
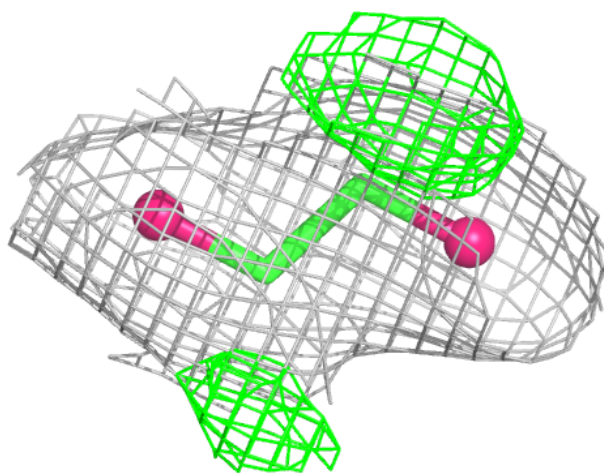
**Electron density around EDO A 502:**

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



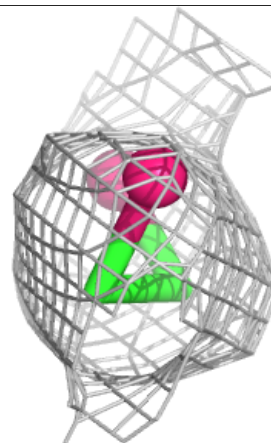
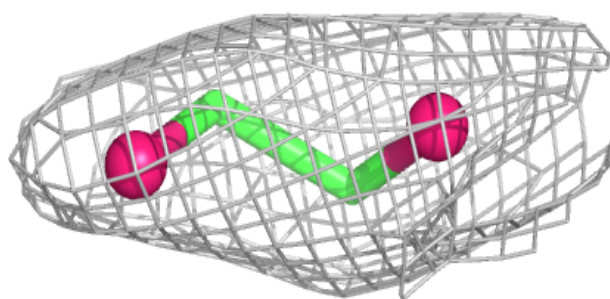
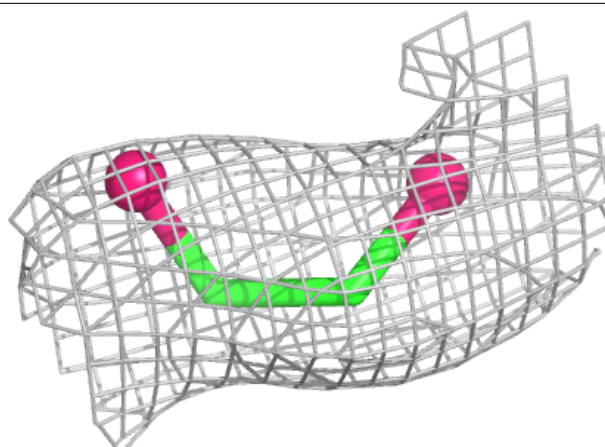
Electron density around EDO C 504:

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



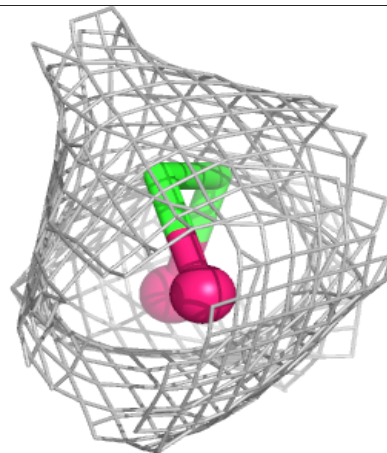
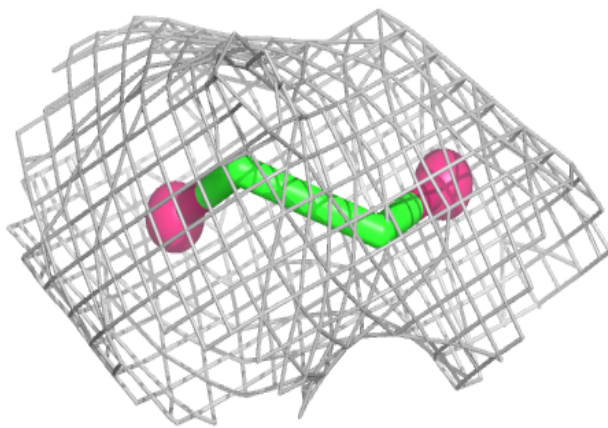
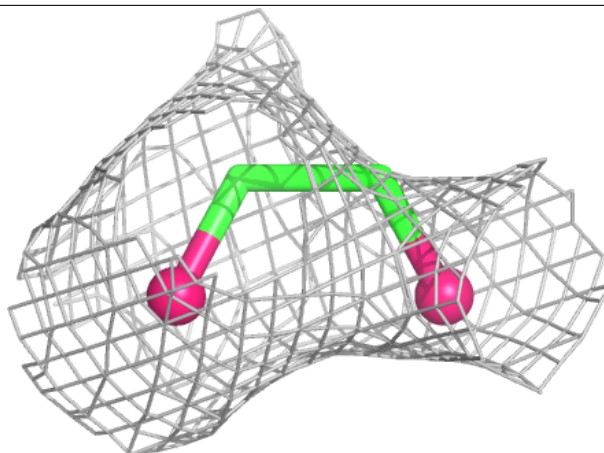
Electron density around EDO D 502:

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



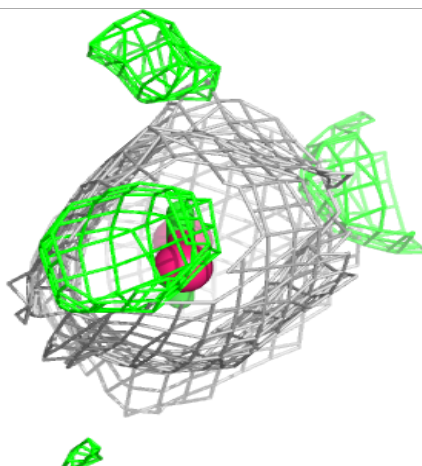
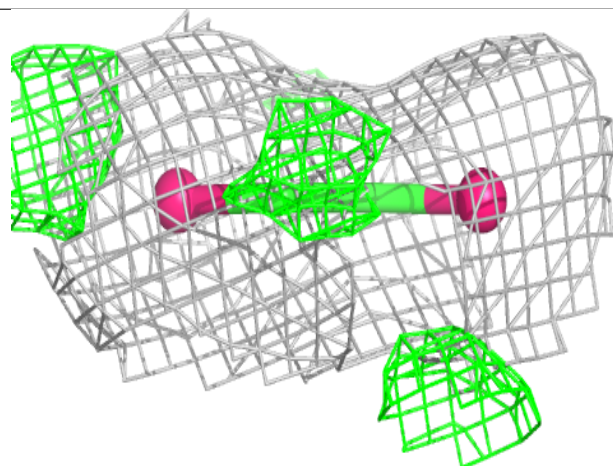
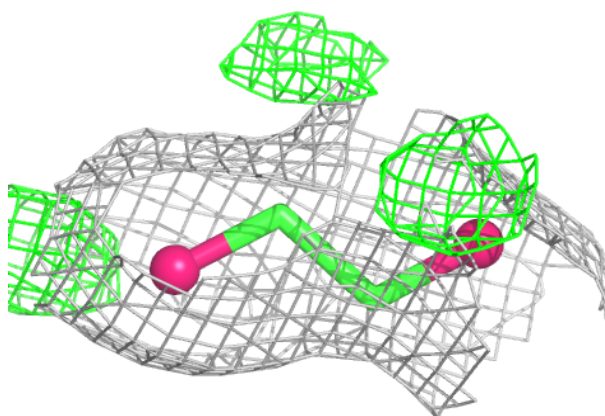
Electron density around EDO C 501:

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



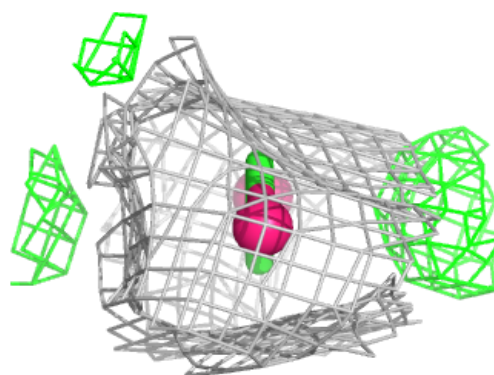
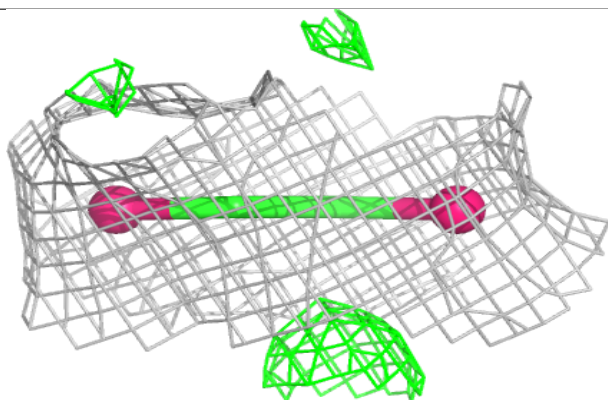
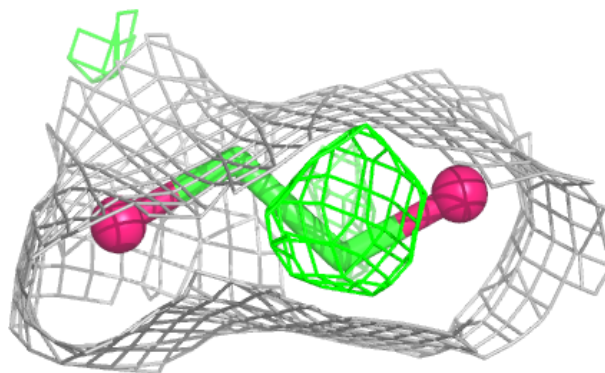
Electron density around EDO D 507:

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

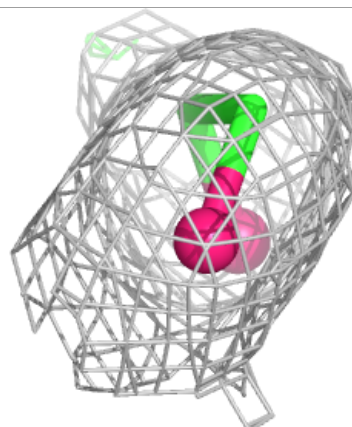
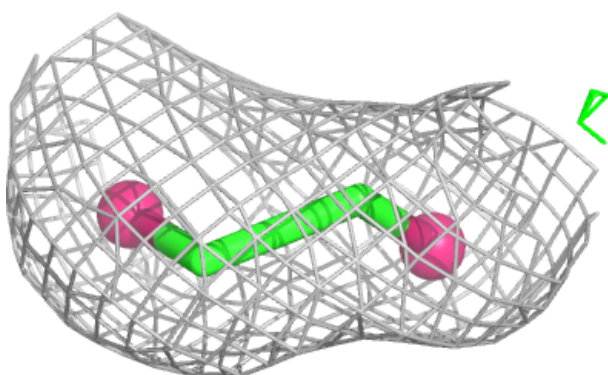
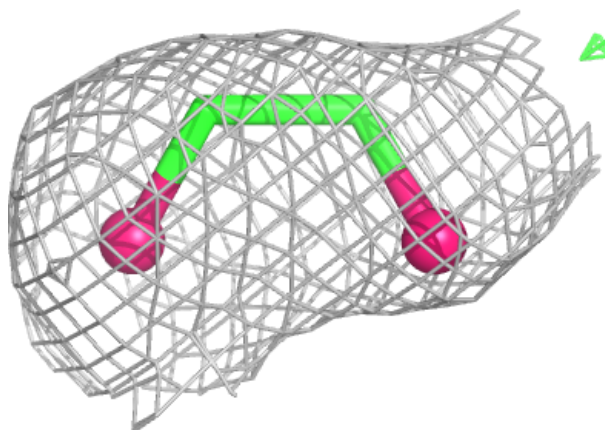


Electron density around EDO B 503:

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

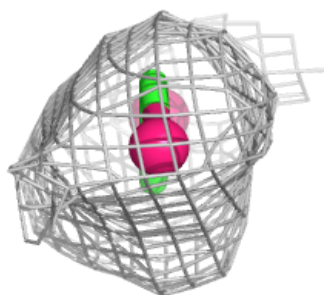
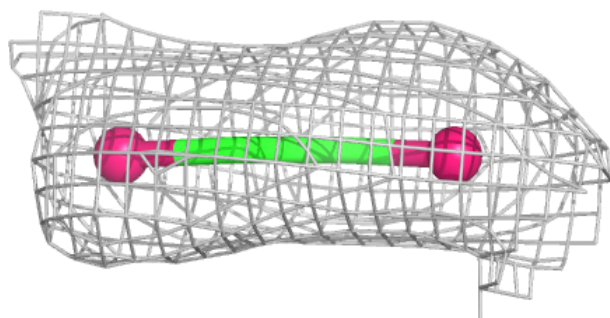
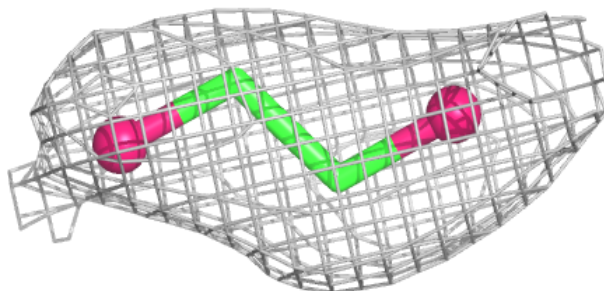
**Electron density around EDO D 505:**

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

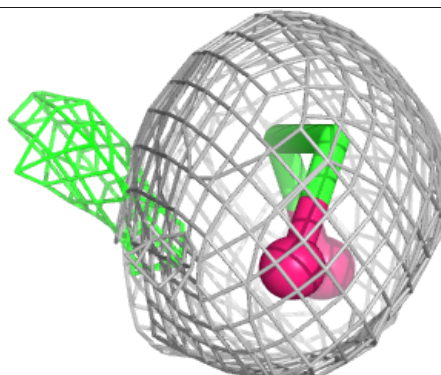
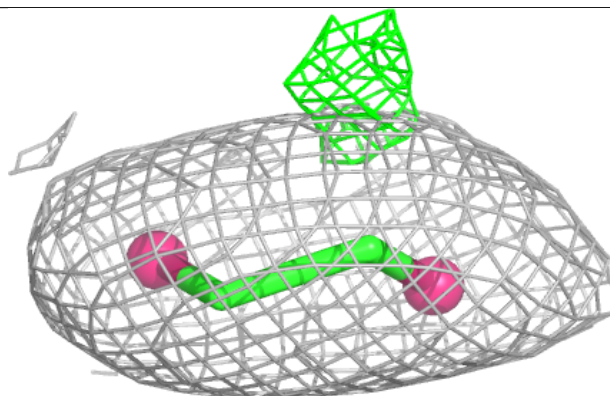
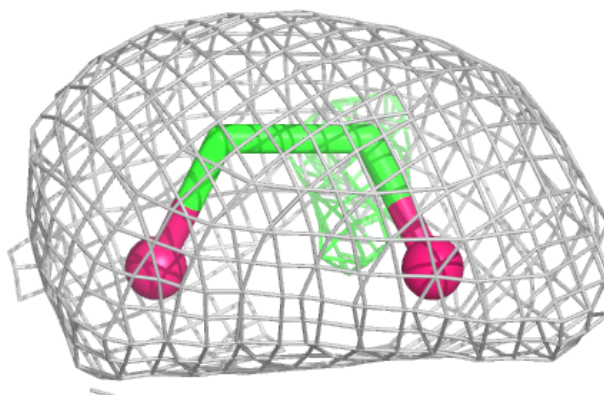


Electron density around EDO C 502:

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

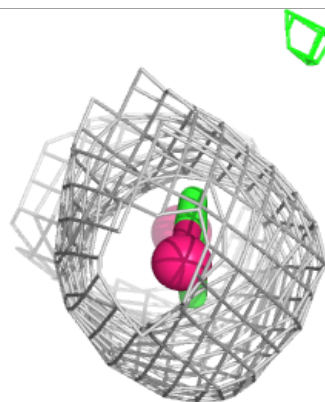
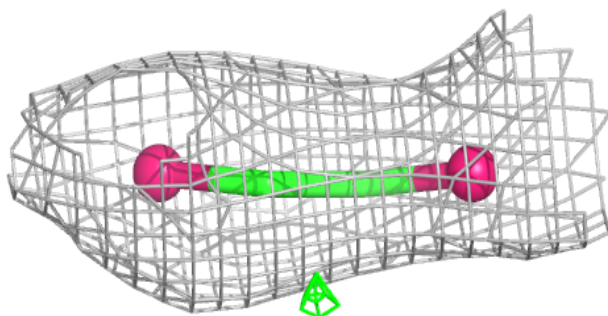
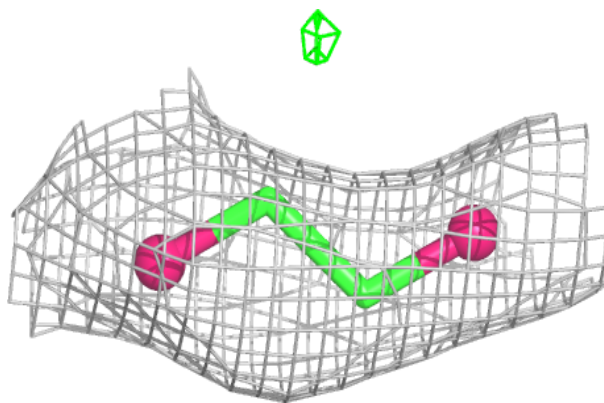
**Electron density around EDO A 501:**

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

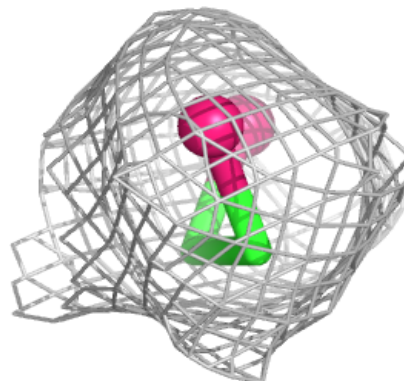
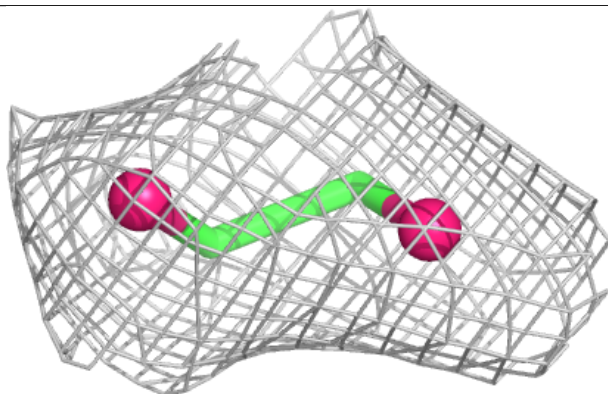
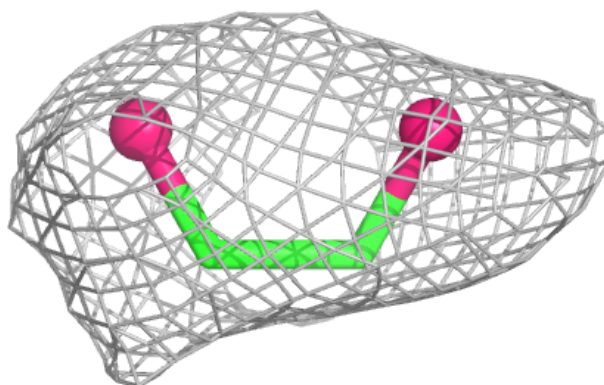


Electron density around EDO B 502:

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

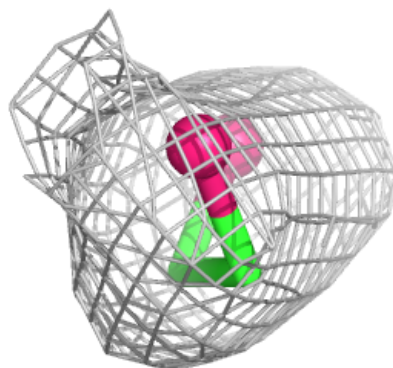
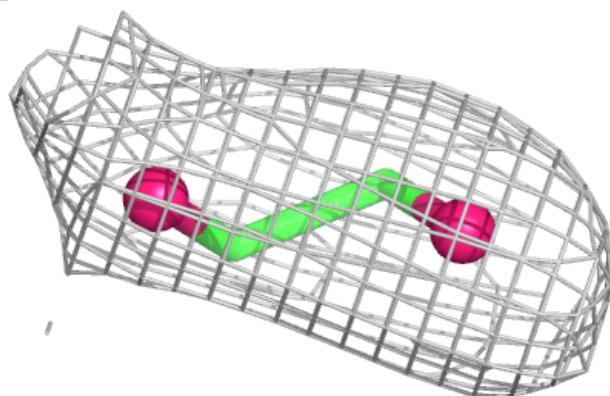
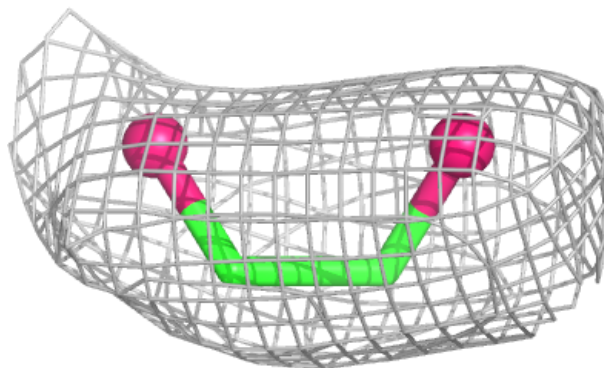
**Electron density around EDO D 508:**

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

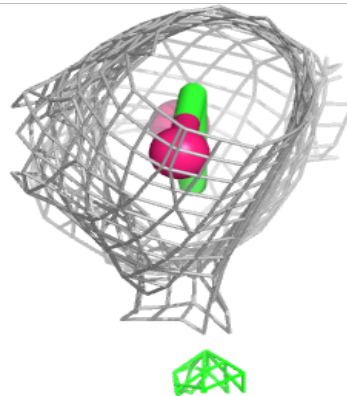
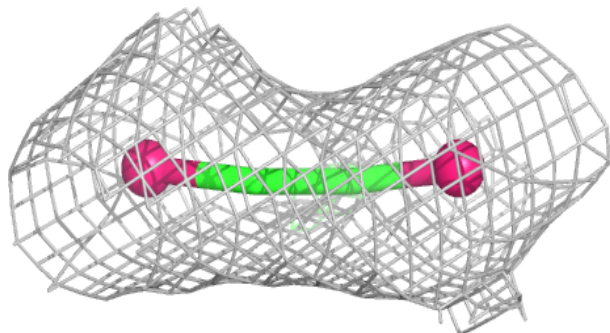
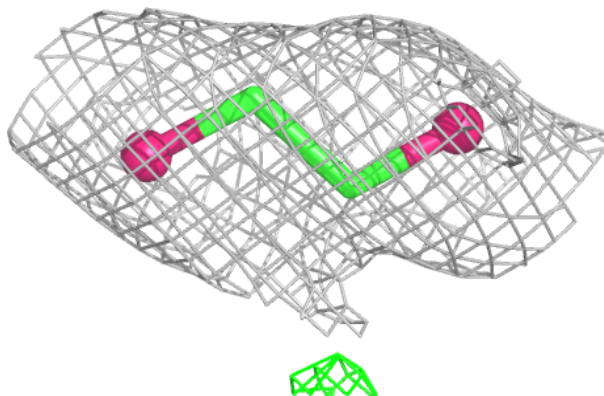


Electron density around EDO A 506:

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

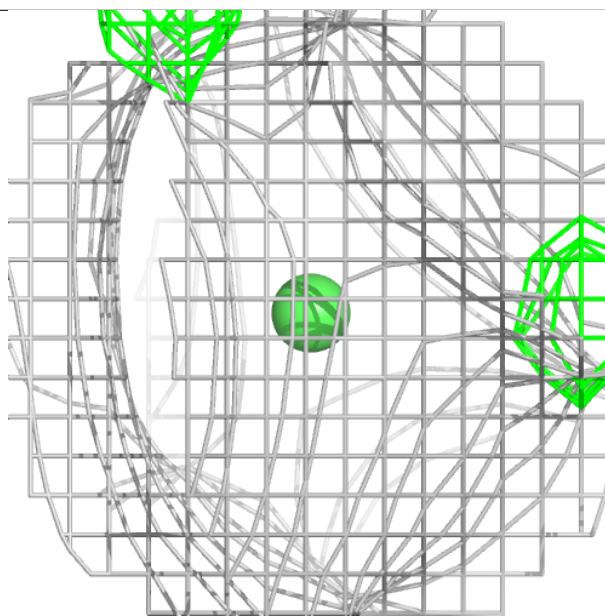
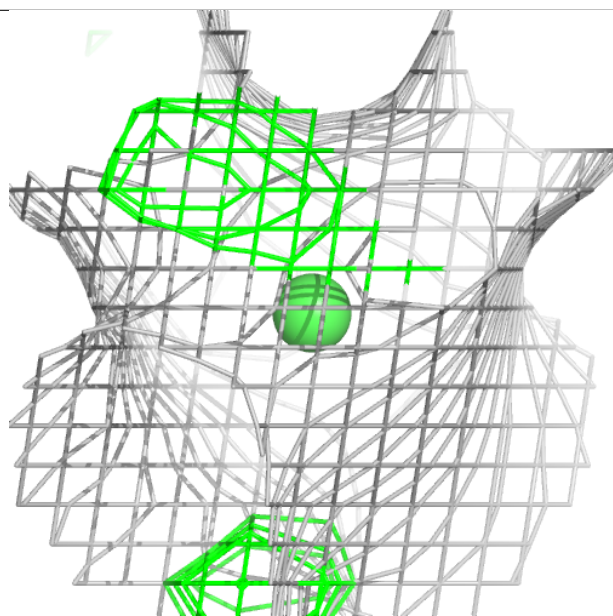
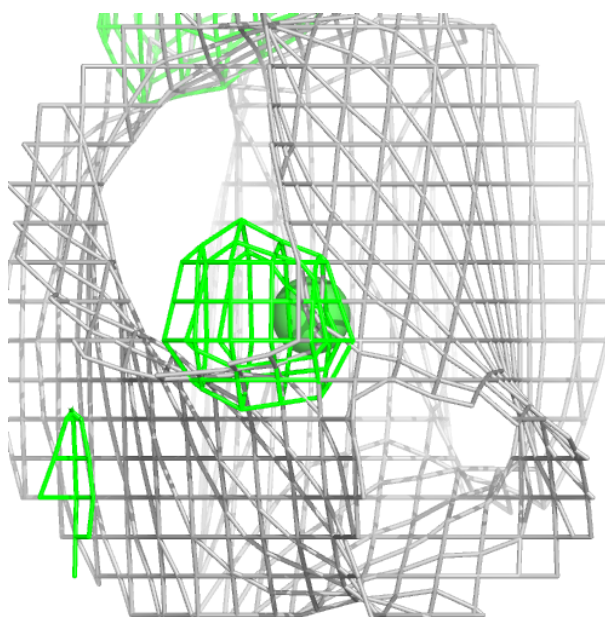
**Electron density around EDO A 505:**

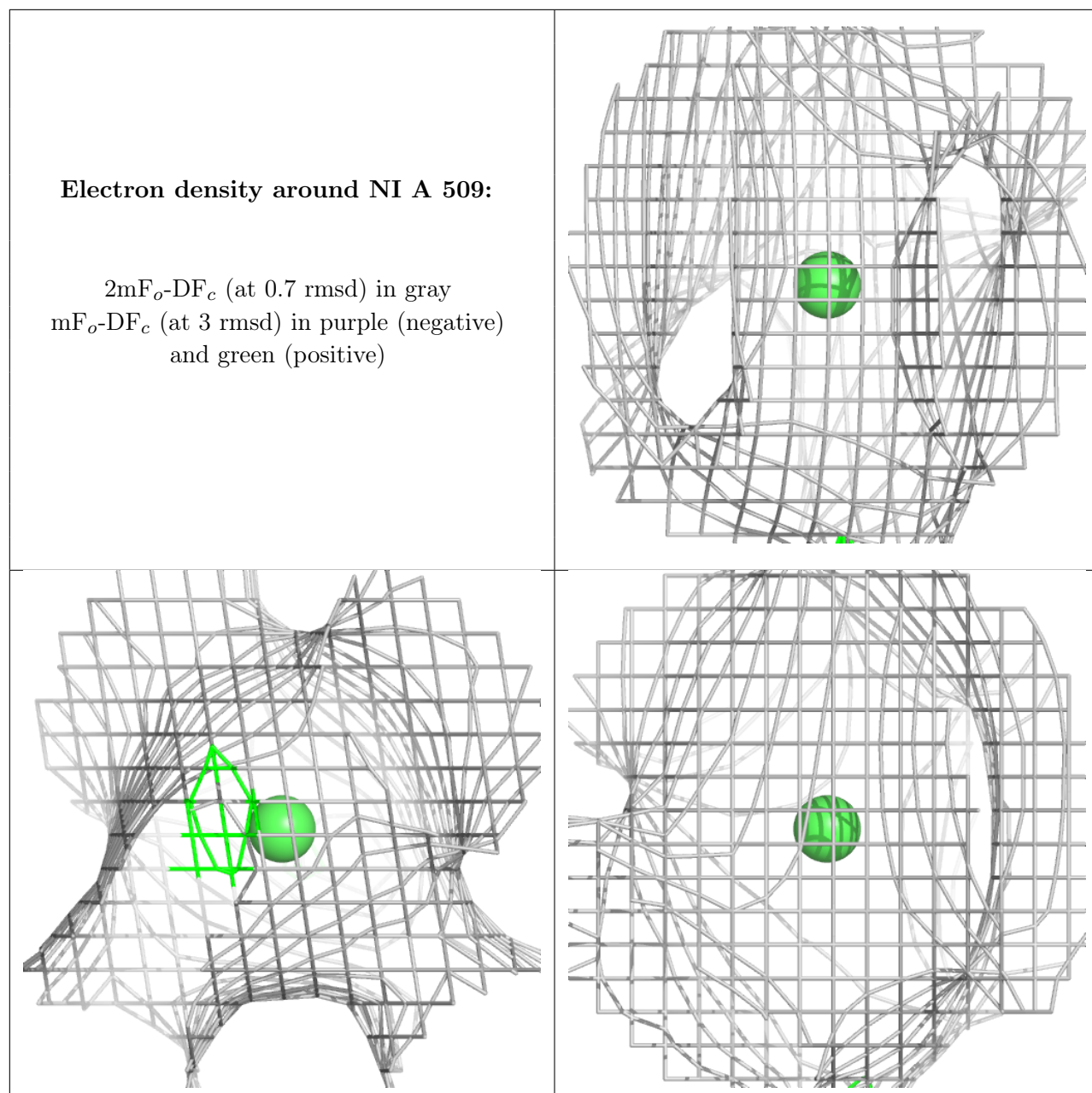
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI B 504:

$2mF_o-DF_c$ (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.