



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:44 AM UTC

PDB ID : 6YJZ / pdb_00006yjz
Title : Crystal structure of mouse pyridoxal kinase in apo form
Authors : Kasaragod, V.B.; Schindelin, H.
Deposited on : 2020-04-05
Resolution : 2.45 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

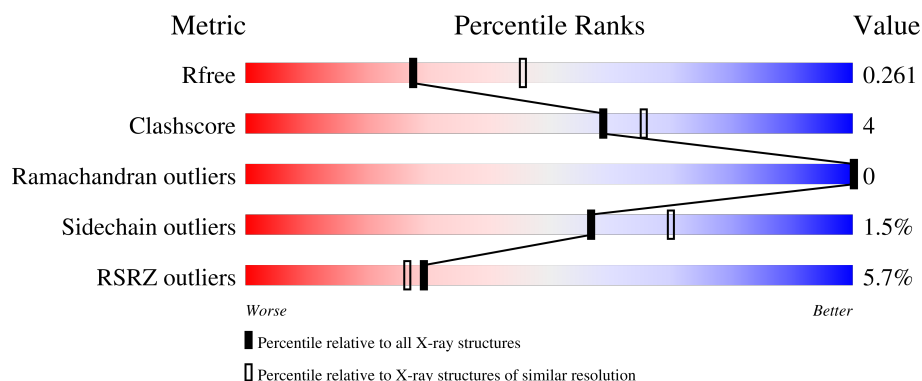
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	314	4% 84% 12% .
1	B	314	5% 85% 12% ..
1	C	314	6% 83% 13% .
1	D	314	8% 84% 12% .

2 Entry composition [i](#)

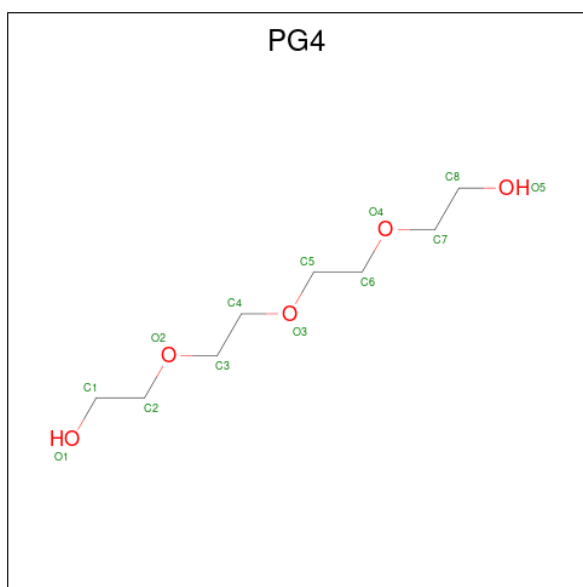
There are 5 unique types of molecules in this entry. The entry contains 19141 atoms, of which 9430 are hydrogens and 0 are deuteriums.

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 Pyridoxal Kinase.

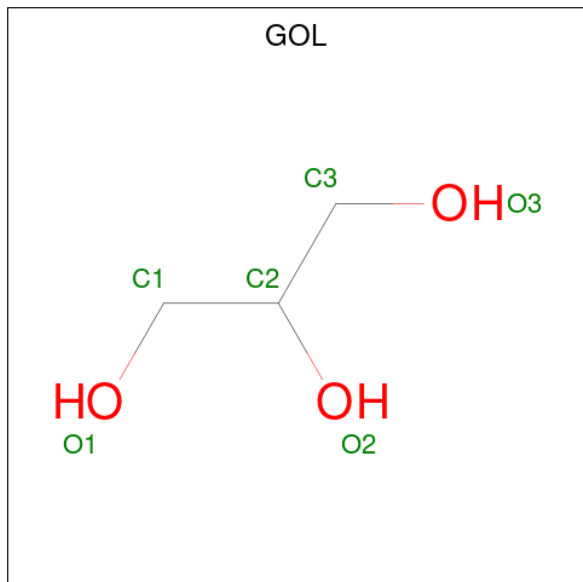
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total	C	H	N	O	S	0	1	0
			4762	1501	2376	417	450	18			
1	B	308	Total	C	H	N	O	S	0	0	0
			4739	1499	2356	415	451	18			
1	C	302	Total	C	H	N	O	S	0	0	0
			4685	1479	2333	413	442	18			
1	D	302	Total	C	H	N	O	S	0	0	0
			4486	1439	2199	389	442	17			

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			31	8	18	5		
2	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

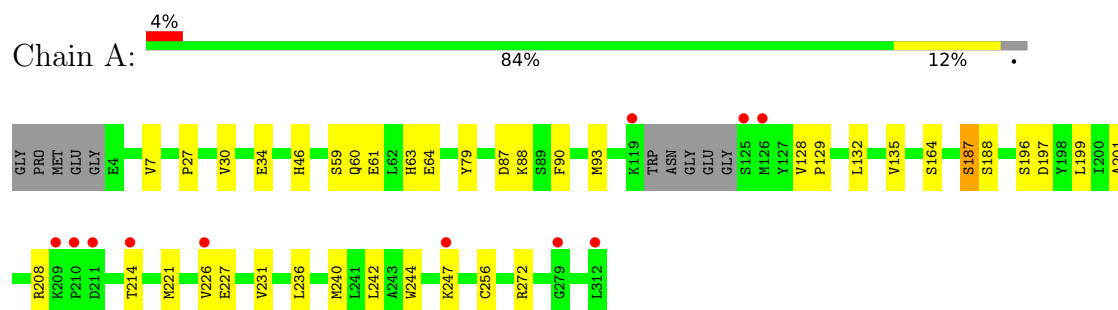
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		
5	B	60	Total	O	0	0
			60	60		
5	C	39	Total	O	0	0
			39	39		
5	D	30	Total	O	0	0
			30	30		

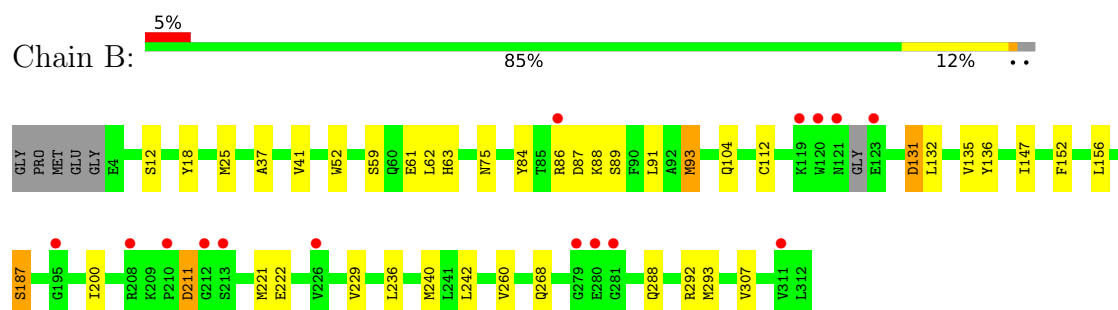
3 Residue-property plots [i](#)

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.

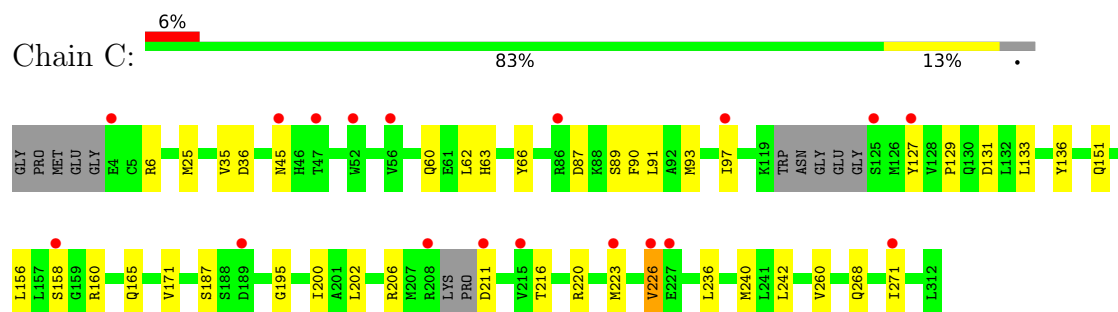
• Molecule 1: Pyridoxal Kinase



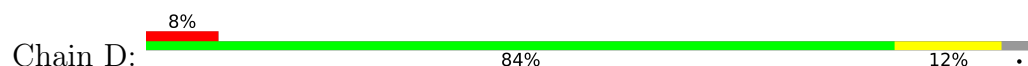
• Molecule 1: Pyridoxal Kinase

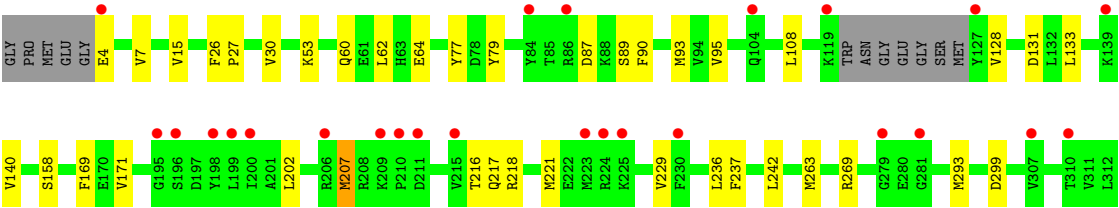


• Molecule 1: Pyridoxal Kinase



• Molecule 1: Pyridoxal Kinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	279.13Å 53.43Å 109.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 2.45 47.32 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.32-2.45) 95.2 (47.32-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.216 , 0.260 0.221 , 0.261	Depositor DCC
R_{free} test set	2930 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.084 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19141	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, EDO, GOL

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	0.77	11/2431 (0.5%)	0.47	0/3288
1	B	0.67	8/2425 (0.3%)	0.42	0/3284
1	C	0.75	5/2392 (0.2%)	0.55	2/3236 (0.1%)
1	D	0.61	2/2328 (0.1%)	0.48	2/3167 (0.1%)
All	All	0.70	26/9576 (0.3%)	0.48	4/12975 (0.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	SER	C-O	-7.72	1.14	1.23
1	A	87	ASP	C-O	-6.95	1.15	1.24
1	B	59	SER	C-O	-6.83	1.16	1.24
1	B	63	HIS	C-O	-6.58	1.16	1.24
1	B	93	MET	C-O	-6.50	1.16	1.24
1	A	64	GLU	C-O	-6.34	1.16	1.24
1	A	93	MET	C-O	-6.32	1.16	1.24
1	B	221	MET	C-O	-6.15	1.16	1.23
1	B	61	GLU	C-O	-5.81	1.17	1.24
1	A	60	GLN	C-O	-5.71	1.17	1.24
1	A	187	SER	C-O	-5.69	1.16	1.23
1	D	60	GLN	C-O	-5.65	1.17	1.24
1	A	201	ALA	C-O	-5.52	1.17	1.24
1	C	151	GLN	C-O	-5.50	1.17	1.24
1	A	196	SER	C-O	-5.47	1.16	1.24
1	B	200	ILE	C-O	-5.42	1.18	1.24
1	B	222	GLU	C-O	-5.42	1.17	1.24
1	A	90	PHE	C-O	-5.38	1.17	1.24
1	C	226	VAL	C-O	-5.30	1.18	1.24
1	A	63	HIS	C-O	-5.23	1.18	1.24
1	A	59	SER	C-O	-5.21	1.18	1.24
1	D	64	GLU	C-O	-5.21	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	GLN	C-O	-5.14	1.18	1.24
1	A	61	GLU	C-O	-5.08	1.18	1.24
1	C	200	ILE	C-O	-5.08	1.18	1.24
1	C	187	SER	C-O	-5.01	1.17	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	LEU	CA-C-N	8.12	129.18	121.46
1	C	202	LEU	C-N-CA	8.12	129.18	121.46
1	D	202	LEU	CA-C-N	5.14	131.48	121.41
1	D	202	LEU	C-N-CA	5.14	131.48	121.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2386	2376	2386	19	1
1	B	2383	2356	2358	23	0
1	C	2352	2333	2340	22	0
1	D	2287	2199	2198	21	1
2	A	26	36	36	1	0
3	A	12	16	16	0	0
3	B	6	8	8	1	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
4	A	16	24	24	0	0
4	B	16	24	24	0	0
4	C	24	36	36	0	0
4	D	4	6	6	0	0
5	A	58	0	0	1	0
5	B	60	0	0	0	0
5	C	39	0	0	2	0
5	D	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9711	9430	9448	84	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:SER:H	1:A:199:LEU:HD21	1.49	0.75
1:C:158:SER:HB3	1:C:171:VAL:HG13	1.80	0.64
1:A:128:VAL:HG22	1:A:129:PRO:HD2	1.81	0.61
1:B:288:GLN:O	1:B:292:ARG:NH2	2.35	0.60
1:A:208:ARG:HG3	1:A:214:THR:HG22	1.83	0.60
2:A:405:PG4:H71	2:A:405:PG4:O3	2.02	0.59
1:C:223:MET:HE3	1:C:260:VAL:HG13	1.87	0.56
1:C:91:LEU:HD11	1:C:136:TYR:CZ	2.41	0.56
1:D:62:LEU:HD22	1:D:90:PHE:CZ	2.40	0.56
1:C:25:MET:HG2	1:C:35:VAL:HG11	1.89	0.55
1:A:244:TRP:CE3	1:A:247:LYS:HD2	2.43	0.54
1:A:187:SER:HA	1:A:199:LEU:HD21	1.88	0.54
1:C:236:LEU:HG	1:C:240:MET:HE2	1.90	0.53
1:C:160:ARG:NH1	5:C:802:HOH:O	2.38	0.53
1:B:75:ASN:ND2	1:B:104:GLN:OE1	2.41	0.53
1:C:91:LEU:HD11	1:C:136:TYR:CE2	2.44	0.53
1:B:236:LEU:HG	1:B:240:MET:HE2	1.92	0.51
1:A:188:SER:N	1:A:199:LEU:HD21	2.23	0.51
1:C:206:ARG:HG2	1:C:216:THR:HG22	1.92	0.51
1:B:91:LEU:HD12	1:B:132:LEU:HD22	1.92	0.51
1:B:87:ASP:OD2	1:B:89:SER:OG	2.29	0.50
1:D:207:MET:HE1	1:D:217:GLN:OE1	2.12	0.50
3:B:502:GOL:HO1	3:B:502:GOL:HO3	1.59	0.50
1:B:87:ASP:CG	1:B:89:SER:HG	2.19	0.50
1:D:95:VAL:CG2	1:D:140:VAL:HG22	2.42	0.50
1:A:187:SER:HA	1:A:199:LEU:CD2	2.41	0.49
1:C:268:GLN:O	1:C:271:ILE:HG22	2.12	0.49
1:B:211:ASP:OD1	1:B:211:ASP:N	2.42	0.49
1:A:7:VAL:HG22	1:A:79:TYR:HB2	1.93	0.49
1:A:46:HIS:CE1	1:A:231:VAL:HG21	2.47	0.49
1:B:131:ASP:N	1:B:131:ASP:OD1	2.46	0.48
1:B:88:LYS:HG3	1:B:135:VAL:HG21	1.95	0.47
1:C:158:SER:CB	1:C:171:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASP:OD2	1:C:89:SER:OG	2.33	0.47
1:A:88:LYS:HG3	1:A:135:VAL:HG21	1.96	0.47
1:C:63:HIS:HB2	1:C:93:MET:SD	2.55	0.47
1:A:236:LEU:HG	1:A:240:MET:HE2	1.97	0.47
1:C:242:LEU:C	1:C:242:LEU:HD23	2.40	0.47
1:C:36:ASP:HA	1:D:15:VAL:O	2.15	0.47
1:B:242:LEU:HD23	1:B:242:LEU:C	2.41	0.46
1:D:269:ARG:NH2	1:D:299:ASP:OD2	2.48	0.46
1:D:27:PRO:O	1:D:30:VAL:HG22	2.15	0.46
1:D:236:LEU:HD22	1:D:293:MET:HE1	1.97	0.46
1:A:128:VAL:HG22	1:A:132:LEU:HD22	1.98	0.46
1:C:93:MET:HE2	1:C:93:MET:HB2	1.88	0.46
1:D:87:ASP:OD1	1:D:89:SER:OG	2.28	0.45
1:D:169:PHE:CD1	1:D:218:ARG:HD3	2.52	0.45
1:D:242:LEU:C	1:D:242:LEU:HD23	2.42	0.45
1:B:84:TYR:OH	1:B:86:ARG:HD2	2.17	0.44
1:B:62:LEU:HD23	1:B:93:MET:HG2	2.00	0.44
1:D:221:MET:HE3	1:D:221:MET:HB2	1.83	0.44
1:A:272:ARG:NH1	5:A:505:HOH:O	2.45	0.44
1:D:77:TYR:O	1:D:108:LEU:HD12	2.18	0.44
1:B:152:PHE:CE2	1:B:156:LEU:HD11	2.54	0.43
1:D:158:SER:HB3	1:D:171:VAL:HG13	2.00	0.43
1:B:229:VAL:O	1:B:229:VAL:HG13	2.19	0.43
1:A:34:GLU:OE1	1:B:18:TYR:OH	2.27	0.43
1:D:237:PHE:HB2	1:D:263:MET:HE3	2.01	0.43
1:D:27:PRO:HA	1:D:30:VAL:HG22	2.01	0.42
1:D:93:MET:HE2	1:D:93:MET:HB2	1.86	0.42
1:A:242:LEU:C	1:A:242:LEU:HD23	2.45	0.42
1:A:226:VAL:O	1:A:226:VAL:HG23	2.20	0.42
1:A:27:PRO:HA	1:A:30:VAL:HG22	2.01	0.42
1:A:27:PRO:O	1:A:30:VAL:HG22	2.19	0.42
1:C:62:LEU:HD22	1:C:90:PHE:CZ	2.55	0.42
1:C:133:LEU:HD22	1:C:156:LEU:HD22	2.02	0.42
1:B:25:MET:CE	1:B:37:ALA:HB2	2.50	0.41
1:B:112:CYS:O	1:B:147:ILE:HA	2.20	0.41
1:D:7:VAL:HG22	1:D:79:TYR:HB2	2.01	0.41
1:D:26:PHE:HB3	1:D:27:PRO:HD3	2.02	0.41
1:B:12:SER:HB2	1:B:41:VAL:HG22	2.02	0.41
1:C:66:TYR:CE1	1:C:97:ILE:HG23	2.56	0.41
1:D:133:LEU:HD12	1:D:133:LEU:O	2.20	0.41
1:A:221:MET:SD	1:A:256:CYS:HB3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:PRO:HB2	1:C:131:ASP:OD1	2.20	0.41
1:B:260:VAL:HG12	1:B:307:VAL:HG21	2.01	0.41
1:C:165:GLN:OE1	1:C:220:ARG:NH1	2.54	0.41
1:B:260:VAL:CG1	1:B:307:VAL:HG21	2.51	0.41
1:B:91:LEU:HD11	1:B:136:TYR:CZ	2.56	0.40
1:B:91:LEU:HD11	1:B:136:TYR:CE2	2.56	0.40
1:D:131:ASP:N	1:D:131:ASP:OD1	2.54	0.40
1:B:52:TRP:CZ3	1:C:195:GLY:HA2	2.57	0.40
1:C:6:ARG:NH2	5:C:801:HOH:O	2.35	0.40
1:D:216:THR:HG21	1:D:218:ARG:CZ	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASP:OD2	1:D:53:LYS:CE[1_554]	2.08	0.12

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	301/314 (96%)	290 (96%)	11 (4%)	0	100	100
1	B	304/314 (97%)	294 (97%)	10 (3%)	0	100	100
1	C	296/314 (94%)	287 (97%)	9 (3%)	0	100	100
1	D	298/314 (95%)	288 (97%)	10 (3%)	0	100	100
All	All	1199/1256 (96%)	1159 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/273 (97%)	263 (99%)	2 (1%)	73	83
1	B	261/273 (96%)	256 (98%)	5 (2%)	50	64
1	C	259/273 (95%)	255 (98%)	4 (2%)	57	70
1	D	245/273 (90%)	241 (98%)	4 (2%)	55	69
All	All	1030/1092 (94%)	1015 (98%)	15 (2%)	57	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	SER
1	A	227	GLU
1	B	131	ASP
1	B	187	SER
1	B	211	ASP
1	B	268	GLN
1	B	293	MET
1	C	45	ASN
1	C	127	TYR
1	C	211	ASP
1	C	226	VAL
1	D	4	GLU
1	D	128	VAL
1	D	207	MET
1	D	229	VAL

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	11	GLN
1	B	60	GLN
1	B	75	ASN
1	B	104	GLN

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Mol	Chain	Res	Type
1	B	308	GLN
1	C	11	GLN
1	C	29	GLN
1	C	51	HIS
1	C	105	ASN
1	C	194	GLN
1	D	282	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	C	706	-	3,3,3	0.39	0	2,2,2	0.57	0
2	PG4	A	401	-	12,12,12	0.53	0	11,11,11	0.37	0
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.31	0
4	EDO	C	704	-	3,3,3	0.44	0	2,2,2	0.33	0
3	GOL	C	701	-	5,5,5	0.86	0	5,5,5	1.04	0
4	EDO	A	403	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	B	501	-	3,3,3	0.43	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	408	-	3,3,3	0.46	0	2,2,2	0.27	0
4	EDO	C	702	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	D	402	-	3,3,3	0.44	0	2,2,2	0.31	0
4	EDO	A	404	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	C	703	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.31	0
3	GOL	A	402	-	5,5,5	0.88	0	5,5,5	1.07	0
4	EDO	A	407	-	3,3,3	0.42	0	2,2,2	0.45	0
3	GOL	D	401	-	5,5,5	0.84	0	5,5,5	1.07	0
2	PG4	A	405	-	12,12,12	0.38	0	11,11,11	0.61	0
4	EDO	C	707	-	3,3,3	0.39	0	2,2,2	0.43	0
4	EDO	B	504	-	3,3,3	0.44	0	2,2,2	0.35	0
3	GOL	A	406	-	5,5,5	0.85	0	5,5,5	1.00	0
4	EDO	C	705	-	3,3,3	0.38	0	2,2,2	0.50	0
3	GOL	B	502	-	5,5,5	0.85	0	5,5,5	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	706	-	-	1/1/1/1	-
2	PG4	A	401	-	-	3/10/10/10	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	C	704	-	-	0/1/1/1	-
3	GOL	C	701	-	-	1/4/4/4	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	B	501	-	-	0/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
4	EDO	C	702	-	-	0/1/1/1	-
4	EDO	D	402	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	C	703	-	-	0/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
3	GOL	A	402	-	-	2/4/4/4	-
4	EDO	A	407	-	-	0/1/1/1	-
3	GOL	D	401	-	-	1/4/4/4	-
2	PG4	A	405	-	-	5/10/10/10	-
4	EDO	C	707	-	-	0/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
3	GOL	A	406	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	705	-	-	0/1/1/1	-
3	GOL	B	502	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	406	GOL	O1-C1-C2-C3
2	A	401	PG4	O2-C3-C4-O3
2	A	405	PG4	O2-C3-C4-O3
3	A	402	GOL	O1-C1-C2-C3
2	A	401	PG4	O4-C7-C8-O5
2	A	405	PG4	O4-C7-C8-O5
3	A	406	GOL	O1-C1-C2-O2
3	D	401	GOL	O2-C2-C3-O3
2	A	405	PG4	C8-C7-O4-C6
2	A	405	PG4	C4-C3-O2-C2
2	A	401	PG4	C5-C6-O4-C7
3	A	402	GOL	O1-C1-C2-O2
2	A	405	PG4	C5-C6-O4-C7
3	C	701	GOL	O2-C2-C3-O3
4	C	706	EDO	O1-C1-C2-O2

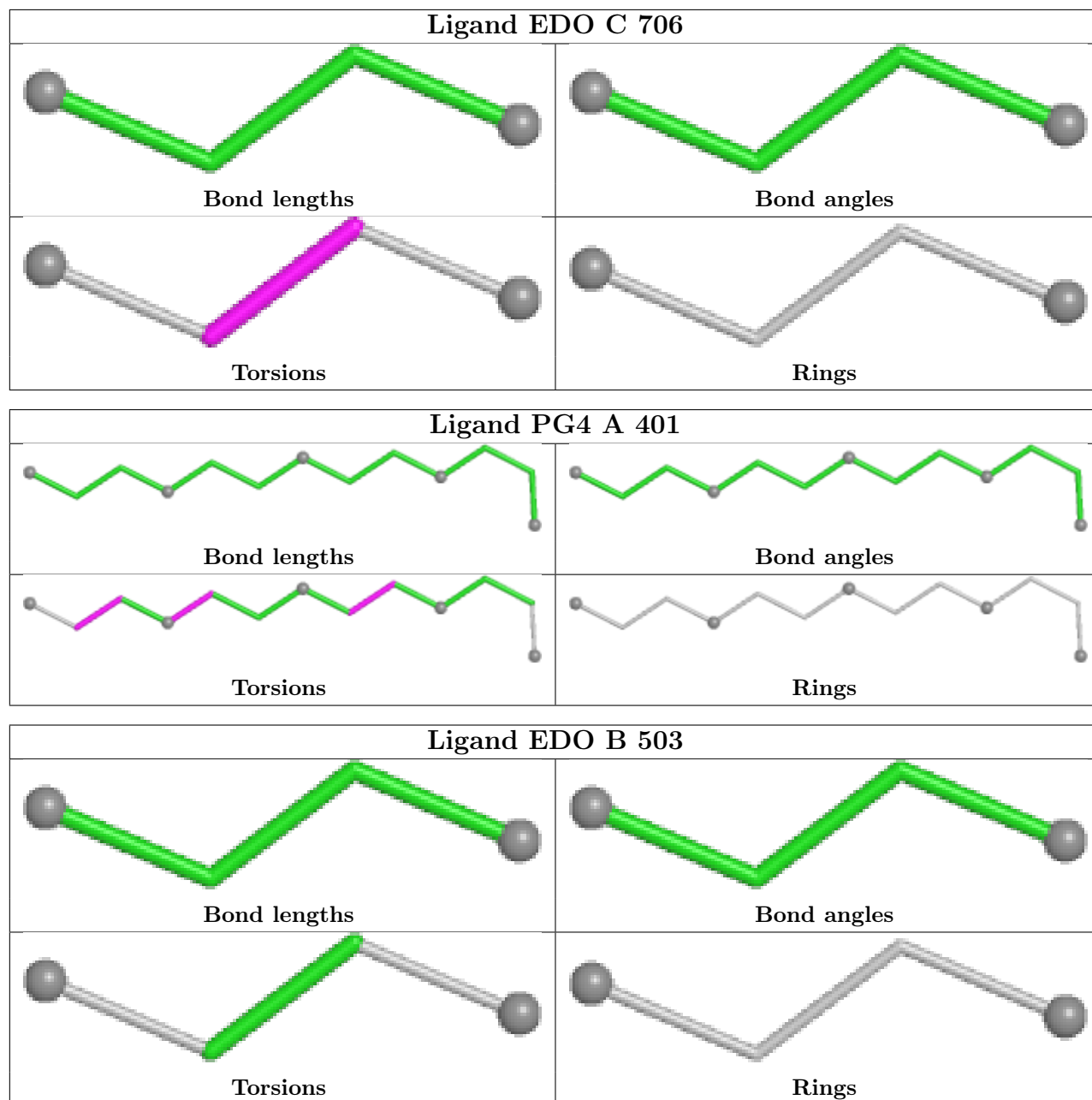
There are no ring outliers.

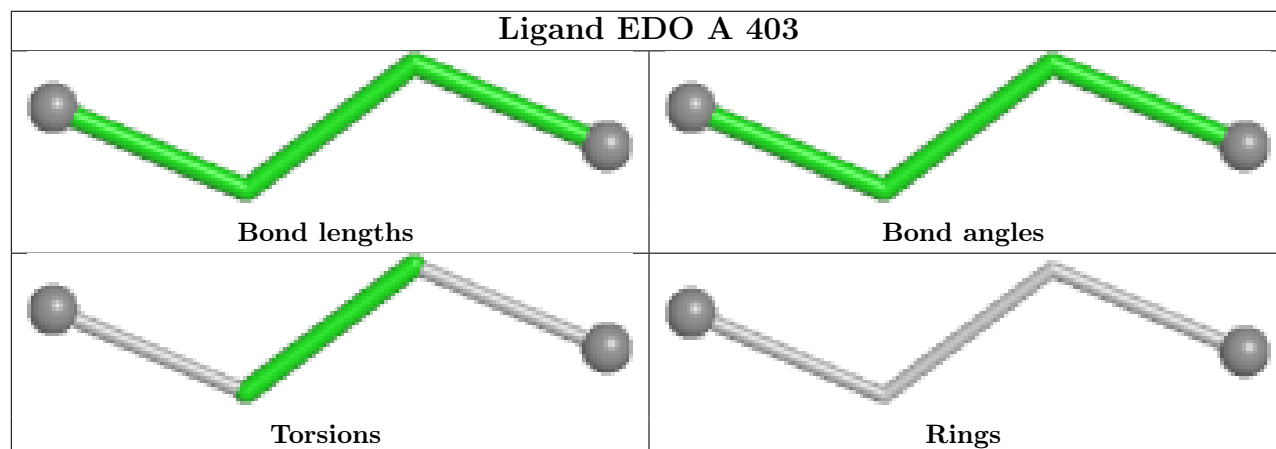
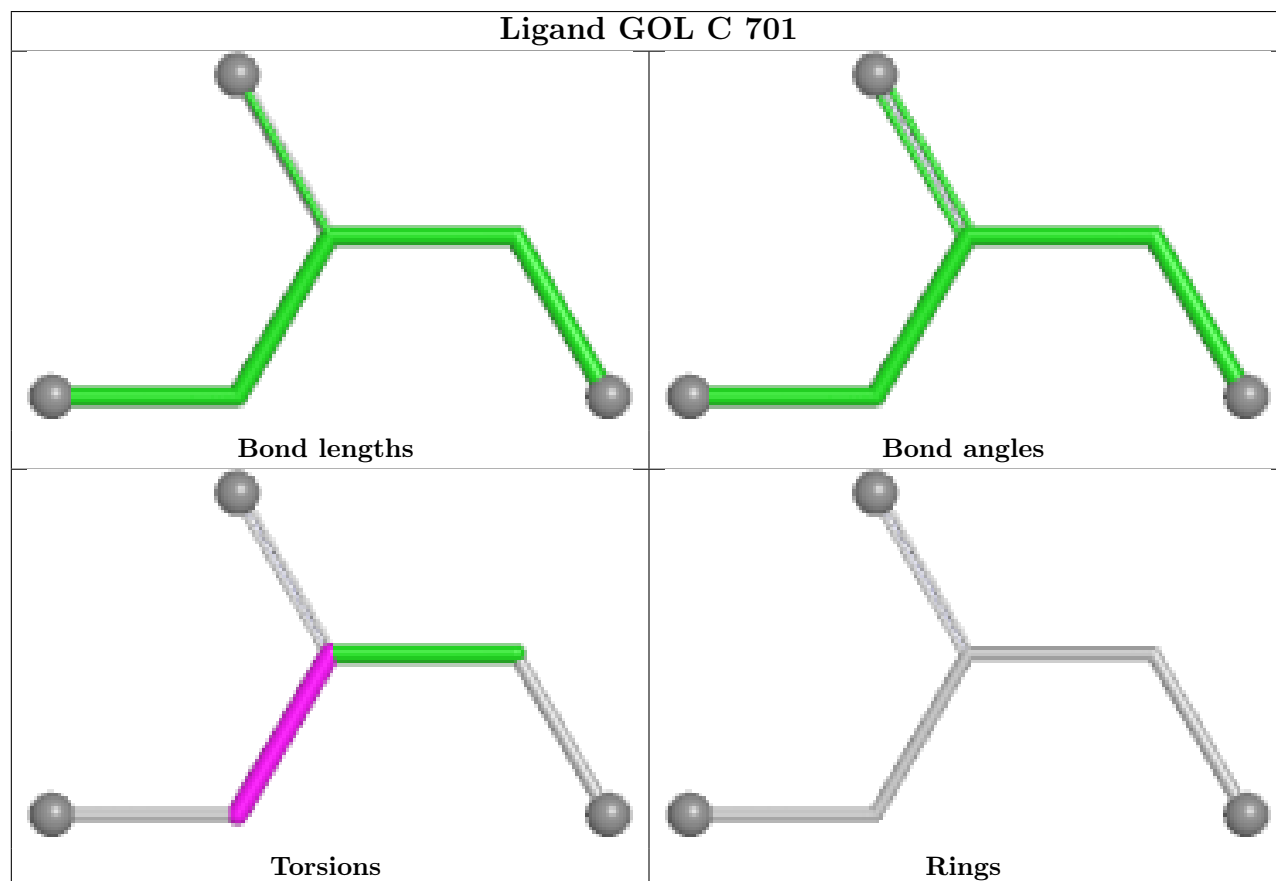
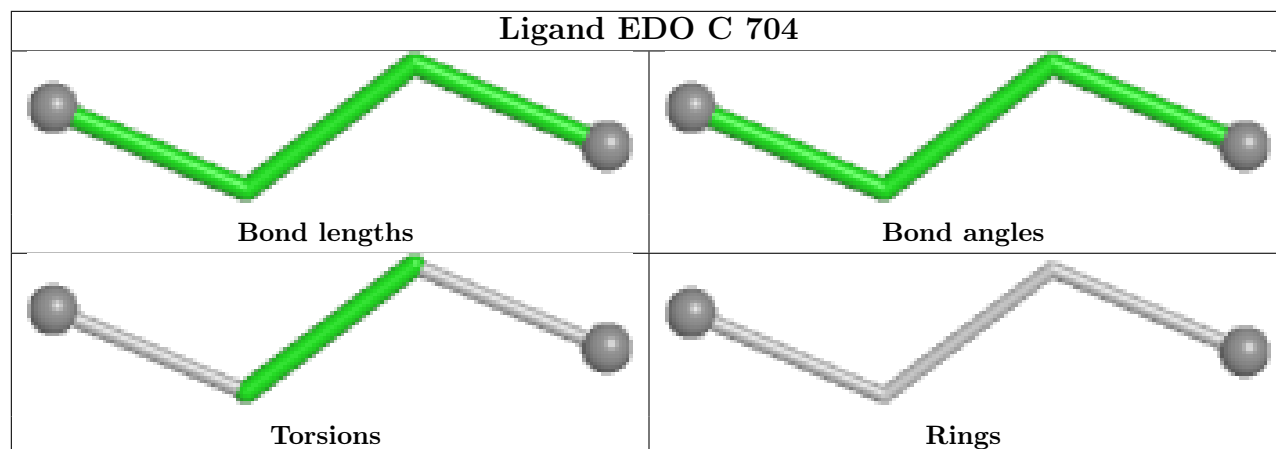
2 monomers are involved in 2 short contacts:

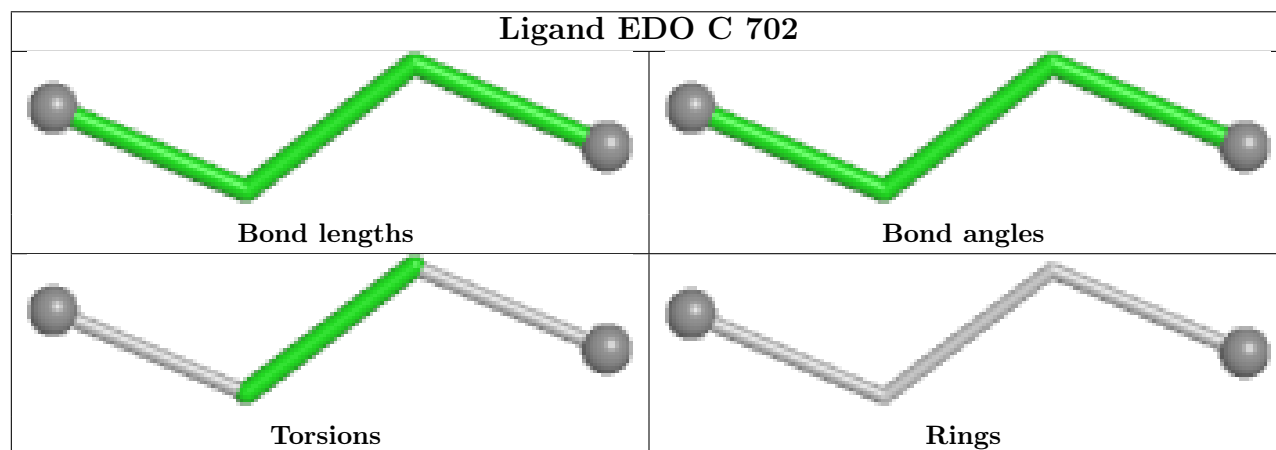
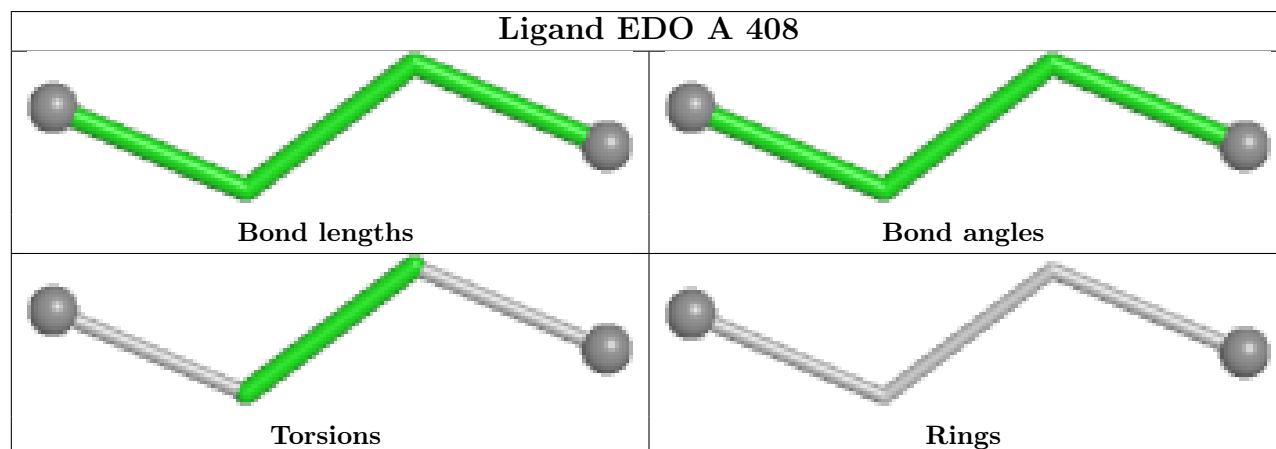
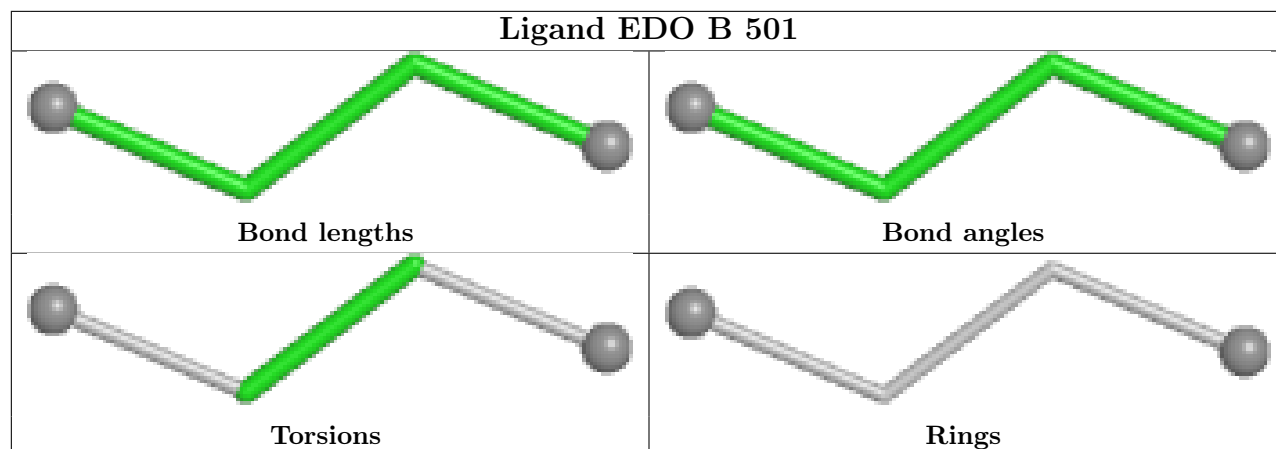
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	PG4	1	0
3	B	502	GOL	1	0

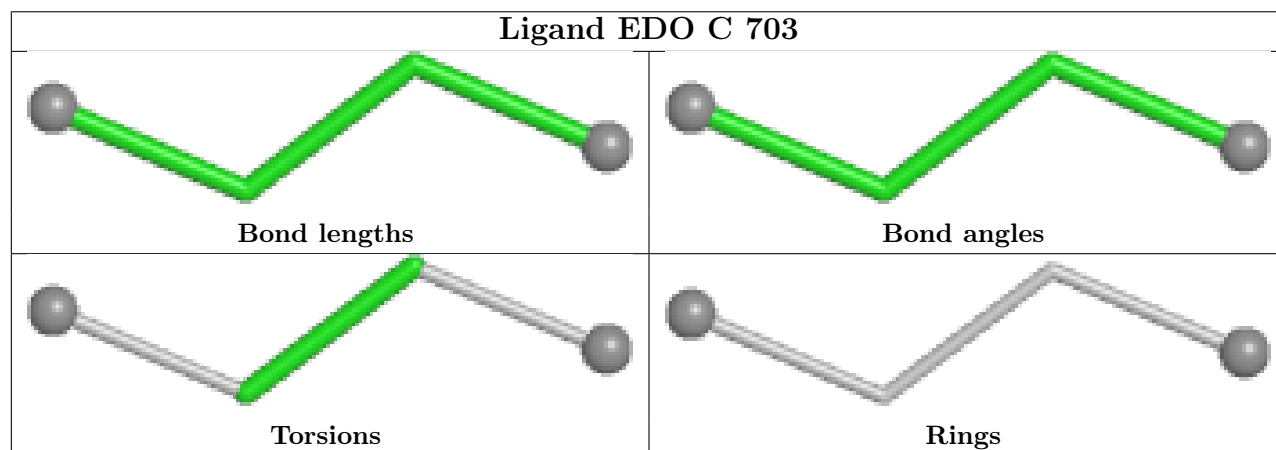
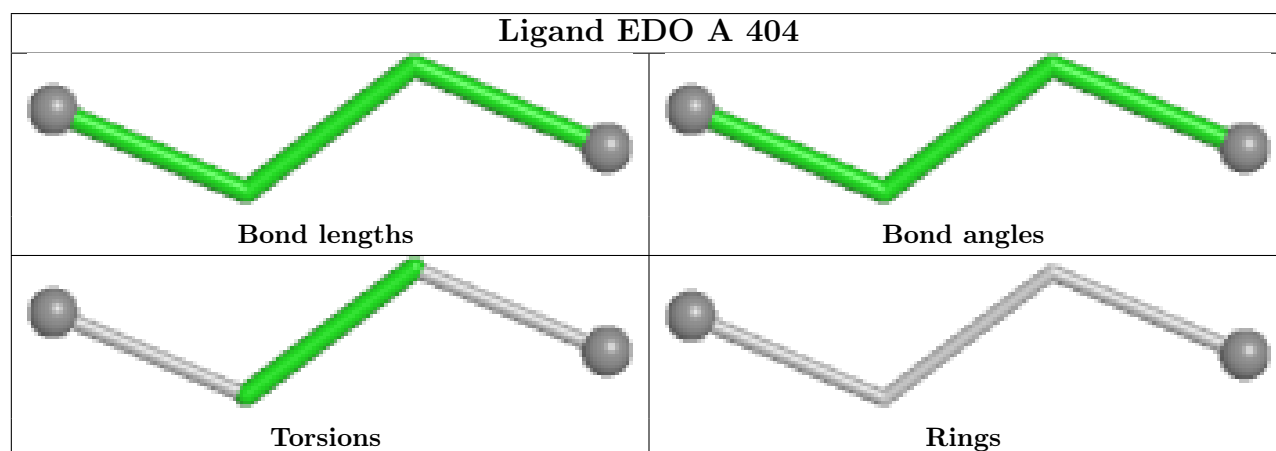
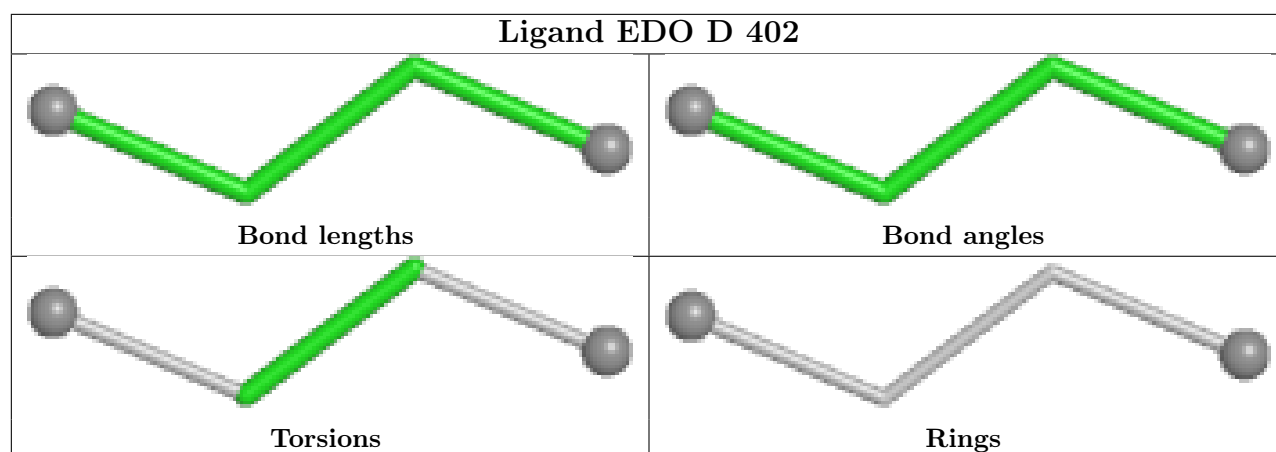
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

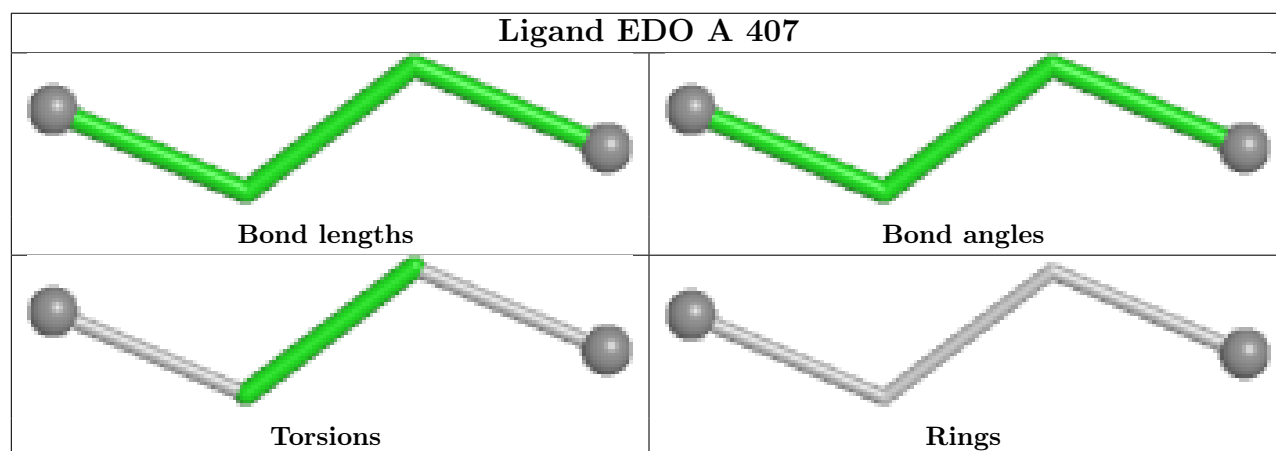
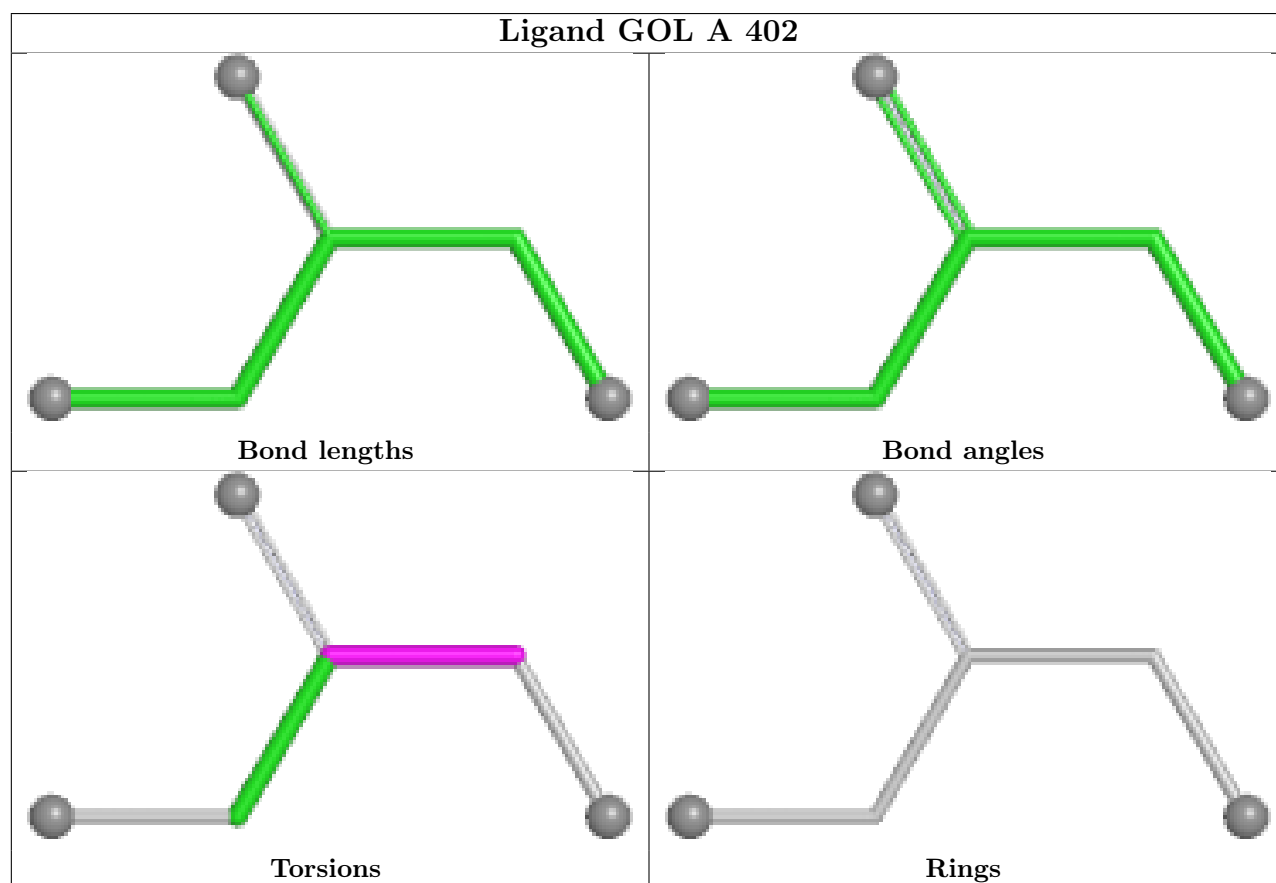
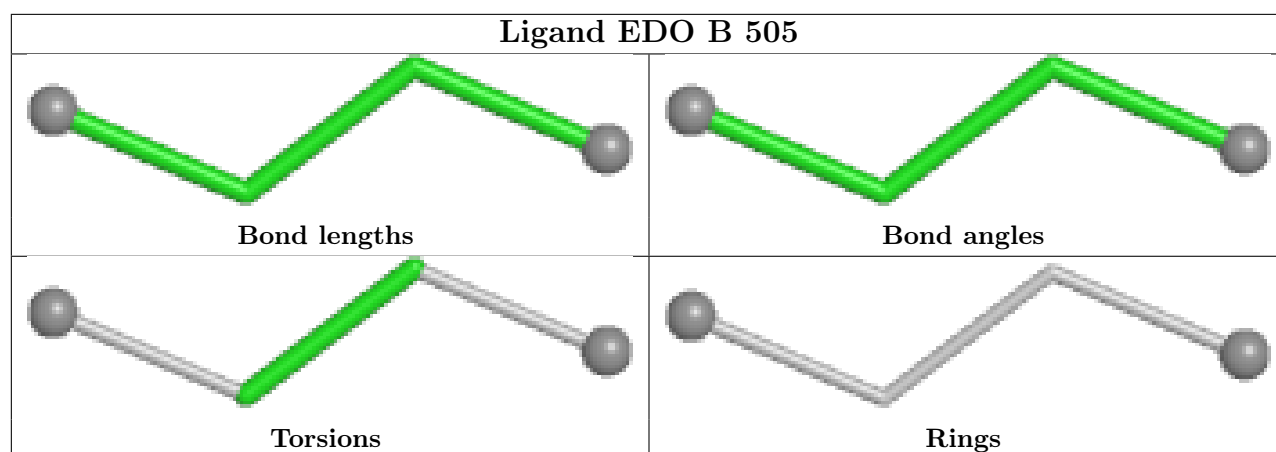
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

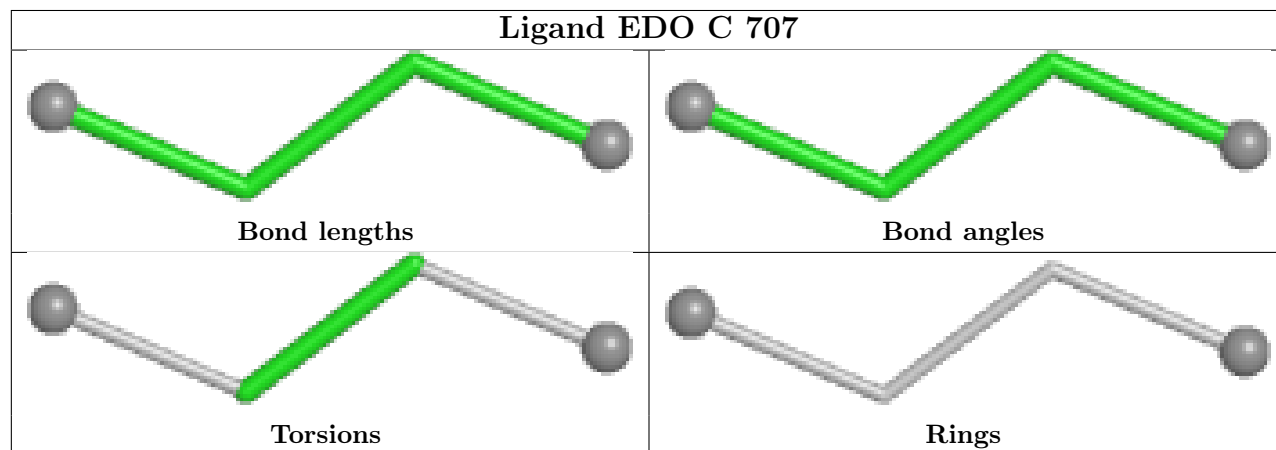
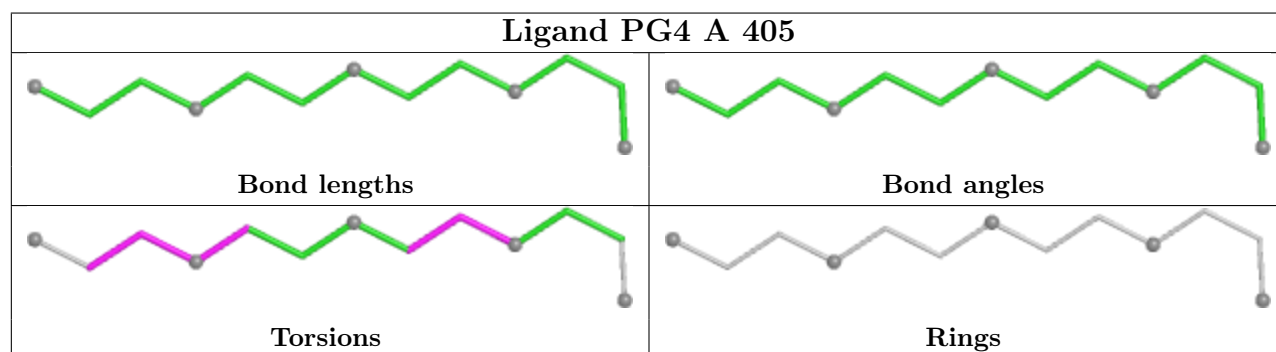
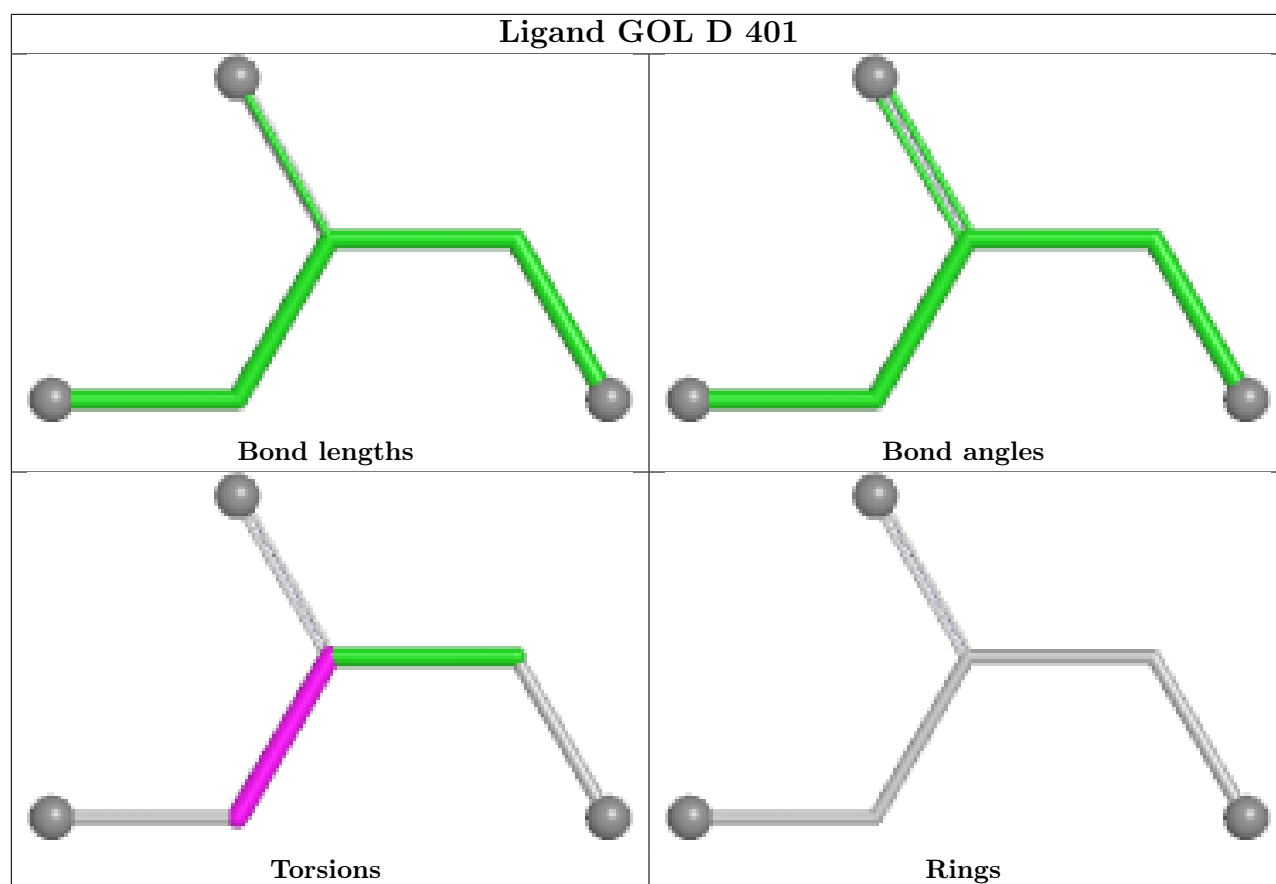


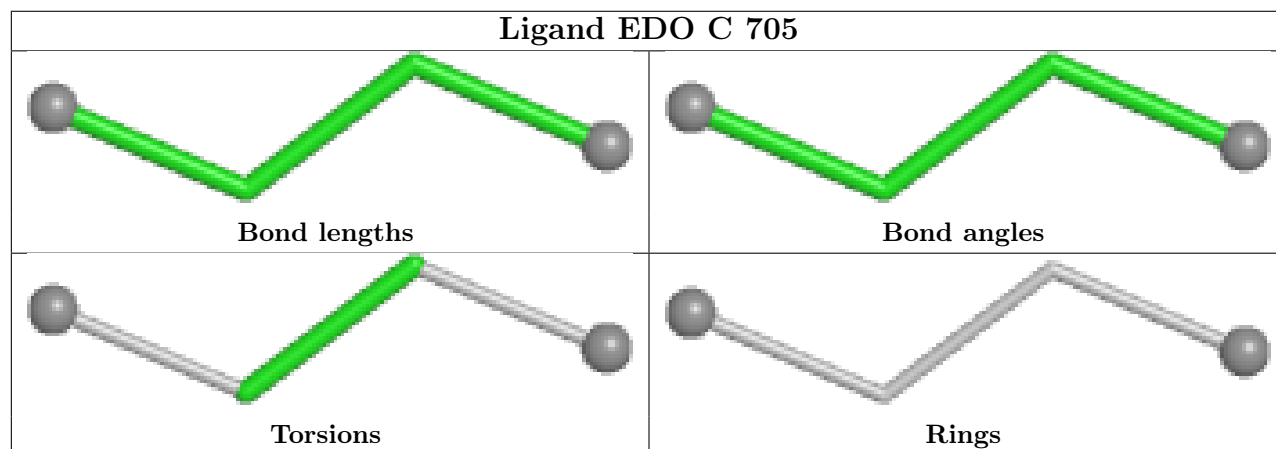
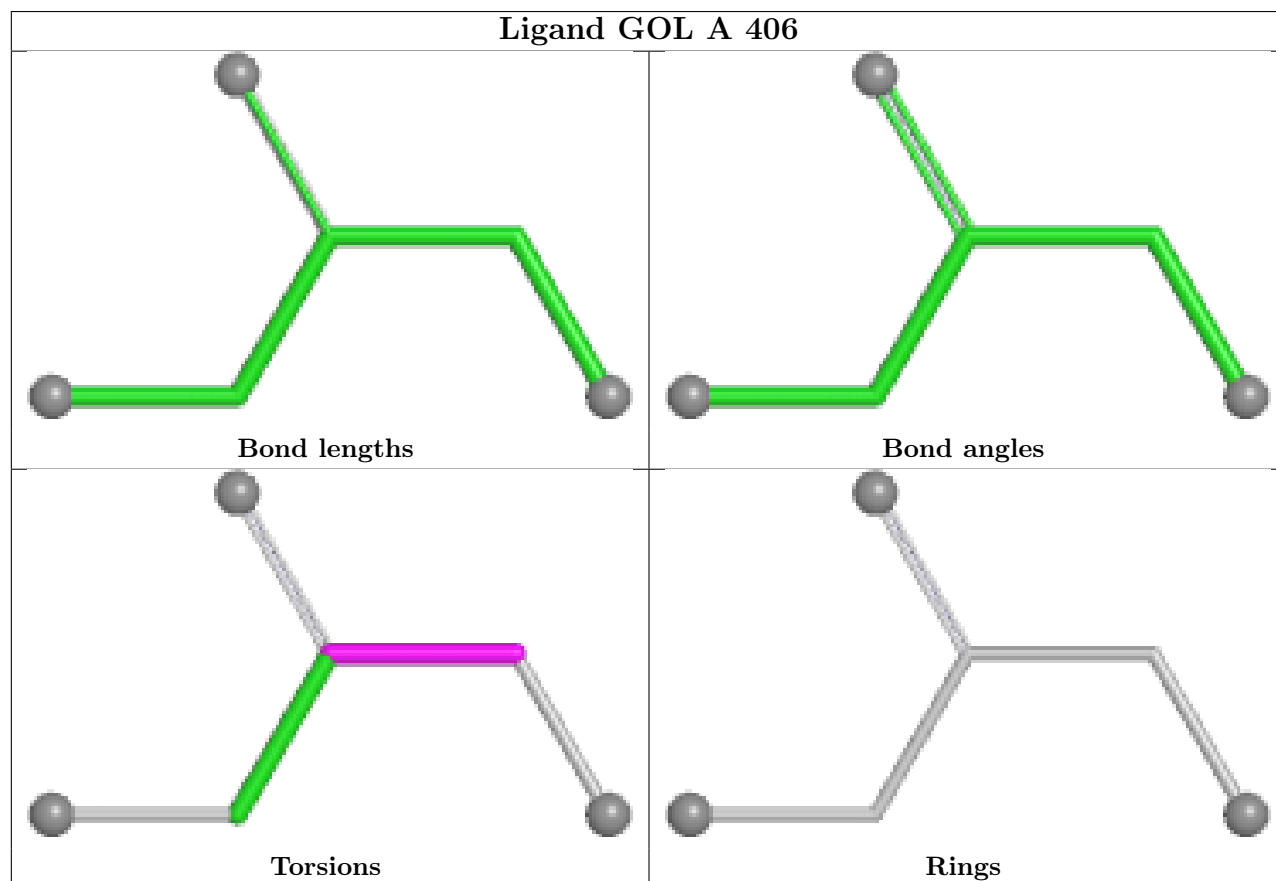
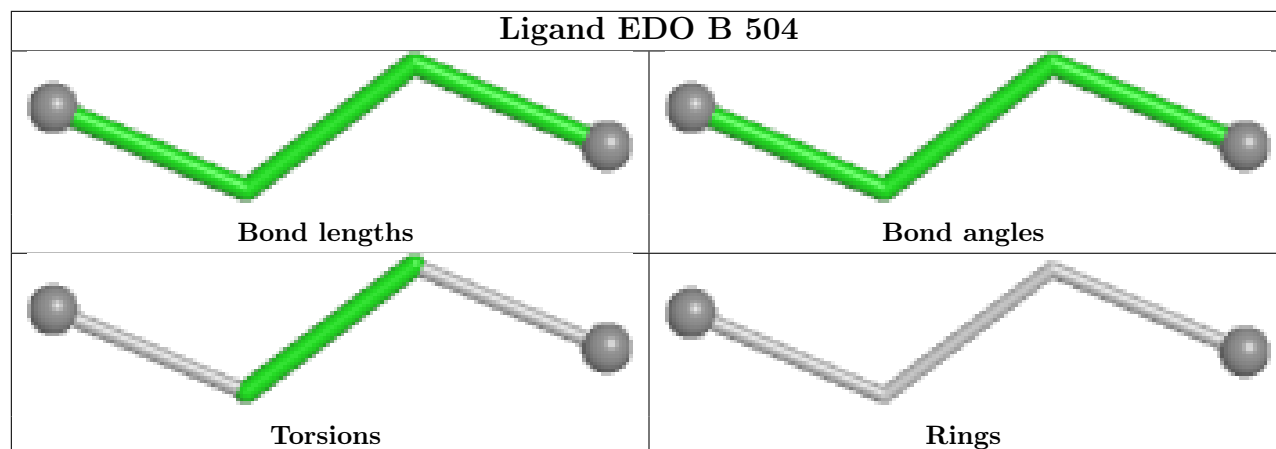


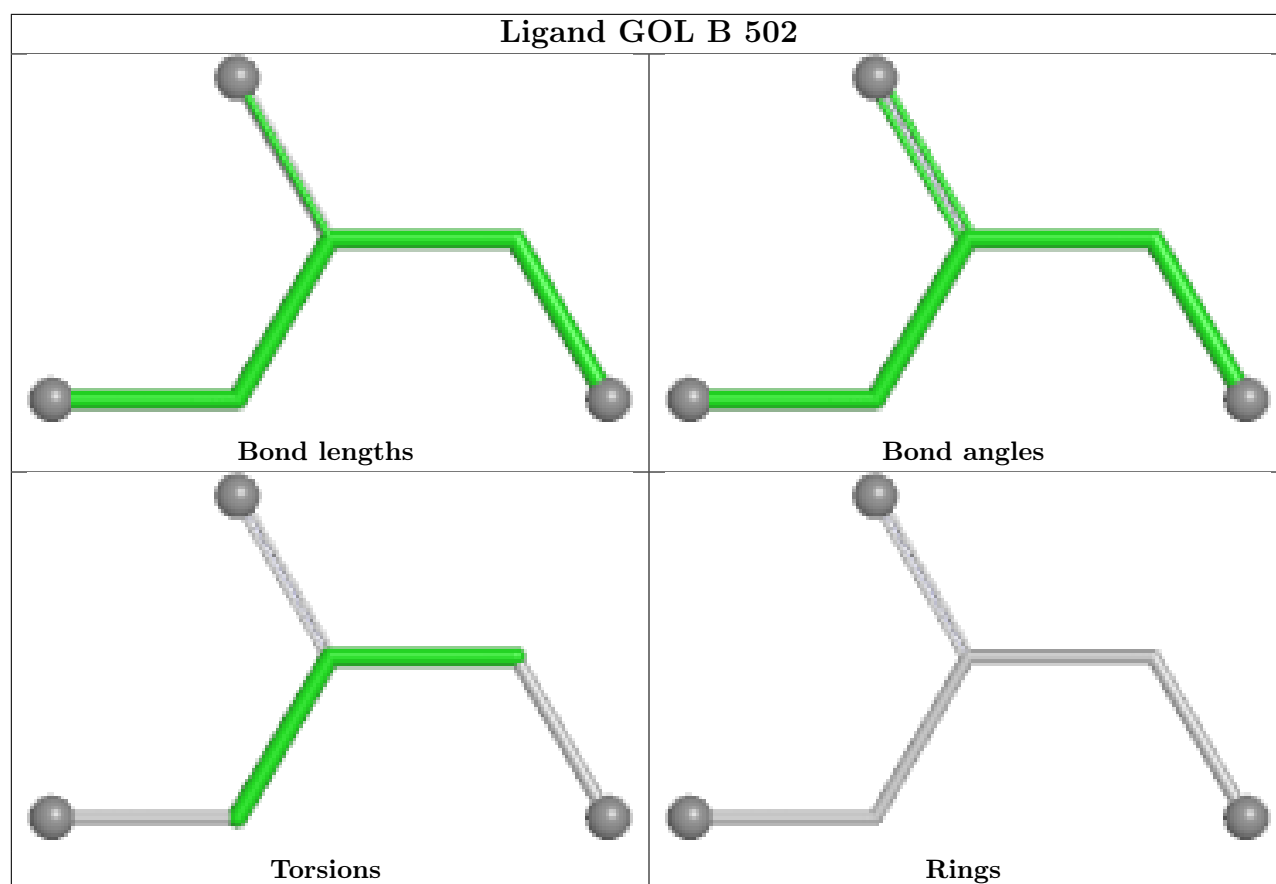












5.7 Other polymers [i](#)

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	304/314 (96%)	0.29	11 (3%)	46 46	36, 55, 89, 125	1 (0%)
1	B	308/314 (98%)	0.33	15 (4%)	35 33	35, 53, 94, 138	0
1	C	302/314 (96%)	0.48	18 (5%)	27 24	43, 62, 87, 103	0
1	D	302/314 (96%)	0.80	25 (8%)	17 15	44, 68, 110, 133	0
All	All	1216/1256 (96%)	0.47	69 (5%)	29 26	35, 60, 98, 138	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	ASN	5.8
1	D	127	TYR	5.6
1	B	123	GLU	4.8
1	B	120	TRP	4.6
1	A	209	LYS	4.4
1	C	4	GLU	4.3
1	B	210	PRO	4.1
1	D	86	ARG	4.0
1	A	226	VAL	3.6
1	D	196	SER	3.6
1	D	198	TYR	3.6
1	B	279	GLY	3.6
1	C	125	SER	3.5
1	B	280	GLU	3.5
1	D	119	LYS	3.5
1	C	223	MET	3.3
1	B	212	GLY	3.3
1	A	119	LYS	3.3
1	A	210	PRO	3.3
1	D	224	ARG	3.3
1	D	225	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	215	VAL	3.1
1	A	126	MET	3.1
1	D	210	PRO	3.1
1	C	227	GLU	3.1
1	D	195	GLY	3.0
1	C	158	SER	3.0
1	A	211	ASP	3.0
1	B	119	LYS	2.9
1	B	281	GLY	2.9
1	C	45	ASN	2.8
1	D	199	LEU	2.8
1	C	215	VAL	2.6
1	A	214	THR	2.6
1	C	86	ARG	2.6
1	D	104	GLN	2.6
1	C	52	TRP	2.5
1	C	208	ARG	2.5
1	D	206	ARG	2.5
1	D	4	GLU	2.5
1	D	211	ASP	2.5
1	D	200	ILE	2.5
1	A	125	SER	2.5
1	D	281	GLY	2.5
1	B	195	GLY	2.4
1	B	208	ARG	2.4
1	D	310	THR	2.4
1	C	47	THR	2.4
1	D	279	GLY	2.4
1	D	223	MET	2.4
1	B	226	VAL	2.4
1	C	271	ILE	2.3
1	B	86	ARG	2.3
1	C	211	ASP	2.3
1	C	127	TYR	2.3
1	D	209	LYS	2.3
1	C	226	VAL	2.3
1	B	213	SER	2.3
1	D	139	LYS	2.3
1	C	56	VAL	2.2
1	D	307	VAL	2.2
1	B	311	VAL	2.2
1	A	247	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	2.1
1	D	230	PHE	2.1
1	A	312	LEU	2.1
1	C	189	ASP	2.1
1	C	97	ILE	2.0
1	D	84	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

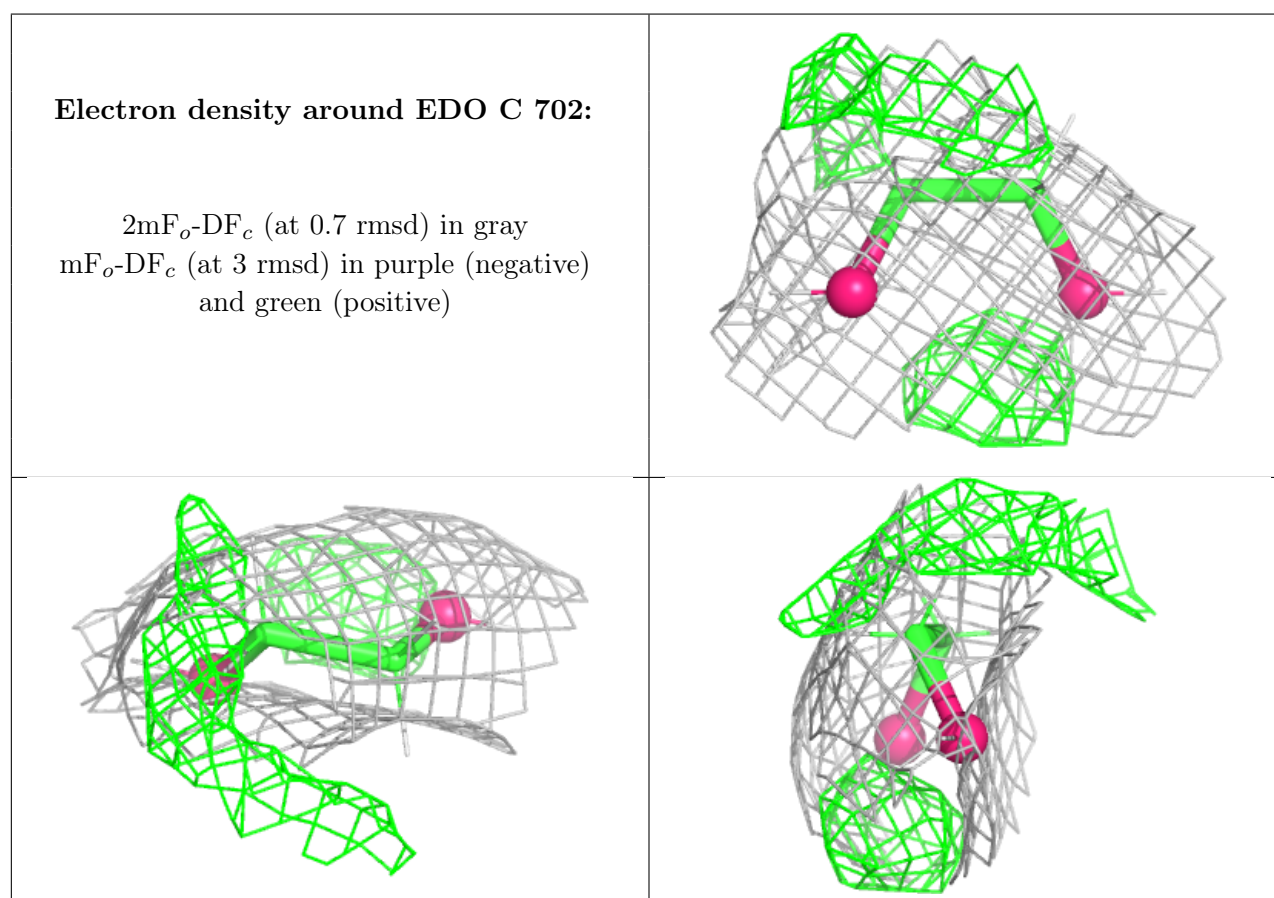
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	C	702	4/4	0.69	0.32	84,102,109,112	0
4	EDO	C	705	4/4	0.72	0.24	87,105,123,148	0
2	PG4	A	405	13/13	0.73	0.23	63,89,107,113	0
4	EDO	B	503	4/4	0.75	0.17	56,68,79,96	0
2	PG4	A	401	13/13	0.76	0.21	65,80,90,92	0
3	GOL	A	406	6/6	0.77	0.16	67,80,94,94	0
4	EDO	A	407	4/4	0.78	0.21	63,76,89,89	0
3	GOL	D	401	6/6	0.79	0.14	62,80,92,100	0
4	EDO	C	707	4/4	0.79	0.32	101,121,126,135	0
4	EDO	C	706	4/4	0.80	0.37	82,110,128,152	0
3	GOL	A	402	6/6	0.82	0.15	65,78,82,85	0
4	EDO	B	501	4/4	0.83	0.13	59,73,82,88	0
4	EDO	A	403	4/4	0.83	0.28	81,97,105,105	0
4	EDO	C	703	4/4	0.85	0.13	73,88,100,100	0
4	EDO	B	505	4/4	0.85	0.20	44,64,77,77	0
4	EDO	A	404	4/4	0.86	0.18	57,69,76,76	0
4	EDO	D	402	4/4	0.87	0.17	63,76,89,89	0

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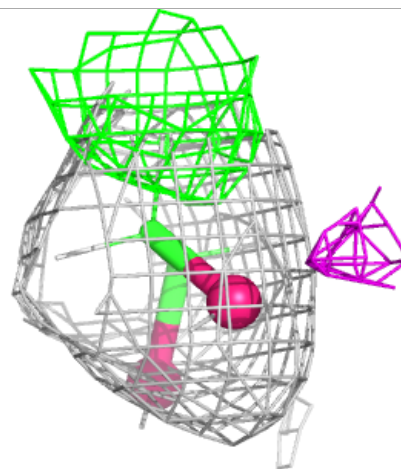
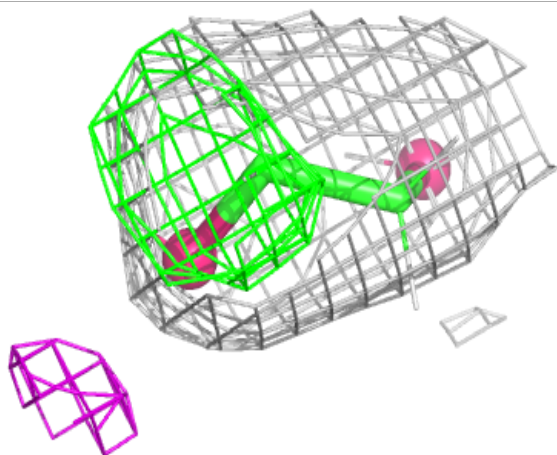
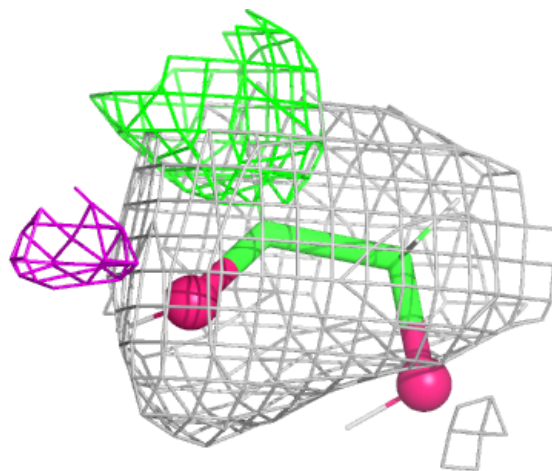
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	502	6/6	0.88	0.15	61,75,91,109	0
4	EDO	C	704	4/4	0.89	0.16	64,78,90,90	0
4	EDO	A	408	4/4	0.90	0.13	38,52,58,63	0
4	EDO	B	504	4/4	0.90	0.17	65,78,85,85	0
3	GOL	C	701	6/6	0.91	0.11	67,81,99,99	0

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.



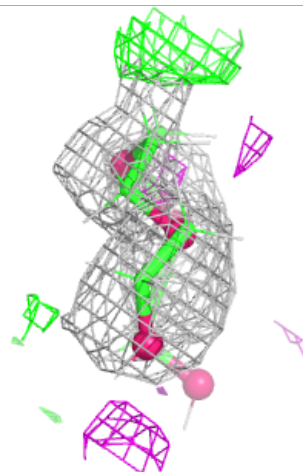
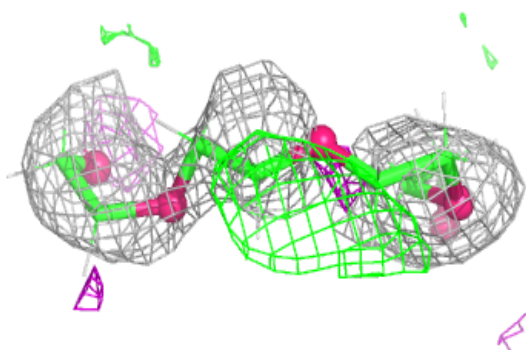
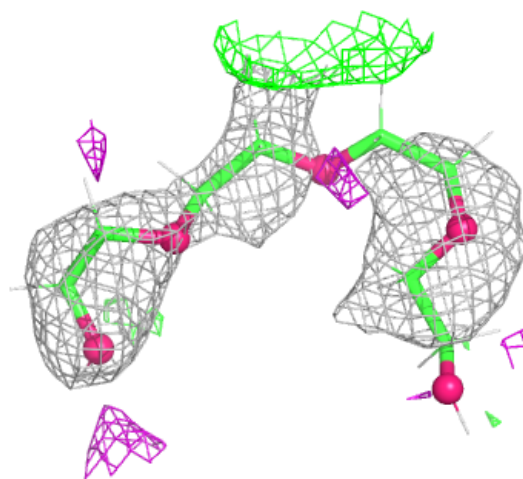
Electron density around EDO C 705:

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



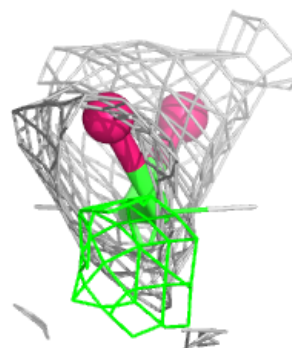
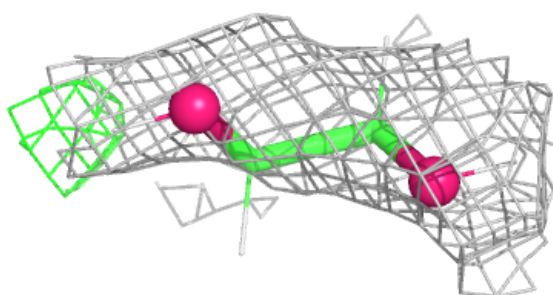
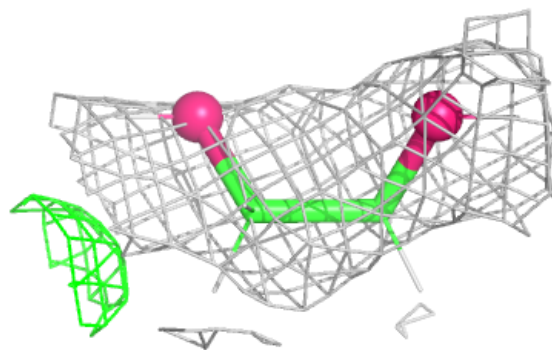
Electron density around PG4 A 405:

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

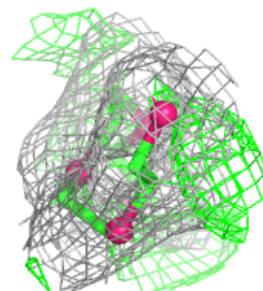
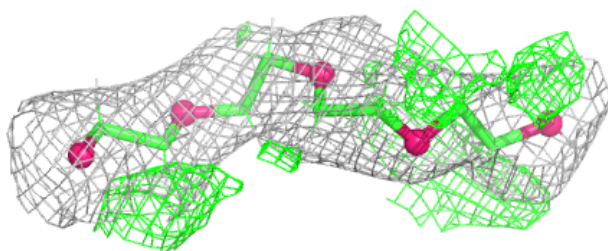
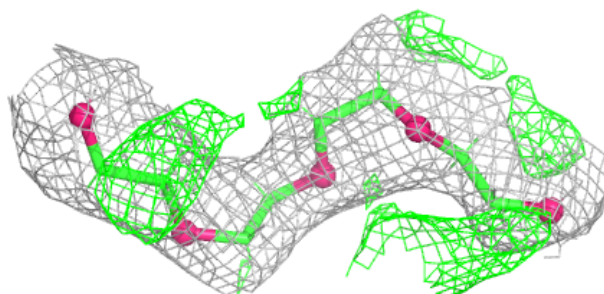


Electron density around EDO B 503:

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

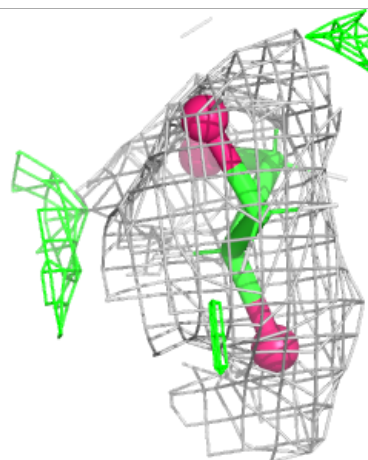
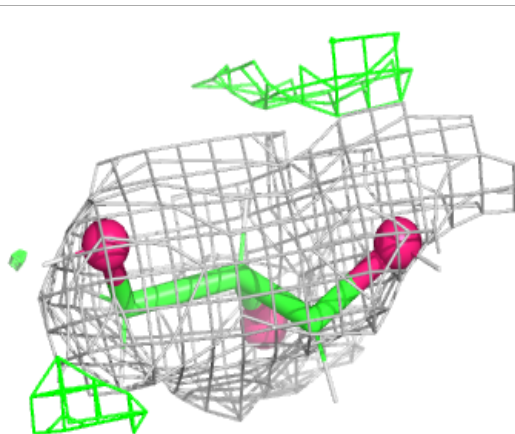
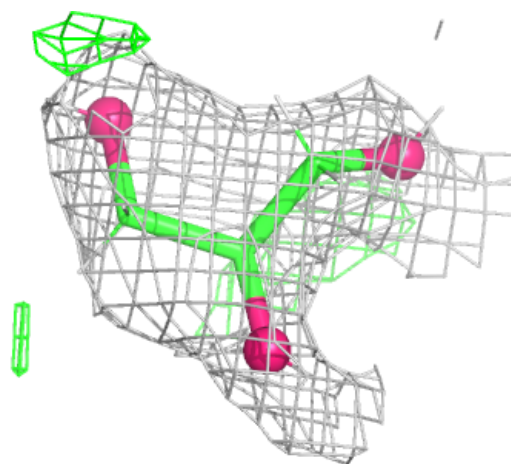
**Electron density around PG4 A 401:**

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



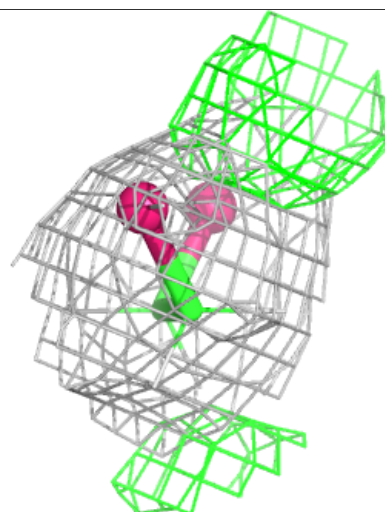
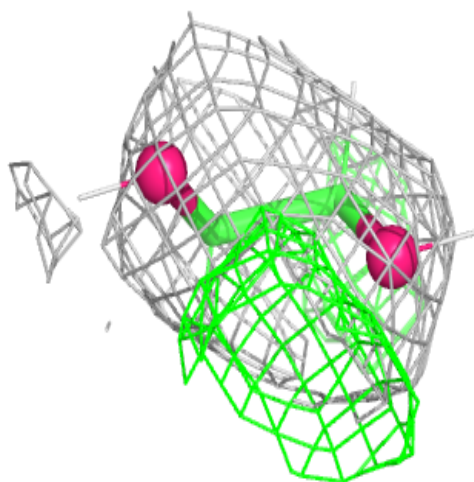
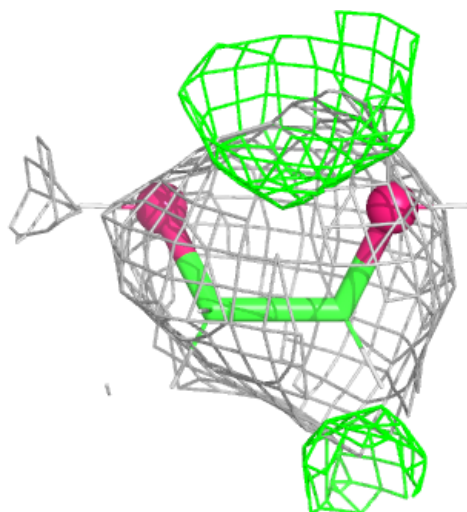
Electron density around GOL A 406:

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



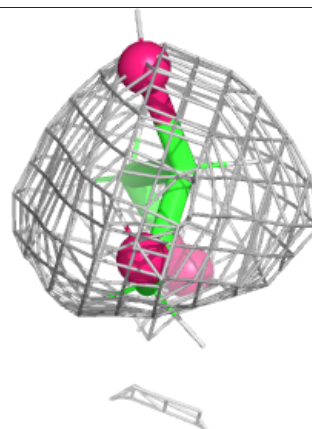
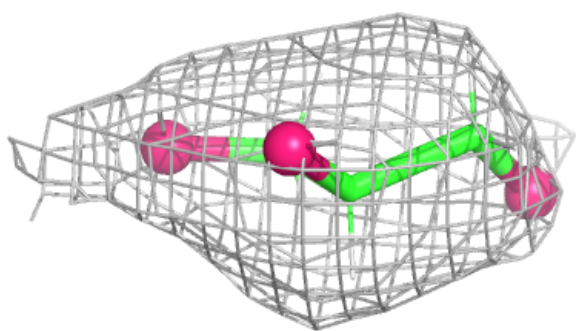
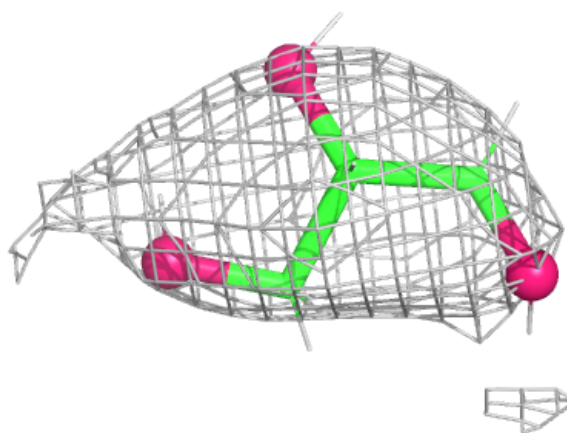
Electron density around EDO A 407:

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

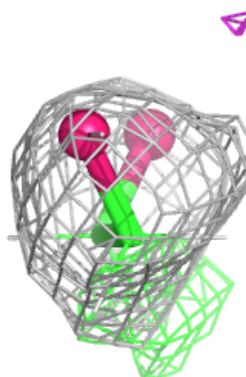
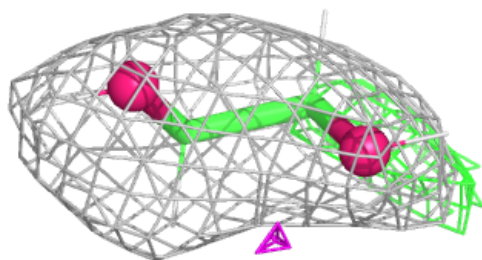
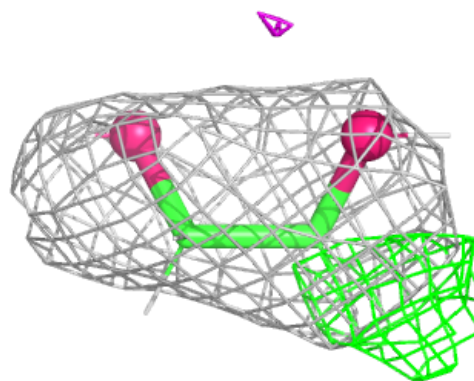


Electron density around GOL D 401:

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

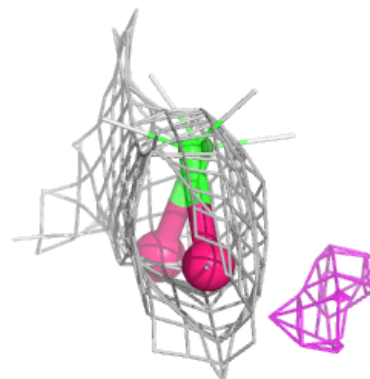
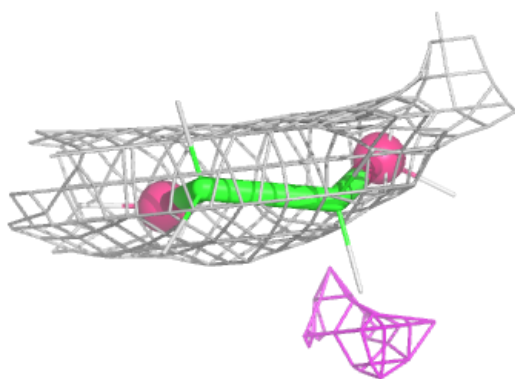
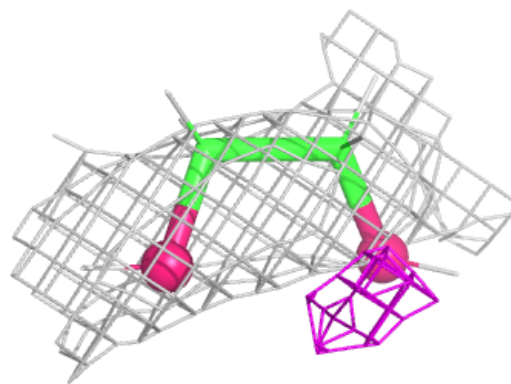
**Electron density around EDO C 707:**

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



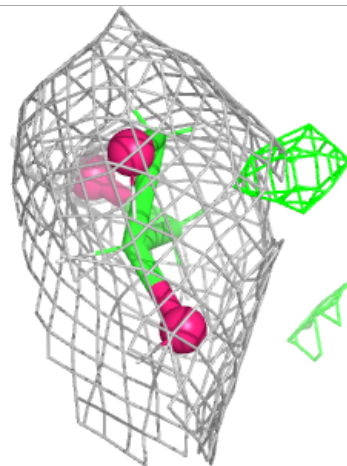
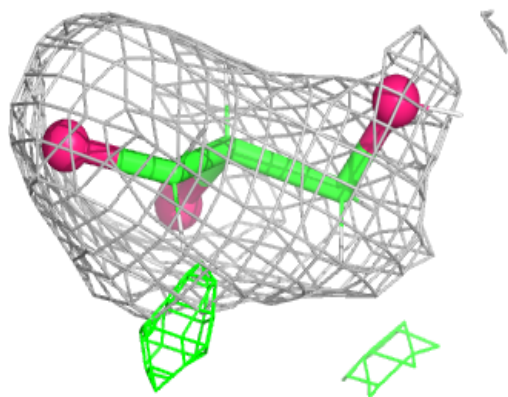
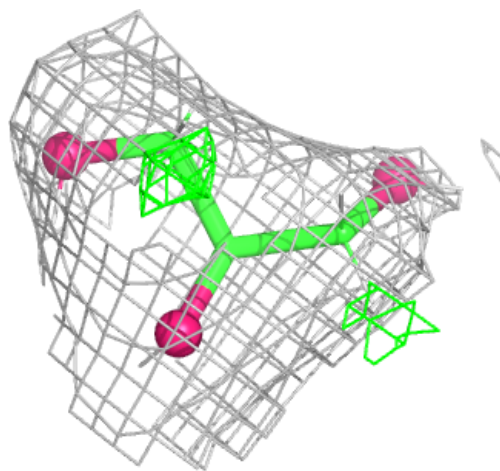
Electron density around EDO C 706:

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



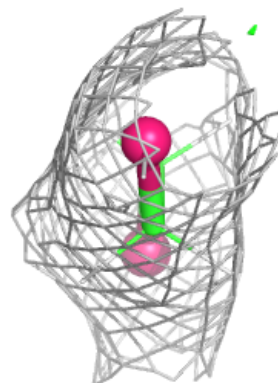
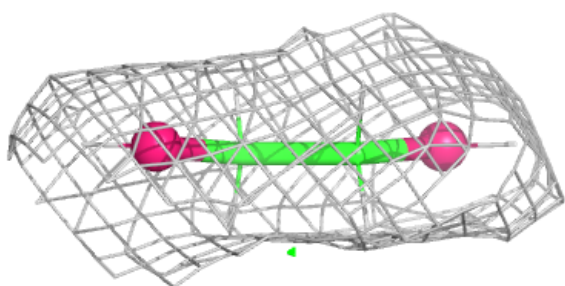
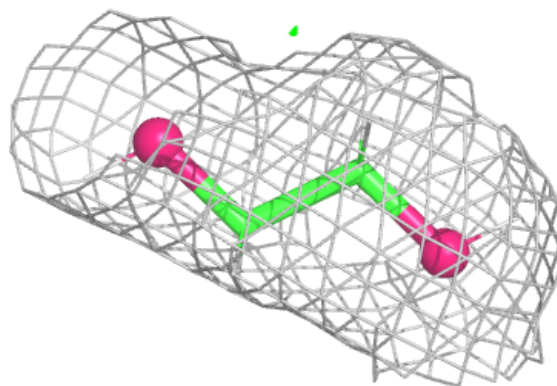
Electron density around GOL A 402:

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

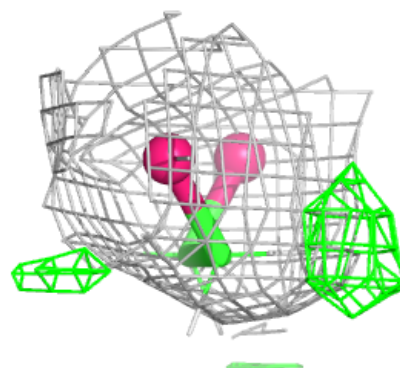
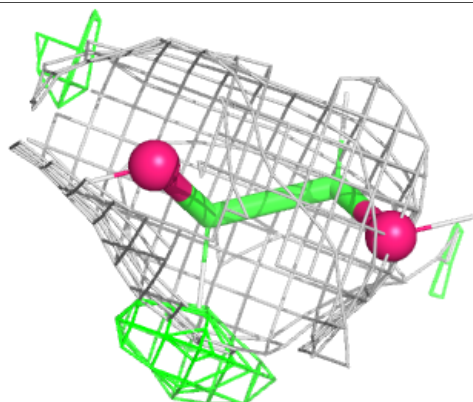
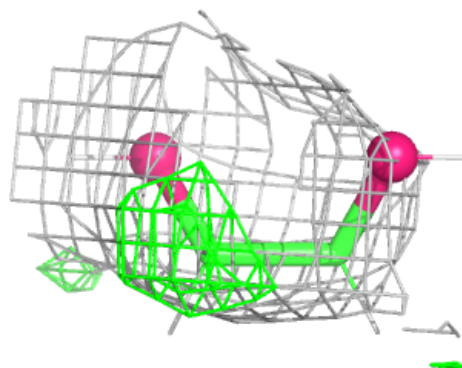


Electron density around EDO B 501:

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

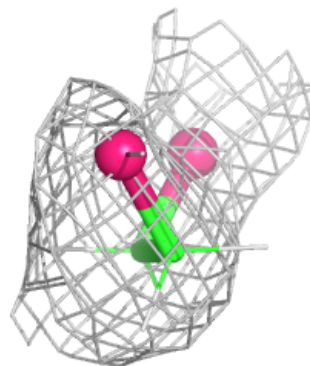
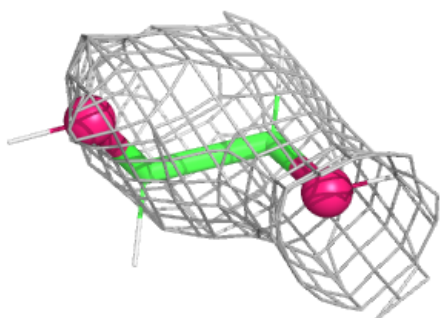
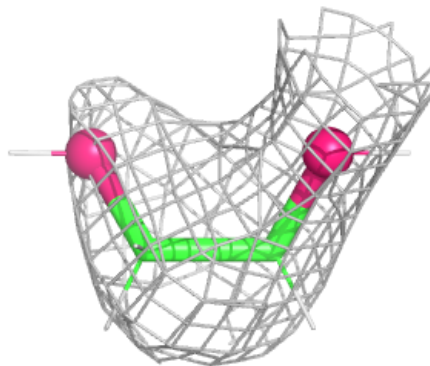
**Electron density around EDO A 403:**

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

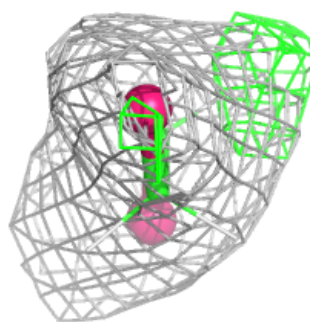
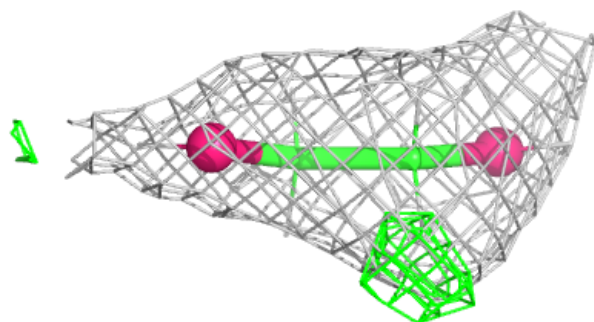
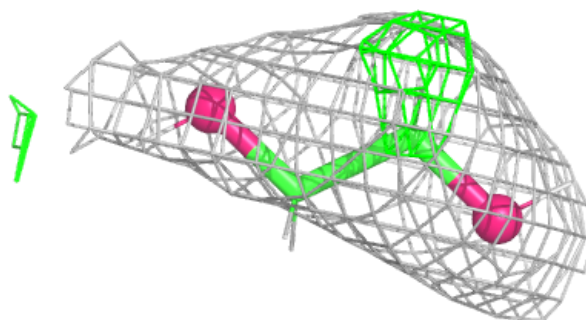


Electron density around EDO C 703:

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

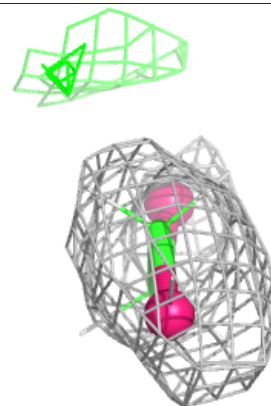
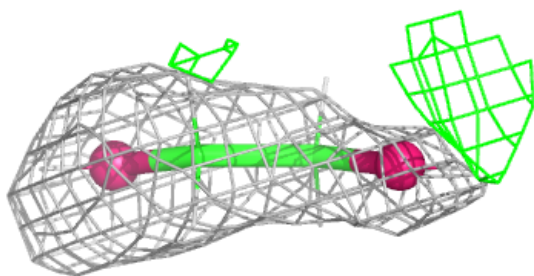
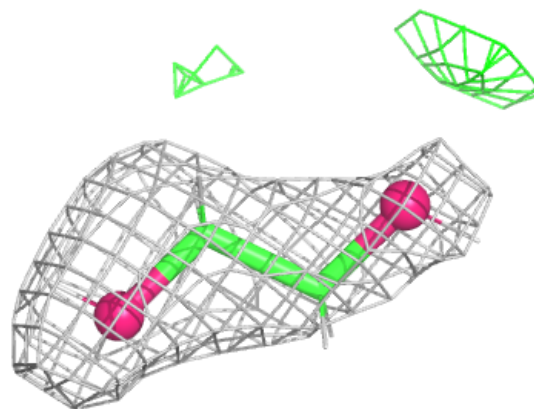
**Electron density around EDO B 505:**

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



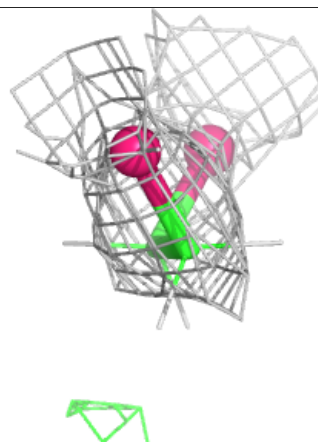
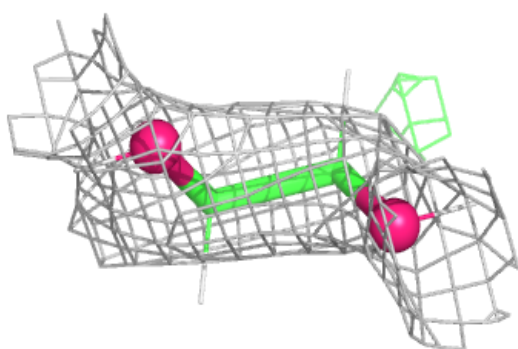
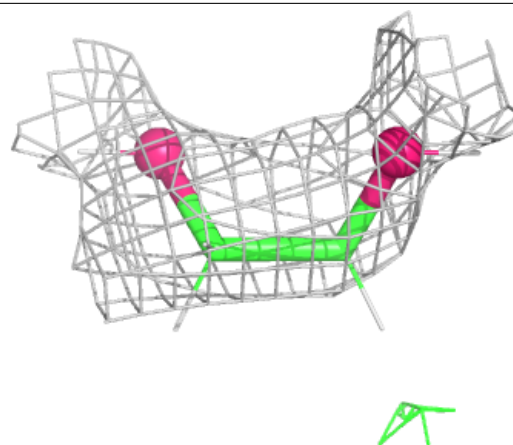
Electron density around EDO A 404:

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



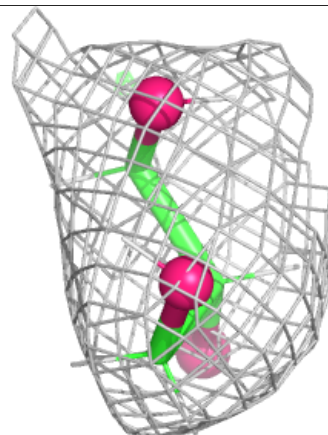
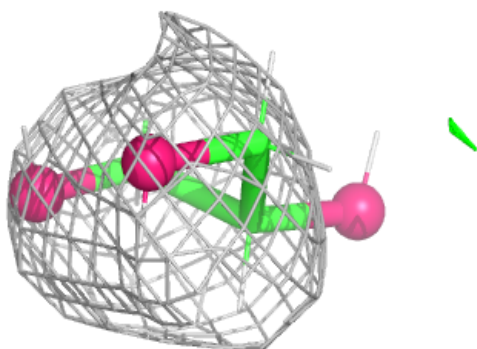
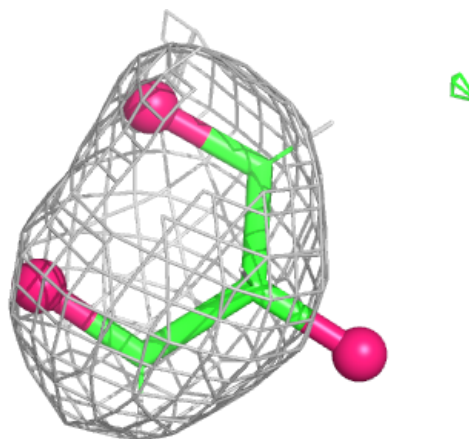
Electron density around EDO D 402:

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



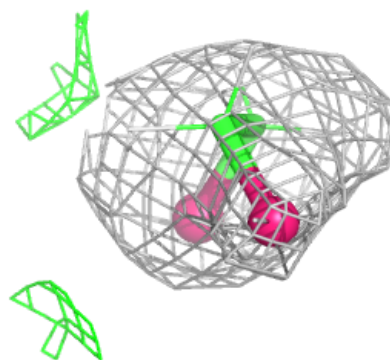
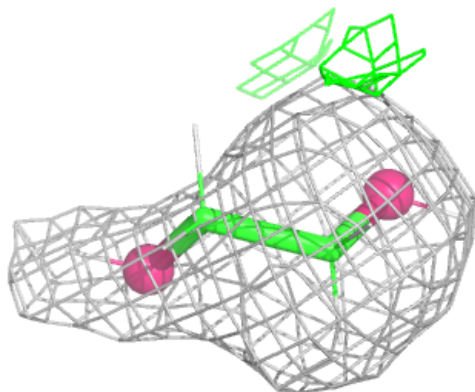
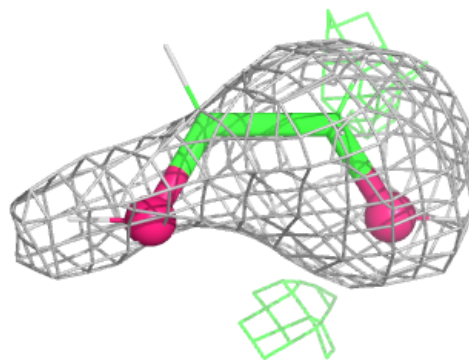
Electron density around GOL B 502:

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



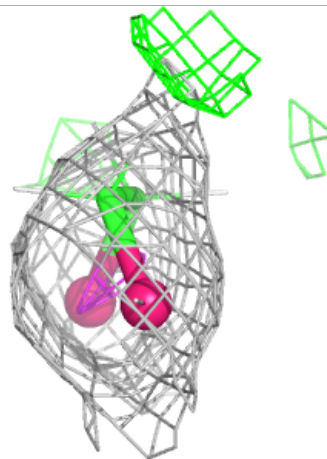
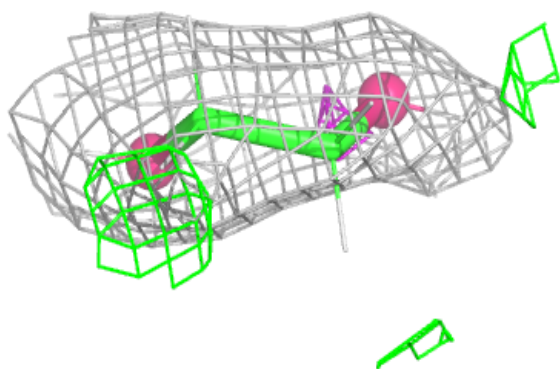
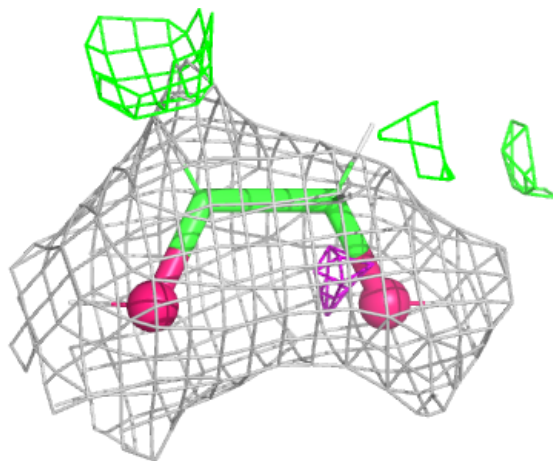
Electron density around EDO C 704:

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



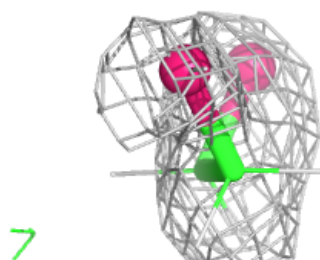
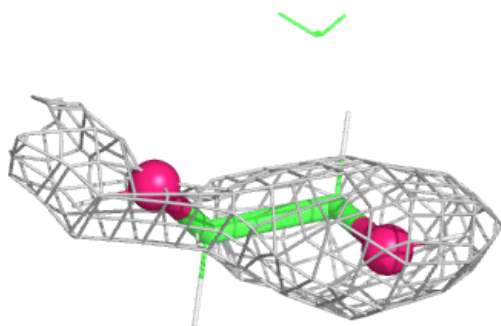
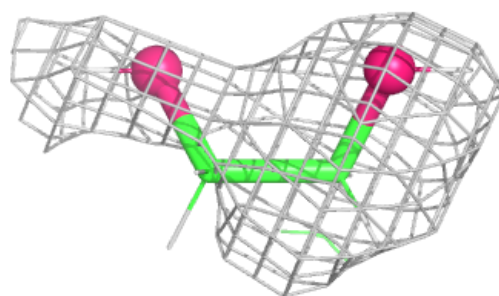
Electron density around EDO A 408:

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

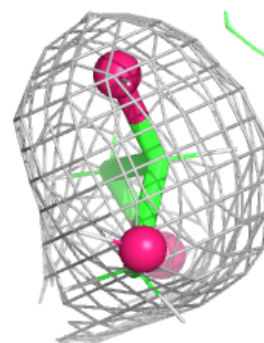
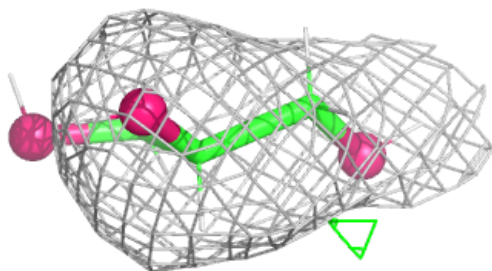
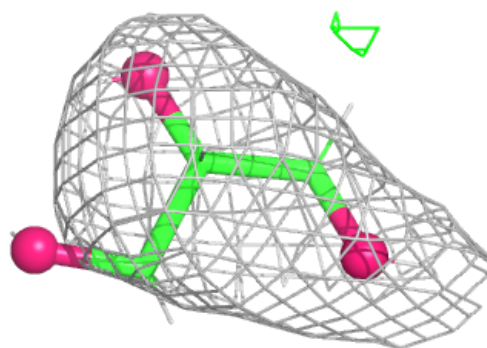


Electron density around EDO B 504:

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

**Electron density around GOL C 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.