



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2022 – 04:42 PM EST

PDB ID : 7SZG  
Title : Structure of the Rieske Non-heme Iron Oxygenase GxtA Pressurized with Xenon  
Authors : Bridwell-Rabb, J.; Liu, J.  
Deposited on : 2021-11-27  
Resolution : 2.69 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.25  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.25

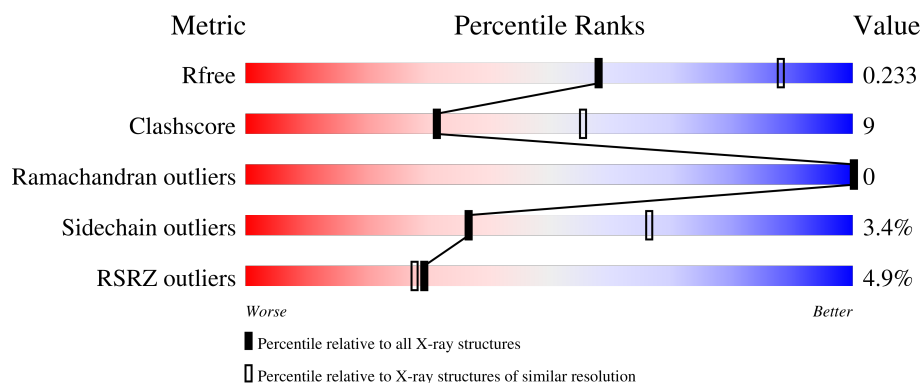
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


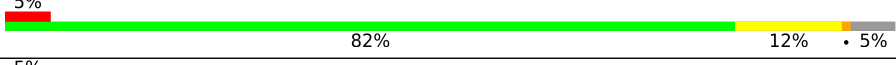

The reported resolution of this entry is 2.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	334	
1	B	334	
1	C	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DTT	A	506	-	-	X	-
6	DTT	B	503	-	-	X	-
6	DTT	C	506	-	-	X	-
7	CL	A	507	-	-	X	-

## 2 Entry composition [i](#)

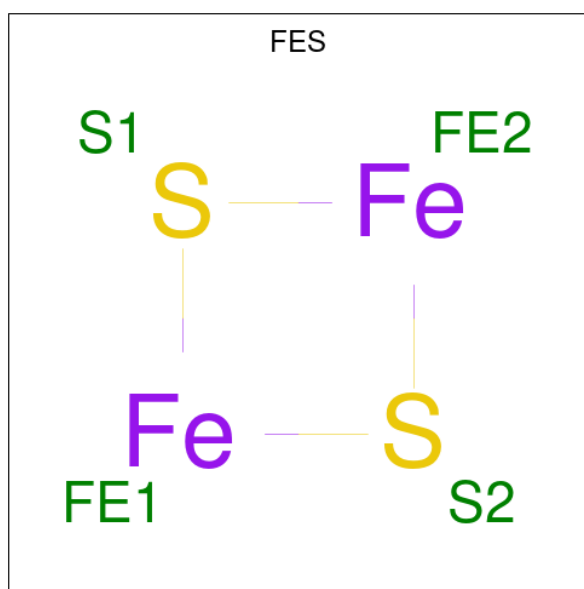
There are 8 unique types of molecules in this entry. The entry contains 8057 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SxtDIOX.

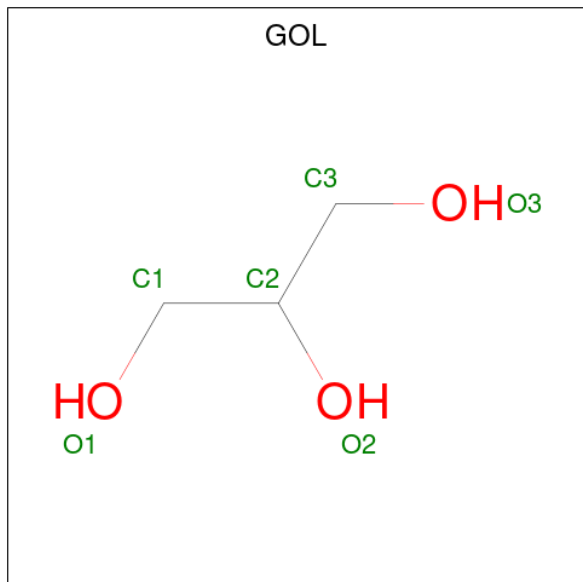
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2532	1609	437	468	18			
1	B	316	Total	C	N	O	S	0	1	0
			2549	1618	439	474	18			
1	C	327	Total	C	N	O	S	0	1	0
			2640	1674	456	491	19			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		

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



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

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

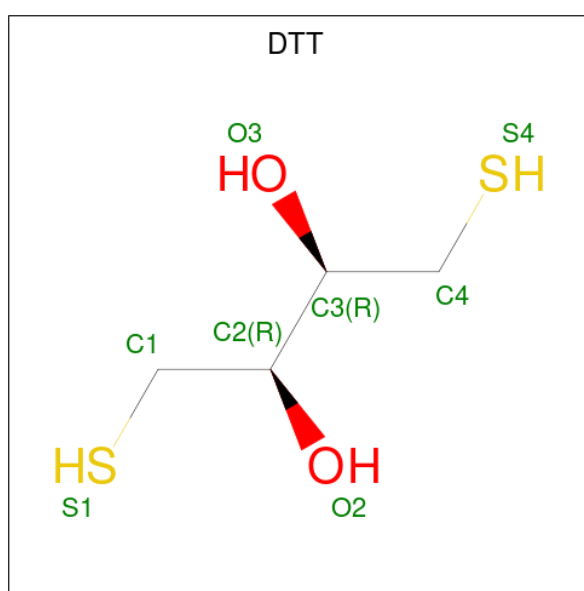
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		
4	B	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		

- Molecule 5 is XENON (three-letter code: XE) (formula: Xe) (labeled as "Ligand of Interest"

by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Xe	0	0
			1	1		
5	B	1	Total	Xe	0	0
			1	1		
5	C	1	Total	Xe	0	0
			1	1		

- Molecule 6 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:  $C_4H_{10}O_2S_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	Cl 1	0	0

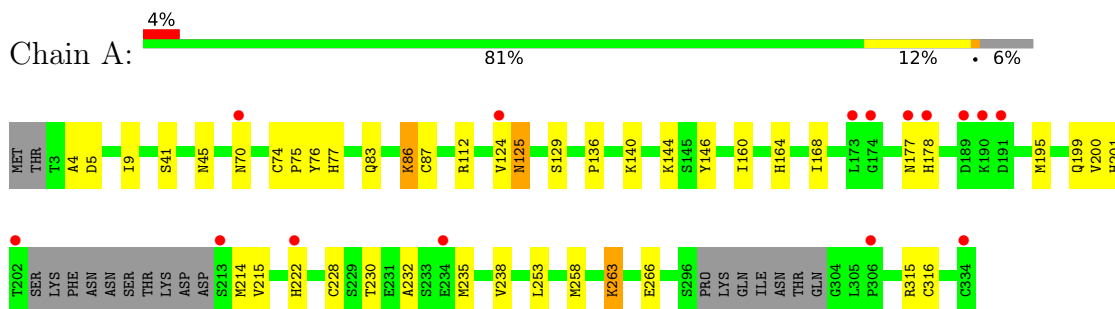
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	85	Total 85	O 85	0	0
8	B	80	Total 80	O 80	0	0
8	C	90	Total 90	O 90	0	0

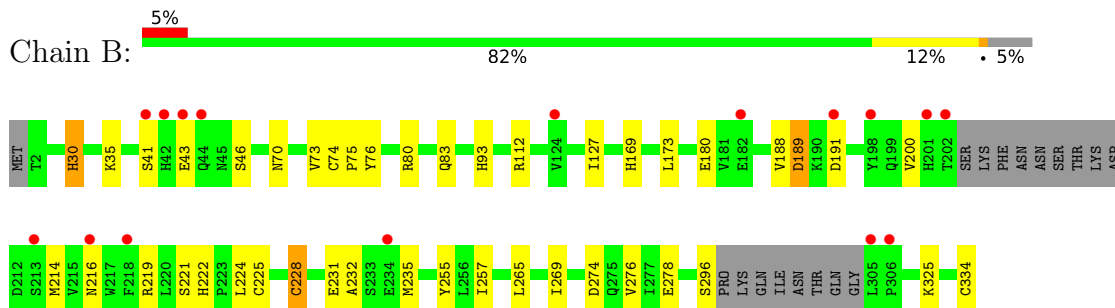
### 3 Residue-property plots [i](#)

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

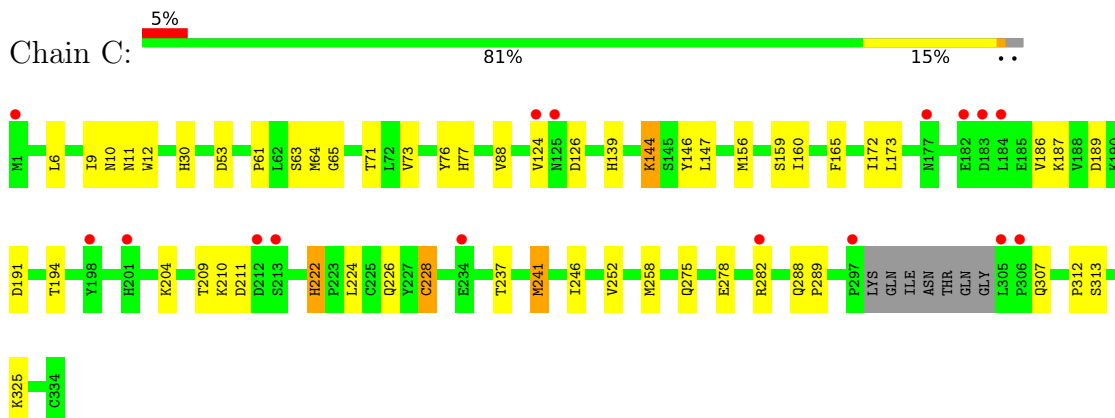
#### • Molecule 1: SxtDIOX



#### • Molecule 1: SxtDIOX



#### • Molecule 1: SxtDIOX





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.73Å 96.93Å 80.81Å 90.00° 106.97° 90.00°	Depositor
Resolution (Å)	48.47 – 2.69 48.47 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.47-2.69) 98.3 (48.47-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.205 , 0.244 0.194 , 0.233	Depositor DCC
$R_{free}$ test set	1534 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, FES, CL, DTT, FE, XE

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	0.55	0/2602	0.76	0/3551
1	B	0.51	0/2619	0.73	0/3575
1	C	0.55	1/2714 (0.0%)	0.74	0/3704
All	All	0.54	1/7935 (0.0%)	0.74	0/10830

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	SER	CA-CB	-5.33	1.45	1.52

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	2532	0	2455	38	0
1	B	2549	0	2468	34	1
1	C	2640	0	2558	51	1
2	A	4	0	0	1	0
2	B	4	0	0	0	0
2	C	4	0	0	1	0
3	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	0	0
3	C	12	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	8	0	9	5	0
6	B	8	0	10	9	0
6	C	8	0	10	13	0
7	A	1	0	0	3	0
7	B	1	0	0	1	0
7	C	1	0	0	0	0
8	A	85	0	0	3	0
8	B	80	0	0	5	0
8	C	90	0	0	14	0
All	All	8057	0	7558	138	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 9.

All (138) 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:172:ILE:HD11	1:C:275:GLN:OE1	1.29	1.31
6:C:506:DTT:H12	8:C:658:HOH:O	1.31	1.24
1:C:228:CYS:SG	6:C:506:DTT:S4	2.33	1.20
1:A:222:HIS:HB3	7:A:507:CL:CL	1.79	1.17
6:B:503:DTT:H2	8:B:603:HOH:O	1.42	1.17
1:A:222:HIS:CB	7:A:507:CL:CL	2.30	1.16
1:B:228:CYS:SG	6:B:503:DTT:S4	2.48	1.11
1:A:124:VAL:HG23	1:A:125:ASN:OD1	1.56	1.05
6:C:506:DTT:H12	6:C:506:DTT:S4	1.98	1.01
1:A:222:HIS:HB2	7:A:507:CL:CL	2.02	0.97
6:B:503:DTT:S4	8:B:603:HOH:O	2.23	0.96
6:C:506:DTT:S4	8:C:647:HOH:O	2.24	0.96
1:C:172:ILE:HD11	1:C:275:GLN:CD	1.87	0.93
1:A:200:VAL:HG13	1:A:214:MET:HB2	1.50	0.92
1:B:200:VAL:HG11	1:B:214:MET:HE3	1.58	0.86
1:B:73:VAL:HG22	1:B:80:ARG:HG2	1.54	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:CYS:SG	6:A:506:DTT:O3	2.35	0.84
1:C:6:LEU:HD12	1:C:9:ILE:CG2	2.09	0.81
6:B:503:DTT:H11	8:B:606:HOH:O	1.82	0.80
1:C:6:LEU:HA	1:C:9:ILE:HG22	1.62	0.79
1:B:222:HIS:HD2	1:B:224:LEU:H	1.31	0.76
1:A:214:MET:HE2	1:A:230:THR:HG22	1.67	0.76
6:C:506:DTT:S4	6:C:506:DTT:C1	2.67	0.74
1:C:307:GLN:HA	8:C:624:HOH:O	1.86	0.74
1:C:228:CYS:SG	8:C:622:HOH:O	2.44	0.74
1:C:228:CYS:HG	6:C:506:DTT:C4	2.00	0.74
1:A:200:VAL:CG1	1:A:214:MET:HB2	2.17	0.74
1:B:274:ASP:O	1:B:278:GLU:HG3	1.86	0.74
6:A:506:DTT:H12	6:A:506:DTT:S4	2.28	0.73
1:B:200:VAL:HG11	1:B:214:MET:CE	2.21	0.70
1:A:214:MET:HE2	1:A:230:THR:CG2	2.21	0.70
1:C:187:LYS:HE2	1:C:194:THR:HB	1.72	0.70
1:B:70:ASN:HD22	1:B:83:GLN:NE2	1.89	0.70
1:A:144:LYS:NZ	8:A:602:HOH:O	2.25	0.69
1:B:30:HIS:CE1	1:B:35:LYS:HG2	2.27	0.69
1:C:228:CYS:SG	6:C:506:DTT:C4	2.81	0.69
1:A:70:ASN:HD22	1:A:83:GLN:NE2	1.91	0.69
1:C:12:TRP:O	1:C:222:HIS:HE1	1.76	0.68
6:C:506:DTT:C1	8:C:658:HOH:O	2.08	0.68
1:B:228:CYS:CB	6:B:503:DTT:S4	2.82	0.67
1:C:246:ILE:HD11	1:C:252:VAL:HG23	1.80	0.64
1:C:61:PRO:HD2	1:C:64:MET:HE3	1.78	0.64
1:C:228:CYS:SG	6:C:506:DTT:H41	2.38	0.64
1:A:199:GLN:NE2	1:A:215:VAL:HG22	2.13	0.64
1:B:43:GLU:HB2	1:B:46:SER:HB3	1.80	0.64
1:B:228:CYS:CB	6:B:503:DTT:HS2	2.10	0.63
1:A:160:ILE:HG23	1:A:316:CYS:SG	2.38	0.63
1:A:263:LYS:O	1:A:263:LYS:HD2	1.98	0.63
1:C:222:HIS:CD2	1:C:224:LEU:H	2.16	0.63
1:C:246:ILE:HD11	1:C:252:VAL:CG2	2.29	0.63
1:A:214:MET:CE	1:A:232:ALA:HB2	2.29	0.62
1:B:200:VAL:CG1	1:B:214:MET:HE3	2.29	0.62
1:C:147:LEU:HD13	1:C:252:VAL:HG22	1.82	0.62
1:A:214:MET:HE1	1:A:232:ALA:HB2	1.82	0.61
1:B:200:VAL:HB	1:B:214:MET:HG3	1.82	0.61
1:C:222:HIS:HD2	1:C:224:LEU:H	1.47	0.61
6:C:506:DTT:H11	8:C:602:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HD3	1:A:87:CYS:O	2.01	0.60
6:C:506:DTT:H2	8:C:619:HOH:O	2.01	0.59
1:C:6:LEU:HD12	1:C:9:ILE:HG22	1.84	0.58
1:B:228:CYS:HB2	6:B:503:DTT:S4	2.42	0.58
1:B:255:TYR:HB3	1:B:257:ILE:HD11	1.86	0.57
6:A:506:DTT:S4	6:A:506:DTT:C1	2.94	0.56
1:B:73:VAL:CG2	1:B:80:ARG:HG2	2.30	0.56
1:C:53:ASP:OD2	1:C:63:SER:OG	2.24	0.55
1:A:238:VAL:HG23	1:A:258:MET:HB2	1.90	0.54
1:C:172:ILE:CD1	1:C:275:GLN:CD	2.70	0.54
1:A:4:ALA:O	1:A:9:ILE:HD11	2.08	0.54
1:B:222:HIS:HB3	1:B:225:CYS:HB2	1.90	0.53
1:B:127:ILE:HD12	1:B:127:ILE:H	1.73	0.53
1:B:200:VAL:CG1	1:B:214:MET:CE	2.86	0.52
1:C:288:GLN:HA	1:C:289:PRO:C	2.29	0.52
1:C:144:LYS:HE3	1:C:146:TYR:CE2	2.45	0.52
1:B:221:SER:N	7:B:507:CL:CL	2.65	0.52
1:C:237:THR:HB	8:C:672:HOH:O	2.08	0.52
1:C:210:LYS:HD2	1:C:210:LYS:H	1.75	0.51
1:B:222:HIS:CD2	1:B:224:LEU:H	2.19	0.51
1:B:74:CYS:SG	1:B:75:PRO:HD2	2.51	0.51
1:C:228:CYS:HB3	8:C:622:HOH:O	2.10	0.50
1:A:263:LYS:HE3	1:A:266:GLU:OE1	2.12	0.50
1:C:10:ASN:HB3	1:C:124:VAL:HG22	1.94	0.50
1:C:147:LEU:HD11	1:C:246:ILE:CD1	2.42	0.49
1:A:199:GLN:NE2	1:A:215:VAL:CG2	2.75	0.49
1:A:45:ASN:O	1:A:45:ASN:OD1	2.31	0.49
1:C:226:GLN:HB3	1:C:241:MET:HE3	1.93	0.49
1:C:77:HIS:HB2	2:C:501:FES:S2	2.53	0.49
6:A:506:DTT:O2	8:A:601:HOH:O	2.20	0.49
1:C:204:LYS:NZ	1:C:209:THR:O	2.46	0.49
1:C:228:CYS:CB	8:C:622:HOH:O	2.60	0.48
1:A:70:ASN:HD22	1:A:83:GLN:HE21	1.60	0.48
1:C:187:LYS:HE3	8:C:684:HOH:O	2.14	0.48
1:C:278:GLU:HG3	3:C:503:GOL:H2	1.96	0.48
1:C:186:VAL:HG23	1:C:186:VAL:O	2.14	0.48
1:B:70:ASN:ND2	1:B:83:GLN:NE2	2.60	0.47
1:B:169:HIS:CE1	1:B:276:VAL:HG13	2.50	0.47
1:C:61:PRO:HG2	1:C:64:MET:CE	2.44	0.47
1:A:160:ILE:CG2	1:A:316:CYS:SG	3.03	0.47
1:A:74:CYS:SG	1:A:75:PRO:HD2	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:PHE:HB3	1:C:173:LEU:O	2.15	0.47
1:C:61:PRO:CD	1:C:64:MET:HE3	2.45	0.46
1:B:216:ASN:ND2	6:B:503:DTT:H41	2.30	0.46
1:A:125:ASN:OD1	1:A:125:ASN:N	2.49	0.46
1:C:186:VAL:O	1:C:186:VAL:CG2	2.63	0.46
6:C:506:DTT:S4	8:C:658:HOH:O	2.61	0.46
1:B:188:VAL:CG1	1:B:188:VAL:O	2.64	0.45
1:C:204:LYS:HE3	1:C:211:ASP:OD1	2.16	0.45
1:A:164:HIS:CD2	1:A:168:ILE:HD11	2.51	0.45
1:B:265:LEU:O	1:B:269:ILE:HG13	2.15	0.45
1:A:5:ASP:C	1:A:9:ILE:HD12	2.37	0.45
6:C:506:DTT:C2	8:C:619:HOH:O	2.62	0.44
1:B:214:MET:HB3	1:B:232:ALA:HB2	1.99	0.44
1:C:144:LYS:HE3	1:C:146:TYR:CZ	2.52	0.44
6:B:503:DTT:C1	8:B:606:HOH:O	2.53	0.44
1:B:188:VAL:O	1:B:188:VAL:HG13	2.19	0.43
1:C:156:MET:O	1:C:160:ILE:HG13	2.18	0.43
1:A:136:PRO:HG2	1:C:71:THR:HG21	2.01	0.43
1:C:228:CYS:HB2	8:C:606:HOH:O	2.19	0.42
1:C:139:HIS:O	1:C:258:MET:HA	2.19	0.42
1:B:219:ARG:HD2	8:B:669:HOH:O	2.19	0.42
1:A:195:MET:HE3	1:A:316:CYS:HB2	2.00	0.42
1:A:214:MET:HE3	1:A:232:ALA:HB2	1.98	0.42
1:C:30[A]:HIS:HB3	1:C:246:ILE:HG23	2.02	0.42
1:C:278:GLU:O	1:C:282:ARG:HG3	2.20	0.42
1:A:4:ALA:O	1:A:9:ILE:CD1	2.67	0.42
6:A:506:DTT:C2	8:A:601:HOH:O	2.68	0.42
1:C:6:LEU:HA	1:C:9:ILE:CG2	2.42	0.42
1:A:146:TYR:HB2	1:A:253:LEU:HB3	2.01	0.42
1:B:255:TYR:HB3	1:B:257:ILE:CD1	2.49	0.41
1:A:77:HIS:HB2	2:A:501:FES:S1	2.60	0.41
1:C:65:GLY:HA3	1:C:73:VAL:O	2.20	0.41
1:B:41:SER:HB2	1:B:46:SER:HB3	2.03	0.41
1:C:189:ASP:OD1	1:C:191:ASP:N	2.45	0.41
1:A:178:HIS:HD1	1:A:201:HIS:CE1	2.39	0.41
1:A:214:MET:HE2	1:A:230:THR:HG21	1.99	0.41
1:B:173:LEU:HD23	1:B:214:MET:HE1	2.03	0.40
1:A:136:PRO:HB2	1:C:88:VAL:HG23	2.03	0.40
1:A:177:ASN:C	1:A:178:HIS:HD2	2.25	0.40
1:B:189:ASP:OD1	1:B:191:ASP:N	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:HIS:CE1	1:C:313:SER:OG[2_656]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/334 (92%)	301 (97%)	8 (3%)	0	100	100
1	B	311/334 (93%)	300 (96%)	11 (4%)	0	100	100
1	C	324/334 (97%)	312 (96%)	12 (4%)	0	100	100
All	All	944/1002 (94%)	913 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/304 (94%)	275 (96%)	10 (4%)	36	65
1	B	288/304 (95%)	277 (96%)	11 (4%)	33	62
1	C	299/304 (98%)	290 (97%)	9 (3%)	41	70
All	All	872/912 (96%)	842 (97%)	30 (3%)	37	66

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	76	TYR
1	A	86	LYS
1	A	112	ARG
1	A	125	ASN
1	A	129	SER
1	A	140	LYS
1	A	235	MET
1	A	263	LYS
1	A	315	ARG
1	B	30	HIS
1	B	76	TYR
1	B	112	ARG
1	B	180	GLU
1	B	189	ASP
1	B	228	CYS
1	B	231	GLU
1	B	235	MET
1	B	296	SER
1	B	325	LYS
1	B	334	CYS
1	C	11	ASN
1	C	76	TYR
1	C	126	ASP
1	C	144	LYS
1	C	222	HIS
1	C	228	CYS
1	C	241	MET
1	C	312	PRO
1	C	325	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	199	GLN
1	A	222	HIS
1	B	30	HIS
1	B	83	GLN
1	B	110	GLN
1	B	222	HIS
1	C	108	HIS
1	C	110	GLN

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Mol	Chain	Res	Type
1	C	222	HIS
1	C	226	GLN
1	C	275	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	503	-	5,5,5	0.08	0	5,5,5	0.33	0
6	DTT	A	506	-	7,7,7	0.24	0	4,8,8	0.50	0
2	FES	C	501	1	0,4,4	-	-	-		
6	DTT	B	503	-	7,7,7	0.22	0	4,8,8	1.17	0
3	GOL	B	502	-	5,5,5	0.09	0	5,5,5	0.34	0
6	DTT	C	506	-	7,7,7	0.34	0	4,8,8	1.55	1 (25%)
2	FES	A	501	1	0,4,4	-	-	-		
3	GOL	C	503	-	5,5,5	0.08	0	5,5,5	0.32	0
3	GOL	C	502	-	5,5,5	0.09	0	5,5,5	0.40	0
2	FES	B	501	1	0,4,4	-	-	-		
3	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	504	-	5,5,5	0.09	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	503	-	-	2/4/4/4	-
2	FES	B	501	1	-	-	0/1/1/1
6	DTT	B	503	-	-	8/8/8/8	-
2	FES	C	501	1	-	-	0/1/1/1
3	GOL	B	502	-	-	3/4/4/4	-
6	DTT	C	506	-	-	5/8/8/8	-
2	FES	A	501	1	-	-	0/1/1/1
3	GOL	C	503	-	-	0/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
6	DTT	A	506	-	-	0/8/8/8	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	506	DTT	C2-C1-S1	-2.39	107.53	114.47

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
3	C	502	GOL	O2-C2-C3-O3
6	B	503	DTT	S1-C1-C2-O2
6	B	503	DTT	S1-C1-C2-C3
6	B	503	DTT	C1-C2-C3-O3
6	B	503	DTT	C1-C2-C3-C4
6	B	503	DTT	O2-C2-C3-O3
6	B	503	DTT	O2-C2-C3-C4

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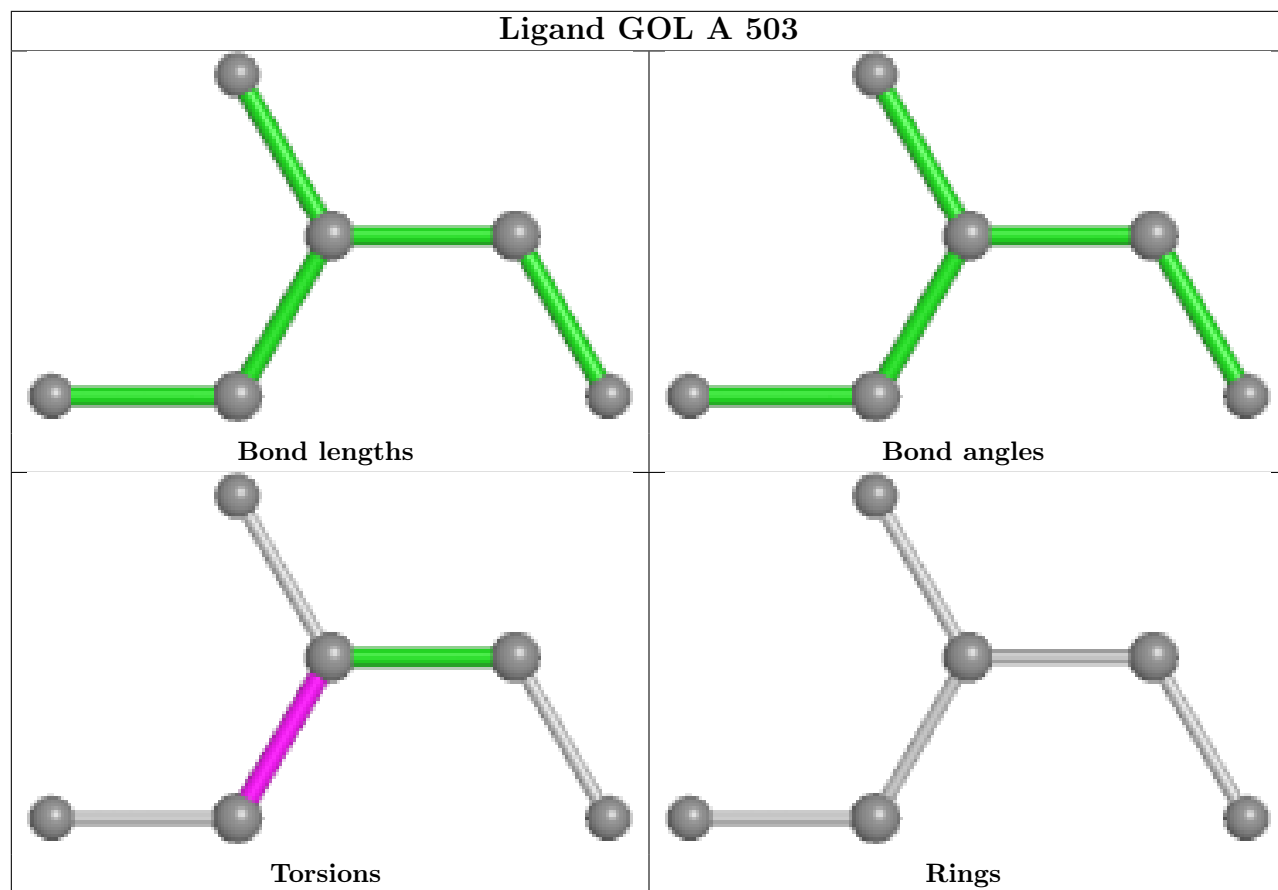
Mol	Chain	Res	Type	Atoms
6	B	503	DTT	C2-C3-C4-S4
6	B	503	DTT	O3-C3-C4-S4
6	C	506	DTT	S1-C1-C2-C3
6	C	506	DTT	C1-C2-C3-C4
6	C	506	DTT	C2-C3-C4-S4
6	C	506	DTT	O3-C3-C4-S4
3	A	503	GOL	O2-C2-C3-O3
3	A	503	GOL	C1-C2-C3-O3
3	B	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3
6	C	506	DTT	O2-C2-C3-O3
3	B	502	GOL	O1-C1-C2-C3
3	A	502	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-O2

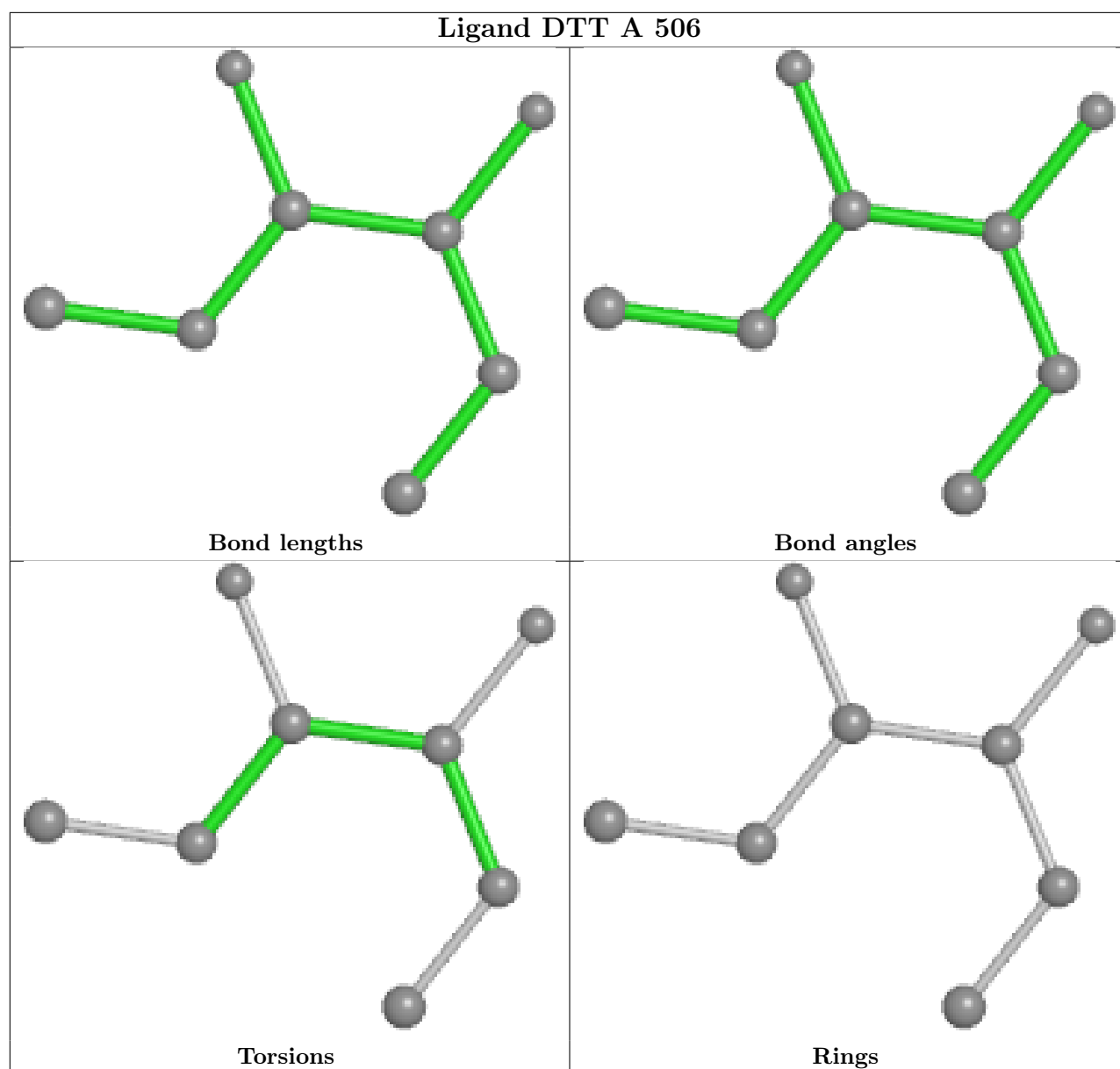
There are no ring outliers.

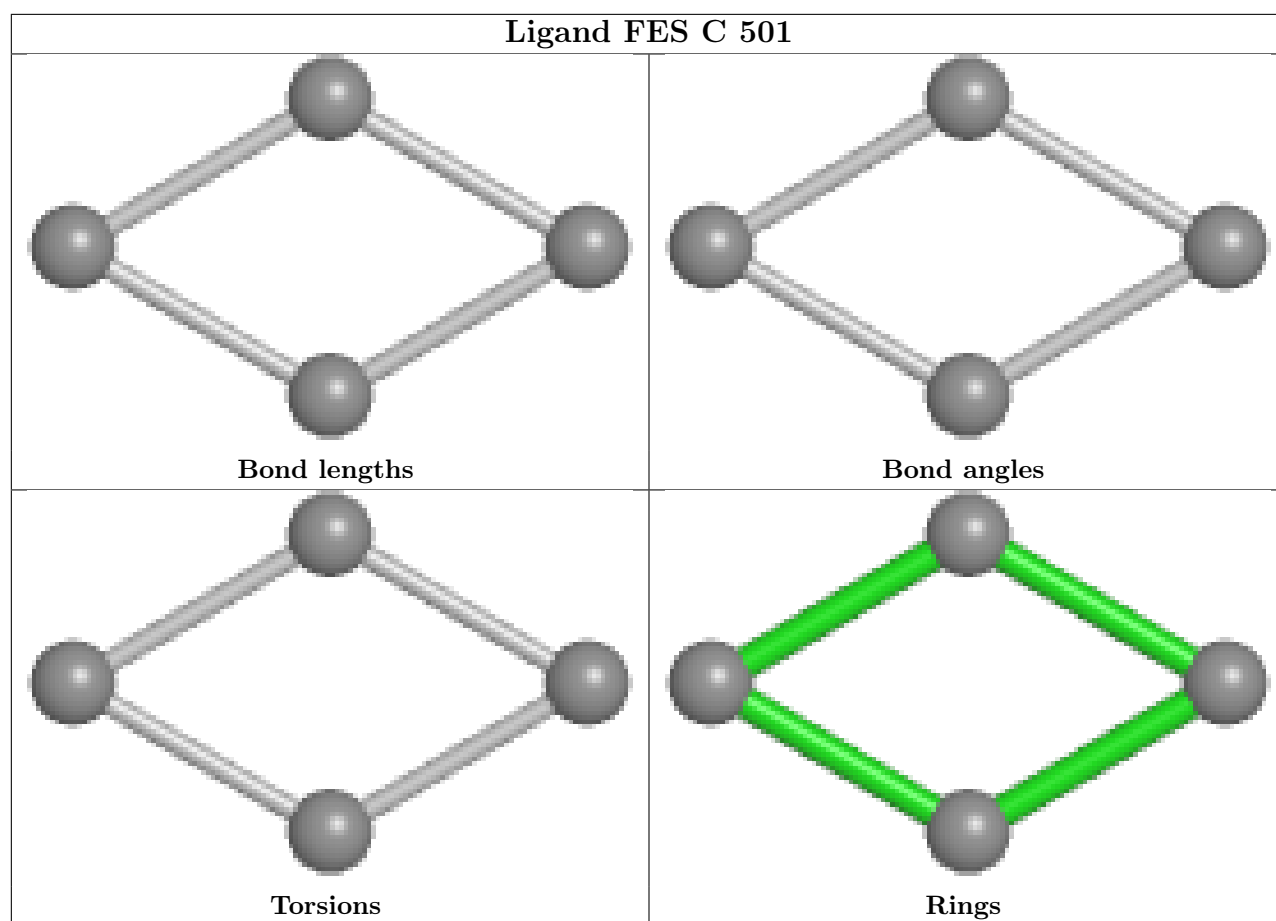
6 monomers are involved in 30 short contacts:

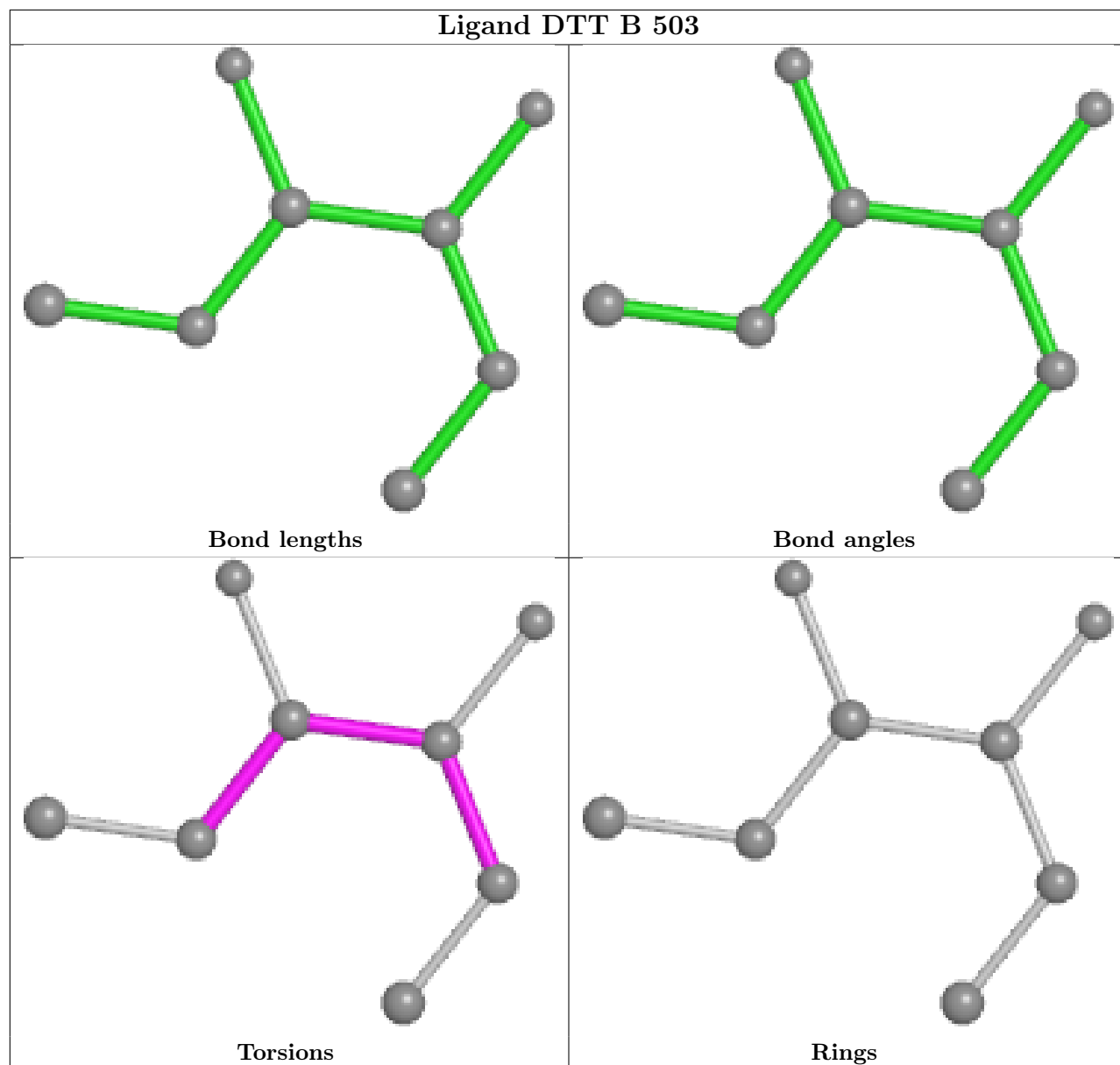
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	506	DTT	5	0
2	C	501	FES	1	0
6	B	503	DTT	9	0
6	C	506	DTT	13	0
2	A	501	FES	1	0
3	C	503	GOL	1	0

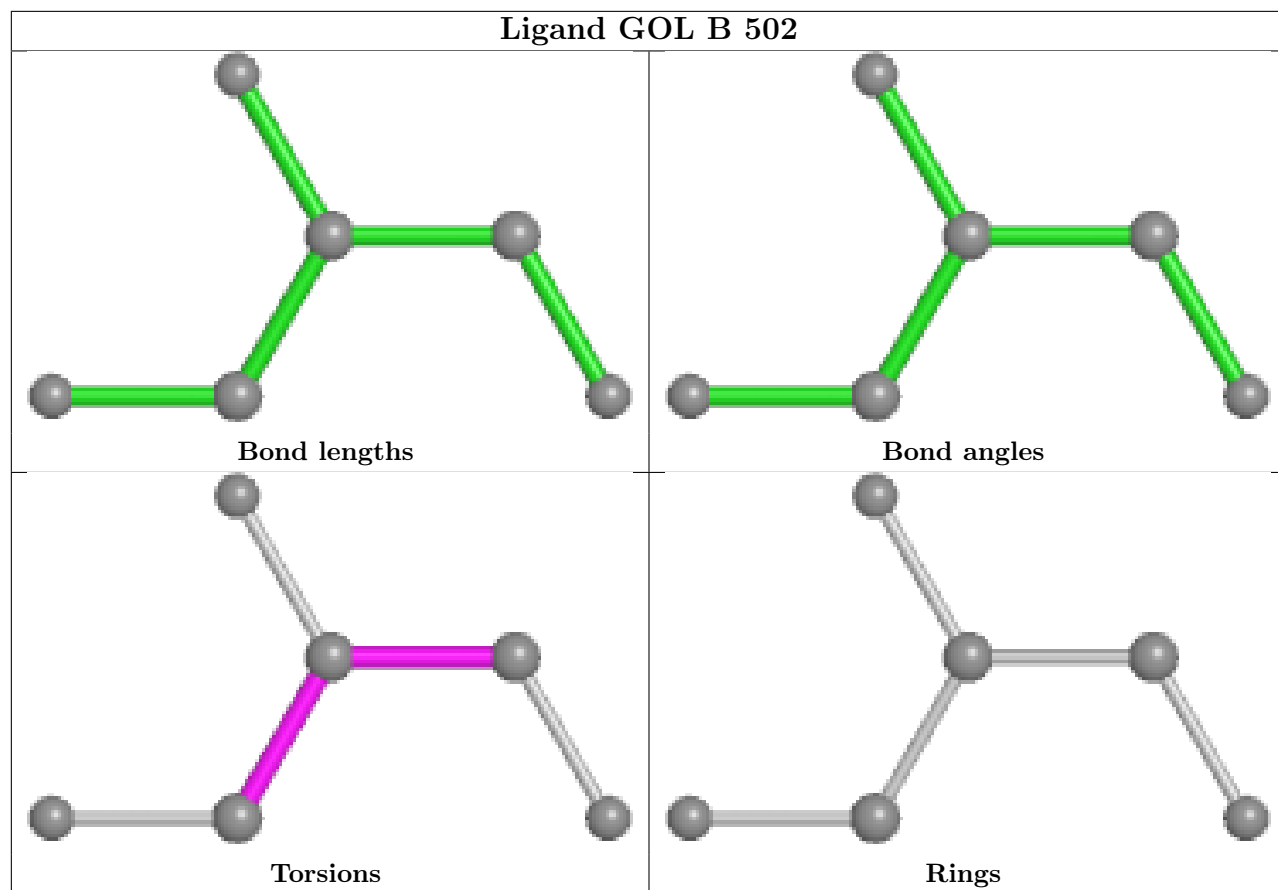
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



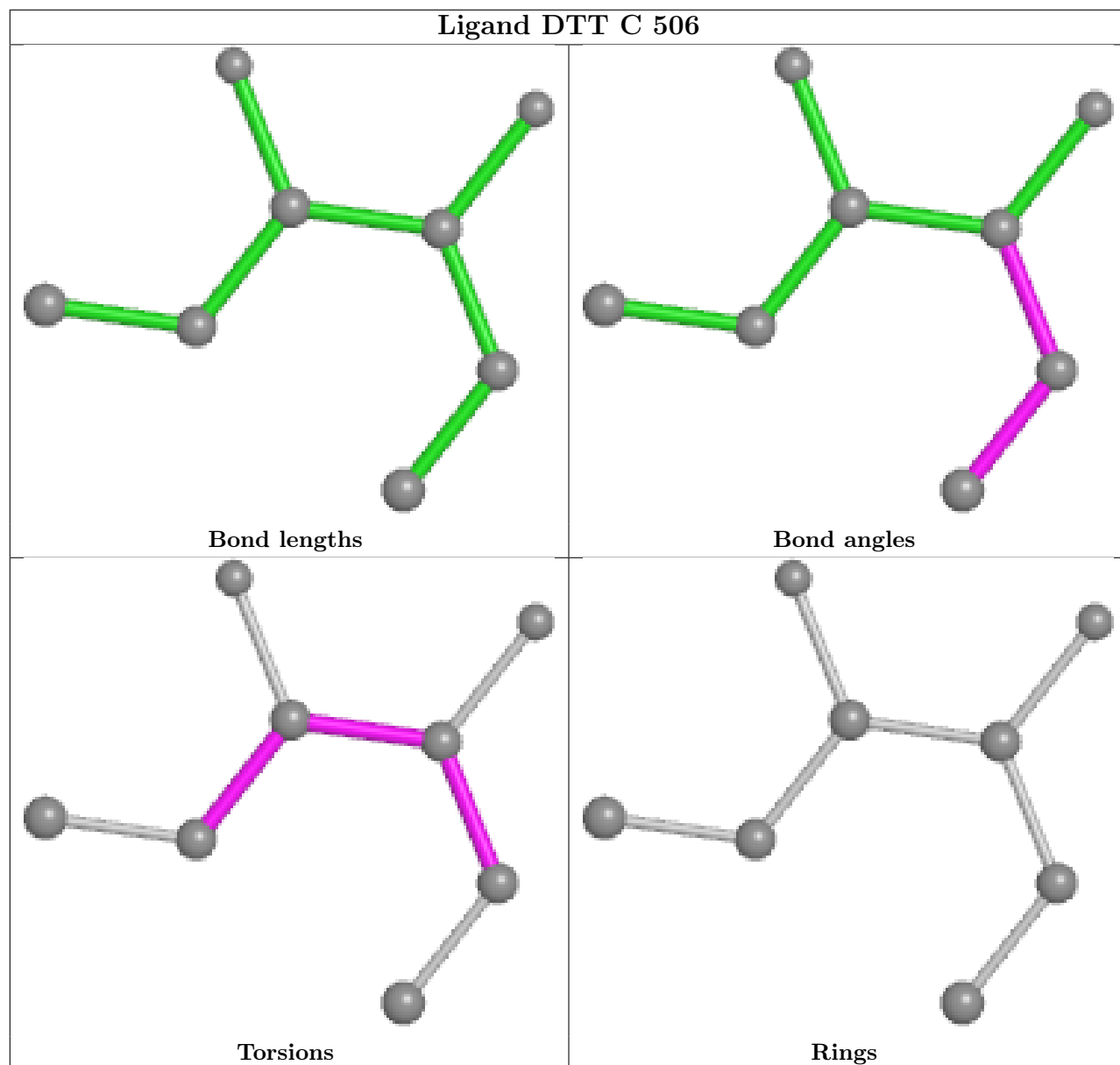


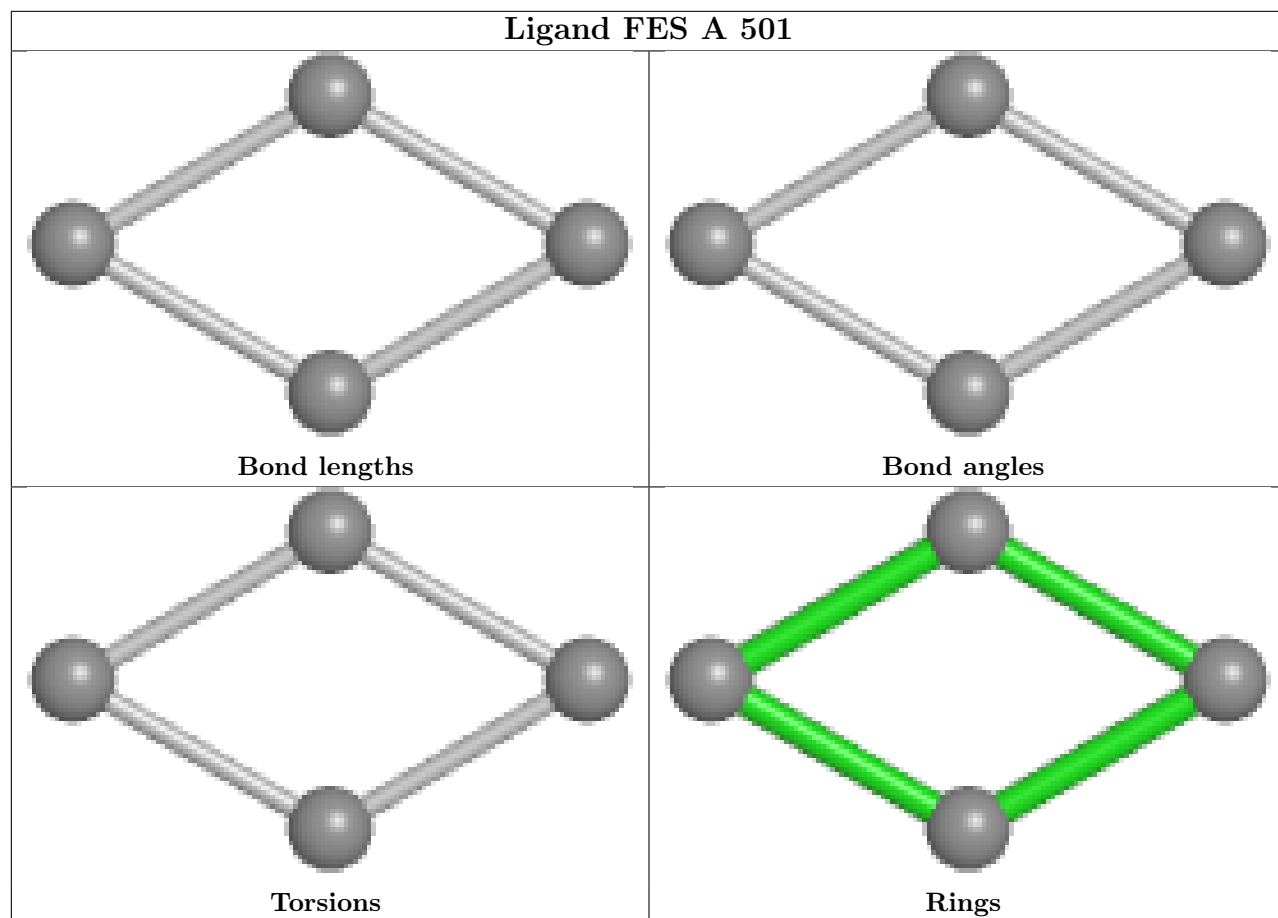


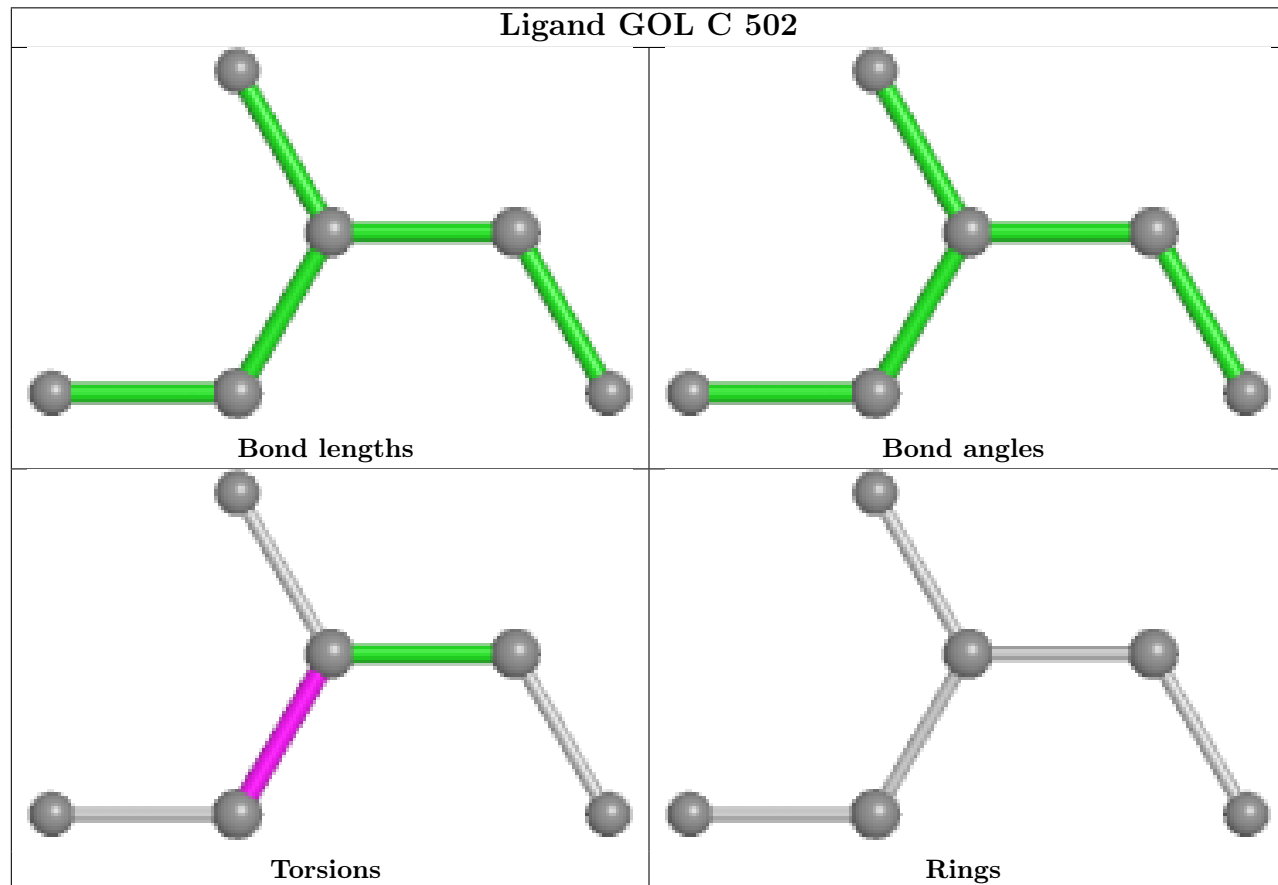
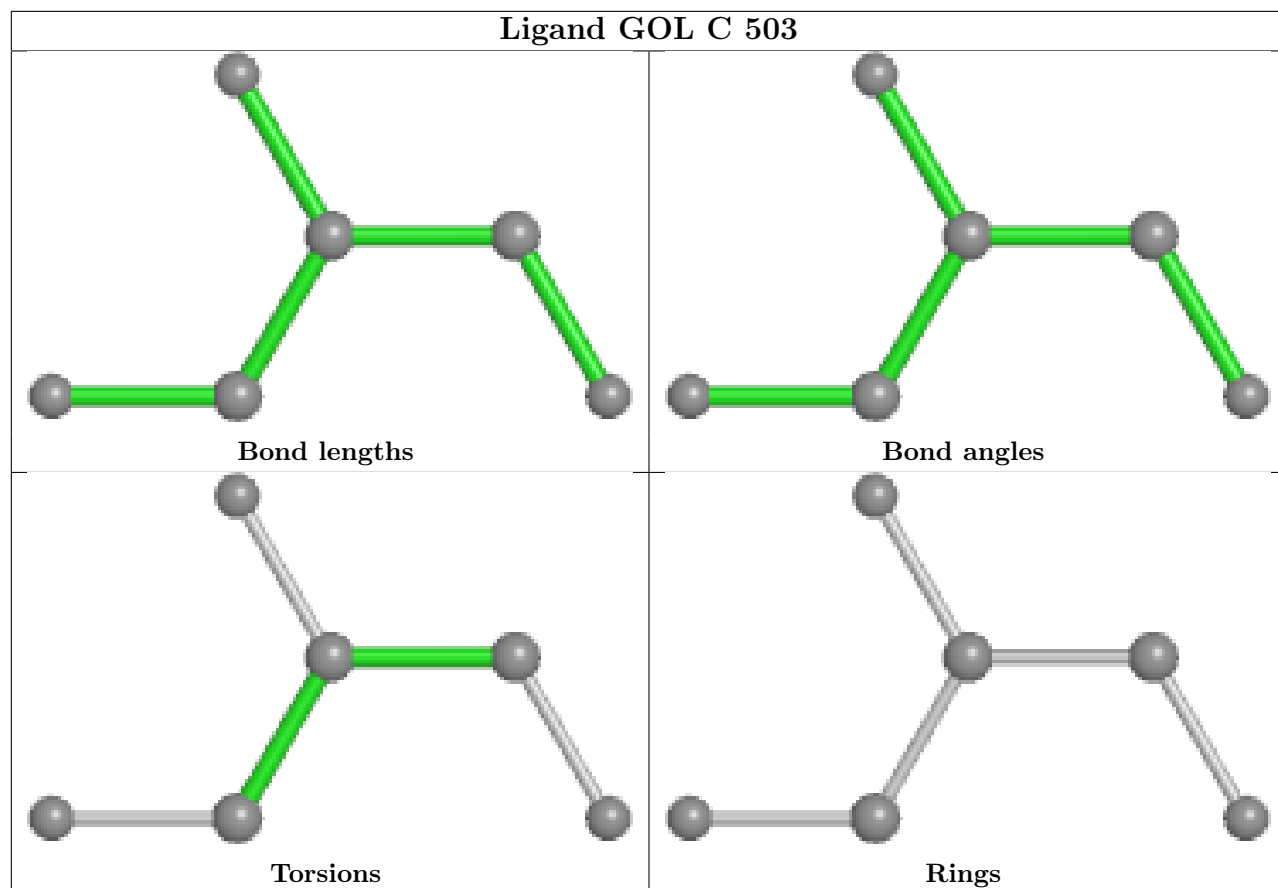


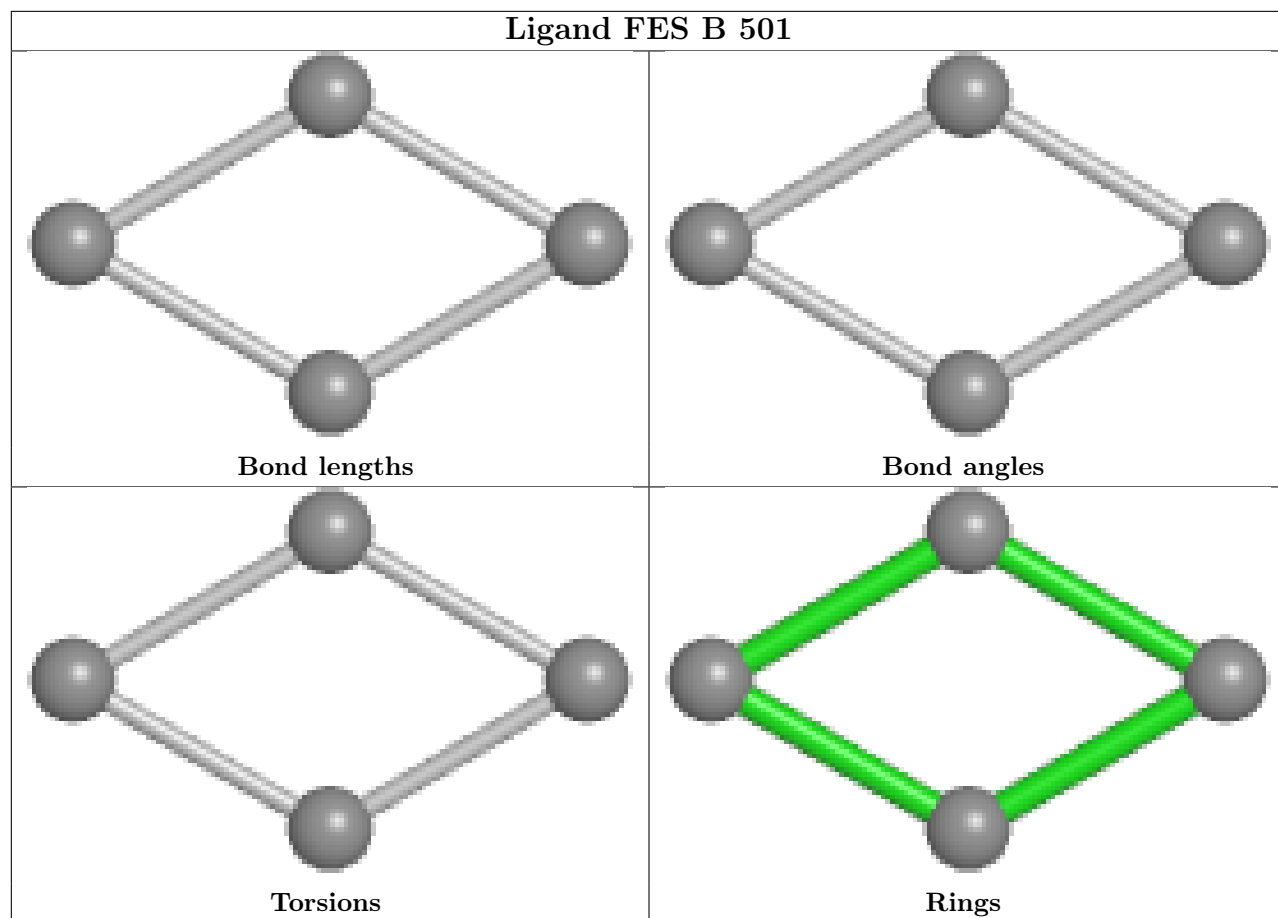


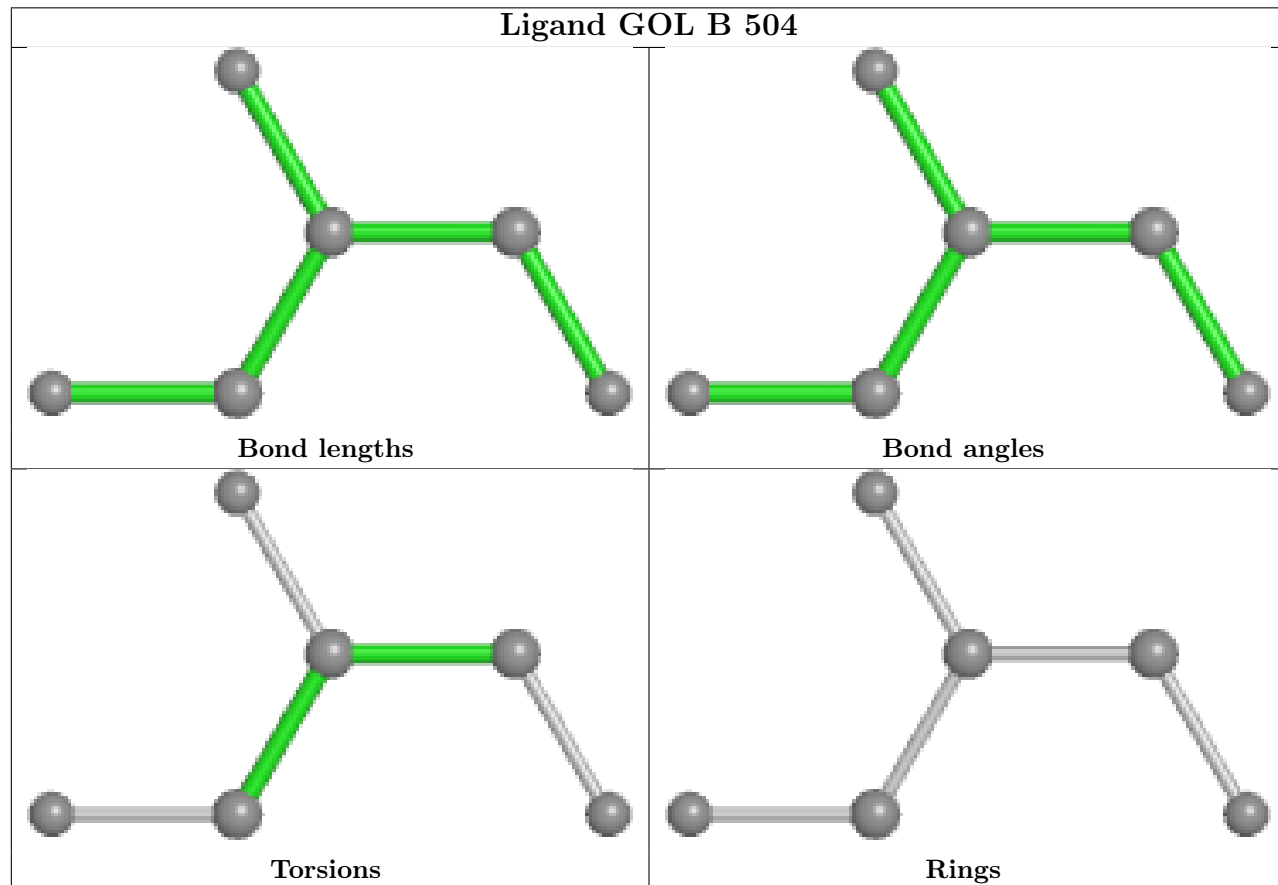
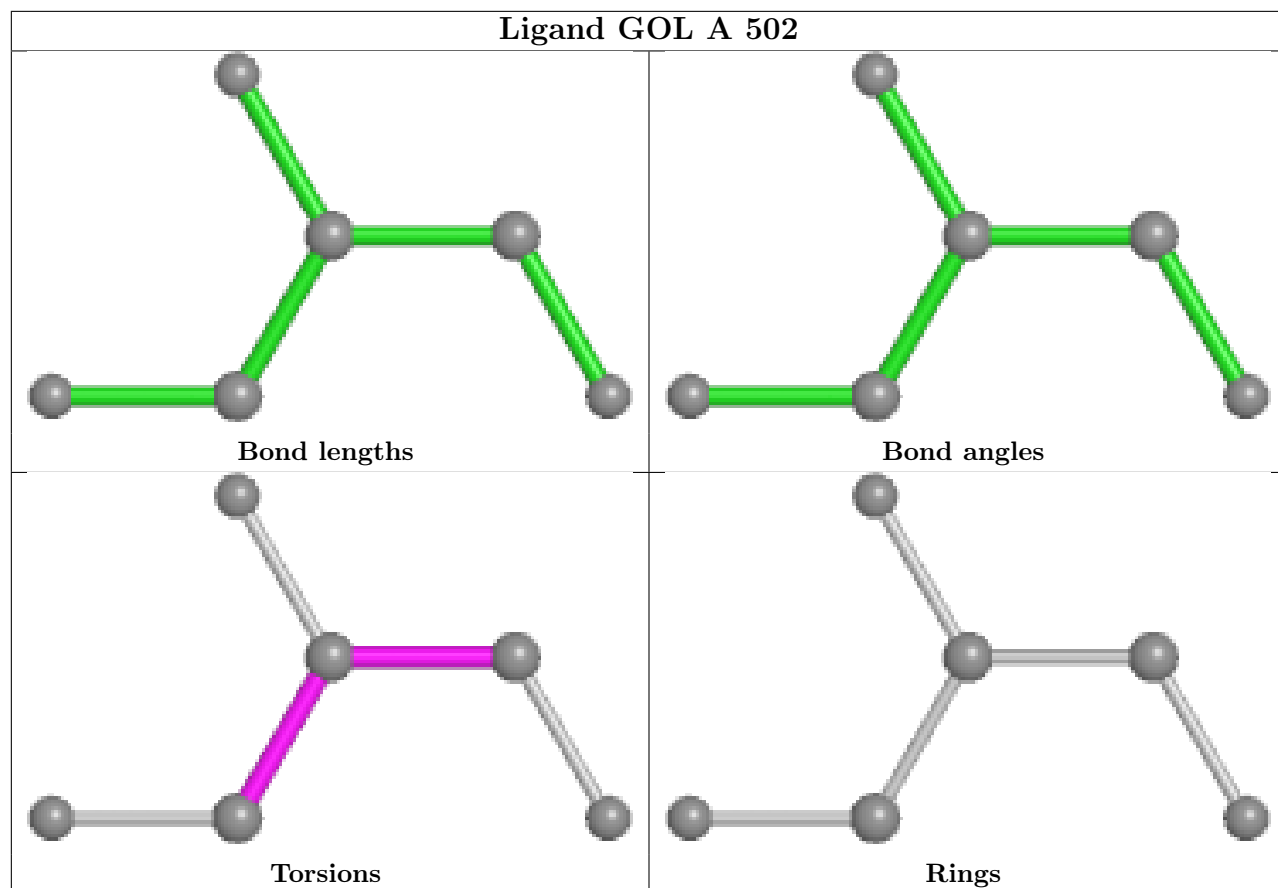












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	315/334 (94%)	0.47	15 (4%)	30 28	32, 46, 71, 102	0
1	B	316/334 (94%)	0.48	16 (5%)	28 26	36, 51, 79, 100	0
1	C	327/334 (97%)	0.46	16 (4%)	29 28	31, 46, 74, 97	0
All	All	958/1002 (95%)	0.47	47 (4%)	29 28	31, 48, 75, 102	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	LYS	4.0
1	C	234	GLU	3.7
1	B	44	GLN	3.6
1	B	42	HIS	3.6
1	A	234	GLU	3.6
1	B	43	GLU	3.3
1	B	234	GLU	3.1
1	B	216	ASN	3.0
1	B	191	ASP	3.0
1	A	202	THR	2.9
1	C	198	TYR	2.9
1	C	306	PRO	2.9
1	C	213	SER	2.9
1	C	182	GLU	2.9
1	C	297	PRO	2.9
1	A	334	CYS	2.8
1	C	177	ASN	2.8
1	C	184	LEU	2.8
1	A	306	PRO	2.6
1	B	202	THR	2.6
1	A	191	ASP	2.6
1	C	1	MET	2.5
1	B	124	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	201	HIS	2.4
1	A	213	SER	2.4
1	A	222	HIS	2.4
1	A	124	VAL	2.4
1	C	183	ASP	2.4
1	C	282	ARG	2.4
1	B	198	TYR	2.4
1	C	305	LEU	2.4
1	A	173	LEU	2.3
1	B	213	SER	2.3
1	A	189	ASP	2.3
1	B	305	LEU	2.3
1	B	201	HIS	2.3
1	B	306	PRO	2.3
1	C	125	ASN	2.2
1	A	177	ASN	2.2
1	A	174	GLY	2.1
1	A	70	ASN	2.1
1	B	218	PHE	2.1
1	C	124	VAL	2.1
1	B	41	SER	2.1
1	C	212	ASP	2.1
1	B	182	GLU	2.0
1	A	178	HIS	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 monosaccharides 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, 95<sup>th</sup> 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.

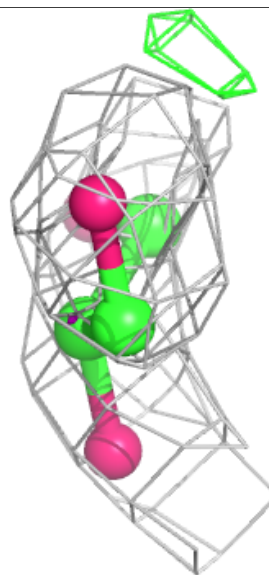
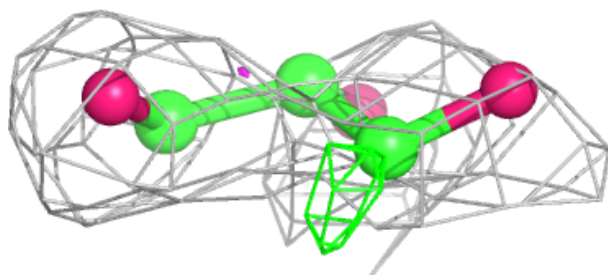
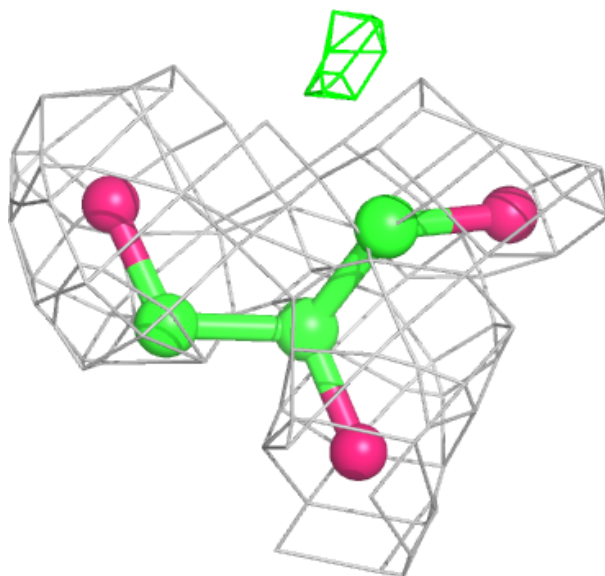


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	504	6/6	0.64	0.32	57,66,69,74	0
3	GOL	A	503	6/6	0.67	0.30	64,77,78,78	0
7	CL	A	507	1/1	0.71	0.20	67,67,67,67	0
3	GOL	C	502	6/6	0.75	0.27	57,63,66,71	0
3	GOL	B	502	6/6	0.75	0.27	54,63,67,67	0
3	GOL	C	503	6/6	0.76	0.19	63,64,67,75	0
7	CL	B	507	1/1	0.77	0.17	71,71,71,71	0
6	DTT	B	503	8/8	0.83	0.24	62,68,75,87	0
6	DTT	A	506	8/8	0.84	0.20	58,73,79,89	0
3	GOL	A	502	6/6	0.89	0.33	54,57,62,68	0
6	DTT	C	506	8/8	0.89	0.22	61,66,71,86	0
7	CL	C	507	1/1	0.95	0.09	47,47,47,47	0
5	XE	B	506	1/1	0.97	0.06	79,79,79,79	1
5	XE	C	505	1/1	0.97	0.08	81,81,81,81	1
2	FES	B	501	4/4	0.97	0.09	42,46,52,53	0
5	XE	A	505	1/1	0.97	0.14	86,86,86,86	1
4	FE	A	504	1/1	0.98	0.07	39,39,39,39	0
2	FES	A	501	4/4	0.98	0.10	36,39,40,44	0
4	FE	B	505	1/1	0.99	0.04	51,51,51,51	0
2	FES	C	501	4/4	0.99	0.13	27,34,35,37	0
4	FE	C	504	1/1	1.00	0.08	49,49,49,49	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.

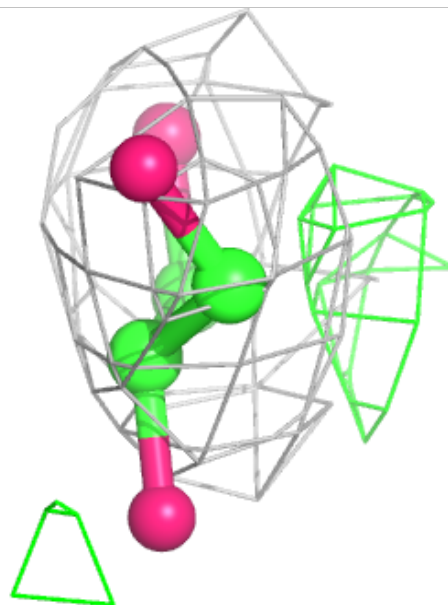
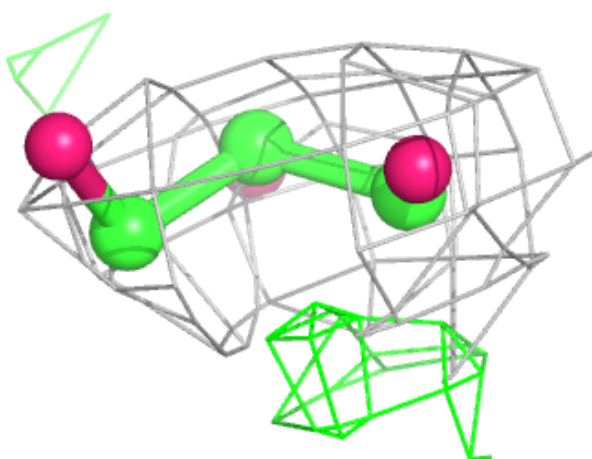
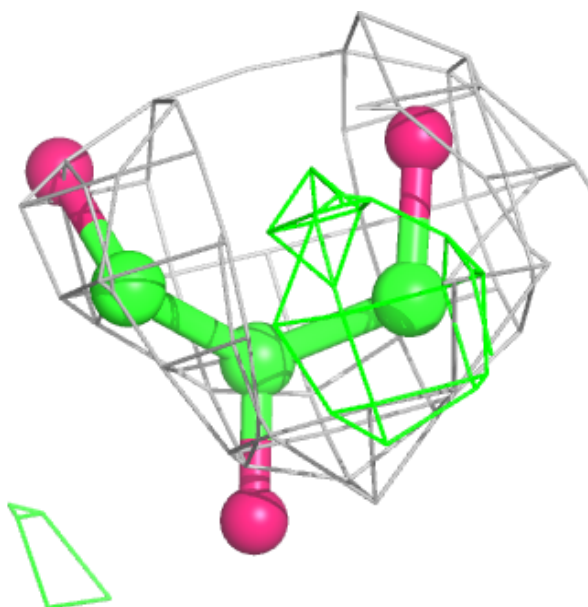
**Electron density around GOL B 504:**

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



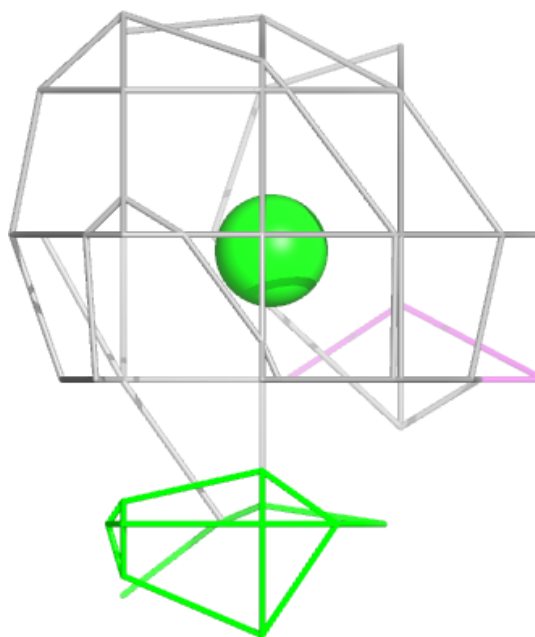
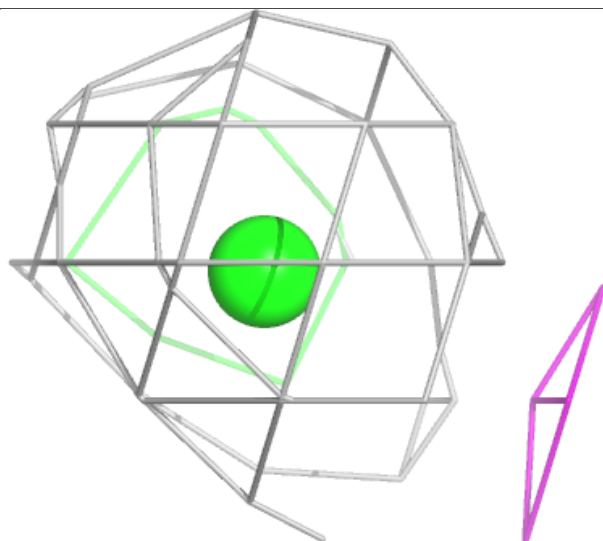
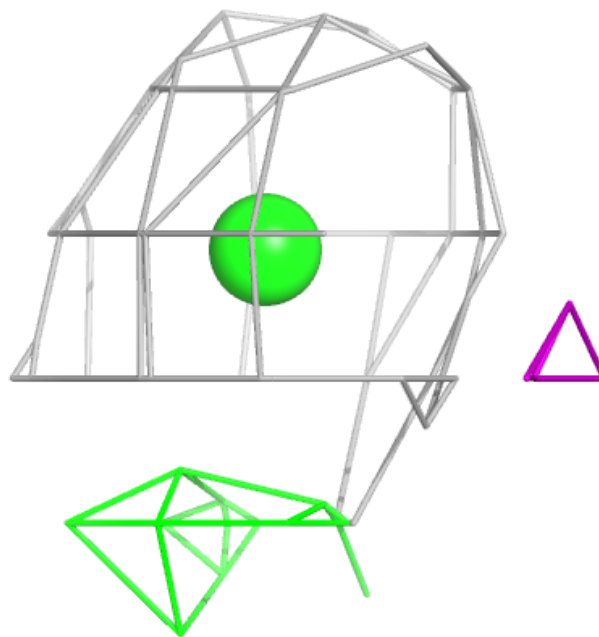
**Electron density around GOL A 503:**

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



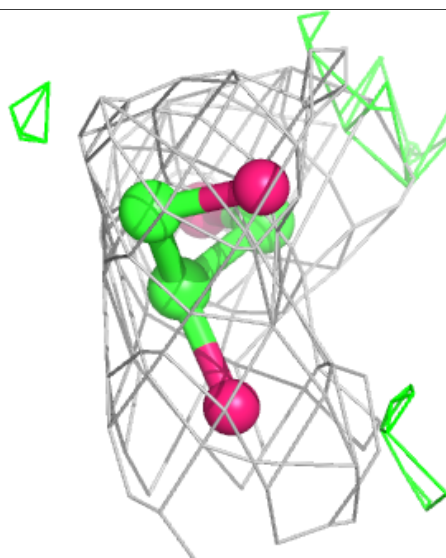
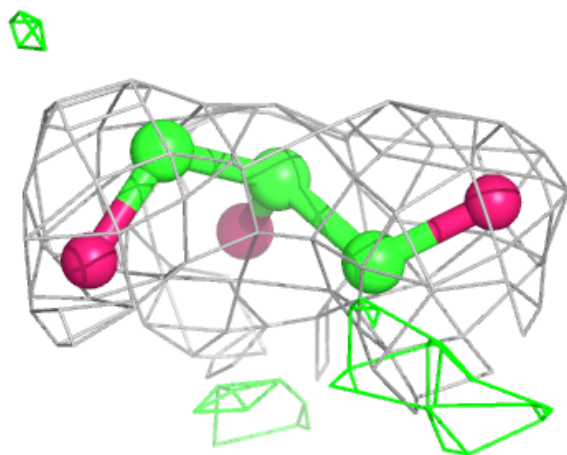
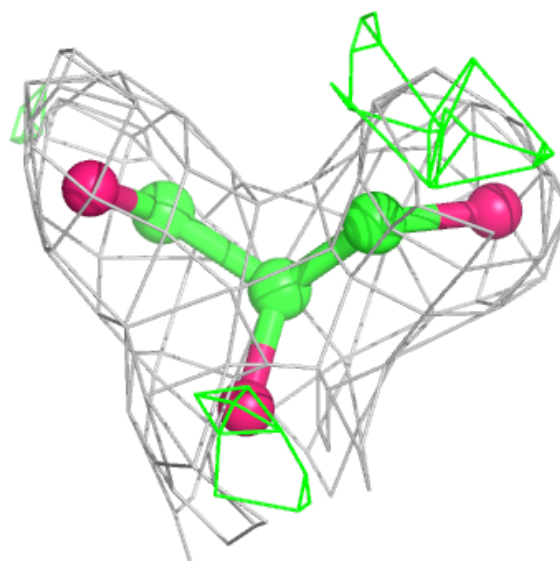
**Electron density around CL A 507:**

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



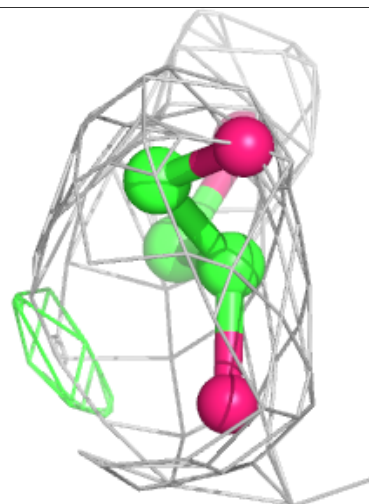
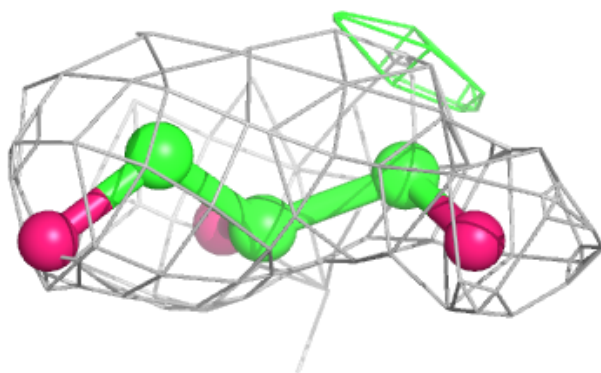
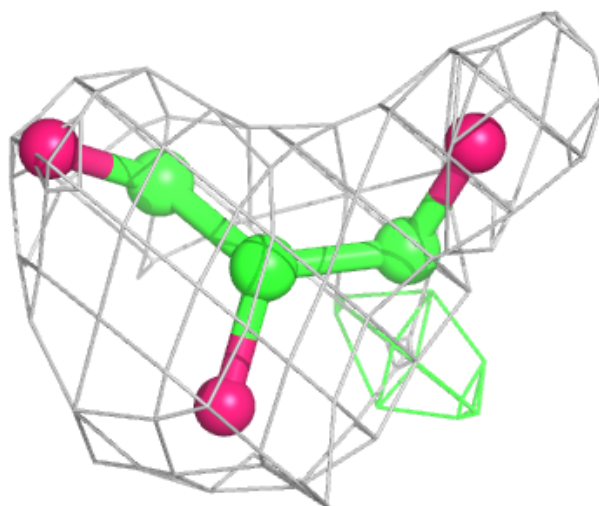
**Electron density around GOL C 502:**

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



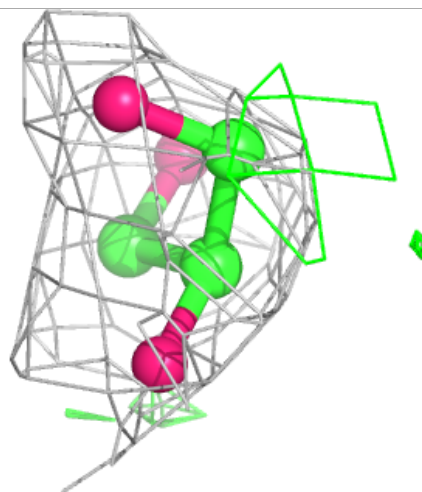
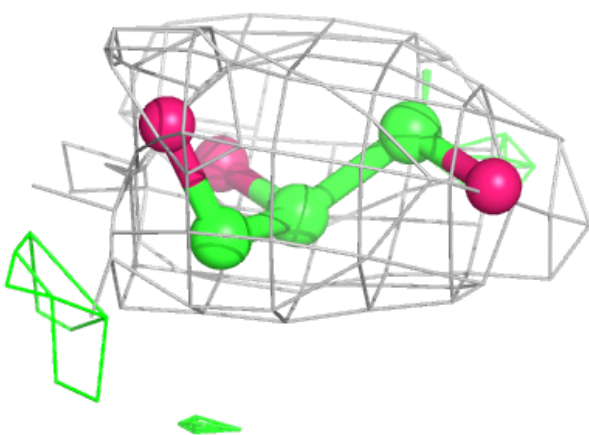
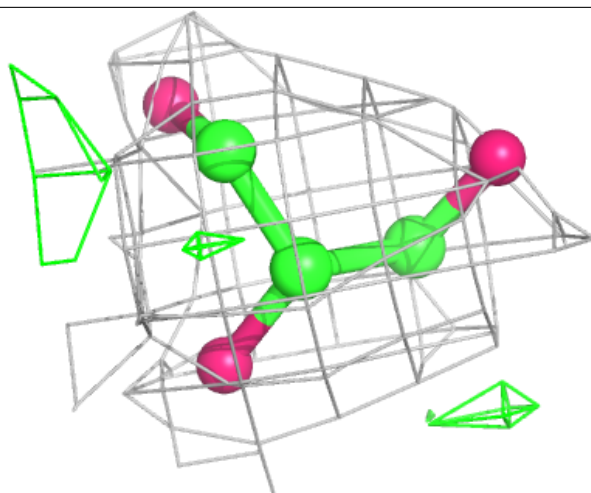
**Electron density around GOL B 502:**

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



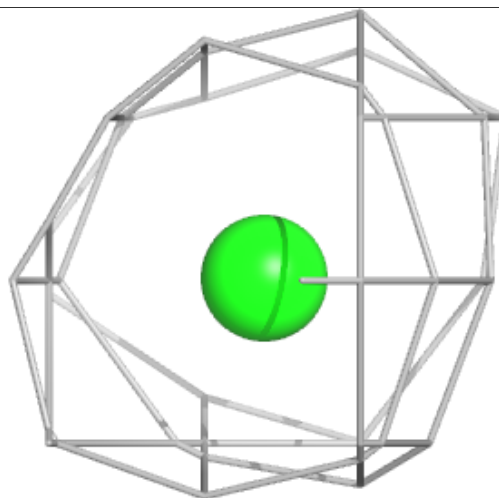
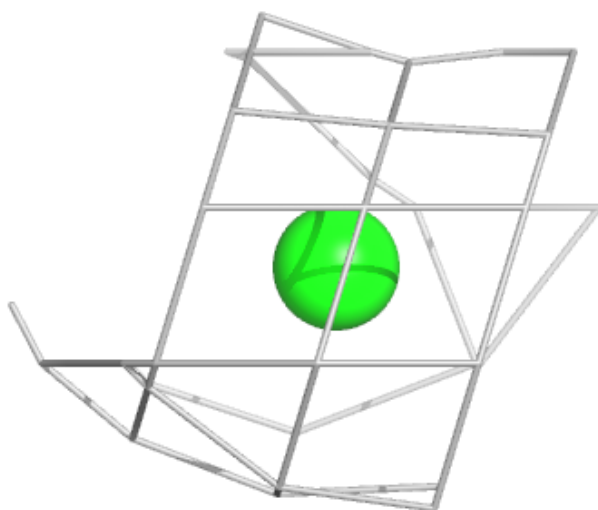
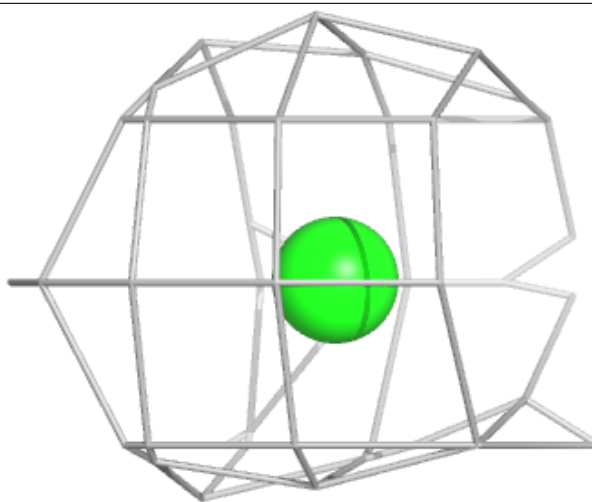
**Electron density around GOL C 503:**

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



**Electron density around CL B 507:**

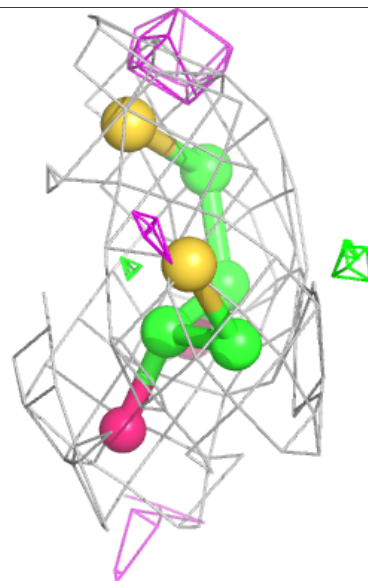
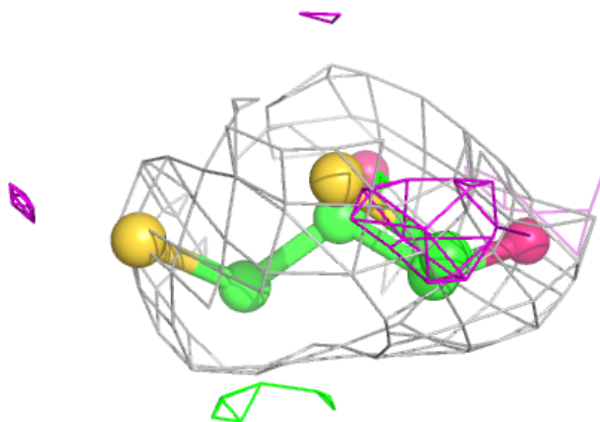
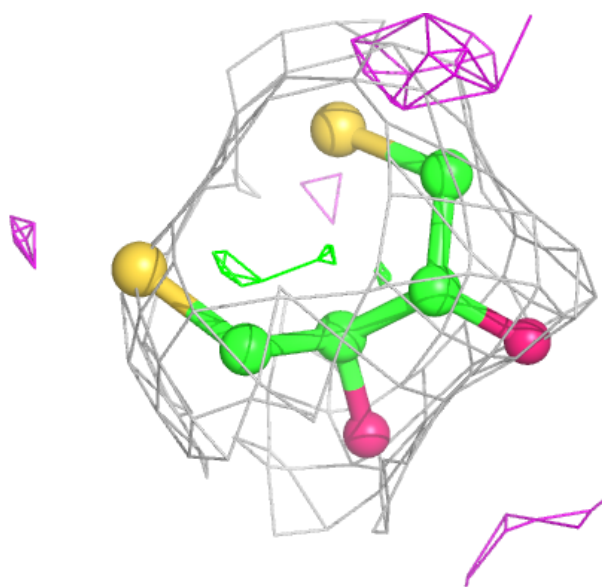
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





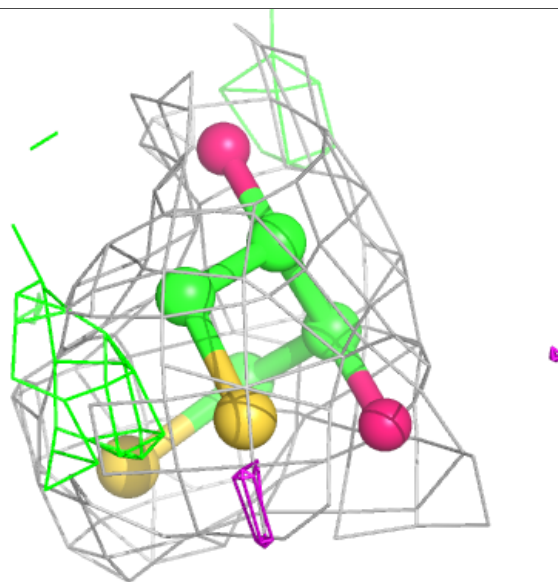
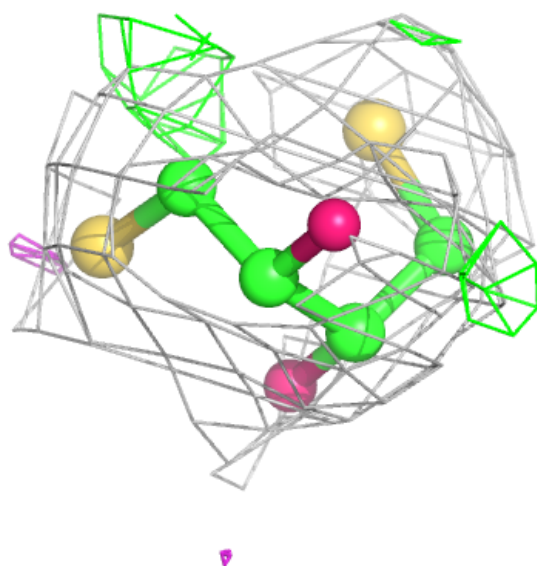
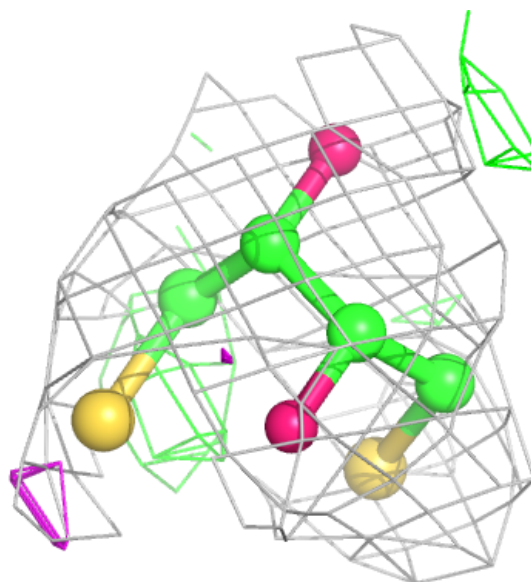
**Electron density around DTT B 503:**

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



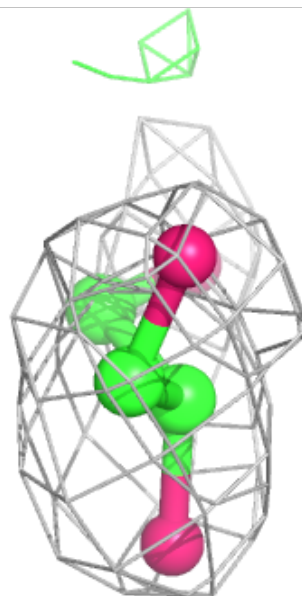
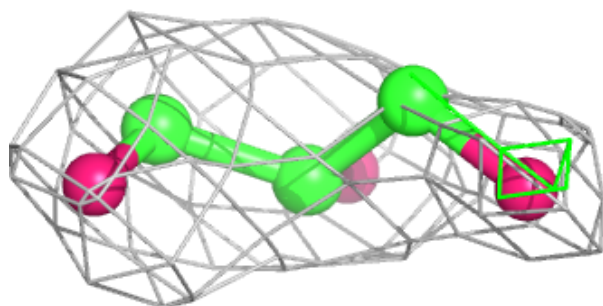
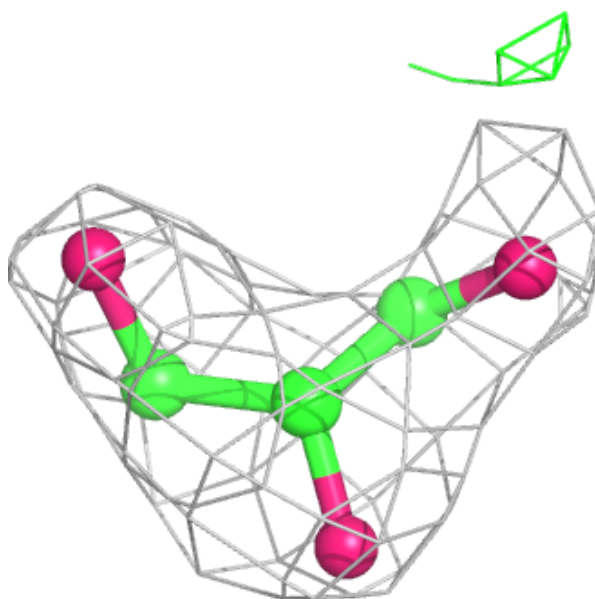
**Electron density around DTT A 506:**

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



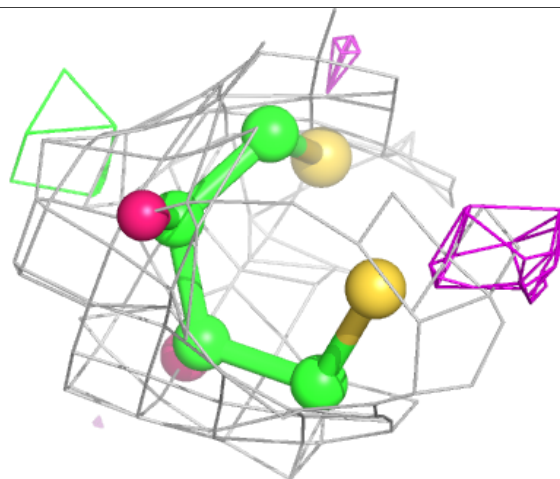
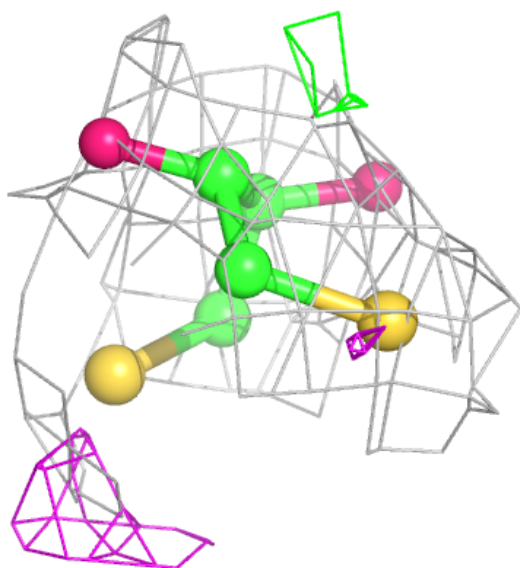
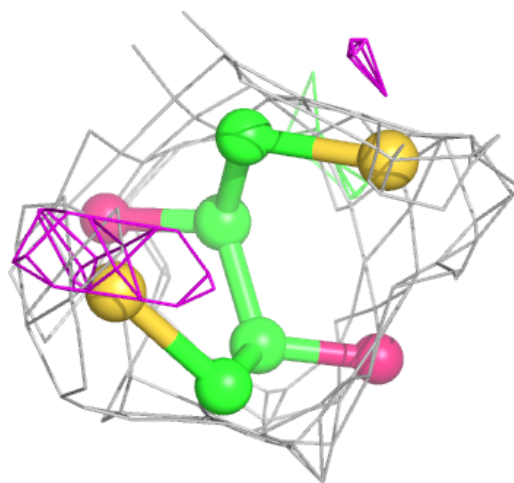
**Electron density around GOL A 502:**

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



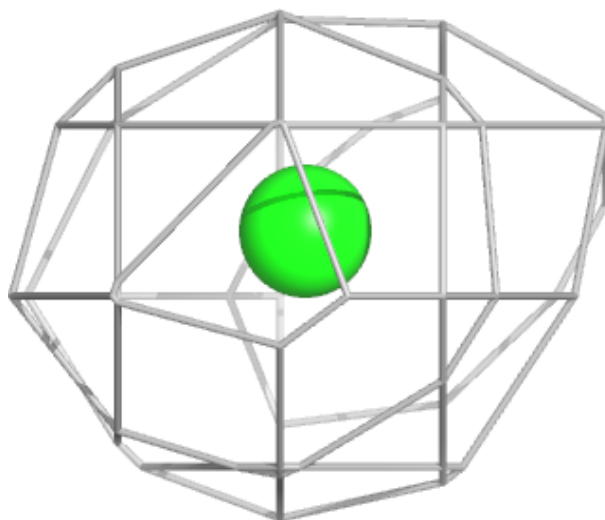
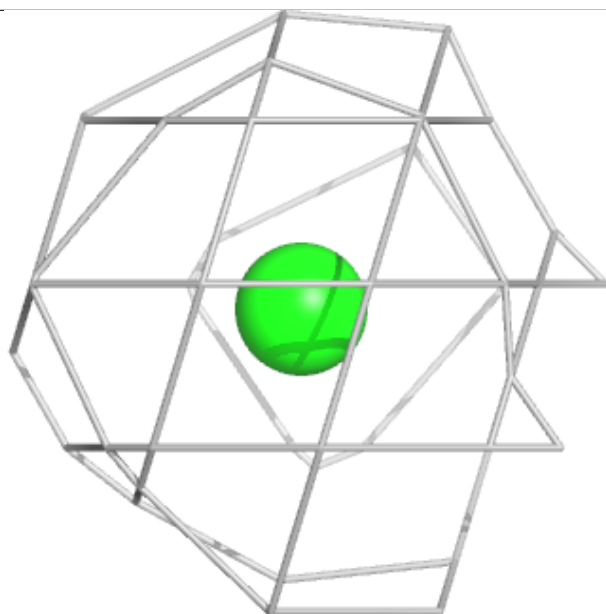
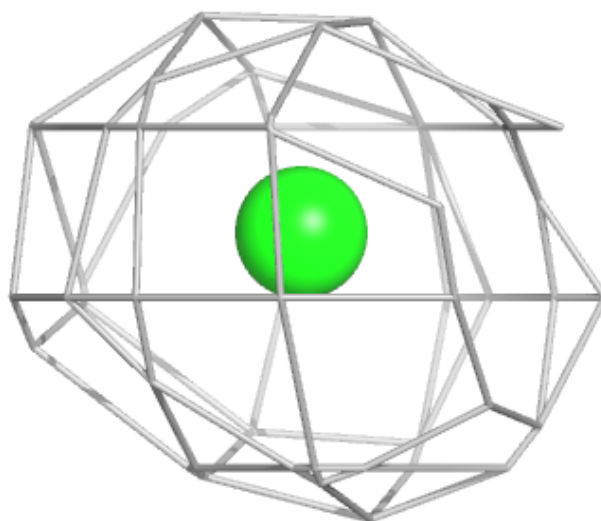
**Electron density around DTT C 506:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



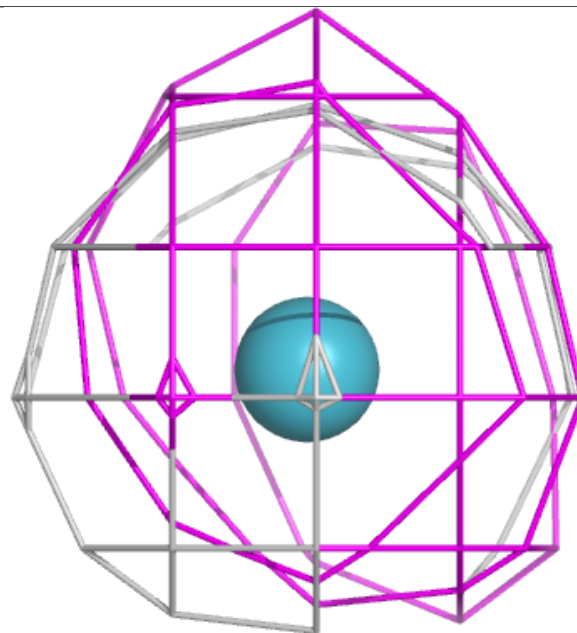
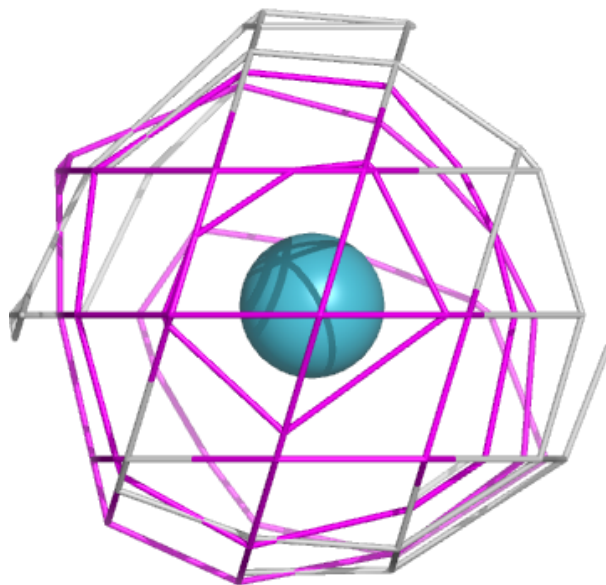
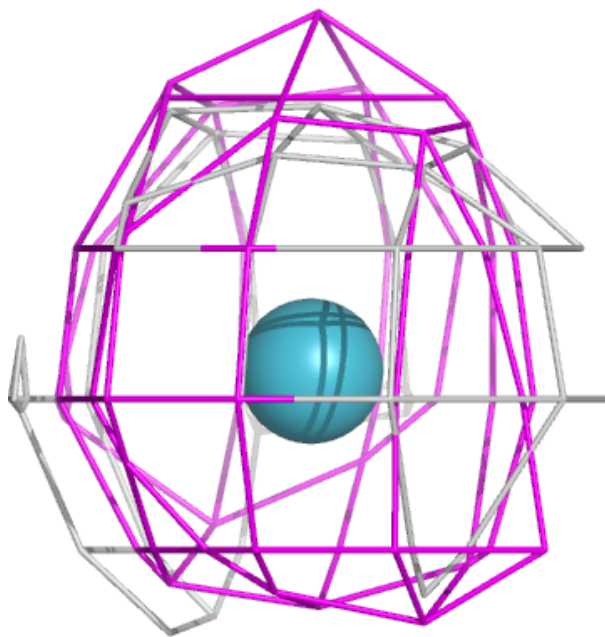
**Electron density around CL C 507:**

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



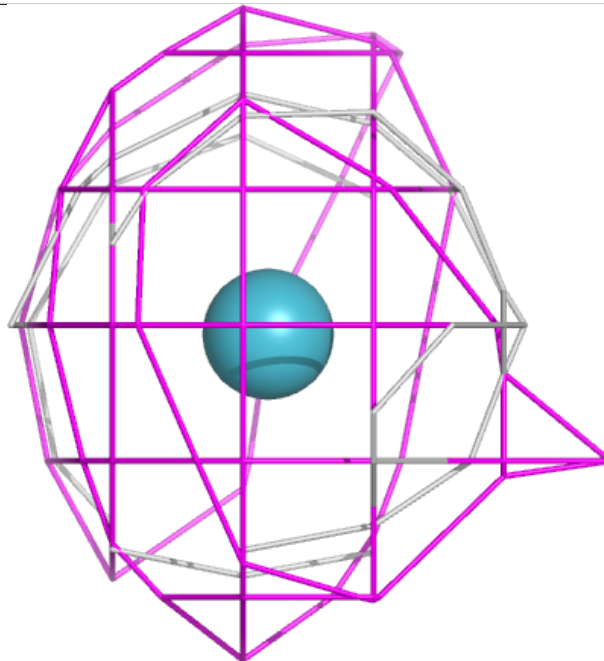
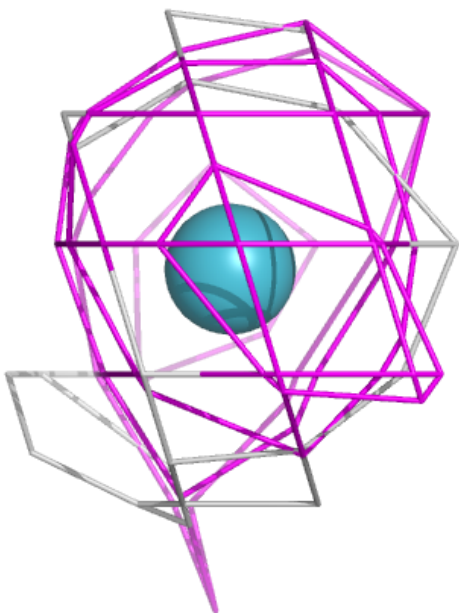
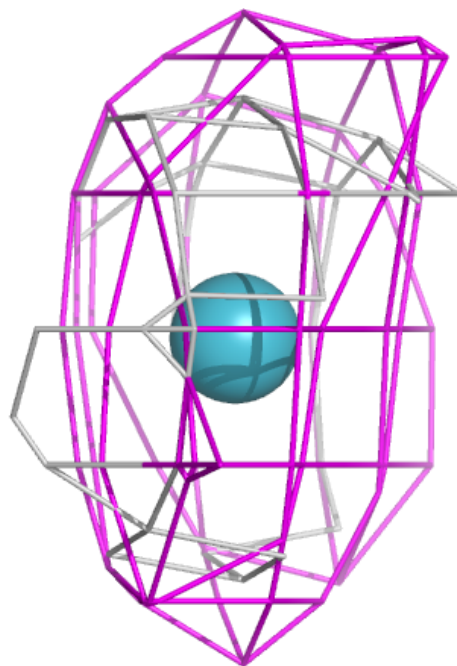
**Electron density around XE B 506:**

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



**Electron density around XE C 505:**

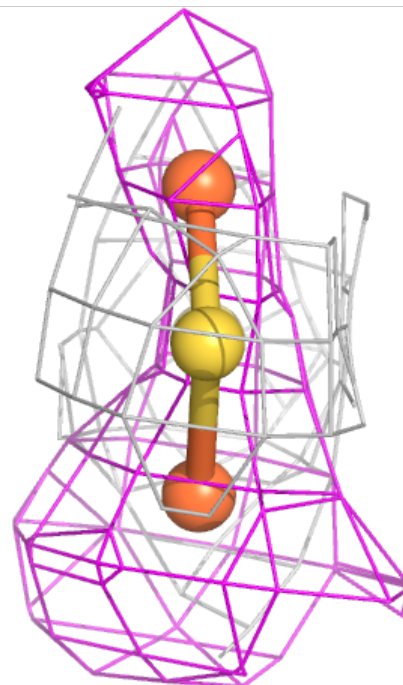
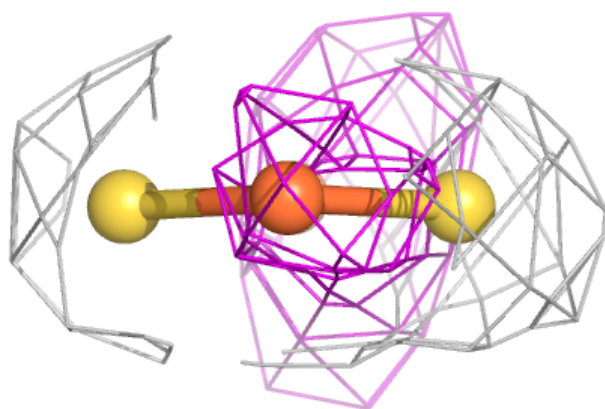
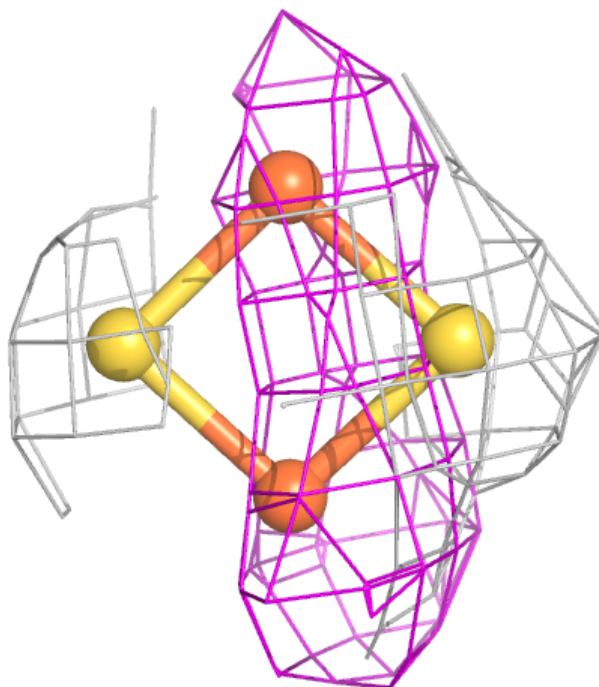
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FES B 501:**

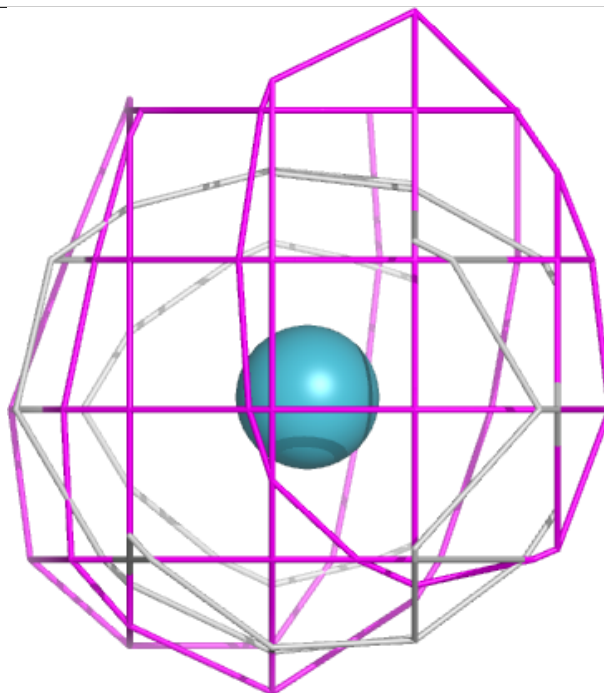
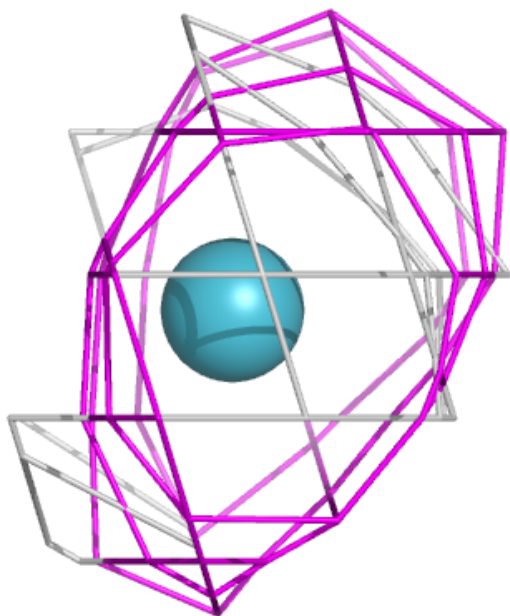
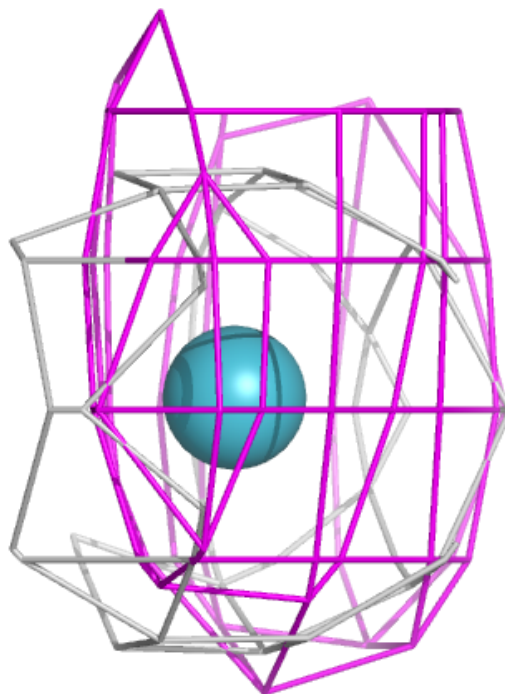
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





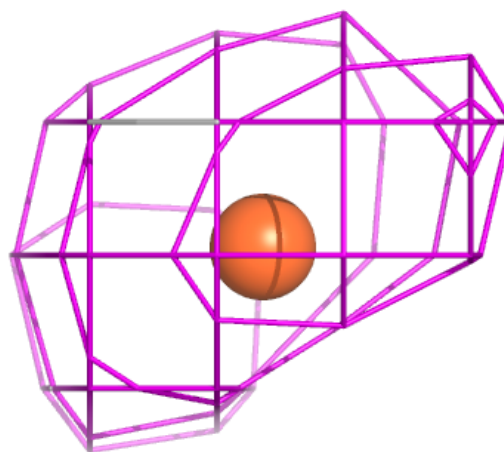
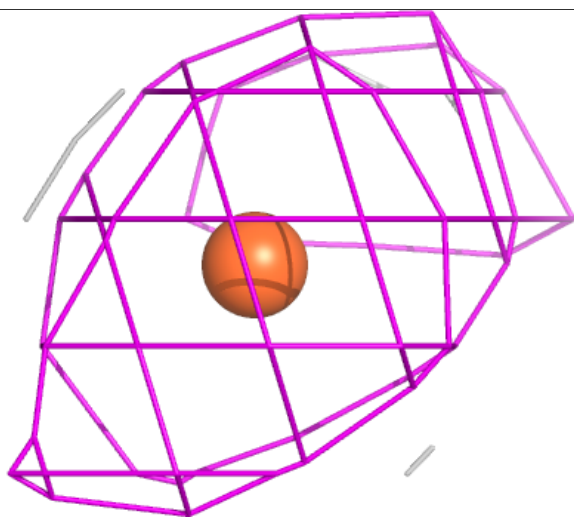
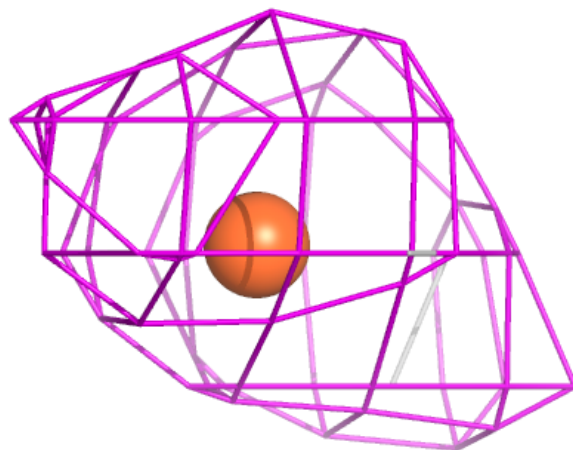
**Electron density around XE A 505:**

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



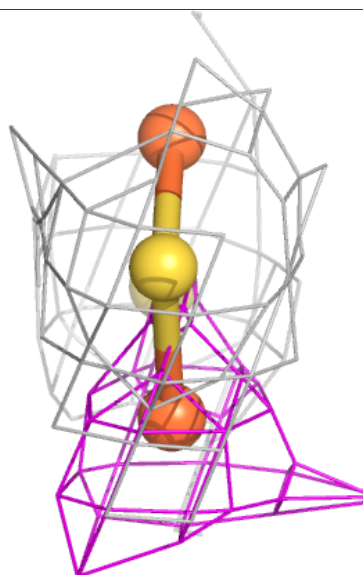
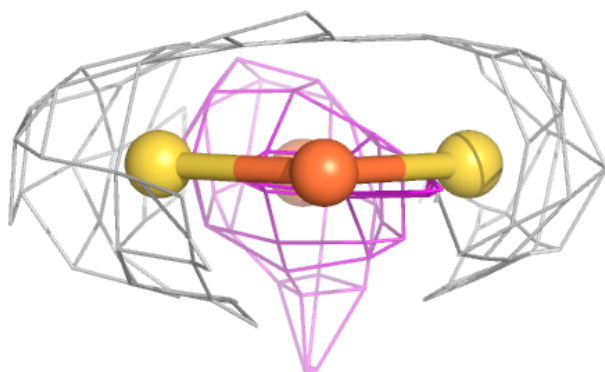
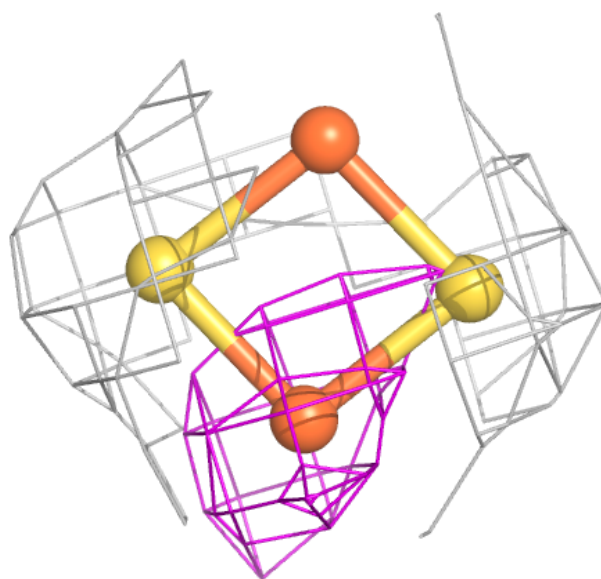
**Electron density around FE A 504:**

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



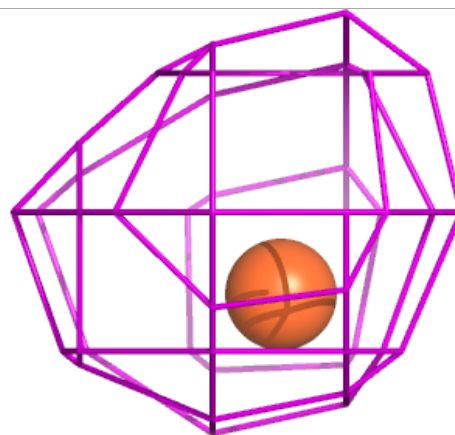
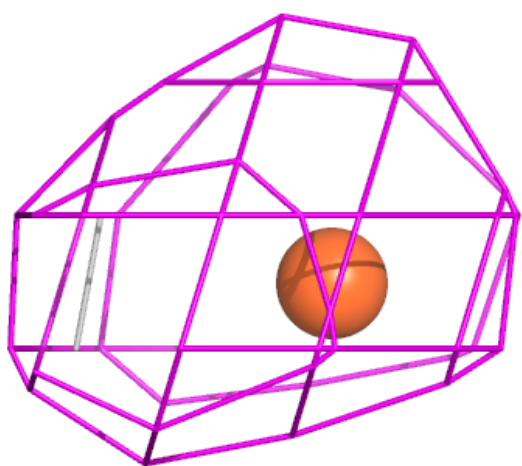
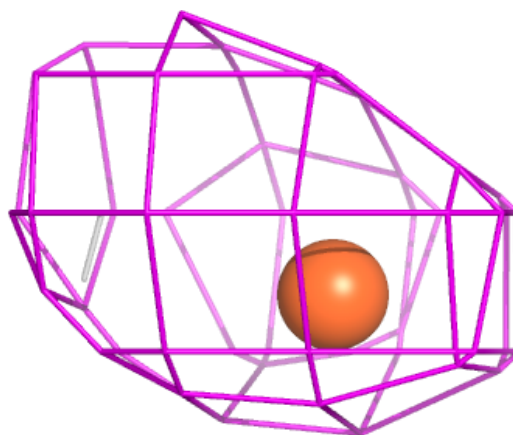
**Electron density around FES A 501:**

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



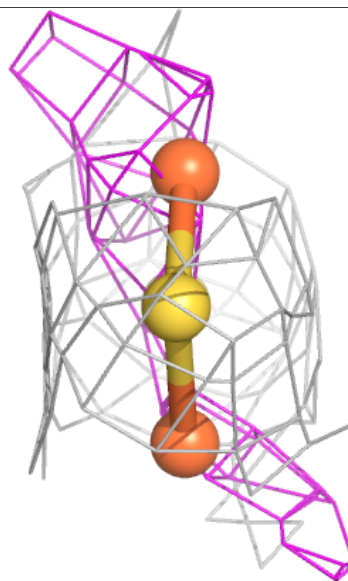
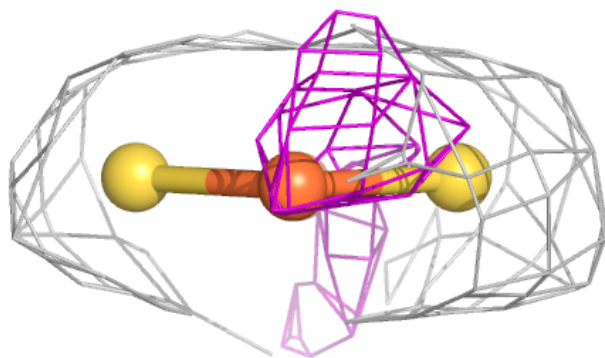
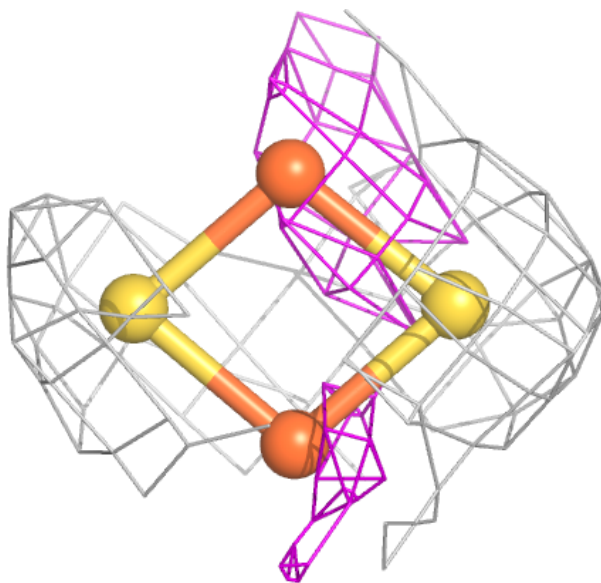
**Electron density around FE B 505:**

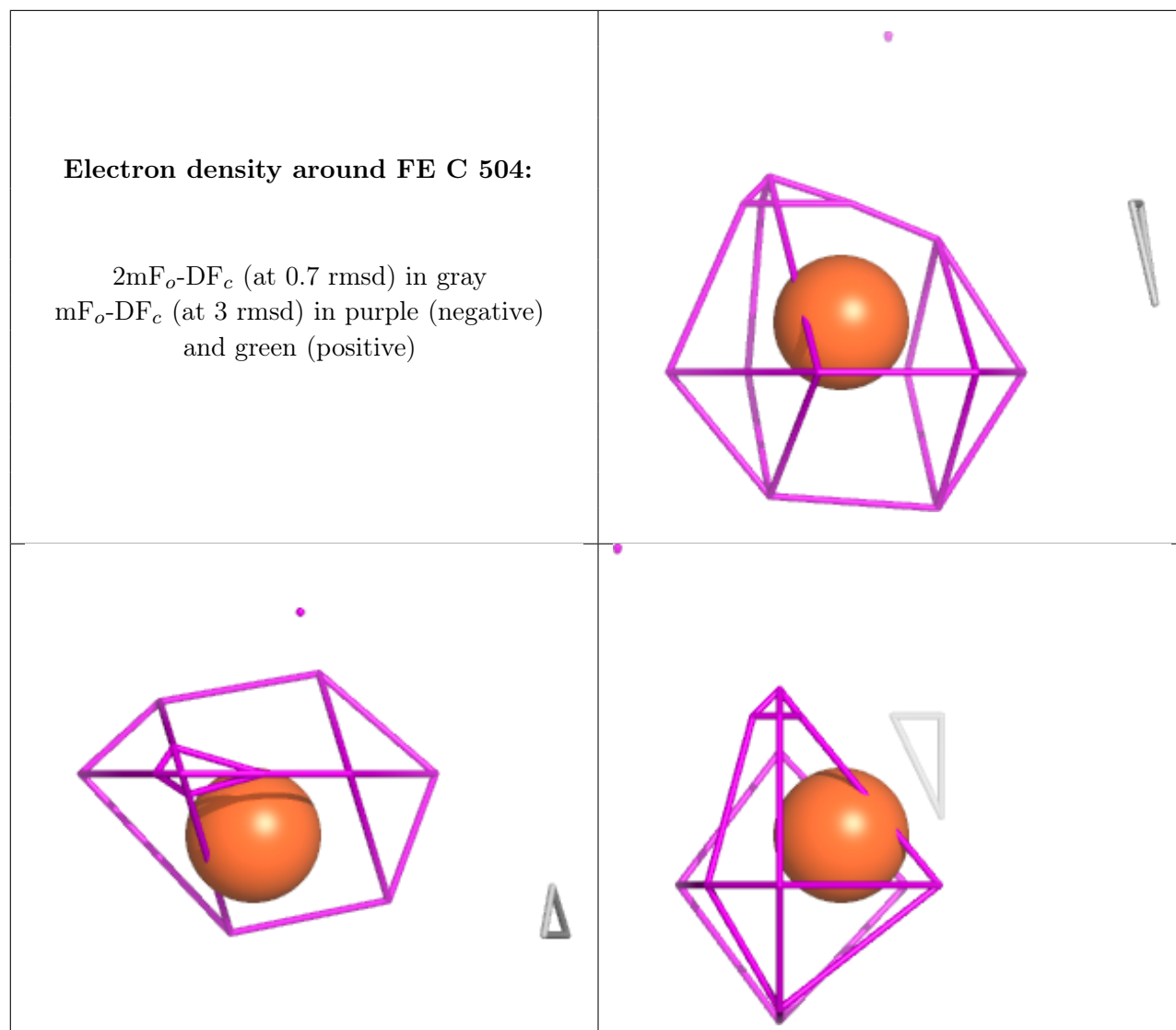
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FES 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.