



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 PM UTC

PDB ID : 8B5K / pdb_00008b5k
Title : Structure of haloalkane dehalogenase DmmarA from Mycobacterium marinum at pH 6.5
Authors : Snajdarova, K.; Marek, M.
Deposited on : 2022-09-23
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

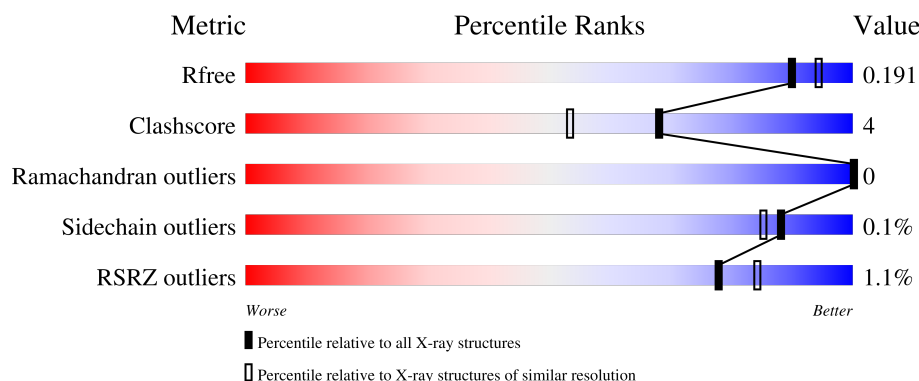
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

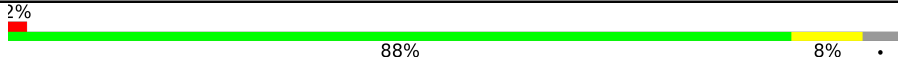
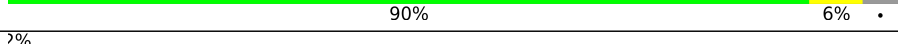
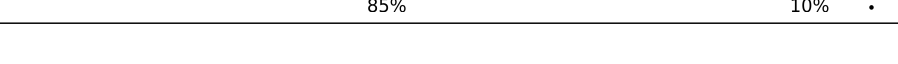
The reported resolution of this entry is 1.85 Å.

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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	296	
1	B	296	
1	C	296	
1	D	296	

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
3	FMT	A	303	-	X	-	-
3	FMT	B	303	-	X	-	-
3	FMT	C	401	-	X	-	-
3	FMT	C	403	-	X	-	-
3	FMT	C	404	-	X	-	-
3	FMT	D	301	-	X	-	-
3	FMT	D	302	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9668 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 Haloalkane dehalogenase DhaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	2	0
			2254	1436	390	419	9			
1	B	284	Total	C	N	O	S	0	1	0
			2250	1433	392	416	9			
1	C	284	Total	C	N	O	S	0	1	0
			2250	1433	392	416	9			
1	D	283	Total	C	N	O	S	0	0	0
			2233	1423	387	414	9			

There are 24 discrepancies between the modelled and reference sequences:

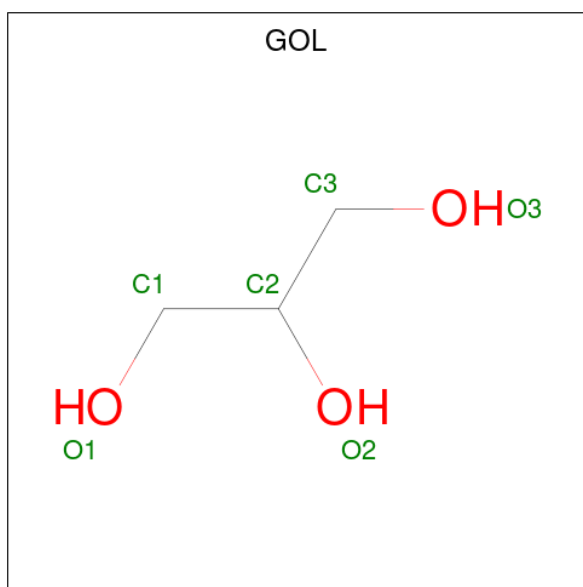
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	HIS	-	expression tag	UNP B2HR89
A	292	HIS	-	expression tag	UNP B2HR89
A	293	HIS	-	expression tag	UNP B2HR89
A	294	HIS	-	expression tag	UNP B2HR89
A	295	HIS	-	expression tag	UNP B2HR89
A	296	HIS	-	expression tag	UNP B2HR89
B	291	HIS	-	expression tag	UNP B2HR89
B	292	HIS	-	expression tag	UNP B2HR89
B	293	HIS	-	expression tag	UNP B2HR89
B	294	HIS	-	expression tag	UNP B2HR89
B	295	HIS	-	expression tag	UNP B2HR89
B	296	HIS	-	expression tag	UNP B2HR89
C	291	HIS	-	expression tag	UNP B2HR89
C	292	HIS	-	expression tag	UNP B2HR89
C	293	HIS	-	expression tag	UNP B2HR89
C	294	HIS	-	expression tag	UNP B2HR89
C	295	HIS	-	expression tag	UNP B2HR89
C	296	HIS	-	expression tag	UNP B2HR89
D	291	HIS	-	expression tag	UNP B2HR89
D	292	HIS	-	expression tag	UNP B2HR89
D	293	HIS	-	expression tag	UNP B2HR89

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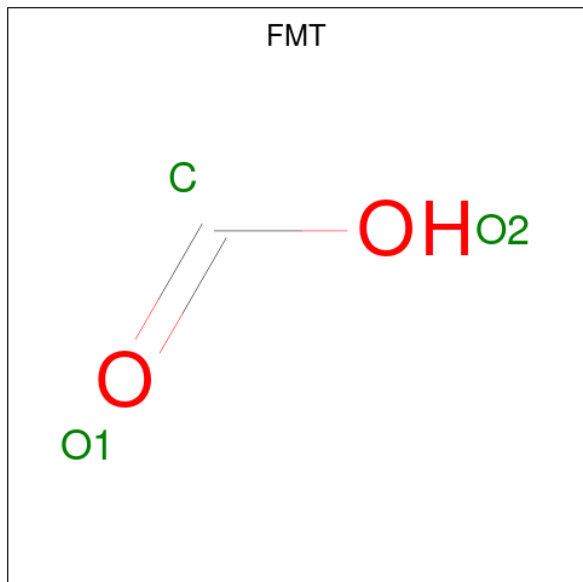
Chain	Residue	Modelled	Actual	Comment	Reference
D	294	HIS	-	expression tag	UNP B2HR89
D	295	HIS	-	expression tag	UNP B2HR89
D	296	HIS	-	expression tag	UNP B2HR89

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2) (labeled as "Ligand of Interest" by depositor).



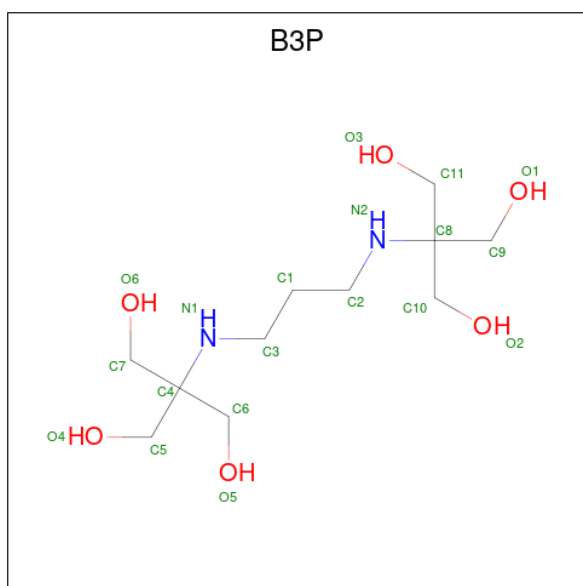
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $\text{C}_4\text{H}_{12}\text{NO}_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			19	11	2	6		

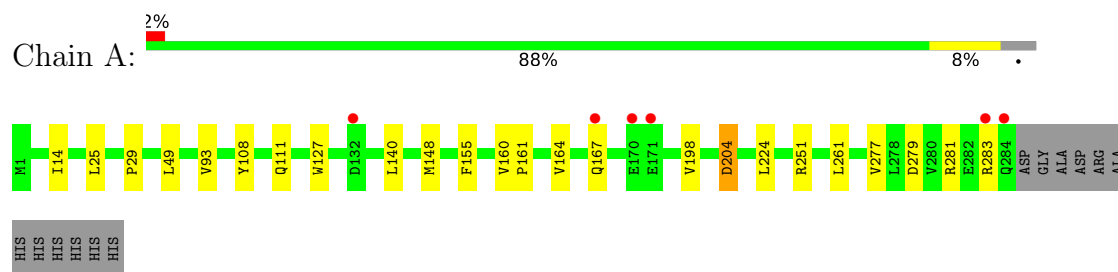
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total 134	O 134	0	0
6	B	156	Total 156	O 156	0	0
6	C	194	Total 194	O 194	0	0
6	D	95	Total 95	O 95	0	0

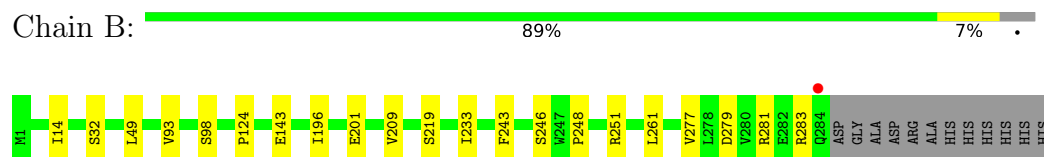
3 Residue-property plots

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.

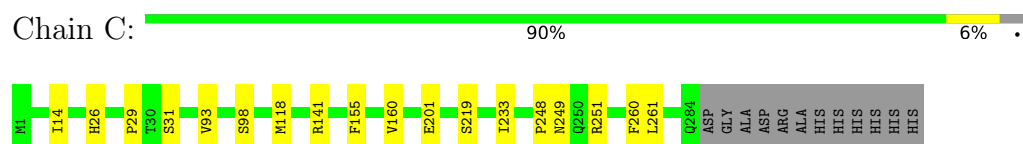
- Molecule 1: Haloalkane dehalogenase DhaA



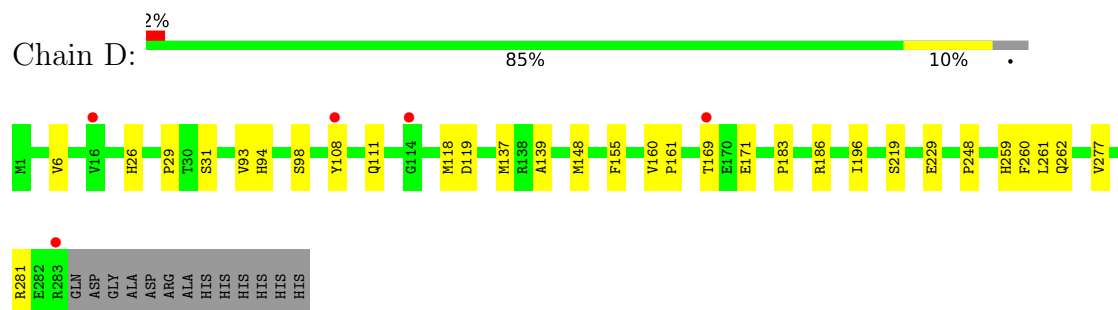
- Molecule 1: Haloalkane dehalogenase DhaA



- Molecule 1: Haloalkane dehalogenase DhaA



- Molecule 1: Haloalkane dehalogenase DhaA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.82Å 61.38Å 106.69Å 90.00° 106.26° 90.00°	Depositor
Resolution (Å)	44.07 – 1.85 44.07 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.07-1.85) 99.7 (44.07-1.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.191 , 0.241 0.194 , 0.191	Depositor DCC
R_{free} test set	4796 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9668	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: FMT, B3P, GOL, TRS

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	0.36	0/2315	0.54	0/3155
1	B	0.34	0/2311	0.54	0/3148
1	C	0.39	0/2311	0.59	0/3148
1	D	0.32	0/2291	0.51	0/3122
All	All	0.35	0/9228	0.55	0/12573

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2200	17	0
1	B	2250	0	2201	14	0
1	C	2250	0	2201	12	0
1	D	2233	0	2180	18	0
2	A	18	0	24	0	0
2	B	12	0	16	2	0
2	C	24	0	32	5	0
3	A	3	0	2	0	0
3	B	3	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	9	0	6	1	0
3	D	6	0	4	0	0
4	C	8	0	12	1	0
5	D	19	0	26	2	0
6	A	134	0	0	2	0
6	B	156	0	0	1	0
6	C	194	0	0	1	0
6	D	95	0	0	1	0
All	All	9668	0	8906	64	0

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

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:THR:HG22	1:D:171:GLU:H	1.59	0.67
1:B:243:PHE:O	1:B:246:SER:HB3	1.96	0.65
1:D:29:PRO:HG3	1:D:155:PHE:HB3	1.83	0.61
1:A:283:ARG:NH2	6:A:401:HOH:O	2.34	0.60
1:A:140:LEU:HD23	1:A:148:MET:HE3	1.85	0.59
1:C:201:GLU:HB3	2:C:406:GOL:H12	1.85	0.58
1:C:219:SER:O	1:C:248:PRO:HG2	2.04	0.57
1:C:233:ILE:HD11	2:C:408:GOL:H2	1.86	0.57
1:D:93:VAL:HB	1:D:98:SER:HA	1.86	0.56
1:B:196:ILE:HD13	2:B:302:GOL:H12	1.88	0.55
1:C:14:ILE:HD11	3:C:401:FMT:H	1.89	0.54
1:A:251:ARG:NH1	1:A:279:ASP:OD2	2.37	0.54
1:A:277:VAL:O	1:A:281:ARG:HG2	2.07	0.53
1:D:229:GLU:HA	1:D:229:GLU:OE1	2.09	0.53
1:B:14:ILE:HD12	1:B:32:SER:HB2	1.91	0.52
1:C:251:ARG:HH11	2:C:405:GOL:H11	1.75	0.52
1:A:224:LEU:HD12	1:A:251:ARG:HG3	1.90	0.51
1:D:137:MET:HE2	1:D:196:ILE:HD12	1.93	0.51
1:A:29:PRO:HG3	1:A:155:PHE:HB3	1.93	0.50
1:D:277:VAL:O	1:D:281:ARG:HG2	2.12	0.50
1:A:160:VAL:O	1:A:164[B]:VAL:HG12	2.13	0.49
1:D:219:SER:O	1:D:248:PRO:HG2	2.13	0.49
1:C:29:PRO:HG3	1:C:155:PHE:HB3	1.95	0.48
1:A:167:GLN:NE2	1:A:167:GLN:H	2.12	0.48
1:C:93:VAL:HB	1:C:98:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:H	1:A:261:LEU:HD23	1.80	0.47
1:B:279:ASP:HB3	1:B:283:ARG:NH1	2.30	0.47
1:B:93:VAL:HB	1:B:98:SER:HA	1.97	0.46
1:A:127:TRP:CE2	1:A:198:VAL:HG11	2.50	0.46
1:D:139:ALA:C	1:D:148:MET:HE1	2.41	0.46
1:C:141:ARG:NH2	2:C:406:GOL:H32	2.31	0.46
5:D:303:B3P:H61	5:D:303:B3P:H31	1.71	0.46
1:D:160:VAL:HA	1:D:260:PHE:CE2	2.50	0.45
1:D:183:PRO:HA	1:D:186:ARG:HD2	1.97	0.45
5:D:303:B3P:N2	6:D:403:HOH:O	2.35	0.45
1:C:249:ASN:O	2:C:405:GOL:H31	2.17	0.45
1:B:233:ILE:HD11	2:B:302:GOL:H2	1.99	0.45
1:B:219:SER:O	1:B:248:PRO:HG2	2.18	0.44
1:D:119:ASP:OD2	1:D:259:HIS:ND1	2.45	0.44
1:A:14:ILE:O	1:A:49:LEU:HA	2.18	0.43
1:B:124:PRO:HD3	1:B:209:VAL:HG12	2.00	0.43
1:B:143:GLU:H	1:B:143:GLU:CD	2.25	0.43
1:B:201:GLU:OE2	6:B:401:HOH:O	2.21	0.43
1:B:277:VAL:O	1:B:281:ARG:HG2	2.18	0.43
1:A:108:TYR:HB3	1:A:111:GLN:HG3	2.00	0.43
1:C:160:VAL:HA	1:C:260:PHE:CE2	2.54	0.43
1:A:167:GLN:H	1:A:167:GLN:CD	2.27	0.43
1:B:251:ARG:NH1	1:B:283:ARG:HH12	2.17	0.42
1:D:160:VAL:HB	1:D:161:PRO:HD3	2.01	0.42
1:D:108:TYR:HB3	1:D:111:GLN:HG3	2.01	0.42
1:B:14:ILE:O	1:B:49:LEU:HA	2.18	0.42
1:D:6:VAL:HG23	1:D:6:VAL:O	2.20	0.42
1:A:160:VAL:HB	1:A:161:PRO:HD3	2.01	0.42
1:C:26:HIS:CD2	1:C:31:SER:HA	2.55	0.42
4:C:407:TRS:H32	6:C:546:HOH:O	2.19	0.42
1:D:261:LEU:HD23	1:D:261:LEU:H	1.84	0.42
1:D:118:MET:HG3	1:D:261:LEU:HD21	2.03	0.41
1:D:26:HIS:CD2	1:D:31:SER:HA	2.56	0.41
1:C:118:MET:HG3	1:C:261:LEU:HD21	2.02	0.40
1:B:261:LEU:H	1:B:261:LEU:HD23	1.87	0.40
1:D:94:HIS:CG	1:D:262:GLN:HE22	2.39	0.40
1:A:25:LEU:HB2	1:A:93:VAL:HG12	2.03	0.40
1:A:164[B]:VAL:HG13	6:A:447:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/296 (96%)	273 (96%)	11 (4%)	0	100	100
1	B	283/296 (96%)	271 (96%)	12 (4%)	0	100	100
1	C	283/296 (96%)	272 (96%)	11 (4%)	0	100	100
1	D	281/296 (95%)	267 (95%)	14 (5%)	0	100	100
All	All	1131/1184 (96%)	1083 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/244 (97%)	235 (99%)	2 (1%)	73	65
1	B	236/244 (97%)	236 (100%)	0	100	100
1	C	236/244 (97%)	236 (100%)	0	100	100
1	D	234/244 (96%)	234 (100%)	0	100	100
All	All	943/976 (97%)	941 (100%)	2 (0%)	88	84

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

Mol	Chain	Res	Type
1	A	204[A]	ASP
1	A	204[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	167	GLN
1	A	210	GLN
1	B	165	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](#)

18 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	$\# Z > 2$
3	FMT	B	303	-	2,2,2	2.96	2 (100%)	1,1,1	1.51	0
2	GOL	C	406	-	5,5,5	0.52	0	5,5,5	0.44	0
3	FMT	C	401	-	2,2,2	2.93	2 (100%)	1,1,1	1.48	0
4	TRS	C	407	-	7,7,7	0.19	0	9,9,9	0.19	0
5	B3P	D	303	-	18,18,18	0.69	0	23,23,23	1.31	3 (13%)
3	FMT	C	404	-	2,2,2	2.88	2 (100%)	1,1,1	1.64	0
3	FMT	C	403	-	2,2,2	2.97	2 (100%)	1,1,1	1.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	D	302	-	2,2,2	2.93	2 (100%)	1,1,1	1.69	0
2	GOL	A	301	-	5,5,5	0.58	0	5,5,5	0.45	0
2	GOL	C	408	-	5,5,5	0.38	0	5,5,5	0.31	0
3	FMT	D	301	-	2,2,2	2.95	2 (100%)	1,1,1	1.46	0
2	GOL	A	302	-	5,5,5	0.50	0	5,5,5	0.32	0
2	GOL	B	302	-	5,5,5	0.47	0	5,5,5	0.55	0
3	FMT	A	303	-	2,2,2	2.92	2 (100%)	1,1,1	1.21	0
2	GOL	A	304	-	5,5,5	0.59	0	5,5,5	0.46	0
2	GOL	B	301	-	5,5,5	0.62	0	5,5,5	0.46	0
2	GOL	C	402	-	5,5,5	0.49	0	5,5,5	0.70	0
2	GOL	C	405	-	5,5,5	0.48	0	5,5,5	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	406	-	-	2/4/4/4	-
4	TRS	C	407	-	-	0/9/9/9	-
5	B3P	D	303	-	-	4/28/28/28	-
2	GOL	A	301	-	-	2/4/4/4	-
2	GOL	C	408	-	-	0/4/4/4	-
2	GOL	A	302	-	-	0/4/4/4	-
2	GOL	B	302	-	-	4/4/4/4	-
2	GOL	A	304	-	-	2/4/4/4	-
2	GOL	B	301	-	-	0/4/4/4	-
2	GOL	C	402	-	-	2/4/4/4	-
2	GOL	C	405	-	-	0/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	FMT	O1-C	3.47	1.41	1.22
3	B	303	FMT	O1-C	3.44	1.41	1.22
3	C	403	FMT	O1-C	3.40	1.40	1.22
3	D	302	FMT	O1-C	3.40	1.40	1.22
3	C	401	FMT	O1-C	3.39	1.40	1.22
3	D	301	FMT	O1-C	3.39	1.40	1.22
3	C	404	FMT	O1-C	3.35	1.40	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	FMT	O2-C	2.47	1.41	1.28
3	D	301	FMT	O2-C	2.44	1.41	1.28
3	C	401	FMT	O2-C	2.38	1.40	1.28
3	B	303	FMT	O2-C	2.38	1.40	1.28
3	D	302	FMT	O2-C	2.37	1.40	1.28
3	C	404	FMT	O2-C	2.33	1.40	1.28
3	A	303	FMT	O2-C	2.24	1.40	1.28

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	303	B3P	C3-N1-C4	-3.44	111.13	116.17
5	D	303	B3P	C2-N2-C8	-2.60	112.36	116.17
5	D	303	B3P	O4-C5-C4	-2.41	106.78	111.68

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	302	GOL	O1-C1-C2-O2
2	B	302	GOL	O1-C1-C2-C3
2	B	302	GOL	C1-C2-C3-O3
2	C	402	GOL	O1-C1-C2-C3
2	C	406	GOL	C1-C2-C3-O3
2	C	406	GOL	O2-C2-C3-O3
5	D	303	B3P	N2-C8-C9-O1
5	D	303	B3P	C10-C8-C9-O1
5	D	303	B3P	C11-C8-C9-O1
2	A	304	GOL	O1-C1-C2-O2
2	A	304	GOL	O1-C1-C2-C3
2	C	402	GOL	O1-C1-C2-O2
5	D	303	B3P	C3-C1-C2-N2
2	B	302	GOL	O2-C2-C3-O3
2	A	301	GOL	O1-C1-C2-C3
2	A	301	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

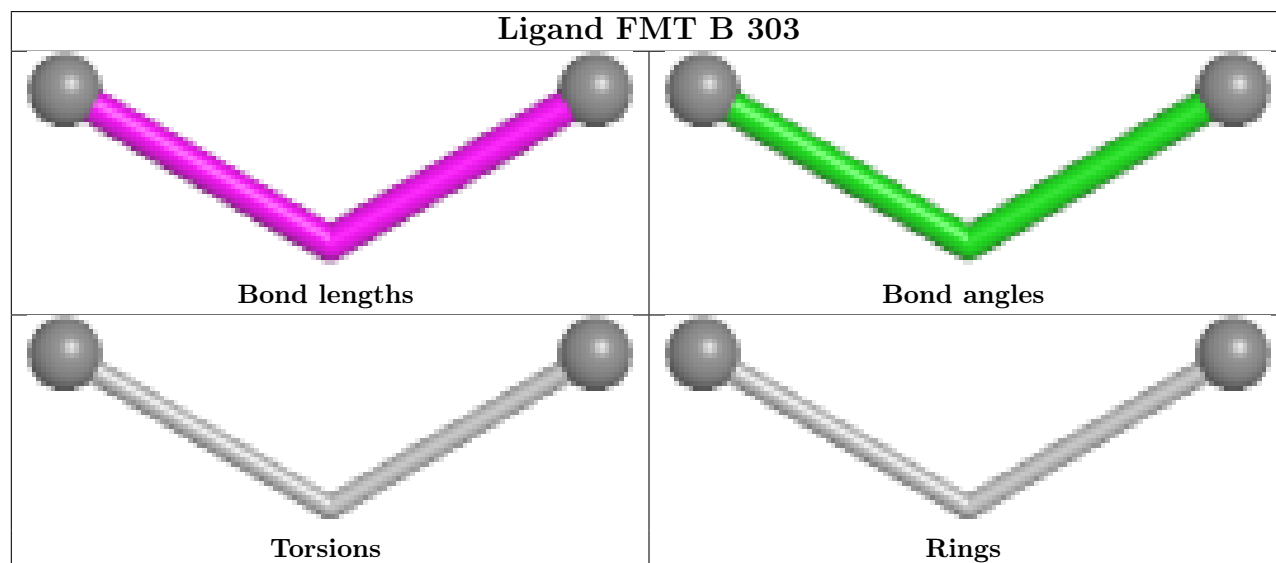
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	406	GOL	2	0

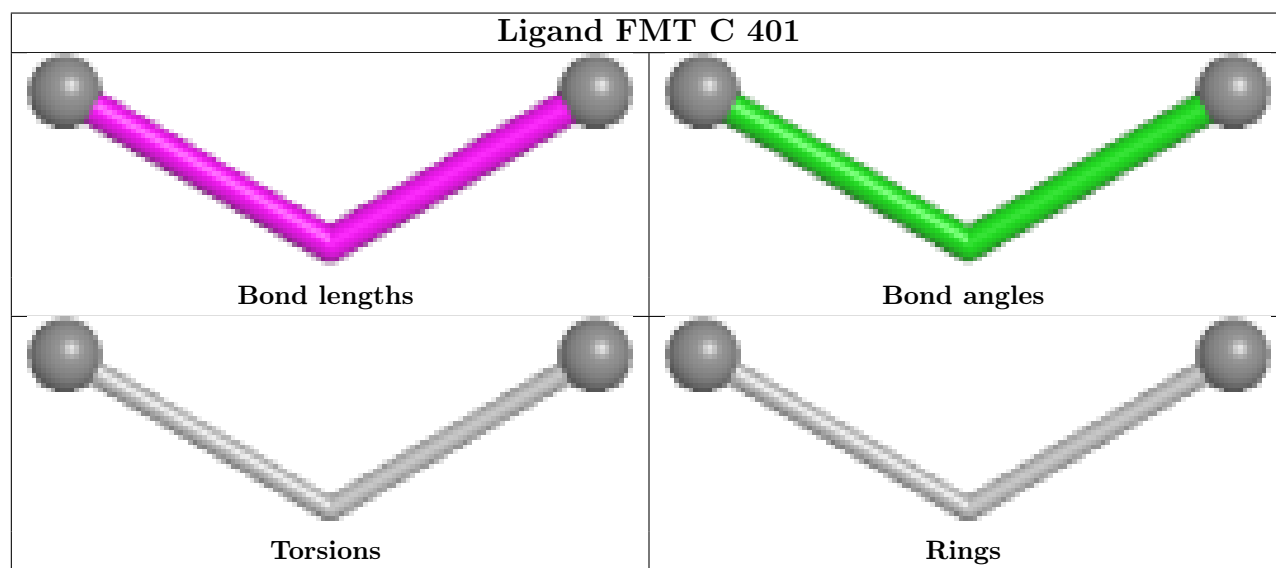
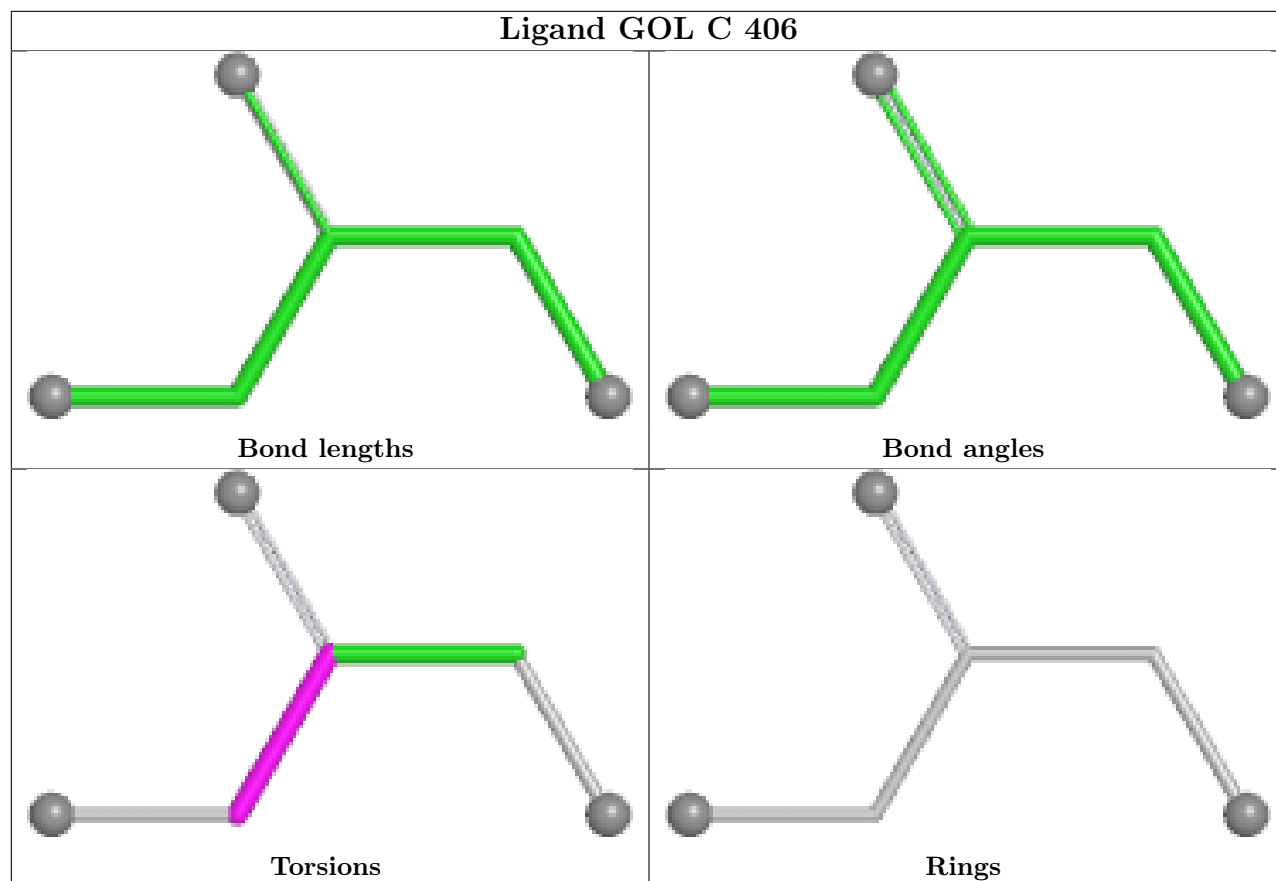
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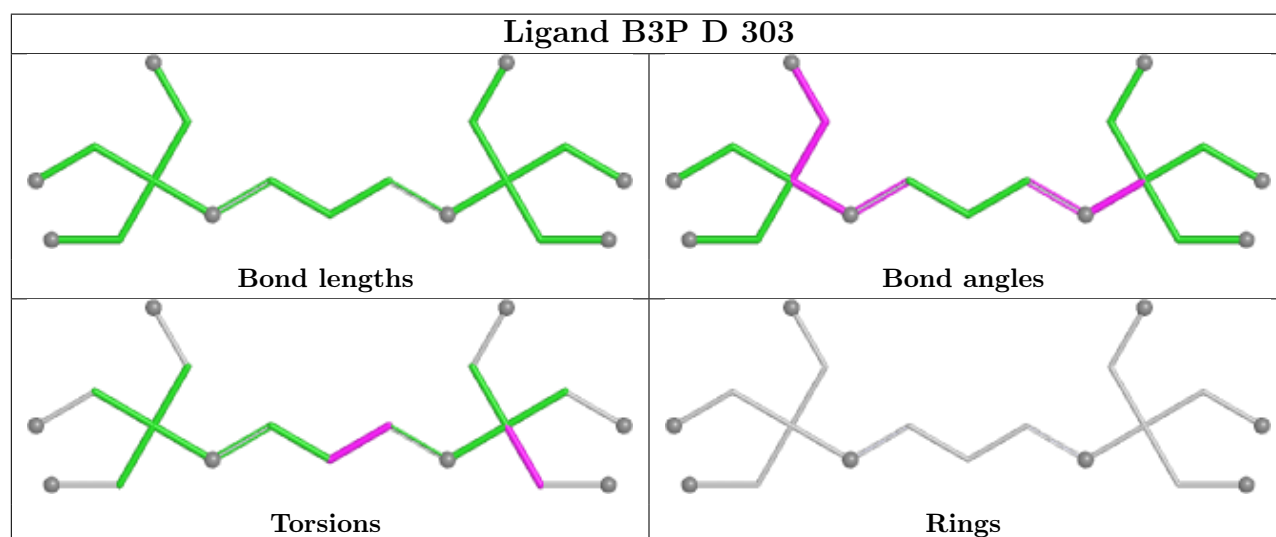
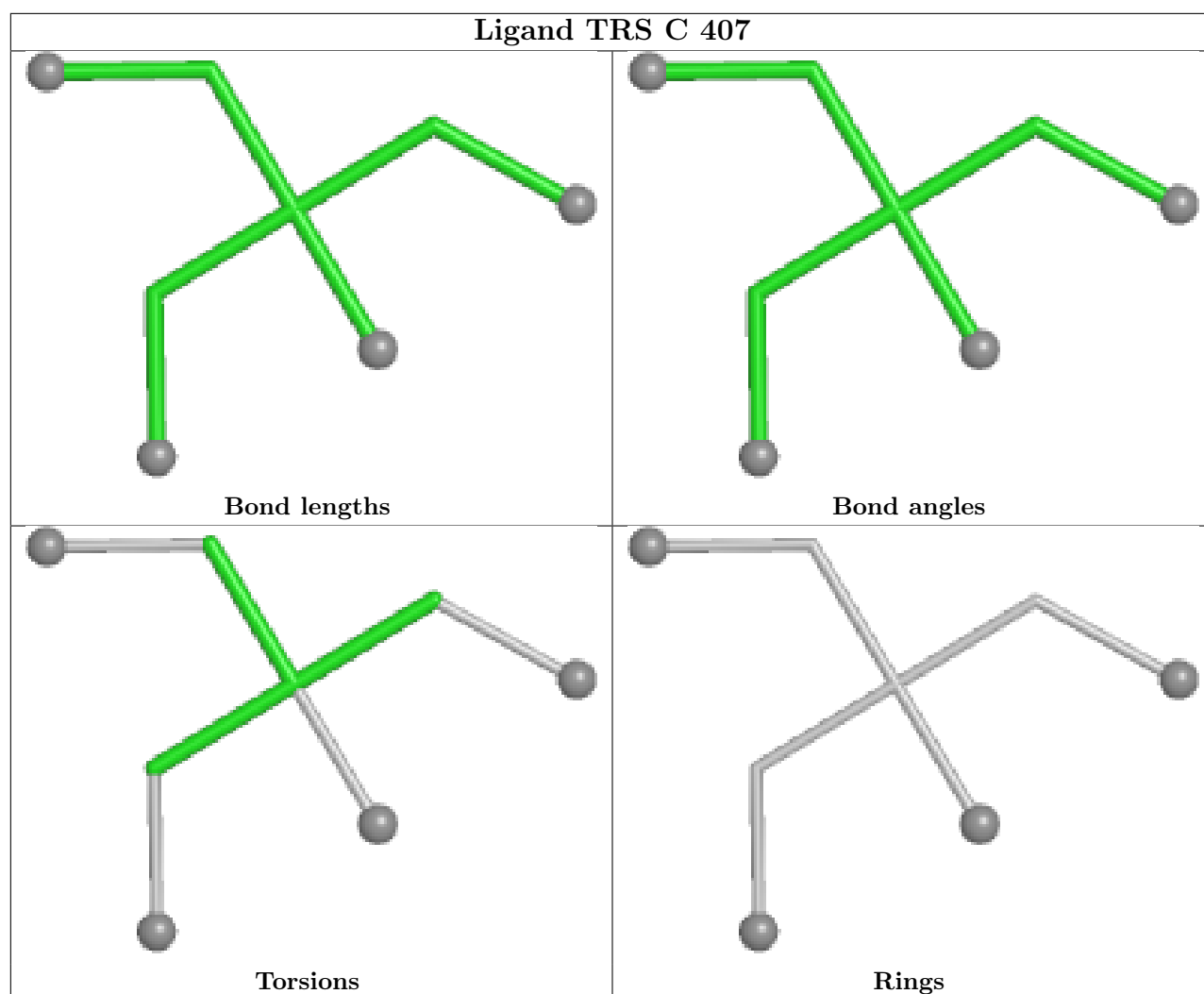
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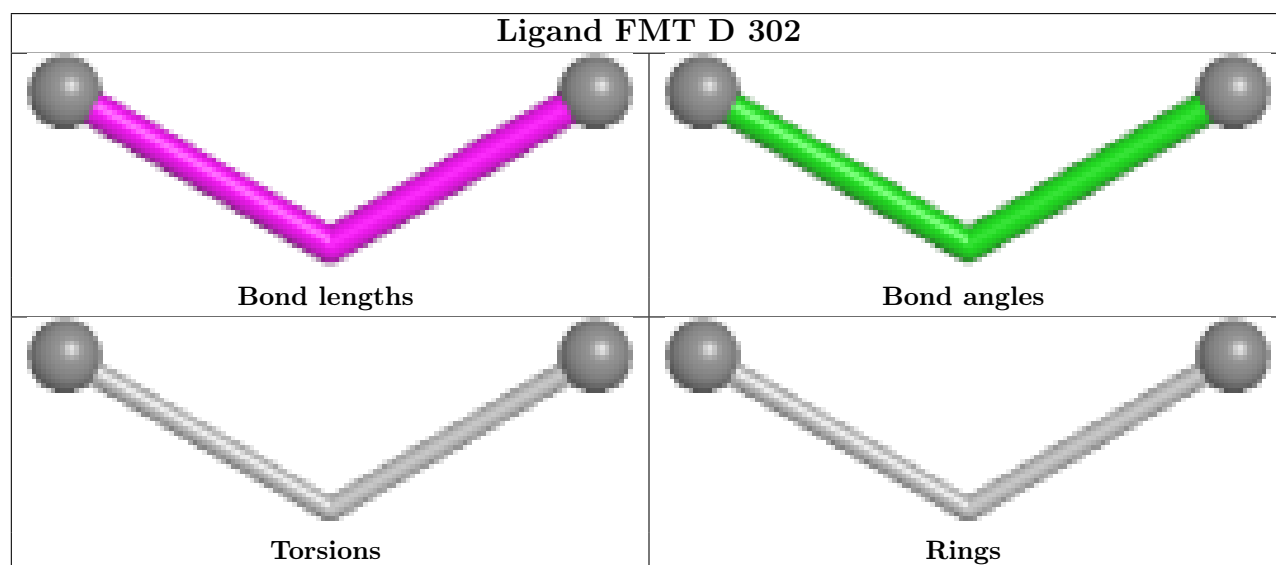
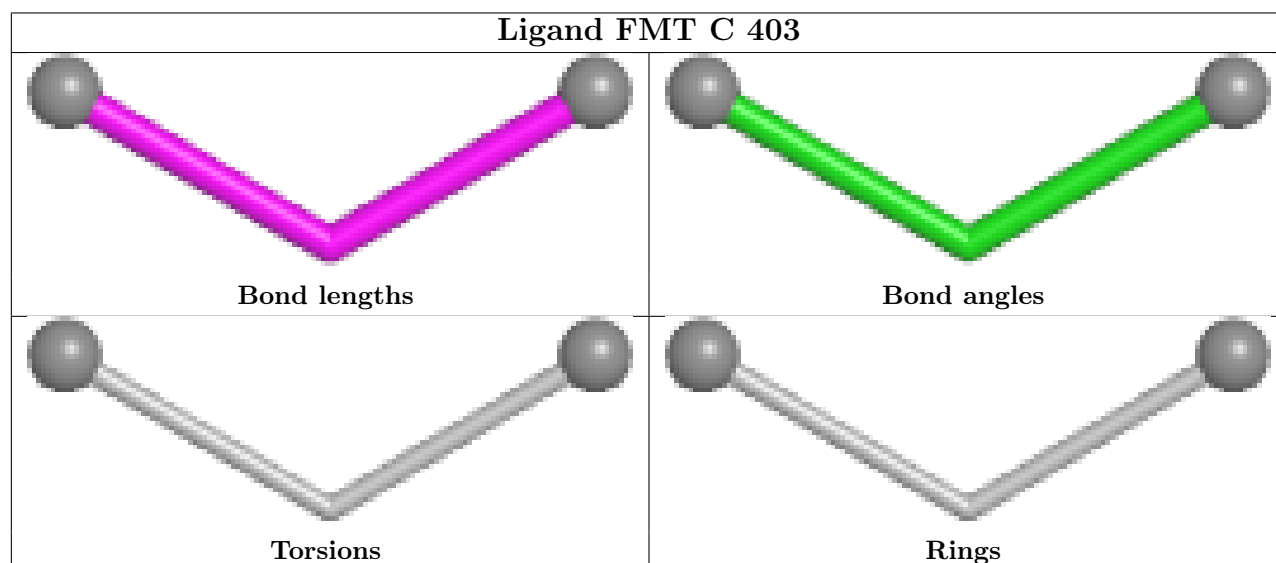
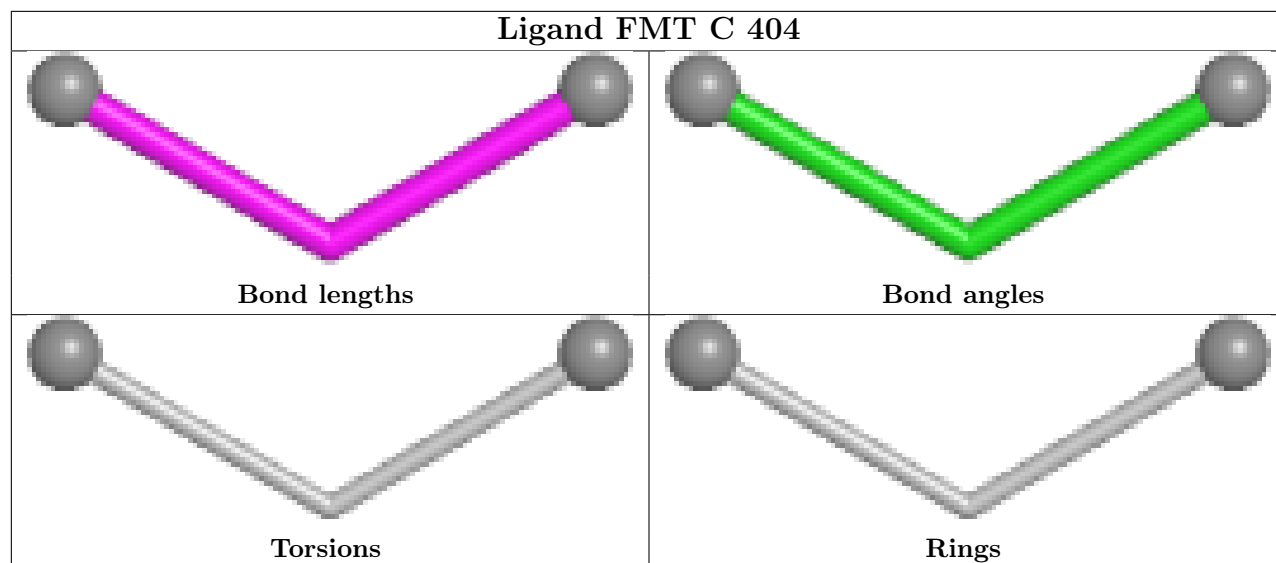
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	FMT	1	0
4	C	407	TRS	1	0
5	D	303	B3P	2	0
2	C	408	GOL	1	0
2	B	302	GOL	2	0
2	C	405	GOL	2	0

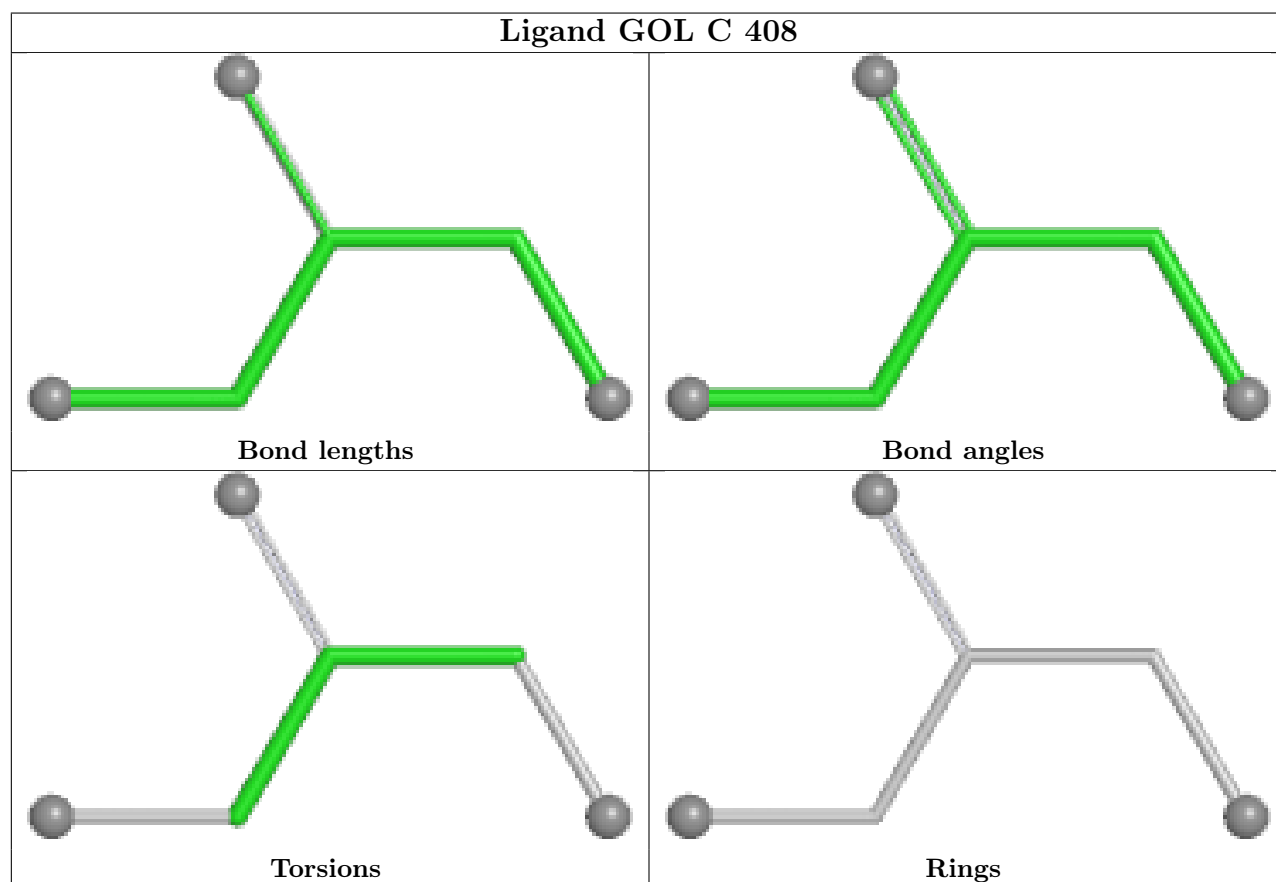
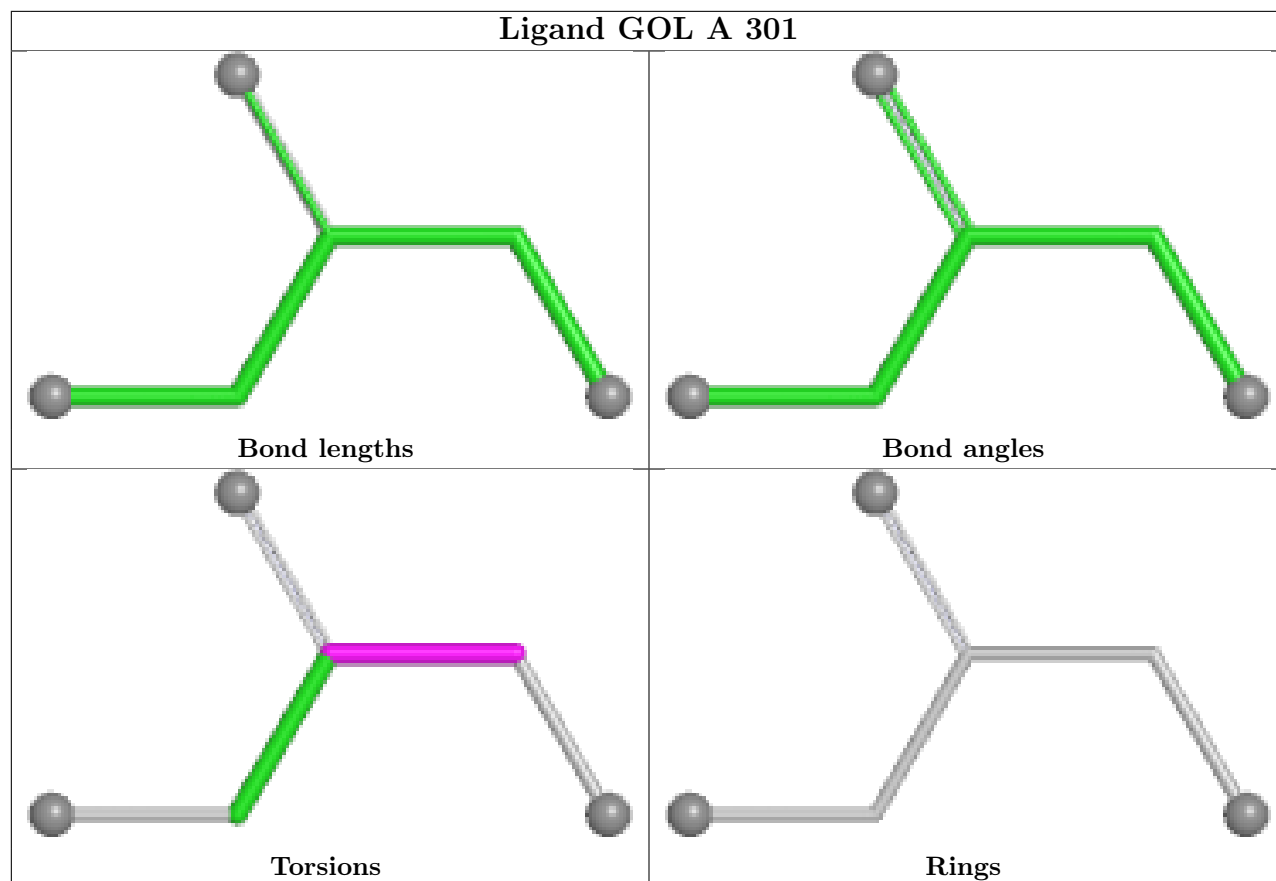
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

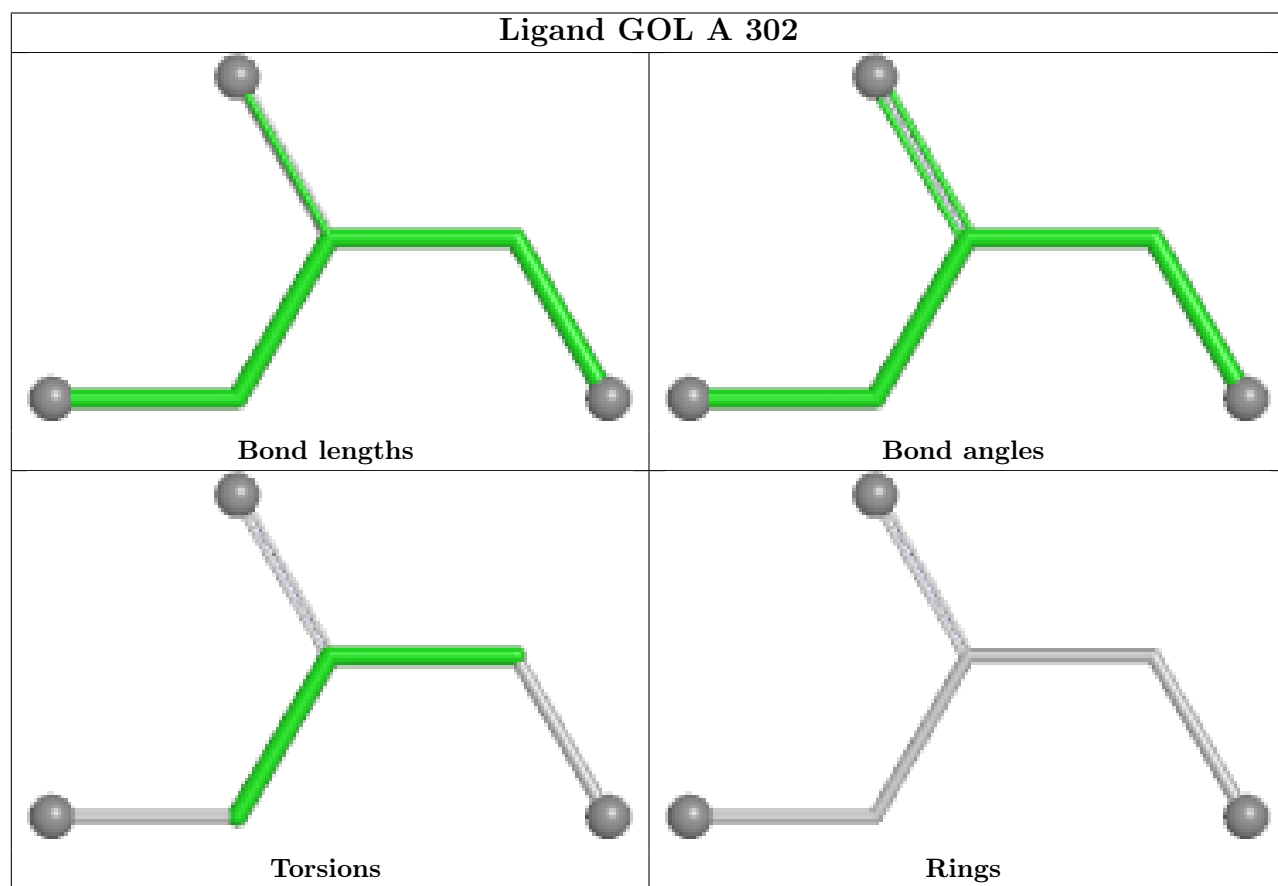
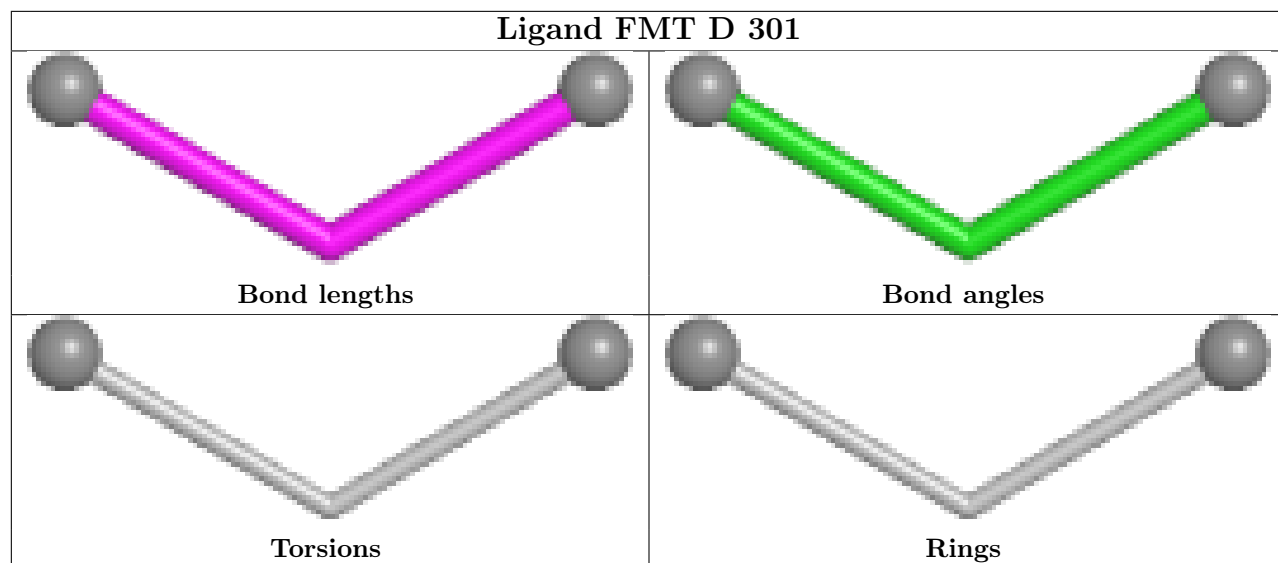


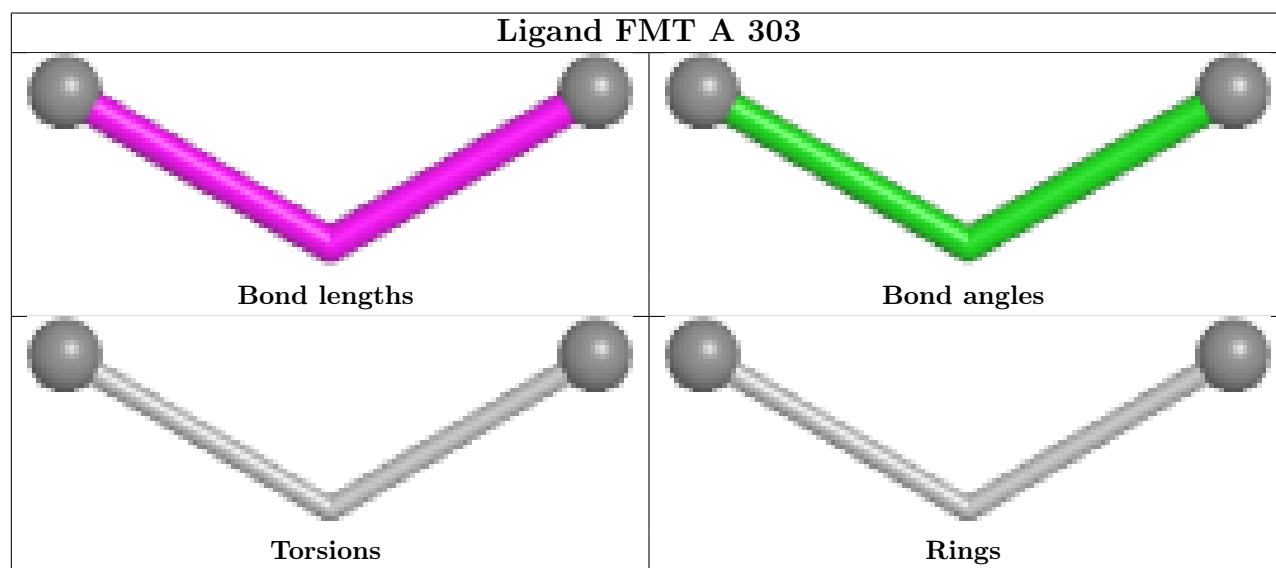
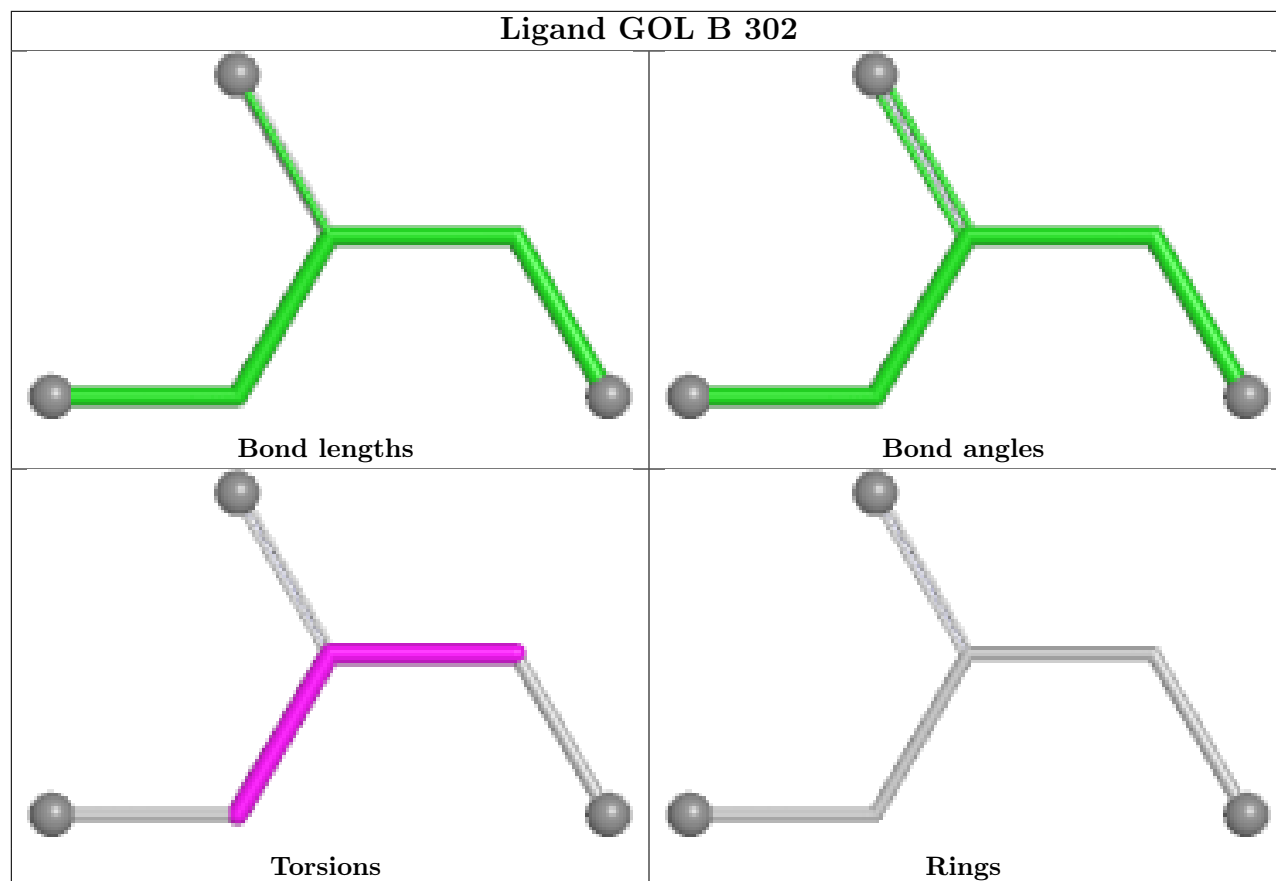


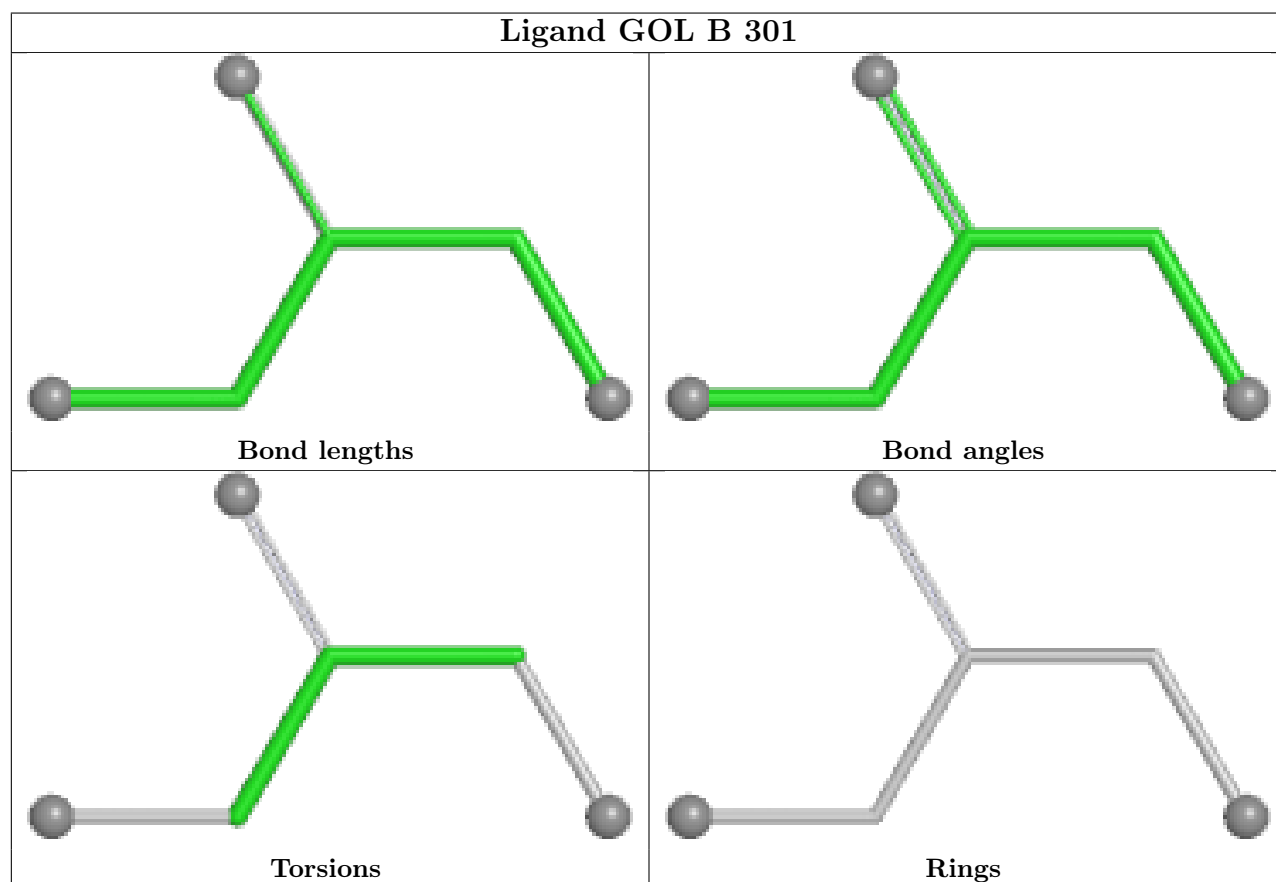
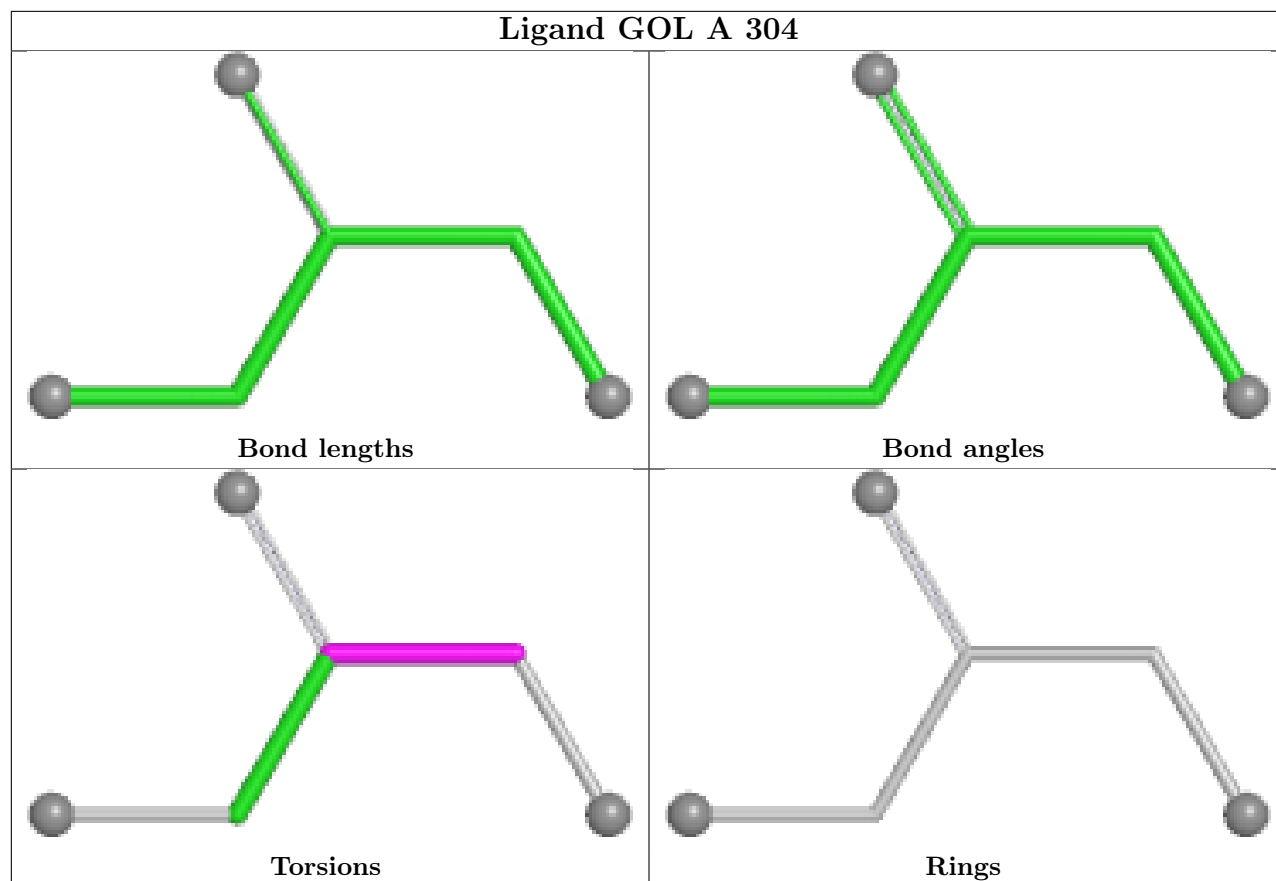


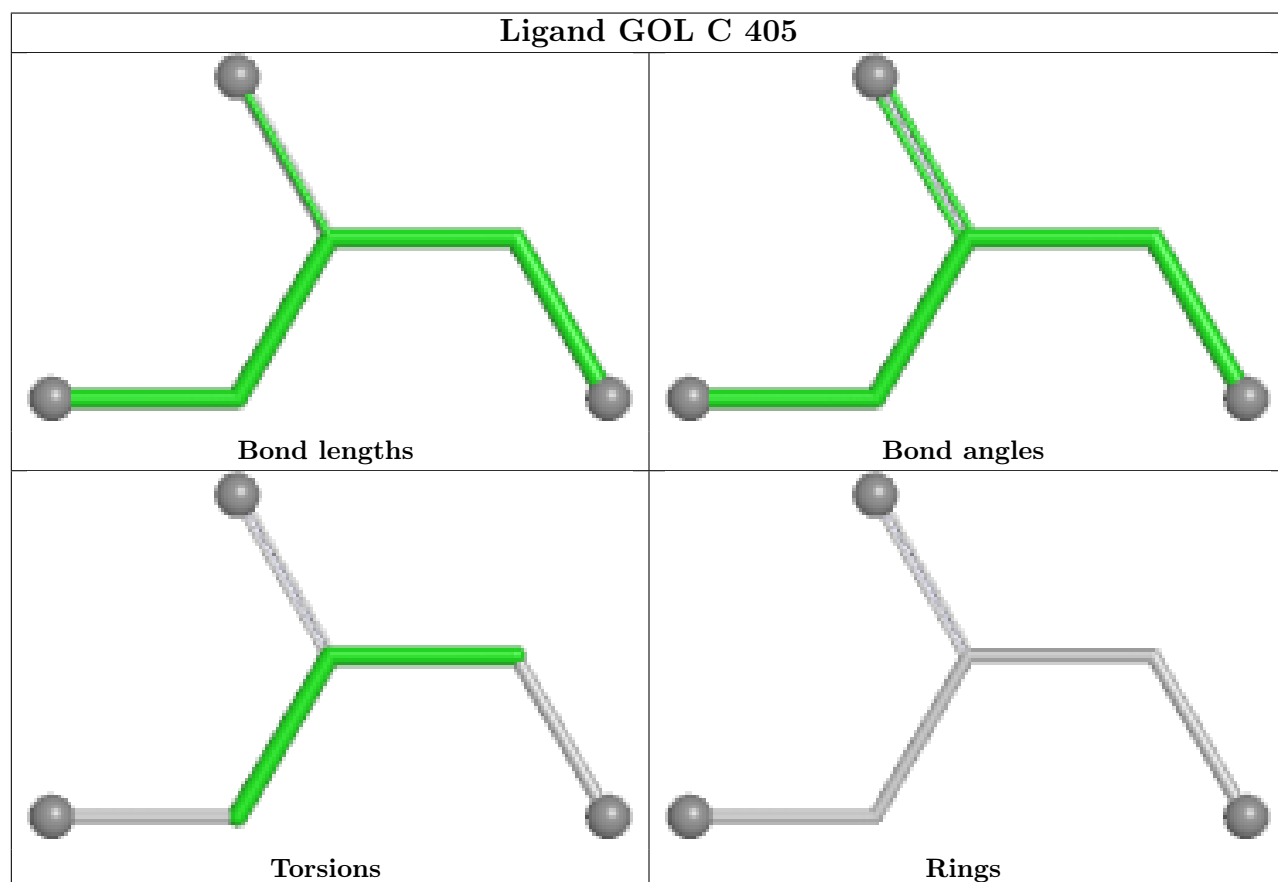
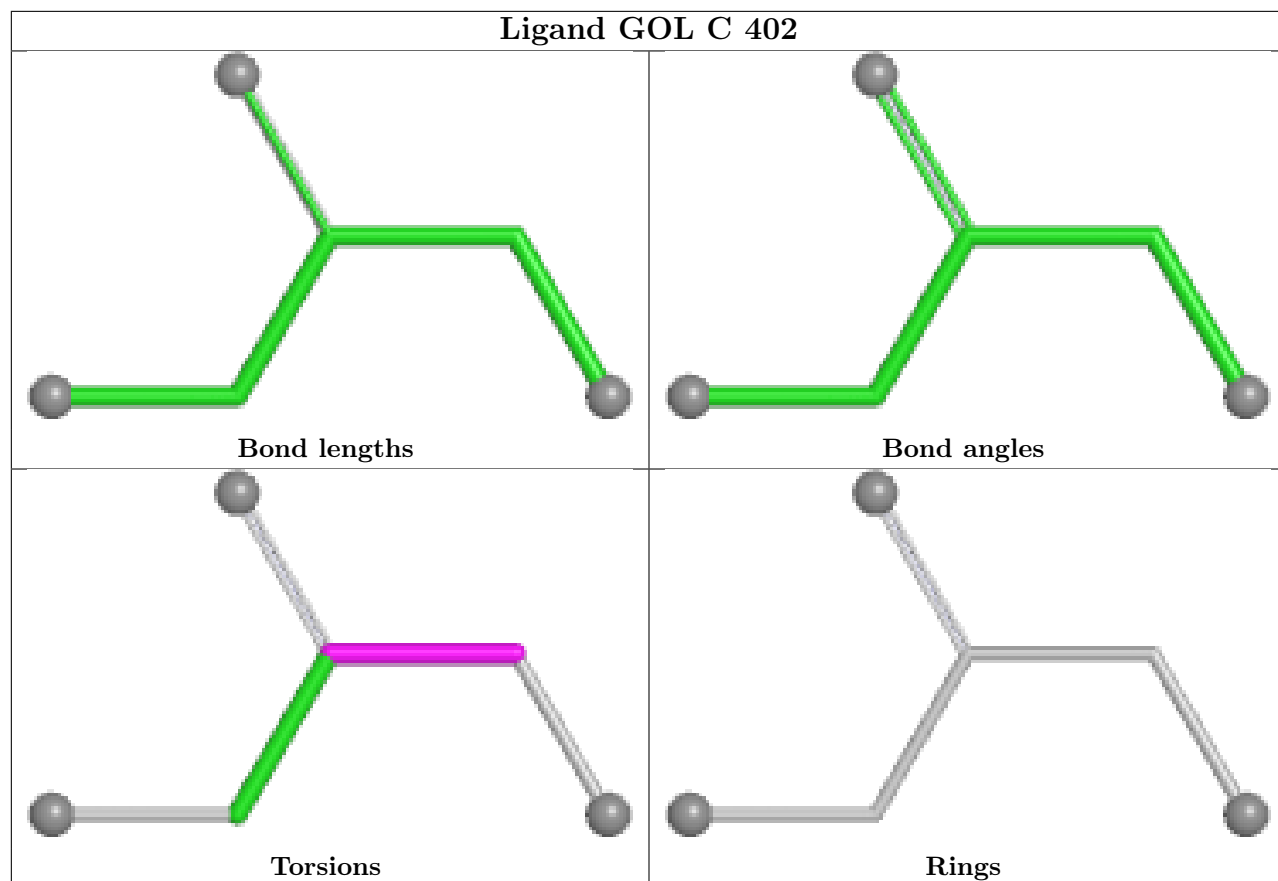












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	284/296 (95%)	0.03	6 (2%) 63 71	13, 25, 37, 71	2 (0%)
1	B	284/296 (95%)	0.05	1 (0%) 88 93	12, 25, 42, 69	1 (0%)
1	C	284/296 (95%)	-0.13	0 100 100	11, 20, 34, 53	1 (0%)
1	D	283/296 (95%)	0.48	5 (1%) 67 75	20, 32, 50, 74	0
All	All	1135/1184 (95%)	0.11	12 (1%) 78 84	11, 25, 44, 74	4 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	283	ARG	2.8
1	B	284	GLN	2.7
1	A	167	GLN	2.6
1	A	171	GLU	2.5
1	A	283	ARG	2.5
1	A	132	ASP	2.4
1	D	108	TYR	2.1
1	A	284	GLN	2.1
1	A	170	GLU	2.0
1	D	114	GLY	2.0
1	D	169	THR	2.0
1	D	16	VAL	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

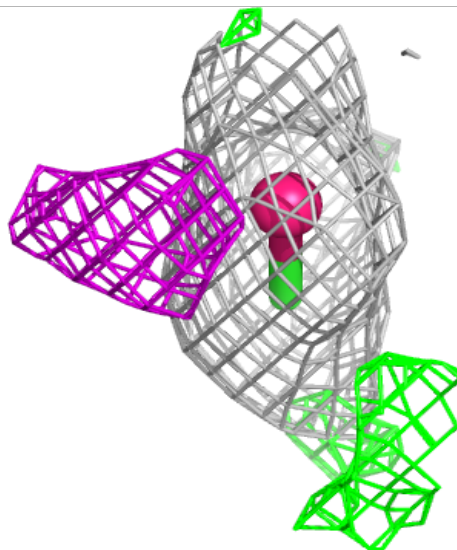
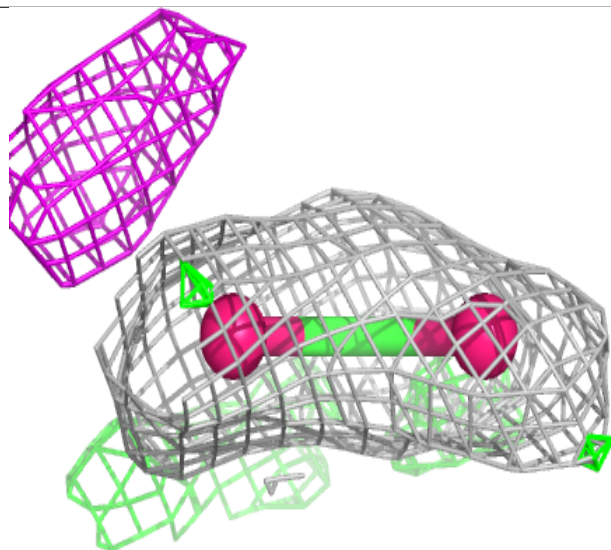
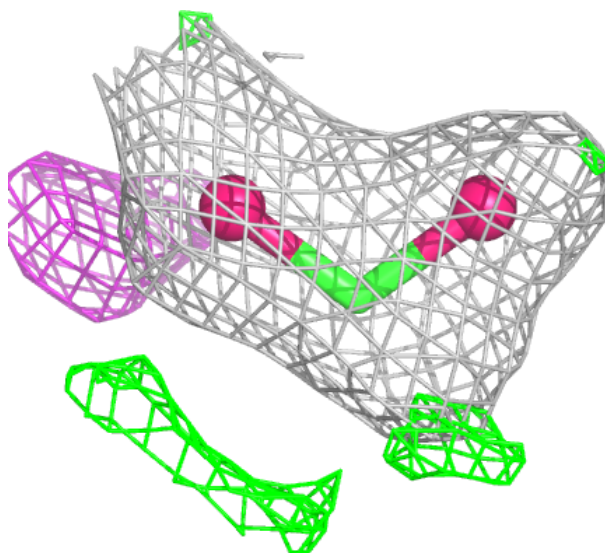
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FMT	D	302	3/3	0.66	0.22	49,49,50,53	0
3	FMT	B	303	3/3	0.72	0.17	50,50,52,53	0
2	GOL	B	302	6/6	0.73	0.19	53,54,56,59	0
2	GOL	C	408	6/6	0.80	0.17	28,41,51,54	0
3	FMT	C	403	3/3	0.81	0.17	46,46,47,52	0
2	GOL	C	405	6/6	0.83	0.14	27,43,44,45	0
4	TRS	C	407	8/8	0.83	0.13	34,41,46,50	0
3	FMT	C	404	3/3	0.85	0.14	52,52,53,55	0
2	GOL	C	406	6/6	0.86	0.13	27,44,50,56	0
3	FMT	D	301	3/3	0.86	0.16	34,34,47,54	0
2	GOL	A	302	6/6	0.89	0.11	27,45,49,49	0
5	B3P	D	303	19/19	0.89	0.11	28,40,54,59	0
2	GOL	A	301	6/6	0.91	0.11	24,38,42,51	0
3	FMT	A	303	3/3	0.91	0.19	31,31,33,36	0
2	GOL	C	402	6/6	0.91	0.10	30,37,41,42	0
2	GOL	B	301	6/6	0.92	0.10	31,38,41,44	0
2	GOL	A	304	6/6	0.92	0.12	37,43,48,52	0
3	FMT	C	401	3/3	0.94	0.16	23,23,35,38	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.

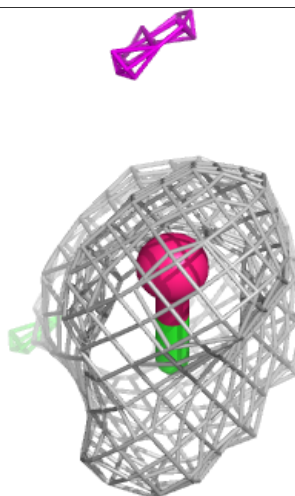
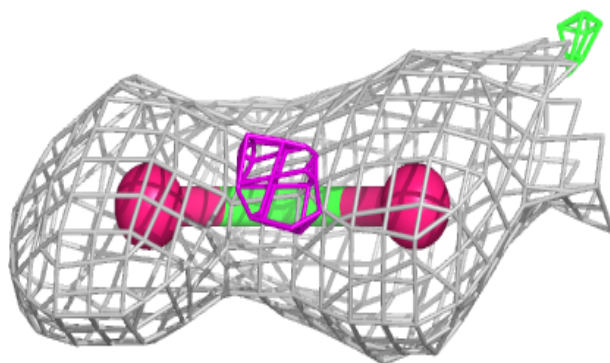
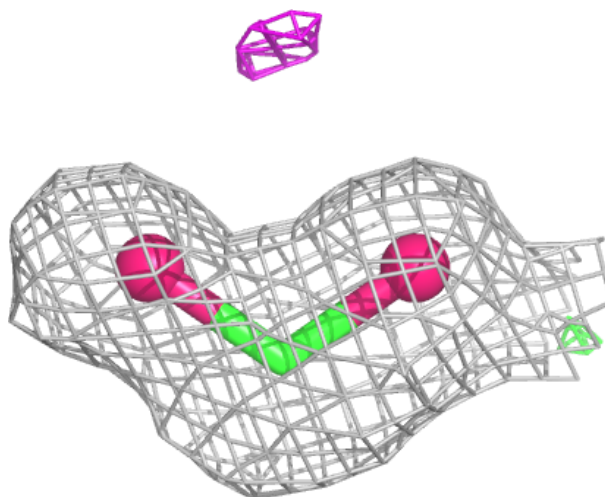
Electron density around FMT D 302:

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



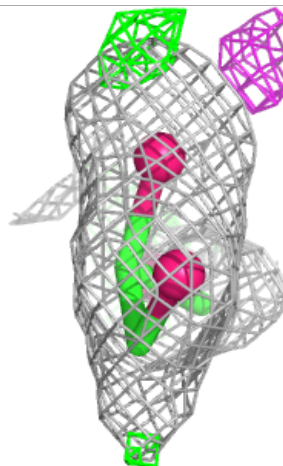
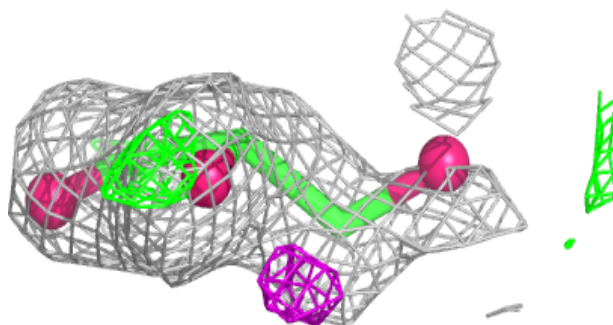
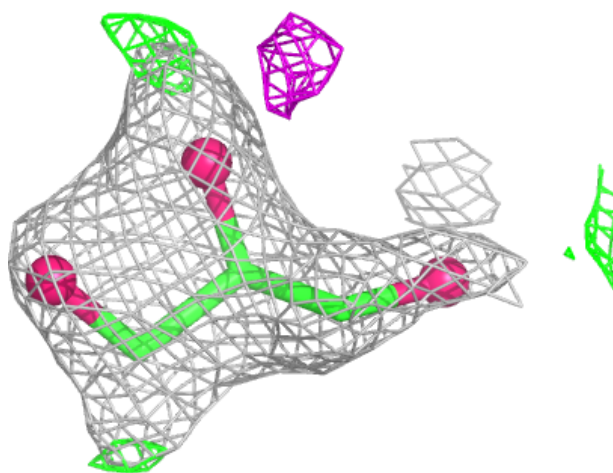
Electron density around FMT B 303:

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



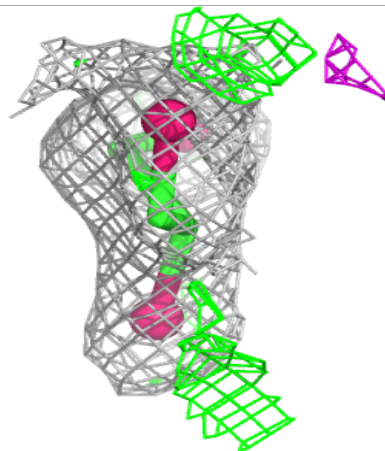
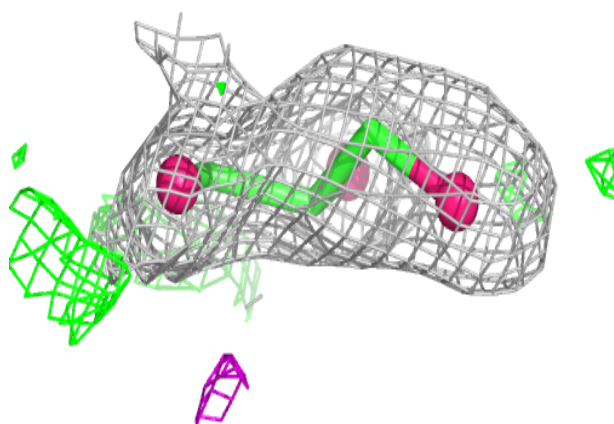
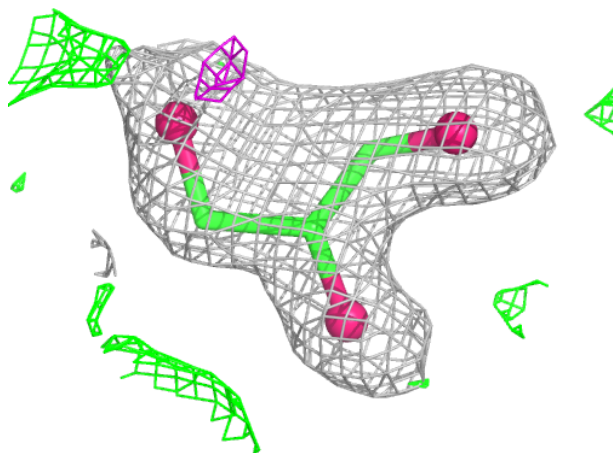
Electron density around GOL B 302:

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



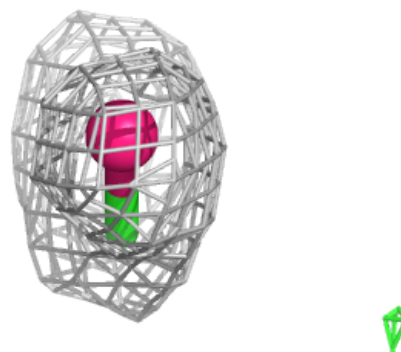
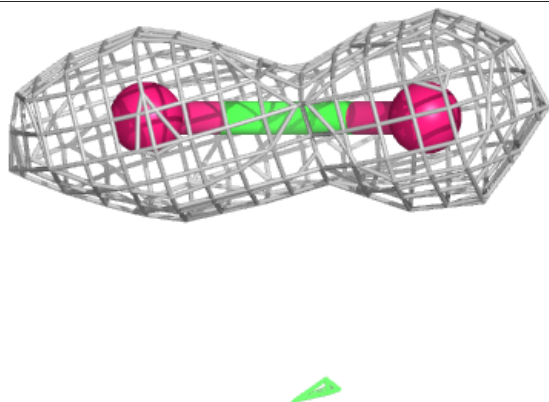
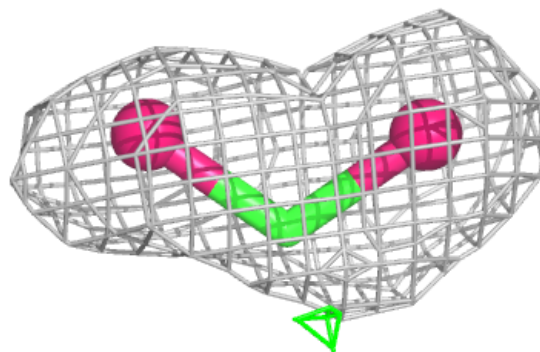
Electron density around GOL C 408:

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and green (positive)



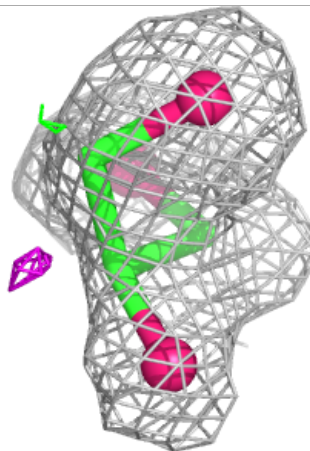
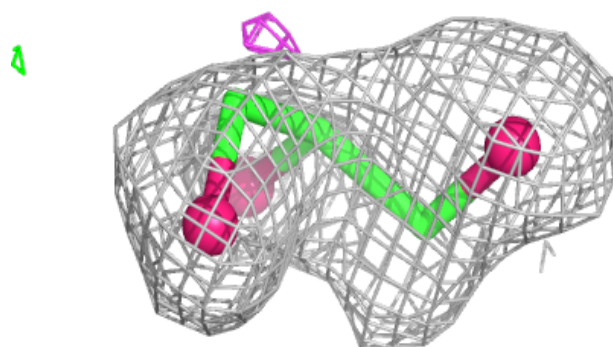
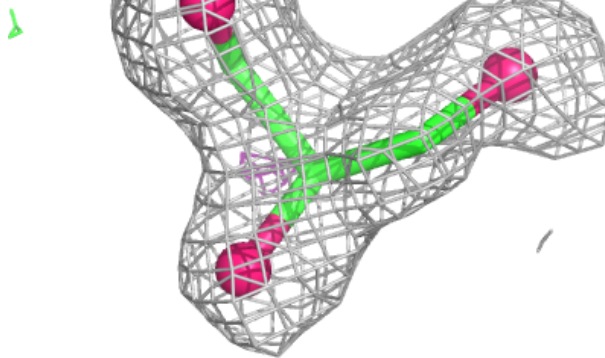
Electron density around FMT C 403:

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



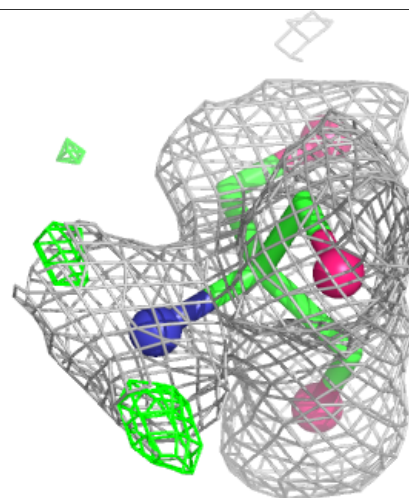
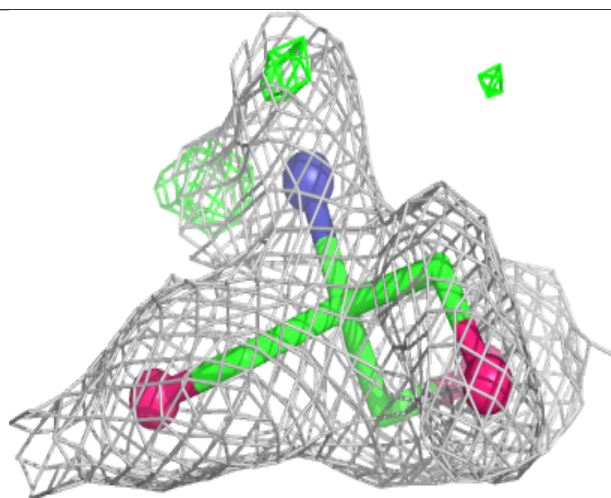
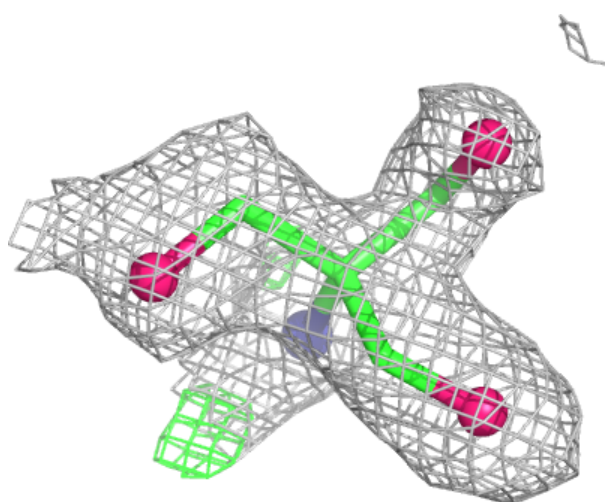
Electron density around GOL C 405:

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



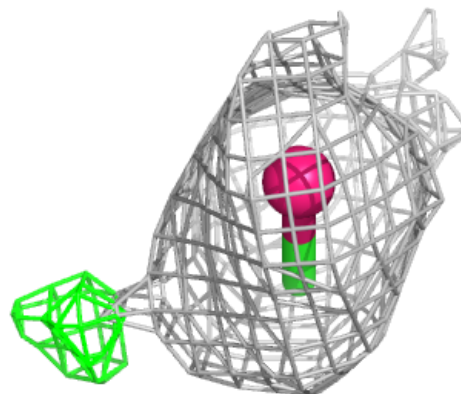
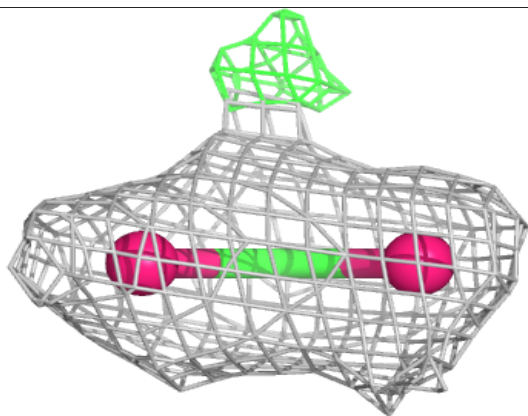
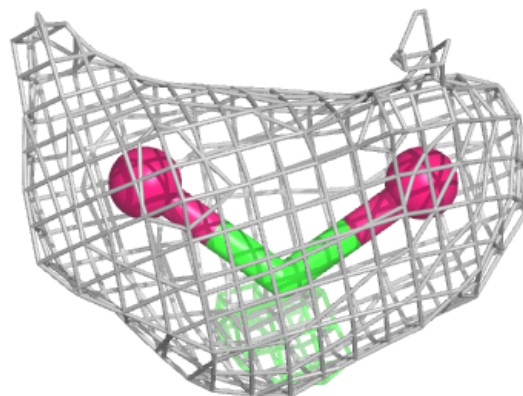
Electron density around TRS C 407:

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

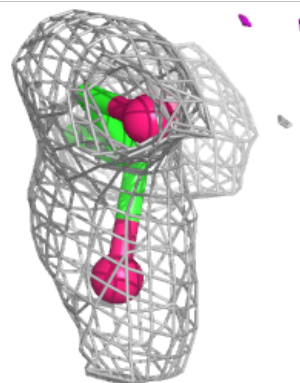
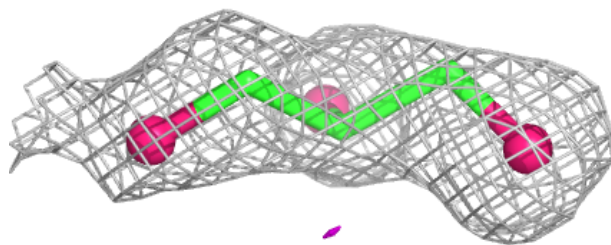
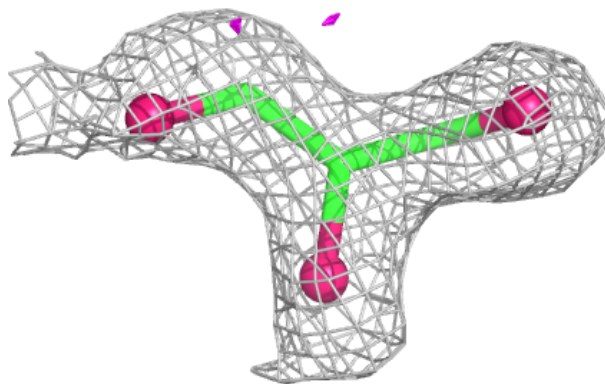


Electron density around FMT C 404:

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

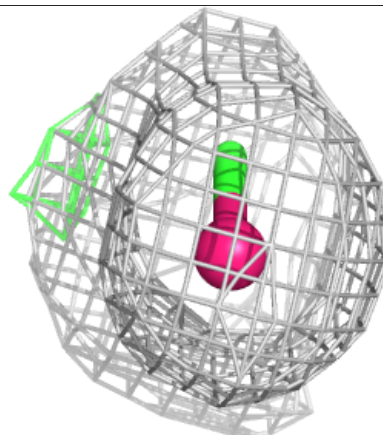
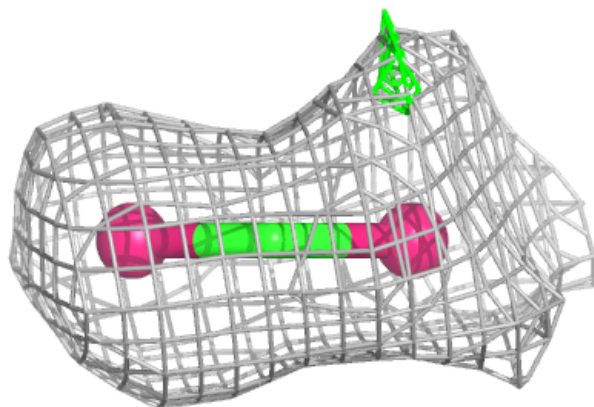
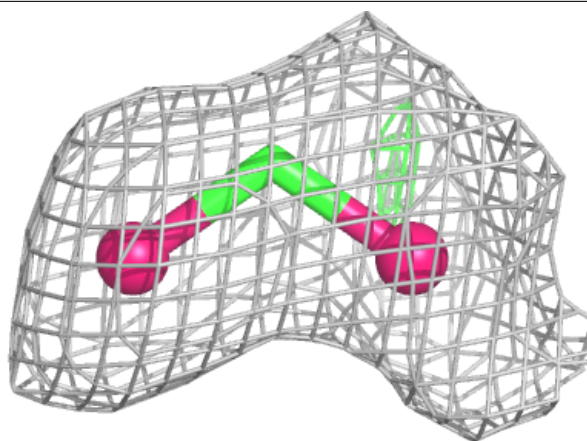
**Electron density around GOL C 406:**

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



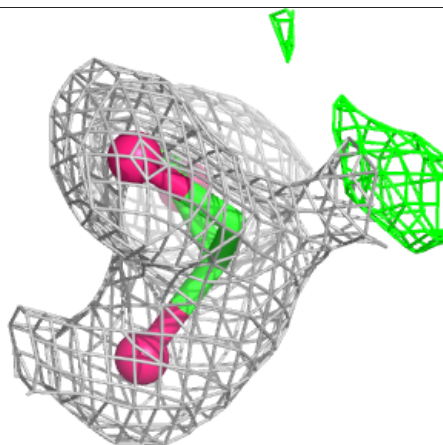
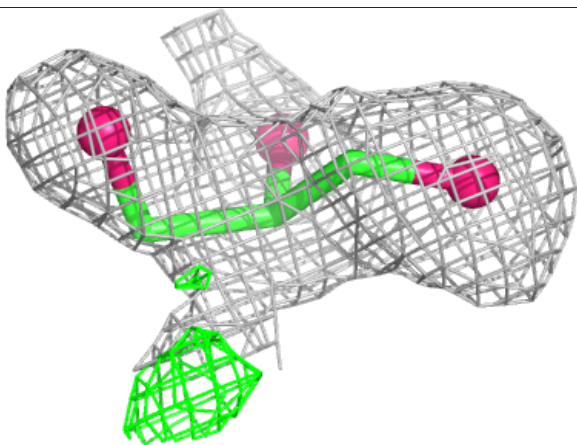
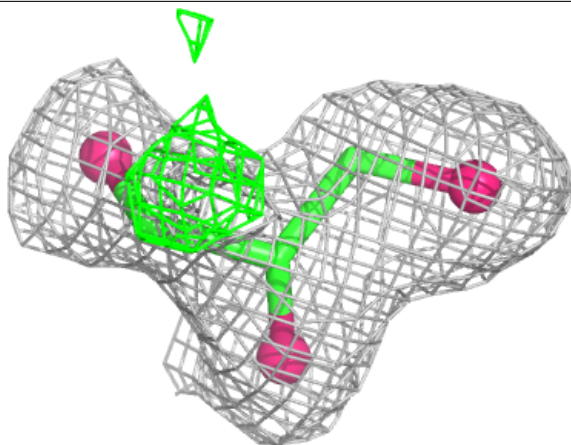
Electron density around FMT D 301:

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

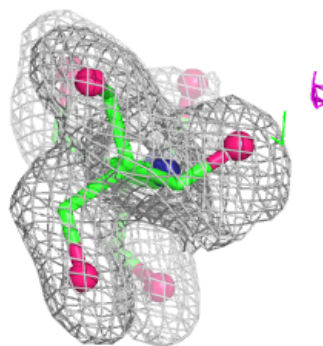
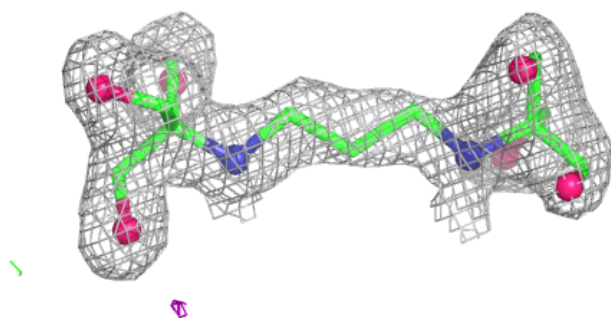
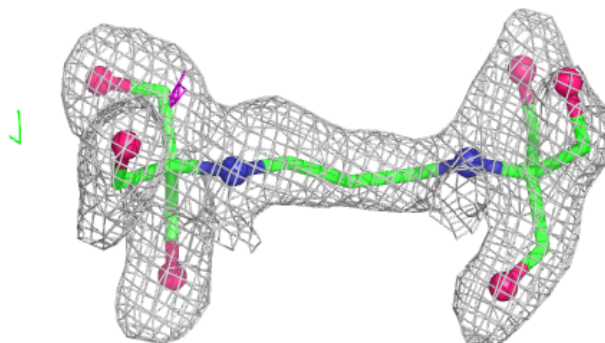


Electron density around GOL A 302:

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

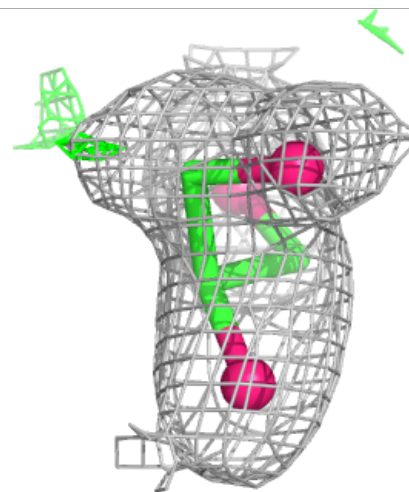
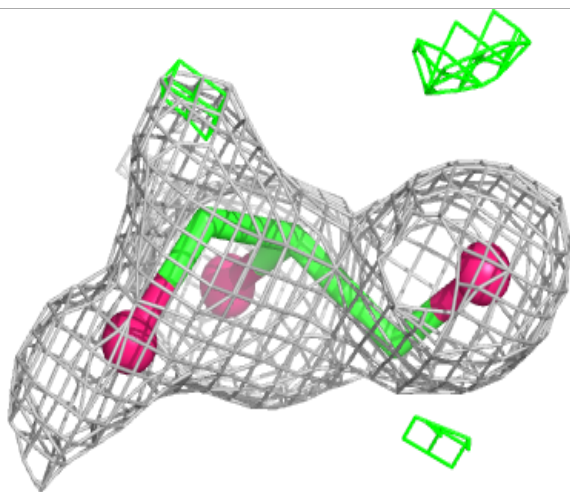
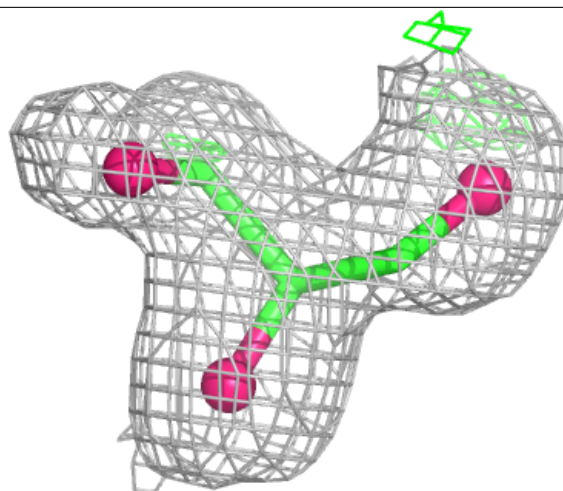
**Electron density around B3P D 303:**

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



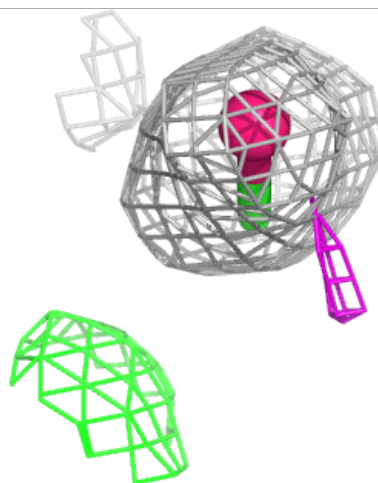
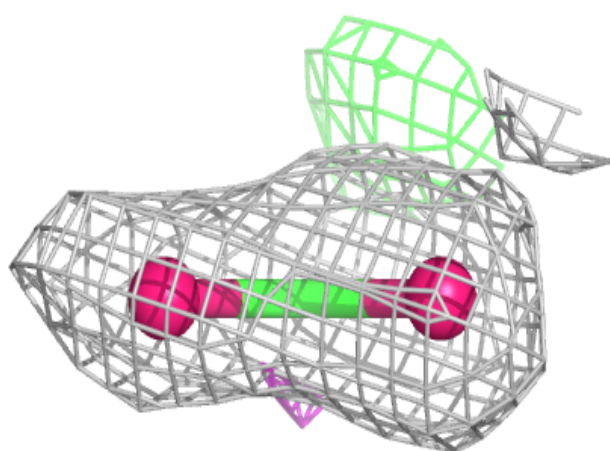
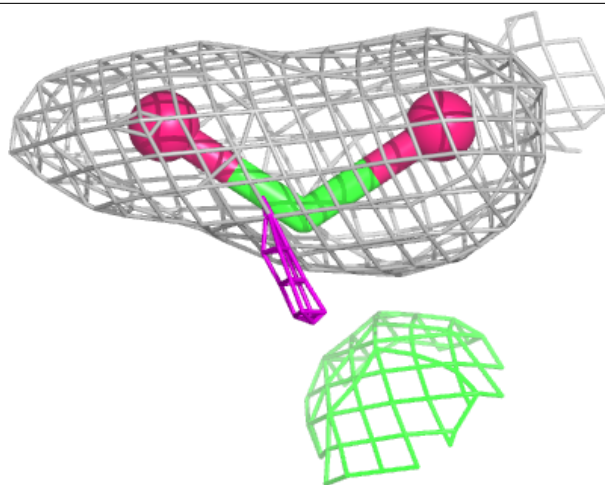
Electron density around GOL A 301:

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



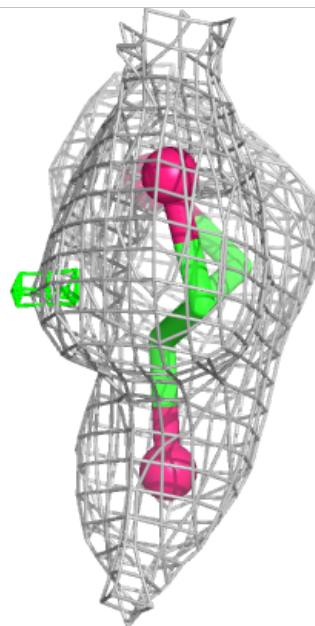
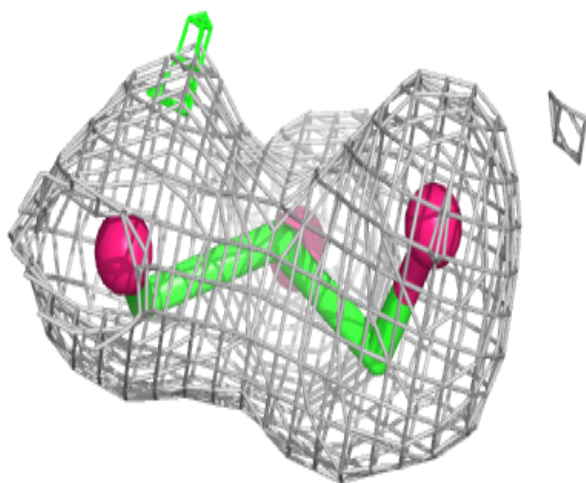
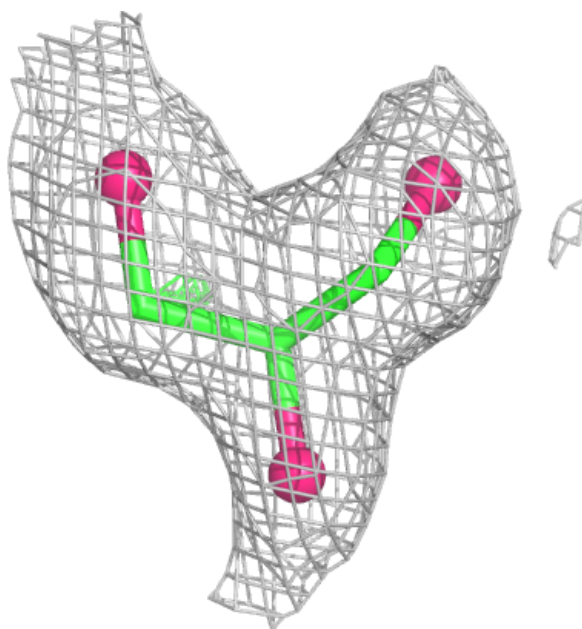
Electron density around FMT A 303:

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



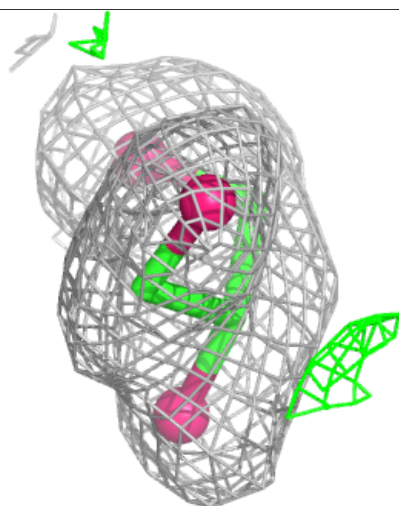
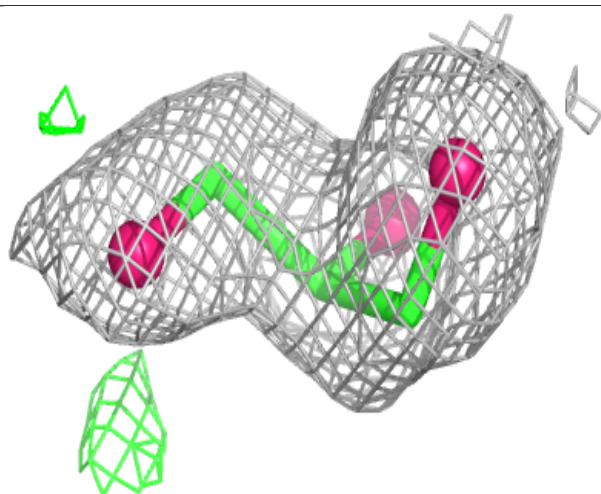
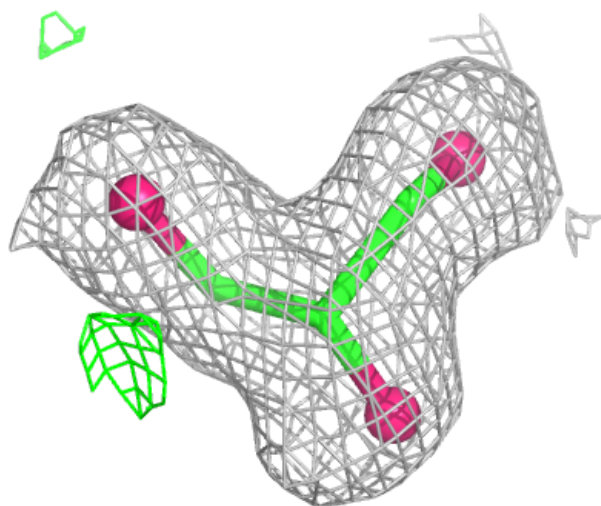
Electron density around GOL C 402:

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



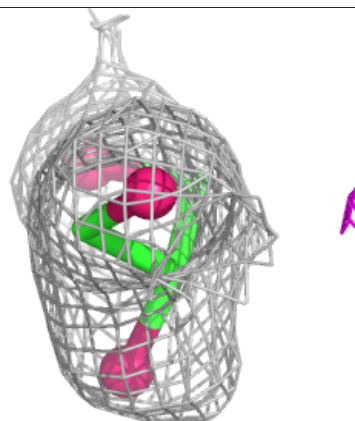
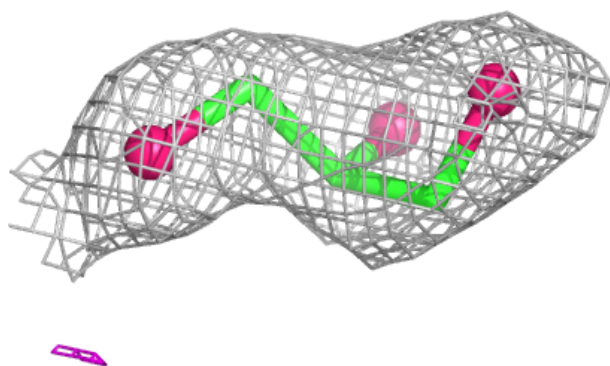
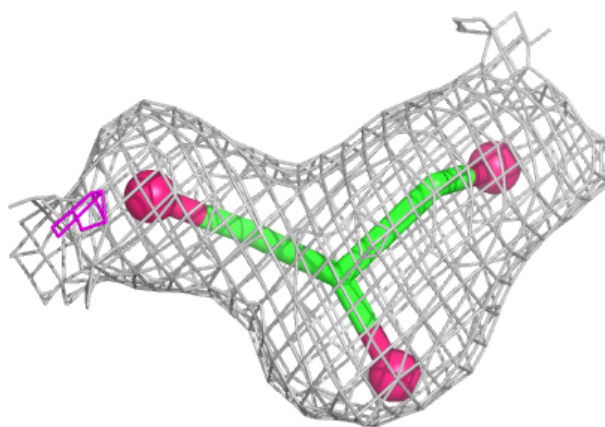
Electron density around GOL B 301:

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

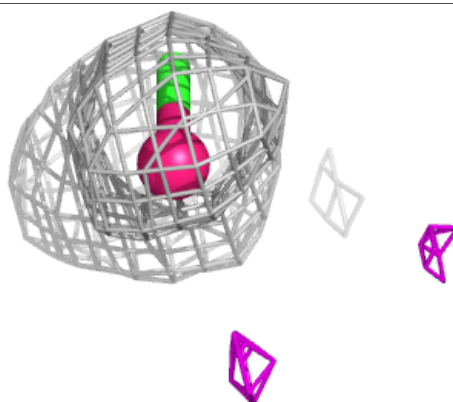
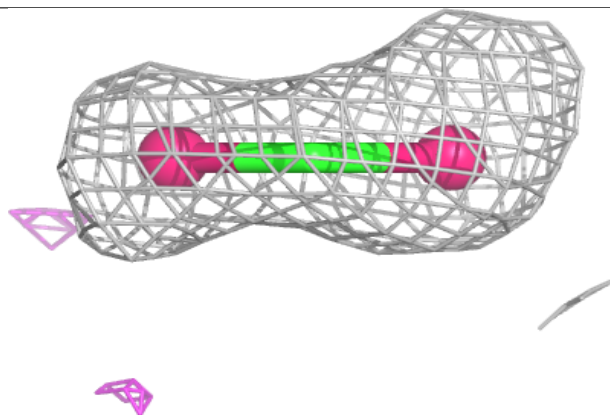
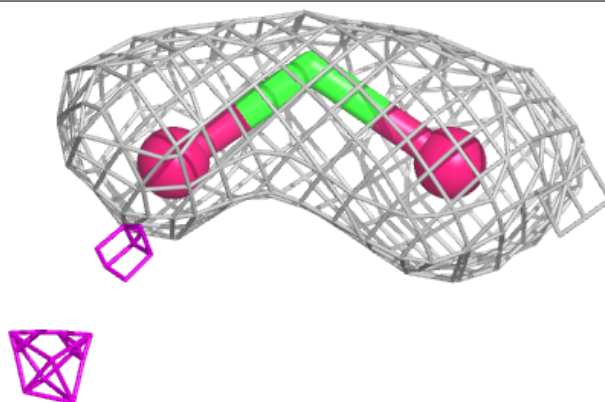


Electron density around GOL A 304:

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

**Electron density around FMT C 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.