



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:52 PM UTC

PDB ID : 7Q89 / pdb_00007q89
Title : OleP mutant G92W in complex with 6DEB
Authors : Savino, C.; Montemiglio, L.C.; Vallone, B.; Exertier, C.; Freda, I.; Gugole, E.
Deposited on : 2021-11-10
Resolution : 2.08 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:

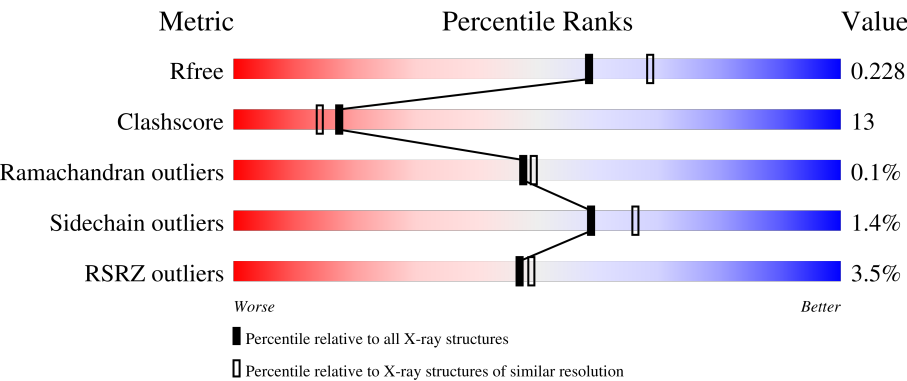
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	408	
1	B	408	
1	C	408	
1	D	408	
1	E	408	

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Mol	Chain	Length	Quality of chain
1	F	408	

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
4	FMT	A	510	-	-	X	-
4	FMT	A	525	-	-	X	-
4	FMT	A	526	-	-	X	-
4	FMT	B	506	-	-	X	-
4	FMT	B	511	-	-	X	-
4	FMT	B	512	-	-	X	-
4	FMT	B	513	-	-	X	-
4	FMT	B	520	-	-	X	-
4	FMT	B	537	-	-	X	-
4	FMT	B	538	-	-	X	-
4	FMT	C	522	-	-	X	-
4	FMT	C	524	-	-	X	-
4	FMT	D	508	-	-	X	-
4	FMT	D	515	-	-	X	-
4	FMT	E	506	-	-	X	-
6	GOL	B	543[A]	-	-	X	-
6	GOL	B	543[B]	-	-	X	-
6	GOL	E	515[A]	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21704 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 Cytochrome P-450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	32	0
			3298	2092	595	596	15			
1	B	402	Total	C	N	O	S	0	33	0
			3331	2113	597	606	15			
1	C	408	Total	C	N	O	S	0	29	0
			3354	2128	598	611	17			
1	D	396	Total	C	N	O	S	0	16	0
			3186	2018	564	589	15			
1	E	395	Total	C	N	O	S	0	9	0
			3141	1985	558	580	18			
1	F	396	Total	C	N	O	S	0	6	0
			3132	1976	556	584	16			

There are 12 discrepancies between the modelled and reference sequences:

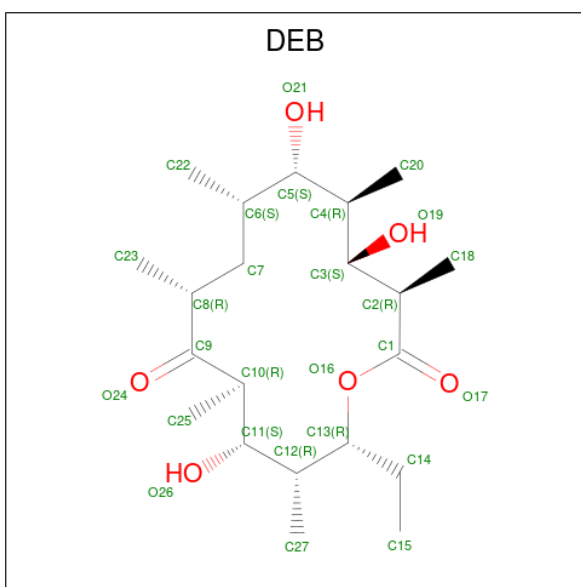
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q59819
A	92	TRP	GLY	engineered mutation	UNP Q59819
B	0	HIS	-	expression tag	UNP Q59819
B	92	TRP	GLY	engineered mutation	UNP Q59819
C	0	HIS	-	expression tag	UNP Q59819
C	92	TRP	GLY	engineered mutation	UNP Q59819
D	0	HIS	-	expression tag	UNP Q59819
D	92	TRP	GLY	engineered mutation	UNP Q59819
E	0	HIS	-	expression tag	UNP Q59819
E	92	TRP	GLY	engineered mutation	UNP Q59819
F	0	HIS	-	expression tag	UNP Q59819
F	92	TRP	GLY	engineered mutation	UNP Q59819

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 6-DEOXYERYTHRONOLIDE B (CCD ID: DEB) (formula: C₂₁H₃₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			27	21	6		
3	B	1	Total	C	O	0	0
			27	21	6		
3	C	1	Total	C	O	0	0
			27	21	6		
3	D	1	Total	C	O	0	0
			27	21	6		
3	E	1	Total	C	O	0	0
			27	21	6		
3	F	1	Total	C	O	0	0
			27	21	6		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 3	C 1	O 2	0	0
4	C	1	Total 3	C 1	O 2	0	0
4	C	1	Total 3	C 1	O 2	0	0
4	C	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	D	1	Total 3	C 1	O 2	0	0
4	E	1	Total 3	C 1	O 2	0	0

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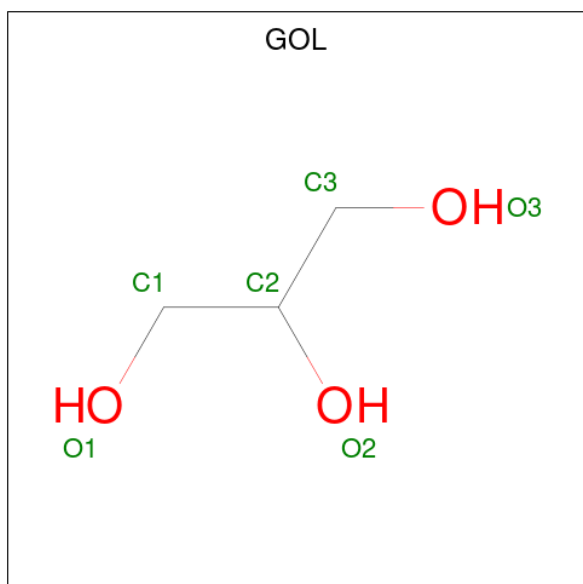
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		
5	B	2	Total	Na	0	0
			2	2		
5	C	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		
5	E	1	Total	Na	0	0
			1	1		
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	1
			12	6	6		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	1
			12	6	6		
6	C	1	Total	C	O	0	1
			12	6	6		
6	C	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	1
			12	6	6		

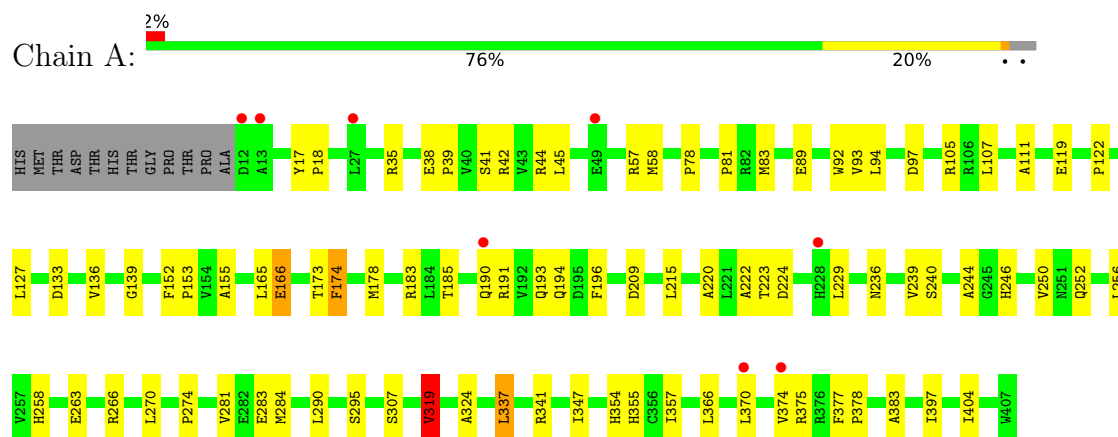
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	301	Total	O	0	0
			301	301		
7	B	258	Total	O	0	0
			258	258		
7	C	308	Total	O	0	0
			308	308		
7	D	169	Total	O	0	0
			169	169		
7	E	146	Total	O	0	0
			146	146		
7	F	157	Total	O	0	0
			157	157		

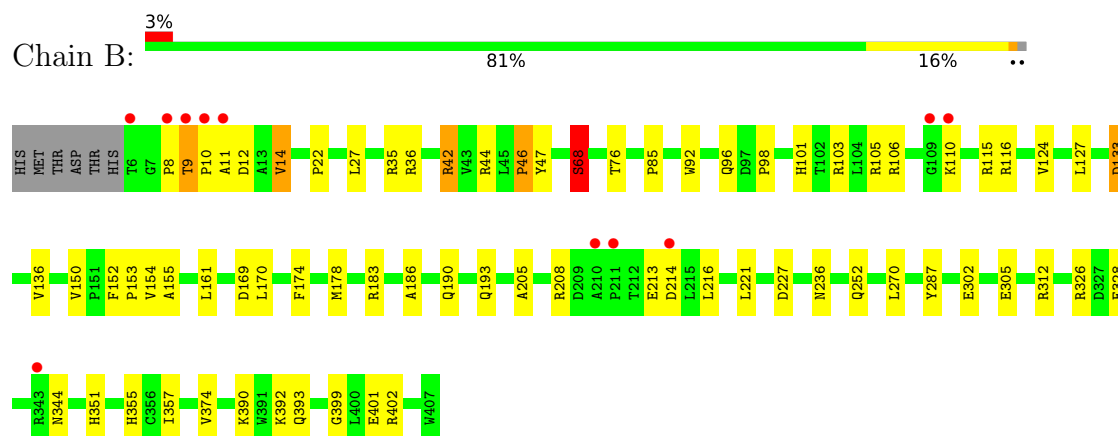
3 Residue-property plots [i](#)

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.

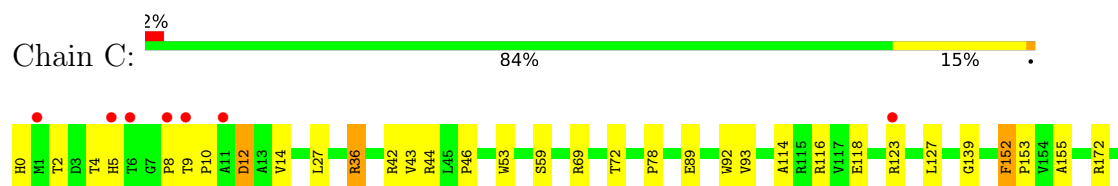
• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450

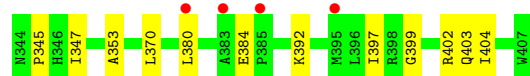


• Molecule 1: Cytochrome P-450

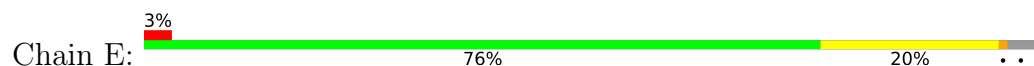




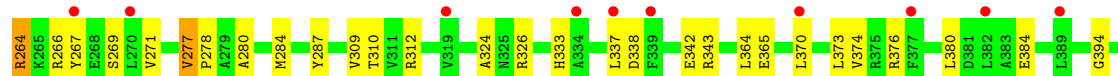
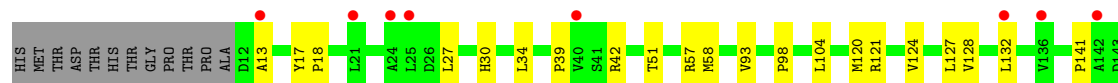
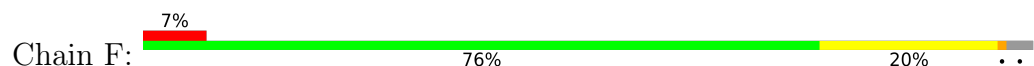
• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450



R402	Q403	I404	V405	S406	W407

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.76Å 110.49Å 159.82Å 90.00° 129.66° 90.00°	Depositor
Resolution (Å)	48.03 – 2.08 48.03 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.03-2.08) 99.8 (48.03-2.08)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.170 , 0.228 0.181 , 0.228	Depositor DCC
R_{free} test set	11825 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21704	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9742e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NA, GOL, DEB, FMT

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	1.16	1/3456 (0.0%)	1.45	13/4701 (0.3%)
1	B	1.19	5/3491 (0.1%)	1.42	9/4750 (0.2%)
1	C	1.17	12/3516 (0.3%)	1.40	10/4785 (0.2%)
1	D	1.19	7/3303 (0.2%)	1.50	15/4499 (0.3%)
1	E	1.13	1/3231 (0.0%)	1.49	4/4400 (0.1%)
1	F	1.12	0/3213	1.51	8/4378 (0.2%)
All	All	1.16	26/20210 (0.1%)	1.46	59/27513 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	ARG	N-CA	7.12	1.55	1.46
1	B	46	PRO	C-O	-6.92	1.15	1.24
1	B	42[A]	ARG	C-O	6.92	1.32	1.23
1	B	42[B]	ARG	C-O	6.92	1.32	1.23
1	B	68	SER	N-CA	6.82	1.54	1.46
1	C	46	PRO	C-O	-6.21	1.17	1.24
1	C	172[A]	ARG	C-O	5.96	1.31	1.24
1	C	172[B]	ARG	C-O	5.96	1.31	1.24
1	C	123	ARG	C-O	5.95	1.31	1.24
1	C	344	ASN	N-CA	5.87	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	PRO	C-O	-5.84	1.16	1.24
1	D	96	GLN	C-O	5.73	1.31	1.24
1	C	395[A]	MET	C-O	-5.68	1.16	1.23
1	C	395[B]	MET	C-O	-5.68	1.16	1.23
1	D	168	ARG	C-O	5.55	1.30	1.24
1	B	22	PRO	C-O	-5.52	1.17	1.23
1	D	280	ALA	C-O	5.45	1.30	1.24
1	D	253	ILE	C-O	5.45	1.30	1.24
1	D	83[A]	MET	C-O	5.35	1.31	1.24
1	D	83[B]	MET	C-O	5.35	1.31	1.24
1	C	59[A]	SER	C-O	5.33	1.30	1.24
1	C	59[B]	SER	C-O	5.33	1.30	1.24
1	D	240	SER	C-O	5.15	1.30	1.24
1	C	152	PHE	N-CA	5.12	1.50	1.46
1	E	85	PRO	C-O	-5.07	1.17	1.24
1	C	123	ARG	CA-C	5.03	1.59	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319[A]	VAL	CA-C-O	-15.77	103.69	120.57
1	A	319[B]	VAL	CA-C-O	-15.77	103.69	120.57
1	B	68	SER	N-CA-C	10.12	132.36	110.80
1	D	83[A]	MET	CA-C-O	9.53	131.31	119.11
1	D	83[B]	MET	CA-C-O	9.53	131.31	119.11
1	B	98	PRO	O-C-N	-9.23	117.07	121.31
1	A	319[A]	VAL	N-CA-C	9.15	121.45	108.36
1	A	319[B]	VAL	N-CA-C	9.15	121.45	108.36
1	B	169	ASP	CA-CB-CG	7.90	120.50	112.60
1	C	172[A]	ARG	CA-C-O	7.36	128.35	120.55
1	C	172[B]	ARG	CA-C-O	7.36	128.35	120.55
1	F	187	ALA	CA-C-N	7.26	130.60	120.29
1	F	187	ALA	C-N-CA	7.26	130.60	120.29
1	D	384	GLU	CB-CA-C	7.06	119.95	109.22
1	B	42[A]	ARG	CA-C-O	7.01	128.90	121.19
1	B	42[B]	ARG	CA-C-O	7.01	128.90	121.19
1	F	277	VAL	N-CA-CB	6.64	115.63	110.45
1	A	78	PRO	CB-CA-C	-6.57	102.52	111.85
1	B	14	VAL	N-CA-CB	6.52	116.15	110.08
1	E	169	ASP	CA-CB-CG	6.50	119.10	112.60
1	D	97	ASP	CA-CB-CG	6.49	119.09	112.60
1	D	22	PRO	N-CA-C	6.12	120.94	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	ASP	CA-C-N	6.09	128.45	120.28
1	D	129	ASP	C-N-CA	6.09	128.45	120.28
1	A	97	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	209	ASP	CB-CA-C	5.81	120.64	110.64
1	C	139	GLY	CA-C-O	-5.81	118.22	122.23
1	B	85	PRO	N-CA-C	5.81	121.78	113.47
1	D	292	SER	O-C-N	5.73	128.28	122.09
1	D	233	GLU	CA-C-N	5.69	127.85	120.56
1	D	233	GLU	C-N-CA	5.69	127.85	120.56
1	F	187	ALA	O-C-N	5.62	127.86	122.07
1	E	231	LYS	CA-C-N	5.55	126.15	119.98
1	E	231	LYS	C-N-CA	5.55	126.15	119.98
1	D	255	ASN	CA-CB-CG	-5.54	107.06	112.60
1	D	94	LEU	N-CA-CB	-5.49	101.77	110.22
1	E	246	HIS	CB-CA-C	5.48	117.83	109.34
1	A	139	GLY	CA-C-N	5.44	128.21	120.49
1	A	139	GLY	C-N-CA	5.44	128.21	120.49
1	C	78	PRO	CB-CA-C	-5.42	104.16	111.85
1	B	227	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	43	VAL	CA-C-O	-5.37	116.32	121.63
1	A	185	THR	CA-C-N	5.35	127.44	120.28
1	A	185	THR	C-N-CA	5.35	127.44	120.28
1	C	123	ARG	CA-C-O	5.35	125.95	119.11
1	D	88	PRO	CA-C-O	-5.34	115.36	121.56
1	A	174	PHE	CA-CB-CG	5.32	119.11	113.80
1	C	204	VAL	N-CA-C	-5.22	105.45	110.72
1	C	196	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	173	THR	CA-C-O	-5.18	115.06	120.55
1	F	13	ALA	CA-C-O	-5.17	115.84	121.84
1	B	133	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	301	THR	N-CA-C	-5.15	106.40	113.30
1	D	301	THR	N-CA-C	-5.15	106.68	113.17
1	F	365	GLU	CA-C-O	-5.12	115.45	120.82
1	F	98	PRO	O-C-N	-5.11	118.96	121.31
1	F	250	VAL	N-CA-C	-5.08	105.37	110.30
1	C	36	ARG	CB-CA-C	-5.06	102.90	110.90
1	D	120	MET	N-CA-C	-5.06	107.11	113.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319[A]	VAL	Mainchain
1	A	319[B]	VAL	Mainchain
1	A	42	ARG	Sidechain
1	B	68	SER	Mainchain

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	3298	0	3371	102	0
1	B	3331	0	3408	97	1
1	C	3354	0	3421	60	1
1	D	3186	0	3212	89	0
1	E	3141	0	3143	78	0
1	F	3132	0	3113	74	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	4	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
3	A	27	0	38	7	0
3	B	27	0	38	2	0
3	C	27	0	38	6	0
3	D	27	0	38	0	0
3	E	27	0	38	0	0
3	F	27	0	38	0	0
4	A	111	0	37	11	0
4	B	111	0	37	23	0
4	C	84	0	28	5	0
4	D	48	0	16	6	0
4	E	33	0	11	3	0
4	F	30	0	10	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	30	0	40	9	0
6	B	18	0	24	14	0
6	C	18	0	24	3	0
6	E	12	0	16	7	0
7	A	301	0	0	6	0
7	B	258	0	0	7	0
7	C	308	0	0	5	0
7	D	169	0	0	4	0
7	E	146	0	0	4	0
7	F	157	0	0	2	0
All	All	21704	0	20319	508	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 13.

All (508) 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:B:236[A]:ASN:OD1	6:B:543[A]:GOL:H2	1.22	1.24
1:B:236[A]:ASN:OD1	6:B:543[A]:GOL:C2	2.04	1.05
1:D:115[A]:ARG:HH11	1:D:115[A]:ARG:CG	1.70	1.04
1:A:92[B]:TRP:HH2	3:A:502:DEB:H223	1.25	1.02
1:B:92:TRP:HA	1:B:236[A]:ASN:ND2	1.74	1.01
1:B:236[A]:ASN:CG	6:B:543[A]:GOL:H2	1.86	1.00
1:C:89[B]:GLU:OE2	1:C:92[B]:TRP:CG	2.16	0.98
1:B:161:LEU:O	1:B:216[B]:LEU:HD13	1.65	0.96
1:B:92:TRP:HA	1:B:236[A]:ASN:HD22	1.27	0.96
1:D:17:TYR:HD2	1:D:83[B]:MET:HE1	1.28	0.94
1:A:92[B]:TRP:HZ3	1:A:240:SER:HG	0.98	0.92
1:B:178[B]:MET:HE1	1:B:193:GLN:HE21	1.35	0.92
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:HG3	1.34	0.91
1:F:266:ARG:NE	1:F:337:LEU:HD12	1.85	0.91
1:A:122:PRO:HB3	1:D:309:VAL:HG22	1.53	0.90
1:E:45:LEU:HD12	1:E:81:PRO:HB2	1.52	0.90
1:A:92[B]:TRP:CH2	3:A:502:DEB:H223	2.07	0.89
1:E:226:ASP:OD2	1:E:229:LEU:HB2	1.71	0.89
1:B:9[A]:THR:HG23	1:B:10[A]:PRO:CD	2.02	0.89
1:A:35[B]:ARG:HE	6:A:545:GOL:H32	1.36	0.88
1:D:267:TYR:CE1	1:D:380:LEU:HD23	2.09	0.88
1:C:89[B]:GLU:OE2	1:C:92[B]:TRP:CD2	2.27	0.87
1:A:92[B]:TRP:CZ2	1:A:94:LEU:HD12	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HB3	1:B:216[B]:LEU:CD1	2.05	0.86
1:A:370:LEU:O	1:A:374:VAL:HG23	1.75	0.85
1:B:9[A]:THR:HG23	1:B:10[A]:PRO:HD2	1.57	0.84
1:D:17:TYR:CD2	1:D:83[B]:MET:HE1	2.12	0.84
1:A:92[B]:TRP:HZ3	1:A:240:SER:OG	1.60	0.84
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:CG	1.90	0.84
1:D:115[A]:ARG:HH11	1:D:115[A]:ARG:HG2	1.42	0.83
1:F:185:THR:OG1	1:F:188:GLU:HG3	1.77	0.83
1:D:115[A]:ARG:HH11	1:D:115[A]:ARG:HG3	1.42	0.82
1:C:92[B]:TRP:HH2	1:C:178:MET:HE1	1.44	0.82
1:B:161:LEU:HB3	1:B:216[B]:LEU:HD11	1.61	0.82
1:F:266:ARG:CZ	1:F:337:LEU:HD12	2.09	0.81
1:E:280:ALA:O	1:E:284[A]:MET:HG3	1.81	0.81
1:F:277:VAL:HG23	1:F:278:PRO:HD3	1.63	0.81
1:D:257:VAL:HG23	1:D:403:GLN:HE22	1.46	0.81
1:F:161:LEU:HD23	1:F:215:LEU:HD12	1.63	0.80
1:F:284[B]:MET:HE1	1:F:370:LEU:HD11	1.60	0.80
1:A:45:LEU:HD12	1:A:81:PRO:HB2	1.62	0.80
1:F:128:VAL:O	1:F:132:LEU:HG	1.82	0.79
1:F:195:ASP:O	1:F:198:VAL:HG22	1.81	0.79
1:C:179[B]:LEU:HD11	3:C:533:DEB:H201	1.64	0.79
1:B:10[B]:PRO:HD3	1:C:360[B]:GLN:OE1	1.83	0.78
1:E:229:LEU:HA	1:E:233[B]:GLU:OE1	1.84	0.77
1:F:262:THR:OG1	7:F:601:HOH:O	2.00	0.77
3:A:502:DEB:H5	6:A:543[A]:GOL:H2	1.66	0.77
1:D:115[A]:ARG:HG3	1:D:115[A]:ARG:NH1	1.98	0.77
1:E:178[A]:MET:HE1	6:E:515[A]:GOL:H32	1.65	0.77
1:A:45:LEU:HD12	1:A:81:PRO:CB	2.14	0.76
1:E:45:LEU:HD12	1:E:81:PRO:CB	2.15	0.76
1:E:51:THR:HG22	4:E:510:FMT:O2	1.85	0.76
1:E:133:ASP:O	1:E:136:VAL:HG22	1.86	0.75
1:B:161:LEU:C	1:B:216[B]:LEU:HD13	2.10	0.75
1:F:333:HIS:HE1	1:F:338:ASP:OD2	1.69	0.75
1:B:105[A]:ARG:HD3	1:B:357:ILE:HD12	1.69	0.75
1:E:256:LEU:HD22	1:E:284[B]:MET:HB3	1.67	0.74
6:C:531[A]:GOL:O3	6:C:531[A]:GOL:O1	2.02	0.74
1:E:370:LEU:O	1:E:374:VAL:HG23	1.87	0.74
1:C:89[B]:GLU:CD	1:C:92[B]:TRP:CE3	2.67	0.73
1:A:92[B]:TRP:HZ2	3:A:502:DEB:HO9	1.30	0.73
1:D:166[B]:GLU:HG3	1:E:228:HIS:NE2	2.04	0.73
1:F:51:THR:O	4:F:505:FMT:O1	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106[A]:ARG:HG3	1:E:106[A]:ARG:NH2	1.96	0.72
1:C:92[B]:TRP:HZ2	3:C:533:DEB:HO9	1.34	0.72
1:D:297:VAL:HG22	1:D:318:VAL:HG22	1.72	0.72
1:B:10[B]:PRO:CD	1:C:360[B]:GLN:OE1	2.37	0.72
1:A:92[B]:TRP:HZ2	1:A:94:LEU:HD12	1.52	0.71
1:B:178[B]:MET:SD	1:B:193:GLN:HG2	2.30	0.71
1:E:178[A]:MET:CE	6:E:515[A]:GOL:H32	2.21	0.71
1:A:119:GLU:OE2	4:A:529:FMT:O2	2.09	0.70
1:B:351:HIS:HD1	4:B:513:FMT:H	1.56	0.70
1:E:207:ARG:HA	1:E:210:ALA:HB3	1.74	0.70
1:A:92[B]:TRP:CE3	6:A:543[B]:GOL:H2	2.27	0.70
1:C:256:LEU:HD22	1:C:284:MET:HB3	1.74	0.70
1:C:92[B]:TRP:HH2	1:C:178:MET:CE	2.04	0.70
3:B:502:DEB:O19	6:B:543[B]:GOL:H31	1.93	0.69
1:D:12:ASP:CG	1:D:44:ARG:HH21	2.00	0.69
1:D:58[B]:MET:HE3	1:D:58[B]:MET:HA	1.74	0.69
1:D:86[A]:THR:HG21	1:D:189:ILE:CG2	2.23	0.69
1:D:115[A]:ARG:CG	1:D:115[A]:ARG:NH1	2.41	0.69
1:A:58[B]:MET:SD	1:A:324:ALA:HB1	2.33	0.69
1:A:92[B]:TRP:CH2	3:A:502:DEB:H5	2.28	0.69
1:B:9[A]:THR:HG23	1:B:10[A]:PRO:HD3	1.73	0.68
4:B:512:FMT:O2	7:B:601:HOH:O	2.11	0.68
1:D:326:ARG:HD3	7:D:672:HOH:O	1.93	0.68
1:C:351:HIS:HE1	7:C:832:HOH:O	1.76	0.68
1:B:105[A]:ARG:NH2	1:B:355:HIS:O	2.26	0.68
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.76	0.68
1:A:127[A]:LEU:HD21	1:A:155:ALA:HB3	1.76	0.67
1:B:236[A]:ASN:OD1	6:B:543[A]:GOL:C1	2.42	0.67
1:D:45:LEU:HD12	1:D:81:PRO:HB2	1.76	0.67
1:F:271:VAL:HG22	1:F:374:VAL:HG13	1.77	0.67
1:A:105[A]:ARG:NH2	1:A:355:HIS:O	2.27	0.67
1:A:92[B]:TRP:HH2	3:A:502:DEB:C22	2.05	0.66
1:A:92[B]:TRP:HE3	1:A:92[B]:TRP:HA	1.59	0.66
2:E:501:HEM:HHC	2:E:501:HEM:HBB2	1.75	0.66
1:F:39:PRO:HB3	1:F:57:ARG:HD2	1.78	0.65
1:B:208:ARG:NH2	7:B:607:HOH:O	2.30	0.65
1:A:122:PRO:CB	1:D:309:VAL:HG22	2.26	0.65
1:F:277:VAL:CG2	1:F:278:PRO:HD3	2.27	0.64
1:F:287:TYR:CG	1:F:337:LEU:HD21	2.31	0.64
1:C:179[B]:LEU:HD11	3:C:533:DEB:C20	2.27	0.64
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89[B]:GLU:CD	1:C:92[B]:TRP:CD2	2.76	0.64
1:F:284[B]:MET:HE1	1:F:370:LEU:CD1	2.26	0.64
1:A:92[B]:TRP:CE3	1:A:92[B]:TRP:HA	2.33	0.64
1:A:283:GLU:HG3	1:A:337:LEU:CD2	2.27	0.63
1:E:64:VAL:HG12	1:E:70:PHE:CZ	2.33	0.63
1:A:178[B]:MET:HE1	1:A:193:GLN:HG2	1.80	0.63
1:A:107:LEU:HD11	1:A:222:ALA:CB	2.29	0.63
1:A:281:VAL:CG2	1:A:370:LEU:HD12	2.29	0.63
1:D:35[B]:ARG:HG3	1:D:57[B]:ARG:HG2	1.81	0.63
1:D:45:LEU:HD11	1:D:318:VAL:HG21	1.79	0.63
1:A:92[B]:TRP:CZ3	6:A:543[B]:GOL:H2	2.35	0.62
1:A:283:GLU:HG3	1:A:337:LEU:HD22	1.80	0.62
4:D:508:FMT:H	1:E:115:ARG:HB3	1.82	0.62
1:D:184:LEU:HB2	1:D:189:ILE:HD11	1.81	0.62
1:E:327:ASP:HB3	1:E:330:VAL:HG12	1.80	0.62
1:D:116:ARG:HB3	1:D:116:ARG:NH1	2.14	0.61
1:D:257:VAL:HG23	1:D:403:GLN:NE2	2.14	0.61
1:A:174:PHE:O	1:A:178[B]:MET:HG2	2.01	0.61
1:F:184:LEU:HB2	1:F:189:ILE:HD11	1.82	0.61
1:F:185:THR:HG1	1:F:188:GLU:HG3	1.62	0.61
1:B:328[A]:GLU:H	4:B:506:FMT:C	2.14	0.61
1:B:328[B]:GLU:H	4:B:506:FMT:C	2.14	0.61
1:A:256:LEU:HD22	1:A:284:MET:HB3	1.81	0.61
1:E:264:ARG:NH2	1:E:380:LEU:O	2.33	0.61
1:B:96:GLN:OE1	4:B:529:FMT:H	2.00	0.61
1:E:213:GLU:N	1:E:213:GLU:OE1	2.34	0.61
1:A:236[B]:ASN:OD1	4:A:538:FMT:H	2.01	0.61
1:B:236[A]:ASN:ND2	6:B:543[A]:GOL:H2	2.16	0.60
1:D:186:ALA:O	1:D:190:GLN:HG3	2.01	0.60
1:C:391:TRP:HB2	4:C:524:FMT:H	1.81	0.60
1:B:9[A]:THR:CG2	1:B:10[A]:PRO:CD	2.78	0.60
1:A:194[B]:GLN:NE2	7:A:611:HOH:O	2.35	0.60
1:A:256:LEU:HD12	1:A:370:LEU:HD11	1.84	0.60
1:E:152:PHE:HB3	1:E:153:PRO:HD3	1.84	0.60
1:A:355:HIS:NE2	4:A:526:FMT:O1	2.35	0.60
1:B:150:VAL:O	1:B:154[A]:VAL:HG12	2.01	0.60
1:D:252[A]:GLN:HE21	1:D:285:LEU:HD23	1.66	0.60
1:B:76:THR:OG1	4:B:507:FMT:O2	2.20	0.59
1:D:256:LEU:HD12	1:D:370[A]:LEU:HD11	1.84	0.59
1:E:104:LEU:HD12	1:E:107:LEU:HD12	1.83	0.59
1:C:14:VAL:HG23	1:C:44[A]:ARG:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:HD22	1:D:83[B]:MET:CE	2.33	0.59
1:F:280:ALA:O	1:F:284[A]:MET:HG3	2.02	0.59
1:F:145:VAL:HA	1:F:149:ALA:HB3	1.85	0.59
1:A:92[B]:TRP:CZ3	1:A:93:VAL:HG12	2.37	0.59
1:F:182:THR:CG2	1:F:394:GLY:HA2	2.33	0.59
1:C:0:HIS:HD2	1:C:2:THR:OG1	1.86	0.59
1:F:182:THR:HG22	1:F:394:GLY:HA2	1.84	0.59
1:C:89[B]:GLU:OE2	1:C:92[B]:TRP:CB	2.51	0.58
1:D:35[B]:ARG:CG	1:D:57[B]:ARG:HG2	2.33	0.58
2:E:501:HEM:HMC1	2:E:501:HEM:HBC2	1.85	0.58
1:D:86[A]:THR:HG21	1:D:189:ILE:HG21	1.85	0.58
1:D:46:PRO:HB2	1:D:47:TYR:CD1	2.39	0.58
1:D:183:ARG:HB3	1:D:184:LEU:HD12	1.84	0.58
1:E:213:GLU:O	1:E:213:GLU:HG2	2.03	0.58
1:D:107:LEU:HD11	1:D:234:ILE:HG12	1.84	0.58
1:D:330:VAL:HG23	1:D:331:PHE:CD2	2.39	0.58
1:E:256:LEU:HD22	1:E:284[A]:MET:HB3	1.84	0.58
1:B:9[B]:THR:O	1:C:114:ALA:HB1	2.03	0.58
1:B:9[A]:THR:CG2	1:B:10[A]:PRO:HD3	2.34	0.57
1:A:111:ALA:CB	1:A:215[A]:LEU:HD21	2.35	0.57
1:A:107:LEU:HD13	1:A:229:LEU:CD1	2.35	0.57
4:B:512:FMT:C	7:B:601:HOH:O	2.53	0.57
1:A:111:ALA:HB2	1:A:215[A]:LEU:HD21	1.85	0.57
1:A:166:GLU:H	1:A:166:GLU:CD	2.11	0.57
1:A:281:VAL:HG22	1:A:370:LEU:HD12	1.85	0.57
1:B:103:ARG:HH12	4:B:538:FMT:H	1.69	0.57
1:A:57[A]:ARG:NH1	1:A:307:SER:CB	2.68	0.57
1:C:14:VAL:HG23	1:C:44[A]:ARG:HG2	1.85	0.57
1:F:30:HIS:O	1:F:34:LEU:HG	2.05	0.57
1:D:152:PHE:HB3	1:D:153:PRO:HD3	1.87	0.56
1:F:195:ASP:O	1:F:198:VAL:CG2	2.52	0.56
1:E:178[A]:MET:CE	6:E:515[A]:GOL:C3	2.84	0.56
1:E:191:ARG:HG2	4:E:506:FMT:H	1.86	0.56
1:E:260:LEU:HG	1:E:284[A]:MET:HE1	1.87	0.56
1:F:342:GLU:O	1:F:343:ARG:HG3	2.06	0.56
1:D:246:HIS:O	1:D:250:VAL:HG23	2.06	0.56
1:A:92[B]:TRP:CZ3	1:A:240:SER:OG	2.46	0.56
1:C:89[B]:GLU:OE2	1:C:92[B]:TRP:HB2	2.05	0.56
1:C:9:THR:N	1:C:10:PRO:CD	2.68	0.55
1:F:287:TYR:CD2	1:F:337:LEU:HD23	2.40	0.55
1:C:89[B]:GLU:CD	1:C:89[B]:GLU:H	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:ARG:NH1	7:E:608:HOH:O	2.38	0.55
1:F:370:LEU:O	1:F:374:VAL:HG23	2.06	0.55
1:D:35[A]:ARG:HD3	1:D:56:THR:O	2.05	0.55
1:B:9[B]:THR:HA	1:C:360[B]:GLN:CD	2.32	0.55
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.37	0.55
1:F:287:TYR:CD2	1:F:337:LEU:CD2	2.90	0.55
1:A:57[A]:ARG:NH1	1:A:307:SER:OG	2.40	0.55
1:C:14:VAL:CG2	1:C:44[A]:ARG:HG2	2.36	0.55
1:F:184:LEU:CB	1:F:189:ILE:HD11	2.36	0.55
1:F:195:ASP:C	1:F:198:VAL:HG22	2.31	0.55
1:A:105[A]:ARG:CD	1:A:357[A]:ILE:HD13	2.37	0.54
1:D:295:SER:OG	1:D:296:PHE:O	2.20	0.54
1:A:35[B]:ARG:HE	6:A:545:GOL:C3	2.15	0.54
1:B:236[A]:ASN:OD1	6:B:543[A]:GOL:H11	2.07	0.54
1:E:45:LEU:HD22	1:E:83:MET:SD	2.48	0.54
1:C:4[A]:THR:HG22	1:C:5:HIS:O	2.08	0.54
1:C:92[B]:TRP:CH2	1:C:178:MET:CE	2.87	0.54
1:A:105[B]:ARG:HG2	1:A:357[B]:ILE:HD11	1.88	0.54
1:B:213:GLU:O	1:B:214[A]:ASP:CG	2.50	0.54
1:B:92:TRP:CD2	6:B:543[B]:GOL:H32	2.43	0.53
1:D:166[B]:GLU:HG3	1:E:228:HIS:CD2	2.44	0.53
1:C:194:GLN:O	1:C:198:VAL:HG23	2.09	0.53
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.90	0.53
1:A:17:TYR:HA	1:A:18:PRO:C	2.33	0.53
1:C:179[B]:LEU:CD1	3:C:533:DEB:C20	2.87	0.53
1:A:58[B]:MET:HG2	1:A:324:ALA:O	2.09	0.53
1:A:92[B]:TRP:CE3	1:A:93:VAL:N	2.77	0.53
1:B:161:LEU:HB3	1:B:216[B]:LEU:HD13	1.90	0.53
1:A:57[A]:ARG:HH11	1:A:307:SER:CB	2.22	0.52
1:D:145:VAL:HA	1:D:149:ALA:HB3	1.89	0.52
1:C:92[B]:TRP:HZ2	3:C:533:DEB:O19	1.90	0.52
1:B:101:HIS:CE1	1:B:105[B]:ARG:HD2	2.44	0.52
1:F:185:THR:O	1:F:189:ILE:HG12	2.09	0.52
1:B:127[A]:LEU:HD21	1:B:155:ALA:HB3	1.90	0.52
1:D:330:VAL:HG23	1:D:331:PHE:CE2	2.45	0.52
1:E:17:TYR:HA	1:E:18:PRO:C	2.34	0.52
1:A:45:LEU:HD12	1:A:81:PRO:HB3	1.91	0.52
1:B:105[A]:ARG:CD	1:B:357:ILE:HD12	2.39	0.52
1:A:107:LEU:HD11	1:A:222:ALA:HB1	1.91	0.52
1:B:46:PRO:HB2	1:B:47:TYR:CD1	2.44	0.51
1:D:178:MET:HE3	1:D:193:GLN:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ARG:C	1:D:184:LEU:HD12	2.34	0.51
1:A:92[B]:TRP:CE3	1:A:92[B]:TRP:CA	2.93	0.51
1:F:266:ARG:O	1:F:269:SER:HB3	2.11	0.51
1:A:92[B]:TRP:CE2	1:A:94:LEU:HB2	2.45	0.51
1:D:17:TYR:CD1	1:D:18:PRO:HA	2.44	0.51
1:D:246:HIS:NE2	1:D:247[B]:GLU:OE2	2.43	0.51
1:F:104:LEU:HB3	1:F:237[A]:MET:CE	2.40	0.51
1:E:35:ARG:NH1	1:E:326:ARG:O	2.44	0.51
1:E:71:SER:OG	1:E:97:ASP:OD2	2.22	0.51
1:C:89[B]:GLU:HB2	7:C:631:HOH:O	2.10	0.51
1:C:283:GLU:HG3	1:C:337:LEU:HD22	1.93	0.51
1:B:9[B]:THR:HA	1:C:360[B]:GLN:OE1	2.10	0.51
1:E:178[B]:MET:HA	1:E:178[B]:MET:HE3	1.91	0.51
1:F:93:VAL:HG21	1:F:237[A]:MET:HE1	1.92	0.51
1:A:45:LEU:HD22	1:A:83:MET:SD	2.51	0.51
1:E:259:LEU:HB2	1:E:284[A]:MET:HE2	1.93	0.51
1:B:9[A]:THR:CB	1:B:10[A]:PRO:CD	2.89	0.51
1:D:194:GLN:O	1:D:198:VAL:HG13	2.11	0.51
1:F:252:GLN:O	1:F:256:LEU:HD13	2.10	0.51
1:B:351:HIS:ND1	4:B:513:FMT:H	2.24	0.51
1:A:105[A]:ARG:HD3	1:A:357[A]:ILE:HD13	1.93	0.51
1:D:104:LEU:O	1:D:107:LEU:HB2	2.10	0.51
1:A:274:PRO:HB2	1:A:375[A]:ARG:NH2	2.26	0.50
1:B:106[A]:ARG:NH1	4:B:537:FMT:C	2.74	0.50
1:D:256:LEU:HD22	1:D:284:MET:HB3	1.93	0.50
1:B:10[B]:PRO:N	1:C:360[B]:GLN:OE1	2.44	0.50
1:E:178[B]:MET:SD	1:E:193:GLN:CG	3.00	0.50
1:A:240:SER:HG	6:A:543[A]:GOL:H31	1.75	0.50
1:B:101:HIS:CE1	1:B:105[B]:ARG:CD	2.95	0.50
1:D:253:ILE:O	1:D:257:VAL:HG22	2.11	0.50
1:E:237[B]:MET:HA	1:E:237[B]:MET:HE2	1.94	0.50
1:F:267:TYR:OH	1:F:373:LEU:O	2.29	0.50
1:B:236[A]:ASN:CG	6:B:543[A]:GOL:C2	2.71	0.50
1:D:34:LEU:O	1:D:38:GLU:C	2.54	0.50
7:A:637:HOH:O	1:D:312:ARG:HD2	2.11	0.50
1:E:172:ARG:NH1	7:E:609:HOH:O	2.38	0.50
1:B:236[A]:ASN:HD21	6:B:543[A]:GOL:C2	2.25	0.50
1:F:264:ARG:NH2	1:F:380:LEU:O	2.41	0.50
1:B:9[A]:THR:OG1	1:B:10[A]:PRO:HD3	2.12	0.49
1:B:393[A]:GLN:NE2	7:B:625:HOH:O	2.44	0.49
1:F:234:ILE:O	1:F:237[B]:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ARG:HD2	7:C:681:HOH:O	2.11	0.49
1:E:331:PHE:CE1	1:E:345:PRO:HD2	2.47	0.49
1:E:178[B]:MET:SD	1:E:193:GLN:HG2	2.53	0.49
1:A:122:PRO:HB3	1:D:309:VAL:CG2	2.36	0.49
1:B:355:HIS:HE2	4:B:511:FMT:C	2.25	0.49
1:D:58[B]:MET:HE1	1:D:347:ILE:HD13	1.94	0.49
1:D:116:ARG:NH1	7:D:613:HOH:O	2.44	0.49
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:CB	2.26	0.49
1:B:14:VAL:HG12	1:C:118:GLU:HG2	1.94	0.49
1:B:183:ARG:HH11	4:B:532:FMT:C	2.26	0.49
1:A:105[B]:ARG:NH1	1:A:357[B]:ILE:HG13	2.28	0.48
1:B:115:ARG:NH1	7:B:627:HOH:O	2.46	0.48
1:C:197[B]:MET:SD	1:C:236:ASN:ND2	2.86	0.48
1:E:123:ARG:NH2	1:E:127[A]:LEU:HD21	2.28	0.48
1:F:58:MET:HE2	1:F:324:ALA:O	2.13	0.48
1:A:281:VAL:HG22	1:A:370:LEU:CD1	2.42	0.48
1:C:93:VAL:HG21	1:C:237[A]:MET:HE1	1.95	0.48
4:A:510:FMT:H	7:A:698:HOH:O	2.13	0.48
1:A:38[A]:GLU:HG2	1:A:41:SER:HB3	1.94	0.48
1:A:375[B]:ARG:HH21	1:A:375[B]:ARG:HG3	1.79	0.48
1:B:236[A]:ASN:ND2	6:B:543[A]:GOL:C2	2.76	0.48
1:E:191:ARG:HG2	4:E:506:FMT:C	2.44	0.48
1:A:366:LEU:O	1:A:370:LEU:HG	2.13	0.48
1:B:186:ALA:O	1:B:190:GLN:HG3	2.14	0.48
1:D:39:PRO:HG3	1:D:57[A]:ARG:CZ	2.43	0.48
1:D:248:THR:O	1:D:252[B]:GLN:HG2	2.13	0.48
1:F:121:ARG:HG3	1:F:364:LEU:HD11	1.96	0.48
1:A:270:LEU:HB3	1:A:374:VAL:HG11	1.95	0.48
1:C:92[B]:TRP:CE3	1:C:92[B]:TRP:HA	2.49	0.48
1:E:58[A]:MET:HE1	1:E:347:ILE:CG2	2.44	0.48
1:D:266:ARG:CZ	1:D:337[A]:LEU:HD12	2.44	0.47
1:D:267:TYR:O	1:D:271:VAL:HG23	2.13	0.47
1:F:127:LEU:HD12	1:F:127:LEU:O	2.14	0.47
1:F:287:TYR:CG	1:F:337:LEU:CD2	2.97	0.47
1:C:354:HIS:NE2	6:C:531[B]:GOL:O3	2.33	0.47
4:D:508:FMT:C	1:E:115:ARG:HB3	2.43	0.47
1:A:290:LEU:O	1:A:397:ILE:HA	2.15	0.47
1:B:103:ARG:O	4:B:537:FMT:H	2.15	0.47
1:D:38:GLU:OE2	4:D:510:FMT:O2	2.32	0.47
1:D:70:PHE:HE2	1:D:304:VAL:HG11	1.79	0.47
1:D:252[B]:GLN:HG3	2:D:501:HEM:CBB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:GLU:C	1:F:343:ARG:HG3	2.39	0.47
1:D:35[A]:ARG:NH2	4:D:515:FMT:O1	2.47	0.47
1:B:178[B]:MET:SD	1:B:193:GLN:CG	3.03	0.47
1:D:17:TYR:CD2	1:D:83[B]:MET:CE	2.92	0.47
1:B:35:ARG:HE	4:B:506:FMT:H	1.79	0.47
1:C:92[B]:TRP:CZ2	3:C:533:DEB:O19	2.62	0.47
1:B:178[B]:MET:HE3	1:B:178[B]:MET:HA	1.97	0.47
1:D:86[A]:THR:CG2	1:D:189:ILE:HB	2.45	0.47
1:C:8:PRO:C	1:C:10:PRO:HD2	2.40	0.47
1:C:152:PHE:HB3	1:C:153:PRO:HD3	1.96	0.47
4:A:535:FMT:C	7:A:608:HOH:O	2.62	0.46
1:F:177:ALA:O	1:F:189:ILE:HD12	2.15	0.46
4:B:524:FMT:C	6:B:542:GOL:H31	2.45	0.46
1:E:178[B]:MET:HE1	1:E:193:GLN:OE1	2.16	0.46
1:A:38[A]:GLU:CD	1:A:41:SER:HB3	2.41	0.46
1:A:239:VAL:HB	6:A:543[B]:GOL:O1	2.15	0.46
1:A:341[B]:ARG:NH1	1:A:341[B]:ARG:HB3	2.30	0.46
1:D:260:LEU:HD11	1:D:370[B]:LEU:HD21	1.97	0.46
1:E:127[B]:LEU:HD21	1:E:155:ALA:HB3	1.98	0.46
1:B:103:ARG:HH12	4:B:538:FMT:C	2.29	0.46
1:F:260:LEU:HG	1:F:284[A]:MET:HE1	1.98	0.46
1:B:133:ASP:O	1:B:136:VAL:HG22	2.16	0.46
1:B:178[B]:MET:HE3	1:B:178[B]:MET:CA	2.46	0.46
1:A:44[A]:ARG:NH2	4:A:519:FMT:O2	2.43	0.46
1:D:402:ARG:HD3	1:D:404:ILE:HG13	1.98	0.46
1:B:110[B]:LYS:HG3	1:B:116:ARG:NH1	2.30	0.46
1:D:46:PRO:HB2	1:D:47:TYR:CE1	2.50	0.46
1:E:213:GLU:O	1:E:213:GLU:CG	2.64	0.46
1:E:320:HIS:HD2	7:E:603:HOH:O	1.99	0.46
1:A:355:HIS:ND1	4:A:525:FMT:C	2.79	0.46
1:F:183:ARG:HB3	1:F:394:GLY:HA3	1.98	0.46
1:F:207:ARG:NH1	7:F:618:HOH:O	2.49	0.46
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.97	0.46
4:A:510:FMT:C	7:A:698:HOH:O	2.64	0.45
1:B:35:ARG:HE	4:B:506:FMT:C	2.29	0.45
1:C:12:ASP:OD1	1:C:12:ASP:N	2.49	0.45
1:D:55:VAL:HG21	1:D:64:VAL:HG21	1.99	0.45
1:E:170:LEU:HD22	1:E:174:PHE:CZ	2.50	0.45
2:F:501:HEM:HBB2	2:F:501:HEM:CMB	2.45	0.45
1:E:92:TRP:CG	6:E:515[A]:GOL:H12	2.50	0.45
1:E:178[B]:MET:SD	1:E:193:GLN:HG3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:PRO:CB	1:F:57:ARG:HD2	2.45	0.45
1:B:42[B]:ARG:H	4:B:520:FMT:C	2.29	0.45
1:C:127:LEU:HD21	1:C:155:ALA:HB3	1.99	0.45
2:D:501:HEM:HAB	2:D:501:HEM:HHC	1.56	0.45
1:F:194:GLN:O	1:F:198:VAL:HG13	2.17	0.45
1:B:42[A]:ARG:H	4:B:520:FMT:C	2.29	0.45
1:D:127:LEU:HD23	1:D:152:PHE:CD1	2.52	0.45
1:F:259:LEU:HB2	1:F:284[A]:MET:CE	2.46	0.45
1:C:72:THR:HG23	6:C:531[B]:GOL:H11	1.99	0.45
1:E:215:LEU:HD23	1:E:215:LEU:HA	1.86	0.45
1:E:186:ALA:O	1:E:190:GLN:HG3	2.17	0.45
1:D:252[B]:GLN:OE1	1:D:252[B]:GLN:HA	2.16	0.45
1:E:33:GLU:HA	1:E:36:ARG:NH2	2.32	0.45
1:B:312[A]:ARG:HB3	1:C:375:ARG:HH21	1.81	0.45
1:B:344:ASN:N	7:B:605:HOH:O	2.24	0.45
1:F:246:HIS:O	1:F:250:VAL:HG23	2.17	0.45
1:B:205:ALA:O	1:B:208:ARG:HG2	2.16	0.44
1:C:283:GLU:HG3	1:C:337:LEU:CD2	2.47	0.44
1:C:305[B]:GLU:HG3	4:C:522:FMT:O1	2.17	0.44
1:A:174:PHE:HB3	1:A:196:PHE:CD2	2.53	0.44
1:D:35[B]:ARG:HG3	1:D:57[B]:ARG:CG	2.44	0.44
1:F:333:HIS:CE1	1:F:338:ASP:OD2	2.60	0.44
1:A:220:ALA:O	1:A:223:THR:HB	2.18	0.44
1:B:92:TRP:HA	1:B:236[A]:ASN:HD21	1.75	0.44
1:B:312[A]:ARG:HB3	1:C:375:ARG:NH2	2.33	0.44
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	2.00	0.44
1:B:305:GLU:HG3	4:B:528:FMT:H	1.99	0.44
1:D:267:TYR:CZ	1:D:380:LEU:HD23	2.50	0.44
1:D:335:ASP:OD1	4:D:515:FMT:O2	2.36	0.44
1:F:168:ARG:O	1:F:172:ARG:HG3	2.17	0.44
1:A:107:LEU:HD11	1:A:222:ALA:HB2	1.99	0.44
1:B:42[A]:ARG:NH2	4:B:515:FMT:O2	2.51	0.44
1:A:92[B]:TRP:CZ2	3:A:502:DEB:H5	2.53	0.44
1:A:383:ALA:HB3	1:A:404:ILE:HG22	1.99	0.44
1:B:106[A]:ARG:NH2	7:B:633:HOH:O	2.50	0.44
1:B:392:LYS:HG2	1:B:401:GLU:HG3	2.00	0.44
1:F:145:VAL:HG21	1:F:402:ARG:HA	1.99	0.44
1:A:246:HIS:O	1:A:250:VAL:HG23	2.17	0.43
1:C:69:ARG:HH12	4:C:522:FMT:C	2.31	0.43
1:A:133:ASP:HA	1:A:136:VAL:HG22	2.00	0.43
1:C:271:VAL:HA	1:C:374:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:LYS:NZ	7:D:612:HOH:O	2.50	0.43
1:E:259:LEU:HB2	1:E:284[A]:MET:CE	2.48	0.43
1:F:267:TYR:CE1	1:F:374:VAL:HG22	2.53	0.43
1:F:380:LEU:HG	1:F:405:VAL:CG1	2.48	0.43
1:A:58[B]:MET:SD	1:A:324:ALA:O	2.75	0.43
1:F:384:GLU:OE1	1:F:402:ARG:NH1	2.51	0.43
1:B:110[B]:LYS:HD2	1:B:110[B]:LYS:HA	1.63	0.43
1:D:17:TYR:HA	1:D:18:PRO:C	2.44	0.43
1:E:178[B]:MET:HE3	1:E:178[B]:MET:CA	2.46	0.43
1:F:148:LEU:O	1:F:152:PHE:HB3	2.18	0.43
1:A:57[A]:ARG:NH1	1:A:307:SER:HB2	2.34	0.43
1:A:58[B]:MET:HE1	1:A:347:ILE:HG23	1.99	0.43
1:B:27:LEU:HD12	1:B:326[A]:ARG:CZ	2.49	0.43
1:B:152:PHE:HB3	1:B:153:PRO:HD3	2.01	0.43
3:B:502:DEB:O19	6:B:543[B]:GOL:C3	2.65	0.43
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	2.00	0.43
1:E:107:LEU:HD11	1:E:229:LEU:HD13	2.00	0.43
1:A:263:GLU:HB2	1:A:266:ARG:HD2	2.00	0.43
1:D:256:LEU:HD13	1:D:284:MET:HE3	2.01	0.43
1:F:27:LEU:HD12	1:F:326:ARG:NH1	2.33	0.43
1:F:141:PRO:HB2	1:F:404:ILE:HG22	1.99	0.43
1:A:152:PHE:HB3	1:A:153:PRO:HD3	2.01	0.43
1:A:377:PHE:N	1:A:378:PRO:HD3	2.34	0.43
1:C:258:HIS:CE1	1:C:262:THR:HG21	2.54	0.43
1:D:343:ARG:HG2	1:D:345:PRO:HD3	1.99	0.43
1:E:231:LYS:O	1:E:235:VAL:HG23	2.18	0.43
1:F:266:ARG:HE	1:F:337:LEU:HD12	1.75	0.43
1:A:35[B]:ARG:HH21	6:A:545:GOL:C1	2.32	0.43
1:E:286:ARG:HD3	1:E:344:ASN:OD1	2.19	0.43
1:F:17:TYR:CD1	1:F:18:PRO:HA	2.53	0.43
1:E:58[B]:MET:HA	1:E:324:ALA:HB1	1.99	0.43
1:B:355:HIS:NE2	4:B:511:FMT:O1	2.46	0.43
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:HB3	1.84	0.43
1:E:128:VAL:HG23	1:E:152:PHE:CE1	2.54	0.43
1:F:120:MET:O	1:F:124:VAL:HG23	2.19	0.43
1:A:89[B]:GLU:HG2	1:A:92[B]:TRP:HB2	2.01	0.42
1:A:105[B]:ARG:NH2	4:A:525:FMT:C	2.82	0.42
1:A:354:HIS:O	1:A:355:HIS:C	2.61	0.42
1:E:46:PRO:HB2	1:E:47:TYR:CD2	2.54	0.42
1:E:178[A]:MET:HE1	6:E:515[A]:GOL:C3	2.40	0.42
1:B:270:LEU:C	1:B:374:VAL:CG1	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LYS:HG3	1:B:399:GLY:O	2.19	0.42
1:C:44[A]:ARG:NE	7:C:603:HOH:O	2.27	0.42
1:C:332:ASP:HB3	4:C:513:FMT:C	2.48	0.42
1:D:166[B]:GLU:CG	1:E:228:HIS:NE2	2.78	0.42
1:D:227:ASP:O	1:D:228:HIS:HB2	2.19	0.42
1:D:392:LYS:HG3	1:D:399:GLY:O	2.19	0.42
1:E:104:LEU:HD12	1:E:107:LEU:CD1	2.49	0.42
1:F:309[A]:VAL:HG12	1:F:310:THR:N	2.34	0.42
1:B:92:TRP:CE3	6:B:543[B]:GOL:H32	2.55	0.42
1:B:106[A]:ARG:CZ	4:B:537:FMT:C	2.97	0.42
1:D:322:ALA:O	1:D:326:ARG:HG2	2.20	0.42
1:E:290:LEU:O	1:E:397:ILE:HA	2.18	0.42
1:A:256:LEU:HD22	1:A:284:MET:CB	2.47	0.42
1:D:101:HIS:HE1	1:D:353:ALA:O	2.02	0.42
1:E:105:ARG:NH2	1:E:355:HIS:O	2.28	0.42
1:F:170:LEU:C	1:F:170:LEU:HD23	2.45	0.42
1:B:8[A]:PRO:HB3	1:B:12:ASP:HB2	2.00	0.42
1:B:390:LYS:HE3	1:B:402[A]:ARG:HH21	1.84	0.42
1:D:219:LEU:O	1:D:222:ALA:HB3	2.20	0.42
1:F:309[A]:VAL:HG12	1:F:310:THR:C	2.44	0.42
1:F:376:ARG:HE	1:F:376:ARG:HB3	1.70	0.42
1:A:375[B]:ARG:HG3	1:A:375[B]:ARG:NH2	2.35	0.42
1:B:174:PHE:O	1:B:178[B]:MET:HG2	2.20	0.42
1:A:240:SER:OG	6:A:543[A]:GOL:H31	2.19	0.42
1:A:295:SER:CB	1:A:319[A]:VAL:HG22	2.49	0.42
1:B:9[A]:THR:OG1	1:B:10[A]:PRO:CD	2.68	0.42
1:B:161:LEU:O	1:B:216[B]:LEU:CD1	2.54	0.42
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.79	0.41
1:E:328:GLU:HB2	7:E:639:HOH:O	2.19	0.41
1:A:355:HIS:HE2	4:A:526:FMT:C	2.32	0.41
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	2.02	0.41
1:A:244:ALA:HB1	2:A:501:HEM:C4C	2.55	0.41
1:B:287:TYR:O	1:B:326[A]:ARG:NH1	2.54	0.41
1:D:188:GLU:OE1	4:D:508:FMT:O1	2.37	0.41
1:F:17:TYR:HA	1:F:18:PRO:C	2.45	0.41
1:A:58[B]:MET:CG	1:A:324:ALA:O	2.68	0.41
1:B:161:LEU:CA	1:B:216[B]:LEU:HD13	2.50	0.41
1:E:308:THR:C	1:E:309:VAL:HG23	2.46	0.41
1:F:271:VAL:CG2	1:F:374:VAL:HG13	2.48	0.41
1:E:178[A]:MET:HE2	6:E:515[A]:GOL:H32	2.02	0.41
1:F:152:PHE:HB3	1:F:153:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:LEU:HA	1:F:262:THR:HG22	2.03	0.41
1:C:266:ARG:O	1:C:269[A]:SER:OG	2.32	0.41
1:D:256:LEU:HD12	1:D:370[A]:LEU:CD1	2.48	0.41
1:E:86:THR:HG21	1:E:189:ILE:HG22	2.02	0.41
1:F:280:ALA:O	1:F:284[B]:MET:HG3	2.19	0.41
1:E:178[A]:MET:HE2	6:E:515[A]:GOL:C3	2.50	0.41
1:A:183:ARG:HD2	4:A:516:FMT:O1	2.21	0.41
1:B:101:HIS:CE1	1:B:105[B]:ARG:HD3	2.56	0.41
1:B:124:VAL:HG13	1:B:152:PHE:HE1	1.86	0.41
1:D:256:LEU:CD1	1:D:370[A]:LEU:HD11	2.51	0.41
1:E:208:ARG:NH1	1:E:223:THR:HG22	2.36	0.41
1:B:11[A]:ALA:O	1:B:44:ARG:NH2	2.54	0.41
1:C:382:LEU:HD12	1:C:382:LEU:HA	1.97	0.41
4:C:524:FMT:H	7:C:727:HOH:O	2.20	0.41
1:A:252:GLN:OE1	1:A:252:GLN:HA	2.21	0.40
1:A:258:HIS:HD2	7:A:765:HOH:O	2.03	0.40
1:F:161:LEU:CD2	1:F:215:LEU:HD12	2.43	0.40
1:D:23:HIS:O	1:D:26:ASP:HB2	2.21	0.40
1:E:354:HIS:O	1:E:355:HIS:C	2.65	0.40
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.91	0.40
1:C:270:LEU:C	1:C:374:VAL:HG11	2.46	0.40
1:D:83[A]:MET:HE3	7:D:614:HOH:O	2.21	0.40
1:D:290:LEU:O	1:D:397:ILE:HA	2.21	0.40
1:E:204:VAL:HG13	1:E:220:ALA:HB2	2.04	0.40
1:F:373:LEU:HD23	1:F:373:LEU:HA	1.91	0.40
1:B:252:GLN:HA	1:B:252:GLN:OE1	2.21	0.40
1:A:256:LEU:CD1	1:A:370:LEU:HD11	2.51	0.40
1:B:170:LEU:HD12	1:B:170:LEU:HA	1.96	0.40
1:C:42[A]:ARG:HG2	1:C:53:TRP:CE3	2.57	0.40
1:D:286:ARG:HG3	1:D:325:ASN:HB3	2.03	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:B:302:GLU:OE2	1:C:208:ARG:NH2[4_556]	2.14	0.06

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	426/408 (104%)	413 (97%)	13 (3%)	0	100	100
1	B	433/408 (106%)	415 (96%)	17 (4%)	1 (0%)	43	44
1	C	435/408 (107%)	426 (98%)	9 (2%)	0	100	100
1	D	410/408 (100%)	388 (95%)	22 (5%)	0	100	100
1	E	402/408 (98%)	385 (96%)	17 (4%)	0	100	100
1	F	400/408 (98%)	375 (94%)	24 (6%)	1 (0%)	36	36
All	All	2506/2448 (102%)	2402 (96%)	102 (4%)	2 (0%)	48	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	264	ARG
1	B	68	SER

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	365/343 (106%)	359 (98%)	6 (2%)	55	62
1	B	369/343 (108%)	365 (99%)	4 (1%)	65	73
1	C	372/343 (108%)	368 (99%)	4 (1%)	65	73
1	D	349/343 (102%)	342 (98%)	7 (2%)	48	54
1	E	341/343 (99%)	334 (98%)	7 (2%)	47	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	339/343 (99%)	334 (98%)	5 (2%)	57	64
All	All	2135/2058 (104%)	2102 (98%)	33 (2%)	59	64

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLU
1	A	190	GLN
1	A	191[A]	ARG
1	A	191[B]	ARG
1	A	224	ASP
1	A	337	LEU
1	B	9[A]	THR
1	B	9[B]	THR
1	B	36	ARG
1	B	221	LEU
1	C	12	ASP
1	C	27[A]	LEU
1	C	27[B]	LEU
1	C	116	ARG
1	D	89	GLU
1	D	94	LEU
1	D	115[A]	ARG
1	D	115[B]	ARG
1	D	207	ARG
1	D	236	ASN
1	D	312	ARG
1	E	42	ARG
1	E	106[A]	ARG
1	E	106[B]	ARG
1	E	183	ARG
1	E	207	ARG
1	E	264	ARG
1	E	326	ARG
1	F	42	ARG
1	F	165	LEU
1	F	183	ARG
1	F	231	LYS
1	F	312	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	HIS
1	A	351	HIS
1	B	193	GLN
1	B	228	HIS
1	C	0	HIS
1	C	190	GLN
1	C	225	ASN
1	C	236	ASN
1	C	393	GLN
1	D	236	ASN
1	E	225	ASN
1	E	340	HIS
1	F	333	HIS
1	F	351	HIS

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](#)

Of 172 ligands modelled in this entry, 8 are monoatomic - leaving 164 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	$\# Z > 2$
4	FMT	B	508	-	2,2,2	0.11	0	1,1,1	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	A	539	-	2,2,2	0.30	0	1,1,1	0.16	0
4	FMT	D	513	-	2,2,2	0.27	0	1,1,1	0.21	0
4	FMT	B	509	-	2,2,2	0.23	0	1,1,1	0.15	0
4	FMT	C	528	-	2,2,2	0.18	0	1,1,1	0.12	0
4	FMT	C	505	-	2,2,2	0.17	0	1,1,1	0.05	0
6	GOL	A	543[B]	-	5,5,5	0.10	0	5,5,5	0.28	0
6	GOL	A	545	-	5,5,5	0.20	0	5,5,5	0.67	0
2	HEM	A	501	1	50,50,50	1.61	10 (20%)	67,82,82	1.76	15 (22%)
4	FMT	A	510	5	2,2,2	0.71	0	1,1,1	0.16	0
4	FMT	F	503	-	2,2,2	0.19	0	1,1,1	0.12	0
4	FMT	F	509	-	2,2,2	0.14	0	1,1,1	0.14	0
4	FMT	B	520	-	2,2,2	0.49	0	1,1,1	0.17	0
4	FMT	F	508	-	2,2,2	0.37	0	1,1,1	0.12	0
4	FMT	D	515	-	2,2,2	0.18	0	1,1,1	0.07	0
4	FMT	A	525	-	2,2,2	0.10	0	1,1,1	0.20	0
4	FMT	A	511	-	2,2,2	0.30	0	1,1,1	0.13	0
4	FMT	A	517	-	2,2,2	0.33	0	1,1,1	0.12	0
6	GOL	A	544	-	5,5,5	0.27	0	5,5,5	0.57	0
6	GOL	B	542	-	5,5,5	0.23	0	5,5,5	0.60	0
6	GOL	A	543[A]	-	5,5,5	0.24	0	5,5,5	0.48	0
4	FMT	E	513	-	2,2,2	0.22	0	1,1,1	0.26	0
4	FMT	C	517	-	2,2,2	0.20	0	1,1,1	0.11	0
4	FMT	E	509	-	2,2,2	0.27	0	1,1,1	0.20	0
4	FMT	F	505	-	2,2,2	0.23	0	1,1,1	0.12	0
6	GOL	B	543[A]	-	5,5,5	0.33	0	5,5,5	0.39	0
4	FMT	B	537	-	2,2,2	0.19	0	1,1,1	0.17	0
4	FMT	A	516	-	2,2,2	0.20	0	1,1,1	0.12	0
4	FMT	B	533	-	2,2,2	0.24	0	1,1,1	0.15	0
4	FMT	C	526	-	2,2,2	0.21	0	1,1,1	0.15	0
4	FMT	A	524	-	2,2,2	0.26	0	1,1,1	0.16	0
4	FMT	A	531	-	2,2,2	0.24	0	1,1,1	0.18	0
4	FMT	B	523	-	2,2,2	0.14	0	1,1,1	0.19	0
4	FMT	A	514	-	2,2,2	0.26	0	1,1,1	0.15	0
4	FMT	A	530	-	2,2,2	0.33	0	1,1,1	0.14	0
3	DEB	C	533	-	27,27,27	0.28	0	37,39,39	0.61	1 (2%)
4	FMT	B	538	-	2,2,2	0.16	0	1,1,1	0.20	0
4	FMT	A	528	-	2,2,2	0.06	0	1,1,1	0.23	0
4	FMT	F	512	-	2,2,2	0.14	0	1,1,1	0.20	0
4	FMT	B	530	-	2,2,2	0.36	0	1,1,1	0.18	0
4	FMT	B	526	-	2,2,2	0.18	0	1,1,1	0.11	0
4	FMT	D	514	-	2,2,2	0.16	0	1,1,1	0.10	0
4	FMT	C	513	-	2,2,2	0.37	0	1,1,1	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	B	507	-	2,2,2	0.33	0	1,1,1	0.15	0
4	FMT	B	516	-	2,2,2	0.17	0	1,1,1	0.10	0
4	FMT	B	532	-	2,2,2	0.25	0	1,1,1	0.15	0
4	FMT	C	523	-	2,2,2	0.17	0	1,1,1	0.11	0
4	FMT	E	507	-	2,2,2	0.14	0	1,1,1	0.09	0
4	FMT	C	522	-	2,2,2	0.27	0	1,1,1	0.20	0
2	HEM	F	501	1	50,50,50	1.53	7 (14%)	67,82,82	1.81	13 (19%)
4	FMT	B	505	-	2,2,2	0.17	0	1,1,1	0.13	0
6	GOL	B	543[B]	-	5,5,5	0.24	0	5,5,5	0.44	0
4	FMT	C	520	-	2,2,2	0.35	0	1,1,1	0.07	0
4	FMT	B	522	-	2,2,2	0.21	0	1,1,1	0.00	0
4	FMT	B	529	-	2,2,2	0.24	0	1,1,1	0.16	0
3	DEB	D	502	-	27,27,27	0.23	0	37,39,39	0.50	0
4	FMT	C	527	-	2,2,2	0.18	0	1,1,1	0.08	0
4	FMT	C	508	-	2,2,2	0.31	0	1,1,1	0.16	0
4	FMT	B	504	-	2,2,2	0.15	0	1,1,1	0.16	0
4	FMT	D	509	-	2,2,2	0.32	0	1,1,1	0.15	0
4	FMT	E	508	-	2,2,2	0.37	0	1,1,1	0.15	0
4	FMT	A	537	-	2,2,2	0.22	0	1,1,1	0.13	0
4	FMT	D	511	-	2,2,2	0.17	0	1,1,1	0.17	0
4	FMT	B	512	-	2,2,2	0.18	0	1,1,1	0.17	0
4	FMT	B	513	-	2,2,2	0.16	0	1,1,1	0.15	0
4	FMT	C	529	-	2,2,2	0.33	0	1,1,1	0.14	0
4	FMT	B	534	-	2,2,2	0.27	0	1,1,1	0.16	0
4	FMT	A	521	-	2,2,2	0.06	0	1,1,1	0.17	0
2	HEM	B	501	1	50,50,50	1.59	10 (20%)	67,82,82	1.89	20 (29%)
4	FMT	A	506	-	2,2,2	0.09	0	1,1,1	0.16	0
4	FMT	C	514	-	2,2,2	0.38	0	1,1,1	0.11	0
4	FMT	D	507	-	2,2,2	0.26	0	1,1,1	0.16	0
4	FMT	E	504	-	2,2,2	0.38	0	1,1,1	0.07	0
4	FMT	C	521	-	2,2,2	0.30	0	1,1,1	0.15	0
4	FMT	A	520	-	2,2,2	0.19	0	1,1,1	0.10	0
4	FMT	B	514	-	2,2,2	0.19	0	1,1,1	0.21	0
3	DEB	E	502	-	27,27,27	0.51	0	37,39,39	0.79	0
4	FMT	A	509	-	2,2,2	0.34	0	1,1,1	0.14	0
4	FMT	B	511	-	2,2,2	0.18	0	1,1,1	0.18	0
4	FMT	B	517	-	2,2,2	0.07	0	1,1,1	0.11	0
4	FMT	A	532	-	2,2,2	0.24	0	1,1,1	0.16	0
4	FMT	D	504	-	2,2,2	0.08	0	1,1,1	0.13	0
4	FMT	A	515	-	2,2,2	0.33	0	1,1,1	0.11	0
4	FMT	C	518	-	2,2,2	0.22	0	1,1,1	0.07	0
4	FMT	A	505	-	2,2,2	0.10	0	1,1,1	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	A	523	-	2,2,2	0.08	0	1,1,1	0.16	0
4	FMT	F	507	-	2,2,2	0.18	0	1,1,1	0.16	0
4	FMT	D	503	-	2,2,2	0.20	0	1,1,1	0.16	0
4	FMT	B	536	-	2,2,2	0.22	0	1,1,1	0.17	0
2	HEM	C	501	1	50,50,50	1.62	12 (24%)	67,82,82	1.91	20 (29%)
2	HEM	D	501	1	50,50,50	1.60	9 (18%)	67,82,82	2.79	33 (49%)
4	FMT	A	538	-	2,2,2	0.14	0	1,1,1	0.13	0
6	GOL	C	532	-	5,5,5	0.14	0	5,5,5	0.32	0
4	FMT	A	533	-	2,2,2	0.37	0	1,1,1	0.11	0
4	FMT	B	510	-	2,2,2	0.21	0	1,1,1	0.14	0
3	DEB	B	502	-	27,27,27	0.51	0	37,39,39	1.07	2 (5%)
4	FMT	F	504	-	2,2,2	0.08	0	1,1,1	0.11	0
4	FMT	A	535	-	2,2,2	0.29	0	1,1,1	0.15	0
4	FMT	B	527	-	2,2,2	0.23	0	1,1,1	0.12	0
4	FMT	B	525	-	2,2,2	0.35	0	1,1,1	0.11	0
4	FMT	D	510	-	2,2,2	0.09	0	1,1,1	0.14	0
4	FMT	E	511	-	2,2,2	0.31	0	1,1,1	0.11	0
4	FMT	C	509	-	2,2,2	0.21	0	1,1,1	0.12	0
4	FMT	C	519	-	2,2,2	0.16	0	1,1,1	0.41	0
4	FMT	D	512	-	2,2,2	0.28	0	1,1,1	0.15	0
6	GOL	C	531[B]	-	5,5,5	0.22	0	5,5,5	0.66	0
4	FMT	A	526	-	2,2,2	0.13	0	1,1,1	0.28	0
4	FMT	C	516	-	2,2,2	0.23	0	1,1,1	0.23	0
4	FMT	B	528	-	2,2,2	0.20	0	1,1,1	0.10	0
4	FMT	A	536	-	2,2,2	0.35	0	1,1,1	0.14	0
4	FMT	D	516	-	2,2,2	0.22	0	1,1,1	0.08	0
4	FMT	C	525	-	2,2,2	0.12	0	1,1,1	0.13	0
4	FMT	A	522	-	2,2,2	0.15	0	1,1,1	0.18	0
4	FMT	C	506	-	2,2,2	0.12	0	1,1,1	0.12	0
4	FMT	D	505	-	2,2,2	0.21	0	1,1,1	0.10	0
4	FMT	E	510	-	2,2,2	0.35	0	1,1,1	0.15	0
6	GOL	E	515[B]	-	5,5,5	0.09	0	5,5,5	0.28	0
4	FMT	D	506	-	2,2,2	0.26	0	1,1,1	0.19	0
4	FMT	C	512	-	2,2,2	0.36	0	1,1,1	0.10	0
4	FMT	A	507	-	2,2,2	0.13	0	1,1,1	0.07	0
4	FMT	A	508	-	2,2,2	0.30	0	1,1,1	0.15	0
4	FMT	C	504	-	2,2,2	0.17	0	1,1,1	0.15	0
6	GOL	C	531[A]	-	5,5,5	0.09	0	5,5,5	0.43	0
4	FMT	B	539	-	2,2,2	0.26	0	1,1,1	0.19	0
4	FMT	F	511	-	2,2,2	0.34	0	1,1,1	0.17	0
4	FMT	A	512	-	2,2,2	0.25	0	1,1,1	0.19	0
4	FMT	C	511	-	2,2,2	0.35	0	1,1,1	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	D	508	-	2,2,2	0.22	0	1,1,1	0.00	0
4	FMT	F	506	-	2,2,2	0.15	0	1,1,1	0.27	0
6	GOL	E	515[A]	-	5,5,5	0.09	0	5,5,5	0.29	0
4	FMT	B	518	-	2,2,2	0.30	0	1,1,1	0.13	0
4	FMT	B	515	-	2,2,2	0.21	0	1,1,1	0.11	0
6	GOL	A	542	-	5,5,5	0.12	0	5,5,5	0.31	0
4	FMT	B	519	-	2,2,2	0.35	0	1,1,1	0.11	0
4	FMT	A	527	-	2,2,2	0.29	0	1,1,1	0.10	0
4	FMT	C	524	-	2,2,2	0.09	0	1,1,1	0.15	0
4	FMT	C	507	-	2,2,2	0.24	0	1,1,1	0.18	0
4	FMT	C	503	-	2,2,2	0.17	0	1,1,1	0.15	0
4	FMT	A	534	-	2,2,2	0.23	0	1,1,1	0.15	0
4	FMT	E	506	-	2,2,2	0.15	0	1,1,1	0.11	0
4	FMT	E	505	-	2,2,2	0.16	0	1,1,1	0.05	0
4	FMT	C	502	-	2,2,2	0.29	0	1,1,1	0.07	0
2	HEM	E	501	1	50,50,50	1.61	10 (20%)	67,82,82	1.79	19 (28%)
4	FMT	B	503	-	2,2,2	0.32	0	1,1,1	0.12	0
4	FMT	A	529	-	2,2,2	0.24	0	1,1,1	0.13	0
4	FMT	E	512	-	2,2,2	0.36	0	1,1,1	0.09	0
4	FMT	B	524	-	2,2,2	0.20	0	1,1,1	0.16	0
4	FMT	A	504	-	2,2,2	0.19	0	1,1,1	0.18	0
4	FMT	C	515	-	2,2,2	0.08	0	1,1,1	0.18	0
4	FMT	D	517	-	2,2,2	0.29	0	1,1,1	0.19	0
4	FMT	A	513	-	2,2,2	0.24	0	1,1,1	0.10	0
4	FMT	A	518	-	2,2,2	0.21	0	1,1,1	0.20	0
4	FMT	B	531	-	2,2,2	0.37	0	1,1,1	0.06	0
4	FMT	B	535	-	2,2,2	0.32	0	1,1,1	0.11	0
4	FMT	A	519	-	2,2,2	0.38	0	1,1,1	0.13	0
4	FMT	C	510	-	2,2,2	0.34	0	1,1,1	0.13	0
4	FMT	B	506	-	2,2,2	0.28	0	1,1,1	0.05	0
4	FMT	D	518	-	2,2,2	0.33	0	1,1,1	0.14	0
4	FMT	E	503	-	2,2,2	0.09	0	1,1,1	0.20	0
4	FMT	F	510	-	2,2,2	0.17	0	1,1,1	0.17	0
3	DEB	F	502	-	27,27,27	0.60	1 (3%)	37,39,39	1.07	2 (5%)
3	DEB	A	502	-	27,27,27	0.26	0	37,39,39	0.55	0
4	FMT	A	503	-	2,2,2	0.27	0	1,1,1	0.08	0
4	FMT	B	521	-	2,2,2	0.22	0	1,1,1	0.09	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	DEB	C	533	-	-	10/50/50/50	0/1/1/1
3	DEB	E	502	-	-	9/50/50/50	0/1/1/1
6	GOL	C	531[A]	-	-	3/4/4/4	-
6	GOL	E	515[A]	-	-	2/4/4/4	-
6	GOL	A	543[B]	-	-	2/4/4/4	-
6	GOL	A	545	-	-	2/4/4/4	-
6	GOL	A	542	-	-	2/4/4/4	-
2	HEM	D	501	1	-	0/14/54/54	-
6	GOL	C	532	-	-	2/4/4/4	-
2	HEM	F	501	1	-	0/14/54/54	-
6	GOL	B	543[B]	-	-	0/4/4/4	-
2	HEM	A	501	1	-	0/14/54/54	-
3	DEB	D	502	-	-	8/50/50/50	0/1/1/1
3	DEB	B	502	-	-	8/50/50/50	0/1/1/1
2	HEM	E	501	1	-	1/14/54/54	-
6	GOL	B	542	-	-	4/4/4/4	-
6	GOL	A	544	-	-	2/4/4/4	-
6	GOL	A	543[A]	-	-	4/4/4/4	-
6	GOL	C	531[B]	-	-	1/4/4/4	-
6	GOL	B	543[A]	-	-	4/4/4/4	-
6	GOL	E	515[B]	-	-	4/4/4/4	-
2	HEM	B	501	1	-	0/14/54/54	-
3	DEB	F	502	-	-	8/50/50/50	0/1/1/1
3	DEB	A	502	-	-	8/50/50/50	0/1/1/1
2	HEM	C	501	1	-	0/14/54/54	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-ND	-4.99	1.79	1.94
2	E	501	HEM	FE-NB	4.72	2.09	1.94
2	F	501	HEM	FE-NC	4.70	2.10	1.95
2	C	501	HEM	FE-NB	4.67	2.09	1.94
2	F	501	HEM	FE-NB	4.38	2.08	1.94
2	D	501	HEM	C1D-ND	-4.24	1.30	1.38
2	A	501	HEM	FE-NC	4.08	2.08	1.95
2	B	501	HEM	FE-NC	3.72	2.07	1.95
2	B	501	HEM	FE-NA	3.71	2.07	1.95
2	F	501	HEM	C1B-NB	-3.70	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NA	3.60	2.07	1.95
2	B	501	HEM	C1D-ND	-3.56	1.31	1.38
2	B	501	HEM	C4C-NC	-3.44	1.33	1.39
2	A	501	HEM	C1B-NB	-3.39	1.34	1.40
2	E	501	HEM	C4D-C3D	3.29	1.50	1.45
2	E	501	HEM	C1B-NB	-3.28	1.34	1.40
2	B	501	HEM	C3D-C2D	-3.26	1.29	1.36
2	E	501	HEM	FE-NC	3.13	2.05	1.95
2	E	501	HEM	C4D-ND	-3.08	1.34	1.40
2	A	501	HEM	FE-NB	3.03	2.04	1.94
2	F	501	HEM	C1C-C2C	-3.02	1.39	1.45
2	A	501	HEM	CMC-C2C	2.98	1.56	1.50
2	C	501	HEM	FE-NC	2.76	2.04	1.95
2	C	501	HEM	C3D-C2D	-2.74	1.30	1.36
2	D	501	HEM	FE-NC	2.72	2.04	1.95
2	A	501	HEM	CHB-C1B	2.70	1.43	1.38
2	A	501	HEM	C1C-NC	-2.67	1.34	1.39
2	B	501	HEM	C4A-NA	-2.66	1.34	1.39
2	D	501	HEM	FE-NA	2.61	2.03	1.95
2	D	501	HEM	CHD-C4C	-2.58	1.33	1.38
2	C	501	HEM	C1A-C2A	-2.53	1.39	1.44
3	F	502	DEB	O24-C9	2.51	1.25	1.21
2	E	501	HEM	C1D-C2D	2.46	1.49	1.44
2	C	501	HEM	C1C-C2C	-2.46	1.40	1.45
2	D	501	HEM	C4B-NB	-2.44	1.34	1.38
2	E	501	HEM	C3C-C4C	-2.40	1.41	1.46
2	C	501	HEM	CMC-C2C	2.40	1.55	1.50
2	A	501	HEM	C2A-C3A	-2.37	1.32	1.38
2	A	501	HEM	C1C-C2C	-2.35	1.40	1.45
2	C	501	HEM	C4A-C3A	-2.34	1.37	1.43
2	E	501	HEM	C1C-C2C	-2.31	1.40	1.45
2	E	501	HEM	C3B-C4B	2.30	1.49	1.44
2	C	501	HEM	C3B-C4B	2.26	1.49	1.44
2	B	501	HEM	C1B-NB	-2.24	1.36	1.40
2	D	501	HEM	CMB-C2B	2.23	1.55	1.50
2	B	501	HEM	CBA-CGA	2.17	1.55	1.50
2	C	501	HEM	C1D-ND	-2.16	1.34	1.38
2	A	501	HEM	CMD-C2D	2.15	1.55	1.50
2	C	501	HEM	C4D-ND	-2.14	1.36	1.40
2	D	501	HEM	C3D-C2D	-2.14	1.32	1.36
2	D	501	HEM	C4C-NC	-2.13	1.35	1.39
2	F	501	HEM	C1D-ND	-2.13	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	O1D-CGD	2.12	1.29	1.22
2	B	501	HEM	CHA-C4D	2.11	1.42	1.38
2	F	501	HEM	CHB-C1B	2.11	1.42	1.38
2	B	501	HEM	C1C-NC	-2.10	1.35	1.39
2	E	501	HEM	C4B-NB	-2.09	1.34	1.38
2	F	501	HEM	C3C-C2C	2.08	1.41	1.37
2	C	501	HEM	C4D-C3D	2.06	1.48	1.45

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CHC-C4B-NB	11.38	136.66	124.42
2	F	501	HEM	CHC-C4B-NB	6.67	131.60	124.42
2	A	501	HEM	CHC-C4B-NB	5.99	130.86	124.42
2	D	501	HEM	CAD-C3D-C4D	5.68	134.60	124.70
2	F	501	HEM	C1B-NB-C4B	5.47	111.69	105.21
2	B	501	HEM	CMD-C2D-C1D	4.92	132.72	125.03
2	D	501	HEM	CHC-C1C-NC	-4.73	119.30	124.45
2	D	501	HEM	CHC-C4B-C3B	-4.63	115.83	125.07
2	E	501	HEM	C3B-C4B-NB	-4.61	106.16	109.47
2	D	501	HEM	O2D-CGD-CBD	4.50	128.23	114.00
2	B	501	HEM	CHC-C4B-NB	4.45	129.22	124.42
2	D	501	HEM	CHD-C1D-ND	4.34	129.09	124.42
2	D	501	HEM	CMD-C2D-C1D	4.28	131.72	125.03
2	D	501	HEM	C3C-C2C-C1C	-4.08	103.19	107.05
2	C	501	HEM	CHC-C1C-NC	-4.05	120.04	124.45
2	D	501	HEM	CHD-C1D-C2D	-4.05	118.64	125.03
2	C	501	HEM	CAD-C3D-C4D	3.85	131.40	124.70
2	A	501	HEM	C1B-NB-C4B	3.82	109.73	105.21
2	C	501	HEM	CMB-C2B-C1B	3.78	130.94	125.03
2	D	501	HEM	CHA-C4D-C3D	-3.77	118.27	125.23
2	A	501	HEM	C3C-C2C-C1C	-3.73	103.52	107.05
2	F	501	HEM	C3B-C4B-NB	-3.65	106.85	109.47
2	C	501	HEM	CHD-C1D-C2D	-3.64	119.29	125.03
2	D	501	HEM	CMB-C2B-C1B	3.63	130.71	125.03
2	D	501	HEM	CHA-C4D-ND	3.60	128.82	124.37
2	C	501	HEM	CHC-C4B-NB	3.57	128.27	124.42
2	C	501	HEM	CAC-C3C-C4C	-3.56	116.33	124.82
2	E	501	HEM	C1B-NB-C4B	3.54	109.40	105.21
2	B	501	HEM	CMA-C3A-C4A	-3.48	120.12	125.42
2	C	501	HEM	CHD-C1D-ND	3.46	128.15	124.42
2	D	501	HEM	CHB-C1B-NB	3.41	128.59	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	CMB-C2B-C1B	3.40	130.34	125.03
2	A	501	HEM	CHC-C1C-NC	-3.29	120.87	124.45
2	E	501	HEM	CHD-C4C-NC	3.27	128.02	124.45
2	C	501	HEM	C1B-NB-C4B	3.26	109.07	105.21
2	E	501	HEM	C4A-C3A-C2A	3.26	110.55	106.82
2	D	501	HEM	C4A-CHB-C1B	-3.24	118.62	126.25
2	C	501	HEM	C1A-CHA-C4D	-3.19	118.75	126.25
2	D	501	HEM	C4D-C3D-C2D	-3.17	102.28	106.89
2	E	501	HEM	CHD-C1D-C2D	-3.16	120.04	125.03
2	E	501	HEM	CHC-C4B-NB	3.11	127.77	124.42
2	F	501	HEM	CHB-C1B-NB	3.09	128.18	124.37
2	B	501	HEM	CHA-C4D-ND	3.07	128.17	124.37
2	E	501	HEM	C4C-C3C-C2C	3.07	109.47	106.81
2	B	501	HEM	C3C-C2C-C1C	-3.04	104.17	107.05
2	B	501	HEM	CHA-C4D-C3D	-3.03	119.63	125.23
2	B	501	HEM	O2A-CGA-O1A	-3.03	115.54	123.33
3	F	502	DEB	C10-C11-C12	3.02	120.30	114.49
3	F	502	DEB	C7-C6-C5	3.02	117.75	110.96
2	A	501	HEM	O2A-CGA-O1A	-3.01	115.60	123.33
2	B	501	HEM	CHC-C1C-NC	-3.00	121.19	124.45
2	A	501	HEM	C4C-C3C-C2C	2.99	109.41	106.81
2	E	501	HEM	CAA-C2A-C1A	2.97	130.75	124.94
2	D	501	HEM	C3B-C4B-NB	-2.93	107.36	109.47
2	D	501	HEM	C4B-C3B-C2B	2.88	109.93	107.28
2	D	501	HEM	O2D-CGD-O1D	-2.85	115.99	123.33
2	B	501	HEM	CHD-C1D-C2D	-2.85	120.53	125.03
2	A	501	HEM	CHD-C1D-ND	2.82	127.46	124.42
2	B	501	HEM	O2D-CGD-CBD	2.82	122.91	114.00
2	C	501	HEM	C3D-C4D-ND	2.78	113.22	110.17
2	A	501	HEM	CMB-C2B-C1B	2.77	129.37	125.03
2	D	501	HEM	CMD-C2D-C3D	-2.76	118.68	126.15
2	E	501	HEM	C2D-C1D-ND	2.76	113.09	109.90
2	B	501	HEM	CMA-C3A-C2A	2.75	131.45	125.62
2	C	501	HEM	O2D-CGD-O1D	-2.75	116.27	123.33
2	F	501	HEM	C1A-CHA-C4D	-2.74	119.80	126.25
2	F	501	HEM	CHA-C4D-C3D	-2.72	120.21	125.23
2	F	501	HEM	CHA-C4D-ND	2.72	127.73	124.37
2	D	501	HEM	O2A-CGA-O1A	-2.70	116.38	123.33
2	B	501	HEM	C1B-NB-C4B	2.66	108.36	105.21
2	B	501	HEM	CAD-C3D-C4D	2.63	129.28	124.70
2	D	501	HEM	CAD-C3D-C2D	-2.59	123.01	127.87
2	B	501	HEM	C2D-C1D-ND	2.59	112.89	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	O2A-CGA-CBA	2.56	122.10	114.00
2	C	501	HEM	C4A-C3A-C2A	2.51	109.69	106.82
2	C	501	HEM	CHA-C4D-C3D	-2.51	120.60	125.23
2	A	501	HEM	CAC-C3C-C4C	-2.50	118.86	124.82
2	D	501	HEM	C1C-CHC-C4B	-2.48	120.75	126.02
2	A	501	HEM	CHD-C1D-C2D	-2.48	121.12	125.03
2	E	501	HEM	CAB-C3B-C2B	-2.48	120.38	128.43
2	D	501	HEM	C3D-C4D-ND	2.47	112.89	110.17
2	F	501	HEM	CHD-C1D-ND	2.47	127.08	124.42
2	C	501	HEM	CHB-C4A-NA	2.45	128.30	123.86
2	F	501	HEM	C3C-C2C-C1C	-2.42	104.76	107.05
2	E	501	HEM	CHB-C1B-NB	2.42	127.36	124.37
2	D	501	HEM	O2A-CGA-CBA	2.42	121.63	114.00
2	B	501	HEM	C1A-CHA-C4D	-2.39	120.62	126.25
2	B	501	HEM	CAC-C3C-C4C	-2.39	119.12	124.82
2	D	501	HEM	C3B-C2B-C1B	-2.38	104.63	106.41
2	D	501	HEM	C4C-CHD-C1D	-2.37	120.99	126.02
2	A	501	HEM	CHD-C4C-NC	2.36	127.03	124.45
2	F	501	HEM	CHA-C1A-NA	2.36	128.14	123.86
2	C	501	HEM	C4C-C3C-C2C	2.36	108.86	106.81
2	B	501	HEM	CAD-CBD-CGD	2.35	119.89	113.67
2	C	501	HEM	C3B-C4B-NB	-2.31	107.81	109.47
2	D	501	HEM	O1D-CGD-CBD	-2.31	115.77	123.09
2	C	501	HEM	C4D-ND-C1D	-2.30	102.49	105.21
2	D	501	HEM	C1A-CHA-C4D	-2.28	120.88	126.25
2	B	501	HEM	CAB-C3B-C2B	2.24	135.71	128.43
3	C	533	DEB	C10-C11-C12	2.22	118.77	114.49
2	E	501	HEM	O2A-CGA-O1A	-2.22	117.61	123.33
3	B	502	DEB	O21-C5-C6	-2.22	105.56	109.79
2	E	501	HEM	CHD-C1D-ND	2.22	126.81	124.42
2	C	501	HEM	C2D-C1D-ND	2.22	112.47	109.90
2	E	501	HEM	C1D-C2D-C3D	-2.18	104.68	106.98
2	A	501	HEM	CMB-C2B-C3B	-2.18	123.15	128.43
2	F	501	HEM	CBD-CAD-C3D	-2.16	106.55	112.53
2	E	501	HEM	C4C-CHD-C1D	-2.16	121.44	126.02
2	A	501	HEM	CHC-C4B-C3B	-2.15	120.79	125.07
2	D	501	HEM	CHB-C1B-C2B	-2.13	120.91	126.95
3	B	502	DEB	O26-C11-C10	2.12	113.70	108.59
2	E	501	HEM	C3C-C2C-C1C	-2.11	105.05	107.05
2	D	501	HEM	CAB-C3B-C4B	-2.11	115.08	124.39
2	B	501	HEM	CMD-C2D-C3D	-2.09	120.50	126.15
2	C	501	HEM	CMD-C2D-C1D	2.08	128.29	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C2C-C1C-NC	2.08	113.49	109.64
2	A	501	HEM	O2A-CGA-CBA	2.07	120.55	114.00
2	C	501	HEM	C3C-C2C-C1C	-2.05	105.11	107.05
2	B	501	HEM	C4D-ND-C1D	-2.05	102.78	105.21
2	E	501	HEM	CBD-CAD-C3D	-2.04	106.89	112.53
2	F	501	HEM	CHD-C1D-C2D	-2.03	121.83	125.03
2	D	501	HEM	CAA-C2A-C1A	2.02	128.89	124.94
2	D	501	HEM	CAB-C3B-C2B	2.02	134.99	128.43
2	A	501	HEM	CAD-C3D-C4D	2.01	128.20	124.70
2	F	501	HEM	CHD-C4C-NC	2.01	126.64	124.45

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	533	DEB	C3-C4-C5-O21
3	C	533	DEB	C20-C4-C5-O21
3	C	533	DEB	O16-C13-C14-C15
6	A	542	GOL	C1-C2-C3-O3
6	A	542	GOL	O2-C2-C3-O3
6	A	543[A]	GOL	O1-C1-C2-C3
6	A	543[B]	GOL	O1-C1-C2-C3
6	A	545	GOL	O1-C1-C2-C3
6	C	531[A]	GOL	O1-C1-C2-C3
6	C	532	GOL	C1-C2-C3-O3
6	E	515[B]	GOL	O1-C1-C2-C3
6	E	515[B]	GOL	C1-C2-C3-O3
6	A	543[B]	GOL	O1-C1-C2-O2
6	C	531[A]	GOL	O1-C1-C2-O2
6	E	515[A]	GOL	O1-C1-C2-O2
6	E	515[B]	GOL	O2-C2-C3-O3
3	A	502	DEB	C3-C4-C5-O21
3	D	502	DEB	C3-C4-C5-O21
3	C	533	DEB	C20-C4-C5-C6
3	C	533	DEB	C3-C4-C5-C6
6	A	544	GOL	O1-C1-C2-C3
6	B	542	GOL	O1-C1-C2-C3
6	B	542	GOL	C1-C2-C3-O3
6	B	543[A]	GOL	O1-C1-C2-C3
6	B	543[A]	GOL	C1-C2-C3-O3
6	C	531[A]	GOL	C1-C2-C3-O3
6	E	515[A]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	E	515[B]	GOL	O1-C1-C2-O2
3	A	502	DEB	C20-C4-C5-O21
3	D	502	DEB	C20-C4-C5-O21
3	E	502	DEB	C18-C2-C3-O19
3	F	502	DEB	C18-C2-C3-O19
3	A	502	DEB	C18-C2-C3-C4
3	B	502	DEB	C18-C2-C3-C4
3	C	533	DEB	C18-C2-C3-C4
3	D	502	DEB	C18-C2-C3-C4
3	E	502	DEB	C18-C2-C3-C4
3	F	502	DEB	C18-C2-C3-C4
6	A	543[A]	GOL	O1-C1-C2-O2
6	B	542	GOL	O2-C2-C3-O3
3	A	502	DEB	C18-C2-C3-O19
3	B	502	DEB	C18-C2-C3-O19
3	C	533	DEB	C18-C2-C3-O19
3	D	502	DEB	C18-C2-C3-O19
6	A	543[A]	GOL	C1-C2-C3-O3
3	E	502	DEB	C3-C4-C5-O21
6	A	544	GOL	O1-C1-C2-O2
6	A	545	GOL	O1-C1-C2-O2
6	B	543[A]	GOL	O2-C2-C3-O3
6	C	531[B]	GOL	O1-C1-C2-O2
6	B	542	GOL	O1-C1-C2-O2
6	B	543[A]	GOL	O1-C1-C2-O2
2	E	501	HEM	C4B-C3B-CAB-CBB
3	F	502	DEB	C3-C4-C5-O21
3	D	502	DEB	C3-C4-C5-C6
6	C	532	GOL	O2-C2-C3-O3
3	B	502	DEB	C3-C4-C5-O21
3	C	533	DEB	C12-C13-C14-C15
3	E	502	DEB	C23-C8-C9-O24
3	A	502	DEB	C1-C2-C3-O19
3	B	502	DEB	C1-C2-C3-O19
3	C	533	DEB	C1-C2-C3-O19
3	D	502	DEB	C1-C2-C3-O19
3	E	502	DEB	C1-C2-C3-O19
3	F	502	DEB	C1-C2-C3-O19
3	D	502	DEB	C20-C4-C5-C6
3	A	502	DEB	C1-C2-C3-C4
3	B	502	DEB	C1-C2-C3-C4
3	C	533	DEB	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	D	502	DEB	C1-C2-C3-C4
3	E	502	DEB	C1-C2-C3-C4
3	F	502	DEB	C1-C2-C3-C4
3	E	502	DEB	C20-C4-C5-O21
3	A	502	DEB	C3-C4-C5-C6
3	A	502	DEB	C20-C4-C5-C6
3	F	502	DEB	C2-C1-O16-C13
3	E	502	DEB	C2-C1-O16-C13
3	F	502	DEB	C7-C8-C9-O24
6	A	543[A]	GOL	O2-C2-C3-O3
3	B	502	DEB	O16-C13-C14-C15
3	B	502	DEB	C3-C4-C5-C6
3	F	502	DEB	C23-C8-C9-O24
3	B	502	DEB	C7-C8-C9-O24
3	E	502	DEB	C7-C8-C9-O24

There are no ring outliers.

48 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	543[B]	GOL	3	0
6	A	545	GOL	3	0
2	A	501	HEM	3	0
4	A	510	FMT	2	0
4	B	520	FMT	2	0
4	D	515	FMT	2	0
4	A	525	FMT	2	0
6	B	542	GOL	1	0
6	A	543[A]	GOL	3	0
4	F	505	FMT	1	0
6	B	543[A]	GOL	9	0
4	B	537	FMT	3	0
4	A	516	FMT	1	0
3	C	533	DEB	6	0
4	B	538	FMT	2	0
4	C	513	FMT	1	0
4	B	507	FMT	1	0
4	B	532	FMT	1	0
4	C	522	FMT	2	0
2	F	501	HEM	3	0
6	B	543[B]	GOL	4	0
4	B	529	FMT	1	0

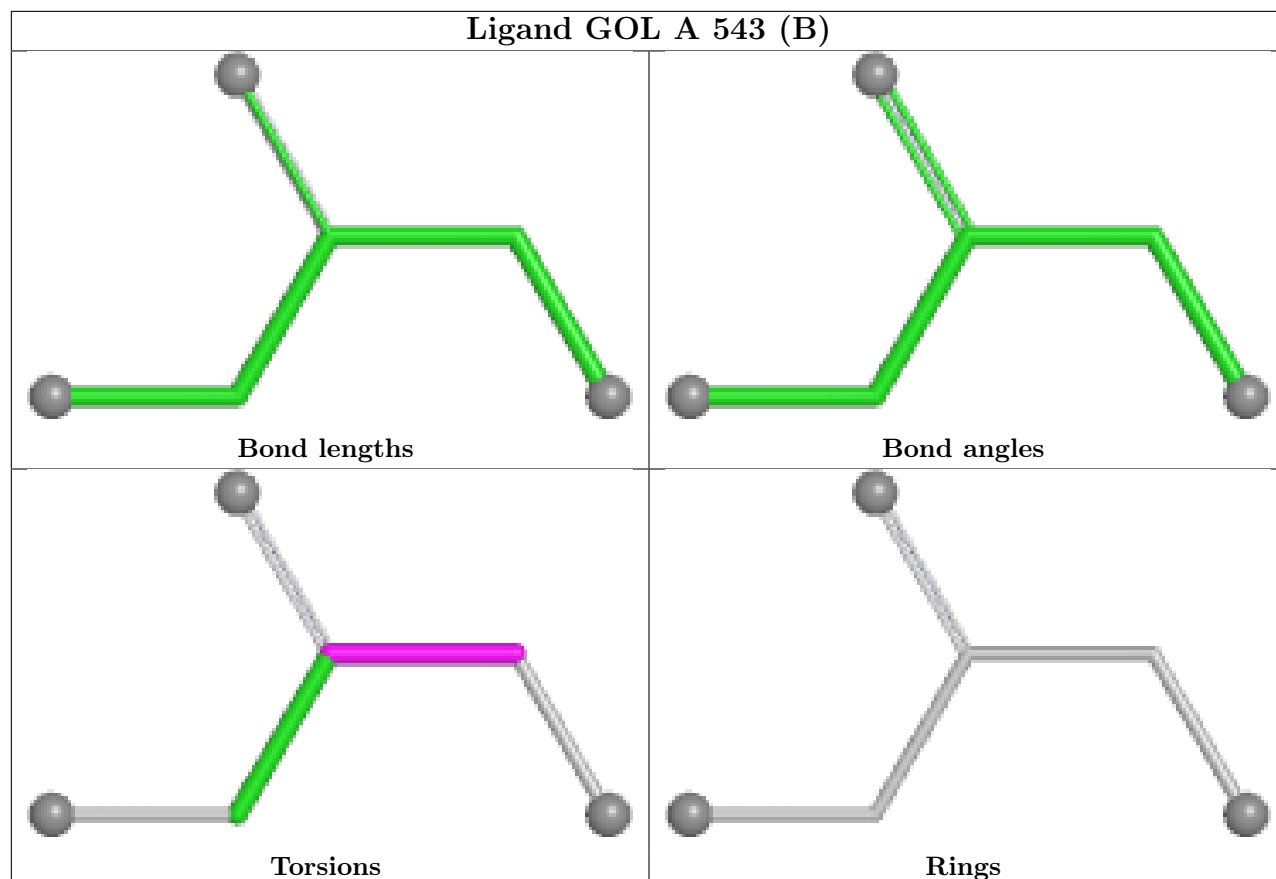
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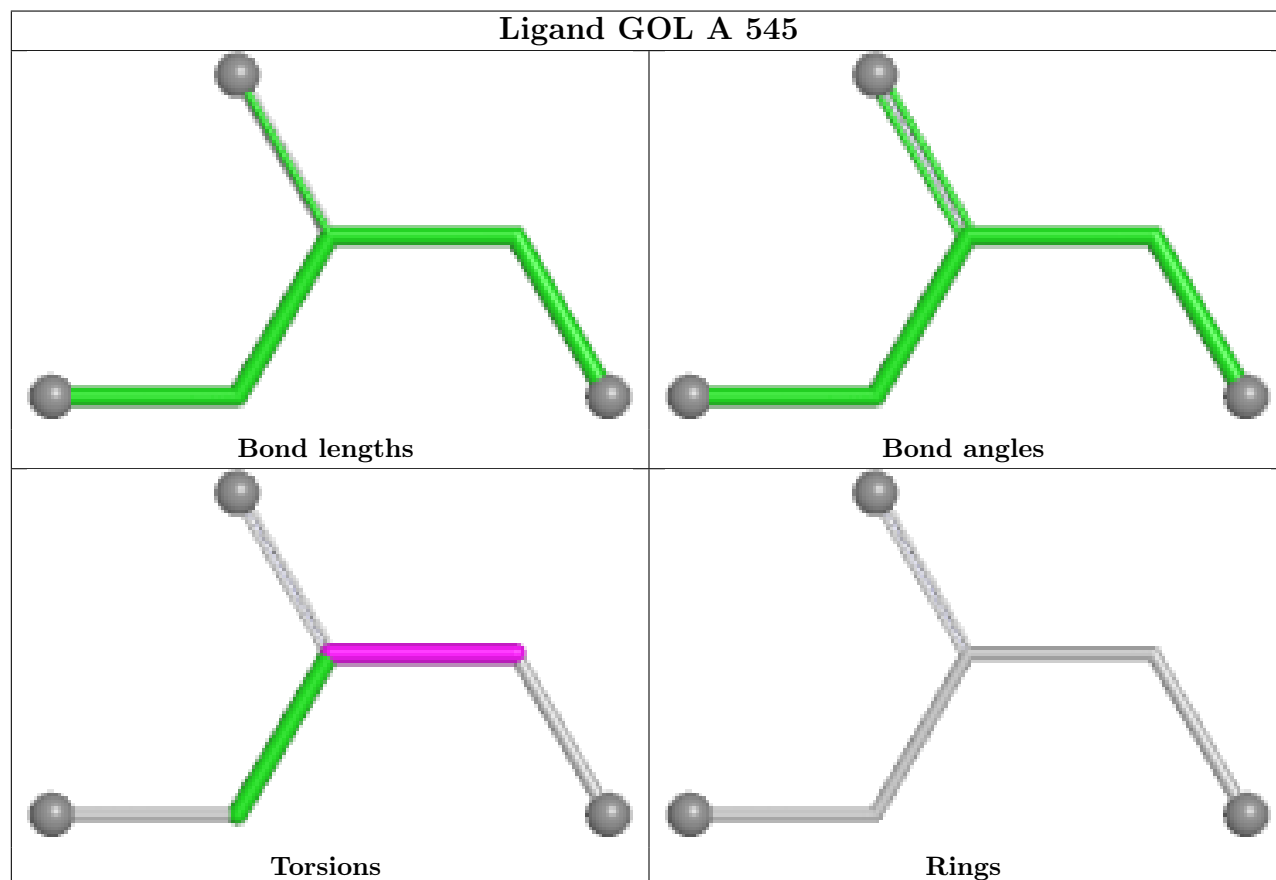
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	512	FMT	2	0
4	B	513	FMT	2	0
2	B	501	HEM	1	0
4	B	511	FMT	2	0
2	C	501	HEM	1	0
2	D	501	HEM	4	0
4	A	538	FMT	1	0
3	B	502	DEB	2	0
4	A	535	FMT	1	0
4	D	510	FMT	1	0
6	C	531[B]	GOL	2	0
4	A	526	FMT	2	0
4	B	528	FMT	1	0
4	E	510	FMT	1	0
6	C	531[A]	GOL	1	0
4	D	508	FMT	3	0
6	E	515[A]	GOL	7	0
4	B	515	FMT	1	0
4	C	524	FMT	2	0
4	E	506	FMT	2	0
2	E	501	HEM	2	0
4	A	529	FMT	1	0
4	B	524	FMT	1	0
4	A	519	FMT	1	0
4	B	506	FMT	4	0
3	A	502	DEB	7	0

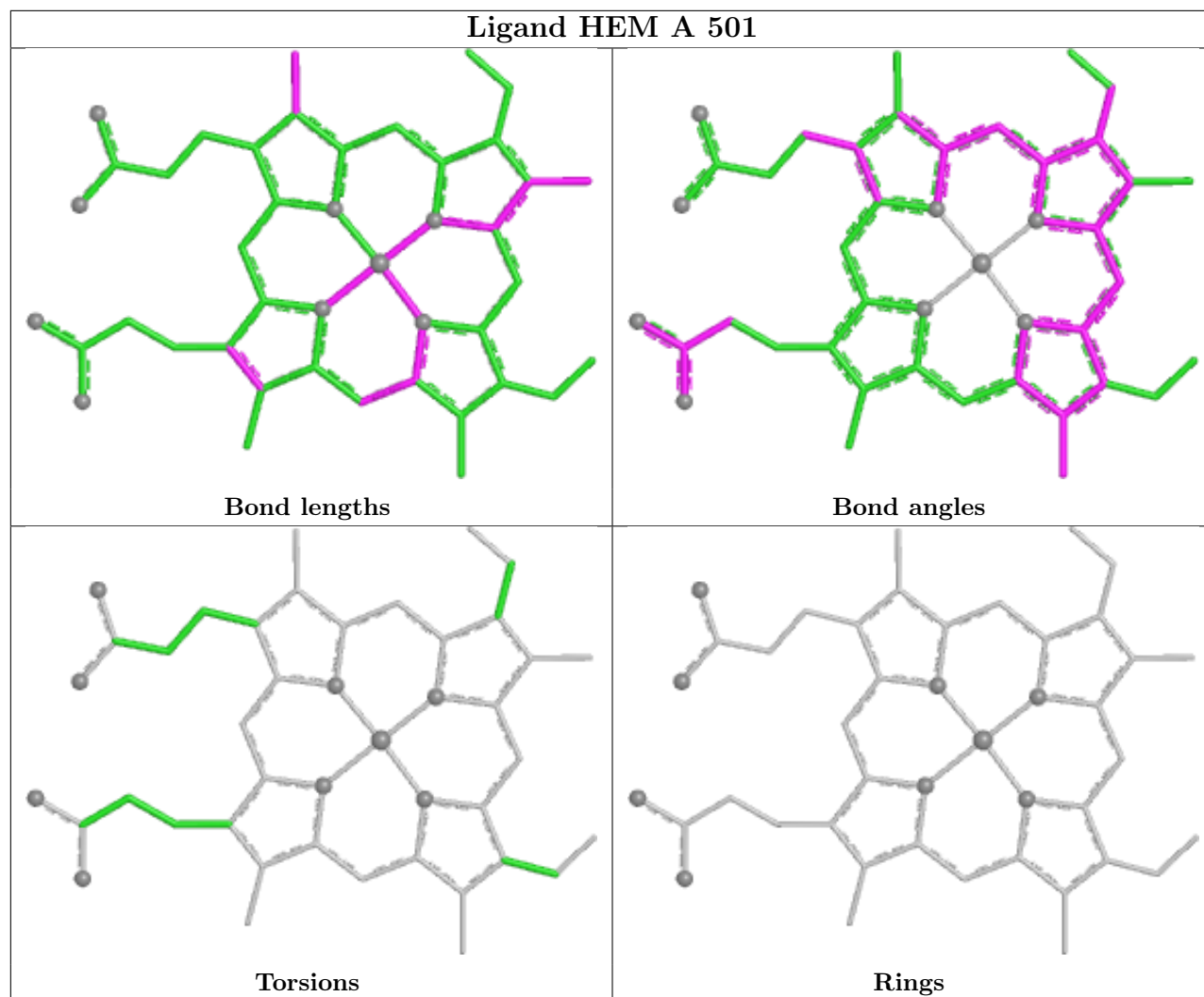
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

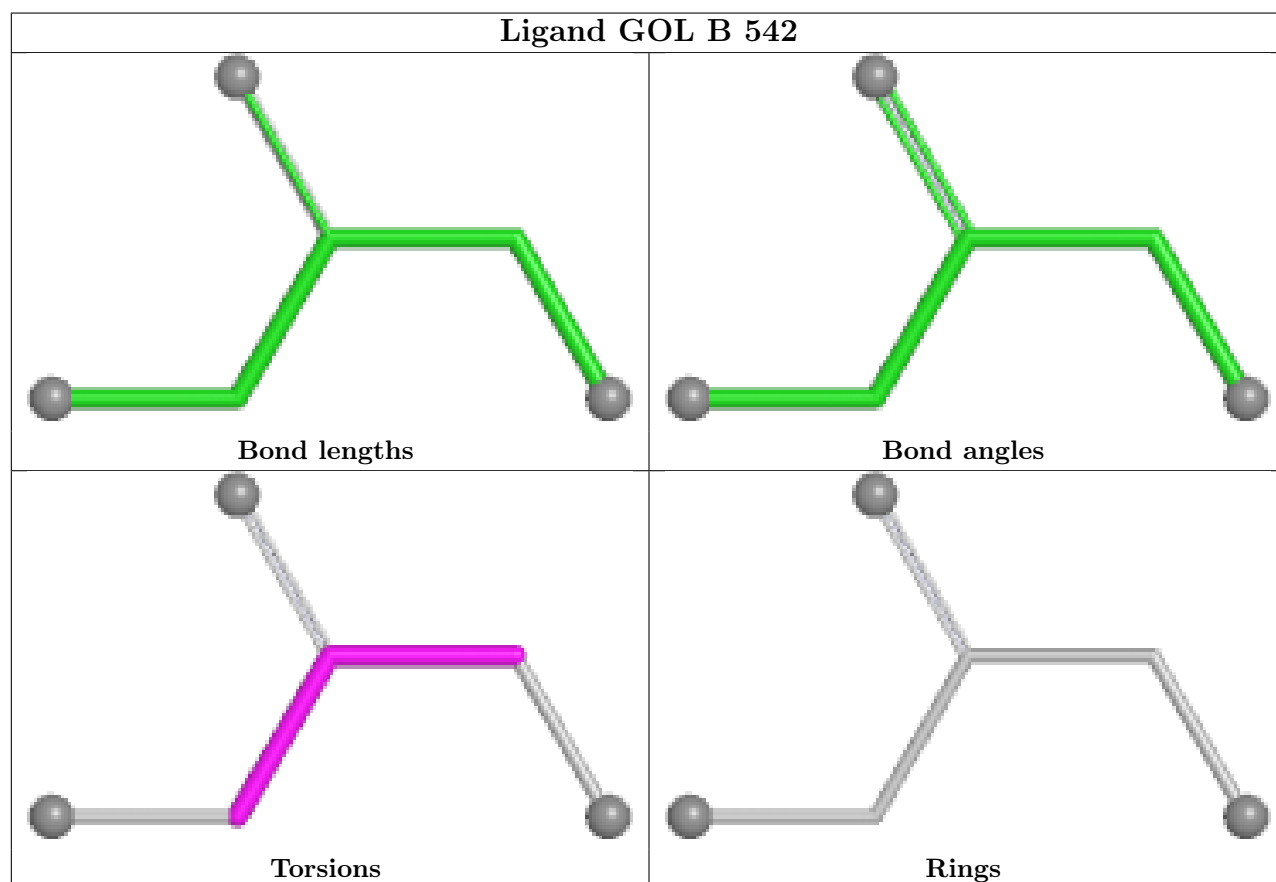
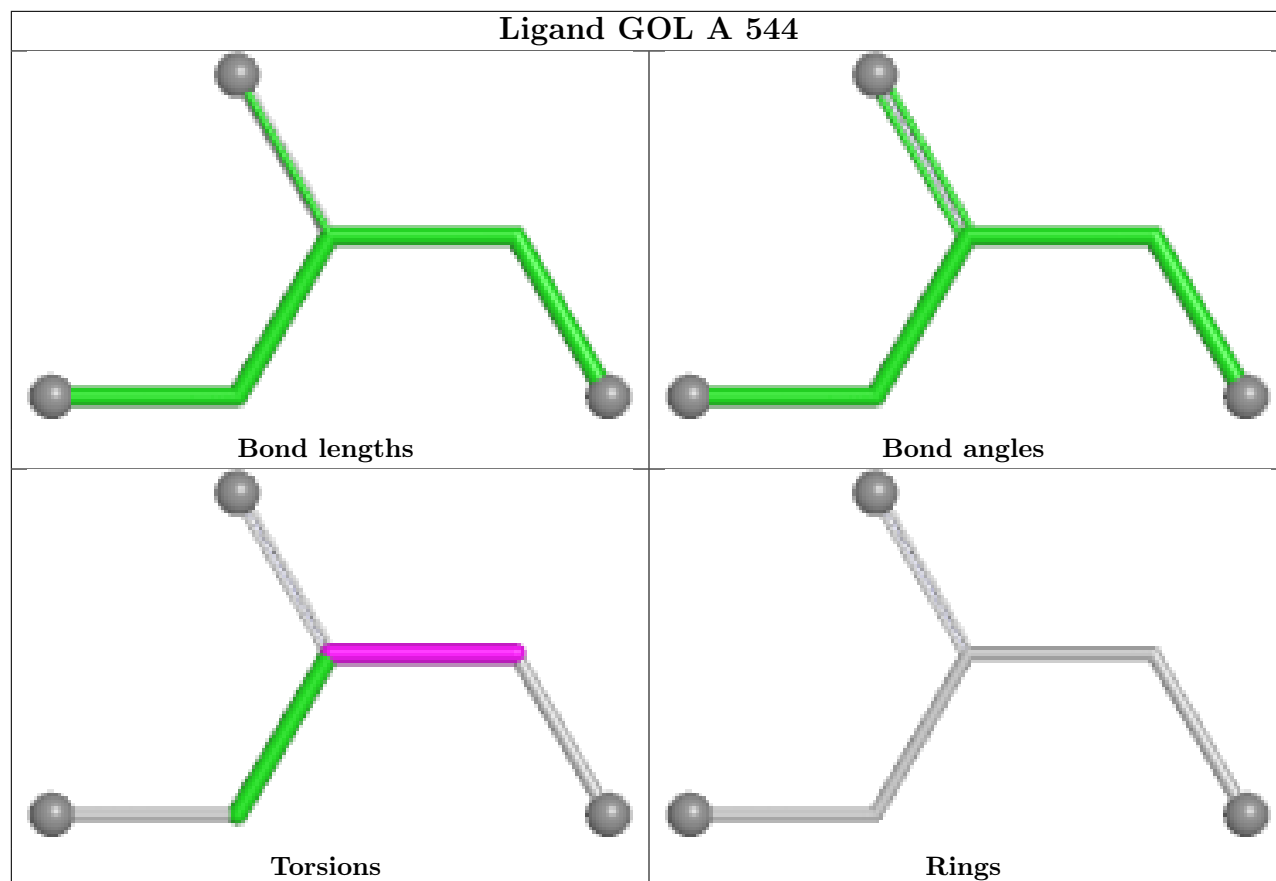
Ligand GOL A 543 (B)



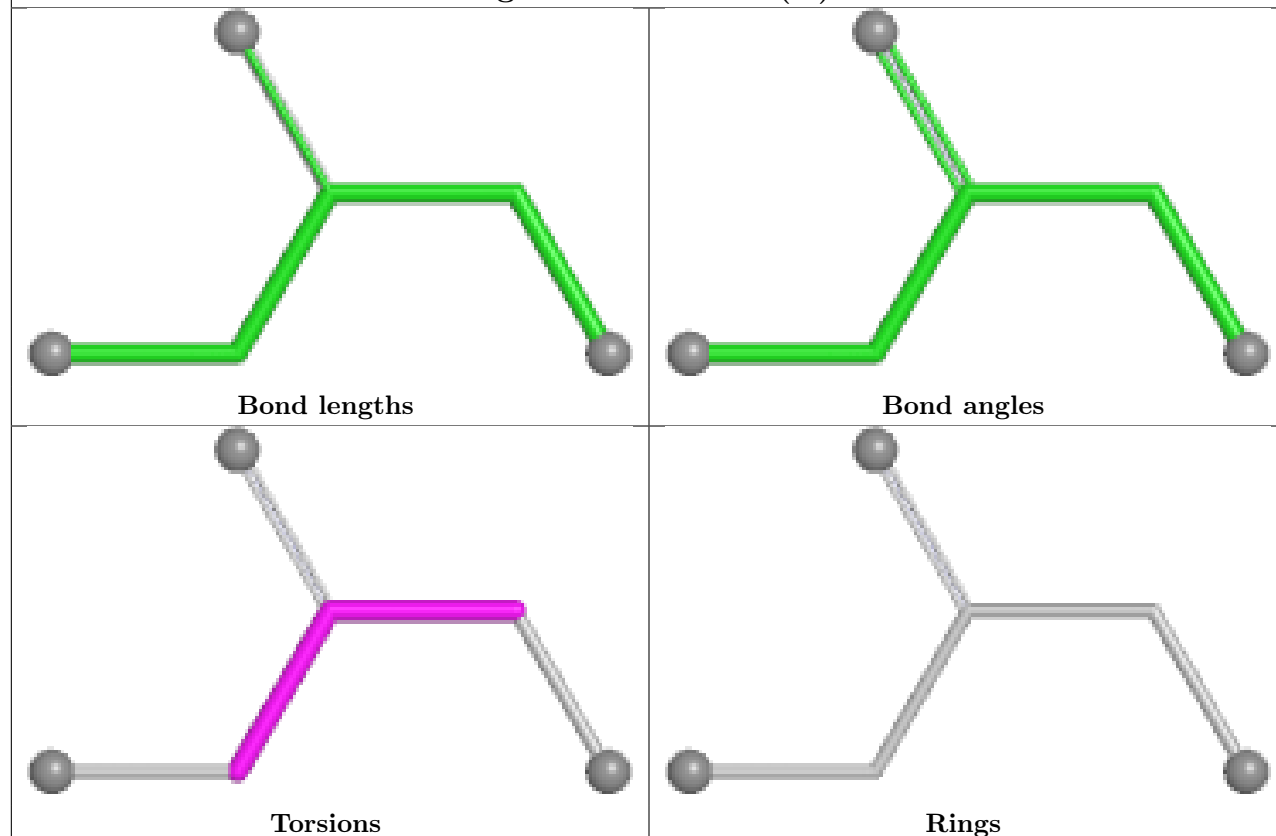
Ligand GOL A 545



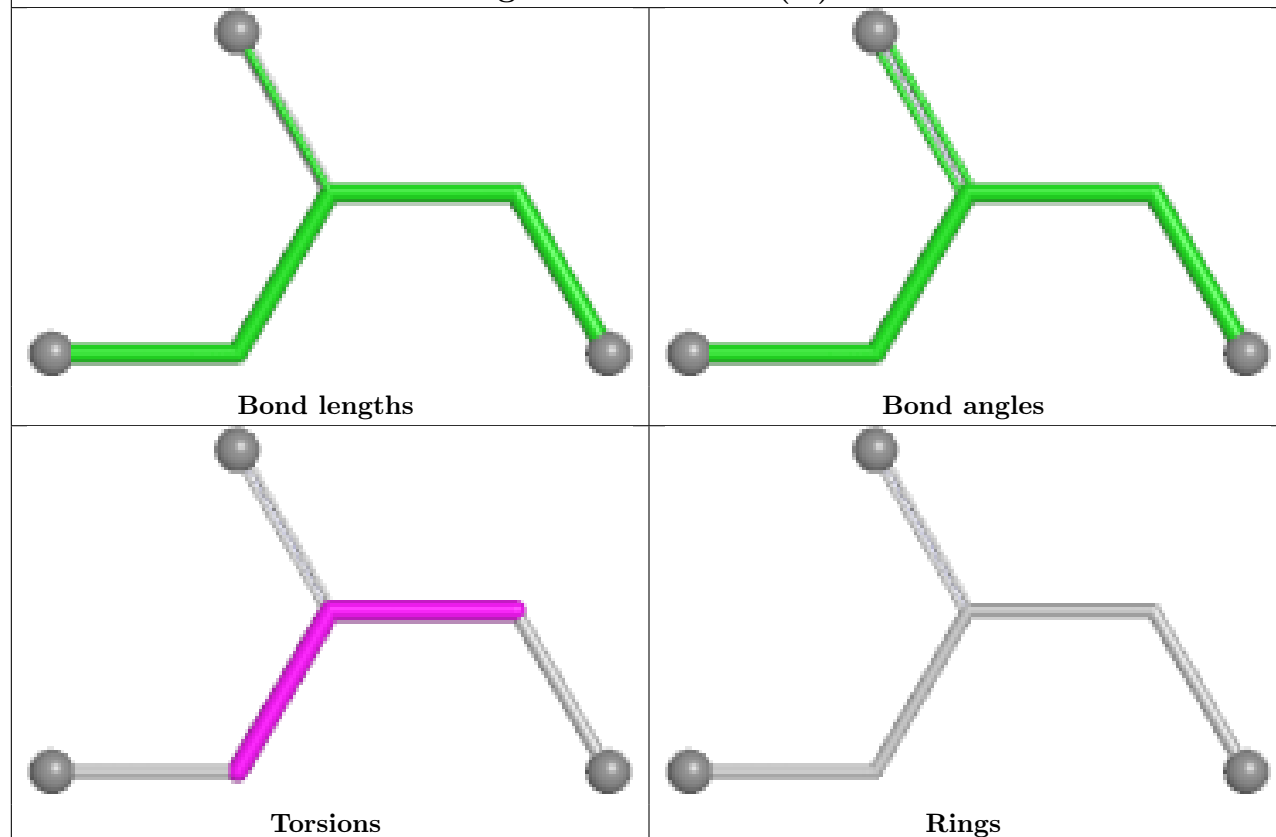


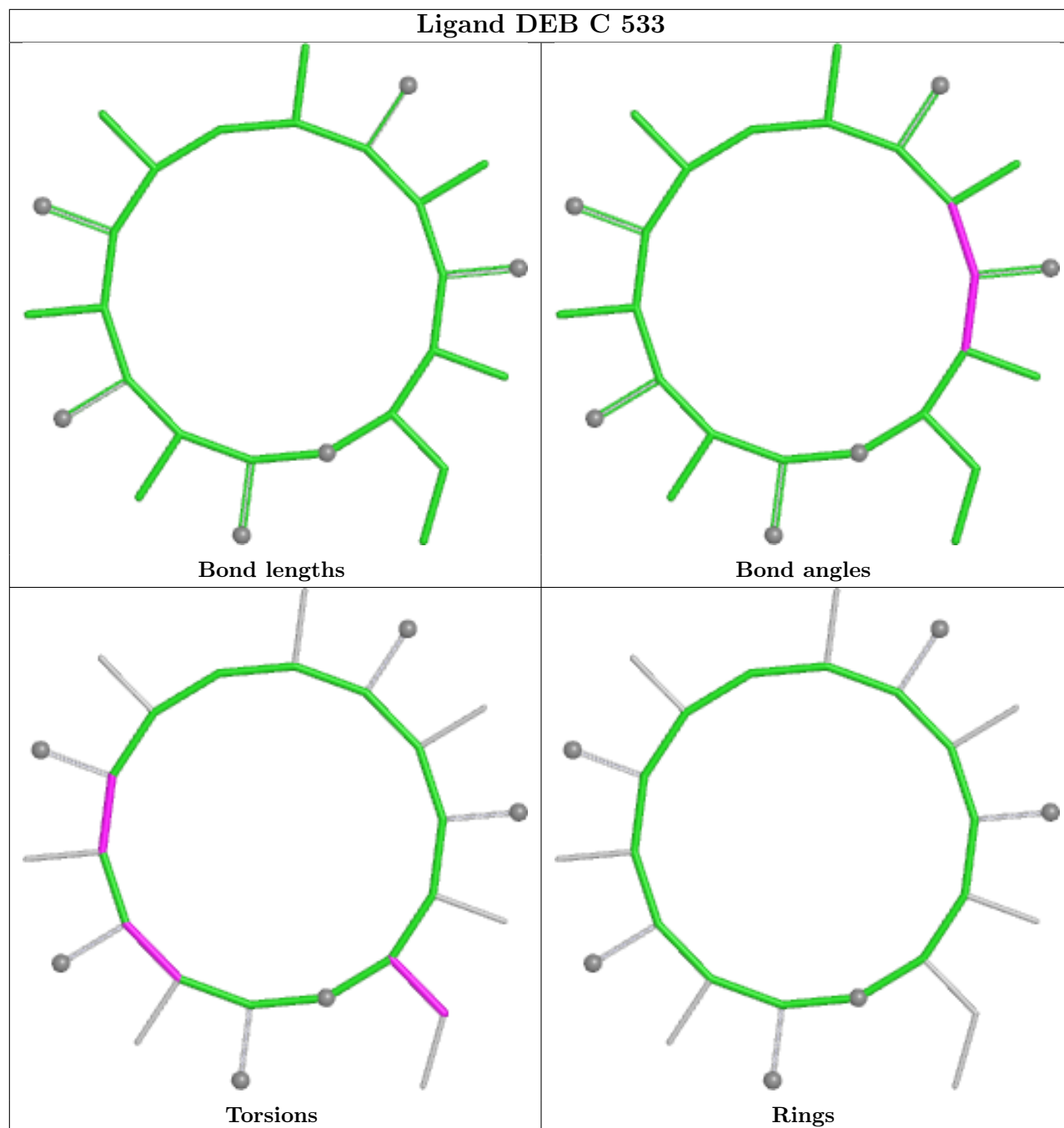


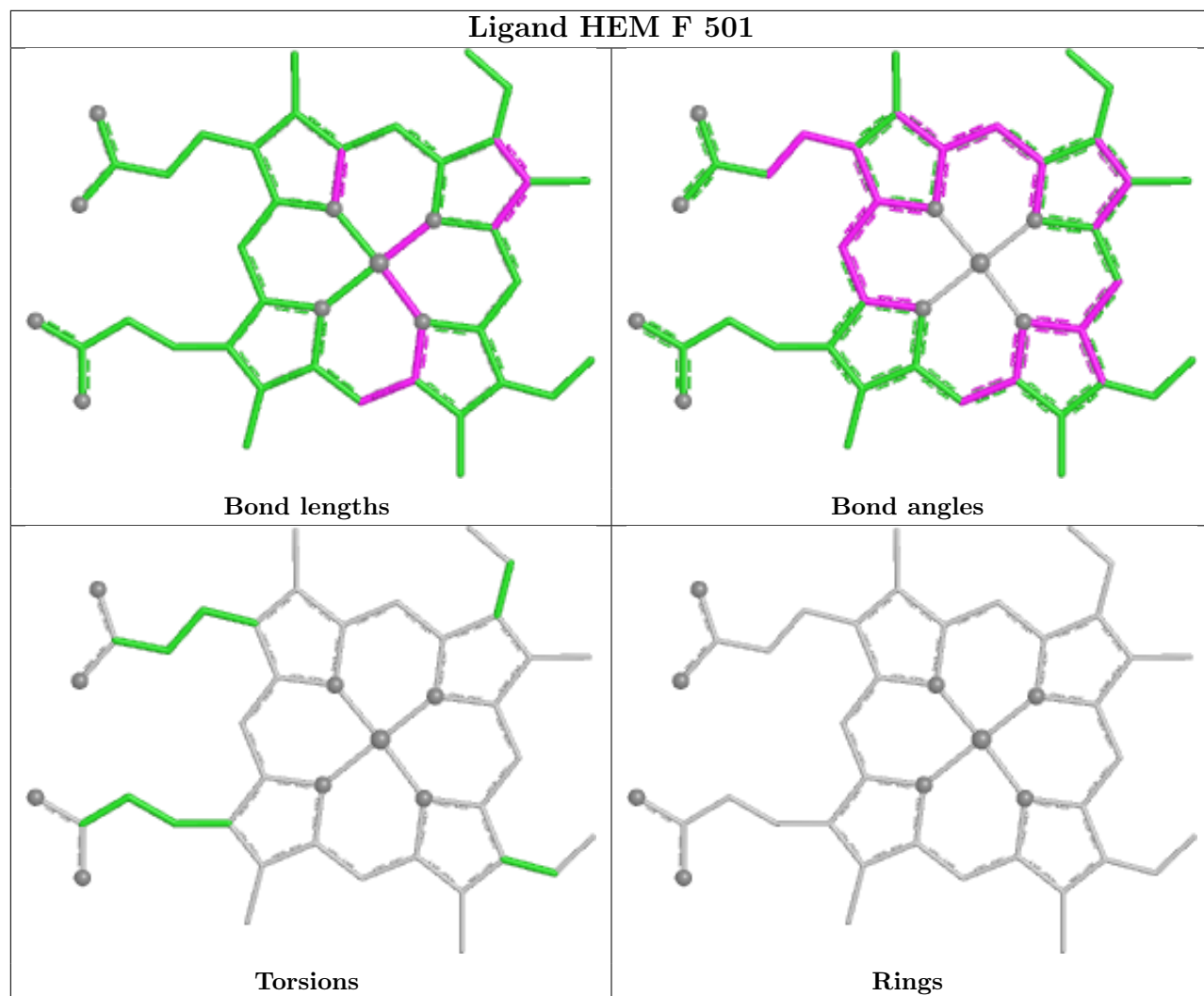
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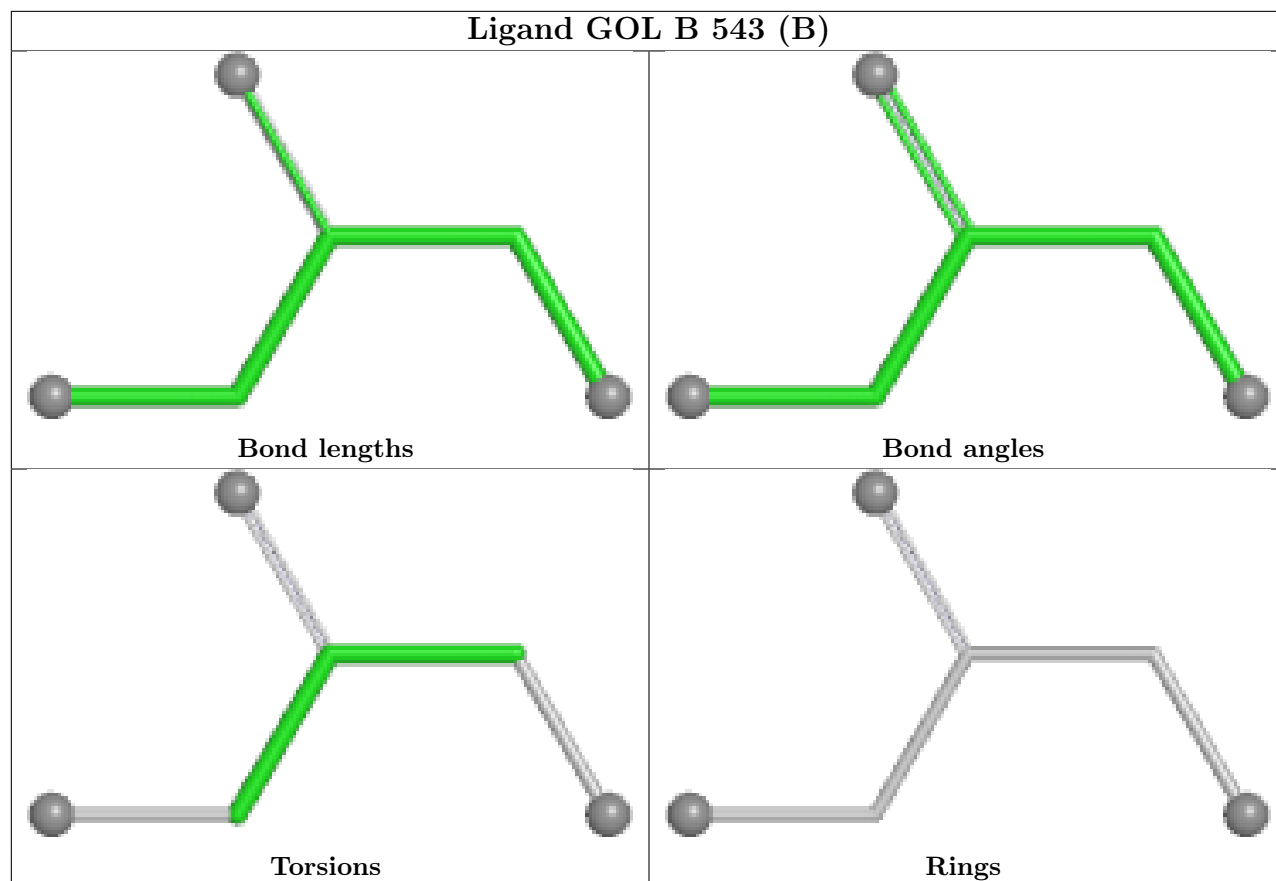


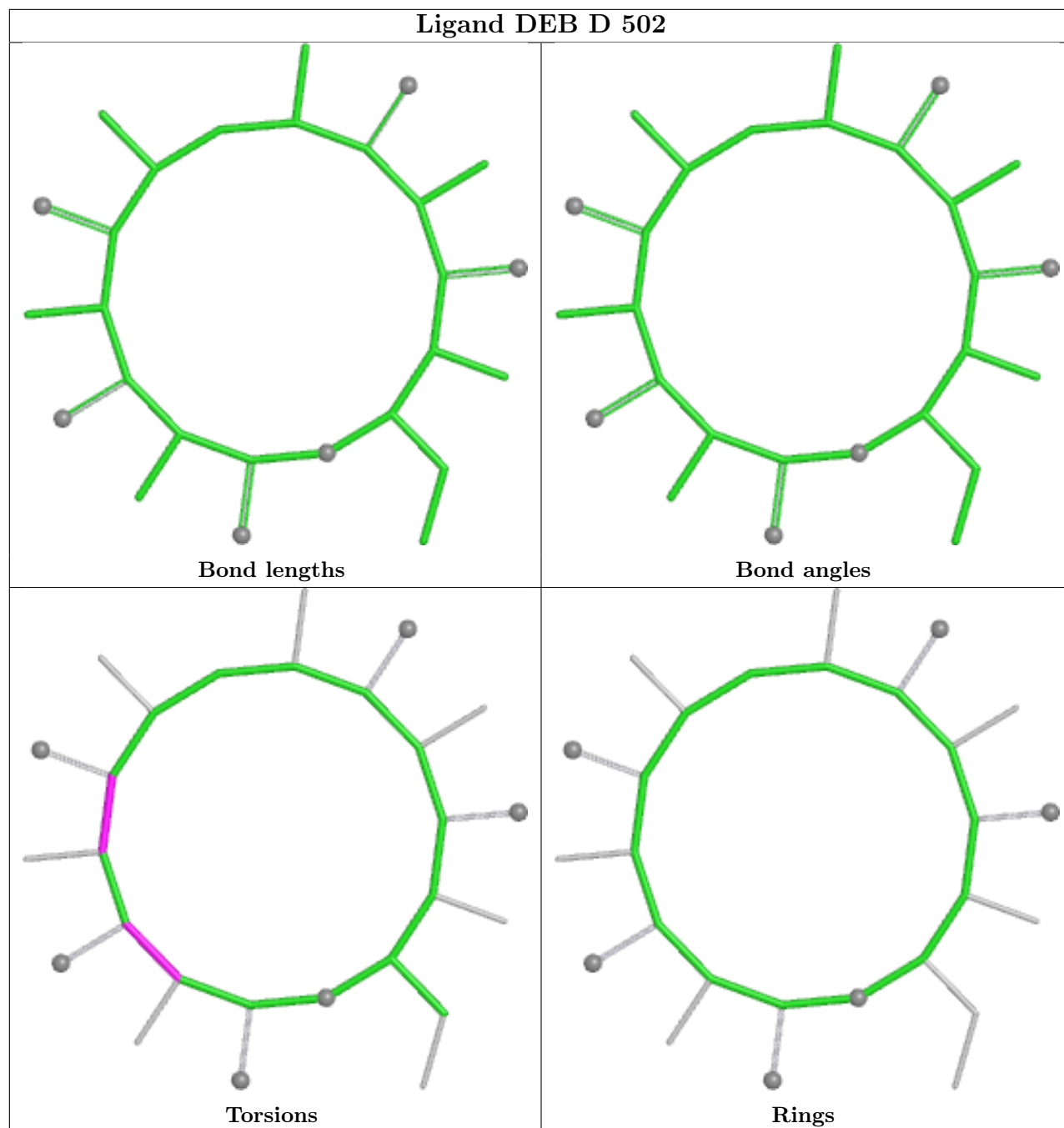
Ligand GOL B 543 (A)

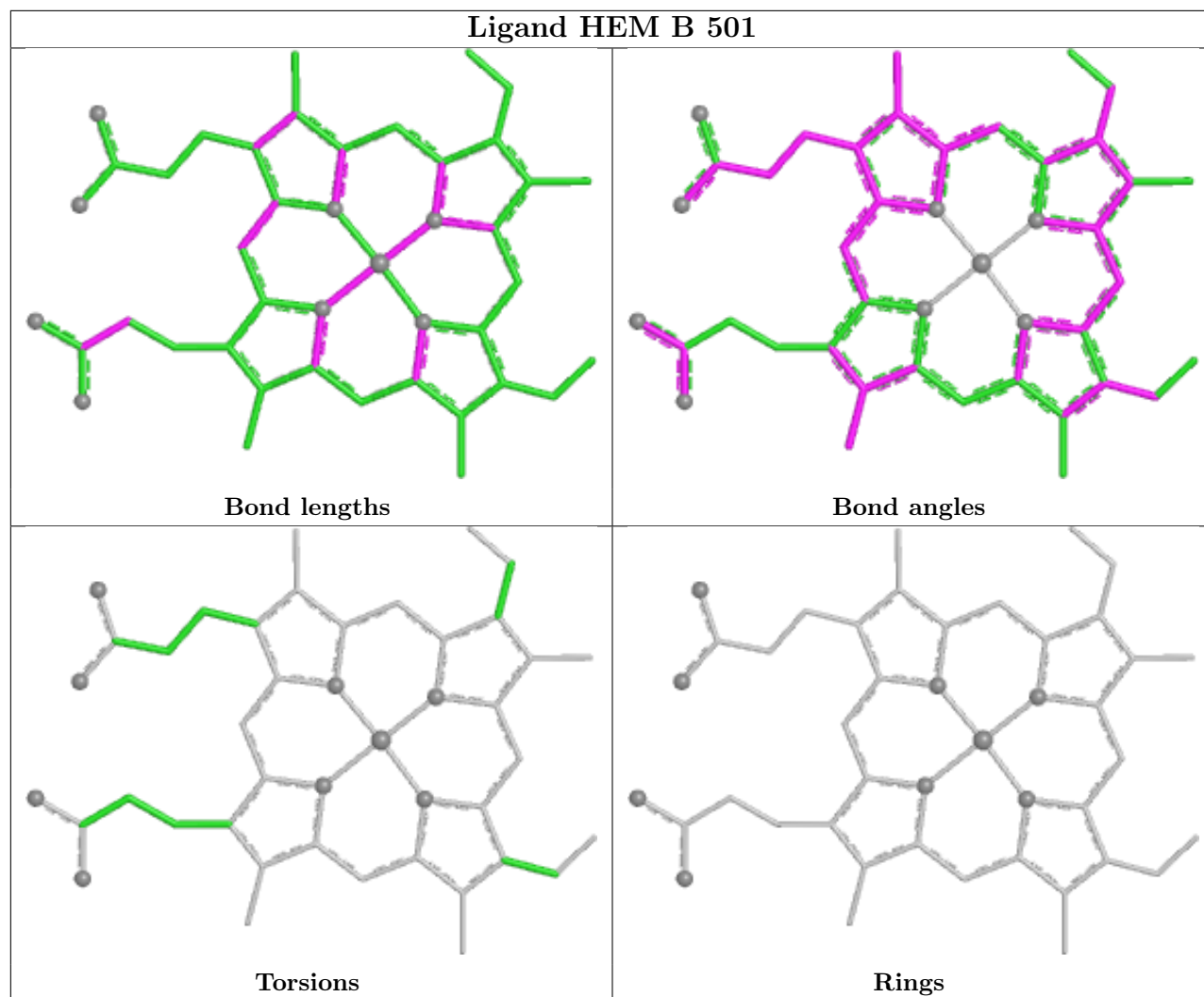




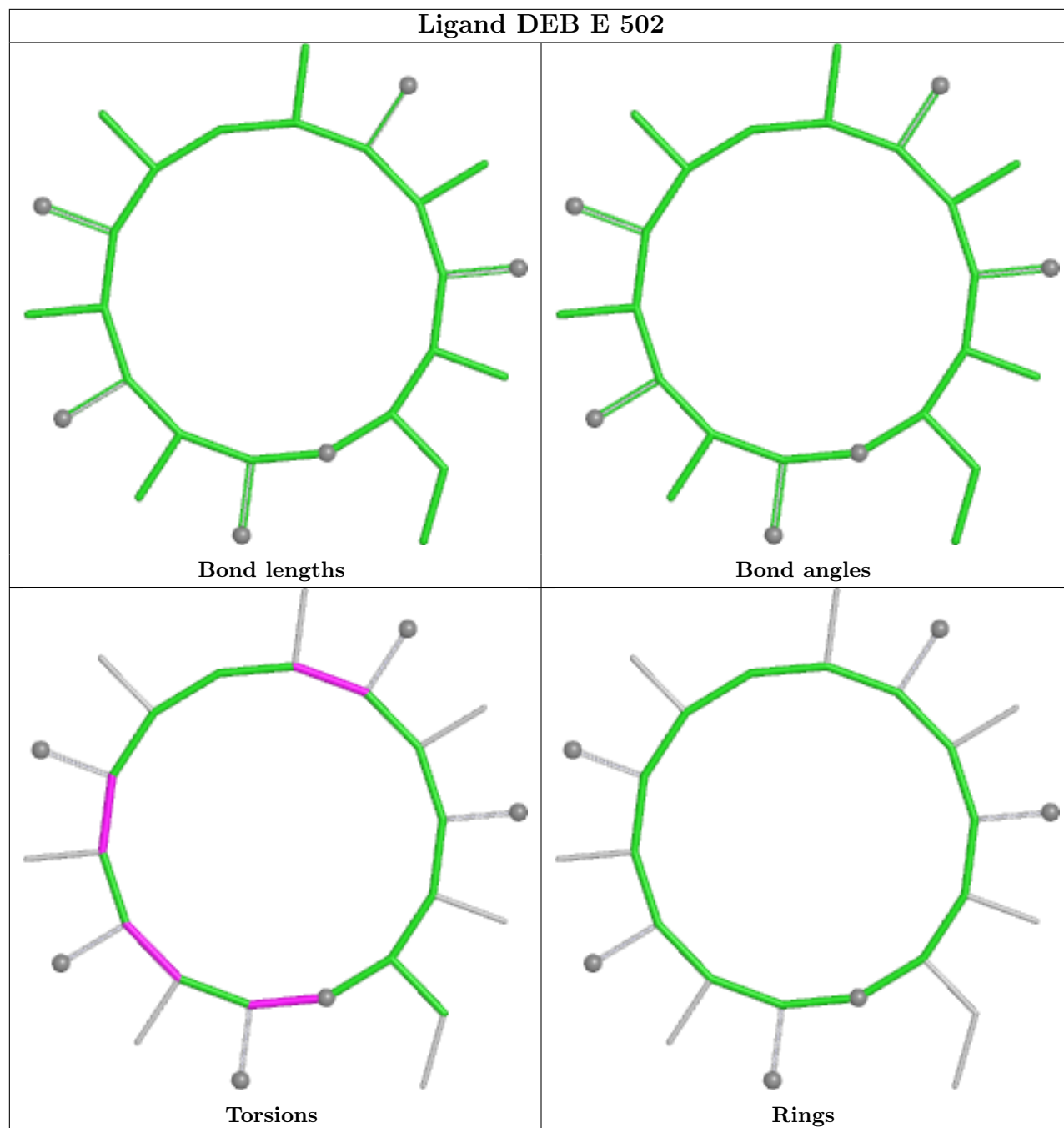


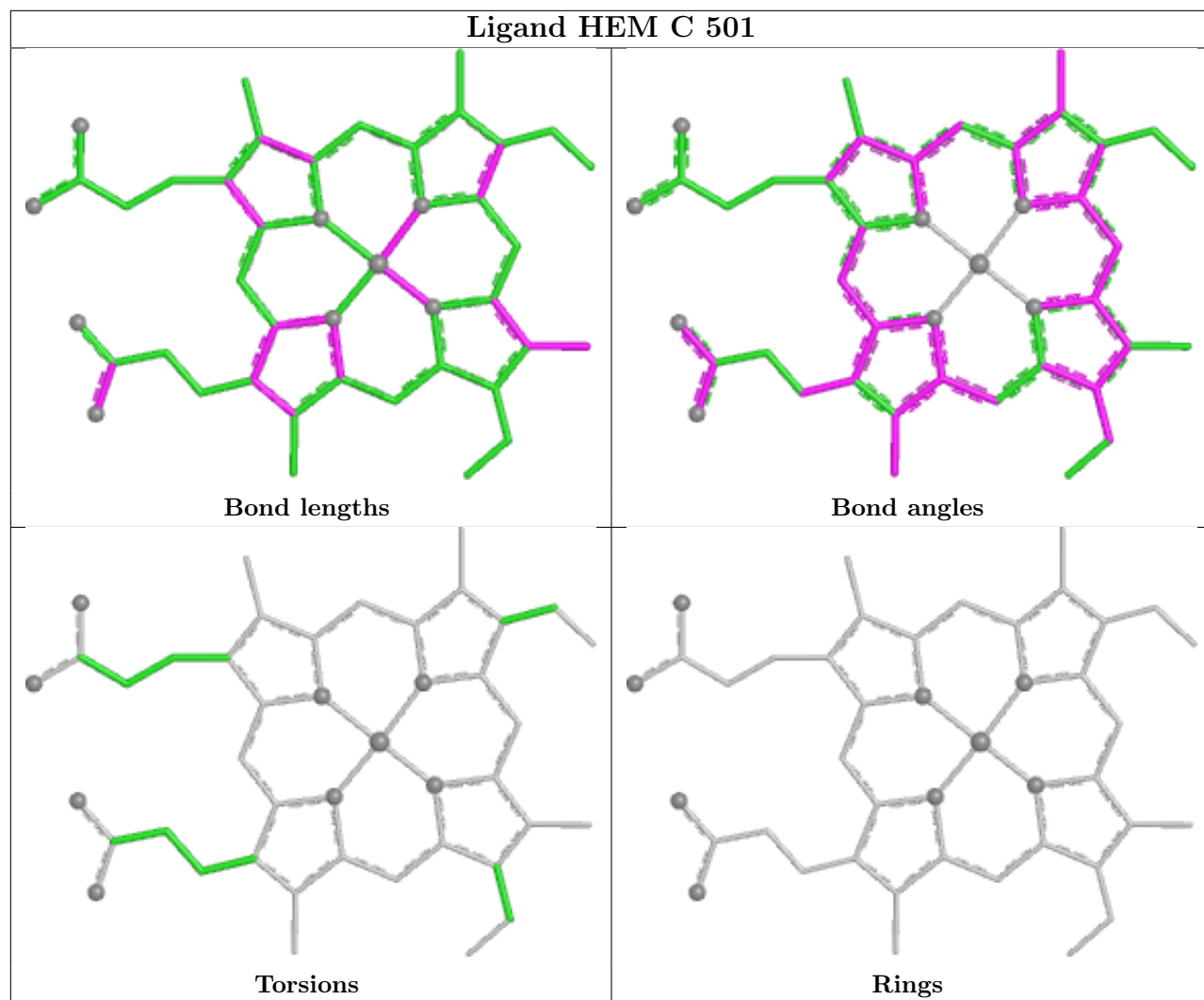


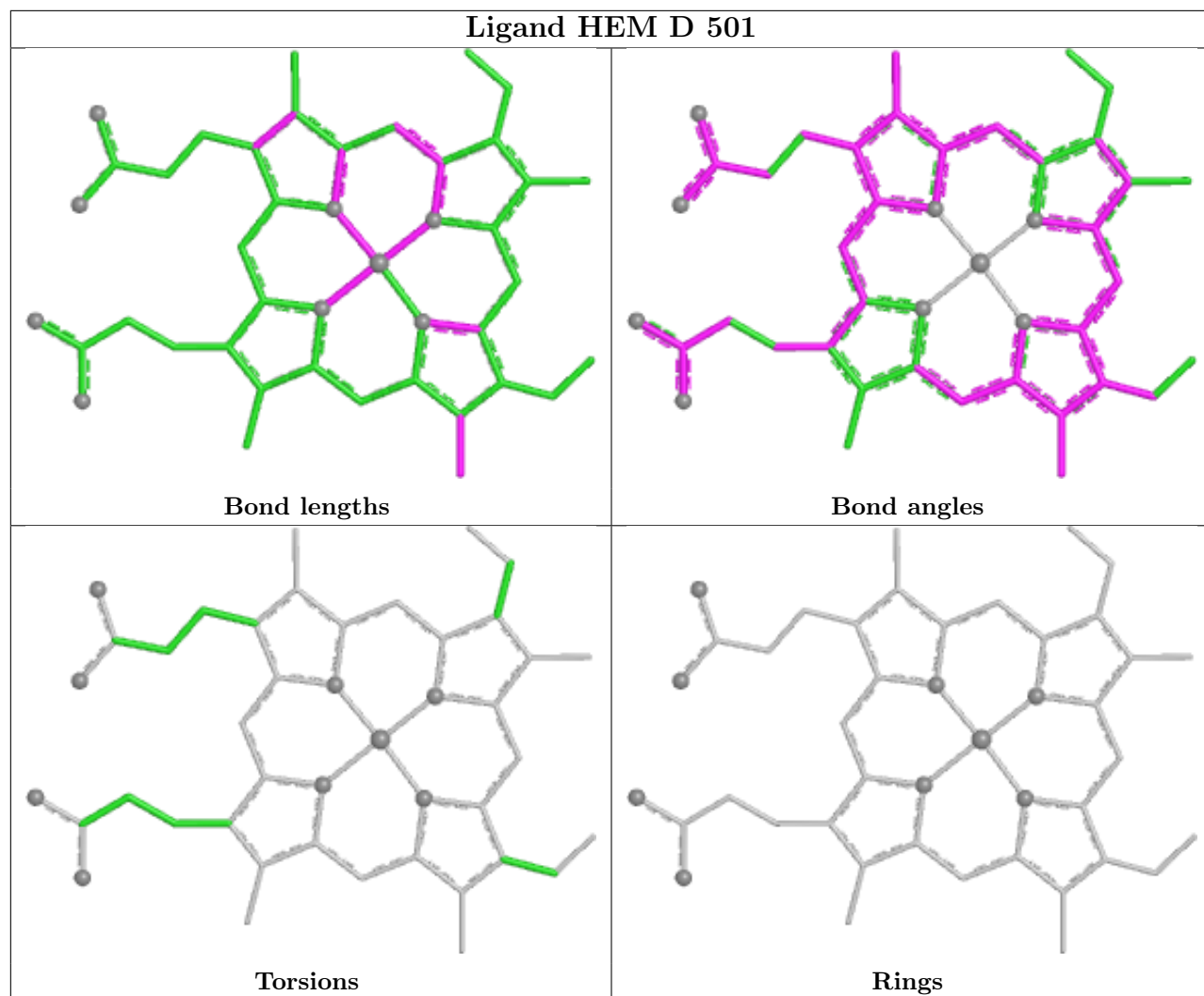


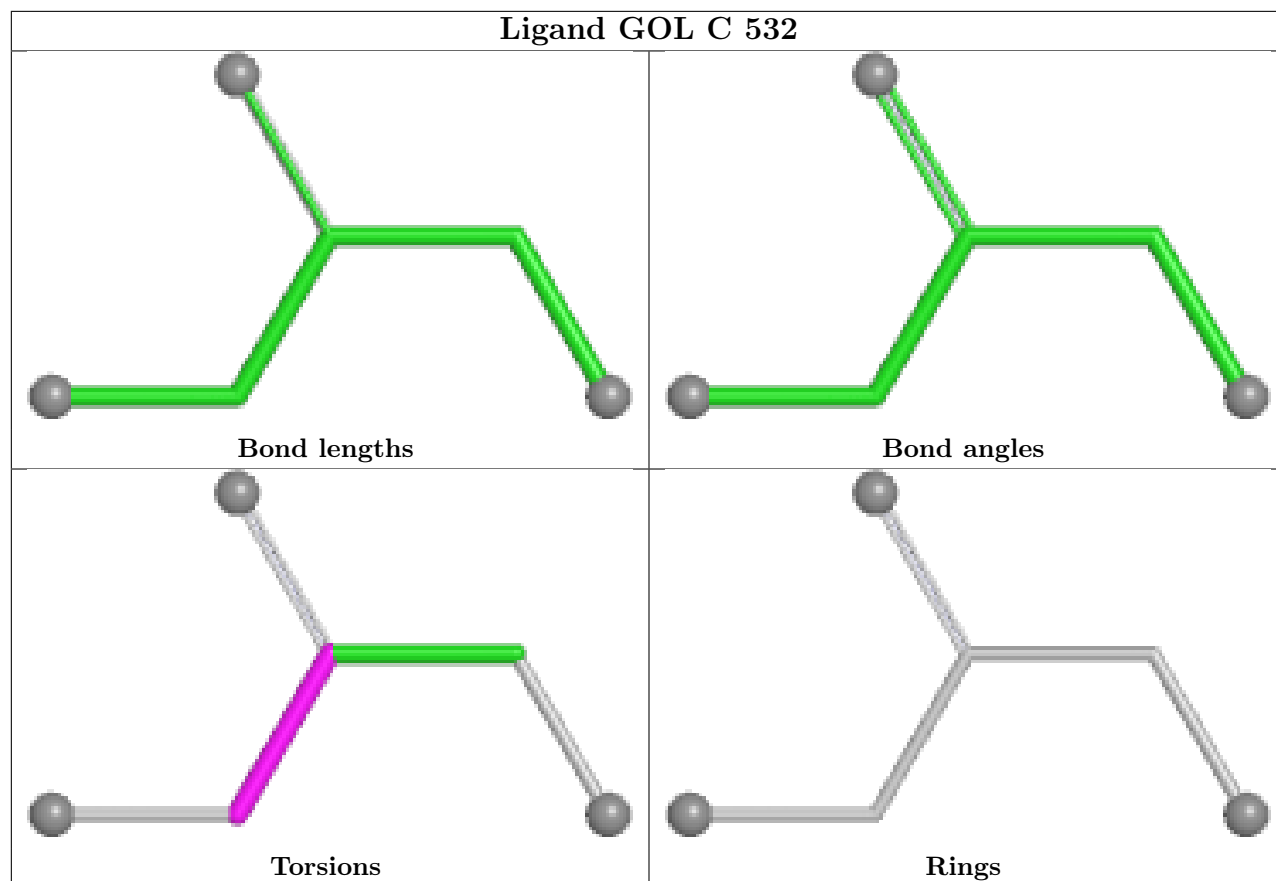


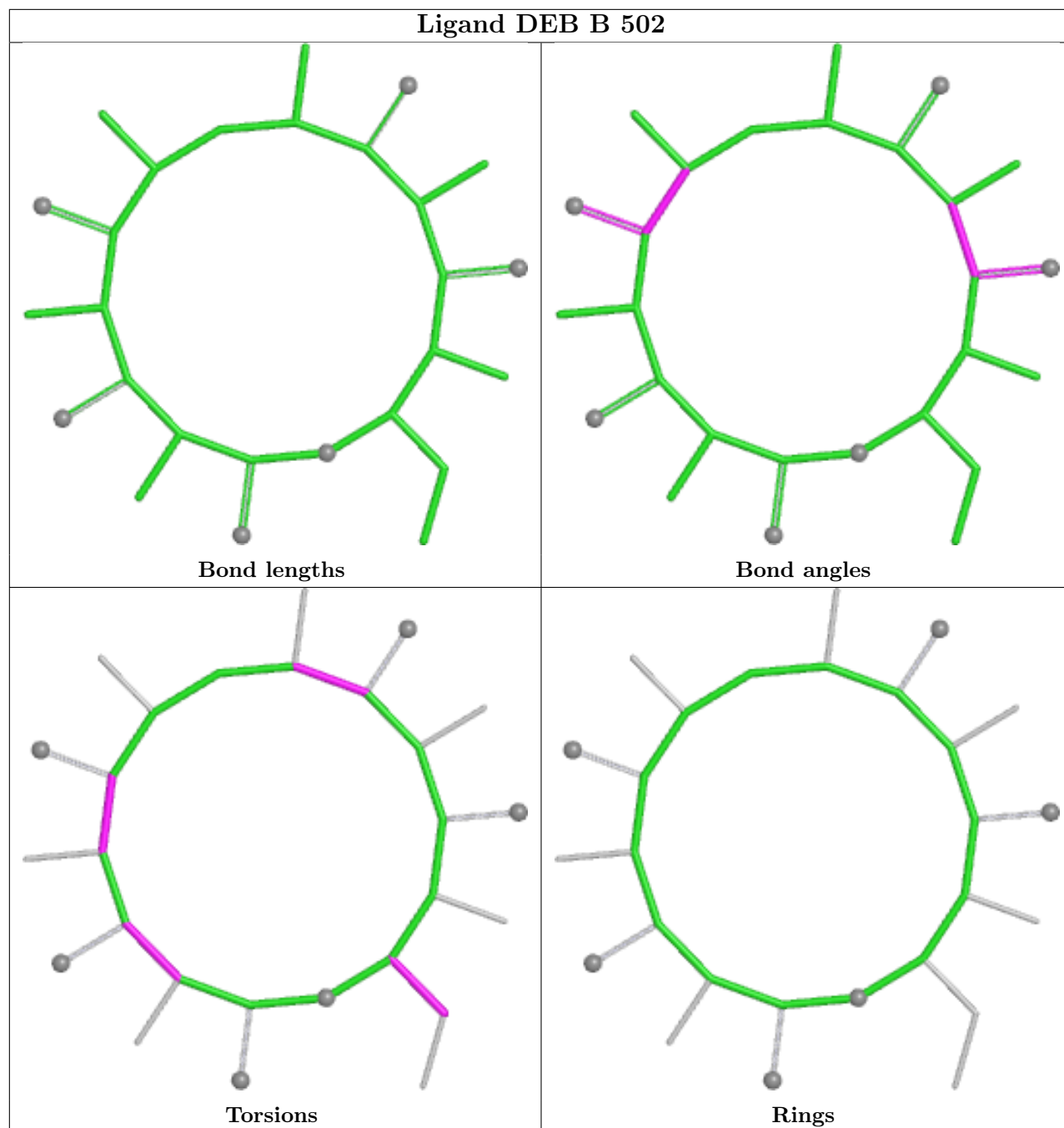
Ligand DEB E 502



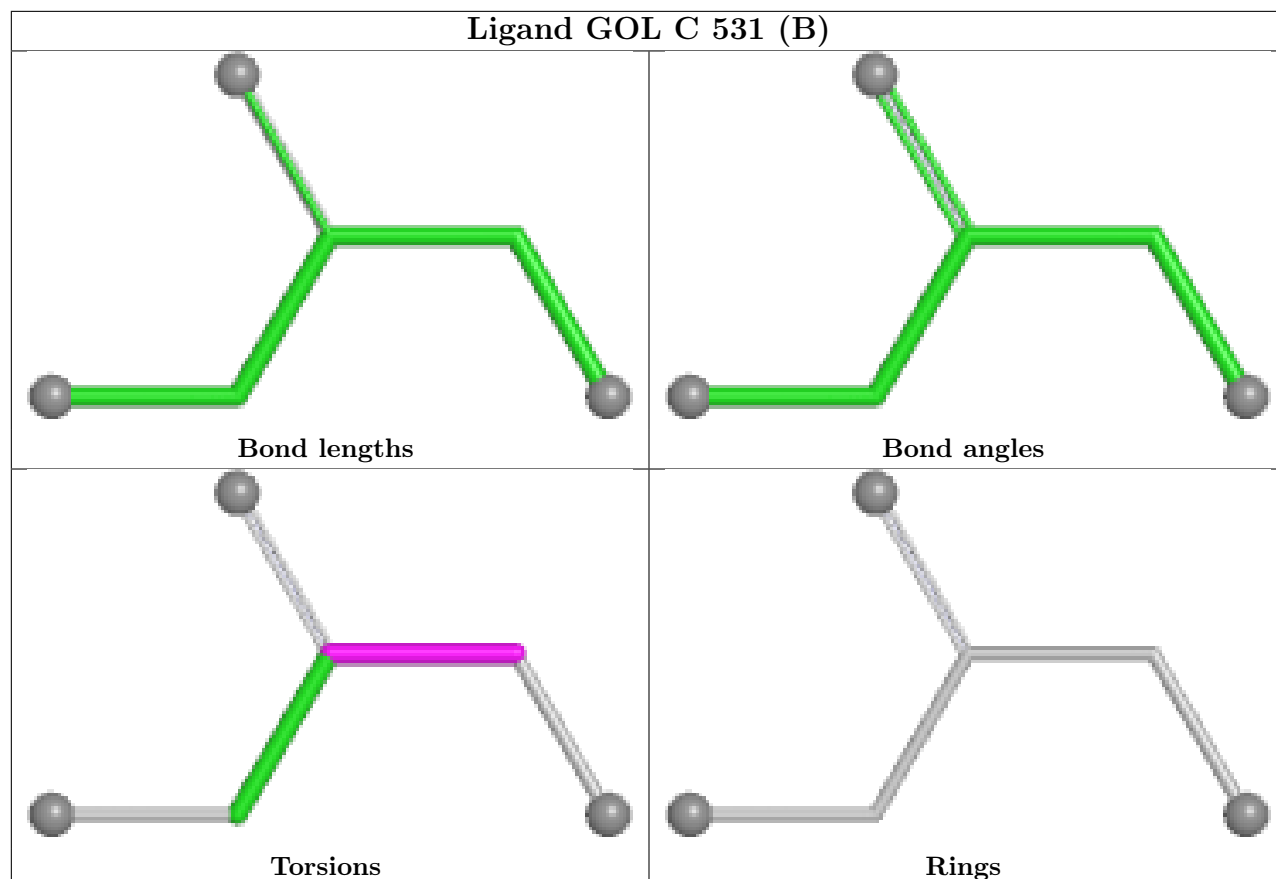




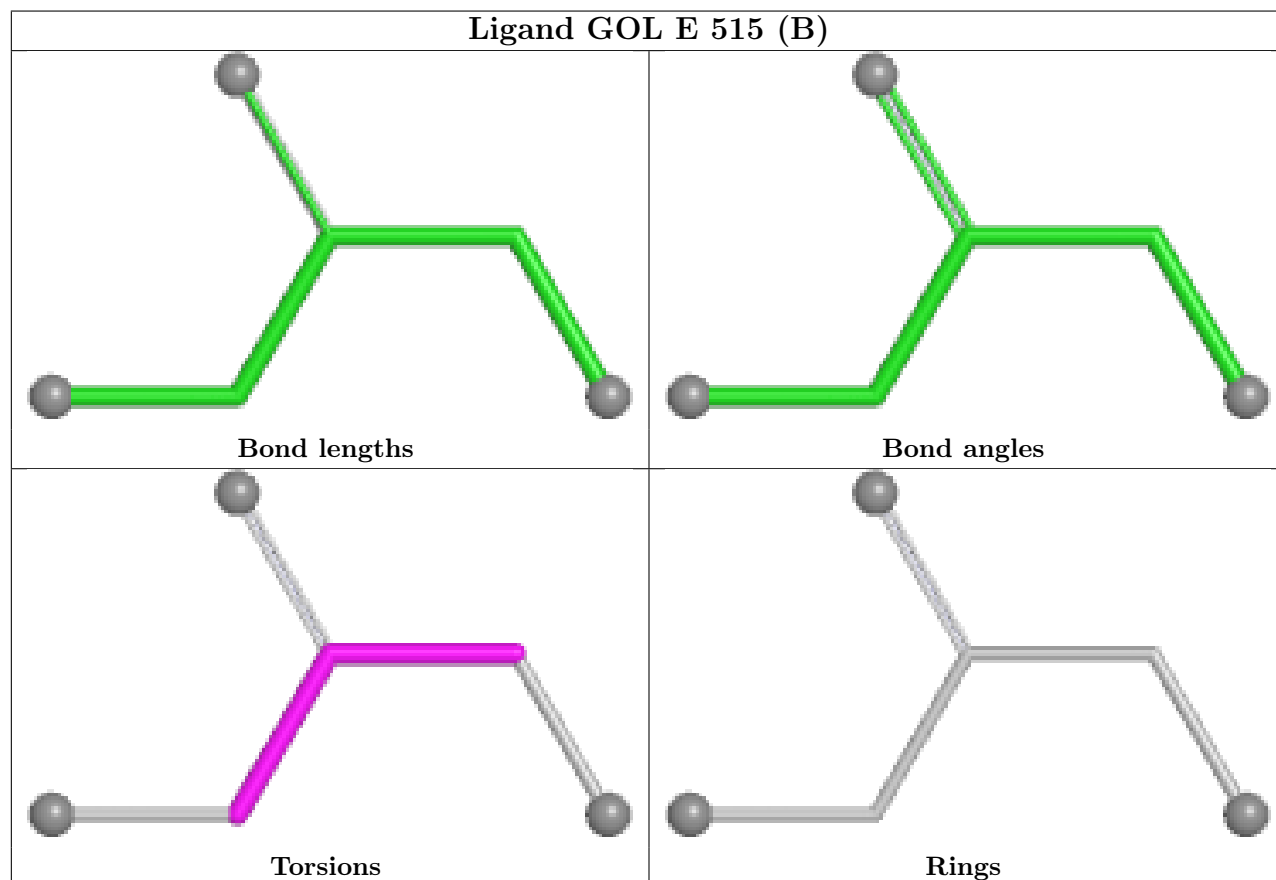




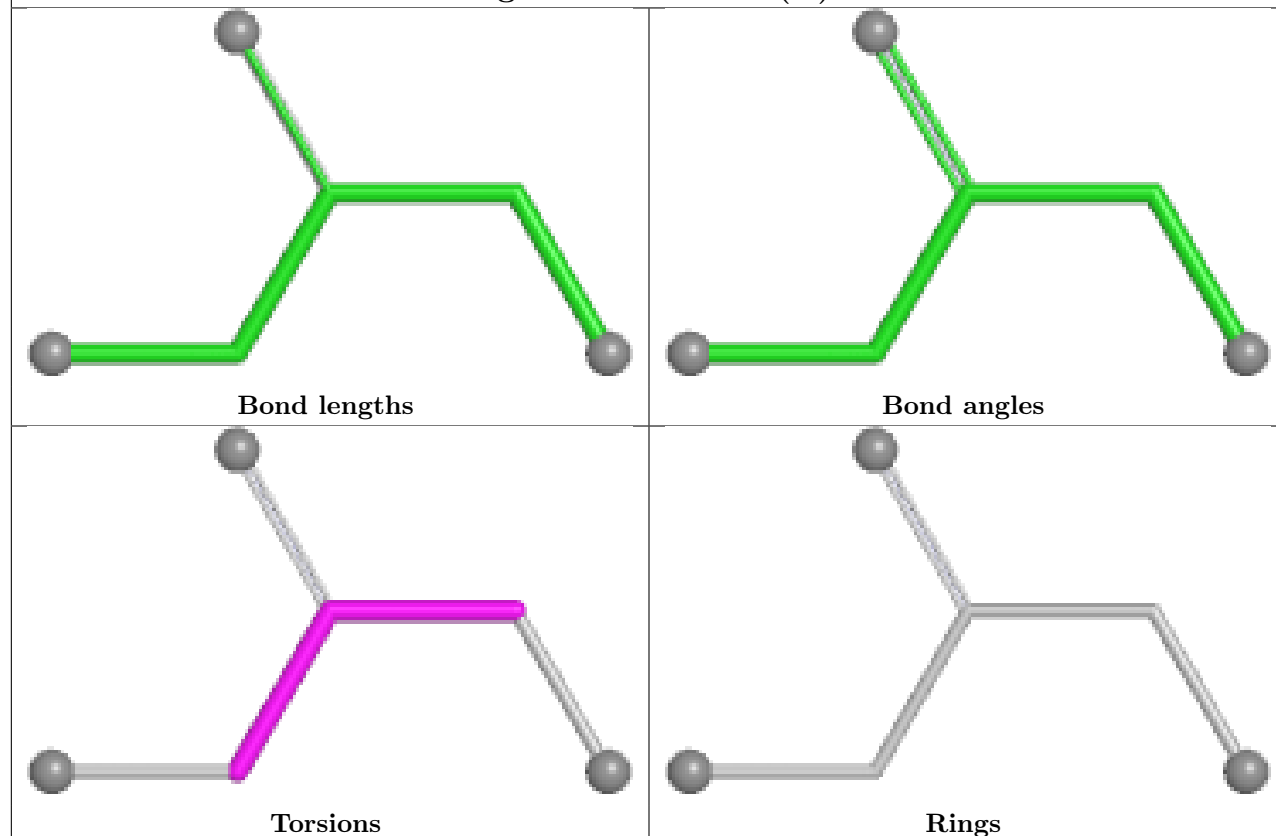
Ligand GOL C 531 (B)



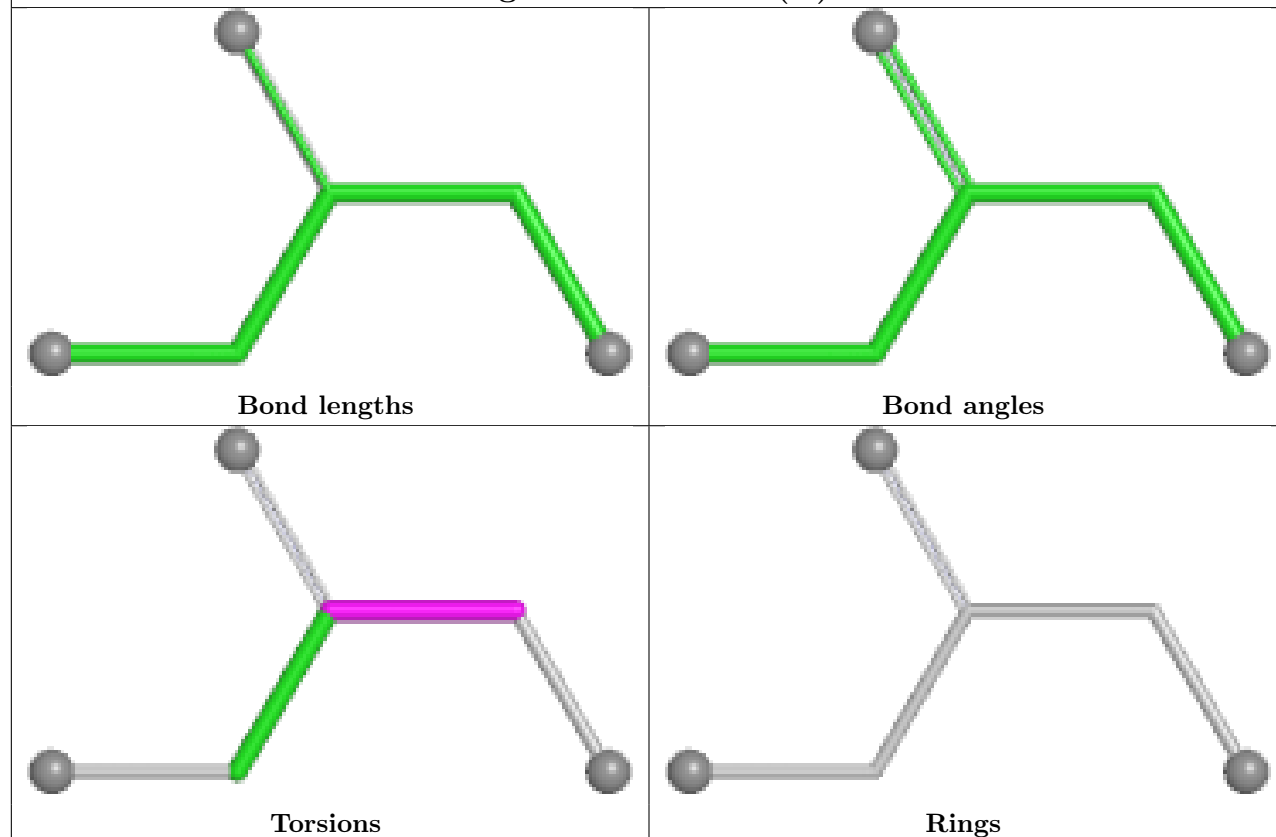
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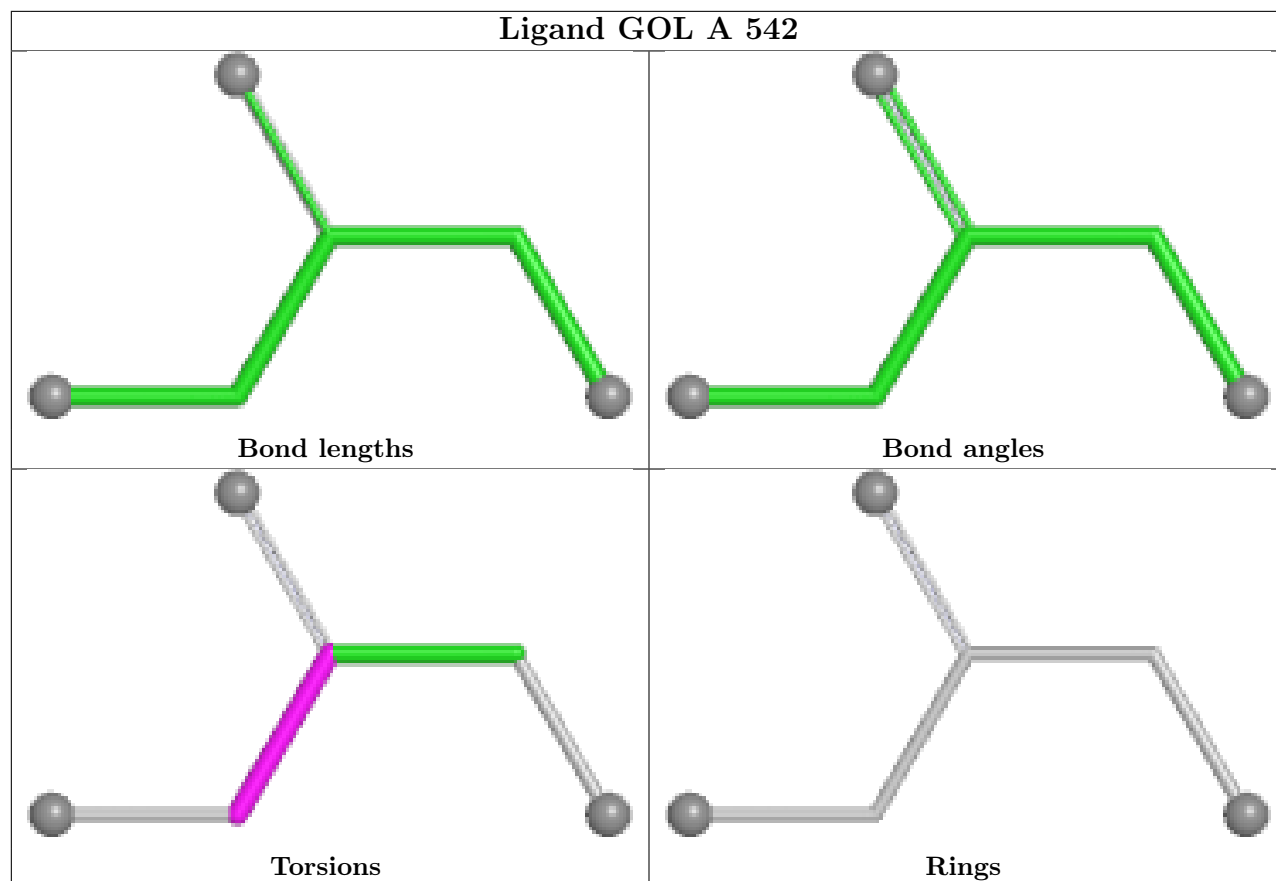


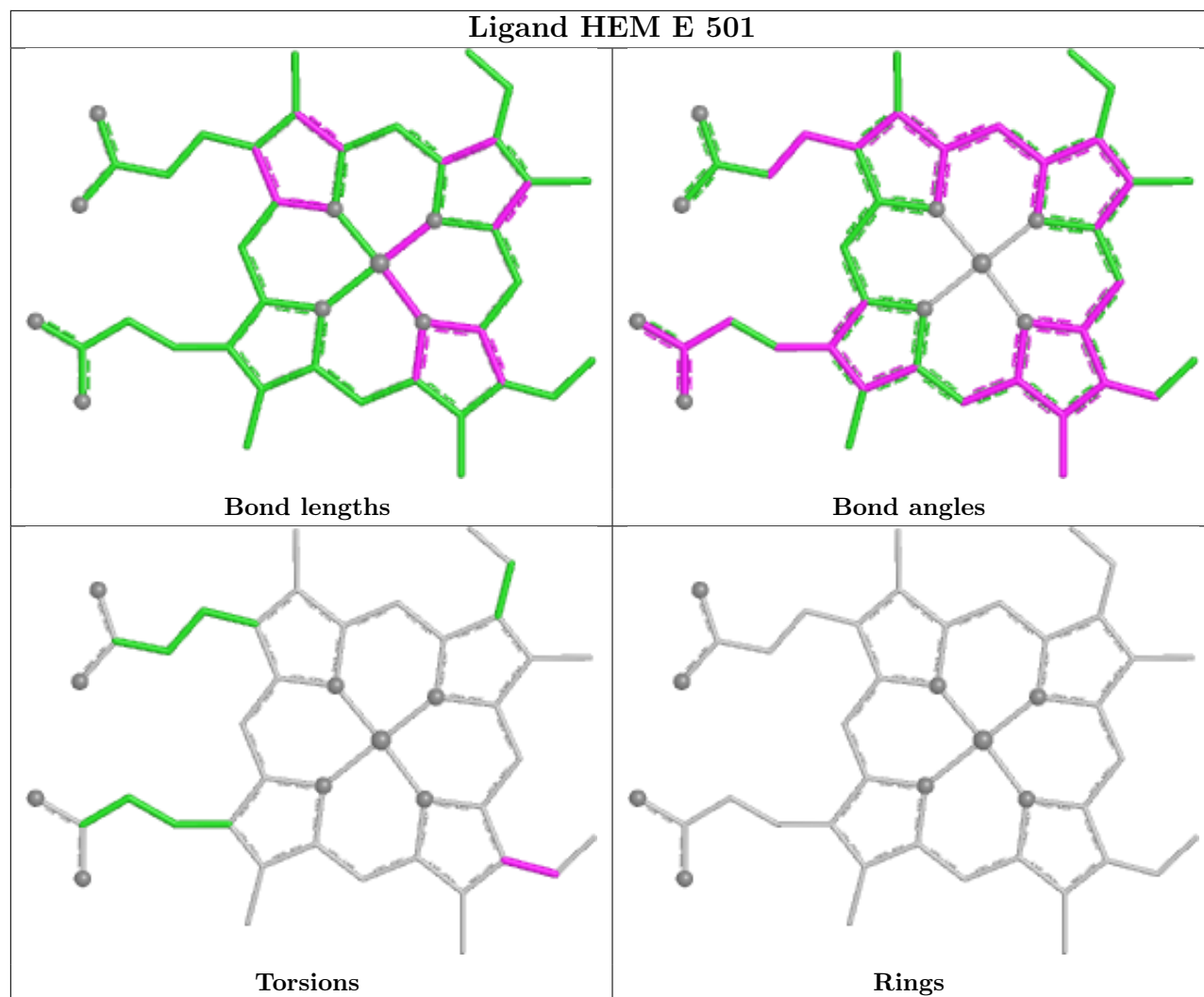
Ligand GOL C 531 (A)



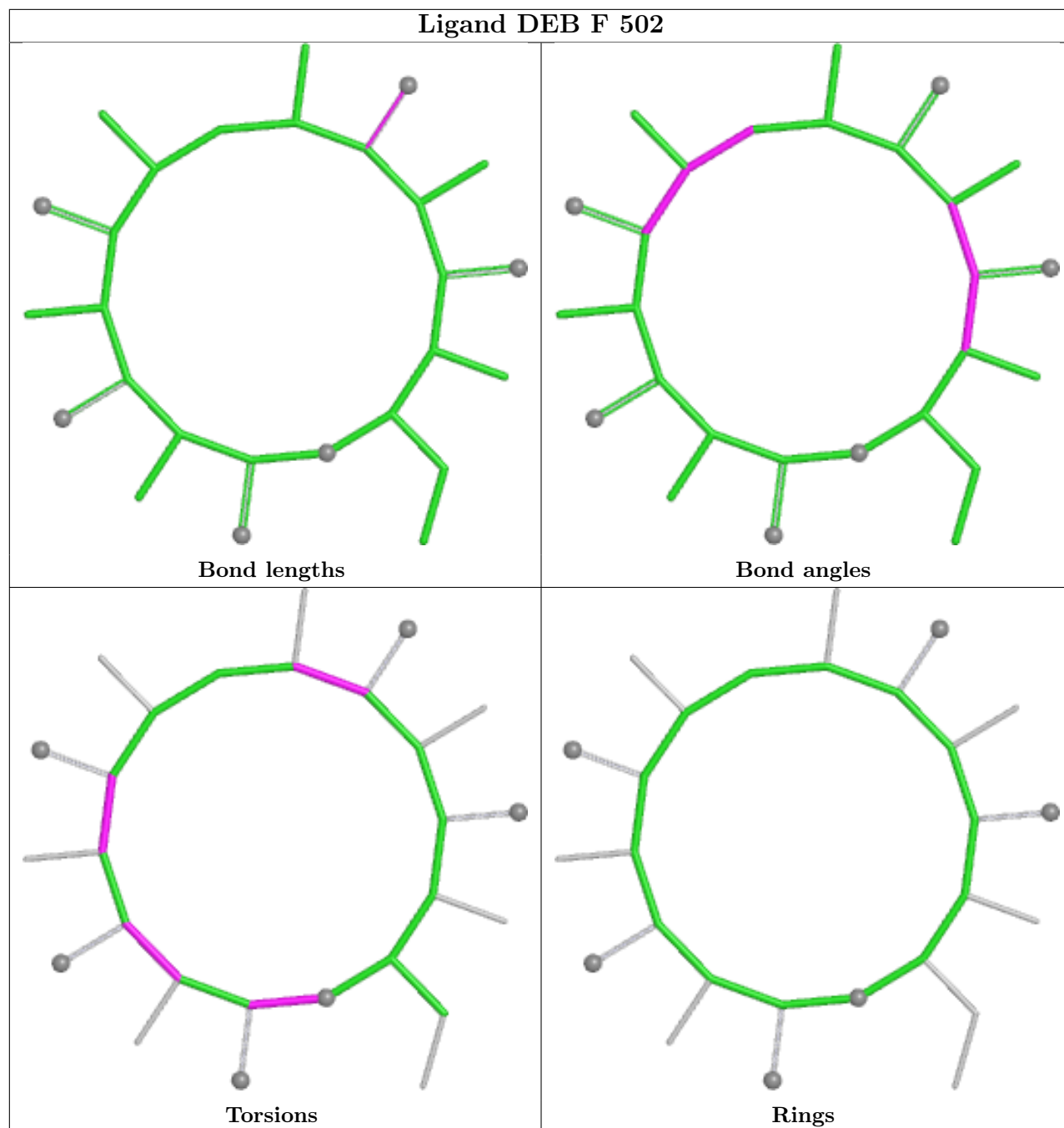
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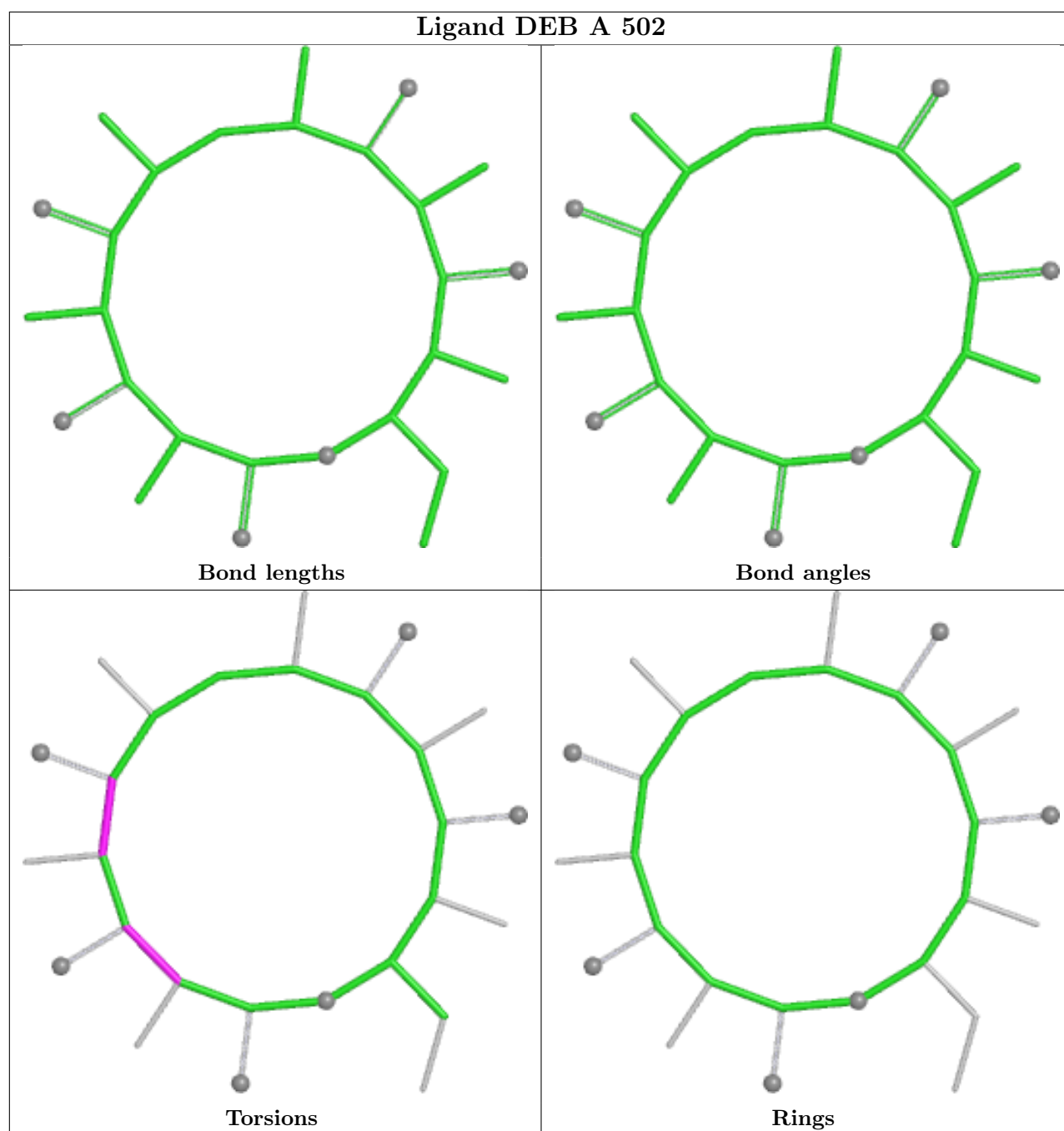






Ligand DEB F 502





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	396/408 (97%)	-0.01	8 (2%) 65 67	20, 46, 70, 110	32 (8%)
1	B	402/408 (98%)	0.16	11 (2%) 56 58	25, 48, 74, 136	33 (8%)
1	C	408/408 (100%)	-0.06	8 (1%) 65 67	22, 45, 70, 145	29 (7%)
1	D	396/408 (97%)	0.53	18 (4%) 38 40	26, 57, 84, 153	16 (4%)
1	E	395/408 (96%)	0.41	11 (2%) 55 57	25, 63, 96, 166	9 (2%)
1	F	396/408 (97%)	0.66	28 (7%) 22 23	25, 68, 107, 127	6 (1%)
All	All	2393/2448 (97%)	0.28	84 (3%) 47 49	20, 54, 95, 166	125 (5%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10[A]	PRO	16.3
1	B	9[A]	THR	10.2
1	B	11[A]	ALA	7.6
1	C	123	ARG	5.2
1	B	8[A]	PRO	5.1
1	C	11	ALA	4.5
1	C	8	PRO	4.1
1	D	16	ALA	3.9
1	E	210	ALA	3.9
1	A	12	ASP	3.7
1	E	204	VAL	3.6
1	D	24	ALA	3.5
1	D	228	HIS	3.4
1	E	13	ALA	3.4
1	F	21	LEU	3.3
1	C	9	THR	3.2
1	E	211	PRO	3.2
1	C	374	VAL	3.1
1	D	14	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	309	VAL	2.9
1	D	330	VAL	2.9
1	F	184	LEU	2.9
1	F	337	LEU	2.9
1	F	370	LEU	2.9
1	D	27	LEU	2.8
1	E	370	LEU	2.8
1	A	13	ALA	2.7
1	F	132	LEU	2.7
1	E	212	THR	2.7
1	E	64	VAL	2.7
1	F	339	PHE	2.6
1	B	109	GLY	2.6
1	A	228	HIS	2.6
1	F	261	LEU	2.6
1	F	136	VAL	2.5
1	C	6	THR	2.5
1	F	185	THR	2.5
1	D	45	LEU	2.5
1	B	210	ALA	2.5
1	F	389	LEU	2.5
1	B	6	THR	2.4
1	F	334	ALA	2.4
1	F	382	LEU	2.4
1	A	374	VAL	2.4
1	F	144	LEU	2.4
1	A	49	GLU	2.3
1	A	27	LEU	2.3
1	B	343[A]	ARG	2.3
1	D	395	MET	2.3
1	C	5	HIS	2.3
1	F	13	ALA	2.3
1	D	21	LEU	2.3
1	E	306	LEU	2.3
1	B	110[A]	LYS	2.3
1	C	1	MET	2.3
1	F	24	ALA	2.3
1	D	380	LEU	2.3
1	B	214[A]	ASP	2.2
1	D	383	ALA	2.2
1	F	142	ALA	2.2
1	F	25	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	407	TRP	2.2
1	F	319	VAL	2.2
1	A	370	LEU	2.2
1	F	270	LEU	2.2
1	D	17	TYR	2.2
1	F	40	VAL	2.1
1	D	229	LEU	2.1
1	F	180	SER	2.1
1	E	330	VAL	2.1
1	D	44	ARG	2.1
1	E	80[A]	THR	2.1
1	F	377	PHE	2.1
1	D	307	SER	2.1
1	A	190	GLN	2.1
1	E	228	HIS	2.1
1	F	267	TYR	2.1
1	F	148	LEU	2.0
1	F	215	LEU	2.0
1	B	211	PRO	2.0
1	D	385	PRO	2.0
1	F	405	VAL	2.0
1	F	256	LEU	2.0
1	D	12	ASP	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	A	534	3/3	0.41	0.21	78,78,93,93	0
4	FMT	A	514	3/3	0.58	0.12	90,90,95,99	0
4	FMT	B	524	3/3	0.61	0.21	73,73,88,91	0
4	FMT	A	504	3/3	0.63	0.10	94,94,106,108	0
4	FMT	B	515	3/3	0.67	0.23	66,66,85,86	0
4	FMT	B	514	3/3	0.67	0.09	90,90,95,98	0
4	FMT	D	507	3/3	0.68	0.17	86,86,95,100	0
4	FMT	E	510	3/3	0.69	0.10	89,89,102,105	0
4	FMT	E	511	3/3	0.70	0.23	92,92,107,121	0
4	FMT	F	511	3/3	0.70	0.13	92,92,98,106	0
4	FMT	A	529	3/3	0.71	0.20	88,88,88,101	0
4	FMT	A	533	3/3	0.71	0.14	84,84,87,100	0
4	FMT	A	508	3/3	0.72	0.11	94,94,104,106	0
4	FMT	F	508	3/3	0.72	0.12	80,80,89,93	0
4	FMT	F	510	3/3	0.72	0.12	92,92,95,97	0
4	FMT	B	536	3/3	0.72	0.22	65,65,73,78	0
4	FMT	C	507	3/3	0.73	0.10	98,98,105,106	0
4	FMT	C	514	3/3	0.73	0.15	88,88,95,108	0
4	FMT	C	513	3/3	0.74	0.11	85,85,99,101	0
4	FMT	A	513	3/3	0.75	0.16	78,78,87,100	0
4	FMT	C	516	3/3	0.75	0.14	75,75,80,81	0
4	FMT	D	503	3/3	0.75	0.19	89,89,93,96	0
4	FMT	D	506	3/3	0.75	0.14	85,85,87,89	0
4	FMT	A	537	3/3	0.75	0.20	75,75,80,94	0
6	GOL	C	532	6/6	0.75	0.14	76,93,96,109	0
4	FMT	B	512	3/3	0.76	0.14	85,85,106,110	0
4	FMT	D	505	3/3	0.76	0.23	86,86,87,94	0
4	FMT	A	531	3/3	0.76	0.11	95,95,101,103	0
4	FMT	B	510	3/3	0.76	0.14	73,73,78,86	0
4	FMT	C	518	3/3	0.76	0.15	73,73,82,94	0
4	FMT	D	516	3/3	0.77	0.17	71,71,92,93	0
4	FMT	D	518	3/3	0.77	0.14	93,93,95,99	0
4	FMT	C	510	3/3	0.77	0.17	86,86,105,106	0
4	FMT	D	511	3/3	0.77	0.20	75,75,83,83	0
4	FMT	A	535	3/3	0.78	0.28	83,83,95,112	0
4	FMT	B	533	3/3	0.78	0.20	91,91,93,97	0
6	GOL	A	544	6/6	0.78	0.18	68,80,81,83	6
4	FMT	C	508	3/3	0.78	0.15	82,82,90,98	0
4	FMT	B	506	3/3	0.79	0.15	64,64,78,79	0
4	FMT	B	529	3/3	0.80	0.12	73,73,88,93	0
4	FMT	A	524	3/3	0.80	0.13	99,99,102,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	B	518	3/3	0.80	0.15	81,81,86,94	0
4	FMT	B	539	3/3	0.80	0.09	91,91,92,97	0
4	FMT	B	503	3/3	0.80	0.12	83,83,83,88	0
4	FMT	A	523	3/3	0.81	0.20	76,76,81,84	0
4	FMT	C	517	3/3	0.81	0.18	60,60,64,84	0
6	GOL	B	542	6/6	0.81	0.13	70,88,89,89	0
4	FMT	D	512	3/3	0.81	0.12	93,93,96,100	0
4	FMT	C	522	3/3	0.82	0.14	87,87,91,93	0
4	FMT	A	516	3/3	0.82	0.15	79,79,90,95	0
6	GOL	A	542	6/6	0.82	0.20	58,72,83,91	0
4	FMT	B	520	3/3	0.82	0.25	78,78,83,96	0
4	FMT	E	512	3/3	0.82	0.13	81,81,92,92	0
4	FMT	A	519	3/3	0.82	0.21	74,74,80,84	0
4	FMT	B	525	3/3	0.83	0.12	86,86,94,101	0
4	FMT	C	521	3/3	0.83	0.13	106,106,107,108	0
4	FMT	F	505	3/3	0.83	0.15	78,78,80,96	0
4	FMT	A	539	3/3	0.83	0.12	86,86,87,89	0
4	FMT	A	538	3/3	0.83	0.22	71,71,72,93	0
4	FMT	B	528	3/3	0.84	0.17	69,69,71,89	0
4	FMT	A	527	3/3	0.84	0.14	79,79,85,87	0
4	FMT	C	520	3/3	0.84	0.14	78,78,83,97	0
4	FMT	A	517	3/3	0.84	0.18	85,85,94,101	0
4	FMT	D	513	3/3	0.84	0.14	82,82,83,89	0
4	FMT	A	512	3/3	0.84	0.17	95,95,108,112	0
4	FMT	C	528	3/3	0.84	0.18	72,72,77,79	0
4	FMT	A	532	3/3	0.84	0.07	102,102,102,106	0
4	FMT	C	504	3/3	0.84	0.22	59,59,63,68	0
4	FMT	C	502	3/3	0.85	0.13	65,65,75,85	0
4	FMT	F	503	3/3	0.85	0.14	76,76,87,92	0
4	FMT	A	520	3/3	0.85	0.23	61,61,74,90	0
4	FMT	B	534	3/3	0.85	0.17	94,94,101,105	0
4	FMT	D	515	3/3	0.85	0.23	68,68,71,80	0
4	FMT	E	506	3/3	0.86	0.17	68,68,73,84	0
4	FMT	F	509	3/3	0.86	0.17	64,64,78,89	0
4	FMT	B	523	3/3	0.86	0.19	64,64,72,79	0
4	FMT	C	523	3/3	0.86	0.18	74,74,87,103	0
4	FMT	B	507	3/3	0.86	0.16	63,63,64,82	0
4	FMT	D	508	3/3	0.86	0.20	64,64,65,76	0
4	FMT	B	513	3/3	0.86	0.16	67,67,87,87	0
4	FMT	F	507	3/3	0.86	0.14	86,86,93,103	0
4	FMT	B	532	3/3	0.87	0.20	84,84,90,92	0
4	FMT	B	521	3/3	0.87	0.16	75,75,79,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	C	511	3/3	0.87	0.08	89,89,99,101	0
4	FMT	D	517	3/3	0.87	0.14	84,84,86,89	0
4	FMT	B	519	3/3	0.87	0.16	79,79,91,92	0
6	GOL	A	545	6/6	0.87	0.15	46,63,70,80	6
4	FMT	E	504	3/3	0.87	0.13	84,84,95,97	0
4	FMT	B	516	3/3	0.87	0.15	68,68,84,86	0
4	FMT	A	522	3/3	0.88	0.11	76,76,77,92	0
4	FMT	B	522	3/3	0.88	0.14	78,78,79,80	0
4	FMT	D	514	3/3	0.88	0.18	69,69,70,86	0
4	FMT	A	518	3/3	0.88	0.15	83,83,88,91	0
4	FMT	C	524	3/3	0.88	0.31	71,71,74,83	0
4	FMT	C	512	3/3	0.88	0.14	76,76,80,87	0
4	FMT	B	508	3/3	0.88	0.09	77,77,93,94	0
4	FMT	A	511	3/3	0.88	0.18	62,62,75,80	0
4	FMT	A	525	3/3	0.88	0.25	73,73,74,77	0
4	FMT	A	515	3/3	0.88	0.15	82,82,94,98	0
4	FMT	C	505	3/3	0.88	0.17	50,50,61,75	0
6	GOL	B	543[A]	6/6	0.88	0.17	36,39,43,45	6
6	GOL	B	543[B]	6/6	0.88	0.17	66,72,80,83	6
4	FMT	B	531	3/3	0.88	0.12	84,84,86,88	0
4	FMT	D	510	3/3	0.89	0.23	66,66,67,79	0
4	FMT	E	503	3/3	0.89	0.18	75,75,84,84	0
4	FMT	C	506	3/3	0.89	0.14	69,69,75,81	0
4	FMT	E	505	3/3	0.89	0.17	55,55,59,74	0
4	FMT	A	528	3/3	0.89	0.15	85,85,88,106	0
4	FMT	E	509	3/3	0.89	0.10	78,78,91,94	0
4	FMT	D	504	3/3	0.89	0.13	58,58,60,64	0
4	FMT	C	503	3/3	0.89	0.19	61,61,71,83	0
4	FMT	C	515	3/3	0.89	0.23	66,66,77,79	0
4	FMT	A	509	3/3	0.89	0.13	86,86,90,92	0
4	FMT	F	504	3/3	0.89	0.19	57,57,64,72	0
3	DEB	D	502	27/27	0.89	0.12	32,42,46,47	0
4	FMT	F	506	3/3	0.90	0.10	74,74,76,84	0
6	GOL	A	543[A]	6/6	0.90	0.14	32,46,51,56	6
6	GOL	A	543[B]	6/6	0.90	0.14	32,40,45,45	6
4	FMT	E	508	3/3	0.90	0.10	91,91,93,96	0
4	FMT	E	513	3/3	0.90	0.18	67,67,71,76	0
3	DEB	C	533	27/27	0.90	0.12	30,37,50,54	0
4	FMT	C	529	3/3	0.90	0.22	83,83,87,101	0
4	FMT	A	536	3/3	0.90	0.12	72,72,79,82	0
4	FMT	F	512	3/3	0.90	0.18	85,85,86,90	0
4	FMT	C	527	3/3	0.91	0.20	50,50,51,73	3

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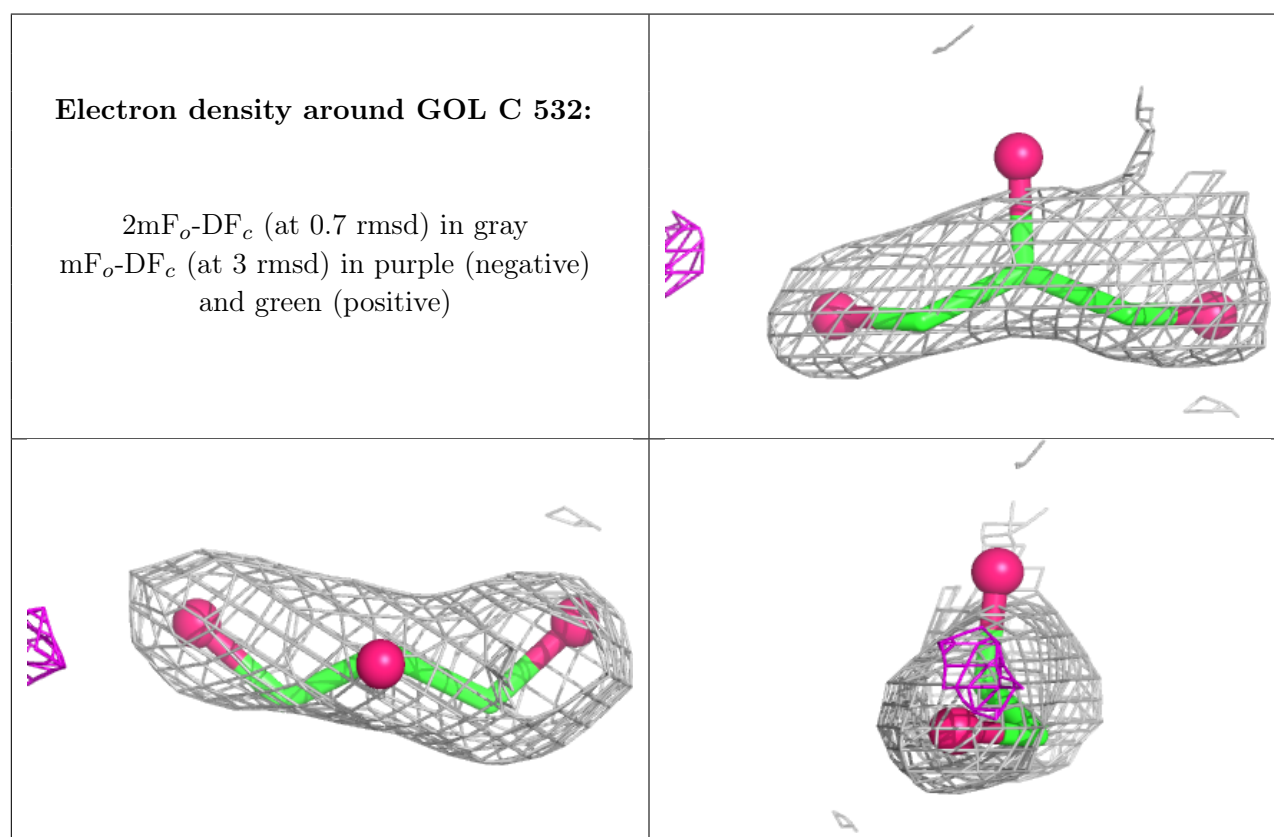
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FMT	A	521	3/3	0.91	0.13	62,62,79,96	0
4	FMT	B	517	3/3	0.91	0.26	61,61,70,75	0
4	FMT	B	535	3/3	0.91	0.18	66,66,72,84	0
4	FMT	A	503	3/3	0.91	0.12	80,80,85,87	0
4	FMT	C	519	3/3	0.91	0.10	52,52,54,61	0
4	FMT	B	537	3/3	0.91	0.15	59,59,83,96	0
4	FMT	B	504	3/3	0.91	0.11	68,68,72,75	0
4	FMT	B	505	3/3	0.91	0.15	70,70,80,90	0
4	FMT	D	509	3/3	0.91	0.12	79,79,81,83	0
4	FMT	A	506	3/3	0.91	0.13	63,63,66,68	0
4	FMT	A	507	3/3	0.91	0.11	63,63,85,89	0
6	GOL	E	515[A]	6/6	0.91	0.14	45,57,59,60	6
6	GOL	E	515[B]	6/6	0.91	0.14	121,125,127,128	6
4	FMT	E	507	3/3	0.92	0.24	59,59,73,85	0
4	FMT	B	526	3/3	0.92	0.14	73,73,73,81	0
4	FMT	B	538	3/3	0.92	0.16	50,50,71,78	0
4	FMT	B	527	3/3	0.92	0.10	74,74,89,93	0
6	GOL	C	531[B]	6/6	0.93	0.17	26,40,43,47	6
4	FMT	A	530	3/3	0.93	0.10	74,74,81,89	0
4	FMT	A	505	3/3	0.93	0.11	65,65,70,79	0
6	GOL	C	531[A]	6/6	0.93	0.17	53,57,60,61	6
4	FMT	C	526	3/3	0.94	0.13	86,86,91,92	0
5	NA	F	513	1/1	0.94	0.11	63,63,63,63	0
4	FMT	A	510	3/3	0.94	0.12	46,46,67,70	0
4	FMT	A	526	3/3	0.94	0.10	58,58,68,70	0
4	FMT	C	509	3/3	0.94	0.10	71,71,73,91	0
3	DEB	E	502	27/27	0.95	0.10	47,53,61,74	0
4	FMT	B	511	3/3	0.95	0.07	62,62,64,66	0
5	NA	A	540	1/1	0.95	0.15	56,56,56,56	0
5	NA	D	519	1/1	0.95	0.14	56,56,56,56	0
4	FMT	C	525	3/3	0.95	0.10	69,69,78,78	0
3	DEB	F	502	27/27	0.95	0.12	56,64,74,83	0
3	DEB	A	502	27/27	0.95	0.09	30,37,50,54	0
4	FMT	B	509	3/3	0.95	0.11	73,73,74,80	0
4	FMT	B	530	3/3	0.95	0.18	52,52,83,96	0
3	DEB	B	502	27/27	0.96	0.08	33,40,51,59	0
5	NA	E	514	1/1	0.96	0.17	63,63,63,63	0
5	NA	B	540	1/1	0.96	0.23	52,52,52,52	0
5	NA	C	530	1/1	0.96	0.13	47,47,47,47	0
5	NA	A	541	1/1	0.97	0.06	47,47,47,47	0
2	HEM	F	501	43/43	0.98	0.07	47,54,64,92	0
2	HEM	D	501	43/43	0.98	0.07	25,36,49,62	0

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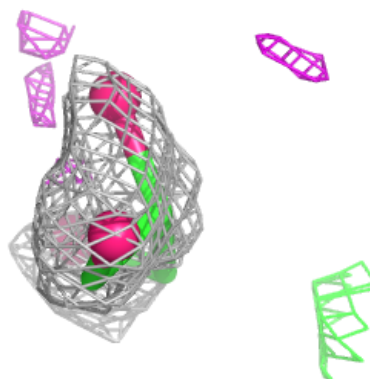
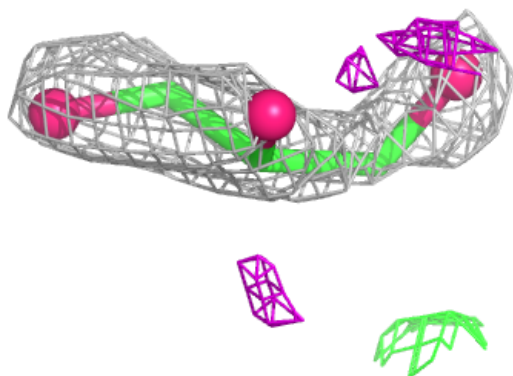
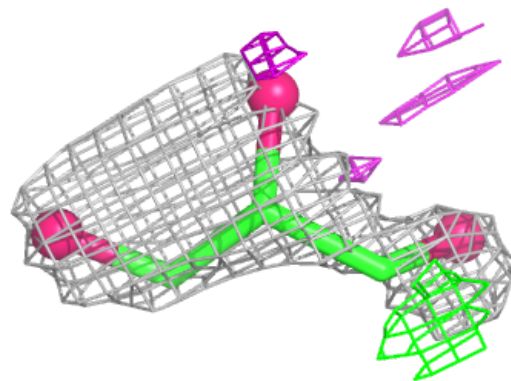
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	B	541	1/1	0.98	0.18	50,50,50,50	0
2	HEM	E	501	43/43	0.98	0.06	39,44,53,66	0
2	HEM	B	501	43/43	0.99	0.06	29,34,45,51	0
2	HEM	C	501	43/43	0.99	0.05	31,36,41,55	0
2	HEM	A	501	43/43	0.99	0.06	29,35,43,61	0

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.



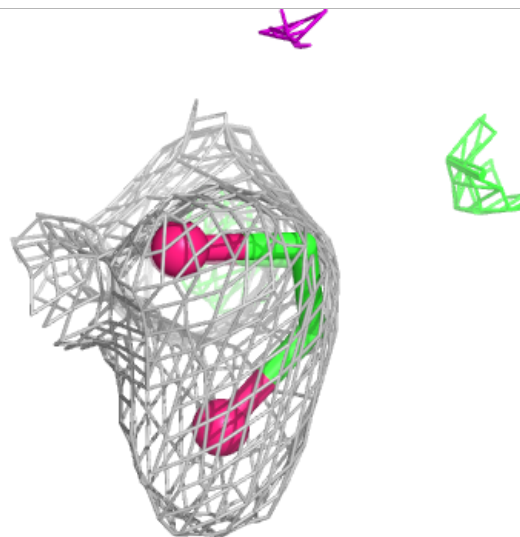
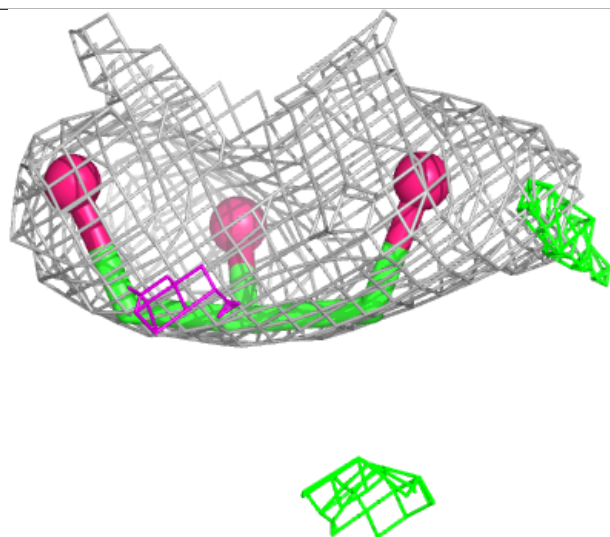
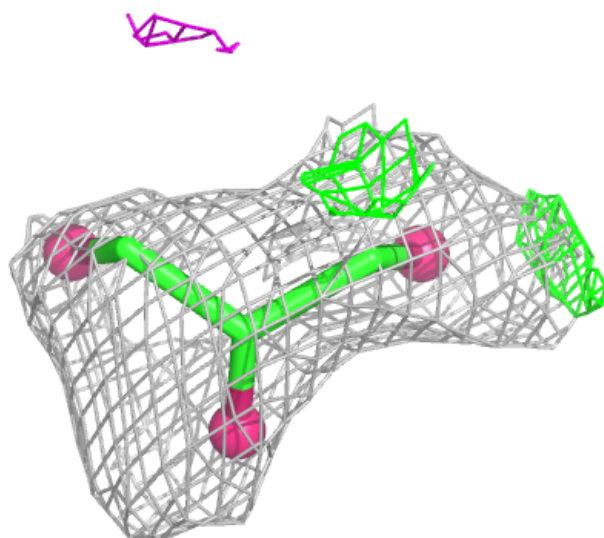
Electron density around GOL A 544:

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



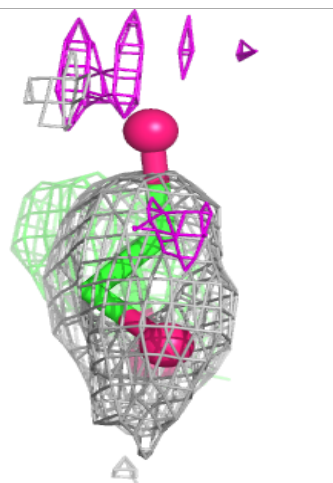
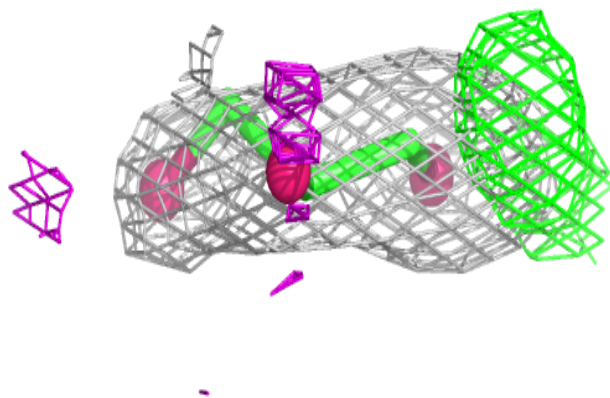
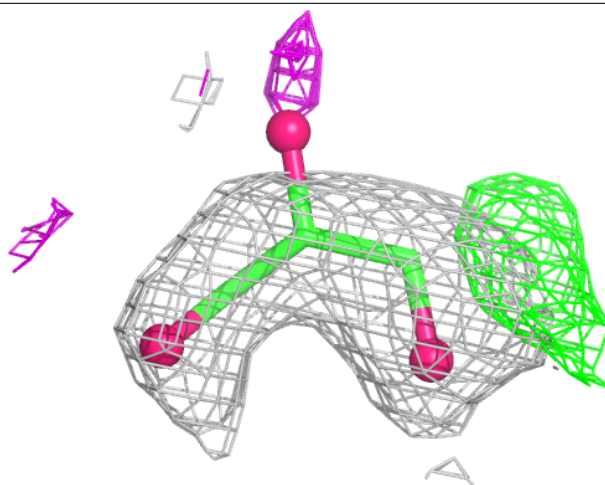
Electron density around GOL B 542:

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



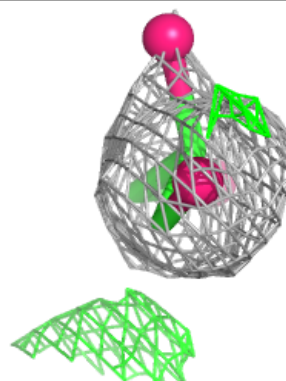
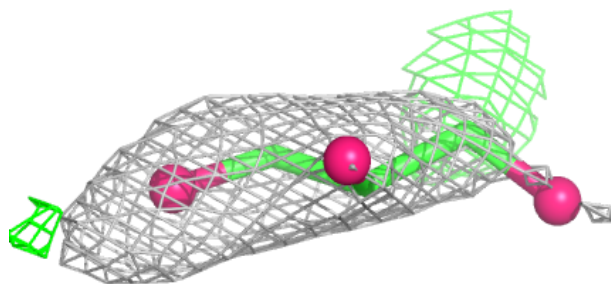
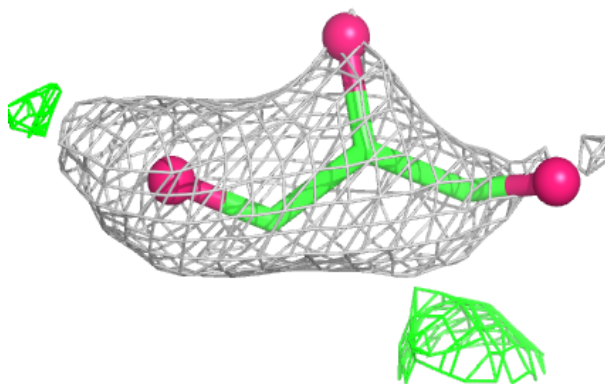
Electron density around GOL A 542:

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

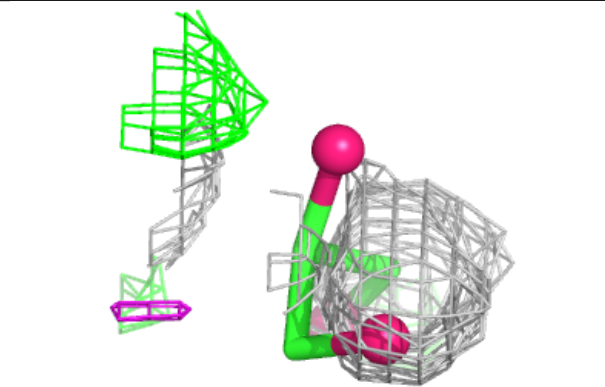
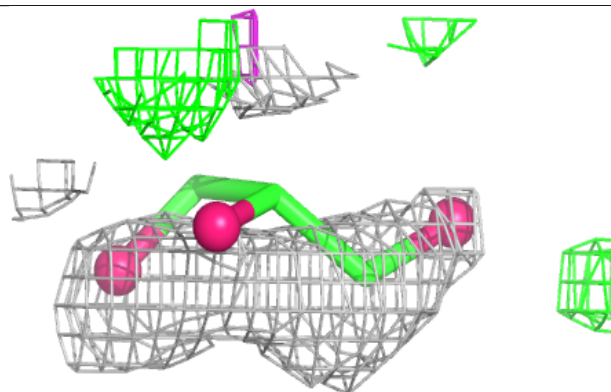
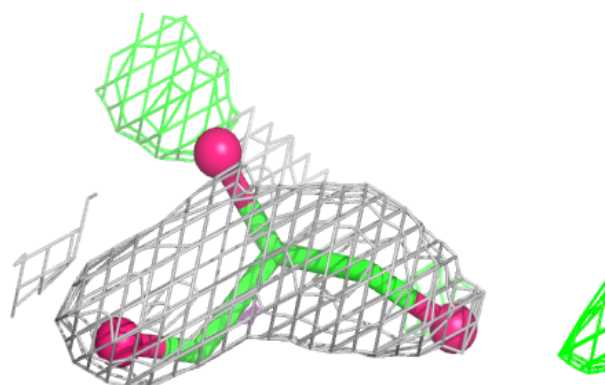


Electron density around GOL A 545:

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

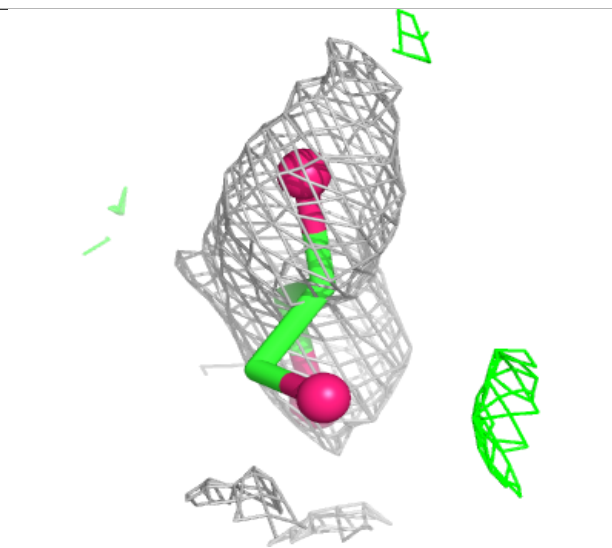
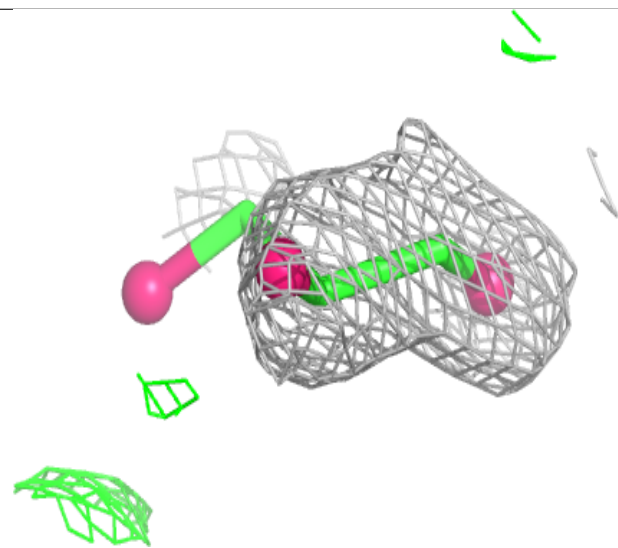
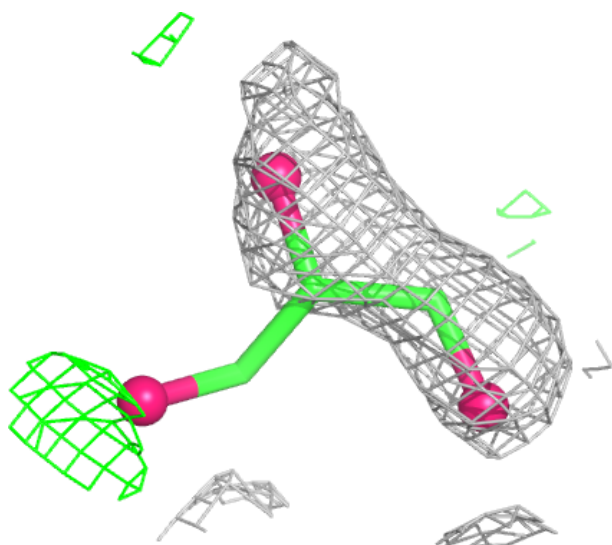
**Electron density around GOL B 543 (A):**

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



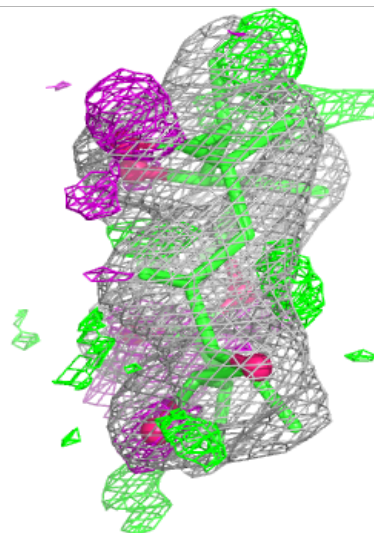
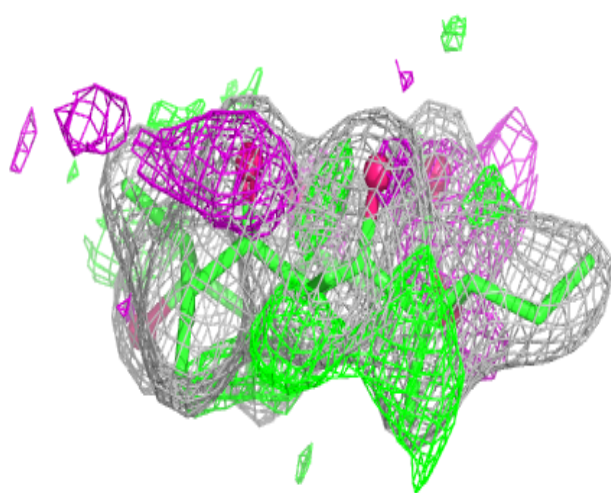
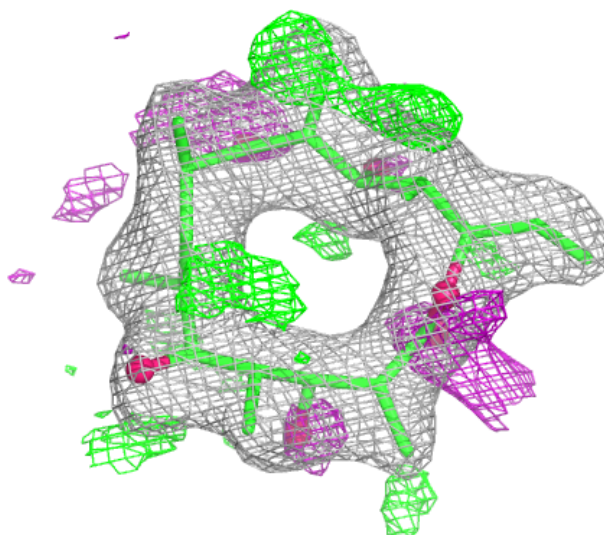
Electron density around GOL B 543 (B):

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



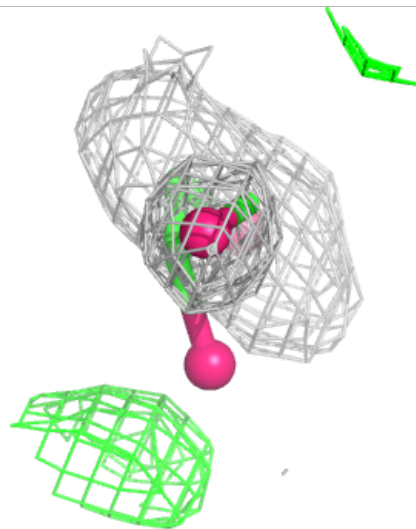
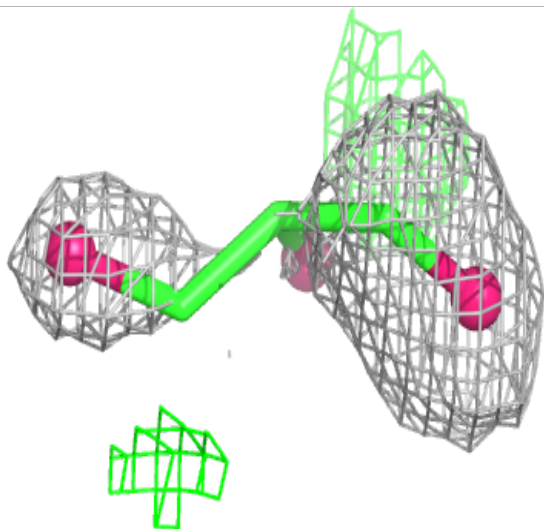
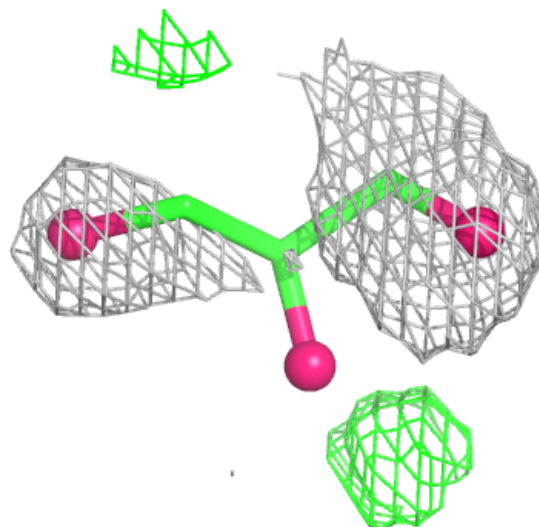
Electron density around DEB D 502:

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



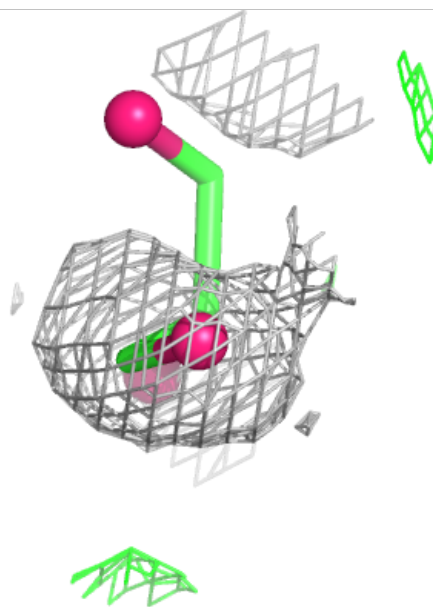
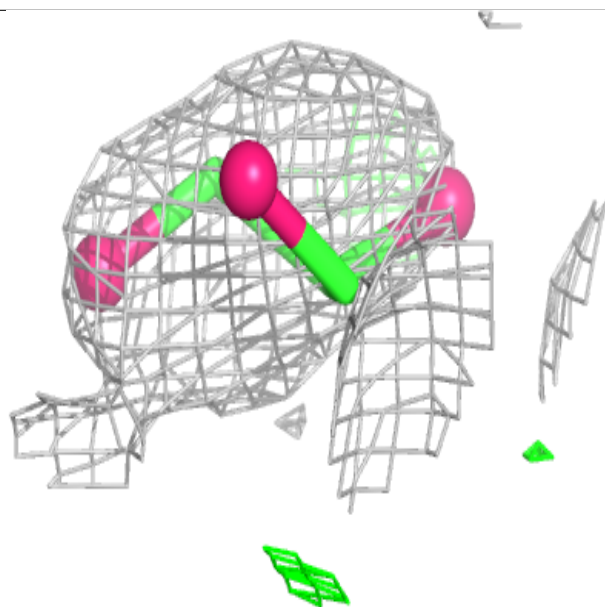
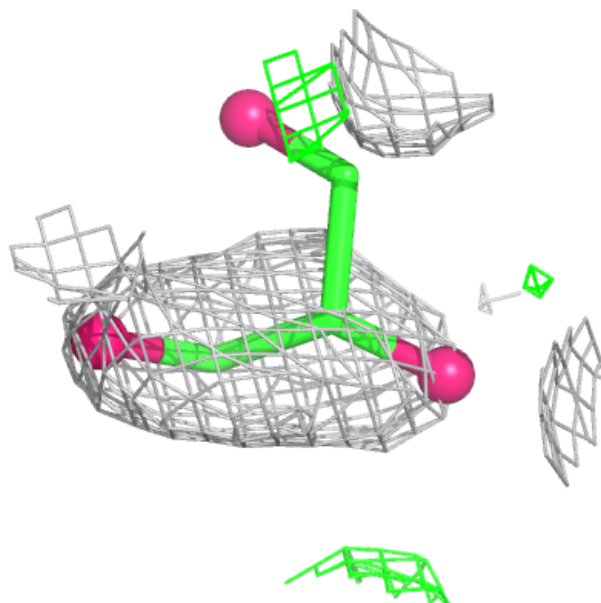
Electron density around GOL A 543 (A):

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



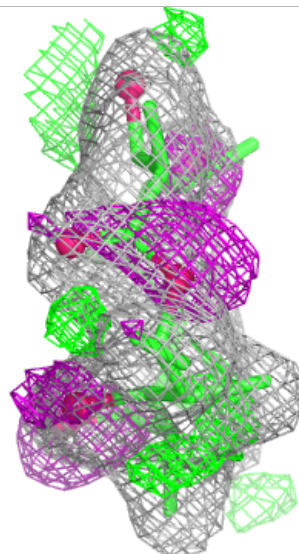
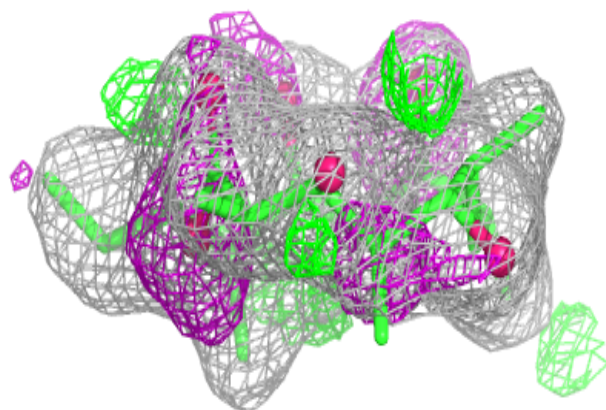
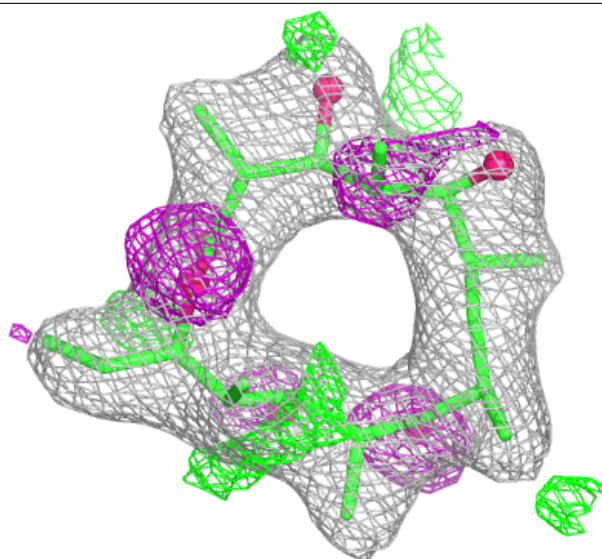
Electron density around GOL A 543 (B):

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



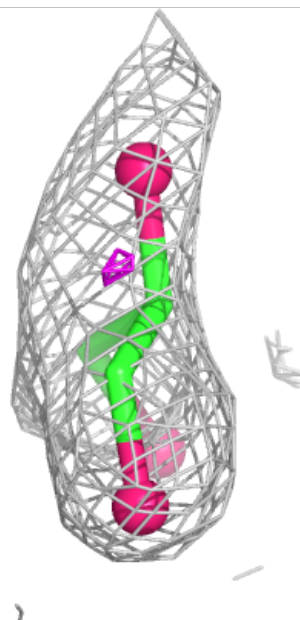
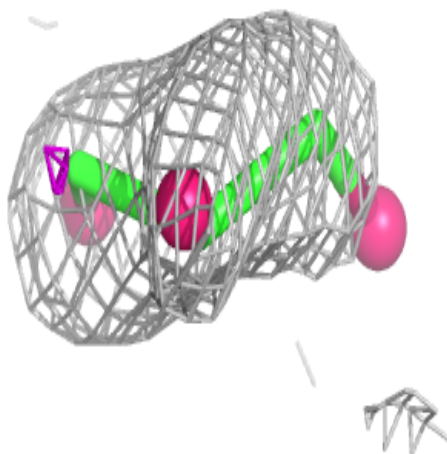
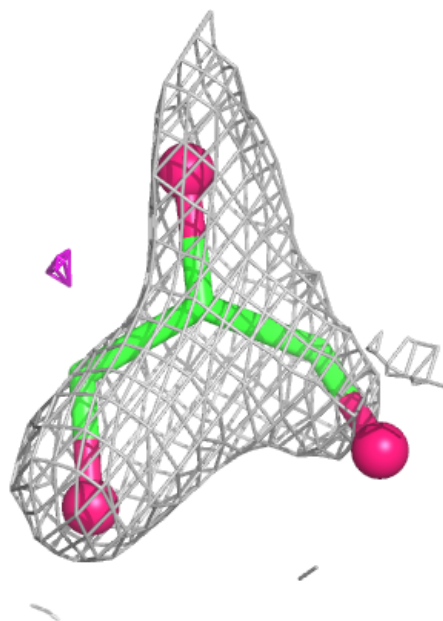
Electron density around DEB C 533:

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



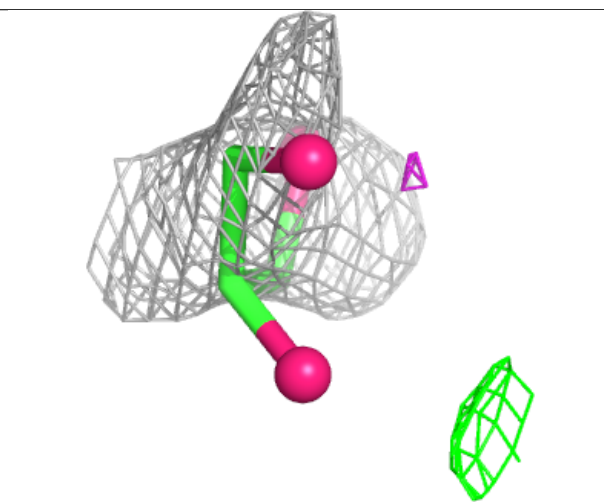
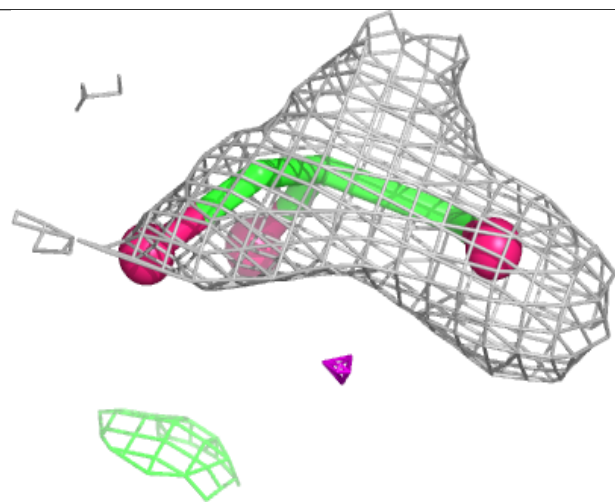
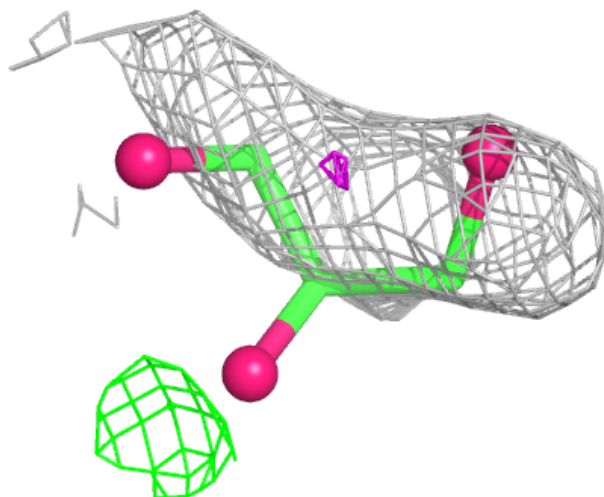
Electron density around GOL E 515 (A):

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



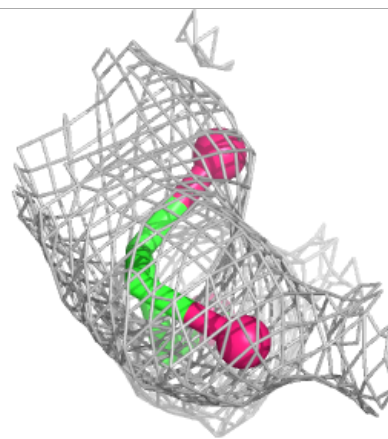
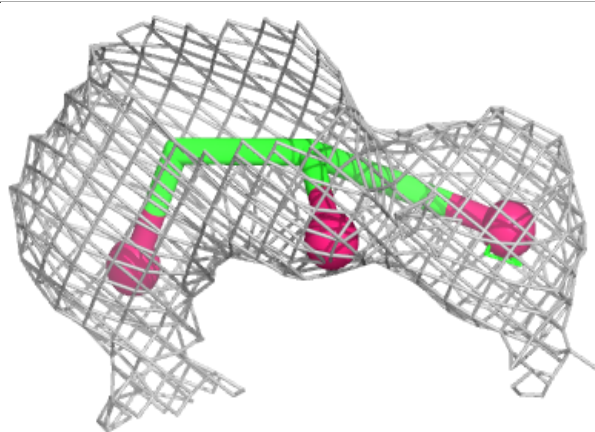
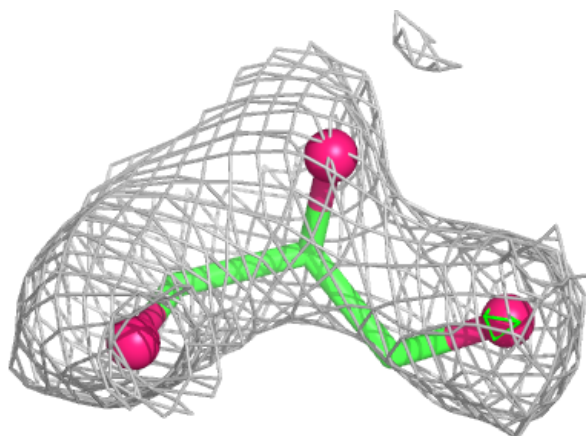
Electron density around GOL E 515 (B):

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



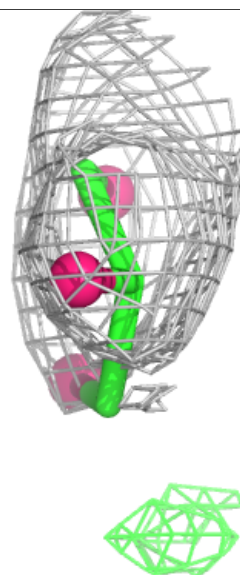
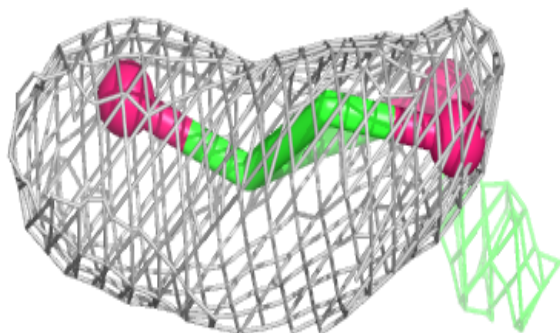
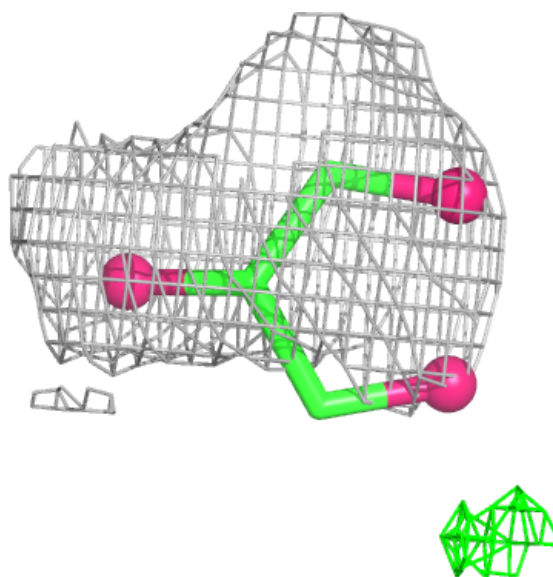
Electron density around GOL C 531 (B):

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



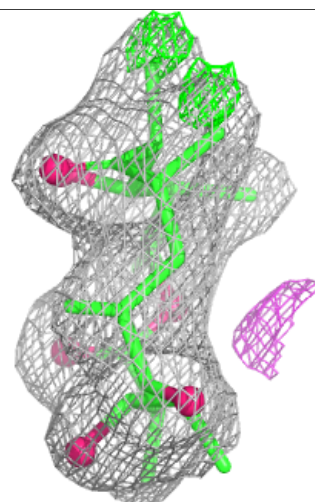
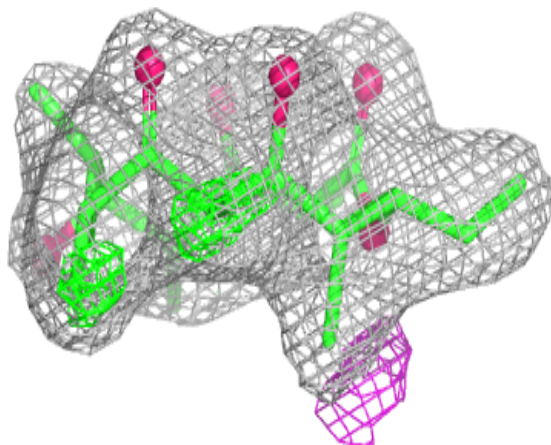
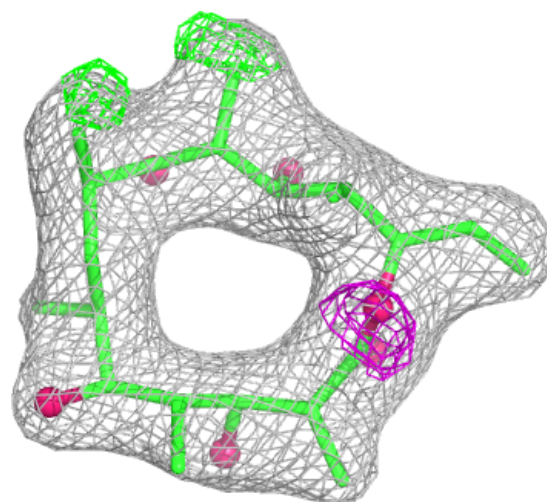
Electron density around GOL C 531 (A):

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



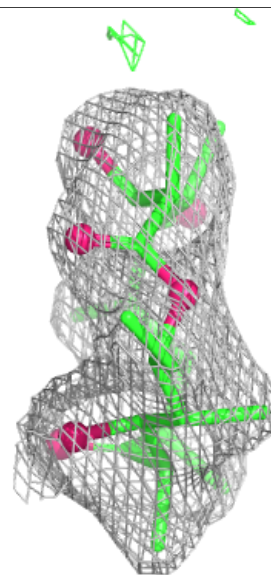
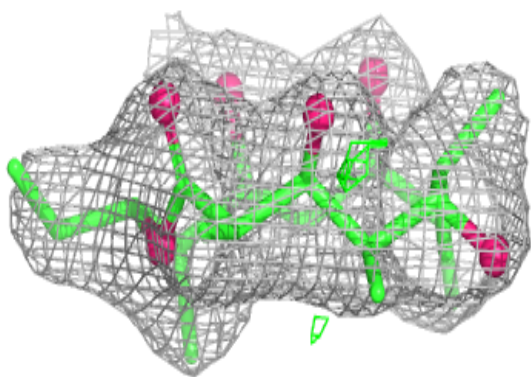
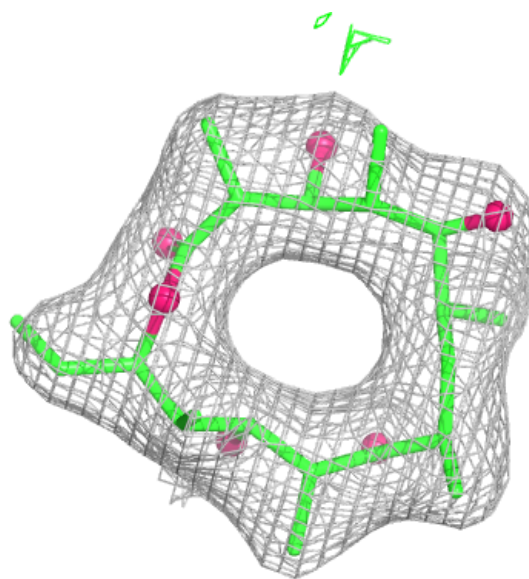
Electron density around DEB E 502:

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



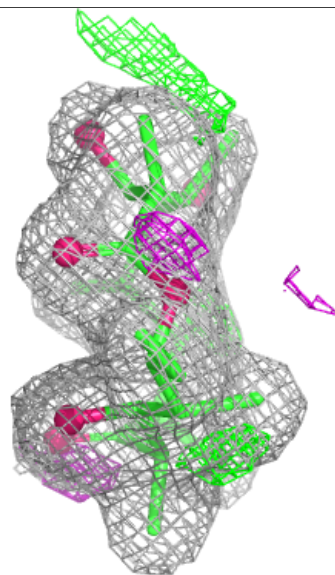
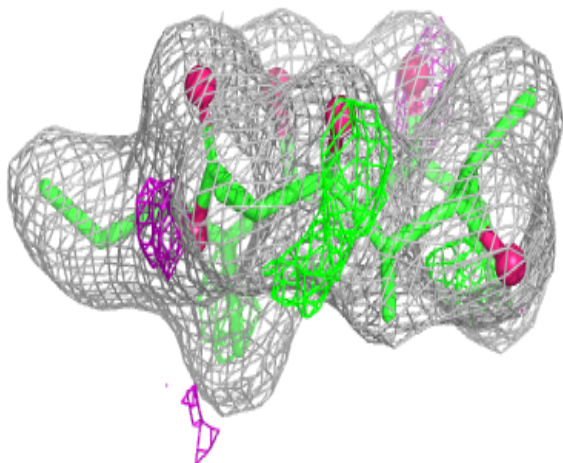
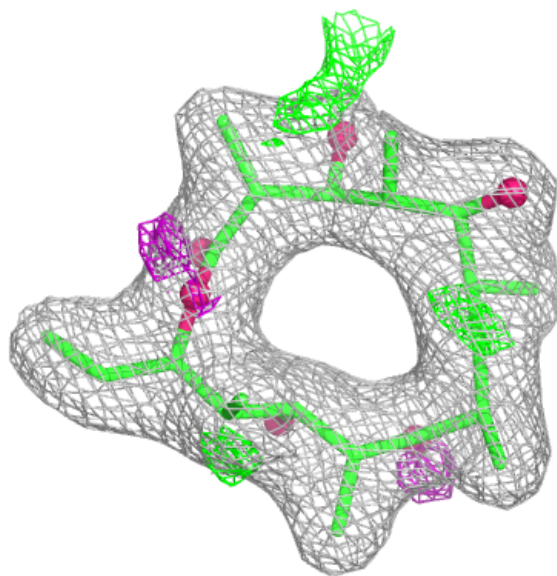
Electron density around DEB F 502:

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



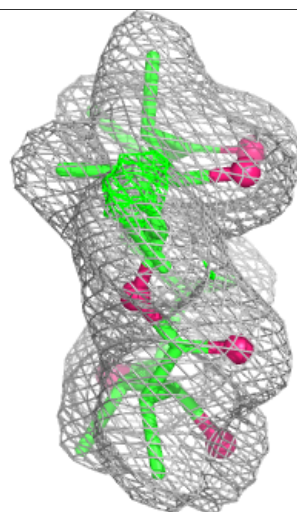
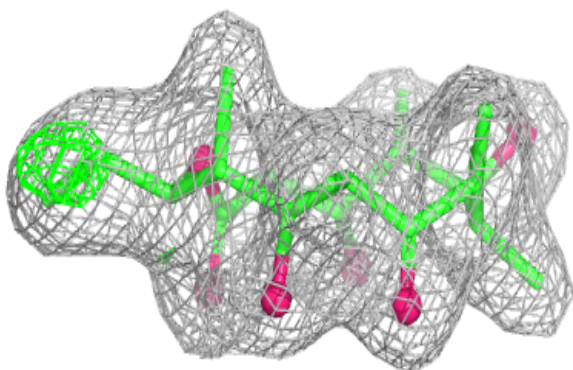
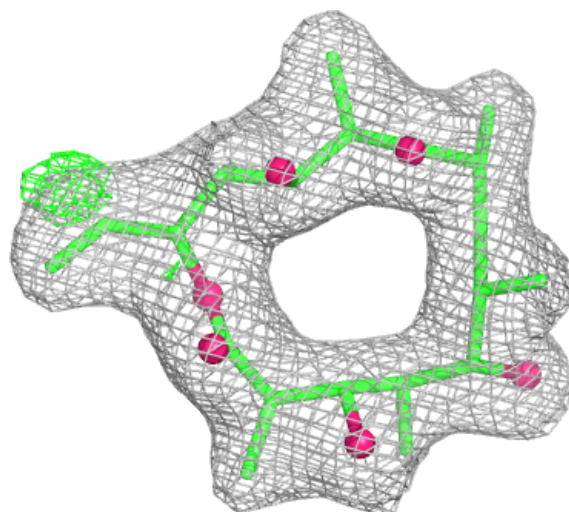
Electron density around DEB A 502:

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



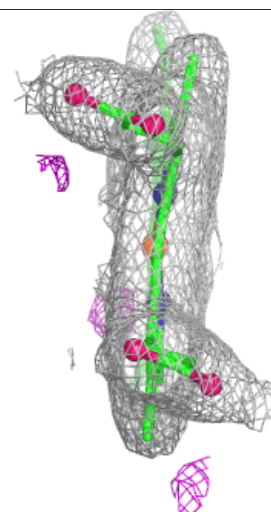
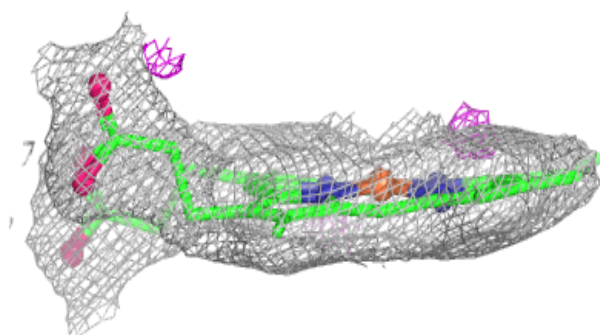
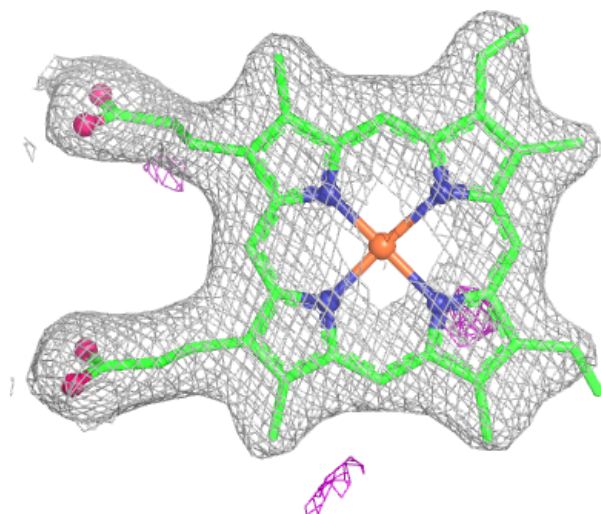
Electron density around DEB B 502:

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



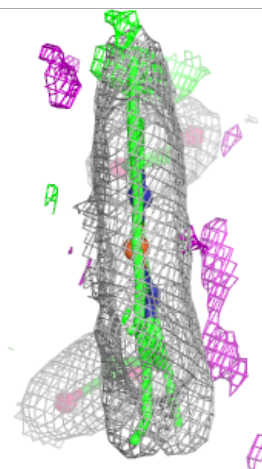
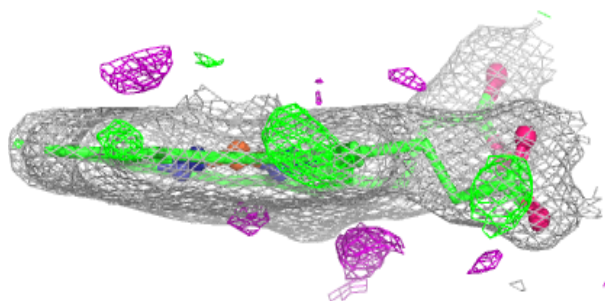
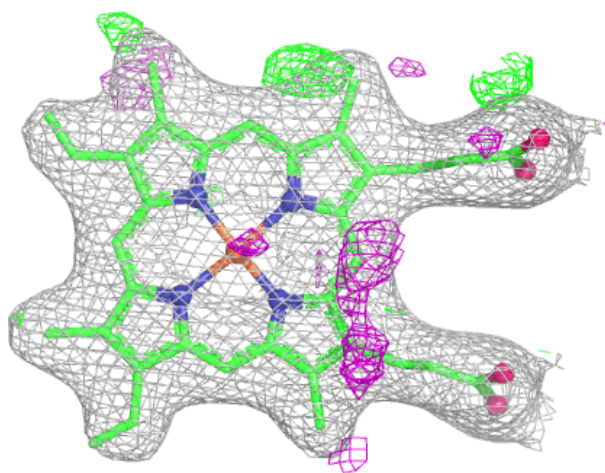
Electron density around HEM F 501:

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



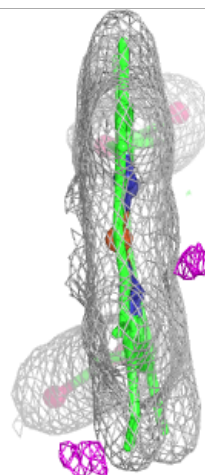
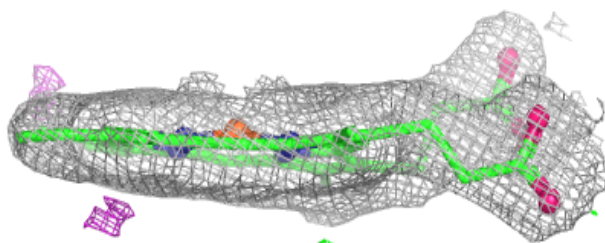
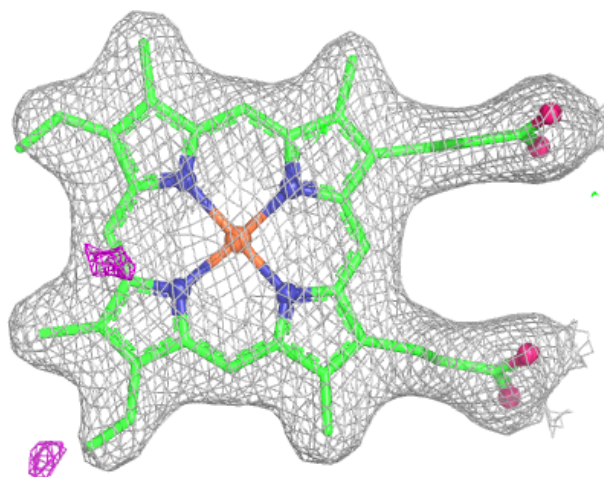
Electron density around HEM D 501:

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



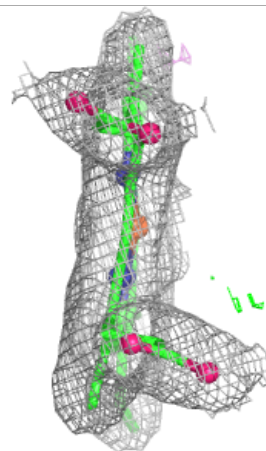
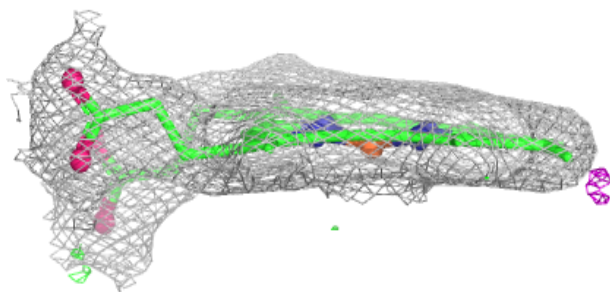
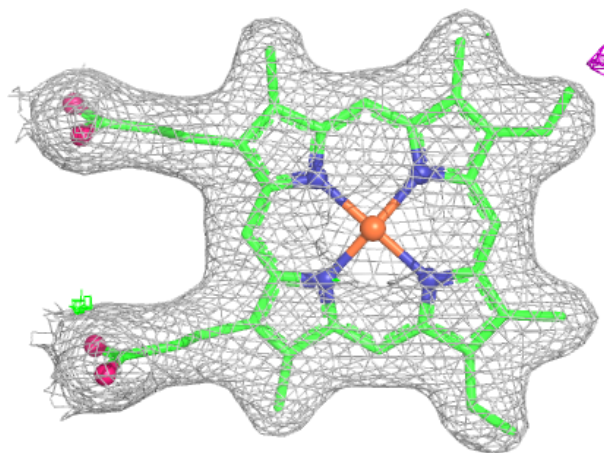
Electron density around HEM E 501:

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



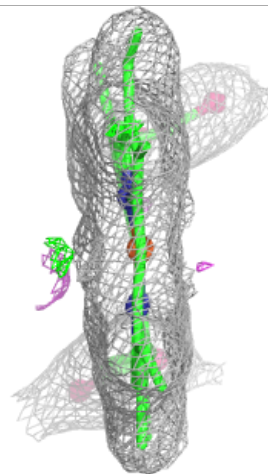
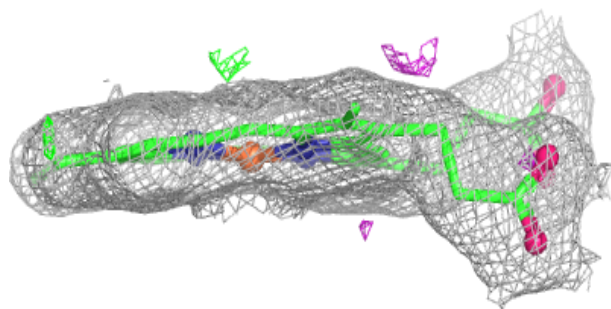
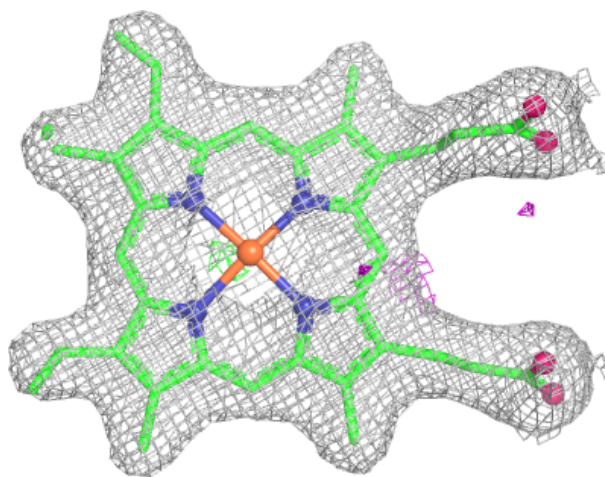
Electron density around HEM B 501:

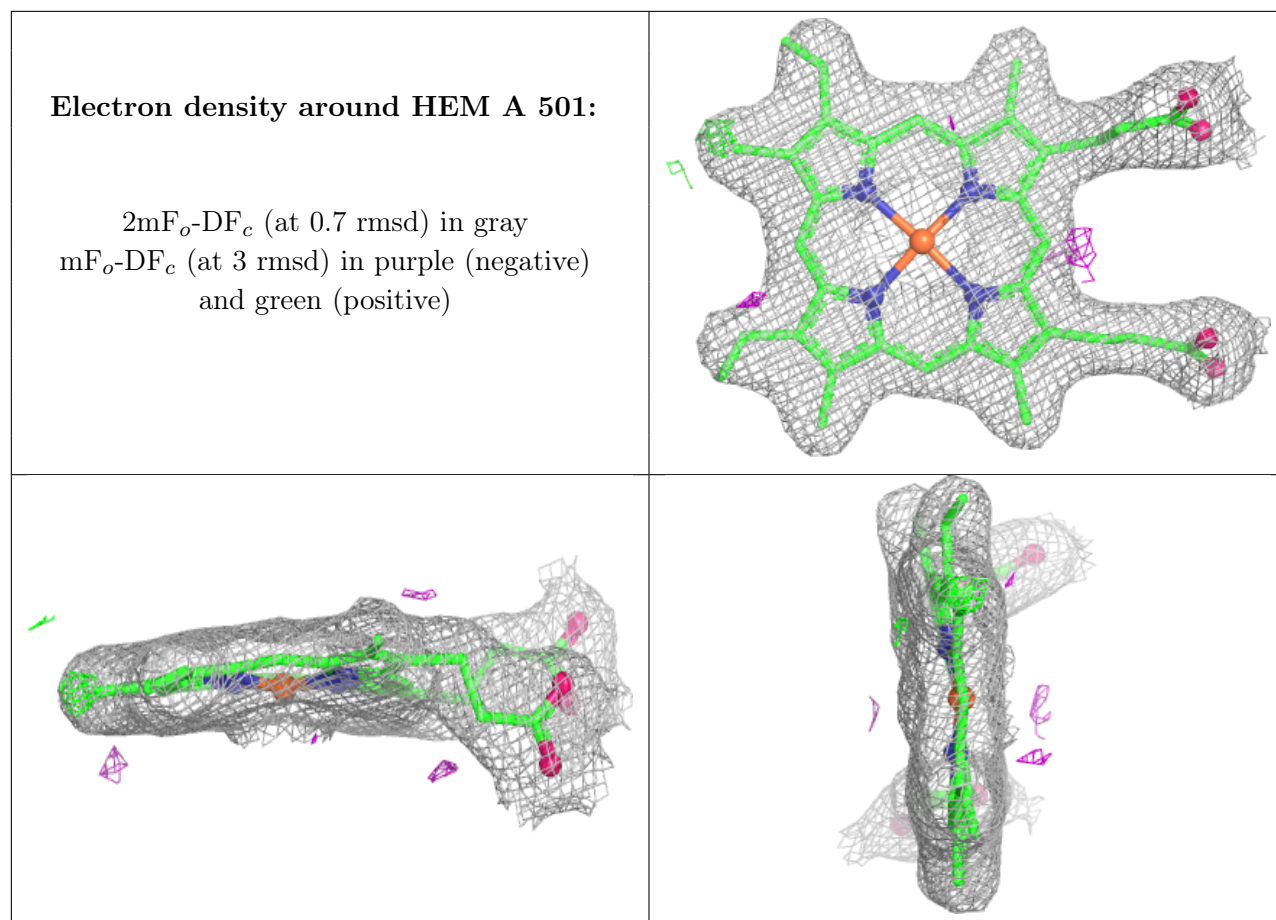
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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.