



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2026 – 12:22 PM JST

PDB ID : 9WTK / pdb\_00009wtk  
Title : Crystal structure of monoalkyl phthalate hydrolase in complex with MBP from Rhodococcus sp. EG-5  
Authors : Aggarwal, S.; Jangid, K.; Singh, S.; Sharma, A.K.; Kumar, P.  
Deposited on : 2025-09-16  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

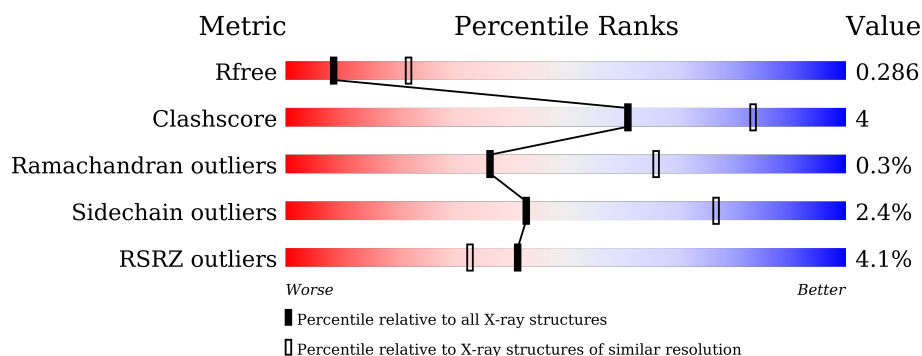
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>
1	B	303	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>..</div> </div> </div>
1	C	303	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
1	D	303	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>.</div> </div> </div>
1	E	303	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
1	F	303	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	303	<div><div></div><div>5%</div><div>78%</div><div>15%</div><div>• 6%</div></div>
1	H	303	<div><div></div><div>5%</div><div>86%</div><div>10%</div><div>• •</div></div>
1	I	303	<div><div></div><div>4%</div><div>84%</div><div>12%</div><div>• •</div></div>
1	J	303	<div><div></div><div>8%</div><div>85%</div><div>11%</div><div>•</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22926 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 Mono-ethylhexylphthalate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2224	1415	382	421	6			
1	B	290	Total	C	N	O	S	0	0	0
			2221	1417	380	418	6			
1	C	289	Total	C	N	O	S	0	0	0
			2209	1408	379	416	6			
1	D	292	Total	C	N	O	S	0	0	0
			2239	1427	385	421	6			
1	E	291	Total	C	N	O	S	0	0	0
			2224	1416	381	421	6			
1	F	289	Total	C	N	O	S	0	0	0
			2213	1410	382	415	6			
1	G	285	Total	C	N	O	S	0	0	0
			2171	1383	373	409	6			
1	H	293	Total	C	N	O	S	0	0	0
			2242	1428	383	425	6			
1	I	293	Total	C	N	O	S	0	0	0
			2244	1430	386	422	6			
1	J	292	Total	C	N	O	S	0	0	0
			2234	1423	382	423	6			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

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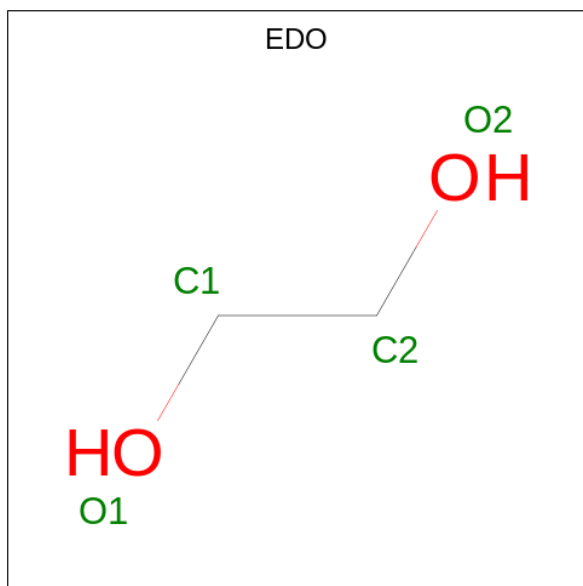
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total C O 7 4 3	0	0
2	I	1	Total C O 7 4 3	0	0
2	I	1	Total C O 7 4 3	0	0
2	I	1	Total C O 7 4 3	0	0
2	J	1	Total C O 7 4 3	0	0
2	J	1	Total C O 7 4 3	0	0
2	J	1	Total C O 7 4 3	0	0
2	J	1	Total C O 7 4 3	0	0
2	J	1	Total C O 7 4 3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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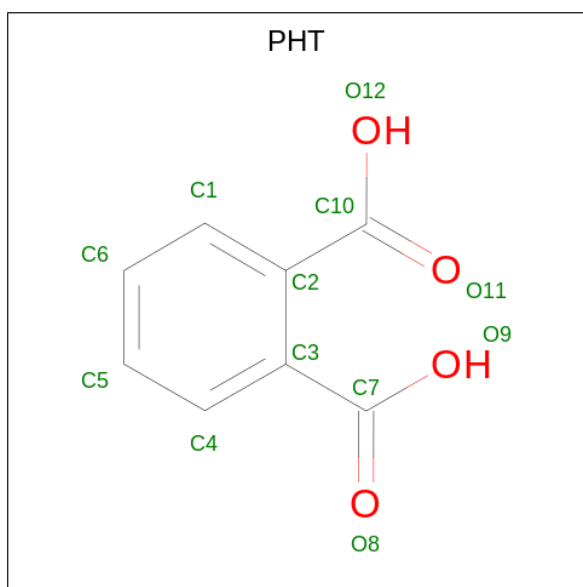
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0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

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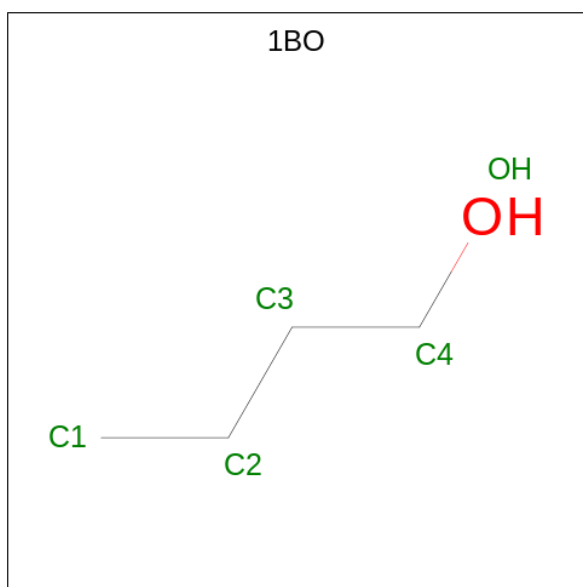
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHTHALIC ACID (CCD ID: PHT) (formula: C<sub>8</sub>H<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



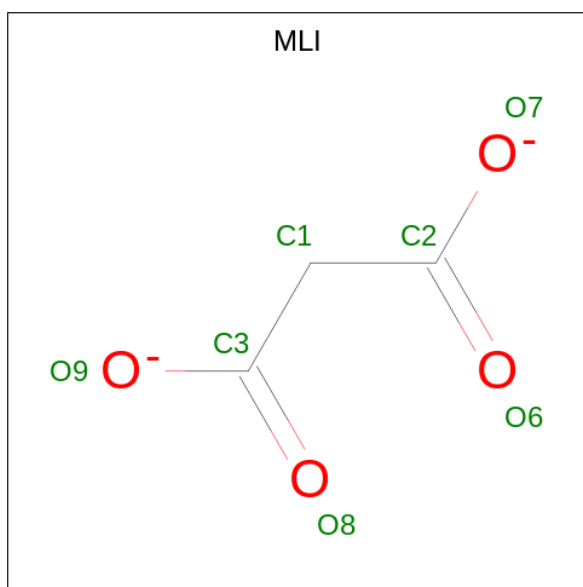
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	8	4		
4	B	1	Total	C	O	0	0
			12	8	4		
4	C	1	Total	C	O	0	0
			12	8	4		
4	D	1	Total	C	O	0	0
			12	8	4		
4	E	1	Total	C	O	0	0
			12	8	4		
4	F	1	Total	C	O	0	0
			12	8	4		
4	G	1	Total	C	O	0	0
			12	8	4		
4	H	1	Total	C	O	0	0
			12	8	4		
4	I	1	Total	C	O	0	0
			12	8	4		
4	J	1	Total	C	O	0	0
			12	8	4		

- Molecule 5 is 1-BUTANOL (CCD ID: 1BO) (formula: C<sub>4</sub>H<sub>10</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	4	1		
5	B	1	Total	C	O	0	0
			5	4	1		
5	D	1	Total	C	O	0	0
			5	4	1		

- Molecule 6 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total	C	O	0	0
			7	3	4		

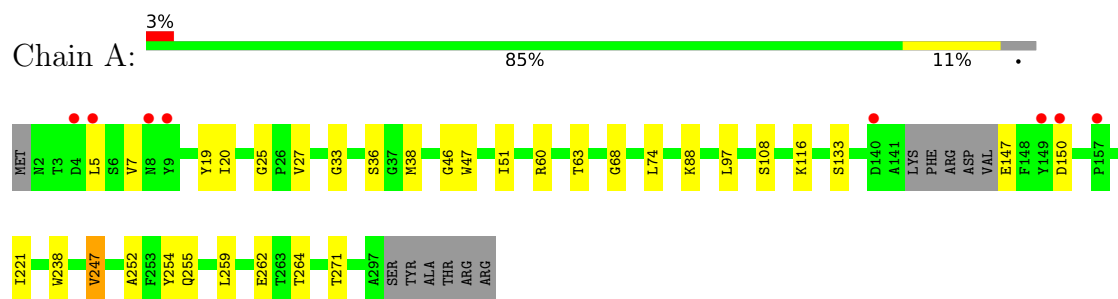
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		
7	F	1	Total	O	0	0
			1	1		
7	G	1	Total	O	0	0
			1	1		
7	H	1	Total	O	0	0
			1	1		

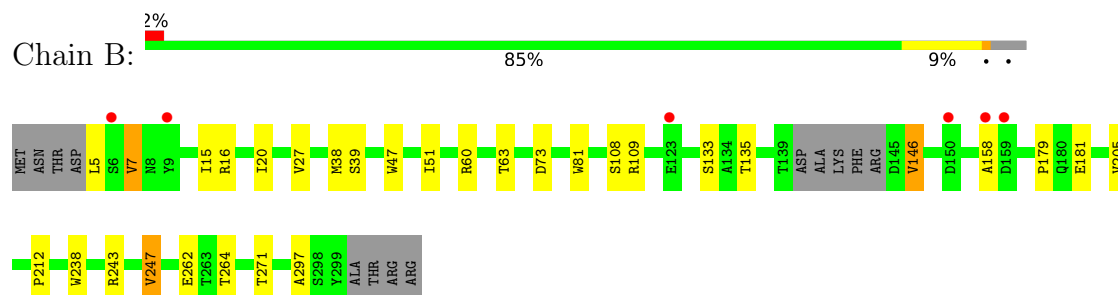
### 3 Residue-property plots [i](#)

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.

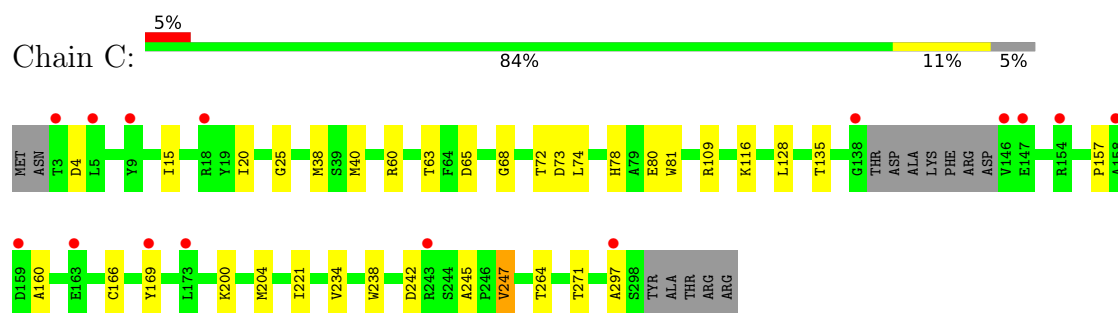
#### • Molecule 1: Mono-ethylhexylphthalate hydrolase



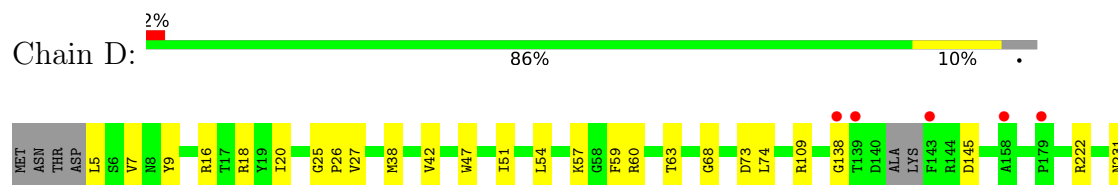
#### • Molecule 1: Mono-ethylhexylphthalate hydrolase



#### • Molecule 1: Mono-ethylhexylphthalate hydrolase

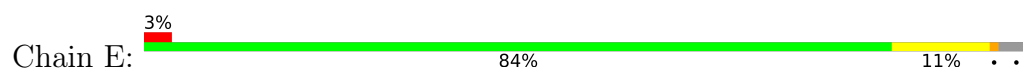


#### • Molecule 1: Mono-ethylhexylphthalate hydrolase

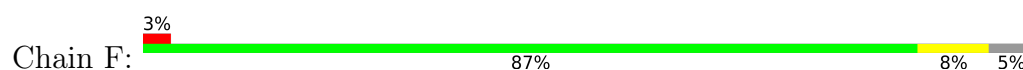




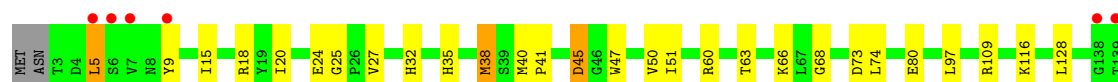
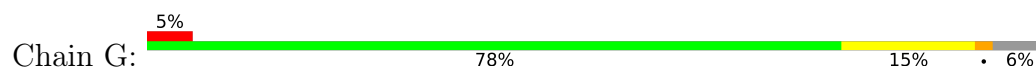
• Molecule 1: Mono-ethylhexylphthalate hydrolase



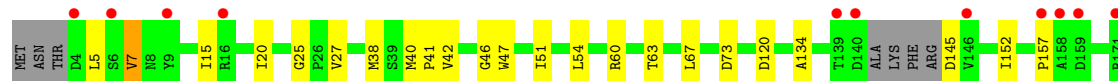
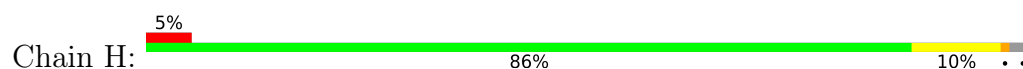
• Molecule 1: Mono-ethylhexylphthalate hydrolase



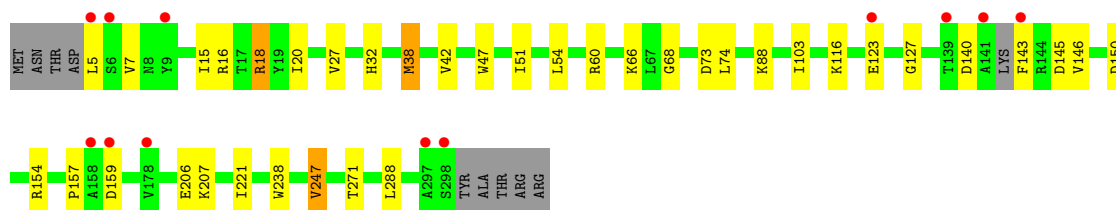
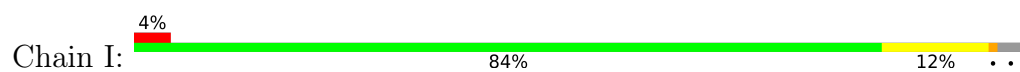
• Molecule 1: Mono-ethylhexylphthalate hydrolase



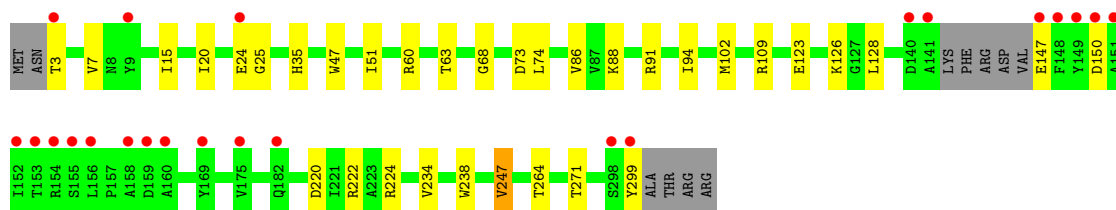
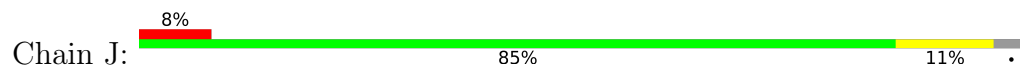
• Molecule 1: Mono-ethylhexylphthalate hydrolase



• Molecule 1: Mono-ethylhexylphthalate hydrolase



- Molecule 1: Mono-ethylhexylphthalate hydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.31Å 244.89Å 192.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.29 – 2.80 24.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.29-2.80) 99.7 (24.29-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.257 , 0.286 0.257 , 0.286	Depositor DCC
$R_{free}$ test set	4988 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	22926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, PEG, 1BO, EDO, PHT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.10	0/2273	0.30	0/3089
1	B	0.11	0/2271	0.31	0/3086
1	C	0.14	0/2258	0.34	0/3068
1	D	0.10	0/2289	0.28	0/3109
1	E	0.10	0/2273	0.30	0/3089
1	F	0.14	0/2262	0.32	0/3072
1	G	0.11	0/2219	0.33	0/3014
1	H	0.11	0/2292	0.30	0/3115
1	I	0.11	0/2294	0.31	0/3116
1	J	0.10	0/2284	0.29	0/3104
All	All	0.11	0/22715	0.31	0/30862

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2224	0	2194	20	0
1	B	2221	0	2195	17	0
1	C	2209	0	2186	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2239	0	2212	19	0
1	E	2224	0	2197	21	0
1	F	2213	0	2192	13	0
1	G	2171	0	2151	30	0
1	H	2242	0	2208	19	0
1	I	2244	0	2217	21	0
1	J	2234	0	2202	19	0
2	A	42	0	60	5	0
2	B	14	0	20	1	0
2	C	21	0	30	2	0
2	D	49	0	70	1	0
2	E	49	0	70	5	0
2	F	35	0	50	2	0
2	G	28	0	40	4	0
2	H	7	0	10	1	0
2	I	28	0	40	2	0
2	J	35	0	50	3	0
3	A	16	0	24	1	0
3	B	52	0	78	3	0
3	C	20	0	30	1	0
3	D	24	0	36	0	0
3	E	16	0	24	3	0
3	F	28	0	42	1	0
3	G	32	0	48	1	0
3	H	20	0	30	3	0
3	I	16	0	24	1	0
3	J	20	0	30	1	0
4	A	12	0	4	1	0
4	B	12	0	4	2	0
4	C	12	0	4	0	0
4	D	12	0	4	1	0
4	E	12	0	4	1	0
4	F	12	0	4	0	0
4	G	12	0	4	1	0
4	H	12	0	4	1	0
4	I	12	0	4	1	0
4	J	12	0	4	0	0
5	A	5	0	10	1	0
5	B	5	0	10	1	0
5	D	5	0	10	1	0
6	F	7	0	2	0	0
6	J	7	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
All	All	22926	0	22834	193	0

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

All (193) 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:I:145:ASP:HB3	4:I:405:PHT:H5	1.42	1.02
1:C:40:MET:HE1	1:C:166:CYS:HA	1.60	0.80
1:C:40:MET:HE3	1:C:169:TYR:HB2	1.68	0.76
1:G:40:MET:HE1	1:G:166:CYS:HA	1.68	0.75
1:H:5:LEU:HG	1:H:7:VAL:HG22	1.73	0.70
1:G:40:MET:HE3	1:G:169:TYR:HB2	1.74	0.69
1:A:46:GLY:HA3	3:A:403:EDO:H11	1.75	0.68
1:G:156:LEU:HD13	1:G:165:ILE:HD13	1.74	0.68
1:B:262:GLU:H	3:B:406:EDO:H12	1.59	0.67
1:G:50:VAL:HG13	1:G:285:VAL:HG22	1.76	0.66
1:D:26:PRO:HD3	1:G:5:LEU:HA	1.78	0.66
1:E:215:GLN:HE22	2:E:409:PEG:H42	1.61	0.65
1:D:231:ASN:HA	2:D:404:PEG:H32	1.79	0.64
1:J:222:ARG:HH22	3:J:412:EDO:H22	1.61	0.64
1:I:38:MET:HG2	2:I:403:PEG:H22	1.80	0.63
1:F:144:ARG:HD2	1:F:147:GLU:HG3	1.80	0.63
1:E:176:THR:HG22	1:E:177:PRO:HD2	1.80	0.62
1:B:5:LEU:HB3	1:B:7:VAL:HG22	1.81	0.61
1:F:286:ARG:NE	1:G:294:ARG:HD3	2.14	0.61
1:F:86:VAL:HG21	3:F:413:EDO:H11	1.84	0.60
1:B:212:PRO:HG3	2:B:403:PEG:H22	1.83	0.59
1:I:146:VAL:HB	2:I:403:PEG:H31	1.83	0.59
1:D:238:TRP:CD1	1:D:247:VAL:HG23	2.38	0.59
1:A:262:GLU:HB3	3:B:409:EDO:H21	1.85	0.58
1:J:109:ARG:HB3	2:J:408:PEG:H11	1.84	0.58
1:J:7:VAL:HG12	1:J:20:ILE:HG12	1.86	0.58
1:E:294:ARG:HH11	2:E:408:PEG:H22	1.68	0.57
1:B:238:TRP:CD1	1:B:247:VAL:HG23	2.38	0.57
1:E:7:VAL:HG12	1:E:20:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG12	1:A:20:ILE:HG12	1.85	0.56
1:C:25:GLY:H	1:C:60:ARG:HB2	1.70	0.56
1:D:5:LEU:HG	1:D:7:VAL:HG13	1.88	0.56
1:E:146:VAL:N	3:E:411:EDO:HO1	2.03	0.56
1:G:35:HIS:HD2	1:G:109:ARG:HE	1.53	0.56
1:D:25:GLY:H	1:D:60:ARG:HB2	1.70	0.56
1:F:36:SER:HB3	2:F:406:PEG:H12	1.88	0.56
1:J:15:ILE:HG23	1:J:73:ASP:HB2	1.88	0.56
2:E:405:PEG:H42	1:H:286:ARG:HD2	1.87	0.55
1:B:108:SER:HA	1:B:133:SER:HA	1.87	0.55
1:D:138:GLY:HA2	1:D:222:ARG:NH2	2.22	0.55
1:I:5:LEU:HD23	1:I:20:ILE:HG21	1.87	0.55
1:J:238:TRP:CD1	1:J:247:VAL:HG23	2.41	0.55
1:G:97:LEU:HD22	2:G:410:PEG:H41	1.88	0.54
1:I:206:GLU:HG2	1:I:207:LYS:HD2	1.89	0.54
1:C:20:ILE:HB	1:C:63:THR:HG22	1.90	0.54
1:G:15:ILE:HG23	1:G:73:ASP:HB2	1.88	0.54
1:A:27:VAL:HG22	1:A:60:ARG:HD3	1.89	0.54
1:J:35:HIS:HA	2:J:408:PEG:H41	1.90	0.54
1:C:78:HIS:HE1	1:C:204:MET:HE2	1.73	0.54
1:B:16:ARG:HD3	1:B:73:ASP:OD2	2.08	0.53
1:G:238:TRP:CD1	1:G:247:VAL:HG23	2.43	0.53
1:A:238:TRP:CD1	1:A:247:VAL:HG23	2.44	0.53
1:E:238:TRP:CD1	1:E:247:VAL:HG23	2.43	0.53
1:H:120:ASP:HB3	2:H:404:PEG:H32	1.91	0.53
1:G:80:GLU:HB3	2:G:409:PEG:H12	1.90	0.52
1:H:238:TRP:CD1	1:H:247:VAL:HG23	2.44	0.52
1:F:25:GLY:H	1:F:60:ARG:HB2	1.73	0.52
1:E:139:THR:HG22	1:E:140:ASP:H	1.75	0.51
1:J:20:ILE:HB	1:J:63:THR:HG22	1.93	0.51
1:D:16:ARG:HD3	1:D:73:ASP:OD2	2.11	0.51
1:J:25:GLY:H	1:J:60:ARG:HB2	1.76	0.51
1:A:147:GLU:HB2	1:A:150:ASP:HB2	1.92	0.51
1:D:9:TYR:CZ	1:D:18:ARG:HG3	2.45	0.51
1:A:108:SER:HA	1:A:133:SER:HA	1.92	0.50
1:I:238:TRP:CD1	1:I:247:VAL:HG23	2.46	0.50
1:H:27:VAL:HG22	1:H:60:ARG:HD3	1.93	0.50
1:H:40:MET:SD	1:H:41:PRO:HD2	2.52	0.50
1:G:27:VAL:HG22	1:G:60:ARG:HD3	1.94	0.50
1:J:88:LYS:HA	1:J:91:ARG:HH11	1.77	0.50
1:C:157:PRO:HG2	1:C:160:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:HIS:HB2	3:I:401:EDO:H12	1.94	0.50
1:F:27:VAL:HG22	1:F:60:ARG:HD3	1.94	0.49
1:G:20:ILE:HB	1:G:63:THR:HG22	1.95	0.49
1:E:15:ILE:HG23	1:E:73:ASP:HB2	1.93	0.49
1:H:47:TRP:O	1:H:51:ILE:HG13	2.12	0.49
1:D:59:PHE:CZ	2:G:401:PEG:H32	2.48	0.49
1:A:254:TYR:CE1	1:A:264:THR:HG22	2.48	0.49
1:G:140:ASP:HA	1:G:249:LEU:HD11	1.94	0.49
1:I:116:LYS:HD3	1:I:221:ILE:HD11	1.94	0.49
1:H:46:GLY:HA3	3:H:402:EDO:H22	1.96	0.48
1:G:116:LYS:HD3	1:G:221:ILE:HD11	1.95	0.48
1:F:20:ILE:HB	1:F:63:THR:HG22	1.96	0.48
1:F:30:LEU:HD23	1:F:105:VAL:HG11	1.95	0.48
1:J:47:TRP:O	1:J:51:ILE:HG13	2.13	0.48
1:A:116:LYS:HD3	1:A:221:ILE:HD11	1.96	0.48
1:E:128:LEU:HB3	1:E:234:VAL:HG22	1.96	0.48
1:A:20:ILE:HB	1:A:63:THR:HG22	1.96	0.48
1:C:15:ILE:HG23	1:C:73:ASP:HB2	1.96	0.48
1:D:26:PRO:HG3	1:G:5:LEU:HD23	1.95	0.48
1:D:109:ARG:HG3	4:D:406:PHT:O11	2.14	0.48
1:J:94:ILE:HG12	1:J:102:MET:HE1	1.96	0.48
2:A:409:PEG:H31	1:H:152:ILE:HA	1.96	0.47
1:B:27:VAL:HG22	1:B:60:ARG:HD3	1.95	0.47
1:A:88:LYS:HE3	1:H:157:PRO:HA	1.96	0.47
1:I:16:ARG:HD3	1:I:73:ASP:OD2	2.14	0.47
1:J:147:GLU:HG2	1:J:150:ASP:HB2	1.97	0.47
1:D:47:TRP:O	1:D:51:ILE:HG13	2.14	0.47
1:G:9:TYR:CZ	1:G:18:ARG:HG3	2.50	0.47
1:H:262:GLU:HB2	3:H:406:EDO:H11	1.95	0.47
1:E:88:LYS:HE2	2:E:402:PEG:H11	1.96	0.47
1:A:25:GLY:H	1:A:60:ARG:HB2	1.81	0.46
1:C:68:GLY:HA2	1:C:74:LEU:HA	1.98	0.46
1:C:128:LEU:HB3	1:C:234:VAL:HG22	1.97	0.46
1:I:15:ILE:HG23	1:I:73:ASP:HB2	1.97	0.46
1:A:33:GLY:HA3	1:A:108:SER:OG	2.15	0.46
1:E:20:ILE:HB	1:E:63:THR:HG22	1.98	0.46
1:H:25:GLY:H	1:H:60:ARG:HB2	1.80	0.46
1:A:47:TRP:O	1:A:51:ILE:HG13	2.15	0.45
1:H:134:ALA:HB3	4:H:405:PHT:H4	1.98	0.45
1:B:47:TRP:O	1:B:51:ILE:HG13	2.15	0.45
1:A:36:SER:N	2:A:410:PEG:H12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:128:LEU:HB3	1:J:234:VAL:HG22	1.97	0.45
1:F:116:LYS:HD3	1:F:221:ILE:HD11	1.99	0.45
3:C:409:EDO:H11	1:D:252:ALA:HB2	1.98	0.45
1:D:54:LEU:HD11	1:D:288:LEU:HD23	1.99	0.45
1:G:254:TYR:CE1	1:G:264:THR:HG22	2.52	0.45
1:D:20:ILE:HB	1:D:63:THR:HG22	1.98	0.45
1:A:68:GLY:HA2	1:A:74:LEU:HA	1.98	0.44
1:B:20:ILE:HB	1:B:63:THR:HG22	1.98	0.44
1:G:116:LYS:HZ3	3:G:404:EDO:H12	1.82	0.44
1:E:25:GLY:H	1:E:60:ARG:HB2	1.83	0.44
1:H:67:LEU:HG	3:H:403:EDO:H21	1.99	0.44
1:E:150:ASP:O	1:E:154:ARG:HG2	2.17	0.44
1:F:54:LEU:HD11	1:F:288:LEU:HD23	1.99	0.44
1:F:240:ARG:O	1:F:247:VAL:HG21	2.18	0.44
1:C:238:TRP:CD1	1:C:247:VAL:HG23	2.53	0.43
1:F:259:LEU:HD21	1:G:247:VAL:HG11	2.00	0.43
1:H:20:ILE:HB	1:H:63:THR:HG22	2.00	0.43
1:F:12:VAL:HG12	2:F:407:PEG:H11	2.00	0.43
1:C:109:ARG:HG2	1:C:135:THR:OG1	2.18	0.43
1:B:15:ILE:HG23	1:B:73:ASP:HB2	2.00	0.43
1:B:179:PRO:HB2	1:B:181:GLU:HG2	2.01	0.43
1:G:45:ASP:OD1	1:G:45:ASP:N	2.51	0.43
1:B:38:MET:HA	5:B:405:1BO:H32	2.01	0.43
1:G:38:MET:SD	4:G:407:PHT:H1	2.58	0.43
1:I:68:GLY:HA2	1:I:74:LEU:HA	2.01	0.43
1:A:36:SER:H	2:A:410:PEG:H12	1.84	0.43
1:B:38:MET:SD	4:B:404:PHT:H1	2.58	0.42
1:G:25:GLY:H	1:G:60:ARG:HB2	1.85	0.42
1:C:81:TRP:CE3	2:C:405:PEG:H32	2.54	0.42
1:G:5:LEU:H	1:G:5:LEU:HG	1.57	0.42
1:C:65:ASP:HB2	1:C:72:THR:OG1	2.19	0.42
1:C:80:GLU:HB3	2:C:406:PEG:H42	2.01	0.42
1:D:27:VAL:HG22	1:D:60:ARG:HD3	2.01	0.42
1:E:262:GLU:HB2	3:E:401:EDO:H11	2.00	0.42
1:J:220:ASP:O	1:J:224:ARG:HG3	2.19	0.42
1:I:54:LEU:HD11	1:I:288:LEU:HD23	2.00	0.42
1:J:126:LYS:HE3	1:J:299:TYR:HB3	2.01	0.42
1:I:18:ARG:C	1:I:18:ARG:HE	2.26	0.42
1:J:68:GLY:HA2	1:J:74:LEU:HA	2.00	0.42
1:D:68:GLY:HA2	1:D:74:LEU:HD23	2.01	0.42
1:G:47:TRP:O	1:G:51:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:HIS:CE1	1:I:66:LYS:HE2	2.55	0.42
1:B:243:ARG:H	3:B:411:EDO:H21	1.85	0.42
1:C:200:LYS:HE3	1:C:200:LYS:HB3	1.57	0.42
1:A:19:TYR:CE2	1:A:97:LEU:HD21	2.55	0.41
1:G:32:HIS:CE1	1:G:66:LYS:HE2	2.55	0.41
1:H:15:ILE:HG23	1:H:73:ASP:HB2	2.02	0.41
1:I:157:PRO:C	1:I:159:ASP:H	2.28	0.41
1:G:128:LEU:HB3	1:G:234:VAL:HG22	2.02	0.41
1:B:109:ARG:HG2	1:B:135:THR:OG1	2.19	0.41
1:A:255:GLN:O	1:A:259:LEU:HD13	2.19	0.41
1:C:242:ASP:HB3	1:C:245:ALA:O	2.20	0.41
1:G:220:ASP:O	1:G:224:ARG:HG3	2.20	0.41
1:J:68:GLY:HA2	1:J:74:LEU:HD23	2.02	0.41
1:B:81:TRP:CD2	1:B:205:VAL:HG21	2.55	0.41
1:J:123:GLU:H	1:J:123:GLU:CD	2.29	0.41
2:A:410:PEG:H21	2:A:410:PEG:H41	1.76	0.41
1:C:116:LYS:HD3	1:C:221:ILE:HD11	2.02	0.41
1:E:27:VAL:HG22	1:E:60:ARG:HD3	2.02	0.41
1:E:47:TRP:O	1:E:51:ILE:HG13	2.21	0.41
1:A:252:ALA:HB2	2:A:401:PEG:H22	2.02	0.41
1:G:40:MET:SD	1:G:41:PRO:HD2	2.61	0.41
1:H:200:LYS:HB3	1:H:200:LYS:HE3	1.81	0.41
1:B:146:VAL:HG13	4:B:404:PHT:H6	2.03	0.41
1:D:42:VAL:HG21	5:D:407:1BO:H31	2.03	0.41
1:E:65:ASP:HB2	1:E:72:THR:OG1	2.21	0.41
4:E:404:PHT:H6	3:E:411:EDO:O1	2.21	0.41
1:G:68:GLY:HA2	1:G:74:LEU:HD23	2.01	0.41
1:H:54:LEU:HD11	1:H:288:LEU:HD23	2.02	0.41
1:I:27:VAL:HG22	1:I:60:ARG:HD3	2.01	0.41
1:I:47:TRP:O	1:I:51:ILE:HG12	2.20	0.41
1:I:123:GLU:H	1:I:123:GLU:CD	2.28	0.41
1:E:57:LYS:HD3	2:E:403:PEG:H41	2.03	0.41
1:D:57:LYS:O	2:G:401:PEG:H31	2.20	0.40
1:I:140:ASP:O	1:I:143:PHE:HA	2.22	0.40
1:I:150:ASP:O	1:I:154:ARG:HG3	2.21	0.40
1:E:134:ALA:HB2	1:E:245:ALA:HB2	2.03	0.40
1:J:86:VAL:HG11	2:J:408:PEG:H31	2.03	0.40
4:A:405:PHT:H4	5:A:406:1BO:H13	2.03	0.40
1:E:294:ARG:HD3	1:H:286:ARG:HD2	2.03	0.40
1:E:126:LYS:O	1:E:295:ARG:HD3	2.22	0.40
1:I:103:ILE:HD12	1:I:127:GLY:HA3	2.03	0.40



There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/303 (95%)	281 (98%)	5 (2%)	1 (0%)	36	66
1	B	286/303 (94%)	274 (96%)	10 (4%)	2 (1%)	18	47
1	C	285/303 (94%)	277 (97%)	6 (2%)	2 (1%)	18	47
1	D	288/303 (95%)	282 (98%)	6 (2%)	0	100	100
1	E	287/303 (95%)	280 (98%)	6 (2%)	1 (0%)	36	66
1	F	285/303 (94%)	278 (98%)	6 (2%)	1 (0%)	30	60
1	G	281/303 (93%)	273 (97%)	7 (2%)	1 (0%)	30	60
1	H	289/303 (95%)	280 (97%)	9 (3%)	0	100	100
1	I	289/303 (95%)	279 (96%)	9 (3%)	1 (0%)	36	66
1	J	288/303 (95%)	281 (98%)	7 (2%)	0	100	100
All	All	2865/3030 (95%)	2785 (97%)	71 (2%)	9 (0%)	36	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	B	158	ALA
1	C	297	ALA
1	G	158	ALA
1	I	7	VAL
1	E	4	ASP
1	C	4	ASP
1	F	297	ALA
1	B	297	ALA

### 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	230/241 (95%)	227 (99%)	3 (1%)	61	86
1	B	230/241 (95%)	224 (97%)	6 (3%)	40	75
1	C	229/241 (95%)	225 (98%)	4 (2%)	53	83
1	D	232/241 (96%)	228 (98%)	4 (2%)	53	83
1	E	231/241 (96%)	226 (98%)	5 (2%)	45	78
1	F	229/241 (95%)	224 (98%)	5 (2%)	45	78
1	G	225/241 (93%)	215 (96%)	10 (4%)	25	59
1	H	232/241 (96%)	224 (97%)	8 (3%)	32	68
1	I	232/241 (96%)	226 (97%)	6 (3%)	40	75
1	J	231/241 (96%)	226 (98%)	5 (2%)	45	78
All	All	2301/2410 (96%)	2245 (98%)	56 (2%)	43	77

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	MET
1	A	247	VAL
1	A	271	THR
1	B	7	VAL
1	B	39	SER
1	B	146	VAL
1	B	247	VAL
1	B	264	THR
1	B	271	THR
1	C	38	MET
1	C	247	VAL
1	C	264	THR
1	C	271	THR
1	D	38	MET
1	D	145	ASP
1	D	247	VAL

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Mol	Chain	Res	Type
1	D	271	THR
1	E	38	MET
1	E	42	VAL
1	E	139	THR
1	E	176	THR
1	E	247	VAL
1	F	18	ARG
1	F	38	MET
1	F	45	ASP
1	F	105	VAL
1	F	271	THR
1	G	5	LEU
1	G	24	GLU
1	G	38	MET
1	G	45	ASP
1	G	140	ASP
1	G	142	LYS
1	G	171	ARG
1	G	247	VAL
1	G	271	THR
1	G	295	ARG
1	H	7	VAL
1	H	38	MET
1	H	42	VAL
1	H	145	ASP
1	H	247	VAL
1	H	264	THR
1	H	271	THR
1	H	295	ARG
1	I	18	ARG
1	I	38	MET
1	I	42	VAL
1	I	88	LYS
1	I	247	VAL
1	I	271	THR
1	J	3	THR
1	J	24	GLU
1	J	247	VAL
1	J	264	THR
1	J	271	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	255	GLN
1	B	8	ASN
1	B	255	GLN
1	C	8	ASN
1	C	22	GLN
1	D	255	GLN
1	E	8	ASN
1	E	180	GLN
1	E	255	GLN
1	F	255	GLN
1	F	267	HIS
1	G	35	HIS
1	G	255	GLN
1	H	255	GLN
1	I	8	ASN
1	J	22	GLN
1	J	255	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

120 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PEG	J	403	-	6,6,6	0.24	0	5,5,5	0.24	0
3	EDO	E	412	-	3,3,3	0.27	0	2,2,2	0.31	0
3	EDO	F	414	-	3,3,3	0.26	0	2,2,2	0.36	0
3	EDO	C	401	-	3,3,3	0.27	0	2,2,2	0.29	0
2	PEG	D	412	-	6,6,6	0.25	0	5,5,5	0.26	0
2	PEG	D	414	-	6,6,6	0.24	0	5,5,5	0.26	0
2	PEG	E	408	-	6,6,6	0.24	0	5,5,5	0.23	0
3	EDO	A	404	-	3,3,3	0.27	0	2,2,2	0.27	0
3	EDO	D	409	-	3,3,3	0.27	0	2,2,2	0.26	0
2	PEG	E	409	-	6,6,6	0.25	0	5,5,5	0.26	0
2	PEG	D	401	-	6,6,6	0.24	0	5,5,5	0.25	0
3	EDO	H	401	-	3,3,3	0.27	0	2,2,2	0.30	0
4	PHT	G	407	-	12,12,12	0.97	0	16,16,16	1.13	1 (6%)
2	PEG	I	407	-	6,6,6	0.23	0	5,5,5	0.26	0
2	PEG	F	408	-	6,6,6	0.25	0	5,5,5	0.23	0
3	EDO	J	411	-	3,3,3	0.27	0	2,2,2	0.29	0
2	PEG	A	411	-	6,6,6	0.24	0	5,5,5	0.27	0
4	PHT	C	403	-	12,12,12	0.95	0	16,16,16	1.35	2 (12%)
2	PEG	J	407	-	6,6,6	0.24	0	5,5,5	0.24	0
3	EDO	G	402	-	3,3,3	0.28	0	2,2,2	0.28	0
3	EDO	B	406	-	3,3,3	0.27	0	2,2,2	0.28	0
4	PHT	B	404	-	12,12,12	0.93	0	16,16,16	1.16	2 (12%)
2	PEG	B	410	-	6,6,6	0.23	0	5,5,5	0.24	0
4	PHT	J	404	-	12,12,12	0.96	0	16,16,16	1.06	2 (12%)
3	EDO	B	417	-	3,3,3	0.27	0	2,2,2	0.29	0
6	MLI	F	405	-	6,6,6	1.64	1 (16%)	7,7,7	1.02	0
2	PEG	G	410	-	6,6,6	0.24	0	5,5,5	0.23	0
3	EDO	I	408	-	3,3,3	0.27	0	2,2,2	0.33	0
2	PEG	B	403	-	6,6,6	0.24	0	5,5,5	0.26	0
2	PEG	I	402	-	6,6,6	0.25	0	5,5,5	0.26	0
3	EDO	A	407	-	3,3,3	0.27	0	2,2,2	0.30	0
6	MLI	J	406	-	6,6,6	1.62	1 (16%)	7,7,7	1.05	0
2	PEG	E	406	-	6,6,6	0.25	0	5,5,5	0.25	0
3	EDO	C	407	-	3,3,3	0.27	0	2,2,2	0.30	0
2	PEG	A	402	-	6,6,6	0.24	0	5,5,5	0.25	0
3	EDO	H	403	-	3,3,3	0.27	0	2,2,2	0.28	0
3	EDO	B	402	-	3,3,3	0.27	0	2,2,2	0.28	0
3	EDO	H	402	-	3,3,3	0.27	0	2,2,2	0.31	0
2	PEG	F	410	-	6,6,6	0.24	0	5,5,5	0.26	0
3	EDO	D	408	-	3,3,3	0.27	0	2,2,2	0.26	0
3	EDO	B	409	-	3,3,3	0.26	0	2,2,2	0.28	0
3	EDO	C	404	-	3,3,3	0.28	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	E	410	-	3,3,3	0.27	0	2,2,2	0.28	0
3	EDO	F	403	-	3,3,3	0.27	0	2,2,2	0.30	0
3	EDO	F	411	-	3,3,3	0.27	0	2,2,2	0.36	0
2	PEG	A	409	-	6,6,6	0.25	0	5,5,5	0.25	0
3	EDO	B	412	-	3,3,3	0.27	0	2,2,2	0.29	0
3	EDO	J	410	-	3,3,3	0.27	0	2,2,2	0.26	0
3	EDO	I	404	-	3,3,3	0.27	0	2,2,2	0.25	0
3	EDO	G	403	-	3,3,3	0.26	0	2,2,2	0.33	0
3	EDO	B	407	-	3,3,3	0.26	0	2,2,2	0.32	0
2	PEG	H	404	-	6,6,6	0.25	0	5,5,5	0.26	0
4	PHT	H	405	-	12,12,12	0.94	0	16,16,16	1.10	2 (12%)
2	PEG	D	402	-	6,6,6	0.24	0	5,5,5	0.25	0
3	EDO	B	416	-	3,3,3	0.27	0	2,2,2	0.28	0
2	PEG	I	406	-	6,6,6	0.24	0	5,5,5	0.24	0
2	PEG	D	411	-	6,6,6	0.25	0	5,5,5	0.25	0
2	PEG	E	407	-	6,6,6	0.24	0	5,5,5	0.22	0
2	PEG	I	403	-	6,6,6	0.25	0	5,5,5	0.37	0
2	PEG	G	401	-	6,6,6	0.25	0	5,5,5	0.34	0
2	PEG	E	405	-	6,6,6	0.24	0	5,5,5	0.20	0
3	EDO	A	403	-	3,3,3	0.26	0	2,2,2	0.34	0
3	EDO	B	411	-	3,3,3	0.26	0	2,2,2	0.27	0
2	PEG	C	405	-	6,6,6	0.24	0	5,5,5	0.23	0
4	PHT	E	404	-	12,12,12	0.93	0	16,16,16	1.09	2 (12%)
2	PEG	C	406	-	6,6,6	0.24	0	5,5,5	0.24	0
2	PEG	A	408	-	6,6,6	0.24	0	5,5,5	0.24	0
2	PEG	C	402	-	6,6,6	0.24	0	5,5,5	0.34	0
3	EDO	B	408	-	3,3,3	0.27	0	2,2,2	0.29	0
3	EDO	C	409	-	3,3,3	0.27	0	2,2,2	0.27	0
3	EDO	D	415	-	3,3,3	0.26	0	2,2,2	0.35	0
3	EDO	H	406	-	3,3,3	0.28	0	2,2,2	0.25	0
4	PHT	A	405	-	12,12,12	0.93	0	16,16,16	1.27	2 (12%)
2	PEG	F	409	-	6,6,6	0.24	0	5,5,5	0.25	0
3	EDO	F	412	-	3,3,3	0.27	0	2,2,2	0.30	0
3	EDO	H	407	-	3,3,3	0.27	0	2,2,2	0.29	0
3	EDO	E	401	-	3,3,3	0.27	0	2,2,2	0.30	0
2	PEG	J	408	-	6,6,6	0.25	0	5,5,5	0.24	0
2	PEG	J	402	-	6,6,6	0.25	0	5,5,5	0.24	0
2	PEG	A	410	-	6,6,6	0.24	0	5,5,5	0.20	0
2	PEG	A	401	-	6,6,6	0.25	0	5,5,5	0.26	0
2	PEG	E	402	-	6,6,6	0.24	0	5,5,5	0.24	0
3	EDO	F	413	-	3,3,3	0.27	0	2,2,2	0.23	0
3	EDO	A	412	-	3,3,3	0.26	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PEG	J	401	-	6,6,6	0.23	0	5,5,5	0.24	0
3	EDO	D	405	-	3,3,3	0.27	0	2,2,2	0.30	0
2	PEG	G	409	-	6,6,6	0.24	0	5,5,5	0.22	0
3	EDO	G	412	-	3,3,3	0.28	0	2,2,2	0.30	0
3	EDO	G	411	-	3,3,3	0.27	0	2,2,2	0.26	0
4	PHT	D	406	-	12,12,12	0.90	0	16,16,16	1.14	2 (12%)
3	EDO	F	404	-	3,3,3	0.27	0	2,2,2	0.26	0
3	EDO	D	403	-	3,3,3	0.27	0	2,2,2	0.29	0
3	EDO	E	411	-	3,3,3	0.25	0	2,2,2	0.40	0
3	EDO	G	405	-	3,3,3	0.27	0	2,2,2	0.30	0
2	PEG	F	406	-	6,6,6	0.24	0	5,5,5	0.25	0
2	PEG	D	413	-	6,6,6	0.24	0	5,5,5	0.25	0
3	EDO	J	405	-	3,3,3	0.26	0	2,2,2	0.30	0
4	PHT	I	405	-	12,12,12	0.95	0	16,16,16	1.19	2 (12%)
3	EDO	B	401	-	3,3,3	0.27	0	2,2,2	0.29	0
2	PEG	D	404	-	6,6,6	0.25	0	5,5,5	0.28	0
3	EDO	G	413	-	3,3,3	0.27	0	2,2,2	0.27	0
2	PEG	F	407	-	6,6,6	0.24	0	5,5,5	0.23	0
3	EDO	D	410	-	3,3,3	0.26	0	2,2,2	0.31	0
3	EDO	C	408	-	3,3,3	0.26	0	2,2,2	0.25	0
3	EDO	B	415	-	3,3,3	0.26	0	2,2,2	0.46	0
4	PHT	F	402	-	12,12,12	0.96	0	16,16,16	1.08	2 (12%)
3	EDO	J	409	-	3,3,3	0.28	0	2,2,2	0.26	0
5	1BO	D	407	-	4,4,4	0.22	0	3,3,3	0.26	0
2	PEG	E	403	-	6,6,6	0.25	0	5,5,5	0.22	0
5	1BO	B	405	-	4,4,4	0.22	0	3,3,3	0.25	0
3	EDO	B	414	-	3,3,3	0.27	0	2,2,2	0.32	0
3	EDO	I	409	-	3,3,3	0.27	0	2,2,2	0.27	0
3	EDO	G	404	-	3,3,3	0.28	0	2,2,2	0.23	0
3	EDO	B	413	-	3,3,3	0.27	0	2,2,2	0.30	0
5	1BO	A	406	-	4,4,4	0.22	0	3,3,3	0.27	0
3	EDO	G	408	-	3,3,3	0.27	0	2,2,2	0.33	0
3	EDO	F	401	-	3,3,3	0.27	0	2,2,2	0.31	0
2	PEG	G	406	-	6,6,6	0.24	0	5,5,5	0.24	0
3	EDO	I	401	-	3,3,3	0.26	0	2,2,2	0.34	0
3	EDO	J	412	-	3,3,3	0.27	0	2,2,2	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	J	403	-	-	1/4/4/4	-
3	EDO	E	412	-	-	0/1/1/1	-
3	EDO	F	414	-	-	0/1/1/1	-
3	EDO	C	401	-	-	1/1/1/1	-
2	PEG	D	412	-	-	0/4/4/4	-
2	PEG	D	414	-	-	1/4/4/4	-
2	PEG	E	408	-	-	0/4/4/4	-
3	EDO	A	404	-	-	0/1/1/1	-
3	EDO	D	409	-	-	0/1/1/1	-
2	PEG	E	409	-	-	1/4/4/4	-
2	PEG	D	401	-	-	1/4/4/4	-
3	EDO	H	401	-	-	0/1/1/1	-
4	PHT	G	407	-	-	4/8/8/8	0/1/1/1
2	PEG	I	407	-	-	2/4/4/4	-
2	PEG	F	408	-	-	4/4/4/4	-
3	EDO	J	411	-	-	1/1/1/1	-
2	PEG	A	411	-	-	3/4/4/4	-
4	PHT	C	403	-	-	4/8/8/8	0/1/1/1
2	PEG	J	407	-	-	2/4/4/4	-
3	EDO	G	402	-	-	0/1/1/1	-
3	EDO	B	406	-	-	0/1/1/1	-
4	PHT	B	404	-	-	8/8/8/8	0/1/1/1
2	PEG	B	410	-	-	1/4/4/4	-
4	PHT	J	404	-	-	6/8/8/8	0/1/1/1
3	EDO	B	417	-	-	0/1/1/1	-
6	MLI	F	405	-	-	4/4/4/4	-
2	PEG	G	410	-	-	2/4/4/4	-
3	EDO	I	408	-	-	1/1/1/1	-
2	PEG	B	403	-	-	1/4/4/4	-
2	PEG	I	402	-	-	1/4/4/4	-
3	EDO	A	407	-	-	0/1/1/1	-
6	MLI	J	406	-	-	2/4/4/4	-
2	PEG	E	406	-	-	0/4/4/4	-
3	EDO	C	407	-	-	1/1/1/1	-
2	PEG	A	402	-	-	2/4/4/4	-
3	EDO	H	403	-	-	1/1/1/1	-
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	H	402	-	-	0/1/1/1	-
2	PEG	F	410	-	-	3/4/4/4	-
3	EDO	D	408	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	409	-	-	1/1/1/1	-
3	EDO	C	404	-	-	0/1/1/1	-
3	EDO	E	410	-	-	1/1/1/1	-
3	EDO	F	403	-	-	0/1/1/1	-
3	EDO	F	411	-	-	0/1/1/1	-
2	PEG	A	409	-	-	3/4/4/4	-
3	EDO	B	412	-	-	0/1/1/1	-
3	EDO	J	410	-	-	0/1/1/1	-
3	EDO	I	404	-	-	1/1/1/1	-
3	EDO	G	403	-	-	0/1/1/1	-
3	EDO	B	407	-	-	1/1/1/1	-
2	PEG	H	404	-	-	1/4/4/4	-
4	PHT	H	405	-	-	8/8/8/8	0/1/1/1
2	PEG	D	402	-	-	1/4/4/4	-
3	EDO	B	416	-	-	1/1/1/1	-
2	PEG	I	406	-	-	1/4/4/4	-
2	PEG	D	411	-	-	0/4/4/4	-
2	PEG	E	407	-	-	1/4/4/4	-
2	PEG	I	403	-	-	1/4/4/4	-
2	PEG	G	401	-	-	1/4/4/4	-
2	PEG	E	405	-	-	4/4/4/4	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	B	411	-	-	1/1/1/1	-
2	PEG	C	405	-	-	2/4/4/4	-
4	PHT	E	404	-	-	6/8/8/8	0/1/1/1
2	PEG	C	406	-	-	3/4/4/4	-
2	PEG	A	408	-	-	0/4/4/4	-
2	PEG	C	402	-	-	0/4/4/4	-
3	EDO	B	408	-	-	1/1/1/1	-
3	EDO	C	409	-	-	0/1/1/1	-
3	EDO	D	415	-	-	0/1/1/1	-
3	EDO	H	406	-	-	0/1/1/1	-
4	PHT	A	405	-	-	4/8/8/8	0/1/1/1
2	PEG	F	409	-	-	3/4/4/4	-
3	EDO	F	412	-	-	0/1/1/1	-
3	EDO	H	407	-	-	1/1/1/1	-
3	EDO	E	401	-	-	1/1/1/1	-
2	PEG	J	408	-	-	2/4/4/4	-
2	PEG	J	402	-	-	1/4/4/4	-
2	PEG	A	410	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	401	-	-	1/4/4/4	-
2	PEG	E	402	-	-	2/4/4/4	-
3	EDO	F	413	-	-	1/1/1/1	-
3	EDO	A	412	-	-	1/1/1/1	-
2	PEG	J	401	-	-	2/4/4/4	-
3	EDO	D	405	-	-	0/1/1/1	-
2	PEG	G	409	-	-	2/4/4/4	-
3	EDO	G	412	-	-	1/1/1/1	-
3	EDO	G	411	-	-	0/1/1/1	-
4	PHT	D	406	-	-	8/8/8/8	0/1/1/1
3	EDO	F	404	-	-	1/1/1/1	-
3	EDO	D	403	-	-	0/1/1/1	-
3	EDO	E	411	-	-	1/1/1/1	-
3	EDO	G	405	-	-	1/1/1/1	-
2	PEG	F	406	-	-	2/4/4/4	-
2	PEG	D	413	-	-	1/4/4/4	-
3	EDO	J	405	-	-	1/1/1/1	-
4	PHT	I	405	-	-	4/8/8/8	0/1/1/1
3	EDO	B	401	-	-	1/1/1/1	-
2	PEG	D	404	-	-	2/4/4/4	-
3	EDO	G	413	-	-	1/1/1/1	-
2	PEG	F	407	-	-	0/4/4/4	-
3	EDO	D	410	-	-	0/1/1/1	-
3	EDO	C	408	-	-	1/1/1/1	-
3	EDO	B	415	-	-	1/1/1/1	-
4	PHT	F	402	-	-	3/8/8/8	0/1/1/1
3	EDO	J	409	-	-	0/1/1/1	-
5	1BO	D	407	-	-	0/2/2/2	-
2	PEG	E	403	-	-	1/4/4/4	-
5	1BO	B	405	-	-	1/2/2/2	-
3	EDO	B	414	-	-	0/1/1/1	-
3	EDO	I	409	-	-	0/1/1/1	-
3	EDO	G	404	-	-	1/1/1/1	-
3	EDO	B	413	-	-	1/1/1/1	-
5	1BO	A	406	-	-	0/2/2/2	-
3	EDO	G	408	-	-	1/1/1/1	-
3	EDO	F	401	-	-	1/1/1/1	-
2	PEG	G	406	-	-	3/4/4/4	-
3	EDO	I	401	-	-	0/1/1/1	-
3	EDO	J	412	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	406	MLI	C1-C3	2.55	1.55	1.51
6	F	405	MLI	C1-C3	2.52	1.54	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	PHT	O8-C7-C3	-3.17	114.25	121.94
4	C	403	PHT	O8-C7-C3	-3.04	114.56	121.94
4	B	404	PHT	O11-C10-C2	-2.68	115.43	121.94
4	H	405	PHT	O8-C7-C3	-2.60	115.62	121.94
4	C	403	PHT	O11-C10-C2	-2.54	115.77	121.94
4	D	406	PHT	O8-C7-C3	-2.53	115.78	121.94
4	I	405	PHT	O11-C10-C2	-2.51	115.84	121.94
4	E	404	PHT	O8-C7-C3	-2.42	116.07	121.94
4	D	406	PHT	O11-C10-C2	-2.39	116.13	121.94
4	F	402	PHT	O11-C10-C2	-2.39	116.13	121.94
4	G	407	PHT	O8-C7-C3	-2.38	116.16	121.94
4	B	404	PHT	O8-C7-C3	-2.33	116.28	121.94
4	E	404	PHT	O11-C10-C2	-2.27	116.43	121.94
4	J	404	PHT	O11-C10-C2	-2.26	116.45	121.94
4	J	404	PHT	O8-C7-C3	-2.25	116.47	121.94
4	A	405	PHT	O11-C10-C2	-2.23	116.52	121.94
4	I	405	PHT	O8-C7-C3	-2.15	116.71	121.94
4	F	402	PHT	O8-C7-C3	-2.11	116.82	121.94
4	H	405	PHT	O11-C10-C2	-2.09	116.86	121.94

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	408	PEG	O2-C3-C4-O4
2	A	409	PEG	O2-C3-C4-O4
2	A	411	PEG	O1-C1-C2-O2
2	A	411	PEG	O2-C3-C4-O4
2	D	413	PEG	O2-C3-C4-O4
2	E	405	PEG	O2-C3-C4-O4
2	I	406	PEG	O2-C3-C4-O4
3	B	408	EDO	O1-C1-C2-O2
3	C	408	EDO	O1-C1-C2-O2
2	E	402	PEG	O2-C3-C4-O4
2	F	406	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	F	410	PEG	O1-C1-C2-O2
2	G	406	PEG	O2-C3-C4-O4
2	B	410	PEG	C1-C2-O2-C3
2	C	406	PEG	O1-C1-C2-O2
2	G	409	PEG	O1-C1-C2-O2
2	J	407	PEG	O1-C1-C2-O2
2	I	407	PEG	O1-C1-C2-O2
3	B	401	EDO	O1-C1-C2-O2
3	C	401	EDO	O1-C1-C2-O2
3	C	407	EDO	O1-C1-C2-O2
3	D	408	EDO	O1-C1-C2-O2
3	E	410	EDO	O1-C1-C2-O2
3	G	413	EDO	O1-C1-C2-O2
3	J	405	EDO	O1-C1-C2-O2
3	J	411	EDO	O1-C1-C2-O2
2	D	402	PEG	O2-C3-C4-O4
2	E	407	PEG	O2-C3-C4-O4
2	F	409	PEG	O2-C3-C4-O4
2	G	406	PEG	O1-C1-C2-O2
2	H	404	PEG	O2-C3-C4-O4
2	J	408	PEG	O2-C3-C4-O4
5	B	405	1BO	C2-C3-C4-OH
2	E	402	PEG	O1-C1-C2-O2
2	A	409	PEG	O1-C1-C2-O2
3	B	411	EDO	O1-C1-C2-O2
3	F	413	EDO	O1-C1-C2-O2
3	G	405	EDO	O1-C1-C2-O2
3	G	412	EDO	O1-C1-C2-O2
3	H	403	EDO	O1-C1-C2-O2
3	I	404	EDO	O1-C1-C2-O2
2	I	407	PEG	C4-C3-O2-C2
4	A	405	PHT	O12-C10-C2-C1
4	B	404	PHT	O11-C10-C2-C1
4	A	405	PHT	O11-C10-C2-C1
2	J	402	PEG	C1-C2-O2-C3
2	I	402	PEG	C4-C3-O2-C2
4	B	404	PHT	O12-C10-C2-C1
2	A	401	PEG	C4-C3-O2-C2
2	A	409	PEG	C4-C3-O2-C2
2	F	408	PEG	C4-C3-O2-C2
2	F	410	PEG	C4-C3-O2-C2
2	J	401	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	J	403	PEG	C4-C3-O2-C2
2	A	411	PEG	C1-C2-O2-C3
2	D	414	PEG	C4-C3-O2-C2
2	G	406	PEG	C4-C3-O2-C2
2	J	407	PEG	C4-C3-O2-C2
2	G	410	PEG	O2-C3-C4-O4
4	J	404	PHT	O12-C10-C2-C1
2	C	406	PEG	C1-C2-O2-C3
2	A	410	PEG	O2-C3-C4-O4
2	F	406	PEG	O2-C3-C4-O4
2	F	408	PEG	O1-C1-C2-O2
2	D	401	PEG	C4-C3-O2-C2
3	B	415	EDO	O1-C1-C2-O2
4	E	404	PHT	O12-C10-C2-C1
4	E	404	PHT	O11-C10-C2-C1
4	J	404	PHT	O11-C10-C2-C1
4	D	406	PHT	C4-C3-C7-O8
2	G	410	PEG	C1-C2-O2-C3
4	D	406	PHT	O11-C10-C2-C1
2	E	405	PEG	O1-C1-C2-O2
2	E	405	PEG	C4-C3-O2-C2
4	D	406	PHT	O12-C10-C2-C1
6	F	405	MLI	C2-C1-C3-O9
6	J	406	MLI	C3-C1-C2-O7
2	C	405	PEG	O2-C3-C4-O4
2	F	410	PEG	O2-C3-C4-O4
4	B	404	PHT	C4-C3-C7-O8
4	D	406	PHT	C4-C3-C7-O9
4	A	405	PHT	O11-C10-C2-C3
2	C	405	PEG	C1-C2-O2-C3
2	J	408	PEG	C4-C3-O2-C2
4	J	404	PHT	O12-C10-C2-C3
4	B	404	PHT	C4-C3-C7-O9
3	J	412	EDO	O1-C1-C2-O2
4	A	405	PHT	O12-C10-C2-C3
4	B	404	PHT	O11-C10-C2-C3
6	F	405	MLI	C3-C1-C2-O7
6	F	405	MLI	C2-C1-C3-O8
6	J	406	MLI	C3-C1-C2-O6
4	C	403	PHT	O11-C10-C2-C1
4	C	403	PHT	O12-C10-C2-C1
4	G	407	PHT	C4-C3-C7-O8

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Mol	Chain	Res	Type	Atoms
4	G	407	PHT	C4-C3-C7-O9
2	E	405	PEG	C1-C2-O2-C3
4	H	405	PHT	C4-C3-C7-O8
4	H	405	PHT	O12-C10-C2-C1
4	H	405	PHT	C4-C3-C7-O9
2	A	410	PEG	C4-C3-O2-C2
2	A	402	PEG	O1-C1-C2-O2
4	H	405	PHT	O11-C10-C2-C1
2	A	402	PEG	C4-C3-O2-C2
2	G	409	PEG	C4-C3-O2-C2
4	E	404	PHT	O12-C10-C2-C3
2	I	403	PEG	C4-C3-O2-C2
4	B	404	PHT	O12-C10-C2-C3
4	J	404	PHT	O11-C10-C2-C3
2	F	408	PEG	C1-C2-O2-C3
6	F	405	MLI	C3-C1-C2-O6
2	G	401	PEG	C4-C3-O2-C2
4	D	406	PHT	O11-C10-C2-C3
4	D	406	PHT	C2-C3-C7-O8
4	E	404	PHT	O11-C10-C2-C3
2	D	404	PEG	O2-C3-C4-O4
2	E	409	PEG	O2-C3-C4-O4
3	B	416	EDO	O1-C1-C2-O2
3	E	411	EDO	O1-C1-C2-O2
3	F	404	EDO	O1-C1-C2-O2
3	G	408	EDO	O1-C1-C2-O2
4	D	406	PHT	C2-C3-C7-O9
4	G	407	PHT	C2-C3-C7-O9
4	J	404	PHT	C4-C3-C7-O9
4	D	406	PHT	O12-C10-C2-C3
2	E	403	PEG	O2-C3-C4-O4
2	F	409	PEG	O1-C1-C2-O2
4	C	403	PHT	O12-C10-C2-C3
4	H	405	PHT	O12-C10-C2-C3
4	J	404	PHT	C4-C3-C7-O8
4	B	404	PHT	C2-C3-C7-O8
4	I	405	PHT	O12-C10-C2-C1
2	B	403	PEG	C4-C3-O2-C2
4	C	403	PHT	O11-C10-C2-C3
4	G	407	PHT	C2-C3-C7-O8
4	H	405	PHT	C2-C3-C7-O8
4	H	405	PHT	C2-C3-C7-O9

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Mol	Chain	Res	Type	Atoms
4	E	404	PHT	C4-C3-C7-O8
4	F	402	PHT	O11-C10-C2-C1
4	F	402	PHT	O12-C10-C2-C1
4	I	405	PHT	O11-C10-C2-C1
4	H	405	PHT	O11-C10-C2-C3
4	E	404	PHT	C4-C3-C7-O9
3	A	412	EDO	O1-C1-C2-O2
3	B	407	EDO	O1-C1-C2-O2
3	B	413	EDO	O1-C1-C2-O2
3	E	401	EDO	O1-C1-C2-O2
2	C	406	PEG	C4-C3-O2-C2
2	D	404	PEG	C1-C2-O2-C3
4	B	404	PHT	C2-C3-C7-O9
4	I	405	PHT	C4-C3-C7-O9
4	I	405	PHT	C4-C3-C7-O8
2	J	401	PEG	C4-C3-O2-C2
4	F	402	PHT	C4-C3-C7-O9
3	B	409	EDO	O1-C1-C2-O2
3	F	401	EDO	O1-C1-C2-O2
3	G	404	EDO	O1-C1-C2-O2
3	H	407	EDO	O1-C1-C2-O2
3	I	408	EDO	O1-C1-C2-O2
2	F	409	PEG	C4-C3-O2-C2

There are no ring outliers.

44 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	408	PEG	1	0
2	E	409	PEG	1	0
4	G	407	PHT	1	0
3	B	406	EDO	1	0
4	B	404	PHT	2	0
2	G	410	PEG	1	0
2	B	403	PEG	1	0
3	H	403	EDO	1	0
3	H	402	EDO	1	0
3	B	409	EDO	1	0
2	A	409	PEG	1	0
2	H	404	PEG	1	0
4	H	405	PHT	1	0
2	I	403	PEG	2	0

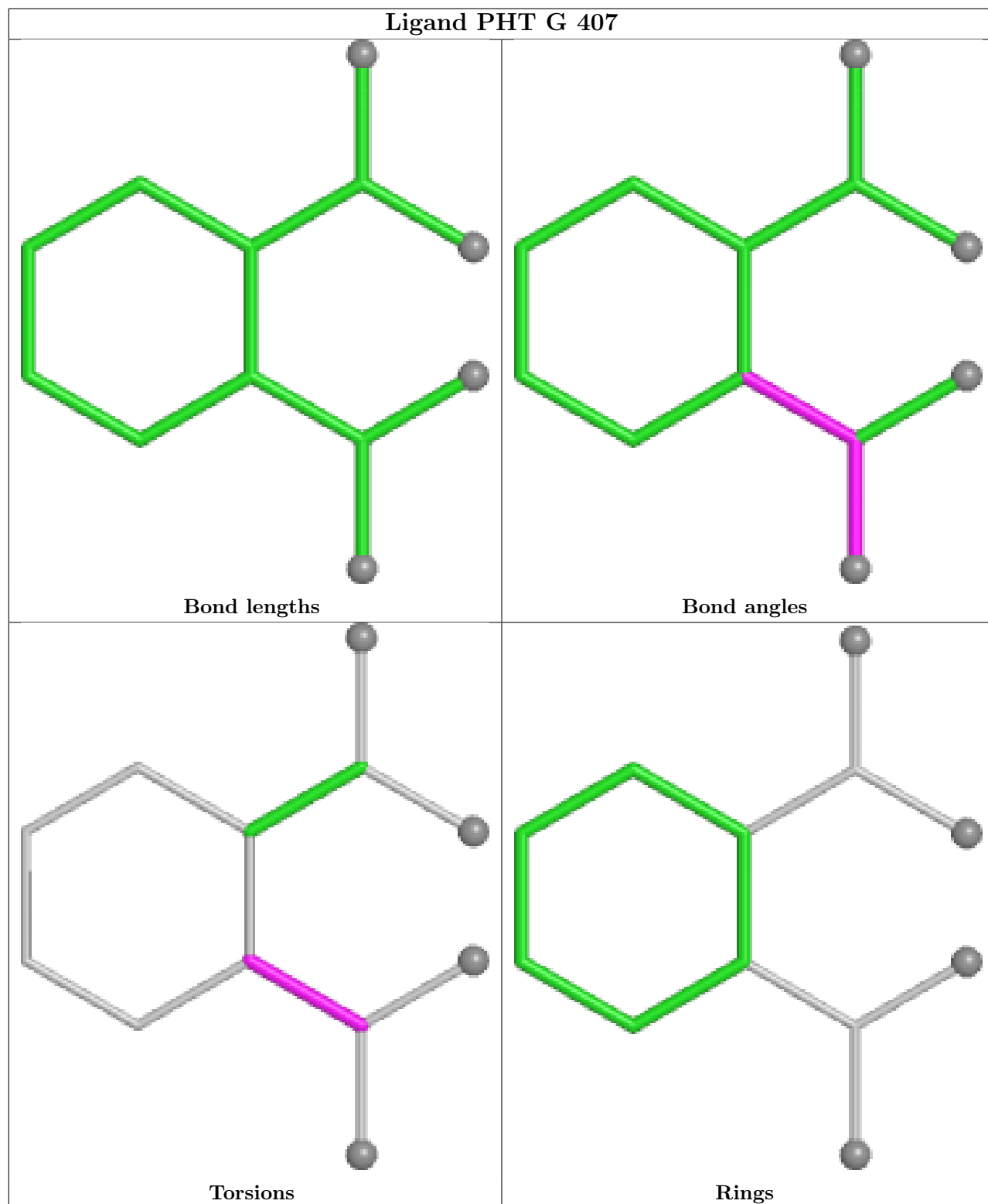
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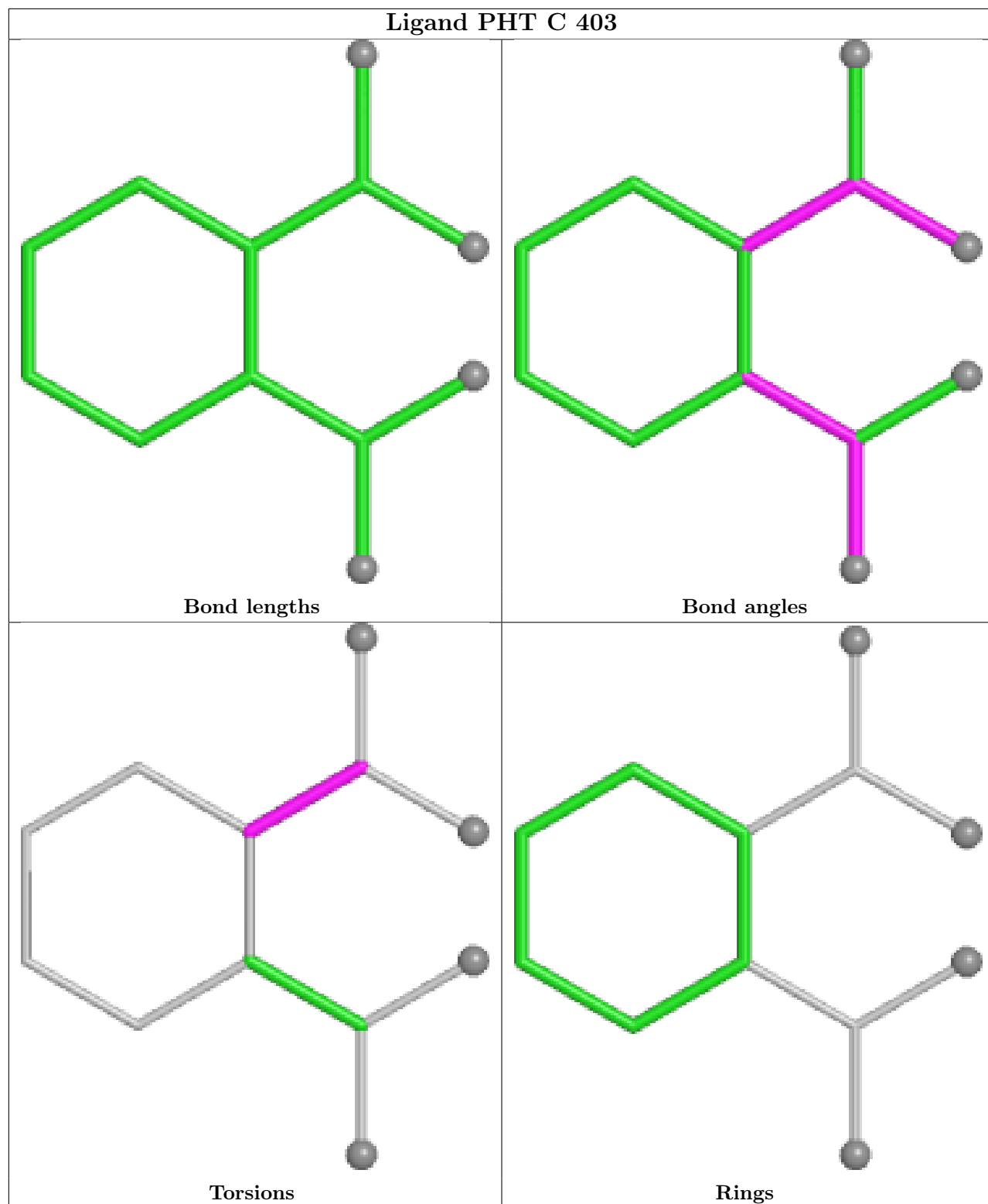
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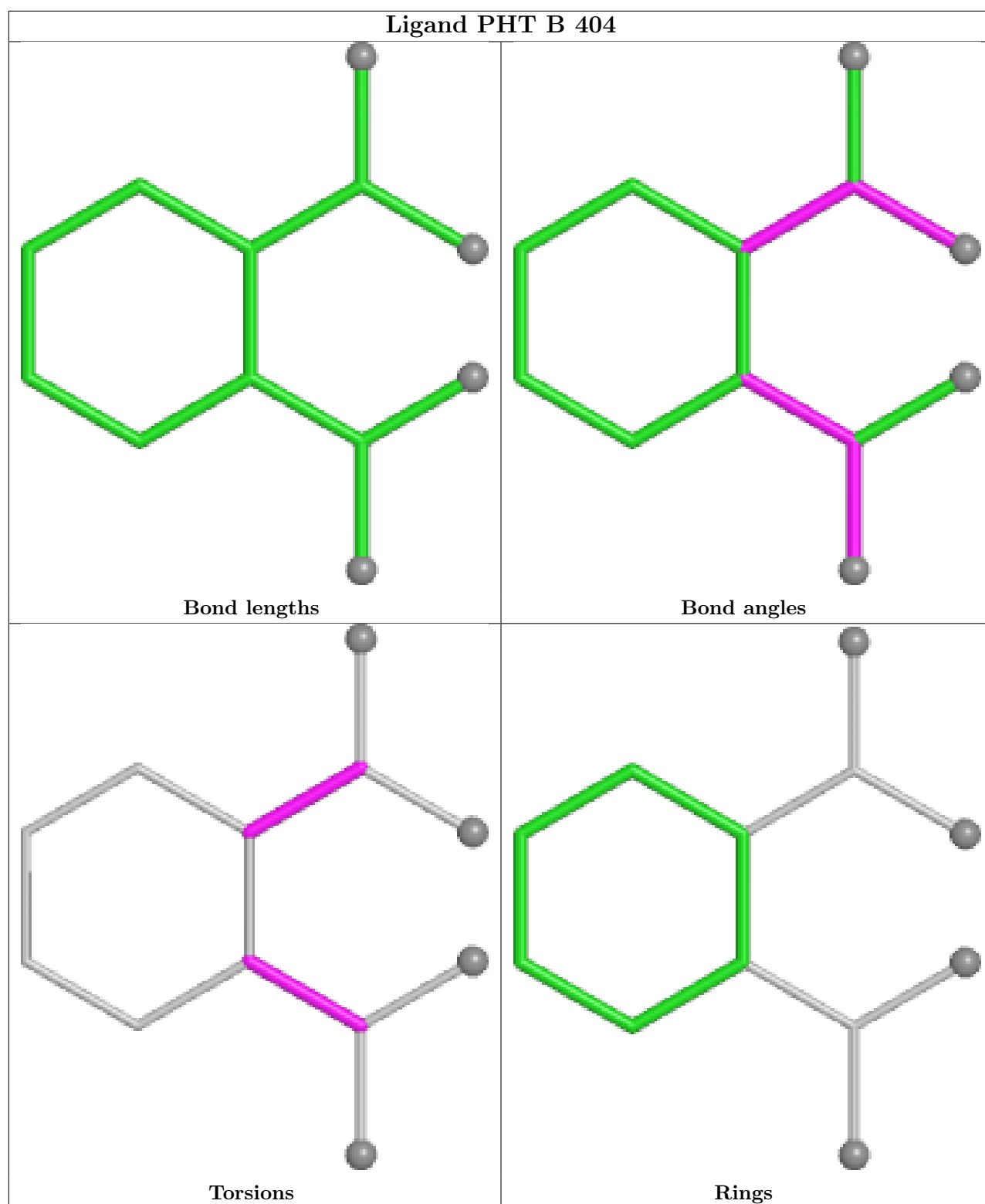
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	PEG	2	0
2	E	405	PEG	1	0
3	A	403	EDO	1	0
3	B	411	EDO	1	0
2	C	405	PEG	1	0
4	E	404	PHT	1	0
2	C	406	PEG	1	0
3	C	409	EDO	1	0
3	H	406	EDO	1	0
4	A	405	PHT	1	0
3	E	401	EDO	1	0
2	J	408	PEG	3	0
2	A	410	PEG	3	0
2	A	401	PEG	1	0
2	E	402	PEG	1	0
3	F	413	EDO	1	0
2	G	409	PEG	1	0
4	D	406	PHT	1	0
3	E	411	EDO	2	0
2	F	406	PEG	1	0
4	I	405	PHT	1	0
2	D	404	PEG	1	0
2	F	407	PEG	1	0
5	D	407	1BO	1	0
2	E	403	PEG	1	0
5	B	405	1BO	1	0
3	G	404	EDO	1	0
5	A	406	1BO	1	0
3	I	401	EDO	1	0
3	J	412	EDO	1	0

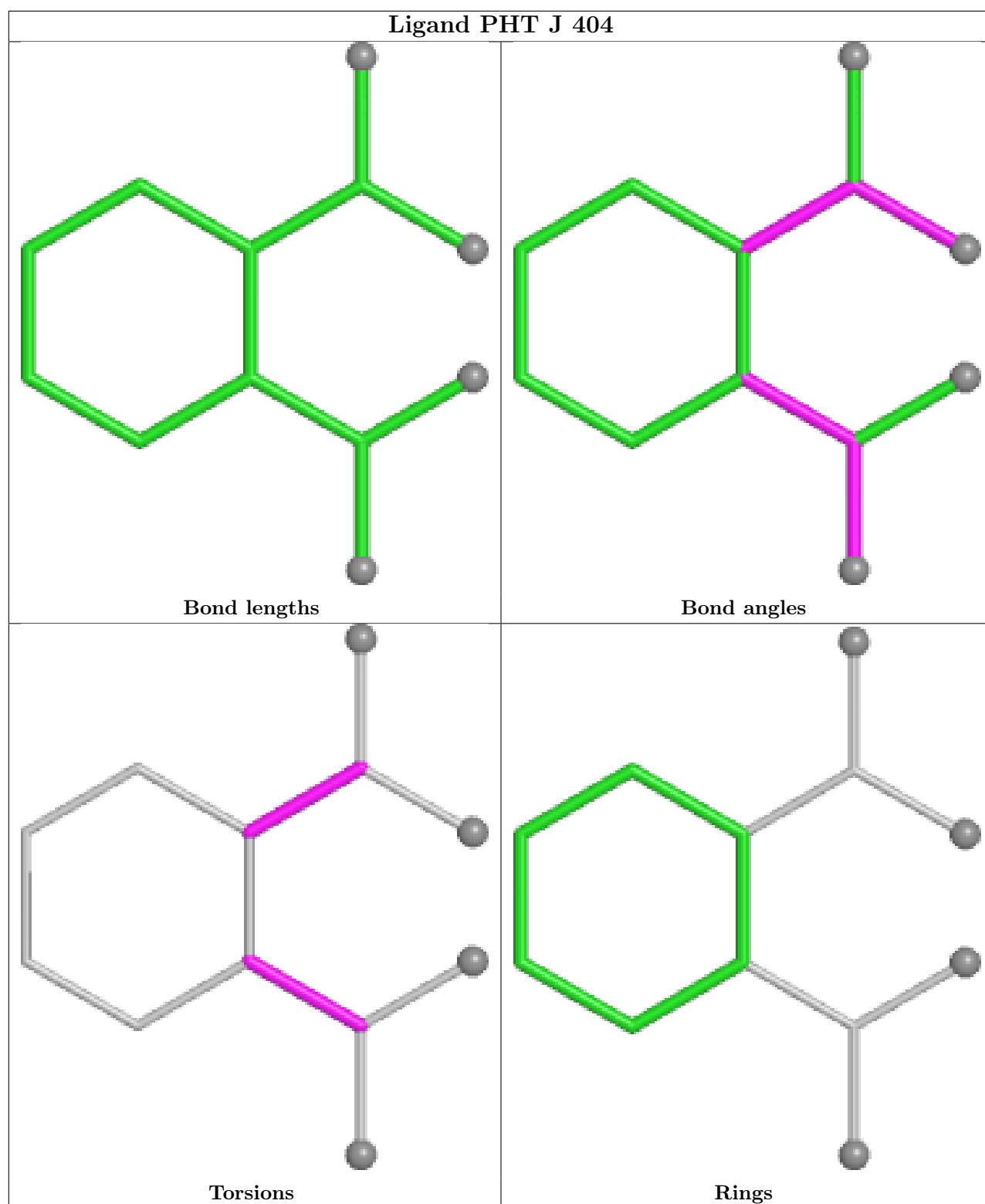
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

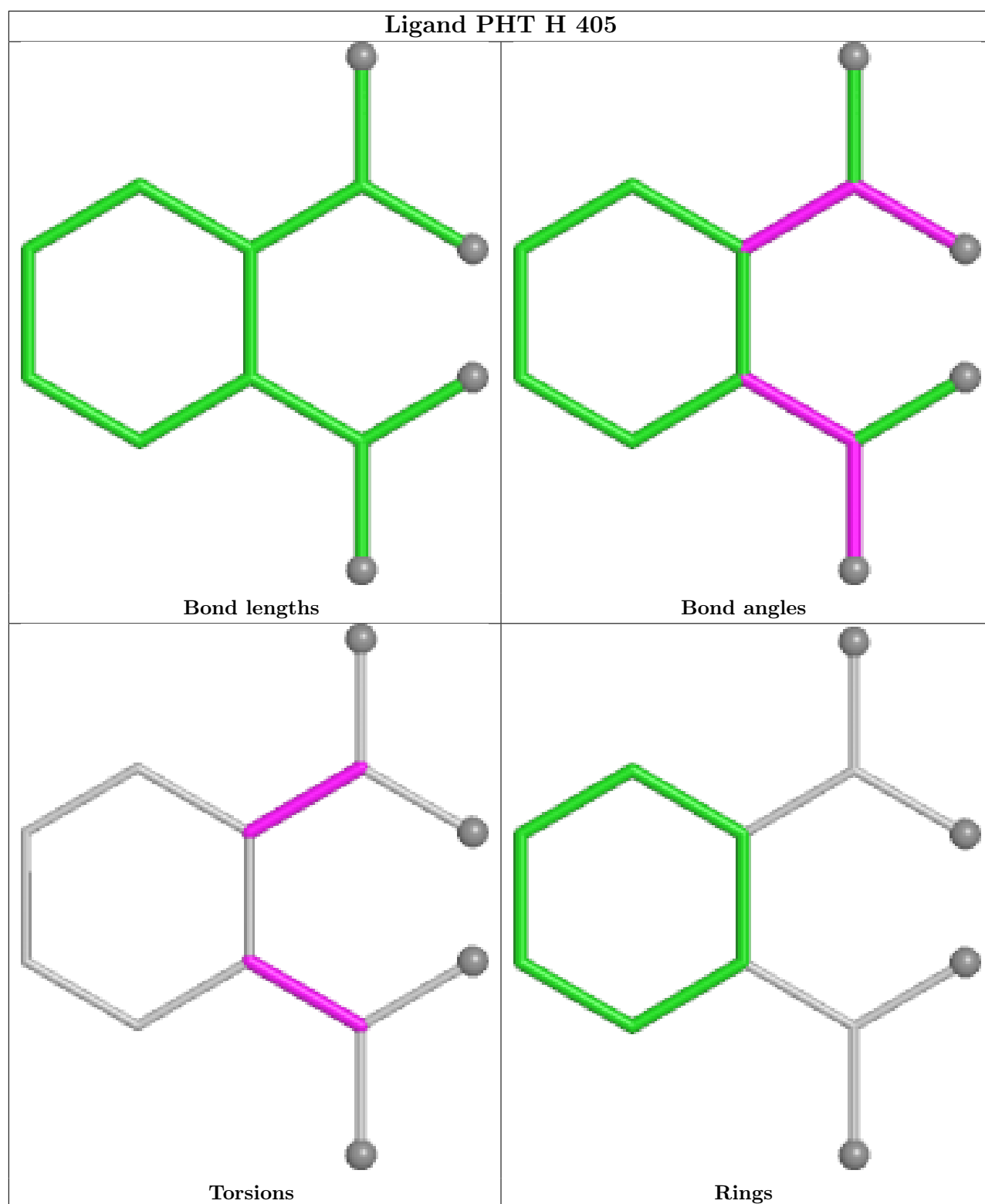


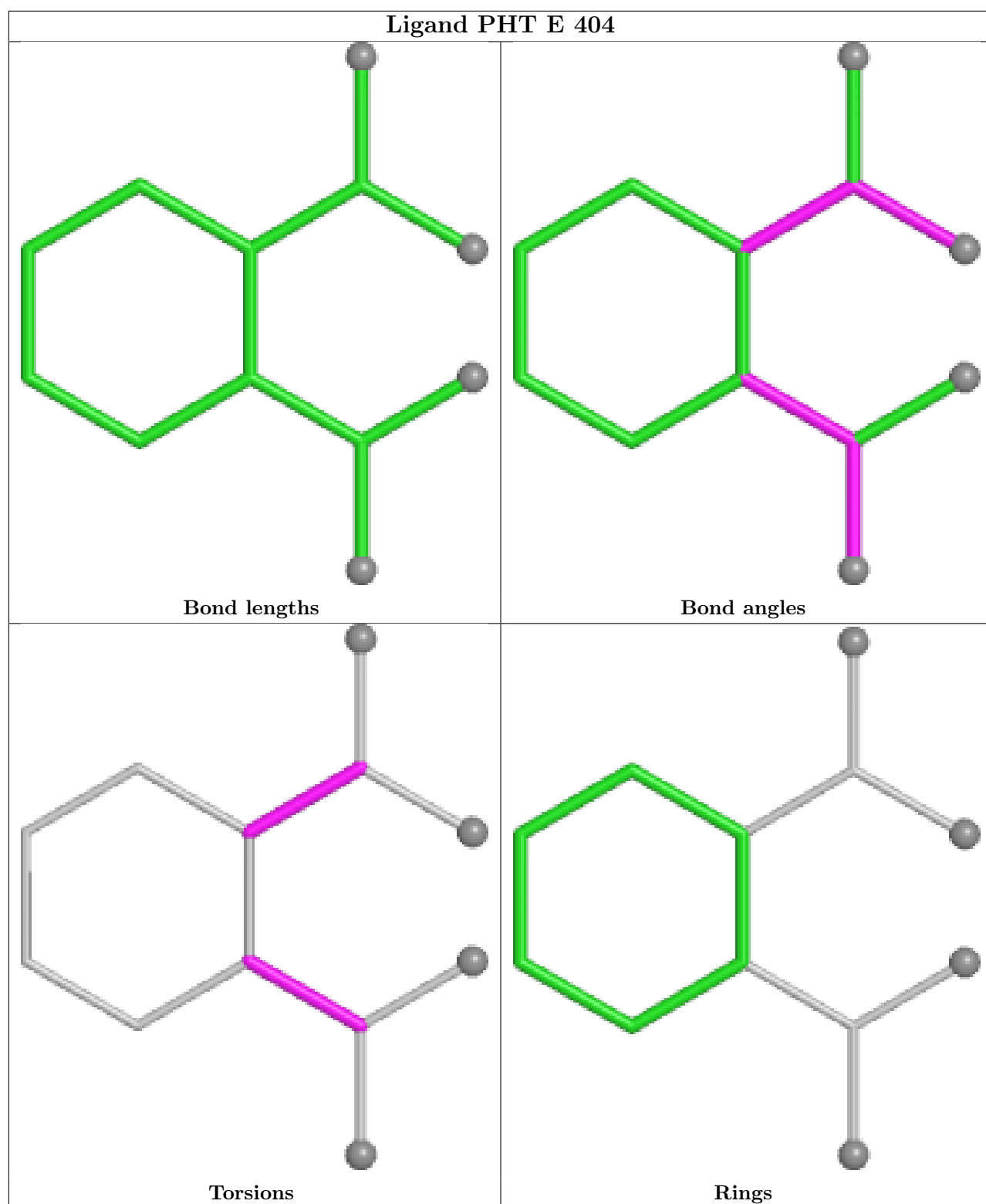


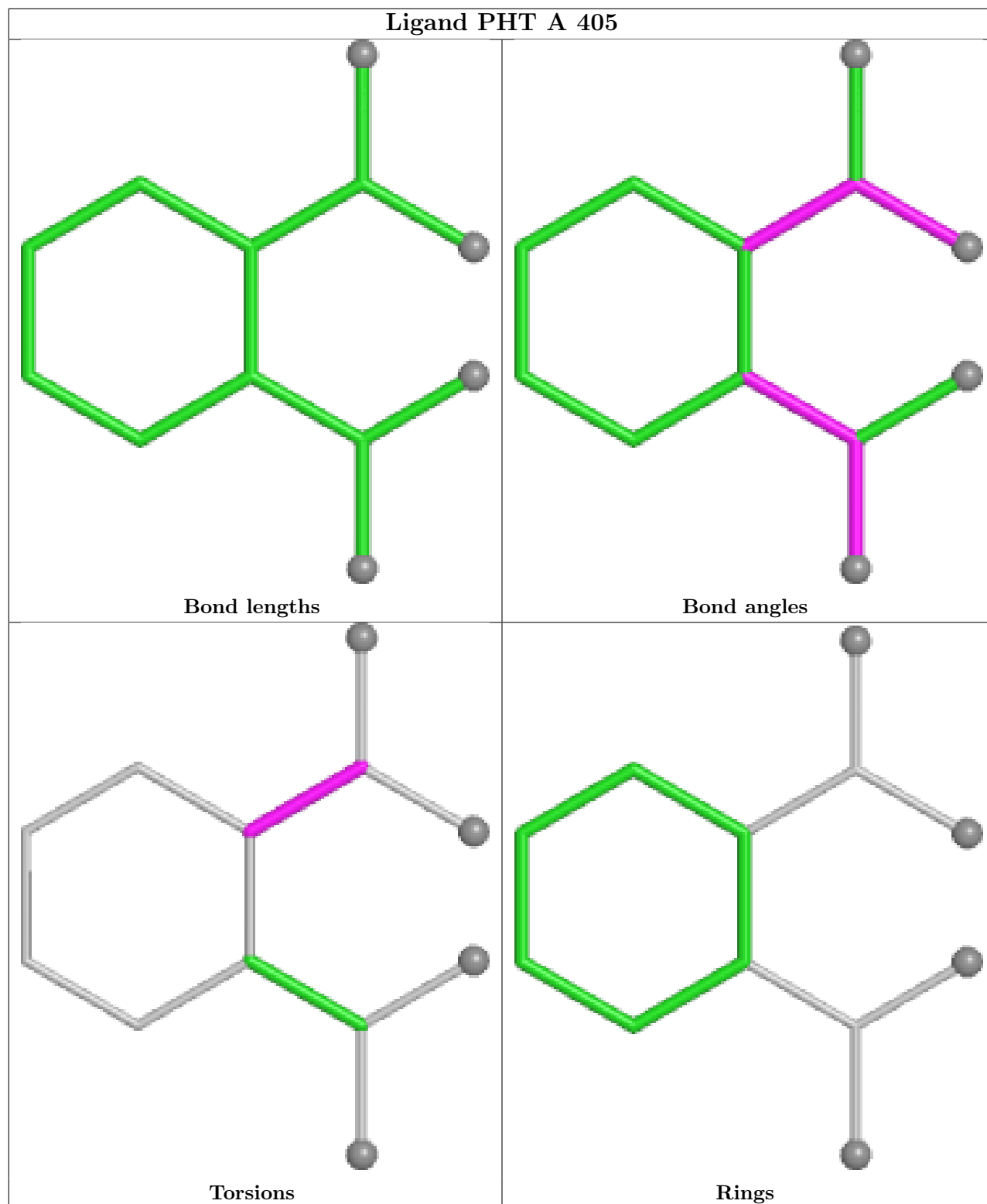


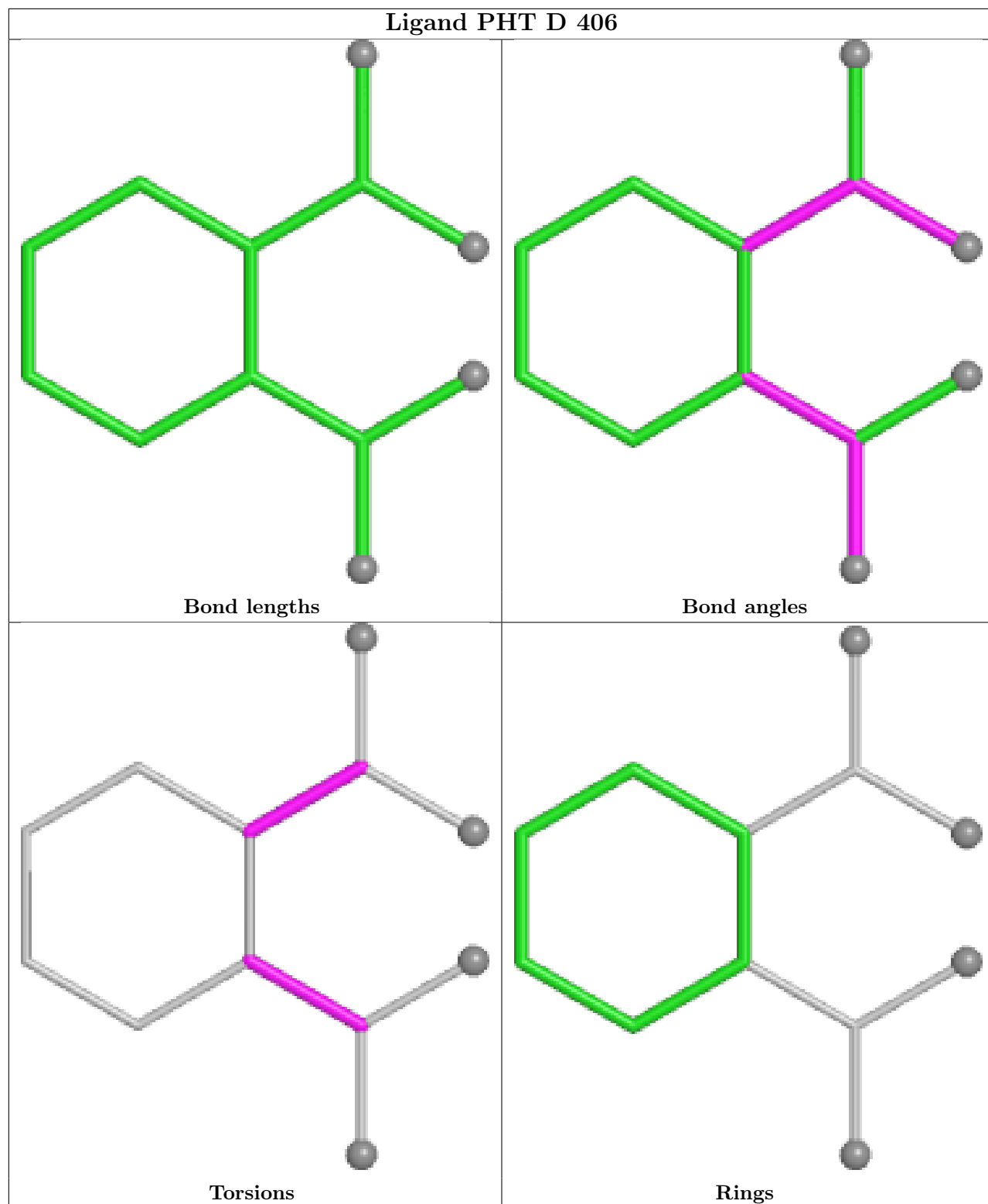




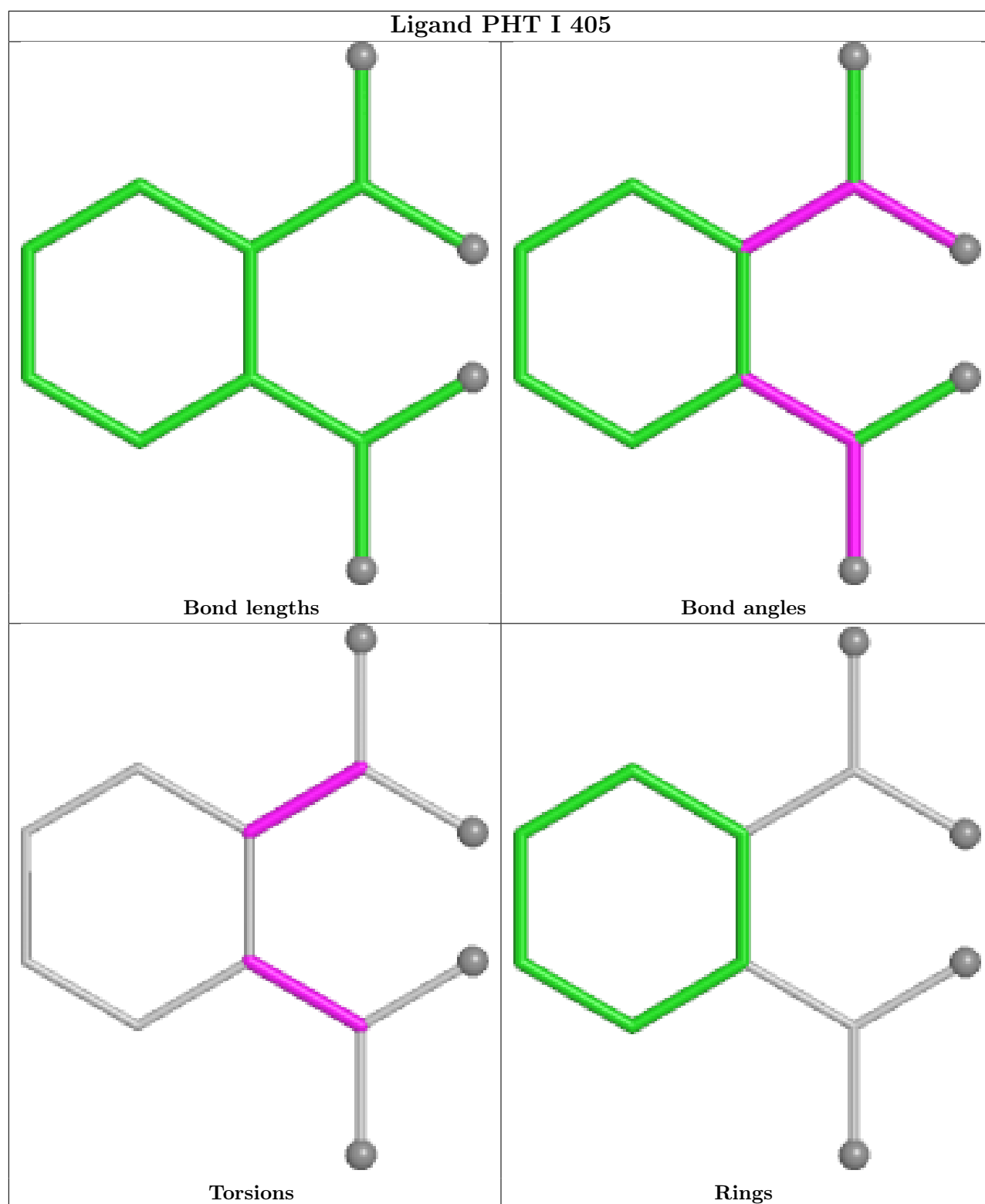


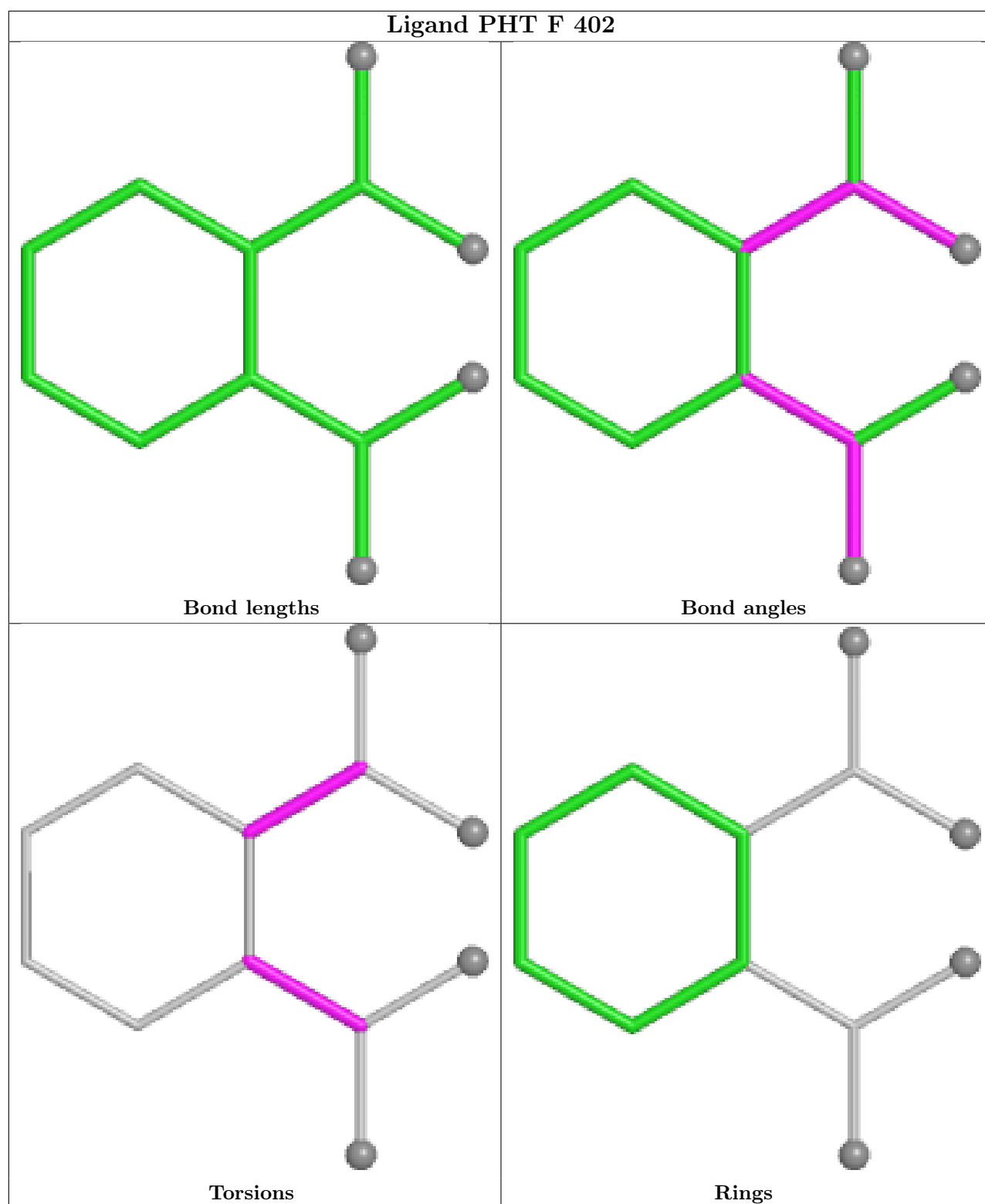


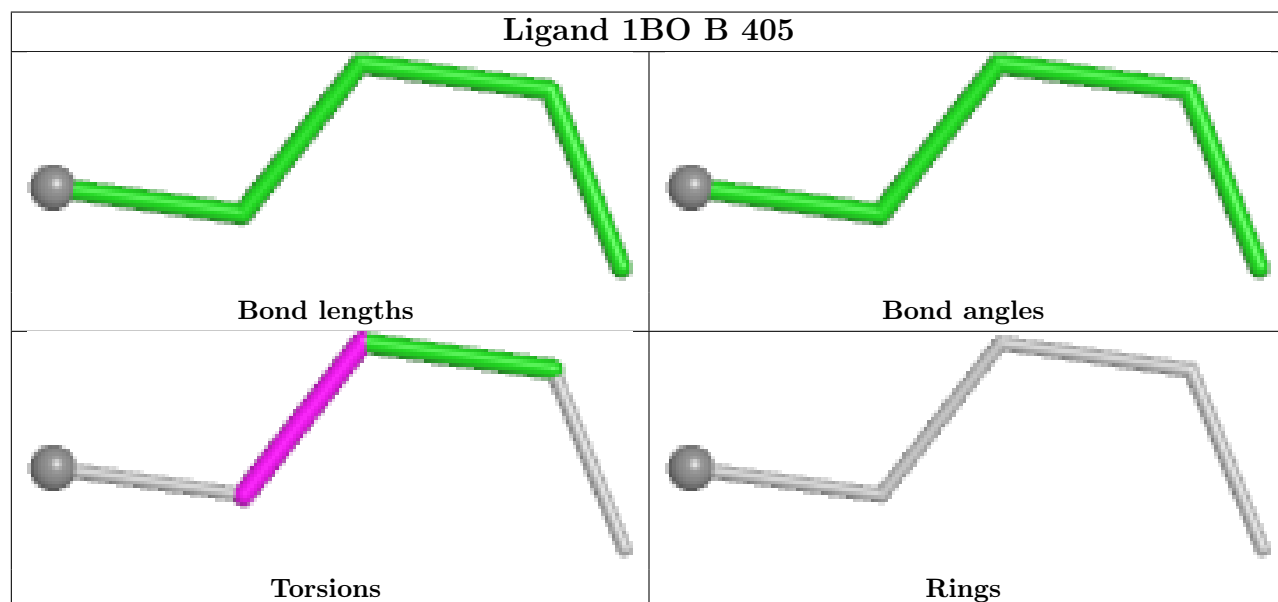
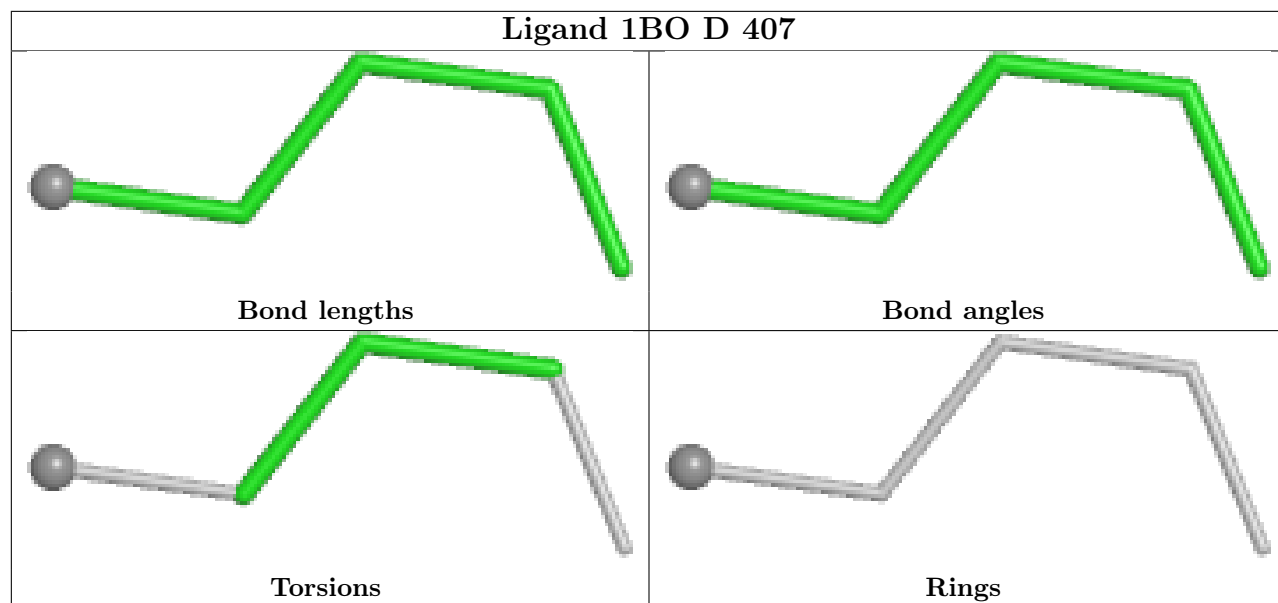


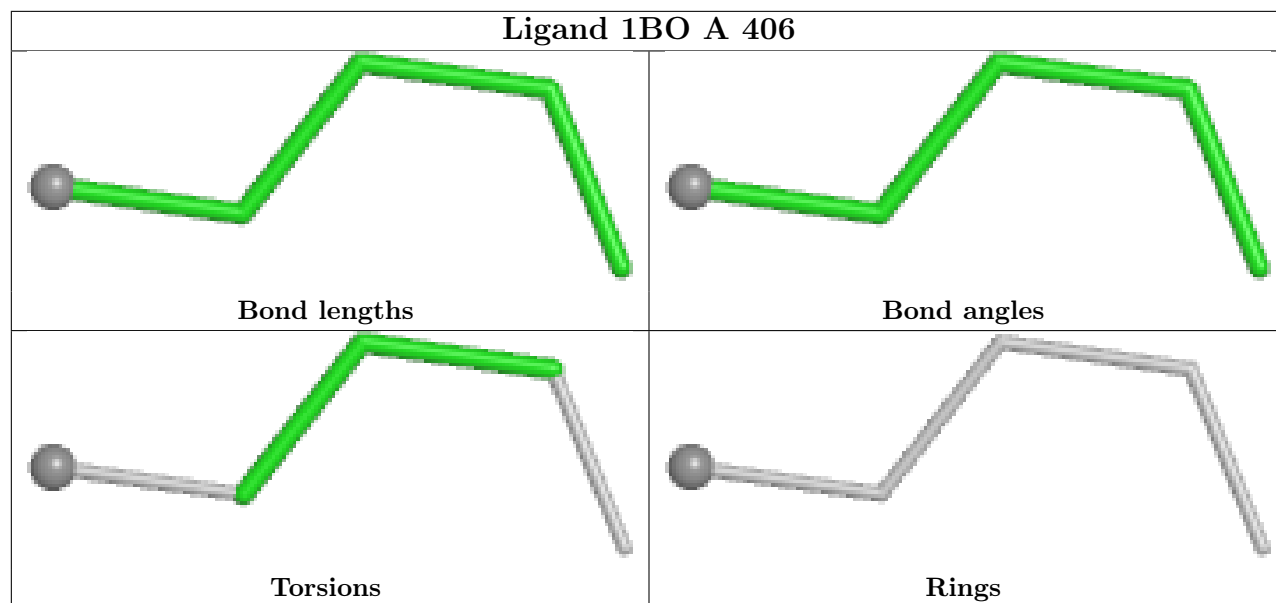












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	291/303 (96%)	0.36	8 (2%) 56 46	10, 14, 32, 53	0
1	B	290/303 (95%)	0.34	6 (2%) 63 54	10, 13, 33, 48	0
1	C	289/303 (95%)	0.39	15 (5%) 33 25	9, 12, 41, 65	0
1	D	292/303 (96%)	0.29	5 (1%) 69 60	9, 12, 30, 61	0
1	E	291/303 (96%)	0.34	10 (3%) 48 39	10, 14, 35, 54	0
1	F	289/303 (95%)	0.35	10 (3%) 47 38	10, 13, 32, 58	0
1	G	285/303 (94%)	0.39	16 (5%) 30 23	10, 14, 34, 57	0
1	H	293/303 (96%)	0.41	14 (4%) 35 28	11, 15, 38, 57	0
1	I	293/303 (96%)	0.41	12 (4%) 41 33	11, 17, 36, 61	0
1	J	292/303 (96%)	0.62	23 (7%) 18 13	13, 19, 52, 81	0
All	All	2905/3030 (95%)	0.39	119 (4%) 41 33	9, 15, 37, 81	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	153	THR	5.1
1	J	149	TYR	4.9
1	G	9	TYR	4.8
1	E	146	VAL	4.6
1	J	9	TYR	4.5
1	H	16	ARG	4.4
1	I	298	SER	4.3
1	H	158	ALA	4.2
1	J	151	ALA	4.2
1	H	171	ARG	4.2
1	C	173	LEU	4.0
1	C	3	THR	4.0
1	F	159	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	6	SER	3.9
1	I	5	LEU	3.8
1	J	150	ASP	3.7
1	A	9	TYR	3.7
1	C	9	TYR	3.7
1	I	143	PHE	3.7
1	B	158	ALA	3.6
1	F	5	LEU	3.6
1	I	158	ALA	3.5
1	H	159	ASP	3.5
1	J	3	THR	3.5
1	J	148	PHE	3.5
1	C	138	GLY	3.4
1	F	9	TYR	3.4
1	I	297	ALA	3.3
1	J	160	ALA	3.2
1	A	150	ASP	3.2
1	J	159	ASP	3.2
1	J	156	LEU	3.1
1	C	147	GLU	3.1
1	D	138	GLY	3.0
1	G	143	PHE	3.0
1	E	9	TYR	3.0
1	B	123	GLU	3.0
1	C	297	ALA	2.9
1	H	299	TYR	2.9
1	H	146	VAL	2.9
1	A	149	TYR	2.8
1	I	141	ALA	2.8
1	H	6	SER	2.8
1	J	24	GLU	2.8
1	J	169	TYR	2.8
1	F	297	ALA	2.8
1	J	154	ARG	2.8
1	F	6	SER	2.8
1	C	158	ALA	2.8
1	J	299	TYR	2.8
1	G	5	LEU	2.8
1	H	9	TYR	2.7
1	C	146	VAL	2.7
1	G	140	ASP	2.7
1	C	163	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	123	GLU	2.7
1	D	143	PHE	2.7
1	H	300	ALA	2.7
1	J	140	ASP	2.7
1	E	181	GLU	2.7
1	G	158	ALA	2.6
1	J	158	ALA	2.6
1	J	182	GLN	2.6
1	J	155	SER	2.6
1	I	9	TYR	2.6
1	F	179	PRO	2.6
1	A	5	LEU	2.6
1	G	159	ASP	2.6
1	J	141	ALA	2.6
1	G	155	SER	2.6
1	E	6	SER	2.5
1	A	4	ASP	2.5
1	E	140	ASP	2.5
1	J	298	SER	2.5
1	E	138	GLY	2.5
1	C	169	TYR	2.5
1	E	224	ARG	2.5
1	I	139	THR	2.5
1	I	159	ASP	2.4
1	C	5	LEU	2.4
1	D	179	PRO	2.4
1	E	24	GLU	2.4
1	G	6	SER	2.4
1	I	178	VAL	2.4
1	B	9	TYR	2.4
1	E	4	ASP	2.3
1	D	158	ALA	2.3
1	E	168	ALA	2.3
1	G	157	PRO	2.3
1	G	139	THR	2.3
1	H	139	THR	2.3
1	B	150	ASP	2.3
1	F	183	ILE	2.3
1	D	139	THR	2.3
1	H	298	SER	2.3
1	H	4	ASP	2.2
1	G	7	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	138	GLY	2.2
1	B	159	ASP	2.2
1	G	138	GLY	2.2
1	F	160	ALA	2.2
1	A	8	ASN	2.2
1	H	157	PRO	2.2
1	G	160	ALA	2.2
1	A	140	ASP	2.1
1	H	140	ASP	2.1
1	F	7	VAL	2.1
1	G	175	VAL	2.1
1	C	159	ASP	2.1
1	G	297	ALA	2.1
1	J	147	GLU	2.1
1	J	152	ILE	2.1
1	C	154	ARG	2.1
1	G	211	GLU	2.1
1	I	6	SER	2.0
1	A	157	PRO	2.0
1	C	243	ARG	2.0
1	C	18	ARG	2.0
1	J	175	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	A	407	4/4	0.59	0.18	31,39,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEG	F	410	7/7	0.69	0.18	34,43,48,65	0
3	EDO	D	403	4/4	0.69	0.20	44,46,47,50	0
2	PEG	E	403	7/7	0.74	0.22	23,37,44,77	0
3	EDO	G	411	4/4	0.76	0.12	11,21,24,25	0
4	PHT	G	407	12/12	0.76	0.28	30,54,71,79	0
2	PEG	H	404	7/7	0.77	0.17	28,36,43,49	0
2	PEG	D	414	7/7	0.78	0.17	21,26,35,42	0
2	PEG	D	401	7/7	0.78	0.17	24,35,43,54	0
2	PEG	F	408	7/7	0.78	0.20	11,21,24,33	0
4	PHT	A	405	12/12	0.79	0.21	31,42,57,60	0
2	PEG	J	401	7/7	0.80	0.15	22,29,31,42	0
2	PEG	D	404	7/7	0.80	0.21	16,22,37,41	0
4	PHT	J	404	12/12	0.80	0.19	18,44,51,56	0
2	PEG	E	405	7/7	0.81	0.21	12,12,23,26	0
3	EDO	I	404	4/4	0.81	0.17	23,23,24,26	0
2	PEG	E	407	7/7	0.81	0.15	10,17,30,32	0
4	PHT	C	403	12/12	0.81	0.26	32,52,72,72	0
3	EDO	D	409	4/4	0.81	0.21	14,17,19,24	0
3	EDO	G	404	4/4	0.81	0.17	12,17,21,22	0
5	1BO	A	406	5/5	0.82	0.20	19,20,26,35	0
3	EDO	F	413	4/4	0.83	0.18	13,15,17,21	0
2	PEG	J	407	7/7	0.83	0.16	20,25,35,38	0
2	PEG	I	402	7/7	0.83	0.22	11,15,34,37	0
3	EDO	A	412	4/4	0.83	0.18	17,20,22,26	0
2	PEG	E	402	7/7	0.83	0.21	12,22,50,62	0
2	PEG	J	403	7/7	0.83	0.18	18,19,22,24	0
4	PHT	D	406	12/12	0.83	0.21	10,22,38,40	0
3	EDO	F	401	4/4	0.83	0.15	20,23,27,28	0
3	EDO	F	404	4/4	0.83	0.14	16,20,25,25	0
3	EDO	F	412	4/4	0.83	0.14	11,12,16,17	0
2	PEG	D	402	7/7	0.84	0.17	20,36,46,50	0
3	EDO	D	408	4/4	0.84	0.18	9,13,25,26	0
4	PHT	H	405	12/12	0.84	0.19	19,34,44,47	0
4	PHT	B	404	12/12	0.84	0.20	9,24,33,39	0
2	PEG	B	410	7/7	0.84	0.13	13,15,21,26	0
2	PEG	I	403	7/7	0.85	0.20	21,34,44,64	0
2	PEG	D	411	7/7	0.85	0.14	14,22,34,43	0
2	PEG	A	401	7/7	0.85	0.14	14,20,30,31	0
4	PHT	E	404	12/12	0.85	0.21	11,34,56,69	0
4	PHT	F	402	12/12	0.85	0.19	14,31,50,67	0
2	PEG	E	406	7/7	0.85	0.16	11,18,29,30	0
3	EDO	E	412	4/4	0.85	0.15	12,16,20,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEG	B	403	7/7	0.85	0.18	23,43,47,56	0
3	EDO	F	403	4/4	0.85	0.15	24,27,32,35	0
3	EDO	I	408	4/4	0.86	0.13	13,15,27,27	0
3	EDO	J	405	4/4	0.86	0.11	17,22,24,34	0
3	EDO	J	411	4/4	0.86	0.14	15,15,23,26	0
3	EDO	B	412	4/4	0.86	0.11	14,20,29,31	0
3	EDO	B	413	4/4	0.86	0.15	12,14,17,29	0
3	EDO	C	401	4/4	0.86	0.15	17,23,25,27	0
3	EDO	C	404	4/4	0.86	0.17	12,19,19,24	0
2	PEG	G	410	7/7	0.86	0.12	10,11,18,19	0
3	EDO	A	404	4/4	0.86	0.16	12,12,13,21	0
3	EDO	G	405	4/4	0.86	0.12	18,25,33,52	0
2	PEG	E	409	7/7	0.86	0.11	10,17,22,24	0
3	EDO	H	401	4/4	0.86	0.18	13,13,13,22	0
2	PEG	G	401	7/7	0.86	0.14	9,9,13,14	0
6	MLI	J	406	7/7	0.86	0.14	21,28,38,41	0
3	EDO	B	417	4/4	0.87	0.11	10,23,23,23	0
2	PEG	A	408	7/7	0.87	0.12	14,22,31,35	0
3	EDO	H	402	4/4	0.87	0.15	12,12,24,25	0
2	PEG	F	407	7/7	0.87	0.14	11,12,20,21	0
3	EDO	B	409	4/4	0.87	0.13	11,11,11,19	0
2	PEG	J	408	7/7	0.87	0.19	16,21,32,32	0
2	PEG	J	402	7/7	0.87	0.16	24,39,43,50	0
3	EDO	E	401	4/4	0.87	0.13	11,14,15,18	0
5	1BO	B	405	5/5	0.87	0.14	14,18,31,37	0
3	EDO	E	411	4/4	0.87	0.16	17,19,19,32	0
4	PHT	I	405	12/12	0.88	0.17	15,27,53,68	0
3	EDO	I	409	4/4	0.88	0.10	14,15,15,15	0
2	PEG	A	402	7/7	0.88	0.13	13,21,25,27	0
3	EDO	B	406	4/4	0.88	0.15	11,14,17,20	0
3	EDO	J	412	4/4	0.88	0.11	16,20,22,23	0
2	PEG	A	409	7/7	0.89	0.19	17,28,39,45	0
2	PEG	E	408	7/7	0.89	0.12	11,20,29,29	0
5	1BO	D	407	5/5	0.89	0.16	10,12,12,17	0
3	EDO	G	412	4/4	0.89	0.12	13,14,15,20	0
2	PEG	I	407	7/7	0.90	0.11	13,23,27,35	0
3	EDO	D	405	4/4	0.90	0.13	25,26,39,40	0
3	EDO	B	402	4/4	0.90	0.13	10,16,24,36	0
2	PEG	F	409	7/7	0.90	0.14	12,12,29,31	0
3	EDO	J	409	4/4	0.90	0.11	19,23,23,24	0
3	EDO	C	407	4/4	0.90	0.12	9,9,9,10	0
3	EDO	C	408	4/4	0.90	0.13	9,13,17,34	0

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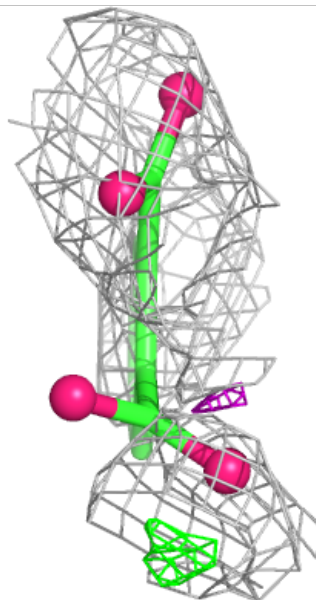
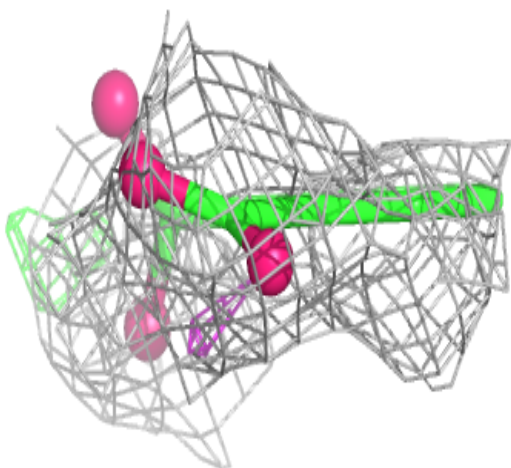
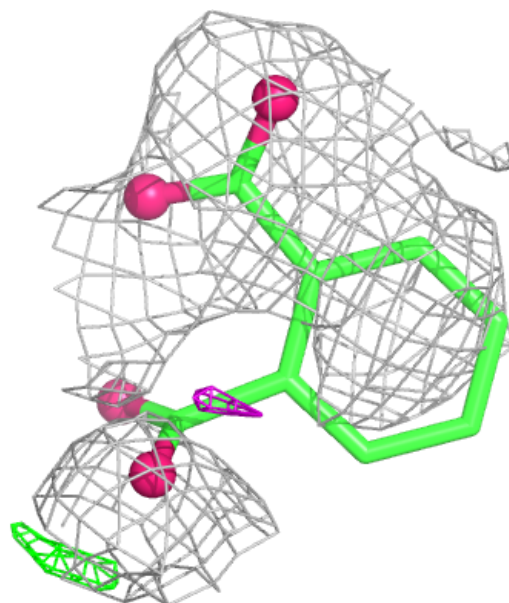
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	F	414	4/4	0.91	0.12	12,12,12,13	0
3	EDO	G	402	4/4	0.91	0.13	10,11,13,15	0
3	EDO	H	403	4/4	0.91	0.12	12,12,12,17	0
2	PEG	I	406	7/7	0.91	0.12	11,12,17,24	0
2	PEG	G	406	7/7	0.91	0.11	10,14,33,37	0
3	EDO	G	408	4/4	0.91	0.14	15,19,29,29	0
3	EDO	B	407	4/4	0.91	0.14	10,12,14,15	0
3	EDO	B	408	4/4	0.91	0.09	9,11,11,17	0
3	EDO	D	415	4/4	0.92	0.12	10,10,10,10	0
2	PEG	C	406	7/7	0.92	0.10	9,9,11,17	0
2	PEG	D	413	7/7	0.92	0.15	12,14,21,25	0
3	EDO	B	416	4/4	0.92	0.11	9,9,10,10	0
3	EDO	G	403	4/4	0.92	0.13	10,10,12,19	0
3	EDO	H	407	4/4	0.92	0.10	11,12,15,26	0
2	PEG	C	402	7/7	0.92	0.12	10,10,15,17	0
3	EDO	A	403	4/4	0.92	0.10	11,11,11,13	0
6	MLI	F	405	7/7	0.92	0.13	11,18,26,27	0
3	EDO	B	411	4/4	0.92	0.10	10,14,15,21	0
3	EDO	G	413	4/4	0.93	0.10	10,10,14,18	0
2	PEG	A	410	7/7	0.93	0.12	11,13,15,21	0
3	EDO	J	410	4/4	0.93	0.10	17,17,19,23	0
2	PEG	F	406	7/7	0.93	0.15	12,12,16,20	0
3	EDO	B	414	4/4	0.93	0.11	13,14,19,27	0
3	EDO	F	411	4/4	0.93	0.10	10,10,14,22	0
3	EDO	I	401	4/4	0.93	0.10	12,12,12,16	0
3	EDO	B	415	4/4	0.93	0.14	11,11,11,17	0
2	PEG	G	409	7/7	0.93	0.12	11,13,19,25	0
2	PEG	D	412	7/7	0.93	0.11	10,12,20,21	0
3	EDO	C	409	4/4	0.94	0.08	9,10,16,20	0
2	PEG	A	411	7/7	0.94	0.11	12,13,23,24	0
2	PEG	C	405	7/7	0.95	0.14	12,14,20,20	0
3	EDO	H	406	4/4	0.96	0.09	12,14,15,23	0
3	EDO	D	410	4/4	0.96	0.07	8,8,8,8	0
3	EDO	B	401	4/4	0.97	0.07	10,10,10,10	0
3	EDO	E	410	4/4	0.97	0.06	11,11,11,11	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.

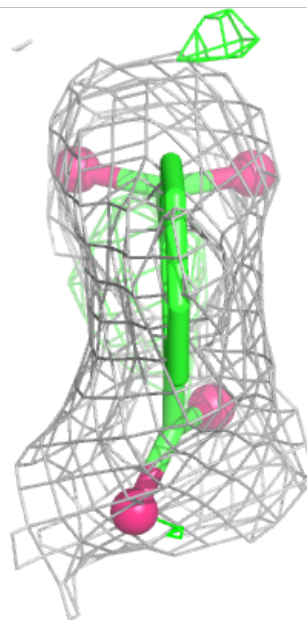
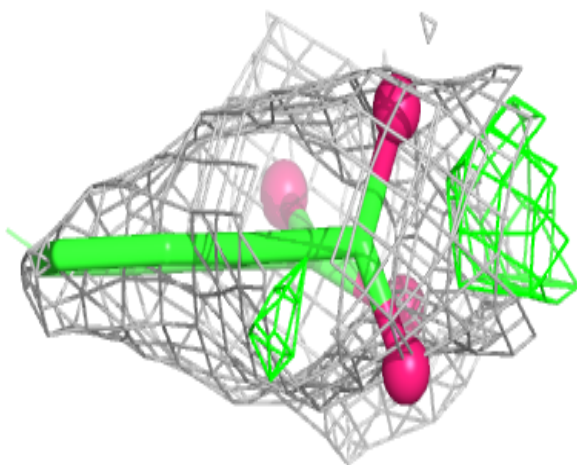
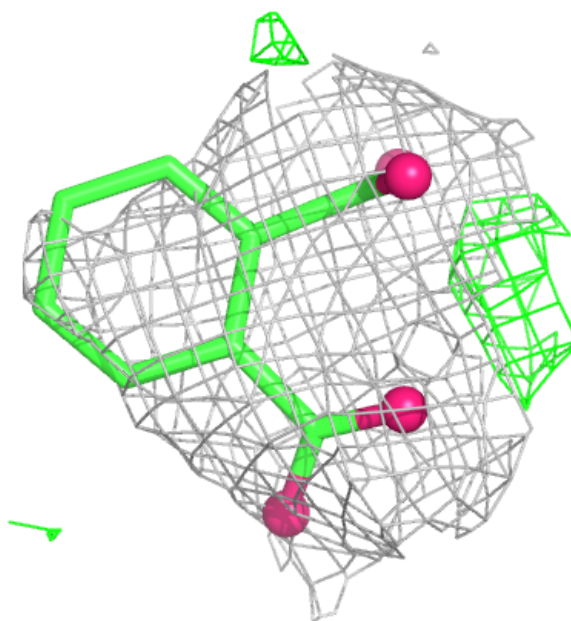
**Electron density around PHT G 407:**

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



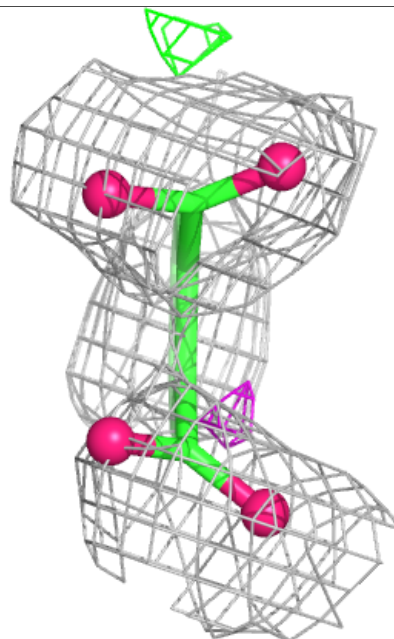
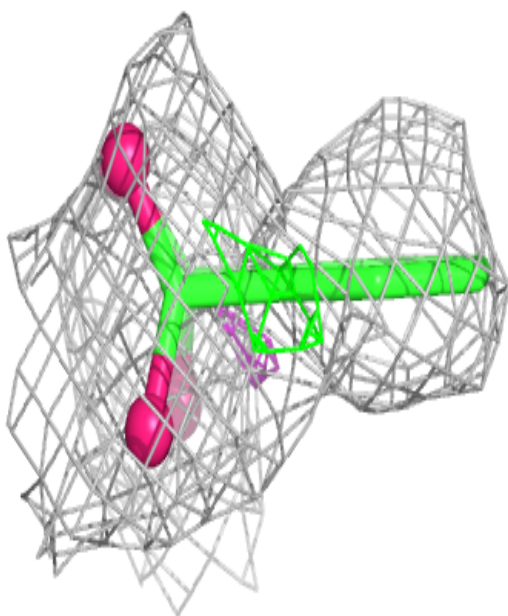
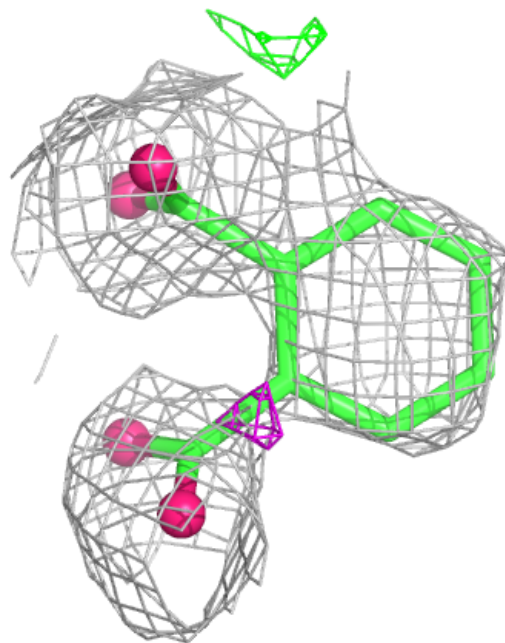
**Electron density around PHT A 405:**

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



**Electron density around PHT J 404:**

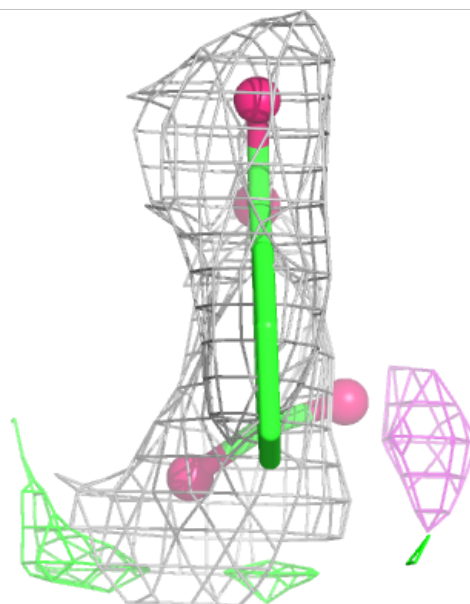
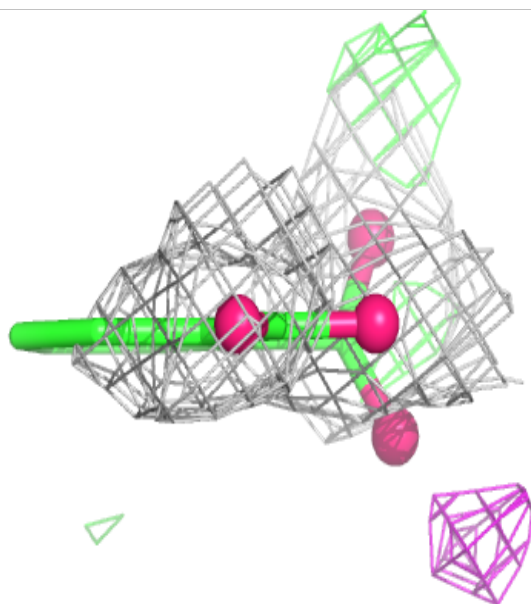
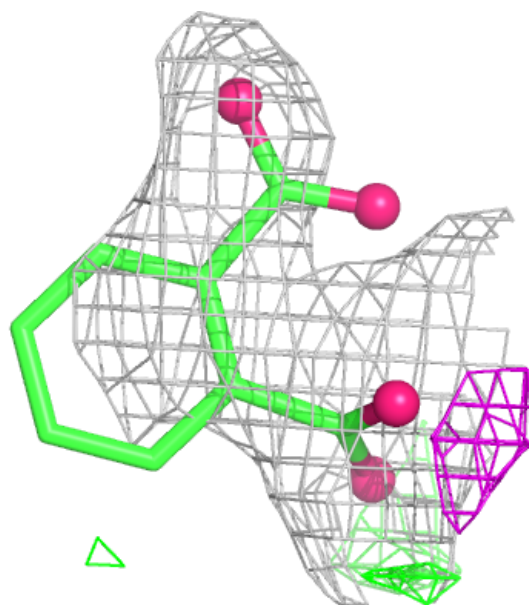
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





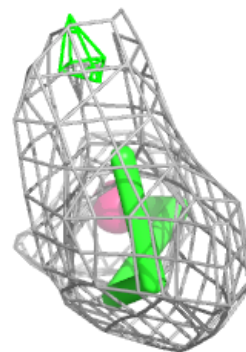
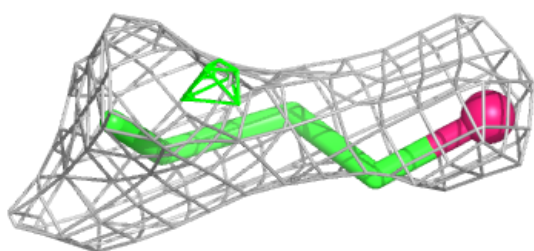
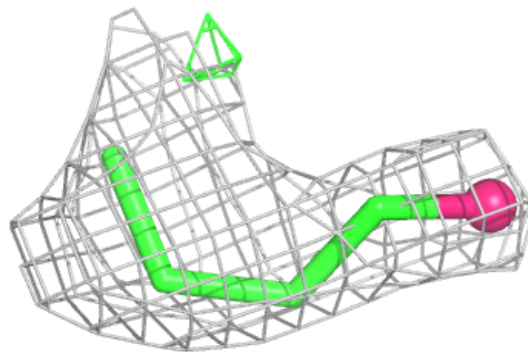
**Electron density around PHT C 403:**

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



**Electron density around 1BO A 406:**

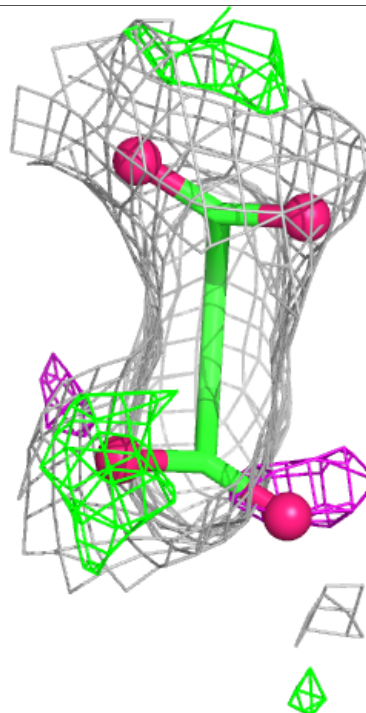
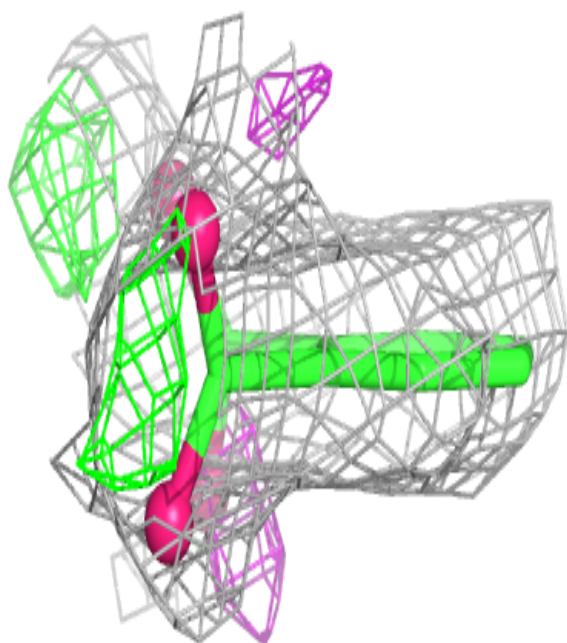
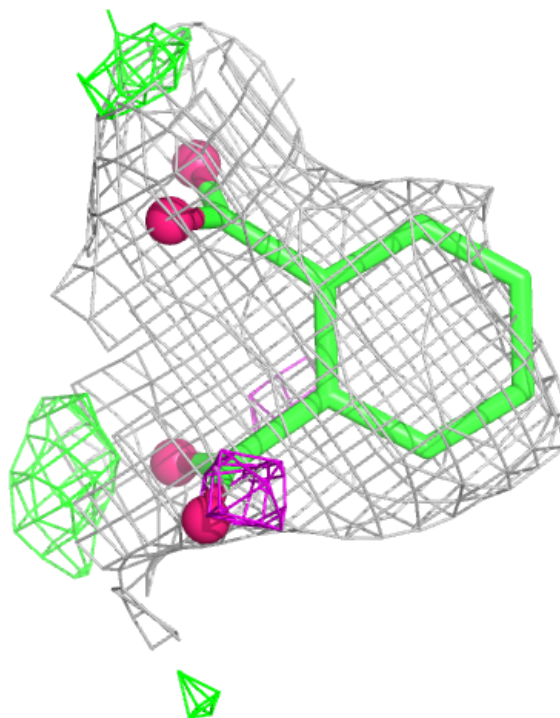
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





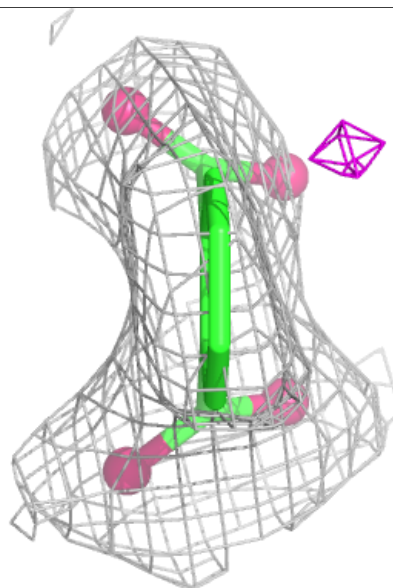
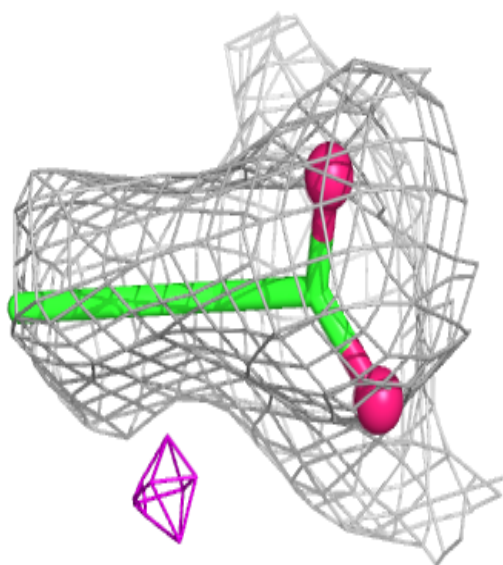
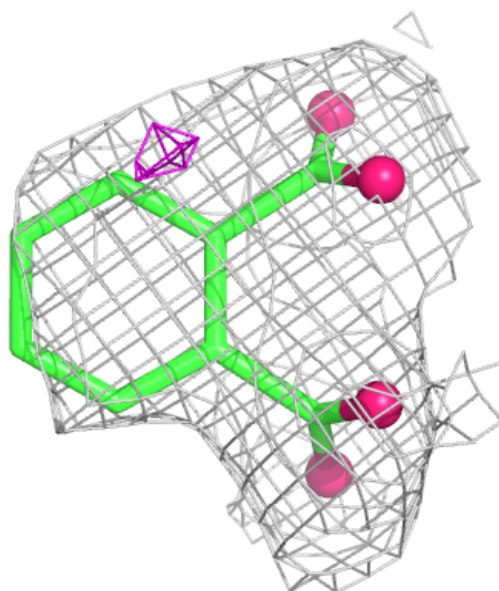
**Electron density around PHT D 406:**

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



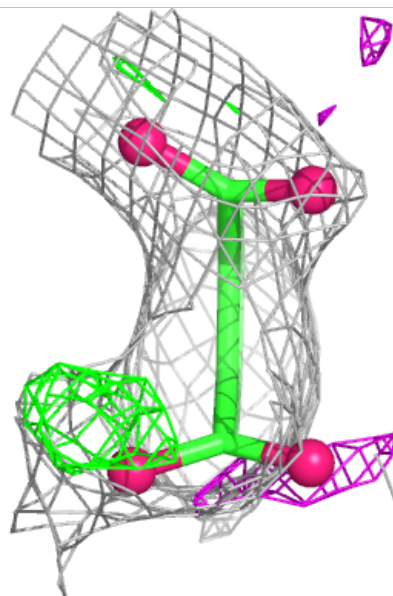
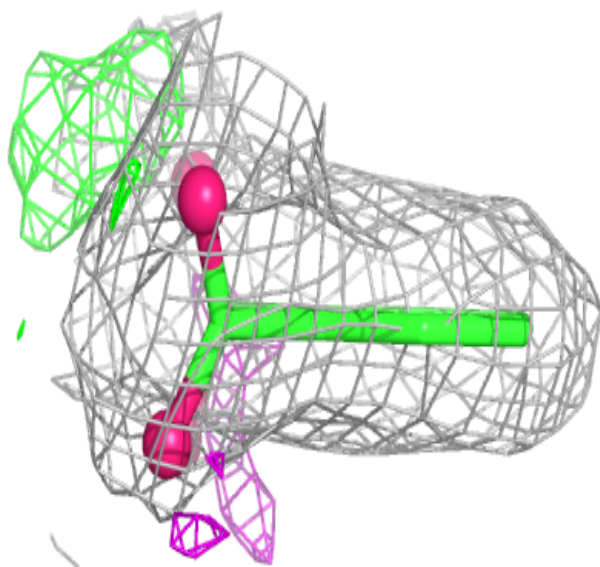
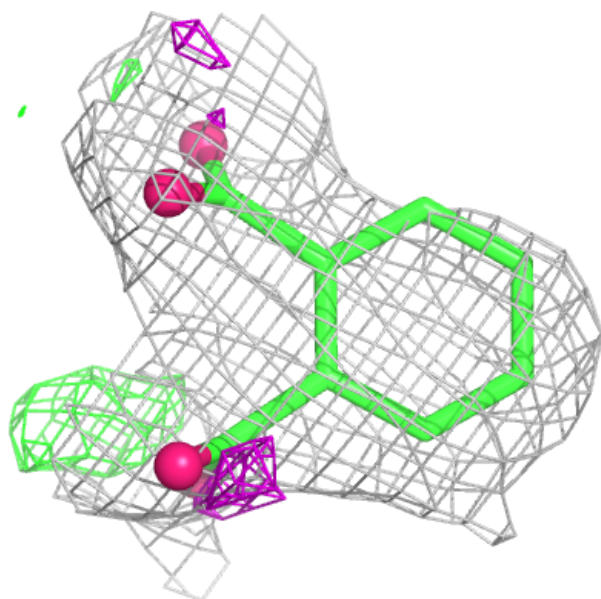
**Electron density around PHT H 405:**

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



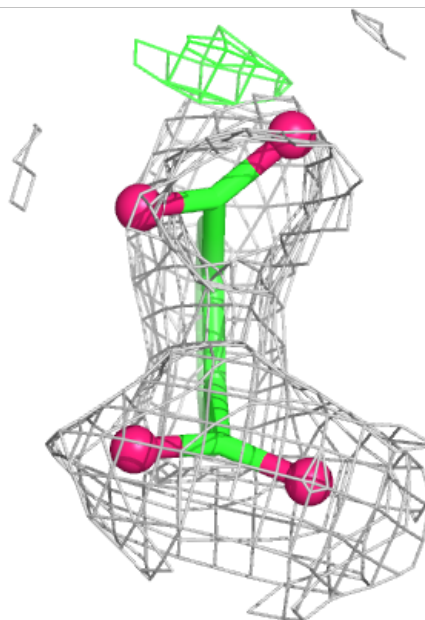
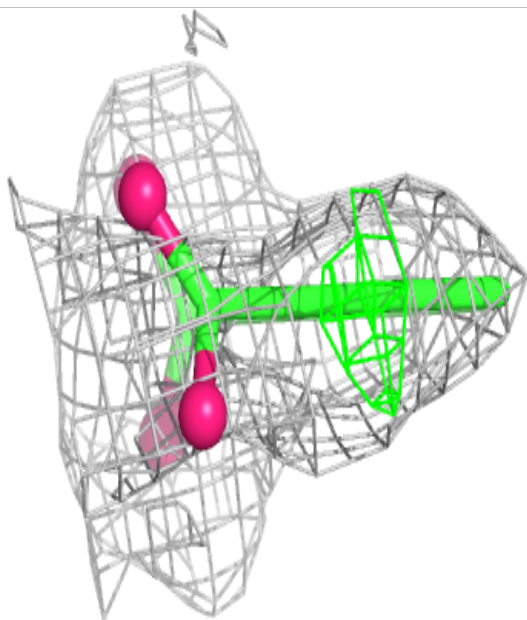
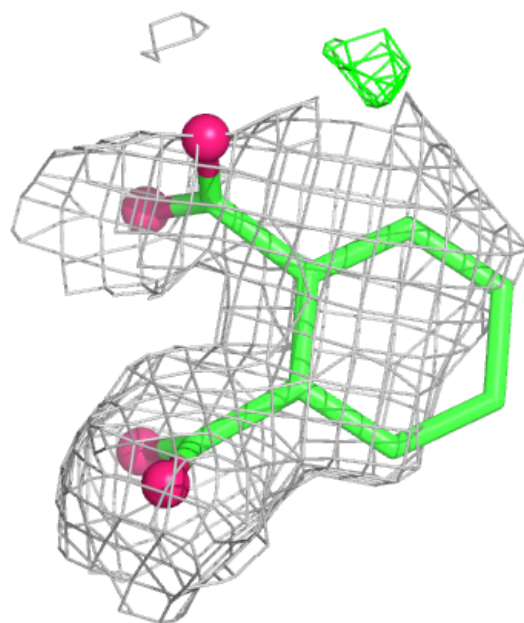
**Electron density around PHT B 404:**

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



**Electron density around PHT E 404:**

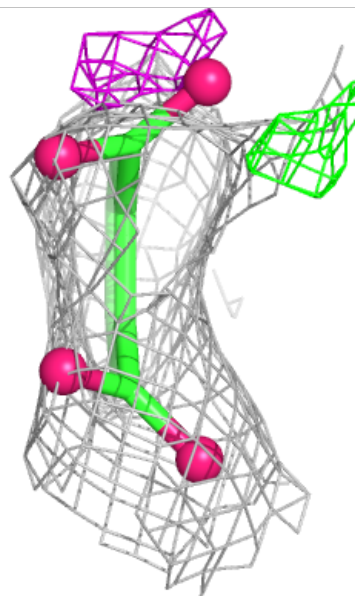
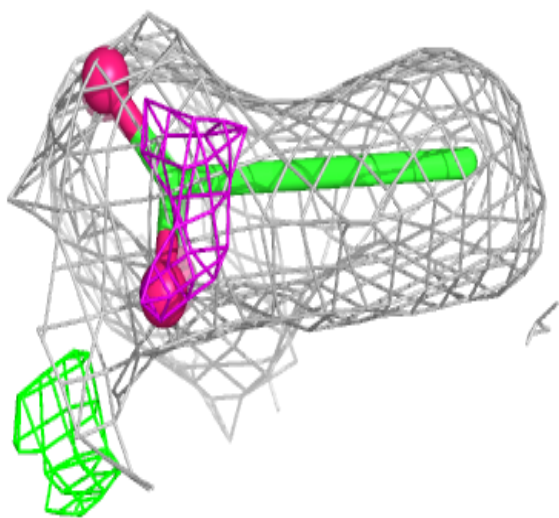
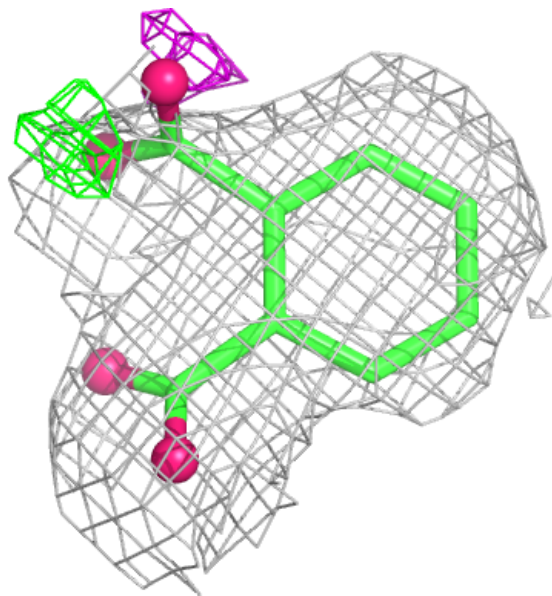
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





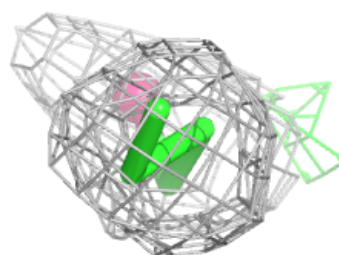
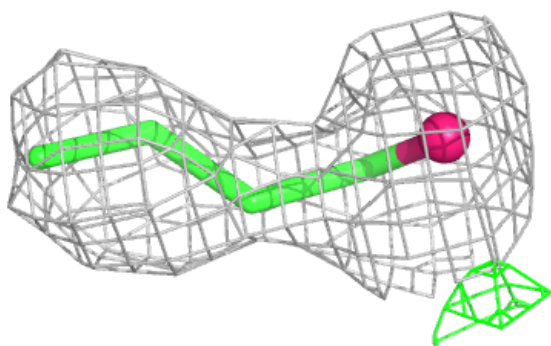
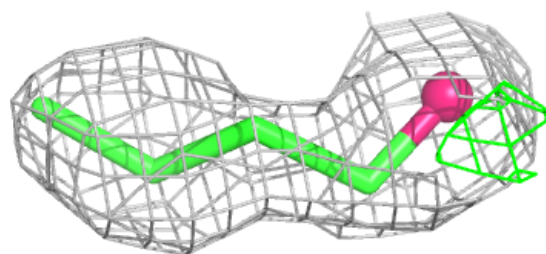
**Electron density around PHT F 402:**

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



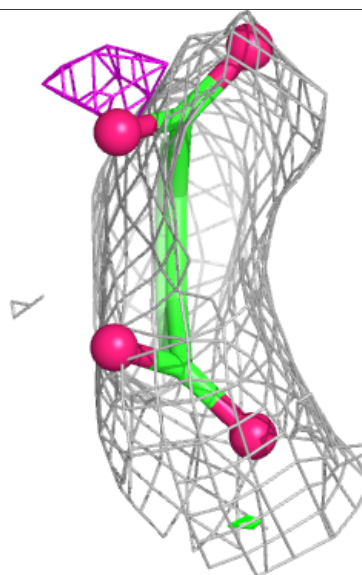
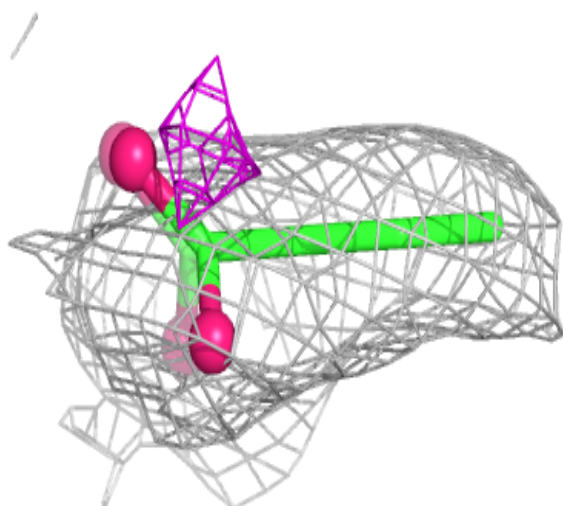
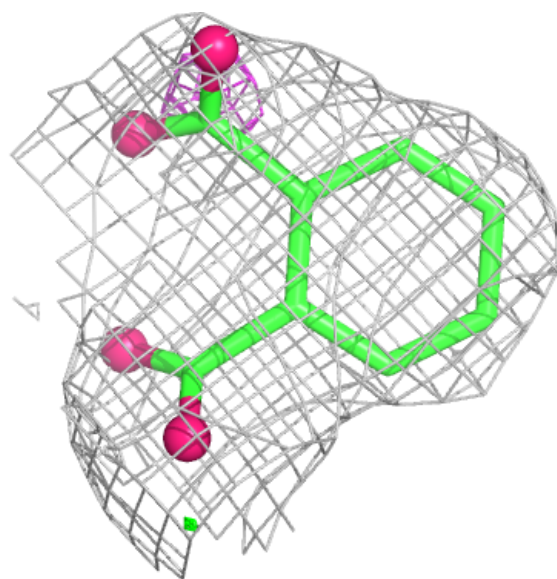
**Electron density around 1BO B 405:**

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



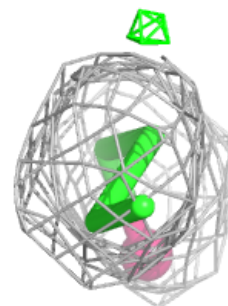
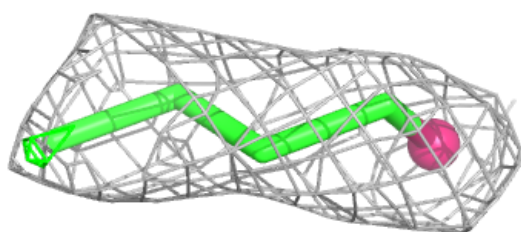
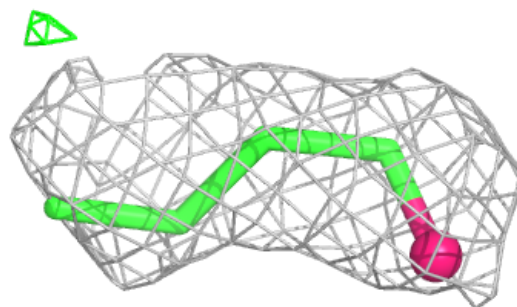
**Electron density around PHT I 405:**

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



**Electron density around 1BO D 407:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.