



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 03:21 AM UTC

PDB ID : 6ZI7 / pdb_00006zi7
Title : Crystal structure of OleP-oleandolide(DEO) bound to L-rhamnose
Authors : Montemiglio, L.C.; Savino, C.; Vallone, B.; Parisi, G.; Freda, I.
Deposited on : 2020-06-25
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

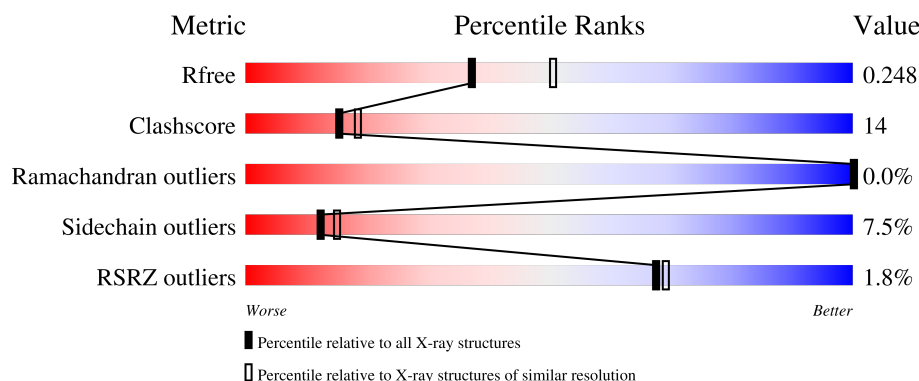
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	407	70%24% . .
1	B	407	% 75%19% . .
1	C	407	% 79%17% . .
1	D	407	2% 69%25% . .
1	E	407	% 70%24% . .

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Mol	Chain	Length	Quality of chain
1	F	407	

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	RAM	A	503[A]	-	-	X	-
4	RAM	A	503[B]	-	-	X	-
4	RAM	B	513	-	-	X	-
4	RAM	D	503	-	-	X	-
5	FMT	A	510	-	-	X	-
5	FMT	A	511	-	-	X	-
5	FMT	A	531	-	-	X	-
5	FMT	A	550	-	-	X	-
5	FMT	A	565	-	-	X	-
5	FMT	B	503	-	-	X	-
5	FMT	B	511	-	-	X	-
5	FMT	B	534	-	-	X	-
5	FMT	C	507	-	-	X	-
5	FMT	C	552	-	-	X	-
5	FMT	D	504	-	-	X	-
5	FMT	D	528	-	-	X	-
5	FMT	E	501	-	-	X	-
5	FMT	F	505	-	-	X	-
5	FMT	F	509	-	-	X	-
5	FMT	F	514	-	-	X	-

2 Entry composition [i](#)

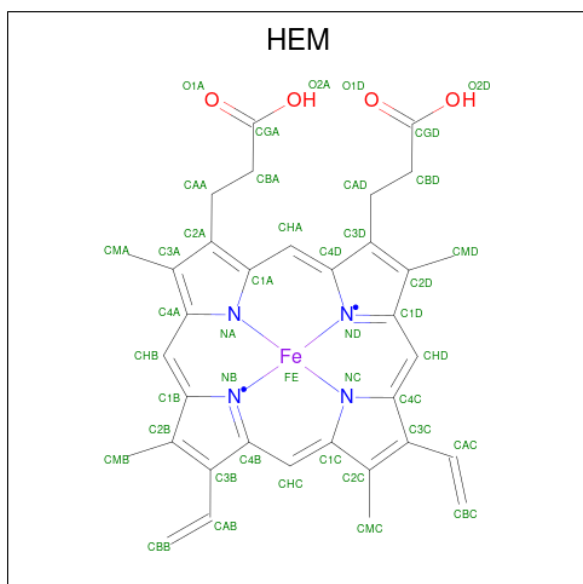
There are 7 unique types of molecules in this entry. The entry contains 22307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

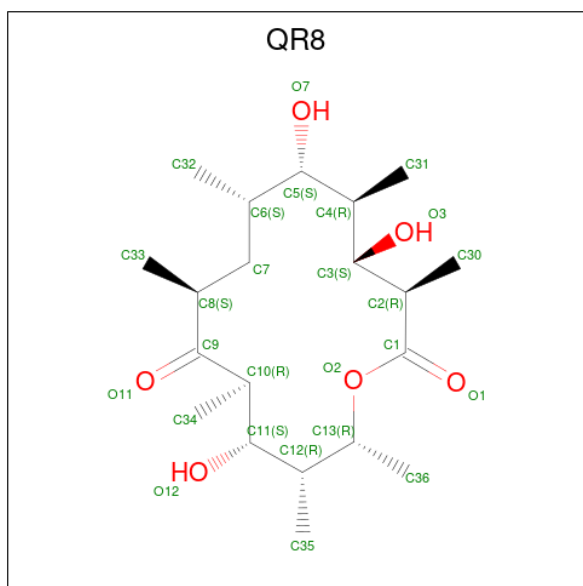
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	36	0
			3303	2099	587	599	18			
1	B	400	Total	C	N	O	S	0	22	0
			3249	2052	574	606	17			
1	C	400	Total	C	N	O	S	0	22	0
			3248	2053	577	603	15			
1	D	400	Total	C	N	O	S	0	42	0
			3372	2142	603	612	15			
1	E	397	Total	C	N	O	S	0	36	0
			3316	2107	591	601	17			
1	F	398	Total	C	N	O	S	0	46	0
			3358	2149	588	606	15			

- 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	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is (3 {R},4 {S},5 {R},6 {S},7 {S},9 {S},11 {R},12 {S},13 {R},14 {R})-3,5,7,9,11,13,14-heptamethyl-4,6,12-tris(oxidanyl)-1-oxacyclotetradecane-2,10-dione (CCD ID: QR8) (formula: C₂₀H₃₆O₆) (labeled as "Ligand of Interest" by depositor).



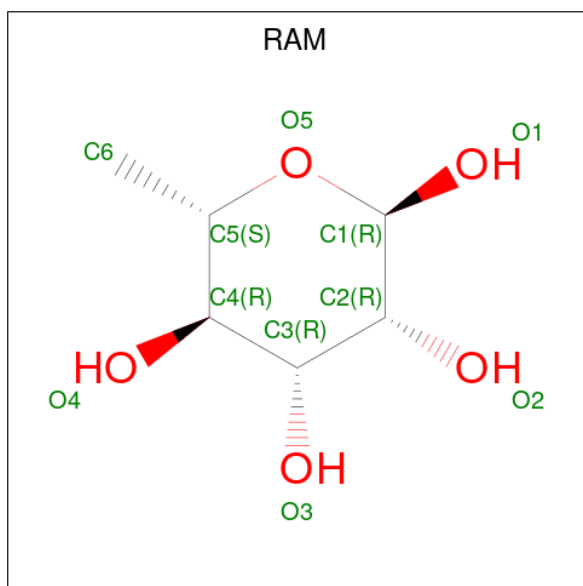
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			26	20	6		
3	B	1	Total	C	O	0	0
			26	20	6		
3	C	1	Total	C	O	0	0
			26	20	6		
3	D	1	Total	C	O	0	0
			26	20	6		
3	E	1	Total	C	O	0	0
			26	20	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			26	20	6		

- Molecule 4 is alpha-L-rhamnopyranose (CCD ID: RAM) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			22	12	10		
4	B	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

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

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

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

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

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

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

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

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

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

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

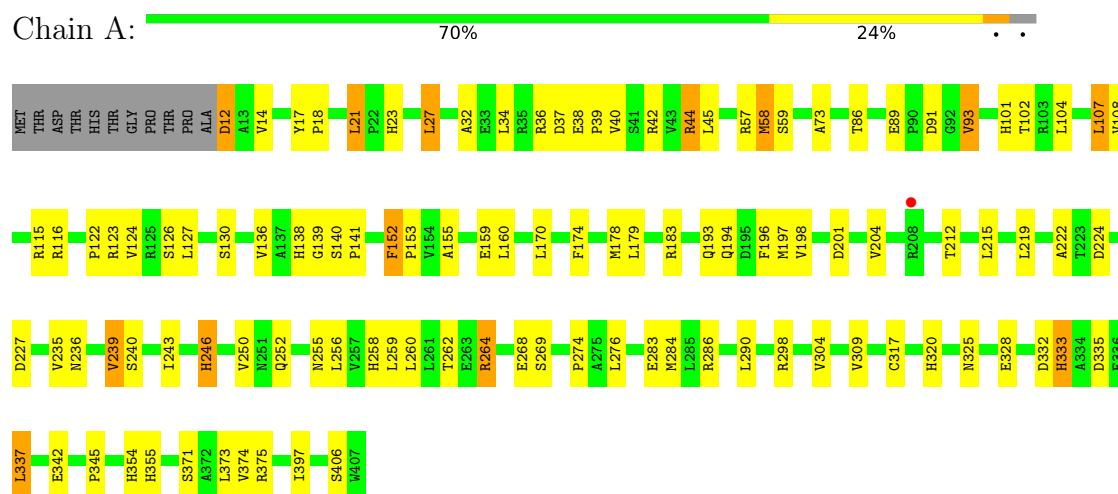
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	260	Total 260	O 260	0	1
7	B	281	Total 281	O 281	0	3
7	C	384	Total 384	O 384	0	3
7	D	158	Total 158	O 158	0	2
7	E	137	Total 137	O 137	0	4
7	F	135	Total 135	O 135	0	2

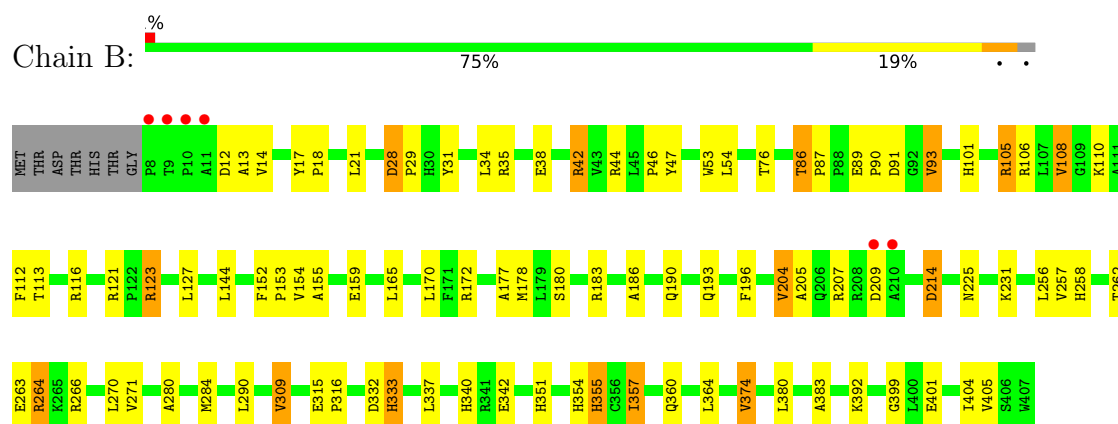
3 Residue-property plots

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

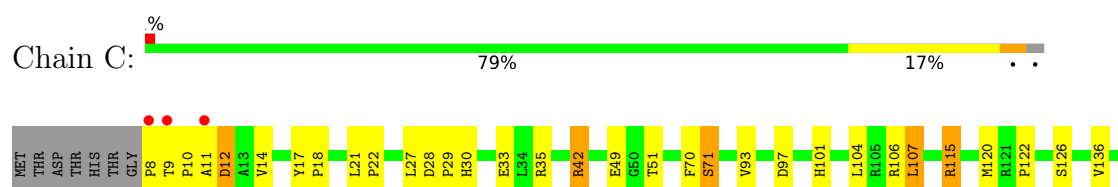
• Molecule 1: Cytochrome P-450

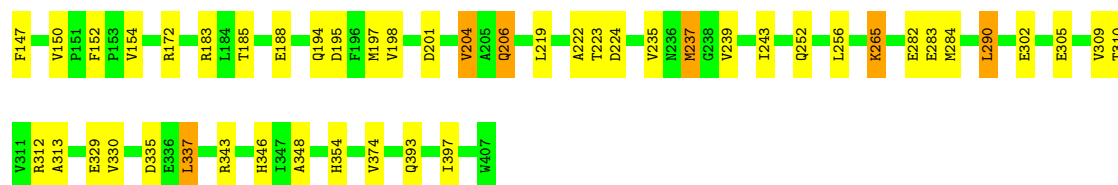


• Molecule 1: Cytochrome P-450

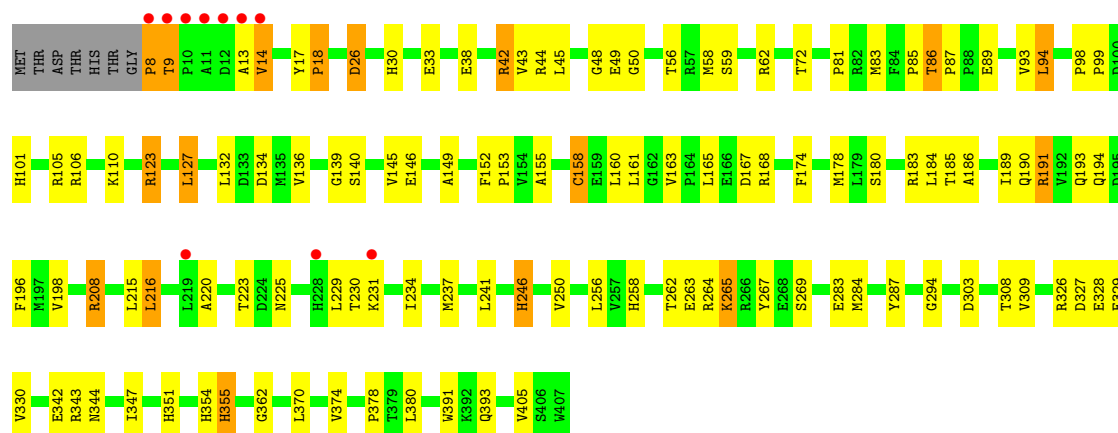


• Molecule 1: Cytochrome P-450

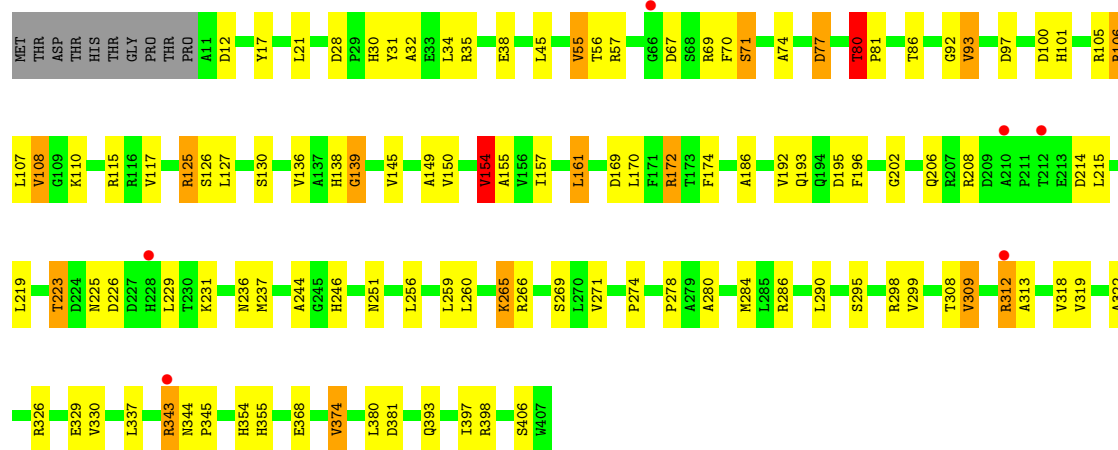




• Molecule 1: Cytochrome P-450

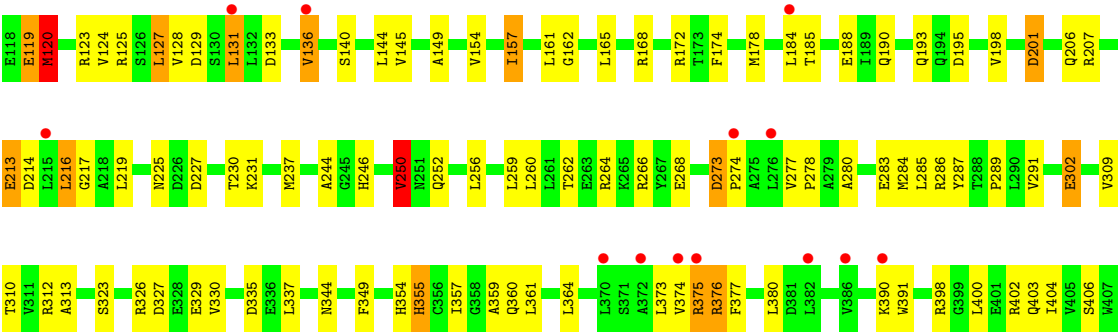


• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.53Å 110.68Å 159.28Å 90.00° 129.46° 90.00°	Depositor
Resolution (Å)	47.92 – 2.28 47.92 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.92-2.28) 99.9 (47.92-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.184 , 0.247 0.190 , 0.248	Depositor DCC
R_{free} test set	14058 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	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*k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22307	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 40.86 % 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 2.5720e-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: NA, RAM, HEM, QR8, 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	1.23	8/3483 (0.2%)	1.50	15/4732 (0.3%)
1	B	1.26	11/3385 (0.3%)	1.51	14/4606 (0.3%)
1	C	1.28	12/3385 (0.4%)	1.49	9/4606 (0.2%)
1	D	1.23	5/3572 (0.1%)	1.51	22/4852 (0.5%)
1	E	1.19	1/3489 (0.0%)	1.52	23/4744 (0.5%)
1	F	1.31	6/3561 (0.2%)	1.70	34/4843 (0.7%)
All	All	1.25	43/20875 (0.2%)	1.54	117/28383 (0.4%)

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	F	0	3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	26[A]	ASP	CA-C	17.62	1.73	1.52
1	F	26[B]	ASP	CA-C	17.62	1.73	1.52
1	A	320	HIS	CE1-NE2	8.94	1.41	1.32
1	F	120[A]	MET	CA-C	7.65	1.63	1.52
1	F	120[B]	MET	CA-C	7.65	1.63	1.52

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	26[A]	ASP	CA-C-O	-21.77	96.66	120.38
1	F	26[B]	ASP	CA-C-O	-21.77	96.66	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	120[A]	MET	N-CA-CB	-15.75	83.88	110.49
1	F	120[B]	MET	N-CA-CB	-15.75	83.88	110.49
1	F	25	LEU	CA-C-N	-14.17	103.44	123.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	213	GLU	Peptide
1	F	26[A]	ASP	Mainchain
1	F	26[B]	ASP	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	3303	0	3379	109	0
1	B	3249	0	3256	64	1
1	C	3248	0	3258	62	0
1	D	3372	0	3458	102	0
1	E	3316	0	3380	76	0
1	F	3358	0	3479	115	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
2	E	43	0	30	3	0
2	F	43	0	30	4	0
3	A	26	0	0	3	0
3	B	26	0	0	1	0
3	C	26	0	0	0	0
3	D	26	0	0	2	0
3	E	26	0	0	0	0
3	F	26	0	0	0	0
4	A	22	0	23	33	0
4	B	11	0	12	11	0
4	D	11	0	12	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	210	0	71	21	1
5	B	108	0	36	9	0
5	C	147	0	49	9	0
5	D	99	0	33	8	0
5	E	42	0	14	2	0
5	F	36	0	12	10	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	260	0	0	9	0
7	B	281	0	0	15	0
7	C	384	0	0	17	0
7	D	158	0	0	6	0
7	E	137	0	0	1	0
7	F	135	0	0	9	0
All	All	22307	0	20652	561	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 14.

The worst 5 of 561 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:E:93[A]:VAL:HG11	1:E:237[A]:MET:CE	1.54	1.37
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:CG2	1.66	1.23
1:F:120[A]:MET:CE	1:F:361[A]:LEU:HD21	1.69	1.22
1:A:197[A]:MET:CE	1:A:235[A]:VAL:HG23	1.73	1.19
1:F:120[A]:MET:HE2	1:F:361[A]:LEU:CD2	1.74	1.18

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:360[B]:GLN:NE2	5:A:567:FMT:O2[3_555]	2.18	0.02

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	430/407 (106%)	418 (97%)	12 (3%)	0	100	100
1	B	421/407 (103%)	407 (97%)	14 (3%)	0	100	100
1	C	420/407 (103%)	406 (97%)	14 (3%)	0	100	100
1	D	440/407 (108%)	409 (93%)	31 (7%)	0	100	100
1	E	431/407 (106%)	410 (95%)	21 (5%)	0	100	100
1	F	442/407 (109%)	413 (93%)	28 (6%)	1 (0%)	43	53
All	All	2584/2442 (106%)	2463 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	273	ASP

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	368/341 (108%)	339 (92%)	29 (8%)	11	14
1	B	358/341 (105%)	333 (93%)	25 (7%)	14	17
1	C	357/341 (105%)	339 (95%)	18 (5%)	22	30
1	D	376/341 (110%)	335 (89%)	41 (11%)	6	6
1	E	368/341 (108%)	329 (89%)	39 (11%)	6	7
1	F	377/341 (111%)	339 (90%)	38 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2204/2046 (108%)	2014 (91%)	190 (9%)	12	11

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	55	VAL
1	E	329[B]	GLU
1	E	93[B]	VAL
1	E	172	ARG
1	E	393[A]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	236	ASN
1	E	206	GLN
1	E	193	GLN
1	E	236	ASN
1	B	393	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](#)

Of 236 ligands modelled in this entry, 6 are monoatomic - leaving 230 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	$\# Z > 2$
5	FMT	C	512	-	2,2,2	0.74	0	1,1,1	0.06	0
5	FMT	D	506	-	2,2,2	0.67	0	1,1,1	0.13	0
5	FMT	A	565	-	2,2,2	0.59	0	1,1,1	0.05	0
5	FMT	B	537	-	2,2,2	0.36	0	1,1,1	0.10	0
5	FMT	B	539	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	D	516	-	2,2,2	0.27	0	1,1,1	0.18	0
5	FMT	B	504	-	2,2,2	0.68	0	1,1,1	0.19	0
5	FMT	A	514	-	2,2,2	0.07	0	1,1,1	0.05	0
5	FMT	C	525	-	2,2,2	0.62	0	1,1,1	0.03	0
5	FMT	E	516	-	2,2,2	0.28	0	1,1,1	0.14	0
4	RAM	D	503	-	11,11,11	1.12	1 (9%)	16,16,16	2.67	9 (56%)
5	FMT	C	509	-	2,2,2	0.56	0	1,1,1	0.02	0
5	FMT	C	530	-	2,2,2	0.29	0	1,1,1	0.14	0
5	FMT	C	533	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	A	512	-	2,2,2	0.37	0	1,1,1	0.13	0
2	HEM	B	501	1	50,50,50	1.78	15 (30%)	67,82,82	1.93	18 (26%)
5	FMT	E	510	-	2,2,2	0.27	0	1,1,1	0.14	0
5	FMT	C	511	-	2,2,2	0.54	0	1,1,1	0.04	0
5	FMT	D	528	-	2,2,2	0.24	0	1,1,1	0.08	0
5	FMT	E	517	-	2,2,2	0.26	0	1,1,1	0.17	0
5	FMT	A	523	-	2,2,2	0.86	0	1,1,1	0.18	0
5	FMT	A	563	-	2,2,2	0.31	0	1,1,1	0.15	0
5	FMT	A	557	-	2,2,2	0.24	0	1,1,1	0.17	0
5	FMT	C	522	-	2,2,2	0.77	0	1,1,1	0.11	0
5	FMT	D	535	-	2,2,2	0.38	0	1,1,1	0.14	0
5	FMT	D	525	-	2,2,2	0.28	0	1,1,1	0.17	0
5	FMT	A	504	-	2,2,2	0.11	0	1,1,1	0.32	0
5	FMT	E	508	-	2,2,2	0.25	0	1,1,1	0.17	0
5	FMT	E	513	-	2,2,2	0.29	0	1,1,1	0.14	0
5	FMT	C	518	-	2,2,2	0.59	0	1,1,1	0.07	0
5	FMT	F	511	-	2,2,2	0.27	0	1,1,1	0.15	0
5	FMT	F	505	-	2,2,2	0.61	0	1,1,1	0.05	0
5	FMT	D	534	-	2,2,2	0.24	0	1,1,1	0.17	0
5	FMT	C	514	-	2,2,2	0.32	0	1,1,1	0.43	0
5	FMT	A	524	-	2,2,2	0.86	0	1,1,1	0.24	0
5	FMT	B	526	-	2,2,2	0.25	0	1,1,1	0.14	0
5	FMT	C	546	-	2,2,2	0.20	0	1,1,1	0.20	0
5	FMT	A	530	-	2,2,2	0.53	0	1,1,1	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	F	515	-	2,2,2	0.28	0	1,1,1	0.17	0
5	FMT	D	523	-	2,2,2	0.26	0	1,1,1	0.17	0
5	FMT	B	516	-	2,2,2	0.26	0	1,1,1	0.15	0
5	FMT	A	538	-	2,2,2	0.55	0	1,1,1	0.06	0
5	FMT	A	564	-	2,2,2	0.31	0	1,1,1	0.11	0
5	FMT	C	539	-	2,2,2	0.35	0	1,1,1	0.11	0
5	FMT	B	511	-	2,2,2	0.42	0	1,1,1	0.00	0
5	FMT	B	538	-	2,2,2	0.31	0	1,1,1	0.10	0
2	HEM	D	501	1	50,50,50	1.98	14 (28%)	67,82,82	2.04	17 (25%)
3	QR8	F	503	-	26,26,26	1.72	3 (11%)	37,38,38	1.63	9 (24%)
5	FMT	F	512	-	2,2,2	0.28	0	1,1,1	0.14	0
5	FMT	A	518	-	2,2,2	0.23	0	1,1,1	0.23	0
5	FMT	D	524	-	2,2,2	0.30	0	1,1,1	0.15	0
5	FMT	D	514	-	2,2,2	0.55	0	1,1,1	0.00	0
5	FMT	A	561	-	2,2,2	0.33	0	1,1,1	0.13	0
5	FMT	A	560	-	2,2,2	0.53	0	1,1,1	0.02	0
5	FMT	A	573	-	2,2,2	0.20	0	1,1,1	0.18	0
5	FMT	E	501	-	2,2,2	0.49	0	1,1,1	0.04	0
5	FMT	A	539	-	2,2,2	0.29	0	1,1,1	0.13	0
5	FMT	F	513	-	2,2,2	0.41	0	1,1,1	0.06	0
5	FMT	C	549	-	2,2,2	0.29	0	1,1,1	0.14	0
5	FMT	D	537	-	2,2,2	0.61	0	1,1,1	0.13	0
5	FMT	A	536	-	2,2,2	0.40	0	1,1,1	0.02	0
5	FMT	B	520	-	2,2,2	0.31	0	1,1,1	0.13	0
5	FMT	D	521	-	2,2,2	0.27	0	1,1,1	0.17	0
5	FMT	D	507	-	2,2,2	0.60	0	1,1,1	0.07	0
5	FMT	C	508	-	2,2,2	0.31	0	1,1,1	0.21	0
5	FMT	B	503	-	2,2,2	1.03	0	1,1,1	0.28	0
5	FMT	B	522	-	2,2,2	0.32	0	1,1,1	0.12	0
5	FMT	F	504	-	2,2,2	0.43	0	1,1,1	0.05	0
5	FMT	B	534	-	2,2,2	0.31	0	1,1,1	0.21	0
3	QR8	A	502	-	26,26,26	1.73	4 (15%)	37,38,38	1.87	10 (27%)
5	FMT	C	531	-	2,2,2	0.26	0	1,1,1	0.15	0
5	FMT	C	551	-	2,2,2	0.24	0	1,1,1	0.15	0
5	FMT	C	515	-	2,2,2	0.87	0	1,1,1	0.15	0
5	FMT	D	532	-	2,2,2	0.19	0	1,1,1	0.17	0
5	FMT	A	531	-	2,2,2	0.61	0	1,1,1	0.07	0
4	RAM	A	503[A]	-	11,11,11	1.32	3 (27%)	16,16,16	3.59	10 (62%)
5	FMT	A	545	-	2,2,2	0.50	0	1,1,1	0.06	0
5	FMT	A	541	-	2,2,2	0.25	0	1,1,1	0.17	0
5	FMT	C	532	-	2,2,2	0.95	0	1,1,1	0.19	0
5	FMT	D	530	-	2,2,2	0.32	0	1,1,1	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	F	507	-	2,2,2	0.47	0	1,1,1	0.14	0
5	FMT	D	533	-	2,2,2	0.27	0	1,1,1	0.07	0
5	FMT	E	514	-	2,2,2	0.34	0	1,1,1	0.09	0
5	FMT	A	555	-	2,2,2	0.51	0	1,1,1	0.03	0
5	FMT	D	505	-	2,2,2	0.70	0	1,1,1	0.06	0
5	FMT	A	550	-	2,2,2	0.36	0	1,1,1	0.18	0
5	FMT	D	508	-	2,2,2	0.30	0	1,1,1	0.04	0
3	QR8	D	502	-	26,26,26	1.67	4 (15%)	37,38,38	1.90	9 (24%)
5	FMT	A	558	-	2,2,2	0.39	0	1,1,1	0.11	0
5	FMT	A	571	-	2,2,2	0.28	0	1,1,1	0.13	0
5	FMT	C	505	-	2,2,2	0.90	0	1,1,1	0.13	0
5	FMT	B	540	-	2,2,2	0.27	0	1,1,1	0.14	0
5	FMT	C	506	-	2,2,2	0.75	0	1,1,1	0.03	0
5	FMT	D	536	-	2,2,2	0.27	0	1,1,1	0.17	0
5	FMT	C	516	-	2,2,2	0.27	0	1,1,1	0.24	0
5	FMT	B	525	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	A	551	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	A	509	-	2,2,2	0.76	0	1,1,1	0.13	0
5	FMT	C	536	-	2,2,2	0.30	0	1,1,1	0.13	0
5	FMT	A	527	-	2,2,2	0.33	0	1,1,1	0.11	0
5	FMT	A	568	-	2,2,2	0.27	0	1,1,1	0.13	0
5	FMT	B	507	-	2,2,2	0.36	0	1,1,1	0.13	0
5	FMT	D	518	-	2,2,2	0.26	0	1,1,1	0.13	0
5	FMT	F	510	-	2,2,2	0.28	0	1,1,1	0.14	0
5	FMT	A	543	-	2,2,2	0.41	0	1,1,1	0.03	0
5	FMT	B	533	-	2,2,2	0.46	0	1,1,1	0.09	0
5	FMT	C	545	-	2,2,2	0.36	0	1,1,1	0.12	0
5	FMT	A	519	-	2,2,2	0.36	0	1,1,1	0.16	0
3	QR8	C	502	-	26,26,26	1.58	3 (11%)	37,38,38	1.79	8 (21%)
5	FMT	A	544	-	2,2,2	0.41	0	1,1,1	0.03	0
5	FMT	B	512	-	2,2,2	0.64	0	1,1,1	0.11	0
5	FMT	A	528	-	2,2,2	0.32	0	1,1,1	0.09	0
5	FMT	F	506	-	2,2,2	0.33	0	1,1,1	0.19	0
5	FMT	A	537	-	2,2,2	0.28	0	1,1,1	0.17	0
5	FMT	C	534	-	2,2,2	0.31	0	1,1,1	0.16	0
5	FMT	C	550	-	2,2,2	0.57	0	1,1,1	0.05	0
4	RAM	B	513	-	11,11,11	1.74	4 (36%)	16,16,16	3.49	9 (56%)
5	FMT	C	535	-	2,2,2	0.30	0	1,1,1	0.14	0
5	FMT	C	541	-	2,2,2	0.31	0	1,1,1	0.12	0
5	FMT	C	503	-	2,2,2	0.76	0	1,1,1	0.18	0
5	FMT	B	527	-	2,2,2	0.27	0	1,1,1	0.14	0
5	FMT	A	506	-	2,2,2	0.97	0	1,1,1	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	A	546	-	2,2,2	0.45	0	1,1,1	0.00	0
5	FMT	A	542	-	2,2,2	0.26	0	1,1,1	0.16	0
5	FMT	D	520	-	2,2,2	0.31	0	1,1,1	0.11	0
5	FMT	D	519	-	2,2,2	0.31	0	1,1,1	0.16	0
5	FMT	D	531	-	2,2,2	0.45	0	1,1,1	0.01	0
5	FMT	A	535	-	2,2,2	0.27	0	1,1,1	0.13	0
5	FMT	A	533	-	2,2,2	0.27	0	1,1,1	0.17	0
5	FMT	C	513	-	2,2,2	0.61	0	1,1,1	0.09	0
5	FMT	A	505	-	2,2,2	0.48	0	1,1,1	0.18	0
5	FMT	B	536	-	2,2,2	0.28	0	1,1,1	0.18	0
5	FMT	C	520	-	2,2,2	0.63	0	1,1,1	0.10	0
5	FMT	A	510	-	2,2,2	0.46	0	1,1,1	0.08	0
5	FMT	A	522	-	2,2,2	0.65	0	1,1,1	0.03	0
5	FMT	B	523	-	2,2,2	0.35	0	1,1,1	0.10	0
5	FMT	C	540	-	2,2,2	0.41	0	1,1,1	0.08	0
5	FMT	F	509	-	2,2,2	0.44	0	1,1,1	0.08	0
2	HEM	C	501	1	50,50,50	1.86	17 (34%)	67,82,82	2.20	26 (38%)
5	FMT	A	529	-	2,2,2	0.27	0	1,1,1	0.15	0
5	FMT	A	532	-	2,2,2	0.38	0	1,1,1	0.08	0
2	HEM	A	501	1	50,50,50	1.68	11 (22%)	67,82,82	2.04	19 (28%)
5	FMT	A	574	-	2,2,2	0.27	0	1,1,1	0.15	0
2	HEM	E	502	1	50,50,50	1.69	9 (18%)	67,82,82	1.68	17 (25%)
5	FMT	C	517	-	2,2,2	0.60	0	1,1,1	0.06	0
5	FMT	B	509	-	2,2,2	0.60	0	1,1,1	0.03	0
5	FMT	A	559	-	2,2,2	0.33	0	1,1,1	0.09	0
5	FMT	B	524	-	2,2,2	0.40	0	1,1,1	0.04	0
5	FMT	A	508	-	2,2,2	0.95	0	1,1,1	0.15	0
5	FMT	A	513	-	2,2,2	0.49	0	1,1,1	0.05	0
5	FMT	B	517	-	2,2,2	0.39	0	1,1,1	0.09	0
5	FMT	B	529	-	2,2,2	0.43	0	1,1,1	0.02	0
5	FMT	B	508	-	2,2,2	0.43	0	1,1,1	0.03	0
5	FMT	C	521	-	2,2,2	0.06	0	1,1,1	0.33	0
5	FMT	A	556	-	2,2,2	0.31	0	1,1,1	0.14	0
5	FMT	C	524	-	2,2,2	0.16	0	1,1,1	0.43	0
5	FMT	C	507	-	2,2,2	0.73	0	1,1,1	0.32	0
5	FMT	C	537	-	2,2,2	0.33	0	1,1,1	0.15	0
5	FMT	A	562	-	2,2,2	0.66	0	1,1,1	0.07	0
5	FMT	B	521	-	2,2,2	0.52	0	1,1,1	0.05	0
5	FMT	A	511	-	2,2,2	0.69	0	1,1,1	0.13	0
5	FMT	B	531	-	2,2,2	0.30	0	1,1,1	0.15	0
5	FMT	A	515	-	2,2,2	0.46	0	1,1,1	0.07	0
5	FMT	A	517	-	2,2,2	0.30	0	1,1,1	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	A	554	-	2,2,2	0.33	0	1,1,1	0.11	0
5	FMT	A	553	-	2,2,2	0.35	0	1,1,1	0.10	0
5	FMT	E	505	-	2,2,2	0.33	0	1,1,1	0.14	0
5	FMT	D	509	-	2,2,2	0.70	0	1,1,1	0.02	0
5	FMT	A	549	-	2,2,2	0.42	0	1,1,1	0.00	0
5	FMT	C	510	-	2,2,2	0.54	0	1,1,1	0.07	0
5	FMT	C	528	-	2,2,2	0.31	0	1,1,1	0.16	0
5	FMT	D	527	-	2,2,2	0.27	0	1,1,1	0.15	0
5	FMT	D	511	-	2,2,2	0.69	0	1,1,1	0.04	0
5	FMT	E	515	-	2,2,2	0.33	0	1,1,1	0.09	0
5	FMT	D	515	-	2,2,2	0.34	0	1,1,1	0.11	0
5	FMT	E	504	-	2,2,2	0.89	0	1,1,1	0.32	0
5	FMT	C	523	-	2,2,2	0.22	0	1,1,1	0.15	0
5	FMT	B	528	-	2,2,2	0.38	0	1,1,1	0.11	0
5	FMT	D	510	-	2,2,2	0.44	0	1,1,1	0.07	0
5	FMT	C	538	-	2,2,2	0.42	0	1,1,1	0.10	0
5	FMT	A	507	-	2,2,2	0.65	0	1,1,1	0.12	0
3	QR8	B	502	-	26,26,26	1.83	4 (15%)	37,38,38	1.77	12 (32%)
5	FMT	A	552	-	2,2,2	0.35	0	1,1,1	0.11	0
5	FMT	A	548	-	2,2,2	0.56	0	1,1,1	0.00	0
5	FMT	A	569	-	2,2,2	0.26	0	1,1,1	0.17	0
5	FMT	A	520	-	2,2,2	0.41	0	1,1,1	0.09	0
5	FMT	C	542	-	2,2,2	0.34	0	1,1,1	0.11	0
3	QR8	E	503	-	26,26,26	1.58	4 (15%)	37,38,38	1.80	12 (32%)
5	FMT	E	512	-	2,2,2	0.30	0	1,1,1	0.12	0
5	FMT	C	552	-	2,2,2	0.31	0	1,1,1	0.15	0
5	FMT	A	572	-	2,2,2	0.26	0	1,1,1	0.14	0
5	FMT	A	547	-	2,2,2	0.33	0	1,1,1	0.12	0
5	FMT	D	526	-	2,2,2	0.33	0	1,1,1	0.13	0
5	FMT	A	567	-	2,2,2	0.32	0	1,1,1	0.13	0
5	FMT	B	530	-	2,2,2	0.19	0	1,1,1	0.17	0
2	HEM	F	502	1	50,50,50	1.59	10 (20%)	67,82,82	1.59	12 (17%)
5	FMT	A	540	-	2,2,2	0.25	0	1,1,1	0.15	0
5	FMT	C	529	-	2,2,2	0.23	0	1,1,1	0.16	0
5	FMT	D	522	-	2,2,2	0.25	0	1,1,1	0.17	0
4	RAM	A	503[B]	-	11,11,11	1.37	2 (18%)	16,16,16	2.61	10 (62%)
5	FMT	A	516	-	2,2,2	0.46	0	1,1,1	0.03	0
5	FMT	B	532	-	2,2,2	0.20	0	1,1,1	0.16	0
5	FMT	C	526	-	2,2,2	0.61	0	1,1,1	0.07	0
5	FMT	B	505	-	2,2,2	0.80	0	1,1,1	0.12	0
5	FMT	F	514	-	2,2,2	0.59	0	1,1,1	0.12	0
5	FMT	E	509	-	2,2,2	0.29	0	1,1,1	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	A	525	-	2,2,2	0.50	0	1,1,1	0.07	0
5	FMT	B	510	-	2,2,2	0.36	0	1,1,1	0.11	0
5	FMT	E	511	-	2,2,2	0.25	0	1,1,1	0.18	0
5	FMT	A	566	-	2,2,2	0.35	0	1,1,1	0.11	0
5	FMT	B	535	-	2,2,2	0.39	0	1,1,1	0.09	0
5	FMT	A	534	-	2,2,2	0.24	0	1,1,1	0.14	0
5	FMT	A	521	-	2,2,2	1.49	1 (50%)	1,1,1	0.30	0
5	FMT	D	504	-	2,2,2	0.87	0	1,1,1	0.12	0
5	FMT	B	518	-	2,2,2	0.26	0	1,1,1	0.16	0
5	FMT	C	548	-	2,2,2	0.30	0	1,1,1	0.17	0
5	FMT	B	514	-	2,2,2	0.77	0	1,1,1	0.11	0
5	FMT	D	517	-	2,2,2	0.24	0	1,1,1	0.16	0
5	FMT	D	529	-	2,2,2	0.31	0	1,1,1	0.18	0
5	FMT	C	519	-	2,2,2	0.67	0	1,1,1	0.05	0
5	FMT	C	504	-	2,2,2	0.87	0	1,1,1	0.42	0
5	FMT	B	506	-	2,2,2	0.68	0	1,1,1	0.13	0
5	FMT	F	501	-	2,2,2	0.30	0	1,1,1	0.10	0
5	FMT	C	547	-	2,2,2	0.38	0	1,1,1	0.08	0
5	FMT	C	543	-	2,2,2	0.33	0	1,1,1	0.10	0
5	FMT	C	544	-	2,2,2	0.45	0	1,1,1	0.01	0
5	FMT	B	519	-	2,2,2	0.26	0	1,1,1	0.17	0
5	FMT	D	512	-	2,2,2	0.48	0	1,1,1	0.05	0
5	FMT	E	506	-	2,2,2	0.37	0	1,1,1	0.01	0
5	FMT	A	570	-	2,2,2	0.22	0	1,1,1	0.16	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	HEM	A	501	1	-	0/14/54/54	-
4	RAM	B	513	-	-	-	0/1/1/1
3	QR8	B	502	-	-	15/48/48/48	0/1/1/1
2	HEM	E	502	1	-	1/14/54/54	-
3	QR8	D	502	-	-	13/48/48/48	0/1/1/1
3	QR8	E	503	-	-	15/48/48/48	0/1/1/1
4	RAM	A	503[A]	-	-	-	0/1/1/1
4	RAM	D	503	-	-	-	0/1/1/1
4	RAM	A	503[B]	-	-	-	0/1/1/1
2	HEM	D	501	1	-	0/14/54/54	-
3	QR8	F	503	-	-	13/48/48/48	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QR8	C	502	-	-	14/48/48/48	0/1/1/1
2	HEM	F	502	1	-	0/14/54/54	-
2	HEM	B	501	1	-	0/14/54/54	-
2	HEM	C	501	1	-	1/14/54/54	-
3	QR8	A	502	-	-	13/48/48/48	0/1/1/1

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	QR8	O2-C13	-6.00	1.37	1.46
2	E	502	HEM	FE-NB	5.89	2.13	1.94
2	D	501	HEM	C1D-ND	-5.87	1.27	1.38
3	C	502	QR8	O2-C13	-5.39	1.38	1.46
3	A	502	QR8	O2-C13	-4.98	1.39	1.46

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CHC-C4B-NB	8.44	133.51	124.42
4	A	503[A]	RAM	O1-C1-C2	-8.37	84.68	108.98
2	A	501	HEM	CHC-C4B-NB	8.31	133.37	124.42
2	C	501	HEM	CHC-C4B-NB	6.95	131.90	124.42
4	A	503[A]	RAM	O3-C3-C2	-6.57	94.89	110.38

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	QR8	C6-C7-C8-C9
3	A	502	QR8	C1-C2-C3-O3
3	B	502	QR8	C6-C7-C8-C9
3	B	502	QR8	C1-C2-C3-O3
3	C	502	QR8	C6-C7-C8-C9

There are no ring outliers.

50 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	512	FMT	1	0
5	A	565	FMT	6	0

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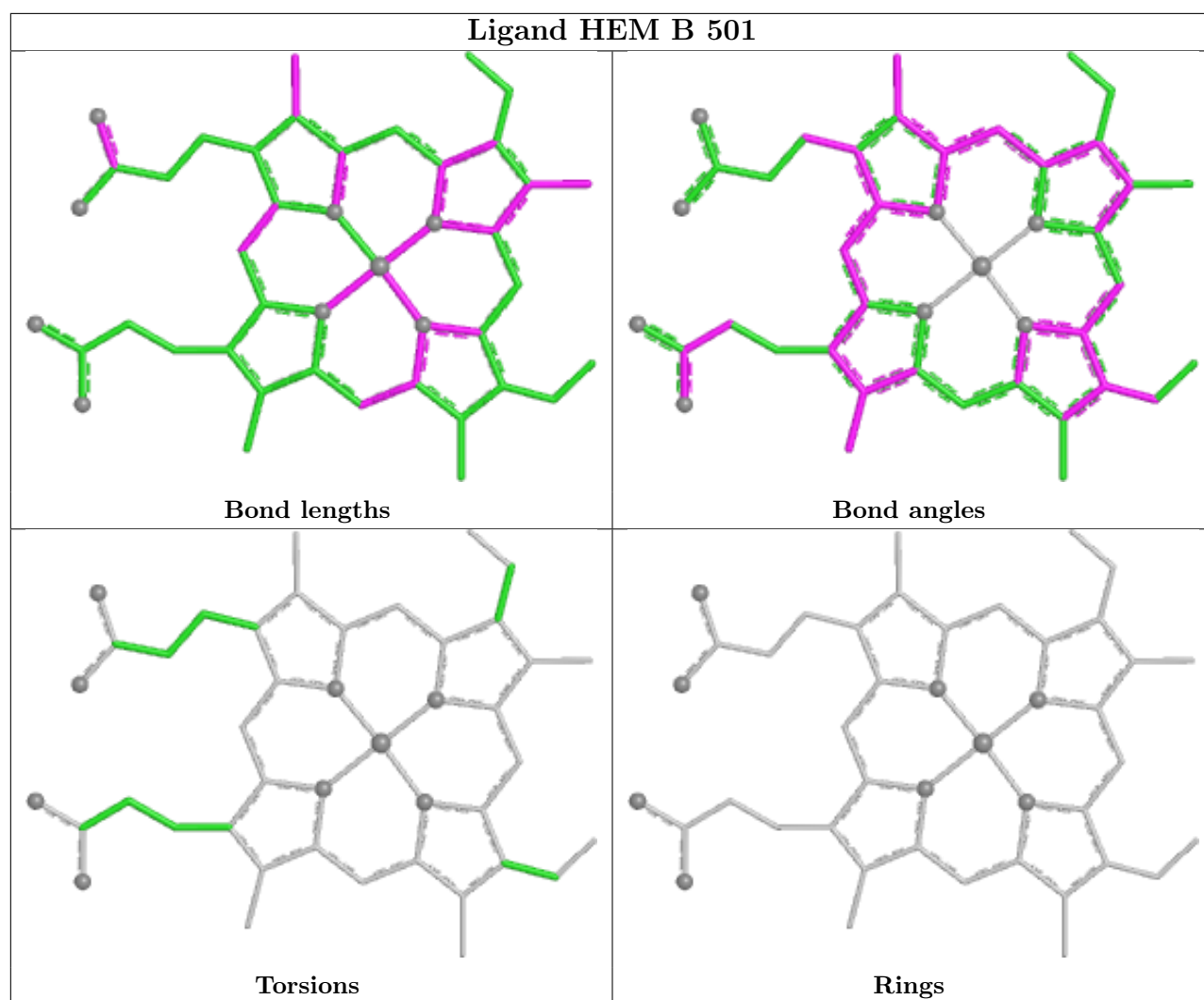
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	514	FMT	1	0
4	D	503	RAM	14	0
2	B	501	HEM	7	0
5	D	528	FMT	2	0
5	A	504	FMT	1	0
5	F	505	FMT	2	0
5	C	514	FMT	1	0
5	A	524	FMT	1	0
5	A	530	FMT	1	0
5	B	511	FMT	2	0
5	B	538	FMT	1	0
2	D	501	HEM	4	0
5	E	501	FMT	2	0
5	D	507	FMT	1	0
5	B	503	FMT	2	0
5	F	504	FMT	1	0
5	B	534	FMT	2	0
3	A	502	QR8	3	0
5	A	531	FMT	2	0
4	A	503[A]	RAM	16	0
5	A	550	FMT	2	0
5	D	508	FMT	1	0
3	D	502	QR8	2	0
5	B	507	FMT	1	0
5	D	518	FMT	1	0
4	B	513	RAM	11	0
5	A	506	FMT	1	0
5	A	546	FMT	1	0
5	A	505	FMT	1	0
5	A	510	FMT	2	0
5	F	509	FMT	2	0
2	C	501	HEM	3	0
2	A	501	HEM	4	0
2	E	502	HEM	3	0
5	C	521	FMT	1	0
5	C	507	FMT	2	0
5	A	511	FMT	2	0
5	C	523	FMT	1	0
3	B	502	QR8	1	0
5	C	552	FMT	2	0
5	A	567	FMT	0	1
2	F	502	HEM	4	0

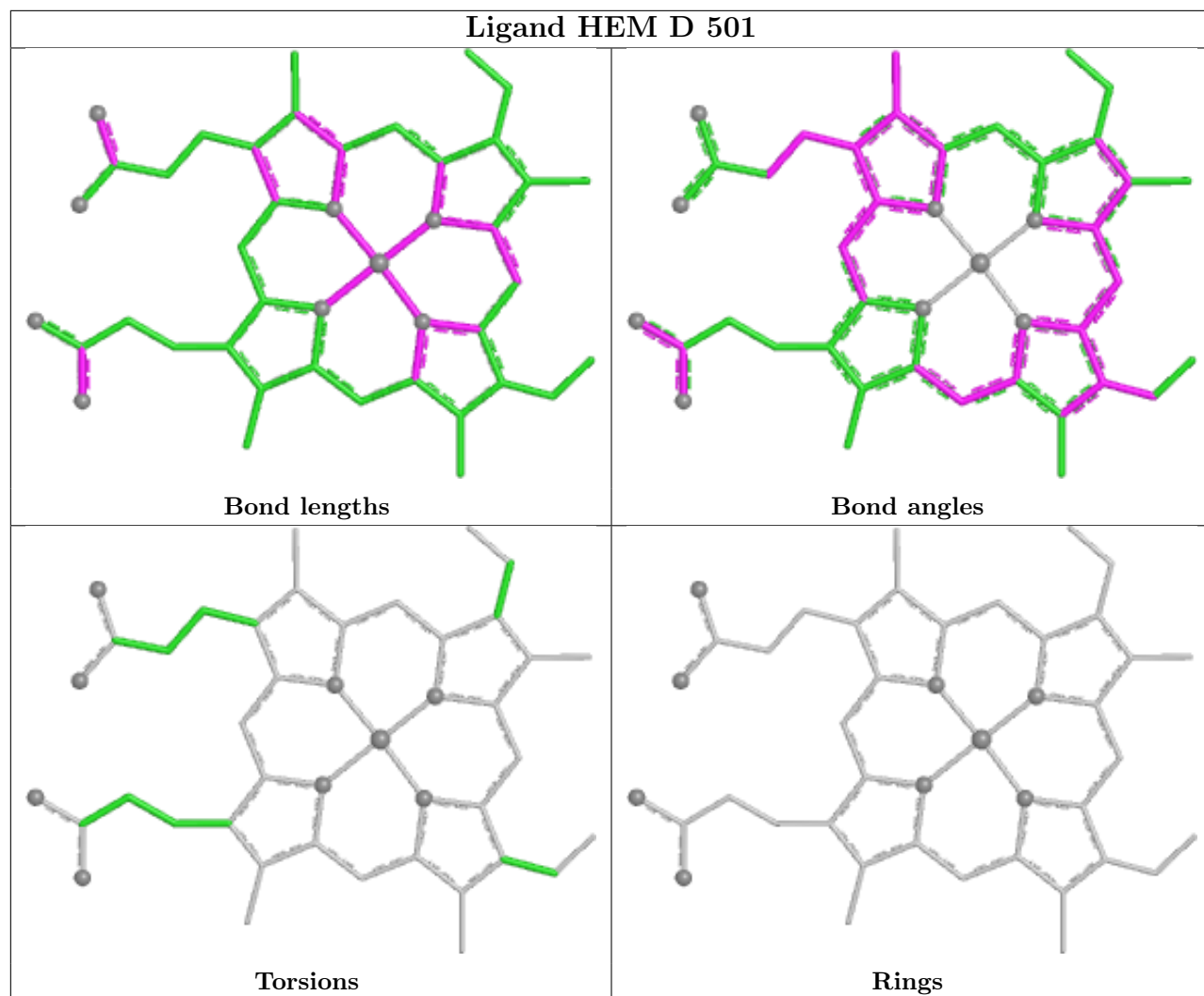
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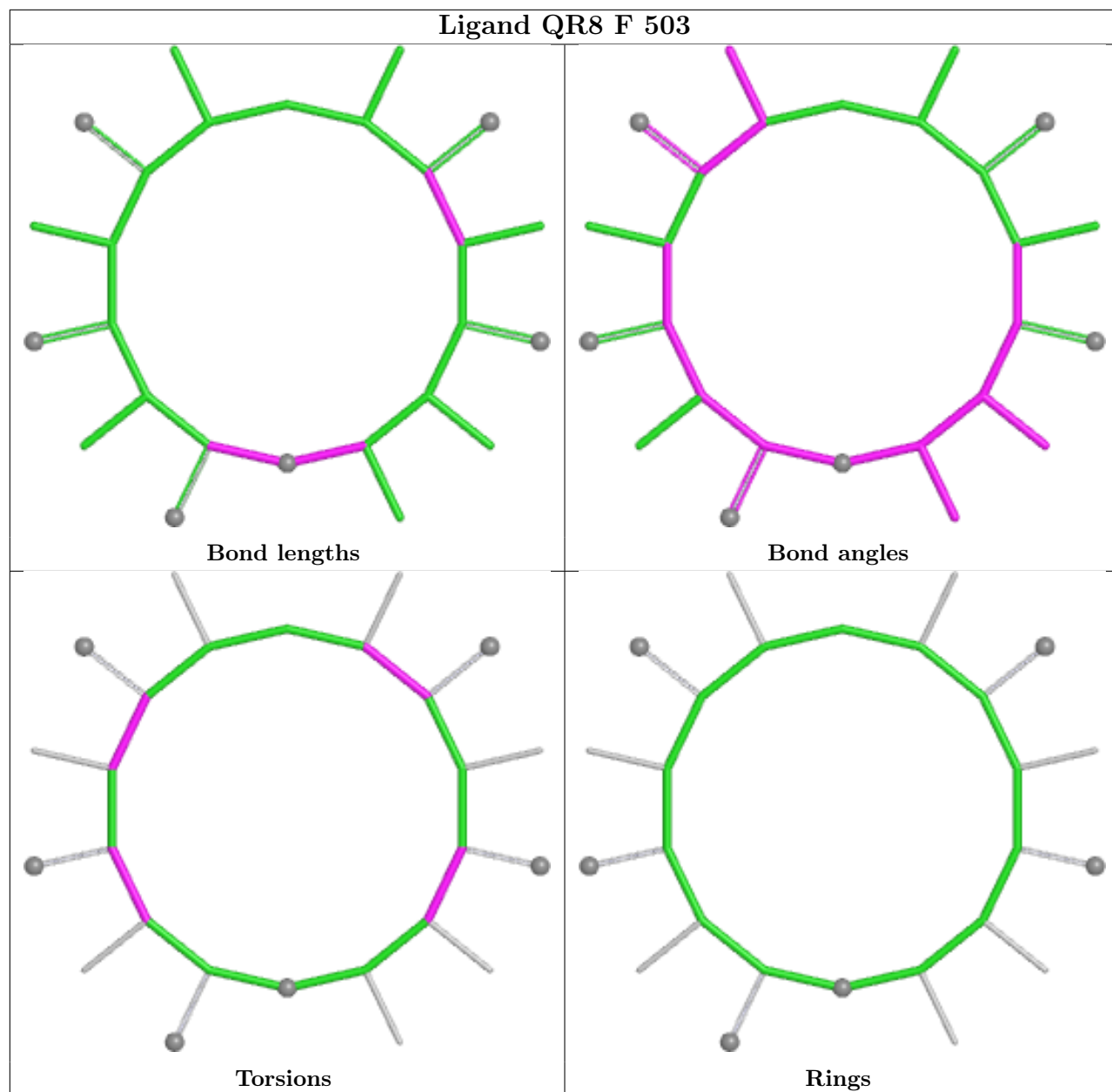
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503[B]	RAM	17	0
5	F	514	FMT	5	0
5	B	510	FMT	1	0
5	D	504	FMT	2	0
5	C	504	FMT	1	0
5	D	512	FMT	1	0

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.

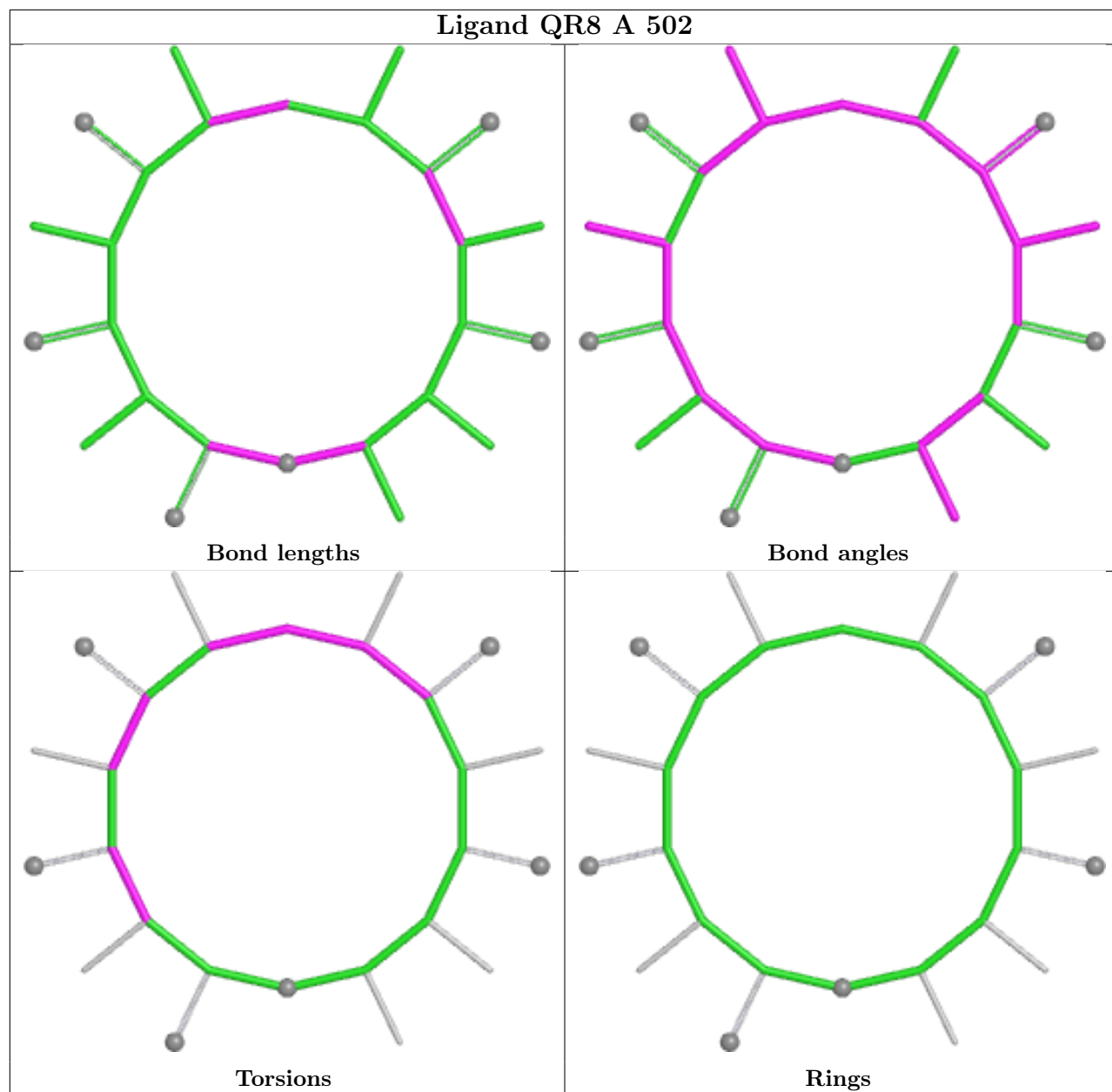


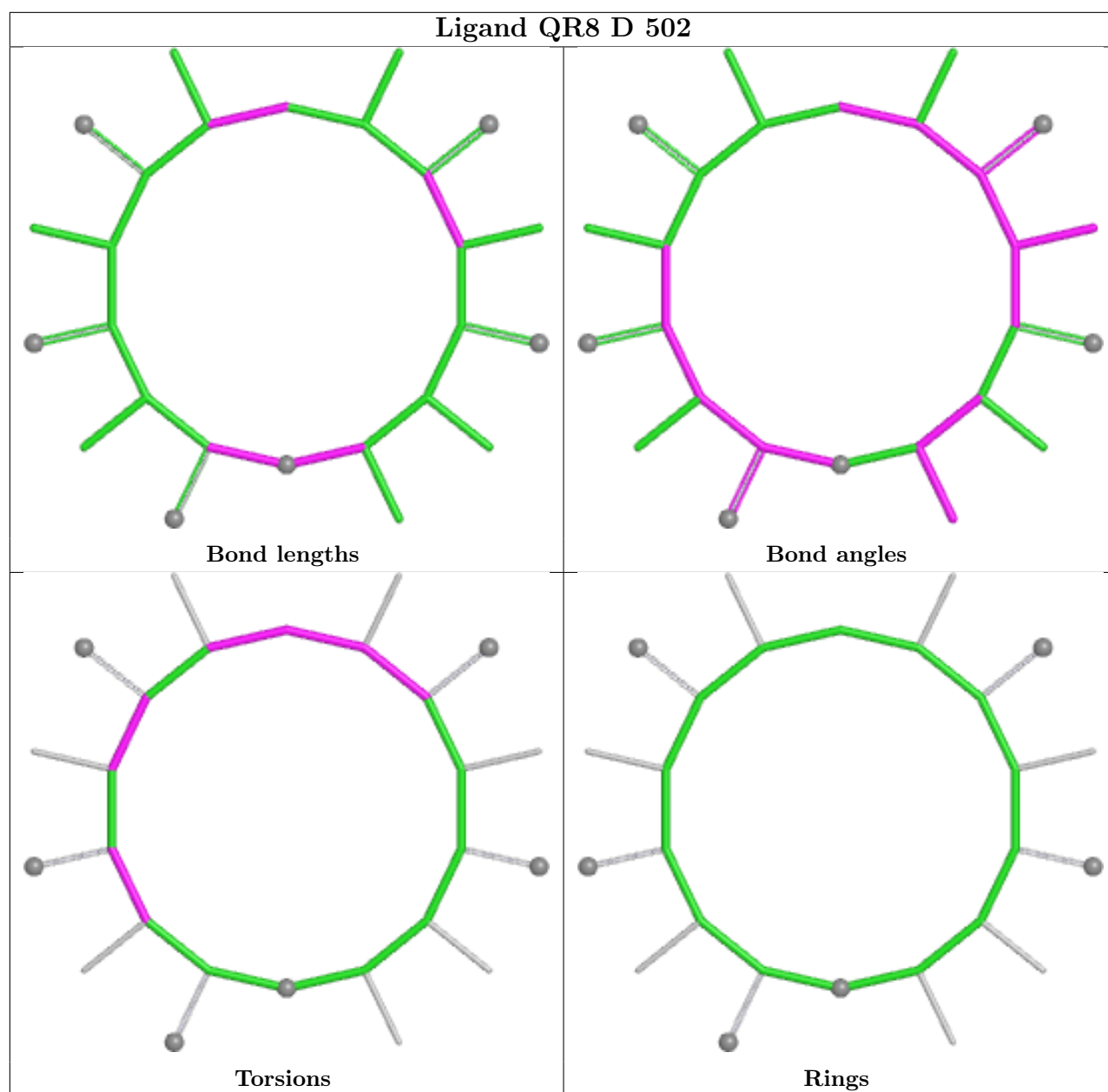


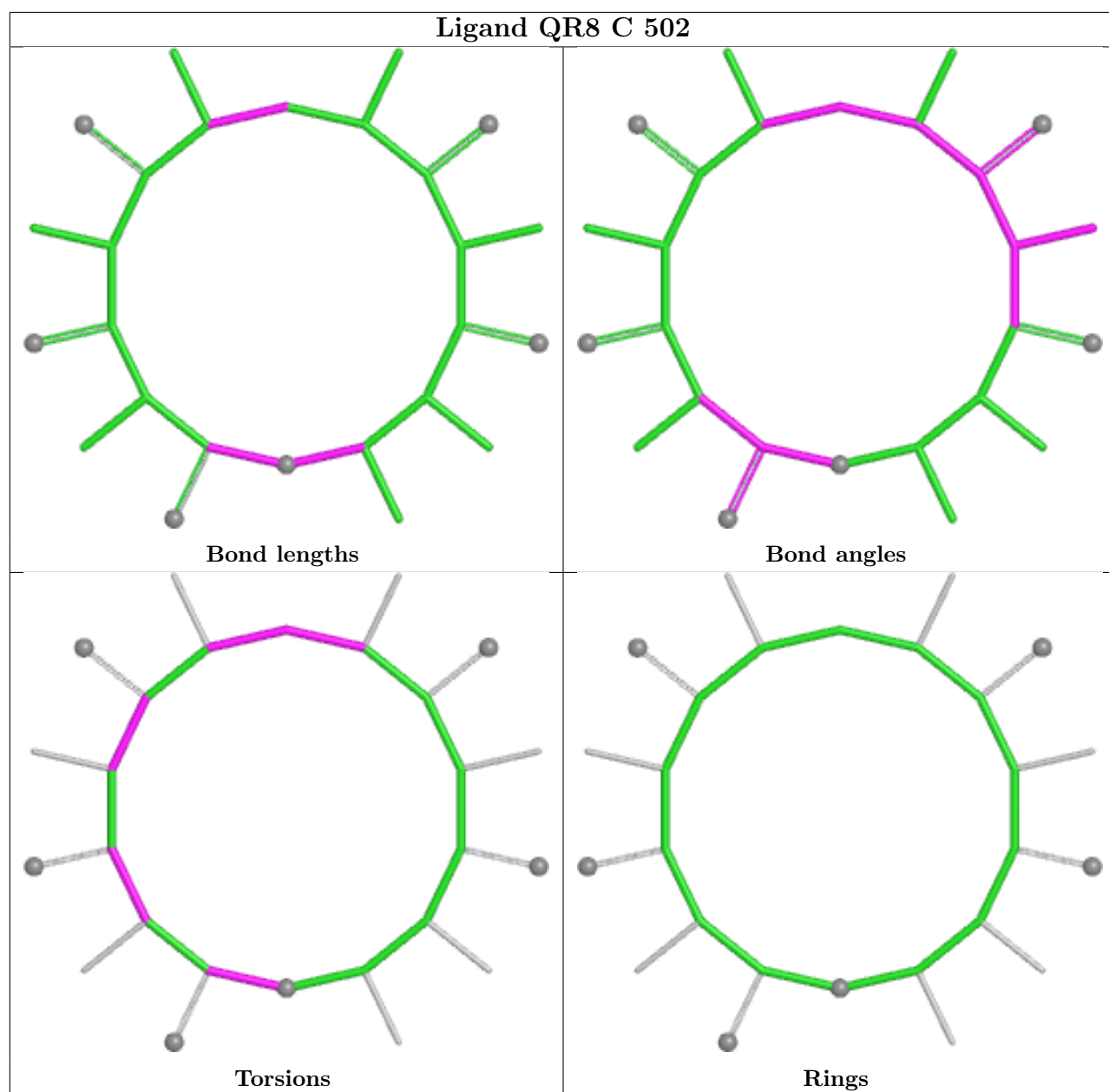
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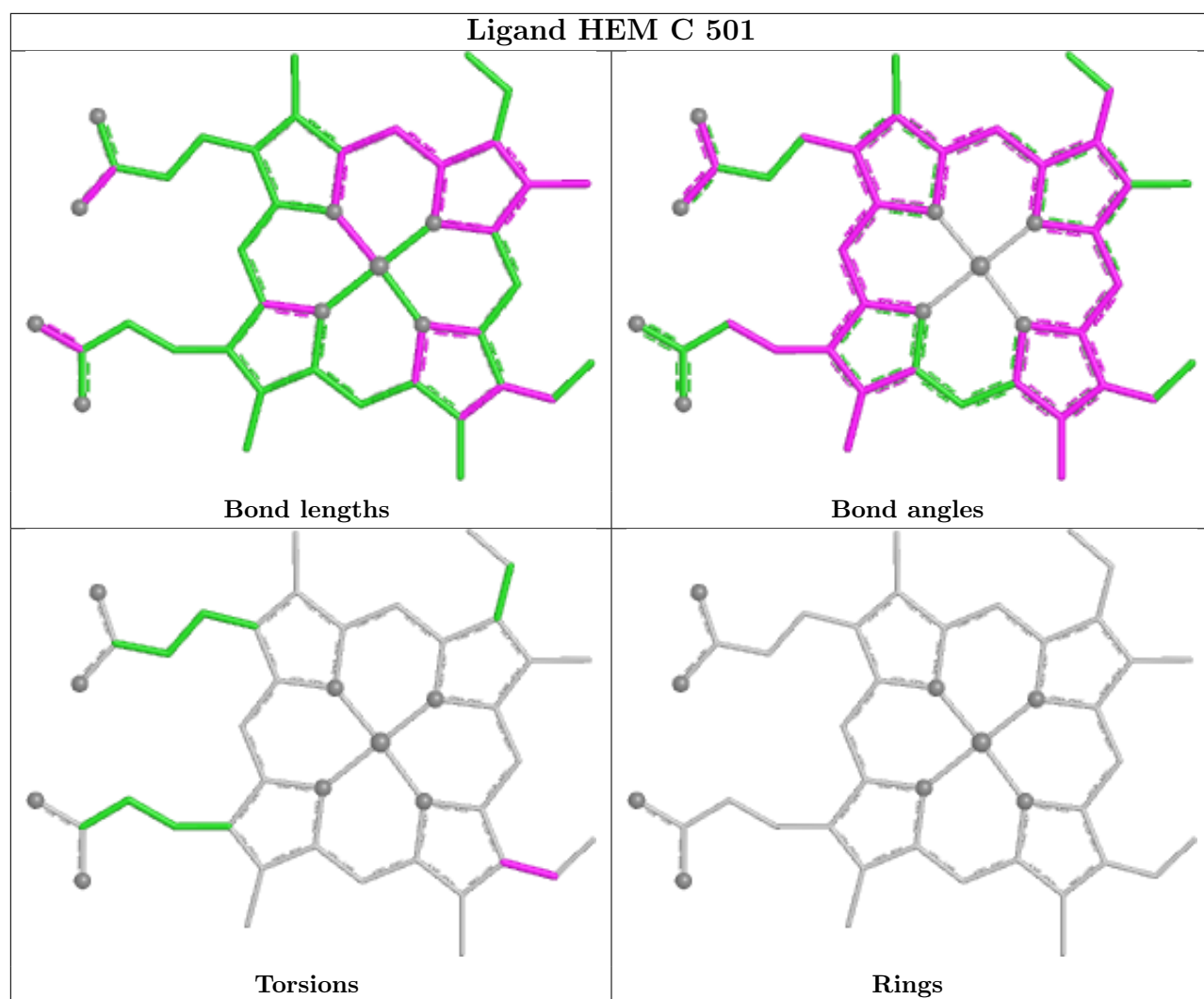


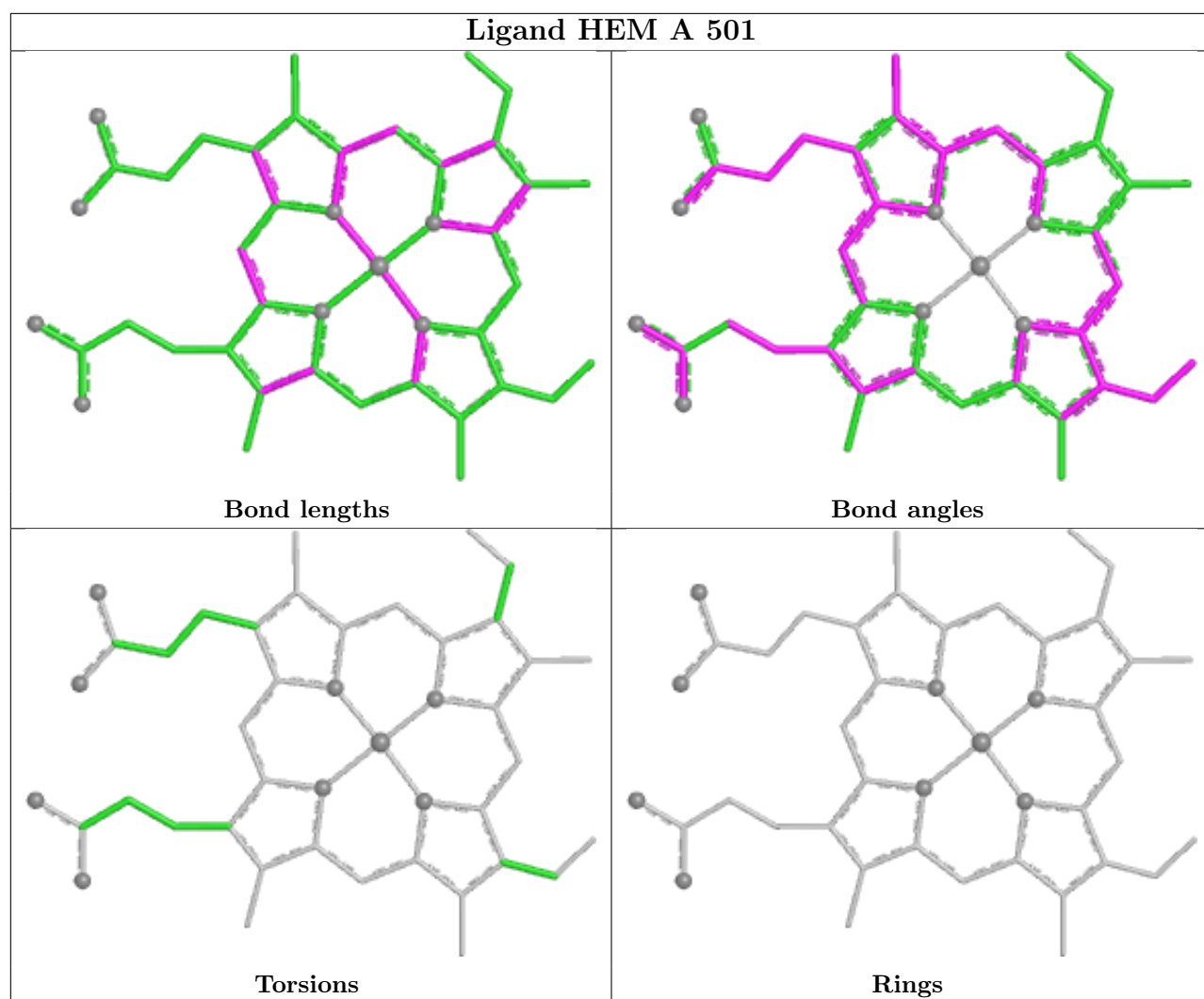
Ligand QR8 A 502

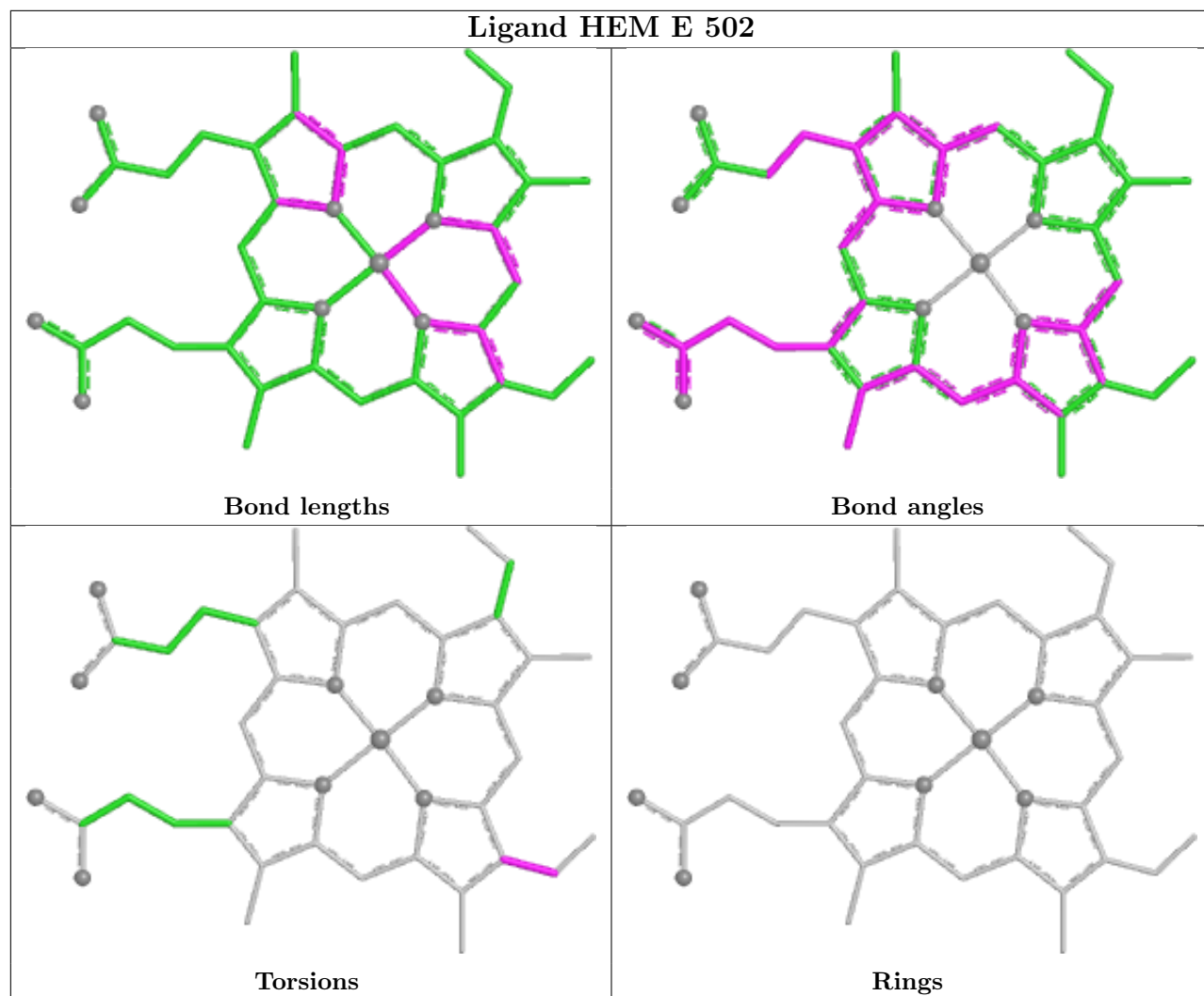




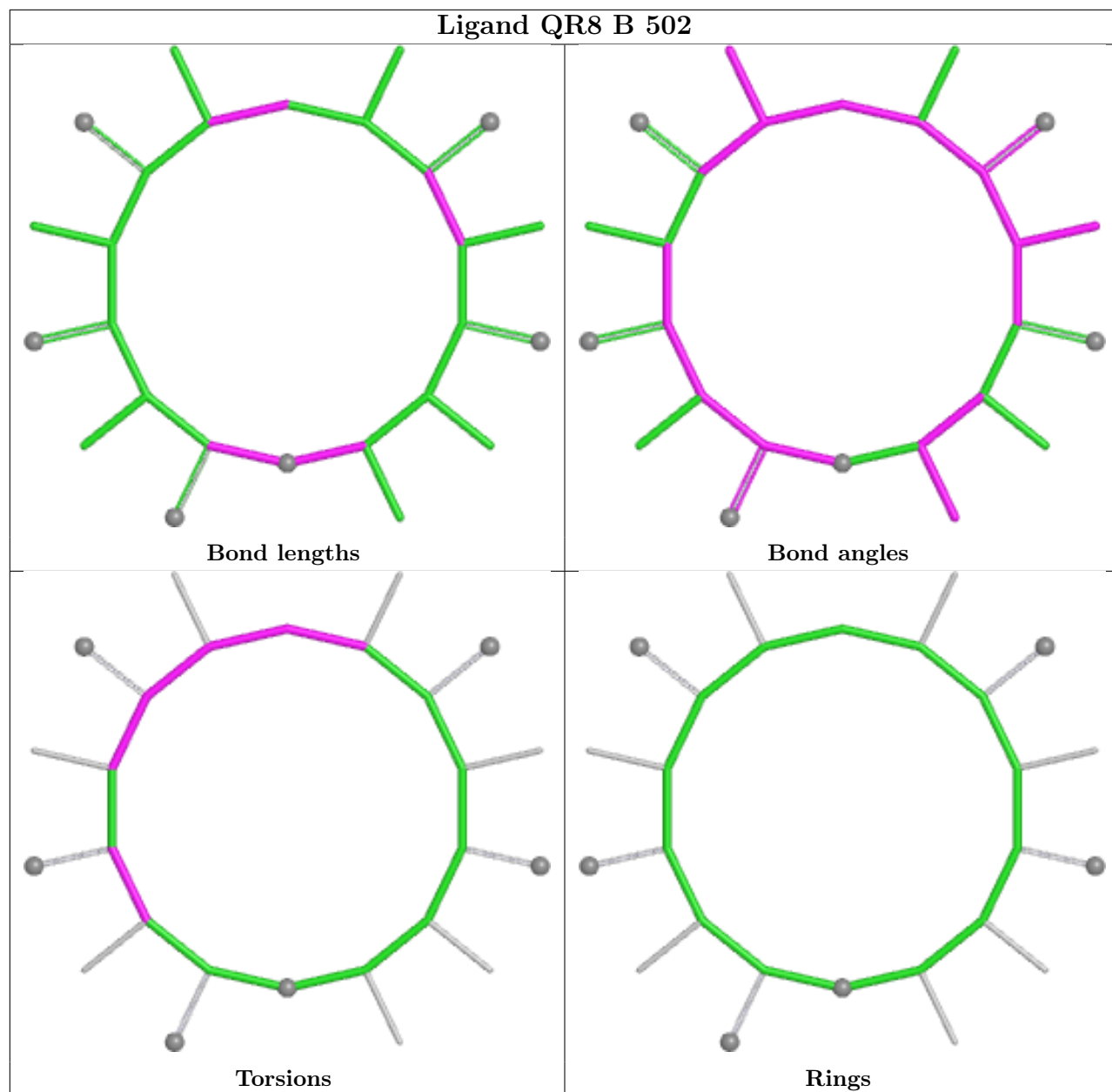




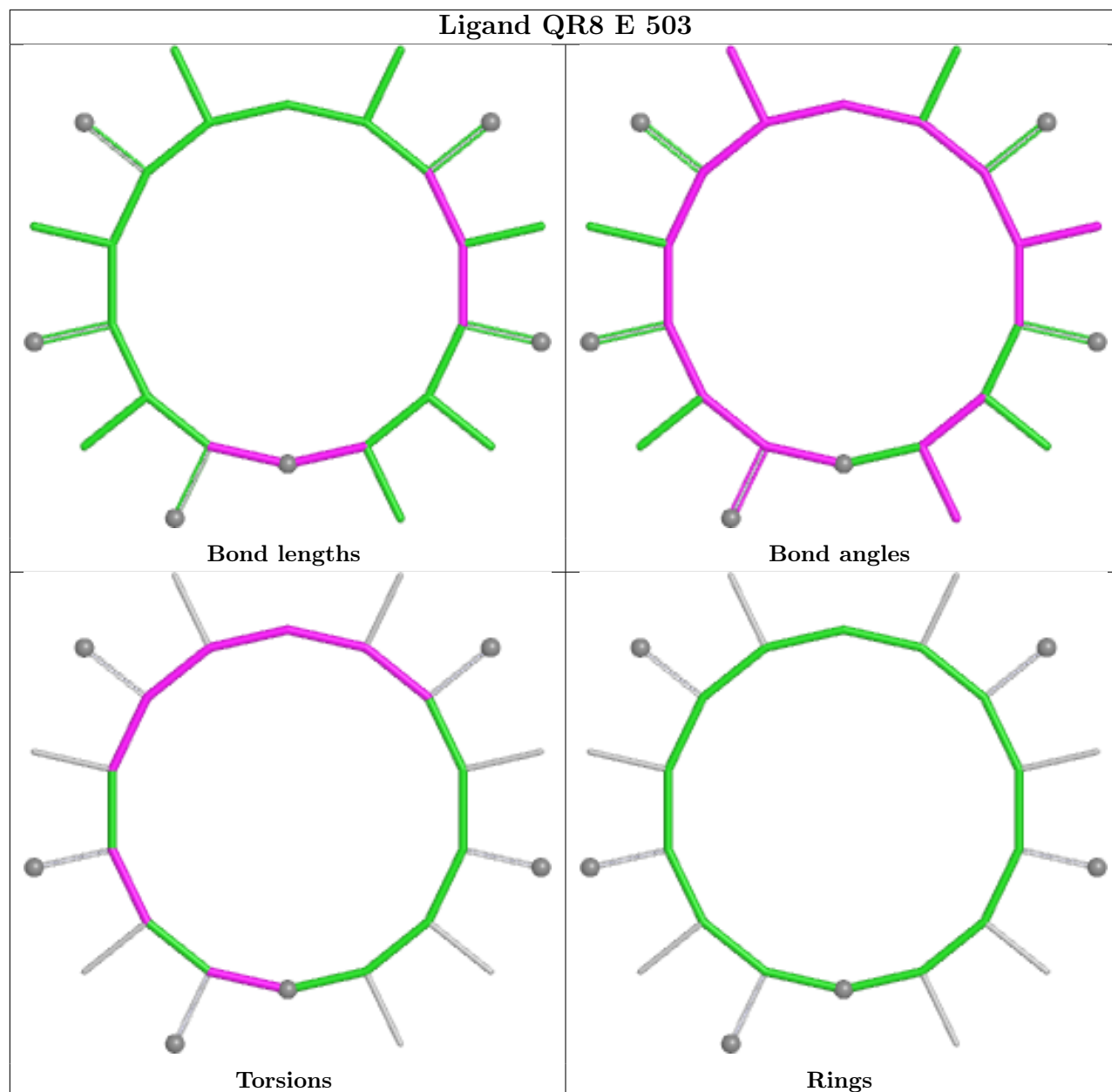


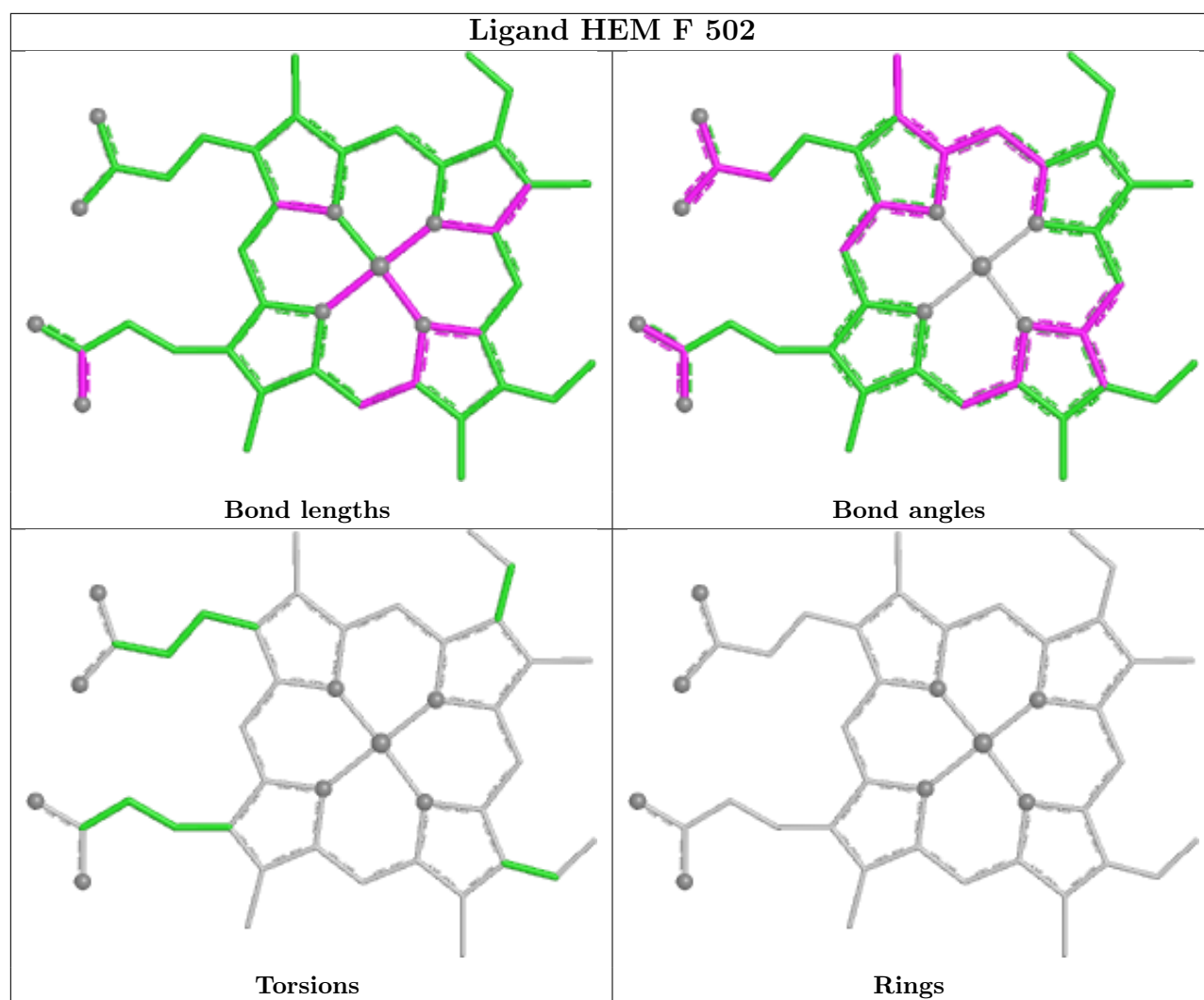


Ligand QR8 B 502



Ligand QR8 E 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/407 (97%)	-0.27	1 (0%) 90 90	19, 46, 69, 103	36 (9%)
1	B	400/407 (98%)	-0.19	6 (1%) 72 73	20, 49, 70, 154	22 (5%)
1	C	400/407 (98%)	-0.43	3 (0%) 82 84	18, 40, 57, 154	22 (5%)
1	D	400/407 (98%)	0.15	10 (2%) 58 60	24, 57, 87, 170	42 (10%)
1	E	397/407 (97%)	0.23	6 (1%) 72 73	31, 61, 91, 147	36 (9%)
1	F	398/407 (97%)	0.50	18 (4%) 38 39	29, 68, 113, 146	46 (11%)
All	All	2391/2442 (97%)	-0.00	44 (1%) 67 69	18, 53, 93, 170	204 (8%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	ALA	7.5
1	B	9	THR	4.9
1	D	10	PRO	4.9
1	D	11	ALA	4.6
1	B	11	ALA	4.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FMT	D	536	3/3	0.31	0.13	111,111,113,115	0
5	FMT	A	551	3/3	0.47	0.14	104,104,113,115	0
5	FMT	A	554	3/3	0.50	0.16	100,100,107,111	0
5	FMT	D	521	3/3	0.52	0.12	102,102,102,104	0
5	FMT	B	527	3/3	0.58	0.14	96,96,99,103	0
5	FMT	E	511	3/3	0.58	0.12	119,119,120,122	0
5	FMT	A	540	3/3	0.59	0.18	105,105,112,114	0
5	FMT	C	528	3/3	0.60	0.11	95,95,95,101	0
5	FMT	C	530	3/3	0.62	0.15	105,105,110,113	0
5	FMT	E	510	3/3	0.63	0.15	95,95,107,108	0
5	FMT	C	546	3/3	0.64	0.16	87,87,88,91	0
5	FMT	D	526	3/3	0.65	0.18	104,104,106,112	0
5	FMT	A	542	3/3	0.65	0.14	102,102,103,104	0
5	FMT	A	529	3/3	0.66	0.12	100,100,107,109	0
5	FMT	A	527	3/3	0.66	0.16	88,88,93,100	0
5	FMT	E	515	3/3	0.66	0.10	103,103,114,115	0
5	FMT	A	571	3/3	0.68	0.15	94,94,108,108	0
5	FMT	D	527	3/3	0.68	0.10	91,91,97,97	0
5	FMT	A	539	3/3	0.68	0.11	101,101,110,111	0
5	FMT	F	510	3/3	0.68	0.11	88,88,98,100	0
5	FMT	A	557	3/3	0.69	0.10	87,87,90,91	0
5	FMT	A	533	3/3	0.69	0.12	87,87,91,92	0
5	FMT	B	520	3/3	0.69	0.11	95,95,102,102	0
5	FMT	A	556	3/3	0.70	0.13	87,87,89,93	0
5	FMT	C	531	3/3	0.71	0.12	102,102,102,106	0
5	FMT	C	535	3/3	0.71	0.16	89,89,112,116	0
5	FMT	B	531	3/3	0.71	0.12	98,98,102,104	0
5	FMT	D	517	3/3	0.71	0.16	114,114,121,129	0
5	FMT	B	533	3/3	0.72	0.22	78,78,79,89	0
5	FMT	B	540	3/3	0.72	0.11	95,95,99,100	0
5	FMT	A	564	3/3	0.72	0.19	90,90,102,105	0
5	FMT	B	532	3/3	0.72	0.10	96,96,99,102	0
5	FMT	C	516	3/3	0.73	0.13	81,81,86,87	0
5	FMT	F	511	3/3	0.73	0.09	101,101,109,109	0
5	FMT	F	512	3/3	0.73	0.11	106,106,112,113	0
5	FMT	B	526	3/3	0.74	0.11	96,96,96,99	0
5	FMT	A	541	3/3	0.74	0.11	92,92,93,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	E	517	3/3	0.74	0.15	95,95,99,100	0
5	FMT	E	509	3/3	0.75	0.10	86,86,101,104	0
5	FMT	C	549	3/3	0.75	0.10	100,100,100,101	0
4	RAM	B	513	11/11	0.75	0.23	50,57,63,64	11
5	FMT	E	508	3/3	0.75	0.09	86,86,89,93	0
5	FMT	A	515	3/3	0.76	0.13	80,80,82,89	0
5	FMT	A	552	3/3	0.76	0.15	83,83,89,92	0
5	FMT	C	548	3/3	0.76	0.13	85,85,91,91	0
5	FMT	D	522	3/3	0.76	0.14	97,97,106,113	0
5	FMT	B	516	3/3	0.77	0.16	100,100,103,107	0
5	FMT	C	526	3/3	0.77	0.14	75,75,80,83	0
5	FMT	A	558	3/3	0.77	0.14	83,83,84,92	0
5	FMT	D	515	3/3	0.78	0.16	79,79,80,88	0
5	FMT	A	517	3/3	0.78	0.09	98,98,106,108	0
5	FMT	D	525	3/3	0.78	0.15	87,87,91,92	0
5	FMT	F	515	3/3	0.78	0.20	101,101,103,108	0
5	FMT	A	572	3/3	0.79	0.18	91,91,97,98	0
5	FMT	B	511	3/3	0.79	0.09	73,73,77,78	0
5	FMT	A	510	3/3	0.79	0.18	75,75,84,85	0
5	FMT	B	518	3/3	0.79	0.14	89,89,104,105	0
5	FMT	A	512	3/3	0.79	0.21	98,98,103,109	0
5	FMT	E	516	3/3	0.79	0.15	90,90,90,96	0
5	FMT	B	525	3/3	0.79	0.15	98,98,105,105	0
5	FMT	A	569	3/3	0.79	0.16	94,94,95,95	0
5	FMT	A	570	3/3	0.79	0.19	92,92,98,98	0
5	FMT	B	528	3/3	0.79	0.15	85,85,86,89	0
5	FMT	A	523	3/3	0.79	0.18	67,67,70,77	0
5	FMT	B	519	3/3	0.80	0.09	100,100,101,104	0
5	FMT	B	517	3/3	0.80	0.15	86,86,94,100	0
5	FMT	D	535	3/3	0.80	0.30	96,96,104,104	0
5	FMT	D	523	3/3	0.80	0.25	85,85,94,95	0
5	FMT	A	538	3/3	0.80	0.18	63,63,75,85	0
5	FMT	B	539	3/3	0.81	0.14	85,85,89,91	0
4	RAM	D	503	11/11	0.81	0.20	58,66,68,68	11
5	FMT	D	530	3/3	0.81	0.19	101,101,109,109	0
5	FMT	B	507	3/3	0.81	0.18	75,75,84,84	0
5	FMT	C	540	3/3	0.81	0.17	74,74,80,83	0
5	FMT	A	545	3/3	0.81	0.24	83,83,87,101	0
5	FMT	C	547	3/3	0.81	0.17	65,65,73,82	0
5	FMT	B	535	3/3	0.81	0.21	88,88,89,94	0
5	FMT	C	523	3/3	0.82	0.17	69,69,75,81	0
5	FMT	A	563	3/3	0.82	0.22	97,97,102,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	D	519	3/3	0.82	0.16	90,90,91,96	0
5	FMT	C	534	3/3	0.82	0.19	88,88,90,92	0
5	FMT	A	560	3/3	0.82	0.20	74,74,81,93	0
5	FMT	C	539	3/3	0.82	0.17	87,87,90,98	0
5	FMT	D	524	3/3	0.82	0.14	111,111,112,116	0
5	FMT	C	551	3/3	0.82	0.28	90,90,94,103	0
5	FMT	D	512	3/3	0.83	0.16	85,85,88,92	0
5	FMT	B	512	3/3	0.83	0.19	68,68,72,74	0
5	FMT	C	510	3/3	0.83	0.12	83,83,84,91	0
5	FMT	C	542	3/3	0.83	0.24	91,91,115,119	0
5	FMT	C	525	3/3	0.83	0.19	90,90,91,94	0
5	FMT	C	518	3/3	0.84	0.17	65,65,72,77	0
5	FMT	D	505	3/3	0.84	0.16	69,69,69,73	0
5	FMT	A	513	3/3	0.84	0.15	75,75,81,88	0
5	FMT	A	537	3/3	0.84	0.10	100,100,109,109	0
5	FMT	A	574	3/3	0.84	0.15	102,102,108,111	0
5	FMT	A	507	3/3	0.84	0.15	69,69,73,76	0
5	FMT	C	506	3/3	0.84	0.20	62,62,69,73	0
5	FMT	B	508	3/3	0.84	0.11	73,73,79,83	0
5	FMT	A	562	3/3	0.84	0.23	55,55,70,72	0
5	FMT	C	508	3/3	0.85	0.18	81,81,87,90	0
5	FMT	C	545	3/3	0.85	0.20	78,78,80,86	0
5	FMT	B	521	3/3	0.85	0.22	66,66,78,84	0
5	FMT	C	537	3/3	0.86	0.19	97,97,109,111	0
5	FMT	B	523	3/3	0.86	0.12	86,86,87,92	0
5	FMT	A	535	3/3	0.86	0.12	89,89,103,109	0
5	FMT	C	541	3/3	0.86	0.11	83,83,85,91	0
5	FMT	A	516	3/3	0.86	0.19	77,77,81,85	0
5	FMT	D	529	3/3	0.86	0.12	76,76,79,82	0
5	FMT	F	509	3/3	0.86	0.15	66,66,67,74	0
4	RAM	A	503[B]	11/11	0.86	0.17	37,41,44,46	11
4	RAM	A	503[A]	11/11	0.86	0.17	34,37,39,44	11
5	FMT	A	548	3/3	0.86	0.23	64,64,65,76	0
5	FMT	C	536	3/3	0.86	0.20	98,98,99,104	0
5	FMT	B	530	3/3	0.87	0.11	71,71,80,93	0
5	FMT	A	549	3/3	0.87	0.27	71,71,87,90	0
5	FMT	E	513	3/3	0.87	0.14	74,74,74,75	0
5	FMT	B	524	3/3	0.87	0.19	68,68,74,78	0
5	FMT	D	516	3/3	0.87	0.20	90,90,91,91	0
5	FMT	A	553	3/3	0.87	0.21	86,86,94,95	0
5	FMT	F	506	3/3	0.87	0.11	74,74,75,76	0
5	FMT	D	518	3/3	0.87	0.10	84,84,96,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	A	536	3/3	0.87	0.20	71,71,71,77	0
5	FMT	A	559	3/3	0.87	0.17	90,90,91,95	0
5	FMT	A	566	3/3	0.87	0.11	87,87,89,96	0
5	FMT	B	529	3/3	0.87	0.18	71,71,71,79	0
5	FMT	A	568	3/3	0.88	0.10	85,85,90,91	0
5	FMT	B	522	3/3	0.88	0.25	76,76,82,90	0
5	FMT	B	536	3/3	0.88	0.14	69,69,76,81	0
5	FMT	B	538	3/3	0.88	0.15	82,82,83,86	0
5	FMT	A	508	3/3	0.88	0.23	74,74,76,83	0
5	FMT	D	511	3/3	0.88	0.27	68,68,73,74	0
5	FMT	A	521	3/3	0.88	0.22	49,49,63,67	0
5	FMT	F	504	3/3	0.88	0.09	78,78,87,91	0
5	FMT	F	505	3/3	0.88	0.18	79,79,84,85	0
5	FMT	A	531	3/3	0.88	0.20	63,63,65,75	0
5	FMT	C	529	3/3	0.88	0.12	84,84,88,92	0
5	FMT	D	531	3/3	0.88	0.14	59,59,65,71	0
5	FMT	C	544	3/3	0.88	0.24	68,68,73,82	0
5	FMT	C	507	3/3	0.88	0.22	60,60,65,68	0
5	FMT	F	513	3/3	0.88	0.28	75,75,79,82	0
5	FMT	A	506	3/3	0.88	0.19	66,66,73,77	0
6	NA	E	507	1/1	0.88	0.16	81,81,81,81	0
5	FMT	D	528	3/3	0.89	0.38	79,79,80,81	0
5	FMT	A	550	3/3	0.89	0.15	64,64,78,80	0
5	FMT	A	528	3/3	0.89	0.16	84,84,84,93	0
5	FMT	C	552	3/3	0.89	0.12	72,72,74,79	0
5	FMT	D	533	3/3	0.89	0.24	70,70,70,73	0
5	FMT	A	520	3/3	0.89	0.16	84,84,87,90	0
5	FMT	D	507	3/3	0.89	0.20	85,85,90,91	0
5	FMT	D	509	3/3	0.89	0.14	66,66,76,76	0
5	FMT	A	547	3/3	0.89	0.21	70,70,73,77	0
5	FMT	A	519	3/3	0.89	0.19	74,74,75,76	0
5	FMT	A	532	3/3	0.89	0.36	76,76,77,85	0
5	FMT	B	514	3/3	0.89	0.16	75,75,80,87	0
5	FMT	E	514	3/3	0.89	0.17	86,86,94,97	0
5	FMT	D	514	3/3	0.90	0.18	60,60,60,71	0
5	FMT	C	504	3/3	0.90	0.15	48,48,52,54	0
5	FMT	C	505	3/3	0.90	0.16	57,57,64,68	0
5	FMT	B	504	3/3	0.90	0.22	69,69,74,80	0
5	FMT	A	561	3/3	0.90	0.11	77,77,83,87	0
5	FMT	B	537	3/3	0.90	0.12	82,82,94,96	0
5	FMT	D	532	3/3	0.90	0.13	79,79,80,84	0
5	FMT	D	520	3/3	0.90	0.10	96,96,100,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	D	534	3/3	0.90	0.10	91,91,91,93	0
5	FMT	A	573	3/3	0.90	0.10	67,67,85,97	0
5	FMT	C	543	3/3	0.90	0.13	82,82,87,92	0
5	FMT	E	501	3/3	0.90	0.14	76,76,78,79	0
5	FMT	E	505	3/3	0.90	0.11	72,72,79,81	0
5	FMT	C	511	3/3	0.90	0.12	68,68,76,80	0
5	FMT	B	509	3/3	0.90	0.12	60,60,62,64	0
5	FMT	A	567	3/3	0.90	0.12	85,85,85,85	0
5	FMT	B	510	3/3	0.91	0.20	86,86,91,92	0
5	FMT	E	512	3/3	0.91	0.15	80,80,81,86	0
5	FMT	C	515	3/3	0.91	0.14	63,63,76,76	0
5	FMT	E	504	3/3	0.91	0.21	63,63,63,74	0
5	FMT	A	504	3/3	0.91	0.15	52,52,56,57	0
5	FMT	D	506	3/3	0.91	0.29	68,68,81,84	0
5	FMT	C	517	3/3	0.91	0.14	70,70,71,74	0
5	FMT	F	501	3/3	0.91	0.11	85,85,86,88	0
5	FMT	C	532	3/3	0.91	0.16	49,49,57,72	0
5	FMT	C	550	3/3	0.92	0.11	57,57,67,70	0
5	FMT	A	511	3/3	0.92	0.17	61,61,66,66	0
5	FMT	A	530	3/3	0.92	0.13	55,55,75,77	0
5	FMT	A	509	3/3	0.92	0.13	61,61,64,71	0
5	FMT	C	503	3/3	0.92	0.15	48,48,55,60	0
5	FMT	A	505	3/3	0.92	0.10	59,59,68,71	0
5	FMT	A	524	3/3	0.92	0.21	60,60,68,74	0
5	FMT	A	565	3/3	0.92	0.22	66,66,82,85	0
5	FMT	A	543	3/3	0.92	0.17	54,54,69,69	0
5	FMT	A	544	3/3	0.92	0.14	67,67,77,81	0
5	FMT	C	509	3/3	0.92	0.17	60,60,67,68	0
5	FMT	A	525	3/3	0.92	0.14	76,76,82,83	0
5	FMT	A	518	3/3	0.92	0.17	58,58,66,71	0
5	FMT	A	514	3/3	0.92	0.23	46,46,48,51	0
6	NA	F	508	1/1	0.92	0.13	59,59,59,59	0
5	FMT	A	546	3/3	0.93	0.17	64,64,73,83	0
5	FMT	C	519	3/3	0.93	0.14	69,69,76,84	0
5	FMT	D	537	3/3	0.93	0.26	48,48,60,65	0
5	FMT	D	504	3/3	0.93	0.17	67,67,71,76	0
5	FMT	F	514	3/3	0.93	0.19	56,56,70,72	0
5	FMT	C	538	3/3	0.93	0.25	58,58,61,64	0
5	FMT	A	555	3/3	0.93	0.18	61,61,65,71	0
5	FMT	C	512	3/3	0.93	0.18	59,59,73,74	0
5	FMT	B	506	3/3	0.94	0.19	63,63,69,71	0
5	FMT	A	534	3/3	0.94	0.10	60,60,72,81	0

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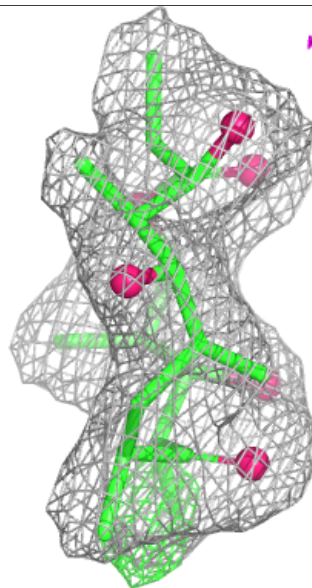
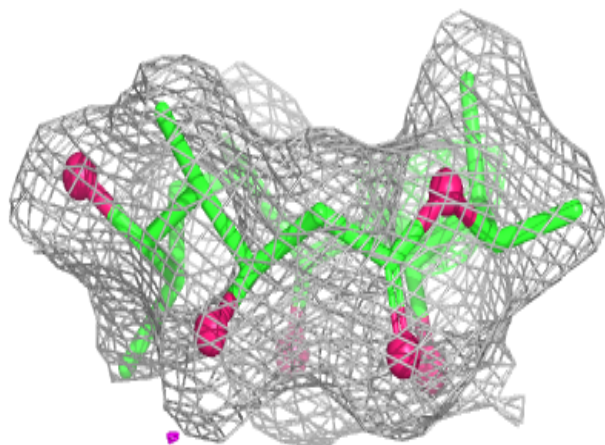
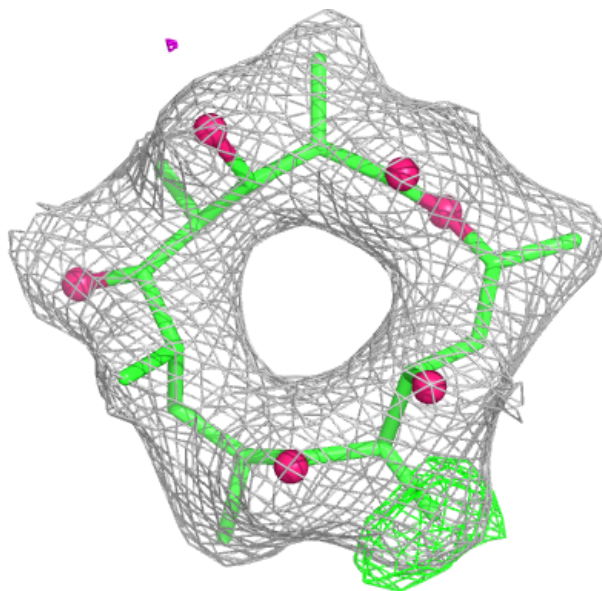
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	B	534	3/3	0.94	0.10	70,70,72,74	0
3	QR8	E	503	26/26	0.94	0.10	46,53,56,57	0
5	FMT	C	520	3/3	0.94	0.19	55,55,66,70	0
5	FMT	C	533	3/3	0.94	0.13	68,68,69,76	0
5	FMT	C	521	3/3	0.94	0.14	59,59,70,87	0
5	FMT	C	513	3/3	0.94	0.23	54,54,62,63	0
5	FMT	C	514	3/3	0.94	0.08	53,53,56,64	0
5	FMT	E	506	3/3	0.94	0.07	70,70,72,74	0
3	QR8	F	503	26/26	0.94	0.10	55,62,66,75	0
5	FMT	D	508	3/3	0.95	0.15	57,57,59,59	0
3	QR8	A	502	26/26	0.95	0.08	33,38,42,43	0
5	FMT	C	522	3/3	0.95	0.22	54,54,62,62	0
5	FMT	A	522	3/3	0.95	0.27	74,74,80,83	0
5	FMT	F	507	3/3	0.95	0.10	66,66,69,72	0
6	NA	A	526	1/1	0.95	0.12	41,41,41,41	0
6	NA	B	515	1/1	0.95	0.19	57,57,57,57	0
6	NA	D	513	1/1	0.95	0.17	54,54,54,54	0
5	FMT	C	524	3/3	0.95	0.11	48,48,49,52	0
5	FMT	B	505	3/3	0.95	0.12	62,62,65,69	0
3	QR8	C	502	26/26	0.96	0.07	30,35,37,42	0
3	QR8	D	502	26/26	0.96	0.08	43,48,51,58	0
5	FMT	D	510	3/3	0.96	0.17	70,70,70,72	0
6	NA	C	527	1/1	0.97	0.08	42,42,42,42	0
3	QR8	B	502	26/26	0.97	0.07	35,41,45,48	0
5	FMT	B	503	3/3	0.97	0.12	53,53,58,63	0
2	HEM	F	502	43/43	0.97	0.09	53,64,75,93	0
2	HEM	B	501	43/43	0.98	0.06	32,36,39,47	0
2	HEM	D	501	43/43	0.98	0.06	36,40,46,49	0
2	HEM	E	502	43/43	0.98	0.07	42,48,54,58	0
2	HEM	C	501	43/43	0.99	0.04	27,30,37,38	0
2	HEM	A	501	43/43	0.99	0.05	29,32,39,41	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.

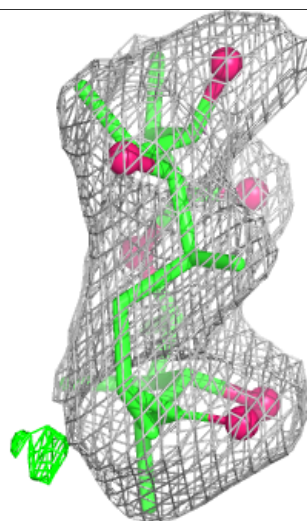
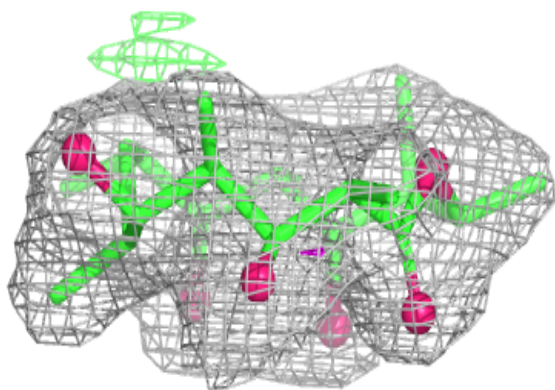
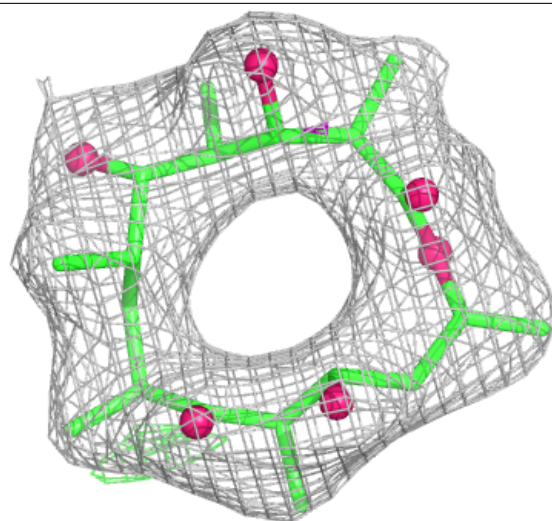
Electron density around QR8 E 503:

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



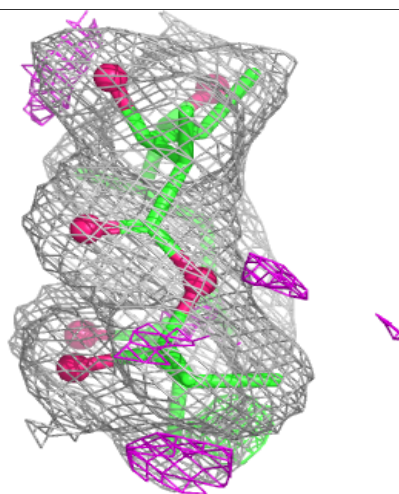
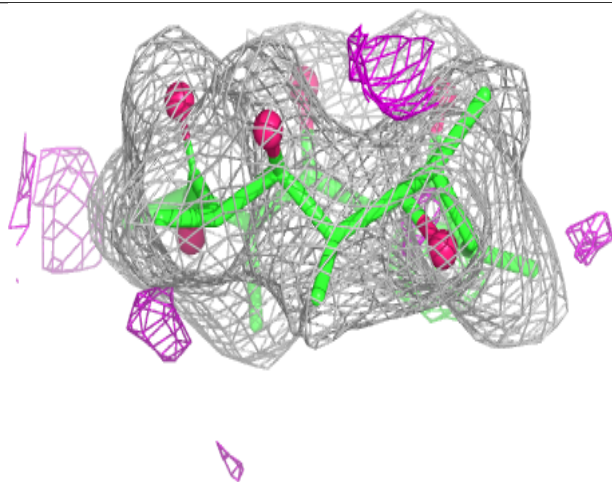
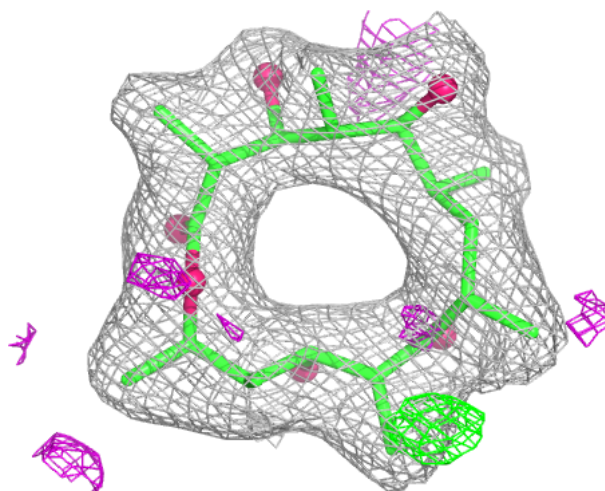
Electron density around QR8 F 503:

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



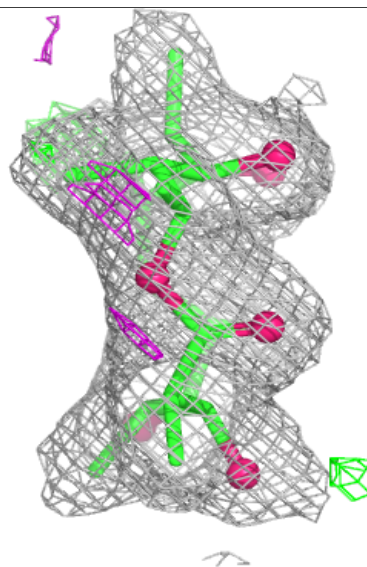
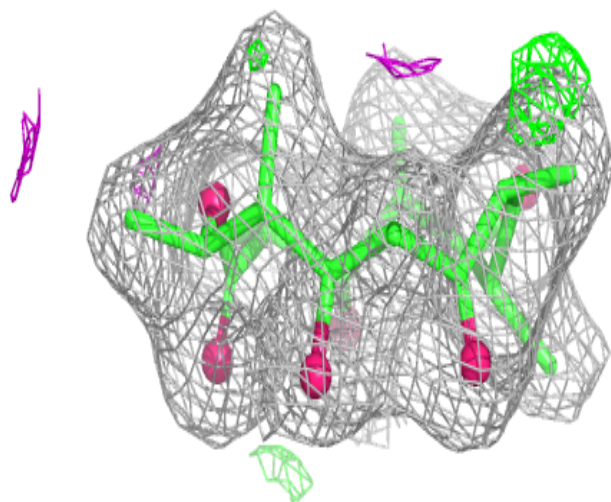
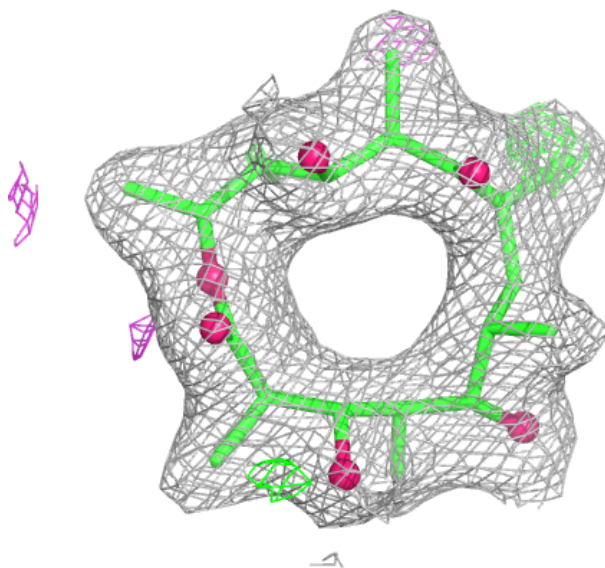
Electron density around QR8 A 502:

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



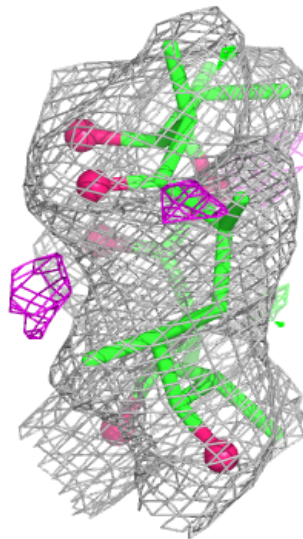
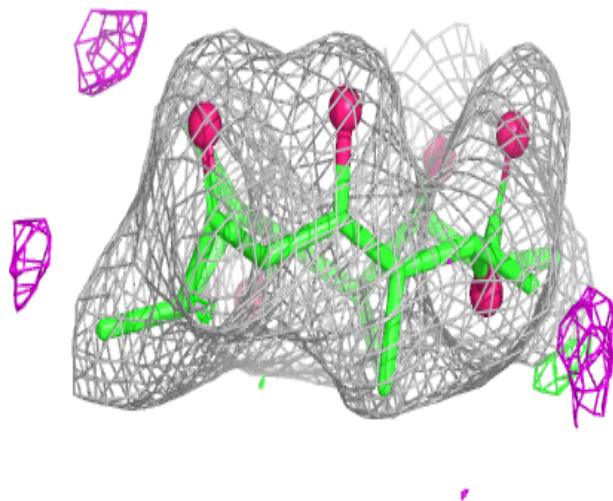
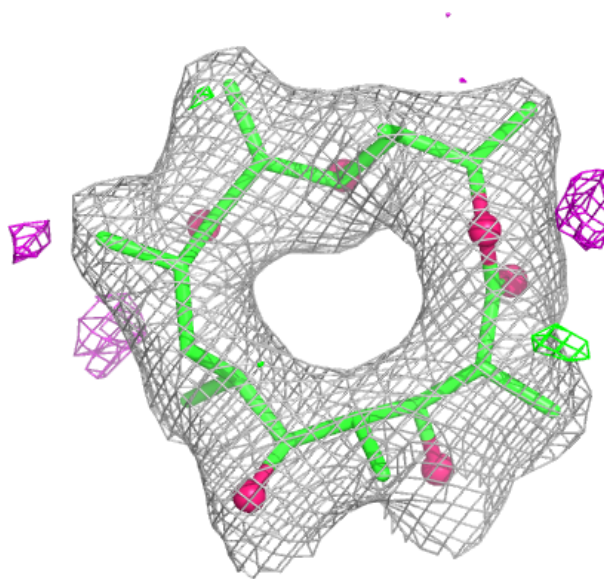
Electron density around QR8 C 502:

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



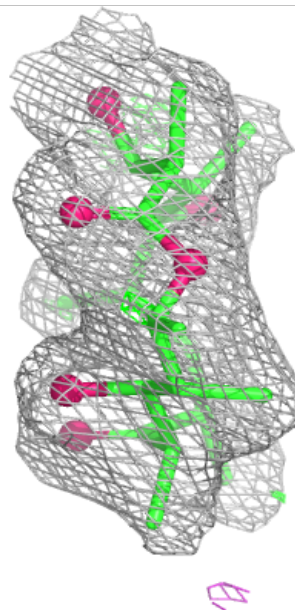
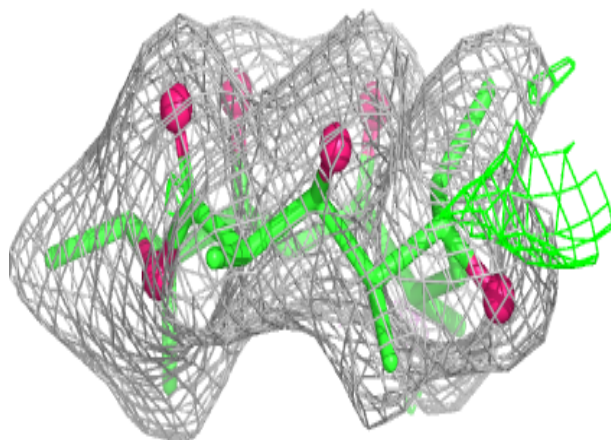
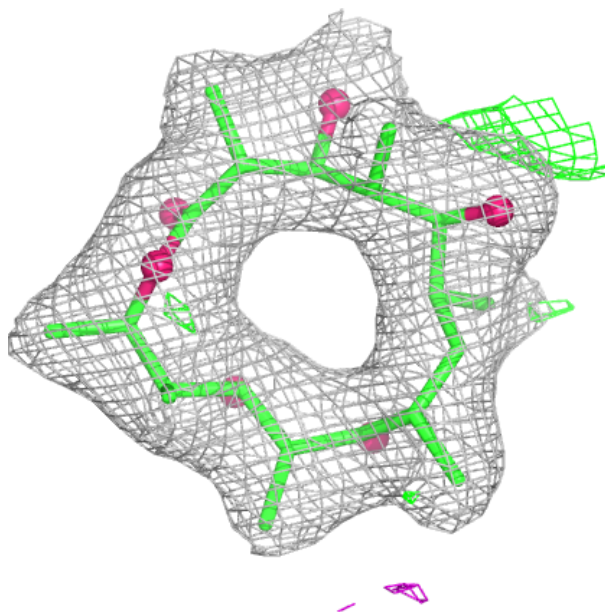
Electron density around QR8 D 502:

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



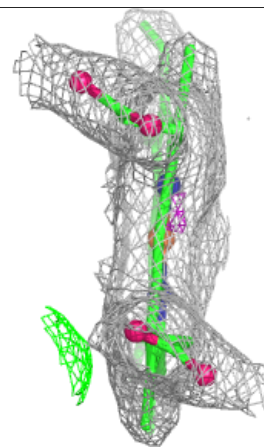
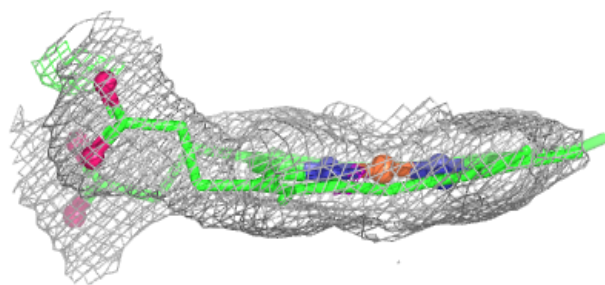
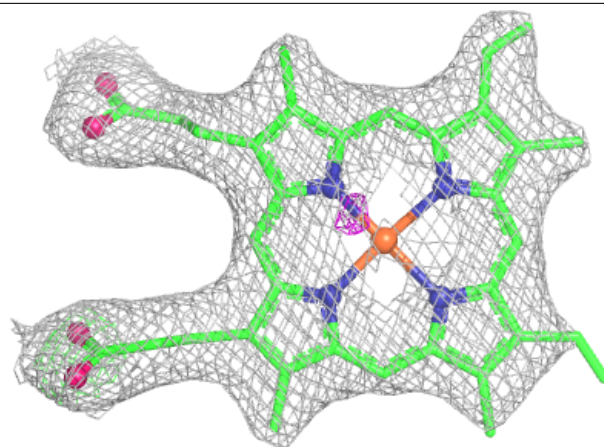
Electron density around QR8 B 502:

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



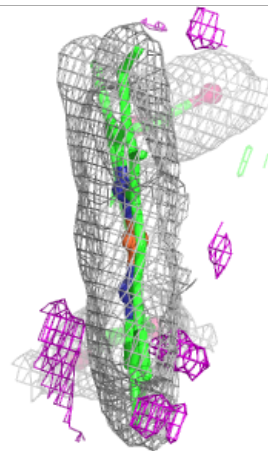
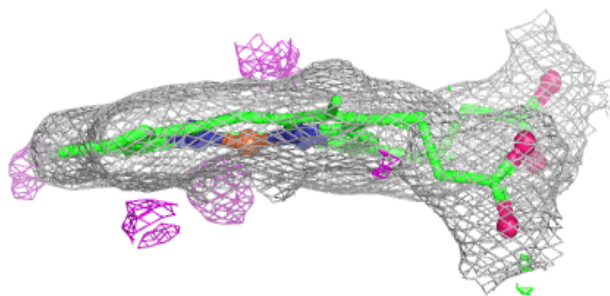
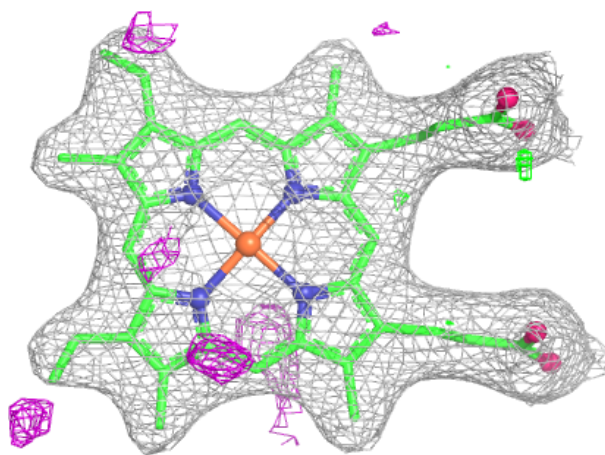
Electron density around HEM F 502:

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



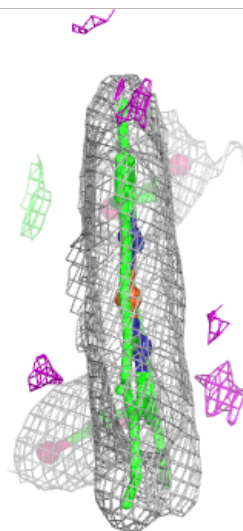
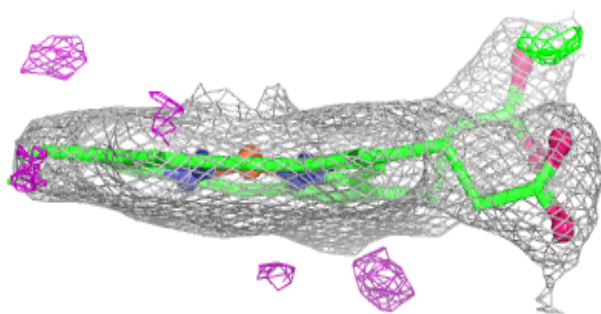
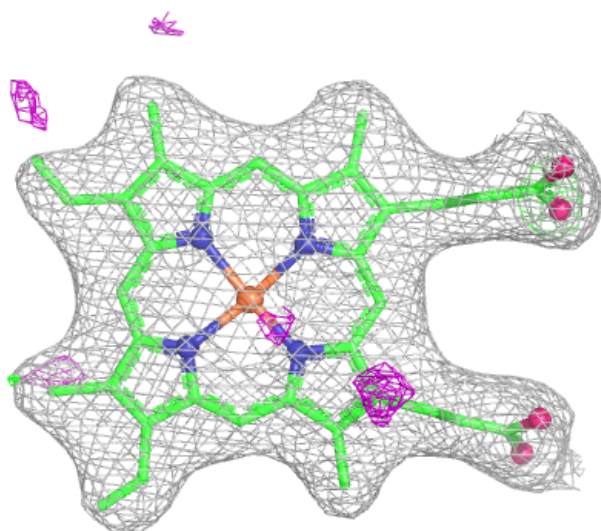
Electron density around HEM B 501:

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



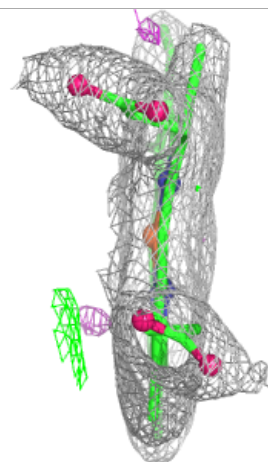
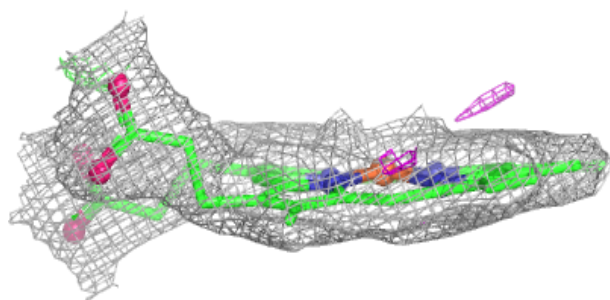
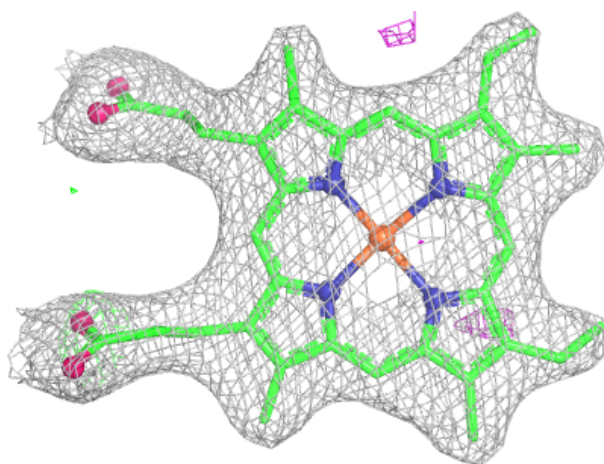
Electron density around HEM D 501:

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



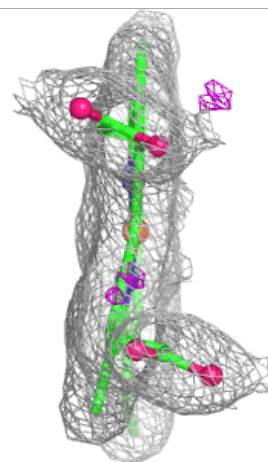
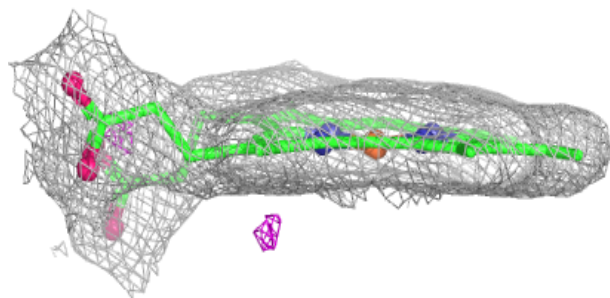
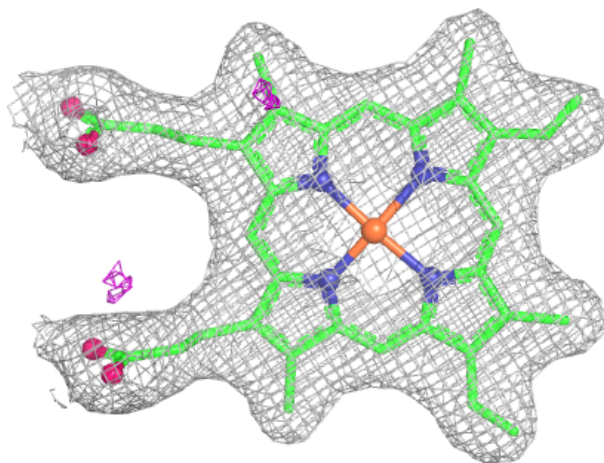
Electron density around HEM E 502:

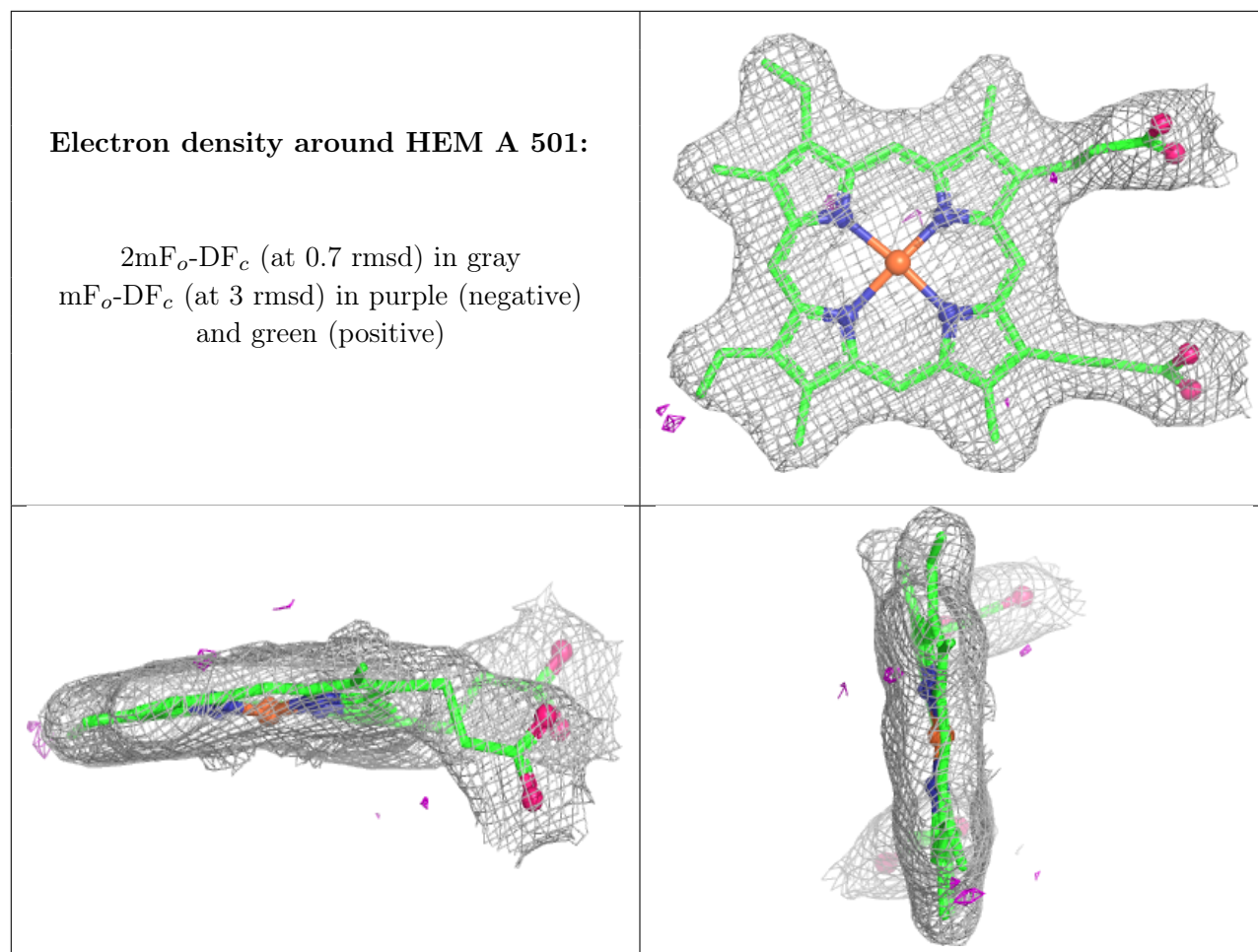
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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 [i](#)

There are no such residues in this entry.