



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:18 AM UTC

PDB ID : 6ZI3 / pdb_00006zi3
Title : Crystal structure of OleP-6DEB bound to L-rhamnose
Authors : Montemiglio, L.C.; Savino, C.; Vallone, B.; Parisi, G.; Freda, I.
Deposited on : 2020-06-24
Resolution : 2.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

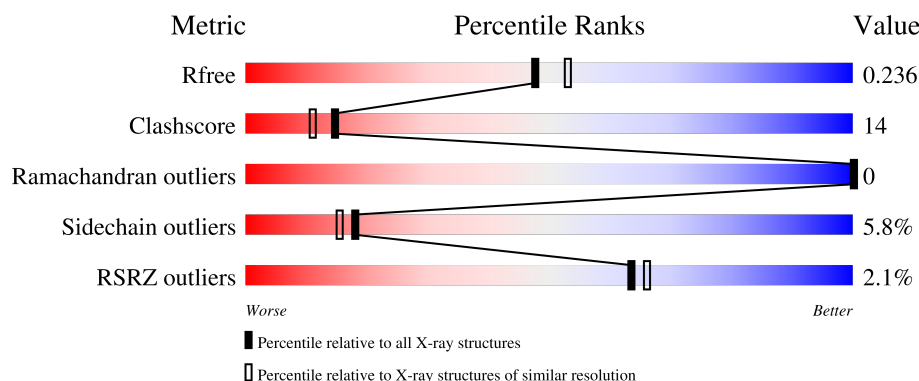
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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

Mol	Chain	Length	Quality of chain
1	A	407	0% 76% 19% ..
1	B	407	2% 77% 17% ..
1	C	407	80% 15% ..
1	D	407	3% 72% 22% ..
1	E	407	2% 74% 19% ..

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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	B	503[A]	-	-	X	-
4	RAM	D	503	-	-	X	-
4	RAM	E	503[A]	-	-	X	-
6	FMT	A	508	-	-	X	-
6	FMT	A	514	-	-	X	-
6	FMT	A	542	-	-	X	-
6	FMT	B	513	-	-	X	-
6	FMT	B	519	-	-	X	-
6	FMT	B	538	-	-	X	-
6	FMT	B	540	-	-	X	-
6	FMT	B	556	-	-	X	-
6	FMT	B	565	-	-	X	-
6	FMT	C	513[B]	-	-	X	-
6	FMT	C	555[B]	-	-	X	-
6	FMT	E	504	-	-	X	-
6	FMT	E	514[B]	-	-	X	-
8	GOL	B	505	-	-	X	-
8	GOL	C	507	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22632 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	397	Total	C	N	O	S	0	60	0
			3451	2210	601	622	18			
1	B	403	Total	C	N	O	S	0	37	0
			3347	2125	598	608	16			
1	C	397	Total	C	N	O	S	0	39	0
			3346	2120	601	609	16			
1	D	396	Total	C	N	O	S	0	53	0
			3425	2190	608	611	16			
1	E	395	Total	C	N	O	S	0	42	0
			3336	2127	596	595	18			
1	F	397	Total	C	N	O	S	0	48	0
			3395	2162	603	616	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q59819
A	2	THR	-	expression tag	UNP Q59819
A	3	ASP	-	expression tag	UNP Q59819
A	4	THR	-	expression tag	UNP Q59819
A	5	HIS	-	expression tag	UNP Q59819
A	6	THR	-	expression tag	UNP Q59819
A	7	GLY	-	expression tag	UNP Q59819
A	8	PRO	-	expression tag	UNP Q59819
A	9	THR	-	expression tag	UNP Q59819
A	10	PRO	-	expression tag	UNP Q59819
B	1	MET	-	initiating methionine	UNP Q59819
B	2	THR	-	expression tag	UNP Q59819
B	3	ASP	-	expression tag	UNP Q59819
B	4	THR	-	expression tag	UNP Q59819
B	5	HIS	-	expression tag	UNP Q59819
B	6	THR	-	expression tag	UNP Q59819
B	7	GLY	-	expression tag	UNP Q59819

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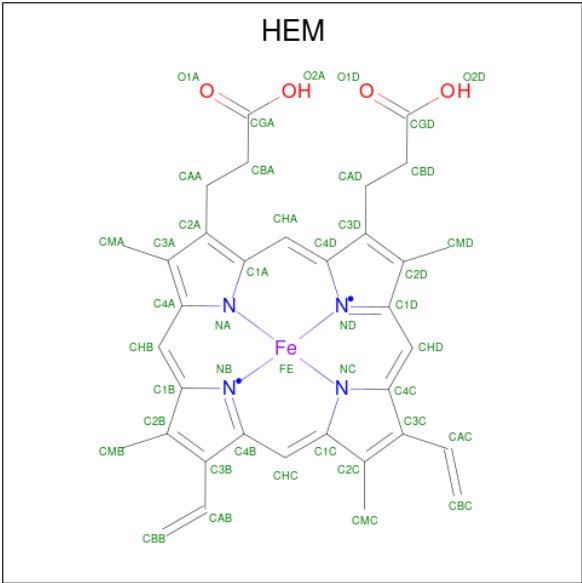
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	PRO	-	expression tag	UNP Q59819
B	9	THR	-	expression tag	UNP Q59819
B	10	PRO	-	expression tag	UNP Q59819
C	1	MET	-	initiating methionine	UNP Q59819
C	2	THR	-	expression tag	UNP Q59819
C	3	ASP	-	expression tag	UNP Q59819
C	4	THR	-	expression tag	UNP Q59819
C	5	HIS	-	expression tag	UNP Q59819
C	6	THR	-	expression tag	UNP Q59819
C	7	GLY	-	expression tag	UNP Q59819
C	8	PRO	-	expression tag	UNP Q59819
C	9	THR	-	expression tag	UNP Q59819
C	10	PRO	-	expression tag	UNP Q59819
D	1	MET	-	initiating methionine	UNP Q59819
D	2	THR	-	expression tag	UNP Q59819
D	3	ASP	-	expression tag	UNP Q59819
D	4	THR	-	expression tag	UNP Q59819
D	5	HIS	-	expression tag	UNP Q59819
D	6	THR	-	expression tag	UNP Q59819
D	7	GLY	-	expression tag	UNP Q59819
D	8	PRO	-	expression tag	UNP Q59819
D	9	THR	-	expression tag	UNP Q59819
D	10	PRO	-	expression tag	UNP Q59819
E	1	MET	-	initiating methionine	UNP Q59819
E	2	THR	-	expression tag	UNP Q59819
E	3	ASP	-	expression tag	UNP Q59819
E	4	THR	-	expression tag	UNP Q59819
E	5	HIS	-	expression tag	UNP Q59819
E	6	THR	-	expression tag	UNP Q59819
E	7	GLY	-	expression tag	UNP Q59819
E	8	PRO	-	expression tag	UNP Q59819
E	9	THR	-	expression tag	UNP Q59819
E	10	PRO	-	expression tag	UNP Q59819
F	1	MET	-	initiating methionine	UNP Q59819
F	2	THR	-	expression tag	UNP Q59819
F	3	ASP	-	expression tag	UNP Q59819
F	4	THR	-	expression tag	UNP Q59819
F	5	HIS	-	expression tag	UNP Q59819
F	6	THR	-	expression tag	UNP Q59819
F	7	GLY	-	expression tag	UNP Q59819
F	8	PRO	-	expression tag	UNP Q59819
F	9	THR	-	expression tag	UNP Q59819

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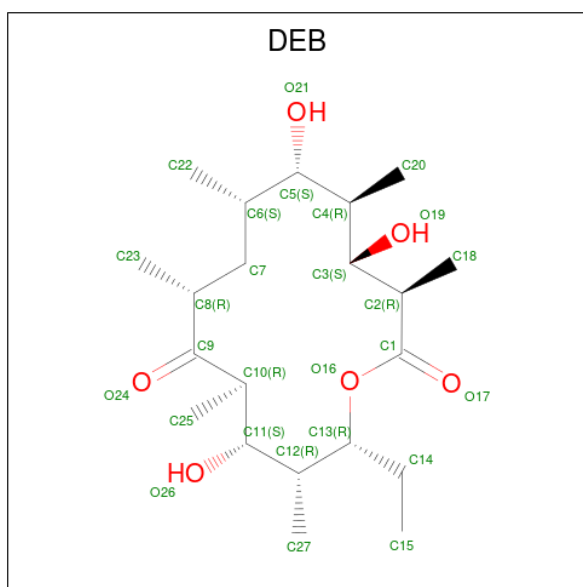
Chain	Residue	Modelled	Actual	Comment	Reference
F	10	PRO	-	expression tag	UNP Q59819

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



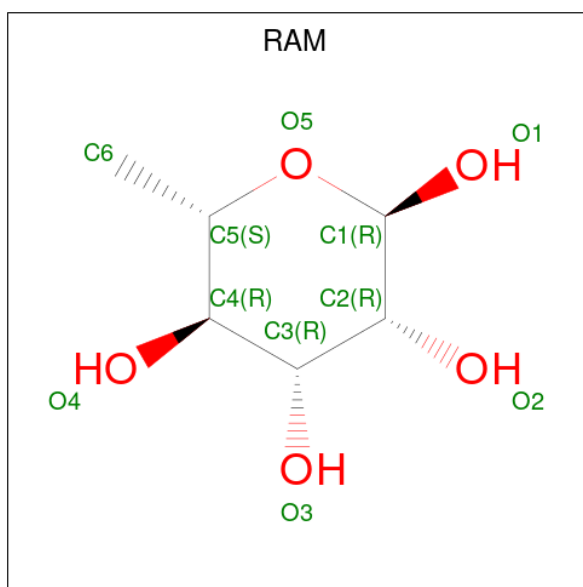
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 6-DEOXYERYTHRONOLIDE B (CCD ID: DEB) (formula: C₂₁H₃₈O₆).



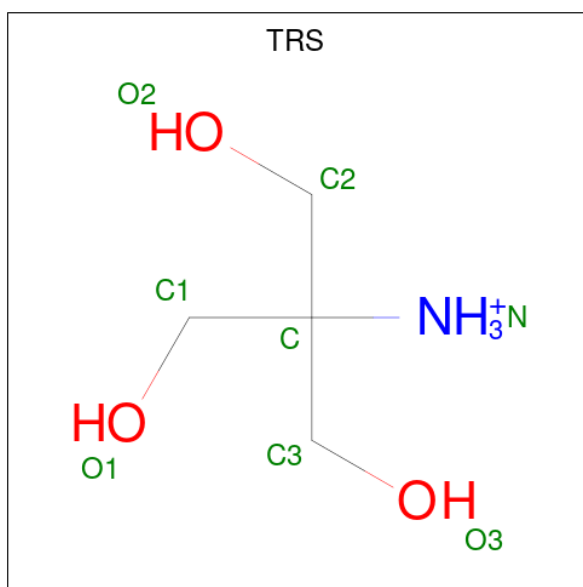
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			27	21	6		
3	B	1	Total	C	O	0	0
			27	21	6		
3	C	1	Total	C	O	0	0
			27	21	6		
3	D	1	Total	C	O	0	0
			27	21	6		
3	E	1	Total	C	O	0	0
			27	21	6		
3	F	1	Total	C	O	0	0
			27	21	6		

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



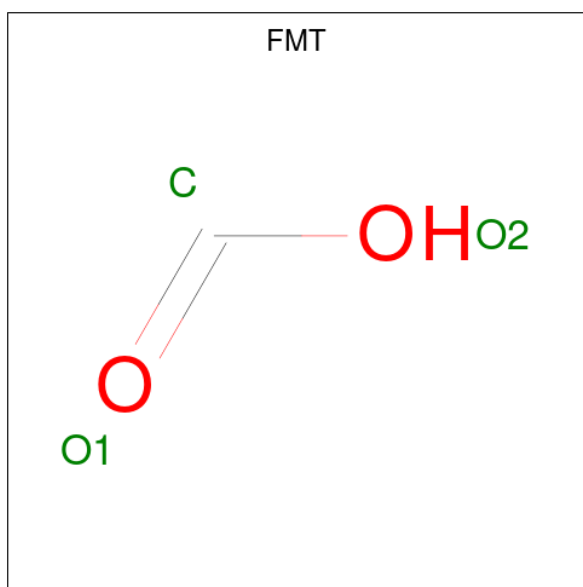
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			11	6	5		
4	B	1	Total	C	O	0	1
			11	6	5		
4	C	1	Total	C	O	0	1
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	1
			11	6	5		
4	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	F	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

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

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

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

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

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

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

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

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

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

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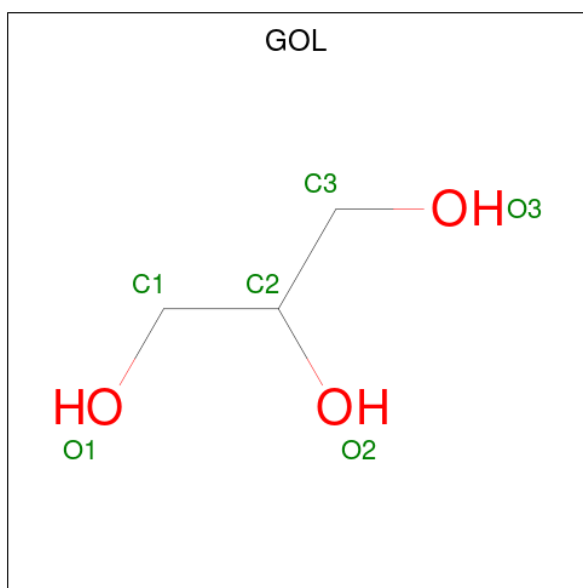
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			3	1	2		
6	F	1	Total	C	O	0	0
			3	1	2		
6	F	1	Total	C	O	0	0
			3	1	2		
6	F	1	Total	C	O	0	0
			3	1	2		
6	F	1	Total	C	O	0	0
			3	1	2		
6	F	1	Total	C	O	0	0
			3	1	2		
6	F	1	Total	C	O	0	0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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	202	Total	O	0	0
			202	202		
9	B	258	Total	O	0	1
			258	258		
9	C	308	Total	O	0	1
			308	308		
9	D	128	Total	O	0	0
			128	128		
9	E	144	Total	O	0	1
			144	144		

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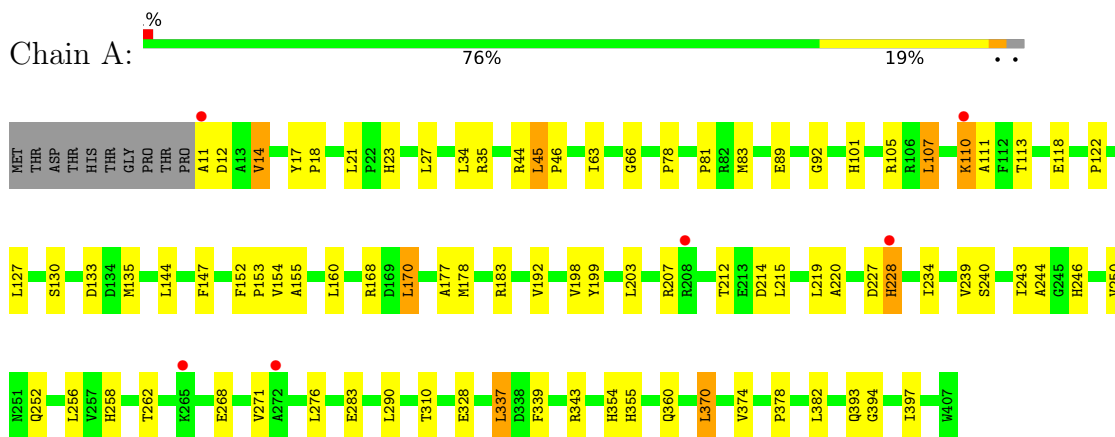
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	119	Total 119	O 119	0	0

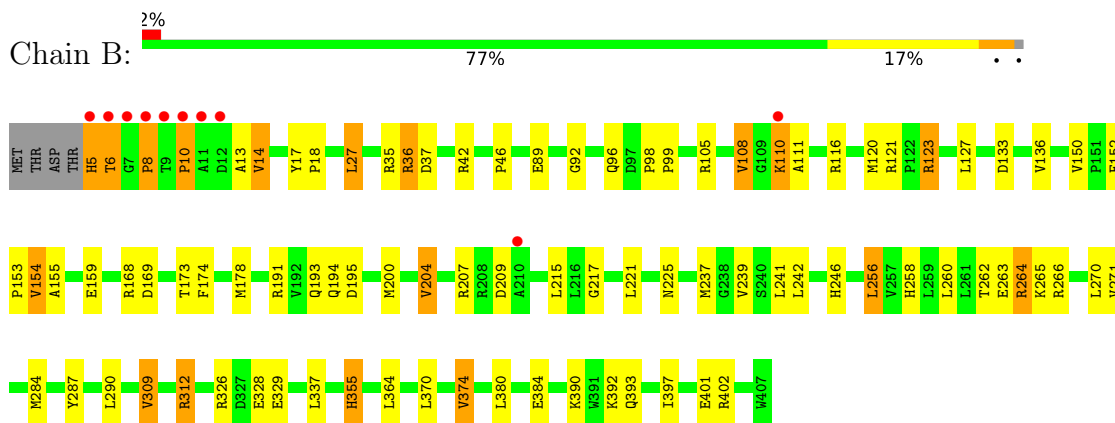
3 Residue-property plots [i](#)

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

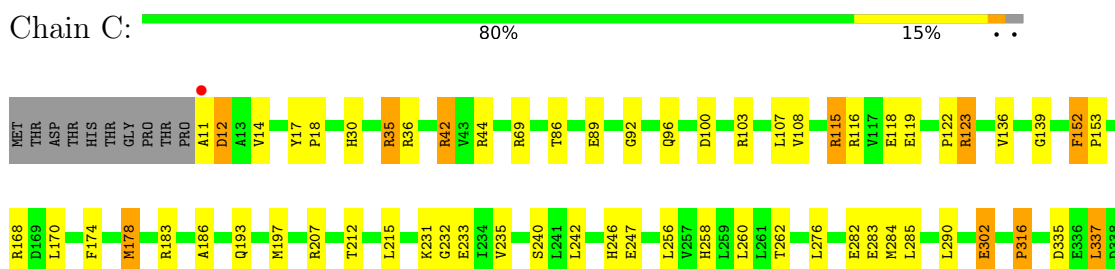
• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450

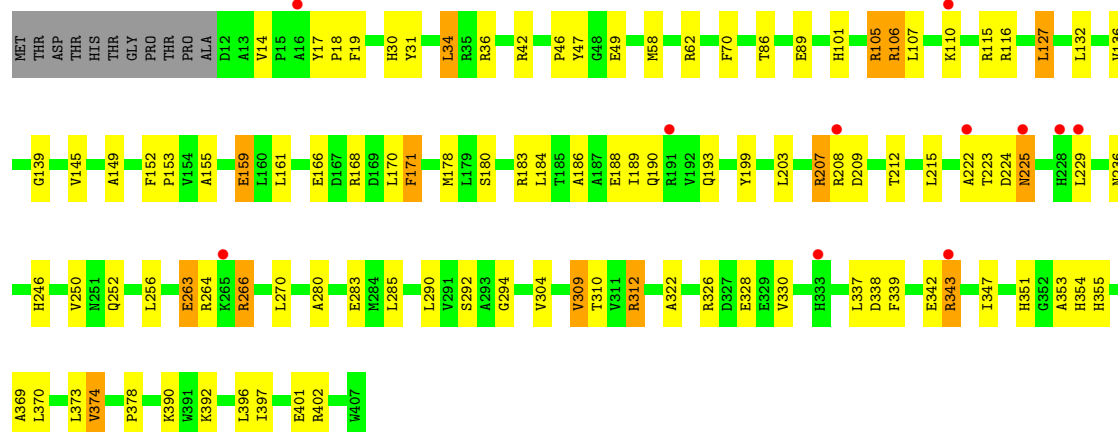


• Molecule 1: Cytochrome P-450

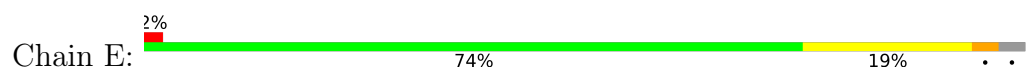




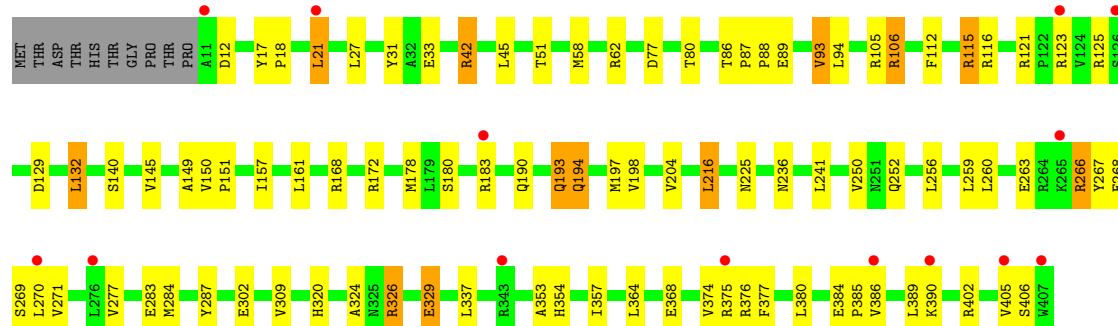
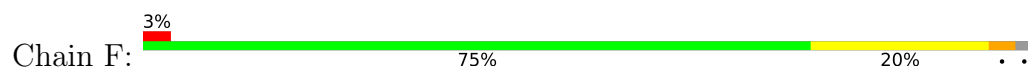
• Molecule 1: Cytochrome P-450



• 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	247.38Å 111.15Å 159.14Å 90.00° 129.40° 90.00°	Depositor
Resolution (Å)	48.09 – 2.08 48.09 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.09-2.08) 99.7 (48.09-2.08)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.172 , 0.225 (Not available) , 0.236	Depositor DCC
R_{free} test set	11824 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22632	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 35.22 % 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 6.0389e-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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.08	3/3685 (0.1%)	1.34	9/5004 (0.2%)
1	B	1.10	3/3529 (0.1%)	1.39	6/4798 (0.1%)
1	C	1.15	2/3519 (0.1%)	1.33	4/4775 (0.1%)
1	D	1.16	5/3657 (0.1%)	1.42	6/4965 (0.1%)
1	E	1.07	2/3534 (0.1%)	1.39	12/4796 (0.3%)
1	F	1.13	2/3612 (0.1%)	1.44	2/4907 (0.0%)
All	All	1.12	17/21536 (0.1%)	1.39	39/29245 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	283	GLU	CD-OE2	12.45	1.49	1.25
1	D	208[A]	ARG	N-CA	8.35	1.56	1.46
1	D	208[B]	ARG	N-CA	8.35	1.56	1.46
1	D	208[A]	ARG	CA-C	7.82	1.62	1.52
1	D	208[B]	ARG	CA-C	7.82	1.62	1.52
1	A	66	GLY	C-O	-6.05	1.15	1.23
1	B	98	PRO	C-O	-6.04	1.19	1.25
1	E	296	PHE	C-O	5.95	1.30	1.23
1	E	14	VAL	N-CA	5.82	1.50	1.46
1	C	35	ARG	CD-NE	-5.54	1.38	1.46
1	A	78	PRO	C-O	-5.37	1.17	1.24
1	C	316	PRO	C-O	-5.23	1.18	1.23
1	B	355	HIS	CE1-NE2	5.18	1.37	1.32
1	F	106	ARG	C-O	-5.16	1.17	1.24
1	B	46	PRO	C-O	-5.13	1.18	1.24
1	A	113	THR	C-O	5.11	1.30	1.23
1	D	396	LEU	C-O	5.02	1.30	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	93	VAL	CB-CA-C	-7.66	102.07	111.88
1	C	35	ARG	CG-CD-NE	-7.13	96.31	112.00
1	E	93	VAL	CB-CA-C	-6.99	102.93	111.88
1	B	173	THR	CA-CB-OG1	-6.96	99.16	109.60
1	C	139	GLY	CA-C-O	-6.26	117.91	122.23
1	B	98	PRO	O-C-N	-6.19	118.46	121.31
1	D	225	ASN	N-CA-C	-6.13	100.83	109.96
1	E	93	VAL	N-CA-CB	6.07	117.25	110.51
1	B	8	PRO	N-CA-C	-5.96	105.25	113.53
1	B	10	PRO	N-CA-C	-5.78	100.56	112.47
1	B	168	ARG	CB-CA-C	-5.78	101.56	110.81
1	A	310	THR	CA-CB-OG1	-5.77	100.95	109.60
1	F	93	VAL	N-CA-CB	5.69	116.82	110.51
1	D	139	GLY	CA-C-O	-5.66	118.32	122.23
1	A	105	ARG	CB-CG-CD	-5.64	98.34	111.30
1	E	301	THR	CA-CB-OG1	-5.60	101.20	109.60
1	C	35	ARG	NE-CZ-NH2	-5.45	114.29	119.20
1	E	67	ASP	CA-C-N	5.39	129.30	120.63
1	E	67	ASP	C-N-CA	5.39	129.30	120.63
1	D	171	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	276[A]	LEU	CA-C-N	5.32	124.59	120.33
1	A	276[A]	LEU	C-N-CA	5.32	124.59	120.33
1	A	276[B]	LEU	CA-C-N	5.32	124.59	120.33
1	A	276[B]	LEU	C-N-CA	5.32	124.59	120.33
1	C	152	PHE	O-C-N	-5.29	116.62	120.27
1	A	23	HIS	CA-CB-CG	-5.21	108.59	113.80
1	E	169	ASP	CA-CB-CG	5.17	117.77	112.60
1	E	154	VAL	N-CA-CB	5.16	118.32	110.58
1	B	169	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	310	THR	CA-CB-OG1	-5.15	101.88	109.60
1	D	292	SER	O-C-N	5.14	127.64	122.09
1	A	34	LEU	CA-C-O	-5.14	115.43	120.82
1	E	105	ARG	CB-CG-CD	-5.13	99.50	111.30
1	D	223	THR	CB-CA-C	5.11	119.27	110.79
1	E	231[A]	LYS	CA-C-N	5.10	125.60	119.94
1	E	231[A]	LYS	C-N-CA	5.10	125.60	119.94
1	E	231[B]	LYS	CA-C-N	5.10	125.60	119.94
1	E	231[B]	LYS	C-N-CA	5.10	125.60	119.94
1	A	360	GLN	N-CA-C	-5.05	105.85	111.36

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	3451	0	3612	68	0
1	B	3347	0	3448	108	0
1	C	3346	0	3420	95	1
1	D	3425	0	3549	113	0
1	E	3336	0	3456	83	1
1	F	3395	0	3494	98	0
2	A	43	0	30	5	0
2	B	43	0	30	2	0
2	C	43	0	30	1	0
2	D	43	0	30	5	0
2	E	43	0	30	7	0
2	F	43	0	30	5	0
3	A	27	0	38	3	0
3	B	27	0	38	0	0
3	C	27	0	38	1	0
3	D	27	0	38	6	0
3	E	27	0	38	4	0
3	F	27	0	38	0	0
4	A	11	0	12	15	0
4	B	11	0	12	7	0
4	C	22	0	24	8	0
4	D	11	0	12	10	0
4	E	11	0	12	12	0
4	F	11	0	12	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
5	F	8	0	12	3	0
6	A	123	0	41	10	0
6	B	189	0	63	17	0
6	C	174	0	56	10	0
6	D	48	0	16	1	0
6	E	33	0	11	5	0
6	F	42	0	14	1	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	B	12	0	16	4	0
8	C	18	0	24	13	0
8	F	6	0	8	1	0
9	A	202	0	0	10	0
9	B	258	0	0	5	0
9	C	308	0	0	13	0
9	D	128	0	0	8	0
9	E	144	0	0	6	0
9	F	119	0	0	3	0
All	All	22632	0	21756	599	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.

All (599) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PRO:HB2	1:B:13:ALA:CB	1.26	1.60
1:B:10:PRO:CB	1:B:13:ALA:HB3	1.25	1.58
1:D:178[B]:MET:HE2	1:D:193[B]:GLN:CG	1.41	1.51
1:C:178[B]:MET:CE	1:C:193[B]:GLN:HA	1.55	1.34
1:D:178[B]:MET:CE	1:D:193[B]:GLN:HG2	1.60	1.30
1:C:178[B]:MET:HE2	1:C:193[B]:GLN:CB	1.69	1.20
1:B:10:PRO:CB	1:B:13:ALA:CB	1.95	1.19
1:E:236:ASN:HD21	4:E:503[A]:RAM:C3	1.55	1.19
1:B:178[B]:MET:CE	1:B:193[B]:GLN:HA	1.73	1.18
1:D:107[B]:LEU:HD11	1:D:229[B]:LEU:HD23	1.17	1.13
1:C:178[B]:MET:HE3	1:C:193[B]:GLN:HA	1.14	1.13
1:F:377[B]:PHE:HB3	1:F:380[B]:LEU:CD1	1.79	1.11
1:C:178[B]:MET:CE	1:C:193[B]:GLN:CA	2.28	1.10
1:C:178[B]:MET:HE2	1:C:193[B]:GLN:HB2	1.19	1.10
1:D:178[B]:MET:CE	1:D:193[B]:GLN:HA	1.82	1.09
1:E:236:ASN:HD21	4:E:503[A]:RAM:H3	1.13	1.08
1:F:270[B]:LEU:HD22	1:F:374[B]:VAL:HG11	1.15	1.08
1:D:343[A]:ARG:HH11	1:D:343[A]:ARG:HB3	1.22	1.05
1:B:193[B]:GLN:HE22	8:B:505:GOL:H12	1.22	1.04
6:E:514[B]:FMT:H	9:E:663[B]:HOH:O	1.58	1.04
1:D:105[A]:ARG:NH1	1:D:355:HIS:O	1.91	1.03
1:C:178[A]:MET:HE1	1:C:193[A]:GLN:HG3	1.06	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129[B]:ASP:OD1	1:F:376[B]:ARG:NH2	1.92	1.02
1:A:240:SER:HA	4:A:503[A]:RAM:H61	1.45	0.99
1:C:178[B]:MET:CE	1:C:193[B]:GLN:CB	2.40	0.99
1:B:326[A]:ARG:NH1	9:B:602:HOH:O	1.95	0.98
1:C:178[A]:MET:HE1	1:C:193[A]:GLN:CG	1.93	0.98
1:C:178[B]:MET:HE3	1:C:193[B]:GLN:CA	1.91	0.98
1:F:125[B]:ARG:NH1	1:F:375[B]:ARG:HH22	1.61	0.98
1:A:256[B]:LEU:HD23	1:A:370[B]:LEU:HD21	1.44	0.97
1:D:390[B]:LYS:CE	1:D:402[B]:ARG:NH2	2.28	0.96
1:C:115[A]:ARG:NH2	1:C:115[A]:ARG:HG3	1.78	0.96
1:B:178[B]:MET:HE3	1:B:193[B]:GLN:HA	1.49	0.95
1:E:57[A]:ARG:HH12	1:E:329[A]:GLU:HG3	1.29	0.94
1:E:172:ARG:NH1	9:E:601:HOH:O	2.01	0.93
1:B:10:PRO:HB3	1:B:13:ALA:CB	1.99	0.93
6:C:513[B]:FMT:O2	9:C:601[B]:HOH:O	1.87	0.93
1:F:377[B]:PHE:HB3	1:F:380[B]:LEU:HD13	1.48	0.93
1:D:390[B]:LYS:HE2	1:D:402[B]:ARG:HH22	1.33	0.91
1:E:35[A]:ARG:HD2	1:E:57[A]:ARG:HG2	1.51	0.90
1:F:377[B]:PHE:CB	1:F:380[B]:LEU:HD13	2.02	0.90
1:C:108:VAL:HG12	1:C:215[B]:LEU:HD11	1.53	0.89
1:A:256[B]:LEU:HD23	1:A:370[B]:LEU:CD2	2.02	0.88
1:C:96:GLN:OE1	4:C:504:RAM:O1	1.92	0.88
1:B:105[A]:ARG:NH2	1:B:355:HIS:O	2.07	0.88
1:B:10:PRO:CB	1:B:13:ALA:HB2	2.03	0.87
1:E:236:ASN:ND2	4:E:503[A]:RAM:H3	1.87	0.87
1:B:178[A]:MET:SD	1:B:193[A]:GLN:HG2	2.14	0.87
1:B:193[B]:GLN:NE2	8:B:505:GOL:H12	1.90	0.87
1:C:119:GLU:OE1	9:C:602:HOH:O	1.93	0.87
2:F:702:HEM:HBB2	2:F:702:HEM:HMB2	1.54	0.87
1:F:357[B]:ILE:HD11	2:F:702:HEM:HMD2	1.56	0.87
1:F:354[B]:HIS:HE1	5:F:705:TRS:O3	1.56	0.86
1:D:107[B]:LEU:HD11	1:D:229[B]:LEU:CD2	2.04	0.86
1:C:115[A]:ARG:HG3	1:C:115[A]:ARG:HH21	1.39	0.86
1:F:270[B]:LEU:CD2	1:F:374[B]:VAL:HG21	2.07	0.85
1:F:377[B]:PHE:CB	1:F:380[B]:LEU:CD1	2.53	0.85
1:A:243:ILE:HD12	4:A:503[A]:RAM:H62	1.57	0.85
1:B:150:VAL:O	1:B:154:VAL:HG13	1.77	0.84
3:E:502:DEB:H203	4:E:503[A]:RAM:C6	2.07	0.84
1:E:44[A]:ARG:HG3	1:E:44[A]:ARG:HH11	1.41	0.84
1:F:268[A]:GLU:HA	1:F:271[A]:VAL:HG12	1.60	0.84
1:E:57[A]:ARG:NH1	1:E:329[A]:GLU:HG3	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30[A]:HIS:NE2	1:D:34[A]:LEU:HD21	1.94	0.82
1:E:236:ASN:ND2	4:E:503[A]:RAM:C3	2.39	0.82
1:C:86[B]:THR:HB	8:C:507:GOL:HO1	1.44	0.82
1:F:260:LEU:HG	1:F:284:MET:HE1	1.62	0.81
1:C:100:ASP:OD2	4:C:504:RAM:O5	1.98	0.81
1:A:89:GLU:HB3	4:A:503[A]:RAM:O2	1.80	0.81
1:B:178[B]:MET:CE	1:B:193[B]:GLN:CA	2.57	0.81
1:E:191:ARG:NH1	9:E:602:HOH:O	2.14	0.80
1:D:178[B]:MET:CE	1:D:193[B]:GLN:CA	2.60	0.79
1:F:377[B]:PHE:HB3	1:F:380[B]:LEU:HD12	1.66	0.78
3:D:502:DEB:O19	4:D:503:RAM:O5	2.01	0.78
1:D:390[B]:LYS:CE	1:D:402[B]:ARG:HH22	1.94	0.77
1:C:178[B]:MET:HE1	1:C:193[B]:GLN:HA	1.62	0.77
1:D:390[B]:LYS:HD2	1:D:402[B]:ARG:HH21	1.48	0.77
1:C:86[A]:THR:OG1	8:C:507:GOL:O1	2.02	0.77
1:C:343:ARG:NH1	6:C:538:FMT:O1	2.17	0.76
1:D:178[B]:MET:HE1	1:D:193[B]:GLN:HA	1.66	0.76
1:D:369:ALA:O	1:D:373[B]:LEU:HD23	1.85	0.76
1:D:178[B]:MET:CE	1:D:193[B]:GLN:CG	2.37	0.76
1:B:178[B]:MET:HE2	1:B:193[B]:GLN:HB2	1.67	0.75
1:A:240:SER:CA	4:A:503[A]:RAM:H61	2.16	0.75
1:E:178[A]:MET:HE2	4:E:503[A]:RAM:H61	1.69	0.74
1:E:280:ALA:O	1:E:284[A]:MET:HG3	1.87	0.74
1:D:390[B]:LYS:CD	1:D:402[B]:ARG:NH2	2.51	0.74
1:B:10:PRO:HA	9:B:726:HOH:O	1.86	0.74
1:E:110[A]:LYS:HG2	1:E:116[A]:ARG:NH1	2.02	0.74
1:A:35[B]:ARG:HE	6:A:514:FMT:C	2.00	0.74
1:F:270[B]:LEU:HD22	1:F:374[B]:VAL:CG1	2.07	0.73
3:E:502:DEB:H203	4:E:503[A]:RAM:H63	1.71	0.73
1:F:384[A]:GLU:OE1	1:F:402:ARG:NH1	2.22	0.73
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.70	0.73
1:F:266:ARG:NH2	1:F:337[B]:LEU:HD12	2.04	0.73
1:F:145:VAL:HA	1:F:149:ALA:HB3	1.71	0.73
1:D:390[B]:LYS:HD2	1:D:402[B]:ARG:NH2	2.03	0.73
1:B:8:PRO:HG3	1:C:282:GLU:HG3	1.70	0.72
1:E:110[A]:LYS:HG2	1:E:116[A]:ARG:HH11	1.55	0.72
1:D:236:ASN:OD1	4:D:503:RAM:O3	2.04	0.72
1:D:224:ASP:OD1	9:D:601:HOH:O	2.07	0.71
1:B:178[B]:MET:HE3	1:B:193[B]:GLN:CA	2.18	0.71
1:D:401[B]:GLU:OE2	9:D:602:HOH:O	2.08	0.71
1:F:354[B]:HIS:CE1	5:F:705:TRS:O3	2.42	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343[B]:ARG:HB3	1:D:343[B]:ARG:HH21	1.55	0.71
2:E:501:HEM:HHC	2:E:501:HEM:HBB2	1.73	0.71
1:C:344:ASN:N	9:C:603:HOH:O	2.03	0.71
1:D:343[A]:ARG:HH11	1:D:343[A]:ARG:CB	2.01	0.71
1:D:322:ALA:O	1:D:326:ARG:HG2	1.91	0.70
2:F:702:HEM:HBB2	2:F:702:HEM:CMB	2.21	0.70
1:E:44[A]:ARG:HG3	1:E:44[A]:ARG:NH1	2.05	0.70
1:D:252[A]:GLN:HE21	1:D:285:LEU:HD23	1.57	0.70
1:F:58[A]:MET:HE3	1:F:62[A]:ARG:NH2	2.05	0.70
1:B:178[A]:MET:HE1	4:B:503[A]:RAM:H2	1.74	0.70
3:D:502:DEB:O19	4:D:503:RAM:C5	2.39	0.69
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.74	0.69
1:F:190[A]:GLN:HE22	1:F:193:GLN:HE21	1.38	0.69
1:E:127[B]:LEU:HD21	1:E:155:ALA:HB3	1.74	0.69
1:D:58[A]:MET:HE1	1:D:347:ILE:HD13	1.73	0.69
1:D:252[B]:GLN:OE1	1:D:252[B]:GLN:HA	1.91	0.69
1:A:127[A]:LEU:HD21	1:A:155:ALA:HB3	1.74	0.69
1:B:193[B]:GLN:HE22	8:B:505:GOL:C1	2.02	0.69
1:D:178[B]:MET:HE3	1:D:193[B]:GLN:HA	1.73	0.69
1:C:260:LEU:CD1	1:C:370[B]:LEU:HD11	2.23	0.69
1:E:256:LEU:HD22	1:E:284[B]:MET:HB3	1.75	0.69
1:E:110[A]:LYS:CG	1:E:116[A]:ARG:NH1	2.56	0.69
1:B:193[B]:GLN:NE2	8:B:505:GOL:C1	2.57	0.68
1:A:228:HIS:HB2	9:A:697:HOH:O	1.93	0.68
1:E:57[A]:ARG:NH1	1:E:329[A]:GLU:CG	2.56	0.68
8:C:507:GOL:H32	6:C:555[B]:FMT:O1	1.93	0.68
1:F:86:THR:HB	1:F:190[B]:GLN:HE22	1.59	0.68
1:C:174:PHE:O	1:C:178[A]:MET:HG2	1.94	0.68
1:C:256:LEU:HD22	1:C:284:MET:HB3	1.77	0.67
1:B:14:VAL:HG11	1:B:42[A]:ARG:HD3	1.75	0.67
1:E:150:VAL:O	1:E:154:VAL:HG13	1.95	0.67
1:C:115[A]:ARG:HH21	1:C:115[A]:ARG:CG	2.06	0.67
1:E:236:ASN:ND2	4:E:503[A]:RAM:O3	2.28	0.67
1:D:390[B]:LYS:CE	1:D:402[B]:ARG:HH21	2.06	0.66
1:B:35[A]:ARG:NH1	6:B:519:FMT:C	2.57	0.66
6:B:540:FMT:C	1:C:115[A]:ARG:NH1	2.58	0.66
1:F:105:ARG:CZ	1:F:357[B]:ILE:HG23	2.26	0.66
1:C:178[B]:MET:HE2	1:C:193[B]:GLN:CG	2.25	0.66
1:B:42[B]:ARG:NE	6:B:556:FMT:O1	2.29	0.66
1:D:106[A]:ARG:NH2	1:D:110[A]:LYS:HZ1	1.93	0.66
1:E:178[B]:MET:SD	1:E:193:GLN:HG2	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125[B]:ARG:NH1	1:F:375[B]:ARG:NH2	2.41	0.66
1:C:233:GLU:OE2	4:C:504:RAM:H5	1.94	0.66
1:D:178[B]:MET:HE2	1:D:193[B]:GLN:CB	2.24	0.66
1:C:123:ARG:NH1	6:C:532:FMT:O1	2.29	0.66
1:F:270[B]:LEU:CD2	1:F:374[B]:VAL:HG11	2.09	0.66
1:D:343[B]:ARG:HH21	1:D:343[B]:ARG:CB	2.09	0.65
3:D:502:DEB:O19	4:D:503:RAM:H61	1.96	0.65
1:D:184:LEU:HB2	1:D:189:ILE:HD11	1.77	0.65
1:B:178[B]:MET:HE2	1:B:193[B]:GLN:CB	2.26	0.65
1:C:108:VAL:CG1	1:C:215[B]:LEU:HD11	2.27	0.65
1:F:129[B]:ASP:OD1	1:F:376[B]:ARG:CZ	2.45	0.65
1:C:178[B]:MET:CE	1:C:193[B]:GLN:HB2	2.08	0.65
1:D:107[B]:LEU:CD1	1:D:229[B]:LEU:HD23	2.11	0.65
1:D:390[B]:LYS:CD	1:D:402[B]:ARG:HH21	2.07	0.65
1:E:333[A]:HIS:HD2	1:E:336[A]:GLU:HB2	1.62	0.65
1:D:178[B]:MET:HE2	1:D:193[B]:GLN:HG3	1.69	0.64
1:C:283:GLU:HG3	1:C:337:LEU:HD22	1.79	0.64
1:B:264[A]:ARG:NH1	1:B:380:LEU:O	2.30	0.64
1:F:353:ALA:HB3	5:F:705:TRS:N	2.13	0.64
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.28	0.64
1:E:333[A]:HIS:CD2	1:E:336[A]:GLU:HB2	2.33	0.63
1:F:267[B]:TYR:CE1	1:F:374[B]:VAL:HG12	2.32	0.63
1:D:178[B]:MET:HE2	1:D:193[B]:GLN:HG2	0.68	0.63
1:E:101[B]:HIS:CD2	1:E:354[B]:HIS:NE2	2.66	0.63
1:D:101[B]:HIS:HE1	1:D:105[B]:ARG:HE	1.46	0.63
1:D:116[B]:ARG:NH2	9:D:603:HOH:O	2.30	0.63
1:E:35[A]:ARG:CD	1:E:57[A]:ARG:HG2	2.27	0.63
1:D:390[B]:LYS:HE2	1:D:402[B]:ARG:NH2	1.99	0.62
1:B:191[B]:ARG:NH2	1:B:194[B]:GLN:OE1	2.32	0.62
6:E:514[B]:FMT:C	9:E:663[B]:HOH:O	2.30	0.62
6:A:515:FMT:H	9:A:678:HOH:O	1.99	0.62
1:B:328:GLU:HB2	6:B:519:FMT:C	2.29	0.62
1:A:183[B]:ARG:NH1	9:A:606:HOH:O	2.28	0.62
1:C:354[B]:HIS:HE1	8:C:505:GOL:O1	1.83	0.62
1:B:178[B]:MET:HE1	1:B:193[B]:GLN:HA	1.75	0.62
1:D:30[A]:HIS:CD2	1:D:34[A]:LEU:HD21	2.34	0.62
1:E:259:LEU:HB2	1:E:284[A]:MET:CE	2.30	0.62
1:B:390[A]:LYS:HZ2	1:B:402[A]:ARG:NH2	1.98	0.61
1:F:125[B]:ARG:HD3	1:F:375[B]:ARG:HH12	1.63	0.61
1:D:390[A]:LYS:CE	1:D:401[A]:GLU:OE2	2.48	0.61
1:F:377[B]:PHE:HB2	1:F:380[B]:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:O	1:A:271[B]:VAL:HG12	2.01	0.61
1:B:384:GLU:OE2	1:B:402[A]:ARG:HD2	2.00	0.61
1:E:105:ARG:NH2	1:E:355:HIS:O	2.23	0.61
1:B:178[A]:MET:HE1	1:B:193[A]:GLN:HG2	1.82	0.61
1:A:14[A]:VAL:HG13	1:A:44[A]:ARG:NH2	2.16	0.61
1:D:390[B]:LYS:HE3	1:D:402[B]:ARG:NH2	2.15	0.61
1:B:178[A]:MET:CE	1:B:193[A]:GLN:HG2	2.31	0.61
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.28	0.60
1:A:122:PRO:HB3	1:D:309:VAL:HG13	1.83	0.60
1:B:390[A]:LYS:NZ	1:B:402[A]:ARG:NH2	2.49	0.60
1:B:178[A]:MET:CE	4:B:503[A]:RAM:H2	2.32	0.60
6:C:513[B]:FMT:C	9:C:601[B]:HOH:O	2.47	0.60
1:C:197[B]:MET:HE1	1:C:232:GLY:O	2.01	0.60
1:A:252:GLN:O	1:A:256[A]:LEU:HG	2.01	0.60
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.84	0.59
6:B:507:FMT:O2	6:B:548:FMT:O2	2.20	0.59
1:A:246:HIS:O	1:A:250[B]:VAL:HG13	2.01	0.59
1:E:326:ARG:NH2	9:E:605:HOH:O	2.35	0.59
1:F:287:TYR:O	1:F:326:ARG:NH2	2.36	0.59
1:F:86:THR:HB	1:F:190[B]:GLN:NE2	2.16	0.59
1:B:326[A]:ARG:HG2	1:B:326[A]:ARG:HH11	1.67	0.59
1:C:42[B]:ARG:NE	9:C:611:HOH:O	2.36	0.59
1:C:36[A]:ARG:NH2	6:C:543:FMT:O1	2.35	0.59
1:D:106[A]:ARG:NH2	1:D:110[A]:LYS:NZ	2.51	0.58
1:F:268[A]:GLU:HA	1:F:271[A]:VAL:CG1	2.33	0.58
1:B:312[A]:ARG:HD2	9:B:714:HOH:O	2.02	0.58
1:D:101[A]:HIS:HD2	9:D:612:HOH:O	1.86	0.58
1:C:108:VAL:HG12	1:C:215[B]:LEU:CD1	2.30	0.58
1:A:170:LEU:C	1:A:170:LEU:HD23	2.29	0.58
1:B:159:GLU:HG2	6:B:565:FMT:H	1.85	0.58
1:D:207:ARG:HD2	1:D:212:THR:OG1	2.03	0.57
1:E:210:ALA:HB1	1:E:211:PRO:CD	2.34	0.57
1:D:264:ARG:NH2	1:D:378:PRO:O	2.37	0.57
1:B:127:LEU:HD21	1:B:155:ALA:HB3	1.85	0.57
1:C:14:VAL:HG23	1:C:44[B]:ARG:HG3	1.86	0.57
1:F:190[A]:GLN:NE2	1:F:193:GLN:HE21	2.00	0.57
1:C:193[A]:GLN:OE1	8:C:507:GOL:H12	2.04	0.57
1:D:58[A]:MET:HE3	1:D:58[A]:MET:HA	1.86	0.57
1:C:335[A]:ASP:OD1	6:C:558:FMT:O2	2.22	0.57
1:C:193[A]:GLN:OE1	8:C:507:GOL:C1	2.53	0.57
1:E:207:ARG:NH2	1:E:214:ASP:OD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:HIS:N	1:B:5:HIS:CD2	2.73	0.56
1:F:140:SER:OG	1:F:406:SER:HA	2.05	0.56
3:E:502:DEB:O19	4:E:503[A]:RAM:H63	2.03	0.56
1:B:260:LEU:HD12	1:B:370[B]:LEU:HD11	1.87	0.56
1:C:89:GLU:HB2	1:C:193[B]:GLN:NE2	2.21	0.56
1:C:12:ASP:HB3	9:C:798:HOH:O	2.04	0.56
1:B:239:VAL:HG11	4:B:503[A]:RAM:O3	2.06	0.56
1:B:256:LEU:HD22	1:B:284:MET:HB3	1.86	0.56
1:C:260:LEU:HD11	1:C:370[B]:LEU:HD11	1.88	0.56
1:E:57[A]:ARG:HH12	1:E:329[A]:GLU:CG	2.09	0.56
1:C:11:ALA:N	9:C:614:HOH:O	2.39	0.55
1:B:108[A]:VAL:CG2	1:B:215:LEU:HD22	2.36	0.55
1:D:58[A]:MET:HE1	1:D:347:ILE:CD1	2.37	0.55
1:D:17[B]:TYR:OH	1:D:294:GLY:N	2.37	0.55
3:D:502:DEB:O19	4:D:503:RAM:C6	2.54	0.55
1:F:270[B]:LEU:HD23	1:F:374[B]:VAL:HG21	1.85	0.55
9:A:721:HOH:O	1:D:312:ARG:HD3	2.05	0.55
3:D:502:DEB:HO9	4:D:503:RAM:C5	2.17	0.55
1:C:30:HIS:HE1	9:C:851:HOH:O	1.88	0.55
1:C:240:SER:OG	4:C:503[A]:RAM:H1	2.07	0.55
1:D:152:PHE:HB3	1:D:153:PRO:HD3	1.87	0.55
1:F:263[A]:GLU:OE2	1:F:263[A]:GLU:HA	2.04	0.55
1:B:35[A]:ARG:NH1	6:B:519:FMT:O1	2.40	0.55
1:C:42[B]:ARG:HD2	9:C:611:HOH:O	2.07	0.55
1:E:17:TYR:HA	1:E:18:PRO:C	2.32	0.55
1:F:58[B]:MET:HE2	1:F:324:ALA:O	2.06	0.55
4:D:503:RAM:H63	9:D:615:HOH:O	2.06	0.54
1:A:243:ILE:HD12	4:A:503[A]:RAM:C6	2.32	0.54
1:C:183[B]:ARG:HD2	1:C:393:GLN:O	2.07	0.54
1:D:246:HIS:O	1:D:250:VAL:HG23	2.07	0.54
1:D:252[A]:GLN:HG3	1:D:256:LEU:HD13	1.89	0.54
1:A:240:SER:HA	4:A:503[A]:RAM:C6	2.28	0.54
1:D:17[A]:TYR:CD1	1:D:19[A]:PHE:CE2	2.95	0.54
1:D:390[A]:LYS:HE2	1:D:401[A]:GLU:OE2	2.07	0.54
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.38	0.54
1:F:375[A]:ARG:HH11	1:F:376[A]:ARG:HG3	1.73	0.54
1:F:268[A]:GLU:CA	1:F:271[A]:VAL:HG12	2.35	0.54
1:B:178[B]:MET:HE2	1:B:193[B]:GLN:HA	1.80	0.54
1:D:17[B]:TYR:HE1	1:D:31[B]:TYR:HH	1.55	0.54
1:A:17:TYR:HA	1:A:18:PRO:C	2.32	0.53
1:E:210:ALA:HB1	1:E:211:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:VAL:HG13	1:C:122:PRO:HB3	1.91	0.53
1:A:118:GLU:HG2	1:D:14:VAL:HG12	1.89	0.53
1:B:174:PHE:O	1:B:178[A]:MET:HG2	2.08	0.53
1:B:209:ASP:HB3	1:F:302:GLU:OE2	2.09	0.53
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.38	0.53
1:F:190[A]:GLN:NE2	1:F:193:GLN:NE2	2.57	0.53
1:A:154:VAL:HG11	1:A:168[B]:ARG:HG3	1.91	0.53
1:C:197[B]:MET:SD	1:C:235:VAL:HG12	2.49	0.53
1:D:89:GLU:HB2	1:D:193[A]:GLN:HE22	1.72	0.53
1:F:241:LEU:HD21	1:F:357[B]:ILE:CD1	2.39	0.52
1:F:384[B]:GLU:HG2	1:F:385:PRO:HD2	1.91	0.52
1:E:71:SER:OG	1:E:97:ASP:OD2	2.27	0.52
1:A:101[B]:HIS:HE1	2:A:501:HEM:O2D	1.92	0.52
1:D:266[B]:ARG:CZ	1:D:337:LEU:HD12	2.40	0.52
3:D:502:DEB:H5	4:D:503:RAM:H5	1.91	0.52
1:E:46:PRO:HB2	1:E:47:TYR:CD2	2.45	0.52
1:D:17[A]:TYR:HA	1:D:18:PRO:C	2.34	0.52
1:F:256:LEU:HD22	1:F:284:MET:HB3	1.92	0.52
1:A:92:GLY:HA2	4:A:503[A]:RAM:H1	1.92	0.52
1:A:177:ALA:HB3	1:A:192:VAL:HG11	1.91	0.52
1:B:42[B]:ARG:CD	6:B:556:FMT:O1	2.57	0.52
1:C:178[B]:MET:CE	1:C:193[B]:GLN:CG	2.85	0.52
2:E:501:HEM:HBB2	2:E:501:HEM:CHC	2.37	0.52
1:F:266:ARG:HD2	1:F:337[A]:LEU:HD23	1.91	0.52
1:C:178[A]:MET:HA	1:C:178[A]:MET:CE	2.39	0.52
1:E:145:VAL:HA	1:E:149:ALA:HB3	1.92	0.52
1:D:101[B]:HIS:CE1	1:D:105[B]:ARG:HG3	2.44	0.52
1:B:108[A]:VAL:HG22	1:B:215:LEU:HD22	1.91	0.52
1:C:89:GLU:N	8:C:507:GOL:O3	2.39	0.52
1:E:178[A]:MET:HE2	4:E:503[A]:RAM:C6	2.38	0.52
1:A:393[A]:GLN:NE2	9:A:601:HOH:O	2.17	0.52
3:A:502:DEB:O19	4:A:503[A]:RAM:O4	2.25	0.52
1:B:17:TYR:HA	1:B:18:PRO:C	2.35	0.52
1:B:242:LEU:O	1:B:246[A]:HIS:HD2	1.92	0.52
1:D:199:TYR:CZ	1:D:203:LEU:HD11	2.45	0.51
1:D:236:ASN:CG	4:D:503:RAM:HO3	2.09	0.51
1:F:270[B]:LEU:HD21	1:F:374[B]:VAL:HG21	1.89	0.51
1:C:89:GLU:HB2	1:C:193[B]:GLN:HE22	1.75	0.51
1:C:178[B]:MET:CE	1:C:193[B]:GLN:HG3	2.40	0.51
1:A:12:ASP:HA	1:A:44[A]:ARG:NH2	2.25	0.51
1:A:92:GLY:CA	4:A:503[A]:RAM:H1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:O	1:C:246[A]:HIS:HD2	1.93	0.51
1:F:180:SER:HB2	1:F:183[A]:ARG:HB2	1.91	0.51
6:B:540:FMT:O1	1:C:115[A]:ARG:NH1	2.43	0.51
1:E:354[B]:HIS:HD2	2:E:501:HEM:O1D	1.94	0.51
1:F:89:GLU:HB3	8:F:704:GOL:H12	1.93	0.51
1:F:129[B]:ASP:CG	1:F:376[B]:ARG:HH21	2.19	0.51
1:A:178[A]:MET:CE	4:A:503[A]:RAM:H4	2.40	0.51
1:E:260:LEU:HG	1:E:284[A]:MET:HE1	1.93	0.51
1:B:27[B]:LEU:CD2	1:B:326[B]:ARG:HG3	2.41	0.50
1:E:333[A]:HIS:CD2	1:E:336[A]:GLU:OE1	2.64	0.50
1:A:246:HIS:O	1:A:250[A]:VAL:HG23	2.11	0.50
6:A:542:FMT:O2	9:A:603:HOH:O	2.18	0.50
1:F:266:ARG:CZ	1:F:337[B]:LEU:HD12	2.40	0.50
1:E:225:ASN:N	1:E:225:ASN:ND2	2.59	0.50
1:C:258:HIS:CE1	1:C:262:THR:HG21	2.47	0.50
6:A:512:FMT:C	6:A:542:FMT:O2	2.60	0.50
1:B:309:VAL:HG13	1:C:122:PRO:CB	2.42	0.50
1:E:31:TYR:CZ	1:E:320:HIS:CD2	3.00	0.50
1:F:241:LEU:CD2	1:F:357[B]:ILE:CD1	2.90	0.50
1:A:337[A]:LEU:HD13	1:A:339:PHE:CE1	2.47	0.50
1:A:17:TYR:O	1:A:46:PRO:HD3	2.12	0.49
1:A:63[B]:ILE:HD13	6:A:505:FMT:O1	2.12	0.49
1:B:209:ASP:CB	1:F:302:GLU:OE2	2.60	0.49
1:C:246[A]:HIS:CE1	1:C:247:GLU:HG2	2.47	0.49
1:B:271:VAL:HA	1:B:374[A]:VAL:HG13	1.94	0.49
1:C:183[B]:ARG:CD	1:C:393:GLN:O	2.61	0.49
1:D:145:VAL:HA	1:D:149:ALA:HB3	1.94	0.49
1:E:170:LEU:HD22	1:E:174:PHE:CZ	2.47	0.49
1:B:239:VAL:CG1	4:B:503[A]:RAM:O3	2.60	0.49
1:E:333[A]:HIS:HD2	1:E:336[A]:GLU:OE1	1.95	0.49
1:D:127:LEU:HD13	1:D:152:PHE:HD1	1.76	0.49
1:D:17[B]:TYR:HE1	1:D:31[B]:TYR:OH	1.96	0.49
1:E:212:THR:O	1:E:212:THR:OG1	2.18	0.49
2:E:501:HEM:HBC2	2:E:501:HEM:HMC2	1.95	0.49
4:E:503[A]:RAM:O2	6:E:506:FMT:C	2.60	0.49
1:F:125[B]:ARG:NH1	1:F:129[B]:ASP:OD2	2.45	0.49
1:A:258:HIS:CE1	1:A:262[A]:THR:HG21	2.48	0.49
1:C:42[B]:ARG:CD	9:C:611:HOH:O	2.60	0.49
1:F:380[A]:LEU:HD11	1:F:405:VAL:HG11	1.94	0.49
1:B:260:LEU:CD1	1:B:370[B]:LEU:HD11	2.43	0.49
1:E:322:ALA:O	1:E:326:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:HA	1:A:271[B]:VAL:HG12	1.95	0.48
1:C:178[A]:MET:HA	1:C:178[A]:MET:HE3	1.94	0.48
1:D:161:LEU:HD23	1:D:215:LEU:HB2	1.94	0.48
1:B:108[B]:VAL:HG21	1:B:237:MET:HE2	1.94	0.48
1:A:107[B]:LEU:HD21	1:A:219:LEU:HD22	1.95	0.48
1:F:77:ASP:HB3	1:F:80:THR:OG1	2.14	0.48
1:B:123:ARG:HE	6:B:565:FMT:C	2.26	0.48
1:D:127:LEU:HD11	1:D:155:ALA:HB3	1.96	0.48
1:E:354[B]:HIS:HE1	9:E:644:HOH:O	1.96	0.48
1:F:375[A]:ARG:HH11	1:F:376[A]:ARG:CG	2.26	0.48
1:A:11:ALA:O	1:A:14[A]:VAL:HG12	2.14	0.48
1:A:101[B]:HIS:HD2	9:A:635:HOH:O	1.96	0.48
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.44	0.48
1:D:343[B]:ARG:CB	1:D:343[B]:ARG:NH2	2.76	0.47
1:E:101[A]:HIS:HE1	2:E:501:HEM:O2D	1.97	0.47
1:E:110[A]:LYS:CG	1:E:116[A]:ARG:HH11	2.21	0.47
1:E:330:VAL:HG22	1:E:331:PHE:CD2	2.49	0.47
1:A:110[A]:LYS:HA	1:A:110[A]:LYS:HD3	1.53	0.47
1:A:45[A]:LEU:HG	1:A:83:MET:SD	2.54	0.47
1:A:283:GLU:HG3	1:A:337[A]:LEU:HD22	1.97	0.47
1:B:10:PRO:CA	1:B:13:ALA:CB	2.85	0.47
1:B:123:ARG:HD2	1:B:123:ARG:O	2.14	0.47
1:F:21[B]:LEU:HD23	1:F:21[B]:LEU:HA	1.78	0.47
1:F:31:TYR:CZ	1:F:320[B]:HIS:CD2	3.03	0.47
1:B:99:PRO:HD2	6:B:508:FMT:O2	2.15	0.47
1:B:270:LEU:HB2	1:B:374[A]:VAL:HG21	1.97	0.47
1:C:339:PHE:N	8:C:506:GOL:O1	2.39	0.47
1:E:343[B]:ARG:CZ	1:E:343[B]:ARG:HB2	2.43	0.47
1:E:30:HIS:CD2	1:E:34[A]:LEU:HD11	2.50	0.47
1:E:174:PHE:O	1:E:178[B]:MET:HG2	2.15	0.47
1:B:287:TYR:CG	1:B:337:LEU:HD13	2.49	0.47
1:F:197:MET:CE	1:F:236[B]:ASN:ND2	2.78	0.47
1:A:122:PRO:CB	1:D:309:VAL:HG13	2.45	0.47
1:C:152:PHE:HB3	1:C:153:PRO:HD3	1.96	0.47
1:D:263[A]:GLU:OE1	1:D:263[A]:GLU:HA	2.15	0.47
1:B:42[B]:ARG:HH21	1:C:118:GLU:CD	2.22	0.46
1:F:259:LEU:HB2	1:F:284:MET:HE2	1.96	0.46
1:B:111:ALA:HA	1:B:116[A]:ARG:HG2	1.96	0.46
1:A:127[B]:LEU:HD11	6:A:543:FMT:C	2.46	0.46
1:C:197[B]:MET:HE2	9:C:700:HOH:O	2.15	0.46
1:F:197:MET:CE	1:F:236[B]:ASN:HD22	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:VAL:O	1:F:389:LEU:HB2	2.16	0.46
1:D:101[B]:HIS:CE1	1:D:105[B]:ARG:HE	2.31	0.46
1:E:152:PHE:HB3	1:E:153:PRO:HD3	1.97	0.46
1:A:239:VAL:HG12	4:A:503[A]:RAM:H63	1.98	0.46
1:D:252[B]:GLN:HG3	2:D:501:HEM:CBB	2.45	0.46
1:D:390[B]:LYS:HE3	1:D:402[B]:ARG:HH21	1.77	0.46
1:D:392:LYS:HG2	1:D:401[B]:GLU:HG3	1.97	0.46
1:E:295:SER:H	1:E:318[B]:VAL:CG2	2.29	0.46
1:C:290:LEU:O	1:C:397:ILE:HA	2.16	0.46
2:E:501:HEM:HHC	2:E:501:HEM:CBB	2.44	0.46
1:C:178[B]:MET:HE1	1:C:193[B]:GLN:HG3	1.97	0.46
1:E:355:HIS:NE2	6:E:504:FMT:O2	2.41	0.46
1:A:382[B]:LEU:HD23	1:A:382[B]:LEU:HA	1.72	0.46
1:B:264[A]:ARG:NH2	9:B:622:HOH:O	2.48	0.46
1:C:354[B]:HIS:CE1	8:C:505:GOL:O1	2.66	0.46
1:D:30[A]:HIS:CD2	1:D:34[A]:LEU:CD2	2.98	0.46
1:E:259:LEU:HB2	1:E:284[A]:MET:HE2	1.97	0.46
1:B:178[B]:MET:HE2	1:B:193[B]:GLN:CA	2.41	0.45
1:B:256:LEU:HD13	1:B:284:MET:HE3	1.98	0.45
1:D:116[B]:ARG:NE	9:D:605:HOH:O	2.38	0.45
1:C:285:LEU:HD13	1:C:349[B]:PHE:CE2	2.51	0.45
1:A:337[A]:LEU:CD1	1:A:339:PHE:CE1	2.99	0.45
1:A:212:THR:OG1	1:A:214:ASP:OD1	2.26	0.45
2:F:702:HEM:HBC2	2:F:702:HEM:CMC	2.47	0.45
1:D:188:GLU:OE2	1:E:115[B]:ARG:HB2	2.16	0.45
1:A:35[A]:ARG:NH2	9:A:602:HOH:O	2.17	0.45
9:A:721:HOH:O	1:D:312:ARG:CD	2.63	0.45
1:B:42[A]:ARG:HD2	1:C:118:GLU:OE2	2.17	0.45
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.69	0.45
1:B:217:GLY:O	1:B:221[B]:LEU:HG	2.16	0.45
1:C:14:VAL:HG23	1:C:44[B]:ARG:CG	2.46	0.45
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.99	0.45
1:D:186:ALA:O	1:D:190[A]:GLN:HG2	2.16	0.45
1:C:86[B]:THR:HB	8:C:507:GOL:O1	2.14	0.45
1:D:115[A]:ARG:HD3	1:D:115[A]:ARG:HA	1.65	0.45
1:D:270:LEU:HB3	1:D:374:VAL:HG21	1.99	0.45
1:E:138[B]:HIS:HD2	1:E:139:GLY:O	1.99	0.45
1:F:252:GLN:O	1:F:256:LEU:HG	2.16	0.45
1:D:178[B]:MET:HE3	1:D:193[B]:GLN:CA	2.37	0.45
1:E:32:ALA:O	1:E:36[A]:ARG:HG2	2.16	0.45
1:A:111:ALA:HB2	1:A:215[B]:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:503[A]:RAM:HO1	6:B:513:FMT:C	2.28	0.45
1:C:246[A]:HIS:HE1	9:C:698:HOH:O	2.00	0.45
1:F:375[A]:ARG:HE	1:F:376[A]:ARG:HG3	1.81	0.45
1:C:35:ARG:HH11	6:C:525:FMT:C	2.30	0.44
4:A:503[A]:RAM:H2	6:A:508:FMT:C	2.46	0.44
1:B:42[B]:ARG:NH2	1:C:118:GLU:CD	2.75	0.44
1:B:42[B]:ARG:NH2	1:C:118:GLU:OE2	2.45	0.44
1:B:89:GLU:HB3	4:B:503[A]:RAM:H1	1.98	0.44
1:C:92:GLY:HA3	4:C:503[A]:RAM:O3	2.18	0.44
1:D:283:GLU:HG3	1:D:337:LEU:CD2	2.47	0.44
1:F:125[B]:ARG:HG2	1:F:368:GLU:OE1	2.16	0.44
1:A:107[A]:LEU:CD1	1:A:234:ILE:HG12	2.47	0.44
1:B:121:ARG:HG3	1:B:364:LEU:HD11	2.00	0.44
3:C:502:DEB:O21	4:C:503[A]:RAM:O1	2.25	0.44
1:E:333[A]:HIS:HD2	1:E:336[A]:GLU:CB	2.28	0.44
1:B:258:HIS:CE1	1:B:262:THR:HG21	2.53	0.44
1:B:329[A]:GLU:CD	9:B:628:HOH:O	2.60	0.44
1:F:375[A]:ARG:HH11	1:F:376[A]:ARG:CD	2.30	0.44
1:D:62:ARG:HH11	1:D:351[B]:HIS:CE1	2.34	0.44
1:F:17:TYR:HA	1:F:18:PRO:C	2.42	0.44
1:A:135[A]:MET:HE3	1:A:147:PHE:HB2	1.99	0.44
1:A:152:PHE:HB3	1:A:153:PRO:HD3	2.00	0.44
1:A:244:ALA:HB1	2:A:501:HEM:C4C	2.53	0.44
1:D:159:GLU:HG3	6:D:514:FMT:C	2.47	0.44
1:E:215:LEU:HA	1:E:215:LEU:HD23	1.69	0.44
1:D:89:GLU:HB2	1:D:193[A]:GLN:NE2	2.32	0.44
1:A:207:ARG:HB2	1:A:220:ALA:CB	2.48	0.44
3:A:502:DEB:H203	4:A:503[A]:RAM:O4	2.18	0.44
1:E:178[B]:MET:HE1	1:E:193:GLN:HG2	1.99	0.44
1:F:121:ARG:HG3	1:F:364:LEU:HD11	1.99	0.44
1:C:69:ARG:HG2	1:C:302[A]:GLU:HG3	2.00	0.43
1:E:57[A]:ARG:NH1	1:E:329[A]:GLU:HB2	2.33	0.43
1:C:170:LEU:HD23	1:C:170:LEU:C	2.42	0.43
1:E:101[B]:HIS:NE2	1:E:354[B]:HIS:CD2	2.86	0.43
1:E:271:VAL:HA	1:E:374:VAL:HG13	2.00	0.43
1:F:42:ARG:NH2	9:F:814:HOH:O	2.50	0.43
1:B:200:MET:O	1:B:204[A]:VAL:HG13	2.18	0.43
1:E:35[A]:ARG:HG2	1:E:57[A]:ARG:HG3	1.99	0.43
1:F:168[B]:ARG:HG2	1:F:172:ARG:HG3	2.00	0.43
1:F:178:MET:HE3	1:F:193:GLN:HG3	2.00	0.43
1:F:375[A]:ARG:NH1	1:F:376[A]:ARG:HG3	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LYS:HG2	1:B:401:GLU:HG3	2.01	0.43
1:D:101[A]:HIS:CD2	9:D:612:HOH:O	2.67	0.43
1:B:13:ALA:O	1:C:115[A]:ARG:NE	2.49	0.43
1:D:236:ASN:OD1	4:D:503:RAM:C3	2.67	0.43
1:A:45[A]:LEU:HD12	1:A:45[A]:LEU:HA	1.87	0.43
1:A:183[B]:ARG:HB2	1:A:394:GLY:O	2.19	0.43
1:B:309:VAL:HG13	1:C:122:PRO:HA	1.99	0.43
2:E:501:HEM:HBC2	2:E:501:HEM:CMC	2.48	0.43
1:F:197:MET:SD	1:F:236[B]:ASN:ND2	2.91	0.43
1:F:216:LEU:HD12	1:F:216:LEU:HA	1.90	0.43
1:B:270:LEU:CB	1:B:374[A]:VAL:HG21	2.49	0.43
1:D:280:ALA:HA	1:D:339:PHE:CD1	2.54	0.43
1:A:354:HIS:O	1:A:355:HIS:C	2.62	0.43
1:E:115[A]:ARG:HE	1:E:115[A]:ARG:HB2	1.56	0.43
1:F:115:ARG:HB2	6:F:706:FMT:C	2.49	0.43
1:B:390[A]:LYS:HZ2	1:B:402[A]:ARG:HH22	1.66	0.42
1:C:86[A]:THR:HG22	1:C:186:ALA:O	2.19	0.42
1:C:107:LEU:HD12	1:C:107:LEU:HA	1.87	0.42
1:D:46:PRO:HB2	1:D:47:TYR:CD2	2.54	0.42
1:D:290:LEU:O	1:D:397:ILE:HA	2.18	0.42
1:E:93:VAL:HG13	1:E:237[A]:MET:SD	2.59	0.42
1:F:161:LEU:O	1:F:216:LEU:HB2	2.19	0.42
4:B:503[A]:RAM:O1	6:B:513:FMT:C	2.66	0.42
1:D:70:PHE:CE2	1:D:304:VAL:HG11	2.54	0.42
1:B:260:LEU:HD11	1:B:370[B]:LEU:HD21	2.02	0.42
1:C:17:TYR:HA	1:C:18:PRO:C	2.44	0.42
1:E:39:PRO:HG2	1:E:308:THR:OG1	2.18	0.42
1:E:327:ASP:HB3	1:E:330:VAL:HG13	2.01	0.42
1:A:271[B]:VAL:HG21	1:A:378:PRO:HB3	2.02	0.42
1:B:8:PRO:HD3	1:C:282:GLU:CD	2.44	0.42
1:B:110[A]:LYS:H	1:B:110[A]:LYS:HD3	1.85	0.42
1:D:107[A]:LEU:HD21	1:D:222:ALA:HB1	2.01	0.42
1:A:63[B]:ILE:HD13	1:A:63[B]:ILE:HA	1.85	0.42
1:B:92:GLY:O	1:B:96:GLN:HG2	2.20	0.42
1:B:328:GLU:HG2	6:B:519:FMT:H	2.00	0.42
1:E:290:LEU:O	1:E:397:ILE:HA	2.19	0.42
1:B:10:PRO:O	1:B:10:PRO:HG2	2.20	0.42
1:D:101[B]:HIS:CD2	1:D:354:HIS:CE1	3.08	0.42
1:D:283:GLU:OE2	1:D:338:ASP:N	2.38	0.42
1:E:207:ARG:HA	1:E:210:ALA:HB3	2.00	0.42
1:A:107[A]:LEU:HD11	1:A:234:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108[A]:VAL:HG22	1:B:215:LEU:CD2	2.50	0.42
1:B:209:ASP:HB2	1:F:302:GLU:HG3	2.01	0.42
1:B:263:GLU:HB2	1:B:266:ARG:HD2	2.01	0.42
1:B:326[A]:ARG:HH11	1:B:326[A]:ARG:CG	2.28	0.42
1:D:19[B]:PHE:CE1	1:D:30[B]:HIS:HD2	2.37	0.42
8:C:507:GOL:O3	6:C:555[B]:FMT:O2	2.37	0.42
1:D:17[B]:TYR:HA	1:D:18:PRO:C	2.44	0.42
1:E:31:TYR:CE1	1:E:320:HIS:CD2	3.08	0.42
1:B:116[A]:ARG:HG3	1:B:120[A]:MET:HE3	2.02	0.42
1:E:355:HIS:HE2	6:E:504:FMT:C	2.33	0.42
1:A:130:SER:O	1:A:133:ASP:HB2	2.20	0.41
1:A:328[A]:GLU:HG2	6:A:514:FMT:H	2.02	0.41
6:B:538:FMT:O1	1:F:106:ARG:NH1	2.47	0.41
1:D:107[A]:LEU:HD12	1:D:107[A]:LEU:HA	1.83	0.41
1:E:104:LEU:HG	1:E:237[B]:MET:HE2	2.02	0.41
1:A:45[B]:LEU:HD12	1:A:81:PRO:CB	2.50	0.41
1:A:240:SER:OG	4:A:503[A]:RAM:H61	2.20	0.41
1:C:207[B]:ARG:HD3	1:C:212:THR:OG1	2.21	0.41
4:C:503[A]:RAM:H5	8:C:507:GOL:O2	2.20	0.41
1:D:170:LEU:C	1:D:170:LEU:HD23	2.45	0.41
1:F:270[B]:LEU:HD21	1:F:277:VAL:CG2	2.50	0.41
1:B:152:PHE:HB3	1:B:153:PRO:HD3	2.01	0.41
1:B:237:MET:HE3	1:B:241:LEU:HG	2.01	0.41
6:B:538:FMT:C	1:F:106:ARG:NH1	2.83	0.41
1:D:270:LEU:CB	1:D:374:VAL:HG21	2.50	0.41
1:E:157:ILE:HG13	1:E:161:LEU:HD22	2.02	0.41
1:A:337[A]:LEU:HD22	1:A:337[A]:LEU:HA	1.88	0.41
3:A:502:DEB:H5	4:A:503[A]:RAM:H5	2.02	0.41
1:B:133:ASP:O	1:B:136:VAL:CG2	2.68	0.41
1:D:115[B]:ARG:HD2	9:D:614:HOH:O	2.20	0.41
1:B:191[A]:ARG:NH1	1:B:195:ASP:OD1	2.53	0.41
1:D:168[A]:ARG:HA	1:D:171:PHE:CZ	2.56	0.41
1:F:150:VAL:HB	1:F:151:PRO:HD3	2.02	0.41
1:A:271[B]:VAL:HA	1:A:374:VAL:HG13	2.03	0.41
1:A:290:LEU:O	1:A:397:ILE:HA	2.21	0.41
1:F:241:LEU:HD21	1:F:357[B]:ILE:HD13	2.03	0.41
1:F:267[A]:TYR:OH	1:F:374[A]:VAL:HA	2.21	0.41
1:A:199:TYR:CZ	1:A:203:LEU:HD11	2.56	0.41
1:C:14:VAL:O	1:C:44[B]:ARG:NE	2.53	0.41
1:C:168:ARG:NH1	9:C:610:HOH:O	2.34	0.41
1:D:180:SER:HB2	1:D:183:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PRO:HB3	1:B:13:ALA:HB2	1.86	0.41
1:C:42[A]:ARG:HH22	1:C:316:PRO:HD2	1.84	0.41
1:C:276:LEU:HD12	1:C:276:LEU:HA	1.95	0.41
1:D:101[A]:HIS:NE2	1:D:353:ALA:O	2.50	0.41
1:F:157:ILE:HD12	1:F:157:ILE:HA	1.91	0.41
1:F:183[A]:ARG:NH2	9:F:805:HOH:O	2.51	0.41
6:A:511:FMT:O1	9:A:604:HOH:O	2.22	0.41
1:D:70:PHE:HE2	1:D:304:VAL:HG11	1.86	0.41
1:D:178[B]:MET:HE2	1:D:193[B]:GLN:CA	2.39	0.41
1:E:21:LEU:HD12	1:E:21:LEU:HA	1.94	0.41
1:E:35[A]:ARG:HD3	1:E:56:THR:O	2.20	0.41
1:F:87:PRO:HA	1:F:88:PRO:HD3	1.93	0.41
1:F:132:LEU:HD12	1:F:132:LEU:HA	1.90	0.41
6:A:508:FMT:O1	6:A:509:FMT:O2	2.39	0.41
1:D:106[A]:ARG:CG	1:D:106[A]:ARG:HH11	2.34	0.41
1:F:197:MET:HE2	1:F:236[B]:ASN:ND2	2.36	0.41
2:F:702:HEM:HMB2	2:F:702:HEM:CBB	2.36	0.41
1:C:178[A]:MET:SD	4:C:503[A]:RAM:C6	3.09	0.40
1:A:135[A]:MET:HE1	1:A:144:LEU:HD12	2.02	0.40
1:B:290:LEU:O	1:B:397:ILE:HA	2.21	0.40
1:E:133:ASP:OD1	1:E:376:ARG:NH2	2.43	0.40
1:F:259:LEU:HB2	1:F:284:MET:CE	2.51	0.40
1:B:6[A]:THR:HG21	1:C:355:HIS:CE1	2.56	0.40
1:B:36:ARG:NH1	1:B:37:ASP:OD2	2.54	0.40
1:E:101[B]:HIS:CD2	1:E:354[B]:HIS:CD2	3.09	0.40
1:B:328:GLU:CB	6:B:519:FMT:C	2.98	0.40
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	2.03	0.40
1:D:58[A]:MET:HE2	1:D:62:ARG:HG3	2.03	0.40
3:E:502:DEB:C20	4:E:503[A]:RAM:H63	2.48	0.40
1:F:194[A]:GLN:NE2	9:F:816:HOH:O	2.54	0.40
8:C:507:GOL:C3	6:C:555[B]:FMT:O1	2.66	0.40
1:F:270[B]:LEU:HD11	1:F:277:VAL:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103[A]:ARG:NH1	1:E:169:ASP:OD2[4_546]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/407 (112%)	440 (97%)	15 (3%)	0	100	100
1	B	438/407 (108%)	425 (97%)	13 (3%)	0	100	100
1	C	434/407 (107%)	428 (99%)	6 (1%)	0	100	100
1	D	447/407 (110%)	428 (96%)	19 (4%)	0	100	100
1	E	435/407 (107%)	413 (95%)	22 (5%)	0	100	100
1	F	443/407 (109%)	424 (96%)	19 (4%)	0	100	100
All	All	2652/2442 (109%)	2558 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/341 (115%)	370 (94%)	22 (6%)	19	16
1	B	374/341 (110%)	345 (92%)	29 (8%)	11	8
1	C	371/341 (109%)	355 (96%)	16 (4%)	26	26
1	D	385/341 (113%)	351 (91%)	34 (9%)	9	6
1	E	373/341 (109%)	347 (93%)	26 (7%)	14	11
1	F	380/341 (111%)	350 (92%)	30 (8%)	11	8
All	All	2275/2046 (111%)	2118 (93%)	157 (7%)	18	11

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14[A]	VAL
1	A	14[B]	VAL
1	A	21	LEU
1	A	27	LEU
1	A	45[A]	LEU
1	A	45[B]	LEU
1	A	107[A]	LEU
1	A	107[B]	LEU
1	A	110[A]	LYS
1	A	110[B]	LYS
1	A	160[A]	LEU
1	A	160[B]	LEU
1	A	170	LEU
1	A	198	VAL
1	A	227[A]	ASP
1	A	227[B]	ASP
1	A	228	HIS
1	A	337[A]	LEU
1	A	337[B]	LEU
1	A	343	ARG
1	A	370[A]	LEU
1	A	370[B]	LEU
1	B	5	HIS
1	B	6[A]	THR
1	B	6[B]	THR
1	B	14	VAL
1	B	27[A]	LEU
1	B	27[B]	LEU
1	B	36	ARG
1	B	108[A]	VAL
1	B	108[B]	VAL
1	B	110[A]	LYS
1	B	110[B]	LYS
1	B	123	ARG
1	B	154	VAL
1	B	204[A]	VAL
1	B	204[B]	VAL
1	B	207	ARG
1	B	225[A]	ASN
1	B	225[B]	ASN
1	B	256	LEU
1	B	264[A]	ARG

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Mol	Chain	Res	Type
1	B	264[B]	ARG
1	B	265[A]	LYS
1	B	265[B]	LYS
1	B	309	VAL
1	B	312[A]	ARG
1	B	312[B]	ARG
1	B	374[A]	VAL
1	B	374[B]	VAL
1	B	393	GLN
1	C	12	ASP
1	C	42[A]	ARG
1	C	42[B]	ARG
1	C	115[A]	ARG
1	C	115[B]	ARG
1	C	116	ARG
1	C	123	ARG
1	C	136	VAL
1	C	178[A]	MET
1	C	178[B]	MET
1	C	231[A]	LYS
1	C	231[B]	LYS
1	C	302[A]	GLU
1	C	302[B]	GLU
1	C	337	LEU
1	C	374	VAL
1	D	34[A]	LEU
1	D	34[B]	LEU
1	D	36[A]	ARG
1	D	36[B]	ARG
1	D	42	ARG
1	D	49[A]	GLU
1	D	49[B]	GLU
1	D	86	THR
1	D	105[A]	ARG
1	D	105[B]	ARG
1	D	106[A]	ARG
1	D	106[B]	ARG
1	D	127	LEU
1	D	132	LEU
1	D	136	VAL
1	D	159	GLU
1	D	166	GLU

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Mol	Chain	Res	Type
1	D	207	ARG
1	D	209	ASP
1	D	225	ASN
1	D	263[A]	GLU
1	D	263[B]	GLU
1	D	266[A]	ARG
1	D	266[B]	ARG
1	D	309	VAL
1	D	312	ARG
1	D	328	GLU
1	D	330	VAL
1	D	342[A]	GLU
1	D	342[B]	GLU
1	D	343[A]	ARG
1	D	343[B]	ARG
1	D	370	LEU
1	D	374	VAL
1	E	14	VAL
1	E	21	LEU
1	E	45	LEU
1	E	93	VAL
1	E	108	VAL
1	E	115[A]	ARG
1	E	115[B]	ARG
1	E	136	VAL
1	E	154	VAL
1	E	161	LEU
1	E	191	ARG
1	E	204	VAL
1	E	207	ARG
1	E	208	ARG
1	E	212	THR
1	E	213	GLU
1	E	225	ASN
1	E	309	VAL
1	E	312[A]	ARG
1	E	312[B]	ARG
1	E	330	VAL
1	E	340[A]	HIS
1	E	340[B]	HIS
1	E	343[A]	ARG
1	E	343[B]	ARG

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Mol	Chain	Res	Type
1	E	374	VAL
1	F	12	ASP
1	F	21[A]	LEU
1	F	21[B]	LEU
1	F	27	LEU
1	F	33	GLU
1	F	42	ARG
1	F	45	LEU
1	F	51	THR
1	F	93	VAL
1	F	94	LEU
1	F	115	ARG
1	F	116	ARG
1	F	123[A]	ARG
1	F	123[B]	ARG
1	F	132	LEU
1	F	193	GLN
1	F	194[A]	GLN
1	F	194[B]	GLN
1	F	198	VAL
1	F	204	VAL
1	F	216	LEU
1	F	225	ASN
1	F	266	ARG
1	F	269	SER
1	F	309	VAL
1	F	326	ARG
1	F	329[A]	GLU
1	F	329[B]	GLU
1	F	390[A]	LYS
1	F	390[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	HIS
1	A	258	HIS
1	A	320	HIS
1	A	340	HIS
1	B	5	HIS
1	B	96	GLN
1	B	258	HIS

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Mol	Chain	Res	Type
1	B	393	GLN
1	C	30	HIS
1	C	206	GLN
1	C	228	HIS
1	C	236	ASN
1	C	258	HIS
1	C	393	GLN
1	D	320	HIS
1	E	193	GLN
1	E	206	GLN
1	E	225	ASN
1	E	236	ASN
1	E	320	HIS
1	F	193	GLN
1	F	351	HIS
1	F	403	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 238 ligands modelled in this entry, 7 are monoatomic - leaving 231 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
6	FMT	B	554	-	2,2,2	0.25	0	1,1,1	0.16	0
6	FMT	B	537	-	2,2,2	0.25	0	1,1,1	0.17	0
6	FMT	C	553	-	2,2,2	0.38	0	1,1,1	0.11	0
6	FMT	B	542	-	2,2,2	0.30	0	1,1,1	0.14	0
6	FMT	D	505	-	2,2,2	0.24	0	1,1,1	0.15	0
6	FMT	E	508	-	2,2,2	0.27	0	1,1,1	0.15	0
6	FMT	F	714	-	2,2,2	0.30	0	1,1,1	0.10	0
8	GOL	B	505	-	5,5,5	0.10	0	5,5,5	0.28	0
6	FMT	B	533	-	2,2,2	0.31	0	1,1,1	0.11	0
6	FMT	A	540	-	2,2,2	0.34	0	1,1,1	0.12	0
6	FMT	C	518	-	2,2,2	0.50	0	1,1,1	0.00	0
4	RAM	E	503[A]	-	11,11,11	0.55	0	16,16,16	1.70	5 (31%)
6	FMT	C	520	-	2,2,2	0.26	0	1,1,1	0.12	0
6	FMT	A	537	-	2,2,2	0.32	0	1,1,1	0.14	0
6	FMT	B	521	-	2,2,2	0.27	0	1,1,1	0.10	0
6	FMT	B	562	-	2,2,2	0.40	0	1,1,1	0.09	0
6	FMT	D	515	-	2,2,2	0.26	0	1,1,1	0.16	0
2	HEM	C	501	1	50,50,50	2.15	17 (34%)	67,82,82	1.83	17 (25%)
6	FMT	B	532	-	2,2,2	0.34	0	1,1,1	0.09	0
6	FMT	E	504	-	2,2,2	0.19	0	1,1,1	0.23	0
6	FMT	F	711	-	2,2,2	0.25	0	1,1,1	0.15	0
6	FMT	C	546	-	2,2,2	0.22	0	1,1,1	0.18	0
6	FMT	D	512	-	2,2,2	0.28	0	1,1,1	0.14	0
6	FMT	D	504	-	2,2,2	0.26	0	1,1,1	0.15	0
6	FMT	F	719	-	2,2,2	0.33	0	1,1,1	0.14	0
6	FMT	C	562	-	2,2,2	0.23	0	1,1,1	0.18	0
6	FMT	A	530	-	2,2,2	0.26	0	1,1,1	0.16	0
6	FMT	A	542	-	2,2,2	0.38	0	1,1,1	0.21	0
6	FMT	C	533	-	2,2,2	0.30	0	1,1,1	0.16	0
6	FMT	C	527	-	2,2,2	0.33	0	1,1,1	0.06	0
6	FMT	B	541	-	2,2,2	0.52	0	1,1,1	0.03	0
6	FMT	C	534	-	2,2,2	0.32	0	1,1,1	0.13	0
6	FMT	D	518	-	2,2,2	0.33	0	1,1,1	0.13	0
6	FMT	B	538	-	2,2,2	0.34	0	1,1,1	0.15	0
6	FMT	D	513	-	2,2,2	0.25	0	1,1,1	0.17	0
6	FMT	E	512	-	2,2,2	0.47	0	1,1,1	0.02	0
6	FMT	B	545	-	2,2,2	0.24	0	1,1,1	0.16	0
6	FMT	B	567	-	2,2,2	0.33	0	1,1,1	0.06	0
6	FMT	B	546	-	2,2,2	0.30	0	1,1,1	0.14	0
6	FMT	A	535	-	2,2,2	0.26	0	1,1,1	0.19	0
6	FMT	A	505	-	2,2,2	0.31	0	1,1,1	0.15	0
6	FMT	B	561	-	2,2,2	0.23	0	1,1,1	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FMT	B	564	-	2,2,2	0.24	0	1,1,1	0.16	0
6	FMT	C	525	-	2,2,2	0.43	0	1,1,1	0.01	0
6	FMT	E	511	-	2,2,2	0.25	0	1,1,1	0.16	0
6	FMT	C	543	-	2,2,2	0.30	0	1,1,1	0.16	0
6	FMT	B	527	-	2,2,2	0.23	0	1,1,1	0.18	0
4	RAM	F	701	-	11,11,11	1.08	0	16,16,16	1.47	1 (6%)
6	FMT	A	507	-	2,2,2	0.27	0	1,1,1	0.16	0
5	TRS	B	504	-	7,7,7	0.31	0	9,9,9	0.61	0
6	FMT	A	533	-	2,2,2	0.31	0	1,1,1	0.14	0
6	FMT	C	522	-	2,2,2	0.23	0	1,1,1	0.07	0
6	FMT	C	550	-	2,2,2	0.34	0	1,1,1	0.10	0
8	GOL	C	505	-	5,5,5	0.13	0	5,5,5	0.24	0
6	FMT	C	541	-	2,2,2	0.35	0	1,1,1	0.08	0
6	FMT	B	509	-	2,2,2	0.42	0	1,1,1	0.13	0
6	FMT	C	521	-	2,2,2	0.29	0	1,1,1	0.14	0
6	FMT	C	545	-	2,2,2	0.25	0	1,1,1	0.15	0
6	FMT	F	708	-	2,2,2	0.30	0	1,1,1	0.11	0
6	FMT	C	516	-	2,2,2	0.34	0	1,1,1	0.18	0
6	FMT	B	524	-	2,2,2	0.37	0	1,1,1	0.09	0
6	FMT	D	516	-	2,2,2	0.30	0	1,1,1	0.15	0
6	FMT	B	558	-	2,2,2	0.26	0	1,1,1	0.17	0
2	HEM	B	501	1	50,50,50	2.15	19 (38%)	67,82,82	1.77	16 (23%)
6	FMT	C	538	-	2,2,2	0.30	0	1,1,1	0.11	0
6	FMT	D	507	-	2,2,2	0.36	0	1,1,1	0.10	0
6	FMT	F	706	-	2,2,2	0.41	0	1,1,1	0.03	0
6	FMT	A	517	-	2,2,2	0.25	0	1,1,1	0.16	0
6	FMT	A	528	-	2,2,2	0.31	0	1,1,1	0.15	0
2	HEM	A	501	1	50,50,50	2.09	19 (38%)	67,82,82	1.89	16 (23%)
6	FMT	B	513	-	2,2,2	0.29	0	1,1,1	0.11	0
6	FMT	C	519	-	2,2,2	0.28	0	1,1,1	0.12	0
6	FMT	E	507	-	2,2,2	0.38	0	1,1,1	0.09	0
6	FMT	E	509	-	2,2,2	0.30	0	1,1,1	0.13	0
6	FMT	A	513	-	2,2,2	0.21	0	1,1,1	0.17	0
6	FMT	A	527	-	2,2,2	0.27	0	1,1,1	0.16	0
6	FMT	B	547	-	2,2,2	0.22	0	1,1,1	0.13	0
6	FMT	C	508	-	2,2,2	0.40	0	1,1,1	0.05	0
6	FMT	C	513[B]	6	2,2,2	0.44	0	1,1,1	0.04	0
6	FMT	B	540	-	2,2,2	0.41	0	1,1,1	0.05	0
6	FMT	D	508	-	2,2,2	0.21	0	1,1,1	0.14	0
6	FMT	F	716	-	2,2,2	0.30	0	1,1,1	0.10	0
6	FMT	C	535	-	2,2,2	0.37	0	1,1,1	0.09	0
6	FMT	C	559	-	2,2,2	0.29	0	1,1,1	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FMT	B	511	-	2,2,2	0.47	0	1,1,1	0.03	0
6	FMT	B	548	-	2,2,2	0.43	0	1,1,1	0.00	0
6	FMT	B	536	-	2,2,2	0.29	0	1,1,1	0.15	0
6	FMT	B	550	-	2,2,2	0.34	0	1,1,1	0.12	0
3	DEB	D	502	-	27,27,27	0.75	1 (3%)	37,39,39	0.83	2 (5%)
6	FMT	F	713	-	2,2,2	0.38	0	1,1,1	0.07	0
6	FMT	A	519	-	2,2,2	0.23	0	1,1,1	0.19	0
5	TRS	A	504	-	7,7,7	0.22	0	9,9,9	0.35	0
6	FMT	A	508	-	2,2,2	0.20	0	1,1,1	0.10	0
6	FMT	B	559	-	2,2,2	0.35	0	1,1,1	0.12	0
3	DEB	E	502	-	27,27,27	0.53	0	37,39,39	0.82	0
6	FMT	C	529	-	2,2,2	0.28	0	1,1,1	0.17	0
6	FMT	A	536	-	2,2,2	0.41	0	1,1,1	0.05	0
6	FMT	B	515	-	2,2,2	0.39	0	1,1,1	0.10	0
6	FMT	C	544	-	2,2,2	0.19	0	1,1,1	0.18	0
5	TRS	F	705	-	7,7,7	0.08	0	9,9,9	0.57	0
6	FMT	C	528	-	2,2,2	0.15	0	1,1,1	0.25	0
6	FMT	C	565	-	2,2,2	0.47	0	1,1,1	0.03	0
6	FMT	B	565	-	2,2,2	0.23	0	1,1,1	0.09	0
6	FMT	C	524	-	2,2,2	0.21	0	1,1,1	0.18	0
6	FMT	E	505	-	2,2,2	0.32	0	1,1,1	0.12	0
6	FMT	B	526	-	2,2,2	0.24	0	1,1,1	0.18	0
2	HEM	D	501	1	50,50,50	2.29	21 (42%)	67,82,82	1.99	18 (26%)
6	FMT	A	525	-	2,2,2	0.29	0	1,1,1	0.14	0
6	FMT	B	534	-	2,2,2	0.33	0	1,1,1	0.11	0
6	FMT	B	518	-	2,2,2	0.32	0	1,1,1	0.13	0
6	FMT	C	558	-	2,2,2	0.60	0	1,1,1	0.05	0
6	FMT	B	563	-	2,2,2	0.23	0	1,1,1	0.17	0
6	FMT	B	556	-	2,2,2	0.26	0	1,1,1	0.13	0
6	FMT	F	718	-	2,2,2	0.40	0	1,1,1	0.12	0
6	FMT	C	560	-	2,2,2	0.26	0	1,1,1	0.15	0
3	DEB	C	502	-	27,27,27	0.81	1 (3%)	37,39,39	0.62	1 (2%)
6	FMT	B	523	-	2,2,2	0.11	0	1,1,1	0.14	0
6	FMT	B	529	-	2,2,2	0.27	0	1,1,1	0.14	0
6	FMT	C	548	-	2,2,2	0.33	0	1,1,1	0.10	0
6	FMT	B	512	-	2,2,2	0.38	0	1,1,1	0.06	0
6	FMT	B	539	-	2,2,2	0.29	0	1,1,1	0.16	0
8	GOL	B	506	-	5,5,5	0.10	0	5,5,5	0.27	0
6	FMT	B	566	-	2,2,2	0.23	0	1,1,1	0.16	0
6	FMT	B	568	-	2,2,2	0.50	0	1,1,1	0.05	0
6	FMT	C	557	-	2,2,2	0.12	0	1,1,1	0.22	0
6	FMT	B	510	-	2,2,2	0.31	0	1,1,1	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FMT	C	555[B]	6	2,2,2	0.41	0	1,1,1	0.04	0
6	FMT	A	518	-	2,2,2	0.24	0	1,1,1	0.17	0
6	FMT	E	506	-	2,2,2	0.45	0	1,1,1	0.06	0
6	FMT	A	520	-	2,2,2	0.30	0	1,1,1	0.12	0
6	FMT	C	556	-	2,2,2	0.36	0	1,1,1	0.02	0
6	FMT	C	514	-	2,2,2	0.24	0	1,1,1	0.17	0
6	FMT	A	544	-	2,2,2	0.26	0	1,1,1	0.17	0
6	FMT	C	551	-	2,2,2	0.28	0	1,1,1	0.15	0
6	FMT	E	514[B]	-	2,2,2	0.22	0	1,1,1	0.17	0
8	GOL	F	704	-	5,5,5	0.11	0	5,5,5	0.29	0
6	FMT	A	531	-	2,2,2	0.34	0	1,1,1	0.14	0
6	FMT	C	554	-	2,2,2	0.30	0	1,1,1	0.14	0
4	RAM	C	504	-	11,11,11	0.41	0	16,16,16	1.02	2 (12%)
6	FMT	B	508	-	2,2,2	0.33	0	1,1,1	0.22	0
6	FMT	D	510	-	2,2,2	0.26	0	1,1,1	0.16	0
6	FMT	D	519	-	2,2,2	0.28	0	1,1,1	0.12	0
6	FMT	A	538	-	2,2,2	0.46	0	1,1,1	0.02	0
6	FMT	B	530	-	2,2,2	0.24	0	1,1,1	0.17	0
6	FMT	B	551	-	2,2,2	0.36	0	1,1,1	0.03	0
6	FMT	B	516	-	2,2,2	0.28	0	1,1,1	0.16	0
6	FMT	A	506	-	2,2,2	0.32	0	1,1,1	0.17	0
6	FMT	C	509	-	2,2,2	0.35	0	1,1,1	0.14	0
6	FMT	F	712	-	2,2,2	0.34	0	1,1,1	0.10	0
6	FMT	A	541	-	2,2,2	0.34	0	1,1,1	0.16	0
3	DEB	B	502	-	27,27,27	0.78	1 (3%)	37,39,39	0.66	0
6	FMT	A	514	-	2,2,2	0.38	0	1,1,1	0.01	0
6	FMT	C	511	-	2,2,2	0.29	0	1,1,1	0.12	0
3	DEB	F	703	-	27,27,27	0.67	1 (3%)	37,39,39	0.60	0
6	FMT	B	552	-	2,2,2	0.25	0	1,1,1	0.17	0
6	FMT	C	512	-	2,2,2	0.26	0	1,1,1	0.18	0
3	DEB	A	502	-	27,27,27	0.55	0	37,39,39	0.87	0
6	FMT	A	543	-	2,2,2	0.25	0	1,1,1	0.16	0
6	FMT	C	547	-	2,2,2	0.34	0	1,1,1	0.14	0
6	FMT	C	552	-	2,2,2	0.26	0	1,1,1	0.16	0
6	FMT	F	707	-	2,2,2	0.40	0	1,1,1	0.07	0
6	FMT	B	569	-	2,2,2	0.28	0	1,1,1	0.18	0
6	FMT	C	517	-	2,2,2	0.28	0	1,1,1	0.21	0
6	FMT	A	522	-	2,2,2	0.47	0	1,1,1	0.01	0
6	FMT	C	530	-	2,2,2	0.32	0	1,1,1	0.16	0
6	FMT	A	521	-	2,2,2	0.19	0	1,1,1	0.18	0
2	HEM	E	501	1	50,50,50	1.98	17 (34%)	67,82,82	1.73	15 (22%)
4	RAM	D	503	-	11,11,11	1.16	0	16,16,16	2.88	12 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FMT	A	512	-	2,2,2	0.48	0	1,1,1	0.00	0
6	FMT	A	516	-	2,2,2	0.30	0	1,1,1	0.15	0
6	FMT	B	549	-	2,2,2	0.25	0	1,1,1	0.16	0
6	FMT	B	535	-	2,2,2	0.32	0	1,1,1	0.10	0
6	FMT	B	514	-	2,2,2	0.29	0	1,1,1	0.15	0
6	FMT	A	534	-	2,2,2	0.22	0	1,1,1	0.20	0
6	FMT	B	553	-	2,2,2	0.29	0	1,1,1	0.17	0
6	FMT	C	526	-	2,2,2	0.47	0	1,1,1	0.06	0
6	FMT	C	523	-	2,2,2	0.28	0	1,1,1	0.17	0
6	FMT	C	536	-	2,2,2	0.25	0	1,1,1	0.09	0
6	FMT	B	507	-	2,2,2	0.23	0	1,1,1	0.20	0
6	FMT	C	542	-	2,2,2	0.31	0	1,1,1	0.13	0
6	FMT	A	532	-	2,2,2	0.30	0	1,1,1	0.15	0
6	FMT	F	717	-	2,2,2	0.32	0	1,1,1	0.11	0
6	FMT	A	539	-	2,2,2	0.30	0	1,1,1	0.14	0
6	FMT	A	515	-	2,2,2	0.56	0	1,1,1	0.00	0
6	FMT	C	549	-	2,2,2	0.25	0	1,1,1	0.17	0
4	RAM	C	503[A]	-	11,11,11	1.04	1 (9%)	16,16,16	3.43	11 (68%)
6	FMT	D	514	-	2,2,2	0.29	0	1,1,1	0.09	0
6	FMT	B	543	-	2,2,2	0.23	0	1,1,1	0.17	0
8	GOL	C	506	-	5,5,5	0.10	0	5,5,5	0.19	0
6	FMT	A	529	-	2,2,2	0.29	0	1,1,1	0.16	0
6	FMT	B	517	-	2,2,2	0.35	0	1,1,1	0.07	0
6	FMT	B	528	-	2,2,2	0.34	0	1,1,1	0.10	0
6	FMT	B	560	-	2,2,2	0.23	0	1,1,1	0.14	0
4	RAM	B	503[A]	-	11,11,11	0.72	0	16,16,16	1.68	3 (18%)
6	FMT	A	511	-	2,2,2	0.18	0	1,1,1	0.17	0
6	FMT	C	510	-	2,2,2	0.32	0	1,1,1	0.12	0
6	FMT	C	537	-	2,2,2	0.34	0	1,1,1	0.16	0
6	FMT	C	540	-	2,2,2	0.28	0	1,1,1	0.15	0
6	FMT	F	709	-	2,2,2	0.31	0	1,1,1	0.15	0
6	FMT	A	545[B]	-	2,2,2	0.11	0	1,1,1	0.20	0
6	FMT	D	506	-	2,2,2	0.31	0	1,1,1	0.12	0
6	FMT	C	532	-	2,2,2	0.28	0	1,1,1	0.15	0
6	FMT	C	563	-	2,2,2	0.37	0	1,1,1	0.13	0
6	FMT	A	523	-	2,2,2	0.41	0	1,1,1	0.01	0
4	RAM	A	503[A]	-	11,11,11	0.73	0	16,16,16	1.30	2 (12%)
6	FMT	B	531	-	2,2,2	0.34	0	1,1,1	0.14	0
6	FMT	B	557	-	2,2,2	0.28	0	1,1,1	0.15	0
2	HEM	F	702	1	50,50,50	1.86	16 (32%)	67,82,82	1.69	15 (22%)
6	FMT	B	520	-	2,2,2	0.31	0	1,1,1	0.12	0
6	FMT	D	509	-	2,2,2	0.40	0	1,1,1	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FMT	B	519	-	2,2,2	0.33	0	1,1,1	0.04	0
6	FMT	B	555	-	2,2,2	0.26	0	1,1,1	0.15	0
6	FMT	F	710	-	2,2,2	0.30	0	1,1,1	0.13	0
6	FMT	D	517	-	2,2,2	0.23	0	1,1,1	0.17	0
6	FMT	F	715	-	2,2,2	0.52	0	1,1,1	0.04	0
8	GOL	C	507	-	5,5,5	0.08	0	5,5,5	0.31	0
6	FMT	B	544	-	2,2,2	0.27	0	1,1,1	0.14	0
6	FMT	C	539	-	2,2,2	0.39	0	1,1,1	0.06	0
6	FMT	A	524	-	2,2,2	0.27	0	1,1,1	0.17	0
6	FMT	B	525	-	2,2,2	0.29	0	1,1,1	0.11	0
6	FMT	A	510	-	2,2,2	0.30	0	1,1,1	0.14	0
6	FMT	A	526	-	2,2,2	0.29	0	1,1,1	0.12	0
6	FMT	E	510	-	2,2,2	0.33	0	1,1,1	0.11	0
6	FMT	A	509	-	2,2,2	0.47	0	1,1,1	0.04	0
6	FMT	C	531	-	2,2,2	0.41	0	1,1,1	0.09	0
6	FMT	E	513	-	2,2,2	0.30	0	1,1,1	0.10	0
6	FMT	C	561	-	2,2,2	0.38	0	1,1,1	0.07	0
6	FMT	C	515	-	2,2,2	0.25	0	1,1,1	0.18	0
6	FMT	C	564	-	2,2,2	0.34	0	1,1,1	0.09	0
6	FMT	B	522	-	2,2,2	0.29	0	1,1,1	0.16	0
6	FMT	D	511	-	2,2,2	0.30	0	1,1,1	0.14	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	B	501	1	-	0/14/54/54	-
2	HEM	A	501	1	-	0/14/54/54	-
8	GOL	B	505	-	-	2/4/4/4	-
4	RAM	C	503[A]	-	-	-	0/1/1/1
4	RAM	E	503[A]	-	-	-	0/1/1/1
8	GOL	F	704	-	-	2/4/4/4	-
2	HEM	C	501	1	-	0/14/54/54	-
8	GOL	C	506	-	-	2/4/4/4	-
3	DEB	D	502	-	-	7/50/50/50	0/1/1/1
5	TRS	A	504	-	-	3/9/9/9	-
4	RAM	C	504	-	-	-	0/1/1/1
4	RAM	B	503[A]	-	-	-	0/1/1/1
3	DEB	E	502	-	-	9/50/50/50	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRS	F	705	-	-	6/9/9/9	-
3	DEB	B	502	-	-	9/50/50/50	0/1/1/1
3	DEB	F	703	-	-	10/50/50/50	0/1/1/1
4	RAM	A	503[A]	-	-	-	0/1/1/1
3	DEB	A	502	-	-	10/50/50/50	0/1/1/1
2	HEM	F	702	1	-	0/14/54/54	-
8	GOL	C	507	-	-	2/4/4/4	-
2	HEM	D	501	1	-	2/14/54/54	-
4	RAM	F	701	-	-	-	0/1/1/1
2	HEM	E	501	1	-	0/14/54/54	-
5	TRS	B	504	-	-	3/9/9/9	-
8	GOL	C	505	-	-	0/4/4/4	-
4	RAM	D	503	-	-	-	0/1/1/1
3	DEB	C	502	-	-	8/50/50/50	0/1/1/1
8	GOL	B	506	-	-	0/4/4/4	-

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C1B-NB	-5.31	1.31	1.40
2	E	501	HEM	C1B-NB	-4.99	1.31	1.40
2	B	501	HEM	C1B-NB	-4.92	1.31	1.40
2	C	501	HEM	C1B-NB	-4.83	1.31	1.40
2	A	501	HEM	C1B-NB	-4.80	1.31	1.40
2	D	501	HEM	FE-ND	-4.80	1.80	1.94
2	F	702	HEM	C1B-NB	-4.44	1.32	1.40
2	C	501	HEM	C3C-C4C	-4.37	1.38	1.46
2	C	501	HEM	C4D-ND	-4.33	1.32	1.40
2	A	501	HEM	C4B-NB	-4.29	1.30	1.38
2	B	501	HEM	C3C-C4C	-4.28	1.38	1.46
2	E	501	HEM	FE-NB	4.22	2.07	1.94
2	A	501	HEM	C3C-C4C	-4.22	1.38	1.46
2	D	501	HEM	C1C-C2C	-4.16	1.37	1.45
2	D	501	HEM	C3C-C4C	-4.14	1.38	1.46
2	C	501	HEM	C4B-NB	-4.13	1.30	1.38
2	D	501	HEM	C4D-ND	-4.06	1.33	1.40
2	F	702	HEM	FE-NB	4.00	2.07	1.94
2	E	501	HEM	C3C-C4C	-4.00	1.39	1.46
2	B	501	HEM	C4B-NB	-3.98	1.31	1.38
2	A	501	HEM	C1C-C2C	-3.92	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C4B-NB	-3.89	1.31	1.38
2	D	501	HEM	C1C-NC	-3.88	1.32	1.39
2	B	501	HEM	FE-NC	3.85	2.07	1.95
2	D	501	HEM	C1D-ND	-3.85	1.31	1.38
2	C	501	HEM	C1C-NC	-3.85	1.32	1.39
2	C	501	HEM	C1C-C2C	-3.83	1.37	1.45
2	D	501	HEM	FE-NC	3.77	2.07	1.95
2	B	501	HEM	C4D-ND	-3.76	1.33	1.40
2	F	702	HEM	C4D-ND	-3.75	1.33	1.40
2	E	501	HEM	C4D-ND	-3.66	1.33	1.40
2	C	501	HEM	FE-NB	3.65	2.06	1.94
2	B	501	HEM	C1C-NC	-3.64	1.32	1.39
2	D	501	HEM	C4C-NC	-3.62	1.32	1.39
2	B	501	HEM	FE-ND	-3.60	1.83	1.94
2	A	501	HEM	C1D-ND	-3.60	1.31	1.38
2	A	501	HEM	C4D-ND	-3.58	1.34	1.40
2	C	501	HEM	FE-NC	3.54	2.06	1.95
2	B	501	HEM	C1C-C2C	-3.49	1.38	1.45
2	E	501	HEM	FE-NC	3.48	2.06	1.95
2	F	702	HEM	C1C-C2C	-3.48	1.38	1.45
2	F	702	HEM	FE-NC	3.48	2.06	1.95
2	B	501	HEM	C1D-ND	-3.46	1.32	1.38
2	E	501	HEM	C4B-NB	-3.43	1.32	1.38
2	A	501	HEM	FE-ND	-3.42	1.84	1.94
2	C	501	HEM	C1D-ND	-3.37	1.32	1.38
2	C	501	HEM	C1A-C2A	-3.37	1.37	1.44
2	B	501	HEM	FE-NB	3.31	2.05	1.94
2	B	501	HEM	C4C-NC	-3.29	1.33	1.39
2	A	501	HEM	FE-NB	3.27	2.05	1.94
2	A	501	HEM	C1C-NC	-3.24	1.33	1.39
2	D	501	HEM	C4A-NA	-3.18	1.33	1.39
2	C	501	HEM	O2A-CGA	-3.14	1.20	1.30
2	E	501	HEM	C1C-C2C	-3.08	1.39	1.45
2	F	702	HEM	C4B-NB	-3.08	1.32	1.38
2	F	702	HEM	C3C-C4C	-3.08	1.40	1.46
2	E	501	HEM	C1D-ND	-3.04	1.32	1.38
2	A	501	HEM	C4C-NC	-3.01	1.33	1.39
2	C	501	HEM	C4C-NC	-3.00	1.34	1.39
2	E	501	HEM	FE-ND	-2.97	1.85	1.94
2	E	501	HEM	C1C-NC	-2.94	1.34	1.39
2	B	501	HEM	C4A-NA	-2.92	1.34	1.39
2	B	501	HEM	O2D-CGD	-2.90	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	O2D-CGD	-2.89	1.21	1.30
2	D	501	HEM	C1A-C2A	-2.86	1.38	1.44
2	F	702	HEM	O2A-CGA	-2.85	1.21	1.30
2	A	501	HEM	O2A-CGA	-2.79	1.21	1.30
2	D	501	HEM	C1B-C2B	-2.78	1.38	1.44
2	A	501	HEM	FE-NC	2.78	2.04	1.95
2	E	501	HEM	O2A-CGA	-2.77	1.21	1.30
2	F	702	HEM	C1D-ND	-2.77	1.33	1.38
2	E	501	HEM	C4C-NC	-2.77	1.34	1.39
2	F	702	HEM	FE-ND	-2.76	1.86	1.94
2	A	501	HEM	O2D-CGD	-2.76	1.21	1.30
2	F	702	HEM	C1A-C2A	-2.74	1.39	1.44
2	E	501	HEM	O2D-CGD	-2.73	1.21	1.30
2	C	501	HEM	C3D-C2D	-2.71	1.30	1.36
2	D	501	HEM	C3D-C2D	-2.71	1.30	1.36
2	C	501	HEM	FE-ND	-2.67	1.86	1.94
2	B	501	HEM	O2A-CGA	-2.66	1.22	1.30
2	F	702	HEM	O2D-CGD	-2.64	1.22	1.30
2	A	501	HEM	C1A-C2A	-2.64	1.39	1.44
2	B	501	HEM	C3D-C2D	-2.61	1.31	1.36
2	F	702	HEM	C4A-NA	-2.60	1.34	1.39
2	B	501	HEM	C1A-C2A	-2.60	1.39	1.44
2	A	501	HEM	C3D-C2D	-2.59	1.31	1.36
2	E	501	HEM	C1A-C2A	-2.58	1.39	1.44
2	D	501	HEM	FE-NB	2.53	2.02	1.94
4	C	503[A]	RAM	O5-C1	-2.53	1.36	1.42
2	D	501	HEM	O2A-CGA	-2.53	1.22	1.30
2	E	501	HEM	C4A-NA	-2.50	1.34	1.39
2	D	501	HEM	O2D-CGD	-2.49	1.22	1.30
2	A	501	HEM	C4A-NA	-2.48	1.34	1.39
2	D	501	HEM	C2A-C3A	-2.46	1.32	1.38
2	E	501	HEM	C1B-C2B	-2.43	1.39	1.44
2	F	702	HEM	C1C-NC	-2.42	1.35	1.39
3	B	502	DEB	O24-C9	-2.41	1.17	1.21
2	C	501	HEM	C2A-C3A	-2.38	1.32	1.38
3	D	502	DEB	O24-C9	-2.29	1.18	1.21
2	F	702	HEM	C4C-NC	-2.27	1.35	1.39
3	F	703	DEB	O24-C9	-2.26	1.18	1.21
3	C	502	DEB	O24-C9	-2.21	1.18	1.21
2	C	501	HEM	C4A-NA	-2.20	1.35	1.39
2	A	501	HEM	C1A-NA	-2.18	1.35	1.39
2	D	501	HEM	CHD-C4C	-2.16	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1A-NA	-2.14	1.35	1.39
2	D	501	HEM	CHA-C1A	-2.14	1.34	1.39
2	B	501	HEM	C1B-C2B	-2.13	1.40	1.44
2	D	501	HEM	C1A-NA	-2.09	1.35	1.39
2	A	501	HEM	C2A-C3A	-2.08	1.33	1.38
2	B	501	HEM	C2A-C3A	-2.07	1.33	1.38
2	F	702	HEM	C3D-C2D	-2.07	1.32	1.36
2	A	501	HEM	C1B-C2B	-2.06	1.40	1.44
2	E	501	HEM	C3D-C2D	-2.04	1.32	1.36

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503[A]	RAM	C3-C4-C5	-8.71	96.57	109.81
2	D	501	HEM	CHC-C4B-NB	7.59	132.60	124.42
2	A	501	HEM	CHC-C4B-NB	6.74	131.68	124.42
2	C	501	HEM	CHC-C4B-NB	6.70	131.63	124.42
2	F	702	HEM	CHC-C4B-NB	5.95	130.82	124.42
2	B	501	HEM	CHC-C4B-NB	5.92	130.79	124.42
2	D	501	HEM	CHD-C1D-ND	5.40	130.23	124.42
2	A	501	HEM	C1B-NB-C4B	4.84	110.94	105.21
4	D	503	RAM	C4-C3-C2	4.77	119.21	110.83
2	C	501	HEM	C1B-NB-C4B	4.73	110.81	105.21
4	C	503[A]	RAM	O5-C1-C2	4.62	118.42	110.30
2	A	501	HEM	CHD-C1D-ND	4.60	129.37	124.42
2	E	501	HEM	C1B-NB-C4B	4.56	110.61	105.21
2	E	501	HEM	CHC-C4B-NB	4.54	129.31	124.42
4	C	503[A]	RAM	O1-C1-O5	-4.52	96.98	110.41
4	F	701	RAM	O5-C1-C2	4.46	118.14	110.30
4	B	503[A]	RAM	C4-C3-C2	4.31	118.39	110.83
2	D	501	HEM	C1B-NB-C4B	4.25	110.24	105.21
2	F	702	HEM	C1B-NB-C4B	4.24	110.22	105.21
2	D	501	HEM	CHA-C4D-ND	4.19	129.56	124.37
2	A	501	HEM	CHD-C1D-C2D	-4.18	118.43	125.03
2	B	501	HEM	C1B-NB-C4B	4.17	110.14	105.21
2	E	501	HEM	C3B-C4B-NB	-4.14	106.50	109.47
2	B	501	HEM	CHD-C1D-ND	4.06	128.80	124.42
2	D	501	HEM	CHD-C1D-C2D	-3.84	118.96	125.03
4	D	503	RAM	C6-C5-C4	-3.80	106.14	113.08
4	D	503	RAM	C1-O5-C5	3.79	120.28	114.37
2	E	501	HEM	CHB-C1B-NB	3.76	129.01	124.37
4	C	503[A]	RAM	O5-C5-C4	-3.72	102.86	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CHA-C4D-ND	3.67	128.91	124.37
4	D	503	RAM	O5-C1-C2	-3.67	103.85	110.30
2	D	501	HEM	C3B-C4B-NB	-3.55	106.92	109.47
4	E	503[A]	RAM	C6-C5-C4	-3.45	106.77	113.08
2	D	501	HEM	CHB-C1B-NB	3.42	128.59	124.37
2	F	702	HEM	CHD-C1D-ND	3.40	128.09	124.42
4	C	503[A]	RAM	C1-C2-C3	3.39	117.28	110.36
2	C	501	HEM	CHD-C1D-ND	3.29	127.96	124.42
4	D	503	RAM	C3-C4-C5	3.23	114.73	109.81
2	A	501	HEM	CHD-C4C-NC	3.21	127.95	124.45
4	C	503[A]	RAM	O4-C4-C3	3.20	117.93	110.38
3	D	502	DEB	C10-C11-C12	3.20	120.65	114.49
4	E	503[A]	RAM	C3-C4-C5	-3.20	104.94	109.81
2	E	501	HEM	CHD-C1D-ND	3.19	127.86	124.42
4	D	503	RAM	O4-C4-C3	3.10	117.68	110.38
2	E	501	HEM	CHA-C4D-ND	3.08	128.18	124.37
2	B	501	HEM	CHD-C1D-C2D	-3.05	120.21	125.03
2	C	501	HEM	CHA-C4D-C3D	-3.05	119.60	125.23
4	D	503	RAM	O5-C5-C6	3.02	113.44	106.74
2	E	501	HEM	CHD-C4C-NC	3.00	127.72	124.45
4	D	503	RAM	O3-C3-C2	-2.95	103.42	110.38
2	D	501	HEM	CAD-C3D-C4D	2.92	129.79	124.70
2	C	501	HEM	CHD-C4C-NC	2.92	127.63	124.45
4	C	503[A]	RAM	C6-C5-C4	2.90	118.39	113.08
2	D	501	HEM	CHA-C4D-C3D	-2.90	119.89	125.23
2	B	501	HEM	CHA-C4D-C3D	-2.89	119.89	125.23
2	A	501	HEM	O2A-CGA-O1A	-2.89	115.90	123.33
2	A	501	HEM	CHB-C1B-NB	2.86	127.91	124.37
2	A	501	HEM	CAD-C3D-C4D	2.86	129.68	124.70
2	F	702	HEM	CHD-C4C-NC	2.84	127.55	124.45
2	A	501	HEM	CHA-C4D-ND	2.83	127.87	124.37
2	E	501	HEM	CHA-C4D-C3D	-2.83	120.01	125.23
2	C	501	HEM	O2A-CGA-O1A	-2.81	116.10	123.33
2	B	501	HEM	O2A-CGA-O1A	-2.78	116.18	123.33
2	F	702	HEM	C1A-CHA-C4D	-2.78	119.72	126.25
2	F	702	HEM	CHB-C1B-NB	2.75	127.77	124.37
4	A	503[A]	RAM	C1-C2-C3	2.75	115.96	110.36
2	B	501	HEM	CAD-C3D-C4D	2.75	129.49	124.70
4	B	503[A]	RAM	C3-C4-C5	2.75	113.99	109.81
2	B	501	HEM	CHB-C1B-NB	2.75	127.77	124.37
2	F	702	HEM	CHA-C4D-ND	2.73	127.74	124.37
2	B	501	HEM	CHD-C4C-NC	2.69	127.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CHA-C4D-ND	2.69	127.69	124.37
2	A	501	HEM	C3B-C4B-NB	-2.68	107.54	109.47
2	C	501	HEM	O2D-CGD-O1D	-2.67	116.47	123.33
4	C	503[A]	RAM	O2-C2-C1	-2.66	103.10	109.25
2	F	702	HEM	C3B-C4B-NB	-2.65	107.56	109.47
2	F	702	HEM	CHD-C1D-C2D	-2.64	120.86	125.03
2	E	501	HEM	CBA-CAA-C2A	2.62	119.78	112.53
2	D	501	HEM	C1A-CHA-C4D	-2.61	120.10	126.25
4	C	503[A]	RAM	O3-C3-C4	2.61	116.53	110.38
2	E	501	HEM	CHD-C1D-C2D	-2.60	120.92	125.03
3	C	502	DEB	C10-C11-C12	2.59	119.47	114.49
2	E	501	HEM	C1A-CHA-C4D	-2.58	120.19	126.25
2	A	501	HEM	C1A-CHA-C4D	-2.57	120.20	126.25
2	A	501	HEM	C4C-CHD-C1D	-2.54	120.63	126.02
2	D	501	HEM	O2A-CGA-O1A	-2.53	116.82	123.33
2	E	501	HEM	O2A-CGA-O1A	-2.53	116.83	123.33
2	C	501	HEM	CHD-C1D-C2D	-2.52	121.04	125.03
2	F	702	HEM	O2A-CGA-O1A	-2.50	116.90	123.33
4	B	503[A]	RAM	C1-O5-C5	-2.47	110.53	114.37
2	B	501	HEM	O2D-CGD-O1D	-2.45	117.03	123.33
2	C	501	HEM	CAD-C3D-C4D	2.44	128.94	124.70
4	E	503[A]	RAM	O5-C1-C2	-2.43	106.02	110.30
2	B	501	HEM	C3B-C4B-NB	-2.43	107.72	109.47
2	C	501	HEM	C3B-C4B-NB	-2.42	107.73	109.47
4	D	503	RAM	O1-C1-O5	2.42	117.60	110.41
2	A	501	HEM	O2D-CGD-O1D	-2.40	117.16	123.33
4	D	503	RAM	O5-C5-C4	2.40	113.87	109.55
4	C	503[A]	RAM	C4-C3-C2	-2.39	106.63	110.83
4	D	503	RAM	O3-C3-C4	-2.38	104.76	110.38
2	C	501	HEM	CBA-CAA-C2A	2.38	119.12	112.53
2	D	501	HEM	C4C-CHD-C1D	-2.36	120.99	126.02
2	D	501	HEM	O2D-CGD-O1D	-2.36	117.27	123.33
2	B	501	HEM	C1A-CHA-C4D	-2.36	120.70	126.25
2	F	702	HEM	C1C-CHC-C4B	-2.31	121.12	126.02
2	D	501	HEM	CHC-C4B-C3B	-2.30	120.47	125.07
3	D	502	DEB	C7-C6-C5	2.30	116.13	110.96
2	C	501	HEM	C3D-C4D-ND	2.30	112.69	110.17
2	C	501	HEM	CHB-C1B-NB	2.28	127.19	124.37
2	B	501	HEM	O2A-CGA-CBA	2.27	121.19	114.00
4	D	503	RAM	C1-C2-C3	-2.26	105.75	110.36
2	C	501	HEM	CHC-C4B-C3B	-2.24	120.61	125.07
2	B	501	HEM	CMD-C2D-C1D	2.23	128.52	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C1A-CHA-C4D	-2.22	121.02	126.25
4	E	503[A]	RAM	O5-C5-C6	2.21	111.65	106.74
4	C	503[A]	RAM	O4-C4-C5	2.18	114.55	109.74
2	F	702	HEM	CAD-C3D-C4D	2.18	128.50	124.70
2	E	501	HEM	CAD-C3D-C4D	2.18	128.49	124.70
2	A	501	HEM	CHC-C4B-C3B	-2.16	120.77	125.07
2	D	501	HEM	O2D-CGD-CBD	2.15	120.78	114.00
2	F	702	HEM	CHA-C4D-C3D	-2.14	121.28	125.23
2	D	501	HEM	O2A-CGA-CBA	2.13	120.72	114.00
2	C	501	HEM	O2A-CGA-CBA	2.10	120.64	114.00
2	F	702	HEM	O2A-CGA-CBA	2.09	120.62	114.00
4	E	503[A]	RAM	C1-O5-C5	-2.09	111.12	114.37
4	C	504	RAM	C1-C2-C3	-2.08	106.11	110.36
2	D	501	HEM	CBA-CAA-C2A	2.06	118.22	112.53
4	C	504	RAM	C4-C3-C2	-2.06	107.22	110.83
2	E	501	HEM	O2D-CGD-O1D	-2.04	118.09	123.33
2	F	702	HEM	O2D-CGD-CBD	2.04	120.43	114.00
2	D	501	HEM	CHD-C4C-NC	2.03	126.67	124.45
2	A	501	HEM	CHA-C4D-C3D	-2.03	121.49	125.23
2	E	501	HEM	C4C-NC-C1C	2.02	109.12	105.82
2	B	501	HEM	C4C-CHD-C1D	-2.02	121.72	126.02
2	A	501	HEM	O2A-CGA-CBA	2.01	120.35	114.00
4	A	503[A]	RAM	C6-C5-C4	-2.00	109.41	113.08

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	DEB	C3-C4-C5-O21
3	B	502	DEB	C3-C4-C5-O21
3	B	502	DEB	O16-C13-C14-C15
3	D	502	DEB	C3-C4-C5-O21
3	D	502	DEB	C20-C4-C5-O21
3	F	703	DEB	C1-C2-C3-O19
3	F	703	DEB	C18-C2-C3-C4
5	A	504	TRS	C2-C-C1-O1
5	A	504	TRS	N-C-C1-O1
5	F	705	TRS	C3-C-C1-O1
5	F	705	TRS	C1-C-C2-O2
5	F	705	TRS	C3-C-C2-O2
5	F	705	TRS	N-C-C2-O2
8	B	505	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	C	506	GOL	O1-C1-C2-C3
8	C	507	GOL	C1-C2-C3-O3
8	F	704	GOL	O1-C1-C2-C3
3	C	502	DEB	C3-C4-C5-O21
3	E	502	DEB	C3-C4-C5-O21
3	F	703	DEB	C3-C4-C5-O21
3	A	502	DEB	C20-C4-C5-O21
3	B	502	DEB	C20-C4-C5-O21
3	C	502	DEB	C20-C4-C5-O21
3	E	502	DEB	C20-C4-C5-O21
8	C	506	GOL	O1-C1-C2-O2
3	A	502	DEB	C18-C2-C3-O19
3	B	502	DEB	C18-C2-C3-O19
3	C	502	DEB	C18-C2-C3-O19
3	E	502	DEB	C18-C2-C3-O19
3	F	703	DEB	C18-C2-C3-O19
3	A	502	DEB	C18-C2-C3-C4
3	E	502	DEB	C18-C2-C3-C4
3	F	703	DEB	C20-C4-C5-O21
8	B	505	GOL	O2-C2-C3-O3
8	C	507	GOL	O2-C2-C3-O3
8	F	704	GOL	O1-C1-C2-O2
3	D	502	DEB	C3-C4-C5-C6
5	A	504	TRS	C3-C-C1-O1
5	F	705	TRS	C2-C-C1-O1
3	B	502	DEB	C18-C2-C3-C4
3	C	502	DEB	C18-C2-C3-C4
3	D	502	DEB	C18-C2-C3-C4
3	D	502	DEB	C20-C4-C5-C6
3	E	502	DEB	C20-C4-C5-C6
3	C	502	DEB	C3-C4-C5-C6
3	A	502	DEB	C3-C4-C5-C6
3	B	502	DEB	C3-C4-C5-C6
3	D	502	DEB	C18-C2-C3-O19
3	A	502	DEB	C20-C4-C5-C6
3	B	502	DEB	C20-C4-C5-C6
3	C	502	DEB	C20-C4-C5-C6
3	F	703	DEB	C20-C4-C5-C6
3	E	502	DEB	C3-C4-C5-C6
3	F	703	DEB	C3-C4-C5-C6
3	B	502	DEB	C12-C13-C14-C15
3	A	502	DEB	C1-C2-C3-O19

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Mol	Chain	Res	Type	Atoms
3	E	502	DEB	C1-C2-C3-O19
3	A	502	DEB	C1-C2-C3-C4
3	F	703	DEB	C1-C2-C3-C4
5	B	504	TRS	C1-C-C2-O2
5	B	504	TRS	C2-C-C3-O3
5	F	705	TRS	N-C-C1-O1
3	A	502	DEB	C23-C8-C9-O24
3	E	502	DEB	C23-C8-C9-O24
3	F	703	DEB	C23-C8-C9-O24
3	A	502	DEB	C7-C8-C9-O24
3	E	502	DEB	C7-C8-C9-O24
3	F	703	DEB	C7-C8-C9-O24
3	C	502	DEB	C23-C8-C9-O24
3	B	502	DEB	C1-C2-C3-O19
3	C	502	DEB	C1-C2-C3-O19
3	D	502	DEB	C1-C2-C3-O19
5	B	504	TRS	N-C-C3-O3
2	D	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

52 monomers are involved in 134 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	505	GOL	4	0
4	E	503[A]	RAM	12	0
2	C	501	HEM	1	0
6	E	504	FMT	2	0
6	A	542	FMT	2	0
6	B	538	FMT	2	0
6	A	505	FMT	1	0
6	C	525	FMT	1	0
6	C	543	FMT	1	0
8	C	505	GOL	2	0
2	B	501	HEM	2	0
6	C	538	FMT	1	0
6	F	706	FMT	1	0
2	A	501	HEM	5	0
6	B	513	FMT	2	0
6	C	513[B]	FMT	2	0
6	B	540	FMT	2	0
6	B	548	FMT	1	0

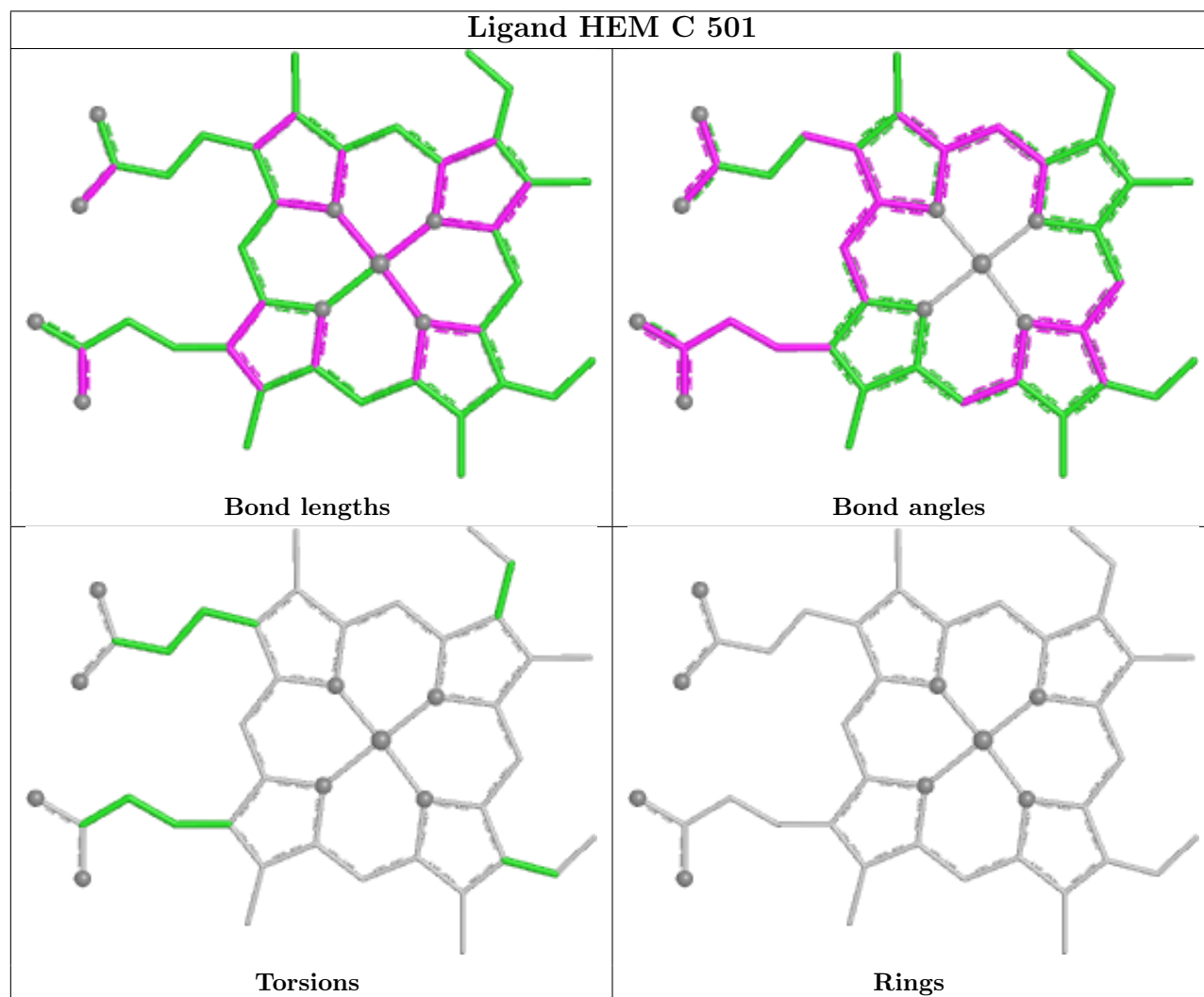
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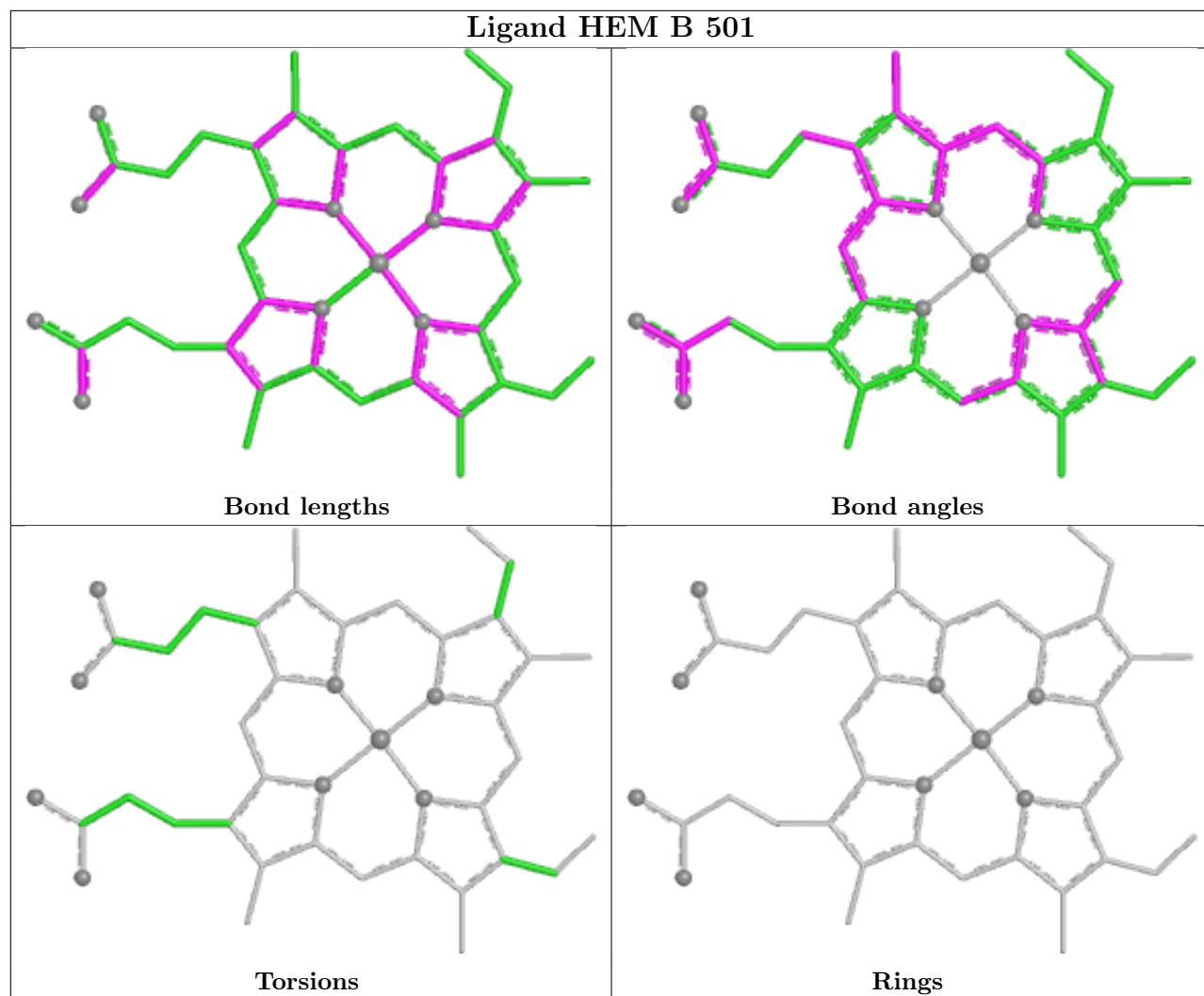
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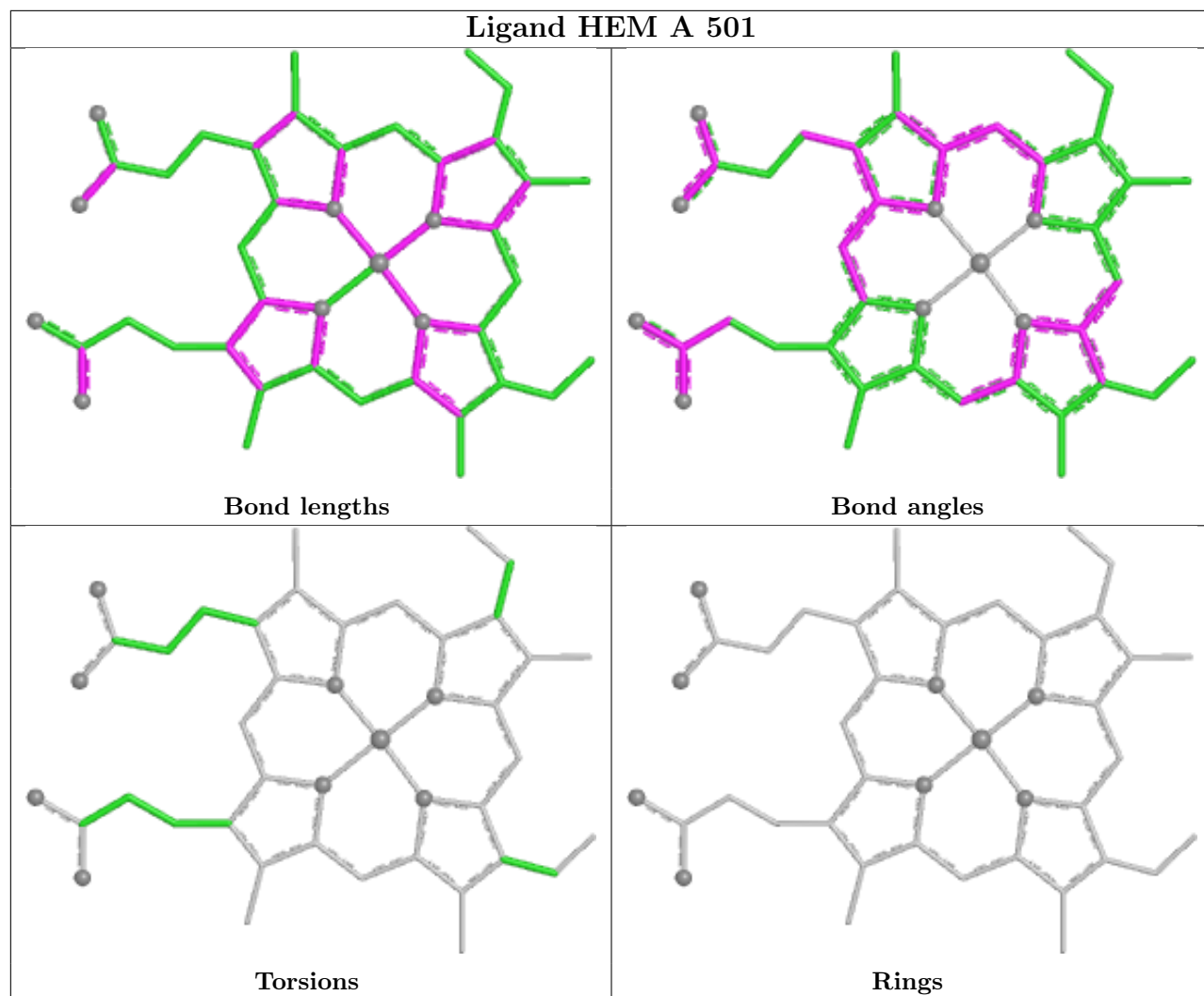
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	DEB	6	0
6	A	508	FMT	2	0
3	E	502	DEB	4	0
5	F	705	TRS	3	0
6	B	565	FMT	2	0
2	D	501	HEM	5	0
6	C	558	FMT	1	0
6	B	556	FMT	2	0
3	C	502	DEB	1	0
6	C	555[B]	FMT	3	0
6	E	506	FMT	1	0
6	E	514[B]	FMT	2	0
8	F	704	GOL	1	0
4	C	504	RAM	3	0
6	B	508	FMT	1	0
6	A	514	FMT	2	0
3	A	502	DEB	3	0
6	A	543	FMT	1	0
2	E	501	HEM	7	0
4	D	503	RAM	10	0
6	A	512	FMT	1	0
6	B	507	FMT	1	0
6	A	515	FMT	1	0
4	C	503[A]	RAM	5	0
6	D	514	FMT	1	0
8	C	506	GOL	1	0
4	B	503[A]	RAM	7	0
6	A	511	FMT	1	0
6	C	532	FMT	1	0
4	A	503[A]	RAM	15	0
2	F	702	HEM	5	0
6	B	519	FMT	5	0
8	C	507	GOL	10	0
6	A	509	FMT	1	0

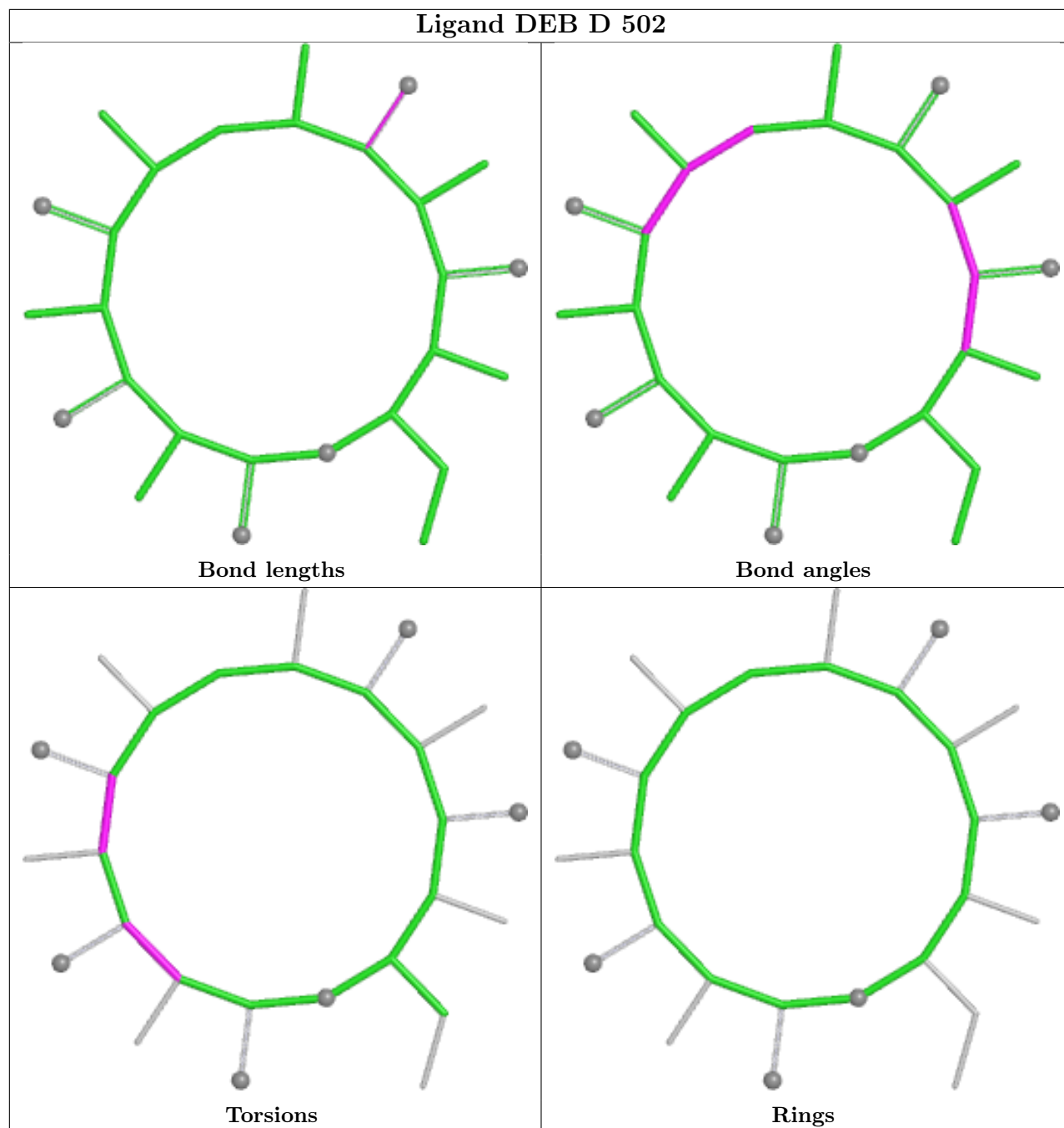
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

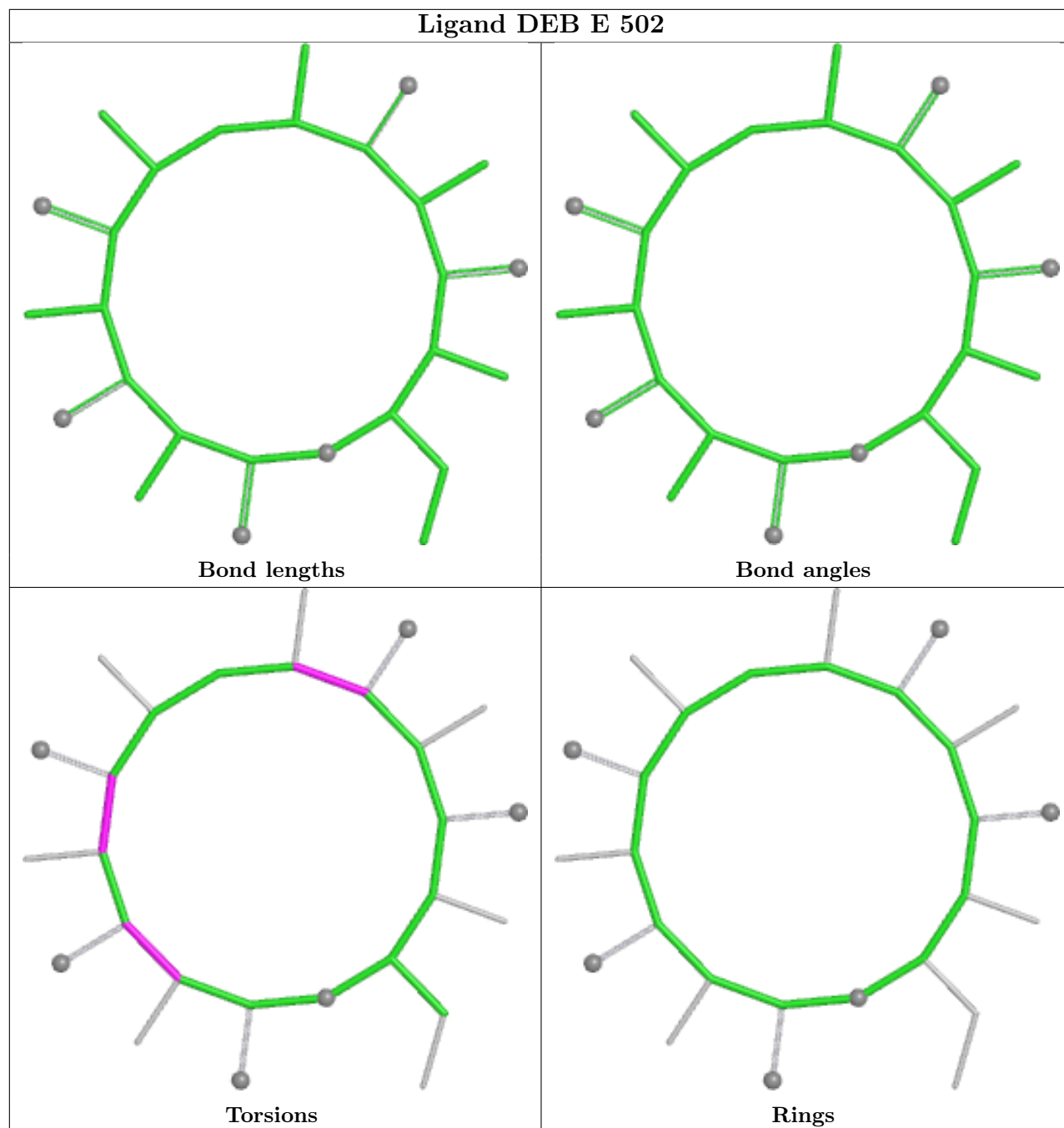


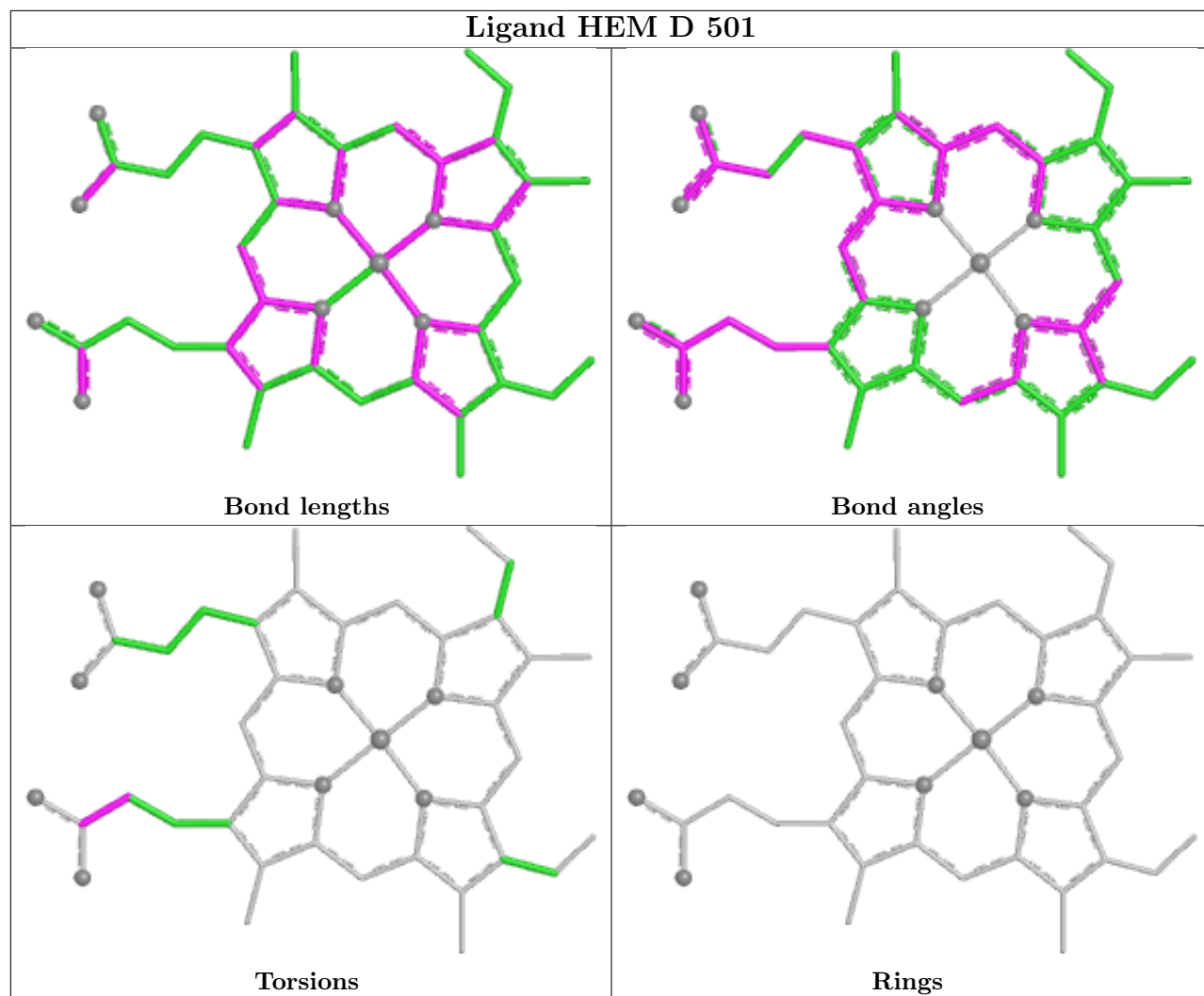


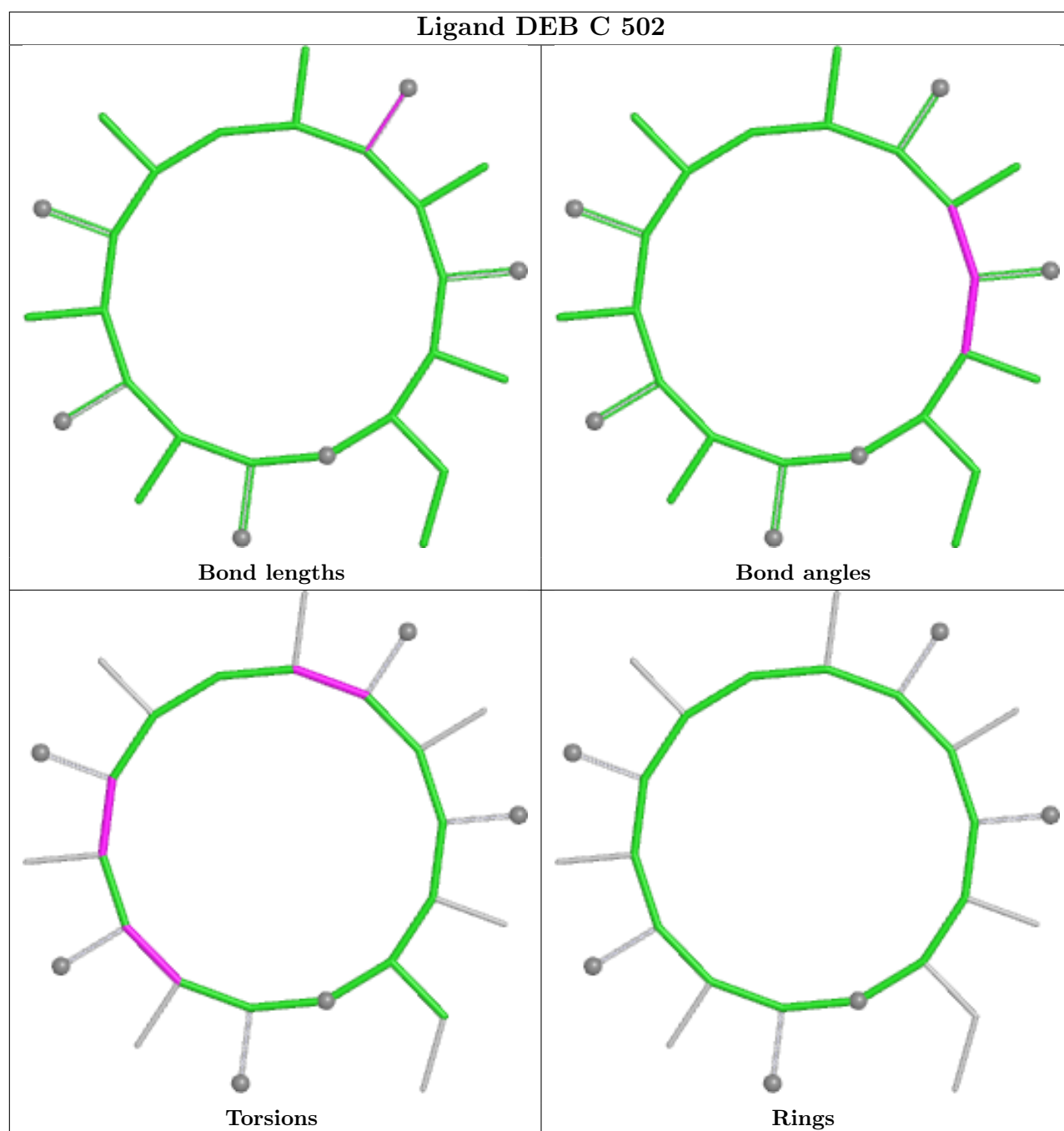


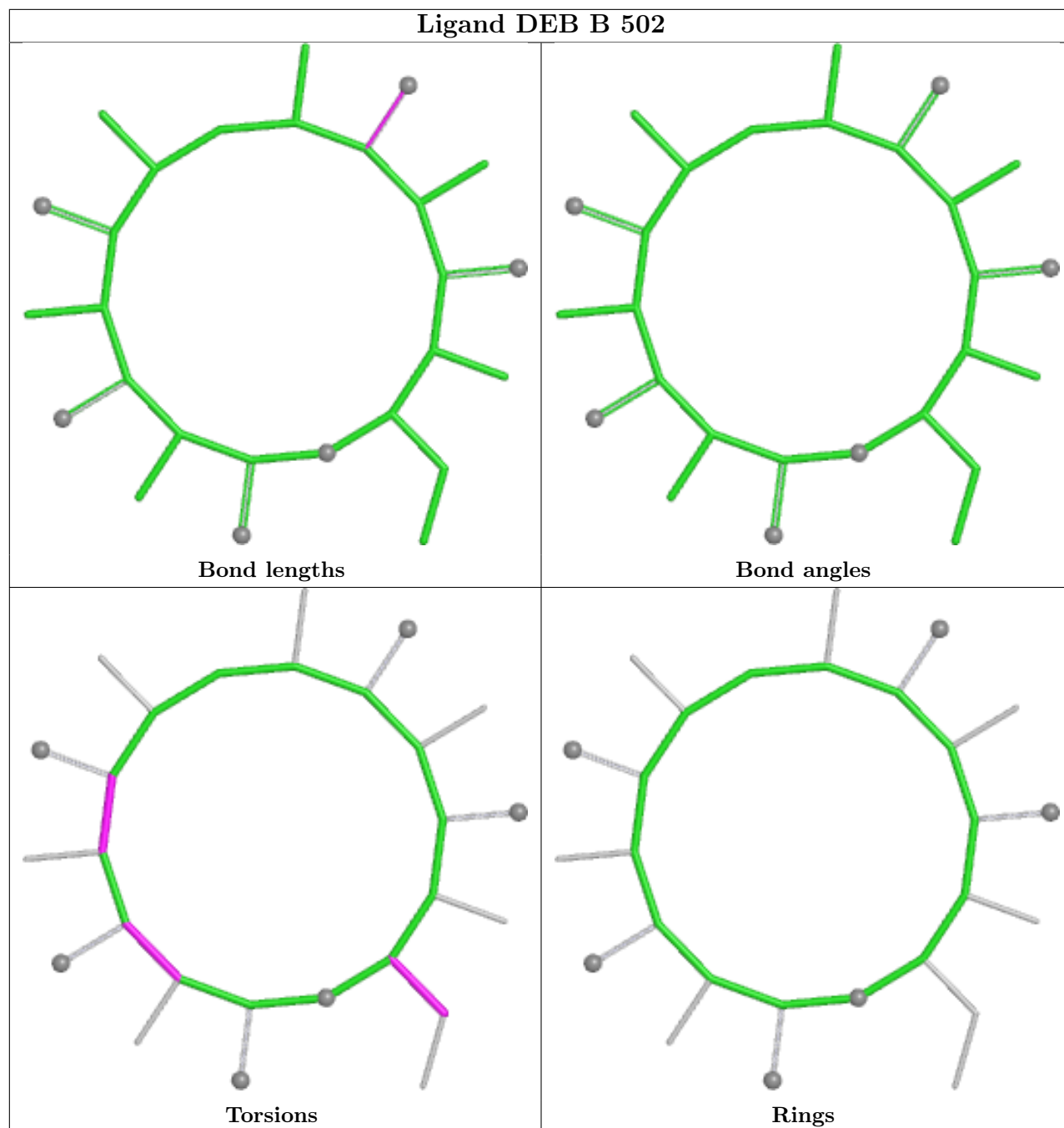


Ligand DEB E 502

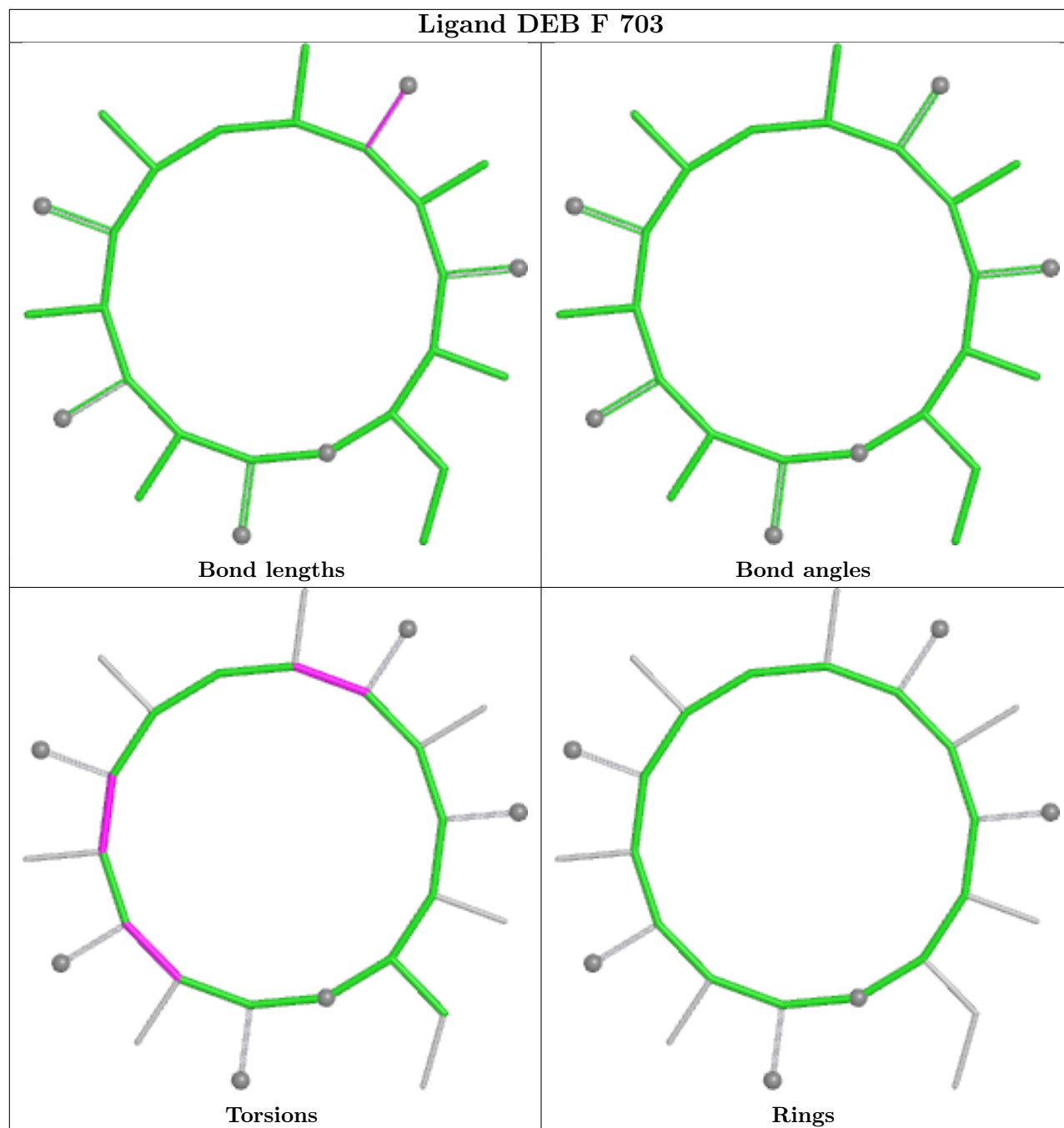


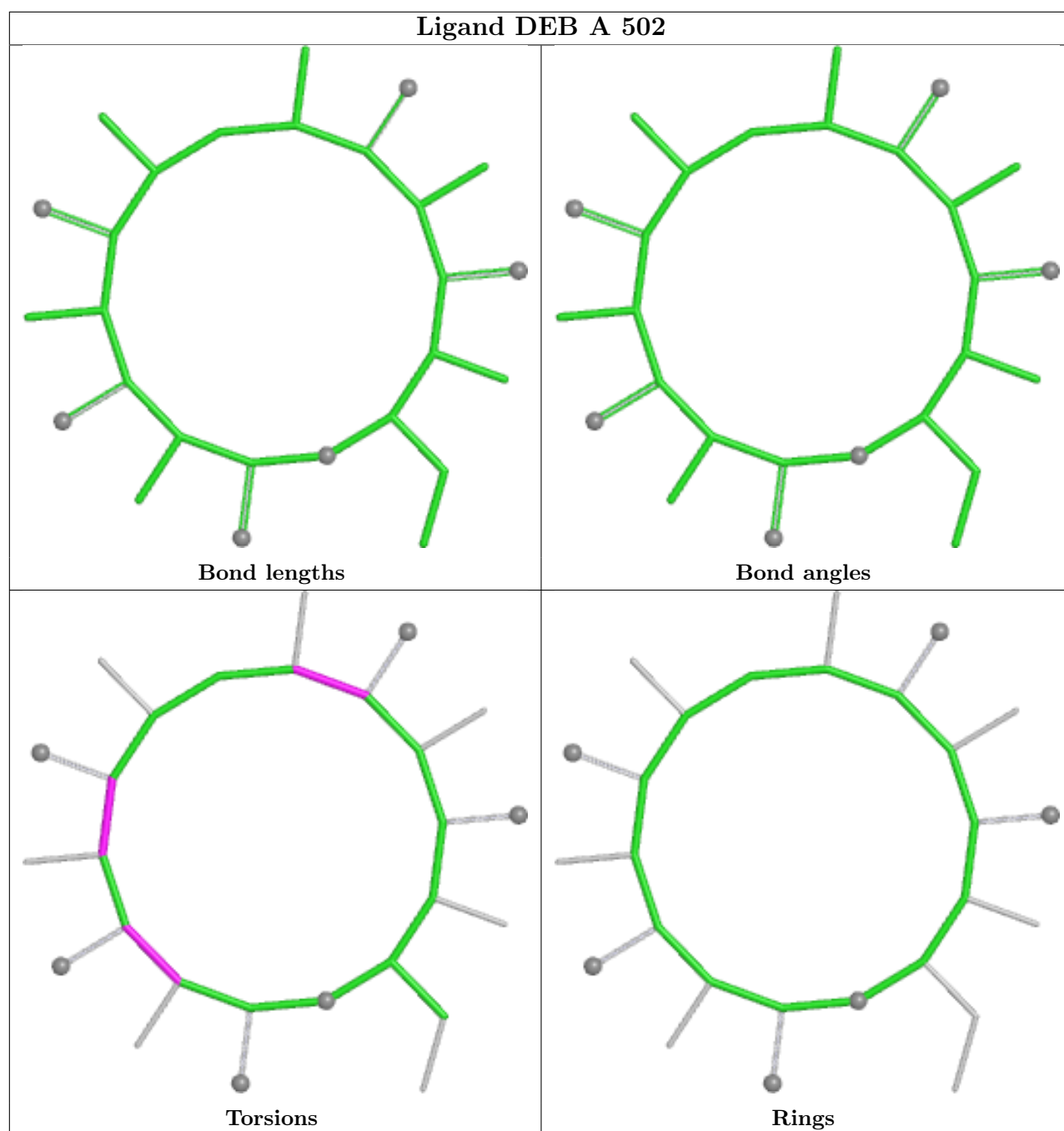


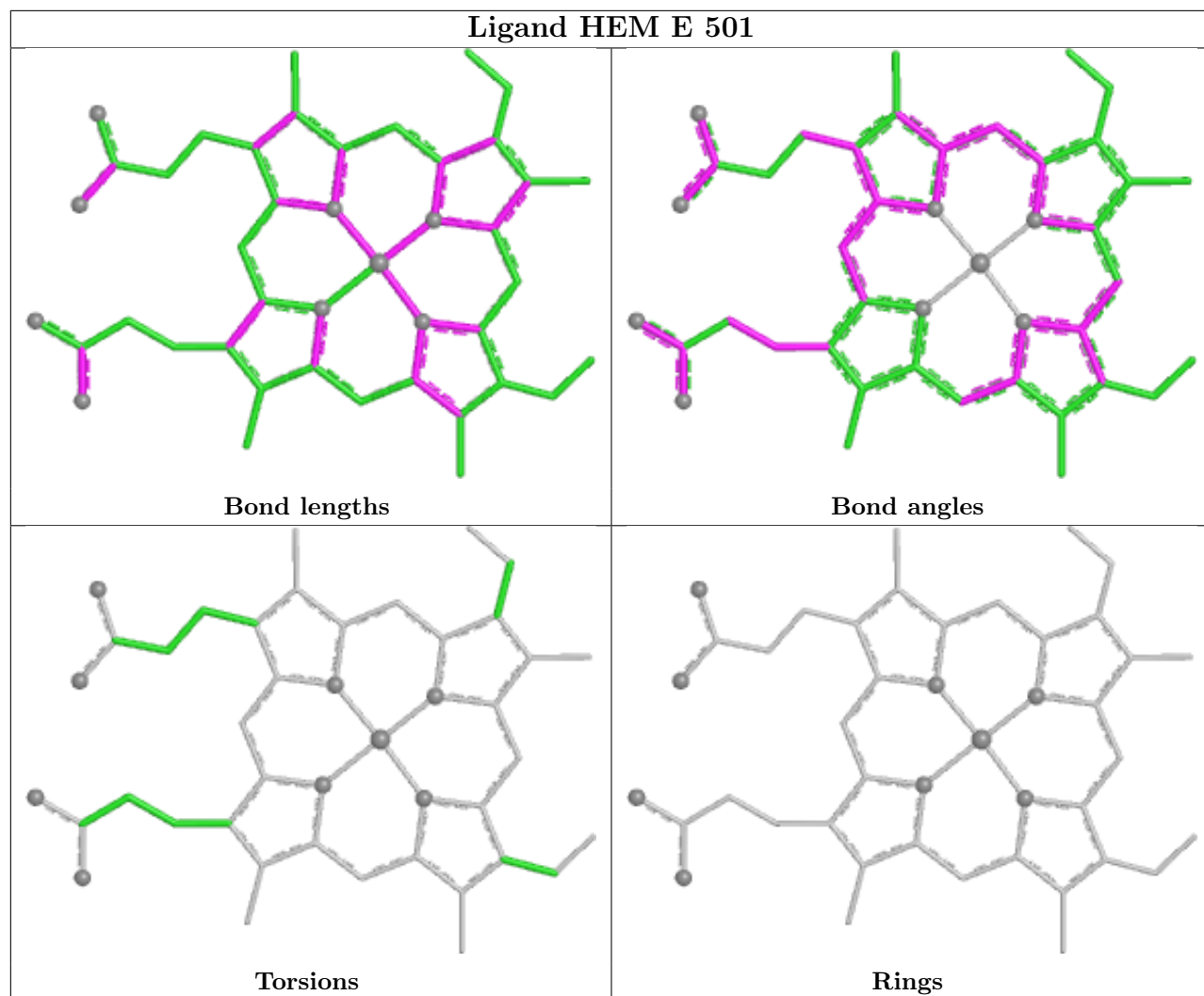


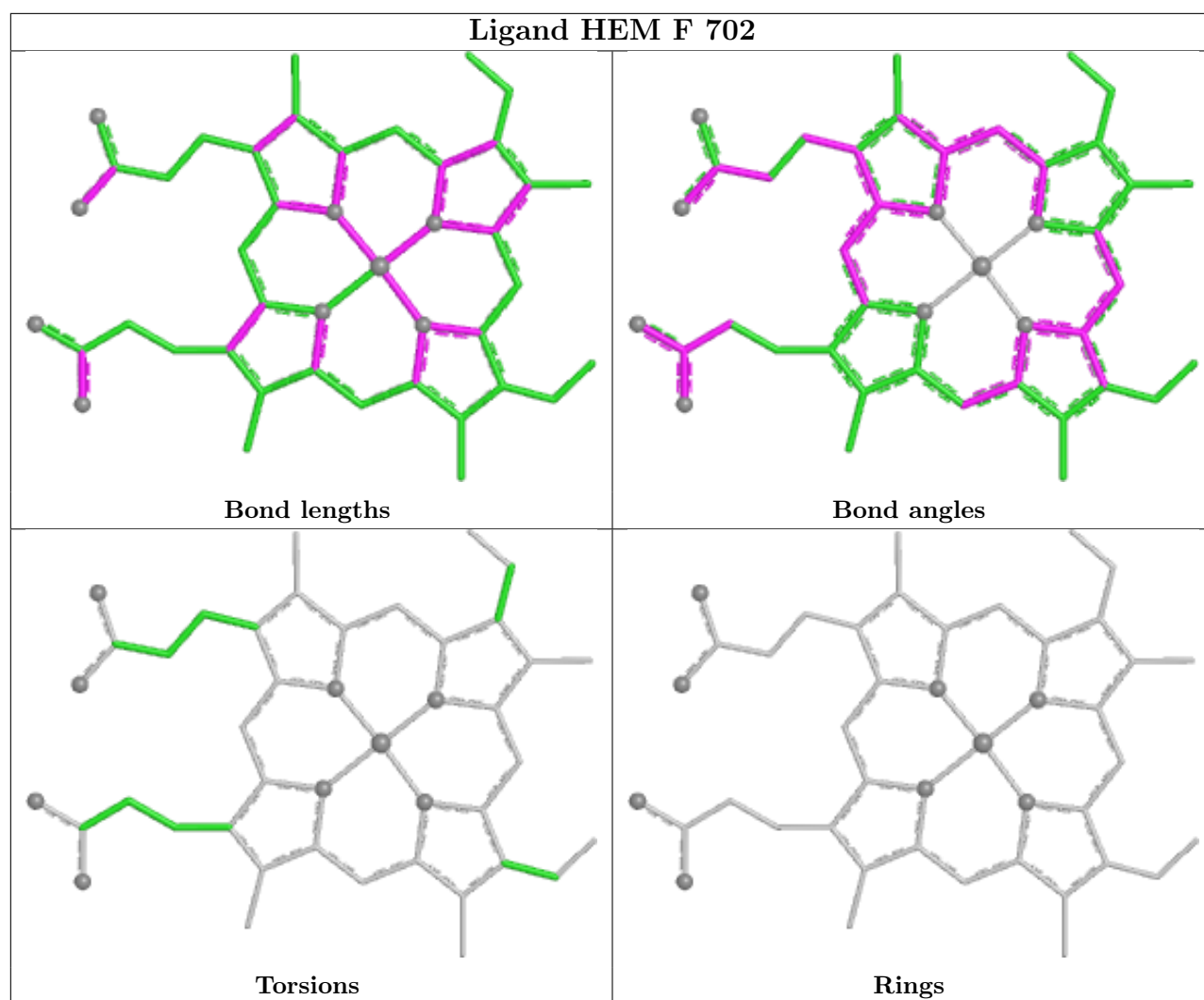


Ligand DEB F 703









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/407 (97%)	-0.09	6 (1%) 72 74	21, 48, 72, 134	60 (15%)
1	B	403/407 (99%)	-0.10	10 (2%) 58 61	22, 47, 72, 134	38 (9%)
1	C	397/407 (97%)	-0.35	1 (0%) 90 91	19, 42, 58, 90	40 (10%)
1	D	396/407 (97%)	0.34	11 (2%) 55 57	23, 61, 84, 119	53 (13%)
1	E	395/407 (97%)	0.21	8 (2%) 65 67	28, 59, 83, 145	42 (10%)
1	F	397/407 (97%)	0.44	14 (3%) 47 49	29, 63, 103, 115	48 (12%)
All	All	2385/2442 (97%)	0.07	50 (2%) 63 66	19, 53, 87, 145	281 (11%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	PRO	5.0
1	A	265[A]	LYS	5.0
1	F	21[A]	LEU	4.5
1	F	11	ALA	4.2
1	B	9	THR	4.0
1	B	7	GLY	3.8
1	B	210	ALA	3.6
1	B	5	HIS	3.6
1	B	6[A]	THR	3.5
1	E	13	ALA	3.4
1	E	211	PRO	3.3
1	D	208[A]	ARG	3.2
1	A	11	ALA	3.2
1	E	231[A]	LYS	3.1
1	E	312[A]	ARG	3.0
1	A	110[A]	LYS	3.0
1	C	11	ALA	3.0
1	B	11	ALA	2.9
1	E	210	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	12[A]	ASP	2.9
1	D	228[A]	HIS	2.9
1	F	123[A]	ARG	2.7
1	F	183[A]	ARG	2.6
1	F	270[A]	LEU	2.6
1	F	390[A]	LYS	2.5
1	D	229[A]	LEU	2.5
1	D	333[A]	HIS	2.4
1	F	126	SER	2.4
1	F	386	VAL	2.4
1	A	228	HIS	2.3
1	D	225	ASN	2.3
1	D	343[A]	ARG	2.3
1	F	276	LEU	2.3
1	D	110[A]	LYS	2.2
1	A	208	ARG	2.2
1	B	10	PRO	2.2
1	F	375[A]	ARG	2.2
1	F	407	TRP	2.2
1	E	212	THR	2.2
1	F	405	VAL	2.2
1	D	191	ARG	2.1
1	E	221[A]	LEU	2.1
1	F	343[A]	ARG	2.1
1	A	272	ALA	2.1
1	B	110[A]	LYS	2.1
1	E	14	VAL	2.1
1	D	16	ALA	2.1
1	D	265[A]	LYS	2.1
1	F	265[A]	LYS	2.0
1	D	222	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
6	FMT	A	525	3/3	0.46	0.11	103,103,110,111	0
6	FMT	C	562	3/3	0.47	0.10	102,102,102,103	0
6	FMT	B	563	3/3	0.49	0.12	102,102,103,103	0
6	FMT	C	546	3/3	0.51	0.10	103,103,106,111	0
6	FMT	D	513	3/3	0.51	0.12	103,103,106,106	0
6	FMT	C	552	3/3	0.53	0.12	107,107,108,110	0
6	FMT	C	549	3/3	0.57	0.09	99,99,106,106	0
6	FMT	A	521	3/3	0.57	0.10	102,102,102,107	0
6	FMT	A	534	3/3	0.60	0.12	86,86,90,93	0
6	FMT	C	540	3/3	0.62	0.10	112,112,117,119	0
6	FMT	A	517	3/3	0.64	0.08	105,105,106,107	0
6	FMT	E	511	3/3	0.66	0.09	108,108,112,113	0
6	FMT	B	530	3/3	0.68	0.12	92,92,97,99	0
6	FMT	B	561	3/3	0.70	0.09	109,109,110,113	0
6	FMT	D	506	3/3	0.70	0.13	104,104,107,110	0
6	FMT	A	516	3/3	0.70	0.15	88,88,90,91	0
6	FMT	B	558	3/3	0.70	0.10	100,100,105,105	0
6	FMT	F	709	3/3	0.71	0.13	84,84,90,90	0
6	FMT	C	545	3/3	0.72	0.09	99,99,103,104	0
4	RAM	C	504	11/11	0.73	0.15	71,78,83,84	11
6	FMT	A	527	3/3	0.73	0.09	97,97,99,101	0
6	FMT	E	508	3/3	0.73	0.08	89,89,94,97	0
6	FMT	B	536	3/3	0.73	0.14	97,97,107,107	0
6	FMT	A	530	3/3	0.73	0.11	103,103,105,108	0
6	FMT	F	711	3/3	0.73	0.13	110,110,112,116	0
6	FMT	A	524	3/3	0.74	0.12	95,95,101,101	0
6	FMT	C	551	3/3	0.75	0.11	101,101,103,103	0
6	FMT	A	526	3/3	0.75	0.10	100,100,103,106	0
6	FMT	B	566	3/3	0.75	0.11	97,97,104,104	0
6	FMT	B	546	3/3	0.77	0.13	86,86,89,94	0
6	FMT	B	549	3/3	0.77	0.11	103,103,104,106	0
6	FMT	C	550	3/3	0.77	0.19	82,82,90,90	0
6	FMT	B	545	3/3	0.78	0.09	101,101,102,102	0
6	FMT	D	515	3/3	0.78	0.11	98,98,101,102	0
6	FMT	A	532	3/3	0.79	0.28	100,100,110,116	0
6	FMT	B	540	3/3	0.79	0.20	76,76,84,87	0
6	FMT	C	547	3/3	0.79	0.15	77,77,95,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	RAM	F	701	11/11	0.79	0.17	103,111,117,120	0
6	FMT	A	506	3/3	0.79	0.18	76,76,86,88	0
6	FMT	C	537	3/3	0.79	0.18	76,76,85,88	0
6	FMT	B	532	3/3	0.79	0.14	87,87,95,97	0
6	FMT	C	560	3/3	0.79	0.19	88,88,89,95	0
6	FMT	F	716	3/3	0.79	0.12	98,98,104,107	0
6	FMT	C	530	3/3	0.80	0.20	81,81,82,88	0
6	FMT	C	533	3/3	0.80	0.14	85,85,90,91	0
6	FMT	B	537	3/3	0.80	0.09	90,90,93,96	0
8	GOL	B	505	6/6	0.80	0.19	100,102,106,107	0
6	FMT	B	557	3/3	0.81	0.14	102,102,102,108	0
4	RAM	B	503[A]	11/11	0.81	0.28	43,50,55,58	11
6	FMT	A	515	3/3	0.81	0.24	59,59,74,83	0
6	FMT	D	511	3/3	0.82	0.14	90,90,96,99	0
6	FMT	A	505	3/3	0.82	0.17	77,77,79,82	0
6	FMT	A	540	3/3	0.82	0.20	86,86,86,94	0
6	FMT	E	507	3/3	0.82	0.23	83,83,86,89	0
6	FMT	A	541	3/3	0.82	0.15	83,83,85,92	0
6	FMT	B	518	3/3	0.82	0.21	81,81,81,88	0
6	FMT	C	554	3/3	0.82	0.24	110,110,114,116	0
6	FMT	B	555	3/3	0.82	0.11	103,103,104,109	0
6	FMT	C	517	3/3	0.82	0.22	75,75,77,84	0
6	FMT	F	717	3/3	0.82	0.10	91,91,100,100	0
6	FMT	F	718	3/3	0.82	0.15	75,75,80,85	0
6	FMT	C	523	3/3	0.82	0.18	84,84,87,95	0
8	GOL	C	507	6/6	0.82	0.25	78,82,88,89	0
6	FMT	A	538	3/3	0.83	0.18	68,68,73,82	0
6	FMT	B	522	3/3	0.83	0.14	74,74,83,84	0
6	FMT	B	542	3/3	0.83	0.09	86,86,88,92	0
6	FMT	C	563	3/3	0.83	0.24	75,75,78,86	0
6	FMT	F	719	3/3	0.83	0.17	95,95,101,102	0
6	FMT	B	533	3/3	0.83	0.13	93,93,94,104	0
6	FMT	B	527	3/3	0.83	0.07	88,88,92,98	0
6	FMT	D	519	3/3	0.84	0.10	89,89,95,98	0
6	FMT	B	508	3/3	0.84	0.13	49,49,65,73	0
6	FMT	A	537	3/3	0.84	0.14	87,87,89,96	0
6	FMT	E	509	3/3	0.84	0.12	88,88,94,95	0
6	FMT	C	544	3/3	0.84	0.15	72,72,78,81	0
6	FMT	F	707	3/3	0.84	0.16	79,79,89,90	0
6	FMT	B	554	3/3	0.84	0.09	96,96,101,103	0
6	FMT	C	510	3/3	0.84	0.14	61,61,82,86	0
6	FMT	F	712	3/3	0.84	0.14	86,86,90,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FMT	F	713	3/3	0.84	0.17	91,91,94,100	0
6	FMT	C	564	3/3	0.84	0.20	92,92,92,97	0
4	RAM	A	503[A]	11/11	0.84	0.24	64,76,87,88	11
6	FMT	B	524	3/3	0.84	0.13	84,84,86,91	0
6	FMT	B	535	3/3	0.84	0.13	75,75,86,89	0
6	FMT	B	560	3/3	0.84	0.15	91,91,91,95	0
6	FMT	D	516	3/3	0.84	0.20	92,92,99,100	0
6	FMT	A	544	3/3	0.85	0.11	88,88,93,93	0
6	FMT	C	565	3/3	0.85	0.23	68,68,74,77	0
6	FMT	A	522	3/3	0.85	0.26	69,69,71,80	0
6	FMT	C	532	3/3	0.85	0.11	89,89,100,100	0
6	FMT	D	512	3/3	0.85	0.12	95,95,103,105	0
4	RAM	C	503[A]	11/11	0.85	0.26	46,56,62,66	11
6	FMT	B	534	3/3	0.85	0.11	75,75,83,87	0
6	FMT	B	552	3/3	0.85	0.18	89,89,95,98	0
6	FMT	B	543	3/3	0.86	0.14	81,81,86,87	0
6	FMT	B	531	3/3	0.86	0.15	92,92,97,103	0
6	FMT	B	513	3/3	0.86	0.22	78,78,89,96	0
6	FMT	A	535	3/3	0.86	0.15	90,90,92,98	0
6	FMT	C	518	3/3	0.86	0.16	53,53,68,76	0
6	FMT	C	553	3/3	0.86	0.17	89,89,90,95	0
6	FMT	B	521	3/3	0.86	0.11	79,79,80,84	0
6	FMT	C	528	3/3	0.86	0.12	60,60,65,84	0
4	RAM	D	503	11/11	0.86	0.21	66,71,75,75	11
6	FMT	A	509	3/3	0.86	0.21	74,74,74,85	0
6	FMT	B	556	3/3	0.86	0.27	88,88,94,98	0
6	FMT	B	526	3/3	0.86	0.13	90,90,94,95	0
6	FMT	F	715	3/3	0.86	0.26	74,74,78,90	0
6	FMT	A	539	3/3	0.86	0.16	106,106,107,109	0
6	FMT	D	510	3/3	0.86	0.16	85,85,91,92	0
6	FMT	B	541	3/3	0.86	0.18	62,62,76,80	0
6	FMT	B	509	3/3	0.86	0.24	69,69,74,80	0
6	FMT	B	562	3/3	0.86	0.14	74,74,87,90	0
6	FMT	D	514	3/3	0.86	0.18	83,83,91,92	0
6	FMT	D	507	3/3	0.87	0.16	88,88,89,93	0
6	FMT	E	512	3/3	0.87	0.19	78,78,80,92	0
6	FMT	B	559	3/3	0.87	0.24	111,111,121,121	0
6	FMT	C	514	3/3	0.87	0.18	81,81,86,87	0
6	FMT	C	538	3/3	0.87	0.12	85,85,85,95	0
6	FMT	A	531	3/3	0.87	0.18	79,79,80,81	0
6	FMT	B	539	3/3	0.87	0.12	83,83,89,91	0
6	FMT	C	561	3/3	0.87	0.14	80,80,101,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FMT	C	521	3/3	0.87	0.14	50,50,67,73	0
6	FMT	D	518	3/3	0.87	0.22	77,77,80,81	0
6	FMT	A	507	3/3	0.87	0.17	71,71,72,73	0
6	FMT	B	525	3/3	0.87	0.16	77,77,82,83	0
5	TRS	B	504	8/8	0.87	0.14	77,85,93,93	0
6	FMT	C	509	3/3	0.87	0.20	76,76,79,83	0
6	FMT	B	548	3/3	0.88	0.22	65,65,85,87	0
6	FMT	B	529	3/3	0.88	0.14	106,106,107,108	0
4	RAM	E	503[A]	11/11	0.88	0.22	71,82,87,87	11
6	FMT	A	533	3/3	0.88	0.15	95,95,96,98	0
6	FMT	B	528	3/3	0.88	0.15	84,84,86,93	0
6	FMT	F	706	3/3	0.88	0.20	65,65,77,78	0
5	TRS	A	504	8/8	0.89	0.14	111,118,119,121	0
6	FMT	B	510	3/3	0.89	0.18	85,85,89,92	0
6	FMT	C	522	3/3	0.89	0.14	82,82,83,83	0
6	FMT	C	543	3/3	0.89	0.13	83,83,86,92	0
6	FMT	C	555[B]	3/3	0.89	0.19	26,26,30,33	3
6	FMT	C	558	3/3	0.89	0.21	57,57,66,79	0
6	FMT	B	553	3/3	0.89	0.13	72,72,84,88	0
6	FMT	A	514	3/3	0.89	0.12	60,60,60,65	0
6	FMT	C	511	3/3	0.89	0.12	82,82,87,88	0
6	FMT	C	531	3/3	0.89	0.14	76,76,88,91	0
6	FMT	B	514	3/3	0.89	0.14	81,81,89,89	0
6	FMT	B	517	3/3	0.89	0.12	74,74,80,80	0
6	FMT	D	504	3/3	0.89	0.18	90,90,94,95	0
6	FMT	D	505	3/3	0.89	0.14	84,84,84,86	0
8	GOL	C	506	6/6	0.89	0.18	86,90,99,102	0
6	FMT	E	510	3/3	0.89	0.09	76,76,84,87	0
6	FMT	C	527	3/3	0.90	0.13	78,78,81,89	0
6	FMT	C	508	3/3	0.90	0.18	79,79,83,88	0
6	FMT	A	523	3/3	0.90	0.19	75,75,81,86	0
6	FMT	C	539	3/3	0.90	0.18	81,81,82,89	0
6	FMT	C	548	3/3	0.90	0.12	63,63,76,78	0
6	FMT	C	515	3/3	0.90	0.10	90,90,92,94	0
6	FMT	D	517	3/3	0.90	0.06	94,94,96,104	0
6	FMT	C	542	3/3	0.90	0.19	94,94,100,102	0
6	FMT	B	568	3/3	0.90	0.18	80,80,85,100	0
6	FMT	E	505	3/3	0.90	0.11	84,84,88,92	0
6	FMT	B	565	3/3	0.91	0.15	85,85,88,92	0
6	FMT	B	512	3/3	0.91	0.19	58,58,72,79	0
6	FMT	B	520	3/3	0.91	0.12	82,82,86,86	0
6	FMT	B	550	3/3	0.91	0.13	82,82,86,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FMT	B	551	3/3	0.91	0.14	73,73,80,82	0
6	FMT	A	518	3/3	0.91	0.13	88,88,94,96	0
6	FMT	B	544	3/3	0.91	0.09	95,95,99,101	0
6	FMT	E	513	3/3	0.91	0.09	86,86,93,95	0
6	FMT	C	512	3/3	0.91	0.11	88,88,93,99	0
6	FMT	A	543	3/3	0.91	0.15	96,96,96,96	0
5	TRS	F	705	8/8	0.91	0.14	50,57,61,62	0
6	FMT	A	536	3/3	0.92	0.17	76,76,81,88	0
6	FMT	A	519	3/3	0.92	0.14	87,87,89,94	0
6	FMT	C	541	3/3	0.92	0.18	69,69,73,77	0
6	FMT	A	545[B]	3/3	0.92	0.18	30,30,37,43	3
6	FMT	C	526	3/3	0.92	0.13	56,56,59,62	0
6	FMT	C	534	3/3	0.92	0.12	69,69,85,86	0
6	FMT	C	535	3/3	0.92	0.15	64,64,77,77	0
6	FMT	B	507	3/3	0.92	0.13	87,87,88,88	0
6	FMT	C	556	3/3	0.92	0.14	66,66,79,82	0
6	FMT	A	528	3/3	0.92	0.18	81,81,99,99	0
6	FMT	E	504	3/3	0.92	0.14	66,66,70,74	0
8	GOL	F	704	6/6	0.92	0.14	74,84,85,94	0
6	FMT	A	529	3/3	0.93	0.14	75,75,77,84	0
6	FMT	A	508	3/3	0.93	0.13	59,59,74,79	0
6	FMT	B	515	3/3	0.93	0.19	73,73,74,82	0
6	FMT	B	564	3/3	0.93	0.12	113,113,115,115	0
6	FMT	D	508	3/3	0.93	0.16	58,58,59,63	0
6	FMT	C	516	3/3	0.93	0.14	68,68,74,75	0
6	FMT	B	538	3/3	0.93	0.23	74,74,77,82	0
6	FMT	F	708	3/3	0.93	0.12	74,74,77,78	0
6	FMT	C	536	3/3	0.93	0.16	77,77,83,86	0
6	FMT	F	710	3/3	0.93	0.12	77,77,80,86	0
6	FMT	B	547	3/3	0.93	0.12	72,72,84,91	0
6	FMT	C	519	3/3	0.93	0.15	71,71,77,78	0
6	FMT	C	520	3/3	0.93	0.10	82,82,84,88	0
6	FMT	F	714	3/3	0.93	0.12	92,92,94,97	0
6	FMT	B	567	3/3	0.93	0.18	64,64,73,74	0
6	FMT	C	559	3/3	0.93	0.13	80,80,81,88	0
6	FMT	B	516	3/3	0.93	0.12	87,87,89,90	0
6	FMT	B	569	3/3	0.93	0.10	81,81,85,86	0
6	FMT	B	511	3/3	0.93	0.14	74,74,79,87	0
6	FMT	A	510	3/3	0.93	0.12	84,84,86,88	0
6	FMT	E	506	3/3	0.93	0.15	58,58,62,70	3
6	FMT	B	519	3/3	0.93	0.12	62,62,72,73	0
6	FMT	C	529	3/3	0.93	0.11	78,78,88,89	0

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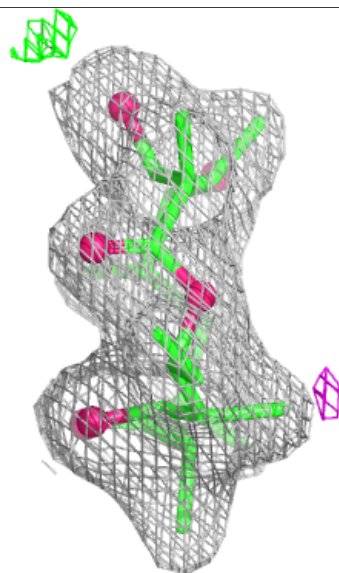
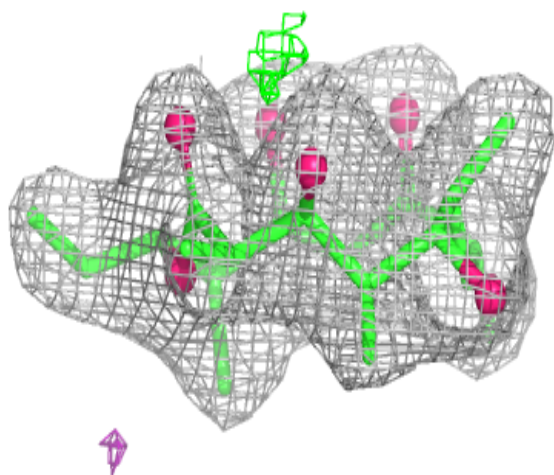
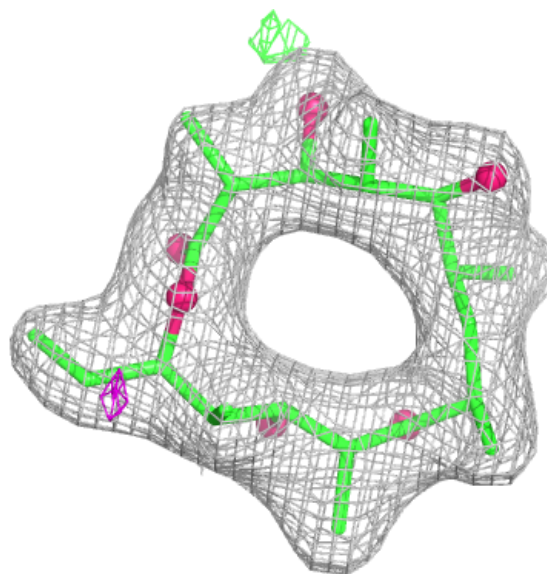
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FMT	A	520	3/3	0.94	0.12	78,78,79,83	0
8	GOL	B	506	6/6	0.94	0.10	76,81,89,96	0
6	FMT	A	542	3/3	0.94	0.26	49,49,60,77	0
7	NA	C	566	1/1	0.94	0.16	43,43,43,43	0
7	NA	E	515	1/1	0.94	0.30	63,63,63,63	0
6	FMT	C	513[B]	3/3	0.95	0.15	45,45,45,53	3
3	DEB	F	703	27/27	0.95	0.10	50,55,59,60	0
7	NA	B	570	1/1	0.95	0.16	53,53,53,53	0
6	FMT	A	511	3/3	0.95	0.14	68,68,80,87	0
7	NA	D	520	1/1	0.95	0.12	62,62,62,62	0
6	FMT	B	523	3/3	0.95	0.11	51,51,52,59	0
7	NA	F	720	1/1	0.95	0.08	56,56,56,56	0
6	FMT	C	524	3/3	0.95	0.10	75,75,77,82	0
6	FMT	E	514[B]	3/3	0.95	0.23	47,47,47,56	3
6	FMT	A	512	3/3	0.95	0.18	60,60,69,75	0
6	FMT	A	513	3/3	0.95	0.15	59,59,62,63	0
3	DEB	E	502	27/27	0.95	0.09	44,49,54,59	0
6	FMT	C	525	3/3	0.96	0.10	52,52,62,66	0
3	DEB	C	502	27/27	0.96	0.07	34,37,41,45	0
8	GOL	C	505	6/6	0.96	0.07	44,48,50,59	0
3	DEB	D	502	27/27	0.96	0.09	46,55,61,65	0
2	HEM	F	702	43/43	0.96	0.10	48,56,71,80	0
7	NA	A	547	1/1	0.96	0.27	66,66,66,66	0
6	FMT	D	509	3/3	0.97	0.09	68,68,71,76	0
3	DEB	A	502	27/27	0.97	0.06	36,42,48,49	0
6	FMT	C	557	3/3	0.97	0.07	48,48,53,53	0
3	DEB	B	502	27/27	0.97	0.07	36,39,45,46	0
2	HEM	A	501	43/43	0.98	0.06	32,36,42,51	0
2	HEM	B	501	43/43	0.98	0.07	32,35,38,49	0
2	HEM	C	501	43/43	0.98	0.06	30,33,37,43	0
2	HEM	D	501	43/43	0.98	0.07	38,43,53,58	0
2	HEM	E	501	43/43	0.98	0.07	39,44,50,55	0
7	NA	A	546	1/1	0.98	0.08	45,45,45,45	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.

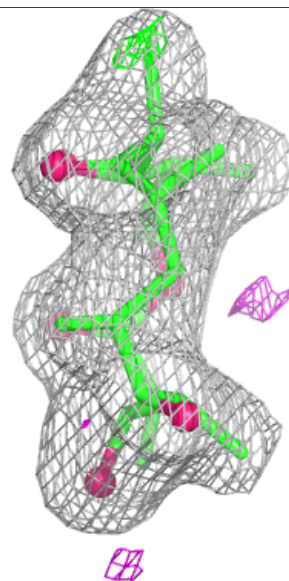
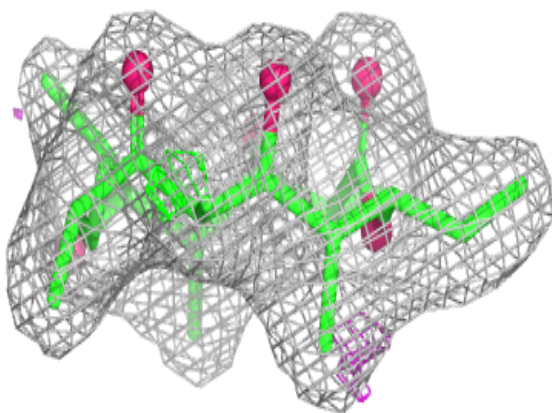
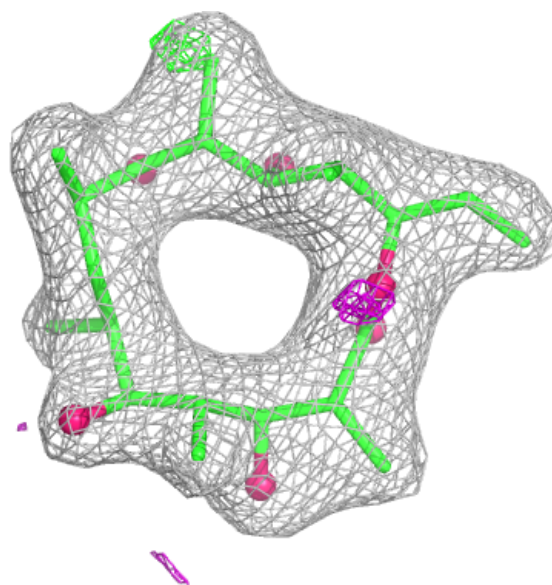
Electron density around DEB F 703:

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



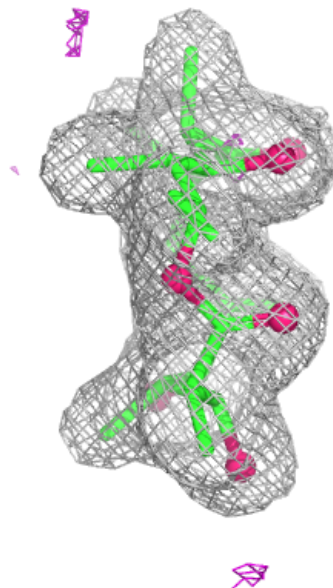
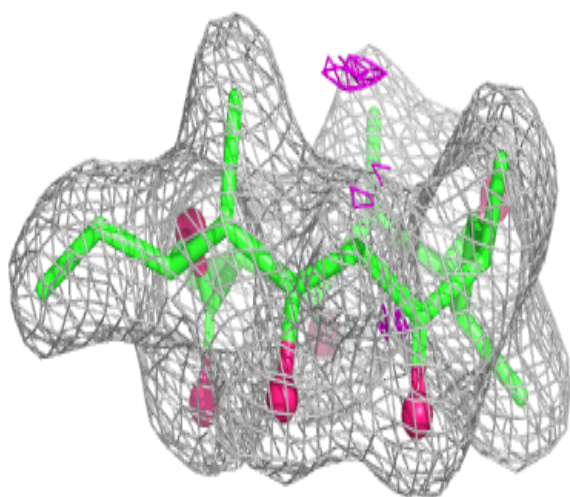
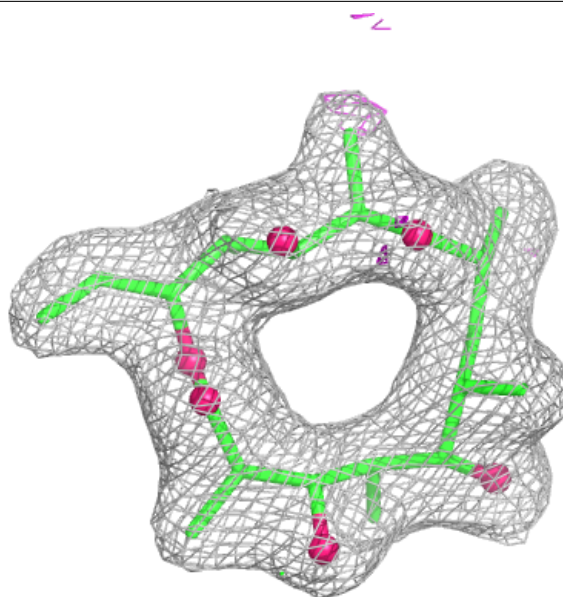
Electron density around DEB E 502:

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



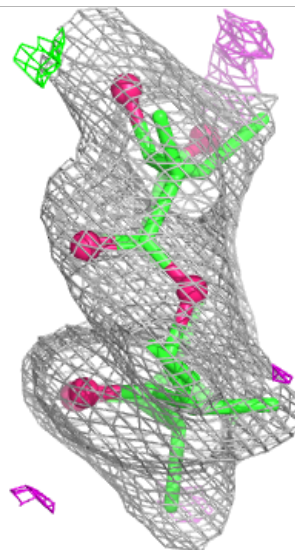
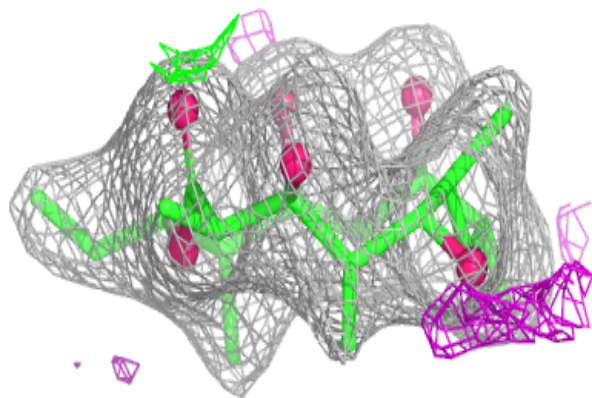
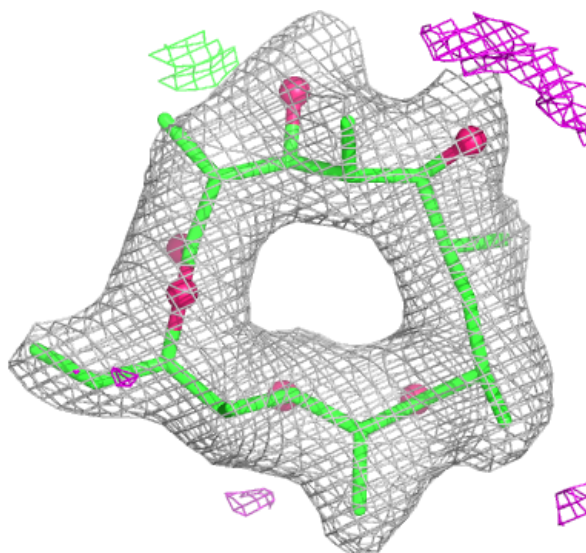
Electron density around DEB C 502:

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



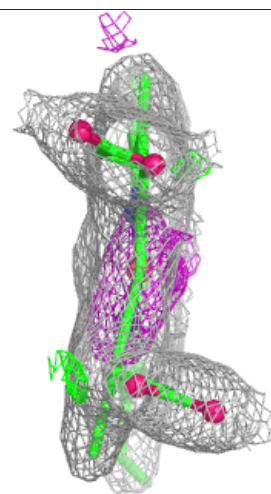
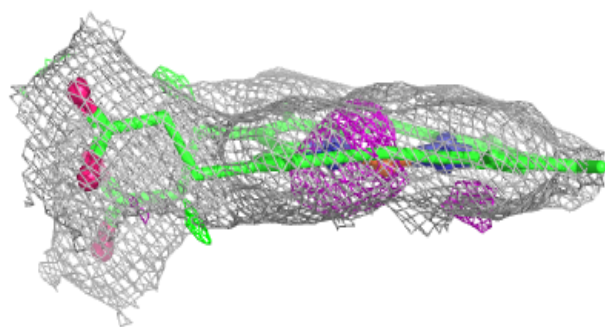
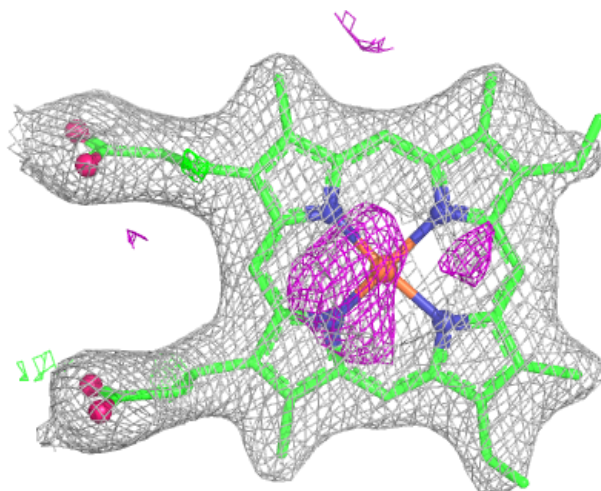
Electron density around DEB D 502:

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



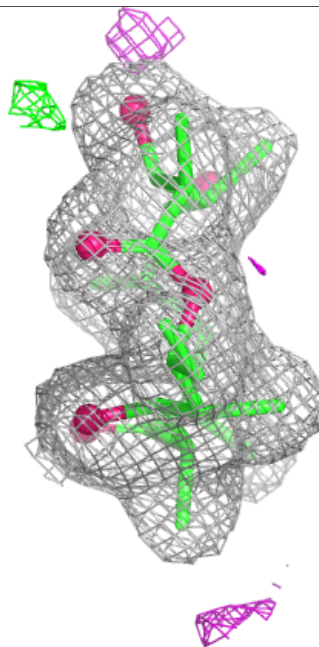
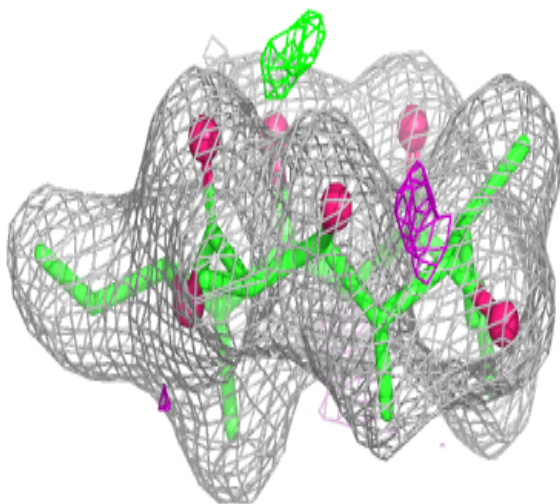
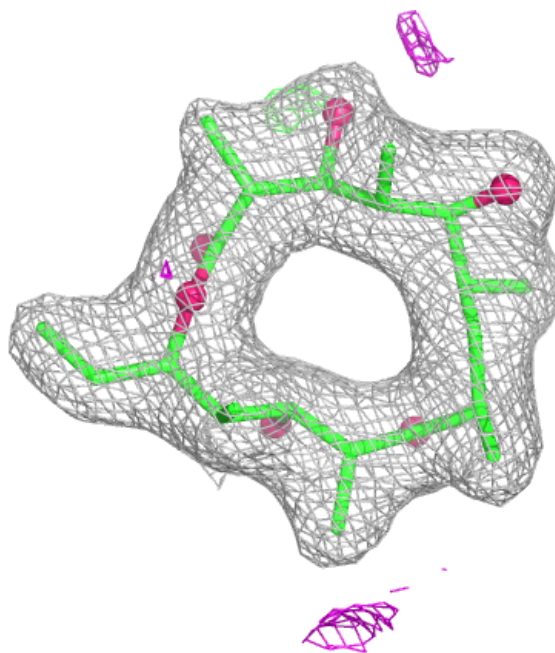
Electron density around HEM F 702:

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



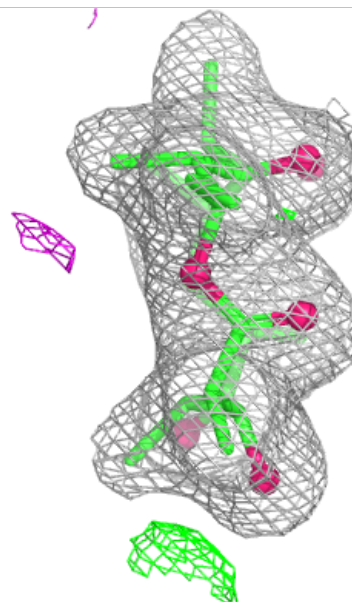
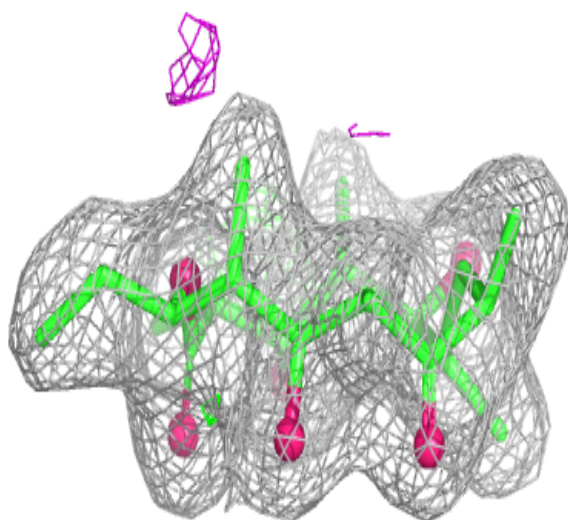
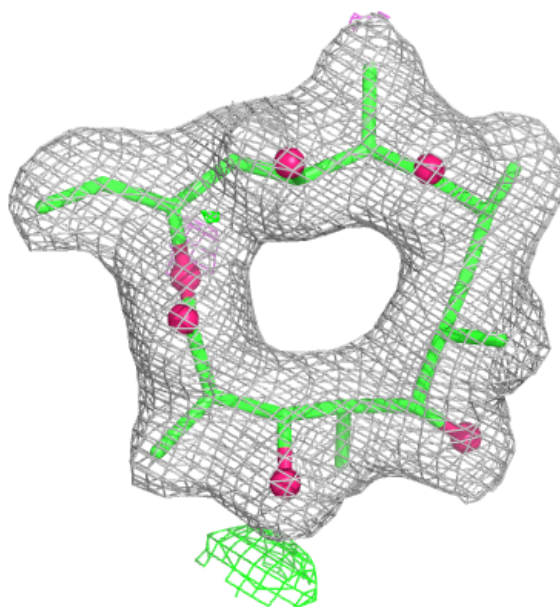
Electron density around DEB A 502:

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



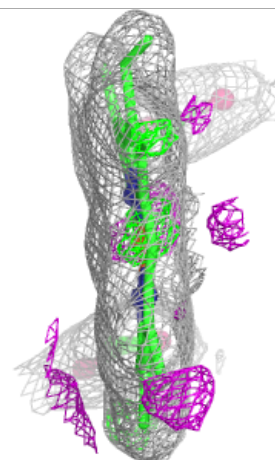
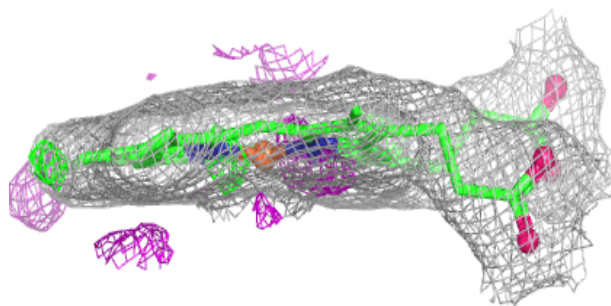
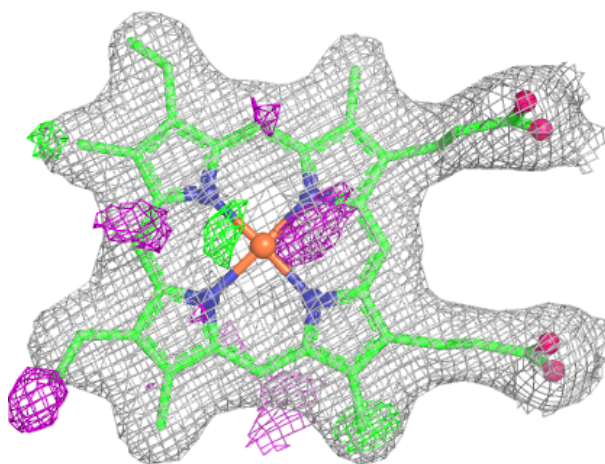
Electron density around DEB B 502:

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



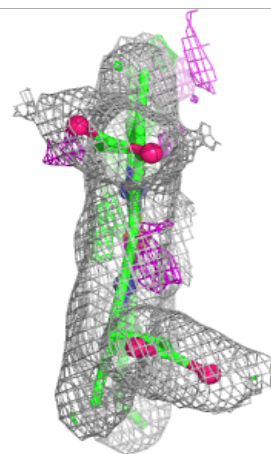
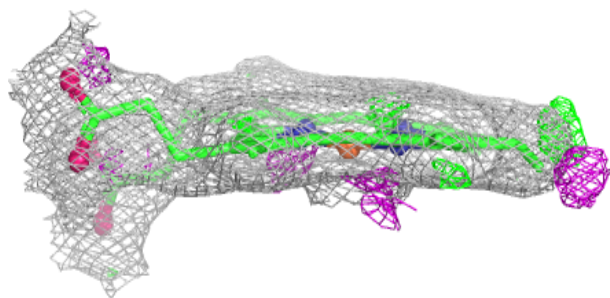
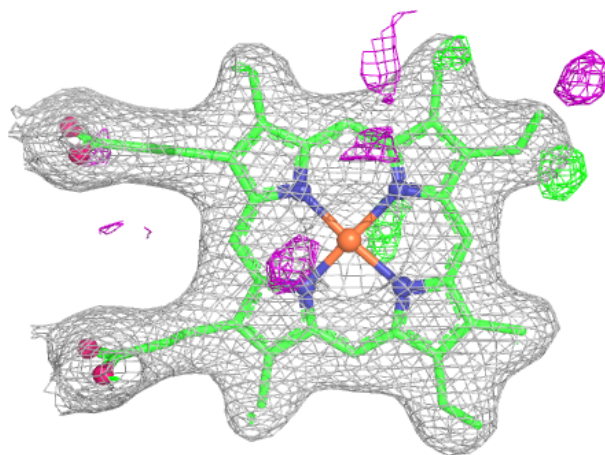
Electron density around HEM A 501:

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



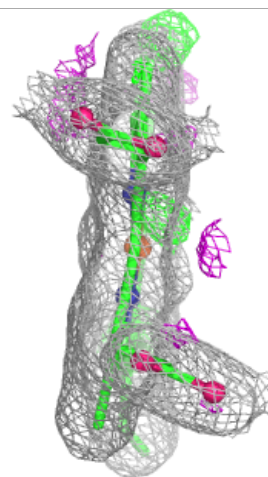
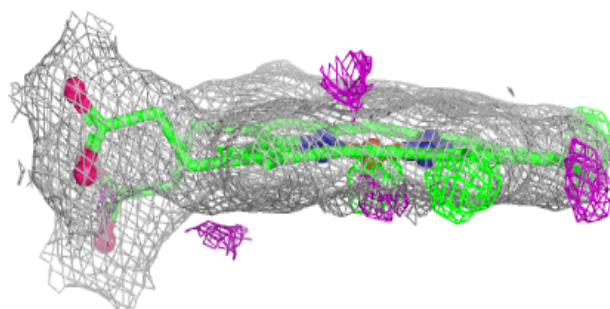
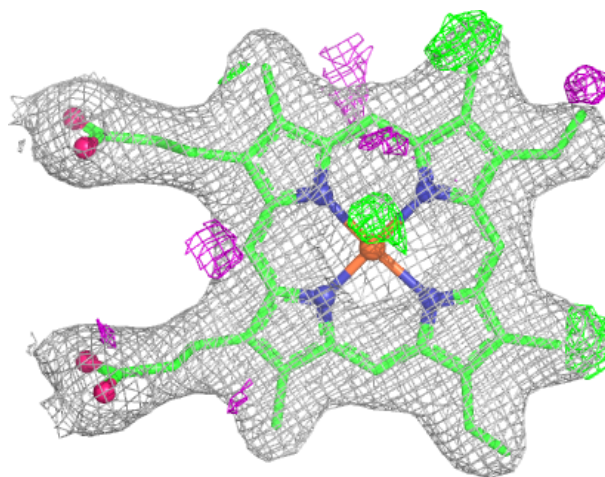
Electron density around HEM B 501:

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



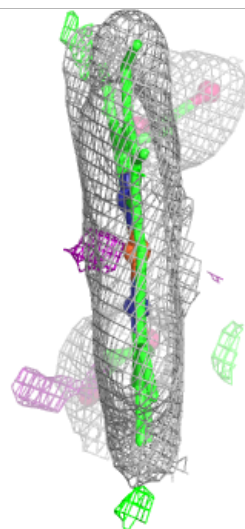
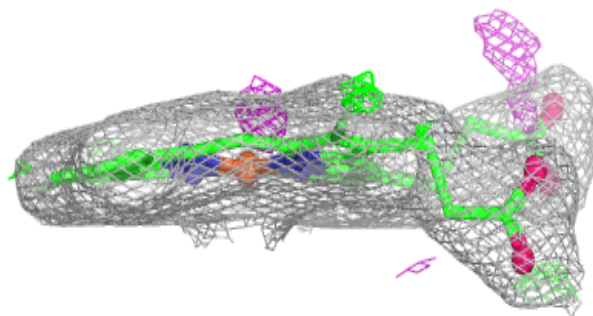
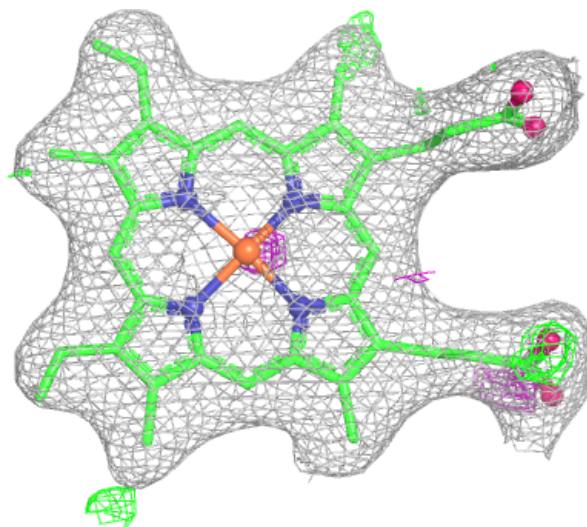
Electron density around HEM C 501:

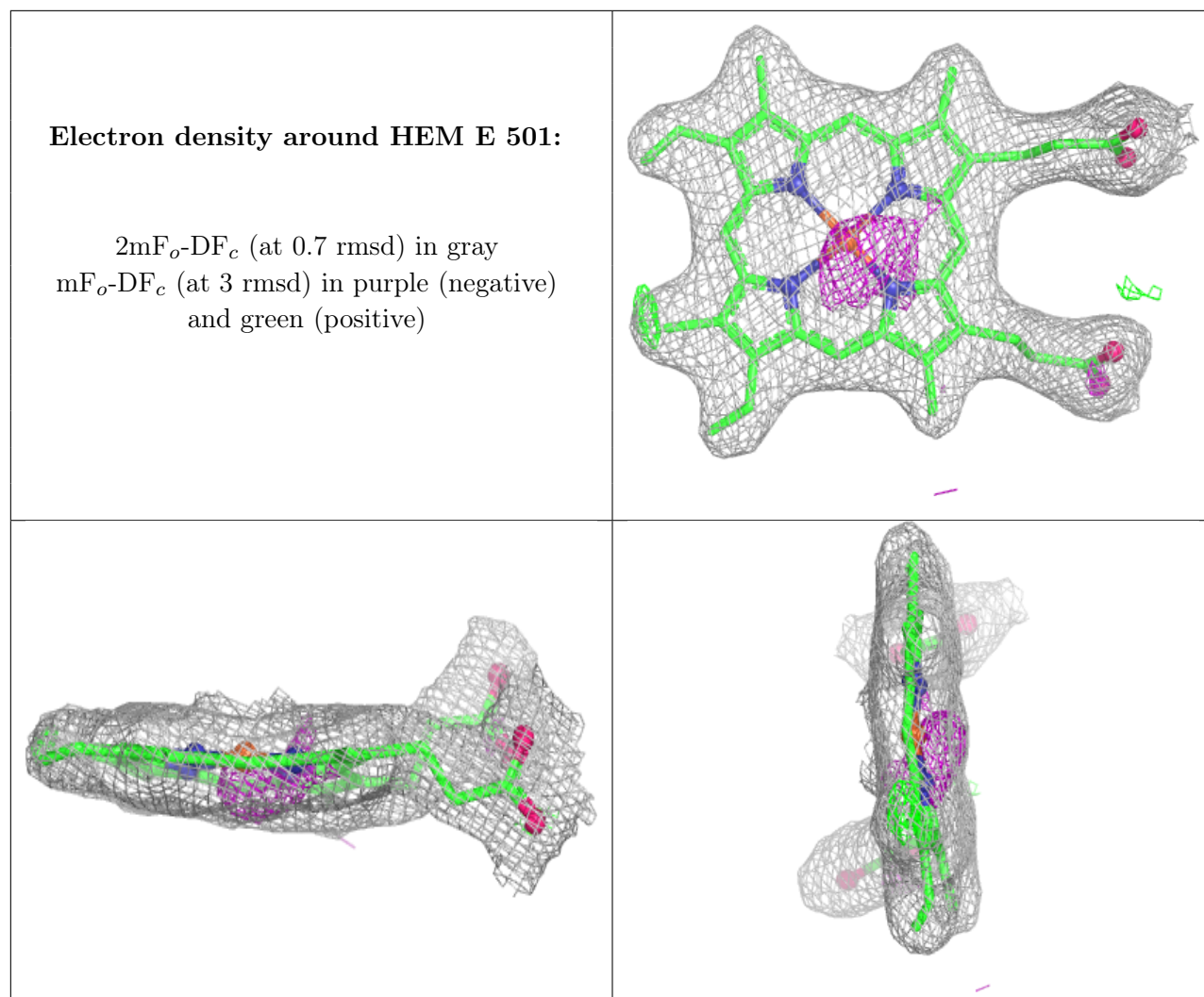
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.