



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:30 AM UTC

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

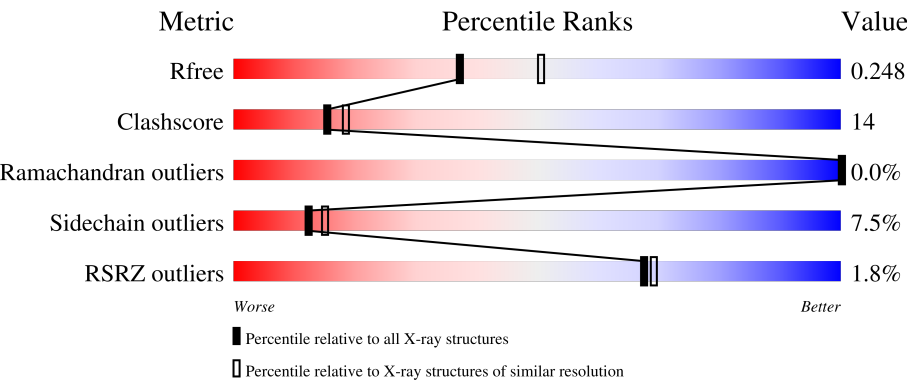
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.28 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	407	70%24% . .
1	B	407	% 75%19% . .
1	C	407	% 79%17% . .
1	D	407	2% 69%25% . .
1	E	407	% 70%24% . .

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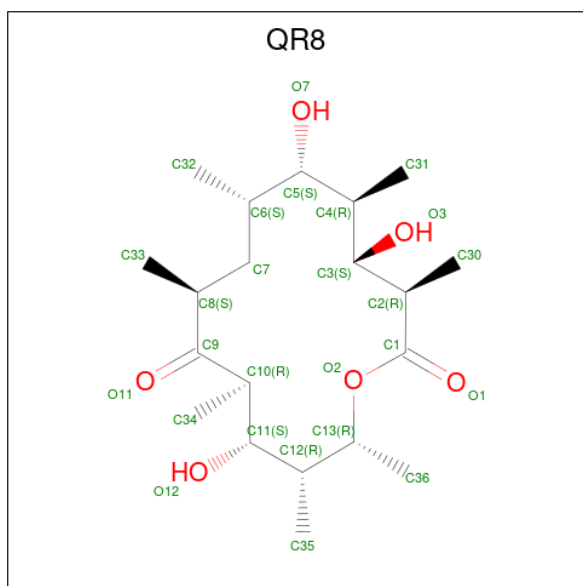
Mol	Chain	Length	Quality of chain
1	F	407	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	RAM	A	503[A]	-	-	X	-
4	RAM	A	503[B]	-	-	X	-
4	RAM	B	513	-	-	X	-
4	RAM	D	503	-	-	X	-
5	FMT	A	510	-	-	X	-
5	FMT	A	511	-	-	X	-
5	FMT	A	531	-	-	X	-
5	FMT	A	550	-	-	X	-
5	FMT	A	565	-	-	X	-
5	FMT	B	503	-	-	X	-
5	FMT	B	511	-	-	X	-
5	FMT	B	534	-	-	X	-
5	FMT	C	507	-	-	X	-
5	FMT	C	552	-	-	X	-
5	FMT	D	504	-	-	X	-
5	FMT	D	528	-	-	X	-
5	FMT	E	501	-	-	X	-
5	FMT	F	505	-	-	X	-
5	FMT	F	509	-	-	X	-
5	FMT	F	514	-	-	X	-

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

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



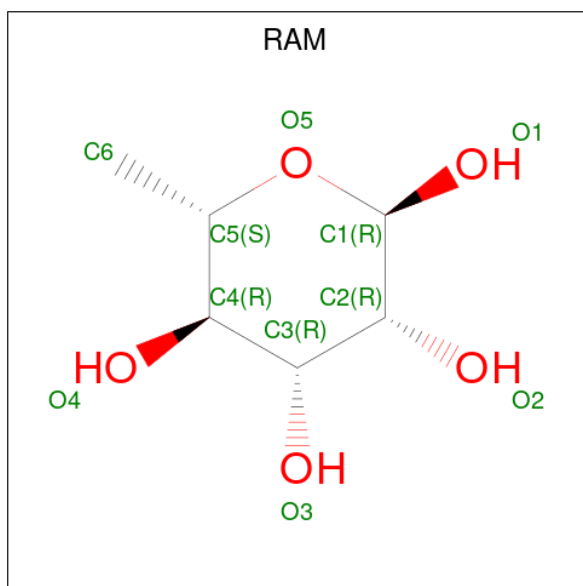
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			26	20	6		
3	B	1	Total	C	O	0	0
			26	20	6		
3	C	1	Total	C	O	0	0
			26	20	6		
3	D	1	Total	C	O	0	0
			26	20	6		
3	E	1	Total	C	O	0	0
			26	20	6		

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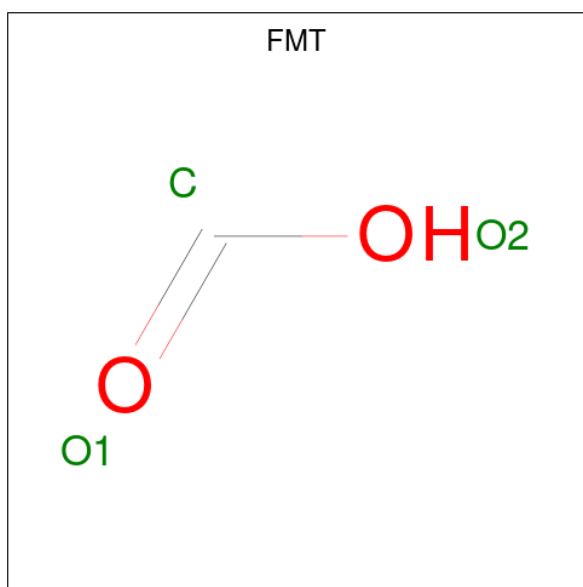
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			26	20	6		

- Molecule 4 is alpha-L-rhamnopyranose (CCD ID: RAM) (formula: $C_6H_{12}O_5$).



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

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

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

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

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

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

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

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

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

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

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

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

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

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

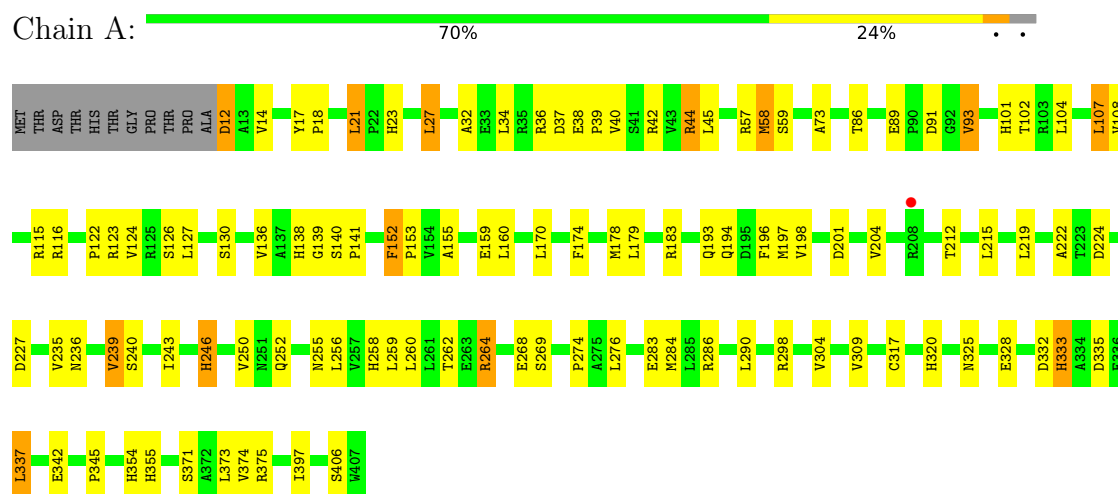
- Molecule 7 is water.

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

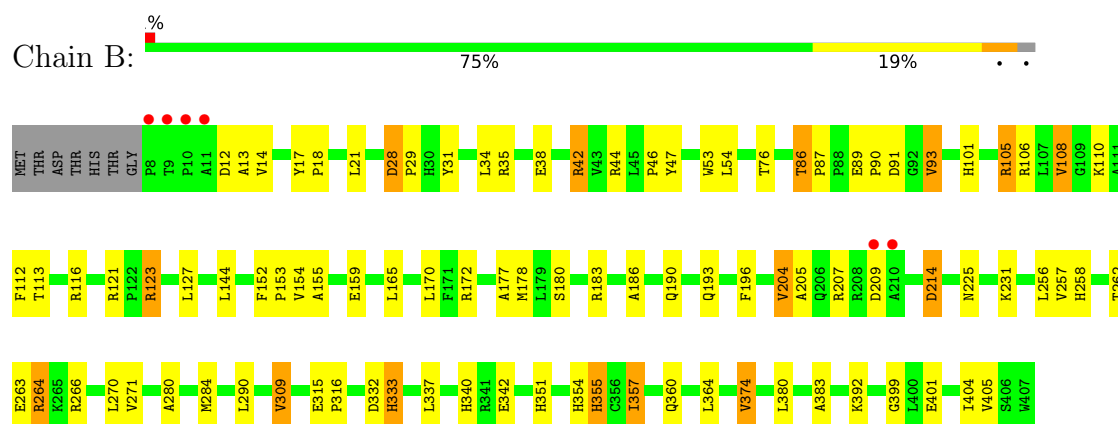
3 Residue-property plots

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

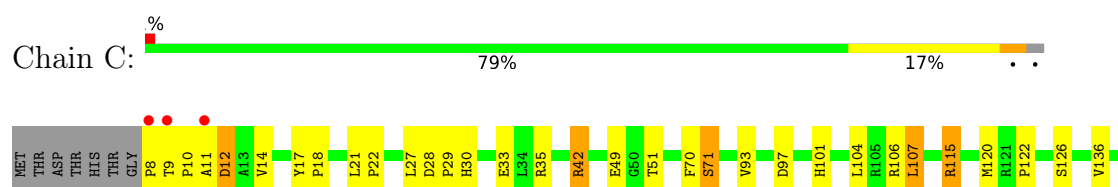
• Molecule 1: Cytochrome P-450

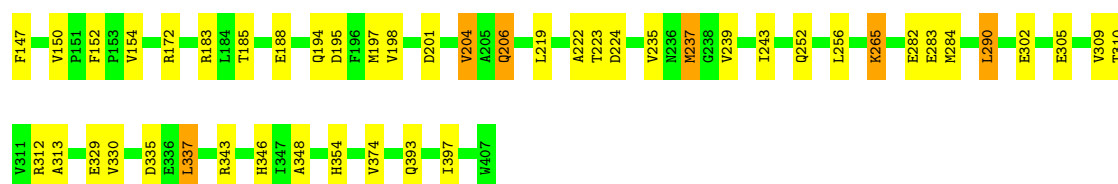


• Molecule 1: Cytochrome P-450

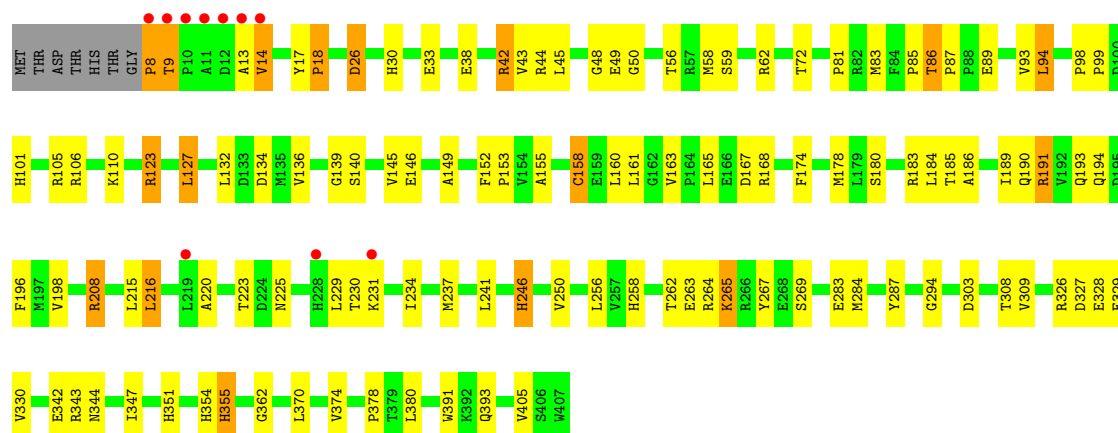


• Molecule 1: Cytochrome P-450

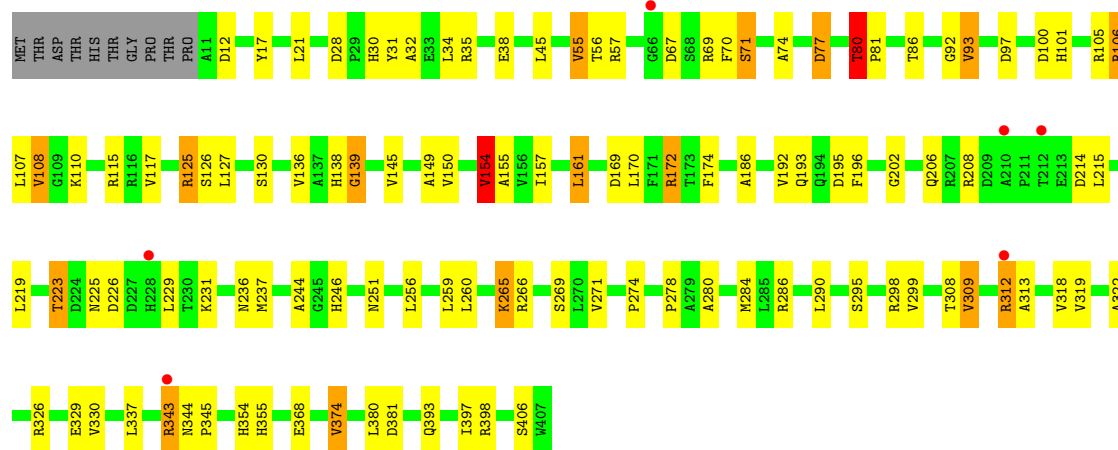




• Molecule 1: Cytochrome P-450

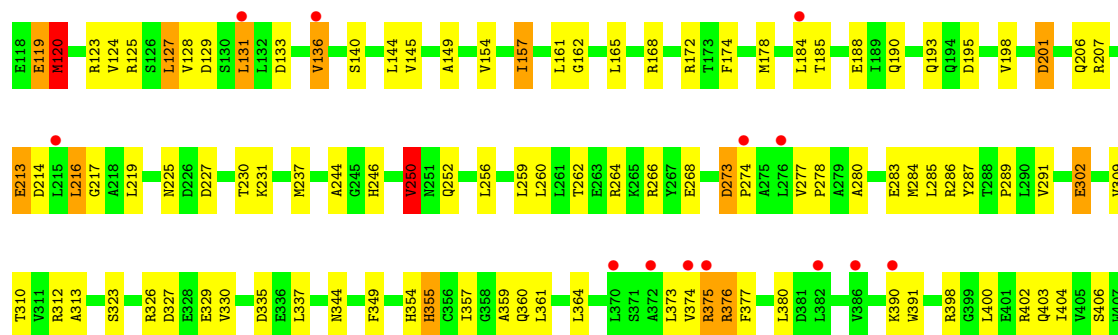


• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.53Å 110.68Å 159.28Å 90.00° 129.46° 90.00°	Depositor
Resolution (Å)	47.92 – 2.28 47.92 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.92-2.28) 99.9 (47.92-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.184 , 0.247 0.190 , 0.248	Depositor DCC
R_{free} test set	14058 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22307	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5720e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, RAM, HEM, QR8, FMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.23	8/3483 (0.2%)	1.50	15/4732 (0.3%)
1	B	1.26	11/3385 (0.3%)	1.51	14/4606 (0.3%)
1	C	1.28	12/3385 (0.4%)	1.49	9/4606 (0.2%)
1	D	1.23	5/3572 (0.1%)	1.51	22/4852 (0.5%)
1	E	1.19	1/3489 (0.0%)	1.52	23/4744 (0.5%)
1	F	1.31	6/3561 (0.2%)	1.70	34/4843 (0.7%)
All	All	1.25	43/20875 (0.2%)	1.54	117/28383 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	26[A]	ASP	CA-C	17.62	1.73	1.52
1	F	26[B]	ASP	CA-C	17.62	1.73	1.52
1	A	320	HIS	CE1-NE2	8.94	1.41	1.32
1	F	120[A]	MET	CA-C	7.65	1.63	1.52
1	F	120[B]	MET	CA-C	7.65	1.63	1.52
1	B	154	VAL	C-O	7.62	1.32	1.24
1	B	357	ILE	C-O	-7.25	1.15	1.24
1	B	31	TYR	C-O	7.12	1.32	1.24
1	C	237[A]	MET	C-O	-7.01	1.16	1.24
1	C	237[B]	MET	C-O	-7.01	1.16	1.24
1	C	239	VAL	C-O	6.97	1.32	1.24
1	C	222	ALA	C-O	-6.86	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	LEU	C-O	6.61	1.31	1.24
1	C	330	VAL	C-O	-6.43	1.17	1.23
1	E	202	GLY	C-O	6.39	1.31	1.23
1	D	355	HIS	CE1-NE2	6.30	1.38	1.32
1	A	130	SER	C-O	6.21	1.31	1.24
1	A	152	PHE	N-CA	6.04	1.50	1.46
1	F	230	THR	C-O	5.89	1.31	1.23
1	C	152	PHE	N-CA	5.88	1.50	1.46
1	A	317	CYS	C-O	5.66	1.30	1.23
1	C	71	SER	CA-CB	-5.65	1.45	1.53
1	A	73	ALA	C-O	5.59	1.31	1.24
1	B	196	PHE	C-O	5.55	1.30	1.24
1	D	158	CYS	C-O	5.51	1.30	1.24
1	B	355	HIS	C-O	-5.46	1.17	1.23
1	F	355	HIS	CE1-NE2	5.45	1.38	1.32
1	A	58	MET	C-O	5.42	1.30	1.24
1	B	34	LEU	C-O	5.37	1.30	1.24
1	B	405	VAL	C-O	5.36	1.29	1.24
1	C	42[A]	ARG	C-O	5.35	1.30	1.23
1	C	42[B]	ARG	C-O	5.35	1.30	1.23
1	D	246	HIS	CE1-NE2	5.33	1.37	1.32
1	D	72	THR	C-O	5.32	1.30	1.24
1	A	255	ASN	C-O	5.30	1.30	1.24
1	D	98	PRO	CA-C	5.29	1.54	1.51
1	C	243	ILE	C-O	5.29	1.29	1.24
1	B	205	ALA	C-O	5.29	1.30	1.24
1	A	12	ASP	N-CA	5.27	1.56	1.46
1	C	154	VAL	C-O	5.21	1.30	1.24
1	B	340	HIS	CE1-NE2	5.06	1.37	1.32
1	B	54	LEU	C-O	5.03	1.30	1.24
1	B	90	PRO	C-O	-5.03	1.17	1.24

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	26[A]	ASP	CA-C-O	-21.77	96.66	120.38
1	F	26[B]	ASP	CA-C-O	-21.77	96.66	120.38
1	F	120[A]	MET	N-CA-CB	-15.75	83.88	110.49
1	F	120[B]	MET	N-CA-CB	-15.75	83.88	110.49
1	F	25	LEU	CA-C-N	-14.17	103.44	123.00
1	F	25	LEU	C-N-CA	-14.17	103.44	123.00
1	F	119	GLU	CA-C-N	-10.40	101.67	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	119	GLU	C-N-CA	-10.40	101.67	121.54
1	B	93	VAL	CB-CA-C	-9.29	100.00	111.88
1	F	26[A]	ASP	CB-CA-C	-9.27	93.68	109.72
1	F	26[B]	ASP	CB-CA-C	-9.27	93.68	109.72
1	D	26	ASP	CA-CB-CG	9.20	121.80	112.60
1	D	139	GLY	CA-C-O	-8.31	114.66	122.39
1	D	98	PRO	O-C-N	-8.20	117.54	121.31
1	F	120[A]	MET	N-CA-C	7.99	127.81	110.80
1	F	120[B]	MET	N-CA-C	7.99	127.81	110.80
1	E	214	ASP	CB-CA-C	-7.52	96.39	110.16
1	F	26[A]	ASP	N-CA-CB	-7.18	99.29	110.57
1	F	26[B]	ASP	N-CA-CB	-7.18	99.29	110.57
1	E	136	VAL	CA-C-O	-7.06	113.37	120.85
1	C	309	VAL	CA-C-O	-6.97	115.10	120.96
1	A	93	VAL	N-CA-CB	6.84	118.10	110.51
1	B	93	VAL	N-CA-CB	6.70	117.95	110.51
1	E	80	THR	CB-CA-C	6.70	120.72	109.67
1	D	56	THR	CA-CB-OG1	-6.61	99.68	109.60
1	F	92	GLY	CA-C-O	-6.49	115.70	121.41
1	A	40	VAL	CA-C-O	-6.47	113.74	120.27
1	B	14	VAL	CB-CA-C	6.45	116.38	110.13
1	D	8	PRO	N-CA-CB	6.43	110.07	103.00
1	D	106	ARG	CB-CA-C	6.23	123.33	110.31
1	E	381	ASP	CA-CB-CG	6.20	118.80	112.60
1	E	195	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	93	VAL	CB-CA-C	-6.10	104.07	111.88
1	B	183	ARG	CB-CA-C	-6.09	99.55	110.70
1	B	105	ARG	CB-CG-CD	-5.97	97.56	111.30
1	F	174	PHE	CA-CB-CG	5.93	119.73	113.80
1	F	273	ASP	CA-C-N	5.89	127.20	119.84
1	F	273	ASP	C-N-CA	5.89	127.20	119.84
1	C	309	VAL	O-C-N	5.88	128.08	122.97
1	E	136	VAL	CA-C-N	5.83	128.09	120.28
1	E	136	VAL	C-N-CA	5.83	128.09	120.28
1	D	303	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	290	LEU	N-CA-C	-5.78	104.89	111.07
1	D	134	ASP	CA-CB-CG	-5.77	106.83	112.60
1	D	294	GLY	O-C-N	5.71	129.93	122.96
1	A	309	VAL	O-C-N	5.69	127.92	122.97
1	D	18	PRO	CA-C-N	5.68	127.89	120.28
1	D	18	PRO	C-N-CA	5.68	127.89	120.28
1	A	375	ARG	CG-CD-NE	-5.66	99.54	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	VAL	CA-C-N	5.65	127.79	120.44
1	D	136	VAL	C-N-CA	5.65	127.79	120.44
1	F	157	ILE	CA-C-O	-5.63	115.10	120.95
1	E	169	ASP	CA-CB-CG	5.59	118.19	112.60
1	F	323	SER	CA-C-N	5.57	128.00	120.38
1	F	323	SER	C-N-CA	5.57	128.00	120.38
1	E	154	VAL	N-CA-CB	5.56	118.10	110.54
1	F	313	ALA	CA-C-O	-5.55	115.67	120.88
1	A	333	HIS	CA-C-N	5.53	128.24	120.28
1	A	333	HIS	C-N-CA	5.53	128.24	120.28
1	E	231	LYS	CA-C-N	5.51	126.22	119.99
1	E	231	LYS	C-N-CA	5.51	126.22	119.99
1	E	223[A]	THR	CA-C-N	5.51	127.93	120.44
1	E	223[A]	THR	C-N-CA	5.51	127.93	120.44
1	E	223[B]	THR	CA-C-N	5.51	127.93	120.44
1	E	223[B]	THR	C-N-CA	5.51	127.93	120.44
1	E	139	GLY	CA-C-O	-5.50	117.28	122.39
1	F	274	PRO	N-CA-CB	5.49	109.02	103.25
1	B	113	THR	CA-C-O	-5.45	115.77	121.55
1	B	271	VAL	CA-C-N	5.45	128.60	120.31
1	B	271	VAL	C-N-CA	5.45	128.60	120.31
1	C	201	ASP	CA-C-N	5.44	125.97	119.94
1	C	201	ASP	C-N-CA	5.44	125.97	119.94
1	E	345	PRO	CA-C-O	-5.43	117.20	121.38
1	C	147	PHE	CA-C-O	-5.41	112.94	119.27
1	F	302	GLU	CB-CG-CD	5.39	121.76	112.60
1	B	91	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	10	PRO	CA-C-N	5.36	128.41	120.91
1	C	10	PRO	C-N-CA	5.36	128.41	120.91
1	B	214	ASP	CB-CA-C	5.36	119.43	110.43
1	E	77	ASP	CB-CA-C	5.34	117.67	109.50
1	F	24	ALA	CA-C-O	-5.32	116.10	122.27
1	C	70	PHE	CA-C-O	-5.32	114.96	120.70
1	D	185	THR	CA-C-N	5.28	127.67	120.54
1	D	185	THR	C-N-CA	5.28	127.67	120.54
1	E	100	ASP	N-CA-C	-5.27	105.62	111.36
1	B	257	VAL	CA-C-O	-5.26	115.79	121.27
1	F	195	ASP	CA-C-O	-5.24	114.87	120.42
1	A	304	VAL	CA-C-O	-5.23	114.73	120.43
1	A	91	ASP	CA-C-N	5.22	124.93	119.92
1	A	91	ASP	C-N-CA	5.22	124.93	119.92
1	F	59	SER	CA-C-N	5.20	127.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	59	SER	C-N-CA	5.20	127.24	120.28
1	F	250	VAL	N-CA-CB	5.19	116.62	110.55
1	D	265[A]	LYS	CA-C-N	5.18	127.53	120.54
1	D	265[A]	LYS	C-N-CA	5.18	127.53	120.54
1	D	265[B]	LYS	CA-C-N	5.18	127.53	120.54
1	D	265[B]	LYS	C-N-CA	5.18	127.53	120.54
1	D	362	GLY	CA-C-O	-5.17	115.41	121.00
1	F	136[A]	VAL	CA-C-N	5.17	127.21	120.28
1	F	136[A]	VAL	C-N-CA	5.17	127.21	120.28
1	F	136[B]	VAL	CA-C-N	5.17	127.21	120.28
1	F	136[B]	VAL	C-N-CA	5.17	127.21	120.28
1	E	108	VAL	N-CA-CB	-5.16	103.62	111.57
1	E	246	HIS	CB-CA-C	5.15	118.16	110.08
1	A	246	HIS	CB-CA-C	5.13	117.29	109.34
1	A	34	LEU	CA-C-O	-5.11	115.45	120.82
1	B	28	ASP	CB-CA-C	5.07	117.26	109.50
1	A	239	VAL	N-CA-C	-5.06	105.56	110.42
1	E	108	VAL	CA-C-N	5.06	125.59	119.98
1	E	108	VAL	C-N-CA	5.06	125.59	119.98
1	F	310	THR	CA-CB-OG1	-5.05	102.02	109.60
1	A	204	VAL	CA-C-O	-5.02	115.85	121.17
1	A	23	HIS	CA-CB-CG	-5.01	108.79	113.80
1	D	308	THR	CA-CB-OG1	-5.01	102.09	109.60
1	C	195	ASP	CA-C-O	-5.00	115.11	120.42
1	D	303	ASP	CA-C-O	-5.00	115.69	121.19
1	B	204	VAL	CA-C-O	-5.00	114.85	120.25

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	213	GLU	Peptide
1	F	26[A]	ASP	Mainchain
1	F	26[B]	ASP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3303	0	3379	109	0
1	B	3249	0	3256	64	1
1	C	3248	0	3258	62	0
1	D	3372	0	3458	102	0
1	E	3316	0	3380	76	0
1	F	3358	0	3479	115	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
2	E	43	0	30	3	0
2	F	43	0	30	4	0
3	A	26	0	0	3	0
3	B	26	0	0	1	0
3	C	26	0	0	0	0
3	D	26	0	0	2	0
3	E	26	0	0	0	0
3	F	26	0	0	0	0
4	A	22	0	23	33	0
4	B	11	0	12	11	0
4	D	11	0	12	14	0
5	A	210	0	71	21	1
5	B	108	0	36	9	0
5	C	147	0	49	9	0
5	D	99	0	33	8	0
5	E	42	0	14	2	0
5	F	36	0	12	10	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	260	0	0	9	0
7	B	281	0	0	15	0
7	C	384	0	0	17	0
7	D	158	0	0	6	0
7	E	137	0	0	1	0
7	F	135	0	0	9	0
All	All	22307	0	20652	561	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (561) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93[A]:VAL:HG11	1:E:237[A]:MET:CE	1.54	1.37
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:CG2	1.66	1.23
1:F:120[A]:MET:CE	1:F:361[A]:LEU:HD21	1.69	1.22
1:A:197[A]:MET:CE	1:A:235[A]:VAL:HG23	1.73	1.19
1:F:120[A]:MET:HE2	1:F:361[A]:LEU:CD2	1.74	1.18
1:B:89:GLU:CB	4:B:513:RAM:H2	1.71	1.17
7:A:715:HOH:O	1:D:13:ALA:HB3	1.41	1.16
1:A:197[A]:MET:CE	1:A:235[A]:VAL:CG2	2.23	1.15
1:E:93[A]:VAL:HG11	1:E:237[A]:MET:HE1	1.18	1.13
1:B:89:GLU:HB3	4:B:513:RAM:H2	1.25	1.11
1:D:89:GLU:HB2	4:D:503:RAM:H62	1.30	1.08
1:E:343[A]:ARG:HH11	1:E:343[A]:ARG:HG2	0.95	1.08
1:F:185[A]:THR:OG1	7:F:601[A]:HOH:O	1.72	1.06
1:C:30[A]:HIS:ND1	1:C:33[A]:GLU:OE2	1.90	1.04
1:D:208[A]:ARG:CB	1:D:208[A]:ARG:HH11	1.72	1.03
1:A:193:GLN:HE21	4:A:503[A]:RAM:H1	1.23	1.00
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:HG23	1.29	0.99
1:B:42[B]:ARG:HG2	1:B:42[B]:ARG:HH21	1.23	0.99
1:E:343[A]:ARG:HG2	1:E:343[A]:ARG:NH1	1.74	0.98
1:E:172:ARG:NH1	7:E:601:HOH:O	1.96	0.97
1:D:193:GLN:CD	4:D:503:RAM:H63	1.90	0.96
1:E:93[A]:VAL:CG1	1:E:237[A]:MET:CE	2.41	0.96
1:F:21:LEU:HD13	1:F:23[B]:HIS:CE1	2.01	0.95
1:D:178:MET:HE2	1:D:193:GLN:HA	1.47	0.94
1:E:280:ALA:O	1:E:284[A]:MET:HG3	1.68	0.94
1:C:335:ASP:HB2	5:C:552:FMT:O2	1.69	0.93
1:D:123[A]:ARG:HG3	1:D:123[A]:ARG:HH11	1.34	0.92
1:D:30[B]:HIS:ND1	1:D:33[B]:GLU:OE2	2.03	0.92
1:B:89:GLU:HB2	4:B:513:RAM:H2	1.51	0.92
1:E:93[A]:VAL:CG1	1:E:237[A]:MET:SD	2.57	0.92
1:A:86:THR:OG1	4:A:503[A]:RAM:H63	1.68	0.91
1:E:93[A]:VAL:HG11	1:E:237[A]:MET:SD	2.11	0.91
1:D:123[A]:ARG:HH11	1:D:123[A]:ARG:CG	1.83	0.90
1:B:42[B]:ARG:HH21	1:B:42[B]:ARG:CG	1.85	0.90
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:CB	2.02	0.89
4:A:503[B]:RAM:O2	5:A:565:FMT:C	2.20	0.89
1:A:193:GLN:NE2	4:A:503[A]:RAM:H1	1.86	0.89
1:D:105:ARG:NH1	1:D:355:HIS:O	2.06	0.88
1:A:197[A]:MET:HE2	1:A:235[A]:VAL:CG2	2.04	0.88
1:C:101[B]:HIS:CE1	1:C:354[B]:HIS:CD2	2.62	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ARG:HG2	1:E:172:ARG:HH11	1.35	0.87
1:F:21:LEU:HD23	1:F:22:PRO:HD2	1.56	0.87
1:C:256:LEU:HD22	1:C:284:MET:HB3	1.57	0.87
1:F:120[A]:MET:HE1	1:F:361[A]:LEU:HD11	1.54	0.87
1:C:185[B]:THR:HG22	7:C:617:HOH:O	1.75	0.86
1:A:345:PRO:HB3	1:D:8:PRO:HA	1.56	0.86
1:B:89:GLU:HB2	4:B:513:RAM:C2	2.06	0.85
1:A:86:THR:OG1	4:A:503[A]:RAM:C6	2.24	0.85
1:D:89:GLU:HB2	4:D:503:RAM:C6	2.06	0.84
1:A:178:MET:HE3	4:A:503[A]:RAM:O2	1.76	0.84
1:E:343[A]:ARG:HH11	1:E:343[A]:ARG:CG	1.85	0.84
1:A:355:HIS:NE2	5:A:504:FMT:O1	2.11	0.84
1:C:30[A]:HIS:CE1	1:C:33[A]:GLU:OE2	2.31	0.83
1:A:335[B]:ASP:OD1	7:A:601:HOH:O	1.96	0.83
1:A:42:ARG:NH2	7:A:603:HOH:O	2.11	0.83
1:F:237[B]:MET:HE3	1:F:237[B]:MET:HA	1.60	0.83
1:A:197[A]:MET:CE	1:A:235[A]:VAL:HG21	2.09	0.82
1:A:39:PRO:CB	1:A:57[B]:ARG:HD3	2.09	0.82
1:F:237[B]:MET:HA	1:F:237[B]:MET:CE	2.09	0.82
1:C:42[B]:ARG:HG2	1:C:42[B]:ARG:HH11	1.45	0.82
3:B:502:QR8:O3	4:B:513:RAM:O4	1.99	0.81
1:F:21:LEU:HD13	1:F:23[B]:HIS:HE1	1.41	0.81
1:F:188[A]:GLU:OE1	7:F:601[A]:HOH:O	1.97	0.81
1:C:106[B]:ARG:NH2	7:C:604:HOH:O	2.12	0.81
1:A:89:GLU:OE2	4:A:503[A]:RAM:O3	1.98	0.80
1:A:39:PRO:HB2	1:A:57[B]:ARG:HD3	1.62	0.80
1:C:188:GLU:HG3	7:C:749:HOH:O	1.82	0.80
3:A:502:QR8:O3	4:A:503[B]:RAM:H2	1.82	0.79
5:A:550:FMT:O2	7:A:602:HOH:O	2.00	0.79
1:C:185[B]:THR:CG2	7:C:617:HOH:O	2.31	0.79
1:A:193:GLN:HE21	4:A:503[A]:RAM:C1	1.97	0.78
1:E:93[A]:VAL:HG13	1:E:237[A]:MET:SD	2.21	0.78
1:D:45:LEU:HD12	1:D:81:PRO:HB2	1.66	0.78
1:B:266:ARG:HD3	7:B:693:HOH:O	1.84	0.77
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:HB	1.67	0.76
1:C:120[A]:MET:CE	7:C:773:HOH:O	2.33	0.76
1:D:208[A]:ARG:HH11	1:D:208[A]:ARG:CG	1.98	0.76
1:B:86[B]:THR:OG1	7:B:602:HOH:O	2.02	0.76
1:A:236:ASN:HD21	4:A:503[B]:RAM:H4	1.50	0.75
1:C:33[A]:GLU:OE1	7:C:601:HOH:O	2.05	0.75
1:F:277:VAL:HG23	1:F:278:PRO:HD3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:VAL:HB	1:C:122:PRO:HB3	1.69	0.75
1:E:125:ARG:HD3	1:E:368:GLU:OE2	1.86	0.75
1:E:256:LEU:HD22	1:E:284[B]:MET:HB3	1.70	0.74
4:A:503[A]:RAM:O4	5:A:565:FMT:C	2.35	0.74
1:E:260:LEU:HG	1:E:284[A]:MET:HE1	1.68	0.74
1:A:101[B]:HIS:CE1	1:A:354[B]:HIS:CD2	2.75	0.74
1:F:27:LEU:HD23	1:F:326[B]:ARG:NE	2.03	0.74
1:F:93[B]:VAL:HG13	1:F:237[B]:MET:SD	2.27	0.74
4:B:513:RAM:H5	7:B:635:HOH:O	1.88	0.73
1:A:197[A]:MET:HE2	1:A:235[A]:VAL:HG21	1.69	0.73
1:D:208[A]:ARG:HH11	1:D:208[A]:ARG:HB2	1.53	0.73
4:A:503[A]:RAM:O4	5:A:565:FMT:H	1.88	0.72
1:F:188[A]:GLU:HB2	7:F:601[A]:HOH:O	1.88	0.72
2:E:502:HEM:HHC	2:E:502:HEM:HBB2	1.72	0.72
1:D:123[A]:ARG:HG3	1:D:123[A]:ARG:NH1	2.01	0.71
1:F:188[A]:GLU:CD	7:F:601[A]:HOH:O	2.33	0.71
1:F:120[A]:MET:HE2	1:F:361[A]:LEU:HD21	0.81	0.71
1:B:42[B]:ARG:HG2	1:B:42[B]:ARG:NH2	1.90	0.71
1:C:126[B]:SER:OG	7:C:603:HOH:O	2.09	0.70
5:C:521:FMT:O1	7:C:602:HOH:O	2.08	0.70
1:D:193:GLN:OE1	4:D:503:RAM:H63	1.91	0.70
1:C:354[B]:HIS:HE1	7:C:636:HOH:O	1.72	0.70
1:D:183[A]:ARG:HD2	1:D:184:LEU:CD1	2.22	0.70
1:B:89:GLU:CB	4:B:513:RAM:C2	2.57	0.69
1:B:354[B]:HIS:HD2	2:B:501:HEM:O1D	1.74	0.69
1:A:178:MET:O	4:A:503[A]:RAM:O1	2.11	0.69
1:B:89:GLU:HB2	4:B:513:RAM:O2	1.91	0.69
1:A:298:ARG:HE	5:A:514:FMT:C	2.06	0.69
1:D:220:ALA:O	1:D:223:THR:OG1	2.09	0.69
1:A:123[B]:ARG:HE	5:A:510:FMT:C	2.06	0.69
1:A:260:LEU:HG	1:A:284[A]:MET:HE1	1.73	0.69
1:C:283:GLU:HG3	1:C:337:LEU:HD22	1.75	0.68
1:D:256[A]:LEU:HD22	1:D:284:MET:HB3	1.76	0.68
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.75	0.68
1:B:170:LEU:HB2	5:F:509:FMT:H	1.76	0.67
1:D:178:MET:CE	1:D:193:GLN:HA	2.24	0.67
1:C:35:ARG:HH11	5:C:504:FMT:C	2.08	0.67
1:B:13:ALA:HB1	1:C:115:ARG:HG2	1.76	0.67
1:A:138[A]:HIS:ND1	1:A:139:GLY:O	2.28	0.67
1:F:260[A]:LEU:HG	1:F:284:MET:HE1	1.76	0.66
1:D:48:GLY:O	7:D:601:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:LEU:O	1:F:284:MET:HE1	1.95	0.66
1:C:30[A]:HIS:NE2	7:C:612:HOH:O	2.29	0.66
1:D:355:HIS:NE2	5:D:508:FMT:O1	2.26	0.65
1:F:93[B]:VAL:CG1	1:F:237[B]:MET:SD	2.84	0.65
1:B:266:ARG:HD2	1:B:337:LEU:HD23	1.79	0.65
1:A:39:PRO:HB3	1:A:57[B]:ARG:HD3	1.79	0.65
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.27	0.65
1:D:230:THR:O	1:D:234:ILE:HD12	1.97	0.65
1:F:24:ALA:HB2	1:F:391:TRP:NE1	2.12	0.64
1:F:133:ASP:O	1:F:136[B]:VAL:HG12	1.96	0.64
5:B:503:FMT:H	7:B:735:HOH:O	1.97	0.63
1:F:24:ALA:HB2	1:F:391:TRP:CD1	2.34	0.63
1:B:392:LYS:HG2	1:B:401[A]:GLU:HG3	1.80	0.63
1:E:17:TYR:HE1	1:E:31:TYR:HH	1.45	0.63
1:A:256:LEU:HD22	1:A:284[A]:MET:HB3	1.81	0.62
1:D:89:GLU:HB3	4:D:503:RAM:H5	1.82	0.62
1:F:390[A]:LYS:NZ	1:F:402[A]:ARG:HE	1.97	0.62
1:C:101[B]:HIS:CE1	1:C:354[B]:HIS:HD2	2.18	0.62
1:B:13:ALA:HB2	5:B:507:FMT:O1	2.00	0.61
1:A:240:SER:HA	4:A:503[B]:RAM:C6	2.31	0.61
1:A:138[A]:HIS:HE1	1:A:141:PRO:O	1.84	0.61
5:D:528:FMT:C	7:D:619:HOH:O	2.47	0.61
1:C:30[A]:HIS:HD1	1:C:33[A]:GLU:CD	2.08	0.61
1:D:178:MET:HE2	1:D:193:GLN:CA	2.26	0.60
1:F:91:ASP:O	5:F:514:FMT:O1	2.19	0.60
1:F:277:VAL:CG2	1:F:278:PRO:HD3	2.30	0.60
1:E:150:VAL:O	1:E:154:VAL:HG13	2.01	0.60
1:F:201:ASP:OD1	7:F:602:HOH:O	2.17	0.60
1:A:243:ILE:HD12	4:A:503[B]:RAM:C6	2.32	0.60
1:B:123:ARG:HD3	5:B:534:FMT:O1	2.01	0.60
3:D:502:QR8:O3	4:D:503:RAM:O1	2.18	0.60
1:D:101[B]:HIS:NE2	1:D:354[B]:HIS:CD2	2.70	0.60
1:D:145:VAL:HA	1:D:149:ALA:HB3	1.84	0.60
1:A:174:PHE:HB3	1:A:196:PHE:CD2	2.37	0.60
1:F:354[B]:HIS:HE1	7:F:626:HOH:O	1.83	0.59
1:A:197[A]:MET:HE2	1:A:235[A]:VAL:HG23	1.66	0.59
1:F:133:ASP:OD1	1:F:376[A]:ARG:NH1	2.34	0.59
1:E:172:ARG:HH11	1:E:172:ARG:CG	2.08	0.59
1:F:103:ARG:HE	5:F:509:FMT:C	2.16	0.59
1:B:86[A]:THR:HG23	7:B:602:HOH:O	2.02	0.59
1:D:127:LEU:HD11	1:D:155:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:ARG:CD	1:E:368:GLU:OE2	2.51	0.59
1:F:112:PHE:HB3	1:F:357:ILE:O	2.02	0.59
1:D:193:GLN:NE2	4:D:503:RAM:H63	2.18	0.59
1:E:290:LEU:O	1:E:397:ILE:HA	2.03	0.58
1:A:12:ASP:HB2	7:A:722:HOH:O	2.03	0.58
1:A:240:SER:HA	4:A:503[B]:RAM:H63	1.86	0.58
1:F:21:LEU:HB3	1:F:23[B]:HIS:NE2	2.19	0.58
1:B:17:TYR:HA	1:B:18:PRO:C	2.29	0.58
1:F:93[A]:VAL:HG23	5:F:514:FMT:C	2.33	0.58
1:A:115[A]:ARG:HD3	7:A:770:HOH:O	2.04	0.57
1:E:93[A]:VAL:HG11	1:E:237[A]:MET:HE2	1.74	0.57
1:E:322:ALA:O	1:E:326:ARG:HG2	2.04	0.57
1:D:101[B]:HIS:CD2	1:D:354[B]:HIS:CD2	2.93	0.57
1:C:335:ASP:HB2	5:C:552:FMT:C	2.33	0.57
1:F:125:ARG:O	1:F:128[B]:VAL:HG12	2.03	0.57
1:D:17:TYR:CD1	1:D:18:PRO:HA	2.39	0.56
1:D:208[A]:ARG:HH11	1:D:208[A]:ARG:HB3	1.67	0.56
1:D:287:TYR:O	1:D:287:TYR:CD1	2.57	0.56
1:C:343[A]:ARG:NH2	7:C:619:HOH:O	2.38	0.56
1:E:312[B]:ARG:HG2	1:E:312[B]:ARG:HH11	1.70	0.56
1:F:244:ALA:HB1	2:F:502:HEM:CHD	2.35	0.56
1:A:243:ILE:HD12	4:A:503[B]:RAM:H61	1.86	0.56
1:F:101[A]:HIS:CE1	1:F:354[A]:HIS:CE1	2.94	0.56
1:C:393[B]:GLN:OE1	7:C:605:HOH:O	2.18	0.56
1:D:208[A]:ARG:CG	1:D:208[A]:ARG:NH1	2.64	0.56
1:F:266:ARG:NH2	1:F:337[B]:LEU:HD12	2.21	0.56
1:C:172:ARG:HH12	5:C:507:FMT:C	2.19	0.55
1:E:74:ALA:HB3	1:E:299:VAL:HB	1.88	0.55
1:F:349:PHE:CE1	1:F:359:ALA:HA	2.40	0.55
1:A:86:THR:OG1	4:A:503[A]:RAM:H61	2.05	0.55
1:D:152:PHE:HB3	1:D:153:PRO:HD3	1.88	0.55
1:D:160:LEU:HG	1:D:215[B]:LEU:HD22	1.88	0.55
1:D:183[A]:ARG:HD2	1:D:184:LEU:HD11	1.87	0.55
1:F:161:LEU:O	1:F:216:LEU:HB2	2.05	0.55
1:E:286:ARG:HD3	1:E:344:ASN:OD1	2.06	0.55
1:A:115[B]:ARG:HH21	1:A:115[B]:ARG:HG3	1.72	0.55
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.89	0.55
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.87	0.55
1:C:93:VAL:HG11	1:C:237[A]:MET:HE1	1.89	0.55
1:A:159:GLU:HG2	5:A:510:FMT:H	1.89	0.55
1:C:305[B]:GLU:OE1	1:C:310:THR:OG1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58[A]:MET:HE1	1:D:347:ILE:HG12	1.88	0.55
1:F:120[A]:MET:CE	1:F:361[A]:LEU:HD11	2.34	0.54
1:E:115:ARG:HB3	5:E:501:FMT:C	2.37	0.54
1:A:283:GLU:HG3	1:A:337:LEU:HD22	1.89	0.54
1:B:105:ARG:HD3	1:B:357:ILE:HD12	1.88	0.54
1:B:264:ARG:NH1	1:B:380:LEU:O	2.40	0.54
1:E:77:ASP:HB3	1:E:80:THR:CG2	2.37	0.54
1:F:286[A]:ARG:HD3	1:F:344:ASN:OD1	2.08	0.54
1:A:36[B]:ARG:HG2	1:A:37:ASP:OD1	2.08	0.54
1:D:158:CYS:HB3	1:D:163:VAL:O	2.08	0.54
1:B:207:ARG:NH2	1:B:214:ASP:OD1	2.40	0.53
1:D:326:ARG:HG3	5:D:507:FMT:H	1.89	0.53
1:E:92:GLY:HA2	1:E:236:ASN:ND2	2.23	0.53
1:A:259:LEU:HB3	1:A:284[A]:MET:HE2	1.91	0.53
1:F:244:ALA:HB1	2:F:502:HEM:C4C	2.43	0.53
1:F:145[B]:VAL:HA	1:F:149:ALA:HB3	1.90	0.53
1:A:274:PRO:O	5:A:550:FMT:O1	2.26	0.53
4:A:503[A]:RAM:HO4	5:A:565:FMT:C	2.18	0.53
1:B:38:GLU:OE1	5:B:510:FMT:O2	2.26	0.53
1:E:266:ARG:HD3	1:E:337:LEU:HD23	1.89	0.53
1:F:145[A]:VAL:HA	1:F:149:ALA:HB3	1.90	0.53
1:F:326[B]:ARG:NH2	1:F:335[B]:ASP:OD2	2.40	0.53
1:A:259:LEU:CB	1:A:284[A]:MET:HE2	2.39	0.53
1:A:38:GLU:HG3	5:A:531:FMT:O2	2.09	0.53
1:A:38:GLU:HG3	5:A:531:FMT:C	2.38	0.53
1:D:89:GLU:CB	4:D:503:RAM:C6	2.84	0.53
1:A:239:VAL:HG12	4:A:503[B]:RAM:H62	1.90	0.53
4:A:503[B]:RAM:O2	5:A:565:FMT:O1	2.25	0.53
1:A:371:SER:HB3	5:A:506:FMT:C	2.39	0.52
1:F:375[B]:ARG:HG2	1:F:376[B]:ARG:HG3	1.89	0.52
1:D:208[A]:ARG:HB2	1:D:208[A]:ARG:NH1	2.23	0.52
1:E:256:LEU:HD22	1:E:284[B]:MET:CB	2.39	0.52
1:B:383:ALA:HB3	1:B:404:ILE:HG22	1.91	0.52
1:C:21:LEU:HD12	1:C:22:PRO:HD2	1.91	0.52
1:E:101[B]:HIS:CD2	1:E:354[B]:HIS:CD2	2.97	0.52
1:F:327:ASP:OD1	1:F:329:GLU:OE1	2.26	0.52
1:F:127[B]:LEU:HD13	7:F:629[B]:HOH:O	2.08	0.52
1:B:35:ARG:NH2	7:B:611:HOH:O	2.43	0.52
1:F:24:ALA:CB	1:F:391:TRP:NE1	2.73	0.52
1:F:289:PRO:HA	5:F:505:FMT:H	1.92	0.52
1:A:127:LEU:HD21	1:A:155:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101[B]:HIS:HE1	2:B:501:HEM:O2D	1.92	0.51
1:E:256:LEU:HD22	1:E:284[A]:MET:HB3	1.91	0.51
1:F:287:TYR:CD1	1:F:337[B]:LEU:HG	2.44	0.51
1:C:28:ASP:OD1	1:C:29:PRO:HD2	2.11	0.51
1:D:89:GLU:CB	4:D:503:RAM:H62	2.21	0.51
1:E:32:ALA:HA	1:E:35[B]:ARG:NH1	2.26	0.51
1:F:21:LEU:HD23	1:F:22:PRO:CD	2.37	0.51
1:F:168[B]:ARG:HH11	1:F:168[B]:ARG:CG	2.22	0.51
1:F:162:GLY:HA3	1:F:214:ASP:OD2	2.11	0.51
1:C:9:THR:CG2	1:C:11:ALA:HB3	2.41	0.51
1:E:145:VAL:HA	1:E:149:ALA:HB3	1.92	0.51
3:A:502:QR8:O3	4:A:503[A]:RAM:H3	2.11	0.50
1:B:193:GLN:CD	4:B:513:RAM:O2	2.53	0.50
1:E:101[B]:HIS:CD2	1:E:354[B]:HIS:NE2	2.79	0.50
1:E:170:LEU:HD22	1:E:174:PHE:CZ	2.46	0.50
1:B:12[B]:ASP:CG	1:B:44:ARG:HH21	2.19	0.50
1:E:256:LEU:HD22	1:E:284[A]:MET:CB	2.39	0.50
1:A:44[B]:ARG:HD2	5:A:511:FMT:C	2.41	0.50
1:D:167:ASP:O	1:D:168:ARG:C	2.54	0.50
1:E:35[A]:ARG:HG2	1:E:57:ARG:HG2	1.92	0.50
1:A:160:LEU:HG	1:A:215[A]:LEU:HD22	1.92	0.50
1:B:172:ARG:HD2	7:B:670:HOH:O	2.10	0.50
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.41	0.50
1:D:9:THR:O	1:D:9:THR:HG22	2.12	0.50
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.93	0.50
1:A:240:SER:CA	4:A:503[B]:RAM:H63	2.42	0.50
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.94	0.50
1:D:193:GLN:HG2	4:D:503:RAM:H4	1.93	0.50
1:D:258[B]:HIS:NE2	1:D:391:TRP:HZ2	2.10	0.50
1:E:251:ASN:HD22	1:E:397:ILE:HD12	1.76	0.50
1:A:32:ALA:HB2	5:A:530:FMT:H	1.94	0.50
1:A:258:HIS:O	1:A:262:THR:HG23	2.12	0.50
1:F:46:PRO:HB2	1:F:47:TYR:CD1	2.47	0.49
1:F:168[A]:ARG:HG2	1:F:172:ARG:HD3	1.93	0.49
1:F:291:VAL:H	5:F:505:FMT:C	2.25	0.49
1:C:393[B]:GLN:CD	7:C:605:HOH:O	2.54	0.49
1:F:42:ARG:HD2	1:F:51:THR:HG23	1.93	0.49
1:D:123[A]:ARG:CG	1:D:123[A]:ARG:NH1	2.54	0.49
1:F:119:GLU:HB3	1:F:120[B]:MET:HE3	1.94	0.49
1:C:42[A]:ARG:NH1	5:C:523:FMT:O2	2.45	0.49
1:C:312:ARG:O	1:C:313:ALA:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401[A]:GLU:OE2	7:B:603[A]:HOH:O	2.19	0.49
1:C:120[A]:MET:HE3	7:C:773:HOH:O	2.03	0.49
1:F:21:LEU:HD22	1:F:23[B]:HIS:CE1	2.47	0.49
1:D:189:ILE:HG21	5:D:504:FMT:C	2.43	0.49
1:E:28:ASP:OD1	1:E:30:HIS:HB2	2.12	0.49
1:B:256:LEU:HD22	1:B:284[B]:MET:HB3	1.94	0.49
1:E:93[A]:VAL:CG1	1:E:237[A]:MET:HE2	2.37	0.49
1:C:14:VAL:HG21	1:C:51[B]:THR:HG23	1.94	0.49
1:F:237[B]:MET:HA	5:F:514:FMT:H	1.95	0.49
1:A:122:PRO:HB3	1:D:309:VAL:HB	1.94	0.48
1:A:240:SER:OG	4:A:503[B]:RAM:C1	2.61	0.48
1:F:252:GLN:OE1	1:F:252:GLN:HA	2.12	0.48
1:D:178:MET:CE	1:D:196:PHE:HB2	2.42	0.48
1:E:251:ASN:HB3	1:E:398:ARG:O	2.12	0.48
1:F:172:ARG:HH11	1:F:172:ARG:HG2	1.78	0.48
1:B:110[B]:LYS:NZ	7:B:605:HOH:O	2.37	0.48
2:E:502:HEM:HBC2	2:E:502:HEM:HMC1	1.96	0.48
1:B:280:ALA:O	1:B:284[A]:MET:HG3	2.14	0.48
1:D:178:MET:HE1	1:D:196:PHE:CB	2.43	0.48
1:A:328:GLU:HB2	5:A:505:FMT:C	2.44	0.48
1:E:35[A]:ARG:HG2	1:E:57:ARG:CG	2.43	0.48
1:E:70:PHE:HB3	1:E:298:ARG:HB3	1.94	0.48
1:E:86:THR:HG22	1:E:186:ALA:HA	1.95	0.48
1:F:24:ALA:CB	1:F:391:TRP:CE2	2.97	0.48
1:F:259:LEU:HB2	1:F:284:MET:CE	2.43	0.48
1:A:44[B]:ARG:HD2	5:A:511:FMT:O2	2.14	0.47
1:A:115[B]:ARG:HH21	1:A:115[B]:ARG:CG	2.26	0.47
1:D:89:GLU:CB	4:D:503:RAM:H5	2.43	0.47
1:D:101[B]:HIS:NE2	1:D:354[B]:HIS:HD2	2.11	0.47
1:A:89:GLU:HB2	4:A:503[B]:RAM:O3	2.13	0.47
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.96	0.47
1:D:208[A]:ARG:CB	1:D:208[A]:ARG:NH1	2.57	0.47
1:F:117:VAL:HG11	1:F:360:GLN:C	2.40	0.47
4:A:503[A]:RAM:O4	5:A:565:FMT:O2	2.27	0.47
1:B:177:ALA:O	1:B:180:SER:HB3	2.14	0.47
5:B:503:FMT:C	7:B:735:HOH:O	2.59	0.47
1:E:271:VAL:HA	1:E:374:VAL:HG13	1.95	0.47
1:A:107[A]:LEU:HD13	1:A:219:LEU:CD2	2.44	0.47
1:D:256[A]:LEU:HD22	1:D:284:MET:CB	2.44	0.47
1:E:380:LEU:HA	1:E:406:SER:O	2.15	0.47
1:E:312[B]:ARG:HH11	1:E:312[B]:ARG:CG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:VAL:O	1:F:120[A]:MET:HG2	2.15	0.47
1:F:206[B]:GLN:HG2	7:F:657:HOH:O	2.15	0.47
1:B:392:LYS:HG3	1:B:399:GLY:O	2.15	0.47
1:C:42[B]:ARG:HH11	1:C:42[B]:ARG:CG	2.23	0.47
1:B:159:GLU:HG2	5:B:534:FMT:O1	2.15	0.47
1:C:185[B]:THR:HG23	1:C:188:GLU:HB3	1.97	0.47
1:D:83:MET:O	7:D:602:HOH:O	2.21	0.47
1:F:27:LEU:HD23	1:F:326[B]:ARG:HE	1.79	0.47
1:D:101[B]:HIS:CD2	1:D:354[B]:HIS:NE2	2.83	0.46
1:F:27:LEU:HD23	1:F:326[B]:ARG:CZ	2.44	0.46
1:A:39:PRO:HB3	1:A:57[B]:ARG:CD	2.43	0.46
1:F:168[B]:ARG:CG	1:F:168[B]:ARG:NH1	2.79	0.46
1:A:240:SER:OG	4:A:503[B]:RAM:H1	2.15	0.46
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.96	0.46
1:B:101[B]:HIS:CE1	1:B:354[B]:HIS:CD2	3.03	0.46
1:C:17:TYR:HA	1:C:18:PRO:C	2.41	0.46
1:C:120[A]:MET:HE2	7:C:773:HOH:O	2.08	0.46
1:D:58[A]:MET:HE1	1:D:347:ILE:CG1	2.46	0.46
1:D:86[A]:THR:HG22	1:D:186:ALA:HA	1.98	0.46
7:A:759:HOH:O	1:D:38:GLU:HG3	2.15	0.46
1:C:219:LEU:O	1:C:223:THR:HG23	2.15	0.46
1:E:115:ARG:HB3	5:E:501:FMT:H	1.97	0.46
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.29	0.46
1:C:206:GLN:HE22	5:C:514:FMT:H	1.81	0.46
1:A:193:GLN:HG2	4:A:503[A]:RAM:O2	2.16	0.46
1:F:93[B]:VAL:HG11	1:F:237[B]:MET:SD	2.57	0.46
1:F:144[B]:LEU:HD23	1:F:144[B]:LEU:HA	1.72	0.46
1:F:287:TYR:CE1	1:F:337[B]:LEU:HG	2.51	0.46
1:B:332:ASP:C	1:B:333[A]:HIS:CG	2.94	0.45
1:E:30:HIS:O	1:E:34[A]:LEU:HG	2.16	0.45
1:A:170:LEU:C	1:A:170:LEU:HD23	2.40	0.45
1:D:190[B]:GLN:HE21	1:D:190[B]:GLN:HA	1.80	0.45
1:E:172:ARG:NH1	1:E:172:ARG:CG	2.73	0.45
1:E:295:SER:H	1:E:318[A]:VAL:CG2	2.29	0.45
1:F:260[B]:LEU:HD12	1:F:260[B]:LEU:HA	1.79	0.45
1:F:361[A]:LEU:HD23	1:F:361[A]:LEU:HA	1.83	0.45
1:F:373:LEU:HD22	1:F:380[B]:LEU:HD11	1.98	0.45
1:F:92:GLY:O	1:F:96:GLN:HG2	2.17	0.45
1:A:152:PHE:HB3	1:A:153:PRO:HD3	1.99	0.45
1:D:123[B]:ARG:HG3	7:D:720:HOH:O	2.17	0.45
1:E:101[B]:HIS:NE2	1:E:354[B]:HIS:CD2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237[A]:MET:HA	5:F:514:FMT:H	1.98	0.45
1:F:237[B]:MET:CE	1:F:237[B]:MET:CA	2.84	0.45
5:B:511:FMT:C	7:B:618:HOH:O	2.63	0.45
1:E:106:ARG:HH11	1:E:106:ARG:CG	2.29	0.45
1:E:138[B]:HIS:HD2	1:E:139:GLY:O	2.00	0.45
1:B:270:LEU:HB2	1:B:374:VAL:HG21	1.98	0.45
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.98	0.45
1:D:94:LEU:HD21	3:D:502:QR8:O12	2.17	0.45
1:A:17:TYR:HA	1:A:18:PRO:C	2.41	0.45
1:A:101[B]:HIS:CE1	1:A:354[B]:HIS:HD2	2.33	0.45
1:A:264:ARG:HG2	1:A:268:GLU:OE2	2.16	0.45
1:A:12:ASP:N	7:A:615:HOH:O	2.49	0.45
1:A:240:SER:HA	4:A:503[B]:RAM:H61	1.98	0.45
1:A:290:LEU:O	1:A:397:ILE:HA	2.17	0.45
3:A:502:QR8:C5	4:A:503[B]:RAM:O5	2.65	0.45
1:C:283:GLU:HG3	1:C:337:LEU:CD2	2.46	0.45
1:C:290:LEU:O	1:C:397:ILE:HA	2.16	0.45
1:D:93:VAL:N	5:D:528:FMT:O2	2.50	0.45
1:D:123[A]:ARG:HD2	5:D:512:FMT:O2	2.17	0.44
1:F:280:ALA:O	1:F:284:MET:HG3	2.17	0.44
1:A:107[B]:LEU:HD21	1:A:222:ALA:CB	2.47	0.44
1:A:243:ILE:HD12	4:A:503[B]:RAM:H62	2.00	0.44
1:C:12[A]:ASP:HB2	1:C:51[A]:THR:CG2	2.47	0.44
1:E:35[A]:ARG:HG3	1:E:56:THR:HB	2.00	0.44
1:F:46:PRO:HB2	1:F:47:TYR:CE1	2.53	0.44
1:A:140:SER:OG	1:A:406:SER:HA	2.17	0.44
1:D:62:ARG:HH11	1:D:351[A]:HIS:CD2	2.35	0.44
1:D:146:GLU:O	7:D:603:HOH:O	2.21	0.44
1:D:178:MET:SD	4:D:503:RAM:O3	2.76	0.44
1:D:327:ASP:OD1	1:D:327:ASP:C	2.60	0.44
1:E:259:LEU:HB2	1:E:284[A]:MET:CE	2.47	0.44
1:E:312[B]:ARG:HG3	1:E:313:ALA:N	2.32	0.44
1:F:184:LEU:HD22	1:F:188[A]:GLU:OE1	2.18	0.44
1:B:315:GLU:HA	1:B:316:PRO:HD3	1.83	0.44
1:F:131[A]:LEU:HD13	1:F:131[A]:LEU:HA	1.74	0.44
1:F:400:LEU:HD13	1:F:403:GLN:CG	2.48	0.44
1:A:138[A]:HIS:CE1	1:A:139:GLY:O	2.71	0.44
1:B:178:MET:HE3	4:B:513:RAM:H1	1.99	0.44
1:D:101[B]:HIS:HE2	1:D:354[B]:HIS:HD2	1.66	0.44
1:D:246:HIS:O	1:D:250:VAL:HG23	2.18	0.44
5:F:504:FMT:C	7:F:628:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD12	1:B:144:LEU:HA	1.89	0.44
1:D:94:LEU:HA	1:D:354[A]:HIS:CE1	2.52	0.44
4:A:503[B]:RAM:H4	4:A:503[B]:RAM:H1	1.63	0.44
5:B:511:FMT:H	7:B:618:HOH:O	2.18	0.44
1:C:256:LEU:HD22	1:C:284:MET:CB	2.37	0.44
1:D:174:PHE:HB3	1:D:196:PHE:CD2	2.53	0.44
1:D:237:MET:HE3	1:D:241:LEU:HG	2.00	0.44
1:F:376[A]:ARG:NH2	1:F:377[A]:PHE:CZ	2.86	0.44
1:B:284[A]:MET:HE3	1:B:337:LEU:HD21	2.00	0.44
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.48	0.44
1:E:127[B]:LEU:HD21	1:E:155:ALA:HB3	1.99	0.43
1:B:354[B]:HIS:HE1	7:B:713:HOH:O	2.00	0.43
1:F:25:LEU:HD23	1:F:25:LEU:N	2.33	0.43
1:F:129[A]:ASP:OD1	1:F:376[A]:ARG:HD2	2.18	0.43
1:F:244:ALA:CB	2:F:502:HEM:CHD	2.96	0.43
1:A:246:HIS:O	1:A:250:VAL:HG23	2.18	0.43
1:C:101[B]:HIS:HE1	2:C:501:HEM:O2D	2.01	0.43
1:C:346[A]:HIS:HD2	1:C:348:ALA:H	1.66	0.43
1:A:258:HIS:CE1	1:A:262:THR:HG21	2.53	0.43
1:D:283:GLU:HA	1:D:344:ASN:HD21	1.82	0.43
1:F:237[B]:MET:CA	1:F:237[B]:MET:HE2	2.48	0.43
1:F:178:MET:HE3	1:F:193:GLN:HG2	2.01	0.43
1:F:214:ASP:HB3	1:F:217:GLY:H	1.82	0.43
1:F:285:LEU:HD23	1:F:285:LEU:HA	1.90	0.43
1:B:263:GLU:O	1:B:266:ARG:HG3	2.18	0.43
1:D:193:GLN:CG	4:D:503:RAM:H4	2.48	0.43
1:D:256[B]:LEU:HD23	1:D:370:LEU:HD11	1.99	0.43
1:F:168[B]:ARG:HH11	1:F:168[B]:ARG:HG2	1.83	0.43
1:A:256:LEU:HD22	1:A:284[B]:MET:HB3	2.00	0.43
1:A:260:LEU:CG	1:A:284[A]:MET:HE1	2.46	0.43
1:B:101[B]:HIS:CE1	2:B:501:HEM:O2D	2.71	0.43
1:B:193:GLN:HG2	4:B:513:RAM:H1	2.00	0.43
1:D:85:PRO:HD2	5:D:504:FMT:O1	2.19	0.43
1:E:55:VAL:HG22	1:E:319:VAL:HG22	2.00	0.43
1:F:283:GLU:HG3	1:F:337[A]:LEU:HD12	2.01	0.43
2:F:502:HEM:HMB2	2:F:502:HEM:HBB2	2.01	0.43
1:B:17:TYR:O	1:B:46:PRO:HD3	2.19	0.43
1:C:8:PRO:N	7:C:639:HOH:O	2.51	0.43
1:C:265[A]:LYS:HZ3	1:C:265[A]:LYS:HG3	1.67	0.43
1:D:264[A]:ARG:NH2	1:D:378:PRO:O	2.51	0.43
1:D:393[B]:GLN:NE2	5:D:518:FMT:O2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101[A]:HIS:CE1	1:F:354[A]:HIS:ND1	2.87	0.43
1:F:123:ARG:CZ	1:F:127[B]:LEU:HD11	2.48	0.43
1:D:180:SER:HB2	1:D:189:ILE:HD11	2.01	0.43
1:D:258[B]:HIS:CD2	1:D:391:TRP:CZ2	3.07	0.43
1:E:215:LEU:HA	1:E:215:LEU:HD23	1.75	0.43
1:B:121:ARG:HG3	1:B:364:LEU:HD11	2.01	0.42
1:A:104:LEU:O	1:A:107[A]:LEU:HB2	2.18	0.42
1:A:332:ASP:O	1:A:333:HIS:C	2.63	0.42
1:B:86[A]:THR:HG22	1:B:186:ALA:HA	2.01	0.42
1:B:127:LEU:HD21	1:B:155:ALA:HB3	2.01	0.42
1:D:44[B]:ARG:HD2	1:D:50:GLY:O	2.19	0.42
1:E:308:THR:O	1:E:309:VAL:HG23	2.19	0.42
1:F:277:VAL:HG23	1:F:278:PRO:CD	2.44	0.42
1:E:157:ILE:HG13	1:E:161:LEU:HD22	2.00	0.42
1:F:283:GLU:OE1	1:F:344:ASN:ND2	2.52	0.42
1:B:46:PRO:HB2	1:B:47:TYR:CD1	2.54	0.42
1:D:380:LEU:HD11	1:D:405:VAL:HG21	2.02	0.42
2:D:501:HEM:HHC	2:D:501:HEM:HAB	1.66	0.42
1:E:226:ASP:HB2	1:E:229:LEU:O	2.19	0.42
1:E:265[A]:LYS:HB2	1:E:265[A]:LYS:NZ	2.35	0.42
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.86	0.42
1:D:89:GLU:HB2	4:D:503:RAM:C5	2.49	0.42
1:F:105:ARG:NH2	1:F:355:HIS:O	2.38	0.42
1:B:351[A]:HIS:HE1	7:B:809:HOH:O	2.03	0.42
1:C:150:VAL:CG2	5:C:507:FMT:H	2.49	0.42
1:D:14:VAL:O	1:D:44[A]:ARG:NH1	2.44	0.42
1:F:225:ASN:ND2	1:F:227:ASP:OD1	2.53	0.42
1:A:101[B]:HIS:HE1	2:A:501:HEM:O2D	2.01	0.42
1:A:193:GLN:HE22	4:A:503[A]:RAM:H63	1.85	0.42
1:B:42[B]:ARG:HD2	1:B:53:TRP:CH2	2.54	0.42
1:E:174:PHE:HB3	1:E:196:PHE:CD2	2.54	0.42
1:A:21:LEU:HD12	5:A:524:FMT:C	2.50	0.42
1:A:212:THR:O	5:A:546:FMT:O1	2.38	0.42
1:A:354[B]:HIS:HE1	7:A:680:HOH:O	2.03	0.42
1:D:99:PRO:HD2	7:D:651:HOH:O	2.20	0.42
1:D:161:LEU:O	1:D:216:LEU:HB2	2.19	0.42
1:D:190[B]:GLN:HE21	1:D:190[B]:GLN:CA	2.32	0.42
1:F:94:LEU:HD12	1:F:94:LEU:HA	1.94	0.42
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.92	0.41
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.86	0.41
1:B:28:ASP:HA	1:B:29:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:GLN:O	5:C:512:FMT:O1	2.38	0.41
1:D:42:ARG:O	1:D:43:VAL:CG1	2.68	0.41
1:D:123[A]:ARG:HH11	1:D:123[A]:ARG:HG2	1.79	0.41
1:F:154:VAL:HG11	1:F:168[A]:ARG:HE	1.84	0.41
1:A:373[B]:LEU:HD12	1:A:373[B]:LEU:HA	1.85	0.41
2:D:501:HEM:HMB2	2:D:501:HEM:HBB2	2.02	0.41
1:E:219:LEU:O	1:E:223[B]:THR:HG23	2.20	0.41
1:F:75:ALA:HA	1:F:80:THR:HG21	2.01	0.41
1:A:107[B]:LEU:HD21	1:A:222:ALA:HB1	2.02	0.41
1:B:258:HIS:CE1	1:B:262:THR:HG21	2.55	0.41
1:F:24:ALA:HB1	1:F:391:TRP:CE2	2.55	0.41
1:F:140:SER:HB2	1:F:406:SER:HA	2.02	0.41
1:A:283:GLU:HG3	1:A:337:LEU:CD2	2.49	0.41
1:C:107:LEU:HD12	1:C:107:LEU:HA	1.80	0.41
1:C:252:GLN:HA	1:C:252:GLN:OE1	2.19	0.41
1:E:45:LEU:HD22	1:E:81:PRO:CB	2.51	0.41
1:F:144[A]:LEU:HD12	1:F:144[A]:LEU:HA	1.92	0.41
1:F:246:HIS:O	1:F:250:VAL:HG12	2.21	0.41
1:A:36[B]:ARG:NE	1:A:37:ASP:OD1	2.54	0.41
1:B:76:THR:OG1	5:B:538:FMT:O2	2.36	0.41
1:D:191[A]:ARG:HD3	1:D:191[A]:ARG:HA	1.58	0.41
1:F:22:PRO:HB3	1:F:398:ARG:NH2	2.36	0.41
1:F:93[B]:VAL:H	5:F:514:FMT:C	2.34	0.41
1:A:286:ARG:HG2	1:A:325:ASN:HB3	2.03	0.41
1:D:101[A]:HIS:HE1	2:D:501:HEM:O2D	2.03	0.41
1:E:71:SER:HB2	1:E:97:ASP:OD2	2.20	0.41
1:E:192:VAL:O	1:E:193:GLN:C	2.63	0.41
1:C:12[A]:ASP:OD1	1:C:12[A]:ASP:N	2.53	0.41
1:C:185[B]:THR:HG23	1:C:188:GLU:CB	2.51	0.41
1:C:282:GLU:OE1	1:C:346[A]:HIS:HE1	2.04	0.41
1:B:108:VAL:HG13	1:B:112:PHE:CE2	2.56	0.40
1:E:67:ASP:OD1	1:E:69:ARG:HG3	2.21	0.40
1:E:244:ALA:CB	2:E:502:HEM:CHD	2.98	0.40
1:E:256:LEU:O	1:E:284[A]:MET:HE1	2.21	0.40
1:F:42:ARG:HD2	1:F:51:THR:CG2	2.51	0.40
1:F:157:ILE:HD12	1:F:157:ILE:HA	1.90	0.40
1:C:71:SER:OG	1:C:97:ASP:OD2	2.22	0.40
1:C:104:LEU:O	1:C:107:LEU:HB2	2.20	0.40
1:A:252:GLN:O	1:A:256:LEU:HG	2.21	0.40
1:C:204:VAL:HG22	7:C:777:HOH:O	2.20	0.40
1:F:124:VAL:HG21	1:F:364:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:MET:O	1:A:59:SER:C	2.65	0.40
1:A:256:LEU:HB3	1:A:284[A]:MET:SD	2.62	0.40
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.91	0.40
1:D:178:MET:HE1	1:D:196:PHE:HB3	2.04	0.40
1:E:77:ASP:HB3	1:E:80:THR:HG23	2.04	0.40
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.90	0.40
1:C:12[A]:ASP:CB	1:C:51[A]:THR:HG21	2.52	0.40
1:C:197:MET:HE1	1:C:235:VAL:HB	2.04	0.40
1:F:17:TYR:HA	1:F:18:PRO:C	2.46	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360[B]:GLN:NE2	5:A:567:FMT:O2[3_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	273	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/341 (108%)	339 (92%)	29 (8%)	11	14
1	B	358/341 (105%)	333 (93%)	25 (7%)	14	17
1	C	357/341 (105%)	339 (95%)	18 (5%)	22	30
1	D	376/341 (110%)	335 (89%)	41 (11%)	6	6
1	E	368/341 (108%)	329 (89%)	39 (11%)	6	7
1	F	377/341 (111%)	339 (90%)	38 (10%)	7	8
All	All	2204/2046 (108%)	2014 (91%)	190 (9%)	12	11

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	21	LEU
1	A	27	LEU
1	A	44[A]	ARG
1	A	44[B]	ARG
1	A	45	LEU
1	A	93	VAL
1	A	102	THR
1	A	107[A]	LEU
1	A	107[B]	LEU
1	A	108[A]	VAL
1	A	108[B]	VAL
1	A	116	ARG
1	A	124	VAL
1	A	126	SER
1	A	136	VAL
1	A	183	ARG
1	A	194[A]	GLN

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Mol	Chain	Res	Type
1	A	194[B]	GLN
1	A	198	VAL
1	A	201	ASP
1	A	227	ASP
1	A	264	ARG
1	A	269	SER
1	A	276	LEU
1	A	337	LEU
1	A	342[A]	GLU
1	A	342[B]	GLU
1	A	374	VAL
1	B	21	LEU
1	B	42[A]	ARG
1	B	42[B]	ARG
1	B	86[A]	THR
1	B	86[B]	THR
1	B	93	VAL
1	B	106	ARG
1	B	108	VAL
1	B	116	ARG
1	B	123	ARG
1	B	190[A]	GLN
1	B	190[B]	GLN
1	B	204	VAL
1	B	209[A]	ASP
1	B	209[B]	ASP
1	B	209[C]	ASP
1	B	225	ASN
1	B	231	LYS
1	B	264	ARG
1	B	309	VAL
1	B	333[A]	HIS
1	B	333[B]	HIS
1	B	342[A]	GLU
1	B	342[B]	GLU
1	B	374	VAL
1	C	12[A]	ASP
1	C	12[B]	ASP
1	C	27	LEU
1	C	49[A]	GLU
1	C	49[B]	GLU
1	C	107	LEU

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Mol	Chain	Res	Type
1	C	115	ARG
1	C	136	VAL
1	C	183	ARG
1	C	198	VAL
1	C	204	VAL
1	C	206	GLN
1	C	265[A]	LYS
1	C	265[B]	LYS
1	C	302	GLU
1	C	329	GLU
1	C	337	LEU
1	C	374	VAL
1	D	9	THR
1	D	14	VAL
1	D	26	ASP
1	D	42	ARG
1	D	49[A]	GLU
1	D	49[B]	GLU
1	D	59	SER
1	D	86[A]	THR
1	D	86[B]	THR
1	D	94	LEU
1	D	110[A]	LYS
1	D	110[B]	LYS
1	D	123[A]	ARG
1	D	123[B]	ARG
1	D	127	LEU
1	D	132	LEU
1	D	140	SER
1	D	165	LEU
1	D	191[A]	ARG
1	D	191[B]	ARG
1	D	208[A]	ARG
1	D	208[B]	ARG
1	D	216	LEU
1	D	225	ASN
1	D	229[A]	LEU
1	D	229[B]	LEU
1	D	231[A]	LYS
1	D	231[B]	LYS
1	D	262	THR
1	D	263[A]	GLU

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Mol	Chain	Res	Type
1	D	263[B]	GLU
1	D	265[A]	LYS
1	D	265[B]	LYS
1	D	269	SER
1	D	329	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	374	VAL
1	E	12	ASP
1	E	21	LEU
1	E	55	VAL
1	E	71	SER
1	E	80	THR
1	E	93[A]	VAL
1	E	93[B]	VAL
1	E	106	ARG
1	E	107	LEU
1	E	108	VAL
1	E	110	LYS
1	E	117	VAL
1	E	125	ARG
1	E	126	SER
1	E	130	SER
1	E	154	VAL
1	E	161	LEU
1	E	172	ARG
1	E	206	GLN
1	E	208	ARG
1	E	225	ASN
1	E	265[A]	LYS
1	E	265[B]	LYS
1	E	269	SER
1	E	274	PRO
1	E	278	PRO
1	E	309	VAL
1	E	312[A]	ARG
1	E	312[B]	ARG
1	E	329[A]	GLU
1	E	329[B]	GLU

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Mol	Chain	Res	Type
1	E	330	VAL
1	E	343[A]	ARG
1	E	343[B]	ARG
1	E	355[A]	HIS
1	E	355[B]	HIS
1	E	374	VAL
1	E	393[A]	GLN
1	E	393[B]	GLN
1	F	21	LEU
1	F	25	LEU
1	F	27	LEU
1	F	44	ARG
1	F	49	GLU
1	F	94	LEU
1	F	115	ARG
1	F	116	ARG
1	F	120[A]	MET
1	F	120[B]	MET
1	F	127[A]	LEU
1	F	127[B]	LEU
1	F	131[A]	LEU
1	F	131[B]	LEU
1	F	165	LEU
1	F	190[A]	GLN
1	F	190[B]	GLN
1	F	198	VAL
1	F	201	ASP
1	F	207	ARG
1	F	213	GLU
1	F	216	LEU
1	F	219	LEU
1	F	231	LYS
1	F	250	VAL
1	F	262	THR
1	F	264	ARG
1	F	268	GLU
1	F	302	GLU
1	F	309	VAL
1	F	312	ARG
1	F	330	VAL
1	F	374	VAL
1	F	375[A]	ARG

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Mol	Chain	Res	Type
1	F	375[B]	ARG
1	F	376[A]	ARG
1	F	376[B]	ARG
1	F	404	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	236	ASN
1	A	258	HIS
1	A	393	GLN
1	B	193	GLN
1	B	258	HIS
1	B	393	GLN
1	C	193	GLN
1	C	206	GLN
1	C	225	ASN
1	C	344	ASN
1	D	96	GLN
1	D	193	GLN
1	D	225	ASN
1	D	236	ASN
1	D	320	HIS
1	E	193	GLN
1	E	206	GLN
1	E	236	ASN
1	E	403	GLN
1	F	193	GLN
1	F	225	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 236 ligands modelled in this entry, 6 are monoatomic - leaving 230 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FMT	C	512	-	2,2,2	0.74	0	1,1,1	0.06	0
5	FMT	D	506	-	2,2,2	0.67	0	1,1,1	0.13	0
5	FMT	A	565	-	2,2,2	0.59	0	1,1,1	0.05	0
5	FMT	B	537	-	2,2,2	0.36	0	1,1,1	0.10	0
5	FMT	B	539	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	D	516	-	2,2,2	0.27	0	1,1,1	0.18	0
5	FMT	B	504	-	2,2,2	0.68	0	1,1,1	0.19	0
5	FMT	A	514	-	2,2,2	0.07	0	1,1,1	0.05	0
5	FMT	C	525	-	2,2,2	0.62	0	1,1,1	0.03	0
5	FMT	E	516	-	2,2,2	0.28	0	1,1,1	0.14	0
4	RAM	D	503	-	11,11,11	1.12	1 (9%)	16,16,16	2.67	9 (56%)
5	FMT	C	509	-	2,2,2	0.56	0	1,1,1	0.02	0
5	FMT	C	530	-	2,2,2	0.29	0	1,1,1	0.14	0
5	FMT	C	533	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	A	512	-	2,2,2	0.37	0	1,1,1	0.13	0
2	HEM	B	501	1	50,50,50	1.78	15 (30%)	67,82,82	1.93	18 (26%)
5	FMT	E	510	-	2,2,2	0.27	0	1,1,1	0.14	0
5	FMT	C	511	-	2,2,2	0.54	0	1,1,1	0.04	0
5	FMT	D	528	-	2,2,2	0.24	0	1,1,1	0.08	0
5	FMT	E	517	-	2,2,2	0.26	0	1,1,1	0.17	0
5	FMT	A	523	-	2,2,2	0.86	0	1,1,1	0.18	0
5	FMT	A	563	-	2,2,2	0.31	0	1,1,1	0.15	0
5	FMT	A	557	-	2,2,2	0.24	0	1,1,1	0.17	0
5	FMT	C	522	-	2,2,2	0.77	0	1,1,1	0.11	0
5	FMT	D	535	-	2,2,2	0.38	0	1,1,1	0.14	0
5	FMT	D	525	-	2,2,2	0.28	0	1,1,1	0.17	0
5	FMT	A	504	-	2,2,2	0.11	0	1,1,1	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	E	508	-	2,2,2	0.25	0	1,1,1	0.17	0
5	FMT	E	513	-	2,2,2	0.29	0	1,1,1	0.14	0
5	FMT	C	518	-	2,2,2	0.59	0	1,1,1	0.07	0
5	FMT	F	511	-	2,2,2	0.27	0	1,1,1	0.15	0
5	FMT	F	505	-	2,2,2	0.61	0	1,1,1	0.05	0
5	FMT	D	534	-	2,2,2	0.24	0	1,1,1	0.17	0
5	FMT	C	514	-	2,2,2	0.32	0	1,1,1	0.43	0
5	FMT	A	524	-	2,2,2	0.86	0	1,1,1	0.24	0
5	FMT	B	526	-	2,2,2	0.25	0	1,1,1	0.14	0
5	FMT	C	546	-	2,2,2	0.20	0	1,1,1	0.20	0
5	FMT	A	530	-	2,2,2	0.53	0	1,1,1	0.05	0
5	FMT	F	515	-	2,2,2	0.28	0	1,1,1	0.17	0
5	FMT	D	523	-	2,2,2	0.26	0	1,1,1	0.17	0
5	FMT	B	516	-	2,2,2	0.26	0	1,1,1	0.15	0
5	FMT	A	538	-	2,2,2	0.55	0	1,1,1	0.06	0
5	FMT	A	564	-	2,2,2	0.31	0	1,1,1	0.11	0
5	FMT	C	539	-	2,2,2	0.35	0	1,1,1	0.11	0
5	FMT	B	511	-	2,2,2	0.42	0	1,1,1	0.00	0
5	FMT	B	538	-	2,2,2	0.31	0	1,1,1	0.10	0
2	HEM	D	501	1	50,50,50	1.98	14 (28%)	67,82,82	2.04	17 (25%)
3	QR8	F	503	-	26,26,26	1.72	3 (11%)	37,38,38	1.63	9 (24%)
5	FMT	F	512	-	2,2,2	0.28	0	1,1,1	0.14	0
5	FMT	A	518	-	2,2,2	0.23	0	1,1,1	0.23	0
5	FMT	D	524	-	2,2,2	0.30	0	1,1,1	0.15	0
5	FMT	D	514	-	2,2,2	0.55	0	1,1,1	0.00	0
5	FMT	A	561	-	2,2,2	0.33	0	1,1,1	0.13	0
5	FMT	A	560	-	2,2,2	0.53	0	1,1,1	0.02	0
5	FMT	A	573	-	2,2,2	0.20	0	1,1,1	0.18	0
5	FMT	E	501	-	2,2,2	0.49	0	1,1,1	0.04	0
5	FMT	A	539	-	2,2,2	0.29	0	1,1,1	0.13	0
5	FMT	F	513	-	2,2,2	0.41	0	1,1,1	0.06	0
5	FMT	C	549	-	2,2,2	0.29	0	1,1,1	0.14	0
5	FMT	D	537	-	2,2,2	0.61	0	1,1,1	0.13	0
5	FMT	A	536	-	2,2,2	0.40	0	1,1,1	0.02	0
5	FMT	B	520	-	2,2,2	0.31	0	1,1,1	0.13	0
5	FMT	D	521	-	2,2,2	0.27	0	1,1,1	0.17	0
5	FMT	D	507	-	2,2,2	0.60	0	1,1,1	0.07	0
5	FMT	C	508	-	2,2,2	0.31	0	1,1,1	0.21	0
5	FMT	B	503	-	2,2,2	1.03	0	1,1,1	0.28	0
5	FMT	B	522	-	2,2,2	0.32	0	1,1,1	0.12	0
5	FMT	F	504	-	2,2,2	0.43	0	1,1,1	0.05	0
5	FMT	B	534	-	2,2,2	0.31	0	1,1,1	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QR8	A	502	-	26,26,26	1.73	4 (15%)	37,38,38	1.87	10 (27%)
5	FMT	C	531	-	2,2,2	0.26	0	1,1,1	0.15	0
5	FMT	C	551	-	2,2,2	0.24	0	1,1,1	0.15	0
5	FMT	C	515	-	2,2,2	0.87	0	1,1,1	0.15	0
5	FMT	D	532	-	2,2,2	0.19	0	1,1,1	0.17	0
5	FMT	A	531	-	2,2,2	0.61	0	1,1,1	0.07	0
4	RAM	A	503[A]	-	11,11,11	1.32	3 (27%)	16,16,16	3.59	10 (62%)
5	FMT	A	545	-	2,2,2	0.50	0	1,1,1	0.06	0
5	FMT	A	541	-	2,2,2	0.25	0	1,1,1	0.17	0
5	FMT	C	532	-	2,2,2	0.95	0	1,1,1	0.19	0
5	FMT	D	530	-	2,2,2	0.32	0	1,1,1	0.11	0
5	FMT	F	507	-	2,2,2	0.47	0	1,1,1	0.14	0
5	FMT	D	533	-	2,2,2	0.27	0	1,1,1	0.07	0
5	FMT	E	514	-	2,2,2	0.34	0	1,1,1	0.09	0
5	FMT	A	555	-	2,2,2	0.51	0	1,1,1	0.03	0
5	FMT	D	505	-	2,2,2	0.70	0	1,1,1	0.06	0
5	FMT	A	550	-	2,2,2	0.36	0	1,1,1	0.18	0
5	FMT	D	508	-	2,2,2	0.30	0	1,1,1	0.04	0
3	QR8	D	502	-	26,26,26	1.67	4 (15%)	37,38,38	1.90	9 (24%)
5	FMT	A	558	-	2,2,2	0.39	0	1,1,1	0.11	0
5	FMT	A	571	-	2,2,2	0.28	0	1,1,1	0.13	0
5	FMT	C	505	-	2,2,2	0.90	0	1,1,1	0.13	0
5	FMT	B	540	-	2,2,2	0.27	0	1,1,1	0.14	0
5	FMT	C	506	-	2,2,2	0.75	0	1,1,1	0.03	0
5	FMT	D	536	-	2,2,2	0.27	0	1,1,1	0.17	0
5	FMT	C	516	-	2,2,2	0.27	0	1,1,1	0.24	0
5	FMT	B	525	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	A	551	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	A	509	-	2,2,2	0.76	0	1,1,1	0.13	0
5	FMT	C	536	-	2,2,2	0.30	0	1,1,1	0.13	0
5	FMT	A	527	-	2,2,2	0.33	0	1,1,1	0.11	0
5	FMT	A	568	-	2,2,2	0.27	0	1,1,1	0.13	0
5	FMT	B	507	-	2,2,2	0.36	0	1,1,1	0.13	0
5	FMT	D	518	-	2,2,2	0.26	0	1,1,1	0.13	0
5	FMT	F	510	-	2,2,2	0.28	0	1,1,1	0.14	0
5	FMT	A	543	-	2,2,2	0.41	0	1,1,1	0.03	0
5	FMT	B	533	-	2,2,2	0.46	0	1,1,1	0.09	0
5	FMT	C	545	-	2,2,2	0.36	0	1,1,1	0.12	0
5	FMT	A	519	-	2,2,2	0.36	0	1,1,1	0.16	0
3	QR8	C	502	-	26,26,26	1.58	3 (11%)	37,38,38	1.79	8 (21%)
5	FMT	A	544	-	2,2,2	0.41	0	1,1,1	0.03	0
5	FMT	B	512	-	2,2,2	0.64	0	1,1,1	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	A	528	-	2,2,2	0.32	0	1,1,1	0.09	0
5	FMT	F	506	-	2,2,2	0.33	0	1,1,1	0.19	0
5	FMT	A	537	-	2,2,2	0.28	0	1,1,1	0.17	0
5	FMT	C	534	-	2,2,2	0.31	0	1,1,1	0.16	0
5	FMT	C	550	-	2,2,2	0.57	0	1,1,1	0.05	0
4	RAM	B	513	-	11,11,11	1.74	4 (36%)	16,16,16	3.49	9 (56%)
5	FMT	C	535	-	2,2,2	0.30	0	1,1,1	0.14	0
5	FMT	C	541	-	2,2,2	0.31	0	1,1,1	0.12	0
5	FMT	C	503	-	2,2,2	0.76	0	1,1,1	0.18	0
5	FMT	B	527	-	2,2,2	0.27	0	1,1,1	0.14	0
5	FMT	A	506	-	2,2,2	0.97	0	1,1,1	0.30	0
5	FMT	A	546	-	2,2,2	0.45	0	1,1,1	0.00	0
5	FMT	A	542	-	2,2,2	0.26	0	1,1,1	0.16	0
5	FMT	D	520	-	2,2,2	0.31	0	1,1,1	0.11	0
5	FMT	D	519	-	2,2,2	0.31	0	1,1,1	0.16	0
5	FMT	D	531	-	2,2,2	0.45	0	1,1,1	0.01	0
5	FMT	A	535	-	2,2,2	0.27	0	1,1,1	0.13	0
5	FMT	A	533	-	2,2,2	0.27	0	1,1,1	0.17	0
5	FMT	C	513	-	2,2,2	0.61	0	1,1,1	0.09	0
5	FMT	A	505	-	2,2,2	0.48	0	1,1,1	0.18	0
5	FMT	B	536	-	2,2,2	0.28	0	1,1,1	0.18	0
5	FMT	C	520	-	2,2,2	0.63	0	1,1,1	0.10	0
5	FMT	A	510	-	2,2,2	0.46	0	1,1,1	0.08	0
5	FMT	A	522	-	2,2,2	0.65	0	1,1,1	0.03	0
5	FMT	B	523	-	2,2,2	0.35	0	1,1,1	0.10	0
5	FMT	C	540	-	2,2,2	0.41	0	1,1,1	0.08	0
5	FMT	F	509	-	2,2,2	0.44	0	1,1,1	0.08	0
2	HEM	C	501	1	50,50,50	1.86	17 (34%)	67,82,82	2.20	26 (38%)
5	FMT	A	529	-	2,2,2	0.27	0	1,1,1	0.15	0
5	FMT	A	532	-	2,2,2	0.38	0	1,1,1	0.08	0
2	HEM	A	501	1	50,50,50	1.68	11 (22%)	67,82,82	2.04	19 (28%)
5	FMT	A	574	-	2,2,2	0.27	0	1,1,1	0.15	0
2	HEM	E	502	1	50,50,50	1.69	9 (18%)	67,82,82	1.68	17 (25%)
5	FMT	C	517	-	2,2,2	0.60	0	1,1,1	0.06	0
5	FMT	B	509	-	2,2,2	0.60	0	1,1,1	0.03	0
5	FMT	A	559	-	2,2,2	0.33	0	1,1,1	0.09	0
5	FMT	B	524	-	2,2,2	0.40	0	1,1,1	0.04	0
5	FMT	A	508	-	2,2,2	0.95	0	1,1,1	0.15	0
5	FMT	A	513	-	2,2,2	0.49	0	1,1,1	0.05	0
5	FMT	B	517	-	2,2,2	0.39	0	1,1,1	0.09	0
5	FMT	B	529	-	2,2,2	0.43	0	1,1,1	0.02	0
5	FMT	B	508	-	2,2,2	0.43	0	1,1,1	0.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	C	521	-	2,2,2	0.06	0	1,1,1	0.33	0
5	FMT	A	556	-	2,2,2	0.31	0	1,1,1	0.14	0
5	FMT	C	524	-	2,2,2	0.16	0	1,1,1	0.43	0
5	FMT	C	507	-	2,2,2	0.73	0	1,1,1	0.32	0
5	FMT	C	537	-	2,2,2	0.33	0	1,1,1	0.15	0
5	FMT	A	562	-	2,2,2	0.66	0	1,1,1	0.07	0
5	FMT	B	521	-	2,2,2	0.52	0	1,1,1	0.05	0
5	FMT	A	511	-	2,2,2	0.69	0	1,1,1	0.13	0
5	FMT	B	531	-	2,2,2	0.30	0	1,1,1	0.15	0
5	FMT	A	515	-	2,2,2	0.46	0	1,1,1	0.07	0
5	FMT	A	517	-	2,2,2	0.30	0	1,1,1	0.16	0
5	FMT	A	554	-	2,2,2	0.33	0	1,1,1	0.11	0
5	FMT	A	553	-	2,2,2	0.35	0	1,1,1	0.10	0
5	FMT	E	505	-	2,2,2	0.33	0	1,1,1	0.14	0
5	FMT	D	509	-	2,2,2	0.70	0	1,1,1	0.02	0
5	FMT	A	549	-	2,2,2	0.42	0	1,1,1	0.00	0
5	FMT	C	510	-	2,2,2	0.54	0	1,1,1	0.07	0
5	FMT	C	528	-	2,2,2	0.31	0	1,1,1	0.16	0
5	FMT	D	527	-	2,2,2	0.27	0	1,1,1	0.15	0
5	FMT	D	511	-	2,2,2	0.69	0	1,1,1	0.04	0
5	FMT	E	515	-	2,2,2	0.33	0	1,1,1	0.09	0
5	FMT	D	515	-	2,2,2	0.34	0	1,1,1	0.11	0
5	FMT	E	504	-	2,2,2	0.89	0	1,1,1	0.32	0
5	FMT	C	523	-	2,2,2	0.22	0	1,1,1	0.15	0
5	FMT	B	528	-	2,2,2	0.38	0	1,1,1	0.11	0
5	FMT	D	510	-	2,2,2	0.44	0	1,1,1	0.07	0
5	FMT	C	538	-	2,2,2	0.42	0	1,1,1	0.10	0
5	FMT	A	507	-	2,2,2	0.65	0	1,1,1	0.12	0
3	QR8	B	502	-	26,26,26	1.83	4 (15%)	37,38,38	1.77	12 (32%)
5	FMT	A	552	-	2,2,2	0.35	0	1,1,1	0.11	0
5	FMT	A	548	-	2,2,2	0.56	0	1,1,1	0.00	0
5	FMT	A	569	-	2,2,2	0.26	0	1,1,1	0.17	0
5	FMT	A	520	-	2,2,2	0.41	0	1,1,1	0.09	0
5	FMT	C	542	-	2,2,2	0.34	0	1,1,1	0.11	0
3	QR8	E	503	-	26,26,26	1.58	4 (15%)	37,38,38	1.80	12 (32%)
5	FMT	E	512	-	2,2,2	0.30	0	1,1,1	0.12	0
5	FMT	C	552	-	2,2,2	0.31	0	1,1,1	0.15	0
5	FMT	A	572	-	2,2,2	0.26	0	1,1,1	0.14	0
5	FMT	A	547	-	2,2,2	0.33	0	1,1,1	0.12	0
5	FMT	D	526	-	2,2,2	0.33	0	1,1,1	0.13	0
5	FMT	A	567	-	2,2,2	0.32	0	1,1,1	0.13	0
5	FMT	B	530	-	2,2,2	0.19	0	1,1,1	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	F	502	1	50,50,50	1.59	10 (20%)	67,82,82	1.59	12 (17%)
5	FMT	A	540	-	2,2,2	0.25	0	1,1,1	0.15	0
5	FMT	C	529	-	2,2,2	0.23	0	1,1,1	0.16	0
5	FMT	D	522	-	2,2,2	0.25	0	1,1,1	0.17	0
4	RAM	A	503[B]	-	11,11,11	1.37	2 (18%)	16,16,16	2.61	10 (62%)
5	FMT	A	516	-	2,2,2	0.46	0	1,1,1	0.03	0
5	FMT	B	532	-	2,2,2	0.20	0	1,1,1	0.16	0
5	FMT	C	526	-	2,2,2	0.61	0	1,1,1	0.07	0
5	FMT	B	505	-	2,2,2	0.80	0	1,1,1	0.12	0
5	FMT	F	514	-	2,2,2	0.59	0	1,1,1	0.12	0
5	FMT	E	509	-	2,2,2	0.29	0	1,1,1	0.16	0
5	FMT	A	525	-	2,2,2	0.50	0	1,1,1	0.07	0
5	FMT	B	510	-	2,2,2	0.36	0	1,1,1	0.11	0
5	FMT	E	511	-	2,2,2	0.25	0	1,1,1	0.18	0
5	FMT	A	566	-	2,2,2	0.35	0	1,1,1	0.11	0
5	FMT	B	535	-	2,2,2	0.39	0	1,1,1	0.09	0
5	FMT	A	534	-	2,2,2	0.24	0	1,1,1	0.14	0
5	FMT	A	521	-	2,2,2	1.49	1 (50%)	1,1,1	0.30	0
5	FMT	D	504	-	2,2,2	0.87	0	1,1,1	0.12	0
5	FMT	B	518	-	2,2,2	0.26	0	1,1,1	0.16	0
5	FMT	C	548	-	2,2,2	0.30	0	1,1,1	0.17	0
5	FMT	B	514	-	2,2,2	0.77	0	1,1,1	0.11	0
5	FMT	D	517	-	2,2,2	0.24	0	1,1,1	0.16	0
5	FMT	D	529	-	2,2,2	0.31	0	1,1,1	0.18	0
5	FMT	C	519	-	2,2,2	0.67	0	1,1,1	0.05	0
5	FMT	C	504	-	2,2,2	0.87	0	1,1,1	0.42	0
5	FMT	B	506	-	2,2,2	0.68	0	1,1,1	0.13	0
5	FMT	F	501	-	2,2,2	0.30	0	1,1,1	0.10	0
5	FMT	C	547	-	2,2,2	0.38	0	1,1,1	0.08	0
5	FMT	C	543	-	2,2,2	0.33	0	1,1,1	0.10	0
5	FMT	C	544	-	2,2,2	0.45	0	1,1,1	0.01	0
5	FMT	B	519	-	2,2,2	0.26	0	1,1,1	0.17	0
5	FMT	D	512	-	2,2,2	0.48	0	1,1,1	0.05	0
5	FMT	E	506	-	2,2,2	0.37	0	1,1,1	0.01	0
5	FMT	A	570	-	2,2,2	0.22	0	1,1,1	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	1	-	0/14/54/54	-
4	RAM	B	513	-	-	-	0/1/1/1
3	QR8	B	502	-	-	15/48/48/48	0/1/1/1
2	HEM	E	502	1	-	1/14/54/54	-
3	QR8	D	502	-	-	13/48/48/48	0/1/1/1
3	QR8	E	503	-	-	15/48/48/48	0/1/1/1
4	RAM	A	503[A]	-	-	-	0/1/1/1
4	RAM	D	503	-	-	-	0/1/1/1
4	RAM	A	503[B]	-	-	-	0/1/1/1
2	HEM	D	501	1	-	0/14/54/54	-
3	QR8	F	503	-	-	13/48/48/48	0/1/1/1
3	QR8	C	502	-	-	14/48/48/48	0/1/1/1
2	HEM	F	502	1	-	0/14/54/54	-
2	HEM	B	501	1	-	0/14/54/54	-
2	HEM	C	501	1	-	1/14/54/54	-
3	QR8	A	502	-	-	13/48/48/48	0/1/1/1

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	QR8	O2-C13	-6.00	1.37	1.46
2	E	502	HEM	FE-NB	5.89	2.13	1.94
2	D	501	HEM	C1D-ND	-5.87	1.27	1.38
3	C	502	QR8	O2-C13	-5.39	1.38	1.46
3	A	502	QR8	O2-C13	-4.98	1.39	1.46
3	D	502	QR8	O2-C13	-4.88	1.39	1.46
2	A	501	HEM	C1B-NB	-4.86	1.31	1.40
2	D	501	HEM	C1B-NB	-4.67	1.32	1.40
2	D	501	HEM	C1C-NC	-4.61	1.30	1.39
2	F	502	HEM	FE-NB	4.58	2.09	1.94
3	F	503	QR8	O2-C13	-4.58	1.39	1.46
2	F	502	HEM	FE-NC	4.42	2.09	1.95
3	E	503	QR8	O2-C13	-4.36	1.39	1.46
2	B	501	HEM	FE-NC	4.31	2.09	1.95
2	E	502	HEM	C4D-ND	-4.12	1.33	1.40
2	C	501	HEM	CHD-C4C	-4.11	1.30	1.38
3	F	503	QR8	O2-C1	4.10	1.43	1.34
2	C	501	HEM	FE-ND	-4.10	1.82	1.94
2	C	501	HEM	C1B-NB	-4.02	1.33	1.40
3	E	503	QR8	O2-C1	3.86	1.43	1.34
2	A	501	HEM	FE-ND	-3.82	1.83	1.94
3	D	502	QR8	C10-C9	-3.77	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1D-ND	-3.59	1.31	1.38
2	E	502	HEM	FE-NC	3.57	2.06	1.95
2	D	501	HEM	C4C-NC	-3.48	1.33	1.39
2	B	501	HEM	C4B-NB	-3.46	1.32	1.38
3	A	502	QR8	O2-C1	3.46	1.42	1.34
3	F	503	QR8	C10-C9	-3.44	1.47	1.52
2	D	501	HEM	C4B-NB	-3.42	1.32	1.38
2	D	501	HEM	FE-NC	3.42	2.06	1.95
2	F	502	HEM	C4D-ND	-3.36	1.34	1.40
3	D	502	QR8	O2-C1	3.34	1.41	1.34
3	B	502	QR8	O2-C1	3.31	1.41	1.34
2	B	501	HEM	C4C-NC	-3.31	1.33	1.39
2	B	501	HEM	CHB-C1B	3.27	1.45	1.38
2	C	501	HEM	C1D-ND	-3.23	1.32	1.38
2	D	501	HEM	FE-NB	3.21	2.04	1.94
2	B	501	HEM	C1C-NC	-3.20	1.33	1.39
3	B	502	QR8	C10-C9	-3.14	1.47	1.52
2	B	501	HEM	FE-NA	3.13	2.05	1.95
4	B	513	RAM	C4-C5	3.07	1.59	1.52
2	D	501	HEM	FE-NA	3.02	2.05	1.95
2	C	501	HEM	C4B-NB	-3.00	1.33	1.38
4	B	513	RAM	O3-C3	2.95	1.50	1.43
3	C	502	QR8	O2-C1	2.93	1.41	1.34
2	F	502	HEM	C1B-NB	-2.91	1.35	1.40
2	A	501	HEM	CHD-C1D	-2.91	1.32	1.39
4	A	503[B]	RAM	C6-C5	-2.84	1.44	1.51
2	E	502	HEM	C3B-C4B	2.81	1.50	1.44
2	F	502	HEM	CHB-C1B	2.75	1.44	1.38
2	A	501	HEM	C1C-NC	-2.73	1.34	1.39
2	B	501	HEM	FE-NB	2.72	2.03	1.94
2	B	501	HEM	C3C-C4C	-2.72	1.41	1.46
2	A	501	HEM	C1D-ND	-2.70	1.33	1.38
2	B	501	HEM	C1C-C2C	-2.65	1.40	1.45
2	D	501	HEM	O2A-CGA	-2.62	1.22	1.30
4	B	513	RAM	C3-C2	2.61	1.59	1.52
2	C	501	HEM	CAB-C3B	-2.61	1.40	1.47
2	C	501	HEM	CMC-C2C	2.59	1.56	1.50
2	A	501	HEM	FE-NB	2.57	2.02	1.94
2	E	502	HEM	C1D-ND	-2.56	1.33	1.38
2	B	501	HEM	CHA-C4D	2.55	1.43	1.38
3	A	502	QR8	C10-C9	-2.54	1.48	1.52
2	F	502	HEM	C1C-NC	-2.54	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503[B]	RAM	O5-C1	2.53	1.49	1.42
2	C	501	HEM	C4C-NC	-2.52	1.34	1.39
2	E	502	HEM	C4B-NB	-2.52	1.33	1.38
2	C	501	HEM	C1A-NA	-2.51	1.34	1.39
3	E	503	QR8	C10-C9	-2.50	1.48	1.52
2	A	501	HEM	C4D-C3D	2.50	1.49	1.45
2	C	501	HEM	O2D-CGD	-2.50	1.22	1.30
3	A	502	QR8	C7-C6	-2.48	1.50	1.54
2	D	501	HEM	CHC-C1C	-2.47	1.33	1.38
2	B	501	HEM	C1B-NB	-2.43	1.36	1.40
2	B	501	HEM	CMC-C2C	2.41	1.55	1.50
2	A	501	HEM	C1C-C2C	-2.41	1.40	1.45
3	D	502	QR8	C7-C6	-2.39	1.50	1.54
3	B	502	QR8	C7-C6	-2.36	1.50	1.54
4	A	503[A]	RAM	C6-C5	-2.35	1.45	1.51
2	D	501	HEM	C4D-C3D	2.35	1.49	1.45
2	A	501	HEM	C3C-C4C	-2.35	1.41	1.46
4	B	513	RAM	C6-C5	2.35	1.57	1.51
2	B	501	HEM	O1D-CGD	2.34	1.29	1.22
4	D	503	RAM	O3-C3	2.29	1.48	1.43
2	A	501	HEM	C4A-C3A	-2.27	1.37	1.43
2	C	501	HEM	C3C-C4C	-2.26	1.42	1.46
2	B	501	HEM	CMD-C2D	-2.26	1.46	1.50
2	C	501	HEM	O1A-CGA	2.25	1.29	1.22
2	E	502	HEM	CHC-C1C	2.21	1.42	1.38
2	C	501	HEM	C1C-NC	-2.21	1.35	1.39
2	D	501	HEM	FE-ND	-2.20	1.88	1.94
2	C	501	HEM	C3C-C2C	2.19	1.41	1.37
2	F	502	HEM	C4B-NB	-2.18	1.34	1.38
2	A	501	HEM	CHA-C1A	-2.18	1.34	1.39
2	F	502	HEM	C1C-C2C	-2.16	1.41	1.45
2	E	502	HEM	C1D-C2D	2.16	1.48	1.44
2	F	502	HEM	O2A-CGA	-2.13	1.23	1.30
2	C	501	HEM	CHD-C1D	-2.13	1.34	1.39
4	A	503[A]	RAM	C1-C2	-2.13	1.47	1.52
4	A	503[A]	RAM	O3-C3	-2.13	1.37	1.43
2	F	502	HEM	FE-NA	2.10	2.02	1.95
2	D	501	HEM	O1D-CGD	2.09	1.28	1.22
2	D	501	HEM	C1D-C2D	2.08	1.48	1.44
5	A	521	FMT	O2-C	2.07	1.39	1.28
3	C	502	QR8	C7-C6	-2.06	1.50	1.54
2	C	501	HEM	C3B-C2B	-2.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	QR8	C10-C11	-2.05	1.49	1.53
2	C	501	HEM	C1C-C2C	-2.05	1.41	1.45
2	E	502	HEM	C1C-NC	-2.04	1.35	1.39

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CHC-C4B-NB	8.44	133.51	124.42
4	A	503[A]	RAM	O1-C1-C2	-8.37	84.68	108.98
2	A	501	HEM	CHC-C4B-NB	8.31	133.37	124.42
2	C	501	HEM	CHC-C4B-NB	6.95	131.90	124.42
4	A	503[A]	RAM	O3-C3-C2	-6.57	94.89	110.38
2	F	502	HEM	CHC-C4B-NB	6.00	130.88	124.42
2	C	501	HEM	CMA-C3A-C4A	5.95	134.49	125.42
4	B	513	RAM	C6-C5-C4	5.72	123.54	113.08
4	B	513	RAM	O3-C3-C2	5.38	123.06	110.38
3	A	502	QR8	C8-C9-C10	-5.09	110.53	119.13
4	B	513	RAM	C4-C3-C2	-4.99	102.06	110.83
2	B	501	HEM	CHC-C4B-NB	4.90	129.70	124.42
2	F	502	HEM	C1B-NB-C4B	4.85	110.95	105.21
4	B	513	RAM	C3-C4-C5	-4.81	102.51	109.81
4	A	503[A]	RAM	O4-C4-C3	4.68	121.40	110.38
3	C	502	QR8	C8-C9-C10	-4.64	111.29	119.13
4	B	513	RAM	O2-C2-C3	4.62	121.27	110.38
2	C	501	HEM	C3C-C2C-C1C	-4.62	102.67	107.05
4	A	503[B]	RAM	C6-C5-C4	-4.54	104.78	113.08
4	B	513	RAM	O3-C3-C4	4.47	120.92	110.38
2	B	501	HEM	C1B-NB-C4B	4.47	110.50	105.21
4	A	503[A]	RAM	C1-O5-C5	4.43	121.27	114.37
3	B	502	QR8	C36-C13-C12	-4.40	108.26	114.46
3	D	502	QR8	C8-C9-C10	-4.24	111.96	119.13
2	C	501	HEM	CMB-C2B-C1B	4.19	131.58	125.03
2	E	502	HEM	C3B-C4B-NB	-4.17	106.48	109.47
4	B	513	RAM	O4-C4-C5	4.08	118.74	109.74
4	D	503	RAM	O1-C1-C2	4.08	120.82	108.98
3	D	502	QR8	O11-C9-C8	4.05	128.61	121.30
4	A	503[B]	RAM	O3-C3-C4	-4.05	100.84	110.38
2	D	501	HEM	CHC-C1C-NC	-4.03	120.06	124.45
2	B	501	HEM	CHD-C1D-ND	4.01	128.74	124.42
2	A	501	HEM	O2A-CGA-O1A	-3.92	113.24	123.33
3	D	502	QR8	C36-C13-C12	-3.91	108.94	114.46
4	D	503	RAM	O5-C1-C2	-3.89	103.46	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	QR8	O11-C9-C8	3.87	128.28	121.30
2	B	501	HEM	CHA-C4D-ND	3.85	129.12	124.37
4	D	503	RAM	O2-C2-C1	3.81	118.04	109.25
2	D	501	HEM	CMD-C2D-C1D	3.81	130.99	125.03
2	C	501	HEM	CHC-C1C-NC	-3.81	120.31	124.45
2	B	501	HEM	CHD-C1D-C2D	-3.80	119.03	125.03
2	D	501	HEM	C1B-NB-C4B	3.76	109.66	105.21
4	D	503	RAM	O3-C3-C2	3.74	119.19	110.38
2	A	501	HEM	CHD-C4C-NC	3.73	128.51	124.45
3	C	502	QR8	C8-C7-C6	3.73	121.78	115.09
4	A	503[B]	RAM	C1-C2-C3	-3.71	102.79	110.36
3	D	502	QR8	C34-C10-C11	3.69	118.95	112.42
3	B	502	QR8	C8-C9-C10	-3.67	112.92	119.13
3	E	503	QR8	C8-C9-C10	-3.66	112.93	119.13
2	D	501	HEM	CHC-C4B-C3B	-3.63	117.82	125.07
2	E	502	HEM	C1B-NB-C4B	3.62	109.49	105.21
2	C	501	HEM	CMA-C3A-C2A	-3.61	117.97	125.62
2	C	501	HEM	CBA-CAA-C2A	3.58	122.44	112.53
2	E	502	HEM	CHB-C1B-NB	3.57	128.78	124.37
3	E	503	QR8	O2-C1-C2	3.53	119.07	111.53
3	E	503	QR8	C36-C13-C12	-3.50	109.53	114.46
4	D	503	RAM	C4-C3-C2	-3.49	104.71	110.83
3	A	502	QR8	C7-C8-C9	3.47	118.64	110.92
2	D	501	HEM	CAD-C3D-C4D	3.46	130.73	124.70
2	A	501	HEM	CHC-C4B-C3B	-3.45	118.18	125.07
3	C	502	QR8	C34-C10-C9	3.45	114.13	108.09
3	F	503	QR8	C32-C6-C5	-3.43	105.24	111.45
2	B	501	HEM	C3C-C2C-C1C	-3.42	103.81	107.05
3	F	503	QR8	O2-C1-C2	3.42	118.83	111.53
2	B	501	HEM	CHA-C4D-C3D	-3.40	118.95	125.23
4	B	513	RAM	C1-C2-C3	3.36	117.21	110.36
2	D	501	HEM	C4A-CHB-C1B	-3.35	118.36	126.25
4	A	503[A]	RAM	O2-C2-C1	-3.35	101.51	109.25
2	A	501	HEM	CAD-C3D-C4D	3.32	130.48	124.70
4	D	503	RAM	C1-C2-C3	-3.30	103.63	110.36
4	A	503[B]	RAM	O5-C1-C2	-3.21	104.65	110.30
2	E	502	HEM	CMA-C3A-C4A	3.18	130.27	125.42
2	B	501	HEM	O2A-CGA-CBA	3.18	124.04	114.00
2	D	501	HEM	CBD-CAD-C3D	-3.17	103.78	112.53
3	E	503	QR8	C32-C6-C7	-3.16	105.89	110.68
2	C	501	HEM	CHD-C1D-ND	3.15	127.81	124.42
3	C	502	QR8	O11-C9-C10	3.15	125.01	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	QR8	O2-C1-C2	3.13	118.22	111.53
3	A	502	QR8	C32-C6-C7	-3.11	105.97	110.68
3	C	502	QR8	C34-C10-C11	3.08	117.87	112.42
3	F	503	QR8	C10-C11-C12	-3.08	108.57	114.49
2	C	501	HEM	C3B-C2B-C1B	-3.07	104.11	106.41
4	A	503[B]	RAM	O3-C3-C2	3.06	117.59	110.38
3	C	502	QR8	O2-C1-O1	-3.05	118.45	123.95
3	F	503	QR8	C36-C13-C12	-3.03	110.19	114.46
3	E	503	QR8	C7-C8-C9	3.02	117.66	110.92
4	B	513	RAM	C1-O5-C5	3.01	119.06	114.37
3	A	502	QR8	C36-C13-C12	-3.01	110.22	114.46
2	B	501	HEM	C1A-CHA-C4D	-3.00	119.19	126.25
2	B	501	HEM	CAD-C3D-C4D	3.00	129.92	124.70
4	A	503[B]	RAM	O1-C1-O5	3.00	119.31	110.41
3	A	502	QR8	C2-C3-C4	-2.99	108.72	114.49
3	D	502	QR8	O2-C1-C2	2.98	117.89	111.53
2	E	502	HEM	CHA-C4D-ND	2.97	128.04	124.37
2	A	501	HEM	C1B-NB-C4B	2.94	108.69	105.21
2	A	501	HEM	CHA-C4D-ND	2.93	128.00	124.37
2	D	501	HEM	CHB-C1B-NB	2.92	127.98	124.37
3	B	502	QR8	C32-C6-C7	-2.91	106.28	110.68
2	C	501	HEM	C1A-CHA-C4D	-2.89	119.44	126.25
3	D	502	QR8	C2-C3-C4	-2.88	108.94	114.49
4	D	503	RAM	O5-C5-C4	-2.86	104.40	109.55
2	B	501	HEM	CMD-C2D-C1D	2.86	129.50	125.03
4	A	503[B]	RAM	C1-O5-C5	-2.85	109.94	114.37
2	B	501	HEM	C4C-C3C-C2C	2.85	109.28	106.81
3	A	502	QR8	C34-C10-C11	2.83	117.43	112.42
3	B	502	QR8	C7-C8-C9	2.83	117.22	110.92
3	A	502	QR8	C32-C6-C5	-2.82	106.34	111.45
3	B	502	QR8	C34-C10-C11	2.81	117.40	112.42
2	F	502	HEM	CMD-C2D-C1D	2.81	129.43	125.03
3	C	502	QR8	O2-C1-C2	2.80	117.52	111.53
3	E	503	QR8	C32-C6-C5	-2.80	106.38	111.45
3	D	502	QR8	C7-C8-C9	2.79	117.13	110.92
2	D	501	HEM	O2A-CGA-O1A	-2.78	116.18	123.33
2	A	501	HEM	C1C-CHC-C4B	-2.78	120.11	126.02
3	C	502	QR8	C7-C8-C9	2.76	117.06	110.92
2	D	501	HEM	CHA-C4D-ND	2.76	127.78	124.37
3	F	503	QR8	C2-C3-C4	-2.75	109.19	114.49
2	E	502	HEM	CHD-C1D-ND	2.73	127.36	124.42
2	B	501	HEM	C4A-C3A-C2A	2.73	109.94	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	QR8	O2-C1-O1	-2.71	119.06	123.95
2	C	501	HEM	C3D-C4D-ND	2.70	113.13	110.17
3	F	503	QR8	C35-C12-C13	-2.70	108.86	112.22
2	C	501	HEM	CHD-C1D-C2D	-2.68	120.80	125.03
2	D	501	HEM	C3C-C2C-C1C	-2.67	104.52	107.05
3	A	502	QR8	O2-C1-C2	2.67	117.23	111.53
3	F	503	QR8	O7-C5-C6	-2.66	104.72	109.79
2	A	501	HEM	CMD-C2D-C1D	2.66	129.19	125.03
2	A	501	HEM	O2D-CGD-CBD	2.66	122.39	114.00
2	E	502	HEM	CBD-CAD-C3D	-2.65	105.20	112.53
2	E	502	HEM	CHD-C1D-C2D	-2.65	120.85	125.03
2	D	501	HEM	CAB-C3B-C2B	2.65	137.03	128.43
4	A	503[A]	RAM	O5-C1-C2	2.64	114.94	110.30
2	C	501	HEM	C3B-C4B-NB	-2.64	107.57	109.47
2	F	502	HEM	CHD-C1D-ND	2.63	127.25	124.42
2	A	501	HEM	C1A-CHA-C4D	-2.63	120.06	126.25
4	D	503	RAM	O4-C4-C5	2.63	115.53	109.74
2	E	502	HEM	CHA-C4D-C3D	-2.60	120.42	125.23
2	E	502	HEM	CBA-CAA-C2A	2.60	119.73	112.53
2	A	501	HEM	CAD-CBD-CGD	2.60	120.56	113.67
2	A	501	HEM	C4A-C3A-C2A	2.60	109.79	106.82
2	E	502	HEM	O2A-CGA-O1A	-2.59	116.67	123.33
3	B	502	QR8	C2-C3-C4	-2.59	109.51	114.49
2	E	502	HEM	CHC-C4B-NB	2.57	127.19	124.42
2	A	501	HEM	CHA-C4D-C3D	-2.57	120.49	125.23
2	C	501	HEM	CAB-C3B-C2B	2.51	136.60	128.43
2	C	501	HEM	C4D-C3D-C2D	-2.50	103.25	106.89
2	C	501	HEM	CHA-C4D-C3D	-2.49	120.63	125.23
3	B	502	QR8	O11-C9-C8	2.49	125.80	121.30
2	C	501	HEM	O2D-CGD-O1D	-2.48	116.95	123.33
3	E	503	QR8	C8-C7-C6	2.47	119.52	115.09
4	A	503[B]	RAM	O5-C5-C6	2.47	112.22	106.74
2	C	501	HEM	CAD-C3D-C4D	2.46	128.98	124.70
2	B	501	HEM	CMA-C3A-C4A	-2.45	121.69	125.42
3	D	502	QR8	C11-C10-C9	-2.44	105.76	110.11
2	F	502	HEM	CHA-C4D-ND	2.42	127.36	124.37
3	F	503	QR8	O2-C1-O1	-2.41	119.59	123.95
2	D	501	HEM	C2D-C1D-ND	2.41	112.69	109.90
2	E	502	HEM	C4A-CHB-C1B	-2.41	120.59	126.25
4	A	503[A]	RAM	C6-C5-C4	-2.40	108.69	113.08
2	C	501	HEM	CHA-C1A-NA	2.39	128.20	123.86
2	A	501	HEM	CHD-C1D-C2D	-2.39	121.26	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	QR8	C8-C7-C6	2.36	119.33	115.09
3	E	503	QR8	C6-C5-C4	-2.36	112.66	116.20
2	E	502	HEM	O2A-CGA-CBA	2.36	121.45	114.00
2	E	502	HEM	CAA-C2A-C1A	2.34	129.52	124.94
2	E	502	HEM	C1D-C2D-C3D	-2.33	104.53	106.98
3	B	502	QR8	C32-C6-C5	-2.32	107.25	111.45
2	D	501	HEM	C1A-CHA-C4D	-2.32	120.80	126.25
2	F	502	HEM	O2A-CGA-O1A	-2.31	117.40	123.33
2	C	501	HEM	C1B-NB-C4B	2.30	107.93	105.21
2	B	501	HEM	C3B-C4B-NB	-2.29	107.82	109.47
2	C	501	HEM	CHC-C4B-C3B	-2.29	120.50	125.07
2	F	502	HEM	CHD-C1D-C2D	-2.29	121.42	125.03
3	E	503	QR8	C34-C10-C9	2.25	112.03	108.09
2	B	501	HEM	C4C-CHD-C1D	-2.25	121.24	126.02
3	D	502	QR8	O2-C1-O1	-2.24	119.91	123.95
3	F	503	QR8	C13-O2-C1	-2.24	114.25	117.55
2	A	501	HEM	CBB-CAB-C3B	-2.23	116.38	127.53
2	E	502	HEM	CHB-C1B-C2B	-2.23	120.62	126.95
2	F	502	HEM	CHC-C4B-C3B	-2.23	120.63	125.07
4	A	503[A]	RAM	C3-C4-C5	-2.22	106.43	109.81
4	A	503[B]	RAM	O5-C5-C4	-2.20	105.59	109.55
2	D	501	HEM	C4D-C3D-C2D	-2.20	103.69	106.89
2	D	501	HEM	CHA-C4D-C3D	-2.20	121.18	125.23
2	C	501	HEM	CAA-C2A-C1A	2.20	129.23	124.94
3	E	503	QR8	C11-C10-C9	-2.19	106.22	110.11
4	A	503[B]	RAM	O2-C2-C3	2.18	115.52	110.38
4	A	503[A]	RAM	O2-C2-C3	2.18	115.52	110.38
2	C	501	HEM	CHA-C1A-C2A	-2.17	120.54	125.30
3	B	502	QR8	C11-C10-C9	-2.17	106.24	110.11
2	B	501	HEM	C1A-C2A-C3A	-2.17	103.51	106.87
2	C	501	HEM	CAB-C3B-C4B	-2.15	114.89	124.39
4	A	503[A]	RAM	O3-C3-C4	2.14	115.43	110.38
2	F	502	HEM	CHD-C4C-NC	2.14	126.79	124.45
2	C	501	HEM	CAC-C3C-C4C	-2.14	119.72	124.82
2	A	501	HEM	CBA-CAA-C2A	2.10	118.35	112.53
2	F	502	HEM	O2D-CGD-O1D	-2.10	117.93	123.33
2	F	502	HEM	O2D-CGD-CBD	2.08	120.56	114.00
2	C	501	HEM	CHD-C4C-NC	2.07	126.71	124.45
3	E	503	QR8	C2-C3-C4	-2.07	110.51	114.49
2	F	502	HEM	CHB-C1B-NB	2.05	126.91	124.37
3	A	502	QR8	C31-C4-C3	-2.04	107.41	111.43
2	A	501	HEM	C2D-C1D-ND	2.04	112.26	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	QR8	O2-C1-O1	-2.03	120.28	123.95
4	D	503	RAM	O2-C2-C3	2.02	115.15	110.38
2	B	501	HEM	CAB-C3B-C2B	2.02	134.99	128.43
2	A	501	HEM	CAB-C3B-C2B	2.00	134.94	128.43

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	QR8	C6-C7-C8-C9
3	A	502	QR8	C1-C2-C3-O3
3	B	502	QR8	C6-C7-C8-C9
3	B	502	QR8	C1-C2-C3-O3
3	C	502	QR8	C6-C7-C8-C9
3	C	502	QR8	C6-C7-C8-C33
3	C	502	QR8	C1-C2-C3-O3
3	D	502	QR8	C6-C7-C8-C9
3	D	502	QR8	C6-C7-C8-C33
3	D	502	QR8	C31-C4-C5-O7
3	D	502	QR8	C3-C4-C5-O7
3	D	502	QR8	C30-C2-C3-C4
3	D	502	QR8	C1-C2-C3-O3
3	E	503	QR8	C6-C7-C8-C9
3	F	503	QR8	C30-C2-C3-C4
3	A	502	QR8	C3-C4-C5-O7
3	B	502	QR8	C3-C4-C5-O7
3	E	503	QR8	C3-C4-C5-O7
3	F	503	QR8	C3-C4-C5-O7
3	C	502	QR8	C3-C4-C5-O7
3	A	502	QR8	C30-C2-C3-O3
3	B	502	QR8	C30-C2-C3-O3
3	C	502	QR8	C30-C2-C3-O3
3	D	502	QR8	C30-C2-C3-O3
3	F	503	QR8	C30-C2-C3-O3
3	A	502	QR8	C30-C2-C3-C4
3	B	502	QR8	C30-C2-C3-C4
3	C	502	QR8	C30-C2-C3-C4
3	A	502	QR8	C31-C4-C5-O7
3	E	503	QR8	C31-C4-C5-O7
3	A	502	QR8	C6-C7-C8-C33
3	E	503	QR8	C6-C7-C8-C33
3	B	502	QR8	C31-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
3	C	502	QR8	C31-C4-C5-O7
3	F	503	QR8	C31-C4-C5-O7
3	E	503	QR8	C30-C2-C3-C4
3	D	502	QR8	C3-C4-C5-C6
3	F	503	QR8	C3-C4-C5-C6
3	B	502	QR8	C5-C6-C7-C8
3	E	503	QR8	C30-C2-C3-O3
3	D	502	QR8	C31-C4-C5-C6
3	F	503	QR8	C7-C8-C9-C10
3	A	502	QR8	C31-C4-C5-C6
3	C	502	QR8	C31-C4-C5-C6
3	F	503	QR8	C31-C4-C5-C6
3	B	502	QR8	C31-C4-C5-C6
3	E	503	QR8	C31-C4-C5-C6
3	B	502	QR8	C3-C4-C5-C6
3	C	502	QR8	C3-C4-C5-C6
3	E	503	QR8	C3-C4-C5-C6
3	A	502	QR8	C32-C6-C7-C8
3	D	502	QR8	C32-C6-C7-C8
3	A	502	QR8	C3-C4-C5-C6
2	E	502	HEM	C4B-C3B-CAB-CBB
3	B	502	QR8	C6-C7-C8-C33
3	E	503	QR8	C1-C2-C3-O3
3	F	503	QR8	C1-C2-C3-O3
3	A	502	QR8	C5-C6-C7-C8
3	D	502	QR8	C5-C6-C7-C8
3	E	503	QR8	C5-C6-C7-C8
3	A	502	QR8	C1-C2-C3-C4
3	B	502	QR8	C1-C2-C3-C4
3	C	502	QR8	C1-C2-C3-C4
3	D	502	QR8	C1-C2-C3-C4
3	E	503	QR8	C1-C2-C3-C4
3	F	503	QR8	C1-C2-C3-C4
3	B	502	QR8	C32-C6-C7-C8
3	E	503	QR8	C32-C6-C7-C8
3	B	502	QR8	O7-C5-C6-C7
3	F	503	QR8	C33-C8-C9-C10
3	B	502	QR8	C4-C5-C6-C7
3	F	503	QR8	C33-C8-C9-O11
3	C	502	QR8	O1-C1-O2-C13
3	E	503	QR8	C4-C5-C6-C7
3	B	502	QR8	C4-C5-C6-C32

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Mol	Chain	Res	Type	Atoms
3	F	503	QR8	O12-C11-C12-C35
3	E	503	QR8	C2-C1-O2-C13
3	A	502	QR8	C33-C8-C9-C10
3	D	502	QR8	C33-C8-C9-C10
3	E	503	QR8	C33-C8-C9-C10
3	C	502	QR8	C32-C6-C7-C8
3	F	503	QR8	C7-C8-C9-O11
2	C	501	HEM	C2B-C3B-CAB-CBB
3	C	502	QR8	C2-C1-O2-C13
3	C	502	QR8	C5-C6-C7-C8

There are no ring outliers.

50 monomers are involved in 138 short contacts:

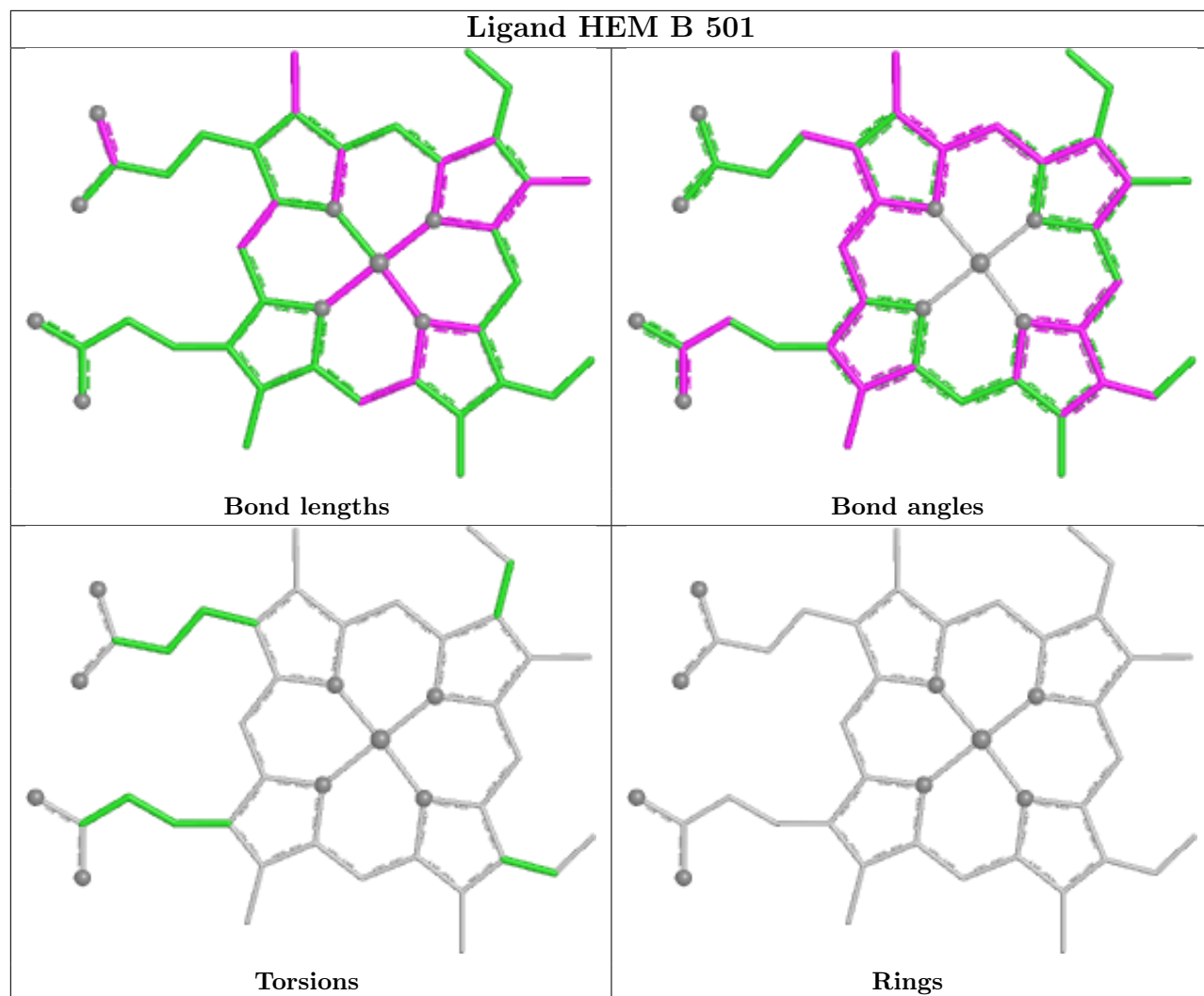
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	512	FMT	1	0
5	A	565	FMT	6	0
5	A	514	FMT	1	0
4	D	503	RAM	14	0
2	B	501	HEM	7	0
5	D	528	FMT	2	0
5	A	504	FMT	1	0
5	F	505	FMT	2	0
5	C	514	FMT	1	0
5	A	524	FMT	1	0
5	A	530	FMT	1	0
5	B	511	FMT	2	0
5	B	538	FMT	1	0
2	D	501	HEM	4	0
5	E	501	FMT	2	0
5	D	507	FMT	1	0
5	B	503	FMT	2	0
5	F	504	FMT	1	0
5	B	534	FMT	2	0
3	A	502	QR8	3	0
5	A	531	FMT	2	0
4	A	503[A]	RAM	16	0
5	A	550	FMT	2	0
5	D	508	FMT	1	0
3	D	502	QR8	2	0
5	B	507	FMT	1	0
5	D	518	FMT	1	0

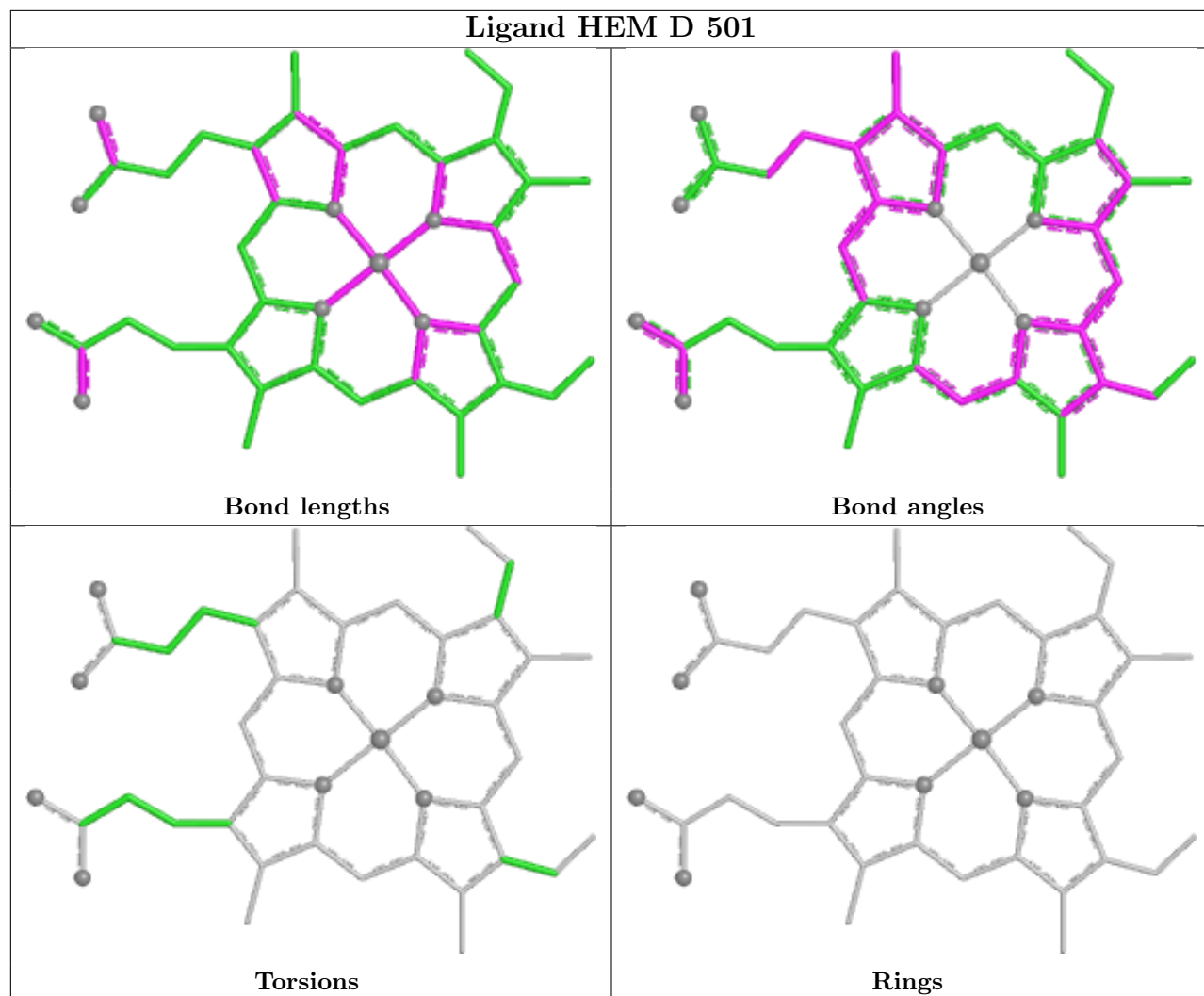
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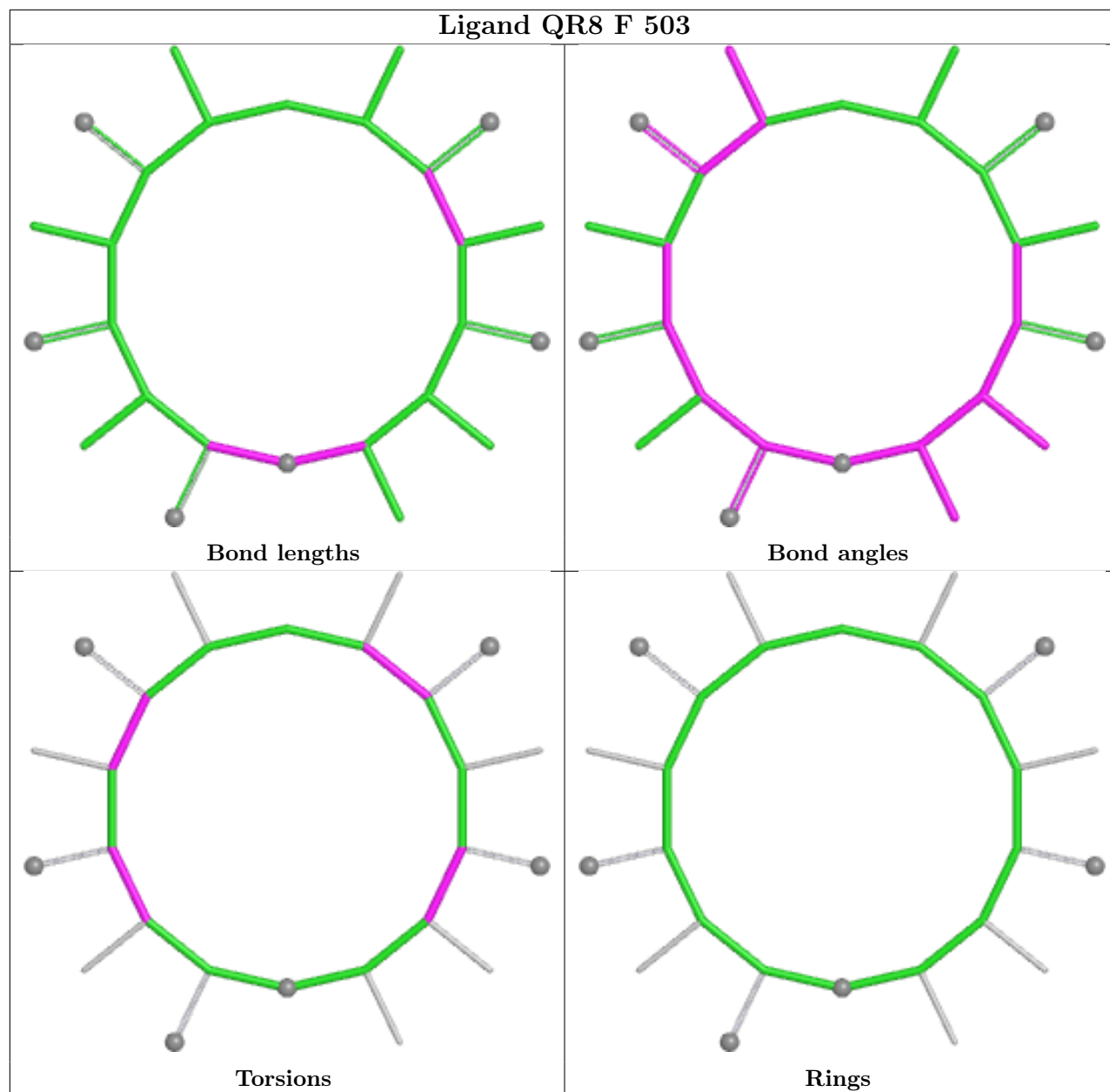
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	513	RAM	11	0
5	A	506	FMT	1	0
5	A	546	FMT	1	0
5	A	505	FMT	1	0
5	A	510	FMT	2	0
5	F	509	FMT	2	0
2	C	501	HEM	3	0
2	A	501	HEM	4	0
2	E	502	HEM	3	0
5	C	521	FMT	1	0
5	C	507	FMT	2	0
5	A	511	FMT	2	0
5	C	523	FMT	1	0
3	B	502	QR8	1	0
5	C	552	FMT	2	0
5	A	567	FMT	0	1
2	F	502	HEM	4	0
4	A	503[B]	RAM	17	0
5	F	514	FMT	5	0
5	B	510	FMT	1	0
5	D	504	FMT	2	0
5	C	504	FMT	1	0
5	D	512	FMT	1	0

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

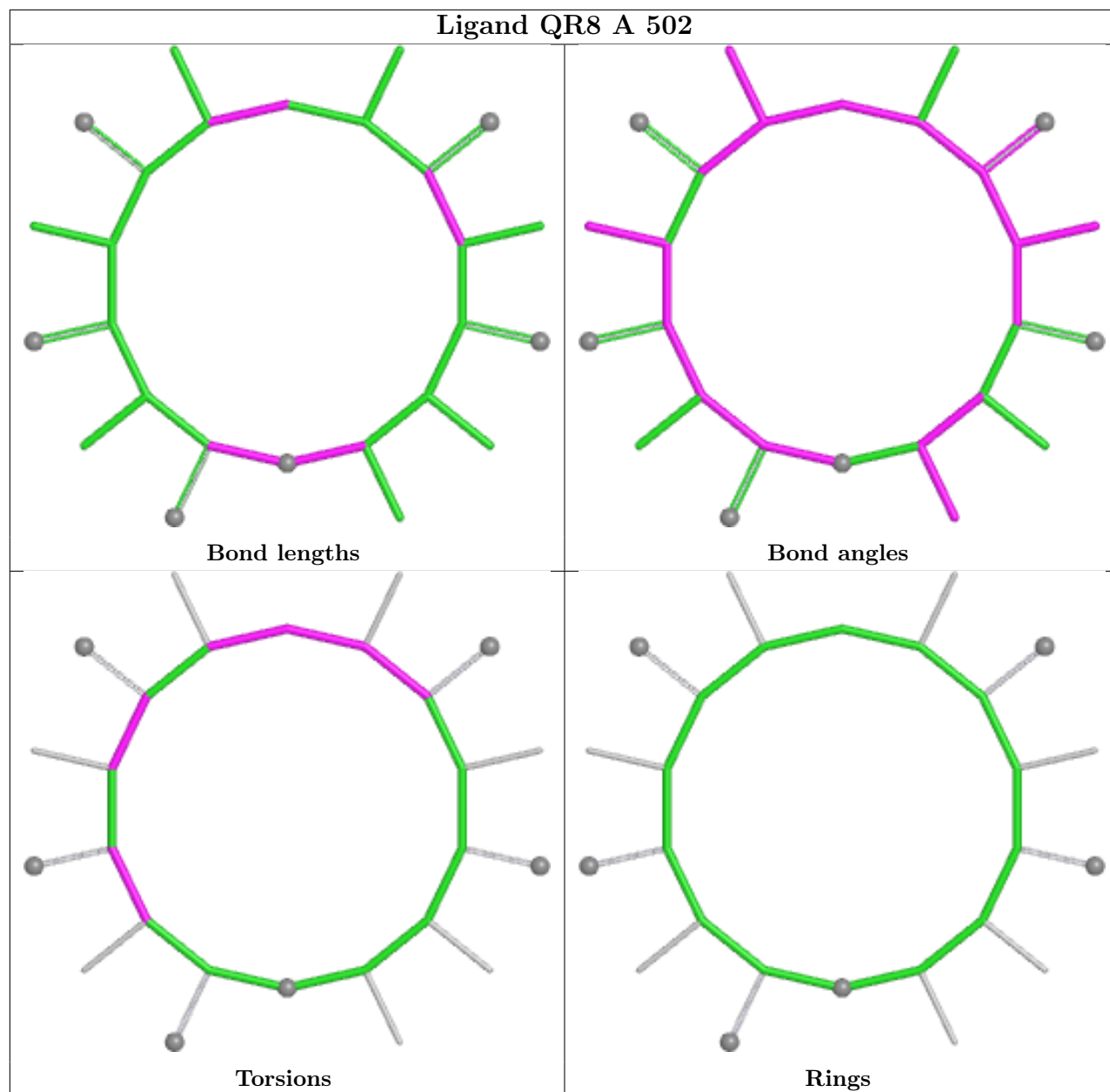




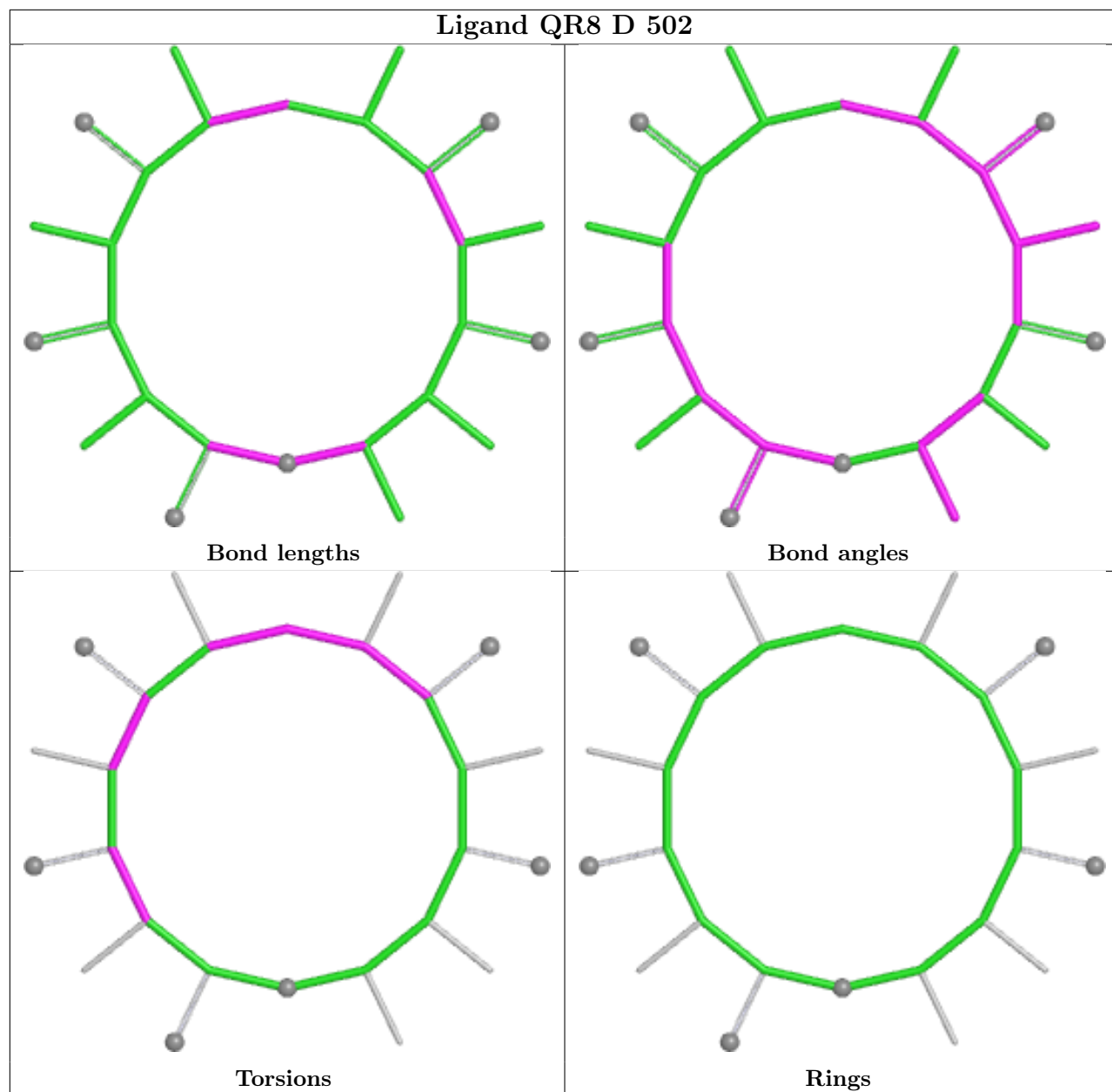
Ligand QR8 F 503

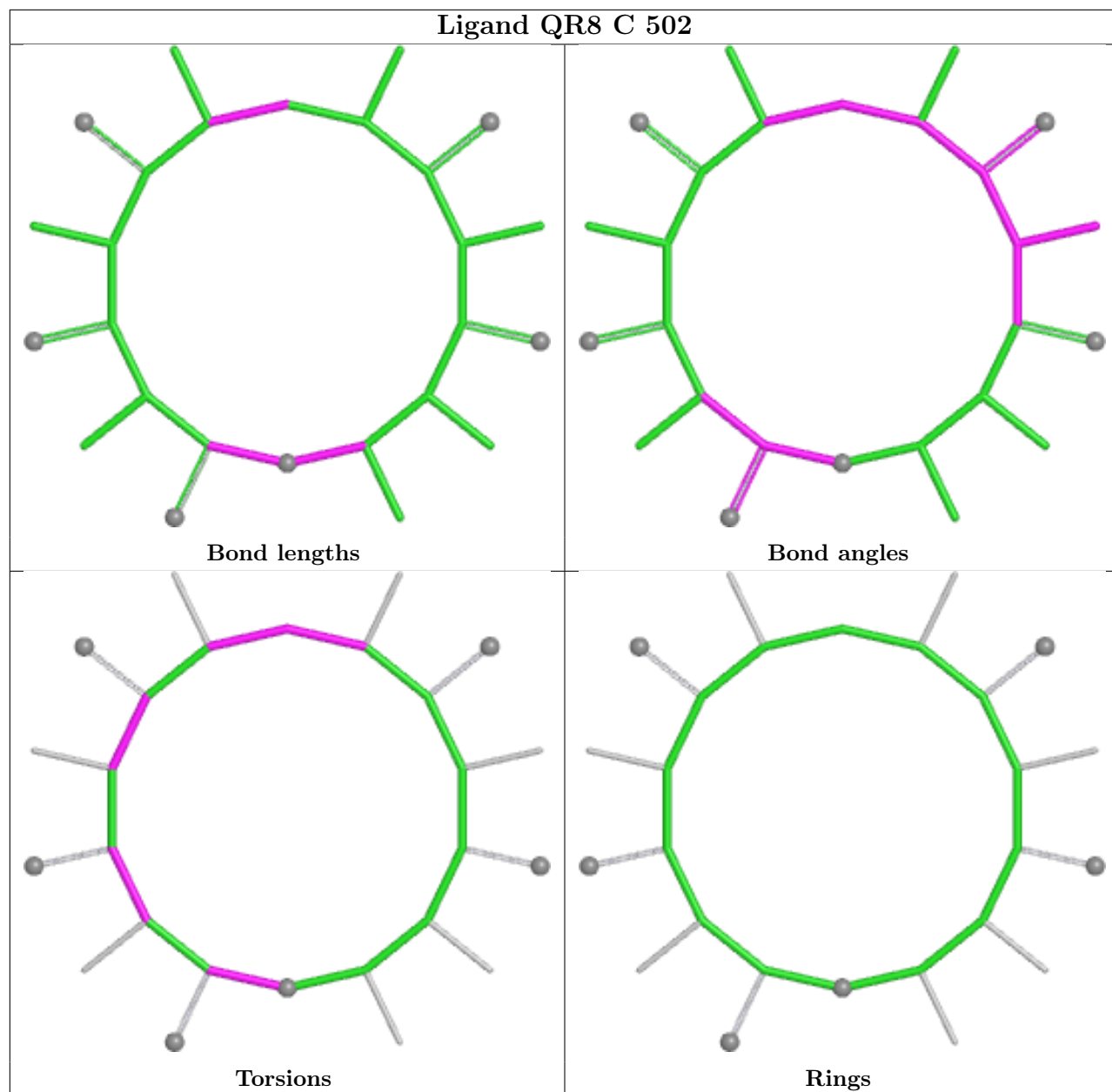


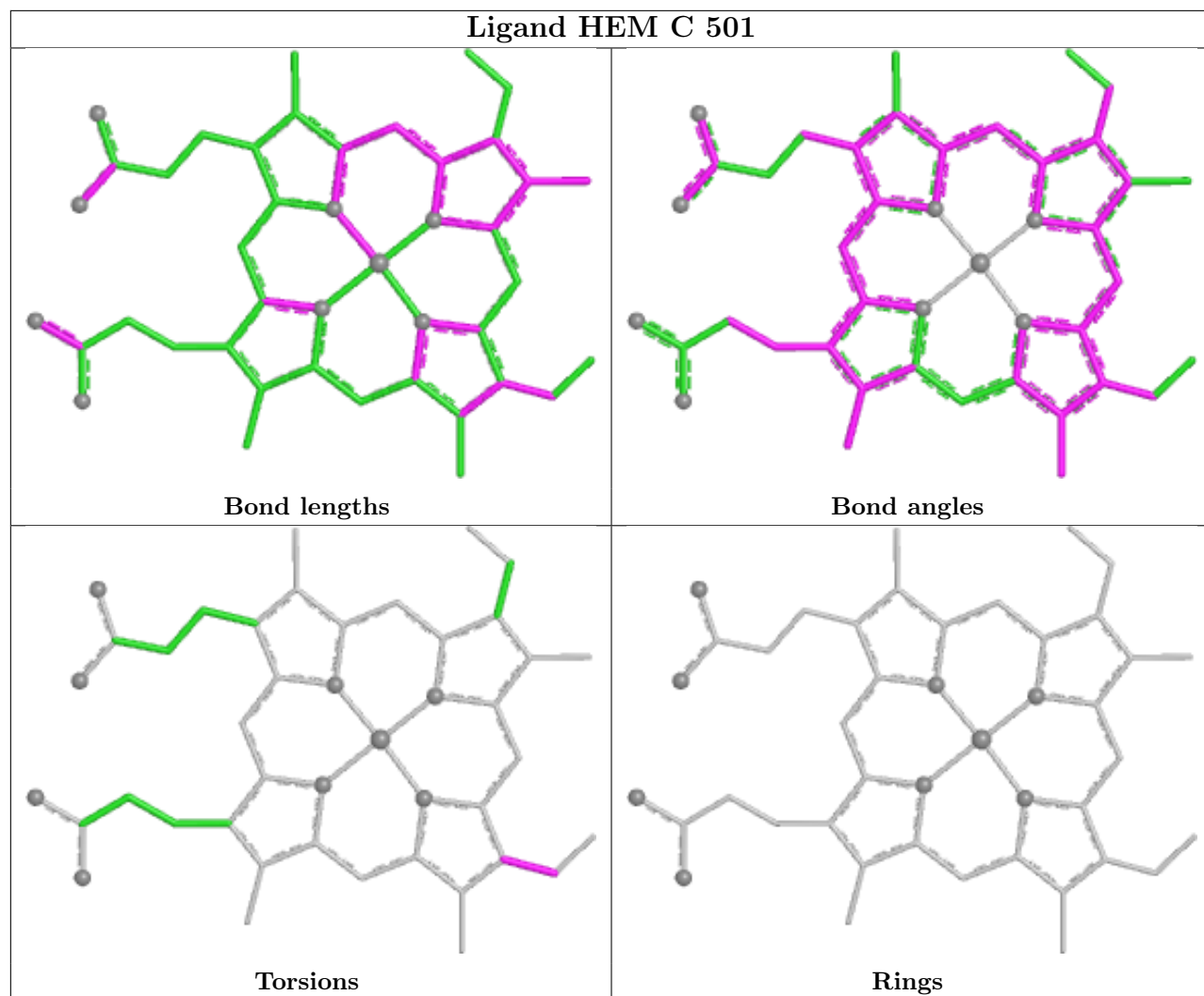
Ligand QR8 A 502

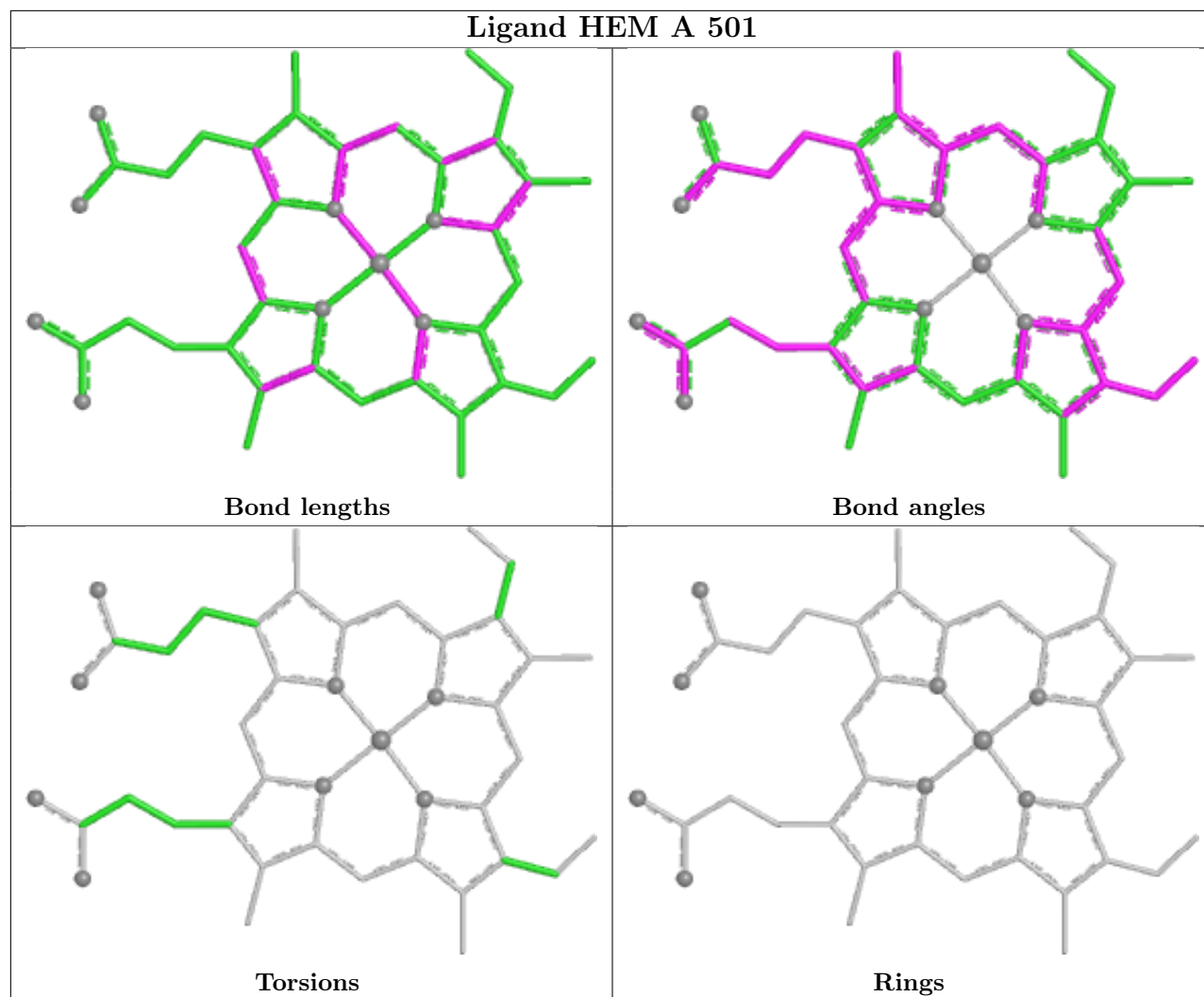


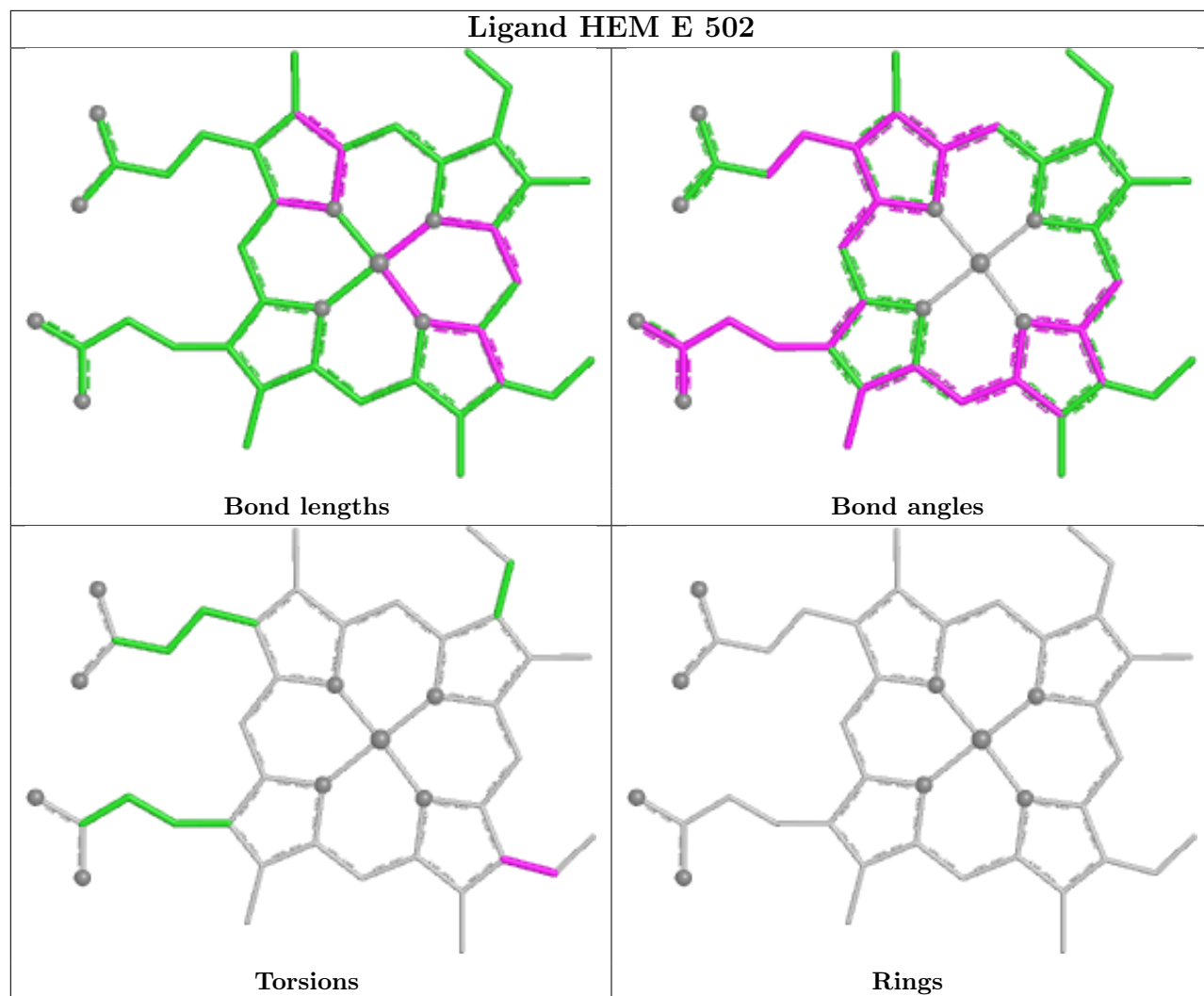
Ligand QR8 D 502

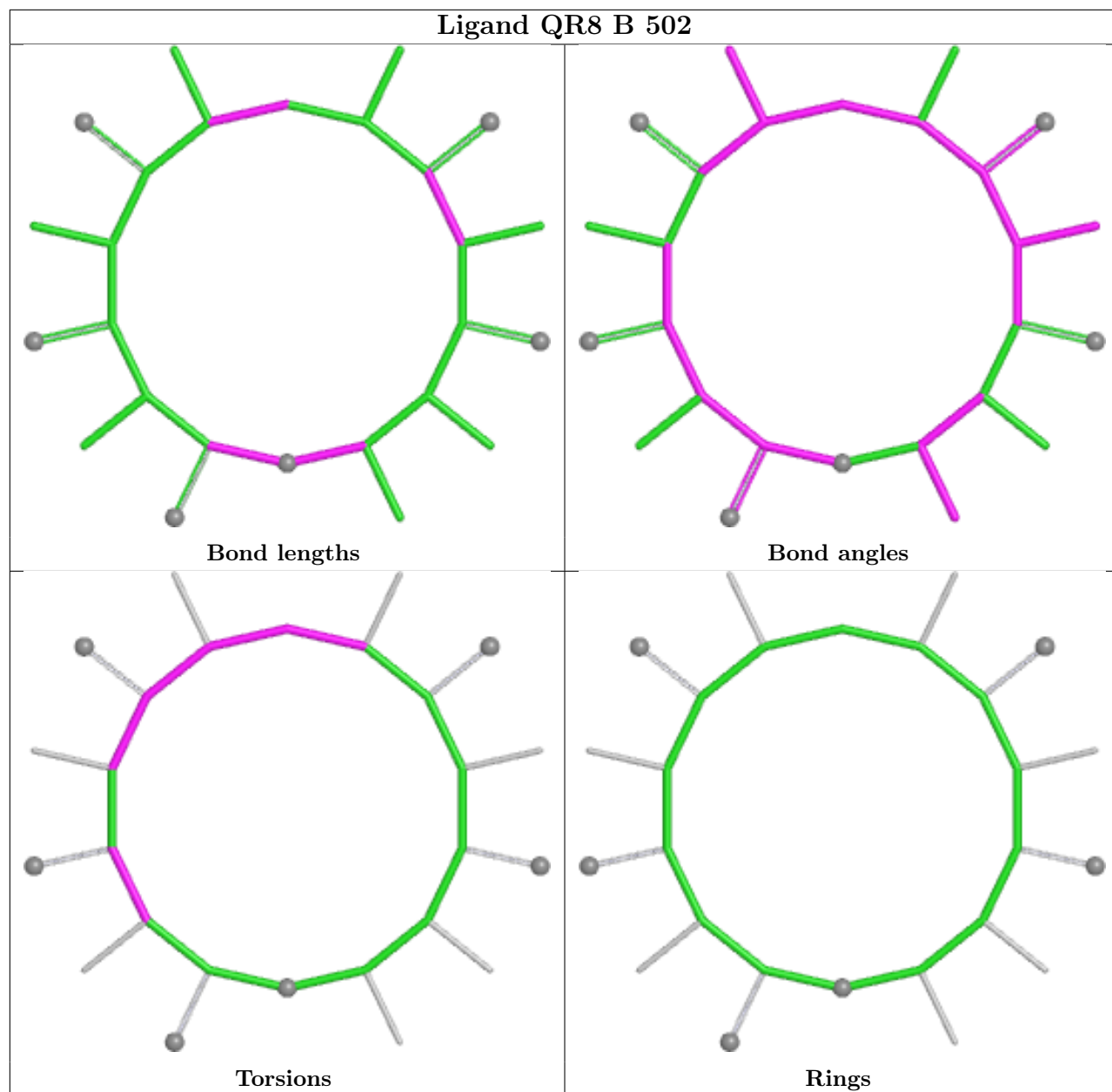




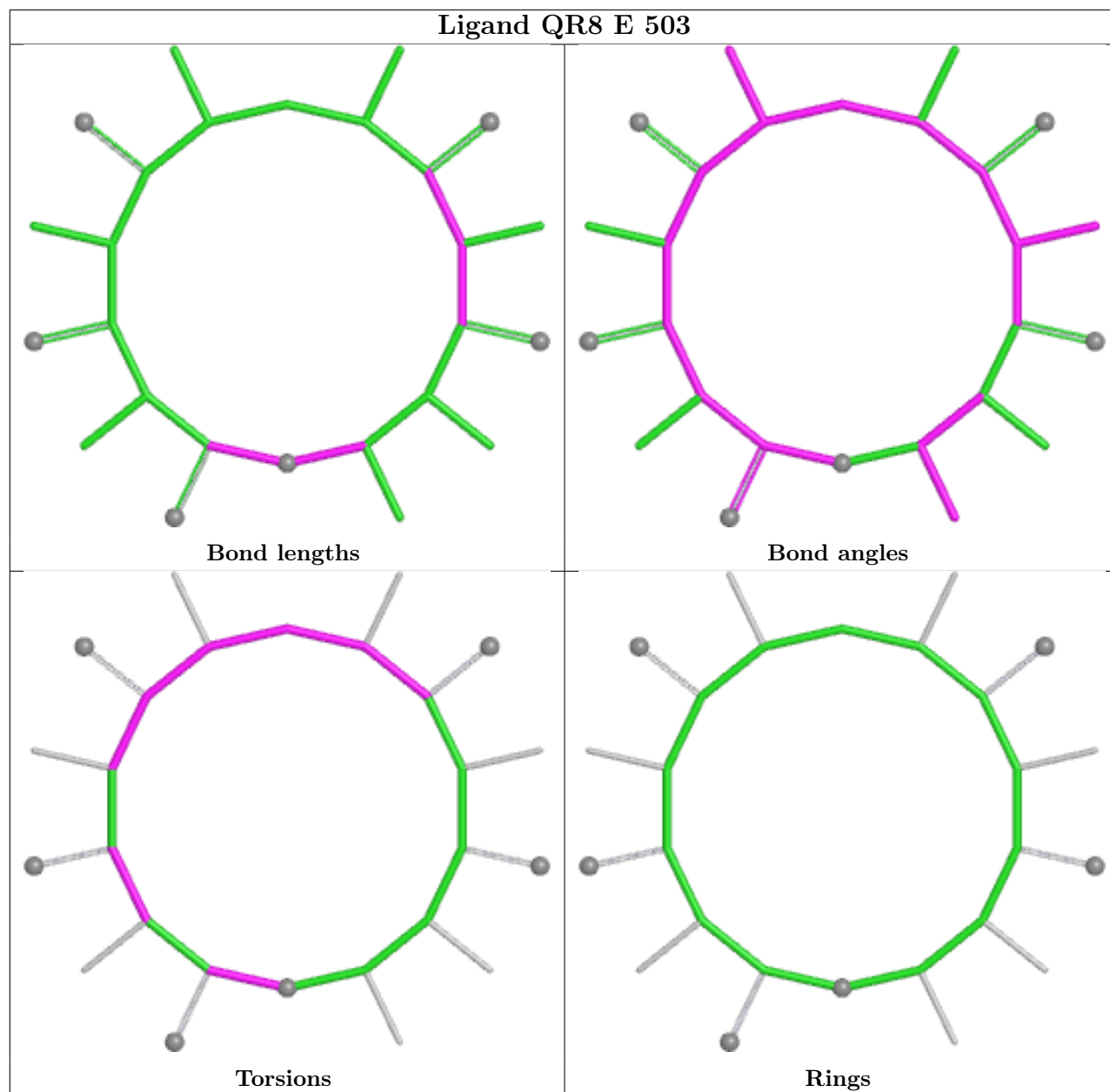


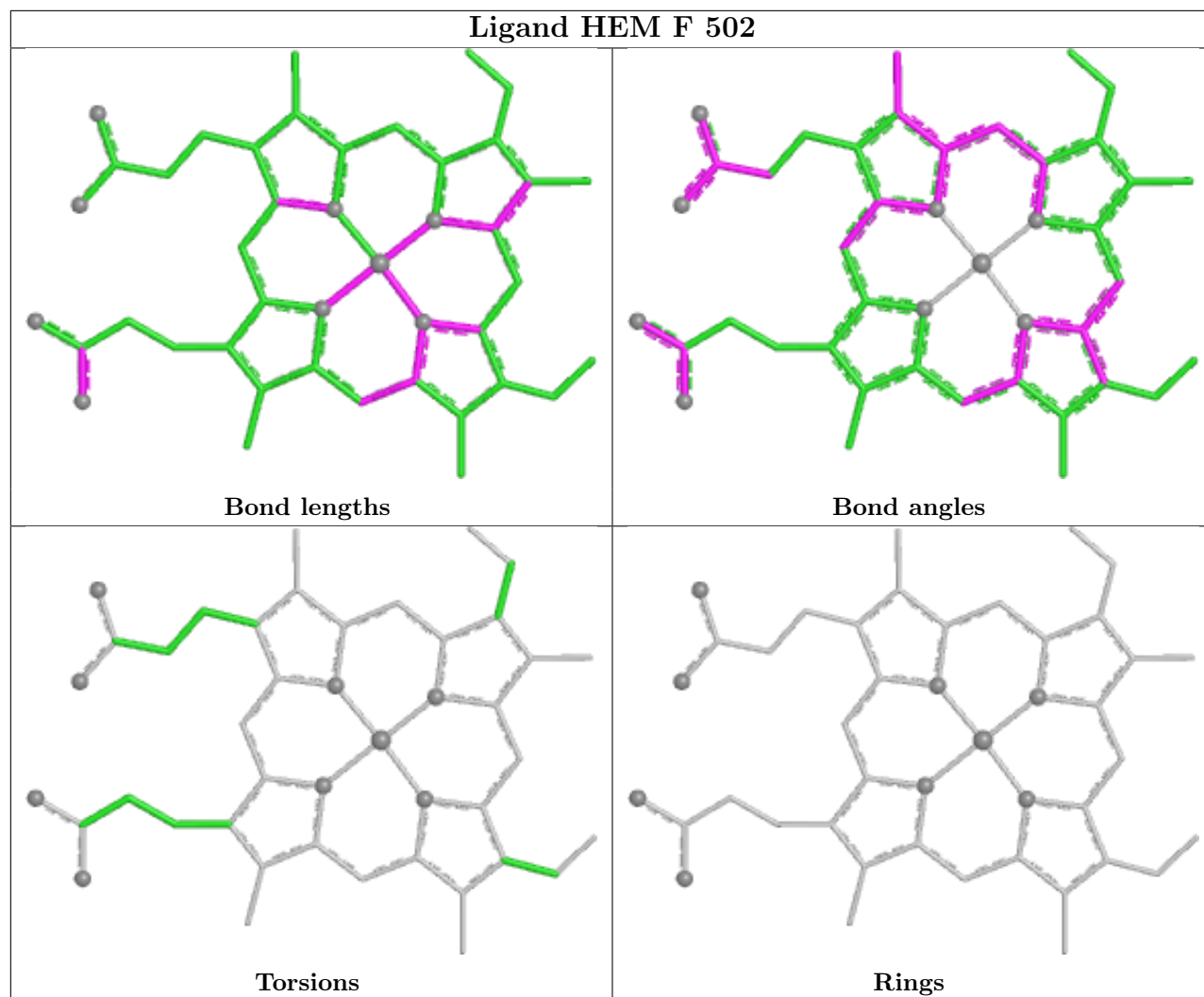






Ligand QR8 E 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	ALA	7.5
1	B	9	THR	4.9
1	D	10	PRO	4.9
1	D	11	ALA	4.6
1	B	11	ALA	4.4
1	F	23[A]	HIS	4.1
1	C	9	THR	3.8
1	D	9	THR	3.7
1	D	228[A]	HIS	3.7
1	F	110[A]	LYS	3.5
1	E	210	ALA	3.4
1	F	386	VAL	3.4
1	F	131[A]	LEU	3.4
1	E	228[A]	HIS	3.3
1	C	8	PRO	3.2
1	D	8	PRO	3.2
1	F	10	PRO	3.2
1	D	12	ASP	3.2
1	F	136[A]	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	8	PRO	2.9
1	E	312[A]	ARG	2.9
1	E	212	THR	2.8
1	F	21	LEU	2.8
1	F	11	ALA	2.8
1	B	10	PRO	2.8
1	F	274	PRO	2.8
1	F	370	LEU	2.8
1	C	11	ALA	2.8
1	F	374	VAL	2.7
1	D	14	VAL	2.6
1	F	276	LEU	2.6
1	F	215	LEU	2.4
1	F	372	ALA	2.4
1	B	210	ALA	2.3
1	F	375[A]	ARG	2.3
1	E	66	GLY	2.2
1	F	390[A]	LYS	2.2
1	D	219	LEU	2.1
1	B	209[A]	ASP	2.1
1	F	184	LEU	2.1
1	F	382[A]	LEU	2.0
1	A	208[A]	ARG	2.0
1	E	343[A]	ARG	2.0
1	D	231[A]	LYS	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($\text{\AA}^2$)	Q<0.9
5	FMT	D	536	3/3	0.31	0.13	111,111,113,115	0
5	FMT	A	551	3/3	0.47	0.14	104,104,113,115	0
5	FMT	A	554	3/3	0.50	0.16	100,100,107,111	0
5	FMT	D	521	3/3	0.52	0.12	102,102,102,104	0
5	FMT	B	527	3/3	0.58	0.14	96,96,99,103	0
5	FMT	E	511	3/3	0.58	0.12	119,119,120,122	0
5	FMT	A	540	3/3	0.59	0.18	105,105,112,114	0
5	FMT	C	528	3/3	0.60	0.11	95,95,95,101	0
5	FMT	C	530	3/3	0.62	0.15	105,105,110,113	0
5	FMT	E	510	3/3	0.63	0.15	95,95,107,108	0
5	FMT	C	546	3/3	0.64	0.16	87,87,88,91	0
5	FMT	D	526	3/3	0.65	0.18	104,104,106,112	0
5	FMT	A	542	3/3	0.65	0.14	102,102,103,104	0
5	FMT	A	529	3/3	0.66	0.12	100,100,107,109	0
5	FMT	A	527	3/3	0.66	0.16	88,88,93,100	0
5	FMT	E	515	3/3	0.66	0.10	103,103,114,115	0
5	FMT	A	571	3/3	0.68	0.15	94,94,108,108	0
5	FMT	D	527	3/3	0.68	0.10	91,91,97,97	0
5	FMT	A	539	3/3	0.68	0.11	101,101,110,111	0
5	FMT	F	510	3/3	0.68	0.11	88,88,98,100	0
5	FMT	A	557	3/3	0.69	0.10	87,87,90,91	0
5	FMT	A	533	3/3	0.69	0.12	87,87,91,92	0
5	FMT	B	520	3/3	0.69	0.11	95,95,102,102	0
5	FMT	A	556	3/3	0.70	0.13	87,87,89,93	0
5	FMT	C	531	3/3	0.71	0.12	102,102,102,106	0
5	FMT	C	535	3/3	0.71	0.16	89,89,112,116	0
5	FMT	B	531	3/3	0.71	0.12	98,98,102,104	0
5	FMT	D	517	3/3	0.71	0.16	114,114,121,129	0
5	FMT	B	533	3/3	0.72	0.22	78,78,79,89	0
5	FMT	B	540	3/3	0.72	0.11	95,95,99,100	0
5	FMT	A	564	3/3	0.72	0.19	90,90,102,105	0
5	FMT	B	532	3/3	0.72	0.10	96,96,99,102	0
5	FMT	C	516	3/3	0.73	0.13	81,81,86,87	0
5	FMT	F	511	3/3	0.73	0.09	101,101,109,109	0
5	FMT	F	512	3/3	0.73	0.11	106,106,112,113	0
5	FMT	B	526	3/3	0.74	0.11	96,96,96,99	0
5	FMT	A	541	3/3	0.74	0.11	92,92,93,96	0
5	FMT	E	517	3/3	0.74	0.15	95,95,99,100	0
5	FMT	E	509	3/3	0.75	0.10	86,86,101,104	0
5	FMT	C	549	3/3	0.75	0.10	100,100,100,101	0
4	RAM	B	513	11/11	0.75	0.23	50,57,63,64	11
5	FMT	E	508	3/3	0.75	0.09	86,86,89,93	0
5	FMT	A	515	3/3	0.76	0.13	80,80,82,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	A	552	3/3	0.76	0.15	83,83,89,92	0
5	FMT	C	548	3/3	0.76	0.13	85,85,91,91	0
5	FMT	D	522	3/3	0.76	0.14	97,97,106,113	0
5	FMT	B	516	3/3	0.77	0.16	100,100,103,107	0
5	FMT	C	526	3/3	0.77	0.14	75,75,80,83	0
5	FMT	A	558	3/3	0.77	0.14	83,83,84,92	0
5	FMT	D	515	3/3	0.78	0.16	79,79,80,88	0
5	FMT	A	517	3/3	0.78	0.09	98,98,106,108	0
5	FMT	D	525	3/3	0.78	0.15	87,87,91,92	0
5	FMT	F	515	3/3	0.78	0.20	101,101,103,108	0
5	FMT	A	572	3/3	0.79	0.18	91,91,97,98	0
5	FMT	B	511	3/3	0.79	0.09	73,73,77,78	0
5	FMT	A	510	3/3	0.79	0.18	75,75,84,85	0
5	FMT	B	518	3/3	0.79	0.14	89,89,104,105	0
5	FMT	A	512	3/3	0.79	0.21	98,98,103,109	0
5	FMT	E	516	3/3	0.79	0.15	90,90,90,96	0
5	FMT	B	525	3/3	0.79	0.15	98,98,105,105	0
5	FMT	A	569	3/3	0.79	0.16	94,94,95,95	0
5	FMT	A	570	3/3	0.79	0.19	92,92,98,98	0
5	FMT	B	528	3/3	0.79	0.15	85,85,86,89	0
5	FMT	A	523	3/3	0.79	0.18	67,67,70,77	0
5	FMT	B	519	3/3	0.80	0.09	100,100,101,104	0
5	FMT	B	517	3/3	0.80	0.15	86,86,94,100	0
5	FMT	D	535	3/3	0.80	0.30	96,96,104,104	0
5	FMT	D	523	3/3	0.80	0.25	85,85,94,95	0
5	FMT	A	538	3/3	0.80	0.18	63,63,75,85	0
5	FMT	B	539	3/3	0.81	0.14	85,85,89,91	0
4	RAM	D	503	11/11	0.81	0.20	58,66,68,68	11
5	FMT	D	530	3/3	0.81	0.19	101,101,109,109	0
5	FMT	B	507	3/3	0.81	0.18	75,75,84,84	0
5	FMT	C	540	3/3	0.81	0.17	74,74,80,83	0
5	FMT	A	545	3/3	0.81	0.24	83,83,87,101	0
5	FMT	C	547	3/3	0.81	0.17	65,65,73,82	0
5	FMT	B	535	3/3	0.81	0.21	88,88,89,94	0
5	FMT	C	523	3/3	0.82	0.17	69,69,75,81	0
5	FMT	A	563	3/3	0.82	0.22	97,97,102,107	0
5	FMT	D	519	3/3	0.82	0.16	90,90,91,96	0
5	FMT	C	534	3/3	0.82	0.19	88,88,90,92	0
5	FMT	A	560	3/3	0.82	0.20	74,74,81,93	0
5	FMT	C	539	3/3	0.82	0.17	87,87,90,98	0
5	FMT	D	524	3/3	0.82	0.14	111,111,112,116	0
5	FMT	C	551	3/3	0.82	0.28	90,90,94,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	D	512	3/3	0.83	0.16	85,85,88,92	0
5	FMT	B	512	3/3	0.83	0.19	68,68,72,74	0
5	FMT	C	510	3/3	0.83	0.12	83,83,84,91	0
5	FMT	C	542	3/3	0.83	0.24	91,91,115,119	0
5	FMT	C	525	3/3	0.83	0.19	90,90,91,94	0
5	FMT	C	518	3/3	0.84	0.17	65,65,72,77	0
5	FMT	D	505	3/3	0.84	0.16	69,69,69,73	0
5	FMT	A	513	3/3	0.84	0.15	75,75,81,88	0
5	FMT	A	537	3/3	0.84	0.10	100,100,109,109	0
5	FMT	A	574	3/3	0.84	0.15	102,102,108,111	0
5	FMT	A	507	3/3	0.84	0.15	69,69,73,76	0
5	FMT	C	506	3/3	0.84	0.20	62,62,69,73	0
5	FMT	B	508	3/3	0.84	0.11	73,73,79,83	0
5	FMT	A	562	3/3	0.84	0.23	55,55,70,72	0
5	FMT	C	508	3/3	0.85	0.18	81,81,87,90	0
5	FMT	C	545	3/3	0.85	0.20	78,78,80,86	0
5	FMT	B	521	3/3	0.85	0.22	66,66,78,84	0
5	FMT	C	537	3/3	0.86	0.19	97,97,109,111	0
5	FMT	B	523	3/3	0.86	0.12	86,86,87,92	0
5	FMT	A	535	3/3	0.86	0.12	89,89,103,109	0
5	FMT	C	541	3/3	0.86	0.11	83,83,85,91	0
5	FMT	A	516	3/3	0.86	0.19	77,77,81,85	0
5	FMT	D	529	3/3	0.86	0.12	76,76,79,82	0
5	FMT	F	509	3/3	0.86	0.15	66,66,67,74	0
4	RAM	A	503[B]	11/11	0.86	0.17	37,41,44,46	11
4	RAM	A	503[A]	11/11	0.86	0.17	34,37,39,44	11
5	FMT	A	548	3/3	0.86	0.23	64,64,65,76	0
5	FMT	C	536	3/3	0.86	0.20	98,98,99,104	0
5	FMT	B	530	3/3	0.87	0.11	71,71,80,93	0
5	FMT	A	549	3/3	0.87	0.27	71,71,87,90	0
5	FMT	E	513	3/3	0.87	0.14	74,74,74,75	0
5	FMT	B	524	3/3	0.87	0.19	68,68,74,78	0
5	FMT	D	516	3/3	0.87	0.20	90,90,91,91	0
5	FMT	A	553	3/3	0.87	0.21	86,86,94,95	0
5	FMT	F	506	3/3	0.87	0.11	74,74,75,76	0
5	FMT	D	518	3/3	0.87	0.10	84,84,96,100	0
5	FMT	A	536	3/3	0.87	0.20	71,71,71,77	0
5	FMT	A	559	3/3	0.87	0.17	90,90,91,95	0
5	FMT	A	566	3/3	0.87	0.11	87,87,89,96	0
5	FMT	B	529	3/3	0.87	0.18	71,71,71,79	0
5	FMT	A	568	3/3	0.88	0.10	85,85,90,91	0
5	FMT	B	522	3/3	0.88	0.25	76,76,82,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	B	536	3/3	0.88	0.14	69,69,76,81	0
5	FMT	B	538	3/3	0.88	0.15	82,82,83,86	0
5	FMT	A	508	3/3	0.88	0.23	74,74,76,83	0
5	FMT	D	511	3/3	0.88	0.27	68,68,73,74	0
5	FMT	A	521	3/3	0.88	0.22	49,49,63,67	0
5	FMT	F	504	3/3	0.88	0.09	78,78,87,91	0
5	FMT	F	505	3/3	0.88	0.18	79,79,84,85	0
5	FMT	A	531	3/3	0.88	0.20	63,63,65,75	0
5	FMT	C	529	3/3	0.88	0.12	84,84,88,92	0
5	FMT	D	531	3/3	0.88	0.14	59,59,65,71	0
5	FMT	C	544	3/3	0.88	0.24	68,68,73,82	0
5	FMT	C	507	3/3	0.88	0.22	60,60,65,68	0
5	FMT	F	513	3/3	0.88	0.28	75,75,79,82	0
5	FMT	A	506	3/3	0.88	0.19	66,66,73,77	0
6	NA	E	507	1/1	0.88	0.16	81,81,81,81	0
5	FMT	D	528	3/3	0.89	0.38	79,79,80,81	0
5	FMT	A	550	3/3	0.89	0.15	64,64,78,80	0
5	FMT	A	528	3/3	0.89	0.16	84,84,84,93	0
5	FMT	C	552	3/3	0.89	0.12	72,72,74,79	0
5	FMT	D	533	3/3	0.89	0.24	70,70,70,73	0
5	FMT	A	520	3/3	0.89	0.16	84,84,87,90	0
5	FMT	D	507	3/3	0.89	0.20	85,85,90,91	0
5	FMT	D	509	3/3	0.89	0.14	66,66,76,76	0
5	FMT	A	547	3/3	0.89	0.21	70,70,73,77	0
5	FMT	A	519	3/3	0.89	0.19	74,74,75,76	0
5	FMT	A	532	3/3	0.89	0.36	76,76,77,85	0
5	FMT	B	514	3/3	0.89	0.16	75,75,80,87	0
5	FMT	E	514	3/3	0.89	0.17	86,86,94,97	0
5	FMT	D	514	3/3	0.90	0.18	60,60,60,71	0
5	FMT	C	504	3/3	0.90	0.15	48,48,52,54	0
5	FMT	C	505	3/3	0.90	0.16	57,57,64,68	0
5	FMT	B	504	3/3	0.90	0.22	69,69,74,80	0
5	FMT	A	561	3/3	0.90	0.11	77,77,83,87	0
5	FMT	B	537	3/3	0.90	0.12	82,82,94,96	0
5	FMT	D	532	3/3	0.90	0.13	79,79,80,84	0
5	FMT	D	520	3/3	0.90	0.10	96,96,100,108	0
5	FMT	D	534	3/3	0.90	0.10	91,91,91,93	0
5	FMT	A	573	3/3	0.90	0.10	67,67,85,97	0
5	FMT	C	543	3/3	0.90	0.13	82,82,87,92	0
5	FMT	E	501	3/3	0.90	0.14	76,76,78,79	0
5	FMT	E	505	3/3	0.90	0.11	72,72,79,81	0
5	FMT	C	511	3/3	0.90	0.12	68,68,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	B	509	3/3	0.90	0.12	60,60,62,64	0
5	FMT	A	567	3/3	0.90	0.12	85,85,85,85	0
5	FMT	B	510	3/3	0.91	0.20	86,86,91,92	0
5	FMT	E	512	3/3	0.91	0.15	80,80,81,86	0
5	FMT	C	515	3/3	0.91	0.14	63,63,76,76	0
5	FMT	E	504	3/3	0.91	0.21	63,63,63,74	0
5	FMT	A	504	3/3	0.91	0.15	52,52,56,57	0
5	FMT	D	506	3/3	0.91	0.29	68,68,81,84	0
5	FMT	C	517	3/3	0.91	0.14	70,70,71,74	0
5	FMT	F	501	3/3	0.91	0.11	85,85,86,88	0
5	FMT	C	532	3/3	0.91	0.16	49,49,57,72	0
5	FMT	C	550	3/3	0.92	0.11	57,57,67,70	0
5	FMT	A	511	3/3	0.92	0.17	61,61,66,66	0
5	FMT	A	530	3/3	0.92	0.13	55,55,75,77	0
5	FMT	A	509	3/3	0.92	0.13	61,61,64,71	0
5	FMT	C	503	3/3	0.92	0.15	48,48,55,60	0
5	FMT	A	505	3/3	0.92	0.10	59,59,68,71	0
5	FMT	A	524	3/3	0.92	0.21	60,60,68,74	0
5	FMT	A	565	3/3	0.92	0.22	66,66,82,85	0
5	FMT	A	543	3/3	0.92	0.17	54,54,69,69	0
5	FMT	A	544	3/3	0.92	0.14	67,67,77,81	0
5	FMT	C	509	3/3	0.92	0.17	60,60,67,68	0
5	FMT	A	525	3/3	0.92	0.14	76,76,82,83	0
5	FMT	A	518	3/3	0.92	0.17	58,58,66,71	0
5	FMT	A	514	3/3	0.92	0.23	46,46,48,51	0
6	NA	F	508	1/1	0.92	0.13	59,59,59,59	0
5	FMT	A	546	3/3	0.93	0.17	64,64,73,83	0
5	FMT	C	519	3/3	0.93	0.14	69,69,76,84	0
5	FMT	D	537	3/3	0.93	0.26	48,48,60,65	0
5	FMT	D	504	3/3	0.93	0.17	67,67,71,76	0
5	FMT	F	514	3/3	0.93	0.19	56,56,70,72	0
5	FMT	C	538	3/3	0.93	0.25	58,58,61,64	0
5	FMT	A	555	3/3	0.93	0.18	61,61,65,71	0
5	FMT	C	512	3/3	0.93	0.18	59,59,73,74	0
5	FMT	B	506	3/3	0.94	0.19	63,63,69,71	0
5	FMT	A	534	3/3	0.94	0.10	60,60,72,81	0
5	FMT	B	534	3/3	0.94	0.10	70,70,72,74	0
3	QR8	E	503	26/26	0.94	0.10	46,53,56,57	0
5	FMT	C	520	3/3	0.94	0.19	55,55,66,70	0
5	FMT	C	533	3/3	0.94	0.13	68,68,69,76	0
5	FMT	C	521	3/3	0.94	0.14	59,59,70,87	0
5	FMT	C	513	3/3	0.94	0.23	54,54,62,63	0

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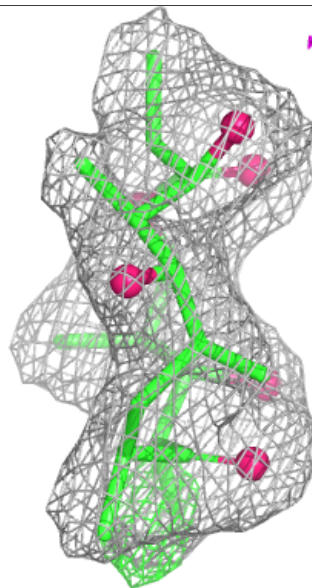
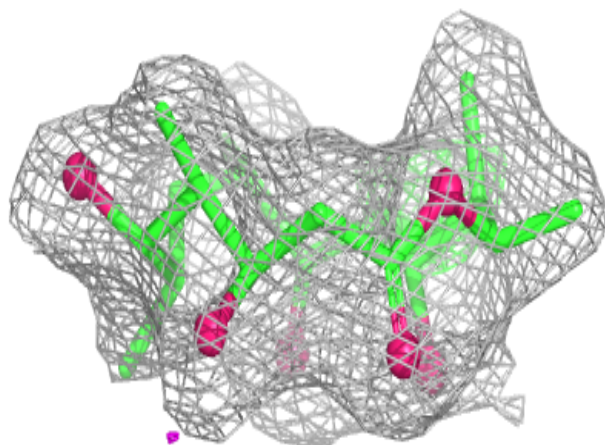
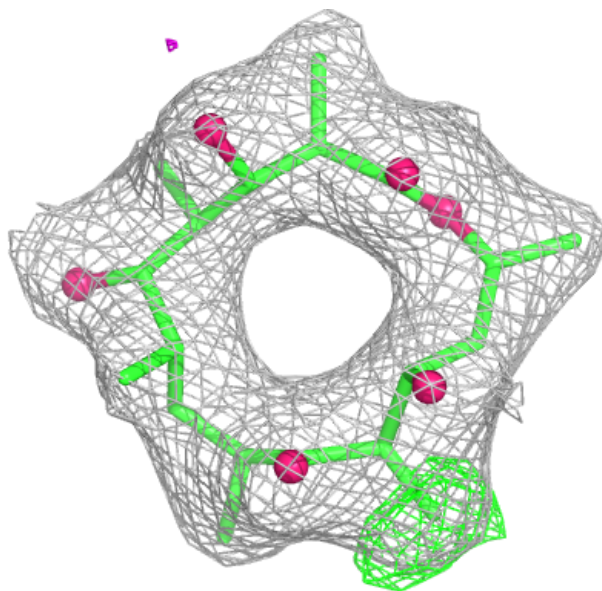
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	C	514	3/3	0.94	0.08	53,53,56,64	0
5	FMT	E	506	3/3	0.94	0.07	70,70,72,74	0
3	QR8	F	503	26/26	0.94	0.10	55,62,66,75	0
5	FMT	D	508	3/3	0.95	0.15	57,57,59,59	0
3	QR8	A	502	26/26	0.95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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

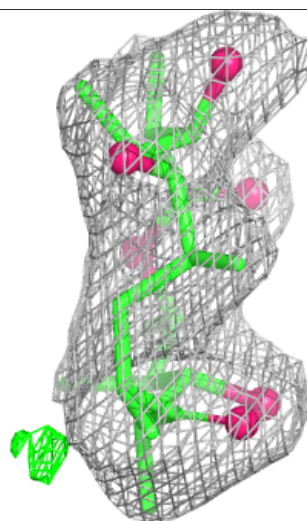
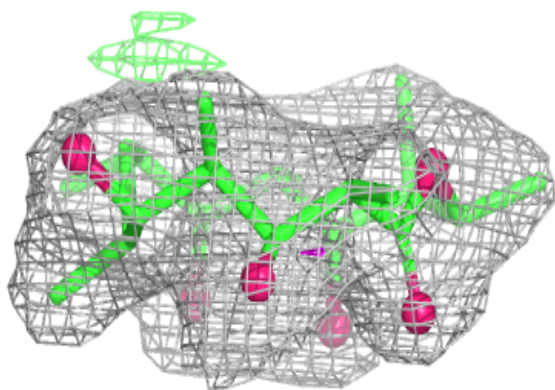
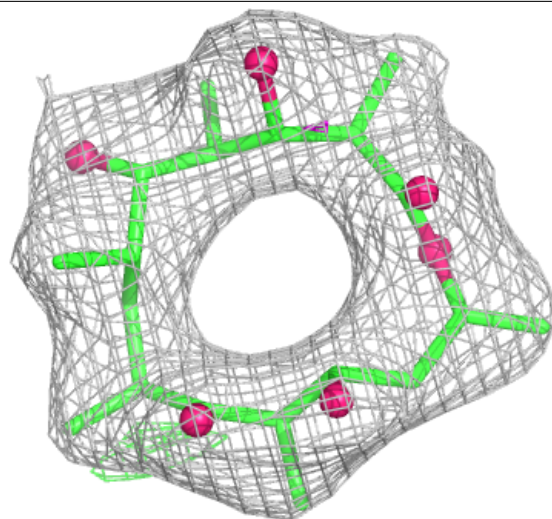
Electron density around QR8 E 503:

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



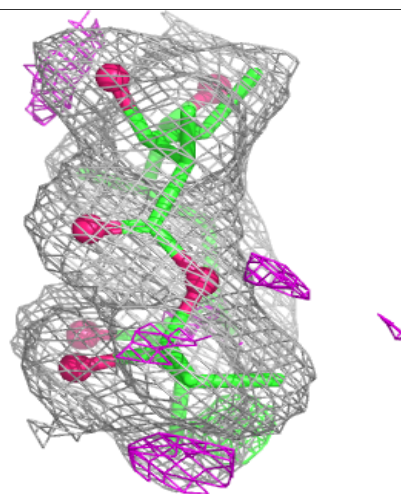
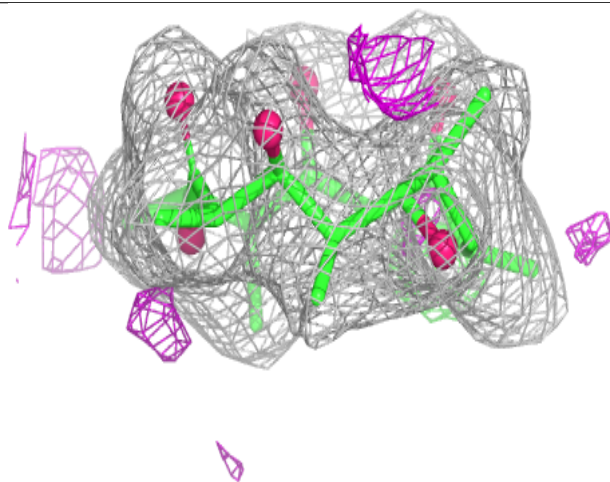
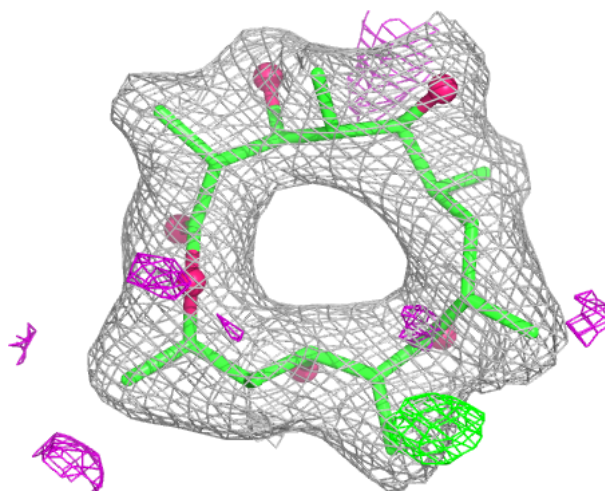
Electron density around QR8 F 503:

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



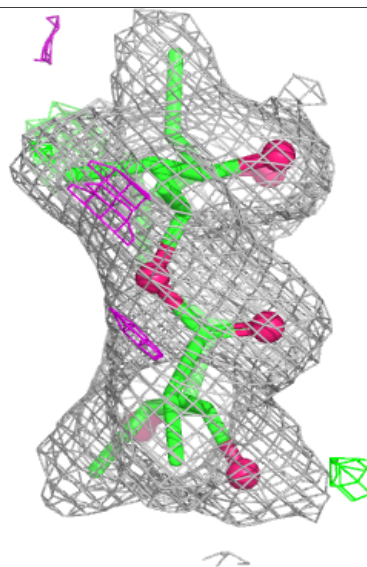
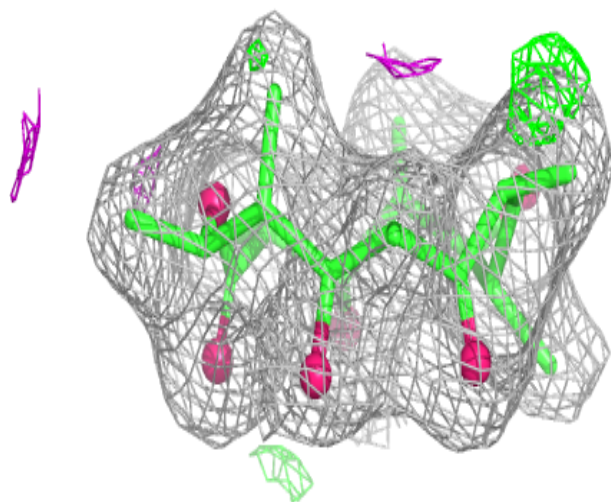
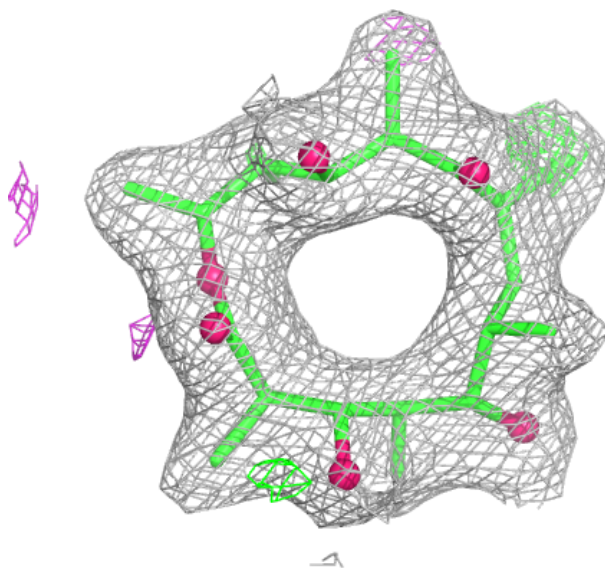
Electron density around QR8 A 502:

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



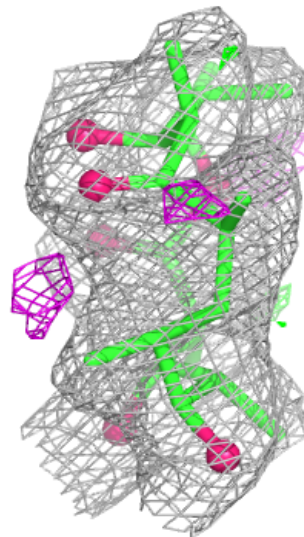
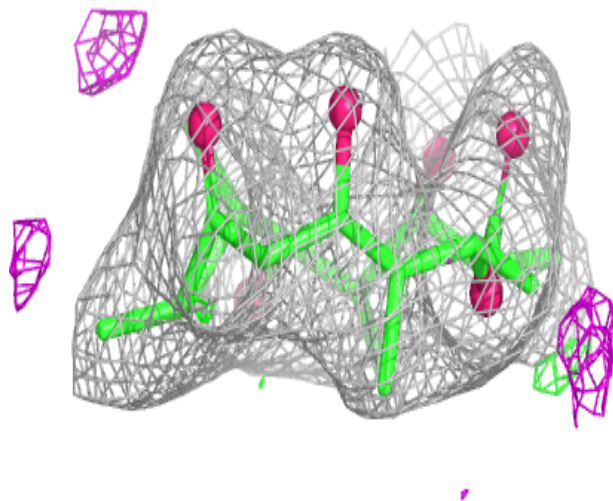
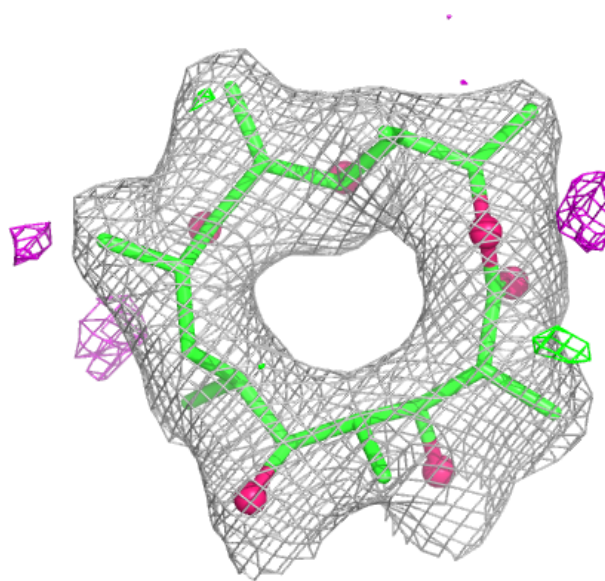
Electron density around QR8 C 502:

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



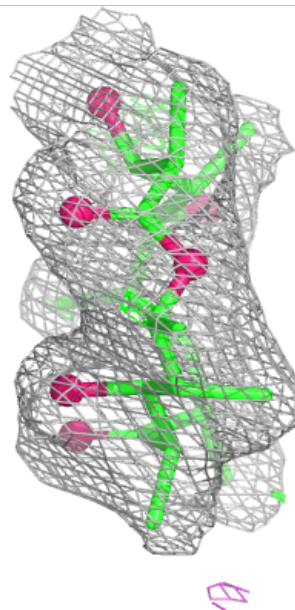
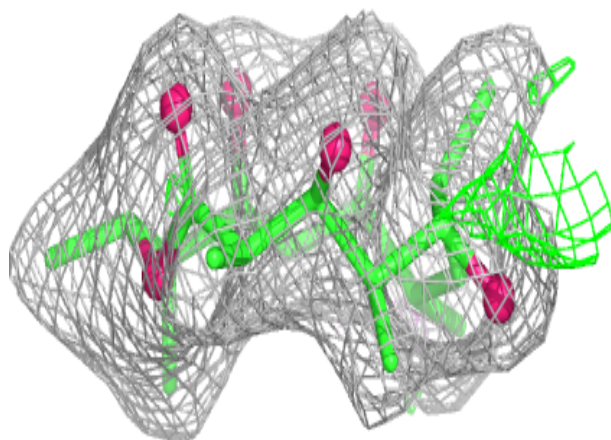
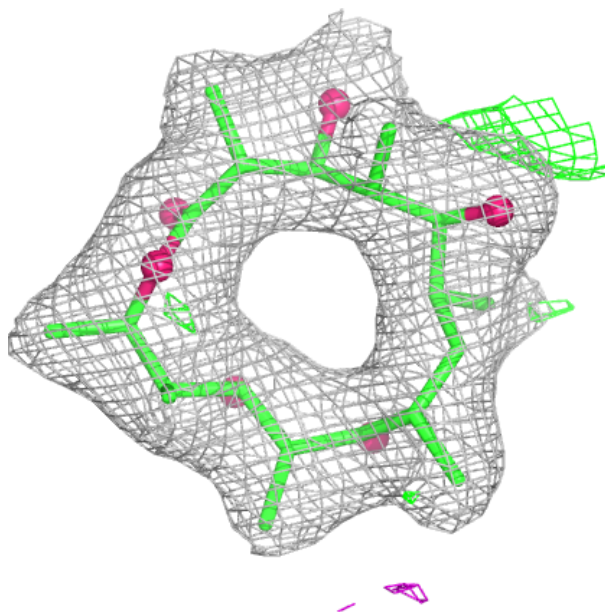
Electron density around QR8 D 502:

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



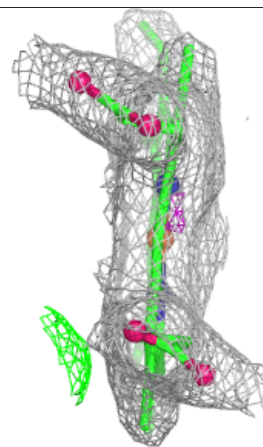
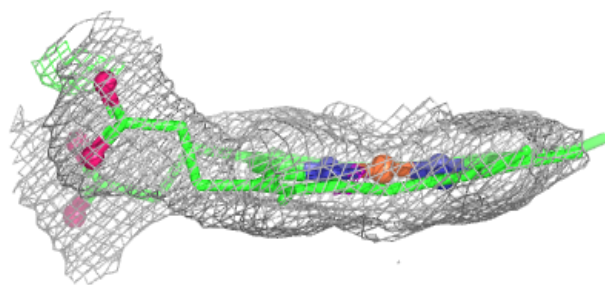
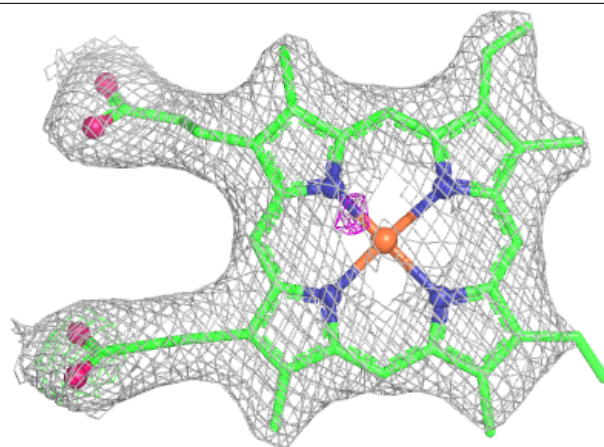
Electron density around QR8 B 502:

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



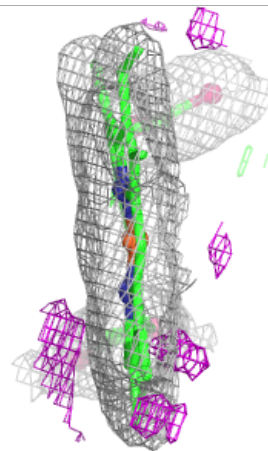
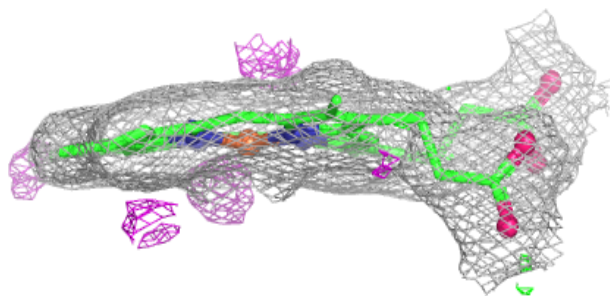
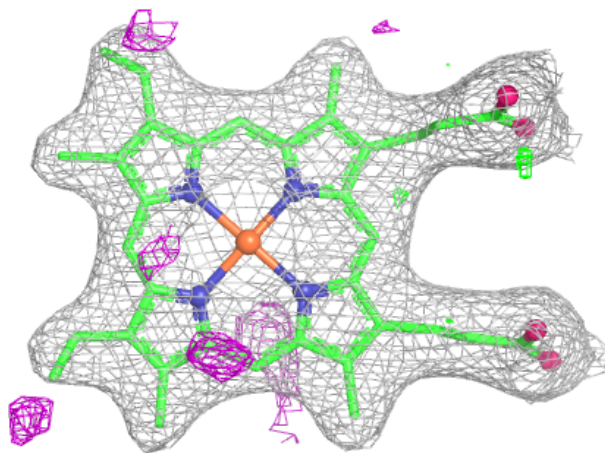
Electron density around HEM F 502:

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



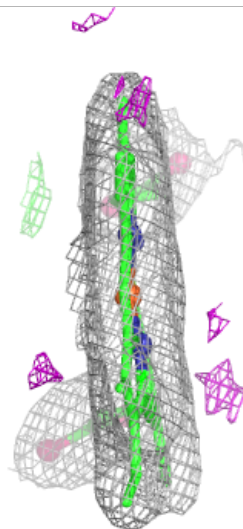
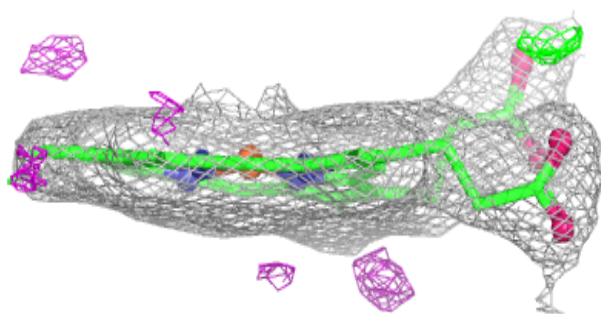
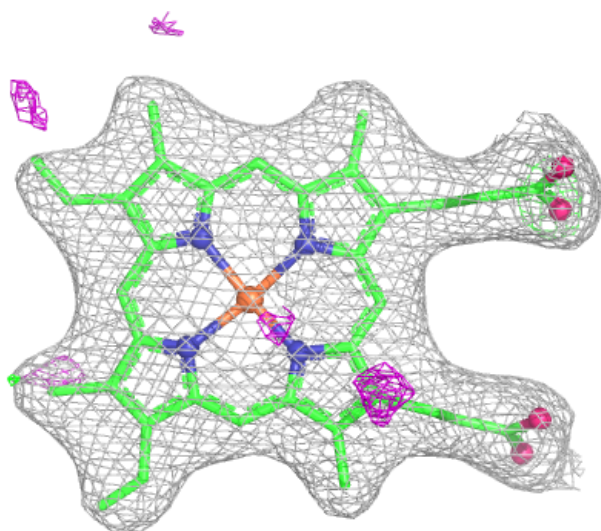
Electron density around HEM B 501:

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



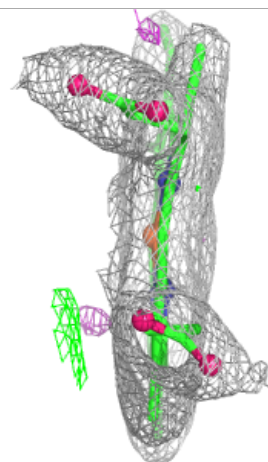
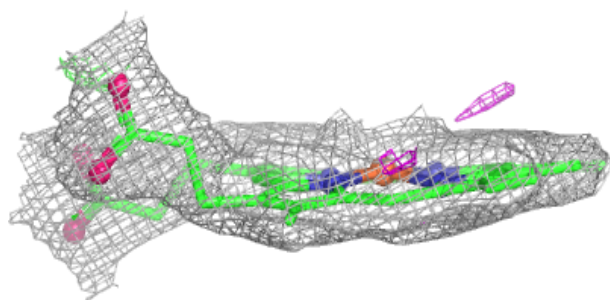
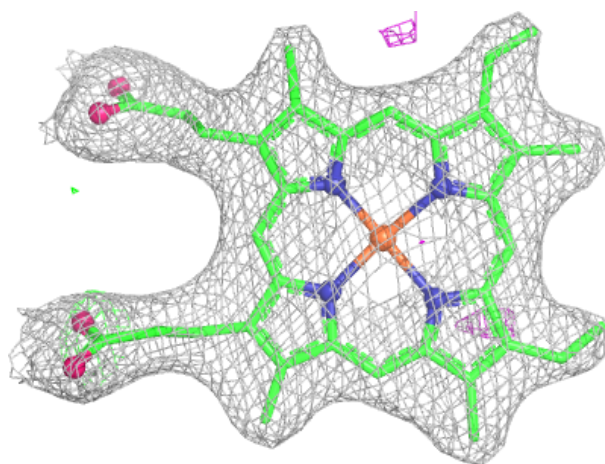
Electron density around HEM D 501:

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



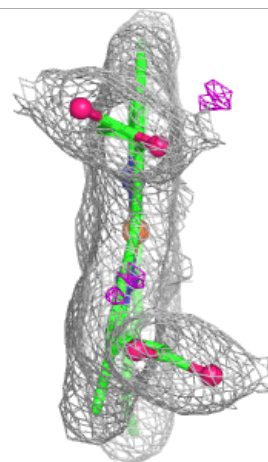
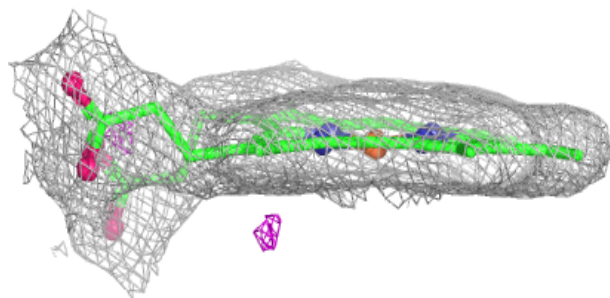
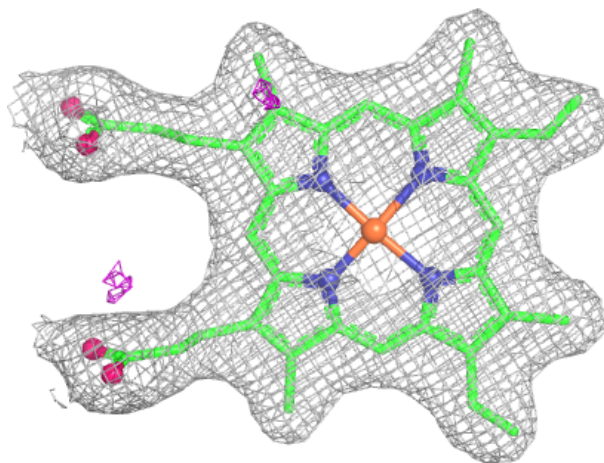
Electron density around HEM E 502:

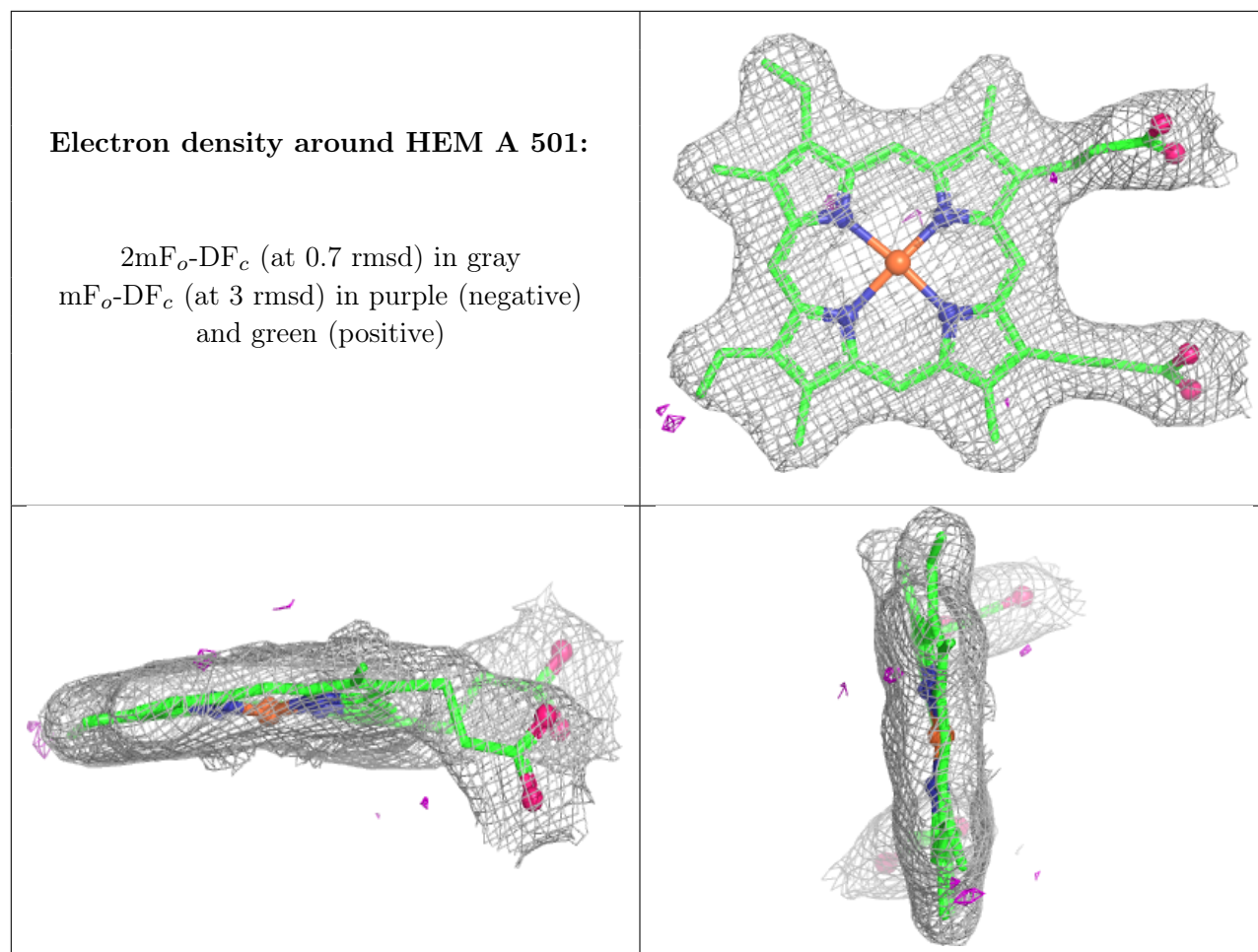
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.