



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:41 am BST

PDB ID : 4QOM  
Title : Bacillus pumilus catalase with pyrogallol bound  
Authors : Loewen, P.C.  
Deposited on : 2014-06-20  
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

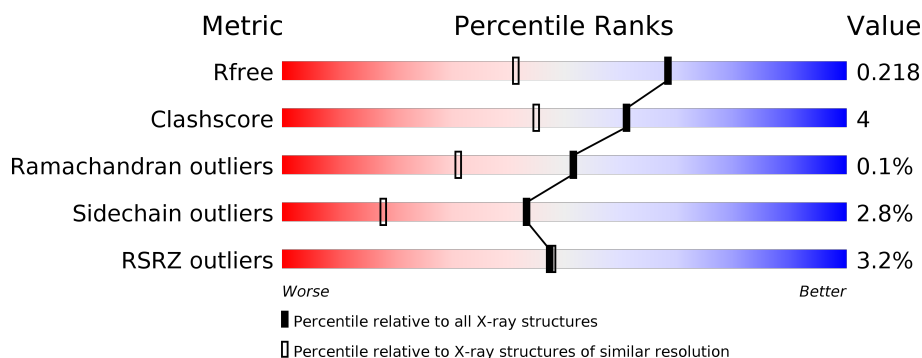
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	491	<div> <div>3%</div> <div>88% 9% ..</div> </div>
1	B	491	<div> <div>2%</div> <div>89% 8% ..</div> </div>
1	C	491	<div> <div>4%</div> <div>89% 9% .</div> </div>
1	D	491	<div> <div>4%</div> <div>88% 9% ..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PYG	A	504	-	-	X	-
3	PYG	B	504	-	X	-	-
3	PYG	C	504	-	-	X	-
3	PYG	D	504	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17977 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	5	0
			3949	2488	692	755	14			
1	B	480	Total	C	N	O	S	0	6	0
			3954	2493	691	754	16			
1	C	480	Total	C	N	O	S	0	6	0
			3962	2498	695	755	14			
1	D	480	Total	C	N	O	S	0	6	0
			3958	2494	692	758	14			

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



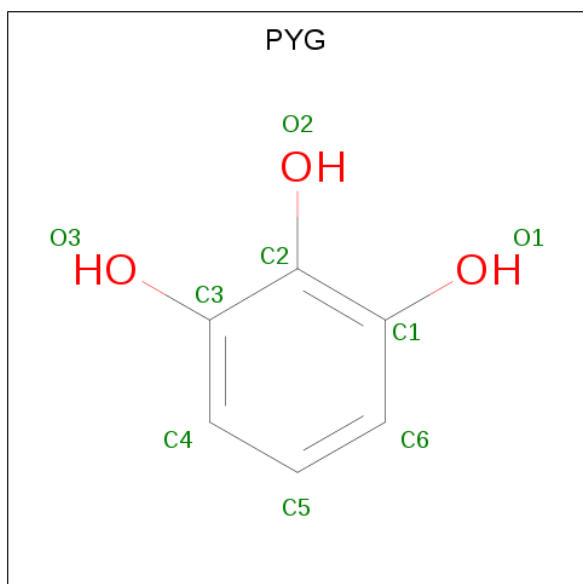
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		

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

- Molecule 3 is BENZENE-1,2,3-TRIOL (three-letter code: PYG) (formula: C<sub>6</sub>H<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			9	6	3		
3	A	1	Total	C	O		
			9	6	3		
3	B	1	Total	C	O		
			9	6	3		
3	B	1	Total	C	O		
			9	6	3		
3	C	1	Total	C	O		
			9	6	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			9	6	3		
3	D	1	Total	C	O	0	0
			9	6	3		
3	D	1	Total	C	O	0	0
			9	6	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		

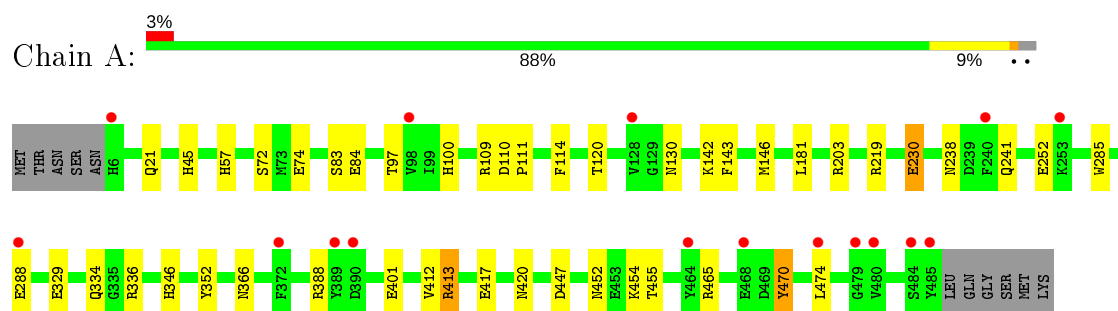
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	436	Total	O	0	0
			436	436		
6	B	424	Total	O	0	0
			424	424		
6	C	446	Total	O	0	0
			446	446		
6	D	424	Total	O	0	0
			424	424		

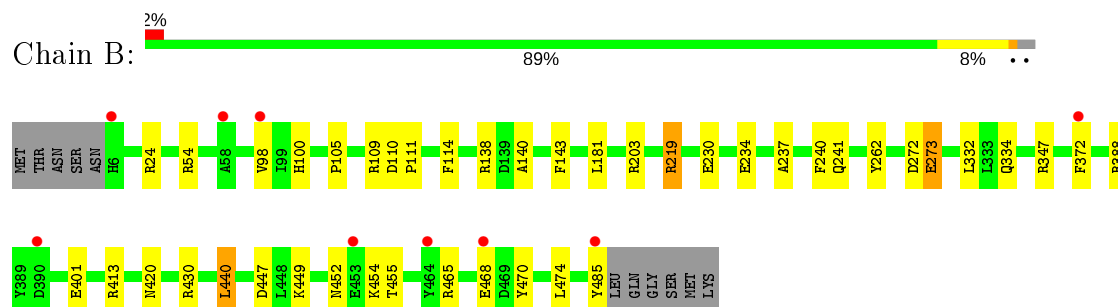
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

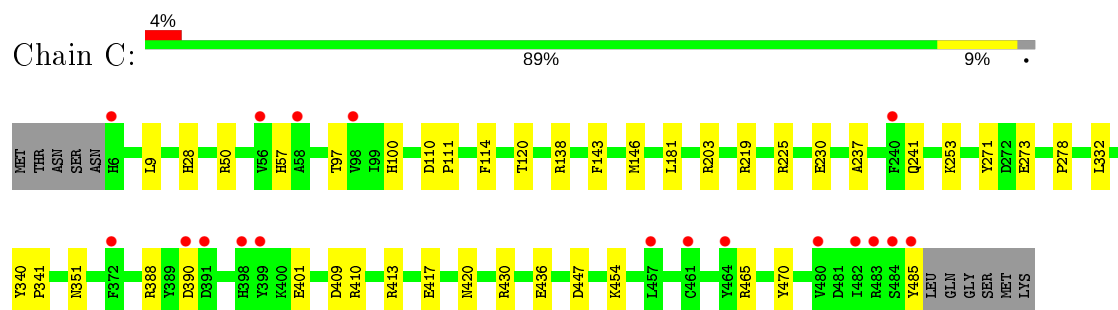
#### • Molecule 1: Catalase



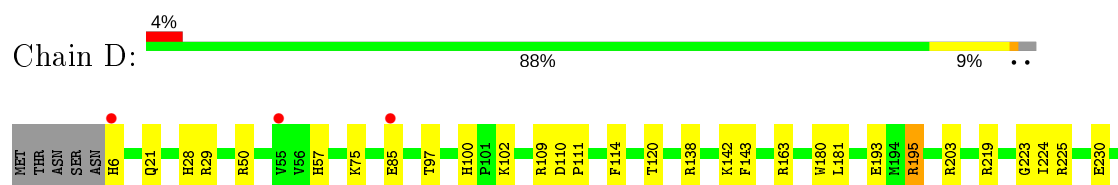
#### • Molecule 1: Catalase

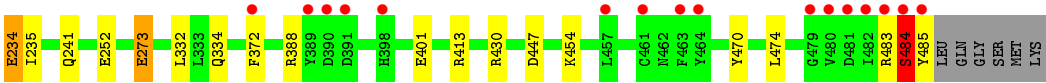


#### • Molecule 1: Catalase



#### • Molecule 1: Catalase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.85Å 109.42Å 103.37Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	103.29 – 1.65 44.29 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.8 (103.29-1.65) 96.8 (44.29-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.178 , 0.210 0.188 , 0.218	Depositor DCC
$R_{free}$ test set	11709 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.075 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CL, NA, PYG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.88	2/4068 (0.0%)	0.95	11/5516 (0.2%)
1	B	0.92	0/4075	0.94	11/5524 (0.2%)
1	C	0.95	0/4080	0.99	16/5531 (0.3%)
1	D	0.89	0/4076	0.94	10/5526 (0.2%)
All	All	0.91	2/16299 (0.0%)	0.95	48/22097 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	TRP	CE3-CZ3	-6.06	1.28	1.38
1	A	329	GLU	CG-CD	5.52	1.60	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	ARG	NE-CZ-NH1	-13.32	113.64	120.30
1	C	225	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	A	465	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	D	203	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	C	465	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	D	413	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	B	203	ARG	NE-CZ-NH2	-8.00	116.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	413	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	A	203	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	C	203	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	203	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	470	TYR	CB-CG-CD2	-7.26	116.64	121.00
1	C	465	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	413	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	C	138	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	D	138	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	109	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	138	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	C	430	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	109	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	203	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	50	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	C	138	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	195	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	D	163	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	A	388	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	430	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	D	430	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	138	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	440	LEU	CB-CG-CD2	5.70	120.70	111.00
1	C	388	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	D	163	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	C	410	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	C	50	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	388	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	413	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	C	470	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	A	329	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	A	252	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	B	24	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	54	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	203	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	C	50	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	440	LEU	CA-CB-CG	5.11	127.06	115.30
1	D	138	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	352	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	B	430	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	484	SER	Peptide

## 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	3949	0	3748	30	1
1	B	3954	0	3761	22	1
1	C	3962	0	3771	22	1
1	D	3958	0	3757	40	2
2	A	86	0	60	13	0
2	B	86	0	60	11	0
2	C	86	0	60	7	0
2	D	86	0	60	10	0
3	A	18	0	9	7	0
3	B	18	0	9	5	0
3	C	18	0	10	5	0
3	D	18	0	9	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	436	0	0	11	0
6	B	424	0	0	5	1
6	C	446	0	0	11	0
6	D	424	0	0	16	0
All	All	17977	0	15314	142	3

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

All (142) 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)
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:HBB2	1.33	1.08
1:C:436:GLU:OE2	6:C:743:HOH:O	1.72	1.05
1:C:454:LYS:HE3	6:C:1045:HOH:O	1.63	0.97
1:C:28:HIS:CE1	6:C:842:HOH:O	2.17	0.95
1:C:28:HIS:ND1	6:C:842:HOH:O	2.00	0.94
2:A:501[A]:HEM:CMB	2:A:501[A]:HEM:HBB2	1.96	0.90
2:B:502[B]:HEM:CMC	2:B:502[B]:HEM:HBC2	2.02	0.90
1:D:195:ARG:CD	1:D:224:ILE:HD11	2.03	0.89
1:D:195:ARG:HD3	1:D:224:ILE:CD1	2.07	0.84
1:B:449:LYS:NZ	6:B:940:HOH:O	1.94	0.82
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:HMC2	1.61	0.80
1:C:219:ARG:HD2	6:C:728:HOH:O	1.83	0.78
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:CMC	2.14	0.76
1:D:180:TRP:HZ3	1:D:195:ARG:HH22	1.32	0.76
1:B:372[A]:PHE:CE2	6:D:904:HOH:O	2.38	0.76
1:D:195:ARG:CG	1:D:224:ILE:HD11	2.16	0.75
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:CMC	2.17	0.75
2:B:501[A]:HEM:HMB2	2:B:501[A]:HEM:HBB2	1.69	0.75
1:A:83:SER:OG	6:A:958:HOH:O	2.04	0.75
1:D:195:ARG:HD3	1:D:224:ILE:HD11	1.66	0.74
2:B:501[A]:HEM:CMB	2:B:501[A]:HEM:HBB2	2.17	0.72
1:D:454:LYS:HE3	6:D:997:HOH:O	1.89	0.72
1:A:181:LEU:HD21	3:A:503:PYG:C6	2.20	0.71
1:C:219:ARG:CD	6:C:728:HOH:O	2.37	0.71
2:A:502[B]:HEM:CMC	2:A:502[B]:HEM:HBC2	2.21	0.70
2:B:502[B]:HEM:HMC1	2:B:502[B]:HEM:HBC2	1.72	0.70
1:B:181:LEU:HD21	3:B:503:PYG:C6	2.21	0.69
1:A:452:ASN:HD22	1:A:455:THR:H	1.41	0.69
2:B:502[B]:HEM:HMC1	2:B:502[B]:HEM:CBG	2.23	0.69
1:B:100:HIS:HE1	6:C:704:HOH:O	1.76	0.68
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:CBB	2.20	0.67
1:B:452:ASN:HD22	1:B:455:THR:H	1.43	0.67
1:D:85:GLU:CD	1:D:85:GLU:H	1.98	0.67
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:HMC2	1.77	0.66
1:D:252:GLU:OE1	6:D:675:HOH:O	2.12	0.66
1:A:45:HIS:HE1	1:C:351:ASN:OD1	1.78	0.66
1:D:181:LEU:HD21	3:D:503:PYG:C6	2.25	0.65
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:HMC2	1.79	0.64
1:B:372[A]:PHE:CD2	6:D:904:HOH:O	2.49	0.64
2:A:502[B]:HEM:HMC1	2:A:502[B]:HEM:HBC2	1.80	0.64
1:D:195:ARG:HD3	1:D:224:ILE:HD13	1.78	0.64
1:A:219:ARG:HD2	6:A:859:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501[A]:HEM:CMC	2:B:501[A]:HEM:HBC2	2.30	0.62
1:D:195:ARG:CD	1:D:224:ILE:CD1	2.71	0.61
1:D:195:ARG:CG	1:D:224:ILE:CD1	2.78	0.61
1:D:219:ARG:CG	6:D:853:HOH:O	2.49	0.60
1:C:111:PRO:HG2	3:C:504:PYG:O1	2.01	0.60
1:D:143:PHE:CZ	3:D:504:PYG:H4	2.37	0.60
1:C:390:ASP:O	6:C:867:HOH:O	2.16	0.59
1:A:219:ARG:HD2	6:A:834:HOH:O	2.02	0.59
1:A:452:ASN:HD21	1:A:454:LYS:HB3	1.68	0.58
1:B:452:ASN:HD21	1:B:454:LYS:HB3	1.67	0.58
1:A:45:HIS:HD2	6:A:686:HOH:O	1.86	0.58
1:C:181:LEU:HD21	3:C:503:PYG:C6	2.34	0.58
2:C:501[A]:HEM:CBC	2:C:501[A]:HEM:HMC2	2.34	0.57
1:D:234:GLU:HG2	6:D:775:HOH:O	2.04	0.57
1:D:483:ARG:O	1:D:484:SER:CB	2.50	0.57
2:D:501[A]:HEM:CMC	2:D:501[A]:HEM:HBC2	2.35	0.57
1:D:234:GLU:CG	6:D:775:HOH:O	2.52	0.56
1:A:334:GLN:HG3	6:D:884:HOH:O	2.05	0.56
2:D:502[B]:HEM:HBC2	2:D:502[B]:HEM:CMC	2.35	0.56
2:B:502[B]:HEM:HMC3	2:B:502[B]:HEM:HBC2	1.86	0.56
2:D:501[A]:HEM:HBB2	2:D:501[A]:HEM:CMB	2.37	0.55
1:D:111:PRO:HG2	3:D:504:PYG:O1	2.05	0.55
1:A:336:ARG:HG3	2:A:502[B]:HEM:HMC3	1.87	0.55
1:C:332:LEU:HD12	2:C:501[A]:HEM:HBB1	1.88	0.55
1:A:100:HIS:HE1	6:D:673:HOH:O	1.88	0.55
1:C:143:PHE:CZ	3:C:504:PYG:H4	2.42	0.55
2:A:501[A]:HEM:CBC	2:A:501[A]:HEM:HMC2	2.36	0.54
1:D:332:LEU:HD12	2:D:501[A]:HEM:HBB1	1.89	0.54
1:B:111:PRO:HG2	3:B:504:PYG:O1	2.08	0.54
2:D:501[A]:HEM:HBB2	2:D:501[A]:HEM:HMB2	1.90	0.54
6:A:803:HOH:O	1:D:100:HIS:HE1	1.92	0.53
1:C:146:MET:HE3	3:C:504:PYG:H5	1.90	0.53
1:A:417:GLU:HG3	1:D:28:HIS:NE2	2.24	0.52
1:A:143:PHE:CZ	3:A:504:PYG:H6	2.43	0.52
1:D:195:ARG:HG3	1:D:224:ILE:CD1	2.40	0.52
1:A:230:GLU:CG	6:A:668:HOH:O	2.58	0.51
3:A:503:PYG:O2	6:A:638:HOH:O	2.19	0.51
2:B:501[A]:HEM:CBB	2:B:501[A]:HEM:HMB2	2.39	0.51
1:A:111:PRO:HG2	3:A:504:PYG:O3	2.11	0.50
1:B:334:GLN:HG3	6:C:705:HOH:O	2.11	0.50
1:B:465:ARG:NE	6:B:929:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:978:HOH:O	1:D:334:GLN:HG3	2.12	0.49
1:B:143:PHE:CZ	3:B:504:PYG:H4	2.47	0.49
1:C:146:MET:CE	3:C:504:PYG:H5	2.43	0.49
1:A:366:ASN:HA	1:C:9[B]:LEU:HD22	1.94	0.49
1:A:219:ARG:CD	6:A:859:HOH:O	2.59	0.48
2:A:502[B]:HEM:HBB2	2:A:502[B]:HEM:CMB	2.43	0.48
1:A:412[A]:VAL:HG12	1:A:413:ARG:N	2.28	0.48
1:B:468:GLU:HG3	6:B:931:HOH:O	2.13	0.48
1:D:29:ARG:NH1	6:D:973:HOH:O	2.47	0.47
1:A:346:HIS:HE1	6:D:904:HOH:O	1.98	0.46
1:D:234:GLU:HG3	1:D:235:ILE:N	2.30	0.46
1:D:195:ARG:HG3	1:D:224:ILE:HG12	1.97	0.46
1:D:6:HIS:HA	6:D:789:HOH:O	2.14	0.46
1:A:146:MET:HE3	3:A:504:PYG:H5	1.96	0.46
1:A:181:LEU:HD21	3:A:503:PYG:C5	2.45	0.46
1:A:230:GLU:HG2	6:A:668:HOH:O	2.14	0.46
1:D:219:ARG:HG2	6:D:853:HOH:O	2.16	0.46
1:C:253:LYS:HE2	1:C:253:LYS:HB3	1.74	0.45
1:D:57:HIS:HA	1:D:97:THR:O	2.16	0.45
1:B:332:LEU:HD12	2:B:501[A]:HEM:HBB1	1.99	0.45
6:B:736:HOH:O	1:C:100:HIS:HE1	1.98	0.45
1:C:219:ARG:HD2	6:C:1000:HOH:O	2.16	0.45
2:A:502[B]:HEM:CMC	2:A:502[B]:HEM:CBC	2.95	0.45
2:D:501[A]:HEM:HMC2	2:D:501[A]:HEM:HBC2	1.99	0.45
1:A:72:SER:HB3	1:A:84:GLU:HA	2.00	0.44
1:A:238:ASN:ND2	6:A:1007:HOH:O	2.26	0.44
1:D:102[B]:LYS:HE3	1:D:102[B]:LYS:HB2	1.62	0.43
1:A:72:SER:OG	1:A:74:GLU:OE1	2.36	0.43
1:B:140:ALA:HA	2:B:501[A]:HEM:HBB1	2.00	0.43
6:C:1045:HOH:O	1:D:388:ARG:HD2	2.19	0.43
1:D:57:HIS:HB2	2:D:501[A]:HEM:HAD2	1.99	0.43
1:B:230:GLU:OE2	1:B:234:GLU:OE2	2.36	0.43
1:C:57:HIS:HA	1:C:97:THR:O	2.18	0.43
1:A:130:ASN:CG	2:A:502[B]:HEM:HMB2	2.40	0.42
1:A:21:GLN:HA	1:D:142:LYS:HD3	2.01	0.42
1:D:109:ARG:NE	6:D:945:HOH:O	2.31	0.42
1:A:146:MET:CE	3:A:504:PYG:H5	2.50	0.42
1:D:483:ARG:O	1:D:484:SER:HB3	2.18	0.42
1:B:181:LEU:HD21	3:B:503:PYG:C5	2.50	0.42
1:B:272:ASP:HB2	6:B:910:HOH:O	2.18	0.42
1:C:340:TYR:HB2	1:C:341:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:HG11	3:B:504:PYG:C6	2.49	0.42
2:A:502[B]:HEM:HMC1	2:A:502[B]:HEM:CBC	2.48	0.41
2:C:501[A]:HEM:HMB2	2:C:501[A]:HEM:HBB2	2.02	0.41
2:C:501[A]:HEM:CMB	2:C:501[A]:HEM:HBB2	2.51	0.41
1:D:225:ARG:HD2	6:D:961:HOH:O	2.20	0.41
1:B:237:ALA:HB2	1:C:237:ALA:HB2	2.02	0.41
2:C:502[B]:HEM:CMB	2:C:502[B]:HEM:HBB2	2.51	0.41
1:D:85:GLU:HG3	6:D:1024:HOH:O	2.19	0.41
1:B:219:ARG:NH2	1:B:262:TYR:OH	2.54	0.41
1:C:271:TYR:HD1	1:C:278:PRO:HD2	1.86	0.41
1:A:142:LYS:HD3	1:D:21:GLN:HA	2.02	0.41
2:D:501[A]:HEM:HMC2	2:D:501[A]:HEM:CBC	2.52	0.40
2:D:502[B]:HEM:CMC	2:D:502[B]:HEM:CBC	2.99	0.40
1:D:193:GLU:HA	1:D:223:GLY:O	2.21	0.40
1:B:105:PRO:HA	1:B:240:PHE:O	2.22	0.40
1:B:347:ARG:O	1:D:372[A]:PHE:HE1	2.05	0.40
2:D:502[B]:HEM:HBC2	2:D:502[B]:HEM:HMC1	2.03	0.40
1:A:57:HIS:HA	1:A:97:THR:O	2.21	0.40

All (3) 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:273:GLU:OE1	1:C:417:GLU:OE2[1_455]	1.69	0.51
1:A:417:GLU:OE2	1:D:273:GLU:OE1[1_455]	2.06	0.14
1:D:225:ARG:NH1	6:B:998:HOH:O[2_655]	2.08	0.12

## 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	483/491 (98%)	471 (98%)	12 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	484/491 (99%)	473 (98%)	11 (2%)	0	100	100
1	C	484/491 (99%)	471 (97%)	13 (3%)	0	100	100
1	D	484/491 (99%)	471 (97%)	12 (2%)	1 (0%)	47	28
All	All	1935/1964 (98%)	1886 (98%)	48 (2%)	1 (0%)	51	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	484	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/432 (99%)	415 (97%)	11 (3%)	46	21
1	B	427/432 (99%)	415 (97%)	12 (3%)	43	18
1	C	427/432 (99%)	416 (97%)	11 (3%)	46	21
1	D	427/432 (99%)	414 (97%)	13 (3%)	41	15
All	All	1707/1728 (99%)	1660 (97%)	47 (3%)	43	18

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	114	PHE
1	A	120	THR
1	A	230	GLU
1	A	241	GLN
1	A	288	GLU
1	A	401	GLU
1	A	420	ASN
1	A	447	ASP
1	A	470	TYR

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Mol	Chain	Res	Type
1	A	474	LEU
1	B	110	ASP
1	B	114	PHE
1	B	219	ARG
1	B	241	GLN
1	B	273	GLU
1	B	401	GLU
1	B	420	ASN
1	B	440	LEU
1	B	447	ASP
1	B	470	TYR
1	B	474	LEU
1	B	485	TYR
1	C	110	ASP
1	C	114	PHE
1	C	120	THR
1	C	230	GLU
1	C	241	GLN
1	C	273	GLU
1	C	401	GLU
1	C	409	ASP
1	C	420	ASN
1	C	447	ASP
1	C	485	TYR
1	D	75	LYS
1	D	110	ASP
1	D	114	PHE
1	D	120	THR
1	D	230	GLU
1	D	234	GLU
1	D	241	GLN
1	D	273	GLU
1	D	401	GLU
1	D	447	ASP
1	D	470	TYR
1	D	474	LEU
1	D	485	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS

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Mol	Chain	Res	Type
1	A	100	HIS
1	A	157	ASN
1	A	226	ASN
1	A	346	HIS
1	A	367	ASN
1	A	420	ASN
1	A	452	ASN
1	B	100	HIS
1	B	157	ASN
1	B	226	ASN
1	B	398	HIS
1	B	420	ASN
1	B	452	ASN
1	C	100	HIS
1	C	226	ASN
1	C	238	ASN
1	C	420	ASN
1	D	100	HIS
1	D	157	ASN
1	D	226	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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
3	PYG	C	504	-	9,9,9	2.72	3 (33%)	12,12,12	2.58	3 (25%)
2	HEM	D	502[B]	1	27,50,50	1.25	3 (11%)	17,82,82	2.45	8 (47%)
2	HEM	A	502[B]	1	27,50,50	1.11	2 (7%)	17,82,82	2.15	8 (47%)
2	HEM	B	501[A]	1,3	27,50,50	1.22	3 (11%)	17,82,82	1.60	3 (17%)
3	PYG	D	504	2	9,9,9	3.12	3 (33%)	12,12,12	2.94	6 (50%)
3	PYG	D	503	-	9,9,9	3.29	2 (22%)	12,12,12	1.68	3 (25%)
3	PYG	B	503	-	9,9,9	3.87	2 (22%)	12,12,12	2.22	3 (25%)
2	HEM	C	502[B]	1	27,50,50	1.15	2 (7%)	17,82,82	2.47	9 (52%)
2	HEM	A	501[A]	1	27,50,50	1.21	4 (14%)	17,82,82	1.90	7 (41%)
2	HEM	B	502[B]	1	27,50,50	1.11	2 (7%)	17,82,82	2.39	9 (52%)
2	HEM	C	501[A]	1	27,50,50	1.02	2 (7%)	17,82,82	2.38	6 (35%)
3	PYG	C	503	-	9,9,9	2.84	2 (22%)	12,12,12	2.30	4 (33%)
3	PYG	A	503	-	9,9,9	3.63	2 (22%)	12,12,12	1.62	3 (25%)
2	HEM	D	501[A]	1,3	27,50,50	1.01	1 (3%)	17,82,82	2.04	7 (41%)
3	PYG	A	504	-	9,9,9	2.87	3 (33%)	12,12,12	1.92	3 (25%)
3	PYG	B	504	2	9,9,9	2.63	3 (33%)	12,12,12	3.07	6 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PYG	C	504	-	-	-	0/1/1/1
2	HEM	D	502[B]	1	-	0/6/54/54	-
2	HEM	A	502[B]	1	-	0/6/54/54	-
2	HEM	B	501[A]	1,3	-	0/6/54/54	-
3	PYG	D	504	2	-	-	0/1/1/1
3	PYG	D	503	-	-	-	0/1/1/1
3	PYG	B	503	-	-	-	0/1/1/1
2	HEM	C	502[B]	1	-	0/6/54/54	-
2	HEM	A	501[A]	1	-	0/6/54/54	-
2	HEM	B	502[B]	1	-	0/6/54/54	-
2	HEM	C	501[A]	1	-	0/6/54/54	-
3	PYG	C	503	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PYG	A	503	-	-	-	0/1/1/1
2	HEM	D	501[A]	1,3	-	0/6/54/54	-
3	PYG	A	504	-	-	-	0/1/1/1
3	PYG	B	504	2	-	-	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	PYG	C3-C2	8.84	1.50	1.40
3	B	503	PYG	C3-C2	8.56	1.50	1.40
3	D	503	PYG	C3-C2	7.67	1.49	1.40
3	B	503	PYG	C1-C2	7.41	1.48	1.40
3	C	503	PYG	C3-C2	6.77	1.48	1.40
3	A	503	PYG	C1-C2	6.05	1.47	1.40
3	D	504	PYG	C1-C2	5.82	1.47	1.40
3	D	504	PYG	C3-C2	5.78	1.46	1.40
3	D	503	PYG	C1-C2	5.77	1.46	1.40
3	A	504	PYG	C3-C2	5.73	1.46	1.40
3	A	504	PYG	C1-C2	5.25	1.46	1.40
3	C	504	PYG	O2-C2	-4.99	1.25	1.37
3	C	504	PYG	C1-C2	4.98	1.46	1.40
3	C	503	PYG	C1-C2	4.25	1.45	1.40
3	B	504	PYG	C1-C2	4.25	1.45	1.40
3	B	504	PYG	C3-C2	4.12	1.44	1.40
3	B	504	PYG	O2-C2	-3.96	1.27	1.37
3	D	504	PYG	O2-C2	-3.71	1.28	1.37
2	A	501[A]	HEM	C3B-C2B	-3.39	1.35	1.40
2	C	502[B]	HEM	C4D-C3D	3.16	1.49	1.42
2	D	501[A]	HEM	C4D-C3D	3.15	1.49	1.42
2	A	502[B]	HEM	C4D-C3D	2.98	1.49	1.42
2	C	501[A]	HEM	C4A-NA	2.85	1.42	1.36
3	C	504	PYG	C3-C2	2.79	1.43	1.40
2	B	502[B]	HEM	C4D-C3D	2.76	1.48	1.42
2	D	502[B]	HEM	C1A-NA	2.70	1.41	1.36
2	C	501[A]	HEM	C4D-C3D	2.61	1.48	1.42
2	D	502[B]	HEM	C3B-C2B	-2.58	1.36	1.40
2	B	501[A]	HEM	C3B-C2B	-2.47	1.36	1.40
2	A	502[B]	HEM	C3B-C2B	-2.43	1.37	1.40
2	B	501[A]	HEM	C4D-C3D	2.40	1.48	1.42
3	A	504	PYG	O3-C3	-2.24	1.31	1.36
2	C	502[B]	HEM	CAA-C2A	-2.24	1.48	1.52
2	A	501[A]	HEM	C3C-C2C	-2.22	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	HEM	C3C-CAC	-2.18	1.43	1.47
2	B	502[B]	HEM	C3B-C2B	-2.16	1.37	1.40
2	B	501[A]	HEM	C3D-C2D	-2.07	1.31	1.37
2	A	501[A]	HEM	C4D-C3D	2.03	1.47	1.42
2	D	502[B]	HEM	C4D-C3D	2.02	1.47	1.42

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	504	PYG	C4-C3-C2	-7.09	112.79	120.06
3	B	504	PYG	C4-C3-C2	-7.03	112.85	120.06
3	C	504	PYG	C4-C3-C2	-5.44	114.48	120.06
2	C	502[B]	HEM	CAD-CBD-CGD	5.07	121.18	112.67
3	B	503	PYG	C6-C1-C2	-5.02	114.92	120.06
3	C	504	PYG	C3-C2-C1	4.92	122.64	119.51
2	C	501[A]	HEM	CAD-CBD-CGD	-4.74	104.72	112.67
3	B	504	PYG	C3-C2-C1	4.61	122.44	119.51
3	C	503	PYG	C6-C1-C2	-4.58	115.37	120.06
2	D	502[B]	HEM	CMB-C2B-C3B	4.44	132.98	124.68
3	D	504	PYG	C3-C2-C1	4.19	122.18	119.51
2	C	502[B]	HEM	CBD-CAD-C3D	-4.16	104.81	112.48
2	A	502[B]	HEM	CAD-CBD-CGD	4.15	119.64	112.67
2	C	501[A]	HEM	CBA-CAA-C2A	-4.02	105.07	112.49
2	D	502[B]	HEM	CBD-CAD-C3D	-3.97	105.17	112.48
3	A	504	PYG	C5-C6-C1	3.93	125.01	120.05
2	D	502[B]	HEM	CAA-CBA-CGA	-3.91	106.12	112.67
2	B	502[B]	HEM	C4C-C3C-C2C	3.89	109.62	106.90
3	B	504	PYG	C5-C4-C3	3.89	124.96	120.05
2	B	502[B]	HEM	CBD-CAD-C3D	-3.86	105.37	112.48
3	B	503	PYG	O1-C1-C2	3.77	127.64	117.90
3	A	504	PYG	C6-C1-C2	-3.75	116.21	120.06
3	D	503	PYG	C6-C1-C2	-3.71	116.26	120.06
2	C	502[B]	HEM	C4C-C3C-C2C	3.69	109.48	106.90
2	C	501[A]	HEM	CMA-C3A-C4A	-3.63	122.89	128.46
2	D	502[B]	HEM	C4A-C3A-C2A	3.57	109.48	107.00
2	C	501[A]	HEM	C4C-C3C-C2C	3.57	109.39	106.90
2	A	502[B]	HEM	C3C-C4C-NC	-3.55	104.25	110.94
2	B	501[A]	HEM	C3B-C4B-NB	-3.53	104.65	109.21
2	B	502[B]	HEM	C3C-C4C-NC	-3.53	104.29	110.94
3	C	503	PYG	C3-C2-C1	3.48	121.72	119.51
2	B	502[B]	HEM	CMD-C2D-C1D	-3.47	123.14	128.46
2	D	501[A]	HEM	CBA-CAA-C2A	-3.40	106.21	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502[B]	HEM	CMD-C2D-C3D	3.40	131.35	124.94
3	D	504	PYG	C5-C4-C3	3.39	124.34	120.05
3	B	504	PYG	O3-C3-C4	3.39	128.54	119.33
2	D	502[B]	HEM	CMD-C2D-C1D	-3.37	123.29	128.46
2	C	501[A]	HEM	CMA-C3A-C2A	3.31	131.18	124.94
2	A	501[A]	HEM	C3B-C4B-NB	-3.30	104.95	109.21
3	C	504	PYG	O3-C3-C4	3.27	128.21	119.33
2	D	501[A]	HEM	CAD-CBD-CGD	-3.20	107.31	112.67
2	D	501[A]	HEM	CMA-C3A-C4A	-3.16	123.61	128.46
2	B	501[A]	HEM	CAD-CBD-CGD	-3.12	107.43	112.67
2	D	501[A]	HEM	CMD-C2D-C1D	-3.11	123.68	128.46
2	C	502[B]	HEM	CMB-C2B-C3B	3.11	130.50	124.68
2	C	502[B]	HEM	CMC-C2C-C3C	3.11	130.49	124.68
2	A	502[B]	HEM	CMD-C2D-C1D	-3.04	123.79	128.46
2	D	502[B]	HEM	CMD-C2D-C3D	3.03	130.65	124.94
2	B	502[B]	HEM	C4A-C3A-C2A	3.02	109.09	107.00
3	C	503	PYG	O1-C1-C2	3.01	125.69	117.90
2	A	502[B]	HEM	CMC-C2C-C3C	3.01	130.31	124.68
3	D	503	PYG	O1-C1-C2	2.97	125.57	117.90
3	B	503	PYG	C5-C6-C1	2.92	123.74	120.05
3	D	504	PYG	O3-C3-C4	2.91	127.25	119.33
2	D	501[A]	HEM	C3B-C4B-NB	-2.86	105.51	109.21
2	D	501[A]	HEM	CMD-C2D-C3D	2.79	130.20	124.94
3	C	503	PYG	C6-C5-C4	2.79	124.20	120.25
3	A	503	PYG	C3-C2-C1	-2.75	117.76	119.51
3	D	504	PYG	C5-C6-C1	-2.75	116.57	120.05
2	A	501[A]	HEM	CBA-CAA-C2A	-2.74	107.43	112.49
2	A	501[A]	HEM	C4C-C3C-C2C	2.72	108.80	106.90
2	A	501[A]	HEM	C3C-C4C-NC	-2.66	105.92	110.94
2	B	502[B]	HEM	CMA-C3A-C4A	-2.62	124.44	128.46
3	A	503	PYG	O3-C3-C2	2.58	124.56	117.90
3	A	503	PYG	O1-C1-C2	2.56	124.50	117.90
2	A	501[A]	HEM	CMD-C2D-C1D	-2.51	124.60	128.46
2	A	502[B]	HEM	C4A-C3A-C2A	2.51	108.74	107.00
2	A	501[A]	HEM	CMA-C3A-C4A	-2.47	124.66	128.46
3	B	504	PYG	O1-C1-C6	2.35	125.73	119.33
2	C	501[A]	HEM	CMB-C2B-C3B	-2.32	120.34	124.68
3	A	504	PYG	C3-C2-C1	-2.30	118.05	119.51
2	C	502[B]	HEM	CMA-C3A-C2A	-2.30	120.61	124.94
2	C	502[B]	HEM	C4A-C3A-C2A	2.27	108.58	107.00
2	B	502[B]	HEM	CAD-CBD-CGD	2.26	116.45	112.67
2	C	502[B]	HEM	CMD-C2D-C1D	-2.25	125.00	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502[B]	HEM	CMB-C2B-C3B	2.23	128.84	124.68
2	D	502[B]	HEM	CMA-C3A-C4A	-2.17	125.12	128.46
2	A	502[B]	HEM	CMD-C2D-C3D	2.15	129.00	124.94
2	B	502[B]	HEM	C1D-C2D-C3D	-2.13	105.51	107.00
2	A	502[B]	HEM	C4C-C3C-C2C	2.12	108.38	106.90
2	D	502[B]	HEM	C3C-C4C-NC	-2.08	107.01	110.94
3	B	504	PYG	C5-C6-C1	-2.06	117.45	120.05
3	D	503	PYG	C5-C6-C1	2.05	122.64	120.05
2	C	502[B]	HEM	C3C-C4C-NC	-2.05	107.08	110.94
3	D	504	PYG	C6-C5-C4	2.03	123.13	120.25
2	B	501[A]	HEM	C3C-C4C-NC	-2.03	107.12	110.94
2	A	501[A]	HEM	CAD-CBD-CGD	-2.02	109.28	112.67
2	D	501[A]	HEM	CMA-C3A-C2A	2.02	128.75	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

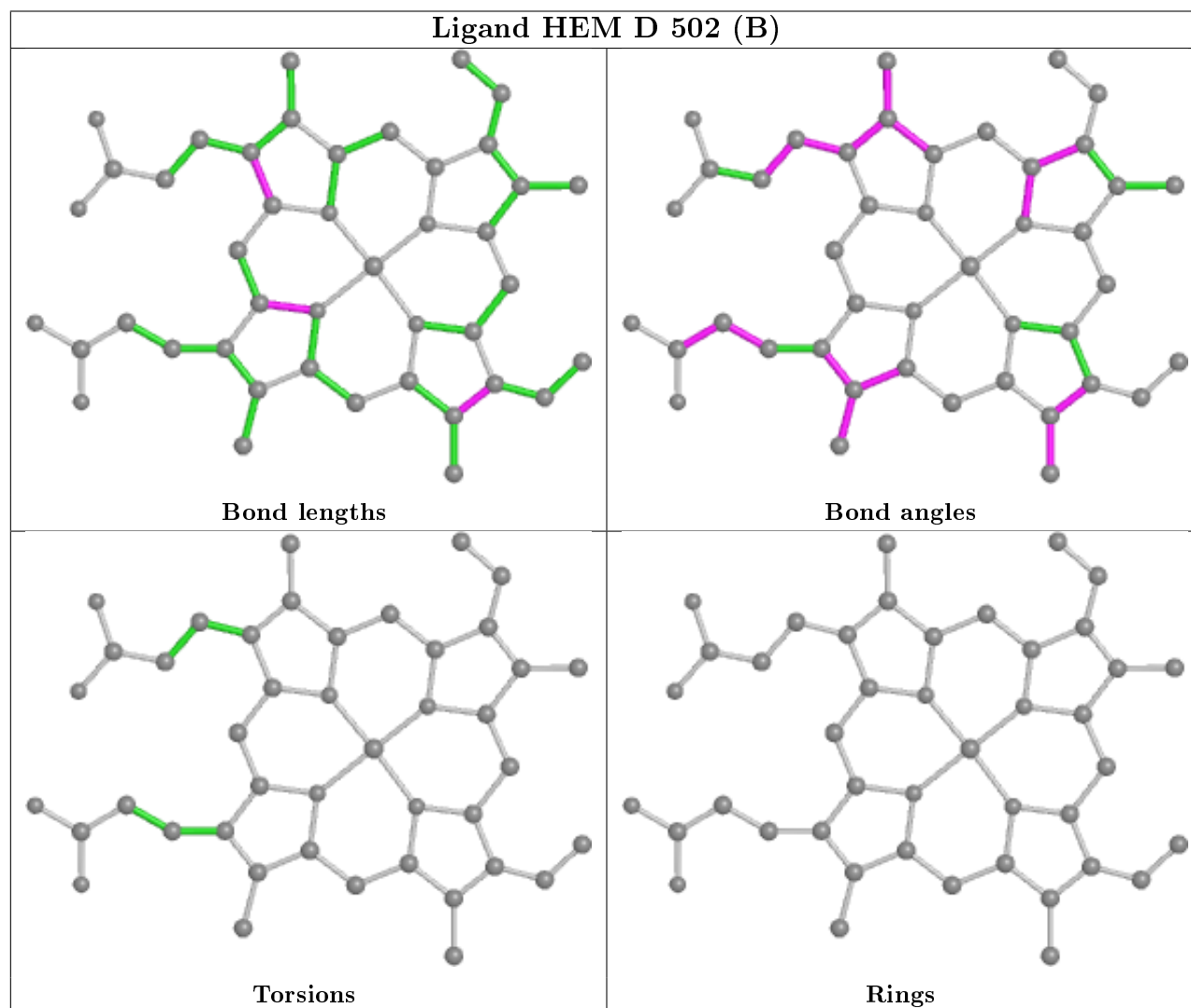
16 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	504	PYG	4	0
2	D	502[B]	HEM	3	0
2	A	502[B]	HEM	7	0
2	B	501[A]	HEM	7	0
3	D	504	PYG	2	0
3	D	503	PYG	1	0
3	B	503	PYG	2	0
2	C	502[B]	HEM	1	0
2	A	501[A]	HEM	6	0
2	B	502[B]	HEM	4	0
2	C	501[A]	HEM	6	0
3	C	503	PYG	1	0
3	A	503	PYG	3	0
2	D	501[A]	HEM	7	0
3	A	504	PYG	4	0
3	B	504	PYG	3	0

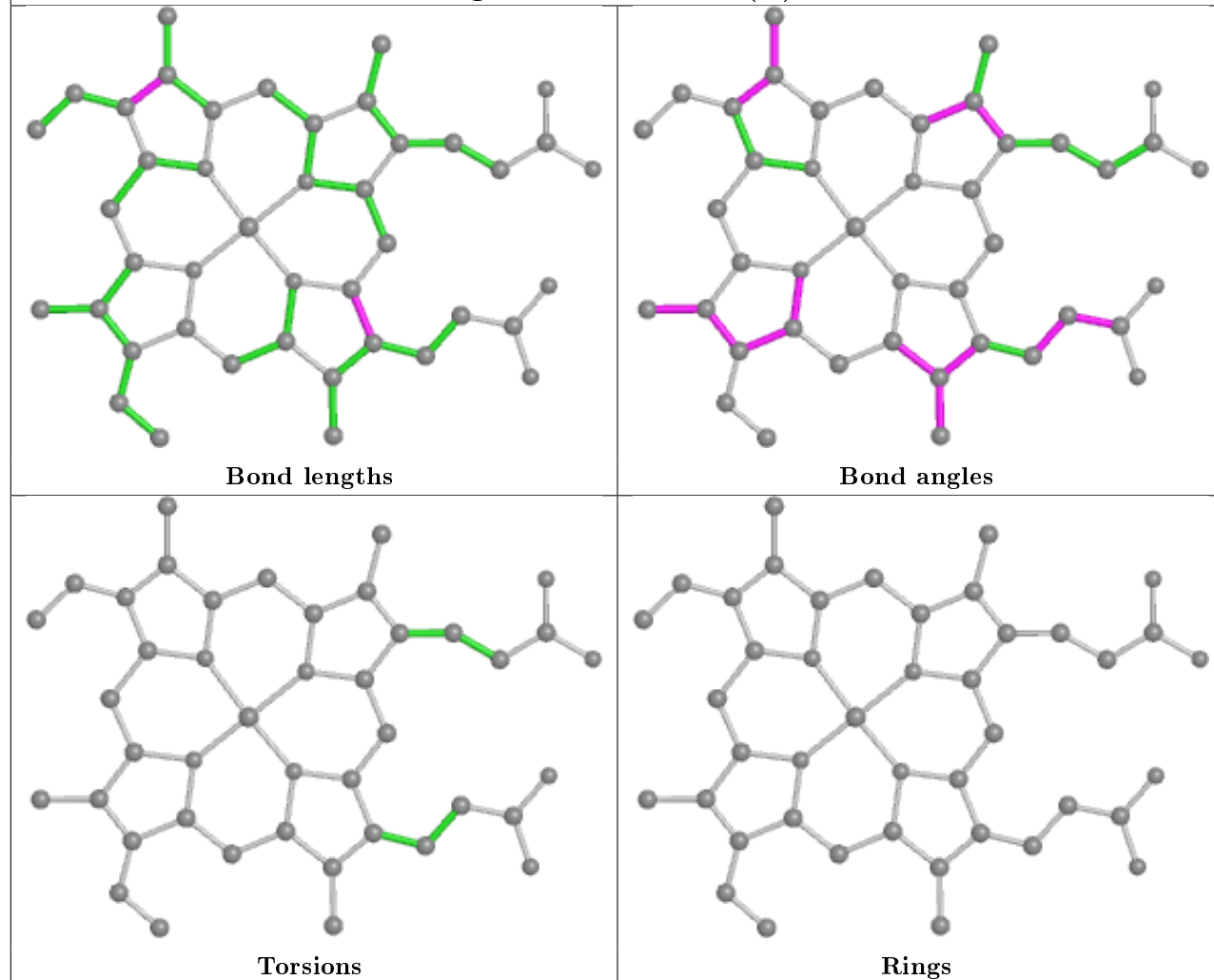
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is



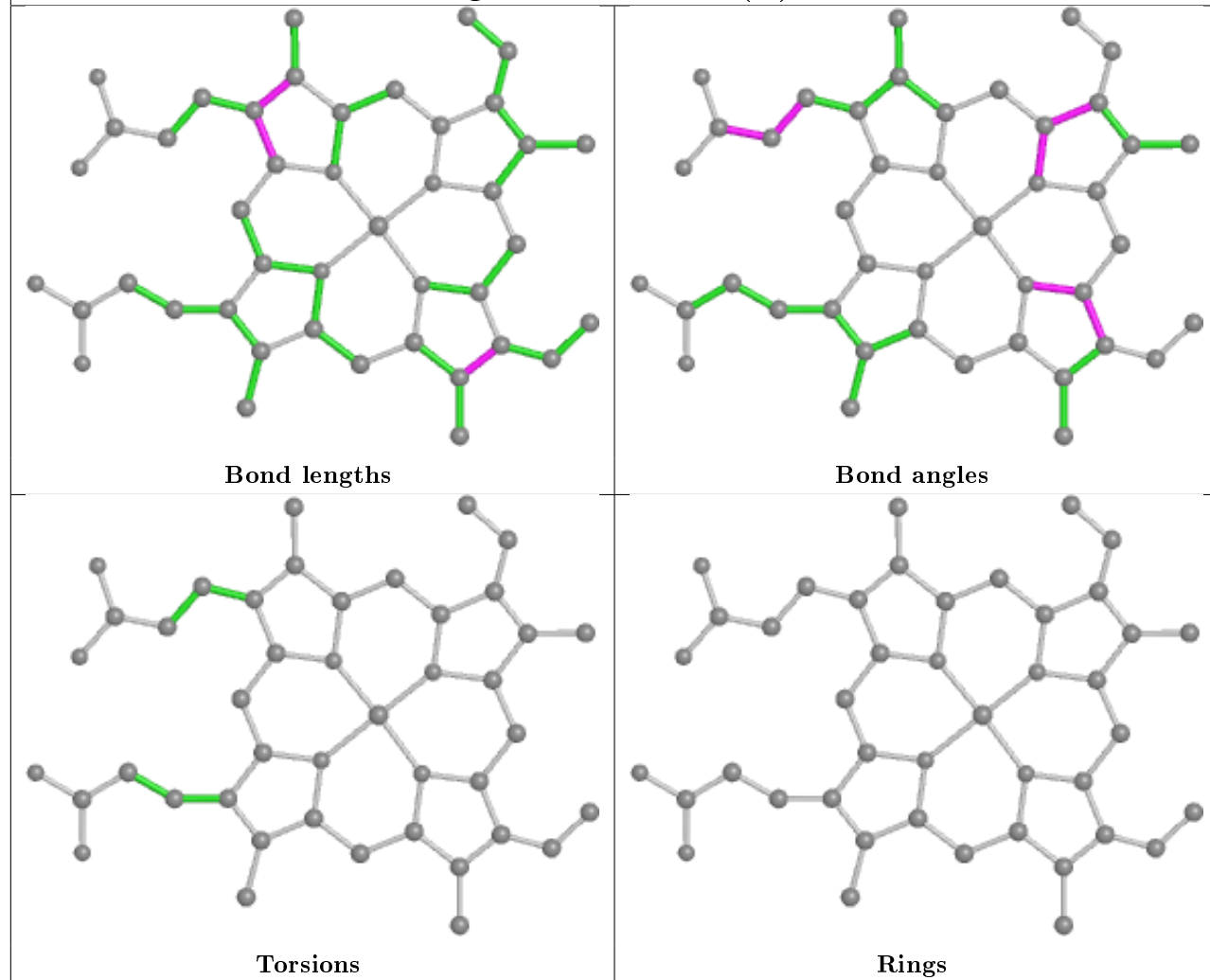
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

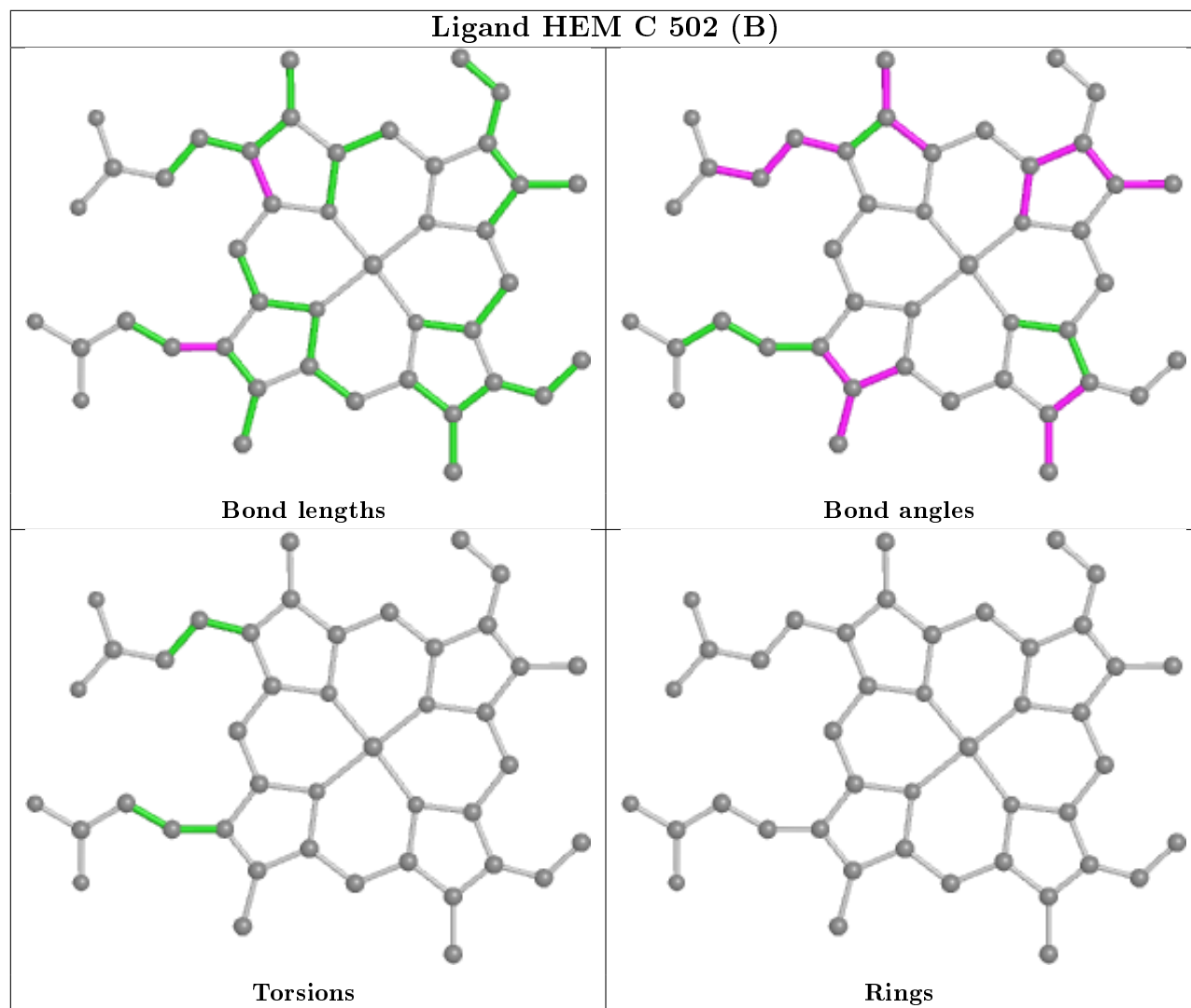


## Ligand HEM A 502 (B)

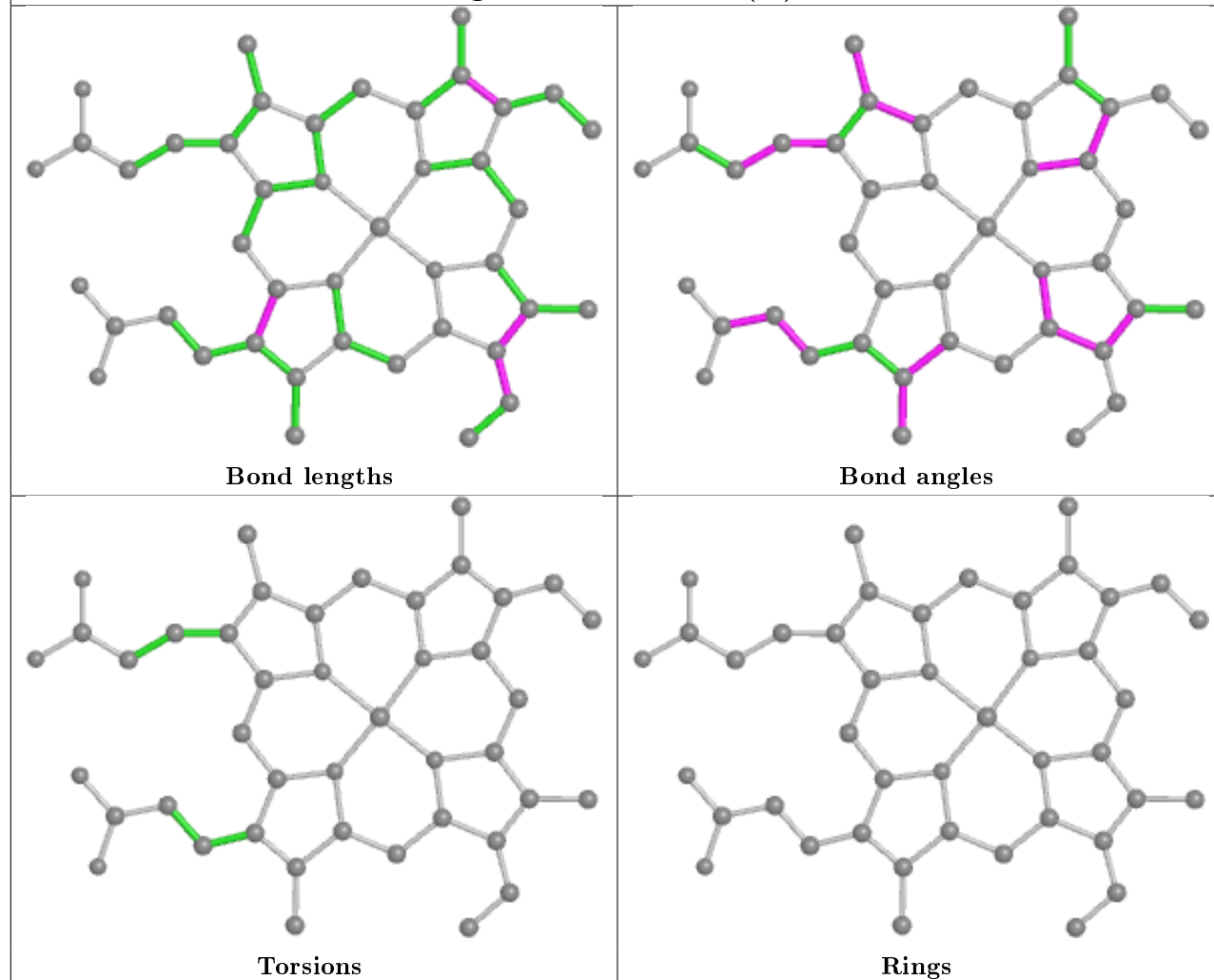


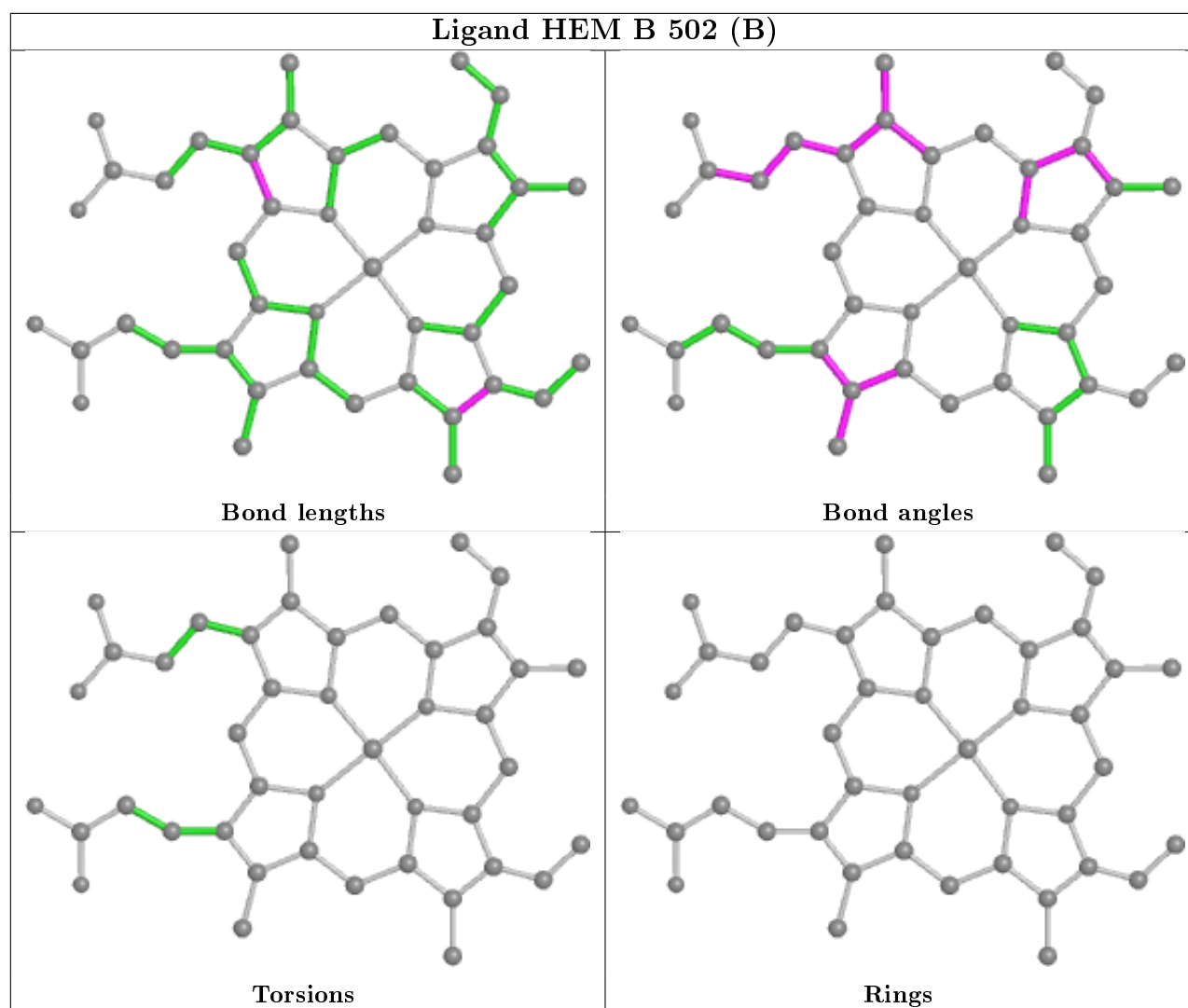
## Ligand HEM B 501 (A)



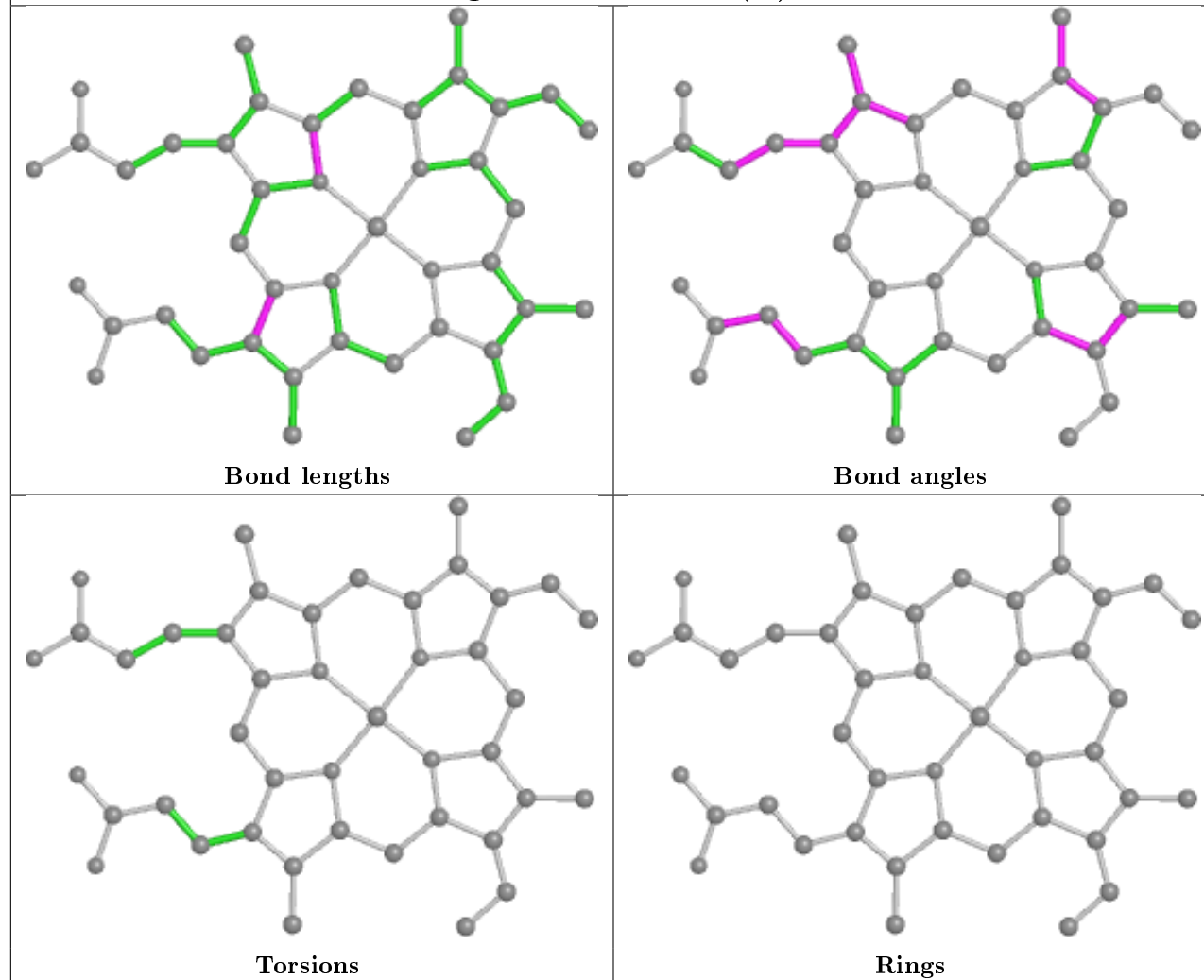


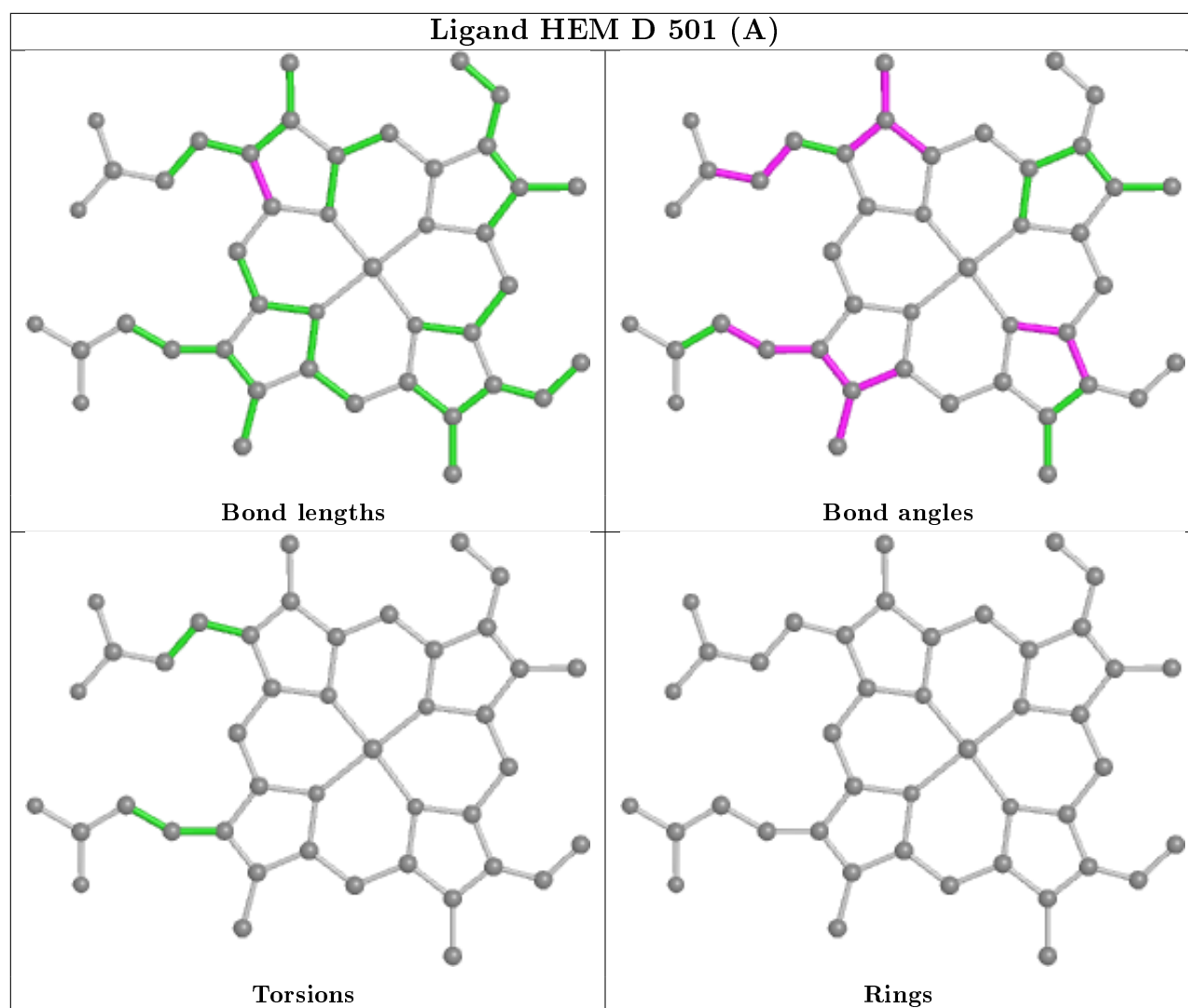
## Ligand HEM A 501 (A)





## Ligand HEM C 501 (A)





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	480/491 (97%)	0.23	16 (3%) 46 47	13, 23, 39, 64	0
1	B	480/491 (97%)	0.09	9 (1%) 66 69	11, 20, 36, 60	0
1	C	480/491 (97%)	0.15	18 (3%) 40 40	12, 18, 34, 70	0
1	D	480/491 (97%)	0.26	19 (3%) 38 38	13, 21, 36, 80	0
All	All	1920/1964 (97%)	0.18	62 (3%) 47 48	11, 21, 36, 80	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	485	TYR	9.6
1	C	485	TYR	8.1
1	D	484	SER	7.6
1	A	485	TYR	7.0
1	C	484	SER	5.4
1	D	483	ARG	5.3
1	B	485	TYR	5.2
1	B	6	HIS	4.9
1	C	6	HIS	4.8
1	D	6	HIS	4.3
1	A	6	HIS	4.3
1	A	484	SER	4.1
1	C	482	ILE	3.9
1	B	372[A]	PHE	3.5
1	D	372[A]	PHE	3.4
1	D	461	CYS	3.3
1	A	98	VAL	3.3
1	C	483	ARG	3.2
1	D	480	VAL	3.2
1	C	56	VAL	3.1
1	C	372[A]	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	482	ILE	3.1
1	B	464	TYR	3.0
1	C	391	ASP	3.0
1	C	240	PHE	3.0
1	A	468	GLU	2.9
1	A	288	GLU	2.9
1	A	372[A]	PHE	2.8
1	A	464	TYR	2.8
1	A	480	VAL	2.8
1	D	481	ASP	2.7
1	C	398	HIS	2.7
1	A	389	TYR	2.7
1	D	479	GLY	2.7
1	B	98	VAL	2.6
1	C	457	LEU	2.6
1	A	253	LYS	2.5
1	D	464	TYR	2.5
1	A	240	PHE	2.5
1	D	457	LEU	2.5
1	D	390	ASP	2.4
1	A	479	GLY	2.4
1	D	85	GLU	2.4
1	A	474	LEU	2.4
1	B	468	GLU	2.4
1	C	480	VAL	2.3
1	D	391	ASP	2.3
1	C	461	CYS	2.3
1	D	55	VAL	2.3
1	C	390	ASP	2.2
1	C	98	VAL	2.1
1	B	390	ASP	2.1
1	C	58	ALA	2.1
1	D	398	HIS	2.1
1	C	399	TYR	2.1
1	C	464	TYR	2.1
1	D	389	TYR	2.1
1	A	128	VAL	2.1
1	A	390	ASP	2.1
1	B	453	GLU	2.1
1	B	58	ALA	2.1
1	D	463	PHE	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 carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

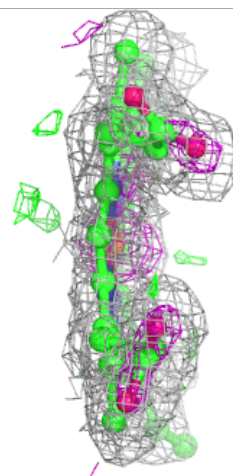
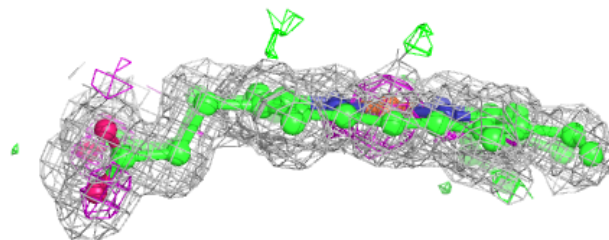
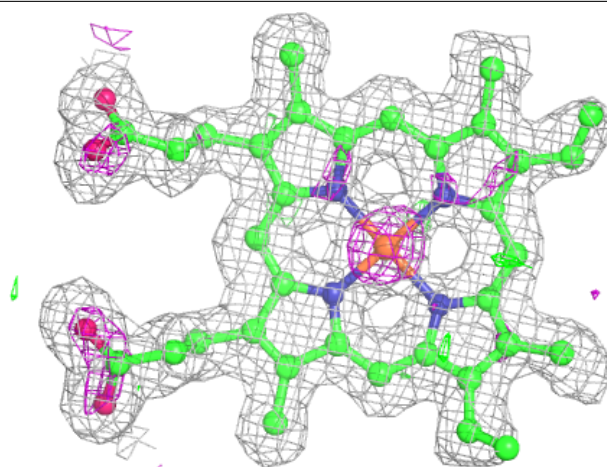
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PYG	A	503	9/9	0.76	0.16	40,42,45,48	0
3	PYG	D	503	9/9	0.81	0.16	33,35,39,41	0
3	PYG	C	503	9/9	0.84	0.17	31,33,36,39	0
3	PYG	B	504	9/9	0.86	0.18	27,31,35,35	0
3	PYG	B	503	9/9	0.88	0.14	34,39,44,50	0
3	PYG	A	504	9/9	0.88	0.17	27,34,35,36	0
3	PYG	D	504	9/9	0.88	0.16	21,32,37,38	0
3	PYG	C	504	9/9	0.90	0.14	20,28,31,32	0
2	HEM	B	501[A]	43/43	0.95	0.12	14,17,19,23	43
2	HEM	C	502[B]	43/43	0.96	0.14	10,12,13,13	43
2	HEM	A	501[A]	43/43	0.96	0.16	13,15,17,18	43
2	HEM	C	501[A]	43/43	0.96	0.13	11,13,14,17	43
2	HEM	A	502[B]	43/43	0.96	0.16	15,16,18,20	43
2	HEM	B	502[B]	43/43	0.96	0.11	10,12,14,14	43
5	NA	B	506	1/1	0.96	0.05	23,23,23,23	0
2	HEM	D	501[A]	43/43	0.96	0.12	14,16,19,23	43
4	CL	C	505	1/1	0.97	0.11	23,23,23,23	0
2	HEM	D	502[B]	43/43	0.97	0.12	11,12,13,13	43
5	NA	A	507	1/1	0.98	0.05	14,14,14,14	0
4	CL	A	506	1/1	0.99	0.04	19,19,19,19	0
4	CL	A	505	1/1	0.99	0.13	23,23,23,23	0
4	CL	B	505	1/1	0.99	0.06	19,19,19,19	0
4	CL	D	505	1/1	0.99	0.05	18,18,18,18	0
4	CL	C	506	1/1	1.00	0.04	19,19,19,19	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.

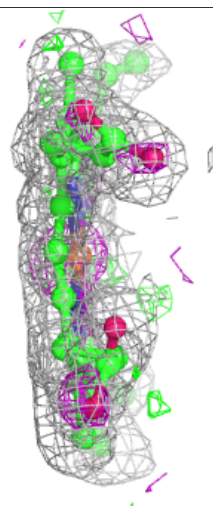
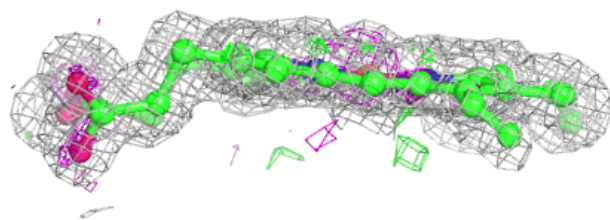
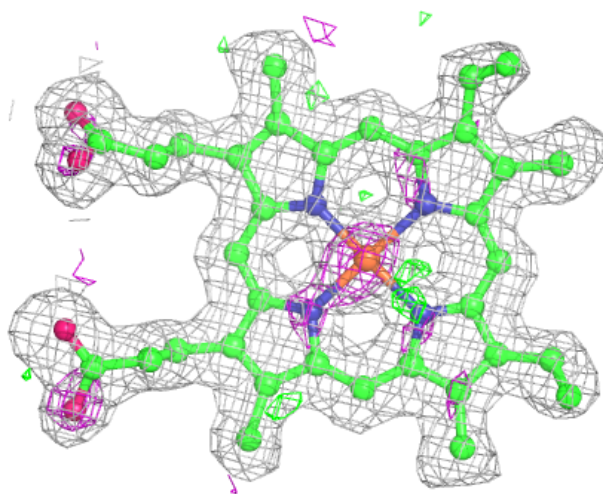
**Electron density around HEM B 501 (A):**

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



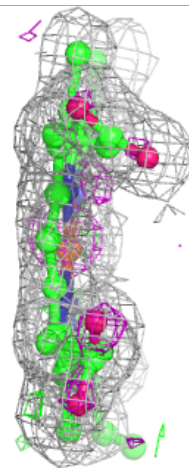
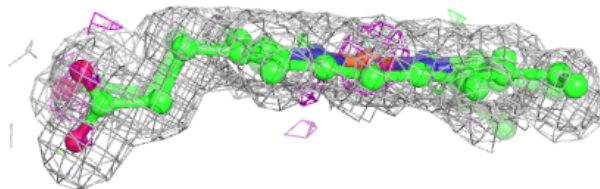
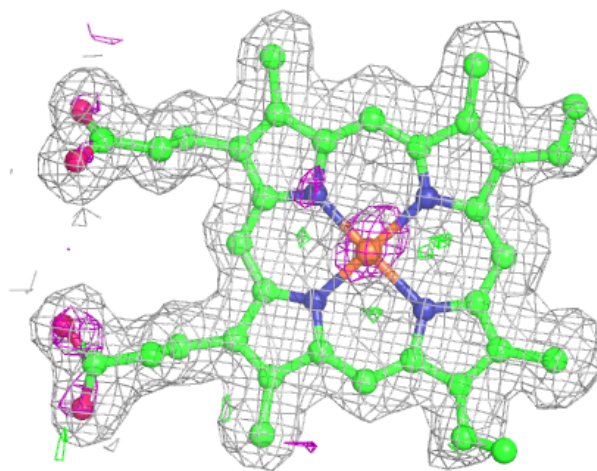
**Electron density around HEM C 502 (B):**

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



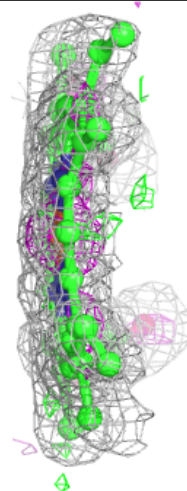
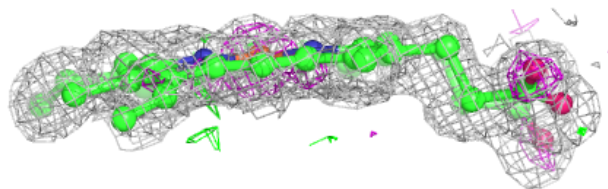
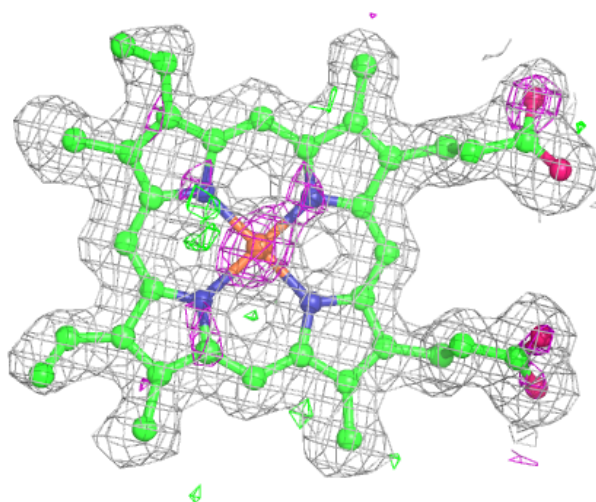
**Electron density around HEM A 501 (A):**

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



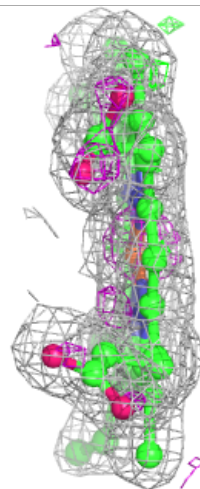
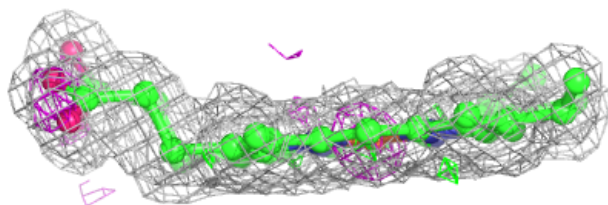
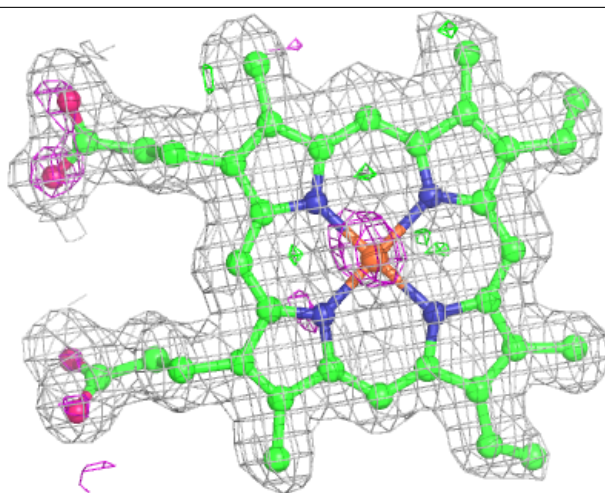
**Electron density around HEM C 501 (A):**

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



**Electron density around HEM A 502 (B):**

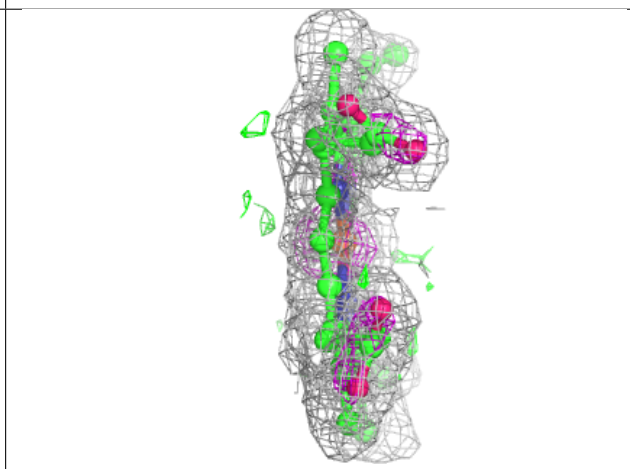
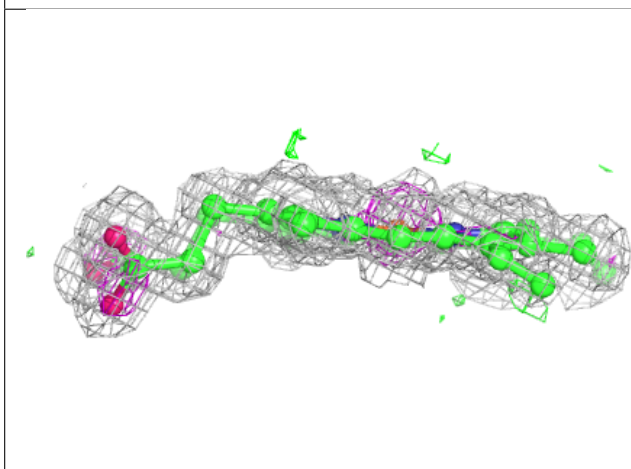
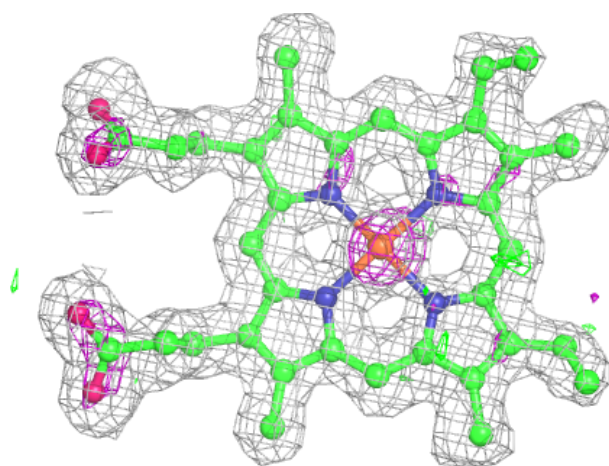
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





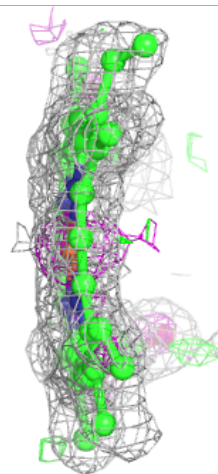
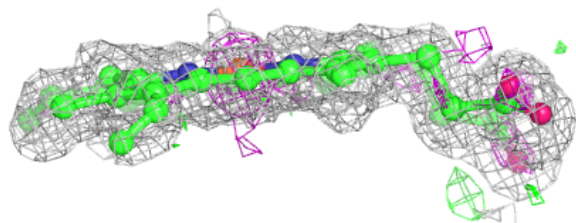
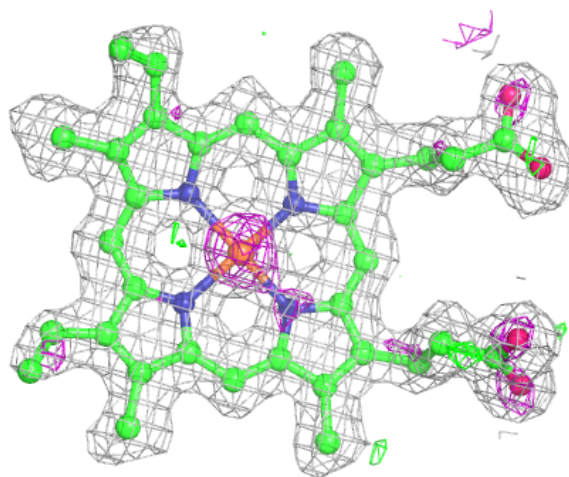
**Electron density around HEM B 502 (B):**

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



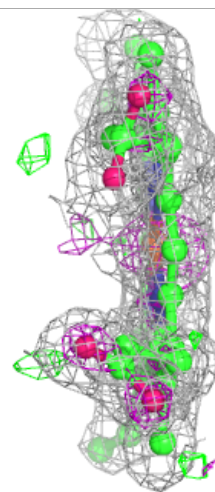
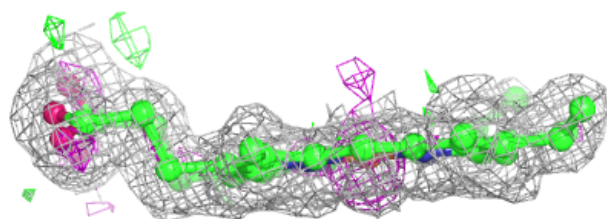
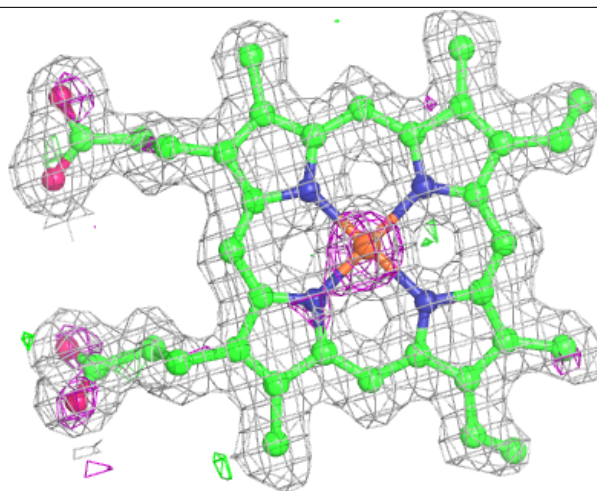
**Electron density around HEM D 501 (A):**

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



**Electron density around HEM D 502 (B):**

$2mF_o-DF_c$  (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.