



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2025 – 02:58 PM EST

PDB ID : 9MZ2 / pdb\_00009mz2  
Title : Structure of human endothelial nitric oxide synthase heme domain bound with  
2-(2-amino-6-fluoro-4-methylquinolin-7-yl)-5-(aminomethyl)phenol  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2025-01-22  
Resolution : 1.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

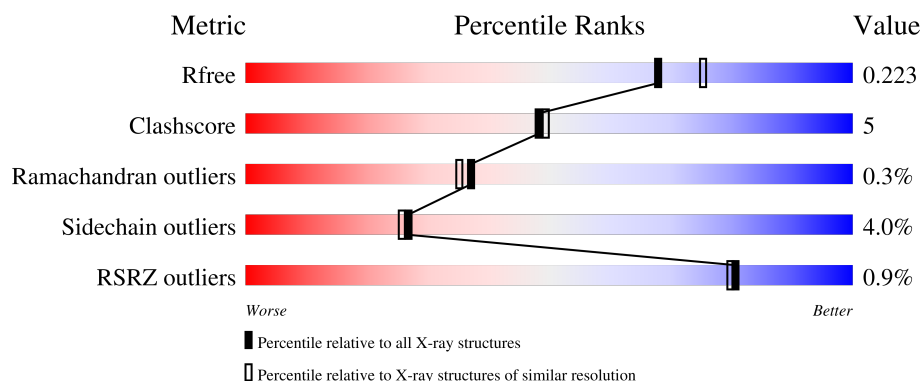
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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))
$R_{free}$	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 81%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>81%</span> <span>9%</span> <span>• 9%</span> </div> </div>
1	B	440	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 78%, yellow 12%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>78%</span> <span>12%</span> <span>• 8%</span> </div> </div>
1	C	440	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 79%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>79%</span> <span>11%</span> <span>• 9%</span> </div> </div>
1	D	440	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 81%, yellow 9%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>81%</span> <span>9%</span> <span>• 9%</span> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	507	-	-	X	-

## 2 Entry composition [i](#)

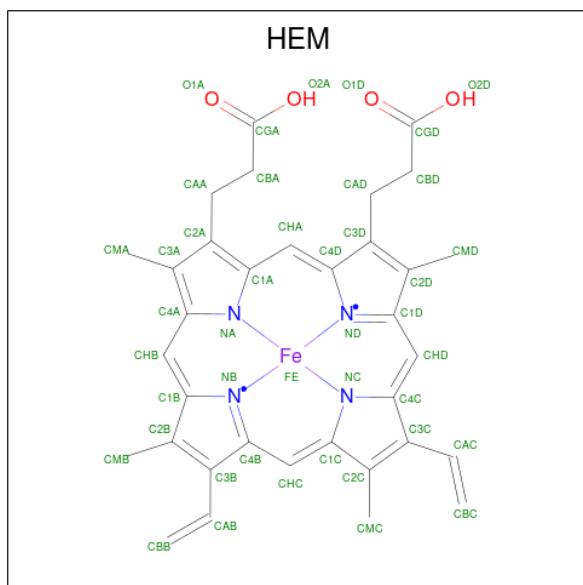
There are 11 unique types of molecules in this entry. The entry contains 13866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			
1	B	403	Total	C	N	O	S	0	2	0
			3226	2054	569	587	16			
1	C	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	D	401	Total	C	N	O	S	0	2	0
			3206	2042	563	585	16			

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



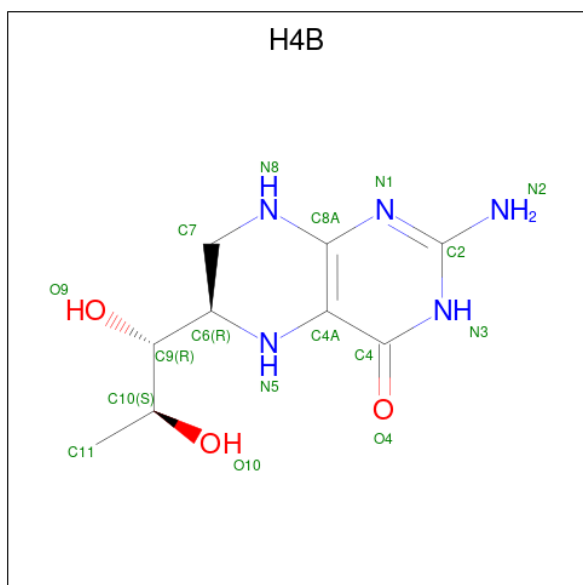
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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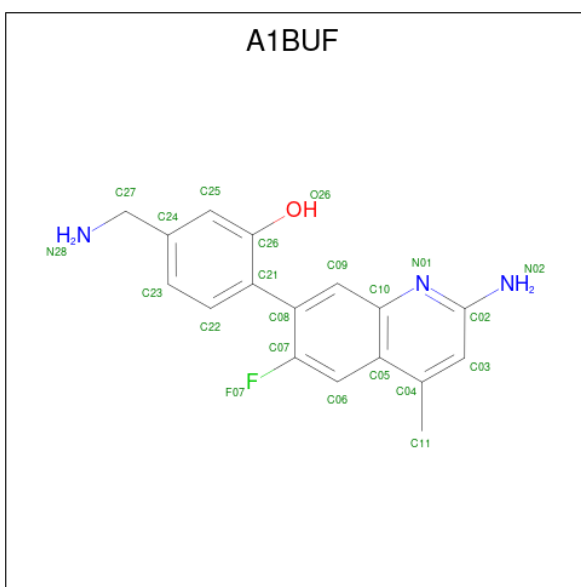
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



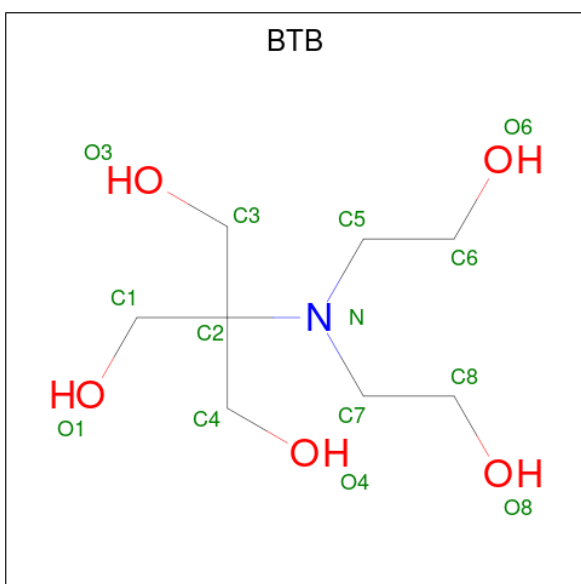
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is (2M)-2-(2-amino-6-fluoro-4-methylquinolin-7-yl)-5-(aminomethyl)phenol (CCD ID: A1BUF) (formula:  $C_{17}H_{16}FN_3O$ ).



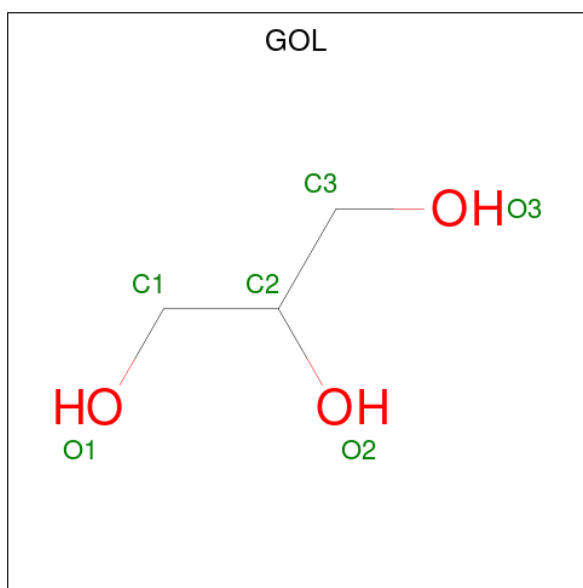
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			22	17	1	3	1		
4	B	1	Total	C	F	N	O	0	0
			22	17	1	3	1		
4	C	1	Total	C	F	N	O	0	0
			22	17	1	3	1		
4	D	1	Total	C	F	N	O	0	0
			22	17	1	3	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula:  $C_8H_{19}NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Gd	0	0
			1	1		
8	B	1	Total	Gd	0	0
			1	1		
8	C	1	Total	Gd	0	0
			1	1		
8	D	1	Total	Gd	0	0
			1	1		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		
9	C	1	Total	Zn	0	0
			1	1		



- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total 1	Ca 1	0	0
10	B	1	Total 1	Ca 1	0	0

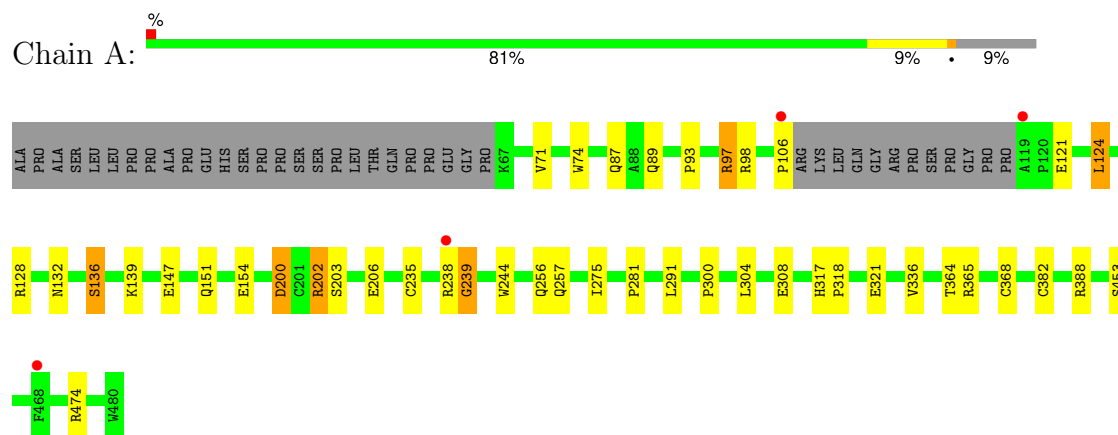
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	123	Total 123	O 123	0	0
11	B	144	Total 144	O 144	0	0
11	C	89	Total 89	O 89	0	0
11	D	153	Total 153	O 153	0	0

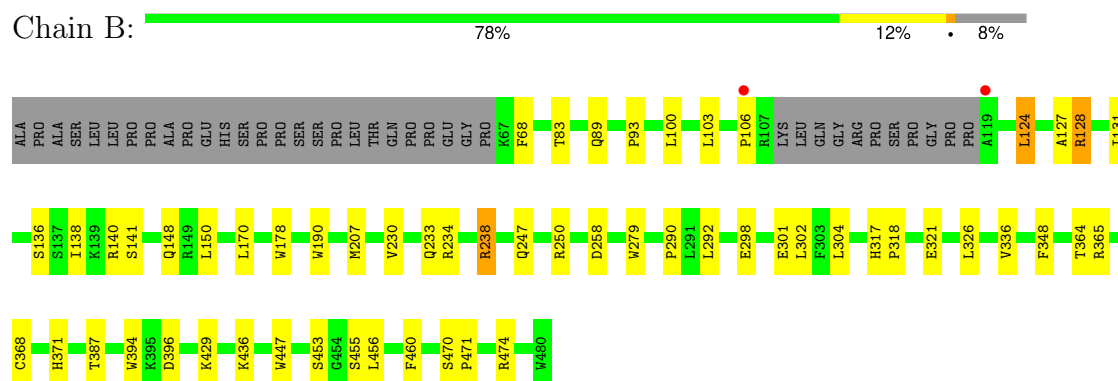
### 3 Residue-property plots

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.

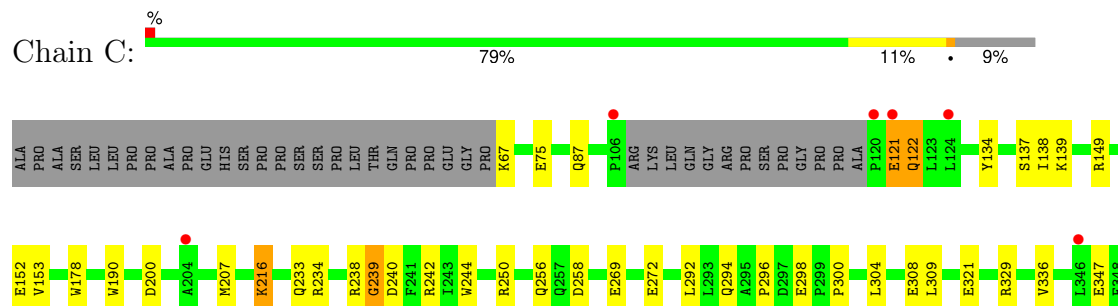
- Molecule 1: Nitric oxide synthase, endothelial



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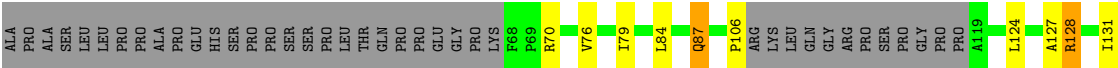
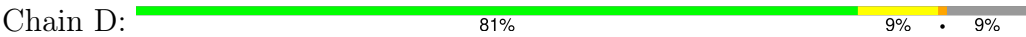


- Molecule 1: Nitric oxide synthase, endothelial





- Molecule 1: Nitric oxide synthase, endothelial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.70Å 152.76Å 108.74Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	38.74 – 1.99 38.74 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.74-1.99) 98.6 (38.74-1.99)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.184 , 0.227 0.181 , 0.223	Depositor DCC
$R_{free}$ test set	6632 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1BUF, CL, HEM, GD, H4B, ZN, GOL, BTB, CA

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	0.28	0/3307	0.48	0/4506
1	B	0.32	0/3324	0.50	0/4528
1	C	0.26	0/3302	0.47	0/4498
1	D	0.31	0/3304	0.50	0/4503
All	All	0.29	0/13237	0.49	0/18035

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	121	GLU	Peptide

### 5.2 Too-close contacts [i](#)

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	3212	0	3116	20	0
1	B	3226	0	3134	37	0
1	C	3207	0	3112	34	0
1	D	3206	0	3108	28	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	2	0
3	B	17	0	15	2	0
3	C	17	0	15	0	0
3	D	17	0	15	2	0
4	A	22	0	0	1	0
4	B	22	0	0	2	0
4	C	22	0	0	2	0
4	D	22	0	0	3	0
5	A	28	0	37	5	0
5	B	28	0	35	6	0
5	C	28	0	38	7	0
5	D	28	0	37	6	0
6	A	18	0	24	1	0
6	B	12	0	16	6	0
6	C	12	0	16	1	0
6	D	12	0	16	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	123	0	0	0	0
11	B	144	0	0	2	0
11	C	89	0	0	3	0
11	D	153	0	0	3	0
All	All	13866	0	12869	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (141) 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)
5:C:504:BTB:O3	5:C:504:BTB:O4	2.01	0.77
1:D:148:GLN:NE2	11:D:601:HOH:O	2.21	0.73
1:B:234:ARG:HA	1:B:238:ARG:HH22	1.53	0.73
1:D:336:VAL:HG21	4:D:503:A1BUF:C07	2.20	0.71
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.72	0.70
3:A:502:H4B:HN5	6:A:508:GOL:H12	1.56	0.70
3:B:502:H4B:HN5	6:B:507:GOL:HO1	1.38	0.68
1:C:292:LEU:HD22	1:C:300:PRO:HB2	1.77	0.66
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.76	0.66
1:B:371:HIS:NE2	6:B:507:GOL:O3	2.25	0.65
1:D:247:GLN:HB2	1:D:250:ARG:HD3	1.78	0.65
5:D:504:BTB:H62	5:D:504:BTB:O8	1.96	0.65
1:D:365:ARG:HH22	6:D:508:GOL:H2	1.61	0.65
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.79	0.64
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.77	0.64
1:C:386:ASP:OD2	1:C:388:ARG:HG2	1.98	0.63
3:D:502:H4B:N5	6:D:508:GOL:O2	2.28	0.63
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.82	0.62
1:A:336:VAL:HG21	4:A:503:A1BUF:C07	2.30	0.61
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.82	0.61
1:A:93:PRO:HG3	1:A:106:PRO:HB3	1.82	0.61
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.82	0.60
1:D:298:GLU:HG3	1:D:299:PRO:HD2	1.82	0.60
1:C:242:ARG:HD2	1:C:349:PRO:HB2	1.83	0.60
1:B:336:VAL:HG21	4:B:503:A1BUF:C07	2.32	0.59
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.83	0.59
1:B:128:ARG:HD3	1:B:150:LEU:HD22	1.84	0.58
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.35	0.58
1:C:134:TYR:O	1:C:137:SER:OG	2.16	0.58
1:C:336:VAL:HG21	4:C:503:A1BUF:C07	2.33	0.58
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.22	0.57
1:A:74:TRP:CB	6:B:507:GOL:H2	2.35	0.56
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.86	0.56
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.87	0.56
1:B:128:ARG:HB2	1:B:128:ARG:NH1	2.20	0.56
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.88	0.56
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.89	0.54
1:A:321:GLU:H	1:A:321:GLU:CD	2.15	0.54
1:C:233:GLN:OE1	11:C:601:HOH:O	2.19	0.54
5:B:505:BTB:O8	5:B:505:BTB:O3	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLU:OE2	5:B:504:BTB:O4	2.26	0.53
2:D:501:HEM:HBA2	4:D:503:A1BUF:C09	2.39	0.53
1:A:124:LEU:HD23	1:A:128:ARG:NH2	2.24	0.53
1:A:200:ASP:OD1	1:A:200:ASP:N	2.32	0.52
1:C:364:THR:O	1:C:368:CYS:HB2	2.10	0.52
1:D:364:THR:O	1:D:368:CYS:HB2	2.09	0.52
1:C:382:CYS:HA	5:C:504:BTB:H11	1.91	0.52
1:A:364:THR:O	1:A:368:CYS:HB2	2.11	0.51
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.23	0.51
1:C:321:GLU:H	1:C:321:GLU:CD	2.19	0.51
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.93	0.50
1:B:124:LEU:HD23	1:B:128:ARG:HH12	1.77	0.49
1:C:216:LYS:HB2	1:C:309:LEU:HD11	1.95	0.49
1:C:75:GLU:HG3	1:D:370:PRO:HG2	1.95	0.49
1:B:364:THR:O	1:B:368:CYS:HB2	2.13	0.49
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.95	0.49
1:B:474:ARG:HD2	11:B:602:HOH:O	2.13	0.48
1:C:258:ASP:N	1:C:258:ASP:OD1	2.45	0.48
1:D:106:PRO:HB3	11:D:670:HOH:O	2.12	0.48
1:D:447:TRP:HA	3:D:502:H4B:N1	2.27	0.48
1:B:447:TRP:HA	3:B:502:H4B:N1	2.28	0.48
1:C:384:ASP:OD1	5:C:504:BTB:O3	2.27	0.48
1:A:74:TRP:HB2	6:B:507:GOL:H2	1.96	0.48
1:C:122:GLN:N	1:C:122:GLN:OE1	2.47	0.48
5:A:505:BTB:H32	5:A:505:BTB:O8	2.14	0.48
1:C:308:GLU:H	1:C:308:GLU:CD	2.22	0.48
1:D:275:ILE:HG12	1:D:281:PRO:HG3	1.95	0.48
1:A:202:ARG:HD2	1:A:206:GLU:OE2	2.14	0.47
1:B:138:ILE:HD12	1:B:140:ARG:HE	1.80	0.47
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.67	0.47
1:C:244:TRP:NE1	1:C:294:GLN:OE1	2.34	0.47
1:C:388:ARG:NH2	11:C:607:HOH:O	2.44	0.47
1:D:298:GLU:CD	5:D:505:BTB:H31	2.39	0.47
1:C:238:ARG:NH1	1:C:296:PRO:HG3	2.30	0.47
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.96	0.47
1:A:235:CYS:SG	1:A:238:ARG:HD3	2.55	0.46
5:A:505:BTB:H62	5:A:505:BTB:H71	1.72	0.46
1:B:234:ARG:HA	1:B:238:ARG:NH2	2.26	0.46
1:B:298:GLU:OE1	5:B:505:BTB:H42	2.16	0.46
5:C:505:BTB:H72	5:C:505:BTB:H41	1.42	0.46
5:D:505:BTB:H11	5:D:505:BTB:H51	1.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.74	0.46
1:B:170:LEU:HD11	1:B:230:VAL:HG11	1.97	0.46
1:B:365:ARG:NH2	6:B:507:GOL:H31	2.30	0.46
5:C:504:BTB:H51	5:C:504:BTB:H32	1.61	0.45
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.45
1:A:453:SER:OG	1:B:396:ASP:OD2	2.33	0.45
1:C:178:TRP:CE3	1:C:190:TRP:HA	2.52	0.45
1:B:387:THR:HA	1:B:394:TRP:CD1	2.52	0.45
5:B:505:BTB:H42	5:B:505:BTB:H72	1.45	0.45
1:D:292:LEU:HD22	1:D:300:PRO:HB2	1.99	0.45
1:B:68:PHE:CD1	1:B:83:THR:HG22	2.52	0.45
1:B:455:SER:HA	1:B:460:PHE:CG	2.52	0.44
1:C:377:GLU:OE1	5:C:505:BTB:O3	2.21	0.44
1:A:244:TRP:CZ2	1:A:300:PRO:HG3	2.52	0.44
1:C:149:ARG:O	1:C:153:VAL:HG22	2.18	0.44
1:C:207:MET:HE2	1:C:207:MET:HB3	1.81	0.44
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.99	0.44
1:C:336:VAL:HG21	4:C:503:A1BUF:F07	2.07	0.44
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.52	0.44
1:A:238:ARG:HG2	1:A:239:GLY:N	2.33	0.44
5:D:505:BTB:O3	5:D:505:BTB:O1	2.29	0.43
1:B:365:ARG:HH22	6:B:507:GOL:H31	1.84	0.43
1:C:269:GLU:O	1:C:272:GLU:HG2	2.18	0.43
1:A:382:CYS:HA	5:A:504:BTB:C1	2.49	0.43
1:D:242:ARG:NH2	1:D:479:PRO:HD3	2.33	0.43
1:B:336:VAL:HG21	4:B:503:A1BUF:F07	2.09	0.43
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.54	0.43
1:C:238:ARG:HD2	1:C:239:GLY:N	2.34	0.43
1:D:365:ARG:HH22	6:D:508:GOL:C2	2.30	0.43
1:B:148:GLN:NE2	11:B:606:HOH:O	2.52	0.43
1:C:455:SER:HA	1:C:460:PHE:CG	2.54	0.42
1:D:250:ARG:HD2	1:D:250:ARG:HA	1.69	0.42
1:D:238:ARG:HG2	1:D:296:PRO:HB3	2.01	0.42
1:A:132:ASN:O	1:A:136:SER:OG	2.38	0.42
1:C:461:HIS:ND1	11:D:602:HOH:O	2.37	0.42
1:D:70:ARG:HD2	1:D:79:ILE:HD13	2.01	0.42
1:B:470:SER:HA	1:B:471:PRO:C	2.45	0.42
1:D:336:VAL:HG21	4:D:503:A1BUF:F07	2.09	0.42
1:C:250:ARG:NH2	11:C:605:HOH:O	2.39	0.42
5:D:504:BTB:H11	5:D:504:BTB:H72	1.79	0.42
1:B:127:ALA:O	1:B:131:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:GLU:CD	1:D:329:ARG:HH21	2.28	0.42
1:D:124:LEU:HD22	1:D:128:ARG:HH12	1.85	0.41
1:B:93:PRO:HG3	1:B:106:PRO:HB3	2.01	0.41
1:C:298:GLU:OE1	6:C:507:GOL:H31	2.19	0.41
5:A:504:BTB:H32	5:A:504:BTB:H51	1.75	0.41
1:B:128:ARG:HB2	1:B:128:ARG:CZ	2.50	0.41
1:A:382:CYS:HA	5:A:504:BTB:H12	2.02	0.41
5:B:504:BTB:H32	5:B:504:BTB:H51	1.72	0.41
1:D:84:LEU:O	1:D:87:GLN:HG2	2.20	0.41
1:D:127:ALA:O	1:D:131:ILE:HG12	2.21	0.41
1:B:298:GLU:OE1	5:B:505:BTB:H72	2.21	0.41
1:C:400:VAL:HG11	1:D:397:LYS:HG2	2.02	0.41
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.55	0.41
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.56	0.41
1:B:453:SER:HB3	1:B:456:LEU:HD12	2.02	0.41
1:C:238:ARG:HH11	1:C:296:PRO:HG3	1.86	0.41
1:D:124:LEU:HB3	1:D:128:ARG:HH22	1.86	0.40
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.87	0.40
1:C:382:CYS:HA	5:C:504:BTB:H31	2.03	0.40

There are no symmetry-related clashes.

## 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	399/440 (91%)	383 (96%)	15 (4%)	1 (0%)	37	35
1	B	401/440 (91%)	393 (98%)	8 (2%)	0	100	100
1	C	398/440 (90%)	381 (96%)	15 (4%)	2 (0%)	25	21
1	D	399/440 (91%)	388 (97%)	10 (2%)	1 (0%)	37	35
All	All	1597/1760 (91%)	1545 (97%)	48 (3%)	4 (0%)	37	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	121	GLU
1	D	144	GLN
1	C	239	GLY
1	A	239	GLY

### 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	342/373 (92%)	321 (94%)	21 (6%)	15	12
1	B	344/373 (92%)	331 (96%)	13 (4%)	28	28
1	C	342/373 (92%)	330 (96%)	12 (4%)	31	31
1	D	342/373 (92%)	332 (97%)	10 (3%)	37	39
All	All	1370/1492 (92%)	1314 (96%)	56 (4%)	27	25

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

Mol	Chain	Res	Type
1	A	71	VAL
1	A	87	GLN
1	A	89	GLN
1	A	97	ARG
1	A	121	GLU
1	A	124	LEU
1	A	136	SER
1	A	139	LYS
1	A	147	GLU
1	A	151	GLN
1	A	154	GLU
1	A	200	ASP
1	A	202	ARG
1	A	203	SER
1	A	256	GLN
1	A	257	GLN

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Mol	Chain	Res	Type
1	A	291	LEU
1	A	304	LEU
1	A	308	GLU
1	A	388	ARG
1	A	474	ARG
1	B	89	GLN
1	B	124	LEU
1	B	128	ARG
1	B	136	SER
1	B	141[A]	SER
1	B	141[B]	SER
1	B	207	MET
1	B	238	ARG
1	B	258	ASP
1	B	301	GLU
1	B	326	LEU
1	B	429	LYS
1	B	436	LYS
1	C	67	LYS
1	C	87	GLN
1	C	122	GLN
1	C	138	ILE
1	C	139	LYS
1	C	152	GLU
1	C	200	ASP
1	C	216	LYS
1	C	240	ASP
1	C	256	GLN
1	C	304	LEU
1	C	329	ARG
1	D	76	VAL
1	D	87	GLN
1	D	128	ARG
1	D	136	SER
1	D	168[A]	SER
1	D	168[B]	SER
1	D	276	GLN
1	D	298	GLU
1	D	326	LEU
1	D	378	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	133	GLN
1	A	151	GLN
1	A	194	GLN
1	A	233	GLN
1	A	277	HIS
1	B	133	GLN
1	B	144	GLN
1	B	148	GLN
1	D	148	GLN
1	D	433	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 12 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	GOL	A	508	-	5,5,5	0.31	0	5,5,5	0.55	0
5	BTB	A	504	8	13,13,13	0.41	0	7,16,16	0.71	0
5	BTB	B	505	-	13,13,13	0.44	0	7,16,16	1.01	0
4	A1BUF	B	503	-	24,24,24	1.38	2 (8%)	34,35,35	1.61	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BTB	B	504	8	13,13,13	0.39	0	7,16,16	0.34	0
6	GOL	A	507	-	5,5,5	0.36	0	5,5,5	0.39	0
6	GOL	D	506	-	5,5,5	0.37	0	5,5,5	0.50	0
6	GOL	C	507	-	5,5,5	0.34	0	5,5,5	0.41	0
5	BTB	D	505	-	13,13,13	0.40	0	7,16,16	0.91	0
5	BTB	D	504	8	13,13,13	0.46	0	7,16,16	0.76	0
3	H4B	D	502	-	16,18,18	0.88	0	14,26,26	2.67	7 (50%)
4	A1BUF	A	503	-	24,24,24	1.41	2 (8%)	34,35,35	1.57	6 (17%)
5	BTB	C	504	8	13,13,13	0.41	0	7,16,16	0.78	0
6	GOL	B	506	-	5,5,5	0.36	0	5,5,5	0.31	0
2	HEM	A	501	1	42,50,50	1.49	5 (11%)	46,82,82	1.88	10 (21%)
2	HEM	C	501	1	42,50,50	1.50	4 (9%)	46,82,82	1.74	13 (28%)
5	BTB	A	505	-	13,13,13	0.83	0	7,16,16	1.08	0
6	GOL	B	507	-	5,5,5	0.28	0	5,5,5	0.76	0
5	BTB	C	505	-	13,13,13	0.52	0	7,16,16	0.80	0
3	H4B	B	502	-	16,18,18	0.70	0	14,26,26	2.51	8 (57%)
2	HEM	D	501	1	42,50,50	1.48	5 (11%)	46,82,82	1.95	14 (30%)
6	GOL	A	506	-	5,5,5	0.32	0	5,5,5	0.91	0
4	A1BUF	D	503	-	24,24,24	1.48	2 (8%)	34,35,35	1.52	6 (17%)
2	HEM	B	501	1	42,50,50	1.50	5 (11%)	46,82,82	1.76	13 (28%)
6	GOL	C	506	-	5,5,5	0.35	0	5,5,5	0.46	0
6	GOL	D	508	-	5,5,5	0.40	0	5,5,5	0.81	0
4	A1BUF	C	503	-	24,24,24	1.39	3 (12%)	34,35,35	1.46	5 (14%)
3	H4B	C	502	-	16,18,18	0.78	0	14,26,26	2.30	5 (35%)
3	H4B	A	502	-	16,18,18	0.86	0	14,26,26	2.53	7 (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
6	GOL	A	508	-	-	4/4/4/4	-
5	BTB	A	504	8	-	3/21/21/21	-
5	BTB	B	505	-	-	10/21/21/21	-
4	A1BUF	B	503	-	-	0/6/18/18	0/3/3/3
5	BTB	B	504	8	-	6/21/21/21	-
6	GOL	A	507	-	-	4/4/4/4	-
6	GOL	D	506	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	507	-	-	2/4/4/4	-
5	BTB	D	505	-	-	15/21/21/21	-
5	BTB	D	504	8	-	8/21/21/21	-
3	H4B	D	502	-	-	2/8/17/17	0/2/2/2
4	A1BUF	A	503	-	-	0/6/18/18	0/3/3/3
5	BTB	C	504	8	-	9/21/21/21	-
6	GOL	B	506	-	-	2/4/4/4	-
2	HEM	A	501	1	-	3/12/54/54	-
2	HEM	C	501	1	-	4/12/54/54	-
5	BTB	A	505	-	-	10/21/21/21	-
6	GOL	B	507	-	-	2/4/4/4	-
5	BTB	C	505	-	-	13/21/21/21	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
2	HEM	D	501	1	-	2/12/54/54	-
6	GOL	A	506	-	-	4/4/4/4	-
4	A1BUF	D	503	-	-	0/6/18/18	0/3/3/3
2	HEM	B	501	1	-	3/12/54/54	-
6	GOL	C	506	-	-	3/4/4/4	-
6	GOL	D	508	-	-	0/4/4/4	-
4	A1BUF	C	503	-	-	0/6/18/18	0/3/3/3
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	A1BUF	C08-C07	5.27	1.48	1.39
4	C	503	A1BUF	C08-C07	4.95	1.47	1.39
4	B	503	A1BUF	C08-C07	4.91	1.47	1.39
4	A	503	A1BUF	C08-C07	4.83	1.47	1.39
2	B	501	HEM	C3C-C2C	-4.10	1.34	1.40
2	D	501	HEM	C3C-CAC	3.64	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.63	1.35	1.40
2	C	501	HEM	C3C-CAC	3.55	1.55	1.47
2	B	501	HEM	C3C-CAC	3.52	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.42	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.38	1.35	1.40
2	A	501	HEM	C3C-CAC	3.31	1.55	1.47
2	C	501	HEM	CAB-C3B	3.25	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CAB-C3B	3.23	1.56	1.47
2	D	501	HEM	C3C-C4C	3.21	1.46	1.41
2	C	501	HEM	C3C-C4C	3.04	1.45	1.41
2	D	501	HEM	CAB-C3B	2.95	1.55	1.47
2	B	501	HEM	CMD-C2D	2.88	1.56	1.50
2	B	501	HEM	CAB-C3B	2.83	1.54	1.47
2	A	501	HEM	C3C-C4C	2.82	1.45	1.41
4	A	503	A1BUF	C06-C07	2.77	1.40	1.35
2	B	501	HEM	C3C-C4C	2.69	1.45	1.41
2	A	501	HEM	CMB-C2B	2.30	1.55	1.50
4	B	503	A1BUF	C06-C07	2.29	1.39	1.35
4	C	503	A1BUF	C05-C10	-2.26	1.38	1.42
2	D	501	HEM	CMA-C3A	2.19	1.56	1.51
4	C	503	A1BUF	C06-C07	2.13	1.39	1.35
4	D	503	A1BUF	C04-C05	-2.00	1.38	1.42

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBA-CAA-C2A	-6.12	102.25	112.54
3	A	502	H4B	C8A-C4A-C4	5.28	119.31	114.50
3	C	502	H4B	C8A-C4A-C4	5.19	119.22	114.50
4	A	503	A1BUF	C21-C08-C07	-5.16	117.78	122.45
2	B	501	HEM	CBA-CAA-C2A	-5.05	104.05	112.54
2	A	501	HEM	CBA-CAA-C2A	-5.05	104.05	112.54
3	B	502	H4B	C8A-C4A-C4	5.00	119.05	114.50
4	B	503	A1BUF	C21-C08-C07	-4.81	118.10	122.45
2	C	501	HEM	C4B-CHC-C1C	4.59	128.62	122.56
3	D	502	H4B	C8A-C4A-C4	4.55	118.64	114.50
4	D	503	A1BUF	C21-C08-C07	-4.34	118.52	122.45
3	D	502	H4B	C2-N3-C4	4.29	121.93	115.96
3	D	502	H4B	N2-C2-N1	4.05	123.29	117.22
3	B	502	H4B	C2-N3-C4	4.05	121.59	115.96
3	D	502	H4B	N1-C2-N3	-4.04	119.29	125.48
4	C	503	A1BUF	C21-C08-C07	-4.01	118.83	122.45
2	A	501	HEM	C4B-CHC-C1C	3.89	127.69	122.56
3	A	502	H4B	C2-N3-C4	3.87	121.35	115.96
2	D	501	HEM	CAD-CBD-CGD	-3.83	103.51	113.67
2	A	501	HEM	C3B-C4B-NB	-3.77	106.76	109.47
2	A	501	HEM	CAD-CBD-CGD	-3.76	103.69	113.67
3	C	502	H4B	C2-N3-C4	3.62	120.99	115.96
3	A	502	H4B	N1-C2-N3	-3.60	119.97	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3B-C2B-C1B	3.46	109.01	106.41
2	D	501	HEM	C4B-CHC-C1C	3.40	127.04	122.56
2	B	501	HEM	CMA-C3A-C4A	-3.39	123.48	128.46
2	C	501	HEM	C3B-C2B-C1B	3.36	108.93	106.41
4	C	503	A1BUF	C05-C10-N01	-3.33	119.27	122.80
3	C	502	H4B	N1-C2-N3	-3.33	120.38	125.48
3	B	502	H4B	N1-C2-N3	-3.30	120.43	125.48
4	D	503	A1BUF	C04-C05-C10	3.21	119.96	118.00
2	A	501	HEM	C3D-C4D-ND	-3.20	106.66	110.17
2	C	501	HEM	CBA-CAA-C2A	-3.18	107.20	112.54
2	D	501	HEM	C4D-ND-C1D	3.12	108.91	105.21
2	A	501	HEM	C1B-NB-C4B	3.12	108.91	105.21
2	D	501	HEM	C3D-C4D-ND	-3.12	106.75	110.17
2	A	501	HEM	C4D-ND-C1D	3.09	108.87	105.21
3	B	502	H4B	C4-C4A-N5	3.06	122.94	118.57
4	B	503	A1BUF	C09-C08-C07	3.06	119.58	116.03
2	B	501	HEM	CMC-C2C-C3C	3.06	130.79	124.68
3	D	502	H4B	C4-C4A-N5	3.04	122.91	118.57
2	C	501	HEM	C1B-NB-C4B	2.93	108.68	105.21
4	D	503	A1BUF	C09-C08-C07	2.87	119.37	116.03
4	C	503	A1BUF	C03-C04-C05	2.84	120.71	117.84
3	D	502	H4B	C2-N1-C8A	2.82	121.28	114.59
2	B	501	HEM	C3D-C4D-ND	-2.82	107.08	110.17
4	A	503	A1BUF	C06-C07-C08	-2.78	119.16	123.59
2	C	501	HEM	C4D-ND-C1D	2.77	108.49	105.21
2	A	501	HEM	C3B-C2B-C1B	2.76	108.49	106.41
2	C	501	HEM	C3B-C4B-NB	-2.75	107.49	109.47
2	B	501	HEM	C4B-CHC-C1C	2.74	126.17	122.56
4	D	503	A1BUF	C05-C10-N01	-2.73	119.91	122.80
2	D	501	HEM	CMC-C2C-C3C	2.67	130.02	124.68
2	C	501	HEM	CAD-CBD-CGD	-2.65	106.63	113.67
2	D	501	HEM	C3B-C4B-NB	-2.65	107.56	109.47
2	B	501	HEM	C4C-CHD-C1D	2.64	126.04	122.56
4	A	503	A1BUF	C05-C10-N01	-2.61	120.03	122.80
3	A	502	H4B	C2-N1-C8A	2.60	120.77	114.59
3	B	502	H4B	C11-C10-C9	-2.59	108.94	112.11
4	A	503	A1BUF	C09-C08-C21	2.59	123.38	117.47
3	A	502	H4B	C11-C10-C9	-2.59	108.95	112.11
4	D	503	A1BUF	C06-C07-C08	-2.58	119.49	123.59
3	C	502	H4B	C2-N1-C8A	2.57	120.71	114.59
2	B	501	HEM	CAD-CBD-CGD	-2.53	106.95	113.67
3	A	502	H4B	N2-C2-N1	2.52	121.01	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C3D-C4D-ND	-2.51	107.42	110.17
4	B	503	A1BUF	C22-C21-C08	-2.50	113.70	118.74
3	B	502	H4B	C2-N1-C8A	2.48	120.48	114.59
2	D	501	HEM	C1B-NB-C4B	2.44	108.10	105.21
2	C	501	HEM	CMA-C3A-C4A	-2.43	124.90	128.46
4	B	503	A1BUF	C06-C07-C08	-2.42	119.74	123.59
3	D	502	H4B	C11-C10-C9	-2.42	109.15	112.11
2	B	501	HEM	C3B-C2B-C1B	2.41	108.22	106.41
2	B	501	HEM	CMA-C3A-C2A	2.38	129.43	124.94
2	C	501	HEM	C4A-C3A-C2A	2.36	108.64	107.00
4	C	503	A1BUF	C09-C08-C21	2.36	122.87	117.47
4	A	503	A1BUF	C09-C08-C07	2.35	118.76	116.03
3	B	502	H4B	N2-C2-N1	2.34	120.73	117.22
2	B	501	HEM	C1B-NB-C4B	2.32	107.96	105.21
3	A	502	H4B	C4-C4A-N5	2.30	121.86	118.57
4	B	503	A1BUF	C05-C10-N01	-2.29	120.37	122.80
2	D	501	HEM	C2D-C1D-ND	-2.28	107.26	109.90
4	C	503	A1BUF	C06-C07-C08	-2.27	119.97	123.59
4	D	503	A1BUF	C06-C05-C10	2.25	121.65	118.99
4	A	503	A1BUF	C04-C05-C10	2.24	119.37	118.00
2	B	501	HEM	CHB-C1B-NB	2.24	127.15	124.37
2	C	501	HEM	CMC-C2C-C3C	2.23	129.13	124.68
2	B	501	HEM	C3B-C4B-NB	-2.19	107.90	109.47
2	D	501	HEM	CHA-C4D-ND	2.15	127.03	124.37
2	B	501	HEM	C4D-ND-C1D	2.14	107.74	105.21
2	C	501	HEM	C2B-C1B-NB	-2.13	107.39	109.84
2	D	501	HEM	CHC-C4B-C3B	2.13	127.83	124.57
3	C	502	H4B	C4-C4A-N5	2.12	121.60	118.57
2	C	501	HEM	C2D-C1D-ND	-2.12	107.46	109.90
2	D	501	HEM	CHB-C1B-NB	2.08	126.95	124.37
3	B	502	H4B	C4A-C4-N3	-2.08	118.65	123.91
2	A	501	HEM	CHB-C1B-NB	2.07	126.93	124.37
4	B	503	A1BUF	C04-C05-C10	2.07	119.26	118.00
4	B	503	A1BUF	C09-C08-C21	2.06	122.19	117.47
2	A	501	HEM	CHC-C4B-C3B	2.06	127.72	124.57
2	D	501	HEM	C2B-C1B-NB	-2.05	107.48	109.84

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	H4B	C7-C6-C9-O9

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Mol	Chain	Res	Type	Atoms
3	B	502	H4B	C7-C6-C9-C10
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	O1-C1-C2-C3
5	A	505	BTB	O1-C1-C2-C4
5	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	B	504	BTB	O1-C1-C2-C3
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	504	BTB	C1-C2-C4-O4
5	B	504	BTB	C3-C2-C4-O4
5	B	504	BTB	N-C2-C4-O4
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C1-C2-N-C7
5	B	505	BTB	C3-C2-N-C5
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C5
5	B	505	BTB	C4-C2-N-C7
5	C	504	BTB	O1-C1-C2-C3
5	C	504	BTB	O1-C1-C2-C4
5	C	504	BTB	O1-C1-C2-N
5	C	504	BTB	C1-C2-C3-O3
5	C	504	BTB	C4-C2-C3-O3
5	C	504	BTB	N-C2-C3-O3
5	C	504	BTB	C1-C2-C4-O4
5	C	504	BTB	C3-C2-C4-O4
5	C	504	BTB	N-C2-C4-O4
5	C	505	BTB	O1-C1-C2-C4
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7

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Mol	Chain	Res	Type	Atoms
5	D	504	BTB	C1-C2-N-C5
5	D	504	BTB	C1-C2-N-C7
5	D	504	BTB	C3-C2-N-C5
5	D	504	BTB	C4-C2-N-C5
5	D	504	BTB	C4-C2-N-C7
5	D	505	BTB	O1-C1-C2-C3
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C4-C2-N-C7
6	A	506	GOL	O1-C1-C2-C3
6	A	507	GOL	C1-C2-C3-O3
6	A	508	GOL	C1-C2-C3-O3
6	C	506	GOL	O1-C1-C2-C3
6	C	507	GOL	O1-C1-C2-C3
6	D	506	GOL	O1-C1-C2-O2
6	D	506	GOL	O1-C1-C2-C3
6	D	506	GOL	C1-C2-C3-O3
6	A	507	GOL	O2-C2-C3-O3
5	D	504	BTB	N-C5-C6-O6
6	A	506	GOL	C1-C2-C3-O3
6	A	507	GOL	O1-C1-C2-C3
6	A	508	GOL	O1-C1-C2-C3
6	B	506	GOL	O1-C1-C2-C3
6	B	507	GOL	O1-C1-C2-C3
5	B	505	BTB	N-C7-C8-O8
2	C	501	HEM	C2A-CAA-CBA-CGA
5	C	505	BTB	N-C7-C8-O8
5	D	505	BTB	N-C5-C6-O6
6	A	506	GOL	O1-C1-C2-O2
6	A	508	GOL	O2-C2-C3-O3
6	C	506	GOL	O1-C1-C2-O2
6	C	507	GOL	O1-C1-C2-O2
6	D	506	GOL	O2-C2-C3-O3
2	B	501	HEM	C4B-C3B-CAB-CBB
3	D	502	H4B	C7-C6-C9-O9
6	A	507	GOL	O1-C1-C2-O2
6	B	506	GOL	O1-C1-C2-O2
5	A	505	BTB	N-C7-C8-O8
6	A	506	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	507	GOL	O1-C1-C2-O2
6	C	506	GOL	O2-C2-C3-O3
2	C	501	HEM	C4B-C3B-CAB-CBB
2	A	501	HEM	C2A-CAA-CBA-CGA
3	B	502	H4B	N5-C6-C9-O9
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C5
5	D	505	BTB	N-C7-C8-O8
3	D	502	H4B	C7-C6-C9-C10
5	C	505	BTB	C3-C2-C4-O4
2	D	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D
6	A	508	GOL	O1-C1-C2-O2
2	D	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O1D
5	C	505	BTB	C4-C2-C3-O3
5	D	504	BTB	C1-C2-C3-O3
5	C	505	BTB	O1-C1-C2-N
5	C	505	BTB	N-C2-C4-O4
5	D	504	BTB	C3-C2-N-C7
5	D	505	BTB	C3-C2-N-C5

There are no ring outliers.

23 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	508	GOL	1	0
5	A	504	BTB	3	0
5	B	505	BTB	4	0
4	B	503	A1BUF	2	0
5	B	504	BTB	2	0
6	C	507	GOL	1	0

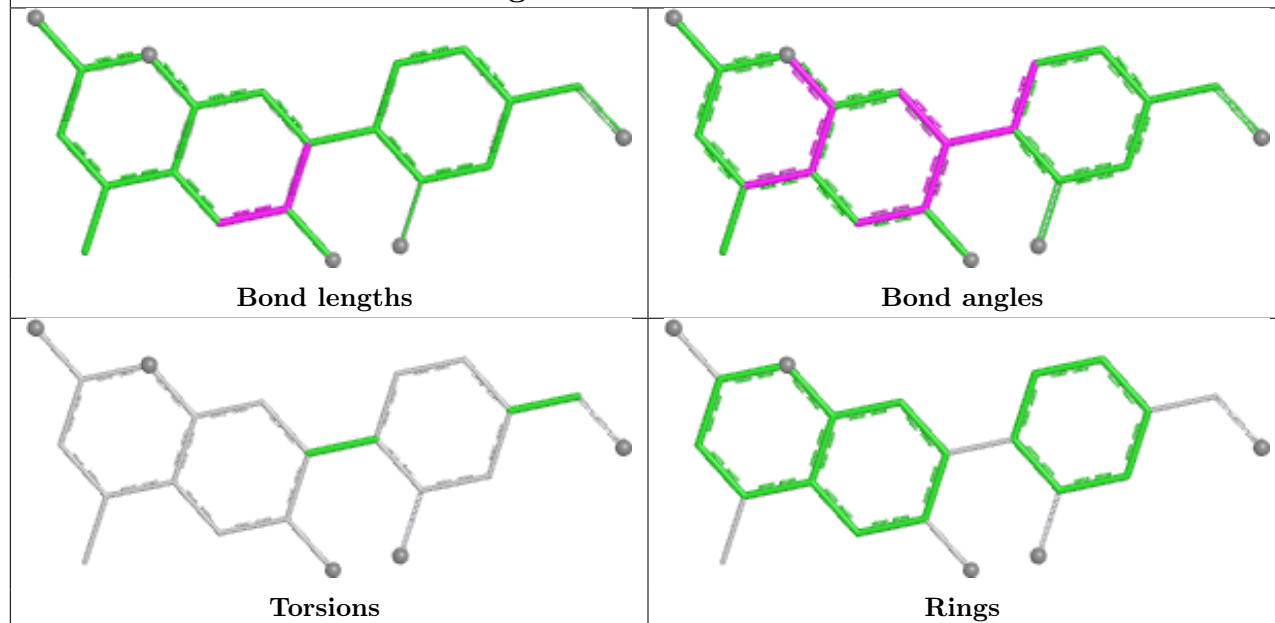
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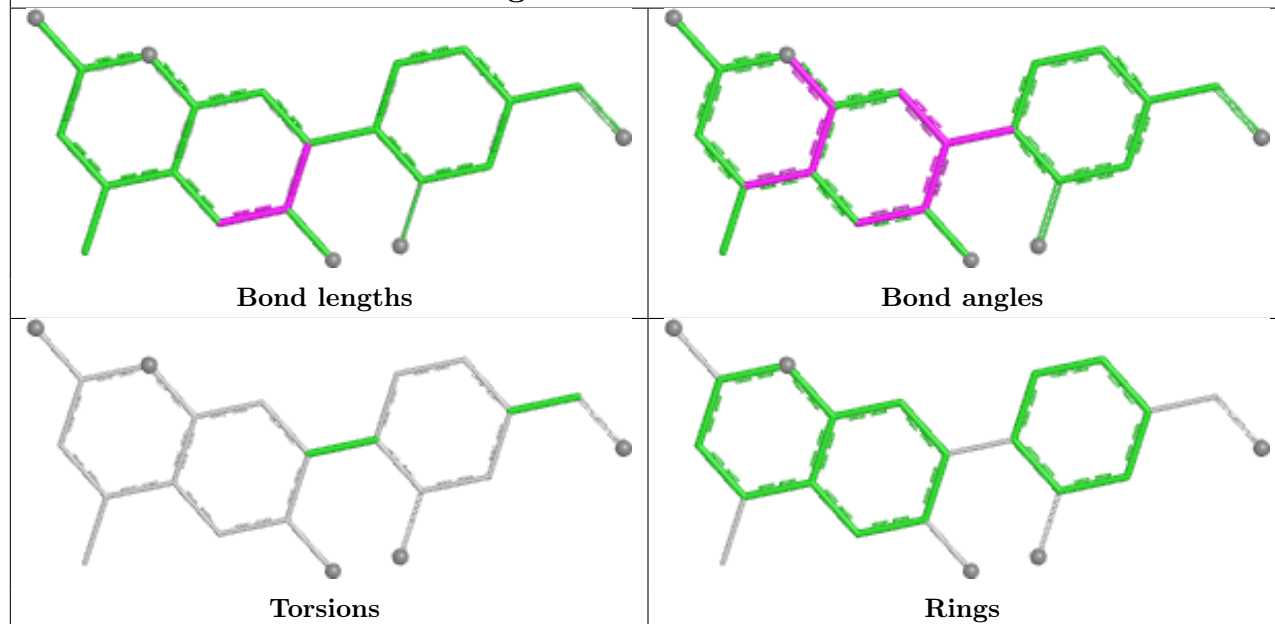
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	505	BTB	3	0
5	D	504	BTB	3	0
3	D	502	H4B	2	0
4	A	503	A1BUF	1	0
5	C	504	BTB	5	0
2	A	501	HEM	2	0
2	C	501	HEM	2	0
5	A	505	BTB	2	0
6	B	507	GOL	6	0
5	C	505	BTB	2	0
3	B	502	H4B	2	0
2	D	501	HEM	3	0
4	D	503	A1BUF	3	0
2	B	501	HEM	2	0
6	D	508	GOL	3	0
4	C	503	A1BUF	2	0
3	A	502	H4B	2	0

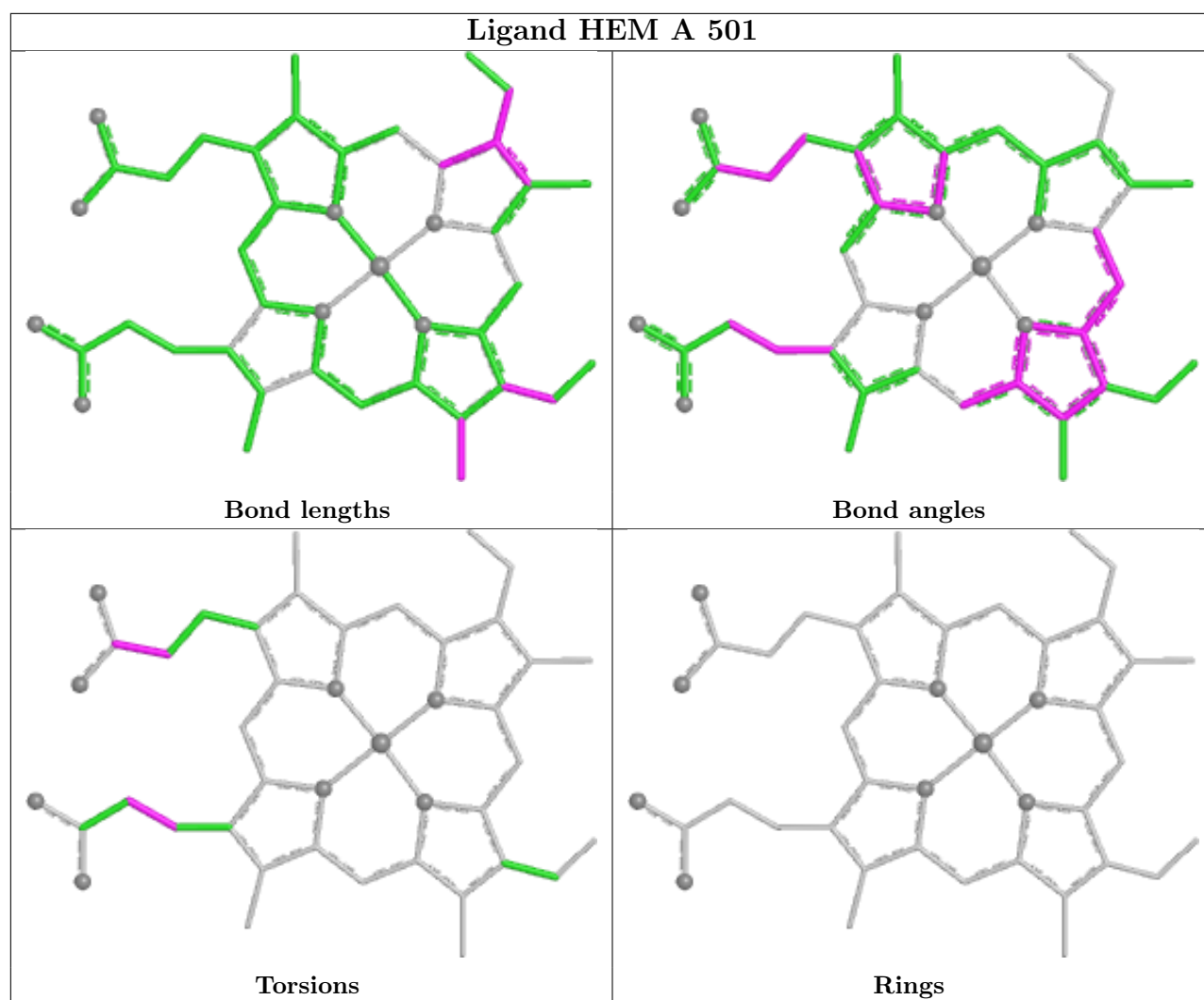
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1BUF B 503

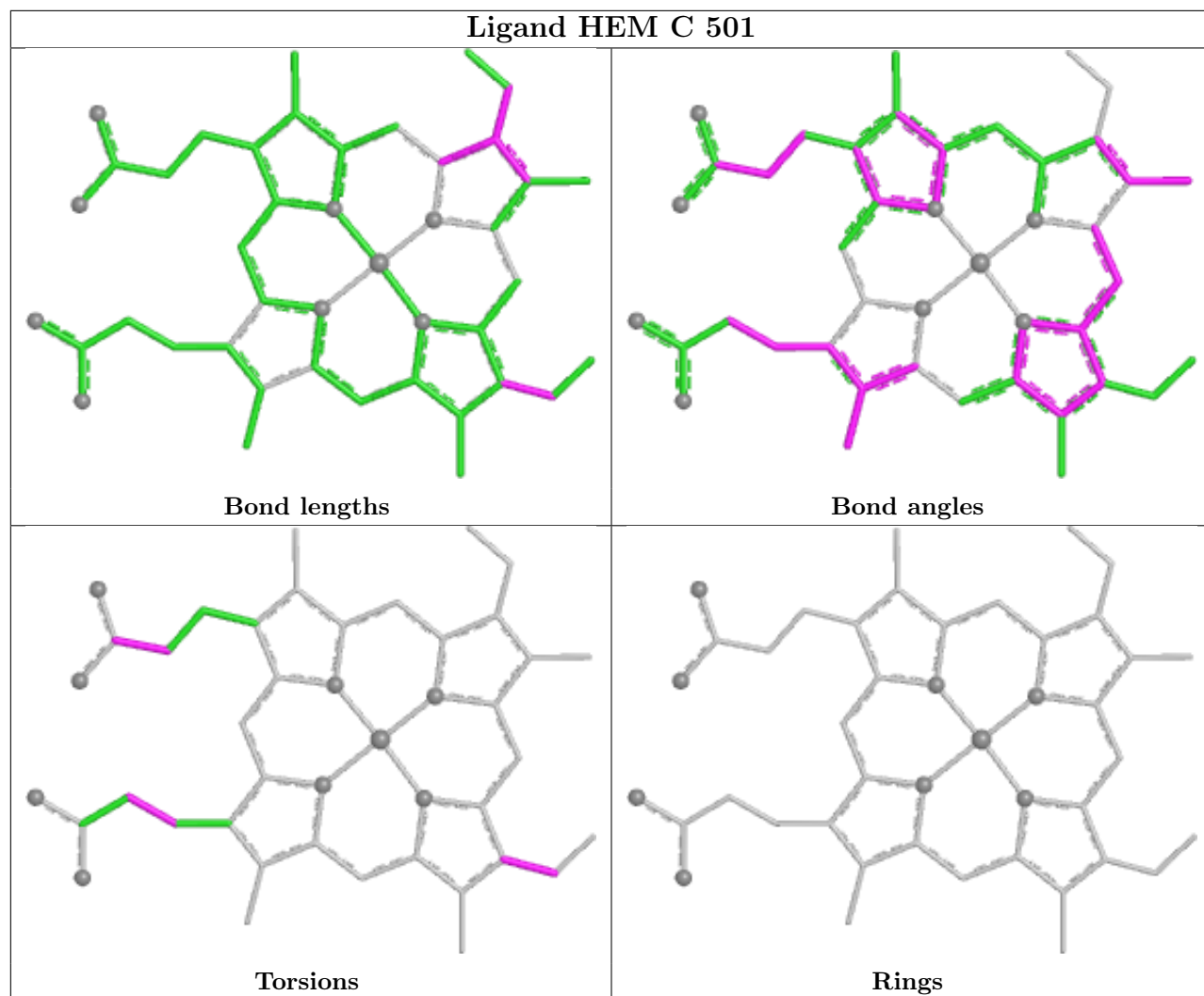


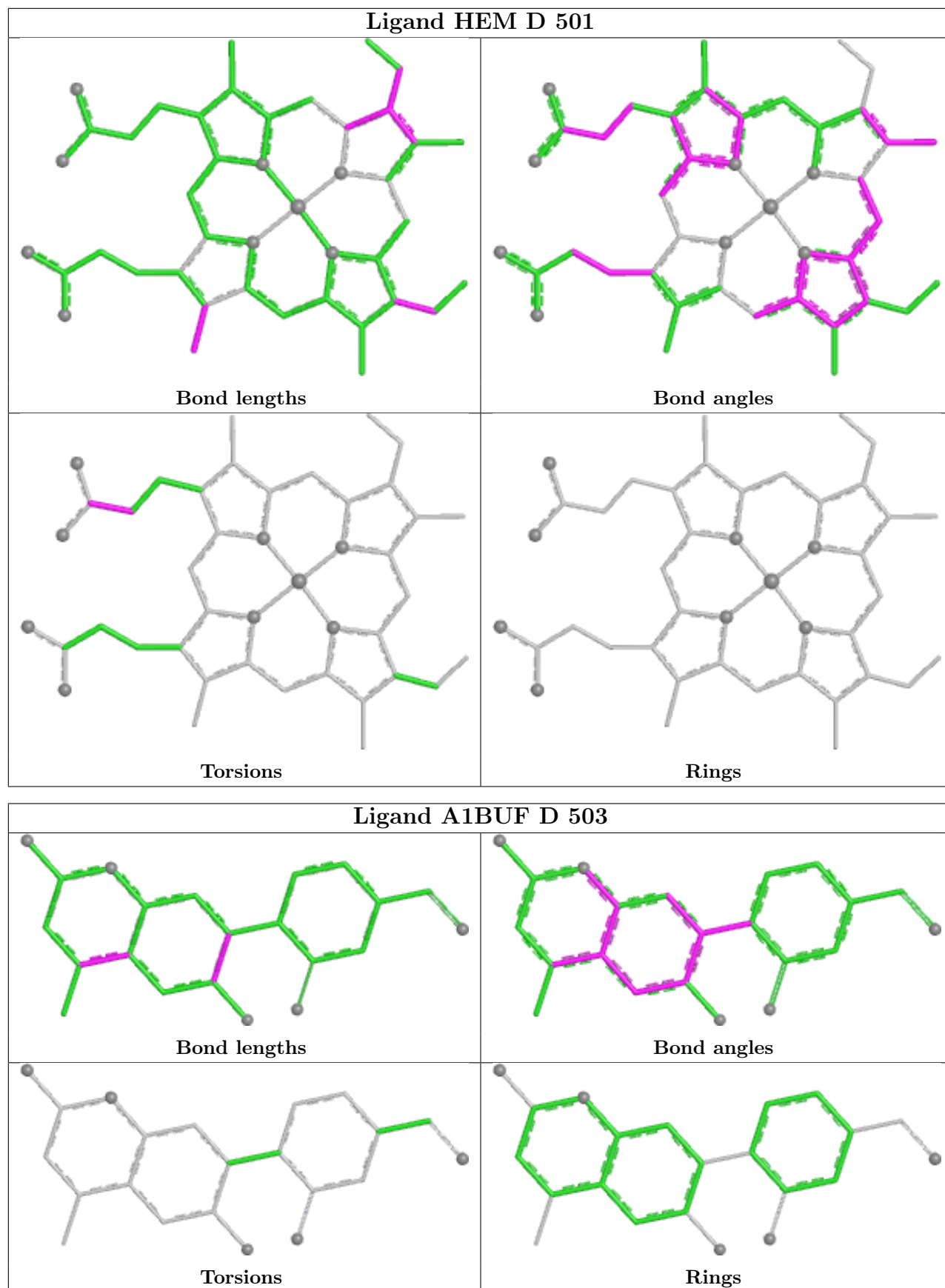
## Ligand A1BUF A 503

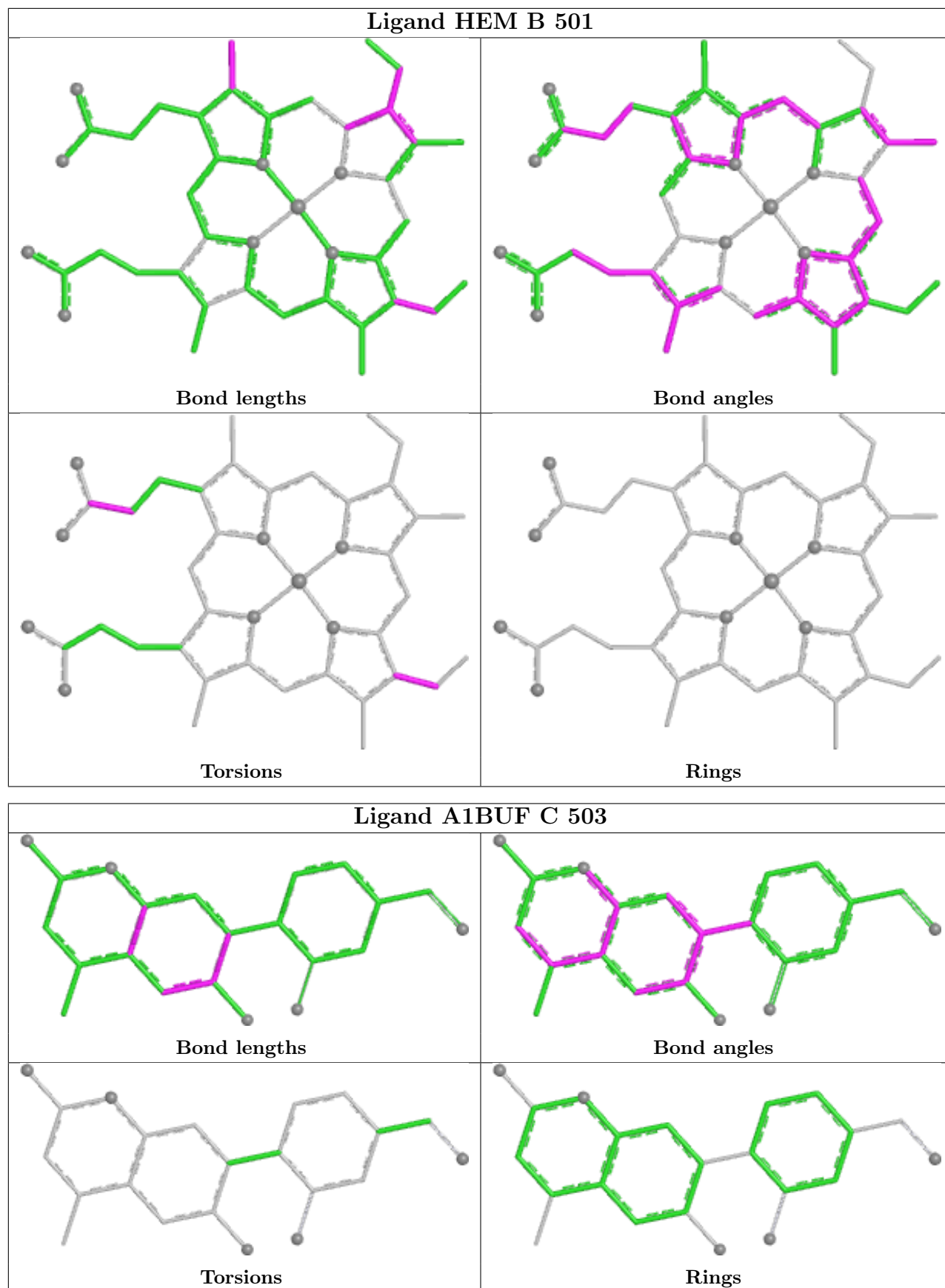












## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	402/440 (91%)	0.17	4 (0%) 79 78	30, 60, 103, 132	1 (0%)
1	B	403/440 (91%)	-0.11	2 (0%) 87 86	32, 50, 87, 130	2 (0%)
1	C	401/440 (91%)	0.27	6 (1%) 71 70	30, 67, 122, 152	1 (0%)
1	D	401/440 (91%)	-0.11	2 (0%) 87 86	34, 50, 84, 114	2 (0%)
All	All	1607/1760 (91%)	0.05	14 (0%) 81 80	30, 56, 105, 152	6 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	ALA	3.3
1	A	106	PRO	3.2
1	D	141[A]	SER	3.2
1	C	121	GLU	3.1
1	C	106	PRO	2.9
1	A	468	PHE	2.9
1	D	142	GLY	2.7
1	C	204	ALA	2.6
1	C	346	LEU	2.4
1	C	120	PRO	2.4
1	A	119	ALA	2.1
1	A	238	ARG	2.1
1	C	124	LEU	2.1
1	B	106	PRO	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	D	506	6/6	0.32	0.17	90,92,97,98	0
6	GOL	A	507	6/6	0.68	0.11	94,102,109,109	0
6	GOL	C	507	6/6	0.75	0.11	89,95,98,99	0
6	GOL	B	506	6/6	0.76	0.10	88,93,95,95	0
6	GOL	D	508	6/6	0.80	0.21	89,96,102,104	0
6	GOL	C	506	6/6	0.83	0.11	71,79,93,98	0
5	BTB	D	505	14/14	0.85	0.12	38,88,93,94	0
5	BTB	C	504	14/14	0.85	0.15	82,105,118,122	0
5	BTB	C	505	14/14	0.85	0.12	80,91,93,97	0
6	GOL	B	507	6/6	0.85	0.17	71,87,89,92	0
5	BTB	A	505	14/14	0.86	0.16	30,77,91,92	0
6	GOL	A	506	6/6	0.89	0.09	51,61,76,78	0
5	BTB	B	505	14/14	0.89	0.10	72,87,98,100	0
5	BTB	B	504	14/14	0.90	0.12	39,80,89,95	0
5	BTB	D	504	14/14	0.91	0.12	39,64,96,96	0
4	A1BUF	C	503	22/22	0.91	0.10	45,58,70,75	0
6	GOL	A	508	6/6	0.91	0.14	81,86,88,91	0
3	H4B	D	502	17/17	0.93	0.09	36,53,59,67	0
3	H4B	B	502	17/17	0.93	0.09	36,47,58,69	0
4	A1BUF	A	503	22/22	0.94	0.08	42,54,64,65	0
4	A1BUF	B	503	22/22	0.94	0.08	33,43,57,59	0
3	H4B	A	502	17/17	0.94	0.09	38,56,69,70	0
5	BTB	A	504	14/14	0.94	0.11	28,83,97,100	0
7	CL	C	508	1/1	0.94	0.11	71,71,71,71	0
3	H4B	C	502	17/17	0.95	0.08	48,59,68,71	0
7	CL	A	509	1/1	0.96	0.08	67,67,67,67	0
4	A1BUF	D	503	22/22	0.96	0.07	35,45,60,82	0
7	CL	D	507	1/1	0.96	0.09	64,64,64,64	0
10	CA	B	510	1/1	0.96	0.06	56,56,56,56	0
7	CL	B	508	1/1	0.97	0.08	67,67,67,67	0
2	HEM	A	501	43/43	0.98	0.07	35,50,63,81	0
8	GD	A	510	1/1	0.98	0.07	92,92,92,92	0

*Continued on next page...*

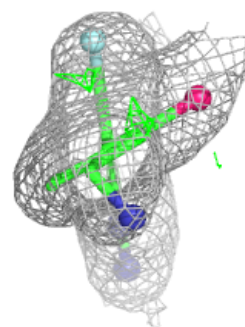
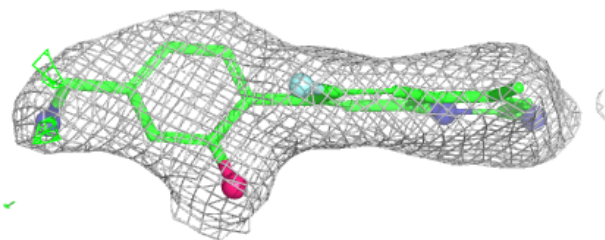
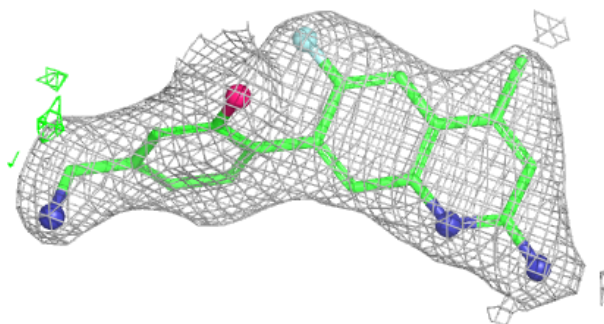
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	GD	B	509	1/1	0.98	0.04	55,55,55,55	0
8	GD	C	509	1/1	0.98	0.06	104,104,104,104	0
8	GD	D	509	1/1	0.98	0.04	53,53,53,53	0
2	HEM	C	501	43/43	0.98	0.07	44,55,68,76	0
2	HEM	B	501	43/43	0.99	0.05	30,36,53,72	0
9	ZN	C	510	1/1	0.99	0.03	49,49,49,49	0
10	CA	A	512	1/1	0.99	0.04	63,63,63,63	0
2	HEM	D	501	43/43	0.99	0.06	30,39,61,70	0
9	ZN	A	511	1/1	1.00	0.02	42,42,42,42	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.

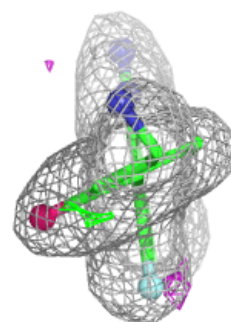
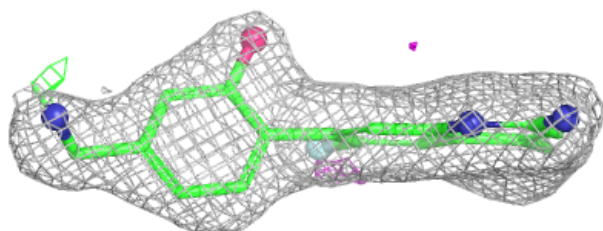
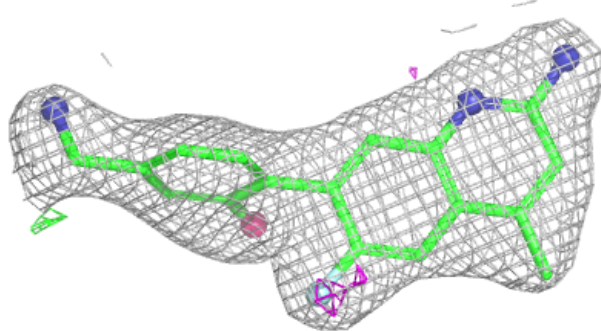
**Electron density around A1BUF C 503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

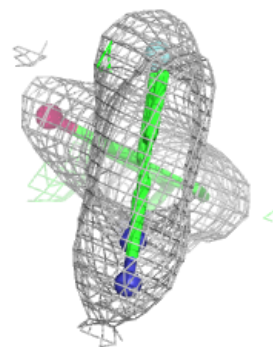
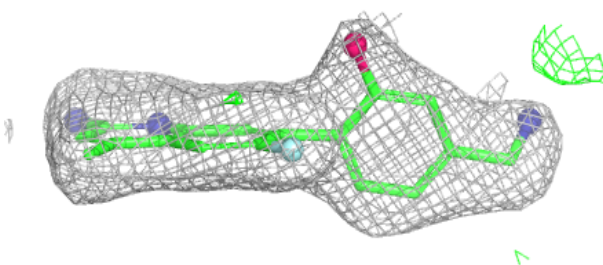
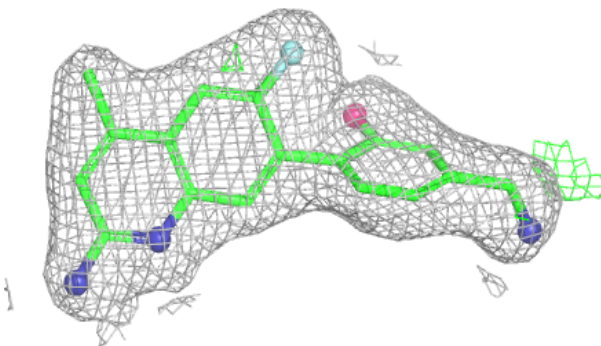


**Electron density around A1BUF A 503:**

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

**Electron density around A1BUF B 503:**

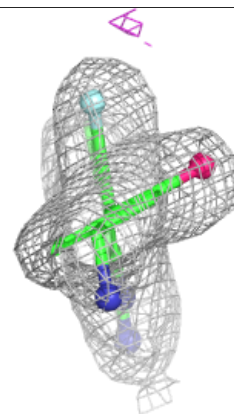
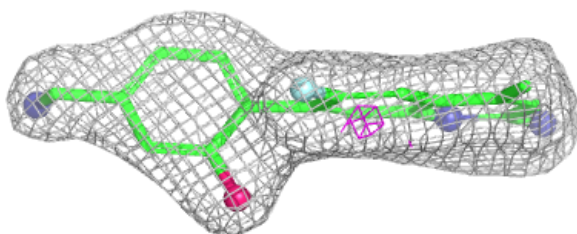
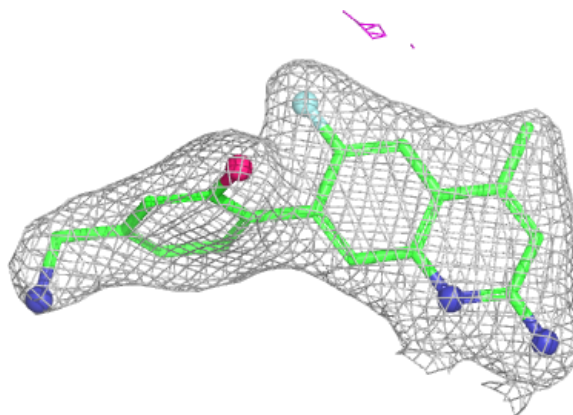
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





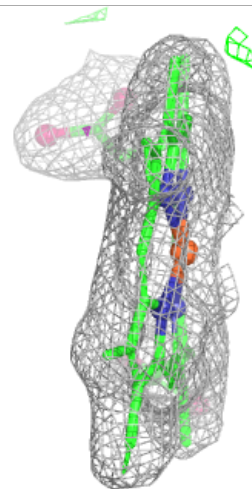
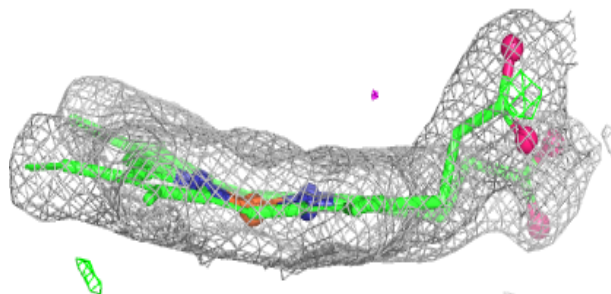
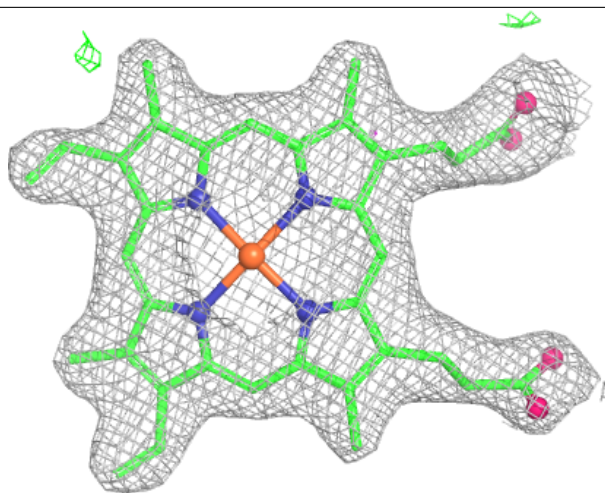
**Electron density around A1BUF D 503:**

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



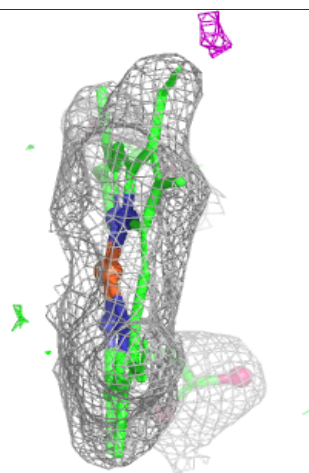
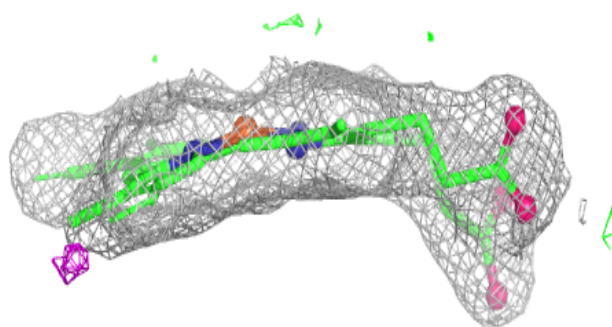
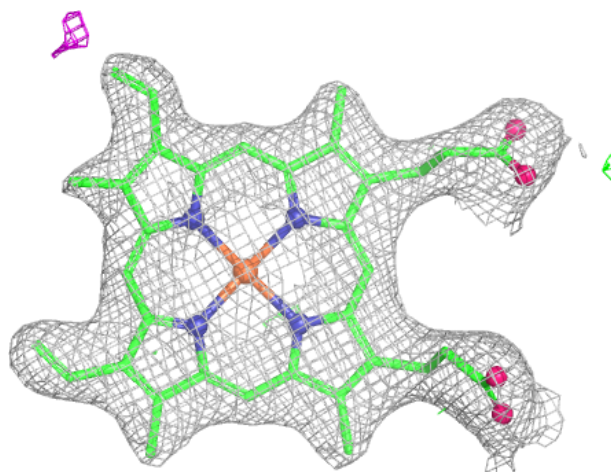
**Electron density around HEM A 501:**

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



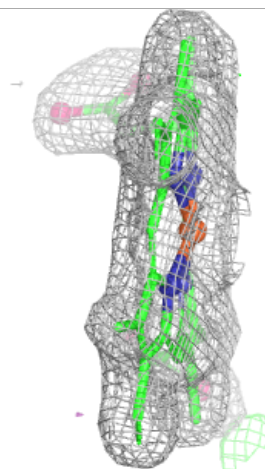
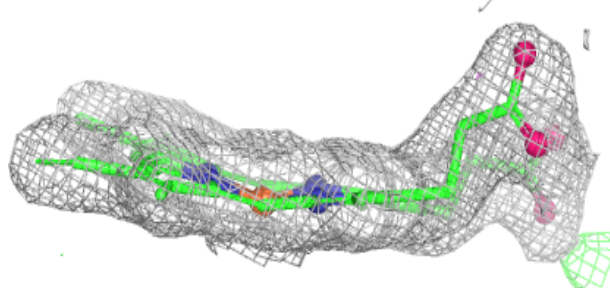
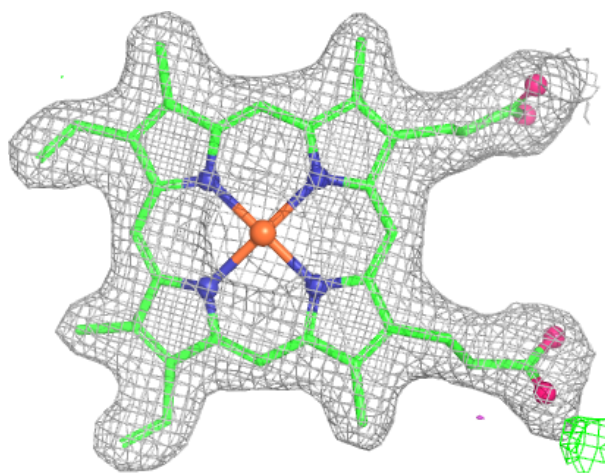
**Electron density around HEM C 501:**

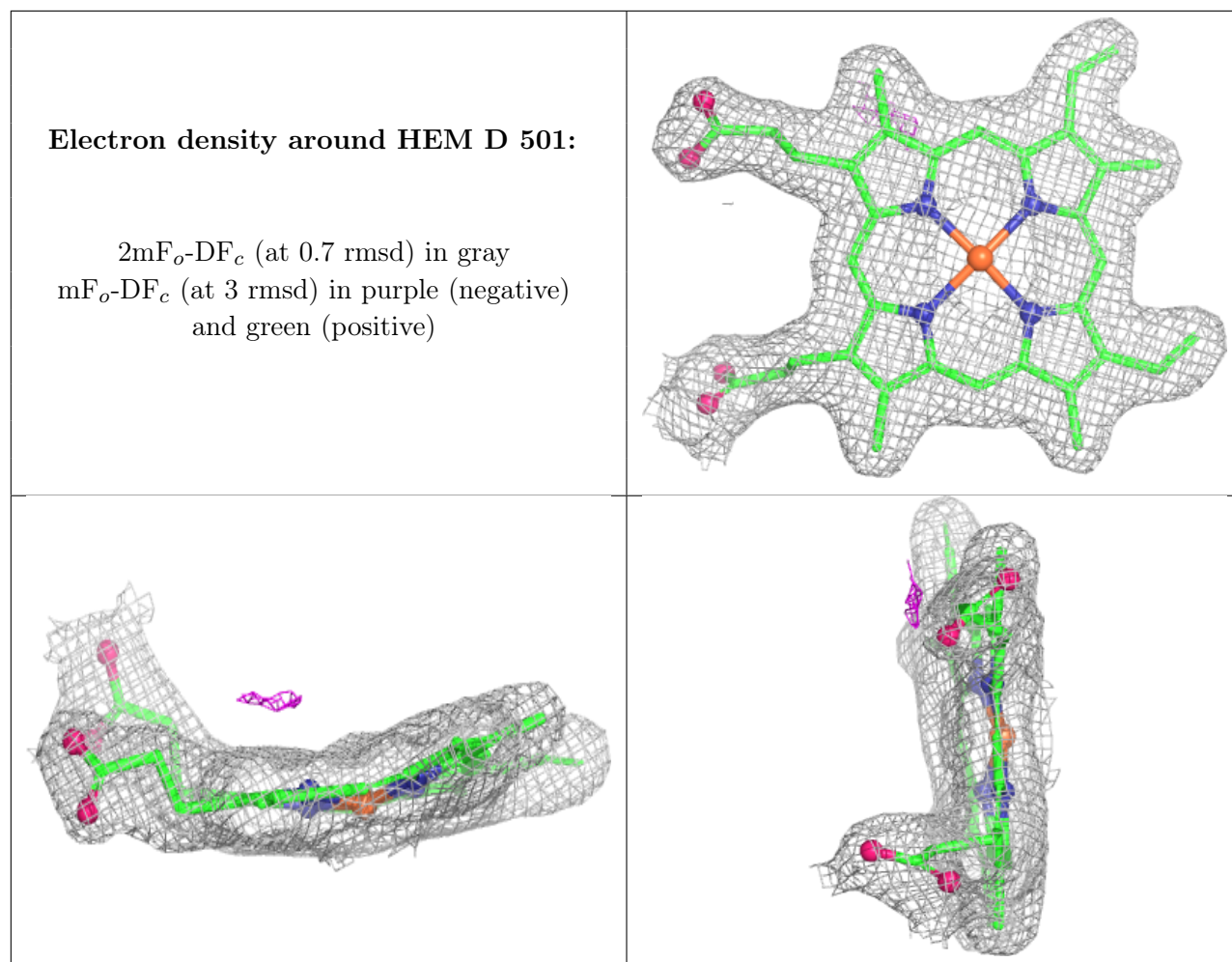
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM B 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.