



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2025 – 02:21 PM EST

PDB ID : 9MZ4 / pdb\_00009mz4  
Title : Structure of human endothelial nitric oxide synthase heme domain bound 7-(3-(aminomethyl)-4-(cyclopropylmethoxy)phenyl)-6-fluoro-4-methylquinolin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2025-01-22  
Resolution : 1.94 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

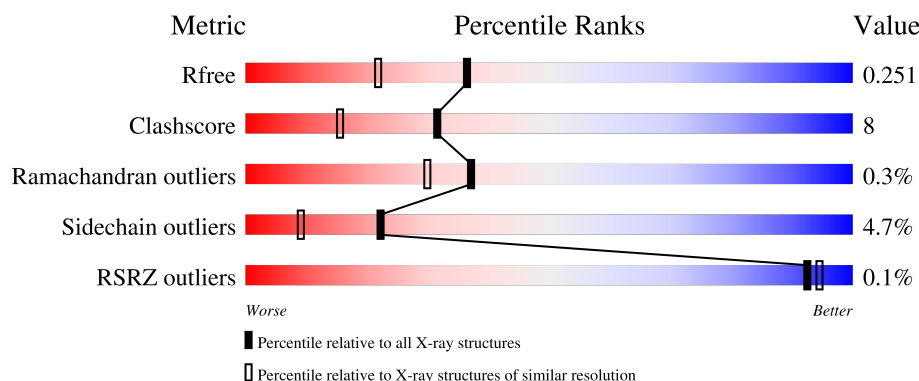
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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>72%</div> <div>18%</div> <div>• 8%</div> </div>
1	B	440	<div> <div>71%</div> <div>21%</div> <div>8%</div> </div>
1	C	440	<div> <div>73%</div> <div>16%</div> <div>• 9%</div> </div>
1	D	440	<div> <div>78%</div> <div>13%</div> <div>9%</div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13932 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	1	0
			3223	2052	569	586	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
			3205	2041	564	584	16			
1	D	402	Total	C	N	O	S	0	3	0
			3220	2051	566	587	16			

There are 4 discrepancies between the modelled and reference sequences:

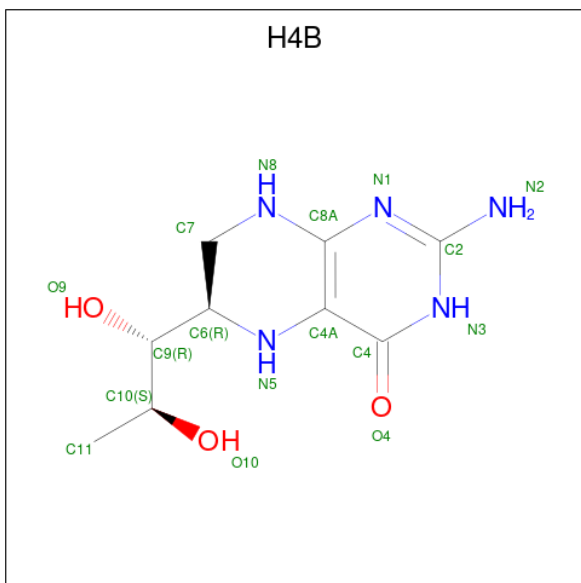
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	conflict	UNP P29474
B	298	GLU	ASP	conflict	UNP P29474
C	298	GLU	ASP	conflict	UNP P29474
D	298	GLU	ASP	conflict	UNP P29474

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



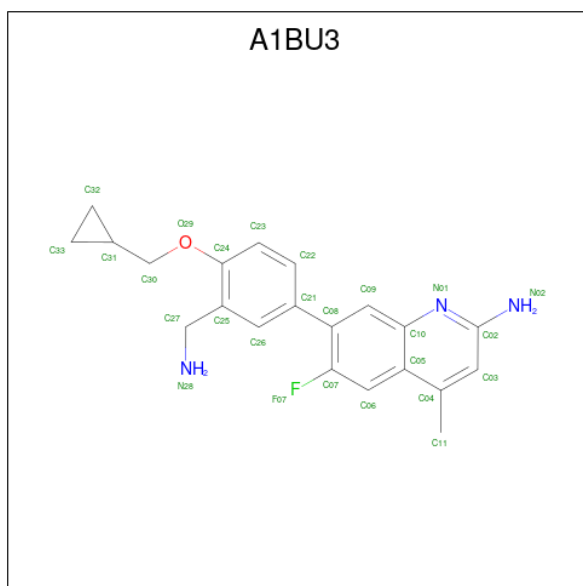
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula:  $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$ ).



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 (7P)-7-[3-(aminomethyl)-4-(cyclopropylmethoxy)phenyl]-6-fluoro-4-methylquinolin-2-amine (CCD ID: A1BU3) (formula: C<sub>21</sub>H<sub>22</sub>FN<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	21	1	3	1		
4	B	1	Total	C	F	N	O	0	0
			26	21	1	3	1		
4	C	1	Total	C	F	N	O	0	0
			26	21	1	3	1		
4	D	1	Total	C	F	N	O	0	0
			26	21	1	3	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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		
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		
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		

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

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

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

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

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

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

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

- Molecule 11 is water.

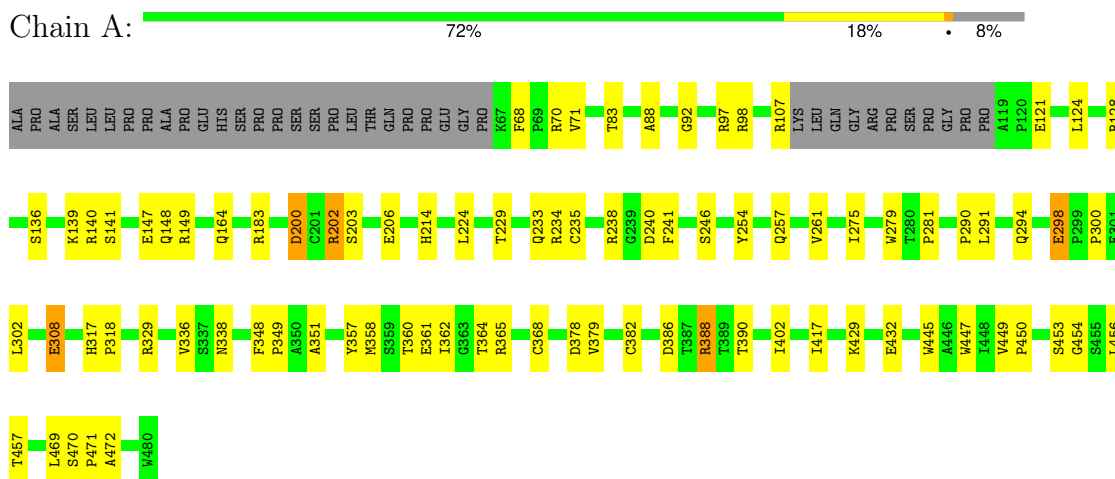
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	116	Total O 116 116	0	0
11	B	188	Total O 188 188	0	0
11	C	77	Total O 77 77	0	0
11	D	155	Total O 155 155	0	0



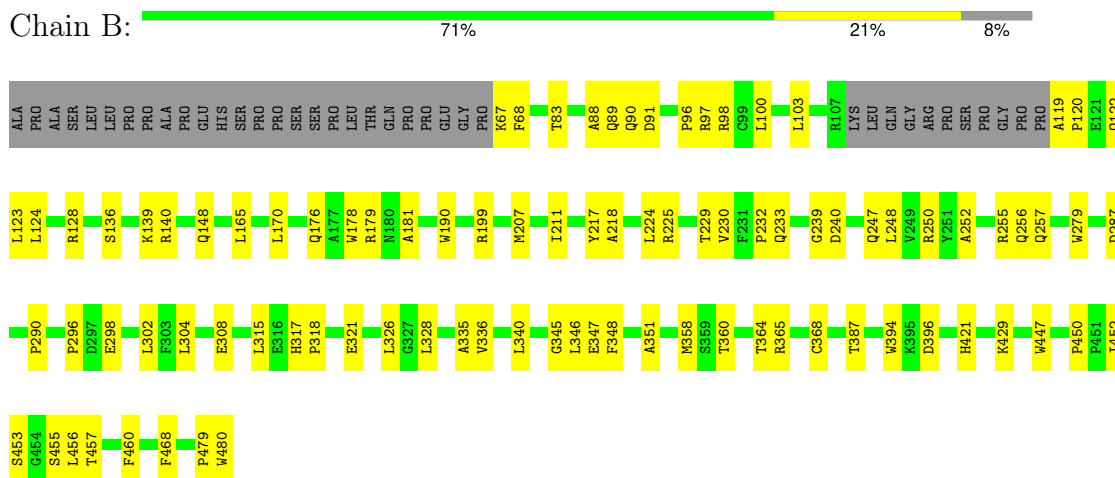
### 3 Residue-property plots

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 3

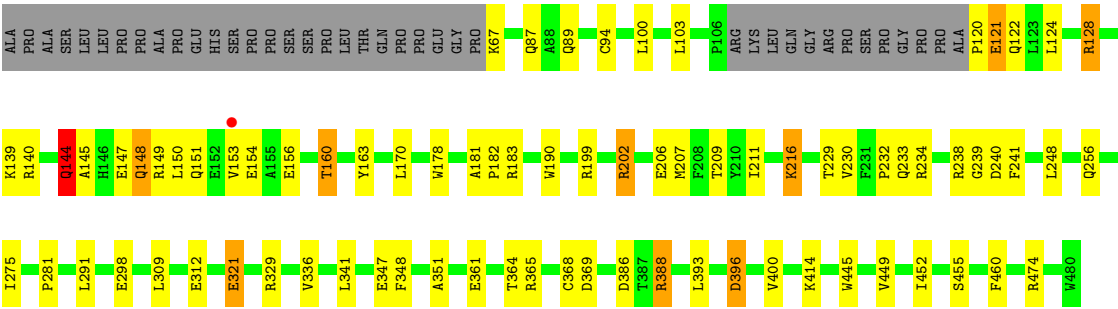


#### • Molecule 1: Nitric oxide synthase 3

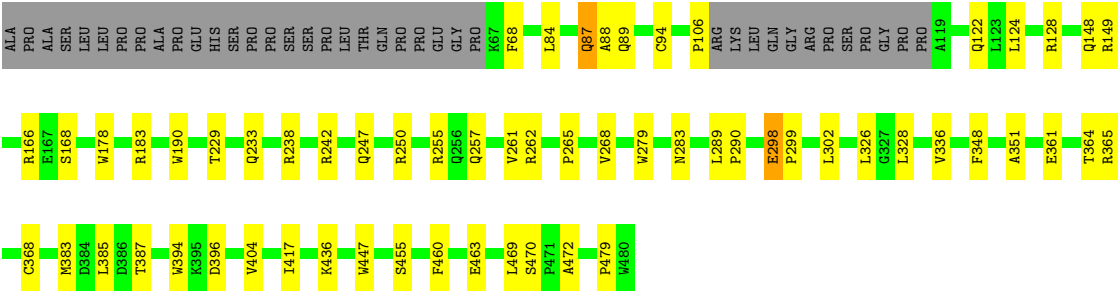
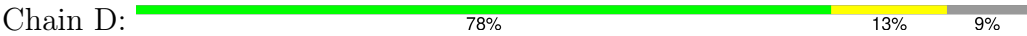


#### • Molecule 1: Nitric oxide synthase 3





● Molecule 1: Nitric oxide synthase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.81Å 151.14Å 107.78Å 90.00° 90.61° 90.00°	Depositor
Resolution (Å)	46.41 – 1.94 46.41 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.41-1.94) 95.5 (46.41-1.94)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.204 , 0.254 0.200 , 0.251	Depositor DCC
$R_{free}$ test set	6921 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.237 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13932	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: CA, A1BU3, GOL, H4B, ZN, HEM, GD, CL, BTB

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	0.29	0/3318	0.52	0/4520
1	B	0.36	0/3324	0.57	0/4528
1	C	0.28	0/3299	0.50	1/4494 (0.0%)
1	D	0.34	0/3321	0.52	0/4525
All	All	0.32	0/13262	0.53	1/18067 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120	PRO	N-CA-CB	6.48	110.13	103.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3223	0	3129	51	0
1	B	3226	0	3134	53	0
1	C	3205	0	3106	46	0
1	D	3220	0	3127	37	0
2	A	43	0	30	7	0
2	B	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	7	0
2	D	43	0	30	5	0
3	A	17	0	15	3	0
3	B	17	0	15	2	0
3	C	17	0	15	3	0
3	D	17	0	15	3	0
4	A	26	0	0	4	0
4	B	26	0	0	2	0
4	C	26	0	0	3	0
4	D	26	0	0	3	0
5	A	28	0	37	6	0
5	B	28	0	36	4	0
5	C	28	0	37	4	0
5	D	28	0	36	2	0
6	A	18	0	24	0	0
6	B	6	0	8	0	0
6	C	12	0	16	1	0
6	D	18	0	24	0	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	1	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	116	0	0	6	0
11	B	188	0	0	5	0
11	C	77	0	0	0	0
11	D	155	0	0	1	0
All	All	13932	0	12894	209	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 8.

All (209) 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:C3	8:C:509:GD:GD	1.92	0.83
1:C:144:GLN:HG3	1:C:145:ALA:N	1.98	0.77
1:D:247:GLN:HB2	1:D:250:ARG:HD3	1.65	0.77
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.69	0.75
5:D:505:BTB:O1	5:D:505:BTB:O3	2.05	0.72
5:D:504:BTB:H62	5:D:504:BTB:O8	1.90	0.71
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.74	0.70
1:D:124:LEU:HB3	1:D:128:ARG:HH22	1.56	0.70
1:A:382:CYS:HA	5:A:504:BTB:H12	1.73	0.69
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.76	0.68
1:A:149:ARG:NH2	1:A:164:GLN:O	2.26	0.68
1:A:183:ARG:HB2	2:A:501:HEM:HBD2	1.76	0.68
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.76	0.67
1:D:255:ARG:HH21	1:D:268:VAL:HG11	1.60	0.67
1:A:200:ASP:OD1	1:A:200:ASP:N	2.26	0.65
1:B:124:LEU:HD22	1:B:128:ARG:HH12	1.60	0.65
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.79	0.64
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.79	0.64
1:A:70:ARG:NH2	11:A:604:HOH:O	2.25	0.63
1:A:429:LYS:NZ	1:A:432:GLU:OE1	2.31	0.62
1:C:321:GLU:H	1:C:321:GLU:CD	2.07	0.62
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.82	0.62
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.82	0.61
1:D:383:MET:HE2	1:D:385:LEU:HD11	1.80	0.61
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.82	0.61
1:D:365:ARG:HH12	3:D:502:H4B:C4	2.14	0.61
1:B:321:GLU:OE2	5:B:504:BTB:O4	2.18	0.61
1:A:279:TRP:HB2	1:A:302:LEU:HD21	1.83	0.61
1:C:336:VAL:HG21	4:C:503:A1BU3:C07	2.32	0.59
2:A:501:HEM:O2A	4:A:503:A1BU3:N28	2.35	0.59
1:C:312:GLU:OE2	1:C:329:ARG:NH2	2.36	0.58
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.85	0.58
1:D:298:GLU:HG3	1:D:299:PRO:HD2	1.86	0.58
1:D:447:TRP:HA	3:D:502:H4B:N1	2.19	0.58
1:C:121:GLU:O	1:C:121:GLU:HG3	2.03	0.58
1:A:336:VAL:HG21	4:A:503:A1BU3:C07	2.34	0.57
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.18	0.56
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.86	0.56
1:B:91:ASP:OD1	11:B:601:HOH:O	2.18	0.56
1:C:94:CYS:HB3	1:D:94:CYS:HB3	1.87	0.56
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.88	0.56
1:A:329:ARG:NH1	11:A:608:HOH:O	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLU:HA	1:C:150:LEU:HD12	1.89	0.55
1:A:364:THR:O	1:A:368:CYS:HB2	2.06	0.55
1:C:386:ASP:OD2	1:C:388:ARG:HG2	2.06	0.55
1:D:242:ARG:NH2	1:D:479:PRO:HD3	2.21	0.55
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.41	0.54
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.43	0.54
1:D:262:ARG:NE	1:D:283:ASN:O	2.35	0.54
5:A:505:BTB:O8	5:A:505:BTB:O3	2.24	0.54
1:B:336:VAL:HG21	4:B:503:A1BU3:C07	2.38	0.54
1:B:90:GLN:HB3	1:B:468:PHE:CD2	2.43	0.53
1:C:103:LEU:HD12	1:D:463:GLU:HB3	1.90	0.53
1:C:341:LEU:HB3	1:C:348:PHE:HB2	1.90	0.53
1:B:181:ALA:HB1	2:B:501:HEM:O1D	2.08	0.53
1:B:447:TRP:HA	3:B:502:H4B:N1	2.24	0.53
1:A:246:SER:HA	1:A:338:ASN:HB3	1.90	0.52
1:D:84:LEU:HD12	1:D:87:GLN:HG3	1.91	0.52
1:D:89:GLN:OE1	1:D:470:SER:N	2.24	0.52
1:A:361:GLU:OE2	4:A:503:A1BU3:N02	2.43	0.52
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.92	0.51
2:D:501:HEM:CGA	3:D:502:H4B:HN3	2.24	0.51
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.92	0.51
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.46	0.51
1:D:279:TRP:CD1	1:D:290:PRO:HG3	2.45	0.51
1:A:257:GLN:HG3	1:C:388:ARG:NH2	2.26	0.51
1:A:294:GLN:HB2	1:A:300:PRO:HB3	1.93	0.51
1:B:364:THR:HG21	1:B:452:ILE:HG23	1.93	0.51
1:B:450:PRO:HG2	1:B:457:THR:HG21	1.92	0.50
1:C:178:TRP:CE3	1:C:190:TRP:HA	2.45	0.50
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.23	0.50
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.93	0.50
1:D:336:VAL:HG21	4:D:503:A1BU3:C07	2.40	0.50
1:B:455:SER:HA	1:B:460:PHE:CG	2.46	0.50
1:A:308:GLU:HG2	1:A:308:GLU:O	2.12	0.50
1:B:365:ARG:HH12	3:B:502:H4B:C4	2.25	0.50
1:A:279:TRP:CG	1:A:290:PRO:HG3	2.47	0.49
1:B:239:GLY:O	1:B:296:PRO:HB3	2.12	0.49
1:A:233:GLN:NE2	11:A:612:HOH:O	2.38	0.49
1:D:364:THR:O	1:D:368:CYS:HB2	2.12	0.49
2:A:501:HEM:CGA	3:A:502:H4B:HN3	2.25	0.49
2:B:501:HEM:O2A	4:B:503:A1BU3:N28	2.45	0.49
1:B:176:GLN:HE22	1:B:179:ARG:HH11	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:OD1	11:A:601:HOH:O	2.20	0.49
2:A:501:HEM:HBA1	4:A:503:A1BU3:C09	2.42	0.49
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.94	0.48
1:A:97:ARG:HG3	1:B:88:ALA:HB3	1.94	0.48
1:A:358:MET:HE3	1:A:360:THR:OG1	2.13	0.48
1:A:447:TRP:HA	3:A:502:H4B:N1	2.28	0.48
1:C:144:GLN:HG3	1:C:145:ALA:H	1.73	0.48
1:A:68:PHE:CD1	1:A:83:THR:HG22	2.48	0.48
1:B:364:THR:O	1:B:368:CYS:HB2	2.14	0.48
1:C:128:ARG:HH11	1:C:128:ARG:HB2	1.78	0.48
1:C:181:ALA:HB1	2:C:501:HEM:HBD1	1.96	0.48
1:A:470:SER:HA	1:A:471:PRO:C	2.38	0.48
1:C:163:TYR:O	1:C:233:GLN:NE2	2.43	0.48
1:D:361:GLU:OE2	4:D:503:A1BU3:N02	2.47	0.48
1:C:149:ARG:O	1:C:153:VAL:HG22	2.14	0.47
1:B:447:TRP:NE1	11:B:606:HOH:O	2.44	0.47
1:C:298:GLU:OE2	6:C:507:GOL:O1	2.29	0.47
1:D:279:TRP:CG	1:D:290:PRO:HG3	2.49	0.47
1:A:257:GLN:HG3	1:C:388:ARG:HH22	1.80	0.47
1:C:364:THR:HG21	1:C:452:ILE:HG23	1.97	0.47
1:A:357:TYR:CD2	1:A:362:ILE:HD11	2.49	0.47
5:C:505:BTB:H72	5:C:505:BTB:H41	1.39	0.47
1:A:445:TRP:CZ2	1:A:449:VAL:HG21	2.50	0.47
1:A:71:VAL:HG12	11:A:631:HOH:O	2.15	0.47
5:A:504:BTB:H72	5:A:504:BTB:H41	1.51	0.46
1:B:298:GLU:OE2	5:B:505:BTB:H31	2.16	0.46
1:C:170:LEU:HD11	1:C:230:VAL:HG11	1.97	0.46
1:C:455:SER:HA	1:C:460:PHE:CG	2.50	0.46
1:C:100:LEU:HB3	1:C:103:LEU:HD22	1.97	0.46
1:D:261:VAL:HG11	1:D:265:PRO:HA	1.97	0.46
1:B:148:GLN:NE2	11:B:611:HOH:O	2.49	0.46
1:B:68:PHE:CD2	1:B:83:THR:HA	2.50	0.46
5:A:505:BTB:H41	5:A:505:BTB:H72	1.42	0.46
1:C:238:ARG:HD2	1:C:239:GLY:N	2.31	0.46
1:D:183:ARG:HB2	2:D:501:HEM:HBD2	1.99	0.45
1:B:170:LEU:HD11	1:B:230:VAL:HG11	1.98	0.45
1:B:315:LEU:HB2	1:B:328:LEU:HB2	1.98	0.45
1:D:124:LEU:O	1:D:128:ARG:NH1	2.50	0.45
1:B:479:PRO:HD2	1:B:480:TRP:CE3	2.51	0.45
1:B:165:LEU:HG	1:B:346:LEU:HD12	1.99	0.45
1:C:199:ARG:O	1:C:232:PRO:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:HB2	1:C:309:LEU:HD11	1.99	0.45
5:C:505:BTB:H51	5:C:505:BTB:H11	1.53	0.45
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.86	0.44
1:B:256:GLN:HA	1:B:256:GLN:OE1	2.18	0.44
1:C:151:GLN:O	1:C:154:GLU:HB2	2.18	0.44
3:C:502:H4B:H113	1:D:463:GLU:HG2	1.99	0.44
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.52	0.44
1:B:308:GLU:H	1:B:308:GLU:CD	2.25	0.44
1:C:275:ILE:HD11	1:C:281:PRO:HB3	2.00	0.44
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.98	0.44
1:D:455:SER:HA	1:D:460:PHE:CB	2.48	0.44
1:B:68:PHE:CD1	1:B:83:THR:HG22	2.52	0.44
2:D:501:HEM:HBA2	4:D:503:A1BU3:C09	2.48	0.44
1:C:361:GLU:OE2	4:C:503:A1BU3:N02	2.51	0.43
1:D:106:PRO:HB3	11:D:670:HOH:O	2.16	0.43
5:C:504:BTB:H11	5:C:504:BTB:H51	1.31	0.43
1:B:340:LEU:HD21	1:B:347:GLU:HG2	2.00	0.43
1:B:387:THR:HA	1:B:394:TRP:CD1	2.54	0.43
5:B:505:BTB:O6	5:B:505:BTB:O8	2.27	0.43
1:B:358:MET:HE3	1:B:360:THR:OG1	2.19	0.43
1:A:445:TRP:CE2	1:A:449:VAL:HG21	2.54	0.43
1:C:211:ILE:HG23	1:C:248:LEU:HD13	2.01	0.43
1:A:235:CYS:SG	1:A:238:ARG:HB3	2.59	0.43
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.53	0.43
2:C:501:HEM:O2A	4:C:503:A1BU3:N28	2.52	0.43
1:C:202:ARG:HA	1:C:241:PHE:HZ	1.84	0.43
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.54	0.43
1:A:202:ARG:HA	1:A:241:PHE:HZ	1.84	0.43
1:D:87:GLN:H	1:D:87:GLN:HG2	1.55	0.43
1:B:455:SER:HA	1:B:460:PHE:CB	2.50	0.42
1:C:156:GLU:O	1:C:160:THR:OG1	2.33	0.42
5:A:505:BTB:H11	5:A:505:BTB:H51	1.71	0.42
1:B:199:ARG:O	1:B:232:PRO:HG3	2.19	0.42
1:C:140:ARG:HA	1:C:140:ARG:HD3	1.81	0.42
1:D:247:GLN:CB	1:D:250:ARG:HD3	2.43	0.42
1:C:229:THR:O	1:C:351:ALA:HA	2.19	0.42
1:D:469:LEU:O	1:D:472:ALA:HB2	2.19	0.42
1:C:445:TRP:CE2	1:C:449:VAL:HG21	2.54	0.42
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.49	0.42
1:A:254:TYR:O	1:A:261:VAL:HA	2.20	0.42
1:C:183:ARG:HB2	2:C:501:HEM:CGD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASP:OD2	1:A:388:ARG:HG3	2.20	0.42
1:B:123:LEU:HD12	1:B:345:GLY:HA3	2.02	0.42
1:C:207:MET:HE2	1:C:207:MET:HB3	1.85	0.42
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.54	0.42
1:C:396:ASP:O	1:C:400:VAL:HG23	2.20	0.42
1:A:298:GLU:H	1:A:298:GLU:HG2	1.69	0.42
1:B:139:LYS:N	1:B:139:LYS:HD2	2.35	0.42
1:B:217:TYR:CZ	1:B:225:ARG:HD2	2.55	0.42
1:A:275:ILE:HD11	1:A:281:PRO:HB3	2.01	0.42
2:A:501:HEM:O1A	11:A:602:HOH:O	2.22	0.42
1:B:252:ALA:N	1:B:287:ASP:O	2.46	0.42
1:B:247:GLN:HA	1:B:335:ALA:O	2.19	0.41
1:D:124:LEU:HB3	1:D:128:ARG:NH2	2.31	0.41
1:A:88:ALA:O	1:B:97:ARG:NH2	2.53	0.41
1:A:469:LEU:O	1:A:472:ALA:HB2	2.20	0.41
2:C:501:HEM:CGA	3:C:502:H4B:HN3	2.33	0.41
1:C:182:PRO:HD2	2:C:501:HEM:O2D	2.20	0.41
1:A:92:GLY:N	1:B:96:PRO:O	2.46	0.41
1:A:128:ARG:CZ	1:A:128:ARG:HB3	2.50	0.41
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.55	0.41
1:C:364:THR:O	1:C:368:CYS:HB2	2.20	0.41
1:B:119:ALA:N	1:B:120:PRO:HD3	2.36	0.41
1:B:218:ALA:O	1:B:224:LEU:HA	2.20	0.41
1:C:145:ALA:HA	1:C:148:GLN:HB3	2.02	0.41
5:B:504:BTB:H61	11:B:723:HOH:O	2.19	0.41
5:A:504:BTB:H12	5:A:504:BTB:H51	1.91	0.41
1:A:390:THR:HB	1:B:421:HIS:HB2	2.03	0.41
1:A:97:ARG:HG2	1:A:98:ARG:HG2	2.02	0.41
1:A:379:VAL:HG21	1:A:402:ILE:HD11	2.02	0.41
1:B:240:ASP:OD2	11:B:602:HOH:O	2.22	0.41
1:D:229:THR:O	1:D:351:ALA:HA	2.20	0.41
1:A:202:ARG:HD2	1:A:206:GLU:OE2	2.21	0.41
1:A:229:THR:O	1:A:351:ALA:HA	2.21	0.41
1:B:211:ILE:HG23	1:B:248:LEU:HD13	2.03	0.41
1:A:214:HIS:CD2	1:A:214:HIS:C	3.00	0.40
1:B:229:THR:O	1:B:351:ALA:HA	2.21	0.40
1:A:240:ASP:CG	1:A:349:PRO:HG3	2.46	0.40
2:B:501:HEM:HHC	2:B:501:HEM:CBB	2.51	0.40
1:C:365:ARG:O	1:C:369:ASP:HB2	2.21	0.40
1:C:393:LEU:HD12	1:D:404:VAL:HG23	2.04	0.40
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:LEU:HD23	1:D:289:LEU:HA	1.86	0.40
1:D:387:THR:HA	1:D:394:TRP:CD1	2.57	0.40
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	400/440 (91%)	382 (96%)	17 (4%)	1 (0%)	37	30
1	B	401/440 (91%)	388 (97%)	12 (3%)	1 (0%)	44	37
1	C	398/440 (90%)	376 (94%)	21 (5%)	1 (0%)	37	30
1	D	401/440 (91%)	391 (98%)	9 (2%)	1 (0%)	44	37
All	All	1600/1760 (91%)	1537 (96%)	59 (4%)	4 (0%)	37	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	GLN
1	B	255	ARG
1	D	88	ALA
1	A	454	GLY

### 5.3.2 Protein sidechains [i](#)

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	343/373 (92%)	324 (94%)	19 (6%)	18	6
1	B	344/373 (92%)	333 (97%)	11 (3%)	34	22
1	C	341/373 (91%)	318 (93%)	23 (7%)	13	3
1	D	344/373 (92%)	332 (96%)	12 (4%)	31	18
All	All	1372/1492 (92%)	1307 (95%)	65 (5%)	22	9

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	121	GLU
1	A	124	LEU
1	A	136	SER
1	A	139	LYS
1	A	140	ARG
1	A	141	SER
1	A	147	GLU
1	A	148	GLN
1	A	200	ASP
1	A	202	ARG
1	A	203	SER
1	A	224	LEU
1	A	234	ARG
1	A	291	LEU
1	A	298	GLU
1	A	308	GLU
1	A	388	ARG
1	A	417	ILE
1	B	67	LYS
1	B	89	GLN
1	B	98	ARG
1	B	122	GLN
1	B	136	SER
1	B	140	ARG
1	B	207	MET
1	B	257	GLN
1	B	326	LEU
1	B	396	ASP
1	B	429	LYS
1	C	67	LYS

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Mol	Chain	Res	Type
1	C	87	GLN
1	C	89	GLN
1	C	121	GLU
1	C	122	GLN
1	C	124	LEU
1	C	128	ARG
1	C	139	LYS
1	C	144	GLN
1	C	148	GLN
1	C	160	THR
1	C	202	ARG
1	C	206	GLU
1	C	209	THR
1	C	216	LYS
1	C	240	ASP
1	C	256	GLN
1	C	291	LEU
1	C	321	GLU
1	C	388	ARG
1	C	396	ASP
1	C	414	LYS
1	C	474	ARG
1	D	68	PHE
1	D	87	GLN
1	D	122	GLN
1	D	148	GLN
1	D	168[A]	SER
1	D	168[B]	SER
1	D	238	ARG
1	D	257	GLN
1	D	298	GLU
1	D	396	ASP
1	D	417	ILE
1	D	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	151	GLN
1	A	164	GLN
1	A	194	GLN

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Mol	Chain	Res	Type
1	B	144	GLN
1	B	148	GLN
1	C	133	GLN
1	C	189	GLN
1	D	194	GLN

### 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	$\# Z  > 2$
5	BTB	B	504	8	13,13,13	0.34	0	7,16,16	0.32	0
2	HEM	B	501	1	42,50,50	1.48	7 (16%)	46,82,82	1.76	16 (34%)
5	BTB	D	504	8	13,13,13	0.40	0	7,16,16	0.57	0
4	A1BU3	A	503	-	29,29,29	0.99	2 (6%)	41,42,42	1.48	6 (14%)
3	H4B	B	502	-	16,18,18	0.73	0	14,26,26	2.40	7 (50%)
6	GOL	C	506	-	5,5,5	0.39	0	5,5,5	0.48	0
5	BTB	B	505	-	13,13,13	0.44	0	7,16,16	0.84	0
5	BTB	A	504	8	13,13,13	0.44	0	7,16,16	1.60	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	506	-	5,5,5	0.34	0	5,5,5	0.36	0
6	GOL	A	508	-	5,5,5	0.37	0	5,5,5	0.44	0
3	H4B	A	502	-	16,18,18	0.75	0	14,26,26	2.29	6 (42%)
4	A1BU3	C	503	-	29,29,29	0.94	2 (6%)	41,42,42	1.52	7 (17%)
3	H4B	D	502	-	16,18,18	0.89	0	14,26,26	2.89	6 (42%)
6	GOL	D	508	-	5,5,5	0.37	0	5,5,5	0.43	0
5	BTB	C	505	-	13,13,13	0.57	0	7,16,16	1.09	1 (14%)
6	GOL	A	507	-	5,5,5	0.37	0	5,5,5	0.31	0
5	BTB	D	505	-	13,13,13	0.44	0	7,16,16	1.20	0
6	GOL	B	506	-	5,5,5	0.33	0	5,5,5	0.38	0
5	BTB	C	504	8	13,13,13	0.52	0	7,16,16	0.60	0
6	GOL	C	507	-	5,5,5	0.39	0	5,5,5	0.34	0
2	HEM	A	501	1	42,50,50	1.50	6 (14%)	46,82,82	1.52	8 (17%)
4	A1BU3	B	503	-	29,29,29	1.05	2 (6%)	41,42,42	1.40	7 (17%)
2	HEM	C	501	1	42,50,50	1.51	6 (14%)	46,82,82	1.62	12 (26%)
2	HEM	D	501	1	42,50,50	1.54	5 (11%)	46,82,82	2.03	15 (32%)
6	GOL	D	506	-	5,5,5	0.33	0	5,5,5	0.46	0
3	H4B	C	502	-	16,18,18	0.85	0	14,26,26	2.39	5 (35%)
5	BTB	A	505	-	13,13,13	0.71	0	7,16,16	1.37	1 (14%)
6	GOL	D	507	-	5,5,5	0.38	0	5,5,5	0.21	0
4	A1BU3	D	503	-	29,29,29	0.93	1 (3%)	41,42,42	1.25	4 (9%)

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
5	BTB	B	504	8	-	7/21/21/21	-
2	HEM	B	501	1	-	3/12/54/54	-
5	BTB	D	504	8	-	5/21/21/21	-
4	A1BU3	A	503	-	-	3/11/13/13	0/4/4/4
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
6	GOL	C	506	-	-	2/4/4/4	-
5	BTB	B	505	-	-	4/21/21/21	-
5	BTB	A	504	8	-	2/21/21/21	-
6	GOL	A	506	-	-	4/4/4/4	-
6	GOL	A	508	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
4	A1BU3	C	503	-	-	3/11/13/13	0/4/4/4
3	H4B	D	502	-	-	1/8/17/17	0/2/2/2
6	GOL	D	508	-	-	2/4/4/4	-
5	BTB	C	505	-	-	16/21/21/21	-
6	GOL	A	507	-	-	2/4/4/4	-
5	BTB	D	505	-	-	4/21/21/21	-
6	GOL	B	506	-	-	2/4/4/4	-
5	BTB	C	504	8	-	12/21/21/21	-
6	GOL	C	507	-	-	0/4/4/4	-
2	HEM	A	501	1	-	1/12/54/54	-
4	A1BU3	B	503	-	-	4/11/13/13	0/4/4/4
2	HEM	C	501	1	-	4/12/54/54	-
2	HEM	D	501	1	-	3/12/54/54	-
6	GOL	D	506	-	-	2/4/4/4	-
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2
5	BTB	A	505	-	-	10/21/21/21	-
6	GOL	D	507	-	-	2/4/4/4	-
4	A1BU3	D	503	-	-	2/11/13/13	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-C2C	-3.95	1.35	1.40
2	B	501	HEM	C3C-C4C	3.93	1.47	1.41
2	D	501	HEM	C3C-C2C	-3.85	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.79	1.35	1.40
2	A	501	HEM	C3C-CAC	3.62	1.55	1.47
2	D	501	HEM	CAB-C3B	3.61	1.57	1.47
2	C	501	HEM	C3C-CAC	3.39	1.55	1.47
2	D	501	HEM	C3C-C4C	3.37	1.46	1.41
2	D	501	HEM	C3C-CAC	3.08	1.54	1.47
2	A	501	HEM	CAB-C3B	3.06	1.55	1.47
2	C	501	HEM	CAB-C3B	3.04	1.55	1.47
2	A	501	HEM	C3C-C4C	2.97	1.45	1.41
2	B	501	HEM	CAB-C3B	2.97	1.55	1.47
2	C	501	HEM	FE-NB	2.93	2.14	1.98
2	B	501	HEM	C3C-C2C	-2.89	1.36	1.40
2	B	501	HEM	C3C-CAC	2.88	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CMD-C2D	2.64	1.56	1.50
4	B	503	A1BU3	C06-C07	2.58	1.40	1.35
2	C	501	HEM	C3C-C4C	2.51	1.45	1.41
4	A	503	A1BU3	C06-C07	2.47	1.39	1.35
2	A	501	HEM	CMB-C2B	2.33	1.55	1.50
4	D	503	A1BU3	C06-C07	2.33	1.39	1.35
2	D	501	HEM	FE-ND	2.32	2.11	1.98
4	A	503	A1BU3	C05-C10	-2.24	1.39	1.42
4	C	503	A1BU3	C05-C10	-2.13	1.39	1.42
2	B	501	HEM	CMB-C2B	2.10	1.55	1.50
4	B	503	A1BU3	C05-C10	-2.07	1.39	1.42
2	B	501	HEM	CMD-C2D	2.06	1.55	1.50
2	C	501	HEM	CMB-C2B	2.05	1.55	1.50
2	B	501	HEM	C4D-ND	-2.02	1.36	1.40
4	C	503	A1BU3	C06-C07	2.00	1.39	1.35

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBA-CAA-C2A	-6.26	102.01	112.54
3	C	502	H4B	C8A-C4A-C4	5.69	119.68	114.50
3	D	502	H4B	C11-C10-C9	-5.62	105.24	112.11
3	D	502	H4B	C8A-C4A-C4	5.61	119.60	114.50
3	B	502	H4B	C8A-C4A-C4	4.99	119.05	114.50
3	A	502	H4B	C8A-C4A-C4	4.85	118.91	114.50
4	A	503	A1BU3	O29-C24-C25	4.79	122.08	115.89
2	B	501	HEM	CMA-C3A-C4A	-4.11	122.43	128.46
3	B	502	H4B	C2-N3-C4	4.06	121.60	115.96
3	D	502	H4B	N1-C2-N3	-3.90	119.50	125.48
4	D	503	A1BU3	O29-C24-C25	3.84	120.86	115.89
2	D	501	HEM	CBD-CAD-C3D	-3.79	102.05	112.53
2	C	501	HEM	C4C-CHD-C1D	3.79	127.56	122.56
2	D	501	HEM	CMA-C3A-C4A	-3.78	122.92	128.46
2	D	501	HEM	C3B-C2B-C1B	3.78	109.25	106.41
2	D	501	HEM	C4B-CHC-C1C	3.70	127.44	122.56
4	B	503	A1BU3	C09-C08-C07	3.67	120.30	116.03
3	D	502	H4B	C2-N3-C4	3.62	121.00	115.96
2	A	501	HEM	C4B-CHC-C1C	3.57	127.27	122.56
3	A	502	H4B	N1-C2-N3	-3.55	120.04	125.48
4	C	503	A1BU3	O29-C24-C25	3.48	120.39	115.89
3	B	502	H4B	N1-C2-N3	-3.42	120.23	125.48
4	C	503	A1BU3	C04-C05-C10	3.36	120.05	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	BTB	O3-C3-C2	3.34	119.25	111.40
4	C	503	A1BU3	C05-C10-N01	-3.32	119.29	122.80
3	C	502	H4B	N1-C2-N3	-3.31	120.41	125.48
3	A	502	H4B	C2-N3-C4	3.29	120.54	115.96
3	C	502	H4B	C2-N3-C4	3.28	120.52	115.96
4	A	503	A1BU3	C05-C10-N01	-3.25	119.36	122.80
2	B	501	HEM	CBA-CAA-C2A	-3.25	107.07	112.54
2	A	501	HEM	CBD-CAD-C3D	-3.25	103.55	112.53
2	B	501	HEM	C4B-CHC-C1C	3.19	126.76	122.56
4	B	503	A1BU3	C32-C31-C30	-2.99	104.86	119.41
2	D	501	HEM	C4D-ND-C1D	2.98	108.73	105.21
2	C	501	HEM	CBD-CAD-C3D	-2.95	104.39	112.53
2	D	501	HEM	C1B-NB-C4B	2.92	108.66	105.21
3	D	502	H4B	C2-N1-C8A	2.90	121.47	114.59
4	A	503	A1BU3	C04-C05-C10	2.84	119.73	118.00
2	C	501	HEM	CMA-C3A-C4A	-2.79	124.37	128.46
3	A	502	H4B	C2-N1-C8A	2.78	121.20	114.59
2	C	501	HEM	C3B-C2B-C1B	2.75	108.47	106.41
4	C	503	A1BU3	C09-C08-C07	2.71	119.19	116.03
4	B	503	A1BU3	C05-C10-N01	-2.65	120.00	122.80
2	D	501	HEM	C2D-C1D-ND	-2.64	106.85	109.90
3	C	502	H4B	C2-N1-C8A	2.64	120.86	114.59
4	A	503	A1BU3	C33-C31-C30	-2.57	106.92	119.41
3	C	502	H4B	N2-C2-N3	2.55	121.05	117.22
2	B	501	HEM	C1B-NB-C4B	2.51	108.19	105.21
2	B	501	HEM	CAD-CBD-CGD	-2.51	107.02	113.67
3	B	502	H4B	C2-N1-C8A	2.50	120.54	114.59
2	D	501	HEM	C3B-C4B-NB	-2.50	107.67	109.47
2	A	501	HEM	C3D-C4D-ND	-2.50	107.43	110.17
2	A	501	HEM	CMC-C2C-C3C	2.49	129.65	124.68
2	D	501	HEM	C2B-C1B-NB	-2.49	106.98	109.84
3	A	502	H4B	N2-C2-N3	2.47	120.93	117.22
3	A	502	H4B	C4-C4A-N5	2.46	122.08	118.57
3	D	502	H4B	N2-C2-N1	2.43	120.86	117.22
2	D	501	HEM	CMA-C3A-C2A	2.40	129.47	124.94
2	A	501	HEM	C3B-C2B-C1B	2.39	108.20	106.41
4	C	503	A1BU3	C33-C31-C30	-2.38	107.83	119.41
4	B	503	A1BU3	C26-C21-C08	-2.38	116.62	120.61
4	D	503	A1BU3	C09-C08-C07	2.37	118.79	116.03
3	B	502	H4B	C4-C4A-N5	2.37	121.95	118.57
2	C	501	HEM	C4A-C3A-C2A	2.37	108.64	107.00
4	C	503	A1BU3	C21-C08-C07	-2.36	119.12	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CAD-C3D-C4D	2.35	128.79	124.70
2	C	501	HEM	CAD-C3D-C2D	-2.32	123.52	127.87
2	C	501	HEM	CHD-C1D-ND	2.31	126.92	124.44
2	B	501	HEM	C4D-ND-C1D	2.30	107.94	105.21
2	B	501	HEM	CAD-C3D-C4D	-2.28	120.72	124.70
5	C	505	BTB	O3-C3-C2	-2.27	106.05	111.40
4	A	503	A1BU3	O29-C24-C23	-2.27	118.99	123.95
2	B	501	HEM	CMA-C3A-C2A	2.27	129.22	124.94
2	B	501	HEM	CBD-CAD-C3D	2.27	118.80	112.53
2	B	501	HEM	CMC-C2C-C3C	2.26	129.21	124.68
2	A	501	HEM	C1B-NB-C4B	2.25	107.87	105.21
2	B	501	HEM	C4C-CHD-C1D	2.25	125.53	122.56
4	B	503	A1BU3	C33-C31-C30	-2.22	108.61	119.41
4	A	503	A1BU3	N02-C02-N01	2.19	120.05	118.24
2	C	501	HEM	C4B-CHC-C1C	2.16	125.41	122.56
2	D	501	HEM	C3D-C4D-ND	-2.16	107.80	110.17
2	C	501	HEM	C4D-ND-C1D	2.15	107.76	105.21
5	A	505	BTB	O1-C1-C2	-2.14	106.37	111.40
2	D	501	HEM	CMB-C2B-C3B	-2.13	123.27	128.43
2	D	501	HEM	CAB-C3B-C2B	-2.13	121.51	128.43
3	B	502	H4B	C4A-C4-N3	-2.12	118.56	123.91
2	B	501	HEM	CMD-C2D-C1D	-2.11	121.73	125.03
4	B	503	A1BU3	C06-C07-C08	-2.11	120.23	123.59
2	B	501	HEM	O1D-CGD-CBD	-2.11	116.40	123.09
2	B	501	HEM	C3B-C4B-NB	-2.10	107.96	109.47
4	C	503	A1BU3	C32-C31-C30	-2.09	109.22	119.41
2	B	501	HEM	O2A-CGA-CBA	2.09	120.61	114.00
2	B	501	HEM	CAD-C3D-C2D	2.08	131.76	127.87
2	A	501	HEM	C3B-C4B-NB	-2.07	107.98	109.47
2	C	501	HEM	CHC-C4B-C3B	2.07	127.73	124.57
4	D	503	A1BU3	C05-C10-N01	-2.06	120.62	122.80
3	B	502	H4B	N2-C2-N3	2.04	120.28	117.22
2	C	501	HEM	C3B-C4B-NB	-2.04	108.00	109.47
4	D	503	A1BU3	C33-C31-C30	-2.04	109.50	119.41
4	B	503	A1BU3	C04-C05-C10	2.03	119.24	118.00
2	A	501	HEM	C4D-ND-C1D	2.01	107.59	105.21
2	D	501	HEM	C4C-CHD-C1D	2.01	125.21	122.56

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2A-CAA-CBA-CGA
2	B	501	HEM	C2D-C3D-CAD-CBD
2	C	501	HEM	C2A-CAA-CBA-CGA
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
3	C	502	H4B	C7-C6-C9-O9
3	C	502	H4B	C7-C6-C9-C10
4	A	503	A1BU3	O29-C30-C31-C32
5	A	504	BTB	C1-C2-C4-O4
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
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	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-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
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-N-C5
5	C	505	BTB	O1-C1-C2-C3
5	C	505	BTB	O1-C1-C2-C4
5	C	505	BTB	O1-C1-C2-N
5	C	505	BTB	C1-C2-C3-O3
5	C	505	BTB	C4-C2-C3-O3
5	C	505	BTB	N-C2-C3-O3
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-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-C7

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Mol	Chain	Res	Type	Atoms
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	O1-C1-C2-N
5	D	504	BTB	N-C5-C6-O6
5	D	505	BTB	O1-C1-C2-C3
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
6	A	506	GOL	O1-C1-C2-C3
6	A	506	GOL	C1-C2-C3-O3
6	D	507	GOL	O1-C1-C2-C3
6	D	508	GOL	C1-C2-C3-O3
6	D	508	GOL	O2-C2-C3-O3
2	B	501	HEM	C4D-C3D-CAD-CBD
5	A	505	BTB	N-C7-C8-O8
6	A	507	GOL	C1-C2-C3-O3
6	C	506	GOL	C1-C2-C3-O3
6	D	506	GOL	O1-C1-C2-C3
6	A	506	GOL	O2-C2-C3-O3
5	C	505	BTB	N-C7-C8-O8
5	D	505	BTB	N-C5-C6-O6
2	C	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C2A-CAA-CBA-CGA
6	A	506	GOL	O1-C1-C2-O2
6	A	507	GOL	O2-C2-C3-O3
6	D	507	GOL	O1-C1-C2-O2
4	C	503	A1BU3	C23-C24-O29-C30
4	C	503	A1BU3	C25-C24-O29-C30
4	A	503	A1BU3	C25-C24-O29-C30
5	B	504	BTB	N-C7-C8-O8
6	C	506	GOL	O2-C2-C3-O3
4	A	503	A1BU3	C23-C24-O29-C30
6	B	506	GOL	O1-C1-C2-O2
6	D	506	GOL	O1-C1-C2-O2
4	B	503	A1BU3	C31-C30-O29-C24
5	B	505	BTB	N-C5-C6-O6
2	C	501	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
5	C	504	BTB	N-C7-C8-O8
4	D	503	A1BU3	C23-C24-O29-C30
5	A	505	BTB	N-C2-C4-O4
5	C	504	BTB	N-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
5	C	504	BTB	C3-C2-N-C5
5	C	504	BTB	C3-C2-N-C7
5	C	504	BTB	C4-C2-N-C5
5	C	504	BTB	C4-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
4	B	503	A1BU3	C23-C24-O29-C30
6	B	506	GOL	O1-C1-C2-C3
2	D	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
4	D	503	A1BU3	C25-C24-O29-C30
4	B	503	A1BU3	C25-C24-O29-C30
5	C	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
3	B	502	H4B	N5-C6-C9-O9
3	C	502	H4B	N5-C6-C9-O9
4	B	503	A1BU3	O29-C30-C31-C32
4	C	503	A1BU3	O29-C30-C31-C32
5	A	504	BTB	N-C2-C4-O4
5	C	504	BTB	C1-C2-N-C7
5	C	505	BTB	N-C2-C4-O4
3	D	502	H4B	O10-C10-C9-O9

There are no ring outliers.

21 monomers are involved in 56 short contacts:

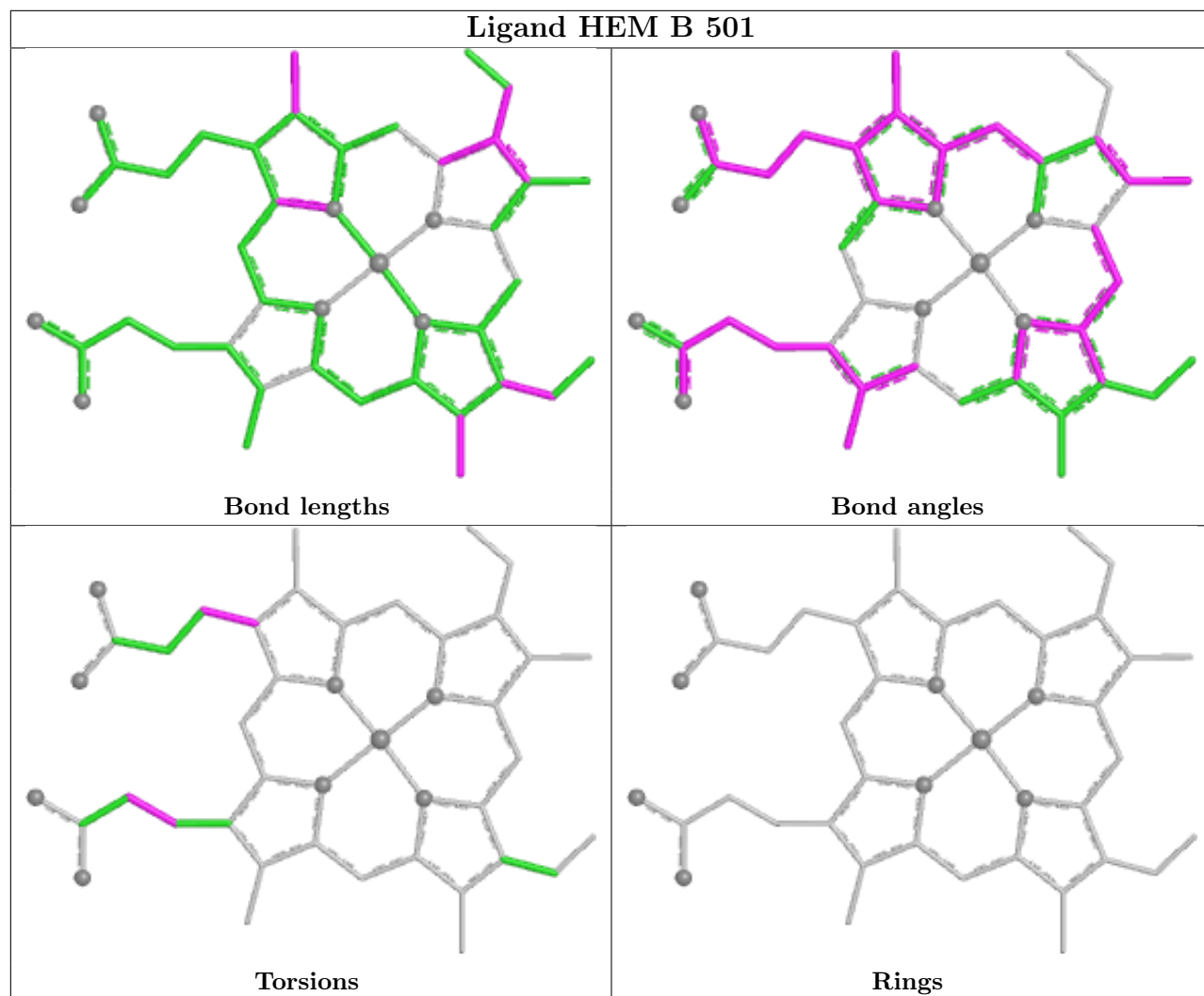
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	BTB	2	0
2	B	501	HEM	5	0
5	D	504	BTB	1	0
4	A	503	A1BU3	4	0
3	B	502	H4B	2	0
5	B	505	BTB	2	0
5	A	504	BTB	3	0
3	A	502	H4B	3	0
4	C	503	A1BU3	3	0
3	D	502	H4B	3	0
5	C	505	BTB	2	0
5	D	505	BTB	1	0
5	C	504	BTB	2	0
6	C	507	GOL	1	0
2	A	501	HEM	7	0
4	B	503	A1BU3	2	0

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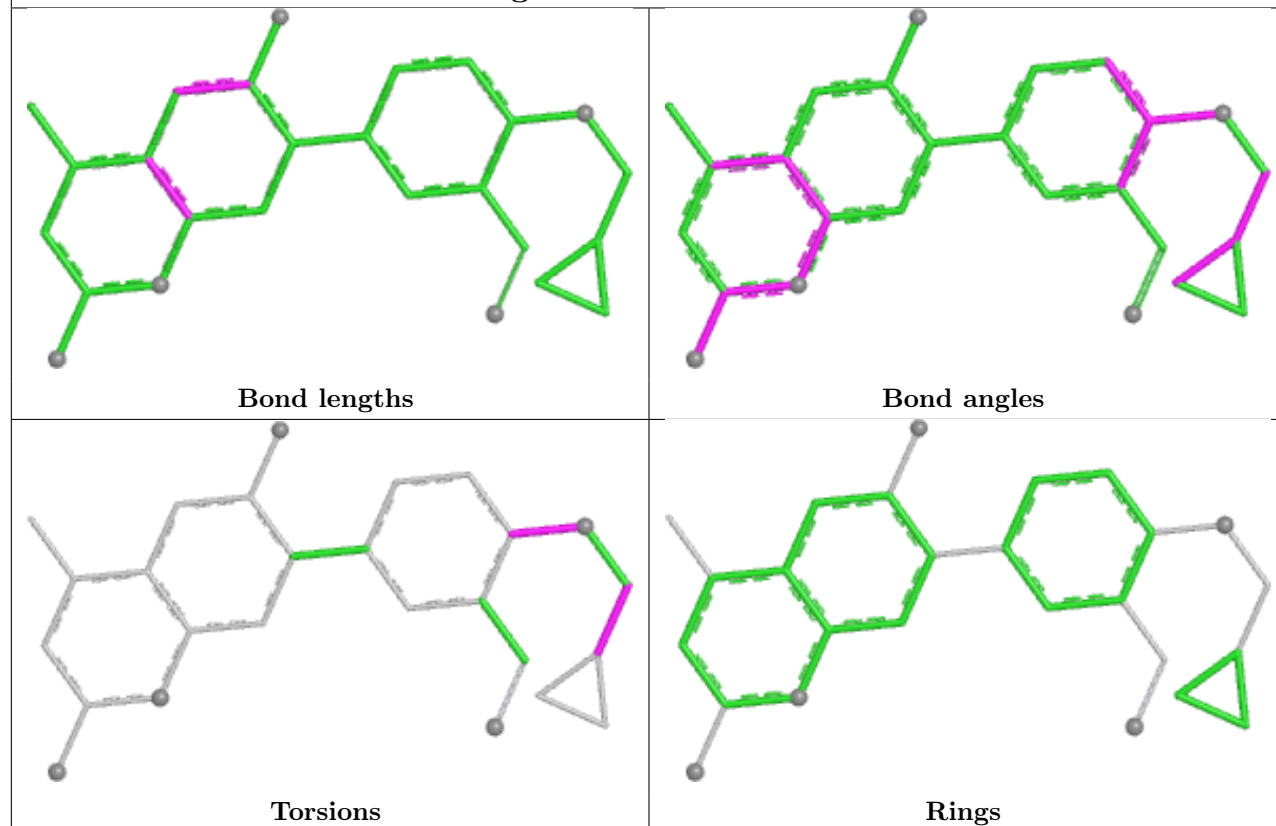
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	7	0
2	D	501	HEM	5	0
3	C	502	H4B	3	0
5	A	505	BTB	3	0
4	D	503	A1BU3	3	0

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.

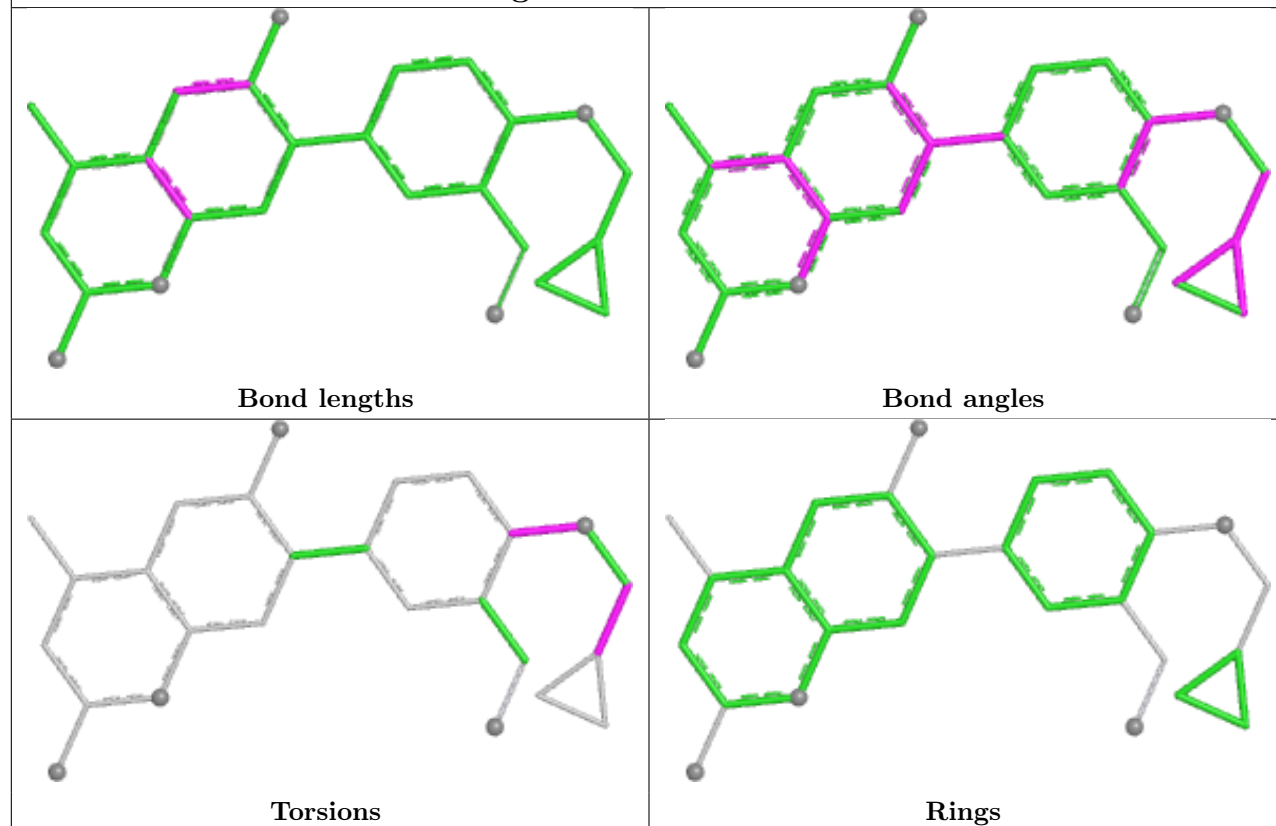


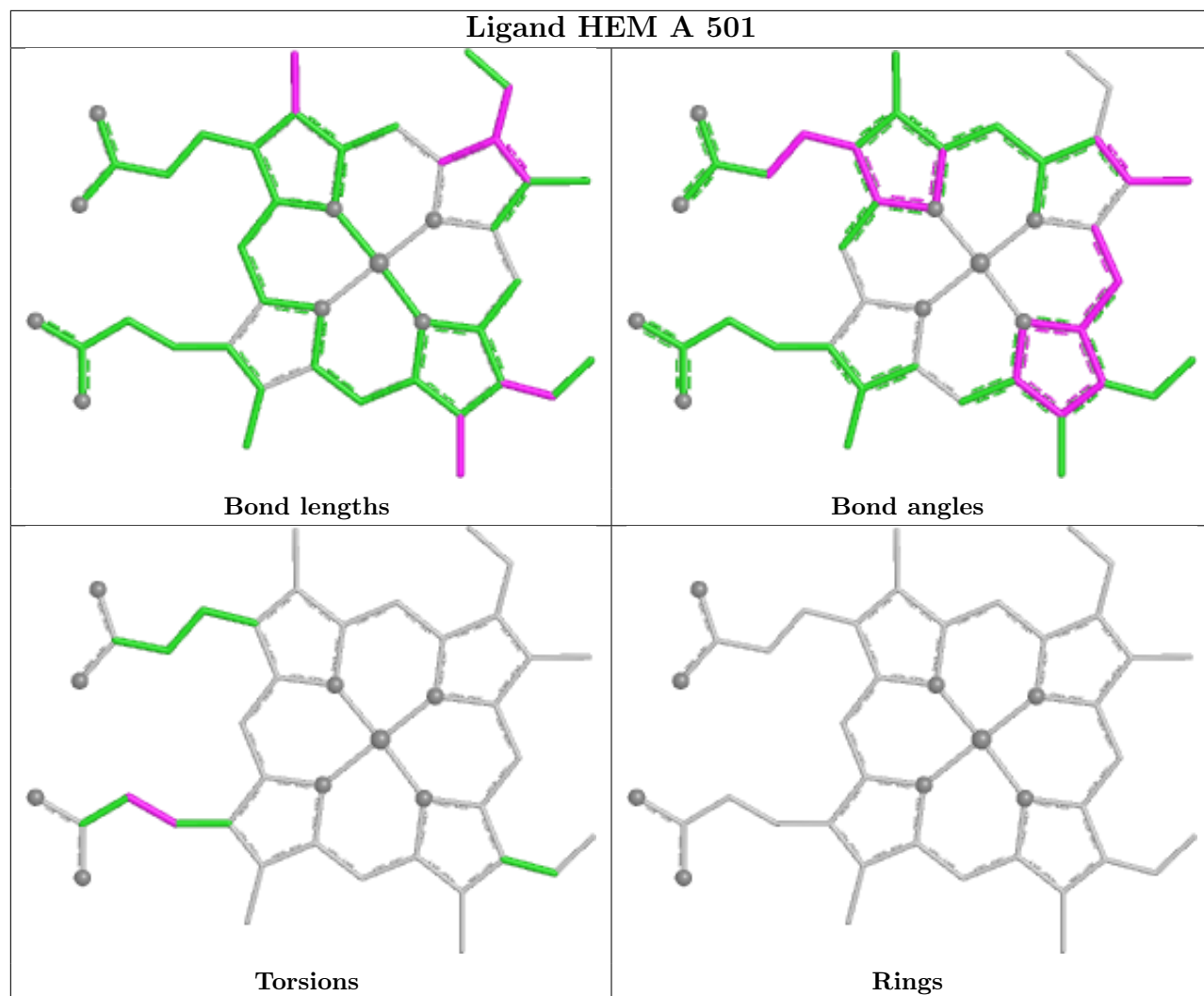


## Ligand A1BU3 A 503

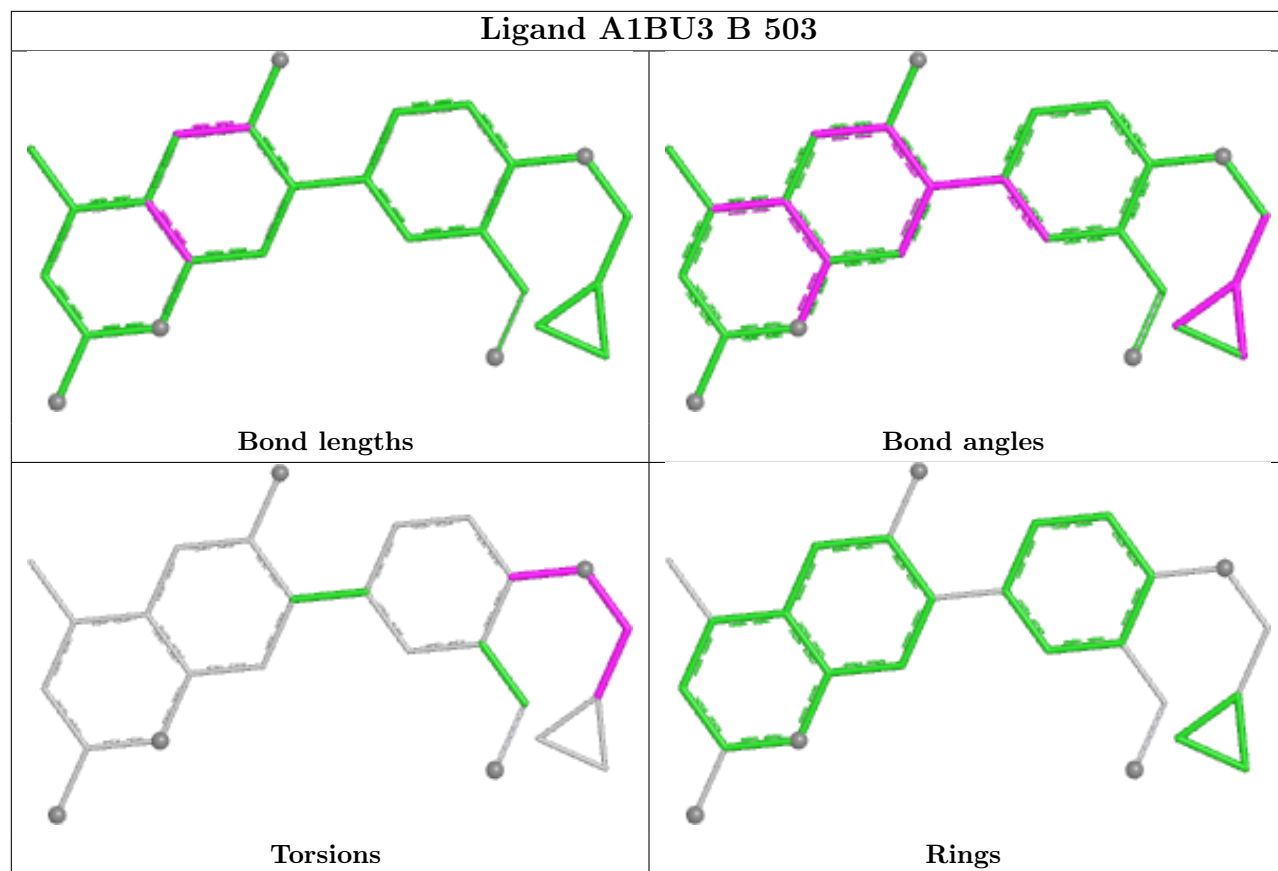


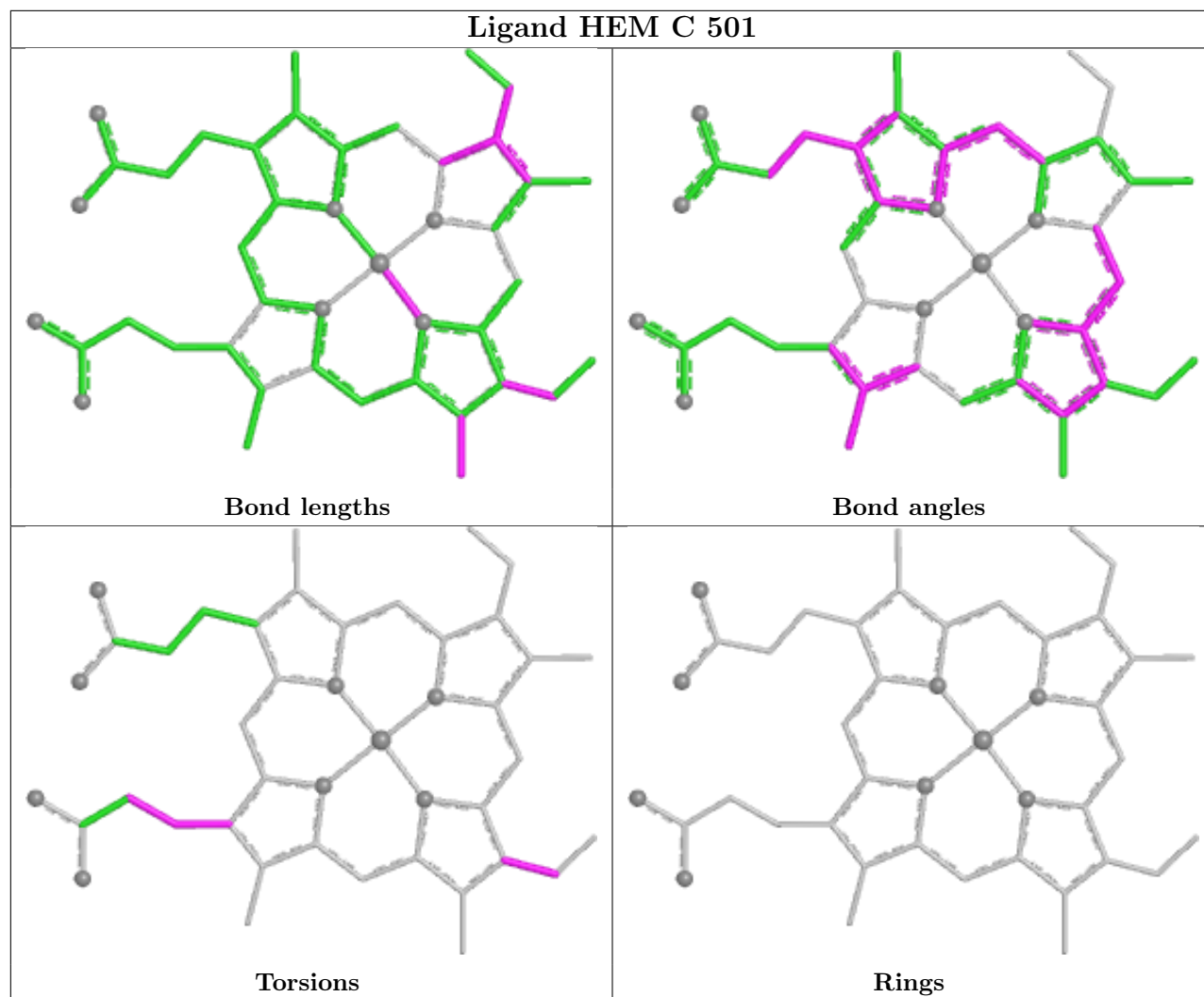
## Ligand A1BU3 C 503

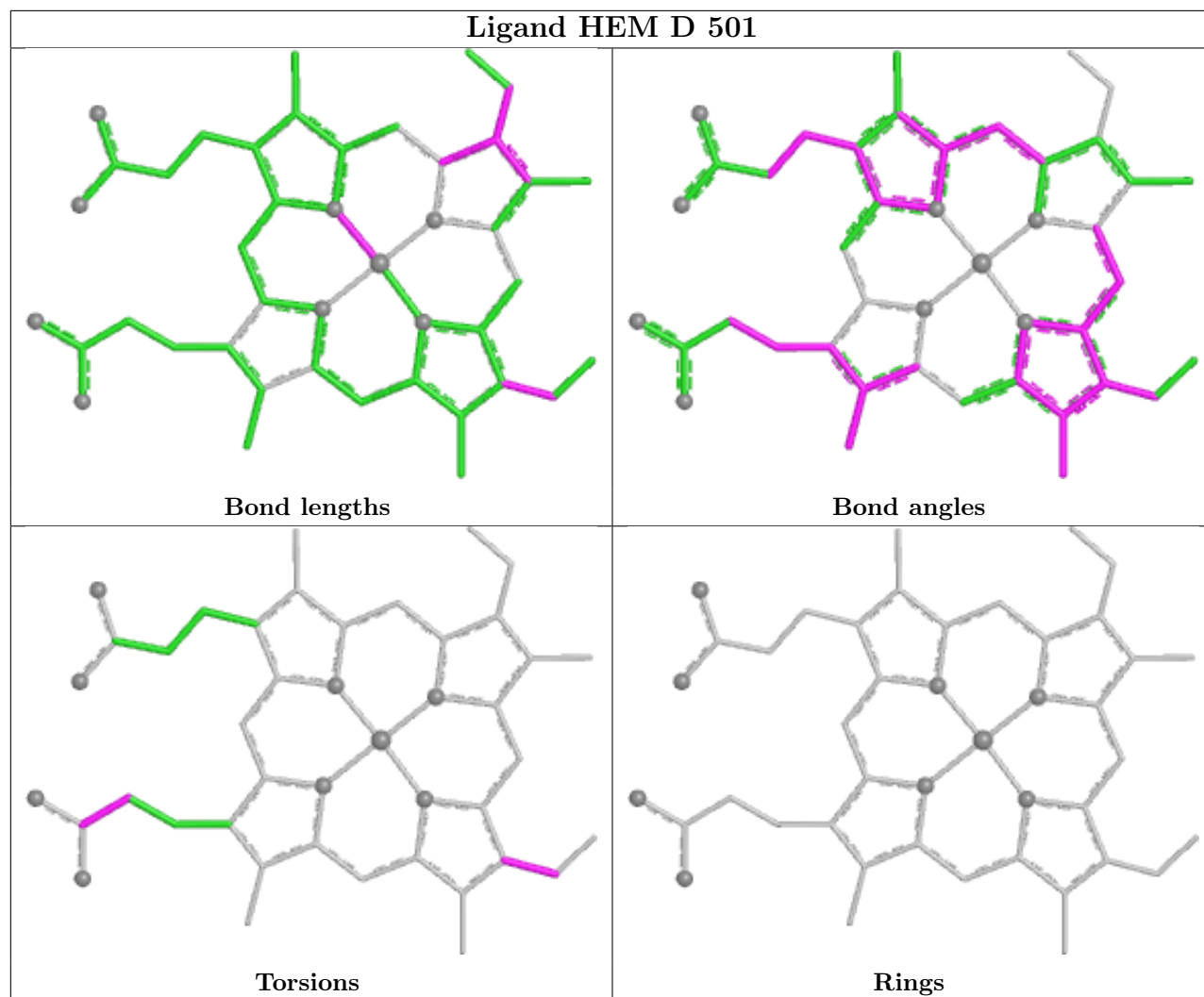


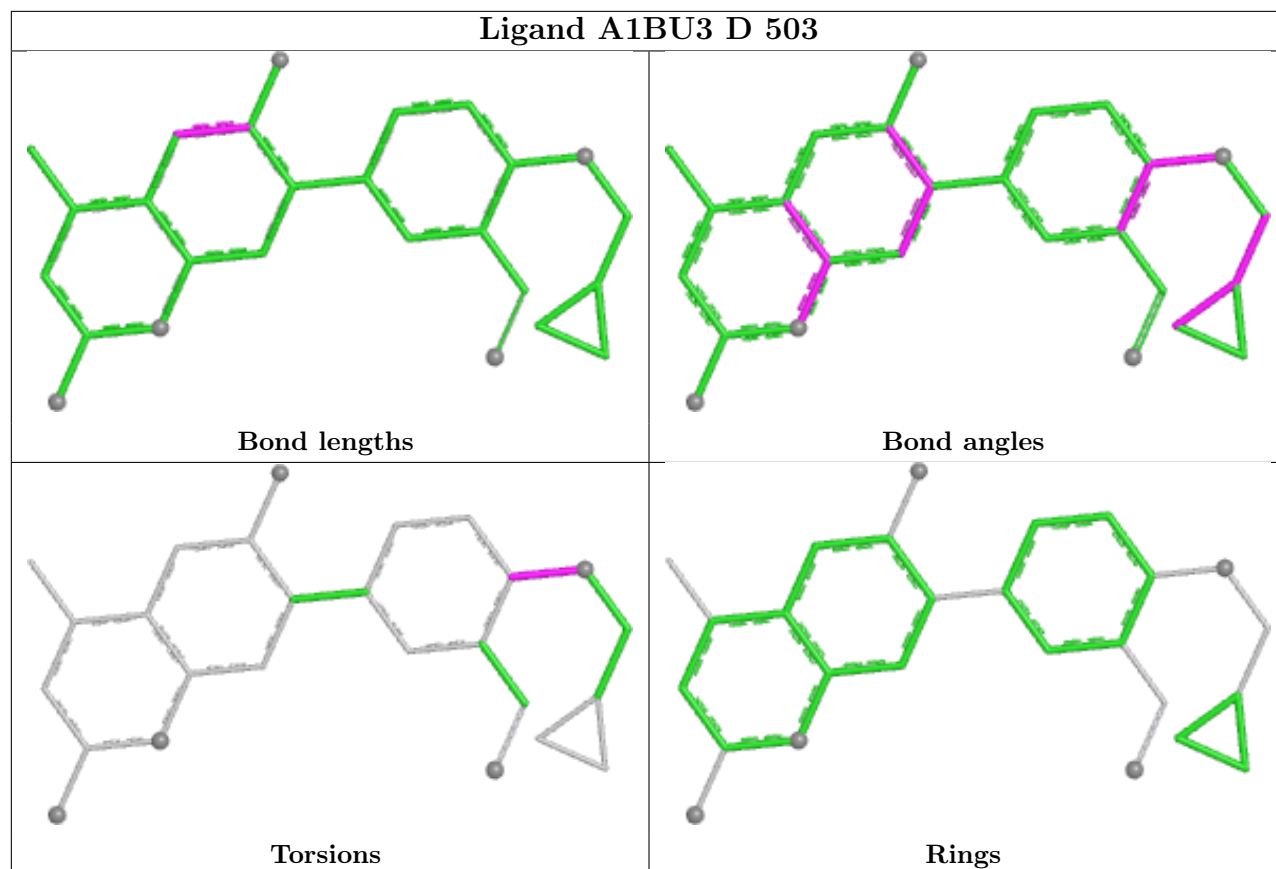


## Ligand A1BU3 B 503









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	403/440 (91%)	-0.92	0	100	100	26, 54, 96, 134	1 (0%)
1	B	403/440 (91%)	-1.08	0	100	100	27, 43, 75, 117	2 (0%)
1	C	401/440 (91%)	-0.69	1 (0%)	92	94	25, 61, 113, 153	1 (0%)
1	D	402/440 (91%)	-1.07	0	100	100	22, 44, 82, 125	3 (0%)
All	All	1609/1760 (91%)	-0.94	1 (0%)	92	94	22, 50, 97, 153	7 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	153	VAL	2.0

### 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	508	6/6	0.91	0.06	69,76,78,81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	507	6/6	0.93	0.06	77,85,85,90	0
6	GOL	C	507	6/6	0.95	0.04	76,82,84,84	0
6	GOL	D	506	6/6	0.95	0.05	76,81,83,86	0
6	GOL	B	506	6/6	0.95	0.05	83,84,87,88	0
5	BTB	B	505	14/14	0.96	0.05	78,88,98,99	0
5	BTB	D	505	14/14	0.96	0.05	58,75,85,86	0
6	GOL	C	506	6/6	0.96	0.05	64,84,87,89	0
5	BTB	C	505	14/14	0.98	0.04	63,77,78,80	0
3	H4B	B	502	17/17	0.98	0.05	42,51,60,65	0
6	GOL	A	506	6/6	0.98	0.04	53,60,65,67	0
3	H4B	C	502	17/17	0.98	0.05	45,59,69,77	0
4	A1BU3	A	503	26/26	0.98	0.06	39,54,65,69	0
4	A1BU3	C	503	26/26	0.98	0.07	45,72,85,90	0
5	BTB	A	505	14/14	0.98	0.05	25,66,77,78	0
3	H4B	A	502	17/17	0.98	0.06	43,58,72,75	0
5	BTB	C	504	14/14	0.98	0.06	72,87,95,100	0
4	A1BU3	D	503	26/26	0.99	0.05	29,47,82,86	0
5	BTB	A	504	14/14	0.99	0.04	27,66,77,80	0
3	H4B	D	502	17/17	0.99	0.04	38,50,60,63	0
6	GOL	A	508	6/6	0.99	0.06	53,76,79,81	0
5	BTB	B	504	14/14	0.99	0.04	40,73,86,89	0
2	HEM	C	501	43/43	0.99	0.05	40,53,74,85	0
4	A1BU3	B	503	26/26	0.99	0.05	28,39,74,76	0
2	HEM	A	501	43/43	0.99	0.04	25,44,69,76	0
6	GOL	D	507	6/6	0.99	0.07	64,70,72,73	0
5	BTB	D	504	14/14	0.99	0.05	31,60,82,96	0
7	CL	A	509	1/1	0.99	0.03	51,51,51,51	0
7	CL	C	508	1/1	0.99	0.05	55,55,55,55	0
2	HEM	D	501	43/43	1.00	0.03	20,31,49,79	0
7	CL	B	507	1/1	1.00	0.03	50,50,50,50	0
2	HEM	B	501	43/43	1.00	0.03	22,31,65,76	0
7	CL	D	509	1/1	1.00	0.02	48,48,48,48	0
8	GD	A	510	1/1	1.00	0.02	88,88,88,88	0
8	GD	B	508	1/1	1.00	0.01	51,51,51,51	0
8	GD	C	509	1/1	1.00	0.01	102,102,102,102	0
8	GD	D	510	1/1	1.00	0.01	46,46,46,46	0
9	ZN	A	511	1/1	1.00	0.02	37,37,37,37	0
9	ZN	C	510	1/1	1.00	0.01	45,45,45,45	0
10	CA	A	512	1/1	1.00	0.02	52,52,52,52	0
10	CA	B	509	1/1	1.00	0.03	45,45,45,45	0

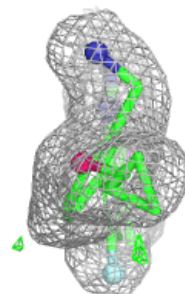
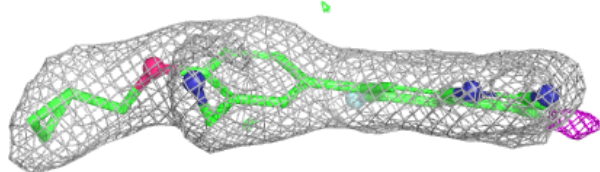
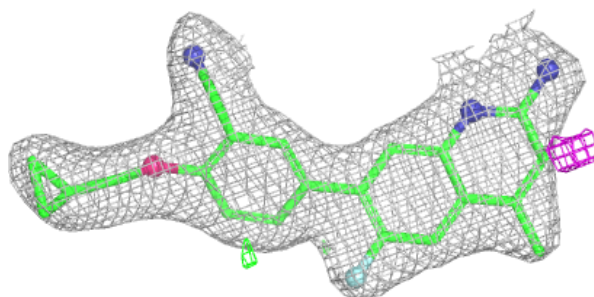
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

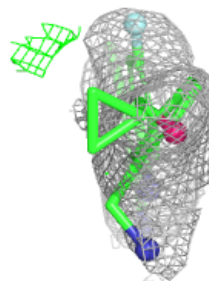
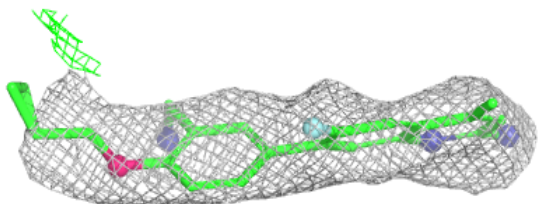
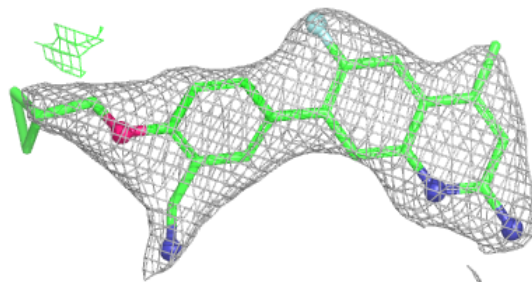
**Electron density around A1BU3 A 503:**

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



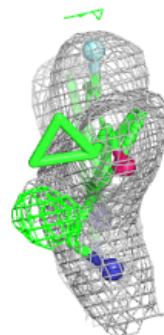
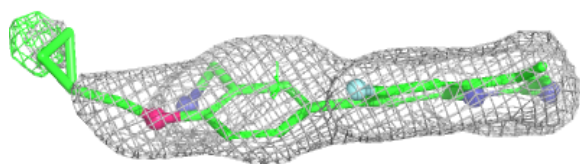
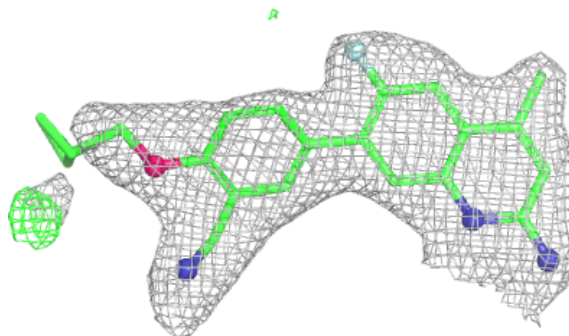
**Electron density around A1BU3 C 503:**

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



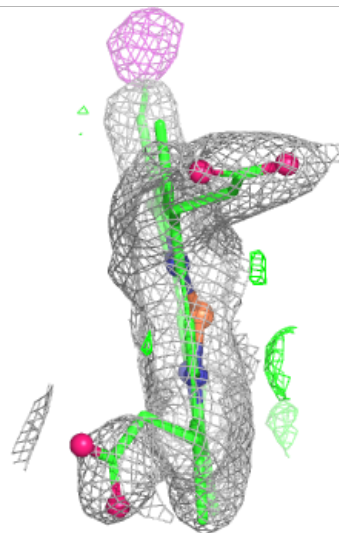
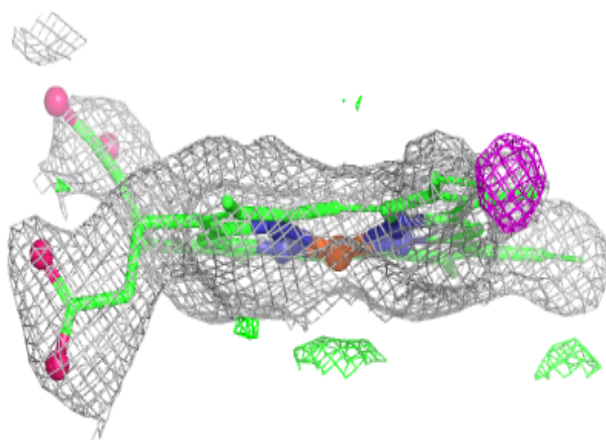
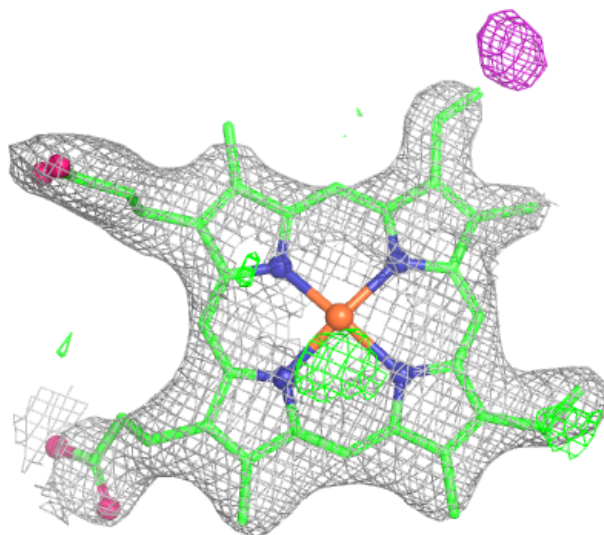
**Electron density around A1BU3 D 503:**

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



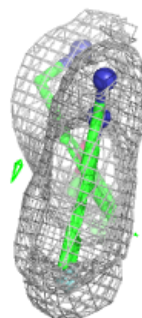
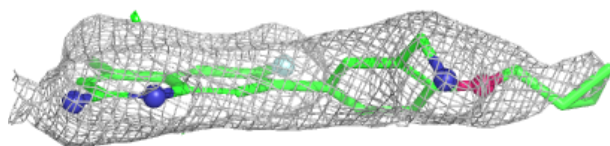
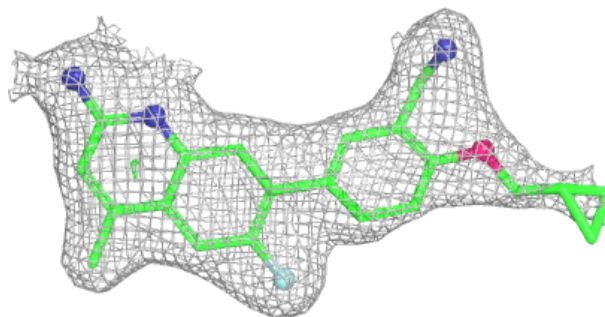
**Electron density around HEM C 501:**

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and green (positive)



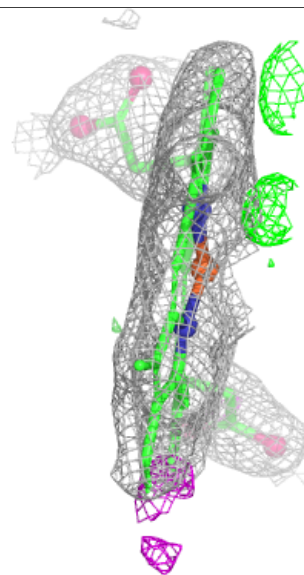
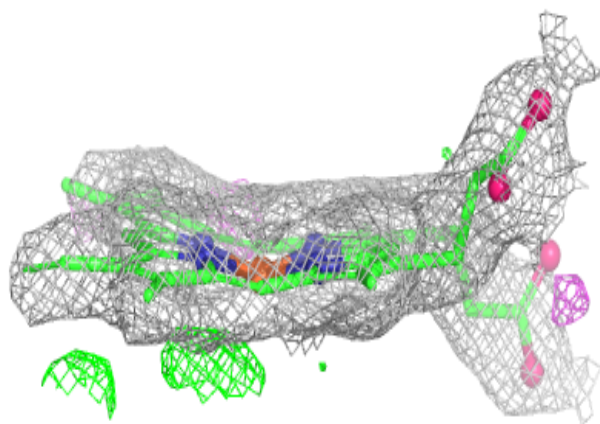
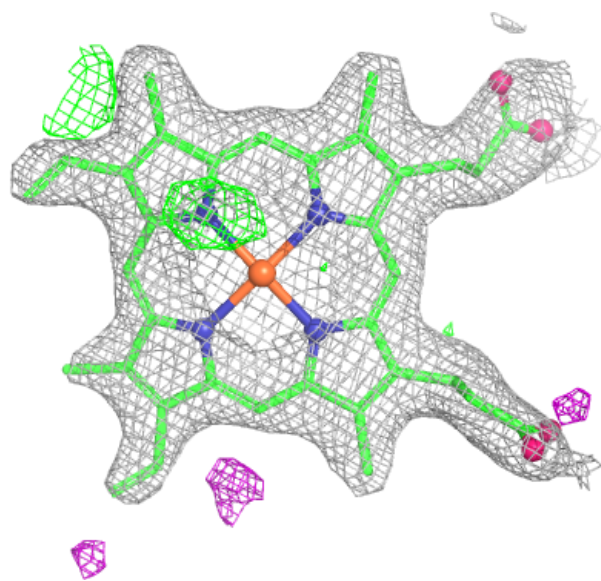
**Electron density around A1BU3 B 503:**

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



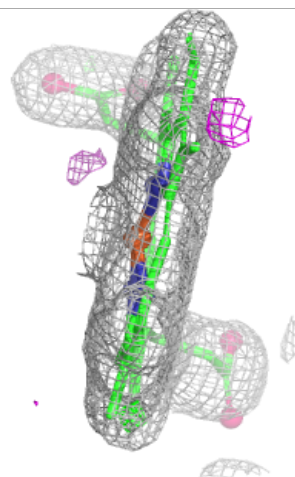
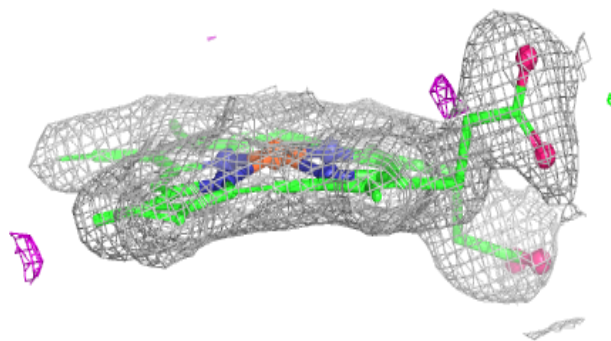
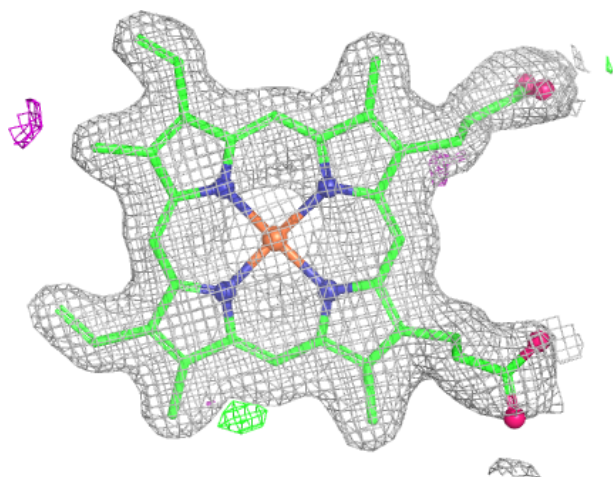
**Electron density around HEM A 501:**

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



**Electron density around HEM D 501:**

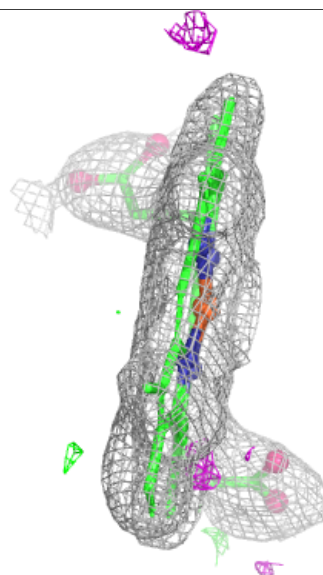
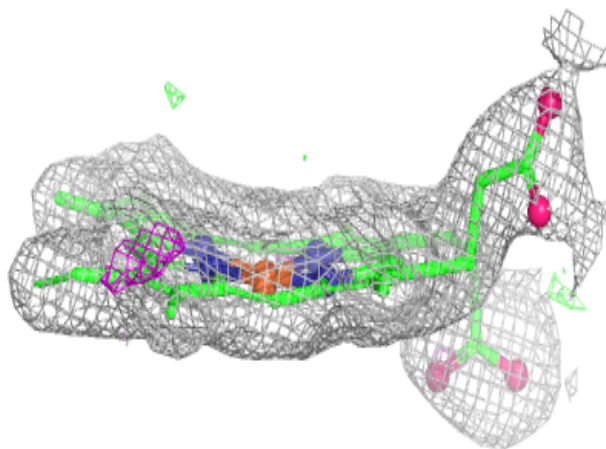
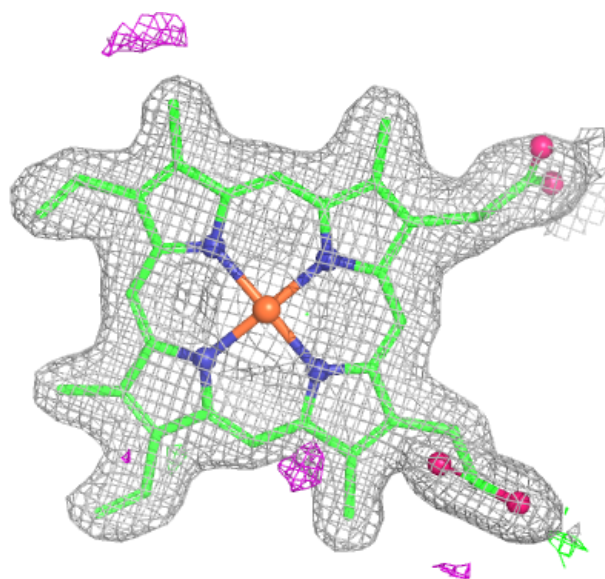
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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.