



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 12:19 PM EDT

PDB ID : 9Q52 / pdb\_00009q52  
Title : Structure of human endothelial nitric oxide synthase heme domain bound with 6-((5-(2-(azetidin-1-yl)ethyl)-2,3-difluorophenxy)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2025-08-20  
Resolution : 2.25 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

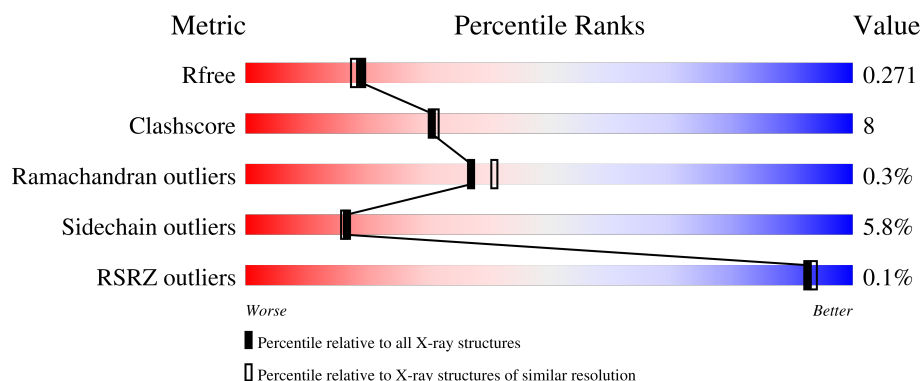
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	440	
1	C	440	
1	D	440	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13527 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	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	B	401	Total	C	N	O	S	0	3	0
			3211	2045	564	586	16			
1	C	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			
1	D	402	Total	C	N	O	S	0	1	0
			3214	2046	567	585	16			

There are 4 discrepancies between the modelled and reference sequences:

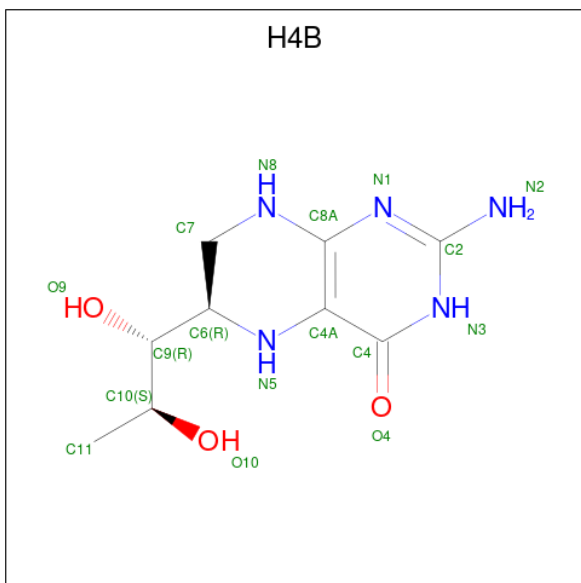
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	conflict	UNP P29474
B	298	GLU	ASP	conflict	UNP P29474
C	298	GLU	ASP	conflict	UNP P29474
D	298	GLU	ASP	conflict	UNP P29474

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



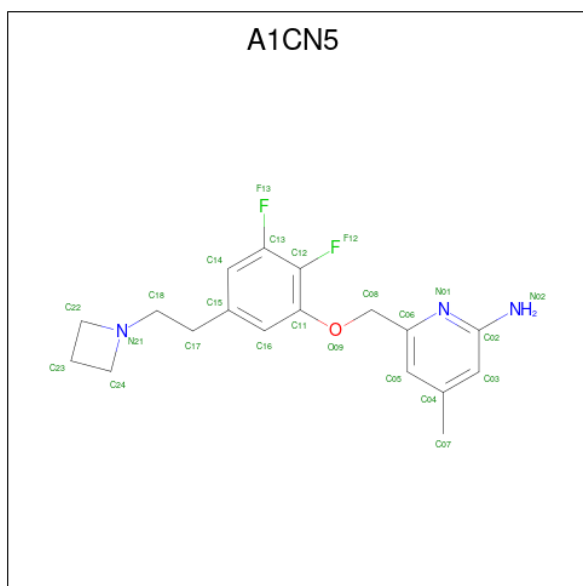
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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 6-({5-[2-(azetidin-1-yl)ethyl]-2,3-difluorophenoxy}methyl)-4-methylpyridin-2-amine (CCD ID: A1CN5) (formula: C<sub>18</sub>H<sub>21</sub>F<sub>2</sub>N<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
			24	18	2	3	1		
4	B	1	Total	C	F	N	O	0	0
			24	18	2	3	1		
4	C	1	Total	C	F	N	O	0	0
			24	18	2	3	1		
4	D	1	Total	C	F	N	O	0	0
			24	18	2	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	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	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	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	C	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 1	Gd 1	0	0
8	B	1	Total 1	Gd 1	0	0
8	C	1	Total 1	Gd 1	0	0
8	D	1	Total 1	Gd 1	0	0

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

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

- Molecule 10 is water.

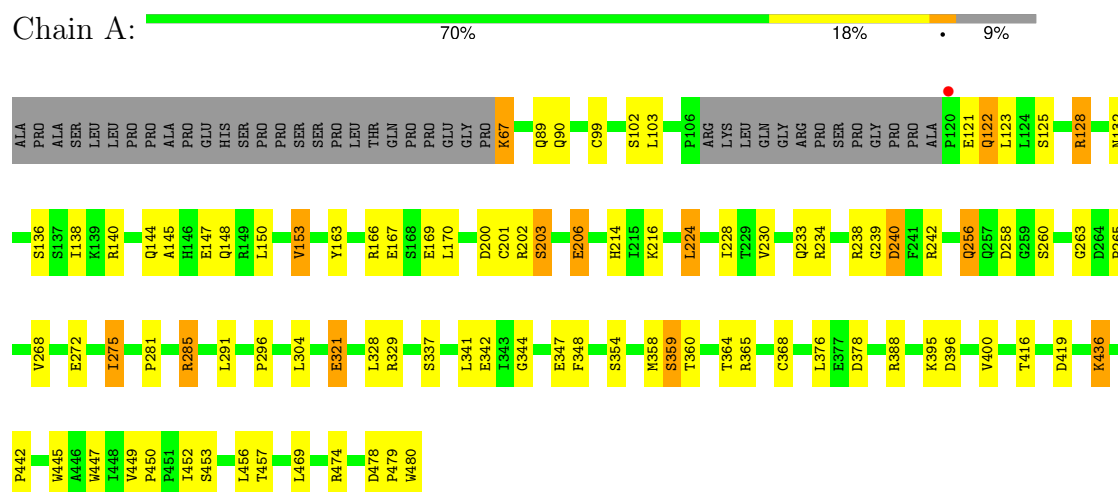
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	30	Total 30	O 30	0	0
10	B	47	Total 47	O 47	0	0
10	C	33	Total 33	O 33	0	0
10	D	45	Total 45	O 45	0	0



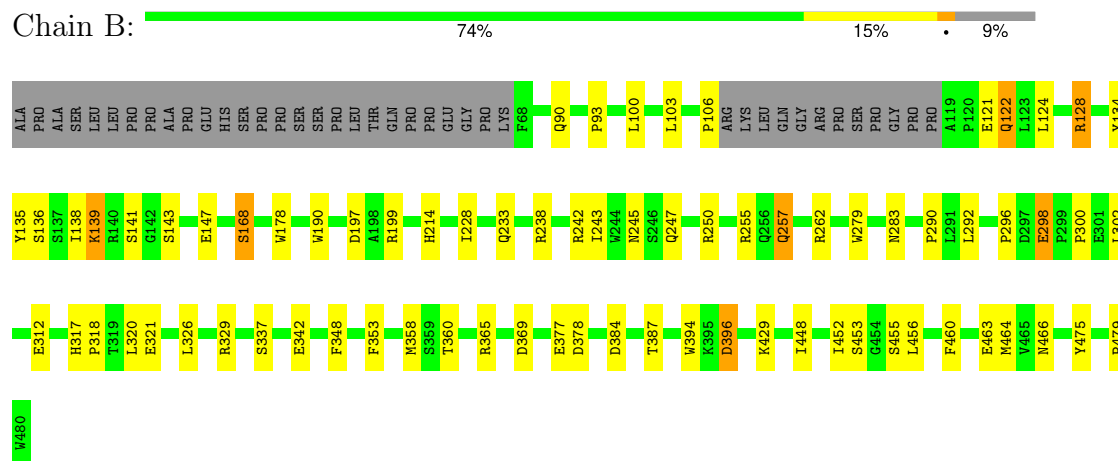
### 3 Residue-property plots

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

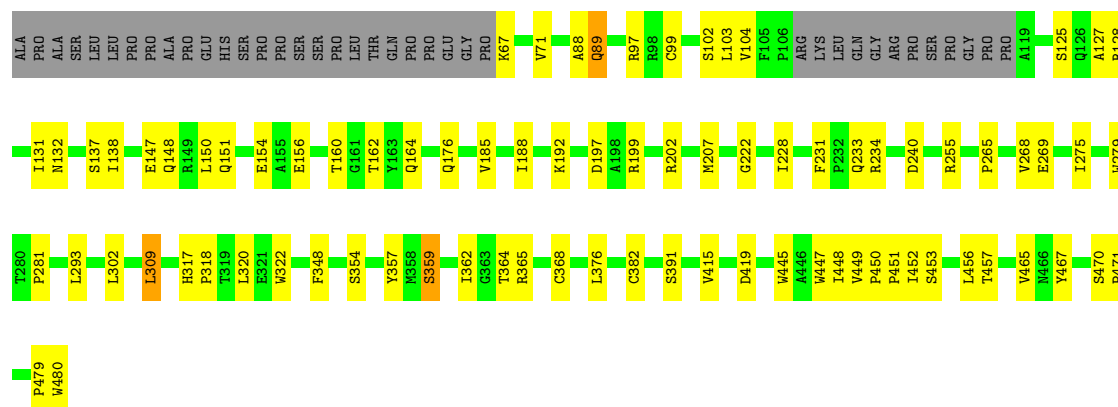


#### • Molecule 1: Nitric oxide synthase 3

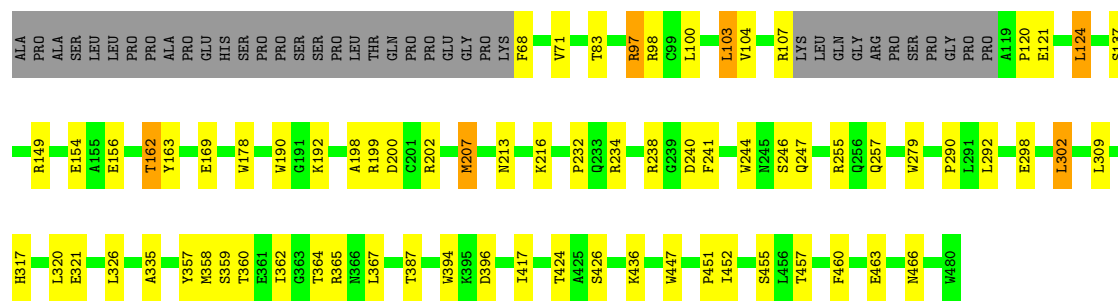


#### • Molecule 1: Nitric oxide synthase 3





- 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, $\alpha$ , $\beta$ , $\gamma$	59.59Å 152.63Å 108.62Å 90.00° 90.64° 90.00°	Depositor
Resolution (Å)	49.22 – 2.25 49.22 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.22-2.25) 96.2 (49.22-2.25)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.211 , 0.275 0.206 , 0.271	Depositor DCC
$R_{free}$ test set	4583 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	1.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.187 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: H4B, GD, BTB, ZN, CL, HEM, A1CN5, GOL

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	0/3302	0.51	0/4498
1	B	0.35	0/3312	0.54	0/4514
1	C	0.31	0/3307	0.50	0/4506
1	D	0.37	0/3309	0.58	0/4509
All	All	0.33	0/13230	0.53	0/18027

There are no bond length outliers.

There are no bond angle outliers.

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	3207	0	3112	54	0
1	B	3211	0	3114	48	0
1	C	3212	0	3116	47	0
1	D	3214	0	3116	44	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
3	A	17	0	15	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
3	C	17	0	15	4	0
3	D	17	0	15	1	0
4	A	24	0	0	0	0
4	B	24	0	0	1	0
4	C	24	0	0	1	0
4	D	24	0	0	1	0
5	A	42	0	56	6	0
5	B	28	0	36	8	0
5	C	42	0	55	5	0
5	D	28	0	36	4	0
6	A	12	0	16	1	0
6	B	6	0	8	0	0
6	C	24	0	32	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	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	30	0	0	2	0
10	B	47	0	0	1	0
10	C	33	0	0	1	0
10	D	45	0	0	2	0
All	All	13527	0	12877	216	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 (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ALA:HB3	1:D:97:ARG:HD2	1.54	0.88
5:B:504:BTB:O3	10:B:601:HOH:O	2.00	0.78
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.64	0.78
1:C:365:ARG:NH1	3:C:502:H4B:N3	2.35	0.75
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:NH2	10:D:601:HOH:O	2.21	0.73
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.70	0.73
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.71	0.71
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.72	0.71
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.05	0.69
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.04	0.69
1:C:128:ARG:O	1:C:132:ASN:ND2	2.27	0.68
1:A:321:GLU:H	1:A:321:GLU:CD	2.02	0.67
2:A:501:HEM:HHA	2:A:501:HEM:HBA1	1.77	0.66
1:D:124:LEU:HD11	1:D:154:GLU:HG3	1.77	0.66
1:C:160:THR:HG23	1:C:162:THR:H	1.61	0.66
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.77	0.65
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.79	0.65
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.79	0.64
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.13	0.64
1:C:99:CYS:HB3	1:D:466:ASN:HB3	1.79	0.64
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.80	0.63
1:C:453:SER:HA	1:D:452:ILE:HG22	1.80	0.62
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.81	0.62
5:B:505:BTB:O3	5:B:505:BTB:O6	2.17	0.62
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.81	0.61
1:C:234:ARG:NH2	1:C:240:ASP:OD2	2.35	0.60
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.37	0.60
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.82	0.60
1:B:136:SER:O	1:B:139:LYS:NZ	2.30	0.59
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.84	0.59
1:C:376:LEU:HB2	10:C:609:HOH:O	2.04	0.58
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.40	0.57
1:A:89:GLN:HG3	1:A:90:GLN:H	1.69	0.56
1:B:292:LEU:HD22	1:B:300:PRO:HB2	1.87	0.56
1:C:156:GLU:O	1:C:160:THR:HG22	2.05	0.56
1:C:382:CYS:HA	5:C:504:BTB:H11	1.88	0.56
1:B:298:GLU:OE2	5:B:505:BTB:O8	2.10	0.56
1:D:387:THR:HA	1:D:394:TRP:CD1	2.41	0.56
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.87	0.55
1:B:124:LEU:HB3	1:B:128:ARG:HH22	1.70	0.55
1:B:257:GLN:H	1:B:257:GLN:CD	2.15	0.55
1:C:156:GLU:OE2	1:C:164:GLN:HG2	2.06	0.55
2:B:501:HEM:O2D	2:B:501:HEM:HHA	2.07	0.54
1:A:128:ARG:O	1:A:132:ASN:ND2	2.40	0.54
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.43	0.54
1:C:467:TYR:HB3	1:D:98:ARG:HB3	1.89	0.54
1:C:102:SER:O	3:C:502:H4B:O10	2.18	0.53
1:A:99:CYS:HB3	1:B:466:ASN:HB3	1.91	0.53
1:B:134:TYR:OH	1:B:168[B]:SER:HB2	2.09	0.53
1:B:134:TYR:OH	1:B:168[A]:SER:HB3	2.07	0.53
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.91	0.53
1:A:238:ARG:NH2	1:A:240:ASP:HA	2.23	0.53
1:B:312:GLU:CD	1:B:329:ARG:HH21	2.17	0.52
1:D:358:MET:HE3	1:D:360:THR:OG1	2.09	0.52
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.91	0.52
1:A:166:ARG:HB2	1:A:169:GLU:CD	2.34	0.52
5:A:505:BTB:O4	5:A:505:BTB:O3	2.24	0.52
1:C:382:CYS:HA	5:C:504:BTB:C1	2.39	0.52
1:D:149:ARG:NH2	1:D:169:GLU:OE1	2.43	0.52
2:C:501:HEM:HBD1	4:C:503:A1CN5:F12	1.99	0.51
1:C:185:VAL:HG23	1:C:448:ILE:HG23	1.93	0.51
1:D:162:THR:OG1	1:D:163:TYR:N	2.42	0.51
2:A:501:HEM:HAD1	10:A:620:HOH:O	2.10	0.51
1:C:104:VAL:HG13	1:C:447:TRP:HH2	1.76	0.51
1:D:321:GLU:OE1	5:D:504:BTB:O8	2.28	0.51
1:A:167:GLU:OE2	6:A:507:GOL:H2	2.11	0.51
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.93	0.51
1:B:122:GLN:CD	1:B:122:GLN:H	2.18	0.51
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.93	0.51
1:D:455:SER:HA	1:D:460:PHE:CG	2.45	0.50
5:B:504:BTB:O3	5:B:504:BTB:O4	2.15	0.50
2:A:501:HEM:HBA1	2:A:501:HEM:CHA	2.40	0.50
1:A:103:LEU:HD12	1:B:463:GLU:HB3	1.93	0.50
1:B:143:SER:O	1:B:147:GLU:HG2	2.12	0.50
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.93	0.49
1:A:145:ALA:HA	1:A:148:GLN:HB2	1.94	0.49
1:A:256:GLN:HB3	1:A:258:ASP:H	1.78	0.49
1:D:298:GLU:CD	5:D:505:BTB:H41	2.38	0.49
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.48	0.49
1:D:298:GLU:OE1	5:D:505:BTB:H52	2.12	0.49
1:D:244:TRP:HB2	1:D:292:LEU:HB2	1.95	0.48
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.49	0.48
1:A:224:LEU:HB2	1:A:416:THR:HB	1.96	0.48
1:A:378:ASP:OD1	10:A:601:HOH:O	2.20	0.48
1:D:357:TYR:CD2	1:D:362:ILE:HD11	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.47	0.48
5:A:506:BTB:H11	5:A:506:BTB:H51	1.71	0.48
1:B:321:GLU:OE1	5:B:504:BTB:O8	2.32	0.48
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.29	0.47
1:B:396:ASP:OD1	1:B:396:ASP:N	2.44	0.47
1:A:453:SER:HA	1:B:452:ILE:HG22	1.95	0.47
1:C:176:GLN:HB2	1:C:471:PRO:HG2	1.96	0.47
1:A:445:TRP:CZ2	1:A:449:VAL:HG21	2.49	0.47
1:B:124:LEU:O	1:B:128:ARG:NH1	2.48	0.47
1:B:358:MET:HE3	1:B:360:THR:OG1	2.15	0.47
2:B:501:HEM:HBD1	4:B:503:A1CN5:F12	2.04	0.47
1:A:102:SER:O	3:A:502:H4B:O10	2.28	0.47
5:B:505:BTB:H11	5:B:505:BTB:H51	1.67	0.47
1:C:265:PRO:O	1:C:268:VAL:HG23	2.14	0.47
1:B:365:ARG:HH12	3:B:502:H4B:C4	2.28	0.47
1:D:100:LEU:HB3	1:D:103:LEU:HD13	1.97	0.47
1:B:250:ARG:HD2	1:B:250:ARG:HA	1.70	0.47
1:C:197:ASP:CG	1:C:199:ARG:HH21	2.23	0.47
1:A:436:LYS:HE3	1:A:436:LYS:HB2	1.68	0.46
1:B:121:GLU:HA	1:B:124:LEU:HD12	1.97	0.46
1:A:67:LYS:HE2	1:A:67:LYS:HB3	1.64	0.46
1:C:309:LEU:HD23	1:C:309:LEU:HA	1.71	0.46
1:B:128:ARG:NH1	1:B:128:ARG:HB2	2.31	0.46
1:B:245:ASN:O	1:B:337:SER:OG	2.33	0.46
3:A:502:H4B:H113	1:B:463:GLU:HG2	1.97	0.46
1:B:448:ILE:HG21	1:B:464:MET:HE1	1.98	0.46
1:A:89:GLN:HG3	1:A:90:GLN:N	2.29	0.45
1:C:451:PRO:HB2	1:D:455:SER:OG	2.16	0.45
1:D:156:GLU:CD	1:D:163:TYR:HA	2.41	0.45
1:A:200:ASP:OD1	1:A:200:ASP:N	2.42	0.45
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.51	0.45
5:C:506:BTB:H62	5:C:506:BTB:O8	2.17	0.45
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.57	0.45
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.97	0.45
2:D:501:HEM:HHA	2:D:501:HEM:O2D	2.17	0.45
1:B:243:ILE:HG21	1:B:337:SER:HB2	1.97	0.45
1:B:262:ARG:NE	1:B:283:ASN:O	2.34	0.45
1:B:455:SER:HA	1:B:460:PHE:CG	2.52	0.45
1:C:447:TRP:CD1	1:C:447:TRP:N	2.85	0.45
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.99	0.45
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:TRP:CE2	1:A:449:VAL:HG21	2.52	0.45
1:A:442:PRO:HG3	1:A:469:LEU:HD12	1.99	0.45
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.98	0.45
1:D:364:THR:HG21	1:D:451:PRO:HB2	1.98	0.45
1:D:247:GLN:HA	1:D:335:ALA:O	2.17	0.44
1:B:228:ILE:HD12	1:B:353:PHE:HB3	2.00	0.44
1:C:447:TRP:CZ2	3:C:502:H4B:H6	2.53	0.44
5:A:505:BTB:H41	5:A:505:BTB:H72	1.70	0.44
1:C:320:LEU:HD13	1:C:322:TRP:CZ2	2.53	0.44
1:C:103:LEU:HA	1:D:463:GLU:HG2	1.99	0.44
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.99	0.43
1:D:198:ALA:O	1:D:232:PRO:HD3	2.18	0.43
1:B:279:TRP:CG	1:B:290:PRO:HG3	2.53	0.43
1:A:138:ILE:HG13	1:A:140:ARG:HB2	2.00	0.43
1:A:202:ARG:O	1:A:203:SER:HB3	2.17	0.43
5:B:504:BTB:H82	5:B:504:BTB:H41	2.01	0.43
1:D:216:LYS:HB3	1:D:216:LYS:HE2	1.74	0.43
1:D:216:LYS:HB2	1:D:309:LEU:HD11	2.01	0.43
5:B:505:BTB:H42	5:B:505:BTB:H72	1.40	0.43
1:C:465:VAL:HG12	1:C:467:TYR:HD1	1.84	0.43
1:C:359:SER:OG	1:C:419:ASP:HA	2.19	0.43
5:C:505:BTB:O4	5:C:505:BTB:H51	2.13	0.43
1:A:163:TYR:OH	1:A:344:GLY:O	2.31	0.43
1:B:429:LYS:HD2	1:B:429:LYS:HA	1.81	0.43
1:A:358:MET:HE3	1:A:360:THR:OG1	2.18	0.43
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.59	0.43
1:B:135:TYR:HA	1:B:138:ILE:HG12	2.01	0.43
1:A:359:SER:OG	1:A:419:ASP:HA	2.19	0.42
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.59	0.42
1:C:89:GLN:HG3	1:C:470:SER:HB2	2.00	0.42
1:D:234:ARG:NH2	1:D:240:ASP:OD2	2.34	0.42
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.38	0.42
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.54	0.42
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.53	0.42
1:A:214:HIS:HE1	1:A:228:ILE:HA	1.85	0.42
1:B:197:ASP:OD2	1:B:199:ARG:NH2	2.41	0.42
1:D:367:LEU:HD23	1:D:367:LEU:HA	1.83	0.42
1:A:240:ASP:H	1:A:296:PRO:HA	1.83	0.42
1:D:292:LEU:HD23	1:D:302:LEU:HD13	2.02	0.42
1:A:122:GLN:H	1:A:122:GLN:HG3	1.57	0.42
1:A:238:ARG:HG2	1:A:239:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.55	0.42
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.32	0.42
1:C:445:TRP:CZ2	1:C:449:VAL:HG21	2.54	0.42
2:D:501:HEM:HBD1	4:D:503:A1CN5:F12	2.10	0.42
1:C:255:ARG:NH1	1:C:268:VAL:HG11	2.34	0.42
5:A:505:BTB:H51	5:A:505:BTB:H11	1.29	0.42
1:D:365:ARG:HH12	3:D:502:H4B:C4	2.32	0.42
1:A:328:LEU:C	1:A:329:ARG:HG3	2.45	0.42
5:C:505:BTB:H32	5:C:505:BTB:H72	1.82	0.42
1:D:68:PHE:CE1	1:D:83:THR:HG22	2.55	0.42
1:D:107:ARG:HA	10:D:617:HOH:O	2.20	0.42
1:A:147:GLU:HA	1:A:150:LEU:HD12	2.02	0.41
1:B:365:ARG:O	1:B:369:ASP:HB2	2.21	0.41
1:A:341:LEU:HB3	1:A:348:PHE:HB2	2.03	0.41
1:A:364:THR:O	1:A:368:CYS:HB2	2.19	0.41
1:D:213:ASN:HA	1:D:216:LYS:HE2	2.01	0.41
1:A:376:LEU:HD23	1:A:395:LYS:HG2	2.02	0.41
1:D:255:ARG:HA	1:D:255:ARG:HD2	1.87	0.41
1:C:147:GLU:HA	1:C:150:LEU:HD12	2.02	0.41
1:D:292:LEU:CD2	1:D:302:LEU:HD13	2.50	0.41
1:A:242:ARG:HG3	1:A:479:PRO:HB3	2.02	0.41
1:B:317:HIS:HB3	1:B:320:LEU:O	2.21	0.41
1:C:450:PRO:HG3	1:C:457:THR:HG21	2.02	0.41
1:D:207:MET:HE3	1:D:241:PHE:HB3	2.03	0.41
1:D:290:PRO:HG2	1:D:302:LEU:HD11	2.00	0.41
1:A:447:TRP:CD1	1:A:447:TRP:N	2.88	0.41
1:C:127:ALA:O	1:C:131:ILE:HG12	2.21	0.41
2:C:501:HEM:HHA	2:C:501:HEM:HBA2	2.02	0.41
1:A:238:ARG:HG2	1:A:239:GLY:N	2.36	0.41
5:A:506:BTB:H72	5:A:506:BTB:H41	1.55	0.41
1:B:214:HIS:CD2	1:B:214:HIS:C	2.98	0.41
1:B:387:THR:HA	1:B:394:TRP:CD1	2.57	0.40
1:D:104:VAL:HG22	1:D:447:TRP:CZ2	2.55	0.40
1:D:317:HIS:HB3	1:D:320:LEU:O	2.20	0.40
1:D:424:THR:OG1	1:D:457:THR:HB	2.22	0.40
1:A:150:LEU:O	1:A:153:VAL:HG23	2.20	0.40
1:B:453:SER:HB3	1:B:456:LEU:HD12	2.02	0.40
1:C:364:THR:HG21	1:C:452:ILE:HG23	2.02	0.40
1:D:98:ARG:O	1:D:98:ARG:HD2	2.20	0.40
1:A:263:GLY:H	1:A:285:ARG:HG3	1.84	0.40
1:A:396:ASP:O	1:A:400:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ASP:O	1:A:480:TRP:N	2.47	0.40
5:A:504:BTB:H32	5:A:504:BTB:H51	1.67	0.40
1:C:188:ILE:HD12	1:C:188:ILE:HA	1.93	0.40
1:D:199:ARG:O	1:D:232:PRO:HG3	2.21	0.40
1:C:222:GLY:O	1:C:415:VAL:HA	2.22	0.40
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.57	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	398/440 (90%)	376 (94%)	19 (5%)	3 (1%)	16	14
1	B	400/440 (91%)	381 (95%)	19 (5%)	0	100	100
1	C	399/440 (91%)	379 (95%)	20 (5%)	0	100	100
1	D	399/440 (91%)	385 (96%)	13 (3%)	1 (0%)	37	41
All	All	1596/1760 (91%)	1521 (95%)	71 (4%)	4 (0%)	37	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	SER
1	A	144	GLN
1	A	260	SER
1	D	120	PRO

### 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	342/373 (92%)	316 (92%)	26 (8%)	11	9
1	B	343/373 (92%)	326 (95%)	17 (5%)	20	22
1	C	342/373 (92%)	324 (95%)	18 (5%)	19	19
1	D	342/373 (92%)	322 (94%)	20 (6%)	17	16
All	All	1369/1492 (92%)	1288 (94%)	81 (6%)	17	15

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	121	GLU
1	A	122	GLN
1	A	123	LEU
1	A	125	SER
1	A	128	ARG
1	A	136	SER
1	A	153	VAL
1	A	206	GLU
1	A	216	LYS
1	A	224	LEU
1	A	240	ASP
1	A	256	GLN
1	A	272	GLU
1	A	275	ILE
1	A	285	ARG
1	A	291	LEU
1	A	304	LEU
1	A	321	GLU
1	A	337	SER
1	A	342	GLU
1	A	354	SER
1	A	359	SER
1	A	388	ARG
1	A	436	LYS
1	A	474	ARG
1	B	90	GLN
1	B	122	GLN

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Mol	Chain	Res	Type
1	B	128	ARG
1	B	139	LYS
1	B	141[A]	SER
1	B	141[B]	SER
1	B	168[A]	SER
1	B	168[B]	SER
1	B	255	ARG
1	B	257	GLN
1	B	298	GLU
1	B	326	LEU
1	B	342	GLU
1	B	377	GLU
1	B	378	ASP
1	B	384	ASP
1	B	396	ASP
1	C	67	LYS
1	C	71	VAL
1	C	89	GLN
1	C	97	ARG
1	C	125	SER
1	C	137	SER
1	C	138	ILE
1	C	148	GLN
1	C	151	GLN
1	C	154	GLU
1	C	192	LYS
1	C	202	ARG
1	C	228	ILE
1	C	269	GLU
1	C	309	LEU
1	C	354	SER
1	C	359	SER
1	C	391	SER
1	D	71	VAL
1	D	97	ARG
1	D	103	LEU
1	D	121	GLU
1	D	124	LEU
1	D	137	SER
1	D	162	THR
1	D	192	LYS
1	D	200	ASP

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Mol	Chain	Res	Type
1	D	207	MET
1	D	238	ARG
1	D	246	SER
1	D	257	GLN
1	D	302	LEU
1	D	326	LEU
1	D	359	SER
1	D	396	ASP
1	D	417	ILE
1	D	426	SER
1	D	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN
1	B	233	GLN
1	C	89	GLN
1	C	151	GLN
1	C	233	GLN
1	C	466	ASN
1	D	126	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 10 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	A	504	8	13,13,13	0.62	0	7,16,16	1.55	1 (14%)
5	BTB	A	506	-	13,13,13	0.38	0	7,16,16	0.57	0
3	H4B	A	502	-	16,18,18	0.94	0	14,26,26	2.39	6 (42%)
6	GOL	C	507	-	5,5,5	0.32	0	5,5,5	0.32	0
4	A1CN5	D	503	-	24,26,26	0.60	0	29,36,36	1.21	1 (3%)
6	GOL	C	509	-	5,5,5	0.29	0	5,5,5	0.53	0
5	BTB	C	504	8	13,13,13	0.48	0	7,16,16	1.19	0
6	GOL	B	506	-	5,5,5	0.39	0	5,5,5	0.11	0
6	GOL	C	508	-	5,5,5	0.43	0	5,5,5	0.85	0
4	A1CN5	A	503	-	24,26,26	0.46	0	29,36,36	1.33	3 (10%)
5	BTB	C	506	-	13,13,13	0.38	0	7,16,16	0.37	0
4	A1CN5	C	503	-	24,26,26	0.49	0	29,36,36	1.42	3 (10%)
5	BTB	B	505	-	13,13,13	0.55	0	7,16,16	1.07	0
5	BTB	B	504	8	13,13,13	0.49	0	7,16,16	1.08	1 (14%)
4	A1CN5	B	503	-	24,26,26	0.48	0	29,36,36	1.11	4 (13%)
3	H4B	C	502	-	16,18,18	0.90	0	14,26,26	2.25	5 (35%)
2	HEM	C	501	1	42,50,50	1.50	6 (14%)	46,82,82	1.61	7 (15%)
3	H4B	B	502	-	16,18,18	0.86	0	14,26,26	2.61	6 (42%)
5	BTB	D	504	8	13,13,13	0.39	0	7,16,16	0.51	0
2	HEM	B	501	1	42,50,50	1.54	5 (11%)	46,82,82	1.65	10 (21%)
6	GOL	A	508	-	5,5,5	0.36	0	5,5,5	0.39	0
6	GOL	C	510	-	5,5,5	0.36	0	5,5,5	0.32	0
2	HEM	D	501	1	42,50,50	1.42	4 (9%)	46,82,82	1.73	11 (23%)
5	BTB	C	505	-	13,13,13	0.49	0	7,16,16	1.13	0
2	HEM	A	501	1	42,50,50	1.55	7 (16%)	46,82,82	1.60	9 (19%)
5	BTB	D	505	-	13,13,13	0.76	0	7,16,16	1.24	1 (14%)
6	GOL	A	507	-	5,5,5	0.32	0	5,5,5	0.74	0
3	H4B	D	502	-	16,18,18	0.79	0	14,26,26	2.35	4 (28%)
5	BTB	A	505	-	13,13,13	0.51	0	7,16,16	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	A	504	8	-	3/21/21/21	-
5	BTB	A	506	-	-	0/21/21/21	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
6	GOL	C	507	-	-	4/4/4/4	-
4	A1CN5	D	503	-	-	1/8/16/16	0/3/3/3
6	GOL	C	509	-	-	2/4/4/4	-
5	BTB	C	504	8	-	10/21/21/21	-
6	GOL	B	506	-	-	2/4/4/4	-
6	GOL	C	508	-	-	1/4/4/4	-
4	A1CN5	A	503	-	-	0/8/16/16	0/3/3/3
5	BTB	C	506	-	-	3/21/21/21	-
4	A1CN5	C	503	-	-	1/8/16/16	0/3/3/3
5	BTB	B	505	-	-	14/21/21/21	-
5	BTB	B	504	8	-	4/21/21/21	-
4	A1CN5	B	503	-	-	0/8/16/16	0/3/3/3
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1	-	4/12/54/54	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
5	BTB	D	504	8	-	4/21/21/21	-
2	HEM	B	501	1	-	4/12/54/54	-
6	GOL	A	508	-	-	2/4/4/4	-
6	GOL	C	510	-	-	0/4/4/4	-
2	HEM	D	501	1	-	3/12/54/54	-
5	BTB	C	505	-	-	11/21/21/21	-
2	HEM	A	501	1	-	6/12/54/54	-
5	BTB	D	505	-	-	5/21/21/21	-
6	GOL	A	507	-	-	4/4/4/4	-
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
5	BTB	A	505	-	-	13/21/21/21	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-4.20	1.34	1.40
2	B	501	HEM	C3C-CAC	3.61	1.55	1.47
2	C	501	HEM	C3C-CAC	3.55	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-3.51	1.35	1.40
2	D	501	HEM	C3C-CAC	3.39	1.55	1.47
2	D	501	HEM	C3C-C2C	-3.36	1.35	1.40
2	A	501	HEM	C3C-CAC	3.34	1.55	1.47
2	B	501	HEM	CAB-C3B	3.23	1.56	1.47
2	A	501	HEM	CAB-C3B	3.16	1.55	1.47
2	C	501	HEM	CAB-C3B	3.12	1.55	1.47
2	B	501	HEM	C3C-C4C	3.08	1.45	1.41
2	C	501	HEM	C3C-C2C	-3.03	1.36	1.40
2	D	501	HEM	CAB-C3B	2.99	1.55	1.47
2	A	501	HEM	C3C-C4C	2.99	1.45	1.41
2	D	501	HEM	C3C-C4C	2.77	1.45	1.41
2	C	501	HEM	C3C-C4C	2.55	1.45	1.41
2	C	501	HEM	FE-NB	2.54	2.12	1.98
2	C	501	HEM	CMB-C2B	2.47	1.55	1.50
2	B	501	HEM	FE-ND	2.36	2.11	1.98
2	A	501	HEM	FE-NB	2.36	2.11	1.98
2	A	501	HEM	CMB-C2B	2.31	1.55	1.50
2	A	501	HEM	CMD-C2D	2.12	1.55	1.50

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	H4B	C8A-C4A-C4	6.06	120.02	114.50
3	A	502	H4B	C8A-C4A-C4	5.96	119.93	114.50
3	D	502	H4B	C8A-C4A-C4	5.31	119.33	114.50
3	C	502	H4B	C8A-C4A-C4	5.12	119.16	114.50
4	C	503	A1CN5	C02-N01-C06	5.07	121.86	118.07
4	D	503	A1CN5	C02-N01-C06	4.69	121.58	118.07
2	A	501	HEM	C4B-CHC-C1C	4.31	128.25	122.56
2	C	501	HEM	C4B-CHC-C1C	4.30	128.23	122.56
2	C	501	HEM	C3B-C4B-NB	-4.24	106.42	109.47
3	B	502	H4B	C11-C10-C9	-4.18	107.00	112.11
4	A	503	A1CN5	C02-N01-C06	4.07	121.12	118.07
2	B	501	HEM	C4C-CHD-C1D	3.85	127.64	122.56
2	B	501	HEM	CBA-CAA-C2A	-3.80	106.14	112.54
2	D	501	HEM	CBA-CAA-C2A	-3.80	106.16	112.54
3	D	502	H4B	C2-N3-C4	3.73	121.15	115.96
3	C	502	H4B	C2-N3-C4	3.66	121.05	115.96
2	D	501	HEM	C4C-CHD-C1D	3.58	127.28	122.56
5	A	504	BTB	O3-C3-C2	3.46	119.54	111.40
2	B	501	HEM	C3B-C2B-C1B	3.46	109.01	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	H4B	N1-C2-N3	-3.46	120.18	125.48
2	D	501	HEM	CMC-C2C-C3C	3.42	131.52	124.68
3	D	502	H4B	N1-C2-N3	-3.35	120.34	125.48
3	B	502	H4B	C2-N3-C4	3.31	120.56	115.96
2	C	501	HEM	C1B-NB-C4B	3.30	109.11	105.21
3	A	502	H4B	C2-N3-C4	3.26	120.50	115.96
3	A	502	H4B	N1-C2-N3	-3.24	120.52	125.48
2	D	501	HEM	C3B-C2B-C1B	3.23	108.84	106.41
3	B	502	H4B	N1-C2-N3	-3.20	120.58	125.48
2	A	501	HEM	C3B-C4B-NB	-3.20	107.17	109.47
2	D	501	HEM	C1B-NB-C4B	3.02	108.78	105.21
2	C	501	HEM	CHC-C4B-C3B	2.93	129.06	124.57
2	B	501	HEM	C4B-CHC-C1C	2.93	126.42	122.56
2	B	501	HEM	C1B-NB-C4B	2.78	108.50	105.21
2	A	501	HEM	C1B-NB-C4B	2.76	108.47	105.21
2	A	501	HEM	C4A-C3A-C2A	2.72	108.89	107.00
2	D	501	HEM	C4D-ND-C1D	2.67	108.36	105.21
5	D	505	BTB	O1-C1-C2	-2.55	105.40	111.40
2	D	501	HEM	C4B-CHC-C1C	2.55	125.92	122.56
3	B	502	H4B	C2-N1-C8A	2.54	120.62	114.59
3	A	502	H4B	C2-N1-C8A	2.51	120.55	114.59
5	B	504	BTB	O1-C1-C2	-2.47	105.58	111.40
2	D	501	HEM	C3B-C4B-NB	-2.45	107.71	109.47
2	A	501	HEM	C3B-C2B-C1B	2.43	108.23	106.41
2	D	501	HEM	CHD-C1D-ND	2.40	127.02	124.44
2	B	501	HEM	C3B-C4B-NB	-2.39	107.75	109.47
2	A	501	HEM	C4D-ND-C1D	2.38	108.03	105.21
3	D	502	H4B	C2-N1-C8A	2.37	120.23	114.59
3	C	502	H4B	C2-N1-C8A	2.37	120.22	114.59
2	C	501	HEM	CMA-C3A-C4A	-2.36	125.00	128.46
2	D	501	HEM	C2B-C1B-NB	-2.34	107.15	109.84
4	B	503	A1CN5	C18-C17-C15	-2.33	105.59	112.15
2	A	501	HEM	C4C-CHD-C1D	2.31	125.61	122.56
4	B	503	A1CN5	N02-C02-N01	2.31	120.30	116.59
4	A	503	A1CN5	N02-C02-N01	2.27	120.24	116.59
2	D	501	HEM	C2D-C1D-ND	-2.22	107.34	109.90
2	C	501	HEM	C4D-ND-C1D	2.22	107.83	105.21
4	C	503	A1CN5	N02-C02-N01	2.17	120.08	116.59
2	A	501	HEM	CMA-C3A-C4A	-2.16	125.29	128.46
3	A	502	H4B	C11-C10-C9	-2.16	109.47	112.11
2	B	501	HEM	C2D-C1D-ND	-2.14	107.43	109.90
2	C	501	HEM	C3B-C2B-C1B	2.13	108.01	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1CN5	O09-C11-C12	2.10	119.09	115.92
3	B	502	H4B	N2-C2-N1	2.09	120.36	117.22
3	C	502	H4B	N2-C2-N3	2.09	120.36	117.22
2	A	501	HEM	CHC-C4B-C3B	2.07	127.73	124.57
2	B	501	HEM	CAD-CBD-CGD	-2.06	108.20	113.67
2	B	501	HEM	C2B-C1B-NB	-2.06	107.47	109.84
4	B	503	A1CN5	C08-C06-C05	-2.04	118.26	121.30
4	B	503	A1CN5	O09-C11-C12	2.03	118.99	115.92
4	C	503	A1CN5	C17-C18-N21	-2.02	106.56	114.39
2	B	501	HEM	C1D-C2D-C3D	2.02	109.11	106.98
3	A	502	H4B	N2-C2-N3	2.01	120.23	117.22

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C2A-CAA-CBA-CGA
3	A	502	H4B	C7-C6-C9-O9
3	A	502	H4B	C7-C6-C9-C10
3	B	502	H4B	C7-C6-C9-O9
3	C	502	H4B	C7-C6-C9-O9
3	C	502	H4B	C7-C6-C9-C10
3	D	502	H4B	C7-C6-C9-O9
3	D	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	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

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Mol	Chain	Res	Type	Atoms
5	B	504	BTB	O1-C1-C2-N
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-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
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	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	N-C2-C3-O3
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-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	C	506	BTB	N-C5-C6-O6
5	D	504	BTB	C1-C2-C3-O3
5	D	504	BTB	C4-C2-C3-O3
5	D	504	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C8-C7-N-C5
6	A	507	GOL	C1-C2-C3-O3
6	B	506	GOL	O1-C1-C2-C3
6	C	507	GOL	O1-C1-C2-C3
6	C	507	GOL	C1-C2-C3-O3
6	C	509	GOL	O1-C1-C2-O2
6	C	509	GOL	O1-C1-C2-C3
2	A	501	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C3D-CAD-CBD-CGD
4	C	503	A1CN5	C15-C17-C18-N21
5	C	505	BTB	N-C5-C6-O6
6	C	507	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C5-C6-O6
5	A	505	BTB	N-C7-C8-O8
5	C	504	BTB	N-C7-C8-O8
2	B	501	HEM	C3D-CAD-CBD-CGD
2	D	501	HEM	C3D-CAD-CBD-CGD
6	A	508	GOL	C1-C2-C3-O3
6	A	507	GOL	O1-C1-C2-O2
6	A	507	GOL	O2-C2-C3-O3
6	B	506	GOL	O1-C1-C2-O2
5	C	505	BTB	N-C7-C8-O8
6	C	507	GOL	O2-C2-C3-O3
5	C	506	BTB	C6-C5-N-C7
6	A	508	GOL	O2-C2-C3-O3
6	C	508	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C7-C8-O8
4	D	503	A1CN5	C12-C11-O09-C08
2	C	501	HEM	C3A-C2A-CAA-CBA
6	A	507	GOL	O1-C1-C2-C3
2	C	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
5	D	505	BTB	C6-C5-N-C2
3	A	502	H4B	N5-C6-C9-O9
3	C	502	H4B	N5-C6-C9-O9
3	D	502	H4B	N5-C6-C9-O9
5	A	505	BTB	N-C2-C4-O4
5	C	504	BTB	O1-C1-C2-N
5	C	505	BTB	C3-C2-N-C5
3	B	502	H4B	C7-C6-C9-C10
5	D	504	BTB	N-C7-C8-O8
5	C	504	BTB	O1-C1-C2-C4
2	B	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A
5	B	504	BTB	C1-C2-C3-O3
3	B	502	H4B	N5-C6-C9-O9

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Mol	Chain	Res	Type	Atoms
5	C	505	BTB	N-C2-C4-O4
5	C	506	BTB	C4-C2-N-C5
2	A	501	HEM	CAD-CBD-CGD-O2D

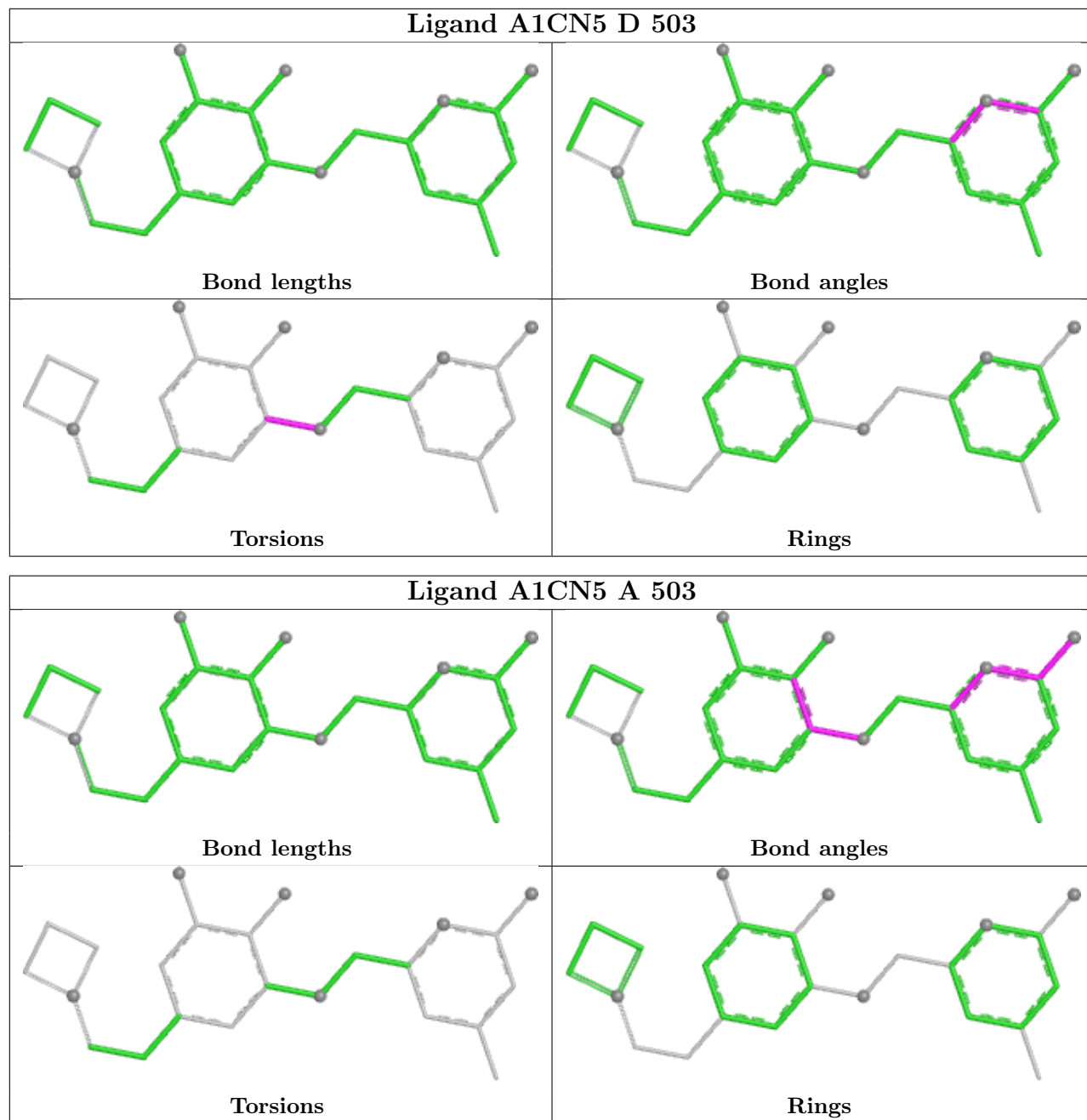
There are no ring outliers.

22 monomers are involved in 51 short contacts:

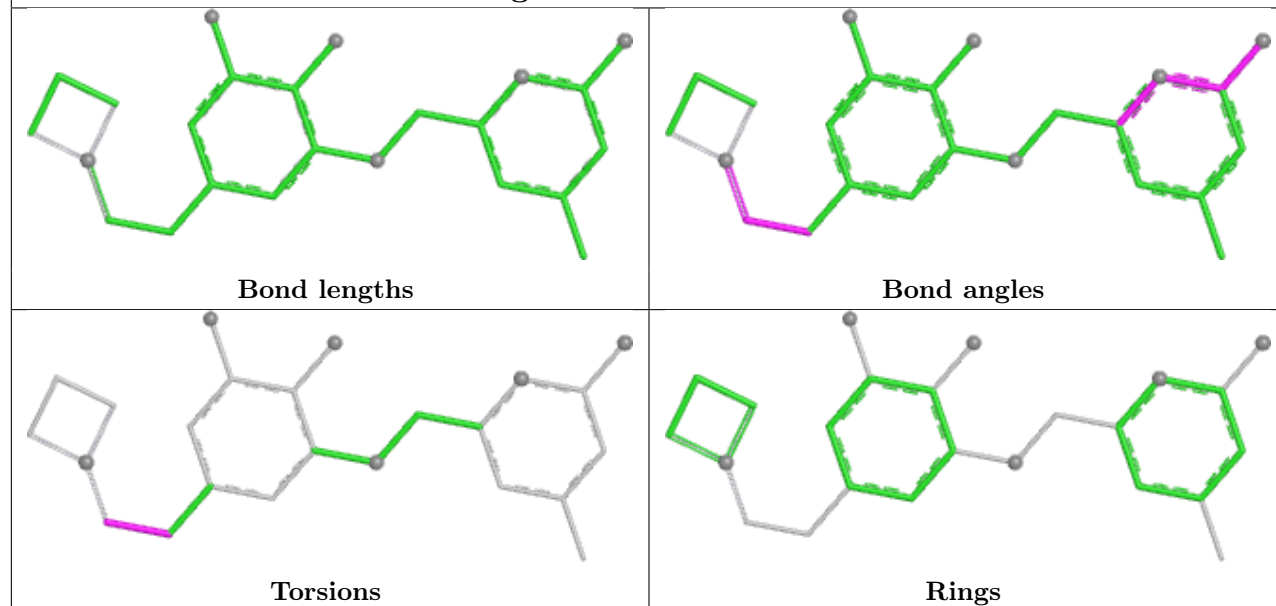
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	BTB	1	0
5	A	506	BTB	2	0
3	A	502	H4B	3	0
4	D	503	A1CN5	1	0
5	C	504	BTB	2	0
5	C	506	BTB	1	0
4	C	503	A1CN5	1	0
5	B	505	BTB	4	0
5	B	504	BTB	4	0
4	B	503	A1CN5	1	0
3	C	502	H4B	4	0
2	C	501	HEM	4	0
3	B	502	H4B	1	0
5	D	504	BTB	2	0
2	B	501	HEM	5	0
2	D	501	HEM	4	0
5	C	505	BTB	2	0
2	A	501	HEM	5	0
5	D	505	BTB	2	0
6	A	507	GOL	1	0
3	D	502	H4B	1	0
5	A	505	BTB	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

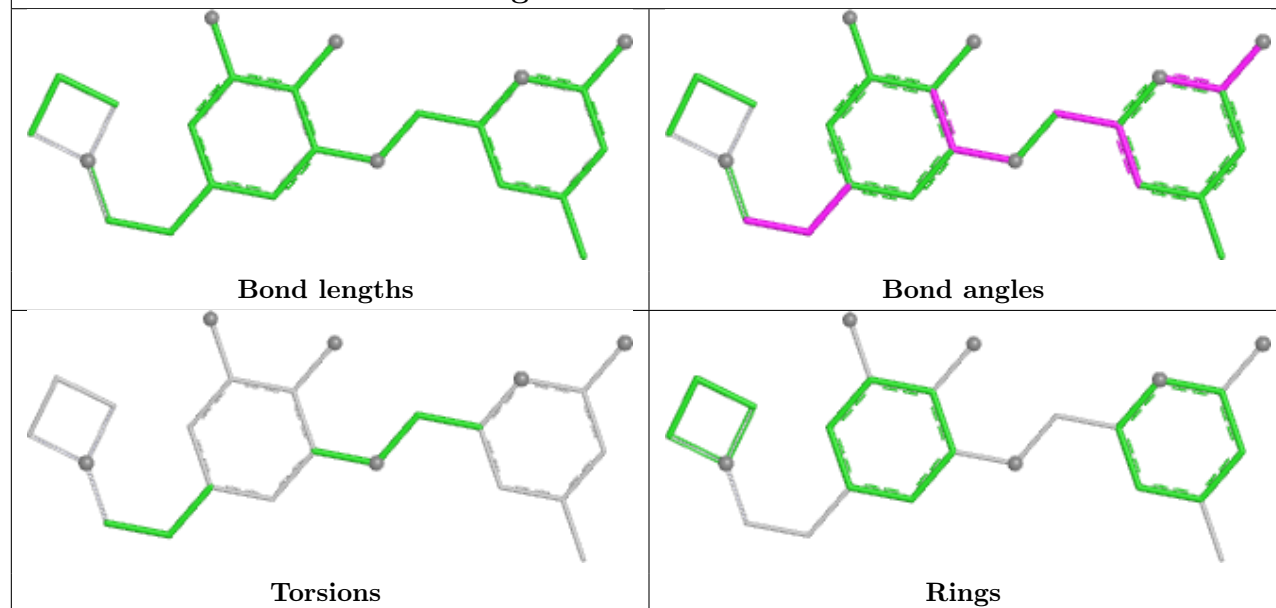
equivalents in the CSD to analyse the geometry.



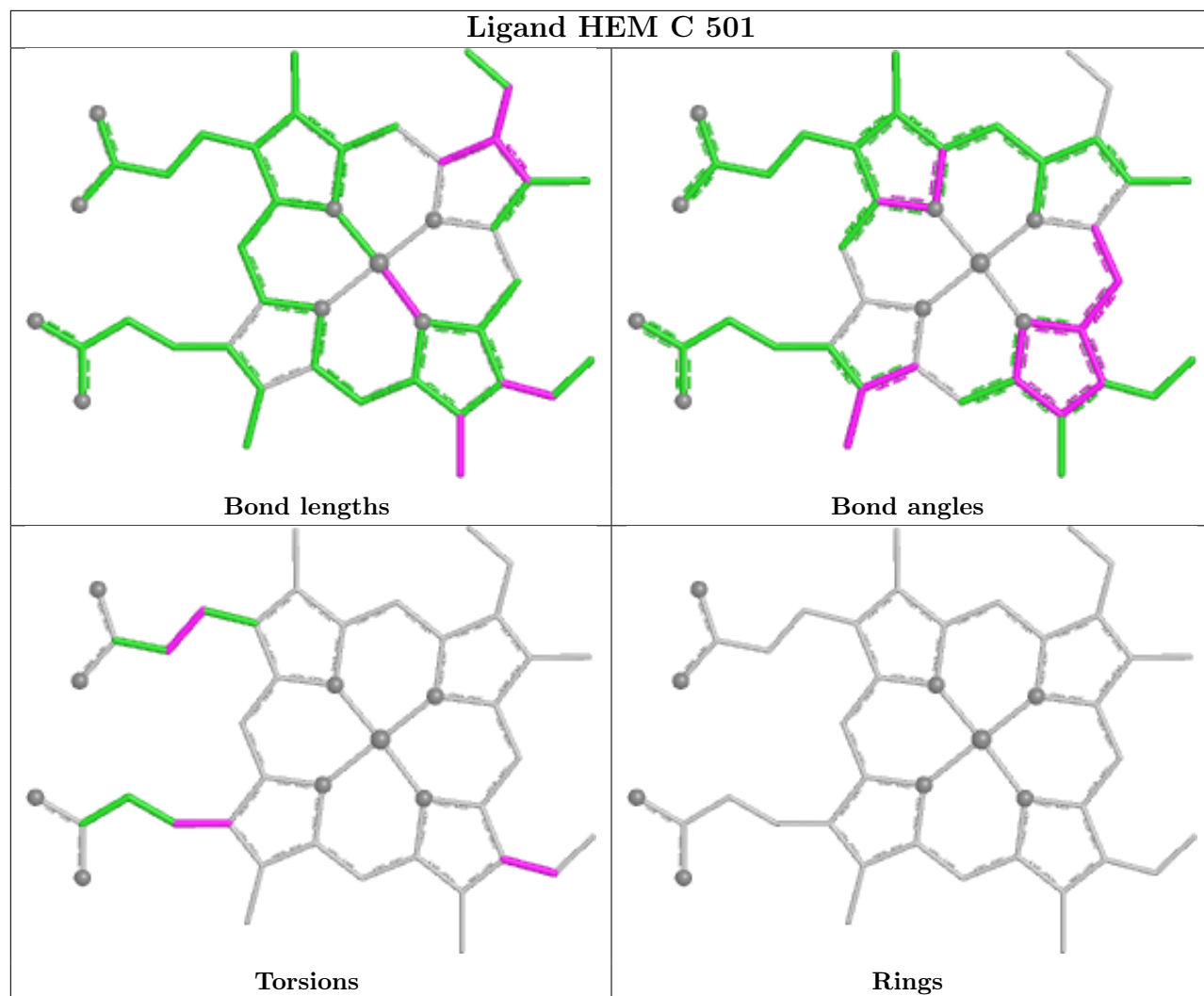
## Ligand A1CN5 C 503

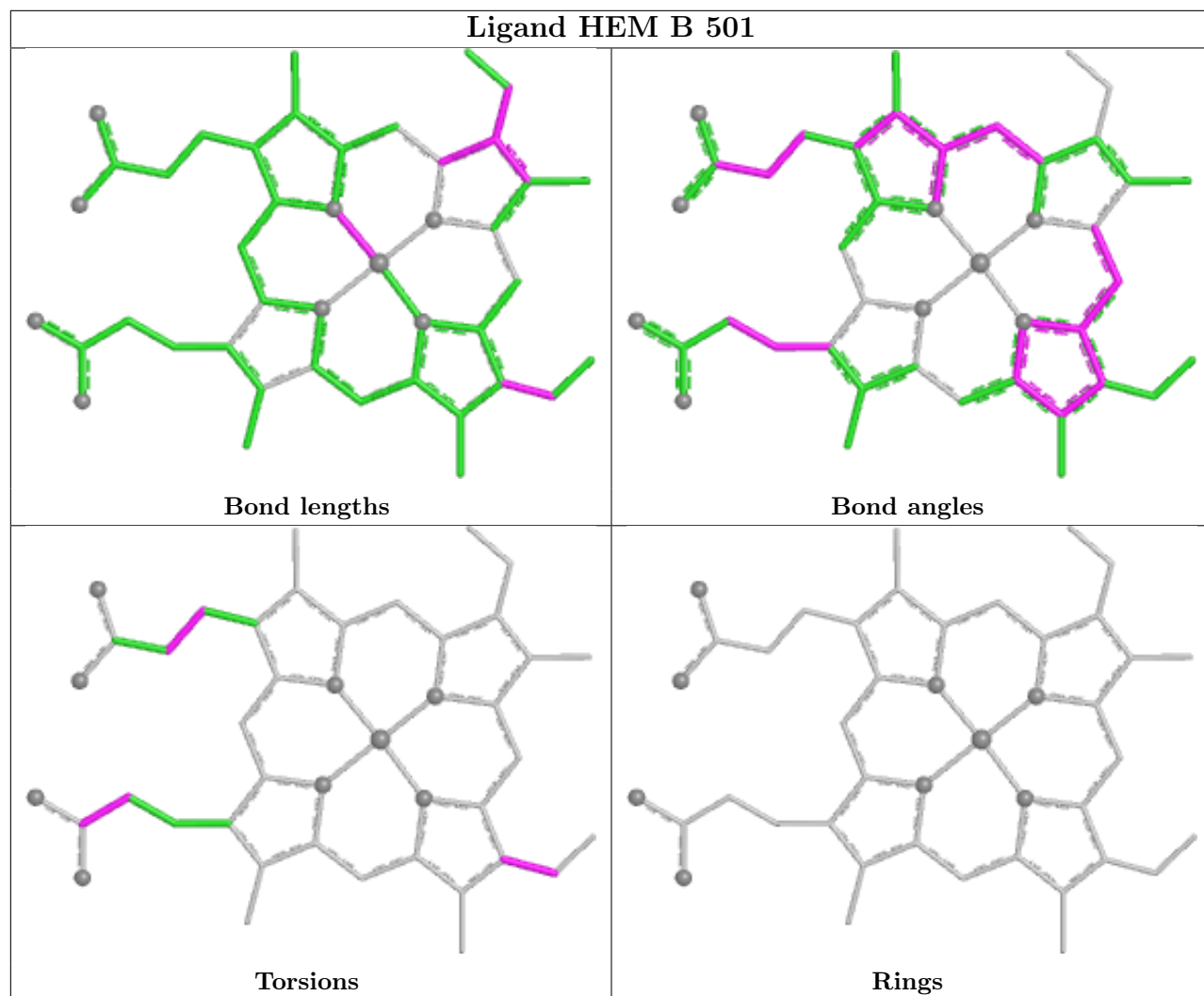


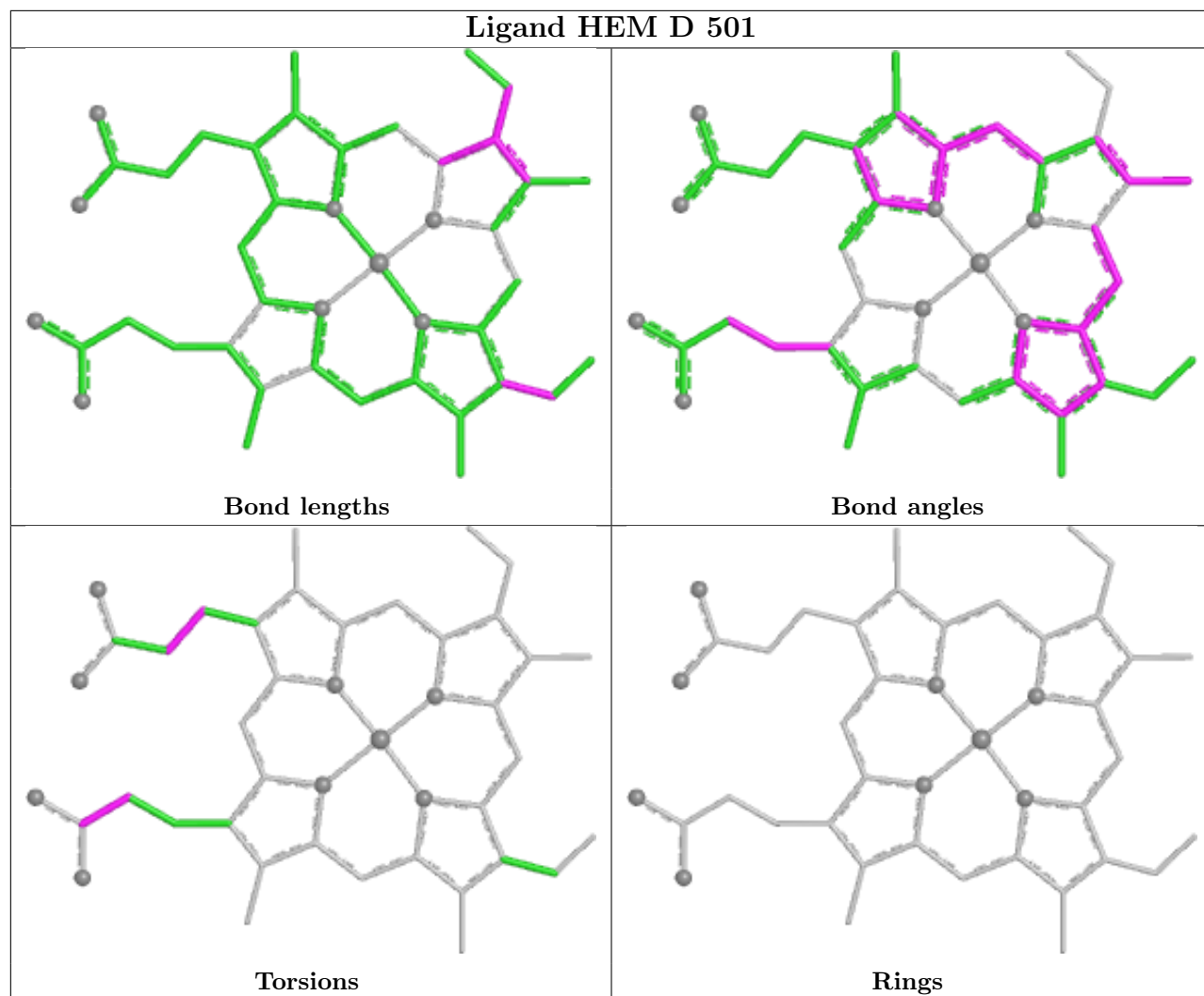
## Ligand A1CN5 B 503

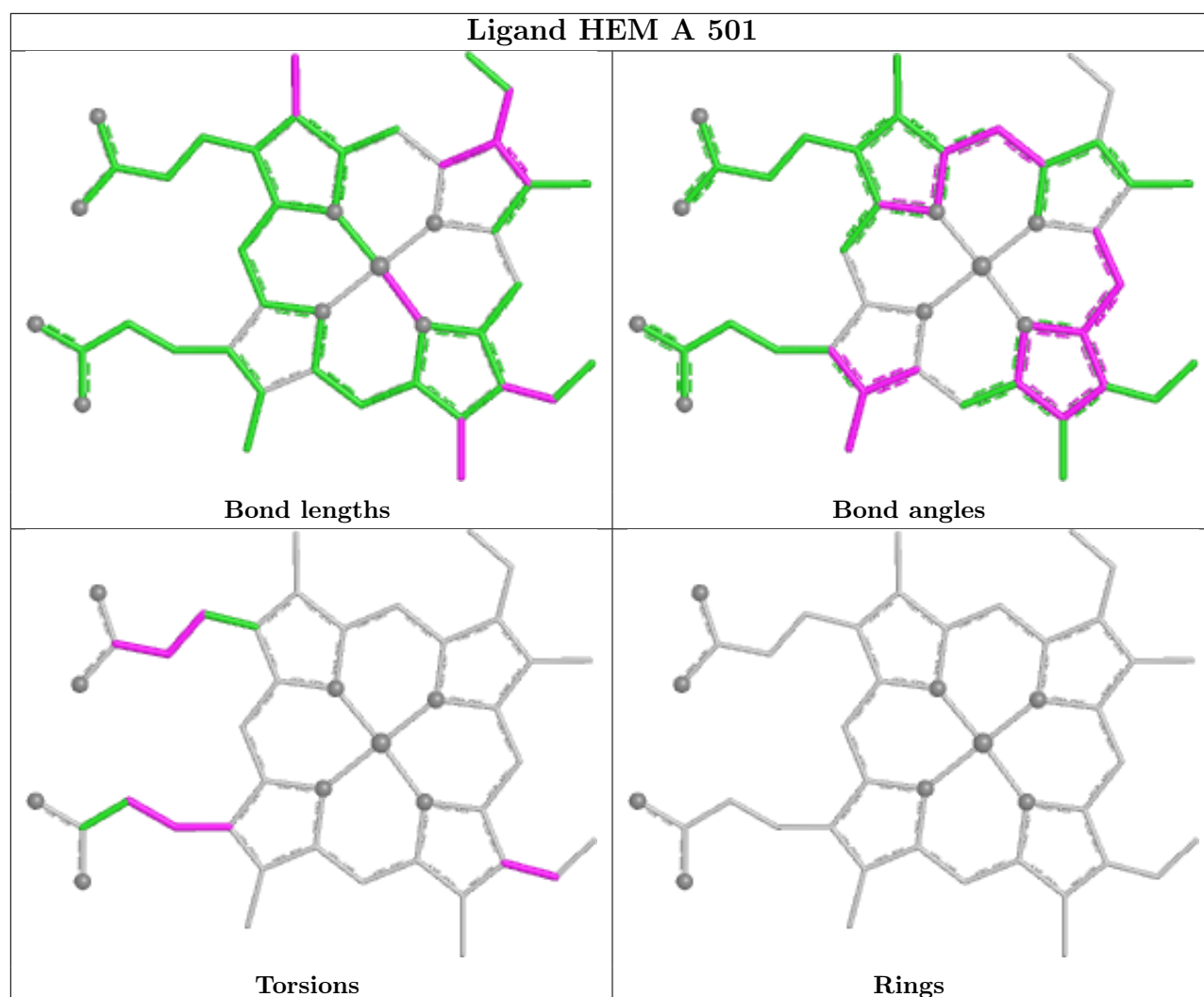












## 5.7 Other polymers [i](#)

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	401/440 (91%)	-0.98	1 (0%) 92 93	39, 76, 125, 153	1 (0%)
1	B	401/440 (91%)	-1.20	0 100 100	29, 58, 103, 146	3 (0%)
1	C	402/440 (91%)	-1.00	0 100 100	41, 73, 121, 148	1 (0%)
1	D	402/440 (91%)	-1.20	0 100 100	38, 58, 92, 147	1 (0%)
All	All	1606/1760 (91%)	-1.10	1 (0%) 92 93	29, 65, 117, 153	6 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	PRO	2.2

### 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	C	509	6/6	0.94	0.06	74,84,91,92	0

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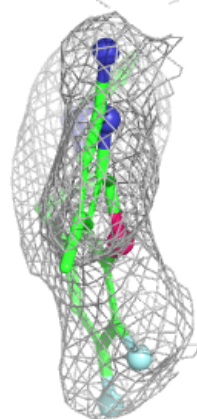
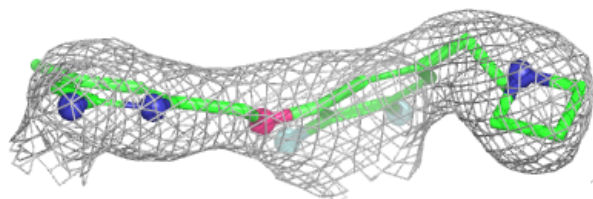
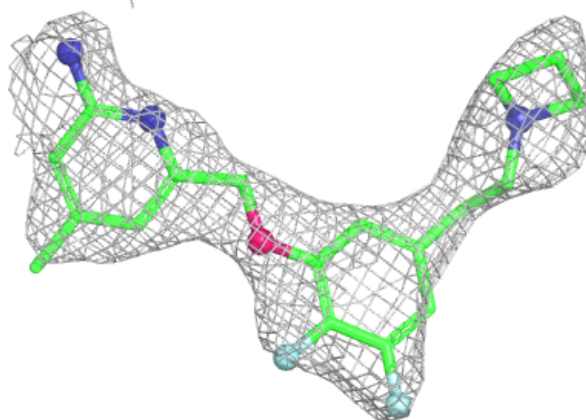
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	C	510	6/6	0.94	0.05	93,101,103,104	0
6	GOL	B	506	6/6	0.97	0.07	78,81,85,93	0
5	BTB	A	506	14/14	0.97	0.06	96,107,113,115	0
5	BTB	D	505	14/14	0.97	0.04	73,85,94,98	0
4	A1CN5	C	503	24/24	0.98	0.07	53,90,98,101	0
5	BTB	A	505	14/14	0.98	0.04	78,90,94,94	0
3	H4B	B	502	17/17	0.98	0.07	72,102,128,130	0
5	BTB	B	505	14/14	0.98	0.03	61,92,99,100	0
5	BTB	C	505	14/14	0.98	0.04	53,75,89,94	0
5	BTB	C	506	14/14	0.98	0.05	101,120,127,128	0
3	H4B	C	502	17/17	0.98	0.09	114,141,151,153	0
6	GOL	A	507	6/6	0.98	0.03	50,84,91,92	0
3	H4B	D	502	17/17	0.98	0.05	60,96,120,121	0
6	GOL	C	507	6/6	0.98	0.03	65,75,83,83	0
4	A1CN5	A	503	24/24	0.98	0.06	55,85,104,106	0
4	A1CN5	B	503	24/24	0.98	0.05	39,66,70,84	0
5	BTB	D	504	14/14	0.99	0.04	55,81,92,95	0
3	H4B	A	502	17/17	0.99	0.08	92,121,143,144	0
5	BTB	B	504	14/14	0.99	0.04	43,59,75,77	0
6	GOL	A	508	6/6	0.99	0.04	45,78,81,86	0
4	A1CN5	D	503	24/24	0.99	0.05	32,70,77,96	0
5	BTB	C	504	14/14	0.99	0.03	49,75,83,86	0
6	GOL	C	508	6/6	0.99	0.04	52,68,72,75	0
5	BTB	A	504	14/14	0.99	0.05	68,99,108,113	0
2	HEM	A	501	43/43	0.99	0.04	56,75,95,110	0
7	CL	A	509	1/1	0.99	0.04	66,66,66,66	0
7	CL	B	507	1/1	0.99	0.04	55,55,55,55	0
7	CL	C	511	1/1	0.99	0.04	63,63,63,63	0
7	CL	D	506	1/1	0.99	0.04	54,54,54,54	0
2	HEM	D	501	43/43	1.00	0.04	35,54,76,91	0
2	HEM	B	501	43/43	1.00	0.03	34,51,69,83	0
2	HEM	C	501	43/43	1.00	0.04	43,64,94,99	0
8	GD	A	510	1/1	1.00	0.01	130,130,130,130	0
8	GD	B	508	1/1	1.00	0.03	59,59,59,59	0
8	GD	C	512	1/1	1.00	0.01	118,118,118,118	0
8	GD	D	507	1/1	1.00	0.01	62,62,62,62	0
9	ZN	A	511	1/1	1.00	0.01	68,68,68,68	0
9	ZN	C	513	1/1	1.00	0.01	61,61,61,61	0

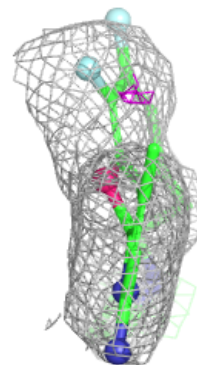
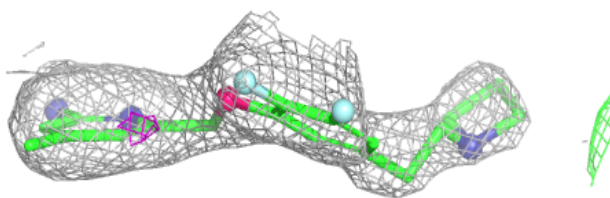
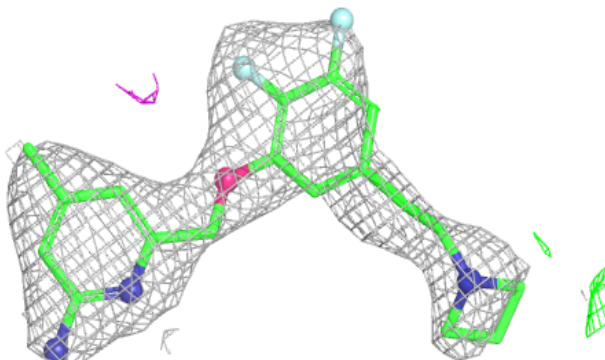
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1CN5 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)

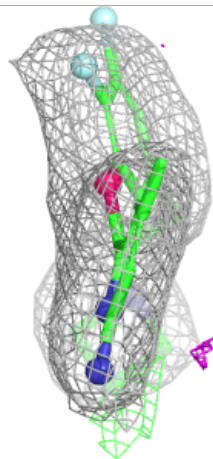
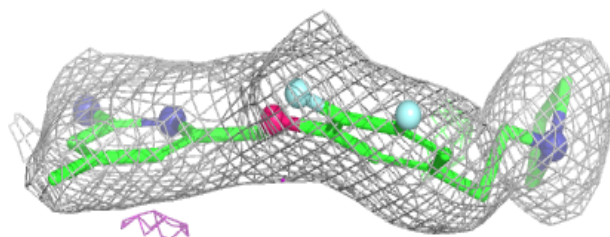
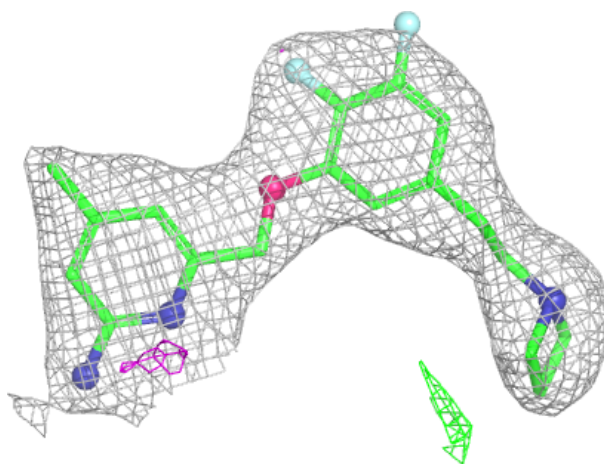
**Electron density around A1CN5 A 503:**

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



**Electron density around A1CN5 B 503:**

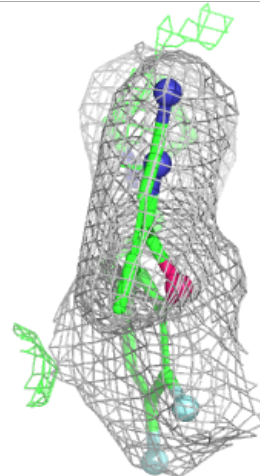
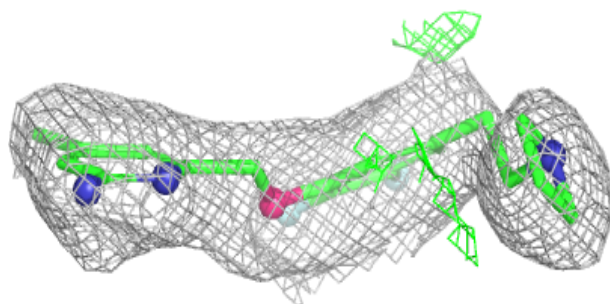
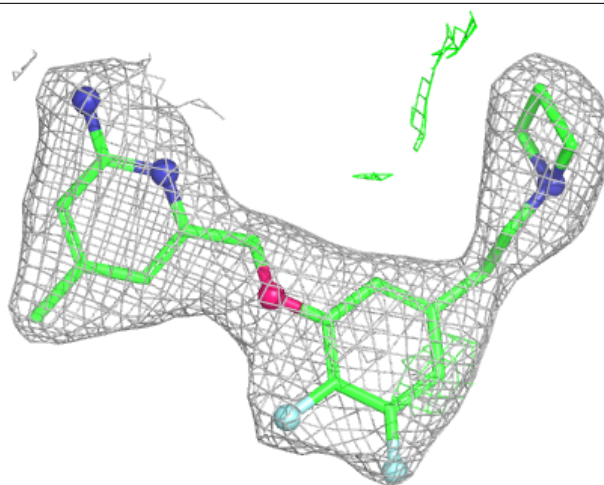
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





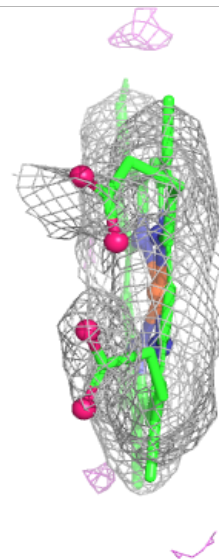
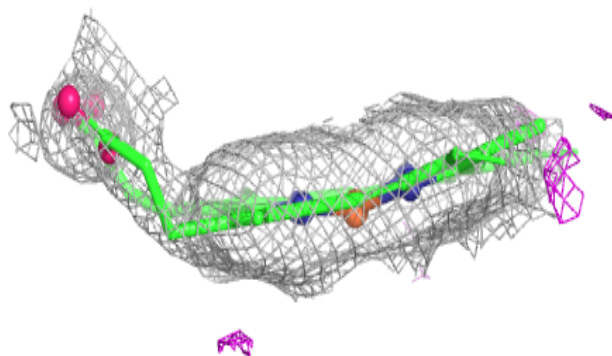
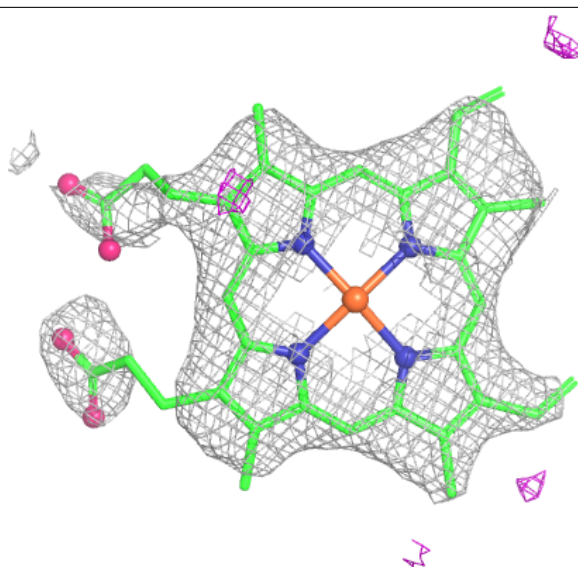
**Electron density around A1CN5 D 503:**

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



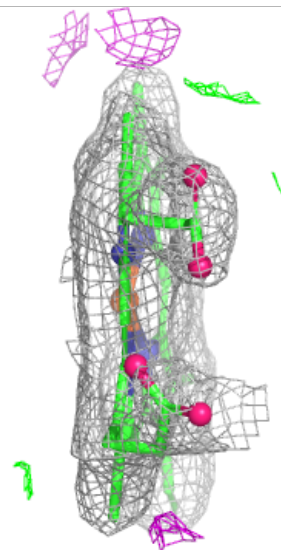
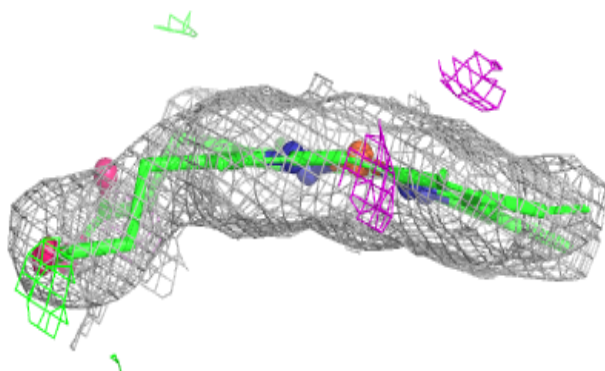
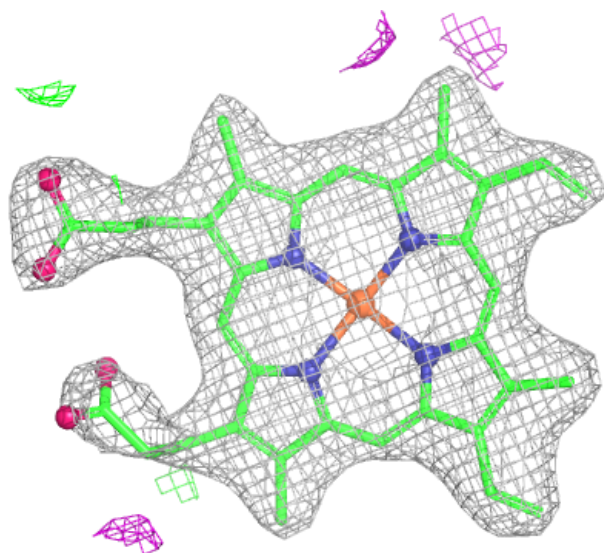
**Electron density around HEM A 501:**

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



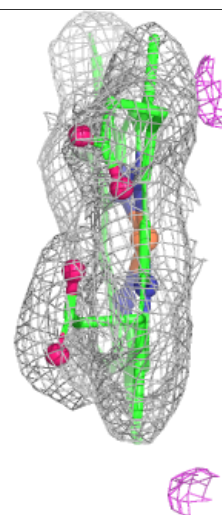
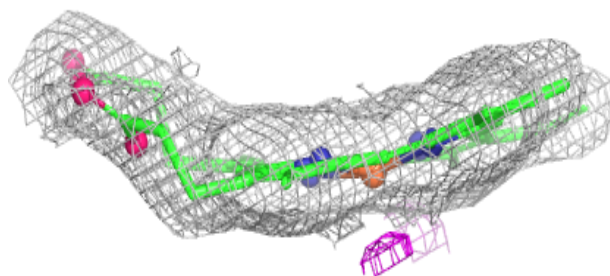
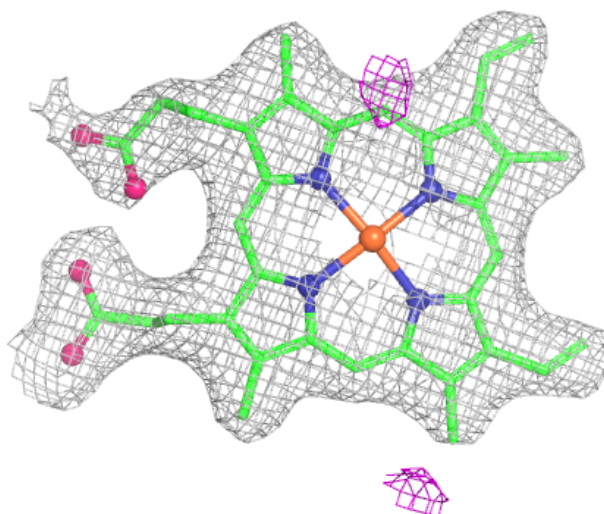
**Electron density around HEM D 501:**

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



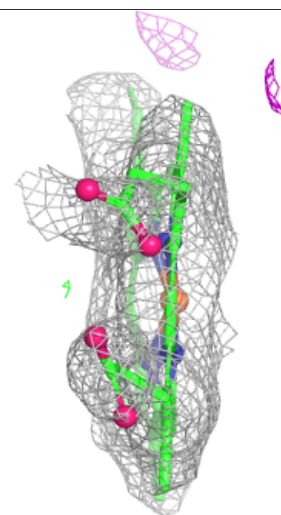
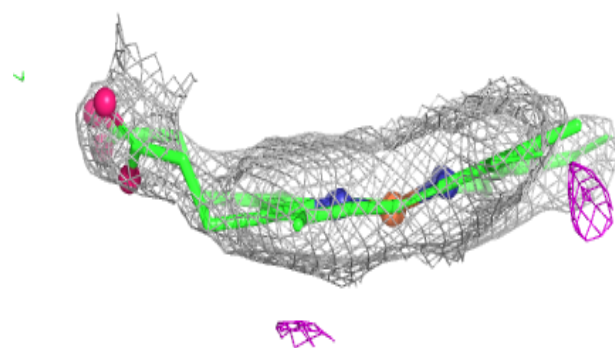
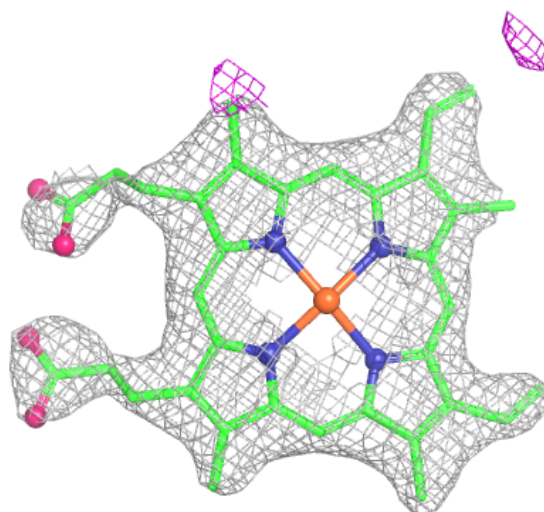
**Electron density around HEM B 501:**

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



**Electron density around HEM C 501:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.