



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 09:18 AM EDT

PDB ID : 6E45  
Title : CRYSTAL STRUCTURE OF HUMAN INDOLEAMINE 2,3-DIOXYGENASE 1 (IDO1) free enzyme in the ferrous state  
Authors : Luo, S.; Tong, L.  
Deposited on : 2018-07-16  
Resolution : 2.00 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

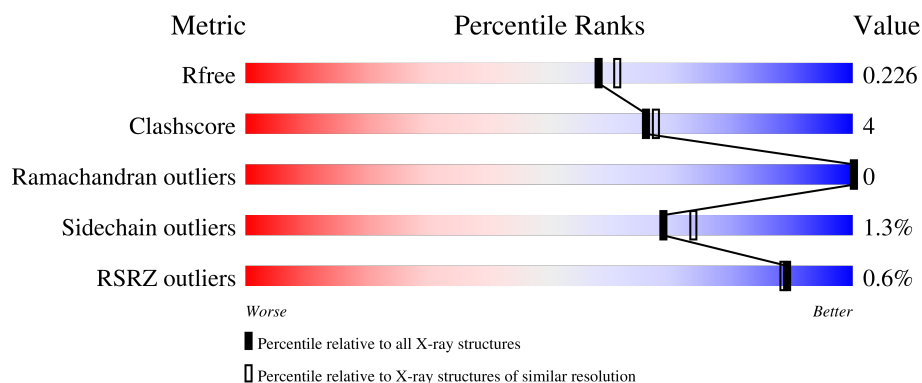
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	405	
1	B	405	
1	C	405	
1	D	405	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	502	-	X	X	-
3	GOL	D	504	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12954 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 Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2911	1873	496	525	17			
1	B	373	Total	C	N	O	S	0	0	0
			2940	1890	502	531	17			
1	C	370	Total	C	N	O	S	0	0	0
			2924	1880	498	529	17			
1	D	369	Total	C	N	O	S	0	0	0
			2915	1875	497	526	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P14902
A	0	GLY	-	expression tag	UNP P14902
A	1	SER	-	expression tag	UNP P14902
A	2	SER	-	expression tag	UNP P14902
A	3	HIS	-	expression tag	UNP P14902
A	4	HIS	-	expression tag	UNP P14902
A	5	HIS	-	expression tag	UNP P14902
A	6	HIS	-	expression tag	UNP P14902
A	7	HIS	-	expression tag	UNP P14902
A	8	HIS	-	expression tag	UNP P14902
A	9	SER	-	expression tag	UNP P14902
A	10	SER	-	expression tag	UNP P14902
A	11	GLY	-	expression tag	UNP P14902
A	12	SER	-	expression tag	UNP P14902
A	13	ALA	-	expression tag	UNP P14902
A	14	ALA	-	expression tag	UNP P14902
A	116	ALA	LYS	engineered mutation	UNP P14902
A	117	ALA	LYS	engineered mutation	UNP P14902
B	-1	MET	-	initiating methionine	UNP P14902
B	0	GLY	-	expression tag	UNP P14902
B	1	SER	-	expression tag	UNP P14902

*Continued on next page...*

*Continued from previous page...*

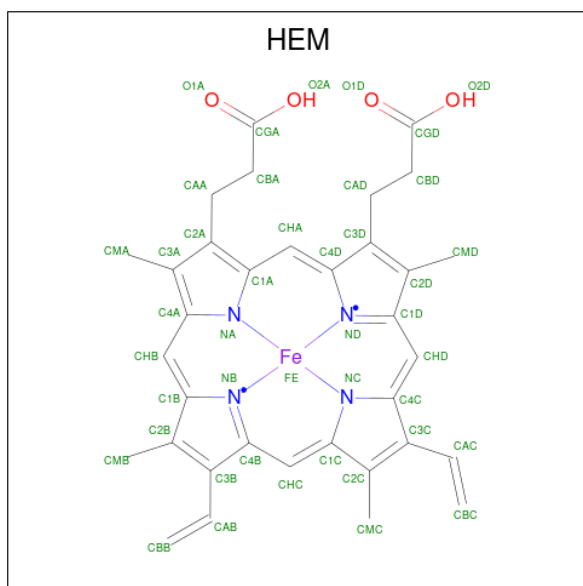
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP P14902
B	3	HIS	-	expression tag	UNP P14902
B	4	HIS	-	expression tag	UNP P14902
B	5	HIS	-	expression tag	UNP P14902
B	6	HIS	-	expression tag	UNP P14902
B	7	HIS	-	expression tag	UNP P14902
B	8	HIS	-	expression tag	UNP P14902
B	9	SER	-	expression tag	UNP P14902
B	10	SER	-	expression tag	UNP P14902
B	11	GLY	-	expression tag	UNP P14902
B	12	SER	-	expression tag	UNP P14902
B	13	ALA	-	expression tag	UNP P14902
B	14	ALA	-	expression tag	UNP P14902
B	116	ALA	LYS	engineered mutation	UNP P14902
B	117	ALA	LYS	engineered mutation	UNP P14902
C	-1	MET	-	initiating methionine	UNP P14902
C	0	GLY	-	expression tag	UNP P14902
C	1	SER	-	expression tag	UNP P14902
C	2	SER	-	expression tag	UNP P14902
C	3	HIS	-	expression tag	UNP P14902
C	4	HIS	-	expression tag	UNP P14902
C	5	HIS	-	expression tag	UNP P14902
C	6	HIS	-	expression tag	UNP P14902
C	7	HIS	-	expression tag	UNP P14902
C	8	HIS	-	expression tag	UNP P14902
C	9	SER	-	expression tag	UNP P14902
C	10	SER	-	expression tag	UNP P14902
C	11	GLY	-	expression tag	UNP P14902
C	12	SER	-	expression tag	UNP P14902
C	13	ALA	-	expression tag	UNP P14902
C	14	ALA	-	expression tag	UNP P14902
C	116	ALA	LYS	engineered mutation	UNP P14902
C	117	ALA	LYS	engineered mutation	UNP P14902
D	-1	MET	-	initiating methionine	UNP P14902
D	0	GLY	-	expression tag	UNP P14902
D	1	SER	-	expression tag	UNP P14902
D	2	SER	-	expression tag	UNP P14902
D	3	HIS	-	expression tag	UNP P14902
D	4	HIS	-	expression tag	UNP P14902
D	5	HIS	-	expression tag	UNP P14902
D	6	HIS	-	expression tag	UNP P14902
D	7	HIS	-	expression tag	UNP P14902

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P14902
D	9	SER	-	expression tag	UNP P14902
D	10	SER	-	expression tag	UNP P14902
D	11	GLY	-	expression tag	UNP P14902
D	12	SER	-	expression tag	UNP P14902
D	13	ALA	-	expression tag	UNP P14902
D	14	ALA	-	expression tag	UNP P14902
D	116	ALA	LYS	engineered mutation	UNP P14902
D	117	ALA	LYS	engineered mutation	UNP P14902

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



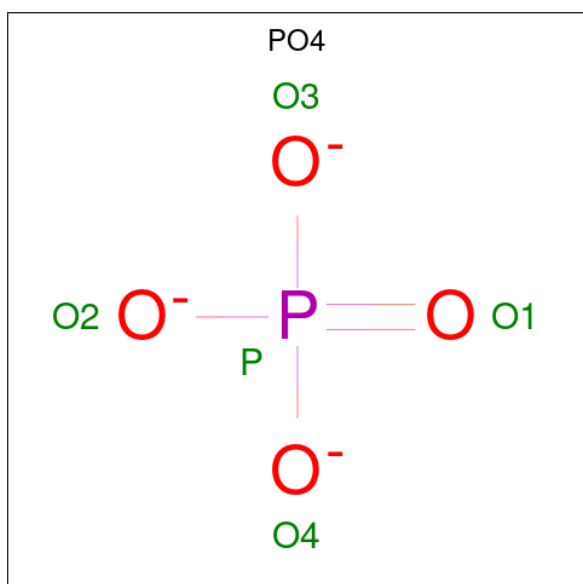
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	218	Total O 218 218	0	0
5	B	281	Total O 281 281	0	0
5	C	254	Total O 254 254	0	0
5	D	294	Total O 294 294	0	0

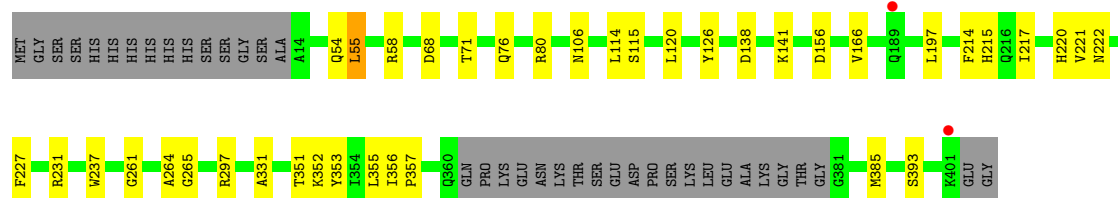


### 3 Residue-property plots


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.

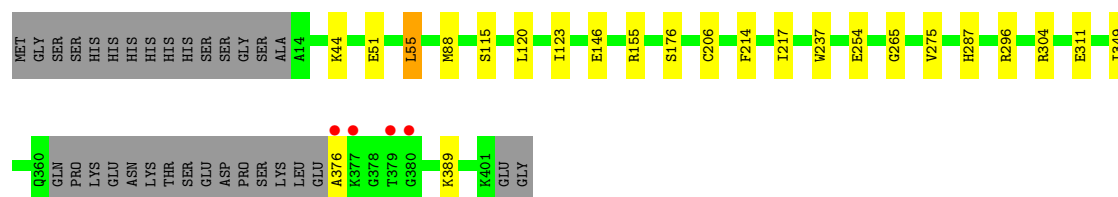
#### • Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain A: 




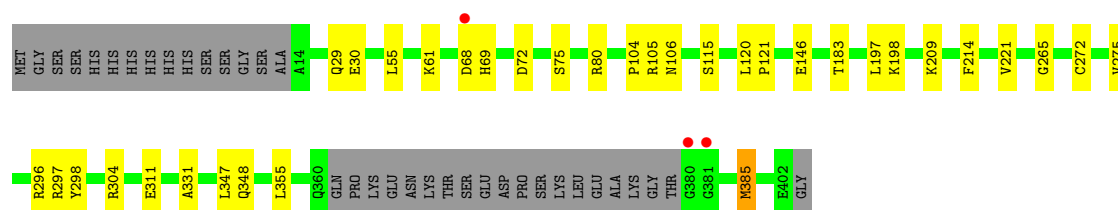
#### • Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain B: 



#### • Molecule 1: Indoleamine 2,3-dioxygenase 1

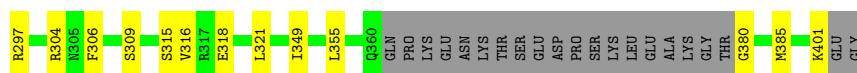
Chain C: 



#### • Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.97Å 196.54Å 116.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.88 – 2.00 65.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (65.88-2.00) 99.4 (65.88-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.189 , 0.226 0.189 , 0.226	Depositor DCC
$R_{free}$ test set	1862 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4311e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, HEM

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	0.59	0/2979	0.56	2/4033 (0.0%)
1	B	0.44	0/3008	0.56	1/4071 (0.0%)
1	C	0.53	1/2992 (0.0%)	0.58	4/4050 (0.1%)
1	D	0.56	1/2983 (0.0%)	0.58	2/4038 (0.0%)
All	All	0.53	2/11962 (0.0%)	0.57	9/16192 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	GLU	CD-OE1	-5.31	1.19	1.25
1	D	235	SER	CB-OG	-5.17	1.35	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	LEU	CB-CG-CD1	-7.20	98.77	111.00
1	D	55	LEU	CA-CB-CG	-7.00	99.20	115.30
1	A	55	LEU	CA-CB-CG	-6.88	99.48	115.30
1	C	55	LEU	CA-CB-CG	-6.60	100.13	115.30
1	B	55	LEU	CA-CB-CG	-6.58	100.16	115.30
1	C	385	MET	CG-SD-CE	6.16	110.06	100.20
1	D	221	VAL	C-N-CA	-5.38	108.24	121.70
1	C	221	VAL	C-N-CA	-5.13	108.89	121.70
1	A	221	VAL	C-N-CA	-5.08	109.00	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2911	0	2921	26	0
1	B	2940	0	2952	18	0
1	C	2924	0	2930	20	0
1	D	2915	0	2924	32	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
3	A	12	0	16	5	0
3	D	18	0	23	6	0
4	B	5	0	0	0	0
4	D	10	0	0	0	0
5	A	218	0	0	6	0
5	B	281	0	0	3	0
5	C	254	0	0	8	0
5	D	294	0	0	6	0
All	All	12954	0	11886	96	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 4.

All (96) 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:D:236:GLY:H	3:D:504:GOL:H12	1.27	0.99
1:D:88:MET:SD	5:D:781:HOH:O	2.39	0.80
1:A:222:ASN:HB3	3:A:503:GOL:H2	1.66	0.78
1:C:105:ARG:NH2	5:C:601:HOH:O	2.17	0.78
1:C:198:LYS:NZ	5:C:602:HOH:O	2.17	0.76
1:A:156:ASP:O	5:A:601:HOH:O	2.08	0.71
1:D:261:GLY:H	3:D:504:GOL:H2	1.55	0.71
1:B:88:MET:HE1	1:B:123:ILE:HG13	1.71	0.71
1:D:62:LEU:CD1	1:D:107:ILE:HD11	2.21	0.71
1:C:146:GLU:HG2	1:D:222:ASN:CB	2.20	0.70
1:D:380:GLY:N	5:D:604:HOH:O	2.26	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:O	1:A:231:ARG:NH1	2.28	0.67
1:A:68:ASP:OD1	5:A:602:HOH:O	2.13	0.66
1:C:146:GLU:HG2	1:D:222:ASN:HB3	1.79	0.65
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.80	0.63
1:D:297:ARG:NH1	5:D:603:HOH:O	2.25	0.63
1:B:376:ALA:N	5:B:602:HOH:O	2.32	0.62
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.81	0.62
1:D:217:ILE:CD1	2:D:501:HEM:HAB	2.29	0.62
1:A:297:ARG:NH1	5:A:603:HOH:O	2.33	0.61
1:B:51:GLU:HG2	1:B:155:ARG:HH21	1.65	0.61
1:C:146:GLU:HG2	1:D:222:ASN:HB2	1.84	0.59
2:C:501:HEM:HMB2	2:C:501:HEM:HBB2	1.83	0.59
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.85	0.59
1:A:220:HIS:HE1	5:A:697:HOH:O	1.88	0.57
1:A:261:GLY:H	3:A:502:GOL:H12	1.70	0.57
1:D:217:ILE:HG21	1:D:349:ILE:HD12	1.90	0.54
1:A:71:THR:HB	1:D:54:GLN:HG2	1.89	0.54
1:A:355:LEU:HD11	1:A:385:MET:HG3	1.89	0.54
1:A:351:THR:HA	1:A:355:LEU:HB2	1.91	0.53
1:D:217:ILE:HD13	2:D:501:HEM:HAB	1.90	0.53
1:D:261:GLY:H	3:D:504:GOL:C2	2.20	0.53
1:A:352:LYS:HD3	1:A:353:TYR:CE1	2.44	0.52
1:D:261:GLY:N	3:D:504:GOL:H2	2.22	0.52
1:C:265:GLY:HA2	2:C:501:HEM:C3D	2.45	0.52
1:B:217:ILE:CD1	2:B:501:HEM:HAB	2.39	0.52
1:D:217:ILE:HD11	2:D:501:HEM:HAB	1.92	0.52
1:D:296:ARG:O	1:D:304:ARG:HD3	2.11	0.51
1:D:236:GLY:H	3:D:504:GOL:C1	2.12	0.51
1:D:265:GLY:HA2	2:D:501:HEM:C3D	2.46	0.50
1:B:254:GLU:HG2	5:B:643:HOH:O	2.10	0.50
1:A:55:LEU:O	1:A:55:LEU:HG	2.06	0.50
1:C:68:ASP:OD1	1:C:69:HIS:ND1	2.44	0.50
1:C:61:LYS:NZ	5:C:609:HOH:O	2.44	0.50
1:B:265:GLY:HA2	2:B:501:HEM:C3D	2.48	0.49
1:C:115:SER:HB3	1:C:120:LEU:O	2.12	0.49
1:D:136:LYS:NZ	5:D:608:HOH:O	2.38	0.49
1:A:166:VAL:HG11	1:A:217:ILE:HG12	1.93	0.49
1:A:54:GLN:O	1:A:58:ARG:HG2	2.14	0.48
1:B:176:SER:HB3	1:B:206:CYS:SG	2.54	0.48
1:D:62:LEU:HD13	1:D:107:ILE:HD11	1.93	0.48
1:B:217:ILE:HD13	2:B:501:HEM:HAB	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:NZ	5:B:608:HOH:O	2.45	0.47
1:C:183:THR:HG21	5:C:602:HOH:O	2.15	0.46
1:A:138:ASP:HB3	1:A:141:LYS:HG3	1.97	0.46
1:B:296:ARG:O	1:B:304:ARG:HD3	2.16	0.46
1:A:197:LEU:HD12	1:A:331:ALA:HB2	1.97	0.46
1:D:15:TYR:HB3	1:D:306:PHE:HB2	1.97	0.46
1:C:121:PRO:HG2	1:C:298:TYR:CD2	2.51	0.45
1:A:115:SER:HB3	1:A:120:LEU:O	2.16	0.45
1:A:265:GLY:HA2	2:A:501:HEM:C3D	2.51	0.45
1:B:275:VAL:HG13	1:B:311:GLU:HG3	1.96	0.45
1:D:321:LEU:HA	1:D:321:LEU:HD23	1.78	0.45
1:D:236:GLY:N	3:D:504:GOL:H12	2.11	0.45
1:A:261:GLY:C	3:A:502:GOL:H31	2.37	0.45
1:D:257:LYS:NZ	5:D:615:HOH:O	2.50	0.44
1:C:106:ASN:HB2	5:C:808:HOH:O	2.17	0.44
1:D:355:LEU:HD11	1:D:385:MET:HG3	1.99	0.43
1:C:197:LEU:HD12	1:C:331:ALA:HB2	2.01	0.43
1:C:275:VAL:CG1	1:C:311:GLU:HG3	2.49	0.43
1:B:217:ILE:HG21	1:B:349:ILE:HD12	2.00	0.42
1:B:44:LYS:HB3	1:B:44:LYS:HE3	1.97	0.42
1:A:76:GLN:HG2	1:A:114:LEU:HD11	1.99	0.42
1:C:29:GLN:NE2	1:C:75:SER:OG	2.53	0.42
1:A:58:ARG:HD3	5:A:632:HOH:O	2.20	0.42
1:A:106:ASN:HB2	5:A:692:HOH:O	2.19	0.42
1:C:348:GLN:NE2	5:C:612:HOH:O	2.47	0.42
1:D:115:SER:HB3	1:D:120:LEU:O	2.20	0.42
1:B:146:GLU:H	1:B:146:GLU:CD	2.23	0.42
1:B:55:LEU:O	1:B:55:LEU:HG	2.11	0.41
1:C:104:PRO:HB2	5:C:808:HOH:O	2.19	0.41
1:D:250:GLU:OE2	5:D:601:HOH:O	2.22	0.41
1:D:401:LYS:HA	1:D:401:LYS:HD3	1.85	0.41
1:C:296:ARG:O	1:C:304:ARG:HD3	2.20	0.41
1:B:51:GLU:HG2	1:B:155:ARG:NH2	2.34	0.41
1:D:315:SER:HB3	1:D:318:GLU:HB2	2.02	0.41
1:B:115:SER:HB3	1:B:120:LEU:O	2.20	0.41
1:C:347:LEU:HD22	1:C:385:MET:SD	2.61	0.41
1:D:188:MET:SD	1:D:316:VAL:HG22	2.61	0.41
1:A:261:GLY:CA	3:A:502:GOL:H31	2.51	0.40
1:C:297:ARG:NH2	5:C:623:HOH:O	2.54	0.40
1:A:261:GLY:HA3	3:A:502:GOL:H11	2.02	0.40
1:A:356:ILE:HB	1:A:357:PRO:HD3	2.04	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:TYR:CD1	1:D:264:ALA:HA	2.56	0.40
1:B:217:ILE:HD11	2:B:501:HEM:HAB	2.03	0.40
1:A:126:TYR:CD1	1:A:264:ALA:HA	2.55	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	364/405 (90%)	356 (98%)	8 (2%)	0	100	100
1	B	369/405 (91%)	364 (99%)	5 (1%)	0	100	100
1	C	366/405 (90%)	358 (98%)	8 (2%)	0	100	100
1	D	365/405 (90%)	357 (98%)	8 (2%)	0	100	100
All	All	1464/1620 (90%)	1435 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	316/346 (91%)	311 (98%)	5 (2%)	62	67
1	B	318/346 (92%)	315 (99%)	3 (1%)	78	83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	317/346 (92%)	312 (98%)	5 (2%)	62	67
1	D	316/346 (91%)	312 (99%)	4 (1%)	69	74
All	All	1267/1384 (92%)	1250 (99%)	17 (1%)	69	74

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	214	PHE
1	A	215	HIS
1	A	237	TRP
1	A	393	SER
1	B	214	PHE
1	B	237	TRP
1	B	287	HIS
1	C	72	ASP
1	C	80	ARG
1	C	209	LYS
1	C	214	PHE
1	C	272	CYS
1	D	209	LYS
1	D	214	PHE
1	D	237	TRP
1	D	309	SER

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

Mol	Chain	Res	Type
1	A	27	ASN
1	A	76	GLN
1	A	220	HIS
1	A	348	GLN
1	C	29	GLN
1	C	191	GLN
1	C	290	GLN
1	C	360	GLN
1	D	189	GLN
1	D	216	GLN
1	D	360	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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$
4	PO4	D	503	-	4,4,4	0.78	0	6,6,6	0.46	0
3	GOL	A	502	-	5,5,5	1.40	2 (40%)	5,5,5	0.71	0
3	GOL	D	505	-	5,5,5	0.77	0	5,5,5	0.57	0
3	GOL	A	503	-	5,5,5	0.62	0	5,5,5	1.44	1 (20%)
4	PO4	D	502	-	4,4,4	0.66	0	6,6,6	0.91	0
3	GOL	D	506	-	5,5,5	0.92	0	5,5,5	1.16	1 (20%)
2	HEM	C	501	1	42,50,50	1.44	5 (11%)	46,82,82	1.49	7 (15%)
2	HEM	D	501	1	42,50,50	1.45	5 (11%)	46,82,82	1.39	10 (21%)
3	GOL	D	504	-	5,5,5	1.21	1 (20%)	5,5,5	1.10	0
2	HEM	B	501	1	42,50,50	1.46	5 (11%)	46,82,82	1.33	7 (15%)
4	PO4	B	502	-	4,4,4	0.78	0	6,6,6	0.32	0
2	HEM	A	501	1	42,50,50	1.47	6 (14%)	46,82,82	1.57	10 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	D	505	-	-	2/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	D	506	-	-	2/4/4/4	-
2	HEM	C	501	1	-	3/12/54/54	-
2	HEM	D	501	1	-	3/12/54/54	-
3	GOL	D	504	-	-	4/4/4/4	-
2	HEM	B	501	1	-	3/12/54/54	-
2	HEM	A	501	1	-	3/12/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-4.13	1.34	1.40
2	D	501	HEM	C3C-C2C	-3.80	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.74	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.59	1.35	1.40
2	D	501	HEM	C3C-CAC	3.34	1.55	1.47
2	B	501	HEM	C3C-CAC	3.21	1.54	1.47
2	A	501	HEM	C3C-CAC	3.17	1.54	1.47
2	C	501	HEM	CAB-C3B	3.07	1.55	1.47
2	B	501	HEM	CAB-C3B	2.97	1.55	1.47
2	A	501	HEM	CAB-C3B	2.90	1.55	1.47
2	C	501	HEM	C3C-CAC	2.88	1.54	1.47
2	D	501	HEM	CAB-C3B	2.86	1.55	1.47
2	D	501	HEM	C3C-C4C	2.72	1.45	1.41
3	A	502	GOL	C3-C2	2.31	1.60	1.51
2	A	501	HEM	FE-ND	2.30	2.10	1.98
2	B	501	HEM	C3C-C4C	2.26	1.44	1.41
2	A	501	HEM	CMD-C2D	2.21	1.55	1.50
2	A	501	HEM	C3C-C4C	2.14	1.44	1.41
2	C	501	HEM	CMB-C2B	2.04	1.55	1.50
2	C	501	HEM	CMD-C2D	2.04	1.54	1.50
3	D	504	GOL	O2-C2	-2.03	1.37	1.43
2	B	501	HEM	CMD-C2D	2.02	1.54	1.50
3	A	502	GOL	C1-C2	2.01	1.59	1.51
2	D	501	HEM	CMB-C2B	2.00	1.54	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4C-CHD-C1D	3.55	127.24	122.56
2	C	501	HEM	CAA-CBA-CGA	-3.37	104.75	113.83
2	A	501	HEM	C1B-NB-C4B	3.04	108.80	105.21
2	D	501	HEM	C4C-CHD-C1D	2.92	126.42	122.56
2	C	501	HEM	CMC-C2C-C3C	2.70	130.09	124.68
2	A	501	HEM	C4A-C3A-C2A	2.70	108.88	107.00
2	C	501	HEM	C1B-NB-C4B	2.69	108.39	105.21
2	B	501	HEM	C4C-CHD-C1D	2.68	126.10	122.56
2	A	501	HEM	C3B-C2B-C1B	2.65	108.40	106.41
2	C	501	HEM	C2C-C3C-C4C	2.59	108.71	106.90
2	A	501	HEM	C2C-C3C-C4C	2.58	108.70	106.90
2	C	501	HEM	C3B-C2B-C1B	2.56	108.33	106.41
2	A	501	HEM	CAA-CBA-CGA	-2.46	107.20	113.83
2	B	501	HEM	C3B-C2B-C1B	2.42	108.23	106.41
2	D	501	HEM	CMC-C2C-C3C	2.41	129.50	124.68
2	B	501	HEM	C4A-C3A-C2A	2.38	108.65	107.00
2	A	501	HEM	C3B-C4B-NB	-2.37	107.77	109.47
2	D	501	HEM	C1B-NB-C4B	2.28	107.91	105.21
2	A	501	HEM	CMC-C2C-C3C	2.28	129.24	124.68
2	D	501	HEM	C3B-C2B-C1B	2.23	108.08	106.41
2	B	501	HEM	CAA-CBA-CGA	-2.22	107.86	113.83
2	A	501	HEM	C4D-ND-C1D	2.22	107.83	105.21
2	D	501	HEM	CMA-C3A-C4A	-2.21	125.21	128.46
2	B	501	HEM	CMC-C2C-C3C	2.21	129.09	124.68
2	B	501	HEM	CMA-C3A-C4A	-2.18	125.26	128.46
2	B	501	HEM	CHB-C1B-NB	2.17	127.06	124.37
2	D	501	HEM	CHB-C1B-NB	2.16	127.05	124.37
2	D	501	HEM	CAA-CBA-CGA	-2.16	108.02	113.83
2	D	501	HEM	C4A-C3A-C2A	2.15	108.49	107.00
3	A	503	GOL	C3-C2-C1	-2.12	104.01	111.80
2	C	501	HEM	CMA-C3A-C4A	-2.12	125.35	128.46
2	C	501	HEM	C4C-CHD-C1D	2.12	125.35	122.56
2	D	501	HEM	C3B-C4B-NB	-2.10	107.96	109.47
2	A	501	HEM	C2B-C1B-NB	-2.06	107.47	109.84
2	D	501	HEM	C1D-C2D-C3D	2.06	109.14	106.98
3	D	506	GOL	C3-C2-C1	-2.04	104.30	111.80

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	C1-C2-C3-O3
3	D	504	GOL	O1-C1-C2-O2
3	D	504	GOL	O1-C1-C2-C3
3	D	505	GOL	C1-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O2-C2-C3-O3
3	A	502	GOL	C1-C2-C3-O3
3	D	506	GOL	O1-C1-C2-C3
3	D	505	GOL	O2-C2-C3-O3
3	D	506	GOL	O1-C1-C2-O2
3	A	503	GOL	O2-C2-C3-O3
3	D	504	GOL	O2-C2-C3-O3
3	D	504	GOL	C1-C2-C3-O3
2	C	501	HEM	CAA-CBA-CGA-O2A
3	A	503	GOL	O1-C1-C2-O2
2	C	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	C3D-CAD-CBD-CGD
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	C3D-CAD-CBD-CGD
2	B	501	HEM	C3D-CAD-CBD-CGD
2	D	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	C3D-CAD-CBD-CGD

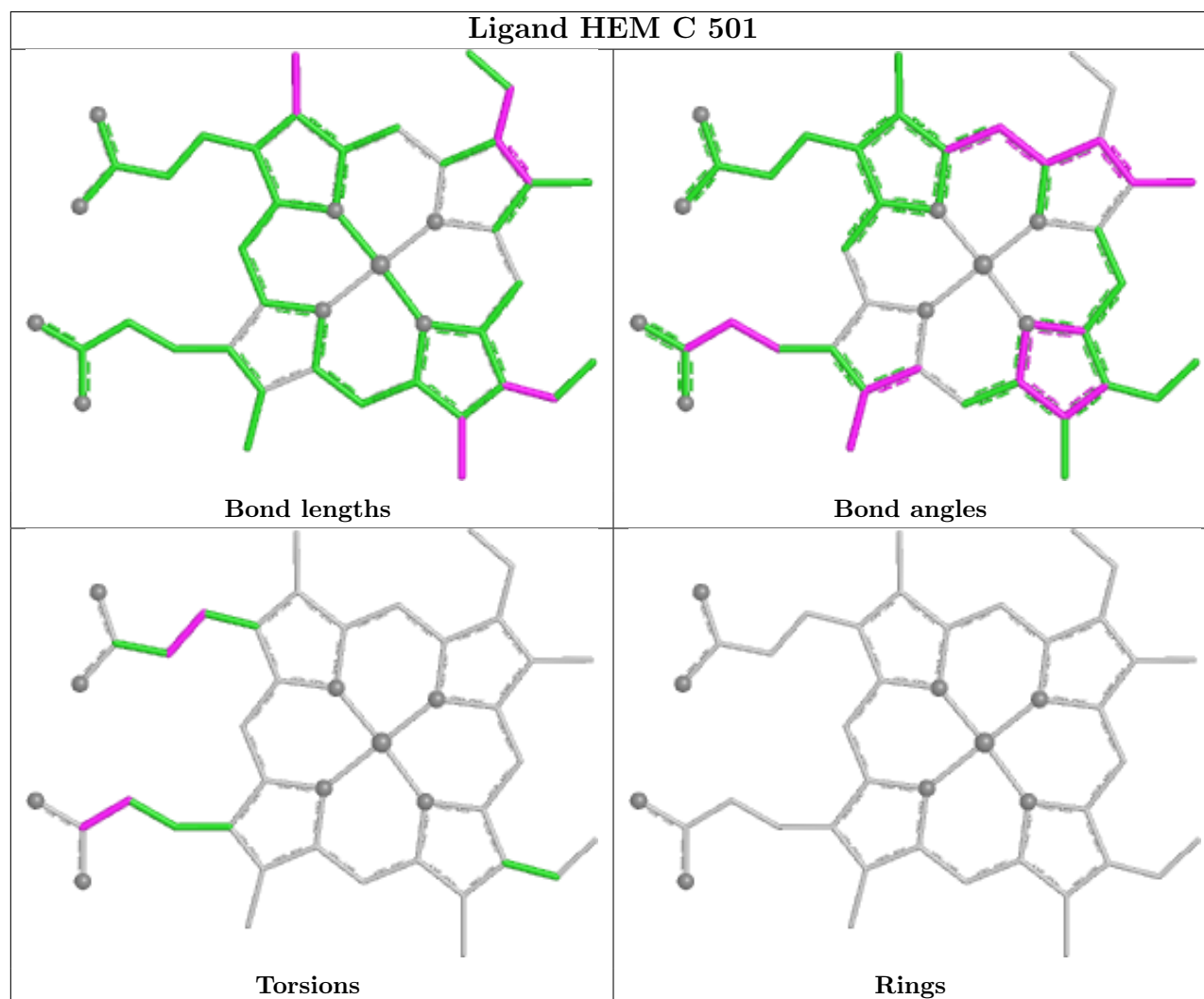
There are no ring outliers.

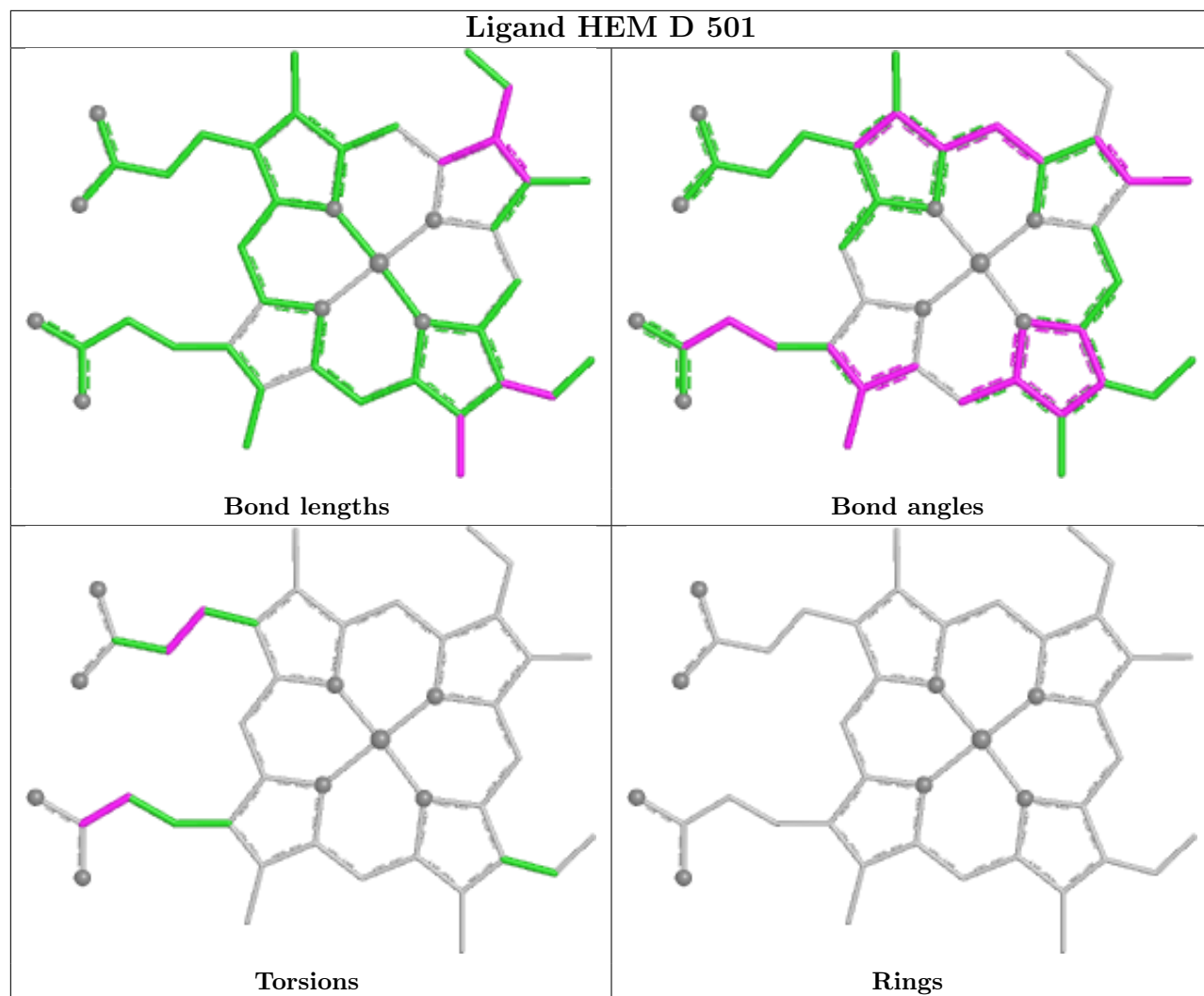
7 monomers are involved in 25 short contacts:

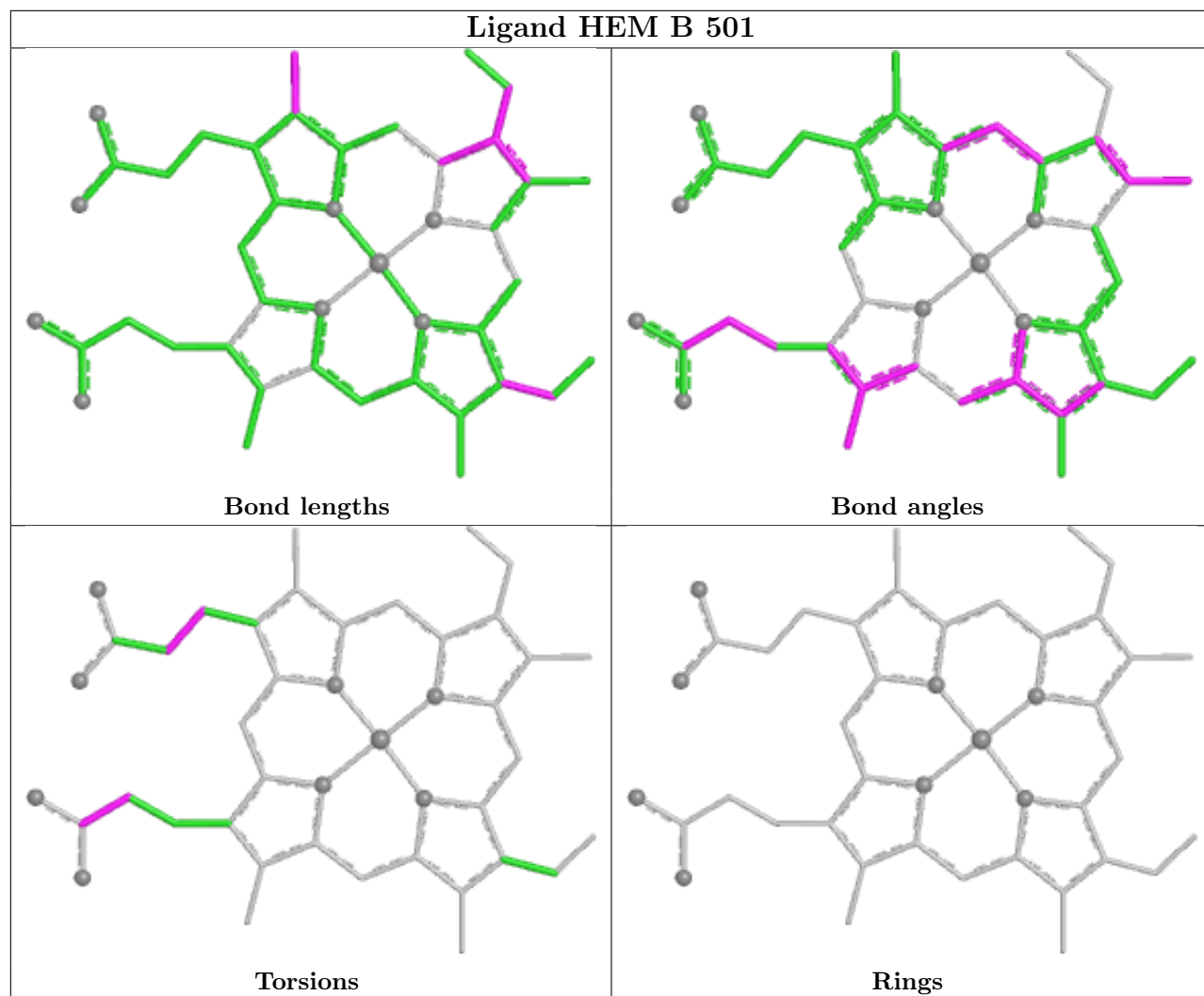
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	4	0
3	A	503	GOL	1	0
2	C	501	HEM	2	0
2	D	501	HEM	5	0
3	D	504	GOL	6	0
2	B	501	HEM	5	0
2	A	501	HEM	2	0

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

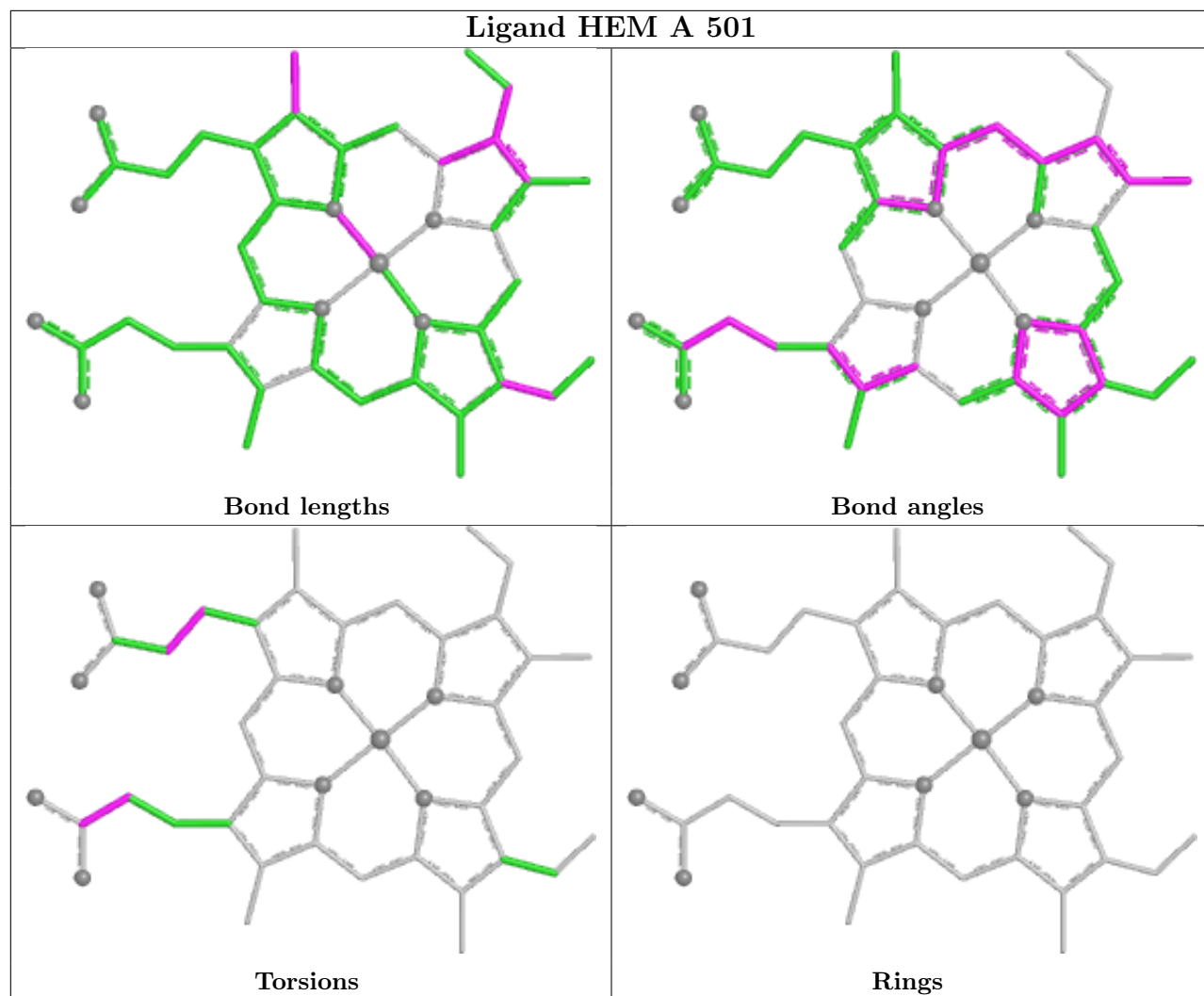
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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	368/405 (90%)	-0.01	2 (0%) 91 90	20, 34, 51, 63	0
1	B	373/405 (92%)	0.02	4 (1%) 80 79	19, 32, 49, 71	0
1	C	370/405 (91%)	-0.04	3 (0%) 86 85	20, 31, 49, 63	0
1	D	369/405 (91%)	0.00	0 100 100	17, 30, 49, 61	0
All	All	1480/1620 (91%)	-0.01	9 (0%) 89 88	17, 32, 50, 71	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	379	THR	6.0
1	A	401	LYS	4.7
1	B	377	LYS	3.8
1	B	376	ALA	3.4
1	B	380	GLY	2.7
1	C	380	GLY	2.7
1	A	189	GLN	2.2
1	C	381	GLY	2.1
1	C	68	ASP	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 monosaccharides in this entry.

## 6.4 Ligands

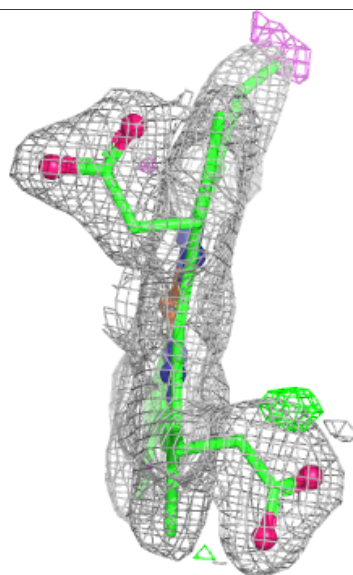
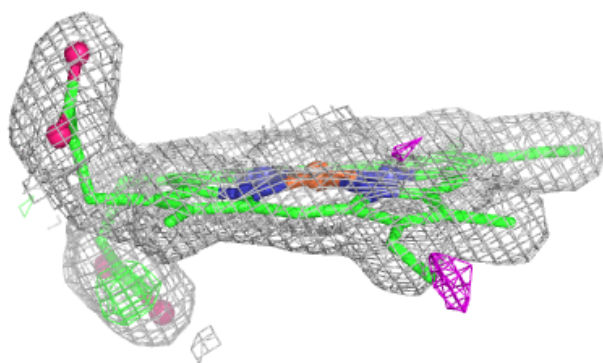
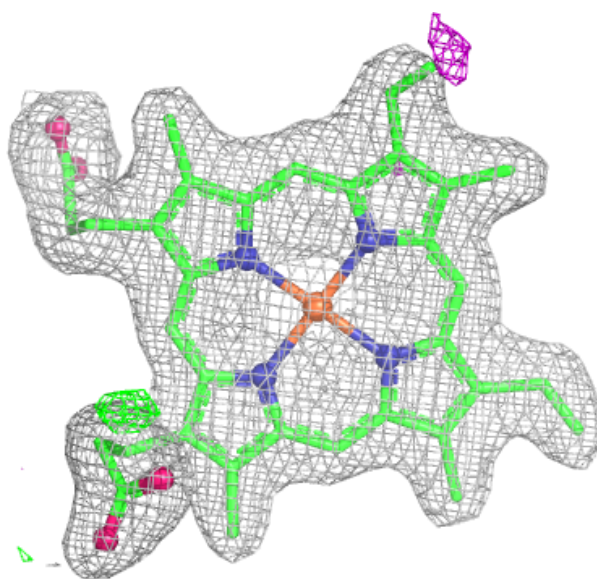
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	502	6/6	0.80	0.35	38,41,47,56	0
3	GOL	A	503	6/6	0.83	0.33	42,46,47,47	0
3	GOL	D	505	6/6	0.83	0.38	46,47,48,49	0
3	GOL	D	504	6/6	0.86	0.43	34,38,40,43	0
4	PO4	D	502	5/5	0.88	0.23	42,43,49,60	0
3	GOL	D	506	6/6	0.92	0.21	40,47,52,54	0
4	PO4	B	502	5/5	0.93	0.20	37,41,51,55	0
4	PO4	D	503	5/5	0.95	0.19	37,41,47,52	0
2	HEM	C	501	43/43	0.97	0.13	25,29,36,42	0
2	HEM	D	501	43/43	0.98	0.12	24,29,34,43	0
2	HEM	B	501	43/43	0.98	0.12	27,31,38,42	0
2	HEM	A	501	43/43	0.98	0.13	28,31,38,50	0

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

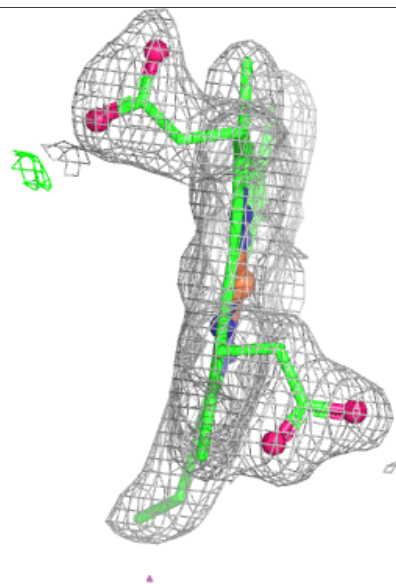
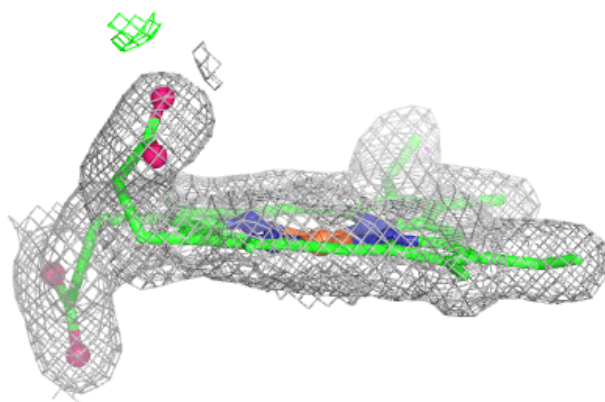
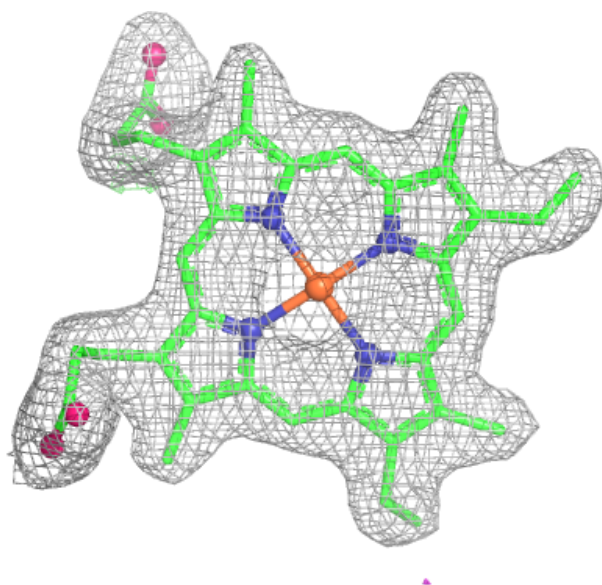
**Electron density around HEM C 501:**

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



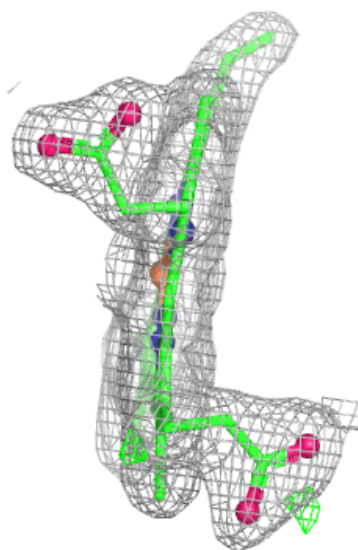
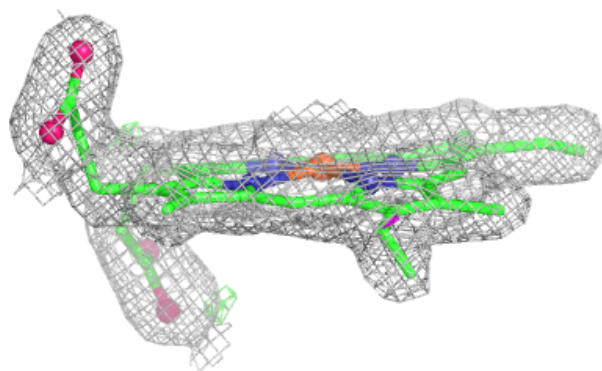
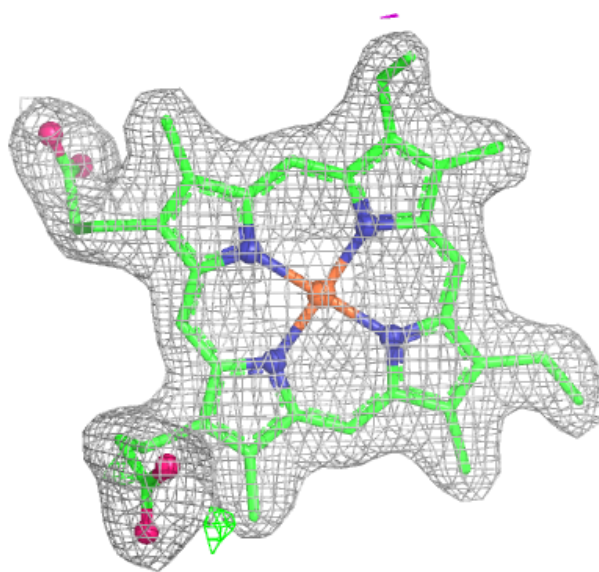
**Electron density around HEM D 501:**

$2mF_o-DF_c$  (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:**

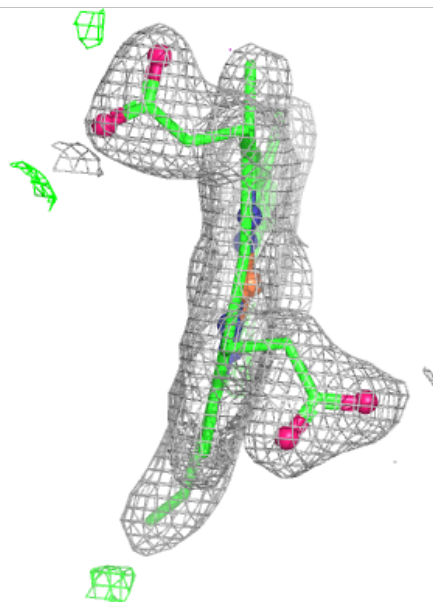
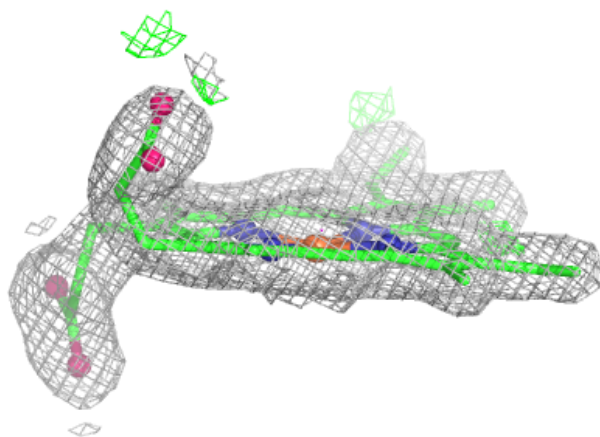
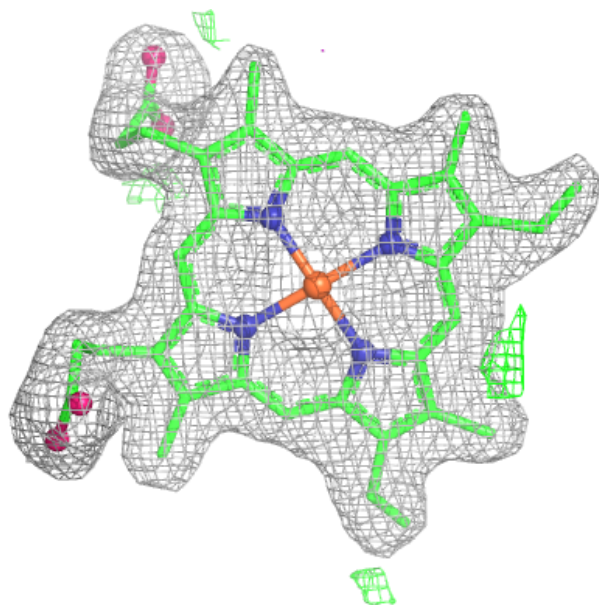
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.