



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:53 am BST

PDB ID : 4LHT  
Title : Crystal Structure of P450cin Y81F mutant, crystallized in 3 mM 1,8-cineole  
Authors : Madrona, Y.; Poulos, T.L.  
Deposited on : 2013-07-01  
Resolution : 2.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

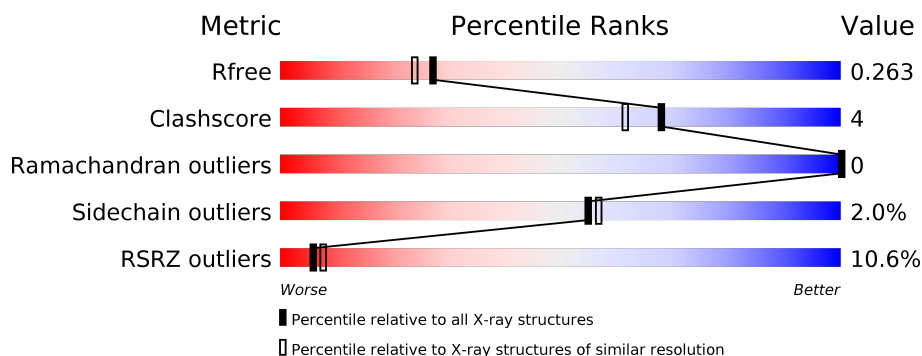
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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

Mol	Chain	Length	Quality of chain
1	A	398	<div> <div>10%</div> <div>89%</div> <div>10% ..</div> </div>
1	B	398	<div> <div>11%</div> <div>89%</div> <div>10% ..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CNL	B	502	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6857 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 P450cin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	1	0
			3146	2007	551	577	11			
1	B	396	Total	C	N	O	S	0	1	0
			3144	2006	548	579	11			

There are 4 discrepancies between the modelled and reference sequences:

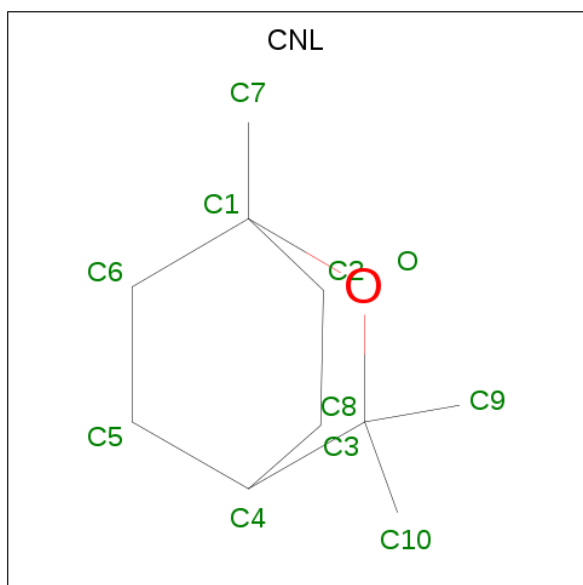
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	INITIATING METHIONINE	UNP Q8VQF6
A	81	PHE	TYR	ENGINEERED MUTATION	UNP Q8VQF6
B	7	MET	-	INITIATING METHIONINE	UNP Q8VQF6
B	81	PHE	TYR	ENGINEERED MUTATION	UNP Q8VQF6

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



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

- Molecule 3 is 1,3,3-TRIMETHYL-2-OXABICYCLO[2.2.2]OCTANE (three-letter code: CNL) (formula: C<sub>10</sub>H<sub>18</sub>O).



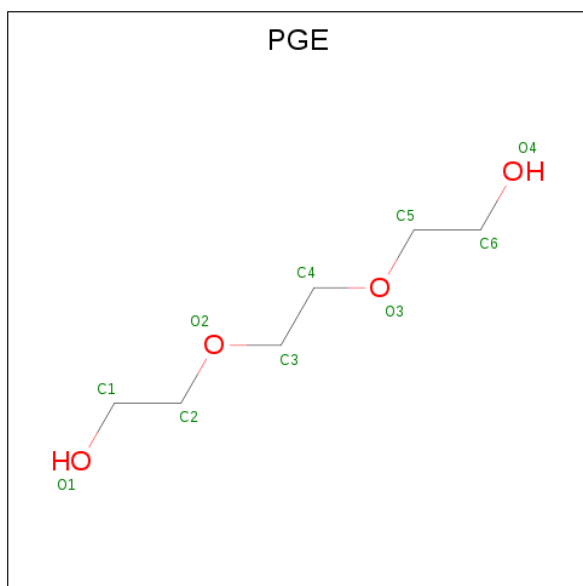
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			11	10	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).

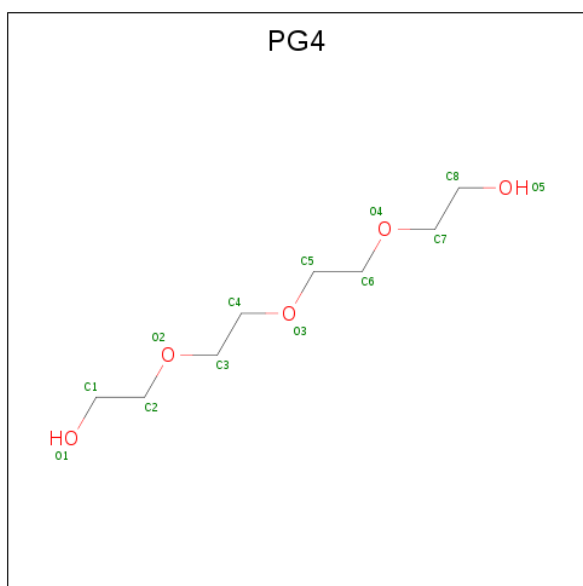


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is water.

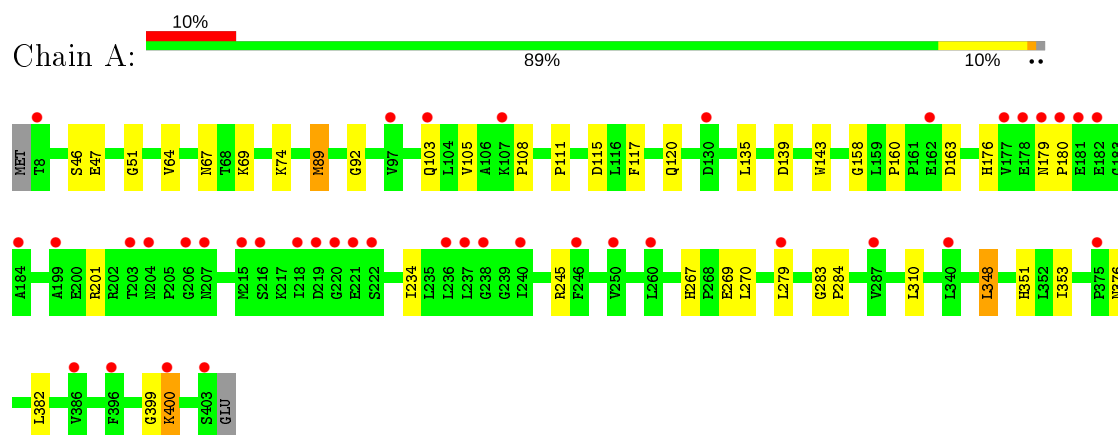
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	210	Total	O	0	0
			210	210		
9	B	213	Total	O	0	0
			213	213		



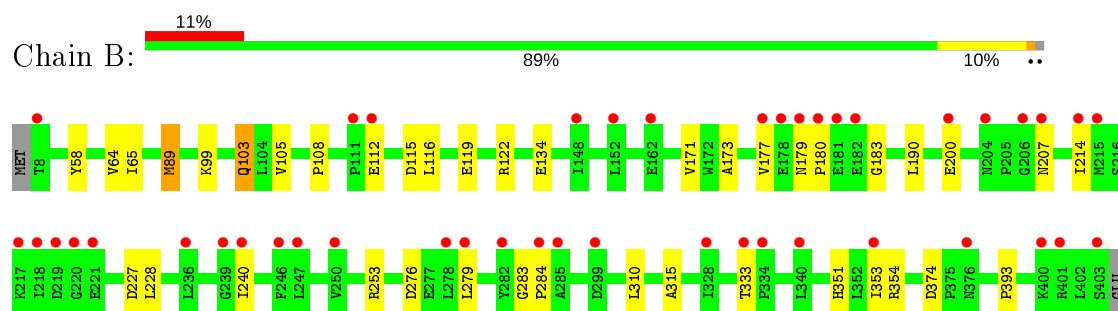
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: P450cin



#### • Molecule 1: P450cin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.46Å 103.71Å 127.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.88 – 2.14 34.69 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.2 (32.88-2.14) 98.2 (34.69-2.14)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.209 , 0.263 0.209 , 0.263	Depositor DCC
$R_{free}$ test set	2553 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6857	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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 36.20 % 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 5.1815e-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: PGE, CL, PG4, SO4, HEM, CNL, PEG

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	0.57	0/3229	0.63	0/4390
1	B	0.59	0/3227	0.63	0/4388
All	All	0.58	0/6456	0.63	0/8778

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

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	3146	0	3106	26	0
1	B	3144	0	3099	24	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	11	0	18	0	0
3	B	11	0	18	0	0
4	A	7	0	10	0	0
5	A	10	0	14	0	0
6	A	5	0	0	0	0
7	A	1	0	0	0	0
8	B	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	210	0	0	3	0
9	B	213	0	0	2	0
All	All	6857	0	6343	48	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 (48) 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:B:276:ASP:OD1	1:B:354:ARG:NH1	2.03	0.91
1:A:267:HIS:HB3	1:A:270:LEU:HD13	1.65	0.77
1:A:201:ARG:NH1	9:A:799:HOH:O	2.08	0.76
1:A:158:GLY:HA3	1:A:201:ARG:HH12	1.54	0.73
1:B:119:GLU:OE1	1:B:122:ARG:NH1	2.24	0.70
1:B:173:ALA:HA	1:B:177:VAL:HG22	1.78	0.64
1:A:67:ASN:OD1	1:A:69:LYS:HG2	1.98	0.62
1:A:269:GLU:HG2	1:A:270:LEU:HD12	1.82	0.61
1:B:227:ASP:OD2	9:B:801:HOH:O	2.16	0.60
1:B:171:VAL:HG21	1:B:240:ILE:HB	1.84	0.60
1:A:376:ASN:ND2	9:A:787:HOH:O	2.39	0.56
1:B:177:VAL:HG21	1:B:183:GLY:HA2	1.88	0.54
1:B:89:MET:HA	1:B:89:MET:HE2	1.90	0.54
1:A:279:LEU:HD11	1:A:353:ILE:HD11	1.91	0.53
1:A:117:PHE:CD1	1:B:119:GLU:HG3	2.44	0.52
1:B:134:GLU:OE1	9:B:776:HOH:O	2.19	0.51
1:B:279:LEU:HD11	1:B:353:ILE:HD11	1.93	0.51
1:A:115:ASP:HB3	1:B:116:LEU:CD2	2.42	0.49
1:B:284:PRO:HD2	2:B:501:HEM:HMB2	1.95	0.49
1:A:111:PRO:HA	1:A:351:HIS:CD2	2.49	0.48
1:A:105:VAL:O	1:A:108:PRO:HD2	2.14	0.47
1:A:234:ILE:HD13	2:A:501:HEM:HMD2	1.96	0.47
1:B:115:ASP:OD1	1:B:351:HIS:HE1	1.96	0.47
1:A:89:MET:HA	1:A:89:MET:HE2	1.97	0.47
1:B:99:LYS:NZ	1:B:103:GLN:OE1	2.47	0.47
1:A:103:GLN:OE1	9:A:790:HOH:O	2.20	0.46
1:A:46:SER:O	1:A:51:GLY:HA2	2.16	0.46
1:B:58:TYR:HA	1:B:315:ALA:HB1	1.97	0.46
1:A:284:PRO:HD2	2:A:501:HEM:HMB2	1.98	0.46
1:A:245:ARG:NE	1:A:245:ARG:HA	2.32	0.45
1:A:139:ASP:O	1:A:143:TRP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:HA	1:B:177:VAL:CG2	2.45	0.44
1:A:160:PRO:HB2	1:A:163:ASP:OD2	2.18	0.43
1:A:283:GLY:HA2	1:A:284:PRO:HD3	1.84	0.43
1:A:176:HIS:CE1	1:A:382:LEU:HD21	2.54	0.42
1:A:74:LYS:HD3	1:A:92:GLY:O	2.19	0.42
1:A:179:ASN:HA	1:A:180:PRO:HD3	1.82	0.42
1:B:253:ARG:HH11	1:B:253:ARG:HD3	1.73	0.42
1:B:105:VAL:O	1:B:108:PRO:HD2	2.20	0.41
1:B:190:LEU:HD23	1:B:190:LEU:C	2.40	0.41
1:B:64:VAL:HG11	1:B:310:LEU:HD21	2.02	0.41
1:A:64:VAL:HG11	1:A:310:LEU:HD21	2.02	0.41
1:A:348:LEU:HD12	2:A:501:HEM:HMD3	2.01	0.41
1:B:179:ASN:HA	1:B:180:PRO:HD3	1.78	0.41
1:A:399:GLY:C	1:A:400:LYS:HD3	2.41	0.41
1:B:283:GLY:HA2	1:B:284:PRO:HD3	1.75	0.41
1:B:374:ASP:HB3	1:B:393:PRO:HB2	2.02	0.41
1:B:214:ILE:HG12	1:B:228:LEU:HD13	2.03	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	395/398 (99%)	388 (98%)	7 (2%)	0	100	100
1	B	395/398 (99%)	388 (98%)	7 (2%)	0	100	100
All	All	790/796 (99%)	776 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/334 (100%)	327 (98%)	6 (2%)	59	60
1	B	333/334 (100%)	326 (98%)	7 (2%)	53	54
All	All	666/668 (100%)	653 (98%)	13 (2%)	55	57

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	89	MET
1	A	120	GLN
1	A	135	LEU
1	A	348	LEU
1	A	400	LYS
1	B	65	ILE
1	B	89	MET
1	B	103	GLN
1	B	112	GLU
1	B	200	GLU
1	B	207	ASN
1	B	333	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CNL	B	502	-	12,12,12	2.60	3 (25%)	19,20,20	1.01	1 (5%)
2	HEM	B	501	1	27,50,50	2.08	6 (22%)	17,82,82	2.05	6 (35%)
3	CNL	A	502	-	12,12,12	2.62	4 (33%)	19,20,20	1.09	1 (5%)
4	PEG	A	503	-	6,6,6	0.81	0	5,5,5	0.56	0
8	PG4	B	503	-	12,12,12	0.83	0	11,11,11	0.37	0
2	HEM	A	501	1	27,50,50	2.05	6 (22%)	17,82,82	2.09	5 (29%)
6	SO4	A	505	-	4,4,4	0.13	0	6,6,6	0.24	0
5	PGE	A	504	-	9,9,9	0.83	0	8,8,8	0.28	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
3	CNL	B	502	-	-	-	0/3/2/2
2	HEM	B	501	1	-	0/6/54/54	-
3	CNL	A	502	-	-	-	0/3/2/2
4	PEG	A	503	-	-	3/4/4/4	-
8	PG4	B	503	-	-	7/10/10/10	-
2	HEM	A	501	1	-	0/6/54/54	-
5	PGE	A	504	-	-	4/7/7/7	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	CNL	O-C8	7.10	1.58	1.45
3	A	502	CNL	O-C8	6.91	1.58	1.45
2	B	501	HEM	C3D-C2D	5.12	1.52	1.37
2	A	501	HEM	C3D-C2D	4.62	1.51	1.37
2	A	501	HEM	C3C-C2C	-4.21	1.34	1.40
2	B	501	HEM	C3B-CAB	4.16	1.56	1.47
2	B	501	HEM	C3C-C2C	-4.06	1.34	1.40
2	B	501	HEM	C3C-CAC	4.05	1.56	1.47
2	A	501	HEM	C3B-CAB	4.02	1.56	1.47
3	A	502	CNL	C5-C4	-3.88	1.43	1.53
2	A	501	HEM	C3C-CAC	3.77	1.55	1.47
3	B	502	CNL	C5-C4	-3.61	1.44	1.53
2	A	501	HEM	C3B-C2B	-3.15	1.36	1.40
2	B	501	HEM	CAA-C2A	2.99	1.56	1.52
2	A	501	HEM	CAA-C2A	2.62	1.55	1.52
2	B	501	HEM	C3B-C2B	-2.55	1.36	1.40
3	A	502	CNL	C2-C3	-2.31	1.48	1.53
3	A	502	CNL	C7-C1	-2.08	1.48	1.52
3	B	502	CNL	C2-C3	-2.01	1.49	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBD-CAD-C3D	-4.90	103.45	112.48
2	A	501	HEM	CMA-C3A-C4A	-3.61	122.91	128.46
2	B	501	HEM	CBD-CAD-C3D	-3.47	106.09	112.48
2	B	501	HEM	CMA-C3A-C4A	-3.38	123.26	128.46
3	A	502	CNL	C10-C8-C9	-3.29	104.91	110.51
2	B	501	HEM	C1D-C2D-C3D	-3.28	104.72	107.00
2	B	501	HEM	CAD-CBD-CGD	-3.16	107.36	112.67
3	B	502	CNL	C10-C8-C9	-3.00	105.40	110.51
2	A	501	HEM	CAD-CBD-CGD	-2.71	108.12	112.67
2	A	501	HEM	C4A-C3A-C2A	2.71	108.88	107.00
2	B	501	HEM	CMB-C2B-C3B	2.54	129.44	124.68
2	B	501	HEM	C4A-C3A-C2A	2.25	108.56	107.00
2	A	501	HEM	CMB-C2B-C3B	2.24	128.87	124.68

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	PEG	O1-C1-C2-O2

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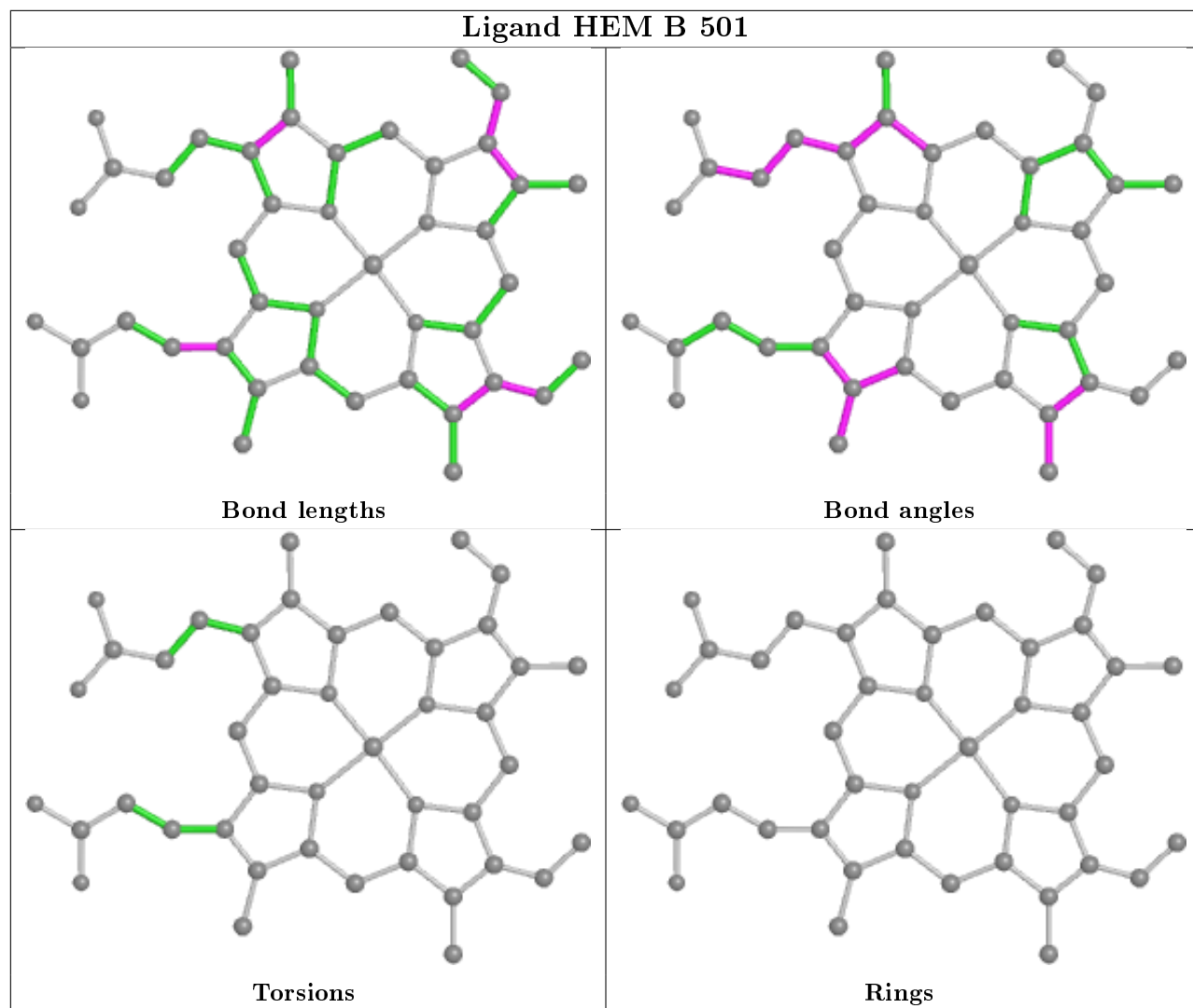
Mol	Chain	Res	Type	Atoms
8	B	503	PG4	O4-C7-C8-O5
8	B	503	PG4	O1-C1-C2-O2
5	A	504	PGE	O3-C5-C6-O4
4	A	503	PEG	C4-C3-O2-C2
4	A	503	PEG	C1-C2-O2-C3
5	A	504	PGE	C1-C2-O2-C3
8	B	503	PG4	C5-C6-O4-C7
8	B	503	PG4	C8-C7-O4-C6
5	A	504	PGE	C4-C3-O2-C2
5	A	504	PGE	C3-C4-O3-C5
8	B	503	PG4	C3-C4-O3-C5
8	B	503	PG4	O3-C5-C6-O4
8	B	503	PG4	C1-C2-O2-C3

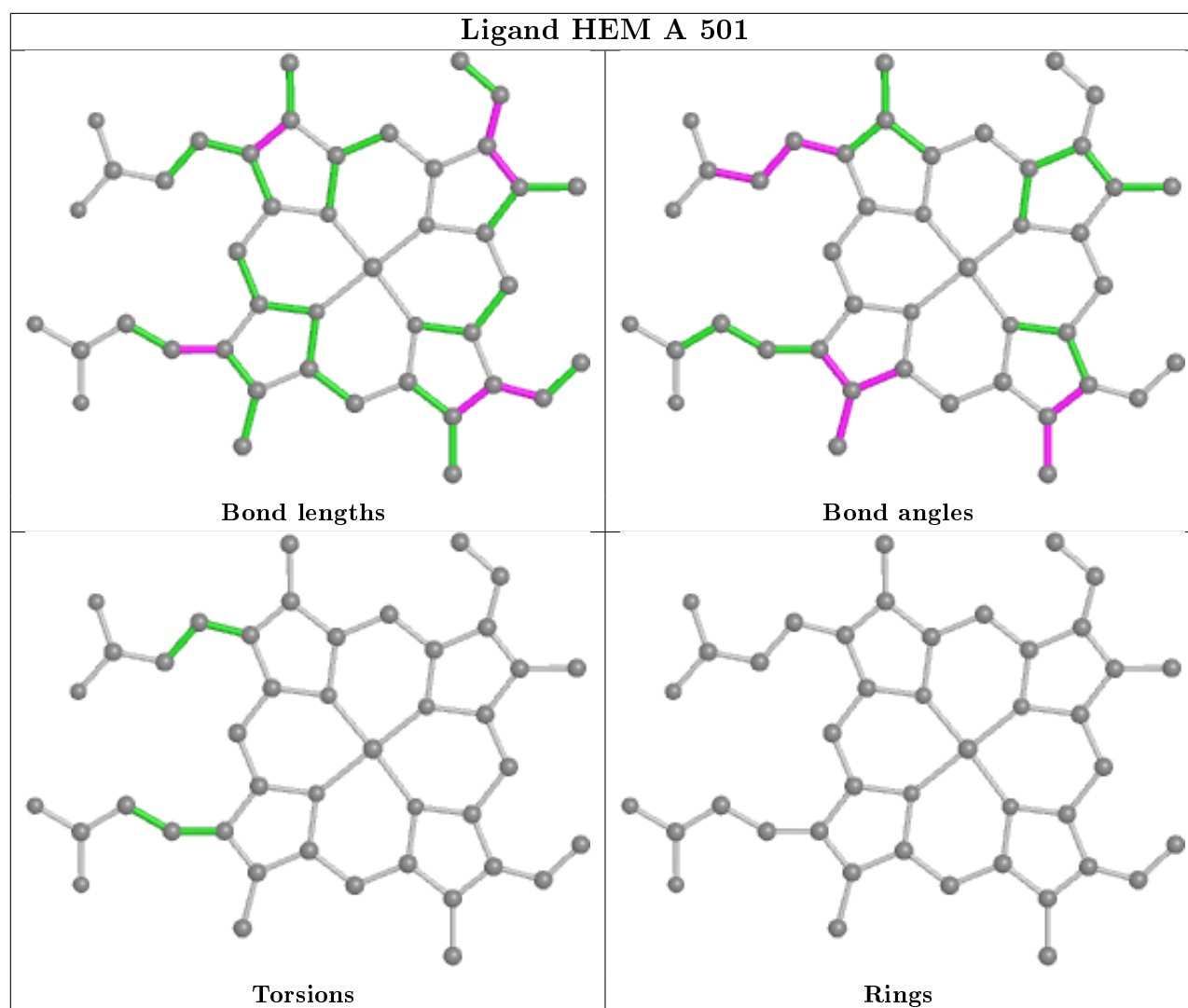
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	1	0
2	A	501	HEM	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	396/398 (99%)	0.85	40 (10%) <b>7</b> <b>9</b>	13, 24, 48, 70	0
1	B	396/398 (99%)	0.81	44 (11%) <b>5</b> <b>6</b>	13, 24, 45, 68	0
All	All	792/796 (99%)	0.83	84 (10%) <b>6</b> <b>8</b>	13, 24, 47, 70	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	VAL	8.6
1	A	8	THR	7.7
1	A	181	GLU	7.2
1	B	8	THR	7.2
1	B	181	GLU	6.5
1	B	177	VAL	6.2
1	A	219	ASP	6.1
1	B	218	ILE	6.0
1	A	221	GLU	5.3
1	A	179	ASN	4.8
1	B	403	SER	4.8
1	A	207	ASN	4.7
1	B	221	GLU	4.7
1	B	219	ASP	4.6
1	B	179	ASN	4.6
1	B	207	ASN	4.5
1	B	334	PRO	4.5
1	B	180	PRO	4.5
1	A	218	ILE	4.3
1	B	220	GLY	4.2
1	B	333	THR	4.2
1	A	204	ASN	4.1
1	B	204	ASN	4.1
1	A	220	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	403	SER	3.9
1	B	299	ASP	3.8
1	A	180	PRO	3.8
1	A	182	GLU	3.7
1	A	400	LYS	3.1
1	A	162	GLU	3.0
1	B	215	MET	3.0
1	A	222	SER	2.8
1	B	178	GLU	2.8
1	A	250	VAL	2.8
1	A	240	ILE	2.8
1	A	279	LEU	2.7
1	B	278	LEU	2.7
1	B	247	LEU	2.7
1	A	215	MET	2.7
1	A	386	VAL	2.7
1	B	282	TYR	2.6
1	B	217	LYS	2.6
1	A	216	SER	2.5
1	A	103	GLN	2.5
1	B	246	PHE	2.5
1	A	97	VAL	2.5
1	A	238	GLY	2.5
1	A	206	GLY	2.4
1	B	284	PRO	2.4
1	A	236	LEU	2.4
1	B	236	LEU	2.3
1	B	162	GLU	2.3
1	B	328	ILE	2.3
1	A	178	GLU	2.3
1	A	237	LEU	2.3
1	B	340	LEU	2.3
1	B	200	GLU	2.3
1	B	400	LYS	2.3
1	B	279	LEU	2.2
1	B	376	ASN	2.2
1	B	250	VAL	2.2
1	A	130	ASP	2.2
1	B	148	ILE	2.1
1	A	340	LEU	2.1
1	B	285	ALA	2.1
1	A	203	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	182	GLU	2.1
1	B	214	ILE	2.1
1	B	240	ILE	2.1
1	A	107	LYS	2.1
1	B	111	PRO	2.1
1	B	112	GLU	2.1
1	A	246	PHE	2.1
1	B	152	LEU	2.0
1	A	260	LEU	2.0
1	A	287	VAL	2.0
1	A	396	PHE	2.0
1	A	375	PRO	2.0
1	A	184	ALA	2.0
1	A	199	ALA	2.0
1	B	353	ILE	2.0
1	B	401	ARG	2.0
1	B	206	GLY	2.0
1	B	239	GLY	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 carbohydrates 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
5	PGE	A	504	10/10	0.70	0.23	49,53,58,58	0
8	PG4	B	503	13/13	0.78	0.19	48,56,75,76	0
3	CNL	B	502	11/11	0.78	0.48	28,32,34,36	6
6	SO4	A	505	5/5	0.86	0.23	76,79,80,82	0
2	HEM	B	501	43/43	0.89	0.20	15,20,23,28	0

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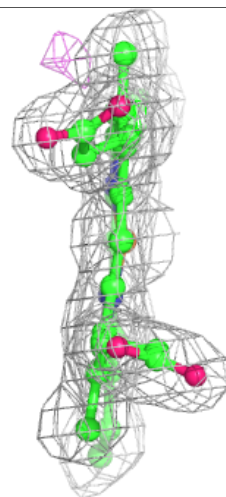
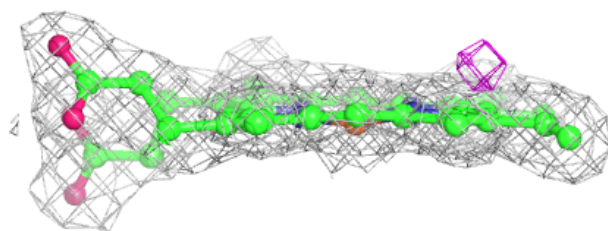
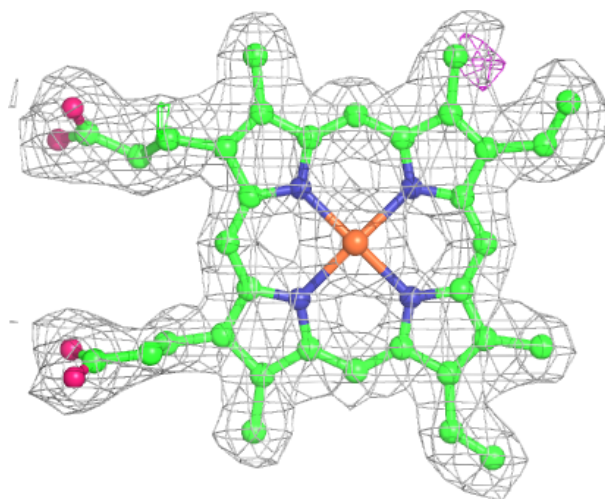
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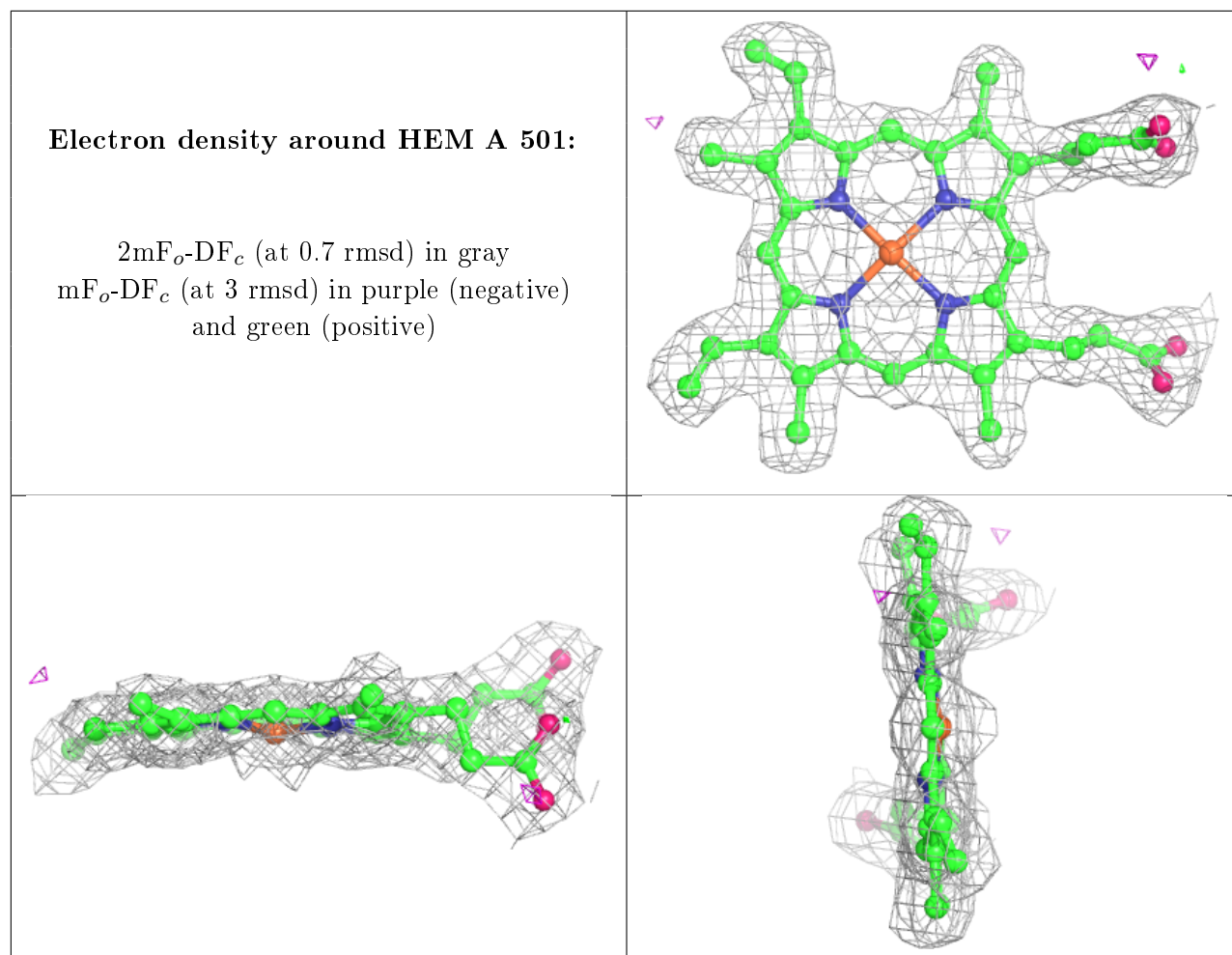
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	A	503	7/7	0.91	0.14	42,42,54,55	0
2	HEM	A	501	43/43	0.91	0.21	12,21,25,27	0
3	CNL	A	502	11/11	0.93	0.60	18,20,23,23	9
7	CL	A	506	1/1	0.99	0.15	24,24,24,24	0

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

**Electron density around HEM B 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.