



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:27 pm BST

PDB ID : 1W0G  
Title : Crystal structure of human cytochrome P450 3A4  
Authors : Williams, P.A.; Cosme, J.; Vinkovic, D.M.; Ward, A.; Angove, H.C.; Day, P.J.;  
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Deposited on : 2004-06-03  
Resolution : 2.73 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

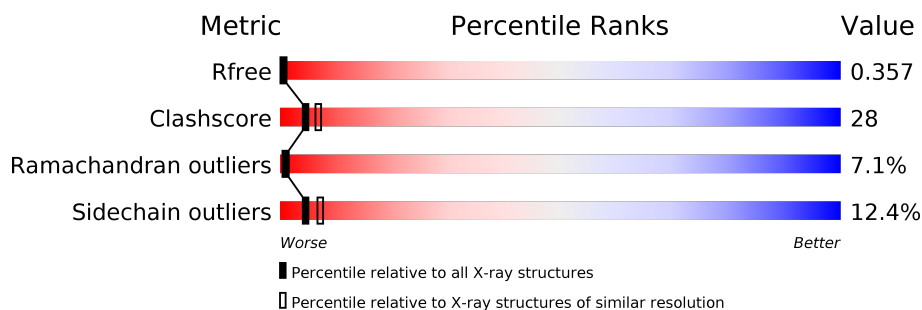
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	485	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3741 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.

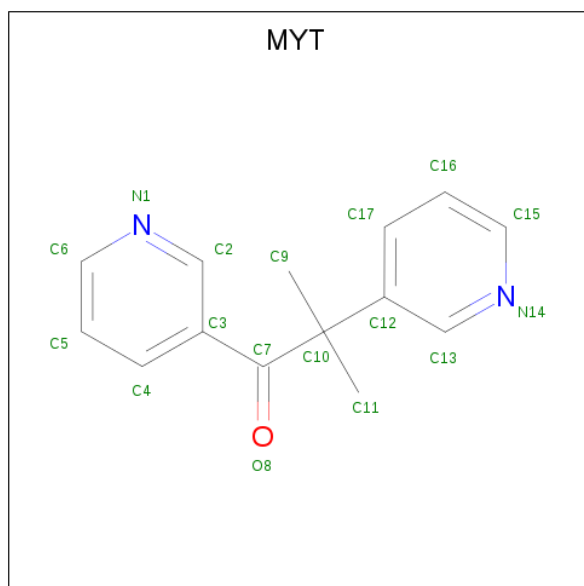
- Molecule 1 is a protein called CYTOCHROME P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	455	3652	2382	597	649	24	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	VAL	TRP	conflict	UNP P08684

- Molecule 2 is METYRAPONE (three-letter code: MYT) (formula: C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	17	14	2	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

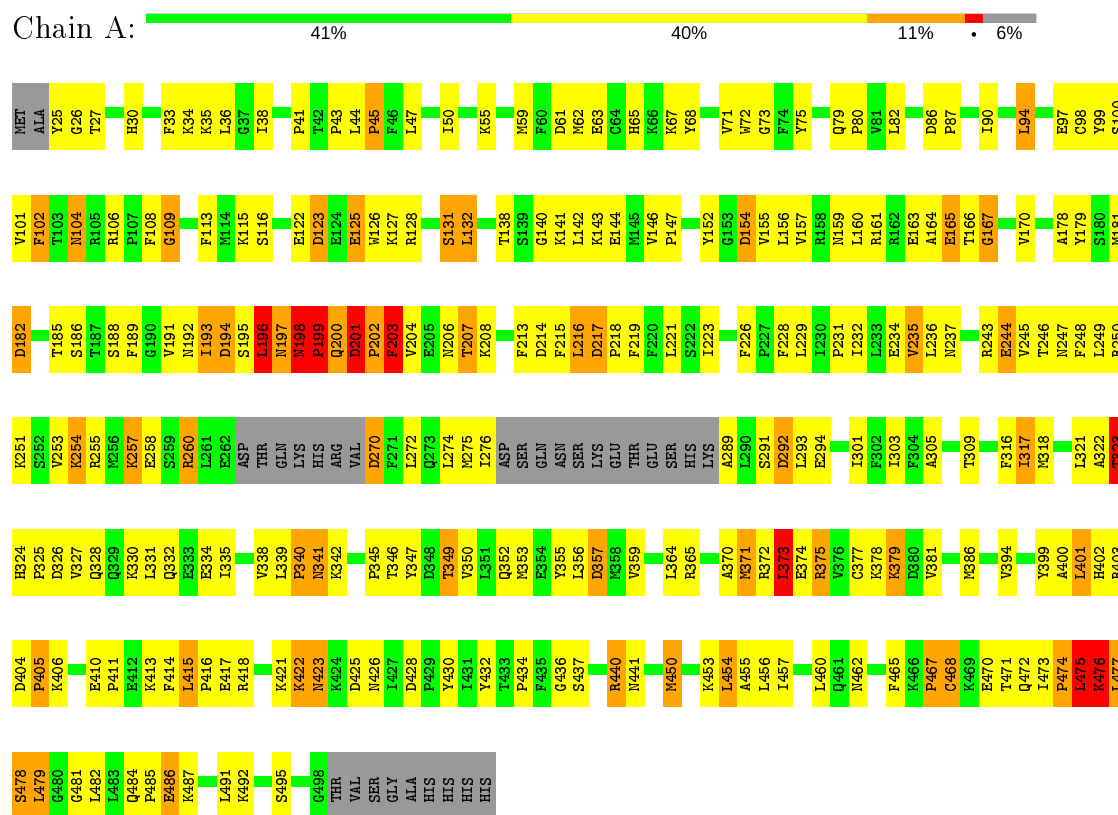
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		

### 3 Residue-property plots

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. 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. 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: CYTOCHROME P450 3A4



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.94Å 100.91Å 131.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 2.73 40.08 – 2.71	Depositor EDS
% Data completeness (in resolution range)	93.9 (81.65-2.73) 91.8 (40.08-2.71)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0003A	Depositor
R, $R_{free}$	0.234 , 0.318 0.374 , 0.357	Depositor DCC
$R_{free}$ test set	652 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.9	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	0.84	EDS
Total number of atoms	3741	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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

### 5.1 Standard geometry

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

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	0.76	0/3742	0.95	18/5063 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	214	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	217	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	475	LEU	CA-CB-CG	7.45	132.44	115.30
1	A	61	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	123	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	357	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	86	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	182	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	326	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	194	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	154	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	270	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	201	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	292	ASP	CB-CG-OD2	5.51	123.25	118.30
1	A	196	LEU	CA-CB-CG	5.47	127.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	373	LEU	N-CA-C	-5.21	96.92	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	421	LYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	PRO	Peptide
1	A	322	ALA	Peptide
1	A	323	THR	Peptide
1	A	33	PHE	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3652	0	3728	210	5
2	A	17	0	14	5	0
3	A	43	0	30	4	0
4	A	29	0	0	5	0
All	All	3741	0	3772	213	5

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 28.

All (213) 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:A:472:GLN:HB2	1:A:476:LYS:HZ1	1.37	0.90
1:A:178:ALA:HB3	1:A:196:LEU:HD12	1.55	0.88
1:A:104:ASN:ND2	1:A:123:ASP:OD1	2.09	0.86
1:A:178:ALA:HB1	1:A:196:LEU:HA	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HE22	1:A:487:LYS:NZ	1.78	0.81
1:A:25:TYR:HB3	4:A:2001:HOH:O	1.82	0.79
1:A:472:GLN:HE22	1:A:487:LYS:HZ3	1.30	0.77
1:A:332:GLN:HA	1:A:335:ILE:HD12	1.69	0.74
1:A:373:LEU:HD21	1:A:436:GLY:HA2	1.69	0.74
1:A:413:LYS:HB2	1:A:415:LEU:HD11	1.70	0.73
1:A:198:ASN:O	1:A:200:GLN:N	2.22	0.72
1:A:276:ILE:N	1:A:276:ILE:HD12	2.05	0.71
1:A:101:VAL:HA	1:A:378:LYS:HG3	1.72	0.71
1:A:146:VAL:HG13	1:A:454:LEU:HD21	1.73	0.70
1:A:178:ALA:CB	1:A:196:LEU:HA	2.21	0.70
1:A:472:GLN:HB2	1:A:476:LYS:NZ	2.05	0.70
1:A:101:VAL:HG22	1:A:102:PHE:CD1	2.26	0.70
1:A:323:THR:O	1:A:324:HIS:CD2	2.47	0.68
1:A:330:LYS:HB3	1:A:355:TYR:CE1	2.30	0.67
1:A:477:LEU:N	1:A:485:PRO:O	2.24	0.67
1:A:345:PRO:HG3	1:A:457:ILE:HG21	1.75	0.67
1:A:357:ASP:HA	1:A:453:LYS:HZ1	1.58	0.66
1:A:479:LEU:HD23	1:A:479:LEU:H	1.60	0.66
1:A:201:ASP:H	1:A:202:PRO:HD3	1.59	0.66
1:A:201:ASP:N	1:A:202:PRO:HD3	2.11	0.66
1:A:55:LYS:HB3	1:A:59:MET:HB2	1.76	0.66
1:A:377:CYS:SG	1:A:379:LYS:O	2.53	0.65
1:A:181:MET:O	1:A:185:THR:HG23	1.97	0.65
1:A:179:TYR:CE1	1:A:455:ALA:HB2	2.31	0.64
1:A:251:LYS:O	1:A:254:LYS:HB3	1.97	0.63
1:A:309:THR:HG21	2:A:1499:MYT:H16	1.79	0.63
1:A:370:ALA:O	1:A:372:ARG:N	2.32	0.63
1:A:185:THR:HG21	1:A:193:ILE:HD11	1.81	0.63
1:A:155:VAL:HG12	1:A:196:LEU:HD22	1.82	0.62
1:A:101:VAL:HG23	1:A:378:LYS:HB2	1.81	0.62
1:A:99:TYR:HD2	1:A:127:LYS:CE	2.13	0.62
1:A:194:ASP:OD2	1:A:198:ASN:ND2	2.27	0.60
1:A:123:ASP:OD1	1:A:378:LYS:NZ	2.31	0.60
1:A:423:ASN:O	1:A:426:ASN:ND2	2.34	0.60
1:A:318:MET:CE	1:A:465:PHE:CD2	2.84	0.60
1:A:62:MET:O	1:A:65:HIS:N	2.35	0.60
1:A:140:GLY:O	1:A:144:GLU:HB2	2.03	0.59
1:A:99:TYR:HD2	1:A:127:LYS:HE2	1.68	0.58
1:A:321:LEU:HD21	1:A:359:VAL:HG11	1.86	0.57
1:A:101:VAL:O	1:A:102:PHE:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HB3	1:A:476:LYS:HE3	1.85	0.57
1:A:357:ASP:HA	1:A:453:LYS:NZ	2.20	0.57
1:A:415:LEU:N	1:A:415:LEU:HD12	2.21	0.56
1:A:178:ALA:HB1	1:A:196:LEU:CA	2.32	0.56
1:A:253:VAL:HG13	1:A:272:LEU:HD21	1.88	0.56
1:A:475:LEU:C	1:A:476:LYS:HD3	2.26	0.55
1:A:472:GLN:CB	1:A:476:LYS:HE3	2.37	0.55
1:A:291:SER:HB3	1:A:294:GLU:CD	2.27	0.55
1:A:164:ALA:O	1:A:167:GLY:N	2.39	0.54
1:A:195:SER:O	1:A:197:ASN:N	2.40	0.54
1:A:228:PHE:O	1:A:231:PRO:HD2	2.08	0.54
1:A:178:ALA:CB	1:A:196:LEU:HD12	2.34	0.54
1:A:482:LEU:HB2	1:A:484:GLN:OE1	2.07	0.54
1:A:25:TYR:CB	4:A:2001:HOH:O	2.49	0.54
1:A:25:TYR:CD1	4:A:2001:HOH:O	2.53	0.54
1:A:47:LEU:HD22	1:A:50:ILE:HD11	1.90	0.54
1:A:400:ALA:O	1:A:401:LEU:C	2.46	0.53
1:A:154:ASP:O	1:A:157:VAL:HG22	2.09	0.53
1:A:159:ASN:HD22	1:A:196:LEU:HD23	1.73	0.53
1:A:189:PHE:O	1:A:260:ARG:NH2	2.42	0.52
1:A:26:GLY:O	1:A:45:PRO:O	2.28	0.52
1:A:146:VAL:N	1:A:147:PRO:CD	2.72	0.52
1:A:94:LEU:HD21	1:A:373:LEU:HD23	1.92	0.52
1:A:138:THR:OG1	1:A:141:LYS:HD3	2.09	0.52
1:A:328:GLN:O	1:A:332:GLN:HG3	2.10	0.52
1:A:485:PRO:O	1:A:486:GLU:CB	2.58	0.52
1:A:156:LEU:HA	1:A:196:LEU:HD21	1.90	0.51
1:A:327:VAL:HG22	1:A:355:TYR:OH	2.10	0.51
1:A:206:ASN:ND2	1:A:248:PHE:CD1	2.78	0.51
1:A:170:VAL:N	1:A:491:LEU:O	2.43	0.51
1:A:338:VAL:HG12	1:A:349:THR:HG22	1.92	0.51
1:A:467:PRO:O	1:A:468:CYS:HB3	2.10	0.51
1:A:272:LEU:C	1:A:272:LEU:HD13	2.31	0.51
1:A:201:ASP:N	1:A:202:PRO:CD	2.74	0.51
1:A:181:MET:SD	1:A:207:THR:HB	2.51	0.50
1:A:243:ARG:HD2	4:A:2017:HOH:O	2.11	0.50
1:A:346:THR:HB	1:A:349:THR:OG1	2.10	0.50
1:A:25:TYR:HD1	4:A:2001:HOH:O	1.94	0.50
1:A:97:GLU:O	1:A:99:TYR:N	2.45	0.50
1:A:97:GLU:HB3	1:A:101:VAL:CG1	2.42	0.50
1:A:404:ASP:O	1:A:406:LYS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HG21	1:A:193:ILE:CD1	2.42	0.50
1:A:106:ARG:HD2	1:A:374:GLU:OE2	2.12	0.49
1:A:126:TRP:CZ2	1:A:440:ARG:HG2	2.47	0.49
1:A:460:LEU:C	1:A:462:ASN:H	2.15	0.49
1:A:243:ARG:HA	1:A:246:THR:OG1	2.12	0.49
1:A:226:PHE:HB2	1:A:229:LEU:HD22	1.94	0.49
1:A:216:LEU:HD22	1:A:481:GLY:CA	2.42	0.49
1:A:128:ARG:NH1	1:A:289:ALA:O	2.46	0.49
1:A:353:MET:O	1:A:356:LEU:HB3	2.13	0.49
1:A:472:GLN:CB	1:A:476:LYS:CE	2.90	0.49
1:A:108:PHE:O	1:A:109:GLY:O	2.30	0.49
2:A:1499:MYT:H4	2:A:1499:MYT:C17	2.43	0.49
1:A:198:ASN:CB	1:A:199:PRO:HD2	2.43	0.49
1:A:160:LEU:HD12	1:A:163:GLU:HB2	1.95	0.49
1:A:101:VAL:HG11	1:A:381:VAL:HG21	1.95	0.49
1:A:159:ASN:ND2	1:A:196:LEU:HD23	2.27	0.49
1:A:359:VAL:HG13	1:A:414:PHE:HZ	1.78	0.49
1:A:178:ALA:O	1:A:182:ASP:CG	2.51	0.48
1:A:441:ASN:HA	3:A:1501:HEM:HBA2	1.95	0.48
1:A:194:ASP:OD1	1:A:196:LEU:HB3	2.13	0.48
1:A:340:PRO:O	1:A:341:ASN:O	2.30	0.48
1:A:471:THR:HG21	1:A:491:LEU:HD23	1.96	0.48
1:A:346:THR:O	1:A:350:VAL:HG23	2.14	0.48
1:A:403:ARG:O	1:A:405:PRO:HD3	2.14	0.48
1:A:475:LEU:O	1:A:476:LYS:HB2	2.14	0.48
1:A:101:VAL:HG22	1:A:102:PHE:HD1	1.78	0.47
1:A:450:MET:SD	1:A:454:LEU:HD22	2.53	0.47
1:A:472:GLN:HB2	1:A:476:LYS:CE	2.44	0.47
1:A:97:GLU:HB3	1:A:101:VAL:HG12	1.96	0.47
1:A:71:VAL:HG13	1:A:82:LEU:HD21	1.96	0.47
1:A:102:PHE:CE2	1:A:394:VAL:HG21	2.50	0.47
1:A:357:ASP:CA	1:A:453:LYS:HZ1	2.25	0.47
1:A:217:ASP:HB2	1:A:218:PRO:CD	2.45	0.47
1:A:415:LEU:CD1	1:A:418:ARG:NH1	2.78	0.46
1:A:338:VAL:HG12	1:A:349:THR:CG2	2.45	0.46
1:A:125:GLU:HA	1:A:125:GLU:OE1	2.15	0.46
1:A:142:LEU:HD11	1:A:450:MET:HG3	1.98	0.46
2:A:1499:MYT:H13	3:A:1501:HEM:C4D	2.50	0.46
1:A:276:ILE:N	1:A:276:ILE:CD1	2.72	0.46
1:A:202:PRO:HB2	1:A:203:PHE:CB	2.46	0.46
1:A:323:THR:O	1:A:324:HIS:CG	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLU:OE1	1:A:355:TYR:HB3	2.16	0.46
1:A:478:SER:HB2	1:A:484:GLN:HG2	1.97	0.46
1:A:257:LYS:HD2	1:A:257:LYS:C	2.36	0.46
1:A:213:PHE:HB2	1:A:215:PHE:CE1	2.50	0.45
1:A:213:PHE:O	1:A:482:LEU:HD21	2.16	0.45
1:A:356:LEU:HD21	1:A:453:LYS:HB3	1.98	0.45
1:A:318:MET:HE1	1:A:465:PHE:CD2	2.51	0.45
1:A:321:LEU:O	1:A:328:GLN:NE2	2.49	0.45
1:A:476:LYS:N	1:A:476:LYS:CD	2.79	0.45
1:A:41:PRO:HD2	1:A:73:GLY:O	2.17	0.45
1:A:305:ALA:HB1	2:A:1499:MYT:N14	2.32	0.45
1:A:421:LYS:O	1:A:422:LYS:CB	2.65	0.45
1:A:204:VAL:O	1:A:208:LYS:HB2	2.17	0.45
1:A:340:PRO:O	1:A:341:ASN:C	2.55	0.45
1:A:339:LEU:O	1:A:340:PRO:C	2.55	0.45
1:A:316:PHE:O	1:A:317:ILE:C	2.54	0.45
1:A:335:ILE:HG12	1:A:353:MET:HE1	1.99	0.44
1:A:59:MET:O	1:A:63:GLU:HG3	2.16	0.44
1:A:62:MET:O	1:A:63:GLU:C	2.56	0.44
1:A:75:TYR:HA	1:A:79:GLN:O	2.17	0.44
1:A:87:PRO:HA	1:A:90:ILE:HB	1.99	0.44
1:A:131:SER:O	1:A:132:LEU:HB2	2.17	0.44
1:A:226:PHE:O	1:A:229:LEU:HB2	2.17	0.44
1:A:260:ARG:HH12	1:A:272:LEU:HD12	1.83	0.44
1:A:386:MET:HE3	1:A:386:MET:HA	2.00	0.44
1:A:203:PHE:O	1:A:203:PHE:HD1	2.01	0.44
1:A:356:LEU:O	1:A:357:ASP:C	2.54	0.44
1:A:460:LEU:O	1:A:462:ASN:N	2.51	0.44
1:A:235:VAL:HG12	1:A:236:LEU:HD22	2.00	0.43
1:A:432:TYR:CZ	1:A:434:PRO:HG3	2.53	0.43
1:A:472:GLN:NE2	1:A:487:LYS:NZ	2.56	0.43
1:A:223:ILE:O	1:A:223:ILE:HG22	2.17	0.43
1:A:470:GLU:O	1:A:472:GLN:HG3	2.19	0.43
1:A:75:TYR:CE2	1:A:80:PRO:HB3	2.54	0.43
1:A:291:SER:HB3	1:A:294:GLU:CG	2.48	0.43
1:A:27:THR:HG22	1:A:45:PRO:HA	1.99	0.43
1:A:415:LEU:HD11	1:A:418:ARG:NH1	2.33	0.43
1:A:470:GLU:O	1:A:472:GLN:N	2.52	0.43
1:A:30:HIS:CE1	1:A:43:PRO:HB2	2.54	0.43
1:A:113:PHE:C	1:A:115:LYS:N	2.71	0.43
1:A:198:ASN:CB	1:A:199:PRO:CD	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:HG21	1:A:456:LEU:HD11	2.01	0.43
1:A:415:LEU:CD1	1:A:418:ARG:HH11	2.32	0.43
1:A:152:TYR:HE2	1:A:186:SER:HG	1.63	0.42
1:A:375:ARG:NH1	3:A:1501:HEM:O2A	2.52	0.42
1:A:364:LEU:O	1:A:365:ARG:C	2.56	0.42
1:A:90:ILE:HG21	1:A:430:TYR:HB3	2.01	0.42
1:A:479:LEU:H	1:A:479:LEU:CD2	2.31	0.42
1:A:251:LYS:HD2	1:A:251:LYS:N	2.34	0.42
1:A:492:LYS:CB	1:A:492:LYS:NZ	2.82	0.42
1:A:152:TYR:OH	1:A:192:ASN:ND2	2.22	0.42
1:A:472:GLN:HB3	1:A:476:LYS:CE	2.47	0.42
1:A:347:TYR:C	1:A:347:TYR:CD1	2.93	0.42
1:A:79:GLN:NE2	1:A:80:PRO:HD2	2.34	0.42
1:A:143:LYS:HA	1:A:146:VAL:HG23	2.02	0.42
1:A:243:ARG:O	1:A:244:GLU:C	2.55	0.42
1:A:330:LYS:HD3	1:A:355:TYR:CE2	2.55	0.42
1:A:179:TYR:CZ	1:A:455:ALA:HB2	2.55	0.42
1:A:189:PHE:CE1	1:A:303:ILE:HD11	2.55	0.42
1:A:219:PHE:CE1	1:A:223:ILE:HD11	2.55	0.42
1:A:476:LYS:N	1:A:476:LYS:HD3	2.35	0.42
1:A:166:THR:O	1:A:167:GLY:C	2.58	0.41
1:A:339:LEU:HD21	1:A:349:THR:HG21	2.02	0.41
1:A:36:LEU:HG	1:A:38:ILE:HD12	2.02	0.41
1:A:68:TYR:HB2	1:A:72:TRP:HB3	2.02	0.41
1:A:219:PHE:CZ	1:A:223:ILE:HD11	2.56	0.41
2:A:1499:MYT:H13	3:A:1501:HEM:ND	2.35	0.41
1:A:206:ASN:HB3	1:A:245:VAL:HG13	2.01	0.41
1:A:113:PHE:C	1:A:115:LYS:H	2.23	0.41
1:A:243:ARG:HG2	1:A:247:ASN:HD21	1.85	0.41
1:A:410:GLU:N	1:A:411:PRO:HD3	2.35	0.41
1:A:198:ASN:HB3	1:A:199:PRO:HD2	2.01	0.41
1:A:104:ASN:HD22	1:A:122:GLU:HB3	1.86	0.41
1:A:161:ARG:O	1:A:165:GLU:N	2.48	0.41
1:A:275:MET:C	1:A:276:ILE:HD12	2.41	0.41
1:A:460:LEU:C	1:A:462:ASN:N	2.73	0.41
1:A:191:VAL:HG12	1:A:193:ILE:HG23	2.02	0.41
1:A:334:GLU:O	1:A:338:VAL:HG23	2.21	0.40
1:A:102:PHE:H	1:A:378:LYS:CG	2.34	0.40
1:A:198:ASN:O	1:A:199:PRO:C	2.58	0.40
1:A:292:ASP:HB3	1:A:293:LEU:HD22	2.03	0.40
1:A:473:ILE:N	1:A:474:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:HZ3	1:A:476:LYS:HG2	1.72	0.40
1:A:485:PRO:O	1:A:486:GLU:HB2	2.21	0.40
1:A:324:HIS:N	1:A:325:PRO:HD3	2.37	0.40
1:A:416:PRO:O	1:A:418:ARG:N	2.55	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:CE2	1:A:226:PHE:CZ[2_775]	1.36	0.84
1:A:232:ILE:CD1	1:A:232:ILE:CD1[4_575]	1.73	0.47
1:A:226:PHE:CE2	1:A:226:PHE:CE2[2_775]	1.85	0.35
1:A:226:PHE:CZ	1:A:226:PHE:CZ[2_775]	2.06	0.14
1:A:228:PHE:CB	1:A:231:PRO:O[4_575]	2.10	0.10

## 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	449/485 (93%)	351 (78%)	66 (15%)	32 (7%)	<b>1</b> <b>1</b>

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	196	LEU
1	A	198	ASN
1	A	199	PRO
1	A	203	PHE
1	A	237	ASN
1	A	255	ARG
1	A	323	THR

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Mol	Chain	Res	Type
1	A	341	ASN
1	A	342	LYS
1	A	467	PRO
1	A	468	CYS
1	A	476	LYS
1	A	486	GLU
1	A	109	GLY
1	A	132	LEU
1	A	167	GLY
1	A	340	PRO
1	A	401	LEU
1	A	422	LYS
1	A	475	LEU
1	A	477	LEU
1	A	371	MET
1	A	402	HIS
1	A	474	PRO
1	A	100	SER
1	A	254	LYS
1	A	417	GLU
1	A	102	PHE
1	A	201	ASP
1	A	405	PRO
1	A	165	GLU

### 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	412/441 (93%)	361 (88%)	51 (12%)	<b>4</b> <b>7</b>

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	35	LYS

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Mol	Chain	Res	Type
1	A	44	LEU
1	A	45	PRO
1	A	67	LYS
1	A	94	LEU
1	A	104	ASN
1	A	116	SER
1	A	125	GLU
1	A	131	SER
1	A	188	SER
1	A	193	ILE
1	A	197	ASN
1	A	198	ASN
1	A	199	PRO
1	A	200	GLN
1	A	203	PHE
1	A	207	THR
1	A	216	LEU
1	A	221	LEU
1	A	234	GLU
1	A	235	VAL
1	A	244	GLU
1	A	249	LEU
1	A	250	ARG
1	A	257	LYS
1	A	258	GLU
1	A	260	ARG
1	A	270	ASP
1	A	274	LEU
1	A	301	ILE
1	A	317	ILE
1	A	331	LEU
1	A	349	THR
1	A	352	GLN
1	A	371	MET
1	A	373	LEU
1	A	375	ARG
1	A	379	LYS
1	A	399	TYR
1	A	415	LEU
1	A	423	ASN
1	A	437	SER
1	A	440	ARG

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Mol	Chain	Res	Type
1	A	450	MET
1	A	454	LEU
1	A	475	LEU
1	A	476	LYS
1	A	478	SER
1	A	479	LEU
1	A	495	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	79	GLN
1	A	104	ASN
1	A	159	ASN
1	A	192	ASN
1	A	197	ASN
1	A	206	ASN
1	A	247	ASN
1	A	324	HIS
1	A	328	GLN
1	A	451	ASN
1	A	472	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
3	HEM	A	1501	1,2	27,50,50	2.25	7 (25%)	17,82,82	1.44	3 (17%)
2	MYT	A	1499	3	17,18,18	1.12	1 (5%)	23,25,25	1.53	4 (17%)

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	HEM	A	1501	1,2	-	0/6/54/54	-
2	MYT	A	1499	3	-	0/16/16/16	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	HEM	C3C-C2C	-5.80	1.32	1.40
3	A	1501	HEM	C3B-C2B	-5.43	1.32	1.40
3	A	1501	HEM	C3D-C2D	4.50	1.51	1.37
3	A	1501	HEM	C3C-CAC	3.59	1.55	1.47
2	A	1499	MYT	C10-C12	-3.55	1.50	1.53
3	A	1501	HEM	C3B-CAB	2.92	1.53	1.47
3	A	1501	HEM	C2A-C3A	-2.33	1.30	1.37
3	A	1501	HEM	C1A-CHA	-2.04	1.35	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1499	MYT	C12-C13-N14	-3.25	121.22	124.09
3	A	1501	HEM	C1D-C2D-C3D	-3.04	104.88	107.00
3	A	1501	HEM	CAD-CBD-CGD	-2.68	108.17	112.67
2	A	1499	MYT	C6-N1-C2	2.62	121.39	116.85
2	A	1499	MYT	C16-C17-C12	-2.56	118.07	120.76
3	A	1501	HEM	C4C-C3C-C2C	2.45	108.61	106.90
2	A	1499	MYT	C13-C12-C10	-2.02	118.79	121.97

There are no chirality outliers.

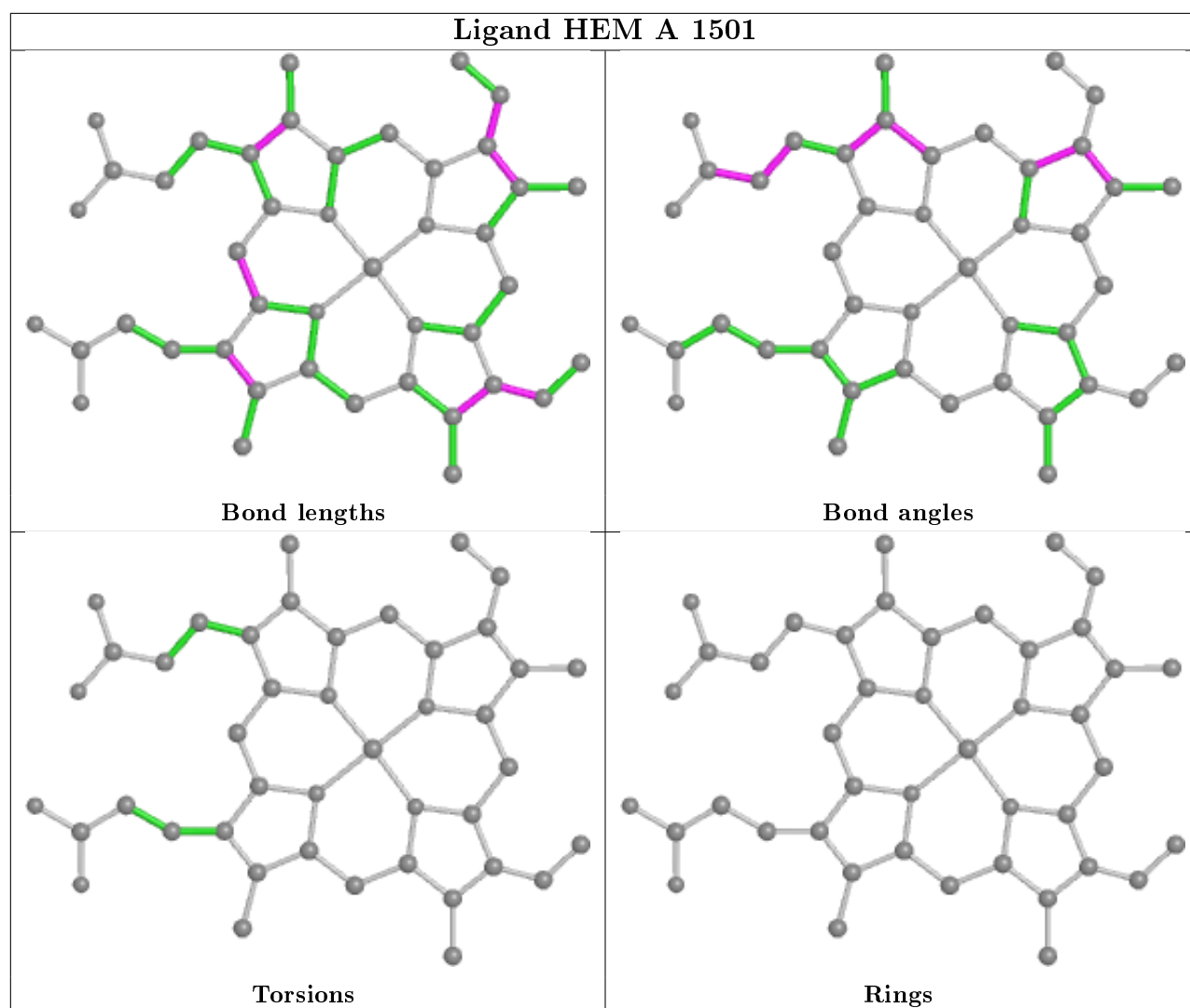
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	HEM	4	0
2	A	1499	MYT	5	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

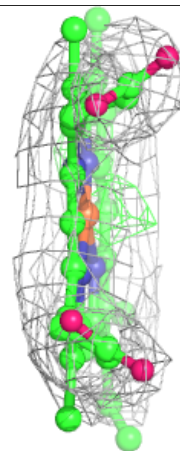
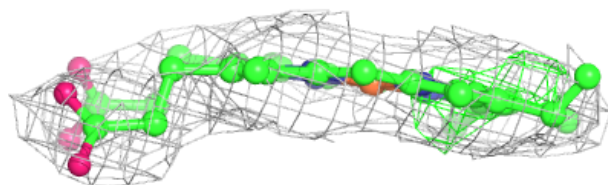
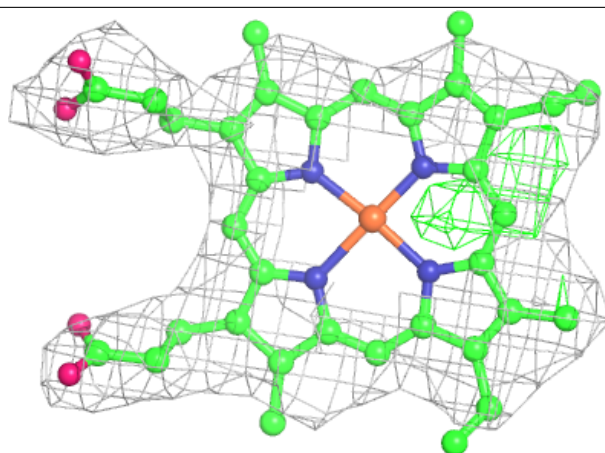
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 A 1501:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.