



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:11 PM EDT

PDB ID : 1ZOA  
Title : Crystal Structure Of A328V Mutant Of The Heme Domain Of P450Bm-3 With N-Palmitoylglycine  
Authors : Hegda, A.; Chen, B.; Haines, D.C.; Bondlela, M.; Mullin, D.; Graham, S.E.; Tomchick, D.R.; Machius, M.; Peterson, J.A.  
Deposited on : 2005-05-12  
Resolution : 1.74 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:

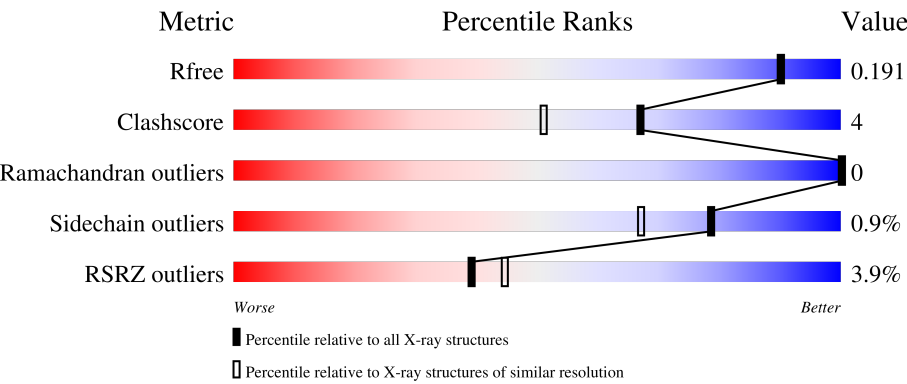
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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 <sub>free</sub>	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 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	473	<div><div>5%</div><div>90%</div><div>6% . .</div></div>
1	B	473	<div><div>3%</div><div>88%</div><div>8% . .</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
4	MES	B	1491	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8501 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 Bifunctional P-450:NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	3	0
			3697	2363	631	686	17			
1	B	457	Total	C	N	O	S	0	4	0
			3705	2369	631	688	17			

There are 8 discrepancies between the modelled and reference sequences:

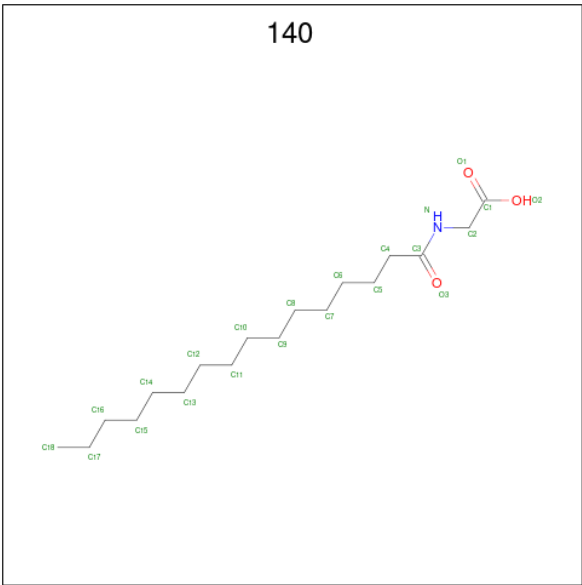
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P14779
A	-1	ALA	-	expression tag	UNP P14779
A	0	MET	-	expression tag	UNP P14779
A	328	VAL	ALA	engineered mutation	UNP P14779
B	-2	GLY	-	expression tag	UNP P14779
B	-1	ALA	-	expression tag	UNP P14779
B	0	MET	-	expression tag	UNP P14779
B	328	VAL	ALA	engineered mutation	UNP P14779

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



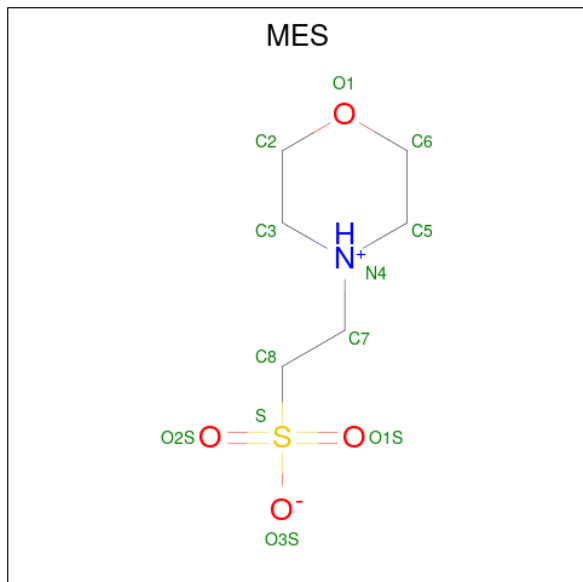
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is N-PALMITOYLGLYCINE (three-letter code: 140) (formula: C<sub>18</sub>H<sub>35</sub>NO<sub>3</sub>).



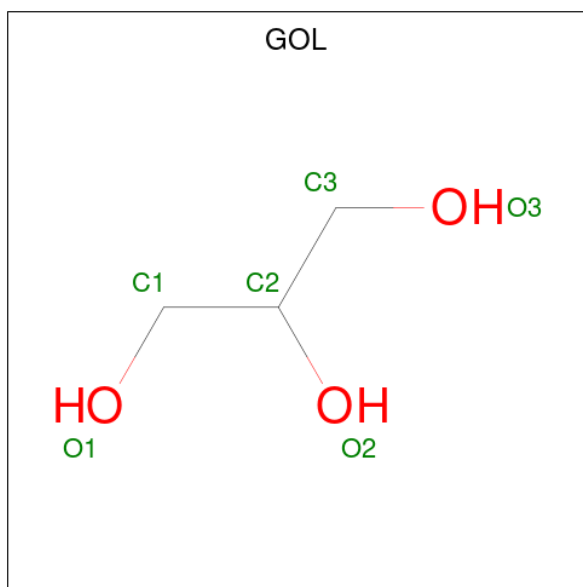
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	18	1	3		
3	B	1	Total	C	N	O	0	0
			22	18	1	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	12	6	1	4	1	0	0
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0

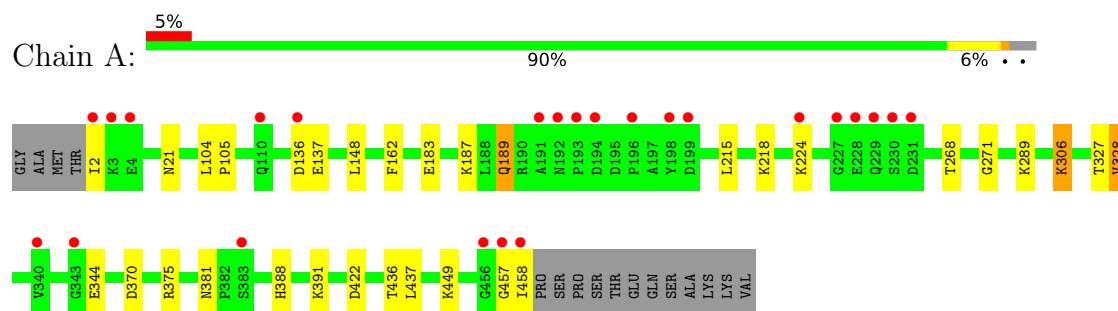
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	472	Total 472	O 472	0	0
6	B	461	Total 461	O 461	0	0

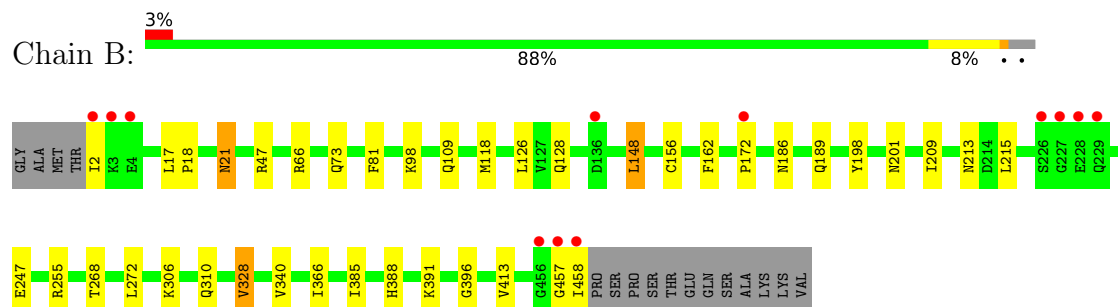
### 3 Residue-property plots [i](#)

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: Bifunctional P-450:NADPH-P450 reductase



- Molecule 1: Bifunctional P-450:NADPH-P450 reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.11Å 148.05Å 63.67Å 90.00° 98.56° 90.00°	Depositor
Resolution (Å)	30.00 – 1.74 39.33 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-1.74) 99.7 (39.33-1.74)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.46 (at 1.74Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.165 , 0.196 0.162 , 0.191	Depositor DCC
$R_{free}$ test set	2196 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: MES, HEM, GOL, 140

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	0.58	0/3782	0.75	2/5113 (0.0%)
1	B	0.59	0/3790	0.76	1/5124 (0.0%)
All	All	0.58	0/7572	0.76	3/10237 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	VAL	N-CA-C	-6.65	93.05	111.00
1	B	328	VAL	N-CA-C	-6.28	94.06	111.00
1	A	137	GLU	N-CA-C	5.54	125.95	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3697	0	3670	29	0
1	B	3705	0	3680	32	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	22	0	34	0	0
3	B	22	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	26	2	0
5	B	12	0	16	0	0
6	A	472	0	0	4	0
6	B	461	0	0	4	0
All	All	8501	0	7520	59	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 (59) 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:457:GLY:O	1:B:458:ILE:HG12	1.63	0.96
1:B:47:ARG:NH1	1:B:73:GLN:HG3	1.85	0.91
1:B:47:ARG:HH11	1:B:73:GLN:HG3	1.37	0.88
1:B:213:ASN:HD22	1:B:255:ARG:HH21	1.27	0.83
1:A:306:LYS:HE3	6:A:1717:HOH:O	1.81	0.80
1:A:183:GLU:OE2	1:A:187[B]:LYS:HE3	1.91	0.70
1:B:310:GLN:HG3	6:B:1715:HOH:O	1.92	0.69
1:A:224:LYS:HG3	6:A:1719:HOH:O	1.94	0.67
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.77	0.66
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.77	0.66
1:B:172:PRO:HB2	6:B:1674:HOH:O	1.98	0.64
1:A:422:ASP:HB2	1:A:449:LYS:CG	2.29	0.62
1:B:186:ASN:HB3	6:B:1922:HOH:O	1.99	0.62
1:A:457:GLY:O	1:A:458:ILE:HB	2.00	0.62
1:A:381:ASN:HD21	1:B:396:GLY:HA2	1.67	0.60
1:A:370:ASP:OD1	1:A:375[B]:ARG:NH2	2.35	0.59
1:B:366:ILE:O	4:B:1491:MES:H71	2.03	0.58
1:A:458:ILE:HG22	1:A:458:ILE:O	2.03	0.58
1:A:268:THR:HG21	1:A:328:VAL:HG23	1.86	0.58
1:B:186:ASN:O	1:B:189:GLN:HG2	2.04	0.57
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.41	0.55
1:B:306:LYS:NZ	1:B:310:GLN:HG2	2.22	0.55
1:B:148:LEU:HD21	1:B:413[A]:VAL:HG21	1.90	0.54
1:A:388:HIS:HD2	1:A:391:LYS:NZ	2.06	0.53
1:A:422:ASP:HB2	1:A:449:LYS:HG3	1.89	0.53
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.74	0.53
1:B:306:LYS:HZ2	1:B:310:GLN:HG2	1.74	0.52
1:B:198:TYR:HA	1:B:201:ASN:HD22	1.74	0.51
1:A:187[B]:LYS:HE2	6:A:1922:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HG21	1:A:328:VAL:CG2	2.41	0.51
1:B:268:THR:HG21	1:B:328:VAL:CG2	2.40	0.51
1:B:126[B]:LEU:C	1:B:126[B]:LEU:HD13	2.32	0.50
1:B:268:THR:HG21	1:B:328:VAL:HG23	1.94	0.50
1:A:289:LYS:HE2	1:B:385:ILE:O	2.12	0.49
1:A:2:ILE:HA	1:A:344:GLU:O	2.13	0.49
1:A:21:ASN:CG	1:A:189:GLN:HE21	2.19	0.45
1:A:306:LYS:H	1:A:306:LYS:NZ	2.14	0.45
1:A:422:ASP:OD2	1:A:449:LYS:HE3	2.16	0.45
1:B:128:GLN:NE2	6:B:1509:HOH:O	2.50	0.45
1:B:98:LYS:HE3	1:B:247:GLU:HB2	1.98	0.45
1:B:306:LYS:NZ	1:B:310:GLN:OE1	2.43	0.44
1:A:104:LEU:N	1:A:105:PRO:CD	2.80	0.44
1:B:366:ILE:O	4:B:1490:MES:H21	2.17	0.43
1:A:271:GLY:HA3	1:A:327:THR:HG21	2.01	0.43
1:B:272:LEU:HD22	2:B:471:HEM:HBB1	1.99	0.43
1:A:215:LEU:HD12	1:A:218:LYS:HE3	2.00	0.43
1:B:81:PHE:HB3	1:B:209:ILE:HG12	2.01	0.43
1:A:457:GLY:O	1:A:458:ILE:CB	2.66	0.42
1:B:118:MET:HE3	1:B:156:CYS:HA	2.02	0.42
1:A:306:LYS:HE2	6:A:1718:HOH:O	2.20	0.42
1:B:66:ARG:NH2	1:B:340:VAL:O	2.53	0.42
1:A:388:HIS:HD2	1:A:391:LYS:HZ3	1.67	0.41
1:B:2:ILE:HD12	1:B:2:ILE:N	2.35	0.41
1:A:422:ASP:HB2	1:A:449:LYS:HG2	2.02	0.41
1:A:436:THR:O	1:A:437:LEU:HB2	2.20	0.41
1:B:17:LEU:HB3	1:B:18:PRO:HD3	2.02	0.41
1:B:118:MET:HB2	1:B:118:MET:HE2	1.81	0.41
1:B:21:ASN:ND2	1:B:189:GLN:OE1	2.55	0.40
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	458/473 (97%)	447 (98%)	11 (2%)	0	100	100
1	B	459/473 (97%)	450 (98%)	9 (2%)	0	100	100
All	All	917/946 (97%)	897 (98%)	20 (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	400/413 (97%)	396 (99%)	4 (1%)	76	63
1	B	402/413 (97%)	399 (99%)	3 (1%)	84	75
All	All	802/826 (97%)	795 (99%)	7 (1%)	78	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	A	148	LEU
1	A	189	GLN
1	A	306	LYS
1	B	21	ASN
1	B	109	GLN
1	B	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	381	ASN
1	A	388	HIS

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Mol	Chain	Res	Type
1	A	403	GLN
1	B	21	ASN
1	B	128	GLN
1	B	189	GLN
1	B	201	ASN
1	B	213	ASN
1	B	403	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
2	HEM	B	471	1	27,50,50	1.77	8 (29%)	17,82,82	2.18	8 (47%)
4	MES	B	1490	-	12,12,12	1.34	2 (16%)	14,16,16	0.67	0
3	140	A	1470	-	18,21,21	0.58	0	19,22,22	0.73	0
2	HEM	A	471	1	27,50,50	1.83	8 (29%)	17,82,82	1.82	8 (47%)
3	140	B	1471	-	18,21,21	0.62	0	19,22,22	0.78	0
5	GOL	B	1480	-	5,5,5	0.61	0	5,5,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	1481	-	5,5,5	0.58	0	5,5,5	0.15	0
4	MES	B	1491	-	12,12,12	1.88	3 (25%)	14,16,16	0.76	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
2	HEM	B	471	1	-	0/6/54/54	-
4	MES	B	1490	-	-	2/6/14/14	0/1/1/1
3	140	A	1470	-	-	8/18/20/20	-
2	HEM	A	471	1	-	0/6/54/54	-
3	140	B	1471	-	-	9/18/20/20	-
5	GOL	B	1480	-	-	2/4/4/4	-
5	GOL	B	1481	-	-	0/4/4/4	-
4	MES	B	1491	-	-	2/6/14/14	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	471	HEM	CBC-CAC	3.77	1.54	1.29
2	B	471	HEM	CBB-CAB	3.70	1.53	1.29
2	B	471	HEM	CBC-CAC	3.67	1.53	1.29
2	B	471	HEM	C3C-CAC	3.58	1.55	1.47
4	B	1491	MES	C3-N4	3.43	1.56	1.46
2	A	471	HEM	C3C-CAC	3.37	1.54	1.47
2	A	471	HEM	C3B-CAB	3.34	1.54	1.47
2	A	471	HEM	CBB-CAB	3.26	1.50	1.29
2	B	471	HEM	C3B-CAB	2.92	1.53	1.47
2	B	471	HEM	CMC-C2C	2.90	1.58	1.51
4	B	1491	MES	C5-N4	2.90	1.54	1.46
2	A	471	HEM	C4D-C3D	2.70	1.48	1.42
2	A	471	HEM	C3C-C2C	-2.63	1.36	1.40
2	B	471	HEM	C4D-C3D	2.49	1.48	1.42
4	B	1490	MES	C3-N4	2.48	1.53	1.46
4	B	1490	MES	C5-N4	2.23	1.53	1.46
2	B	471	HEM	C3B-C2B	-2.17	1.37	1.40
2	A	471	HEM	CMC-C2C	2.15	1.56	1.51
2	A	471	HEM	C4B-NB	2.04	1.40	1.36
4	B	1491	MES	C8-S	2.02	1.80	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	471	HEM	C1D-ND	2.02	1.40	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	471	HEM	CAA-CBA-CGA	4.19	119.70	112.67
2	B	471	HEM	CMA-C3A-C4A	-3.01	123.84	128.46
2	B	471	HEM	CBD-CAD-C3D	-2.98	106.99	112.48
2	B	471	HEM	CMB-C2B-C3B	2.82	129.96	124.68
2	B	471	HEM	CMA-C3A-C2A	2.78	130.18	124.94
2	A	471	HEM	CMB-C2B-C3B	2.74	129.81	124.68
2	A	471	HEM	CMC-C2C-C3C	2.70	129.73	124.68
2	A	471	HEM	CMD-C2D-C1D	-2.63	124.42	128.46
2	B	471	HEM	CMC-C2C-C3C	2.61	129.56	124.68
2	A	471	HEM	CMD-C2D-C3D	2.42	129.51	124.94
2	A	471	HEM	CBD-CAD-C3D	-2.34	108.16	112.48
2	B	471	HEM	CMD-C2D-C1D	-2.30	124.93	128.46
2	A	471	HEM	CMA-C3A-C4A	-2.28	124.96	128.46
2	B	471	HEM	CMD-C2D-C3D	2.27	129.21	124.94
2	A	471	HEM	C4C-C3C-C2C	2.16	108.41	106.90
2	A	471	HEM	CAA-CBA-CGA	2.11	116.22	112.67

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1471	140	O3-C3-C4-C5
3	A	1470	140	C5-C6-C7-C8
5	B	1480	GOL	O1-C1-C2-C3
3	B	1471	140	N-C3-C4-C5
3	A	1470	140	C13-C14-C15-C16
3	B	1471	140	C11-C12-C13-C14
3	B	1471	140	C13-C14-C15-C16
3	B	1471	140	C7-C8-C9-C10
3	B	1471	140	C12-C13-C14-C15
3	A	1470	140	C11-C10-C9-C8
3	A	1470	140	C11-C12-C13-C14
3	B	1471	140	C10-C11-C12-C13
3	B	1471	140	C5-C6-C7-C8
4	B	1490	MES	C8-C7-N4-C3
4	B	1490	MES	C8-C7-N4-C5
4	B	1491	MES	C8-C7-N4-C3

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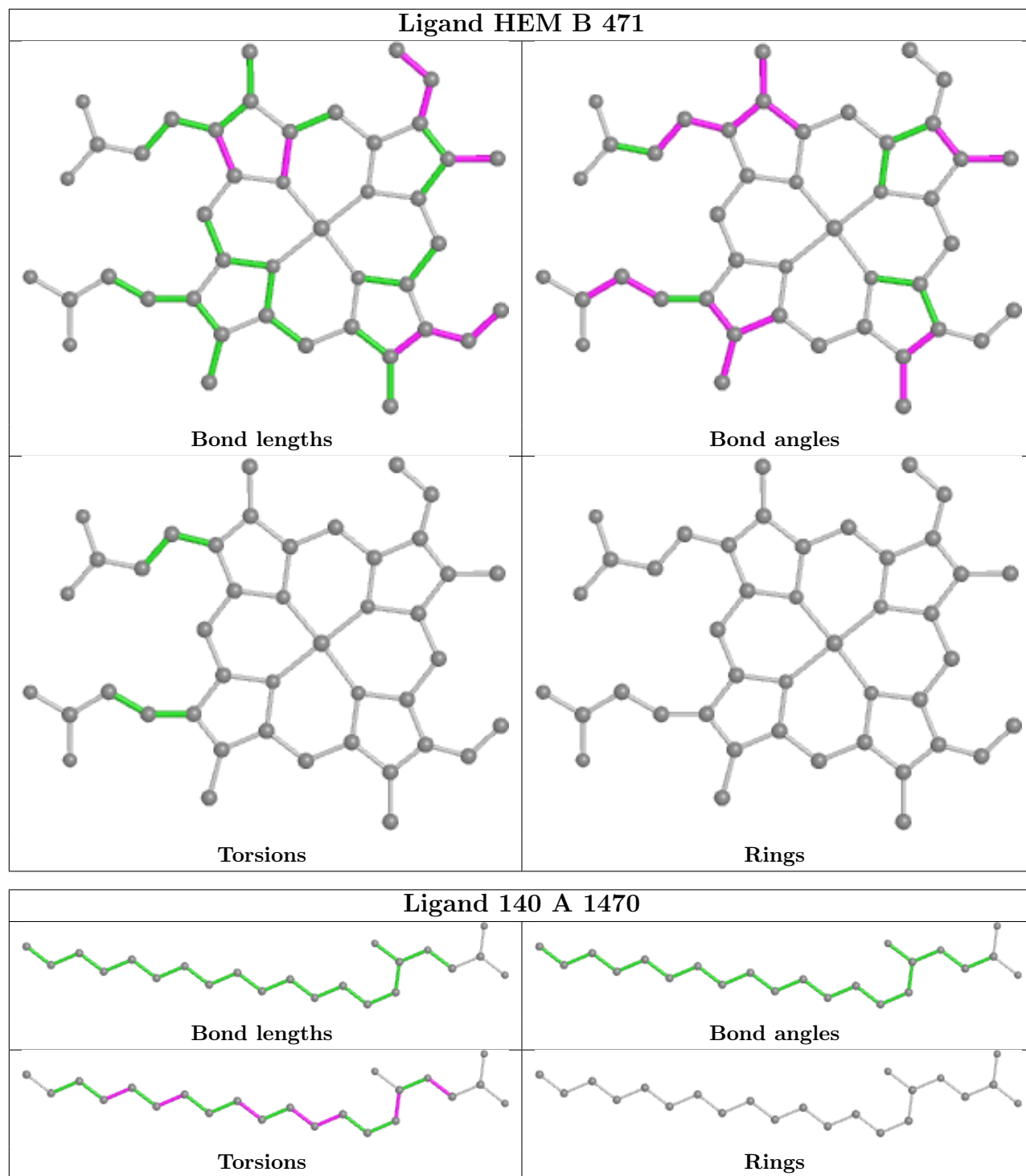
Mol	Chain	Res	Type	Atoms
4	B	1491	MES	C8-C7-N4-C5
3	A	1470	140	N-C3-C4-C5
3	A	1470	140	O3-C3-C4-C5
5	B	1480	GOL	O1-C1-C2-O2
3	A	1470	140	C6-C7-C8-C9
3	B	1471	140	C4-C5-C6-C7
3	A	1470	140	C1-C2-N-C3

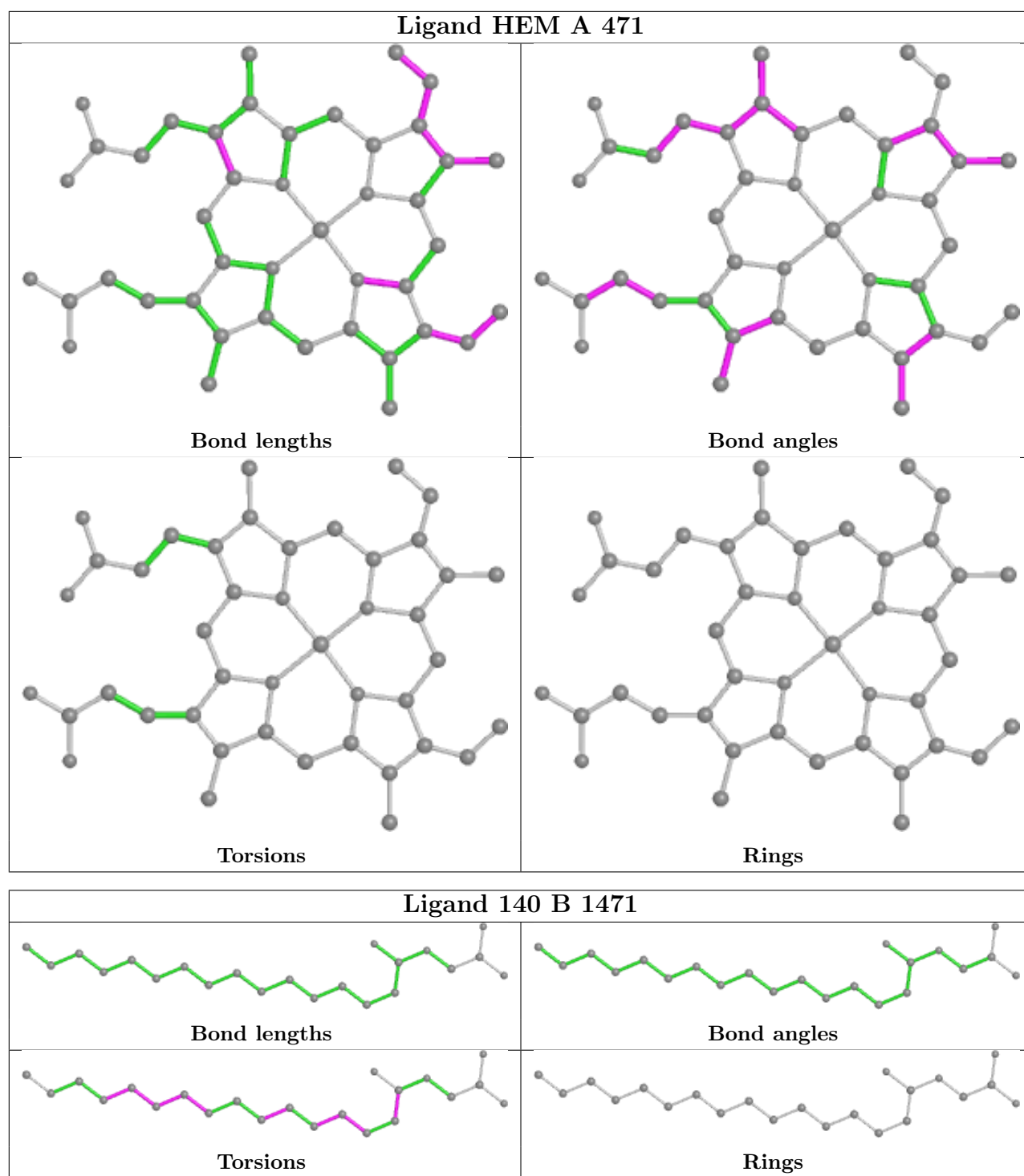
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	471	HEM	1	0
4	B	1490	MES	1	0
4	B	1491	MES	1	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 ⓘ

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	457/473 (96%)	0.01	24 (5%) 26 31	11, 20, 40, 50	0
1	B	457/473 (96%)	-0.10	12 (2%) 56 61	11, 19, 35, 50	0
All	All	914/946 (96%)	-0.04	36 (3%) 39 45	11, 19, 39, 50	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	ILE	13.3
1	B	2	ILE	12.3
1	A	2	ILE	10.6
1	A	227	GLY	6.9
1	A	3	LYS	5.5
1	B	458	ILE	5.4
1	B	227	GLY	5.4
1	A	228	GLU	4.4
1	B	457	GLY	4.3
1	B	4	GLU	4.3
1	A	4	GLU	3.8
1	A	229	GLN	3.4
1	B	3	LYS	3.3
1	A	196	PRO	3.1
1	B	229	GLN	2.9
1	A	192	ASN	2.9
1	A	198	TYR	2.9
1	A	457	GLY	2.9
1	B	136	ASP	2.9
1	B	172	PRO	2.8
1	A	456	GLY	2.7
1	A	383	SER	2.7
1	A	231	ASP	2.7
1	A	340	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	194	ASP	2.6
1	B	228	GLU	2.5
1	A	199	ASP	2.4
1	A	136	ASP	2.3
1	B	456	GLY	2.3
1	A	191	ALA	2.2
1	A	193	PRO	2.2
1	B	226	SER	2.2
1	A	343	GLY	2.1
1	A	110	GLN	2.0
1	A	224	LYS	2.0
1	A	230	SER	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 [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.

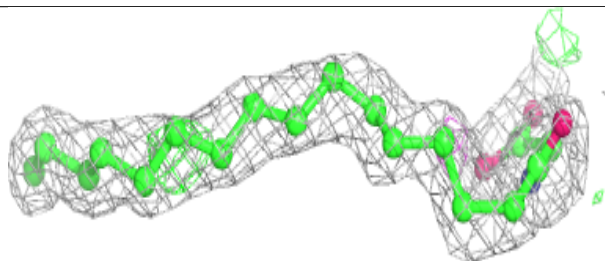
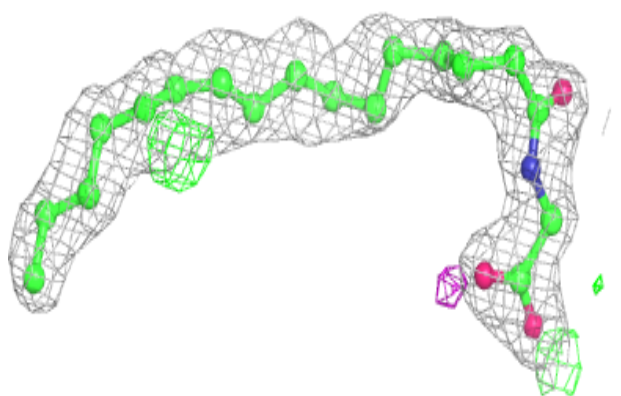
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MES	B	1491	12/12	0.46	0.46	60,62,71,72	0
5	GOL	B	1480	6/6	0.66	0.34	50,53,55,55	0
5	GOL	B	1481	6/6	0.72	0.24	51,55,56,56	0
4	MES	B	1490	12/12	0.76	0.33	49,51,66,68	0
3	140	A	1470	22/22	0.87	0.14	25,32,37,38	0
3	140	B	1471	22/22	0.88	0.16	23,32,35,38	0
2	HEM	A	471	43/43	0.98	0.09	8,12,18,30	0
2	HEM	B	471	43/43	0.98	0.09	9,12,18,27	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.

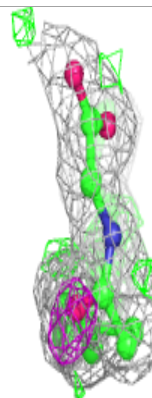
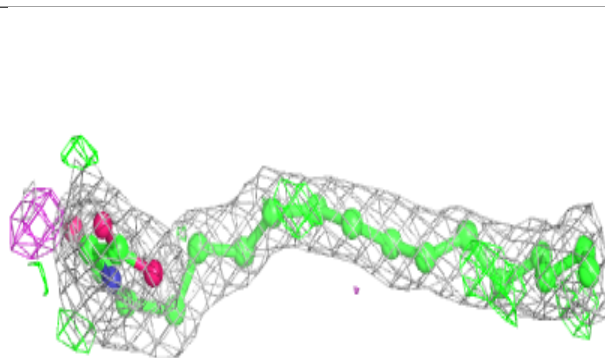
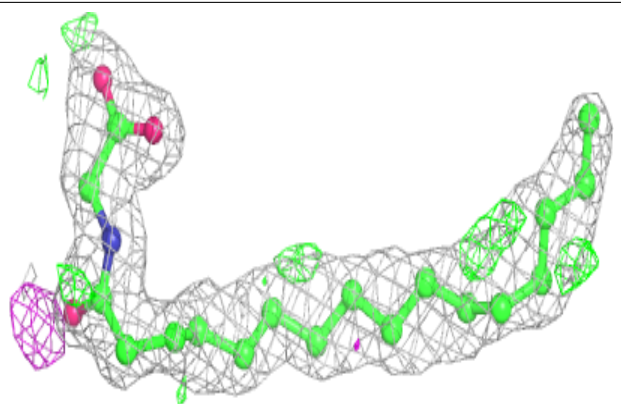
**Electron density around 140 A 1470:**

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



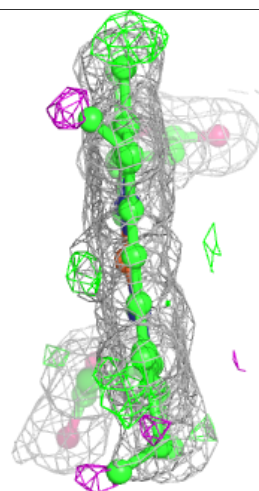
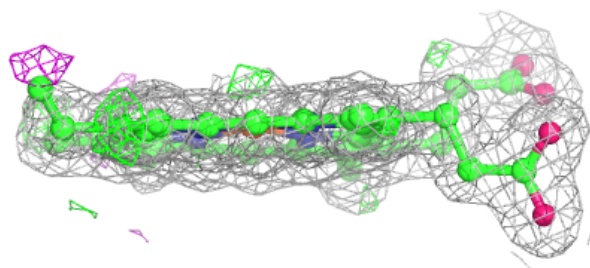
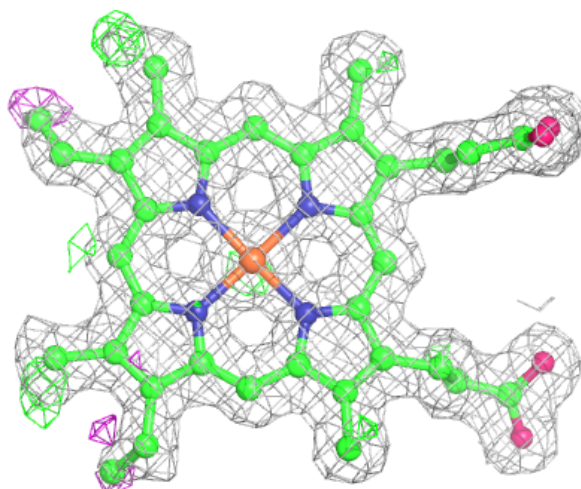
**Electron density around 140 B 1471:**

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



**Electron density around HEM A 471:**

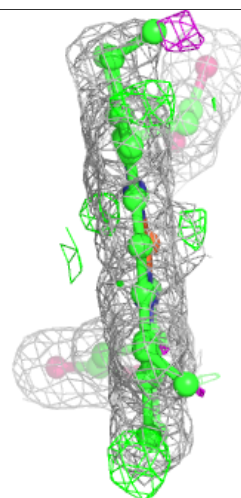
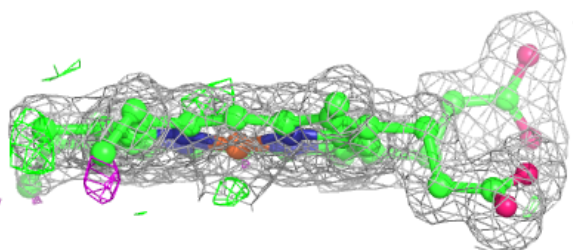
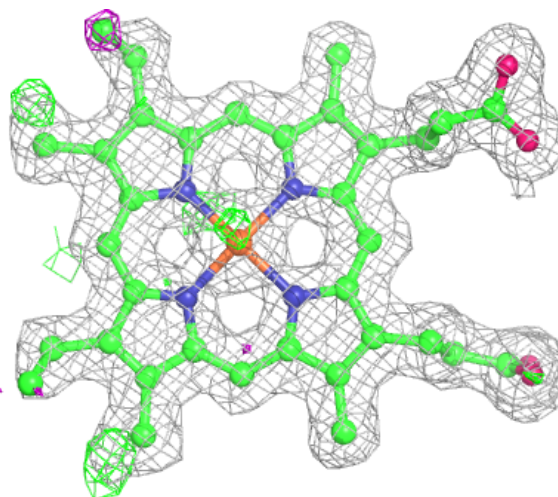
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM B 471:**

$2mF_o-DF_c$  (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.