Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 10:38 AM EDT

PDB ID	:	1ZO9
Title	:	Crystal Structure Of The Wild Type Heme Domain Of P450BM-3 with N-palmitoylmethionine
Authors	:	Hegda, A.; Chen, B.; Tomchick, D.R.; Bondlela, M.; Haines, D.C.; Schaffer, N.; Machius, M.; Graham, S.E.; Peterson, J.A.
Deposited on	:	2005-05-12
Resolution	:	1.70 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

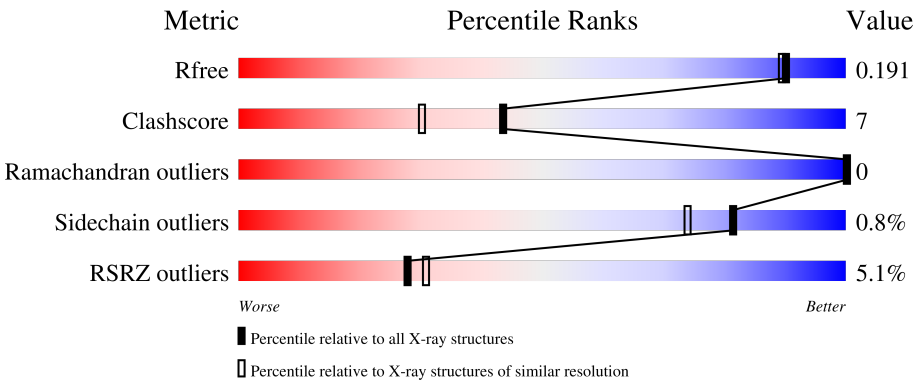
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 >=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 <=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	7% 84% 12% ·
1	B	473	3% 89% 7% ·

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	GOL	A	1478	-	-	-	X
4	GOL	A	1481	-	-	-	X
4	GOL	B	1479	-	-	X	-
5	MES	B	1491	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8853 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.

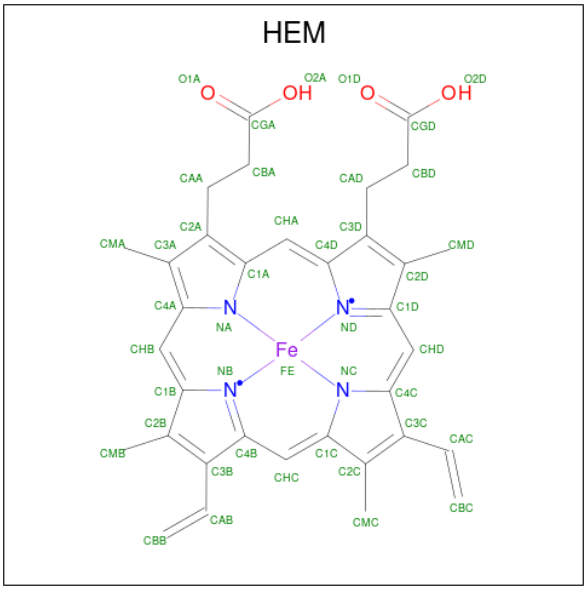
- Molecule 1 is a protein called Bifunctional P-450:NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	458	3768	2406	645	698	19	0	11	0
1	B	458	3767	2403	645	702	17	0	10	0

There are 6 discrepancies between the modelled and reference sequences:

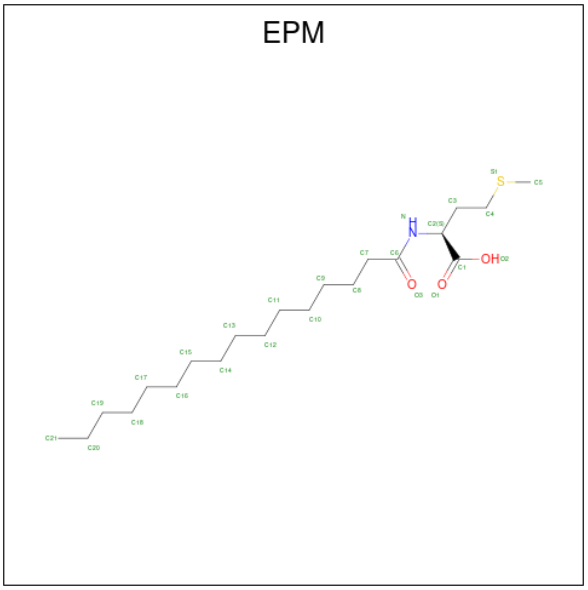
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P14779
A	-1	ALA	-	expression tag	UNP P14779
A	0	MET	-	expression tag	UNP P14779
B	-2	GLY	-	expression tag	UNP P14779
B	-1	ALA	-	expression tag	UNP P14779
B	0	MET	-	expression tag	UNP P14779

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



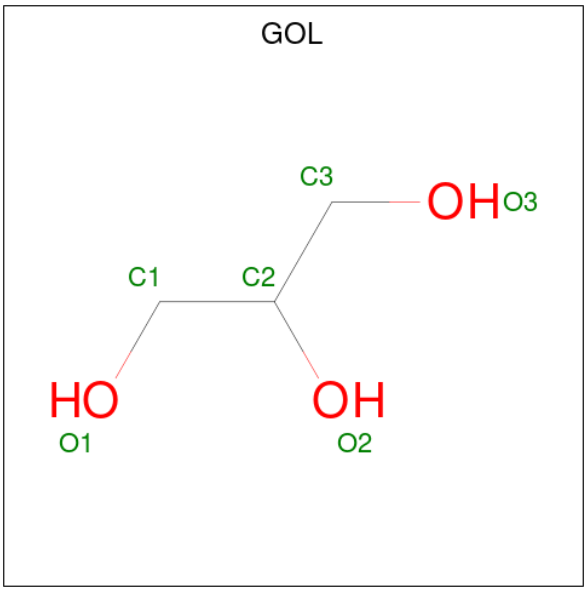
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is N-PALMITOYL-L-METHIONINE (three-letter code: EPM) (formula: $C_{21}H_{41}NO_3S$).



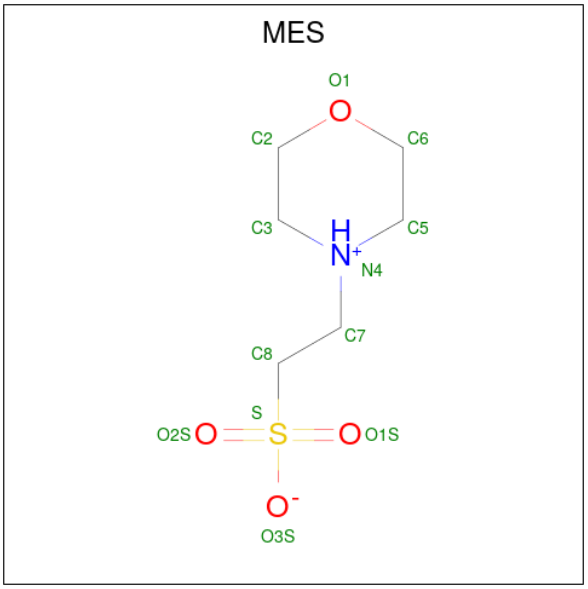
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	26	21	1	3	1	0	0
			Total	C	N	O	S		
3	B	1	26	21	1	3	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 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		
5	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
5	B	1	12	6	1	4	1	0	0

- Molecule 6 is water.

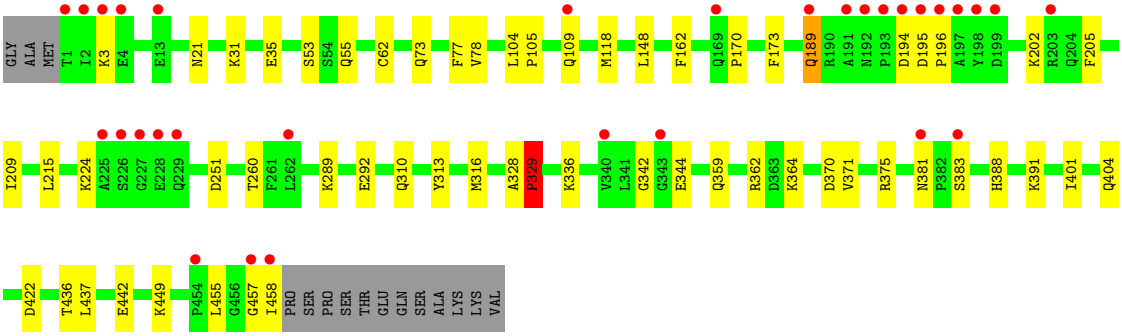
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	533	533	533	0	0
			Total	O		
6	B	539	539	539	0	0

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.

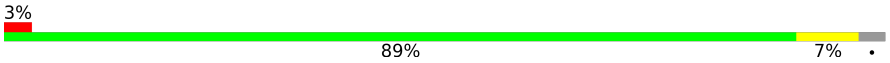
• Molecule 1: Bifunctional P-450:NADPH-P450 reductase

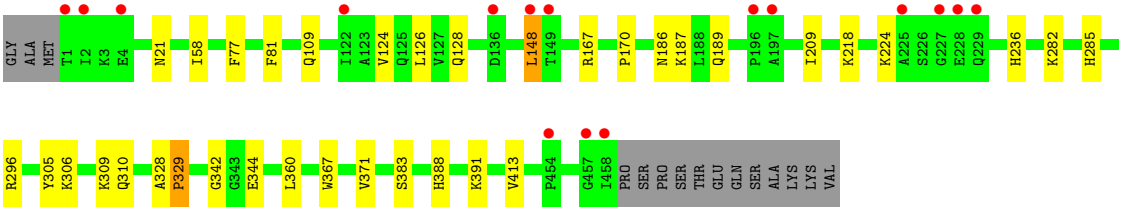
Chain A:



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

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.04Å 147.81Å 63.60Å 90.00° 98.60° 90.00°	Depositor
Resolution (Å)	29.60 – 1.70 29.59 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.60-1.70) 79.6 (29.59-1.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.164 , 0.199 0.154 , 0.191	Depositor DCC
R_{free} test set	5673 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8853	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: HEM, GOL, MES, EPM

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	0.53	0/3853	0.71	2/5206 (0.0%)
1	B	0.53	0/3852	0.72	2/5206 (0.0%)
All	All	0.53	0/7705	0.71	4/10412 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	328	ALA	N-CA-C	-7.10	91.83	111.00
1	A	328	ALA	N-CA-C	-6.96	92.22	111.00
1	B	329	PRO	N-CA-C	5.51	126.42	112.10
1	A	329	PRO	N-CA-C	5.43	126.23	112.10

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	3768	0	3751	66	0
1	B	3767	0	3733	36	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	26	0	40	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	40	0	0
4	A	66	0	88	14	0
4	B	18	0	24	6	0
5	B	24	0	26	1	0
6	A	533	0	0	16	0
6	B	539	0	0	11	0
All	All	8853	0	7762	105	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 7.

All (105) 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:457:GLY:O	1:A:458:ILE:HB	1.66	0.95
1:B:306[B]:LYS:HD3	6:B:1642:HOH:O	1.70	0.89
1:A:224:LYS:HA	1:A:224:LYS:HE2	1.57	0.87
1:A:422:ASP:HB2	1:A:449[A]:LYS:HG3	1.58	0.86
1:B:218:LYS:HE2	6:B:1947:HOH:O	1.79	0.82
1:A:189:GLN:HG3	6:A:1930:HOH:O	1.79	0.81
1:B:309:LYS:HD3	4:B:1474:GOL:H2	1.64	0.77
1:B:306[A]:LYS:HZ1	1:B:310:GLN:HG3	1.51	0.76
1:B:282:LYS:HD2	4:B:1479:GOL:H12	1.69	0.74
1:A:364:LYS:HE3	4:A:1475:GOL:H12	1.72	0.72
1:A:292:GLU:OE2	4:A:1473:GOL:H11	1.90	0.71
1:B:128[B]:GLN:HE21	1:B:128[B]:GLN:HA	1.54	0.71
4:A:1476:GOL:H32	6:A:1635:HOH:O	1.92	0.70
1:B:170:PRO:HG3	6:B:1774:HOH:O	1.92	0.69
1:A:21:ASN:HA	1:A:189:GLN:HG2	1.76	0.68
1:A:388:HIS:HA	1:A:391[B]:LYS:HD3	1.75	0.67
1:A:224:LYS:HE3	6:A:1818:HOH:O	1.94	0.66
4:A:1473:GOL:H12	6:B:1926:HOH:O	1.93	0.66
1:A:329:PRO:HD2	3:A:1470:EPM:H121	1.79	0.65
1:B:285:HIS:HB3	5:B:1491:MES:H21	1.79	0.64
1:A:381:ASN:HB3	6:A:1926:HOH:O	1.97	0.64
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.80	0.64
1:A:78:VAL:HG11	3:A:1470:EPM:H191	1.81	0.63
1:A:310[B]:GLN:NE2	6:A:1682:HOH:O	2.32	0.62
1:B:282:LYS:HD2	4:B:1479:GOL:H31	1.80	0.62
1:B:306[A]:LYS:NZ	1:B:310:GLN:HG3	2.12	0.62
1:A:455:LEU:O	4:A:1472:GOL:H11	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:OD1	4:A:1478:GOL:H11	2.01	0.61
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.37	0.59
1:A:388:HIS:HD2	1:A:391[A]:LYS:NZ	2.01	0.59
1:A:383:SER:HB3	6:A:1816:HOH:O	2.05	0.56
1:A:260:THR:HA	3:A:1470:EPM:H211	1.86	0.56
1:A:458:ILE:HG23	6:A:1966:HOH:O	2.05	0.56
1:A:458:ILE:CG2	6:A:1966:HOH:O	2.54	0.56
1:A:457:GLY:O	1:A:458:ILE:CB	2.47	0.56
4:A:1472:GOL:H2	6:A:1829:HOH:O	2.06	0.56
1:A:195:ASP:OD1	1:A:196:PRO:HD2	2.07	0.55
1:B:282:LYS:O	4:B:1479:GOL:H32	2.08	0.54
4:A:1481:GOL:H11	6:A:1970:HOH:O	2.08	0.54
1:A:224:LYS:HE2	1:A:224:LYS:CA	2.34	0.53
1:B:306[B]:LYS:HE3	6:B:1758:HOH:O	2.07	0.53
1:A:455:LEU:HB3	4:A:1472:GOL:O1	2.08	0.53
1:A:310[A]:GLN:HG2	1:A:310[A]:GLN:O	2.09	0.53
1:A:31[B]:LYS:O	1:A:35:GLU:HG3	2.09	0.52
1:B:236:HIS:CD2	6:B:1937:HOH:O	2.62	0.52
1:A:388:HIS:HD2	1:A:391[B]:LYS:NZ	2.07	0.52
1:A:53:SER:HB3	1:A:359:GLN:HB3	1.92	0.51
1:A:31[A]:LYS:O	1:A:35:GLU:HG3	2.10	0.51
1:A:173:PHE:CD1	1:A:215:LEU:HD22	2.45	0.51
1:B:306[A]:LYS:HZ1	1:B:310:GLN:CG	2.23	0.51
1:B:126[B]:LEU:C	1:B:126[B]:LEU:HD13	2.31	0.51
1:A:170:PRO:HG3	6:A:1864:HOH:O	2.11	0.51
1:B:296[A]:ARG:NH2	6:B:1675:HOH:O	2.43	0.51
1:A:162:PHE:CZ	1:A:215:LEU:HD21	2.47	0.50
1:B:77:PHE:CE1	1:B:187:LYS:HE2	2.46	0.50
1:A:62:CYS:SG	1:A:391[A]:LYS:HE2	2.52	0.50
1:A:404[B]:GLN:H	1:A:404[B]:GLN:CD	2.14	0.50
1:B:309:LYS:HA	4:B:1474:GOL:H2	1.92	0.50
1:A:342:GLY:O	1:A:344:GLU:HG3	2.12	0.50
1:B:282:LYS:CD	4:B:1479:GOL:H31	2.42	0.49
1:B:342:GLY:O	1:B:344:GLU:HG3	2.12	0.49
1:A:118[A]:MET:HG3	6:A:1665:HOH:O	2.13	0.49
1:B:186[A]:ASN:O	1:B:189:GLN:HG2	2.13	0.49
1:B:306[B]:LYS:HD3	1:B:306[B]:LYS:H	1.78	0.49
1:B:148:LEU:HD21	1:B:413[B]:VAL:HG21	1.94	0.49
1:A:422:ASP:HB2	1:A:449[A]:LYS:CG	2.37	0.48
1:A:336:LYS:HZ3	4:A:1483:GOL:C1	2.26	0.48
1:B:109:GLN:NE2	1:B:305:TYR:OH	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLN:NE2	1:A:109:GLN:HA	2.29	0.48
1:B:167:ARG:HD3	6:B:1762:HOH:O	2.14	0.47
1:A:449[A]:LYS:HG2	6:A:1775:HOH:O	2.13	0.47
1:A:205:PHE:O	1:A:209:ILE:HG13	2.14	0.47
1:B:306[B]:LYS:HD3	1:B:306[B]:LYS:N	2.30	0.47
1:A:73:GLN:HG3	1:A:77:PHE:CE2	2.50	0.47
1:A:3:LYS:HD2	1:A:344:GLU:OE1	2.16	0.46
1:B:81:PHE:HB3	1:B:209:ILE:HG12	1.98	0.46
1:B:224:LYS:HD2	6:B:1998:HOH:O	2.14	0.46
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.98	0.46
1:B:186[B]:ASN:O	1:B:189:GLN:HG2	2.16	0.45
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.98	0.45
1:A:370:ASP:OD1	1:A:375[B]:ARG:NH2	2.48	0.44
1:A:388:HIS:HD2	1:A:391[A]:LYS:HZ2	1.66	0.44
1:A:404[B]:GLN:H	1:A:404[B]:GLN:NE2	2.16	0.44
1:A:370:ASP:OD1	1:A:375[B]:ARG:NH1	2.50	0.43
1:A:383:SER:CB	6:A:1816:HOH:O	2.65	0.43
1:A:422:ASP:HB3	1:A:449[A]:LYS:HE2	2.00	0.43
1:A:442:GLU:HG3	6:A:1971:HOH:O	2.17	0.43
1:A:109:GLN:NE2	6:A:1677:HOH:O	2.52	0.43
1:A:55:GLN:OE1	4:A:1484:GOL:H32	2.19	0.43
1:A:289:LYS:NZ	1:B:383:SER:O	2.51	0.43
1:B:124:VAL:O	1:B:128[B]:GLN:HG2	2.18	0.43
1:A:313:TYR:HA	1:A:316[A]:MET:SD	2.60	0.42
1:B:224:LYS:HG3	6:B:1856:HOH:O	2.20	0.42
1:A:104:LEU:N	1:A:105:PRO:CD	2.82	0.42
1:B:58:ILE:HD12	1:B:360:LEU:HD13	1.99	0.42
1:A:371:VAL:CG2	4:A:1475:GOL:H32	2.50	0.42
1:A:404[B]:GLN:CD	1:A:404[B]:GLN:N	2.72	0.42
1:A:436:THR:O	1:A:437:LEU:HB2	2.19	0.42
1:A:55:GLN:HE22	4:A:1484:GOL:H32	1.85	0.41
1:A:401:ILE:O	1:A:404[B]:GLN:NE2	2.52	0.41
1:A:422:ASP:CB	1:A:449[A]:LYS:HE2	2.50	0.41
1:A:362:ARG:O	4:A:1475:GOL:H11	2.21	0.41
1:A:109:GLN:HA	1:A:109:GLN:HE21	1.86	0.41
1:A:194:ASP:HA	1:A:202:LYS:NZ	2.37	0.40
1:B:306[B]:LYS:CE	6:B:1758:HOH:O	2.69	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	467/473 (99%)	453 (97%)	14 (3%)	0	100	100
1	B	466/473 (98%)	453 (97%)	13 (3%)	0	100	100
All	All	933/946 (99%)	906 (97%)	27 (3%)	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	408/412 (99%)	405 (99%)	3 (1%)	84	77
1	B	408/412 (99%)	405 (99%)	3 (1%)	84	77
All	All	816/824 (99%)	810 (99%)	6 (1%)	81	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	189	GLN
1	A	329	PRO
1	B	21	ASN
1	B	148	LEU
1	B	329	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	110	GLN
1	A	206	GLN
1	A	381	ASN
1	A	388	HIS
1	A	403	GLN
1	B	21	ASN
1	B	92	HIS
1	B	109	GLN
1	B	189	GLN
1	B	201	ASN
1	B	206	GLN
1	B	236	HIS
1	B	310	GLN
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)

20 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	GOL	A	1475	-	5,5,5	0.70	0	5,5,5	0.20	0
2	HEM	A	471	1	41,50,50	1.85	11 (26%)	45,82,82	1.32	5 (11%)
4	GOL	A	1473	-	5,5,5	0.51	0	5,5,5	0.21	0
4	GOL	A	1481	-	5,5,5	0.60	0	5,5,5	0.20	0
5	MES	B	1490	-	12,12,12	1.24	1 (8%)	14,16,16	0.77	0
2	HEM	B	471	1	41,50,50	2.05	13 (31%)	45,82,82	1.31	8 (17%)
4	GOL	B	1474	-	5,5,5	0.47	0	5,5,5	0.21	0
4	GOL	A	1476	-	5,5,5	0.52	0	5,5,5	0.19	0
4	GOL	A	1485	-	5,5,5	0.28	0	5,5,5	0.36	0
4	GOL	A	1480	-	5,5,5	0.69	0	5,5,5	0.16	0
4	GOL	B	1477	-	5,5,5	0.43	0	5,5,5	0.21	0
3	EPM	B	1471	-	25,25,25	0.95	1 (4%)	27,27,27	1.17	1 (3%)
3	EPM	A	1470	-	25,25,25	0.96	2 (8%)	27,27,27	1.05	2 (7%)
5	MES	B	1491	-	12,12,12	1.63	2 (16%)	14,16,16	0.73	0
4	GOL	A	1484	-	5,5,5	0.39	0	5,5,5	0.22	0
4	GOL	A	1482	-	5,5,5	0.49	0	5,5,5	0.26	0
4	GOL	B	1479	-	5,5,5	0.60	0	5,5,5	0.17	0
4	GOL	A	1478	-	5,5,5	0.65	0	5,5,5	0.13	0
4	GOL	A	1472	-	5,5,5	0.49	0	5,5,5	0.24	0
4	GOL	A	1483	-	5,5,5	0.23	0	5,5,5	0.26	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
4	GOL	A	1475	-	-	2/4/4/4	-
2	HEM	A	471	1	-	2/12/54/54	-
4	GOL	A	1473	-	-	2/4/4/4	-
4	GOL	A	1481	-	-	2/4/4/4	-
5	MES	B	1490	-	-	2/6/14/14	0/1/1/1
2	HEM	B	471	1	-	2/12/54/54	-
4	GOL	B	1474	-	-	2/4/4/4	-
4	GOL	A	1476	-	-	2/4/4/4	-
4	GOL	A	1485	-	-	2/4/4/4	-
4	GOL	A	1480	-	-	0/4/4/4	-
4	GOL	B	1477	-	-	2/4/4/4	-
3	EPM	B	1471	-	-	6/27/27/27	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPM	A	1470	-	-	7/27/27/27	-
5	MES	B	1491	-	-	0/6/14/14	0/1/1/1
4	GOL	A	1484	-	-	0/4/4/4	-
4	GOL	A	1482	-	-	2/4/4/4	-
4	GOL	B	1479	-	-	2/4/4/4	-
4	GOL	A	1478	-	-	2/4/4/4	-
4	GOL	A	1472	-	-	2/4/4/4	-
4	GOL	A	1483	-	-	2/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	471	HEM	C3C-CAC	5.11	1.58	1.47
2	B	471	HEM	CBB-CAB	4.97	1.55	1.30
2	A	471	HEM	CBB-CAB	4.90	1.54	1.30
2	A	471	HEM	C3C-CAC	4.04	1.56	1.47
2	B	471	HEM	CBC-CAC	3.69	1.53	1.29
2	A	471	HEM	CBC-CAC	3.53	1.52	1.29
2	B	471	HEM	CBD-CGD	-3.50	1.42	1.50
5	B	1491	MES	C5-N4	3.40	1.56	1.46
2	A	471	HEM	CBD-CAD	3.19	1.62	1.52
3	A	1470	EPM	C2-C1	3.02	1.60	1.52
2	B	471	HEM	CBD-CAD	3.01	1.61	1.52
2	B	471	HEM	C4D-C3D	3.01	1.50	1.45
5	B	1491	MES	C3-N4	2.80	1.54	1.46
3	B	1471	EPM	C2-C1	2.78	1.59	1.52
2	A	471	HEM	CBA-CGA	-2.64	1.44	1.50
2	A	471	HEM	CHB-C1B	2.63	1.41	1.35
2	B	471	HEM	O2A-CGA	-2.61	1.22	1.30
2	B	471	HEM	CHB-C1B	2.60	1.41	1.35
2	A	471	HEM	CBD-CGD	-2.58	1.44	1.50
2	B	471	HEM	C3C-C2C	-2.57	1.36	1.40
2	B	471	HEM	CBA-CGA	-2.53	1.44	1.50
2	B	471	HEM	CHA-C4D	2.52	1.41	1.35
2	B	471	HEM	CMC-C2C	2.44	1.57	1.51
2	A	471	HEM	C2C-C1C	2.40	1.48	1.42
2	A	471	HEM	CHA-C4D	2.37	1.41	1.35
5	B	1490	MES	C5-N4	2.33	1.53	1.46
2	A	471	HEM	O1A-CGA	2.17	1.29	1.22
2	B	471	HEM	C4D-ND	-2.12	1.36	1.40
3	A	1470	EPM	O2-C1	-2.10	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	471	HEM	C4D-C3D	2.10	1.48	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	471	HEM	CMC-C2C-C3C	3.66	131.53	124.68
3	B	1471	EPM	C3-C2-N	-3.60	103.59	110.88
2	B	471	HEM	CMC-C2C-C3C	3.18	130.63	124.68
2	A	471	HEM	O2A-CGA-CBA	3.11	124.02	114.03
3	A	1470	EPM	C3-C2-N	-2.92	104.96	110.88
2	B	471	HEM	O2A-CGA-CBA	2.56	122.25	114.03
2	B	471	HEM	CMA-C3A-C4A	-2.51	124.60	128.46
2	A	471	HEM	O1A-CGA-CBA	-2.51	115.01	123.08
2	A	471	HEM	C4B-CHC-C1C	2.40	125.72	122.56
2	B	471	HEM	CBB-CAB-C3B	-2.31	116.11	127.62
2	B	471	HEM	C4C-CHD-C1D	2.24	125.51	122.56
2	A	471	HEM	CBB-CAB-C3B	-2.23	116.53	127.62
2	B	471	HEM	CMA-C3A-C2A	2.19	129.08	124.94
2	B	471	HEM	C4B-CHC-C1C	2.06	125.28	122.56
3	A	1470	EPM	O2-C1-C2	2.03	120.14	113.40
2	B	471	HEM	O2D-CGD-CBD	2.00	120.46	114.03

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1472	GOL	O1-C1-C2-O2
4	A	1472	GOL	O1-C1-C2-C3
4	A	1473	GOL	O1-C1-C2-O2
4	A	1473	GOL	O1-C1-C2-C3
4	A	1475	GOL	O1-C1-C2-C3
4	A	1476	GOL	O1-C1-C2-C3
4	A	1481	GOL	O1-C1-C2-C3
4	A	1483	GOL	O1-C1-C2-C3
4	A	1485	GOL	O1-C1-C2-C3
4	B	1474	GOL	O1-C1-C2-O2
4	B	1474	GOL	O1-C1-C2-C3
3	B	1471	EPM	C10-C11-C12-C13
3	A	1470	EPM	C10-C11-C12-C13
3	A	1470	EPM	C12-C13-C14-C15
4	A	1478	GOL	O1-C1-C2-C3
4	A	1482	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	1477	GOL	O1-C1-C2-C3
4	B	1479	GOL	O1-C1-C2-C3
4	A	1475	GOL	O1-C1-C2-O2
4	A	1482	GOL	O1-C1-C2-O2
4	A	1483	GOL	O1-C1-C2-O2
4	A	1485	GOL	O1-C1-C2-O2
4	B	1479	GOL	O1-C1-C2-O2
3	A	1470	EPM	C16-C17-C18-C19
3	B	1471	EPM	C12-C13-C14-C15
3	B	1471	EPM	O3-C6-C7-C8
4	A	1476	GOL	O1-C1-C2-O2
4	A	1481	GOL	O1-C1-C2-O2
4	B	1477	GOL	O1-C1-C2-O2
3	B	1471	EPM	N-C6-C7-C8
3	B	1471	EPM	C9-C10-C11-C12
3	A	1470	EPM	O3-C6-C7-C8
5	B	1490	MES	C8-C7-N4-C5
3	A	1470	EPM	N-C6-C7-C8
3	A	1470	EPM	C9-C10-C11-C12
4	A	1478	GOL	O1-C1-C2-O2
3	B	1471	EPM	C15-C16-C17-C18
3	A	1470	EPM	C6-C7-C8-C9
2	B	471	HEM	CAD-CBD-CGD-O1D
2	B	471	HEM	CAD-CBD-CGD-O2D
2	A	471	HEM	CAD-CBD-CGD-O1D
2	A	471	HEM	CAD-CBD-CGD-O2D
5	B	1490	MES	C8-C7-N4-C3

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1475	GOL	3	0
4	A	1473	GOL	2	0
4	A	1481	GOL	1	0
4	B	1474	GOL	2	0
4	A	1476	GOL	1	0
3	A	1470	EPM	3	0
5	B	1491	MES	1	0
4	A	1484	GOL	2	0
4	B	1479	GOL	4	0
4	A	1478	GOL	1	0

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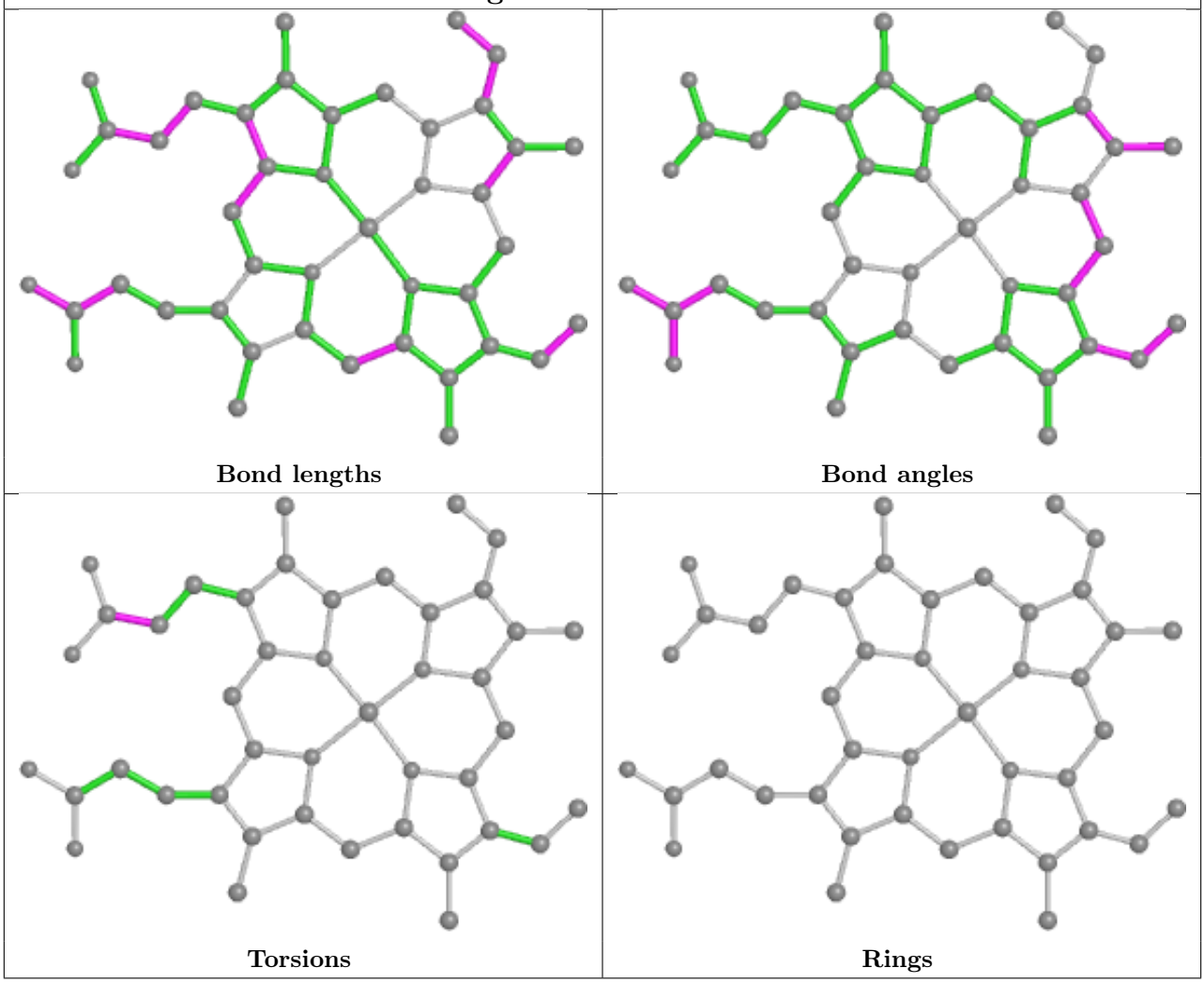
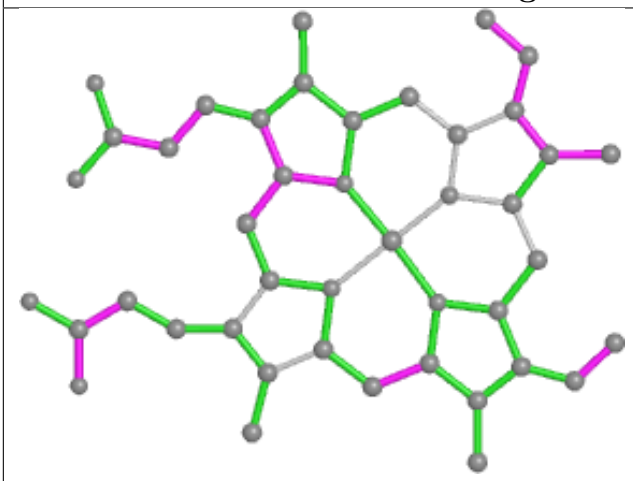
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1472	GOL	3	0
4	A	1483	GOL	1	0

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

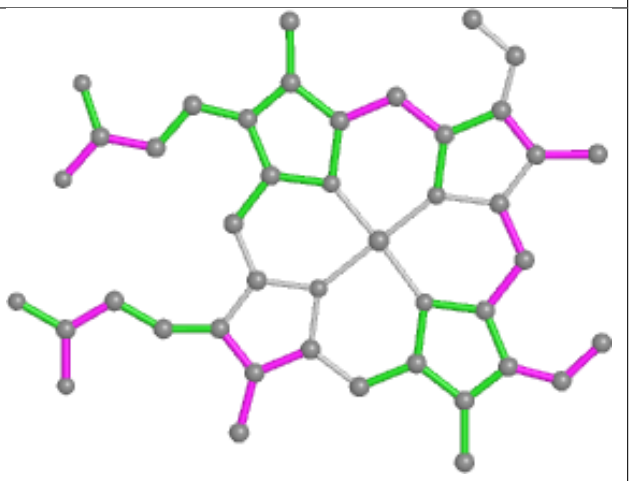
Ligand HEM A 471



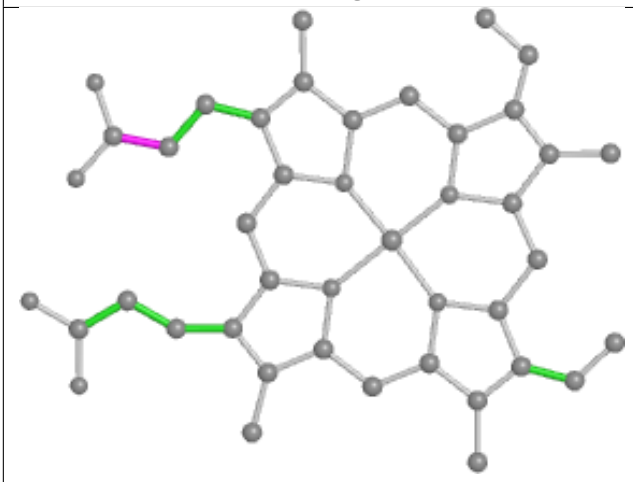
Ligand HEM B 471



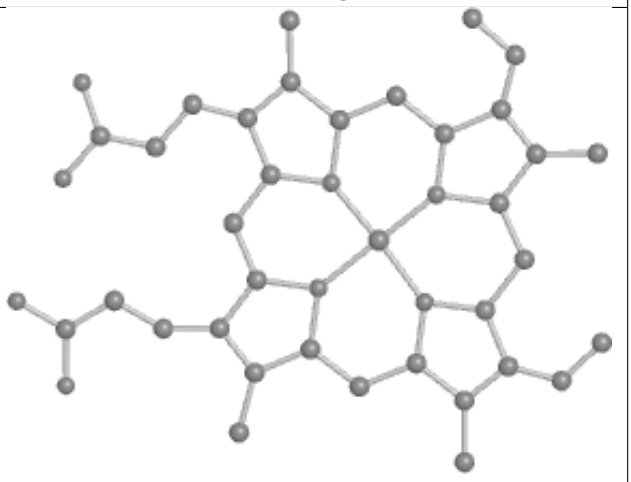
Bond lengths



Bond angles

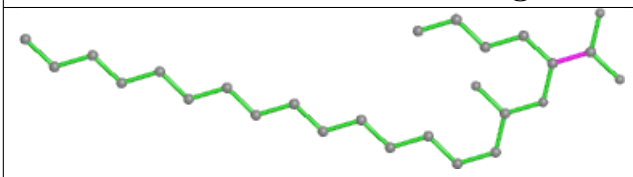


Torsions

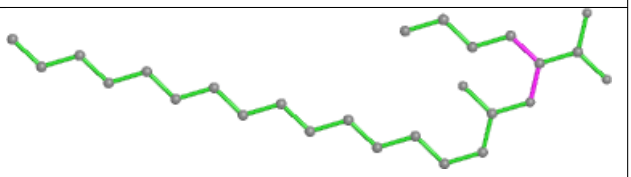


Rings

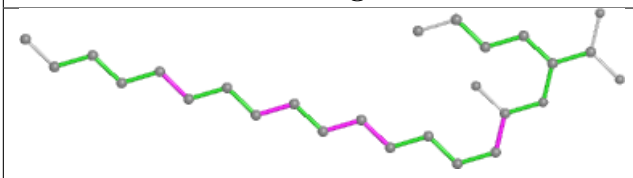
Ligand EPM B 1471



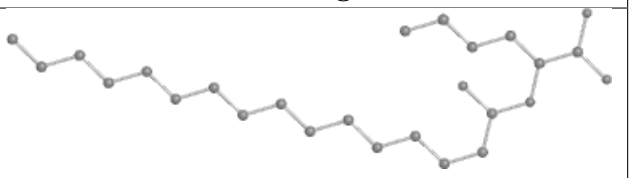
Bond lengths



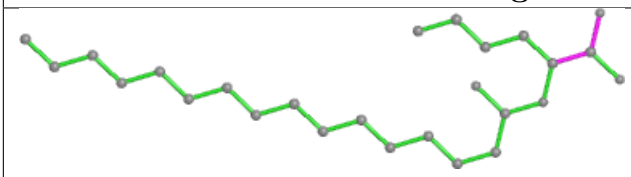
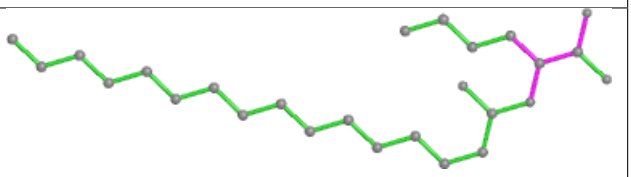
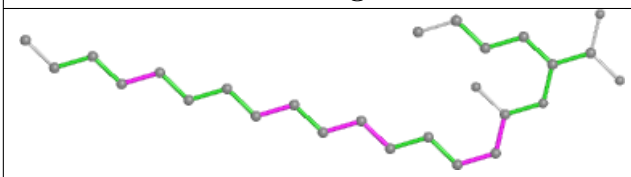
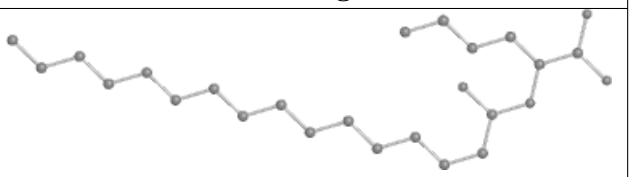
Bond angles



Torsions



Rings

Ligand EPM A 1470	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95th 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^2)	Q<0.9
1	A	458/473 (96%)	0.16	31 (6%)	17	19	14, 21, 46, 70	0
1	B	458/473 (96%)	0.02	16 (3%)	44	49	15, 21, 37, 63	0
All	All	916/946 (96%)	0.09	47 (5%)	28	31	14, 21, 42, 70	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	ILE	11.9
1	B	227	GLY	11.1
1	A	227	GLY	9.7
1	A	2	ILE	9.5
1	A	1	THR	7.9
1	B	458	ILE	7.7
1	B	1	THR	6.7
1	B	2	ILE	6.5
1	B	229	GLN	6.3
1	A	196	PRO	5.6
1	B	457	GLY	5.2
1	A	198	TYR	5.0
1	A	228	GLU	4.7
1	A	197	ALA	4.5
1	A	229	GLN	4.3
1	B	228	GLU	4.2
1	B	4	GLU	4.2
1	A	225	ALA	4.2
1	A	193	PRO	4.1
1	B	225	ALA	3.9
1	A	195	ASP	3.7
1	A	383	SER	3.5
1	A	457	GLY	3.4
1	A	192	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	191	ALA	3.1
1	A	3	LYS	2.9
1	B	454	PRO	2.9
1	A	189	GLN	2.7
1	A	109	GLN	2.6
1	B	196	PRO	2.6
1	A	381	ASN	2.6
1	B	136	ASP	2.5
1	A	194	ASP	2.5
1	A	4	GLU	2.5
1	A	226	SER	2.4
1	A	343	GLY	2.4
1	A	203	ARG	2.3
1	A	340	VAL	2.3
1	A	13	GLU	2.3
1	A	262	LEU	2.3
1	A	454	PRO	2.2
1	B	197	ALA	2.2
1	B	148	LEU	2.2
1	B	149	THR	2.1
1	A	199	ASP	2.1
1	B	122	ILE	2.1
1	A	169	GLN	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, 95th 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.

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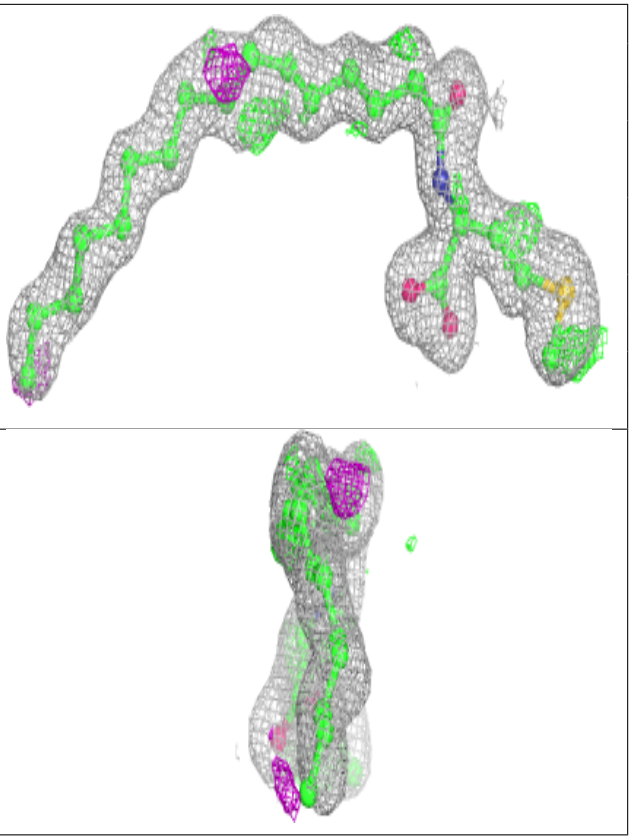
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

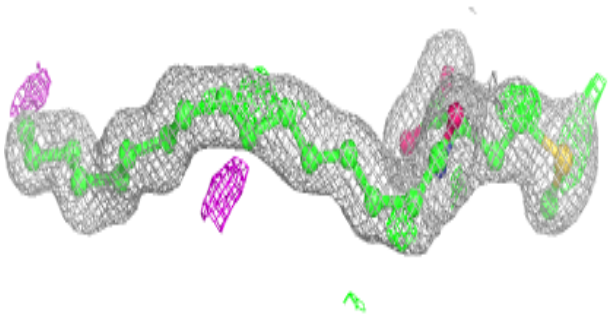
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MES	B	1491	12/12	0.51	0.51	53,57,69,73	0
4	GOL	A	1478	6/6	0.58	0.45	53,55,56,57	0
4	GOL	B	1479	6/6	0.67	0.28	50,52,53,57	0
4	GOL	B	1474	6/6	0.70	0.21	39,47,49,49	0
4	GOL	A	1475	6/6	0.72	0.28	40,46,46,47	0
4	GOL	A	1472	6/6	0.72	0.25	49,52,53,56	0
4	GOL	A	1481	6/6	0.72	0.48	41,47,48,49	0
4	GOL	A	1473	6/6	0.74	0.24	46,51,53,54	0
4	GOL	A	1482	6/6	0.74	0.20	29,45,50,53	0
4	GOL	A	1485	6/6	0.74	0.30	28,46,48,54	0
4	GOL	A	1476	6/6	0.75	0.39	49,50,51,55	0
4	GOL	A	1484	6/6	0.75	0.27	41,47,50,50	0
5	MES	B	1490	12/12	0.82	0.26	43,47,65,66	0
4	GOL	A	1483	6/6	0.82	0.26	40,50,51,55	0
4	GOL	B	1477	6/6	0.83	0.16	51,53,54,56	0
4	GOL	A	1480	6/6	0.88	0.12	23,37,39,39	0
3	EPM	A	1470	26/26	0.92	0.15	23,29,33,39	0
3	EPM	B	1471	26/26	0.93	0.13	21,28,31,36	0
2	HEM	B	471	43/43	0.96	0.10	14,17,19,31	0
2	HEM	A	471	43/43	0.97	0.11	14,17,19,29	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 EPM A 1470:

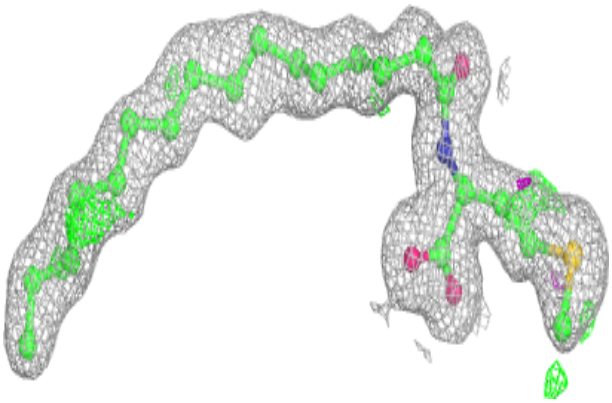
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

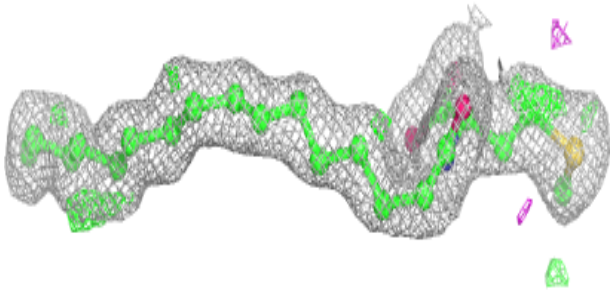


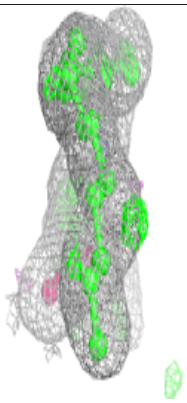


Electron density around EPM B 1471:

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

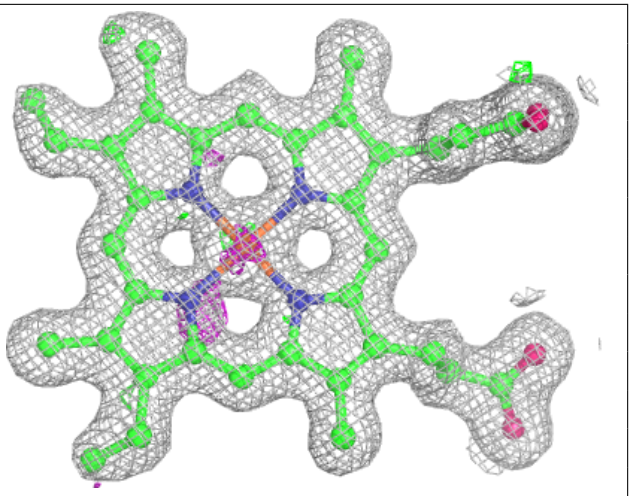


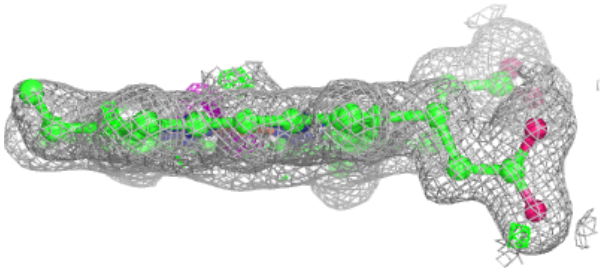


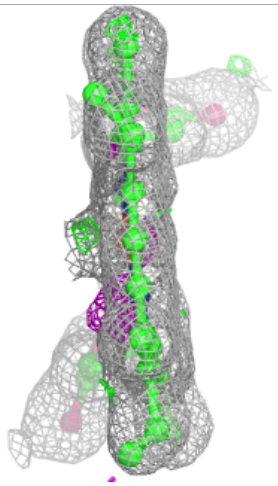


Electron density around HEM B 471:

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

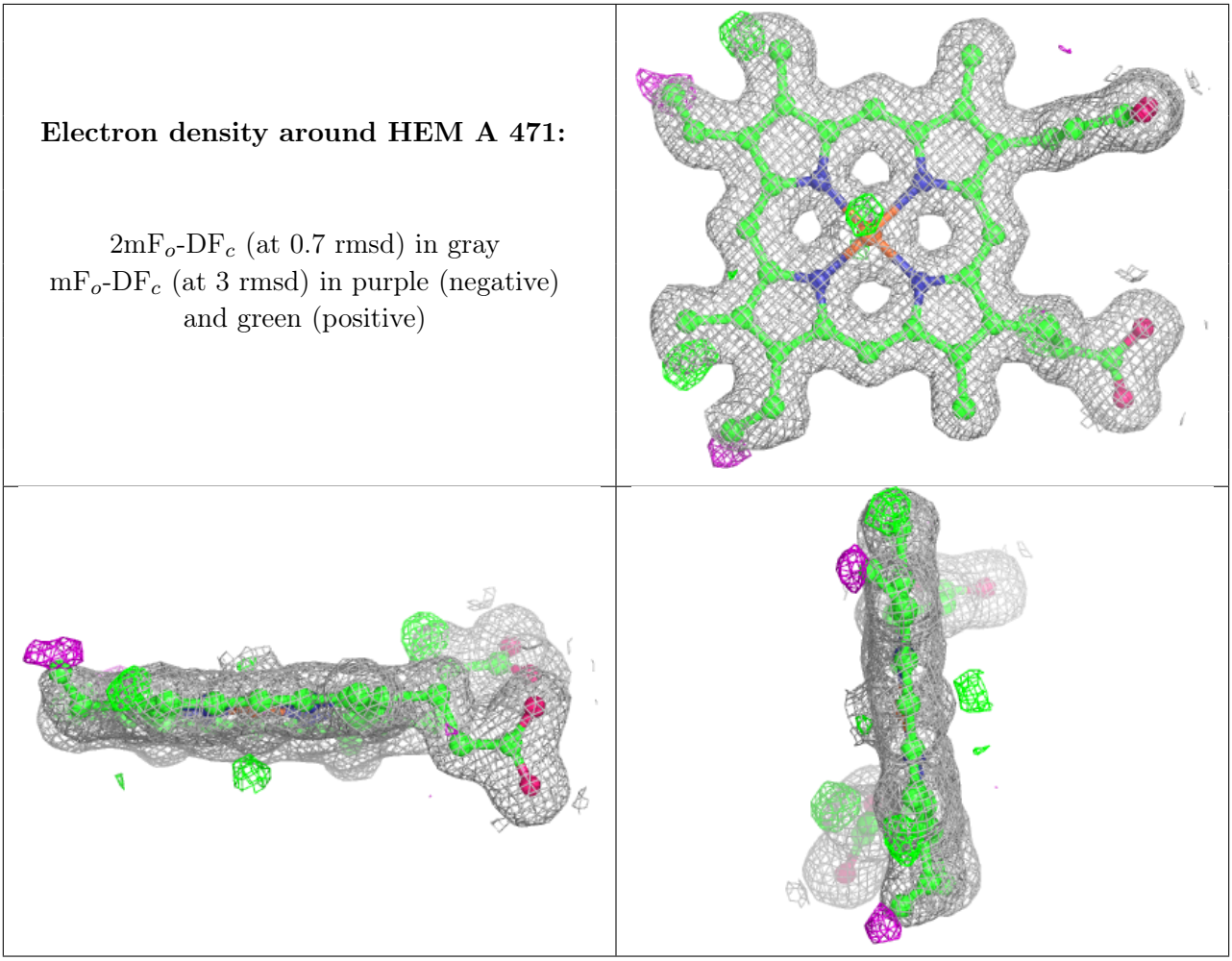






Electron density around HEM A 471:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.