



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:04 PM UTC

PDB ID : 9IST / pdb_00009ist
Title : Crystal Structure of Cytochrome P450BM3 VI-18A12 Mutant Heme Domain
with N-Decanoyl-L-Homoserine Lactone
Authors : Yokoyama, Y.; Sugimoto, H.; Shoji, O.
Deposited on : 2024-07-18
Resolution : 2.27 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

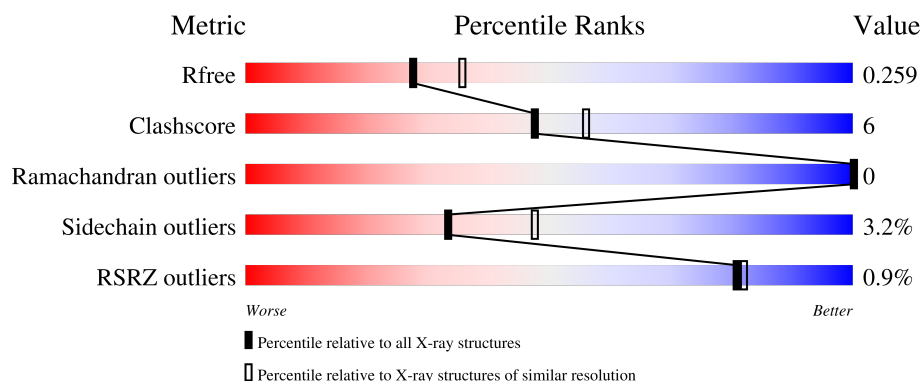
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 $\leq 5\%$. 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	455	 84% 15% .
1	B	455	 84% 14% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7882 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.

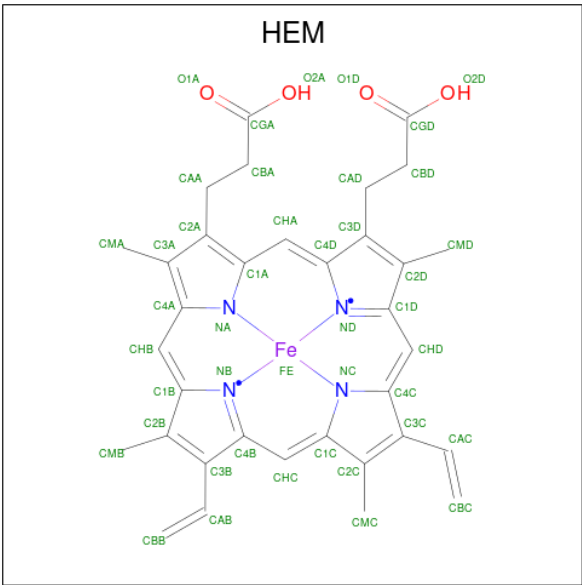
- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3676	2353	621	685	17			
1	B	455	Total	C	N	O	S	0	0	0
			3676	2353	621	685	17			

There are 10 discrepancies between the modelled and reference sequences:

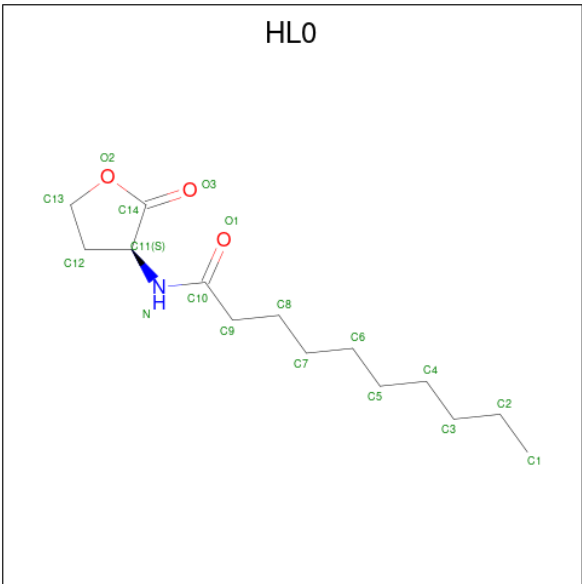
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	VAL	PRO	engineered mutation	UNP P14779
A	47	TRP	ARG	engineered mutation	UNP P14779
A	49	LEU	THR	engineered mutation	UNP P14779
A	74	VAL	ALA	engineered mutation	UNP P14779
A	188	PRO	LEU	engineered mutation	UNP P14779
B	25	VAL	PRO	engineered mutation	UNP P14779
B	47	TRP	ARG	engineered mutation	UNP P14779
B	49	LEU	THR	engineered mutation	UNP P14779
B	74	VAL	ALA	engineered mutation	UNP P14779
B	188	PRO	LEU	engineered mutation	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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-[(3S)-2-oxotetrahydrofuran-3-yl]decanamide (CCD ID: HL0) (formula: C₁₄H₂₅NO₃) (labeled as "Ligand of Interest" by depositor).



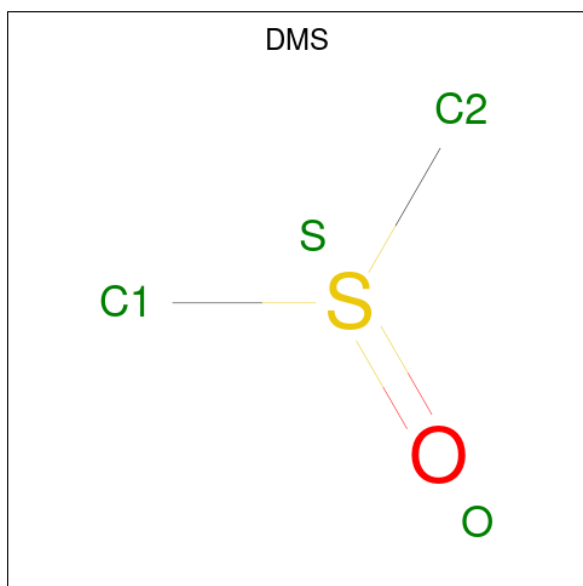
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	14	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			18	14	1	3		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

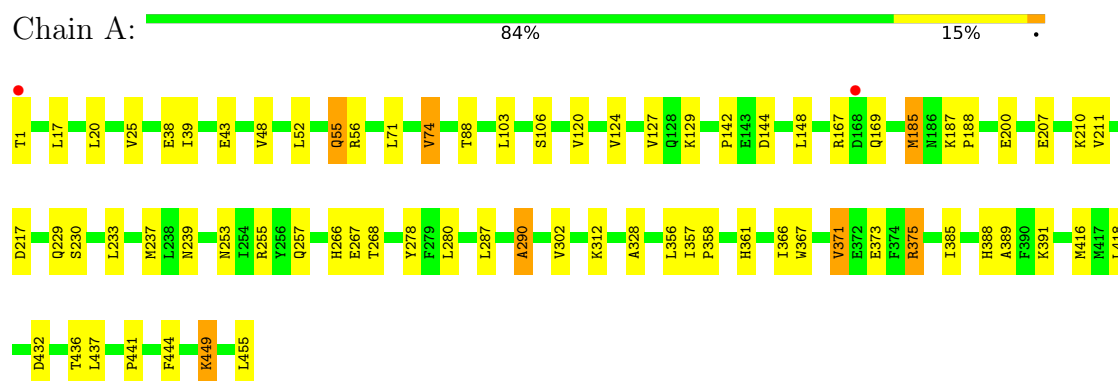
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	182	Total	O	0	0
			182	182		
6	B	176	Total	O	0	0
			176	176		

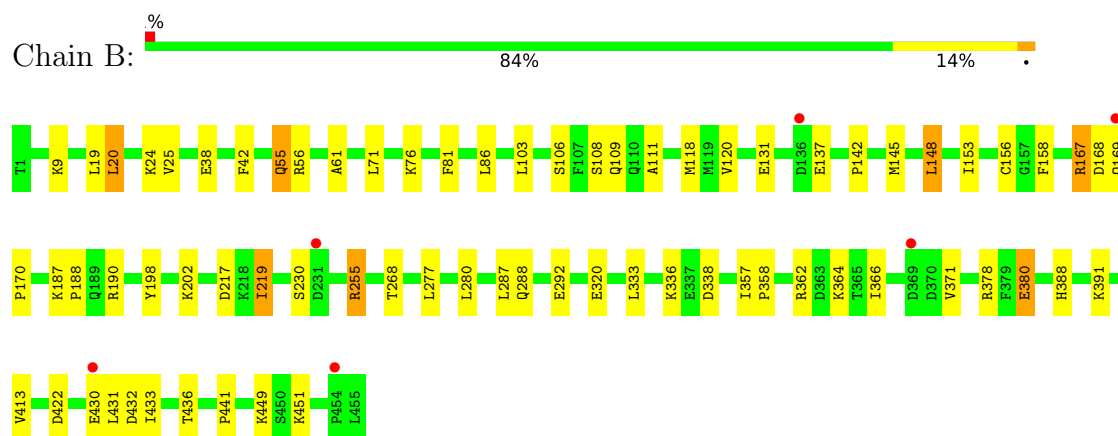
3 Residue-property plots

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

- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.48Å 148.78Å 61.37Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	47.00 – 2.27 47.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.00-2.27) 97.5 (47.00-2.27)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.259 0.195 , 0.259	Depositor DCC
R_{free} test set	2326 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7882	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 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DMS, GOL, HEM, HLO

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	1.06	0/3763	1.45	6/5089 (0.1%)
1	B	1.06	0/3763	1.46	8/5089 (0.2%)
All	All	1.06	0/7526	1.46	14/10178 (0.1%)

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	B	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	GLU	N-CA-C	-6.33	104.43	111.71
1	B	168	ASP	N-CA-C	-5.84	104.13	112.13
1	A	356	LEU	CA-C-N	5.78	123.88	120.24
1	A	356	LEU	C-N-CA	5.78	123.88	120.24
1	A	290	ALA	CA-C-N	5.68	127.90	120.28
1	A	290	ALA	C-N-CA	5.68	127.90	120.28
1	A	432	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	148	LEU	CA-C-O	-5.61	114.93	120.82
1	B	338	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	436	THR	N-CA-C	-5.49	103.48	108.75
1	B	81	PHE	CA-CB-CG	5.35	119.15	113.80
1	B	170	PRO	CA-C-N	5.17	127.57	120.39
1	B	170	PRO	C-N-CA	5.17	127.57	120.39
1	A	437	LEU	N-CA-C	-5.08	105.93	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	378	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3676	0	3648	38	0
1	B	3676	0	3648	41	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	18	0	25	0	0
3	B	18	0	25	0	0
4	A	4	0	6	1	0
4	B	4	0	6	0	0
5	A	12	0	16	0	0
5	B	30	0	40	5	0
6	A	182	0	0	0	0
6	B	176	0	0	4	0
All	All	7882	0	7474	84	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 6.

All (84) 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:74:VAL:HG13	1:A:185:MET:HE2	1.64	0.80
5:B:505:GOL:H2	6:B:624:HOH:O	1.87	0.74
1:A:373:GLU:OE2	1:A:375:ARG:HD3	1.90	0.72
1:B:145:MET:HA	1:B:145:MET:HE2	1.74	0.69
1:B:422:ASP:OD1	1:B:451:LYS:HE2	1.95	0.66
1:A:268:THR:HG21	4:A:503:DMS:O	1.96	0.66
1:B:217:ASP:OD1	1:B:255:ARG:HD3	1.98	0.63
1:A:38:GLU:OE2	1:A:56:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HD22	1:B:42:PHE:CZ	2.37	0.59
1:B:167:ARG:HD3	1:B:169:GLN:O	2.03	0.59
1:B:137:GLU:OE2	6:B:601:HOH:O	2.17	0.59
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.85	0.58
1:A:17:LEU:HD12	1:A:20:LEU:HD12	1.88	0.56
1:B:38:GLU:OE2	1:B:56:ARG:NH1	2.39	0.55
1:B:20:LEU:HG	1:B:25:VAL:HG13	1.88	0.54
1:B:55:GLN:HG2	1:B:366:ILE:CD1	2.38	0.54
1:B:198:TYR:O	1:B:202:LYS:HG3	2.08	0.53
1:B:288:GLN:NE2	1:B:292:GLU:OE1	2.41	0.53
1:A:217:ASP:OD1	1:A:255:ARG:HD3	2.09	0.52
1:B:86:LEU:HD11	1:B:103:LEU:HD12	1.91	0.52
1:A:55:GLN:HG3	1:A:56:ARG:N	2.25	0.52
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.92	0.51
1:B:61:ALA:O	1:B:333:LEU:HD13	2.10	0.51
1:B:55:GLN:CG	1:B:366:ILE:HD11	2.40	0.51
1:A:38:GLU:CD	1:A:56:ARG:HH11	2.21	0.49
1:A:55:GLN:HG2	1:A:366:ILE:HD11	1.93	0.49
1:B:362:ARG:HA	1:B:371:VAL:HG21	1.94	0.49
1:B:333:LEU:HD21	5:B:508:GOL:H12	1.95	0.48
1:B:320:GLU:HA	1:B:320:GLU:OE1	2.13	0.48
5:B:505:GOL:C2	6:B:624:HOH:O	2.53	0.48
1:A:71:LEU:HD21	1:A:88:THR:O	2.12	0.48
1:A:229:GLN:HE22	1:A:239:ASN:HD21	1.62	0.48
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.96	0.48
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.96	0.48
1:A:142:PRO:HG3	1:A:441:PRO:O	2.13	0.48
1:A:207:GLU:O	1:A:211:VAL:HG23	2.14	0.48
1:B:55:GLN:HG2	1:B:366:ILE:HD11	1.96	0.48
1:A:233:LEU:O	1:A:237:MET:HG3	2.14	0.47
1:B:9:LYS:HG3	1:B:19:LEU:HD21	1.96	0.47
1:A:267:GLU:OE1	1:A:436:THR:OG1	2.30	0.47
1:A:449:LYS:HD3	1:A:449:LYS:HA	1.81	0.46
1:A:43:GLU:HG2	1:A:48:VAL:HG22	1.97	0.45
1:A:124:VAL:HG13	1:A:455:LEU:HD13	1.99	0.45
1:B:362:ARG:HA	1:B:371:VAL:CG2	2.46	0.45
1:B:333:LEU:CD2	5:B:508:GOL:H11	2.46	0.45
1:A:169:GLN:H	1:A:169:GLN:CD	2.25	0.45
1:A:357:ILE:N	1:A:358:PRO:CD	2.80	0.45
1:B:108:SER:O	1:B:111:ALA:HB3	2.16	0.45
1:B:333:LEU:CD2	5:B:508:GOL:C1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:HA	1:A:312:LYS:HD2	1.76	0.44
1:B:109:GLN:N	6:B:620:HOH:O	2.51	0.44
1:B:158:PHE:CE2	1:B:219:ILE:HD13	2.53	0.44
1:B:431:LEU:HD21	1:B:433:ILE:HD11	2.00	0.44
1:A:253:ASN:O	1:A:257:GLN:HG2	2.18	0.44
1:B:187:LYS:N	1:B:188:PRO:CD	2.81	0.44
1:A:129:LYS:NZ	1:A:144:ASP:OD1	2.50	0.44
1:B:190:ARG:HG2	1:B:198:TYR:CZ	2.53	0.44
1:A:148:LEU:HD23	1:A:148:LEU:C	2.43	0.43
1:B:71:LEU:O	1:B:76:LYS:HE3	2.18	0.43
1:A:388:HIS:HA	1:A:391:LYS:HD3	2.00	0.43
1:A:290:ALA:HB1	1:A:418:LEU:HD13	2.01	0.43
1:B:153:ILE:HD12	1:B:153:ILE:HA	1.81	0.43
1:A:278:TYR:HA	1:A:444:PHE:CZ	2.54	0.43
1:A:367:TRP:HB2	1:A:371:VAL:HG23	2.01	0.43
1:B:357:ILE:N	1:B:358:PRO:CD	2.83	0.42
2:B:501:HEM:CMC	2:B:501:HEM:HBC2	2.48	0.42
1:B:103:LEU:O	1:B:106:SER:HB2	2.19	0.42
1:A:39:ILE:HD12	1:A:52:LEU:HD21	2.01	0.42
1:A:103:LEU:O	1:A:106:SER:HB2	2.19	0.42
1:A:266:HIS:ND1	1:A:267:GLU:OE2	2.48	0.42
1:A:127:VAL:HG21	1:A:416:MET:HE2	2.01	0.42
1:A:357:ILE:HG22	1:A:361:HIS:CE1	2.55	0.41
1:B:148:LEU:HD21	1:B:413:VAL:HG21	2.02	0.41
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.92	0.41
1:B:391:LYS:HA	1:B:391:LYS:HD2	1.88	0.41
1:B:142:PRO:HG3	1:B:441:PRO:O	2.20	0.41
1:B:118:MET:HE1	1:B:156:CYS:HA	2.03	0.41
1:A:280:LEU:HD22	1:A:287:LEU:HA	2.03	0.41
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	2.02	0.41
1:B:268:THR:HB	2:B:501:HEM:C3B	2.56	0.41
1:B:24:LYS:NZ	1:B:432:ASP:OD1	2.54	0.40
1:B:280:LEU:HD22	1:B:287:LEU:HA	2.02	0.40
1:A:187:LYS:N	1:A:188:PRO:CD	2.85	0.40
1:A:328:ALA:O	1:A:357:ILE:HD12	2.22	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	453/455 (100%)	434 (96%)	19 (4%)	0	100	100
1	B	453/455 (100%)	433 (96%)	20 (4%)	0	100	100
All	All	906/910 (100%)	867 (96%)	39 (4%)	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	400/400 (100%)	387 (97%)	13 (3%)	33	47
1	B	400/400 (100%)	387 (97%)	13 (3%)	33	47
All	All	800/800 (100%)	774 (97%)	26 (3%)	33	47

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	25	VAL
1	A	55	GLN
1	A	74	VAL
1	A	167	ARG
1	A	185	MET
1	A	200	GLU
1	A	210	LYS

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Mol	Chain	Res	Type
1	A	230	SER
1	A	371	VAL
1	A	375	ARG
1	A	385	ILE
1	A	449	LYS
1	B	20	LEU
1	B	55	GLN
1	B	120	VAL
1	B	131	GLU
1	B	167	ARG
1	B	219	ILE
1	B	230	SER
1	B	255	ARG
1	B	336	LYS
1	B	364	LYS
1	B	380	GLU
1	B	430	GLU
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	206	GLN
1	A	229	GLN
1	A	236	HIS
1	B	55	GLN
1	B	204	GLN
1	B	359	GLN
1	B	397	GLN
1	B	404	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	A	501	1,4	50,50,50	1.64	9 (18%)	67,82,82	1.83	13 (19%)
5	GOL	A	505	-	5,5,5	0.19	0	5,5,5	0.38	0
2	HEM	B	501	1,4	50,50,50	1.61	6 (12%)	67,82,82	1.74	15 (22%)
5	GOL	B	504	-	5,5,5	0.20	0	5,5,5	0.31	0
5	GOL	B	508	-	5,5,5	0.28	0	5,5,5	0.74	0
3	HL0	B	502	-	18,18,18	0.42	0	17,21,21	0.71	0
4	DMS	A	503	2	3,3,3	0.32	0	3,3,3	0.35	0
5	GOL	B	507	-	5,5,5	0.23	0	5,5,5	0.48	0
4	DMS	B	503	2	3,3,3	0.34	0	3,3,3	0.25	0
5	GOL	A	504	-	5,5,5	0.12	0	5,5,5	0.19	0
3	HL0	A	502	-	18,18,18	0.43	0	17,21,21	0.62	0
5	GOL	B	505	-	5,5,5	0.13	0	5,5,5	0.30	0
5	GOL	B	506	-	5,5,5	0.17	0	5,5,5	0.41	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	A	501	1,4	-	3/14/54/54	-
5	GOL	A	505	-	-	1/4/4/4	-
2	HEM	B	501	1,4	-	4/14/54/54	-
5	GOL	B	504	-	-	3/4/4/4	-
5	GOL	B	508	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HL0	B	502	-	-	2/13/23/23	0/1/1/1
5	GOL	B	507	-	-	0/4/4/4	-
5	GOL	A	504	-	-	2/4/4/4	-
3	HL0	A	502	-	-	6/13/23/23	0/1/1/1
5	GOL	B	505	-	-	0/4/4/4	-
5	GOL	B	506	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NB	4.93	2.10	1.94
2	A	501	HEM	FE-NB	4.83	2.09	1.94
2	A	501	HEM	FE-NC	4.42	2.09	1.95
2	B	501	HEM	C1B-NB	-4.37	1.32	1.40
2	B	501	HEM	FE-NC	3.78	2.07	1.95
2	A	501	HEM	C4D-ND	-3.55	1.34	1.40
2	A	501	HEM	C1B-NB	-3.34	1.34	1.40
2	B	501	HEM	C1C-C2C	-2.95	1.39	1.45
2	B	501	HEM	C4B-NB	-2.89	1.33	1.38
2	A	501	HEM	C1D-ND	-2.75	1.33	1.38
2	B	501	HEM	C4D-ND	-2.70	1.35	1.40
2	A	501	HEM	C4B-NB	-2.68	1.33	1.38
2	A	501	HEM	C3C-C4C	-2.44	1.41	1.46
2	A	501	HEM	C4C-NC	-2.25	1.35	1.39
2	A	501	HEM	C1C-C2C	-2.18	1.41	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHC-C4B-NB	6.37	131.28	124.42
2	A	501	HEM	C1B-NB-C4B	5.22	111.39	105.21
2	B	501	HEM	CHD-C1D-ND	5.20	130.02	124.42
2	B	501	HEM	CHC-C4B-NB	4.39	129.15	124.42
2	B	501	HEM	CHA-C4D-ND	3.97	129.28	124.37
2	A	501	HEM	CHD-C1D-C2D	-3.90	118.88	125.03
2	B	501	HEM	O2A-CGA-CBA	3.78	125.95	114.00
2	B	501	HEM	CAD-C3D-C4D	3.76	131.24	124.70
2	A	501	HEM	CHD-C1D-ND	3.35	128.03	124.42
2	B	501	HEM	C1B-NB-C4B	3.27	109.08	105.21
2	A	501	HEM	O2A-CGA-CBA	3.01	123.51	114.00
2	A	501	HEM	C3B-C4B-NB	-2.97	107.33	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4B-C3B-C2B	-2.85	104.66	107.28
2	A	501	HEM	CHA-C1A-NA	2.78	128.90	123.86
2	B	501	HEM	O1A-CGA-CBA	-2.73	114.44	123.09
2	B	501	HEM	CHA-C4D-C3D	-2.67	120.30	125.23
2	A	501	HEM	C2D-C1D-ND	2.66	112.98	109.90
2	B	501	HEM	CAD-C3D-C2D	-2.65	122.91	127.87
2	B	501	HEM	CHD-C1D-C2D	-2.62	120.88	125.03
2	A	501	HEM	O1A-CGA-CBA	-2.59	114.87	123.09
2	B	501	HEM	CBD-CAD-C3D	-2.51	105.60	112.53
2	B	501	HEM	C1A-CHA-C4D	-2.51	120.35	126.25
2	A	501	HEM	C3C-C2C-C1C	-2.32	104.85	107.05
2	A	501	HEM	CAD-C3D-C4D	2.28	128.67	124.70
2	A	501	HEM	CHC-C1C-NC	-2.28	121.97	124.45
2	B	501	HEM	CMD-C2D-C1D	2.18	128.44	125.03
2	A	501	HEM	CBD-CAD-C3D	-2.08	106.77	112.53
2	B	501	HEM	O2D-CGD-CBD	2.07	120.54	114.00

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	GOL	O1-C1-C2-C3
5	B	504	GOL	C1-C2-C3-O3
5	B	508	GOL	C1-C2-C3-O3
5	B	508	GOL	O2-C2-C3-O3
5	A	504	GOL	O1-C1-C2-O2
3	A	502	HL0	C4-C5-C6-C7
3	A	502	HL0	C7-C8-C9-C10
5	B	504	GOL	O2-C2-C3-O3
5	B	506	GOL	C1-C2-C3-O3
3	B	502	HL0	C1-C2-C3-C4
3	A	502	HL0	C3-C4-C5-C6
3	A	502	HL0	C2-C3-C4-C5
3	A	502	HL0	C1-C2-C3-C4
3	A	502	HL0	C6-C7-C8-C9
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D
5	A	505	GOL	O1-C1-C2-O2
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O1D
5	B	504	GOL	O1-C1-C2-O2

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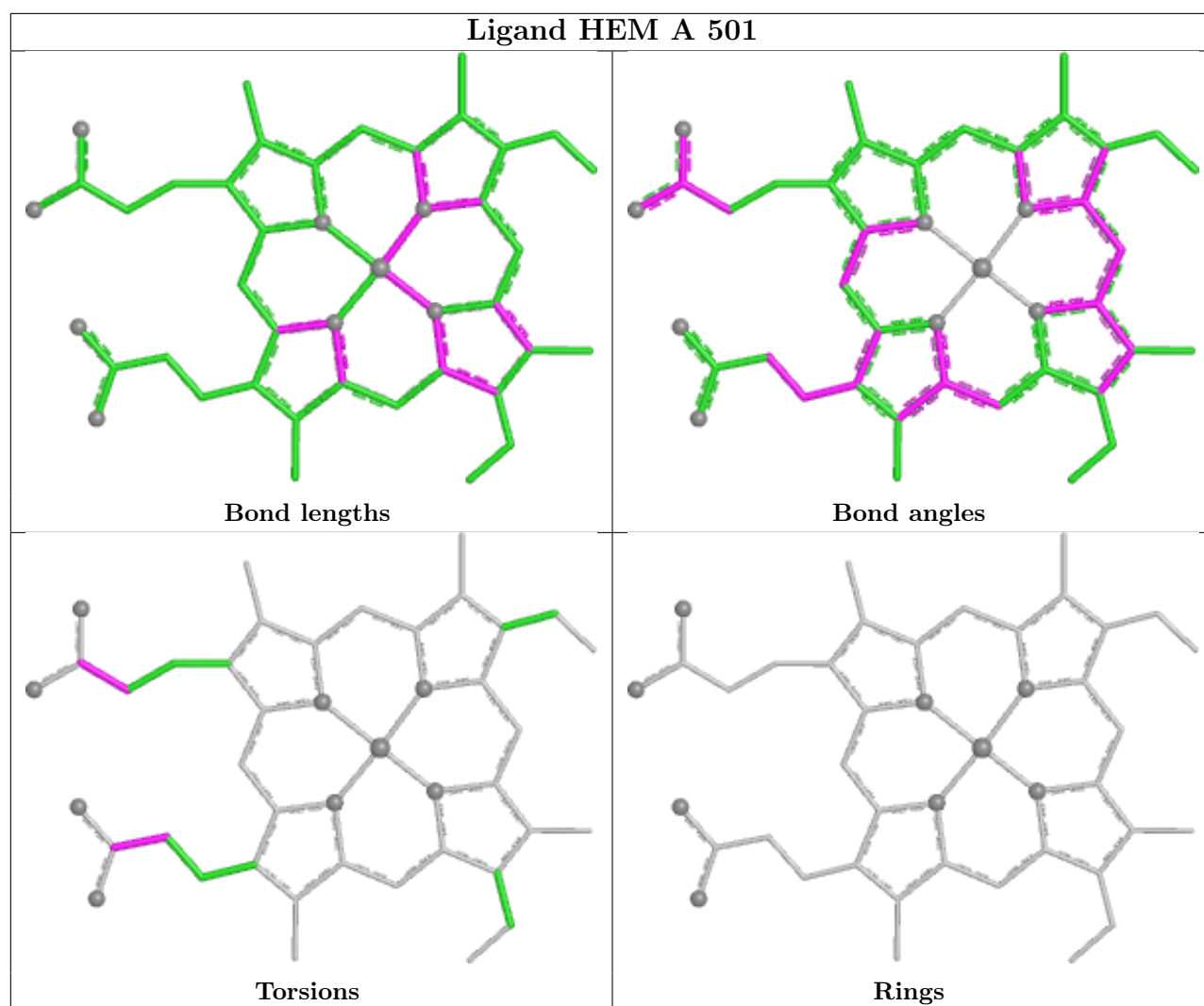
Mol	Chain	Res	Type	Atoms
5	B	506	GOL	O2-C2-C3-O3
2	B	501	HEM	CAA-CBA-CGA-O1A
3	B	502	HL0	C5-C6-C7-C8
2	A	501	HEM	CAA-CBA-CGA-O2A

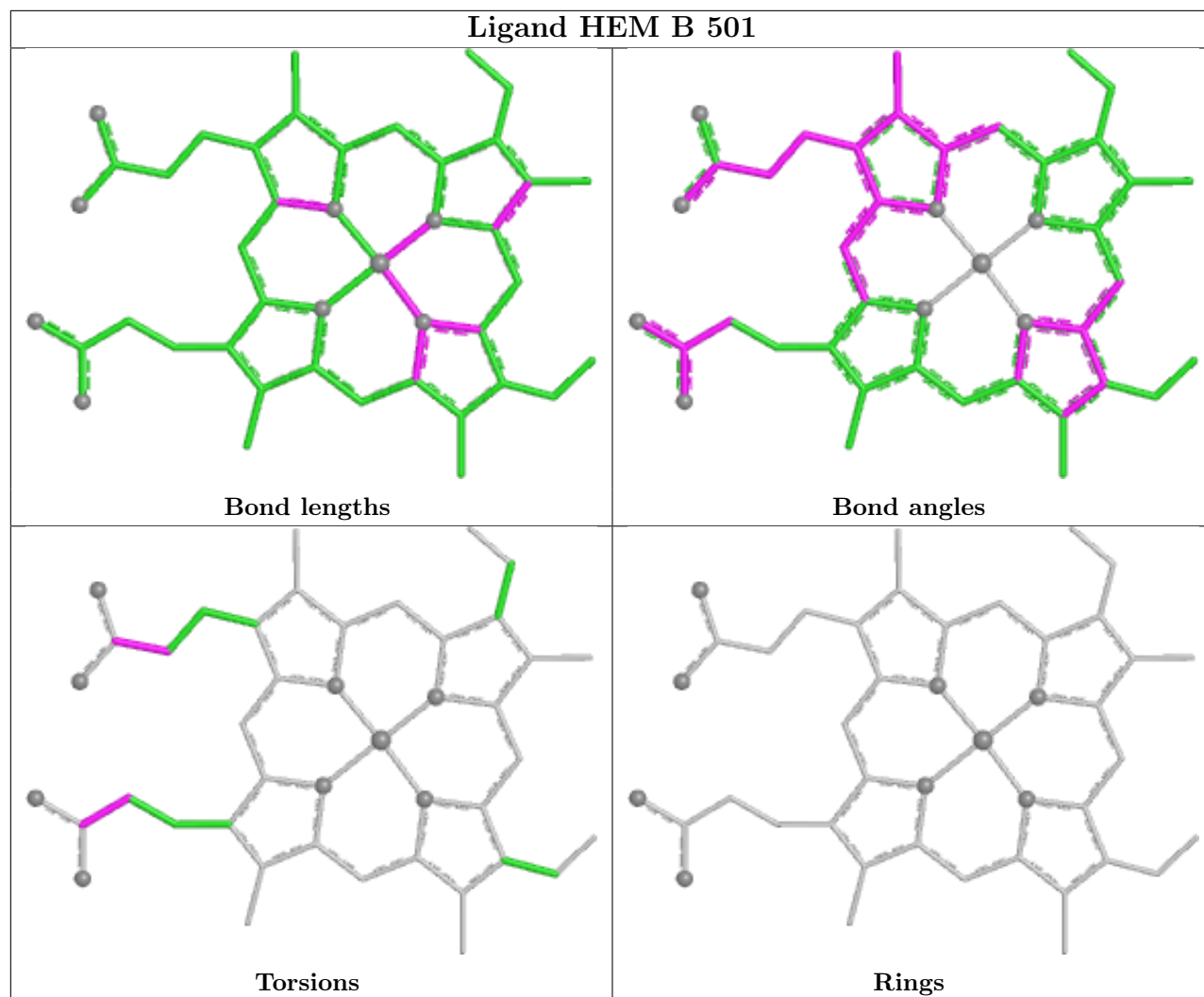
There are no ring outliers.

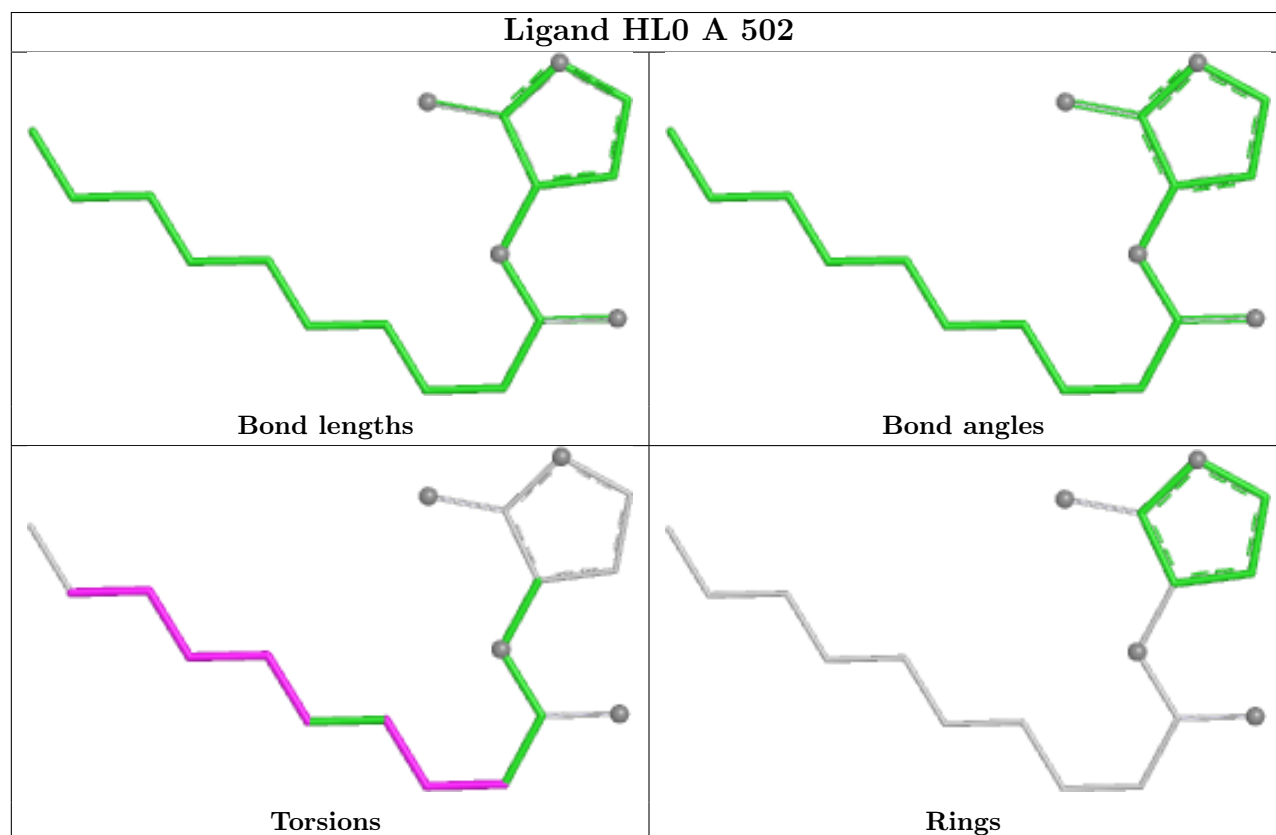
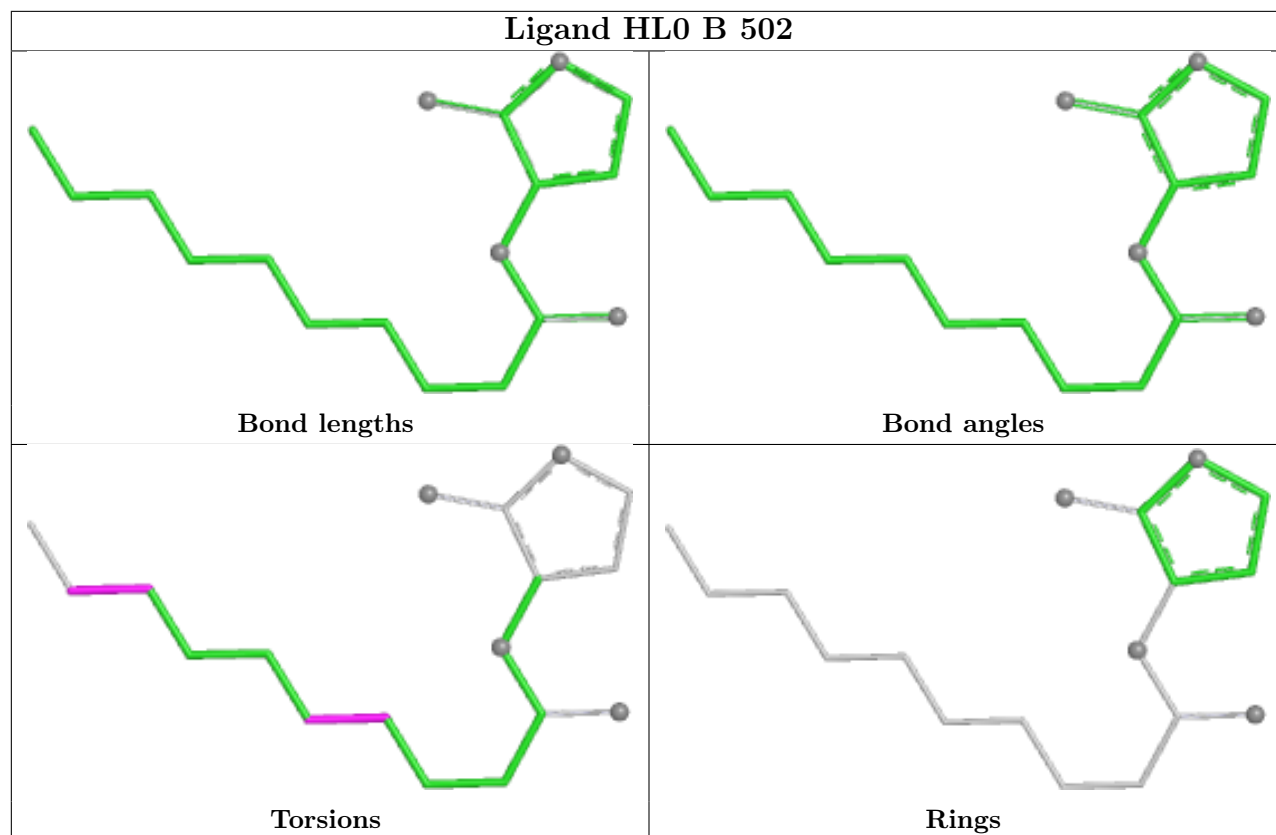
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	1	0
2	B	501	HEM	3	0
5	B	508	GOL	3	0
4	A	503	DMS	1	0
5	B	505	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	455/455 (100%)	-0.19	2 (0%) 88 89	16, 24, 40, 72	0
1	B	455/455 (100%)	-0.18	6 (1%) 75 76	15, 23, 39, 64	0
All	All	910/910 (100%)	-0.18	8 (0%) 81 82	15, 23, 40, 72	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	454	PRO	3.0
1	B	136	ASP	2.7
1	B	369	ASP	2.5
1	A	168	ASP	2.3
1	A	1	THR	2.2
1	B	231	ASP	2.1
1	B	430	GLU	2.1
1	B	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 oligosaccharides 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,

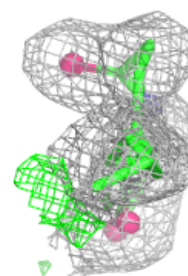
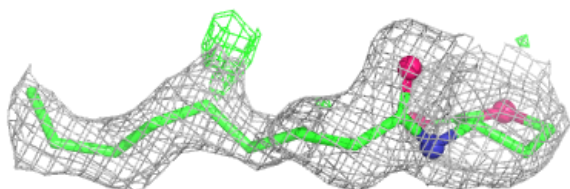
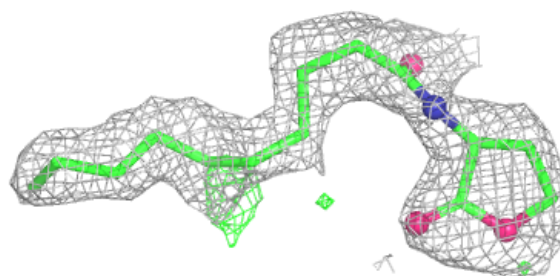
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	507	6/6	0.85	0.14	34,38,40,41	0
5	GOL	A	504	6/6	0.87	0.13	37,39,46,50	0
3	HL0	A	502	18/18	0.87	0.16	31,51,61,61	0
5	GOL	B	508	6/6	0.90	0.10	20,25,26,27	0
5	GOL	B	506	6/6	0.92	0.09	29,30,31,38	0
5	GOL	B	504	6/6	0.93	0.09	25,28,31,31	0
3	HL0	B	502	18/18	0.93	0.10	25,33,45,46	0
5	GOL	A	505	6/6	0.96	0.07	26,28,31,31	0
5	GOL	B	505	6/6	0.97	0.05	19,21,22,25	0
4	DMS	A	503	4/4	0.97	0.08	24,24,25,25	0
2	HEM	A	501	43/43	0.98	0.06	15,18,24,29	0
4	DMS	B	503	4/4	0.98	0.08	25,26,27,28	0
2	HEM	B	501	43/43	0.98	0.06	14,16,18,22	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.

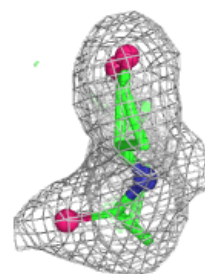
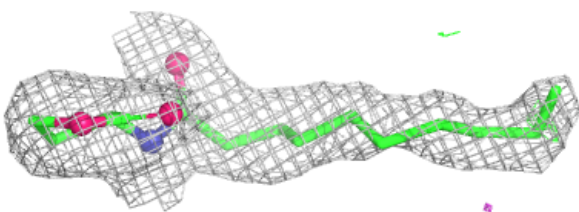
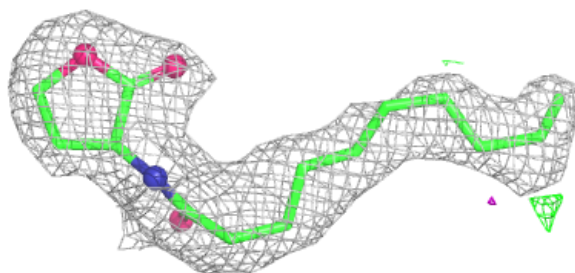
Electron density around HL0 A 502:

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



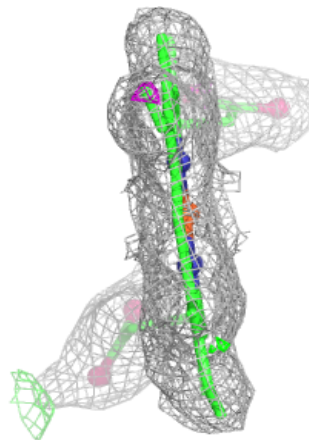
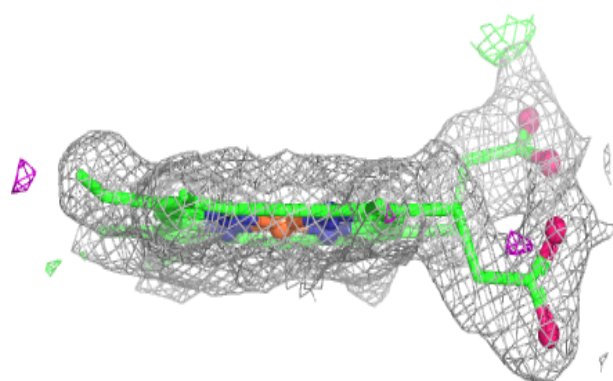
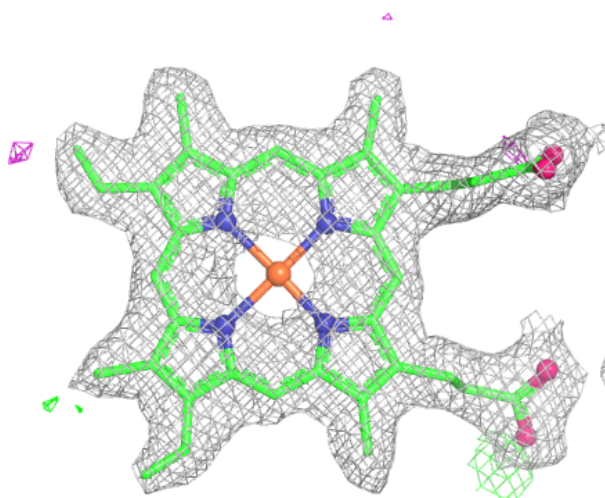
Electron density around HL0 B 502:

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



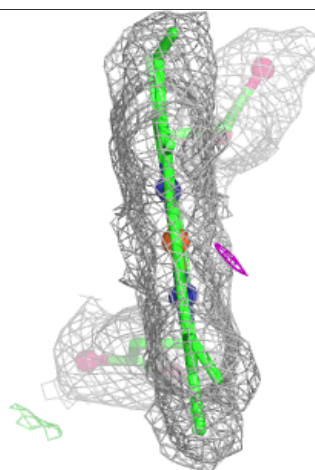
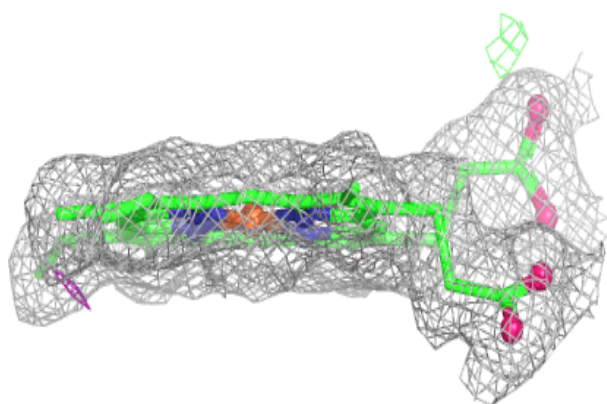
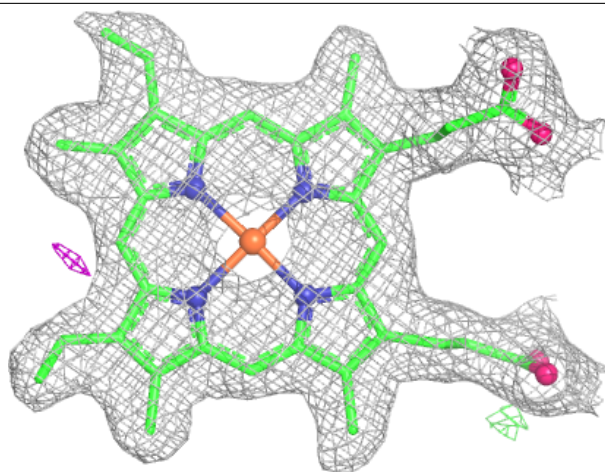
Electron density around HEM A 501:

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



Electron density around HEM B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.