Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 12:12 PM EDT

PDB ID	:	3NLF / pdb_00003nlf
Title	:	Structure of endothelial nitric oxide synthase heme domain complexed with 6-{{(3'R,4'S)-3'-[2"-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine
Authors	:	Ji, H.; Delker, S.L.; Li, H.; Martasek, P.; Roman, L.; Poulos, T.L.; Silverman, R.B.
Deposited on	:	2010-06-21
Resolution	:	2.32 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 (1)) were used in the production of this report:

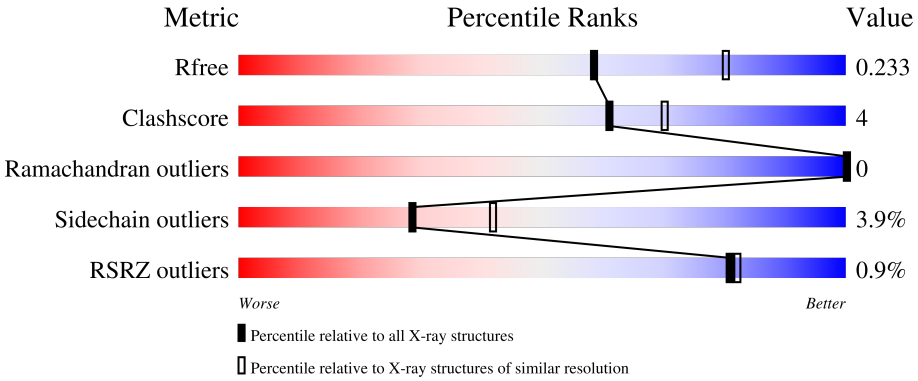
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	444	% 82% 7% • 9%
1	B	444	% 82% 8% • 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6952 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.

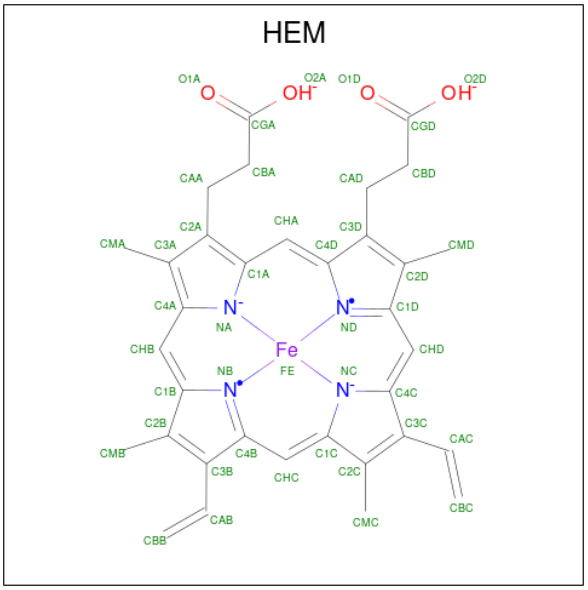
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3209	2041	564	588	16			
1	B	403	Total	C	N	O	S	0	0	0
			3209	2040	566	587	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

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



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

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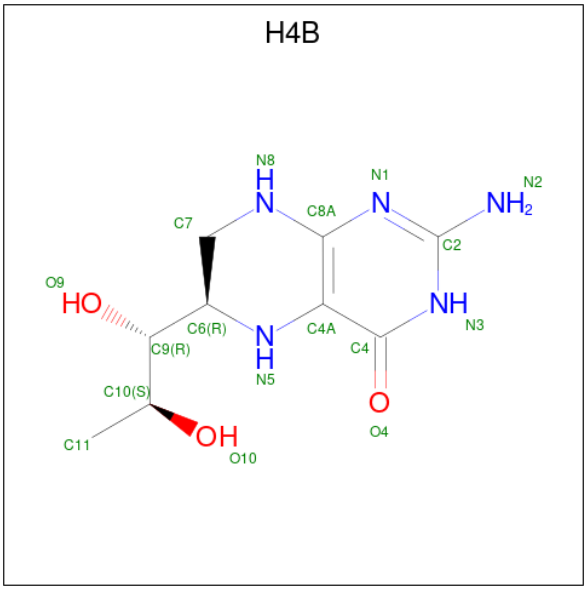
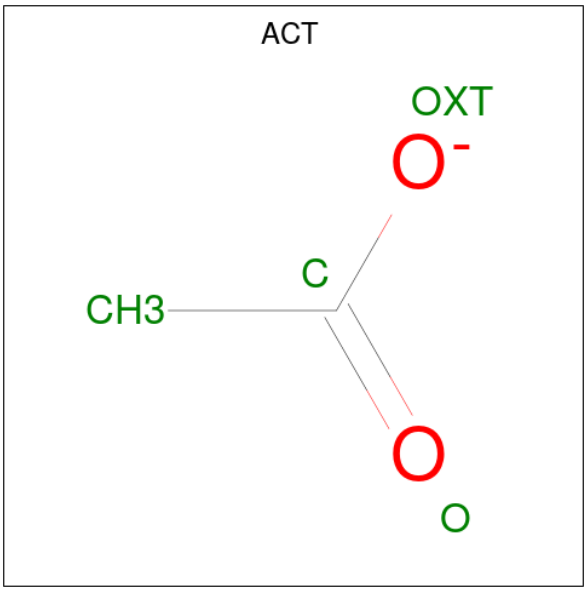
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



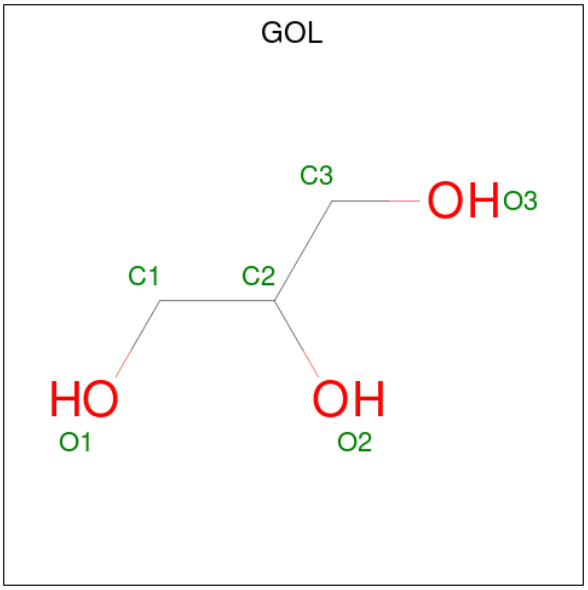
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			17	9	5	3			
3	B	1	Total	C	N	O		0	0
			17	9	5	3			

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



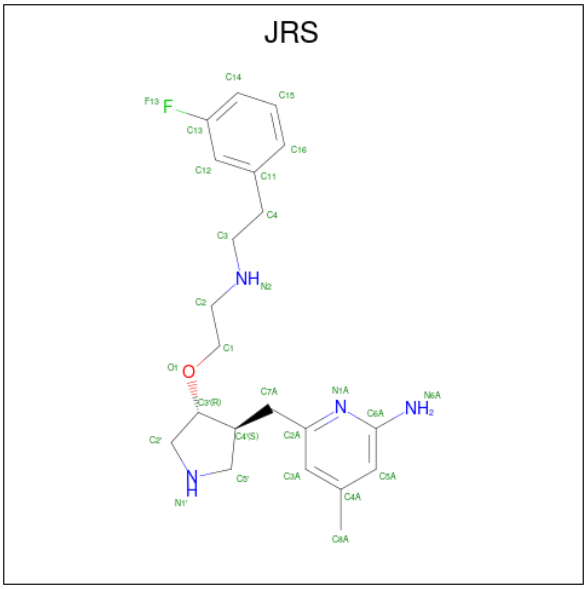
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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



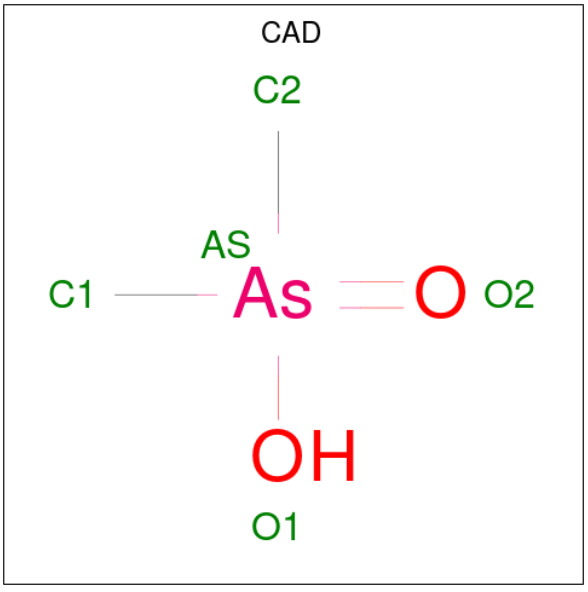
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is 6-{[(3S,4R)-4-(2-{[2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (CCD ID: JRS) (formula: $C_{21}H_{29}FN_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
6	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

- Molecule 7 is CACODYLIC ACID (CCD ID: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total As C 3 1 2	0	0
7	B	1	Total As C 3 1 2	0	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	0

- Molecule 9 is water.

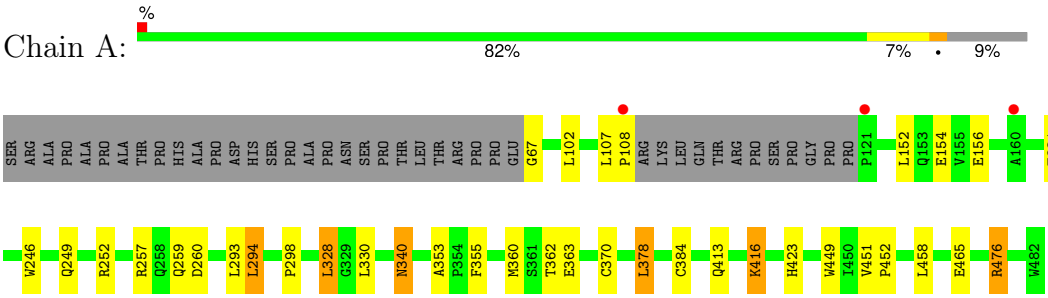
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	171	Total O 171 171	0	0
9	B	162	Total O 162 162	0	0

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.

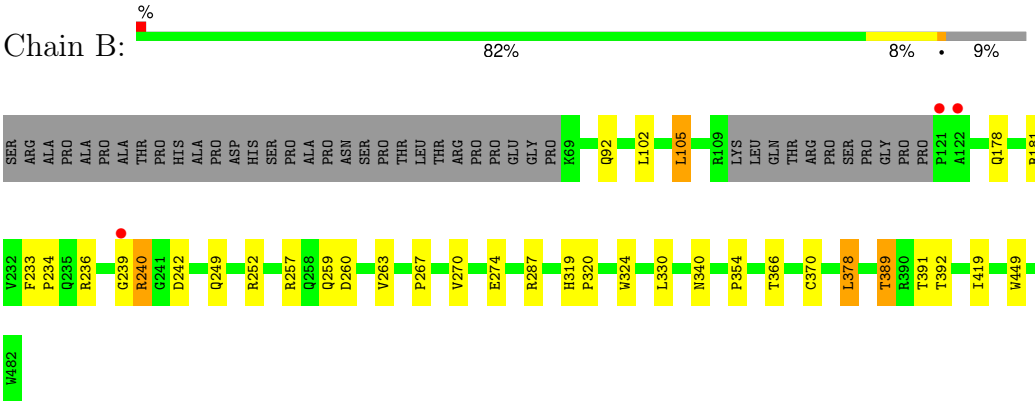
- Molecule 1: Nitric oxide synthase, endothelial

Chain A:



- Molecule 1: Nitric oxide synthase, endothelial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.12Å 107.05Å 157.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.19 – 2.32 38.19 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.19-2.32) 99.4 (38.19-2.32)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.174 , 0.224 0.183 , 0.233	Depositor DCC
R_{free} test set	2160 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6952	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAD, H4B, JRS, ACT, GOL, ZN, HEM

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	0.69	0/3299	0.84	2/4494 (0.0%)
1	B	0.67	0/3298	0.83	1/4491 (0.0%)
All	All	0.68	0/6597	0.84	3/8985 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	240	ARG	N-CA-C	7.61	119.71	108.60
1	A	67	GLY	CA-C-N	6.82	126.85	119.89
1	A	67	GLY	C-N-CA	6.82	126.85	119.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3209	0	3115	24	0
1	B	3209	0	3117	24	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
3	A	17	0	15	2	0
3	B	17	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
6	A	27	0	29	2	0
6	B	27	0	29	2	0
7	A	3	0	0	1	0
7	B	3	0	0	1	0
8	A	1	0	0	0	0
9	A	171	0	0	2	0
9	B	162	0	0	5	0
All	All	6952	0	6402	54	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 (54) 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)
2:B:500:HEM:HMC2	2:B:500:HEM:HBC2	1.58	0.83
1:A:476:ARG:HH11	1:A:476:ARG:HG3	1.43	0.81
1:A:476:ARG:HH11	1:A:476:ARG:CG	1.98	0.76
1:A:476:ARG:HG3	1:A:476:ARG:NH1	2.06	0.67
1:B:324:TRP:HB2	7:B:950:CAD:C1	2.27	0.65
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.43	0.65
1:A:378:LEU:HB2	9:A:1003:HOH:O	2.00	0.61
2:B:500:HEM:HBA1	6:B:800:JRS:H7AA	1.83	0.59
1:B:366:THR:O	1:B:370:CYS:HB2	2.03	0.59
1:B:477:TYR:CE1	6:B:800:JRS:H15	2.38	0.59
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.86	0.57
1:B:239:GLY:C	9:B:1131:HOH:O	2.47	0.57
1:B:270:VAL:O	1:B:274:GLU:HG3	2.05	0.57
1:A:257:ARG:HD2	9:A:1058:HOH:O	2.07	0.55
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.89	0.55
1:B:240:ARG:HA	9:B:1131:HOH:O	2.08	0.53
1:A:360:MET:HE3	1:A:362:THR:OG1	2.08	0.53
1:A:340:ASN:H	1:A:340:ASN:HD22	1.56	0.53
1:B:236:ARG:CD	1:B:242:ASP:OD1	2.57	0.52
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.50	0.52
1:B:236:ARG:HD3	1:B:242:ASP:CG	2.35	0.52
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:HB2	1:B:252:ARG:HG2	1.93	0.51
1:B:449:TRP:HA	3:B:600:H4B:N1	2.26	0.50
1:A:384:CYS:CB	7:A:950:CAD:AS	3.20	0.50
1:B:378:LEU:HB2	9:B:1004:HOH:O	2.12	0.49
1:A:449:TRP:HA	3:A:600:H4B:N1	2.29	0.47
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.96	0.47
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.96	0.47
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.96	0.46
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.45	0.46
1:A:152:LEU:O	1:A:156:GLU:HG2	2.17	0.45
1:B:240:ARG:N	9:B:1131:HOH:O	2.49	0.44
1:B:223:ARG:HB2	1:B:223:ARG:HH11	1.83	0.44
1:A:355:PHE:CD1	2:A:500:HEM:CAC	3.01	0.43
1:B:236:ARG:HD3	1:B:242:ASP:OD1	2.19	0.43
1:A:413:GLN:O	1:A:416:LYS:HE3	2.18	0.43
1:B:263:VAL:HG11	1:B:267:PRO:HA	2.01	0.43
1:B:389:THR:O	1:B:389:THR:CG2	2.66	0.43
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.41	0.43
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.54	0.42
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.82	0.42
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.20	0.42
1:A:363:GLU:OE1	6:A:800:JRS:N1A	2.53	0.42
2:B:500:HEM:HMC2	2:B:500:HEM:CBC	2.40	0.42
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.90	0.41
2:A:500:HEM:HBA1	6:A:800:JRS:H7AA	2.02	0.41
1:A:231:THR:O	1:A:353:ALA:HA	2.20	0.41
1:B:287:ARG:HD3	9:B:1129:HOH:O	2.20	0.41
1:A:355:PHE:CD1	2:A:500:HEM:HAC	2.55	0.41
1:A:423:HIS:HB2	1:B:392:THR:HB	2.03	0.41
3:A:600:H4B:O4	5:A:880:GOL:O2	2.37	0.40
1:B:231:THR:O	1:B:354:PRO:HD2	2.20	0.40
1:A:328:LEU:HB3	1:A:330:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/444 (90%)	390 (98%)	10 (2%)	0	100	100
1	B	399/444 (90%)	393 (98%)	6 (2%)	0	100	100
All	All	799/888 (90%)	783 (98%)	16 (2%)	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	343/377 (91%)	330 (96%)	13 (4%)	29	43
1	B	343/377 (91%)	329 (96%)	14 (4%)	27	40
All	All	686/754 (91%)	659 (96%)	27 (4%)	28	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	154	GLU
1	A	240	ARG
1	A	259	GLN
1	A	260	ASP
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	416	LYS
1	A	458	LEU
1	A	476	ARG
1	B	92	GLN

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Mol	Chain	Res	Type
1	B	102	LEU
1	B	105	LEU
1	B	223	ARG
1	B	257	ARG
1	B	259	GLN
1	B	260	ASP
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	389	THR
1	B	391	THR
1	B	419	ILE
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	196	GLN
1	A	278	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	A	478	GLN
1	B	178	GLN
1	B	215	ASN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN
1	B	478	GLN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	A	880	-	5,5,5	0.47	0	5,5,5	0.55	0
5	GOL	B	880	-	5,5,5	0.44	0	5,5,5	0.88	0
4	ACT	B	860	-	3,3,3	0.81	0	3,3,3	0.76	0
3	H4B	A	600	-	17,18,18	0.70	0	14,26,26	2.09	7 (50%)
7	CAD	B	950	1	0,2,4	-	-	0,1,6	-	-
2	HEM	B	500	1	50,50,50	1.96	12 (24%)	67,82,82	1.39	10 (14%)
7	CAD	A	950	1	0,2,4	-	-	0,1,6	-	-
6	JRS	A	800	-	28,29,29	0.79	0	29,38,38	1.45	4 (13%)
3	H4B	B	600	-	17,18,18	0.93	1 (5%)	14,26,26	1.98	5 (35%)
6	JRS	B	800	-	28,29,29	0.59	0	29,38,38	1.51	2 (6%)
4	ACT	A	860	-	3,3,3	0.83	0	3,3,3	0.81	0
2	HEM	A	500	1	50,50,50	1.83	10 (20%)	67,82,82	1.20	7 (10%)

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
5	GOL	A	880	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	880	-	-	2/4/4/4	-
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
2	HEM	B	500	1	-	5/14/54/54	-
6	JRS	A	800	-	-	1/13/23/23	0/3/3/3
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
6	JRS	B	800	-	-	2/13/23/23	0/3/3/3
2	HEM	A	500	1	-	4/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C2D	7.36	1.52	1.36
2	A	500	HEM	C3D-C2D	6.44	1.50	1.36
2	B	500	HEM	FE-ND	4.85	2.09	1.94
2	A	500	HEM	FE-NC	4.71	2.10	1.95
2	B	500	HEM	FE-NC	4.70	2.10	1.95
2	A	500	HEM	FE-ND	4.48	2.08	1.94
2	B	500	HEM	FE-NA	3.70	2.07	1.95
2	B	500	HEM	FE-NB	3.34	2.05	1.94
2	A	500	HEM	CAB-C3B	3.04	1.55	1.47
2	B	500	HEM	CAB-C3B	2.99	1.55	1.47
2	A	500	HEM	CAC-C3C	2.93	1.55	1.47
2	B	500	HEM	CAC-C3C	2.84	1.55	1.47
2	B	500	HEM	CMB-C2B	2.66	1.56	1.50
2	A	500	HEM	FE-NB	2.65	2.03	1.94
2	A	500	HEM	FE-NA	2.62	2.03	1.95
2	A	500	HEM	CMA-C3A	2.35	1.55	1.50
2	B	500	HEM	CMD-C2D	2.33	1.55	1.50
3	B	600	H4B	C7-C6	2.23	1.54	1.52
2	B	500	HEM	CMA-C3A	2.18	1.55	1.50
2	A	500	HEM	CMD-C2D	2.15	1.55	1.50
2	A	500	HEM	CMB-C2B	2.14	1.55	1.50
2	B	500	HEM	C2A-C3A	-2.06	1.33	1.38
2	B	500	HEM	O1D-CGD	2.01	1.28	1.22

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	800	JRS	C6A-N1A-C2A	5.80	122.41	118.07
3	A	600	H4B	C2-N1-C8A	4.52	121.33	113.36
2	B	500	HEM	CBA-CAA-C2A	-4.12	101.13	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	C4D-ND-C1D	4.11	110.08	105.21
3	B	600	H4B	C2-N1-C8A	4.09	120.58	113.36
2	A	500	HEM	C4D-ND-C1D	3.76	109.66	105.21
6	A	800	JRS	C6A-N1A-C2A	3.58	120.75	118.07
2	A	500	HEM	CMD-C2D-C1D	3.28	130.17	125.03
2	B	500	HEM	CMD-C2D-C1D	3.26	130.12	125.03
6	A	800	JRS	C14-C13-C12	-3.12	119.11	123.23
3	B	600	H4B	C4A-C4-N3	3.01	120.39	112.13
3	A	600	H4B	C4A-C4-N3	2.94	120.20	112.13
6	A	800	JRS	C7A-C2A-N1A	2.84	120.05	116.57
2	A	500	HEM	CHB-C1B-NB	2.77	127.80	124.37
3	A	600	H4B	C4-C4A-N5	2.77	123.81	116.27
2	B	500	HEM	CBD-CAD-C3D	-2.71	105.04	112.53
3	A	600	H4B	O4-C4-C4A	-2.60	120.98	127.26
2	B	500	HEM	C3B-C4B-NB	-2.60	107.60	109.47
2	A	500	HEM	CAD-C3D-C4D	2.58	129.20	124.70
3	B	600	H4B	C4-C4A-N5	2.44	122.92	116.27
2	B	500	HEM	C1D-C2D-C3D	-2.40	104.45	106.98
3	B	600	H4B	C2-N3-C4	-2.40	120.77	125.11
2	B	500	HEM	C1B-NB-C4B	2.30	107.94	105.21
3	A	600	H4B	C2-N3-C4	-2.25	121.03	125.11
3	B	600	H4B	O4-C4-C4A	-2.19	121.97	127.26
3	A	600	H4B	N3-C2-N1	-2.17	119.36	123.32
2	B	500	HEM	CAD-C3D-C4D	2.12	128.39	124.70
2	B	500	HEM	C2A-C1A-NA	-2.10	107.82	110.15
3	A	600	H4B	N2-C2-N3	2.09	121.17	116.76
2	A	500	HEM	CHD-C4C-NC	2.05	126.69	124.45
6	B	800	JRS	C3A-C2A-N1A	-2.04	120.40	122.73
2	A	500	HEM	CAD-CBD-CGD	-2.04	108.26	113.67
6	A	800	JRS	C3A-C2A-N1A	-2.03	120.42	122.73
2	A	500	HEM	O1D-CGD-CBD	-2.02	116.68	123.09
2	B	500	HEM	C3B-C2B-C1B	2.01	107.92	106.41

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	880	GOL	C1-C2-C3-O3
5	A	880	GOL	O2-C2-C3-O3
5	B	880	GOL	C1-C2-C3-O3
2	A	500	HEM	C2A-CAA-CBA-CGA
6	B	800	JRS	C1-C2-N2-C3

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Mol	Chain	Res	Type	Atoms
5	B	880	GOL	O2-C2-C3-O3
2	A	500	HEM	C3D-CAD-CBD-CGD
6	B	800	JRS	C4-C3-N2-C2
6	A	800	JRS	O1-C1-C2-N2
2	A	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	C3D-CAD-CBD-CGD
2	B	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAD-CBD-CGD-O2D
2	B	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAD-CBD-CGD-O1D

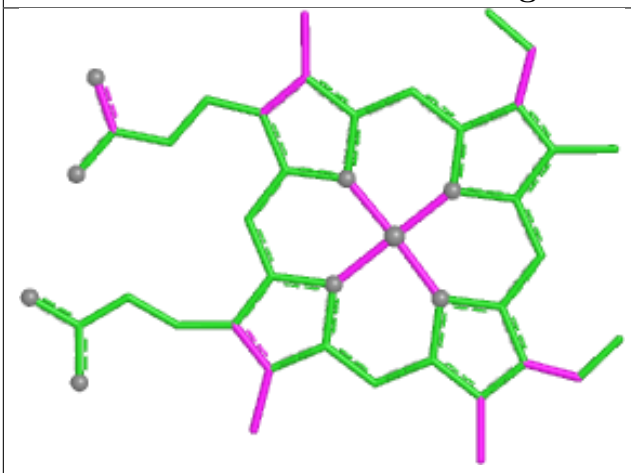
There are no ring outliers.

9 monomers are involved in 16 short contacts:

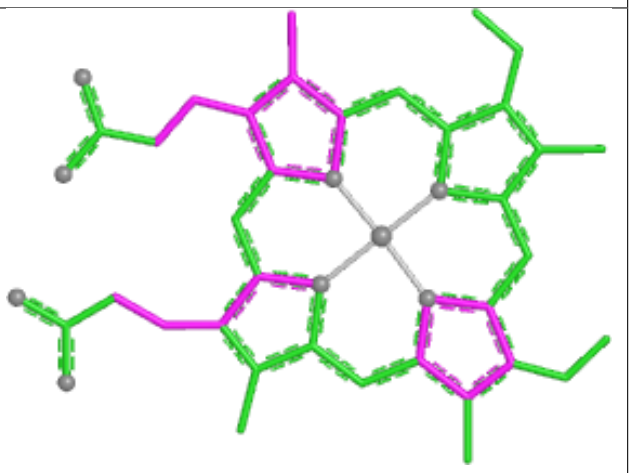
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	880	GOL	1	0
3	A	600	H4B	2	0
7	B	950	CAD	1	0
2	B	500	HEM	5	0
7	A	950	CAD	1	0
6	A	800	JRS	2	0
3	B	600	H4B	1	0
6	B	800	JRS	2	0
2	A	500	HEM	4	0

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.

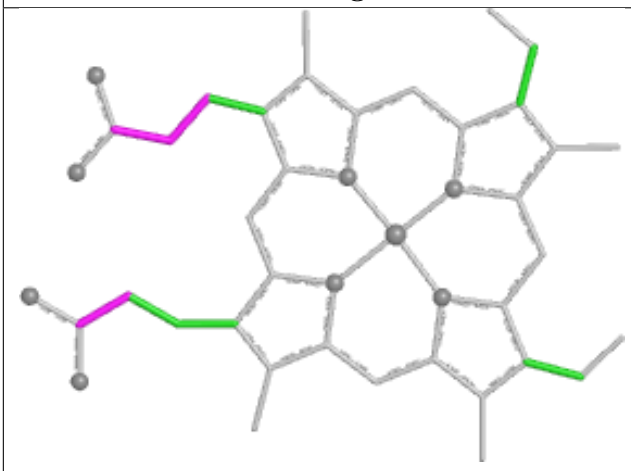
Ligand HEM B 500



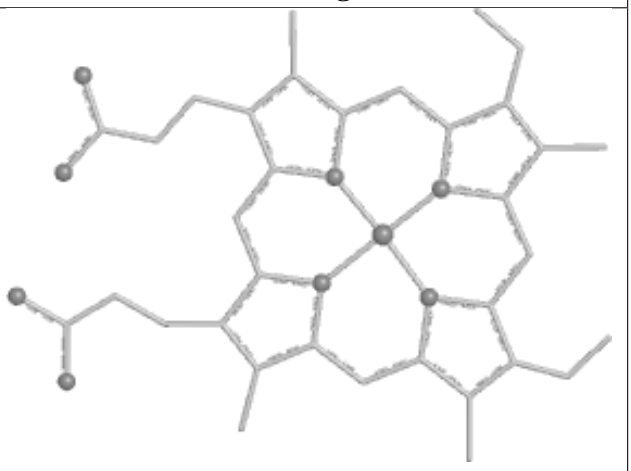
Bond lengths



Bond angles

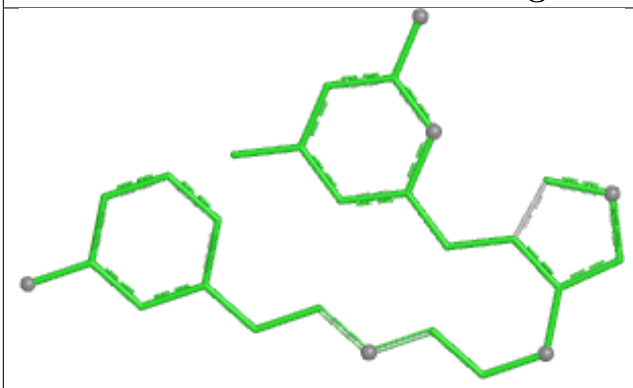


Torsions



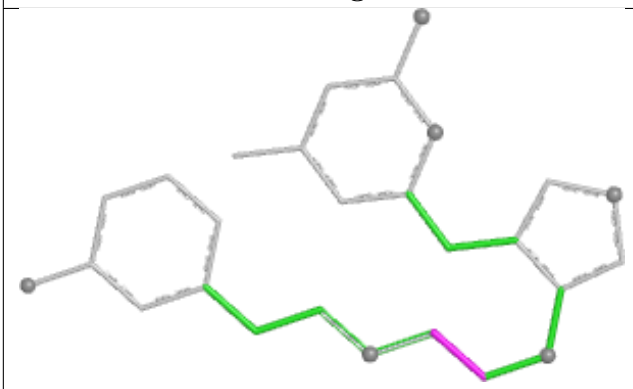
Rings

Ligand JRS A 800

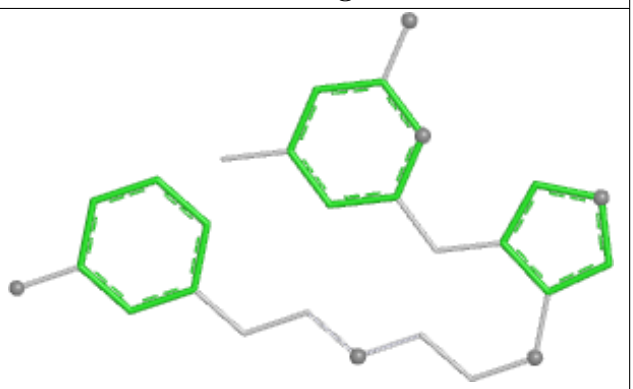


Bond lengths

Bond angles

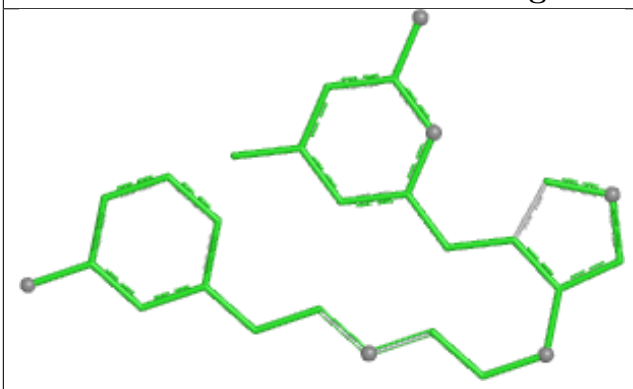


Torsions

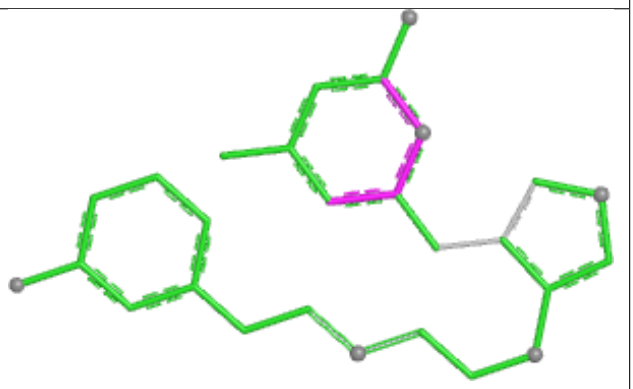


Rings

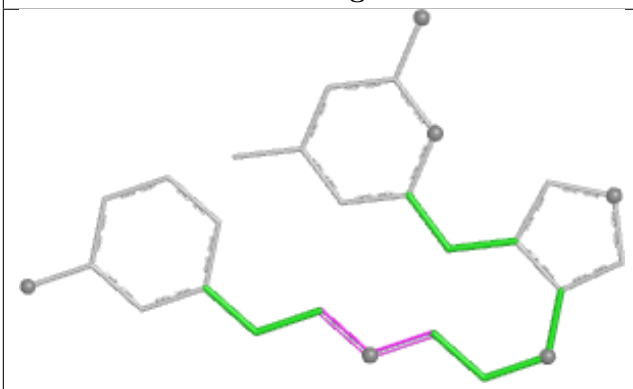
Ligand JRS B 800



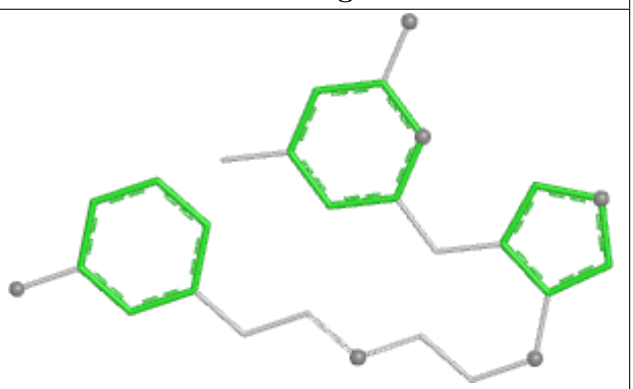
Bond lengths



Bond angles

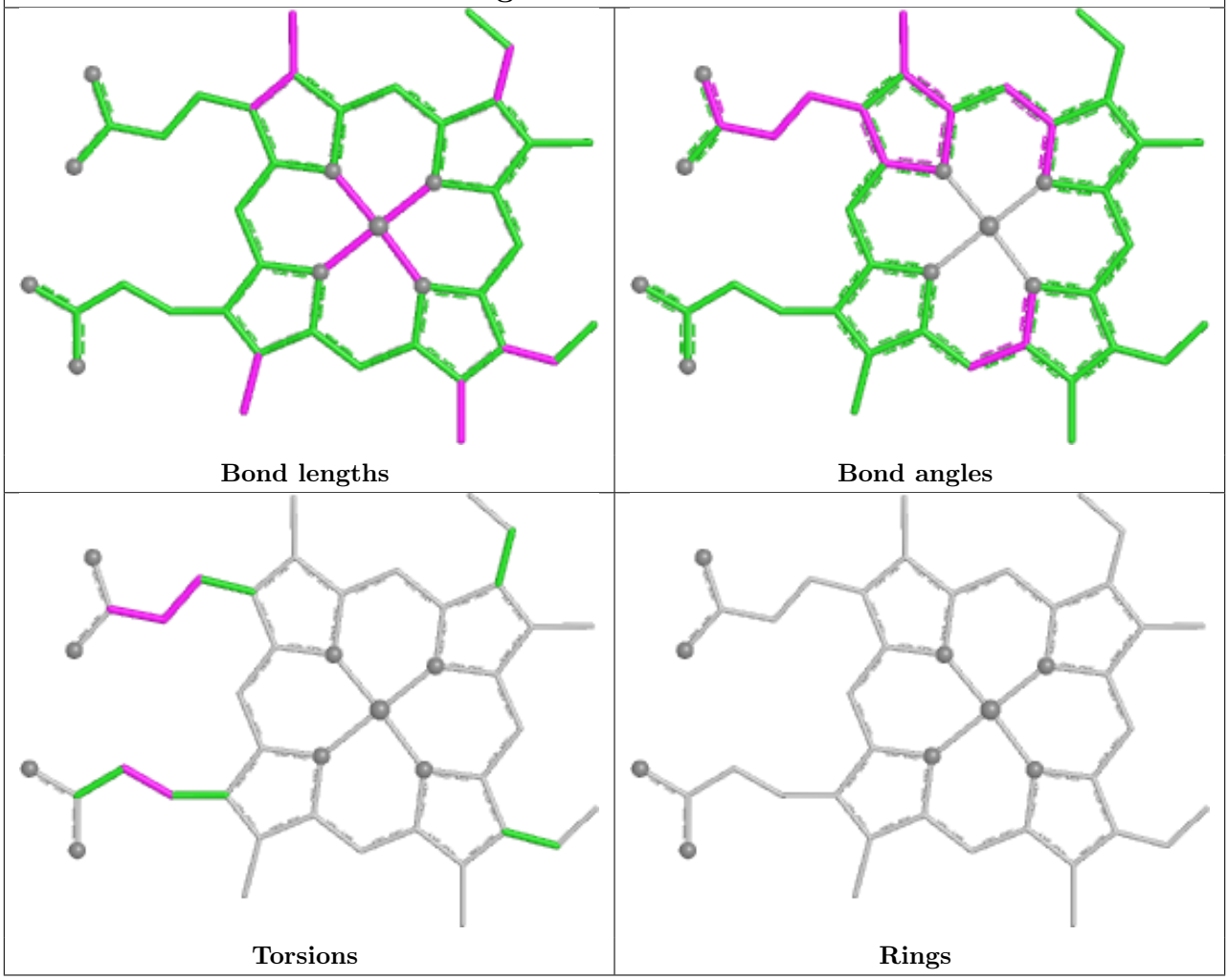


Torsions



Rings

Ligand HEM A 500



5.7 Other polymers

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^{th} 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	404/444 (90%)	-0.23	4 (0%)	79	81	22, 35, 59, 77	0
1	B	403/444 (90%)	-0.19	3 (0%)	84	85	22, 37, 60, 79	0
All	All	807/888 (90%)	-0.21	7 (0%)	81	82	22, 36, 59, 79	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	PRO	4.1
1	B	121	PRO	3.3
1	A	108	PRO	3.2
1	A	239	GLY	2.9
1	A	160	ALA	2.4
1	B	239	GLY	2.3
1	B	122	ALA	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

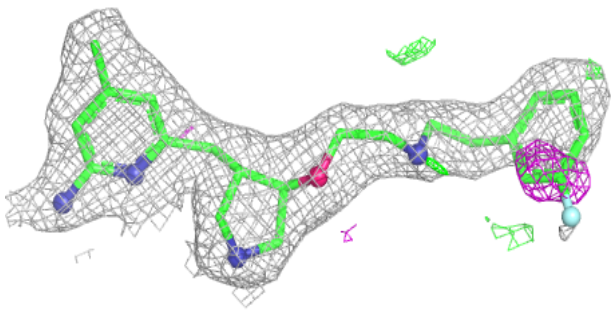
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

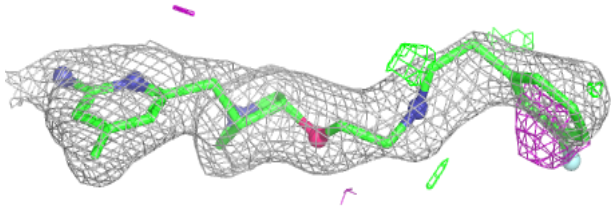
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	880	6/6	0.91	0.11	40,43,44,44	0
4	ACT	B	860	4/4	0.92	0.12	44,45,45,47	0
5	GOL	B	880	6/6	0.93	0.10	41,42,42,43	0
6	JRS	A	800	27/27	0.93	0.12	21,35,71,72	0
6	JRS	B	800	27/27	0.93	0.11	30,35,70,71	0
4	ACT	A	860	4/4	0.94	0.09	44,44,44,46	0
3	H4B	B	600	17/17	0.95	0.06	23,26,28,30	0
3	H4B	A	600	17/17	0.96	0.05	24,29,31,32	0
2	HEM	A	500	43/43	0.98	0.06	21,25,43,47	0
2	HEM	B	500	43/43	0.98	0.06	22,27,43,48	0
7	CAD	A	950	3/5	0.98	0.10	58,58,58,59	0
7	CAD	B	950	3/5	0.98	0.09	56,56,58,59	0
8	ZN	A	900	1/1	1.00	0.02	28,28,28,28	0

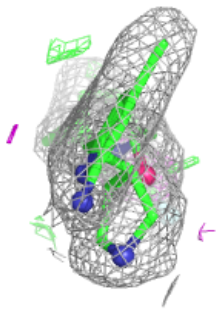
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JRS A 800:

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

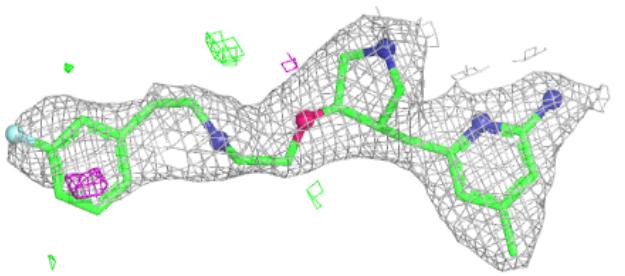


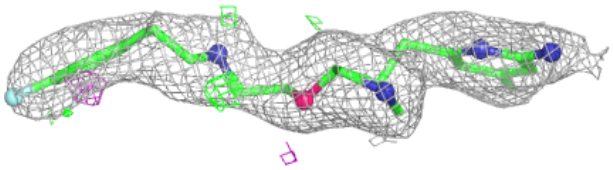


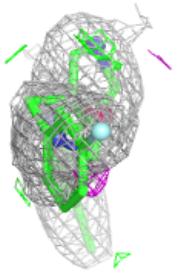


Electron density around JRS B 800:

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

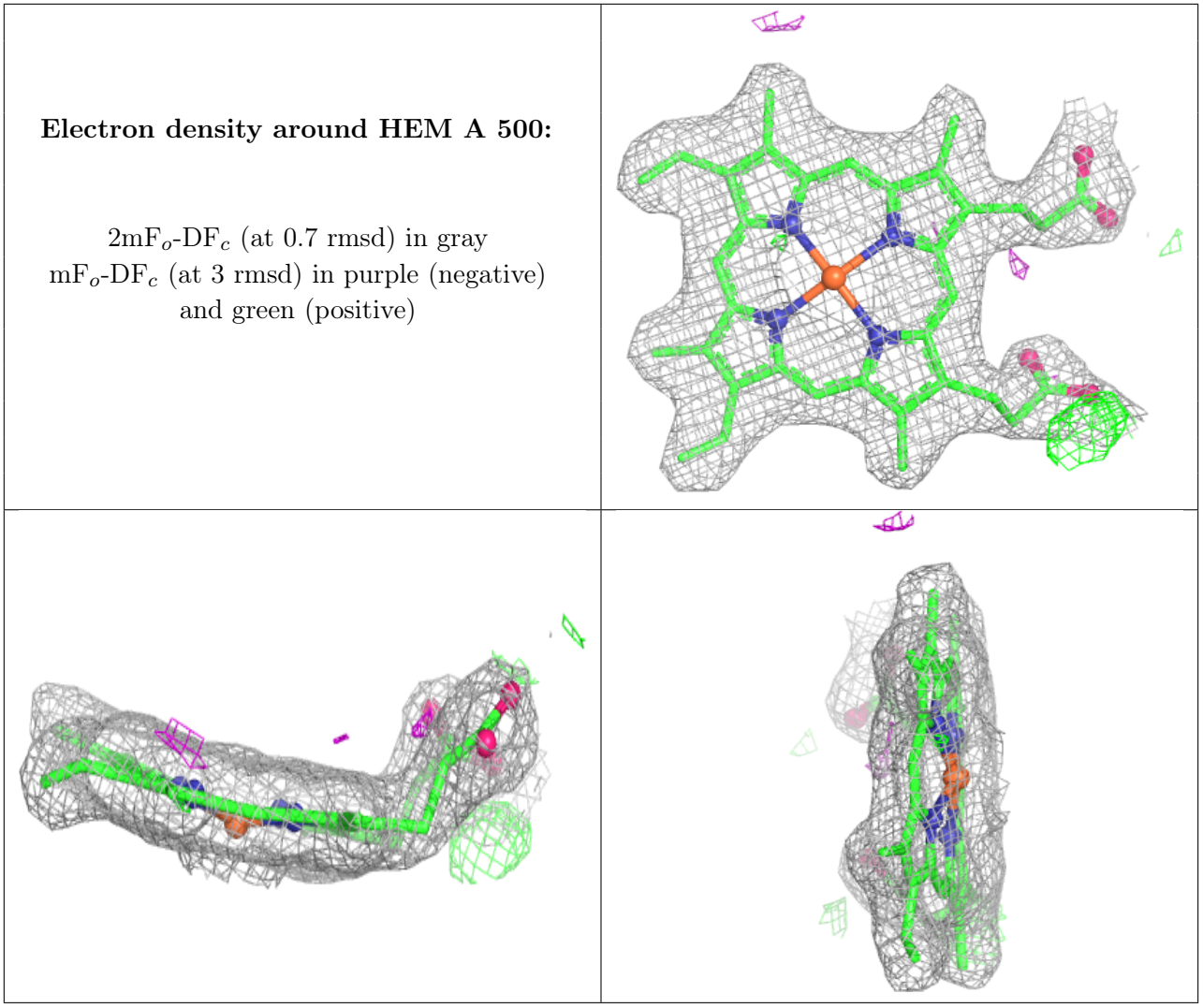






Electron density around HEM A 500:

$2mF_o$-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 500:

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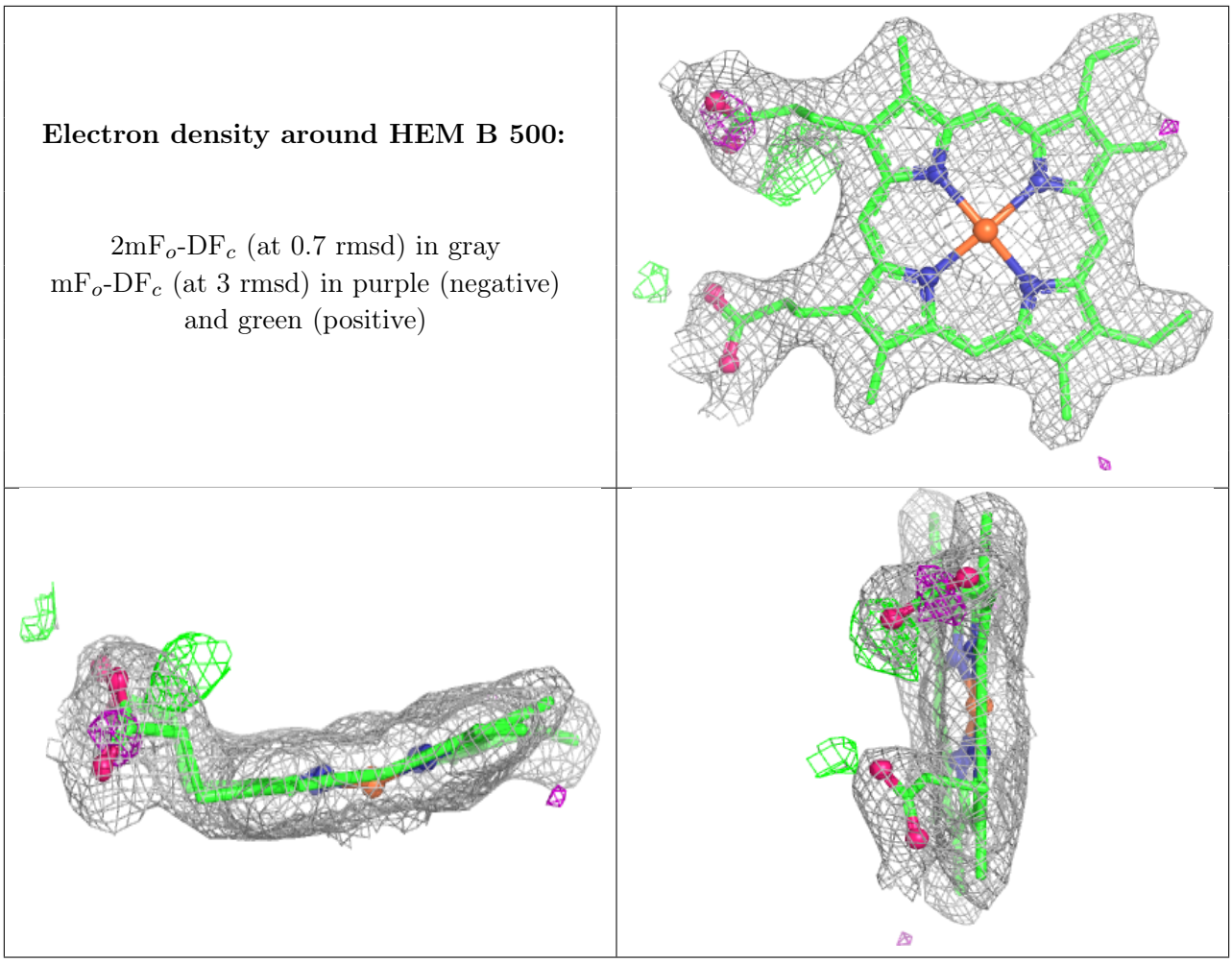
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.