Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 04:36 PM EST

PDB ID	:	3DQS
Title	:	Structure of endothelial NOS heme domain in complex with a inhibitor (+-)-N1-{cis-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}-N2-(4'-chlorobenzyl)ethane-1,2-diamine
Authors	:	Igarashi, J.; Li, H.; Poulos, T.L.
Deposited on	:	2008-07-09
Resolution	:	2.03 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:

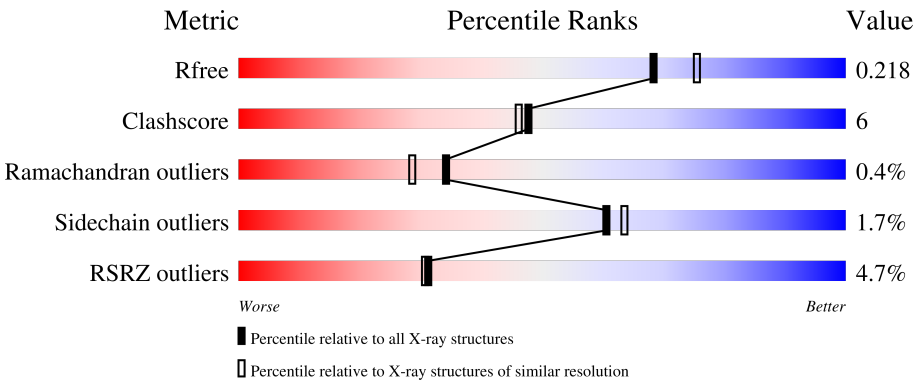
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	416	7% 86% 10% • •
1	B	416	2% 85% 11% • •

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7115 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.

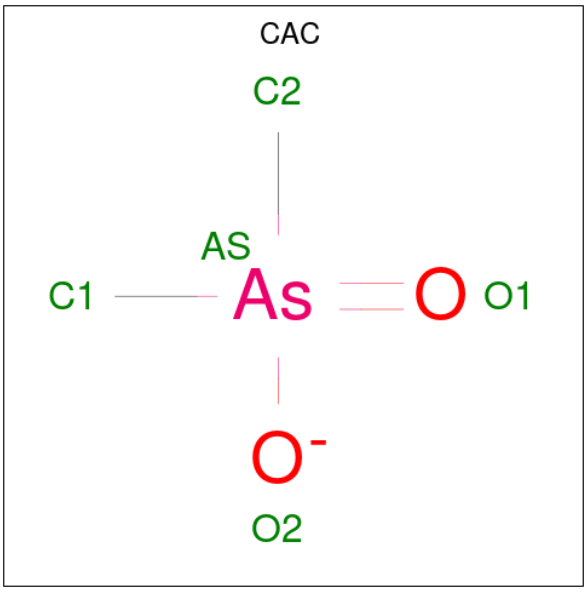
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3216	2046	565	589	16	0	0	0
1	B	402	3202	2035	565	586	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	variant	UNP P29473
B	100	ARG	CYS	variant	UNP P29473

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



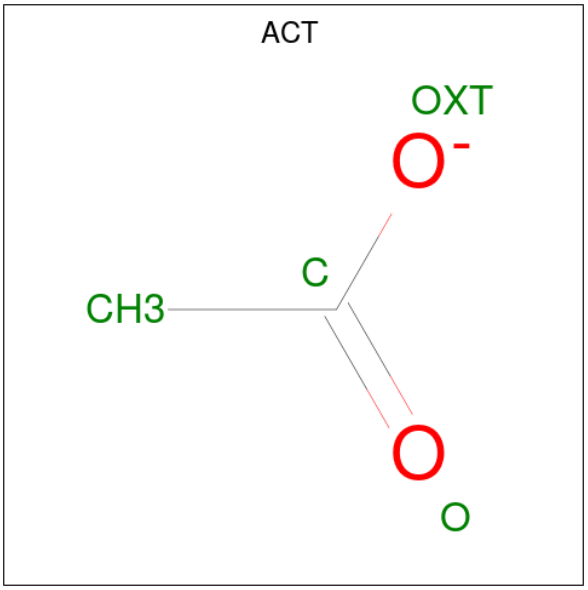
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	C		
2	A	1	3	1	2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

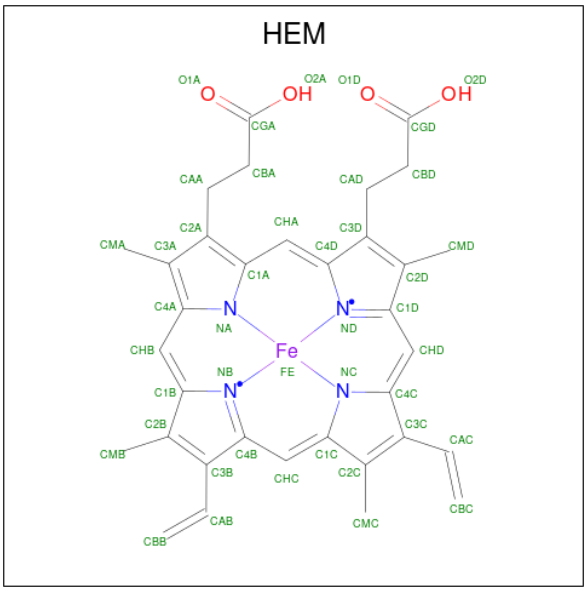


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

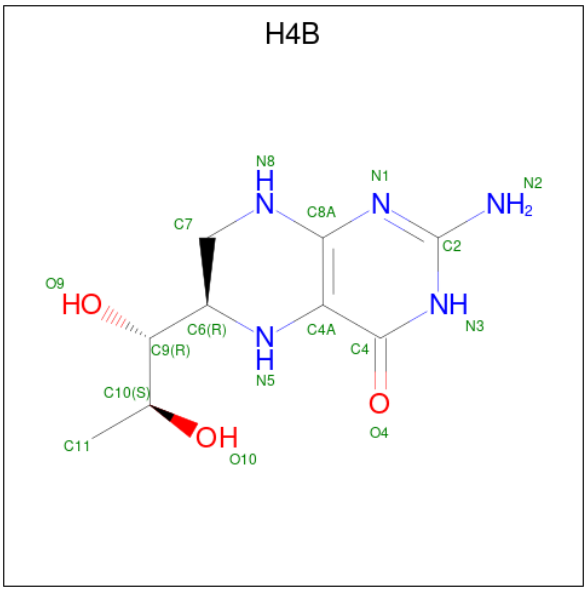
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 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		
5	A	1	48	37	1	4	6	0	1
			Total	C	Fe	N	O		
5	B	1	48	37	1	4	6	0	1

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



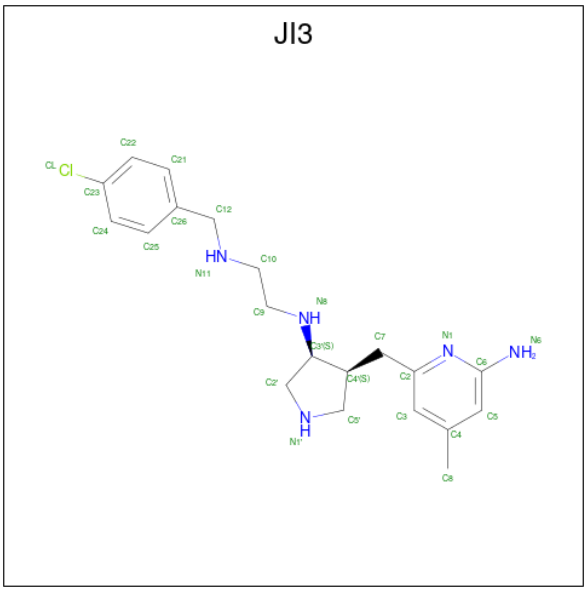
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	17	9	5	3	0	0

Continued on next page...

Continued from previous page...

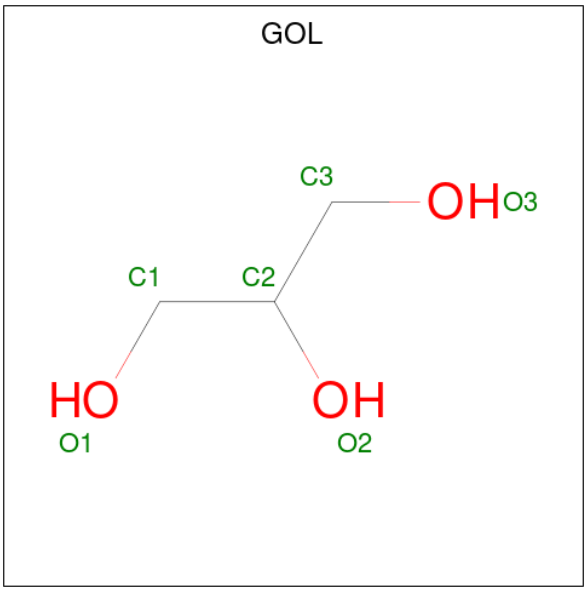
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	17	9	5	3	0	0

- Molecule 7 is N-{(3S,4S)-4-[(6-AMINO-4-METHYLPYRIDIN-2-YL)METHYL]PYRROLIDIN-3-YL}-N'-(4-CHLOROBENZYL)ETHANE-1,2-DIAMINE (three-letter code: JI3) (formula: $C_{20}H_{28}ClN_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	N		
7	A	1	26	20	1	5	0	0
			Total	C	Cl	N		
7	B	1	26	20	1	5	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

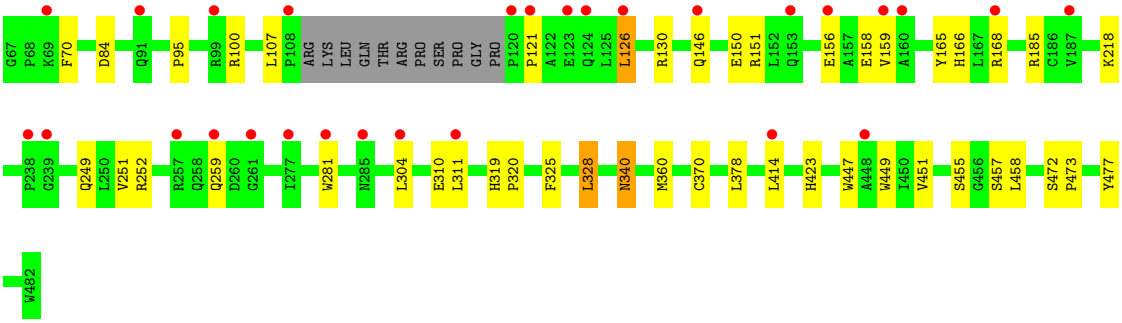
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	250	250	250	0	0
			Total	O		
9	B	238	238	238	0	0

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.

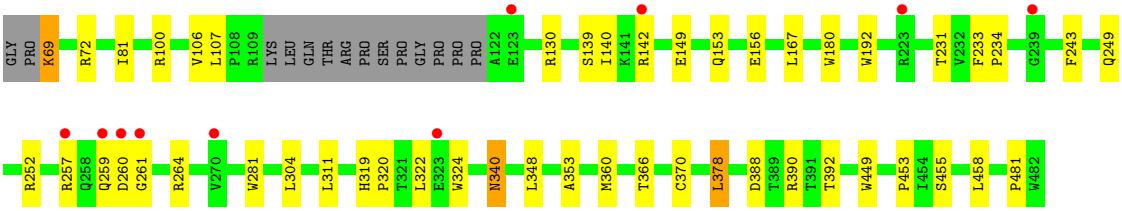
• Molecule 1: Nitric oxide synthase, endothelial

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	57.96Å 106.84Å 156.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 – 2.03 48.45 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.45-2.03) 99.1 (48.45-2.01)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.227 0.190 , 0.218	Depositor DCC
R_{free} test set	3211 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.9	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	7115	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 3.72% 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: CAC, ACT, ZN, JI3, HEM, H4B, GOL

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	0.42	0/3307	0.66	1/4506 (0.0%)
1	B	0.43	0/3290	0.66	2/4480 (0.0%)
All	All	0.43	0/6597	0.66	3/8986 (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	360	MET	N-CA-C	-6.14	94.43	111.00
1	A	360	MET	N-CA-C	-5.90	95.06	111.00
1	B	243	PHE	N-CA-C	-5.41	96.40	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3216	0	3121	37	0
1	B	3202	0	3109	38	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	48	0	8	2	0
5	B	48	0	8	1	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	26	0	28	3	0
7	B	26	0	28	5	0
8	A	6	0	8	0	0
8	B	6	0	8	1	0
9	A	250	0	0	4	0
9	B	238	0	0	2	0
All	All	7115	0	6354	78	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 (78) 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:126:LEU:HD11	1:A:156:GLU:HG2	1.45	0.98
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.68	0.75
1:B:249:GLN:HB2	1:B:252:ARG:HD3	1.71	0.72
1:A:126:LEU:HD12	1:A:130:ARG:NE	2.08	0.69
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.78	0.66
1:A:249:GLN:HB2	1:A:252:ARG:HG3	1.83	0.61
1:A:310:GLU:HB2	9:A:1027:HOH:O	1.99	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.42	0.60
1:B:340:ASN:HD22	1:B:340:ASN:H	1.49	0.60
5:A:700[A]:HEM:O2D	7:A:800:JI3:H101	2.01	0.59
1:A:126:LEU:HD12	1:A:130:ARG:HE	1.66	0.59
5:B:700[A]:HEM:O2D	7:B:800:JI3:H101	2.04	0.58
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.45	0.57
1:A:340:ASN:H	1:A:340:ASN:HD22	1.52	0.57
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.87	0.57
1:B:106:VAL:HG21	8:B:880:GOL:H12	1.85	0.57
1:A:146:GLN:O	1:A:150:GLU:HG3	2.07	0.55
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.37	0.54
1:B:69:LYS:N	1:B:69:LYS:HZ3	2.06	0.53
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.89	0.53
1:A:259:GLN:HB2	9:A:1113:HOH:O	2.10	0.52
1:A:378:LEU:HB2	9:A:910:HOH:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:HD21	7:B:800:JI3:H24	1.92	0.52
1:A:126:LEU:HD11	1:A:156:GLU:CG	2.31	0.51
1:B:340:ASN:HD22	1:B:340:ASN:N	2.07	0.51
1:B:264:ARG:HH11	1:B:264:ARG:HG3	1.76	0.50
1:B:366:THR:O	1:B:370:CYS:HB2	2.12	0.50
1:B:130:ARG:HH21	1:B:156:GLU:CD	2.12	0.50
1:A:158:GLU:HG2	1:A:165:TYR:HA	1.94	0.49
1:B:149:GLU:O	1:B:153:GLN:HG3	2.12	0.49
1:A:449:TRP:HA	6:A:760:H4B:N1	2.27	0.49
1:B:449:TRP:HA	6:B:760:H4B:N1	2.27	0.48
1:B:340:ASN:H	1:B:340:ASN:ND2	2.11	0.48
1:A:107:LEU:HD21	7:A:800:JI3:H24	1.96	0.48
1:A:126:LEU:O	1:A:130:ARG:HG3	2.15	0.47
1:A:340:ASN:HD22	1:A:340:ASN:N	2.11	0.47
1:A:472:SER:HA	1:A:473:PRO:C	2.35	0.47
1:B:231:THR:O	1:B:353:ALA:HA	2.14	0.47
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.42	0.47
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.97	0.46
1:B:107:LEU:HD21	7:B:800:JI3:C24	2.45	0.46
1:A:251:VAL:O	1:A:252:ARG:HG2	2.16	0.45
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.52	0.45
1:B:257:ARG:NH1	1:B:261:GLY:O	2.49	0.45
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.52	0.45
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.47	0.44
1:A:151:ARG:HD3	1:A:168:ARG:CZ	2.48	0.44
1:A:477:TYR:OH	5:A:700[A]:HEM:O1D	2.25	0.44
1:B:378:LEU:HB2	9:B:909:HOH:O	2.18	0.44
1:A:423:HIS:HB2	1:B:392:THR:HB	2.00	0.43
1:B:130:ARG:NH2	1:B:156:GLU:OE1	2.33	0.43
1:A:130:ARG:NH1	1:A:156:GLU:OE1	2.51	0.43
1:A:166:HIS:HD2	9:A:1092:HOH:O	1.99	0.43
1:A:325:PHE:O	1:A:328:LEU:HB2	2.17	0.43
1:B:69:LYS:N	1:B:69:LYS:HE2	2.34	0.43
1:A:126:LEU:HD12	1:A:130:ARG:CZ	2.48	0.43
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.53	0.43
1:A:447:TRP:CE2	1:A:451:VAL:HG21	2.53	0.42
1:B:264:ARG:HG3	1:B:264:ARG:NH1	2.34	0.42
1:A:70:PHE:HB3	1:A:84:ASP:O	2.19	0.42
1:A:340:ASN:H	1:A:340:ASN:ND2	2.17	0.42
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.55	0.42
1:A:126:LEU:HD23	1:A:159:VAL:HG11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLN:H	1:B:259:GLN:HG3	1.57	0.42
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.55	0.41
1:B:140:ILE:CD1	1:B:142:ARG:HD2	2.45	0.41
1:B:72:ARG:NH1	9:B:945:HOH:O	2.53	0.41
1:B:130:ARG:NH2	1:B:156:GLU:CD	2.74	0.41
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.55	0.41
1:B:69:LYS:N	1:B:69:LYS:CE	2.84	0.41
1:B:72:ARG:NE	1:B:81:ILE:HD13	2.36	0.41
1:B:388:ASP:OD1	1:B:390:ARG:HB2	2.21	0.41
1:A:455:SER:HB3	1:A:458:LEU:HD12	2.02	0.41
1:A:457:SER:OG	1:B:453:PRO:HB2	2.21	0.40
1:B:281:TRP:HB2	1:B:304:LEU:HD21	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	401/416 (96%)	388 (97%)	12 (3%)	1 (0%)	47	43
1	B	398/416 (96%)	386 (97%)	10 (2%)	2 (0%)	29	22
All	All	799/832 (96%)	774 (97%)	22 (3%)	3 (0%)	34	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PRO
1	B	260	ASP
1	B	481	PRO

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	344/354 (97%)	338 (98%)	6 (2%)	60	63
1	B	342/354 (97%)	336 (98%)	6 (2%)	59	61
All	All	686/708 (97%)	674 (98%)	12 (2%)	60	63

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	PRO
1	A	100	ARG
1	A	126	LEU
1	A	328	LEU
1	A	340	ASN
1	A	414	LEU
1	B	69	LYS
1	B	100	ARG
1	B	139	SER
1	B	311	LEU
1	B	340	ASN
1	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	153	GLN
1	A	191	GLN
1	A	259	GLN
1	A	279	HIS
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	124	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	GLN
1	B	222	ASN
1	B	278	GLN
1	B	279	HIS
1	B	340	ASN
1	B	405	ASN
1	B	413	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)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	HEM	B	700[A]	-	41,50,50	1.26	5 (12%)	45,82,82	1.81	4 (8%)
8	GOL	A	880	-	5,5,5	0.21	0	5,5,5	0.27	0
7	JI3	B	800	-	26,28,28	2.37	11 (42%)	30,37,37	2.12	6 (20%)
2	CAC	A	850	-	0,2,4	-	-	0,1,6	-	-
2	CAC	B	850	-	0,2,4	-	-	0,1,6	-	-
5	HEM	A	700[A]	-	41,50,50	1.41	6 (14%)	45,82,82	1.58	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACT	B	860	-	3,3,3	0.93	0	3,3,3	0.80	0
6	H4B	B	760	-	16,18,18	2.05	3 (18%)	11,26,26	4.29	8 (72%)
8	GOL	B	880	-	5,5,5	0.16	0	5,5,5	0.20	0
5	HEM	B	700[B]	-	41,50,50	1.26	5 (12%)	45,82,82	1.93	6 (13%)
3	ACT	A	860	-	3,3,3	0.97	0	3,3,3	0.78	0
6	H4B	A	760	-	16,18,18	2.13	5 (31%)	11,26,26	4.41	9 (81%)
5	HEM	A	700[B]	-	41,50,50	1.41	6 (14%)	45,82,82	1.68	6 (13%)
7	JI3	A	800	-	26,28,28	2.51	10 (38%)	30,37,37	2.13	6 (20%)

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	HEM	B	700[A]	-	-	3/12/54/54	-
7	JI3	B	800	-	-	3/12/22/22	0/3/3/3
5	HEM	A	700[A]	-	-	0/12/54/54	-
6	H4B	B	760	-	-	0/8/17/17	0/2/2/2
8	GOL	B	880	-	-	2/4/4/4	-
5	HEM	B	700[B]	-	-	6/12/54/54	-
8	GOL	A	880	-	-	2/4/4/4	-
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	HEM	A	700[B]	-	-	1/12/54/54	-
7	JI3	A	800	-	-	0/12/22/22	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	760	H4B	C4-N3	5.63	1.42	1.33
6	B	760	H4B	C4-N3	5.15	1.42	1.33
7	A	800	JI3	C7-C4'	5.12	1.60	1.53
7	A	800	JI3	C3-C4	4.88	1.47	1.39
7	A	800	JI3	C5-C4	4.76	1.46	1.39
7	B	800	JI3	C7-C4'	4.70	1.60	1.53
7	B	800	JI3	C5-C4	4.55	1.46	1.39
7	A	800	JI3	C5-C6	4.44	1.46	1.39
7	B	800	JI3	C5-C6	4.32	1.46	1.39
6	B	760	H4B	C4A-N5	4.30	1.46	1.38
7	B	800	JI3	C3-C4	4.26	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	760	H4B	C4A-N5	3.87	1.45	1.38
7	A	800	JI3	C3-C2	3.87	1.45	1.38
7	A	800	JI3	C2-N1	3.64	1.40	1.34
7	B	800	JI3	C3-C2	3.42	1.44	1.38
5	A	700[A]	HEM	C3C-CAC	-3.12	1.41	1.47
5	A	700[B]	HEM	C3C-CAC	-3.12	1.41	1.47
5	A	700[A]	HEM	CAB-C3B	-3.11	1.39	1.47
5	A	700[B]	HEM	CAB-C3B	-3.11	1.39	1.47
5	B	700[A]	HEM	C3C-C2C	-3.08	1.36	1.40
5	B	700[B]	HEM	C3C-C2C	-3.08	1.36	1.40
6	B	760	H4B	C6-N5	3.02	1.51	1.45
5	A	700[A]	HEM	CHA-C4D	2.97	1.42	1.35
5	A	700[B]	HEM	CHA-C4D	2.97	1.42	1.35
7	B	800	JI3	C24-C23	2.93	1.43	1.38
5	A	700[A]	HEM	CHB-C1B	2.88	1.42	1.35
5	A	700[B]	HEM	CHB-C1B	2.88	1.42	1.35
6	A	760	H4B	C6-N5	2.87	1.51	1.45
7	B	800	JI3	C2-N1	2.83	1.39	1.34
7	A	800	JI3	C22-C23	2.62	1.43	1.38
7	B	800	JI3	C25-C24	2.52	1.43	1.38
7	B	800	JI3	C6-N1	2.51	1.39	1.35
7	A	800	JI3	C24-C23	2.49	1.42	1.38
5	B	700[A]	HEM	CHB-C1B	2.42	1.41	1.35
5	B	700[B]	HEM	CHB-C1B	2.42	1.41	1.35
5	B	700[A]	HEM	C3C-CAC	-2.40	1.42	1.47
5	B	700[B]	HEM	C3C-CAC	-2.40	1.42	1.47
7	B	800	JI3	C22-C23	2.33	1.42	1.38
5	A	700[A]	HEM	CAA-C2A	2.30	1.55	1.52
5	A	700[B]	HEM	CAA-C2A	2.30	1.55	1.52
5	A	700[A]	HEM	C4A-NA	2.28	1.40	1.36
5	A	700[B]	HEM	C4A-NA	2.28	1.40	1.36
7	B	800	JI3	C22-C21	2.23	1.42	1.38
6	A	760	H4B	C7-N8	2.22	1.48	1.44
7	A	800	JI3	C25-C24	2.21	1.42	1.38
5	B	700[A]	HEM	C4A-NA	2.17	1.40	1.36
5	B	700[B]	HEM	C4A-NA	2.17	1.40	1.36
5	B	700[A]	HEM	CHA-C4D	2.06	1.40	1.35
5	B	700[B]	HEM	CHA-C4D	2.06	1.40	1.35
6	A	760	H4B	C8A-N1	2.03	1.38	1.34
7	A	800	JI3	C6-N1	2.01	1.38	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	700[A]	HEM	CBA-CAA-C2A	-9.82	95.87	112.62
5	B	700[B]	HEM	CBA-CAA-C2A	-9.82	95.87	112.62
6	A	760	H4B	C8A-C4A-C4	9.39	122.92	114.57
6	B	760	H4B	C8A-C4A-C4	9.30	122.83	114.57
7	A	800	JI3	C6-N1-C2	7.95	124.12	118.10
7	B	800	JI3	C6-N1-C2	7.84	124.04	118.10
5	A	700[A]	HEM	CBA-CAA-C2A	-7.37	100.05	112.62
5	A	700[B]	HEM	CBA-CAA-C2A	-7.37	100.05	112.62
6	A	760	H4B	C2-N3-C4	5.82	125.18	115.93
6	B	760	H4B	C2-N3-C4	5.53	124.72	115.93
7	A	800	JI3	C4-C3-C2	-5.30	116.85	120.32
6	A	760	H4B	N1-C2-N3	-5.05	117.50	125.42
7	B	800	JI3	C4-C3-C2	-4.91	117.10	120.32
6	B	760	H4B	N1-C2-N3	-4.78	117.92	125.42
6	A	760	H4B	C4A-C4-N3	-3.73	113.42	124.01
6	B	760	H4B	N2-C2-N1	3.57	122.81	117.25
6	B	760	H4B	C4A-C4-N3	-3.57	113.86	124.01
6	A	760	H4B	N2-C2-N1	3.56	122.79	117.25
6	A	760	H4B	C2-N1-C8A	3.54	122.47	114.54
6	B	760	H4B	C2-N1-C8A	3.48	122.34	114.54
5	B	700[B]	HEM	CAD-C3D-C4D	3.45	130.69	124.66
6	A	760	H4B	C4-C4A-N5	-3.43	116.24	119.12
6	B	760	H4B	C4-C4A-N5	-3.41	116.26	119.12
5	A	700[A]	HEM	C4C-CHD-C1D	3.15	126.71	122.56
5	A	700[B]	HEM	C4C-CHD-C1D	3.15	126.71	122.56
5	B	700[B]	HEM	CAD-C3D-C2D	-2.98	122.32	127.88
5	A	700[A]	HEM	CMD-C2D-C1D	2.97	129.57	125.04
5	A	700[B]	HEM	CMD-C2D-C1D	2.97	129.57	125.04
5	B	700[A]	HEM	C4B-CHC-C1C	2.96	126.47	122.56
5	B	700[B]	HEM	C4B-CHC-C1C	2.96	126.47	122.56
6	B	760	H4B	C4A-N5-C6	-2.85	113.40	121.16
5	A	700[B]	HEM	CBD-CAD-C3D	2.76	120.31	112.63
7	A	800	JI3	C3-C4-C5	2.76	121.38	118.09
7	B	800	JI3	C3-C4-C5	2.75	121.37	118.09
7	B	800	JI3	C2'-C3'-N8	-2.72	108.89	113.73
5	B	700[A]	HEM	C4C-CHD-C1D	2.72	126.15	122.56
5	B	700[B]	HEM	C4C-CHD-C1D	2.72	126.15	122.56
5	A	700[A]	HEM	C4B-CHC-C1C	2.71	126.14	122.56
5	A	700[B]	HEM	C4B-CHC-C1C	2.71	126.14	122.56
6	A	760	H4B	C4A-N5-C6	-2.61	114.05	121.16
7	A	800	JI3	C2'-C3'-N8	-2.42	109.42	113.73
6	A	760	H4B	O9-C9-C6	2.40	114.71	108.98
5	A	700[A]	HEM	C4A-C3A-C2A	-2.37	105.35	107.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	700[B]	HEM	C4A-C3A-C2A	-2.37	105.35	107.00
7	A	800	JI3	C3-C2-N1	-2.29	120.48	122.90
7	A	800	JI3	C26-C12-N11	-2.28	106.90	112.80
7	B	800	JI3	N6-C6-N1	2.26	120.07	116.49
7	B	800	JI3	C3-C2-N1	-2.05	120.72	122.90
5	B	700[A]	HEM	C2C-C3C-C4C	-2.02	105.49	106.90
5	B	700[B]	HEM	C2C-C3C-C4C	-2.02	105.49	106.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	880	GOL	O1-C1-C2-C3
8	B	880	GOL	O1-C1-C2-O2
7	B	800	JI3	C26-C12-N11-C10
8	A	880	GOL	O1-C1-C2-O2
5	B	700[A]	HEM	C4B-C3B-CAB-CBB
5	B	700[B]	HEM	C4B-C3B-CAB-CBB
7	B	800	JI3	N11-C10-C9-N8
7	B	800	JI3	C2'-C3'-N8-C9
5	B	700[B]	HEM	CAD-CBD-CGD-O2D
5	B	700[B]	HEM	CAD-CBD-CGD-O1D
8	A	880	GOL	O1-C1-C2-C3
5	B	700[A]	HEM	CAA-CBA-CGA-O2A
5	B	700[B]	HEM	CAA-CBA-CGA-O2A
5	B	700[A]	HEM	CAA-CBA-CGA-O1A
5	B	700[B]	HEM	CAA-CBA-CGA-O1A
5	B	700[B]	HEM	C3D-CAD-CBD-CGD
5	A	700[B]	HEM	CAD-CBD-CGD-O2D

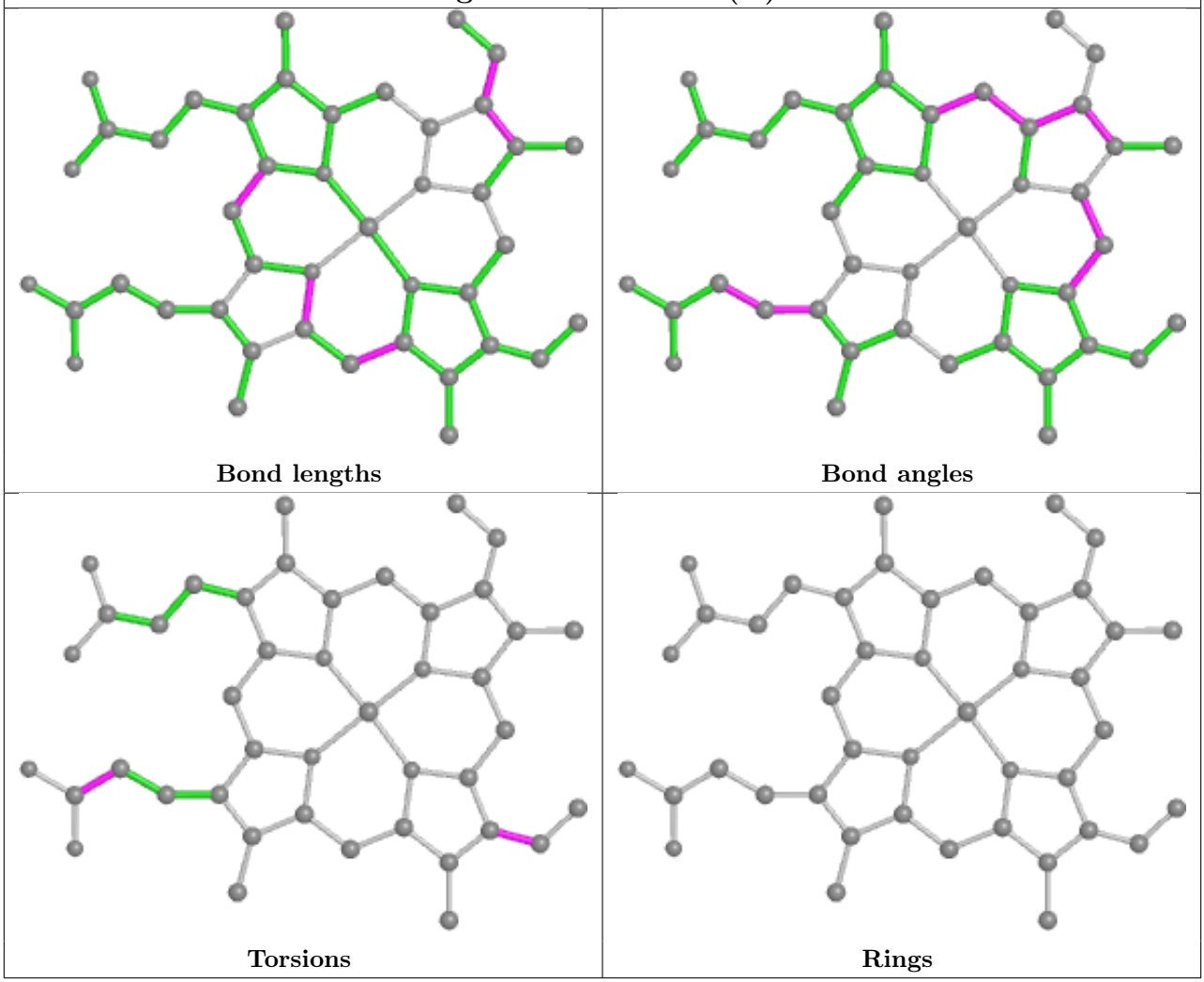
There are no ring outliers.

7 monomers are involved in 12 short contacts:

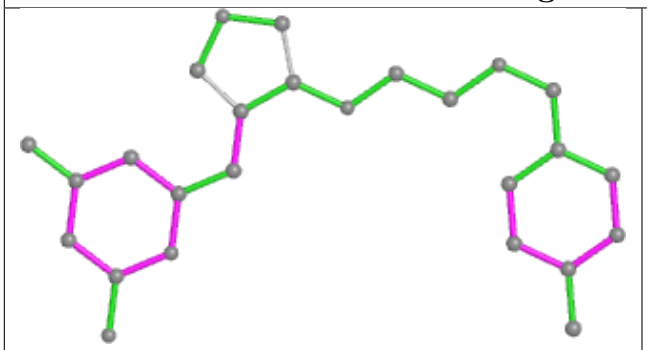
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700[A]	HEM	1	0
7	B	800	JI3	5	0
5	A	700[A]	HEM	2	0
6	B	760	H4B	1	0
8	B	880	GOL	1	0
6	A	760	H4B	1	0
7	A	800	JI3	3	0

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.

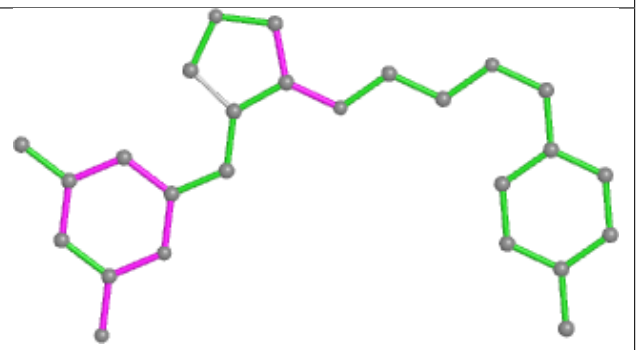
Ligand HEM B 700 (A)



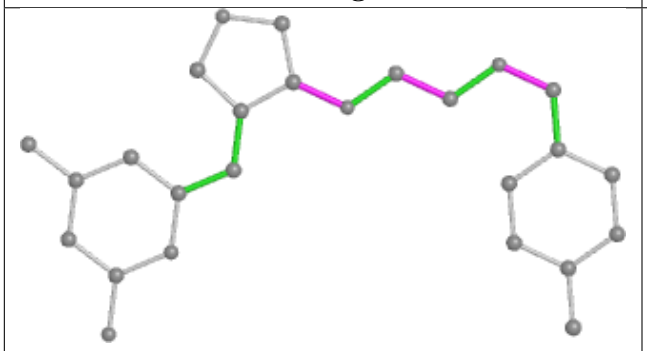
Ligand JI3 B 800



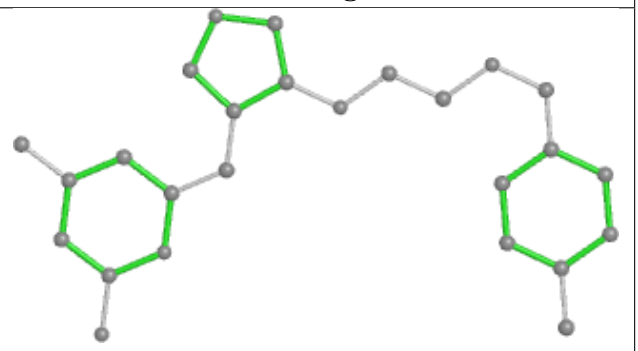
Bond lengths



Bond angles

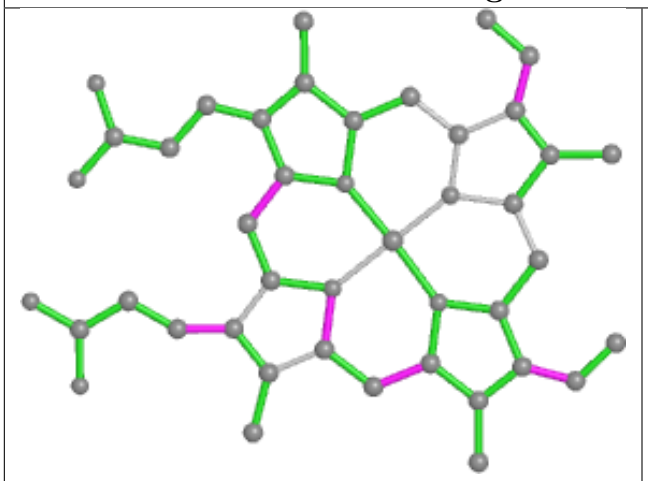


Torsions

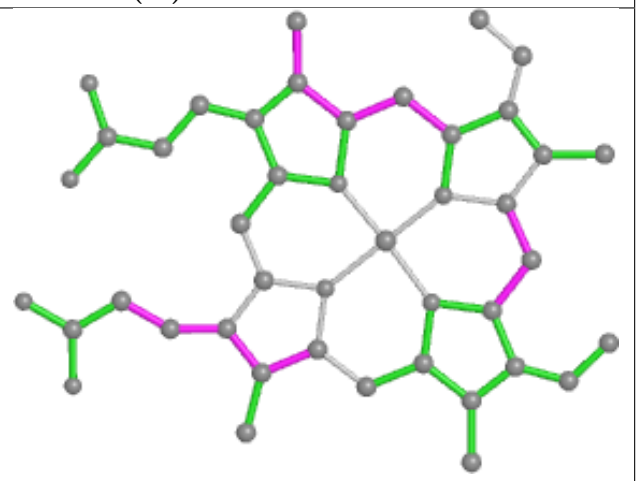


Rings

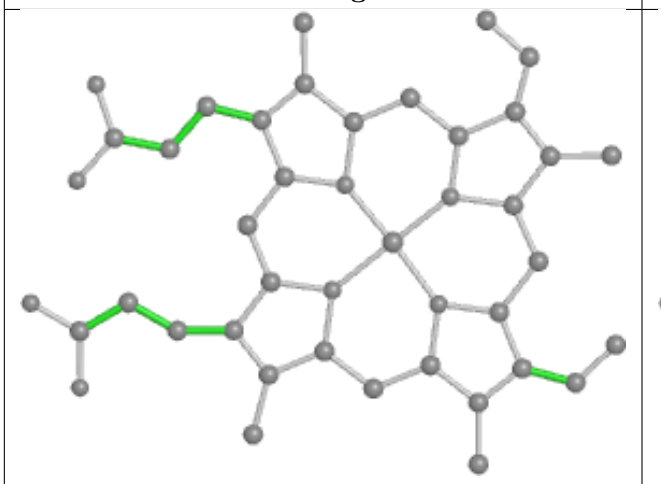
Ligand HEM A 700 (A)



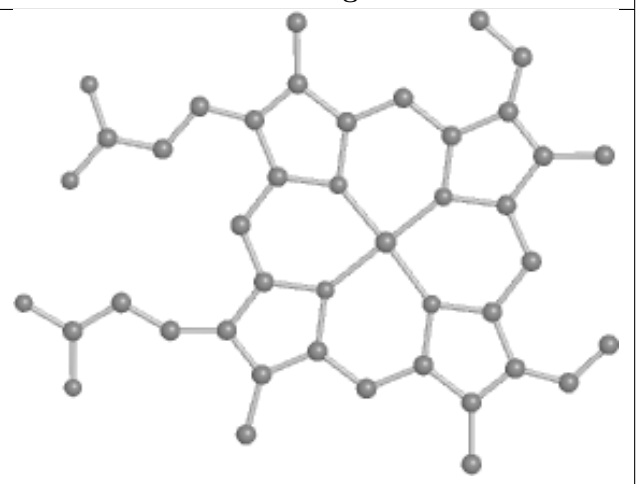
Bond lengths



Bond angles

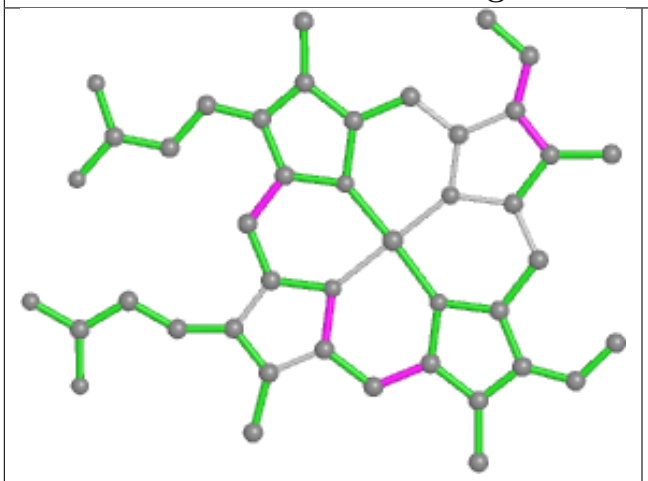


Torsions

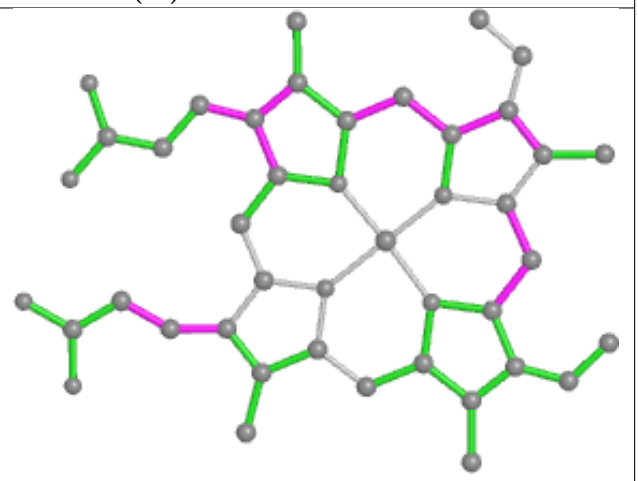


Rings

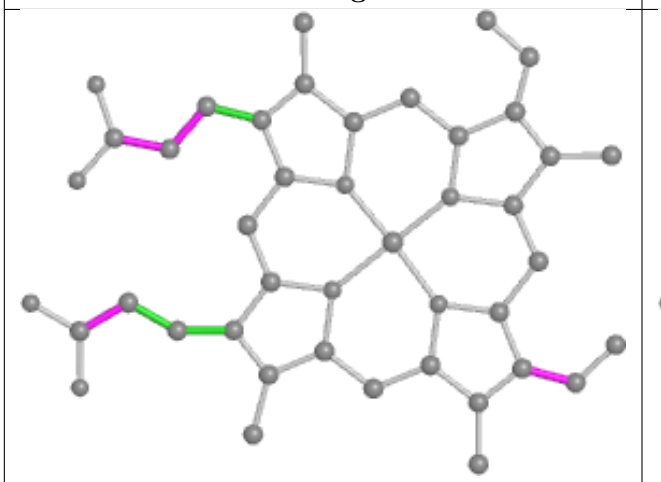
Ligand HEM B 700 (B)



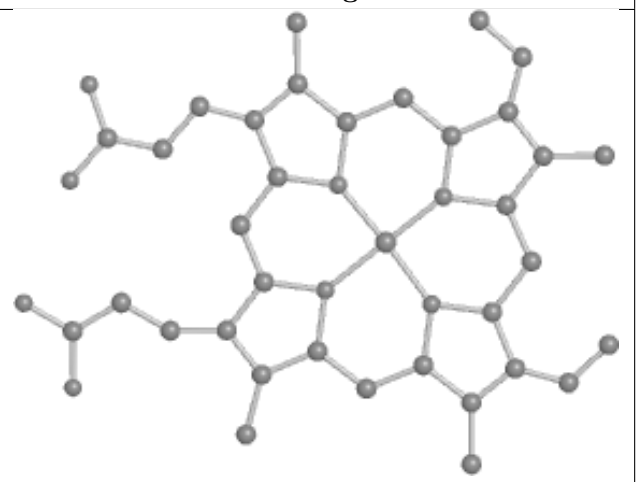
Bond lengths



Bond angles

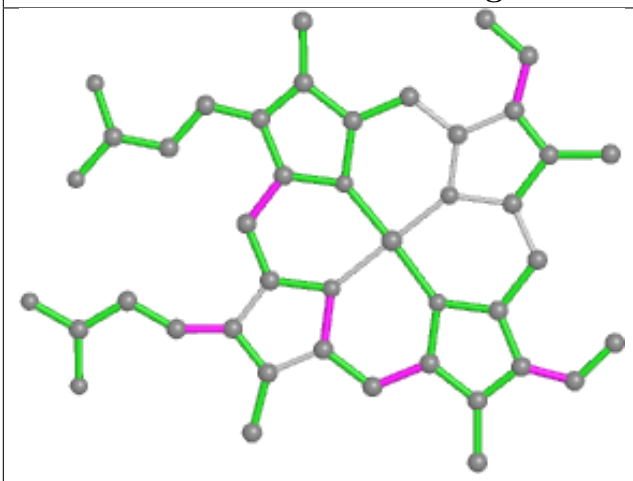


Torsions

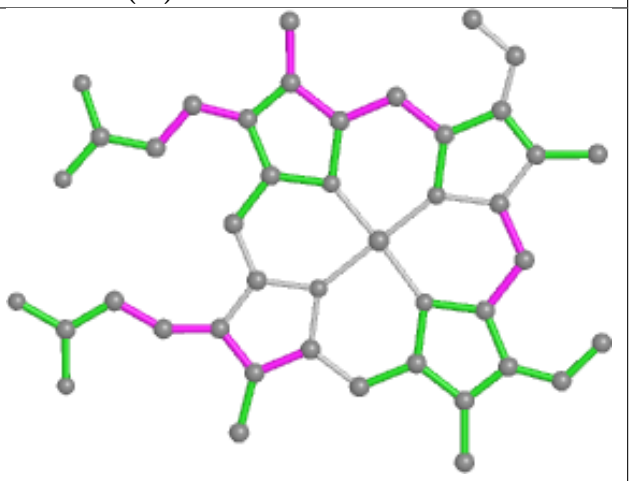


Rings

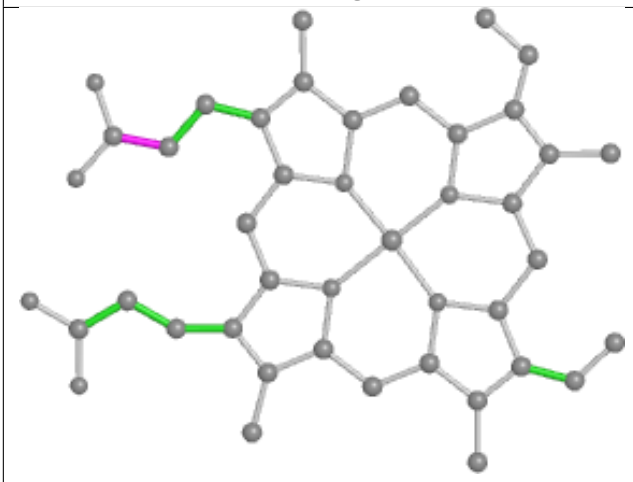
Ligand HEM A 700 (B)



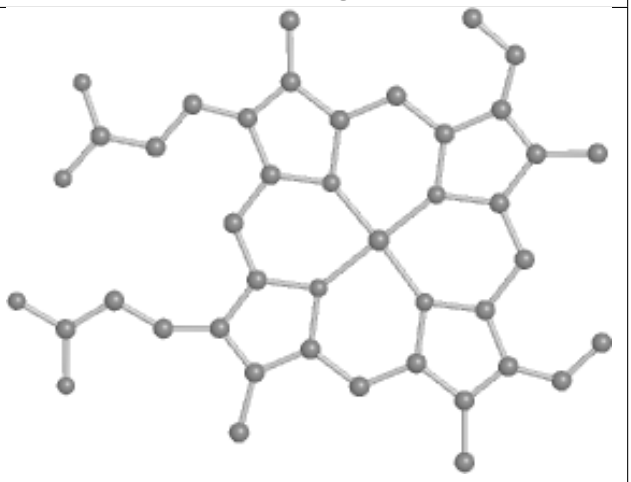
Bond lengths



Bond angles

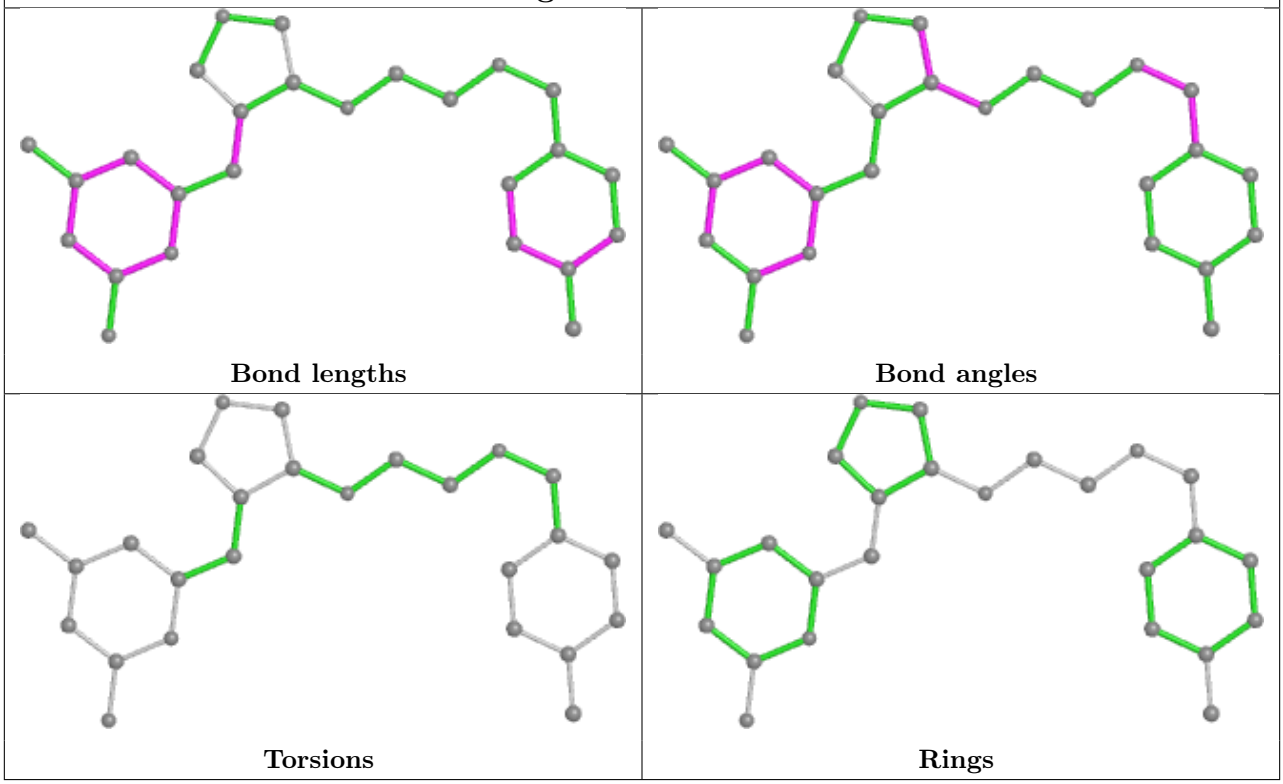


Torsions



Rings

Ligand JI3 A 800



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	405/416 (97%)	0.36	28 (6%)	16	16	24, 34, 54, 77	0
1	B	402/416 (96%)	0.17	10 (2%)	57	57	25, 37, 54, 67	0
All	All	807/832 (96%)	0.26	38 (4%)	31	31	24, 36, 54, 77	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	6.6
1	A	259	GLN	5.3
1	A	120	PRO	4.7
1	A	239	GLY	3.4
1	A	160	ALA	3.2
1	B	260	ASP	3.1
1	A	123	GLU	3.1
1	B	142	ARG	2.9
1	A	121	PRO	2.9
1	A	153	GLN	2.9
1	B	257	ARG	2.8
1	B	261	GLY	2.8
1	A	126	LEU	2.7
1	B	239	GLY	2.7
1	A	285	ASN	2.7
1	A	277	ILE	2.6
1	A	99	ARG	2.6
1	A	146	GLN	2.6
1	B	323	GLU	2.6
1	A	69	LYS	2.5
1	A	124	GLN	2.5
1	B	123	GLU	2.4
1	A	159	VAL	2.4
1	A	238	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	261	GLY	2.3
1	A	257	ARG	2.3
1	A	311	LEU	2.3
1	A	281	TRP	2.3
1	A	156	GLU	2.2
1	A	187	VAL	2.2
1	A	168	ARG	2.2
1	A	108	PRO	2.2
1	B	223	ARG	2.1
1	A	304	LEU	2.1
1	A	91	GLN	2.1
1	A	414	LEU	2.1
1	A	448	ALA	2.0
1	B	270	VAL	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	B	880	6/6	0.87	0.25	50,52,52,53	0
7	JI3	B	800	26/26	0.88	0.18	30,36,53,56	0
7	JI3	A	800	26/26	0.88	0.22	25,34,55,59	0
8	GOL	A	880	6/6	0.90	0.25	48,50,50,51	0
6	H4B	B	760	17/17	0.95	0.16	33,34,34,34	0
5	HEM	A	700[A]	43/43	0.97	0.21	23,25,30,33	5
5	HEM	A	700[B]	43/43	0.97	0.21	23,25,29,30	5
6	H4B	A	760	17/17	0.97	0.15	30,31,33,33	0
3	ACT	B	860	4/4	0.97	0.13	42,42,42,43	0

Continued on next page...

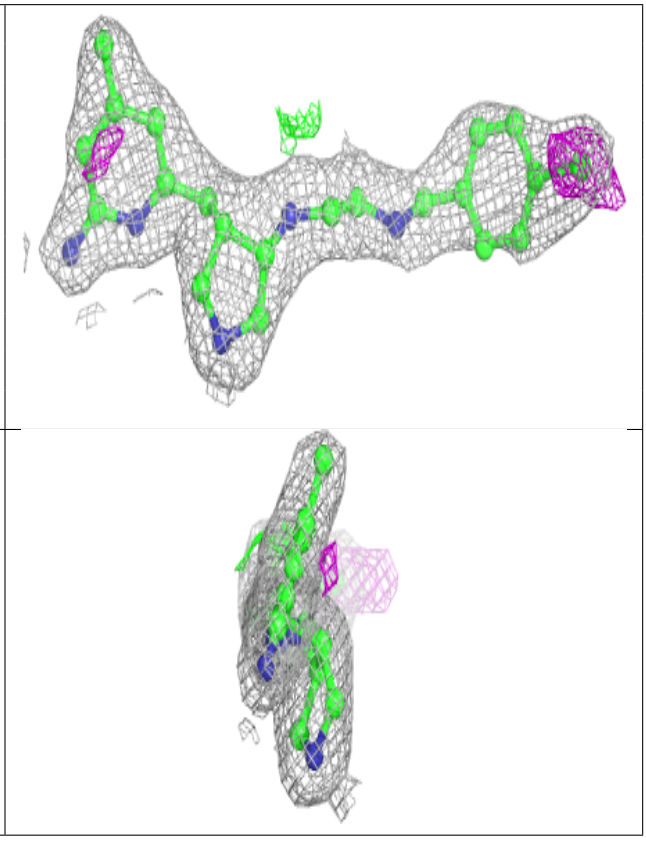
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CAC	B	850	3/5	0.98	0.13	56,56,56,56	0
3	ACT	A	860	4/4	0.98	0.13	41,41,42,42	0
5	HEM	B	700[A]	43/43	0.98	0.14	26,28,34,35	5
5	HEM	B	700[B]	43/43	0.98	0.14	26,28,32,34	5
2	CAC	A	850	3/5	0.98	0.10	44,44,45,48	0
4	ZN	A	900	1/1	1.00	0.10	29,29,29,29	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.

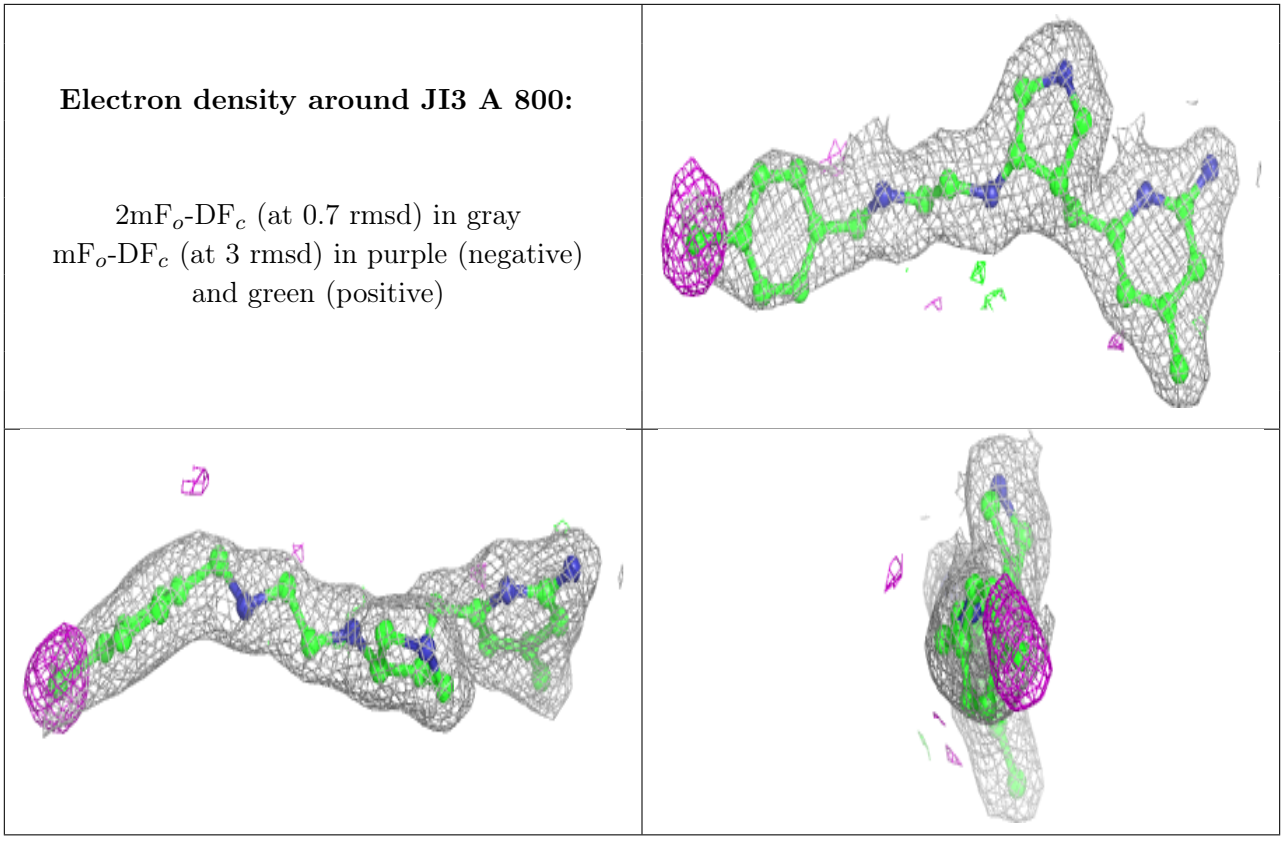
Electron density around JI3 B 800:

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



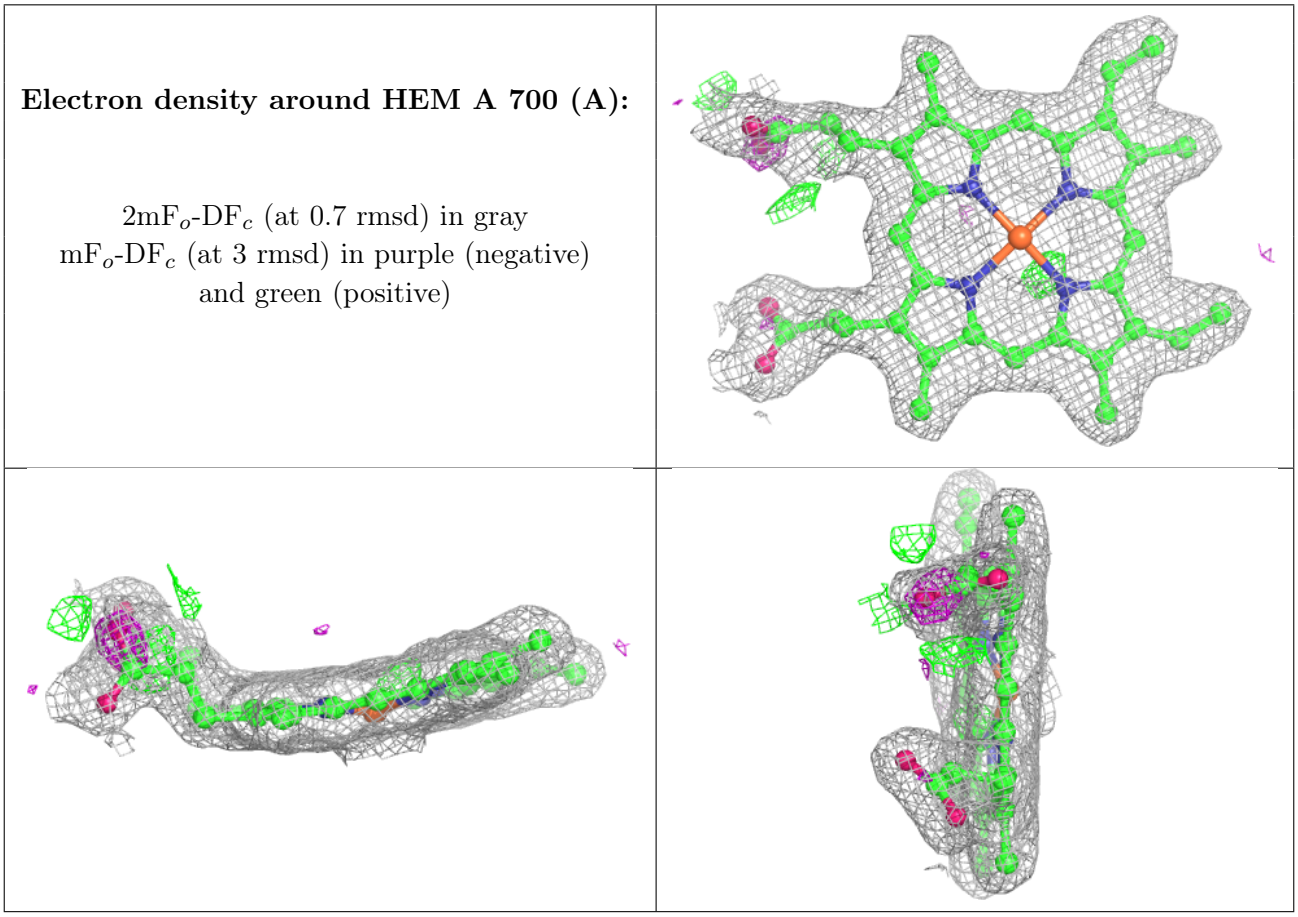
Electron density around JI3 A 800:

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



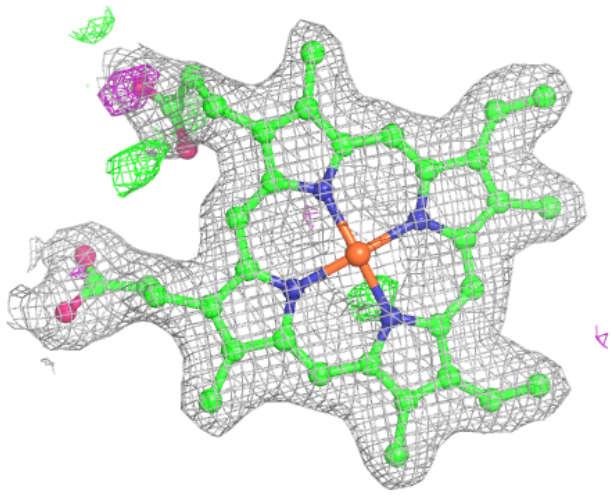
Electron density around HEM A 700 (A):

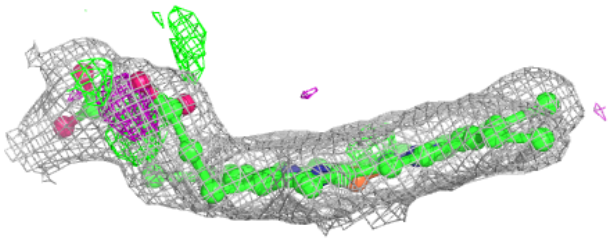
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

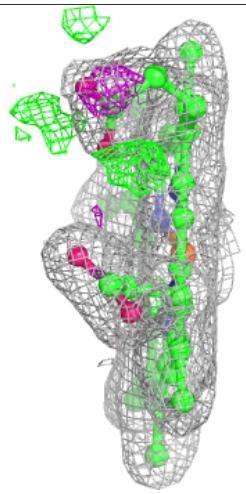


Electron density around HEM A 700 (B):

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

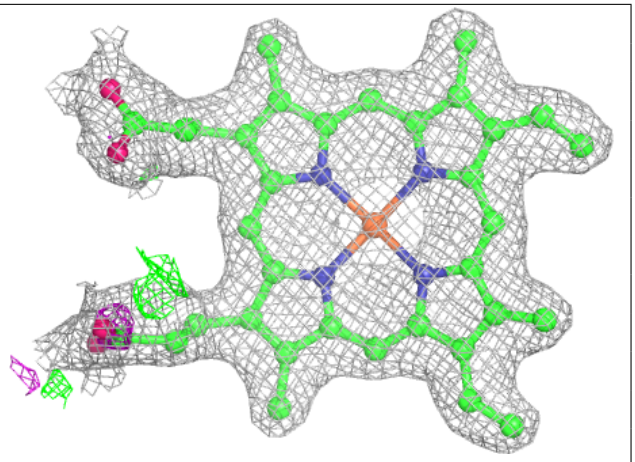


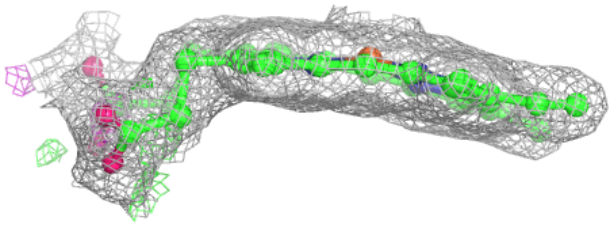


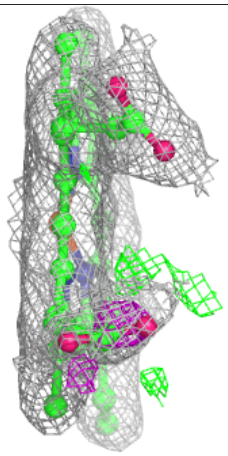


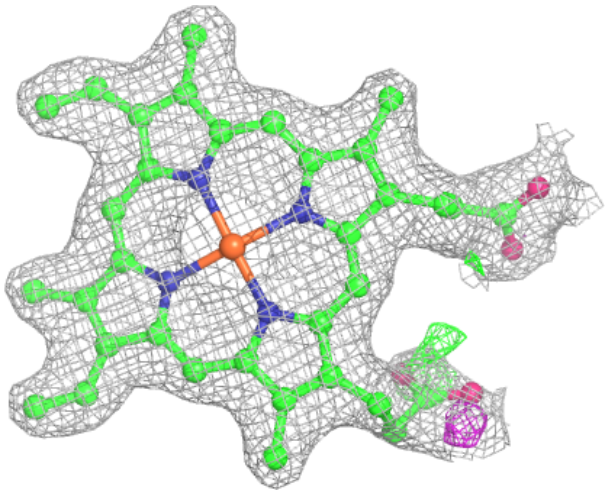
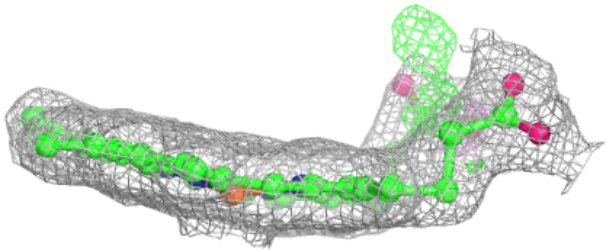
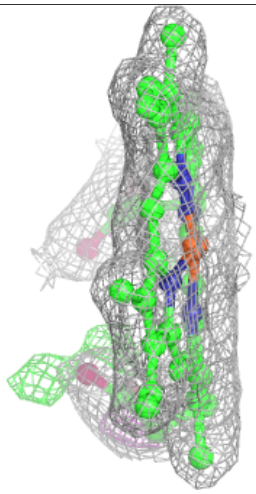
Electron density around HEM B 700 (A):

$2mF_o$-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 700 (B): $2mF_o$-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.