Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 11:06 PM EDT

PDB ID	:	6AUY
Title	:	Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with 4-Methyl-6-(3-(3-(methylamino)propyl)phenethyl)pyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2017-09-01
Resolution	:	1.92 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:

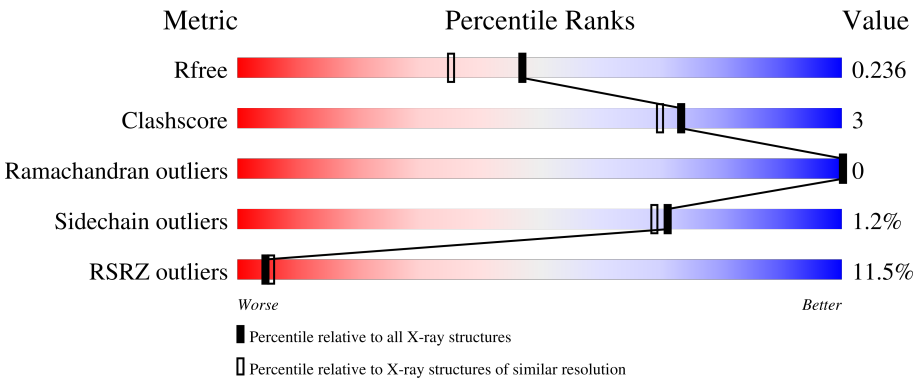
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	421	8%, 90%, 9%
1	B	421	14%, 89%, 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7385 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.

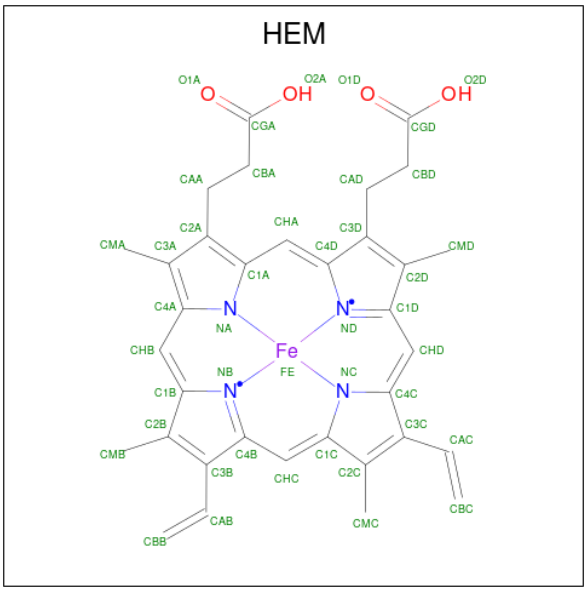
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3387	2169	576	620	22	0	2	0
1	B	409	3339	2139	569	610	21	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

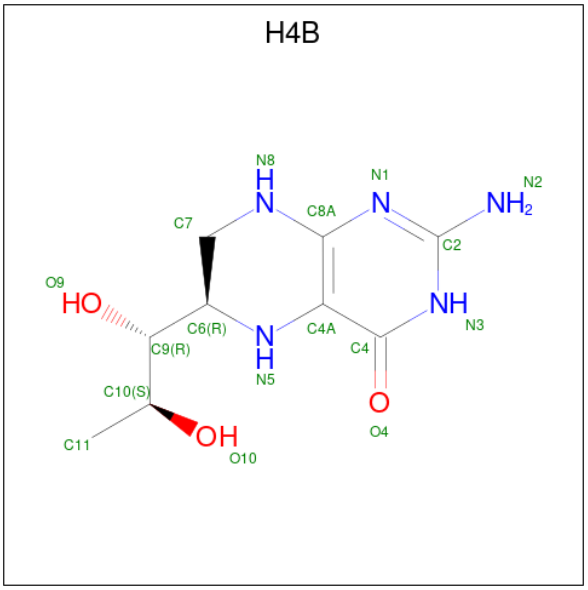
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475

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



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

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

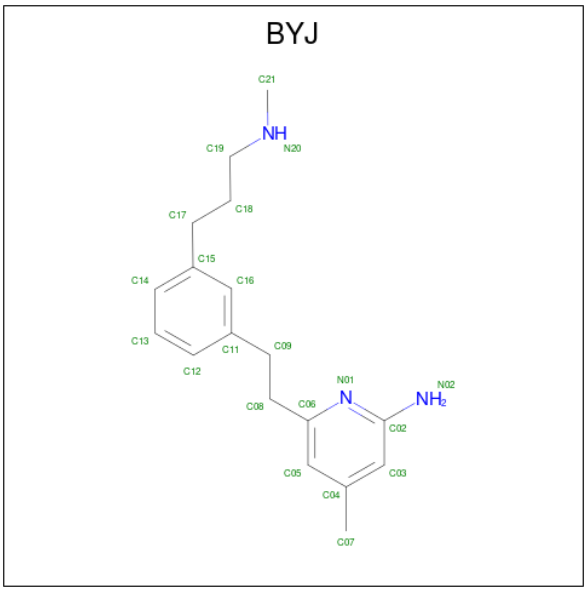


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	9	5	3	0	0
3	B	1	17	9	5	3	0	0

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

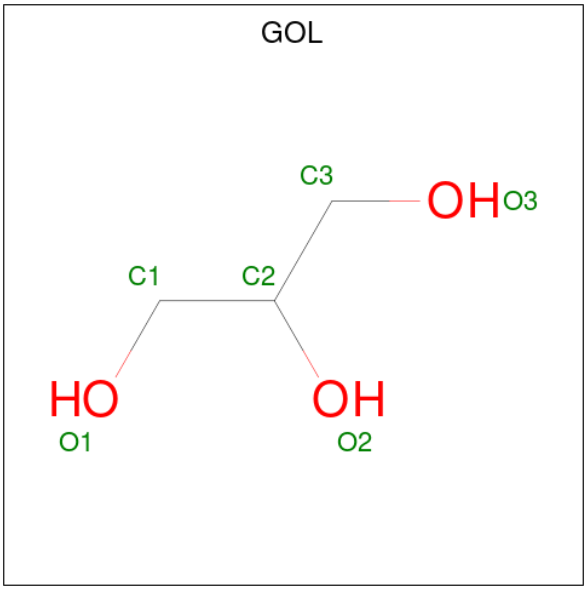
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 is 4-methyl-6-(2-{3-[3-(methylamino)propyl]phenyl}ethyl)pyridin-2-amine (three-letter code: BYJ) (formula: $C_{18}H_{25}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	A	1	21	18	3	0	0
5	B	1	21	18	3	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is water.

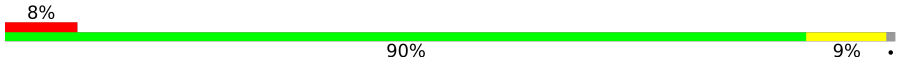
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	283	283	283	0	0
			Total	O		
7	B	189	189	189	0	0

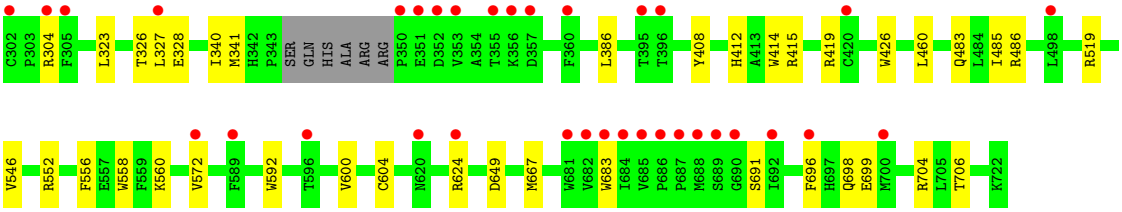
3 Residue-property plots (i)

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, brain

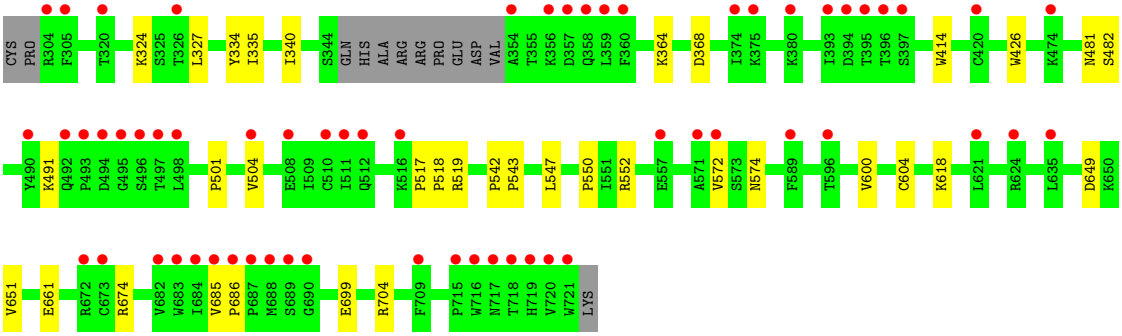
Chain A:





• Molecule 1: Nitric oxide synthase, brain

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	52.52Å 122.03Å 165.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.10 – 1.92 39.10 – 1.92	Depositor EDS
% Data completeness (in resolution range)	93.8 (39.10-1.92) 94.3 (39.10-1.92)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.186 , 0.236 0.190 , 0.236	Depositor DCC
R_{free} test set	3792 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7385	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: GOL, H4B, HEM, ZN, BYJ

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	0.37	0/3490	0.52	0/4735
1	B	0.35	0/3440	0.48	0/4668
All	All	0.36	0/6930	0.50	0/9403

There are no bond length outliers.

There are no bond angle outliers.

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	3387	0	3296	20	0
1	B	3339	0	3249	21	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	1	0	0	0	0
5	A	21	0	0	3	0
5	B	21	0	0	2	0
6	A	12	0	16	1	0
6	B	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	283	0	0	1	0
7	B	189	0	0	1	0
All	All	7385	0	6667	45	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 3.

All (45) 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:A:801:HEM:HBD2	5:A:804:BYJ:C13	2.17	0.74
1:A:326:THR:HG21	1:A:706:THR:HG22	1.71	0.71
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.78	0.65
1:B:572:VAL:HG21	5:B:803:BYJ:C13	2.28	0.63
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.84	0.60
1:A:572:VAL:HG21	5:A:804:BYJ:C13	2.31	0.59
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.84	0.59
1:A:415:ARG:HH22	6:A:805:GOL:H31	1.69	0.58
1:A:552:ARG:NH1	1:A:649:ASP:OD1	2.40	0.53
1:B:364:LYS:NZ	1:B:368:ASP:OD2	2.40	0.52
2:B:801:HEM:HBD2	5:B:803:BYJ:C13	2.40	0.52
1:A:483:GLN:HB2	1:A:486:ARG:HG3	1.93	0.51
1:B:501:PRO:HA	1:B:504:VAL:HG23	1.93	0.51
1:B:661:GLU:HG3	7:B:1012:HOH:O	2.10	0.51
1:A:460:LEU:HD12	1:A:592:TRP:HB3	1.94	0.50
1:B:552:ARG:NH1	1:B:649:ASP:OD1	2.45	0.50
1:A:519:ARG:NH2	7:A:906:HOH:O	2.44	0.49
2:A:801:HEM:HBD2	5:A:804:BYJ:C14	2.42	0.49
1:A:552:ARG:HH12	1:A:649:ASP:CG	2.16	0.49
1:B:327:LEU:HB2	1:B:704:ARG:HG2	1.94	0.48
1:A:667:MET:HE1	1:A:698:GLN:HG2	1.95	0.47
1:B:674:ARG:HH21	6:B:804:GOL:H2	1.79	0.47
1:A:304:ARG:HG3	1:A:323:LEU:HD11	1.96	0.46
1:B:482:SER:HA	1:B:574:ASN:HB3	1.98	0.46
1:A:485:ILE:HD13	1:A:546:VAL:HG13	1.98	0.46
1:A:691:SER:HA	1:A:696:PHE:CG	2.51	0.46
1:A:699:GLU:HB3	1:B:340:ILE:HD13	1.98	0.45
1:B:491:LYS:HA	1:B:491:LYS:HD2	1.81	0.45
1:B:542:PRO:HA	1:B:543:PRO:HD3	1.81	0.45
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.53	0.44
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:VAL:O	1:B:604:CYS:HB2	2.19	0.43
1:A:327:LEU:HD11	1:A:704:ARG:NH1	2.34	0.43
1:B:547:LEU:HD21	1:B:651:VAL:HG22	2.00	0.43
1:B:334:TYR:C	1:B:335:ILE:HG13	2.40	0.42
1:B:327:LEU:HD12	1:B:704:ARG:HG2	2.02	0.42
1:B:517:PRO:HA	1:B:518:PRO:HD3	1.95	0.41
1:B:685:VAL:HA	1:B:686:PRO:HD3	1.90	0.41
1:B:550:PRO:HG2	1:B:552:ARG:NH2	2.35	0.41
1:A:408:TYR:CE1	1:A:412:HIS:CE1	3.09	0.41
1:A:419:ARG:HD3	1:A:683:TRP:CD2	2.55	0.41
1:B:550:PRO:O	1:B:552:ARG:NH2	2.53	0.41
1:A:556:PHE:HB3	1:A:558:TRP:CE2	2.56	0.41
1:A:340:ILE:HD13	1:B:699:GLU:HB3	2.03	0.40
1:A:600:VAL:O	1:A:604:CYS:HB2	2.22	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	413/421 (98%)	406 (98%)	7 (2%)	0	100	100
1	B	407/421 (97%)	397 (98%)	10 (2%)	0	100	100
All	All	820/842 (97%)	803 (98%)	17 (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	373/376 (99%)	368 (99%)	5 (1%)	69	66
1	B	367/376 (98%)	363 (99%)	4 (1%)	73	72
All	All	740/752 (98%)	731 (99%)	9 (1%)	71	69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	GLU
1	A	341	MET
1	A	386	LEU
1	A	560	LYS
1	A	624	ARG
1	B	324	LYS
1	B	481	ASN
1	B	519	ARG
1	B	618	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#\|Z\| > 2$
6	GOL	A	806	-	5,5,5	0.36	0	5,5,5	0.35	0
3	H4B	B	802	-	16,18,18	0.82	0	11,26,26	2.62	5 (45%)
2	HEM	B	801	1	41,50,50	1.91	6 (14%)	45,82,82	1.83	11 (24%)
5	BYJ	A	804	-	22,22,22	0.40	0	28,28,28	1.58	3 (10%)
6	GOL	A	805	-	5,5,5	0.34	0	5,5,5	0.26	0
6	GOL	B	804	-	5,5,5	0.36	0	5,5,5	0.21	0
3	H4B	A	802	-	16,18,18	0.72	0	11,26,26	2.49	5 (45%)
5	BYJ	B	803	-	22,22,22	0.30	0	28,28,28	1.38	3 (10%)
2	HEM	A	801	1	41,50,50	1.80	6 (14%)	45,82,82	1.96	10 (22%)
6	GOL	B	805	-	5,5,5	0.47	0	5,5,5	0.33	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
6	GOL	A	806	-	-	4/4/4/4	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
2	HEM	B	801	1	-	2/12/54/54	-
5	BYJ	A	804	-	-	3/10/10/10	0/2/2/2
6	GOL	A	805	-	-	2/4/4/4	-
6	GOL	B	804	-	-	2/4/4/4	-
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
5	BYJ	B	803	-	-	3/10/10/10	0/2/2/2
2	HEM	A	801	1	-	4/12/54/54	-
6	GOL	B	805	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3D-C2D	7.51	1.52	1.36
2	A	801	HEM	C3D-C2D	6.77	1.51	1.36
2	A	801	HEM	C3C-C2C	-3.88	1.35	1.40
2	B	801	HEM	C3C-C2C	-3.75	1.35	1.40
2	B	801	HEM	C3C-CAC	3.48	1.54	1.47
2	A	801	HEM	C3C-CAC	3.33	1.54	1.47
2	A	801	HEM	CAB-C3B	2.94	1.55	1.47
2	B	801	HEM	FE-NB	2.90	2.11	1.96
2	B	801	HEM	CAB-C3B	2.72	1.54	1.47
2	B	801	HEM	CMB-C2B	2.27	1.55	1.50
2	A	801	HEM	FE-ND	2.24	2.07	1.96
2	A	801	HEM	CMB-C2B	2.02	1.55	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	CBA-CAA-C2A	-6.26	101.94	112.62
2	B	801	HEM	C4D-ND-C1D	5.91	111.18	105.07
5	A	804	BYJ	C02-N01-C06	5.71	122.43	118.10
2	A	801	HEM	CAD-C3D-C4D	5.30	133.93	124.66
3	B	802	H4B	C8A-C4A-C4	5.03	119.04	114.57
3	A	802	H4B	C8A-C4A-C4	4.81	118.84	114.57
2	A	801	HEM	C4D-ND-C1D	4.54	109.76	105.07
5	B	803	BYJ	C02-N01-C06	4.18	121.27	118.10
2	B	801	HEM	CBA-CAA-C2A	-4.00	105.79	112.62
2	A	801	HEM	CAD-C3D-C2D	-3.87	120.68	127.88
5	A	804	BYJ	C05-C06-N01	-3.86	118.81	122.90
3	B	802	H4B	C2-N3-C4	3.65	121.73	115.93
2	B	801	HEM	C4B-CHC-C1C	3.63	127.35	122.56
2	B	801	HEM	CAD-C3D-C4D	3.58	130.92	124.66
5	B	803	BYJ	C05-C06-N01	-3.40	119.30	122.90
3	B	802	H4B	N1-C2-N3	-3.38	120.12	125.42
3	A	802	H4B	C4-C4A-N5	3.25	121.85	119.12
5	B	803	BYJ	C08-C06-N01	3.23	120.76	115.95
3	A	802	H4B	C2-N3-C4	3.20	121.02	115.93
3	A	802	H4B	N1-C2-N3	-2.93	120.82	125.42
2	A	801	HEM	CMD-C2D-C1D	2.84	129.36	125.04
2	B	801	HEM	CHD-C1D-ND	2.82	127.49	124.43
3	B	802	H4B	C4-C4A-N5	2.74	121.42	119.12
2	A	801	HEM	C4B-CHC-C1C	2.74	126.17	122.56
2	B	801	HEM	CMA-C3A-C4A	-2.73	124.27	128.46
2	A	801	HEM	CMA-C3A-C4A	-2.61	124.44	128.46
2	A	801	HEM	CMC-C2C-C3C	2.54	129.43	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	C3B-C2B-C1B	2.52	108.36	106.49
2	B	801	HEM	C4C-CHD-C1D	2.52	125.88	122.56
3	B	802	H4B	C2-N1-C8A	2.51	120.16	114.54
3	A	802	H4B	C2-N1-C8A	2.43	119.98	114.54
2	B	801	HEM	CAD-C3D-C2D	-2.38	123.44	127.88
5	A	804	BYJ	C08-C06-N01	2.25	119.30	115.95
2	B	801	HEM	CMD-C2D-C1D	2.07	128.19	125.04
2	A	801	HEM	CHD-C1D-ND	2.02	126.62	124.43
2	B	801	HEM	C1B-NB-C4B	2.00	107.14	105.07
2	B	801	HEM	CMC-C2C-C3C	2.00	128.43	124.68

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	805	GOL	O1-C1-C2-C3
6	A	806	GOL	O1-C1-C2-C3
6	A	806	GOL	C1-C2-C3-O3
6	B	804	GOL	O1-C1-C2-C3
6	B	805	GOL	O1-C1-C2-C3
6	A	806	GOL	O1-C1-C2-O2
6	B	804	GOL	O1-C1-C2-O2
2	A	801	HEM	C4D-C3D-CAD-CBD
5	A	804	BYJ	C15-C17-C18-C19
6	A	805	GOL	O1-C1-C2-O2
6	A	806	GOL	O2-C2-C3-O3
6	B	805	GOL	O1-C1-C2-O2
2	A	801	HEM	C2D-C3D-CAD-CBD
5	B	803	BYJ	C06-C08-C09-C11
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C2A-CAA-CBA-CGA
5	A	804	BYJ	C14-C15-C17-C18
5	A	804	BYJ	C16-C15-C17-C18
5	B	803	BYJ	C14-C15-C17-C18
5	B	803	BYJ	C16-C15-C17-C18
2	B	801	HEM	C4B-C3B-CAB-CBB
2	A	801	HEM	C3D-CAD-CBD-CGD

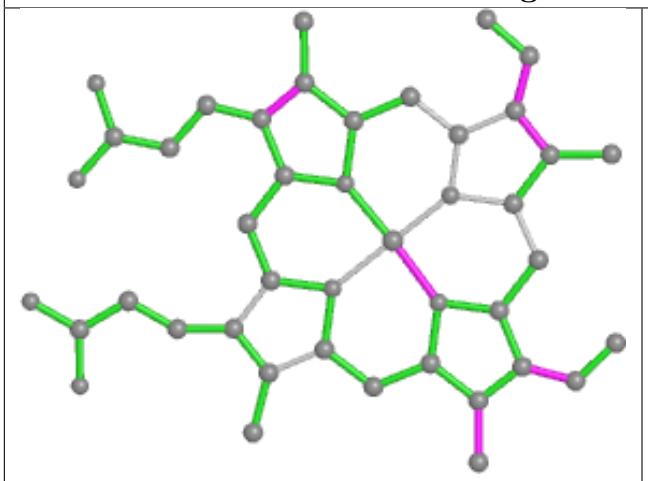
There are no ring outliers.

6 monomers are involved in 10 short contacts:

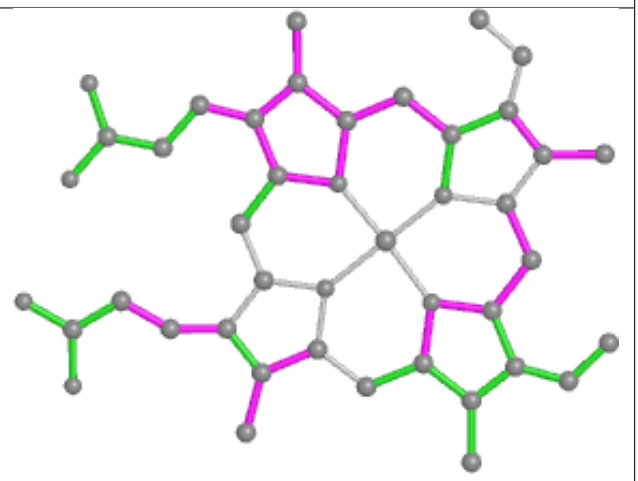
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	2	0
5	A	804	BYJ	3	0
6	A	805	GOL	1	0
6	B	804	GOL	1	0
5	B	803	BYJ	2	0
2	A	801	HEM	4	0

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.

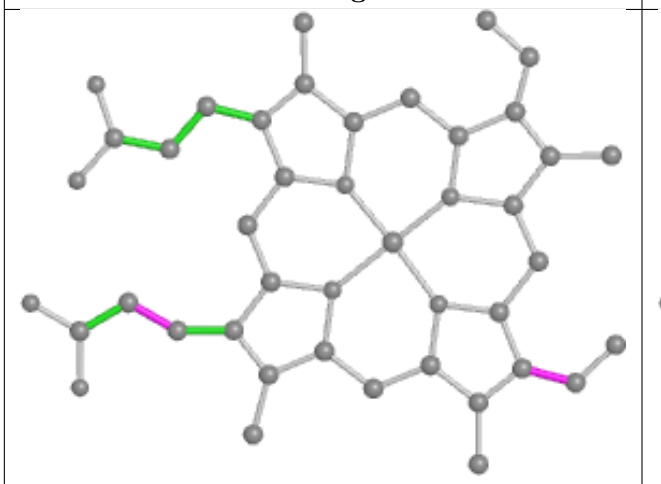
Ligand HEM B 801



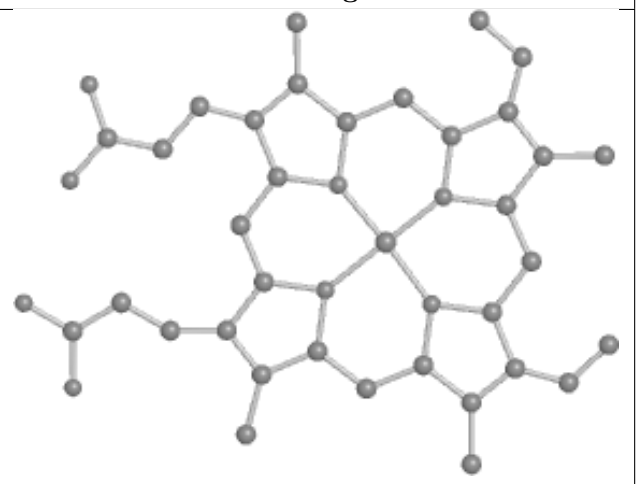
Bond lengths



Bond angles

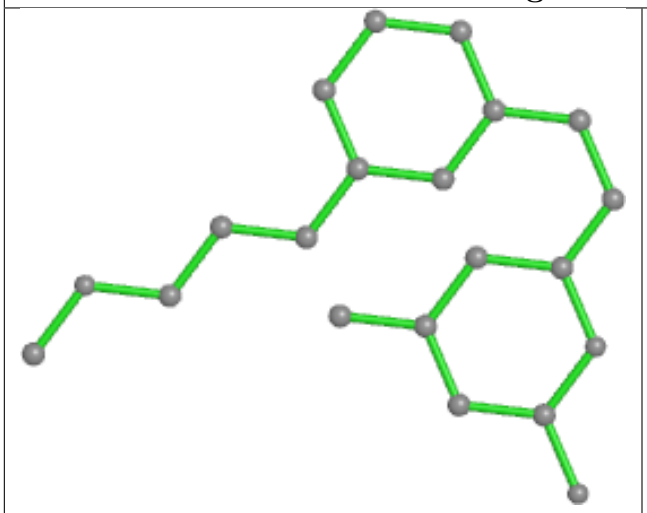


Torsions

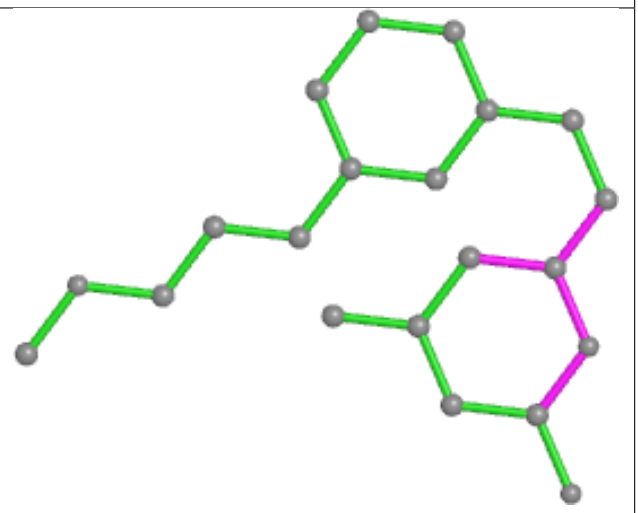


Rings

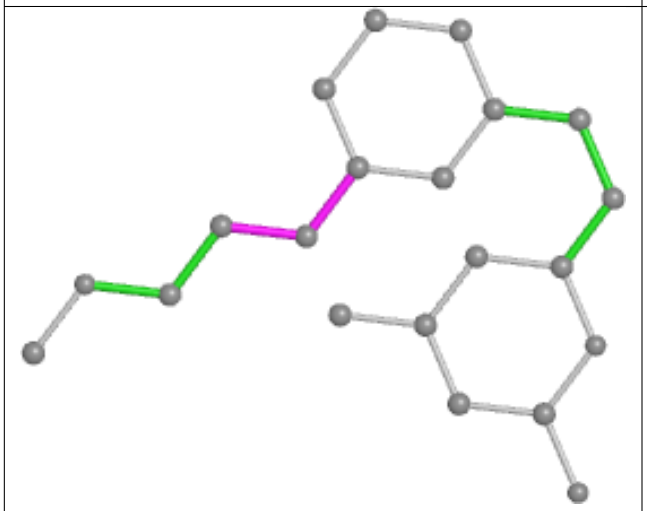
Ligand BYJ A 804



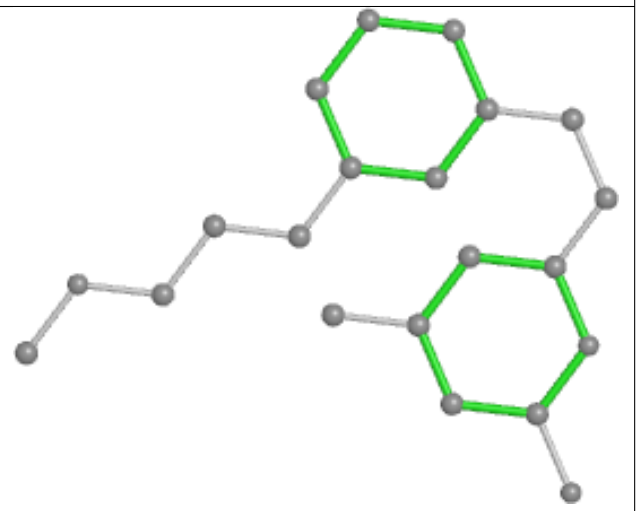
Bond lengths



Bond angles

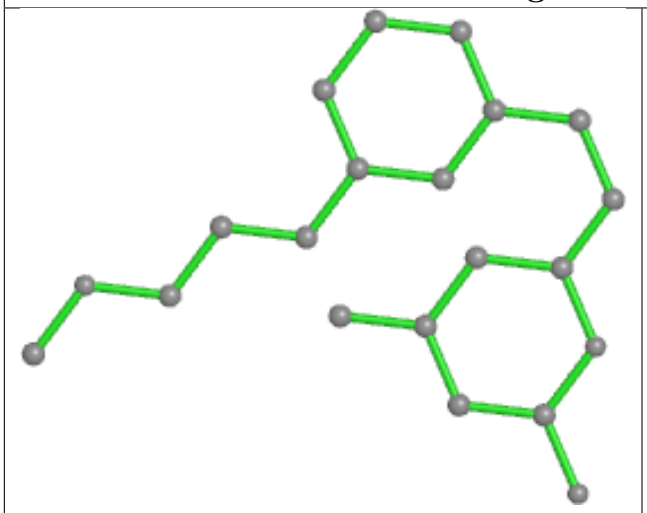


Torsions

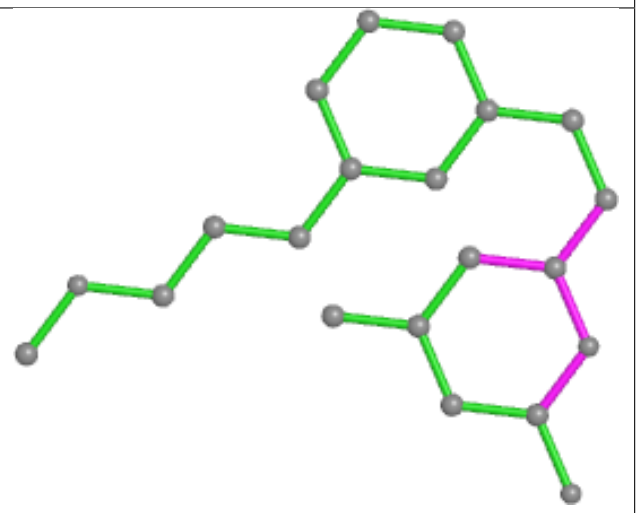


Rings

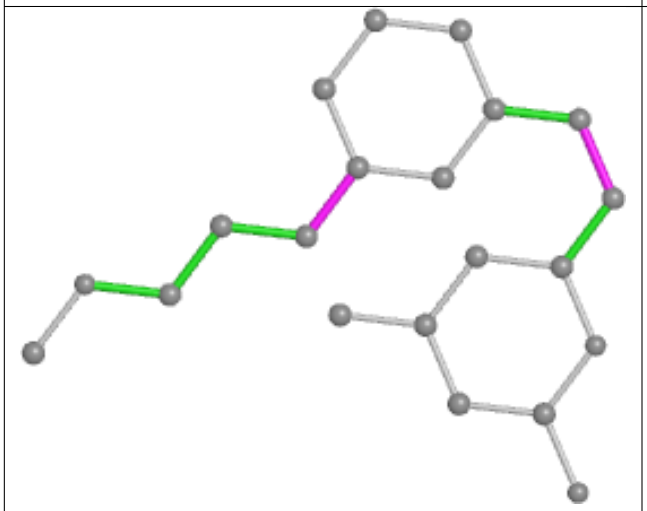
Ligand BYJ B 803



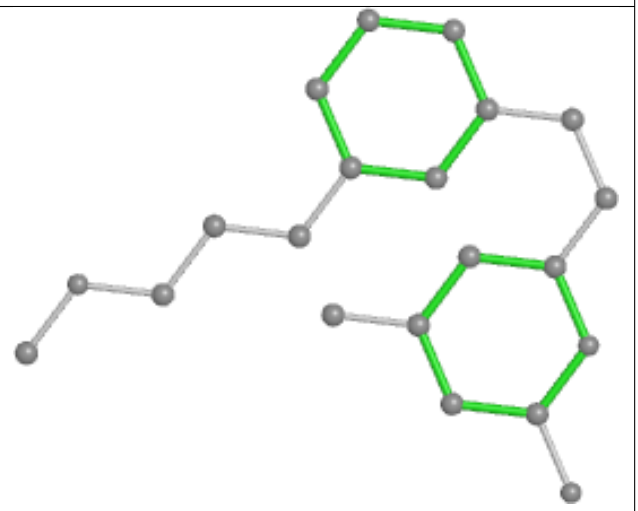
Bond lengths



Bond angles

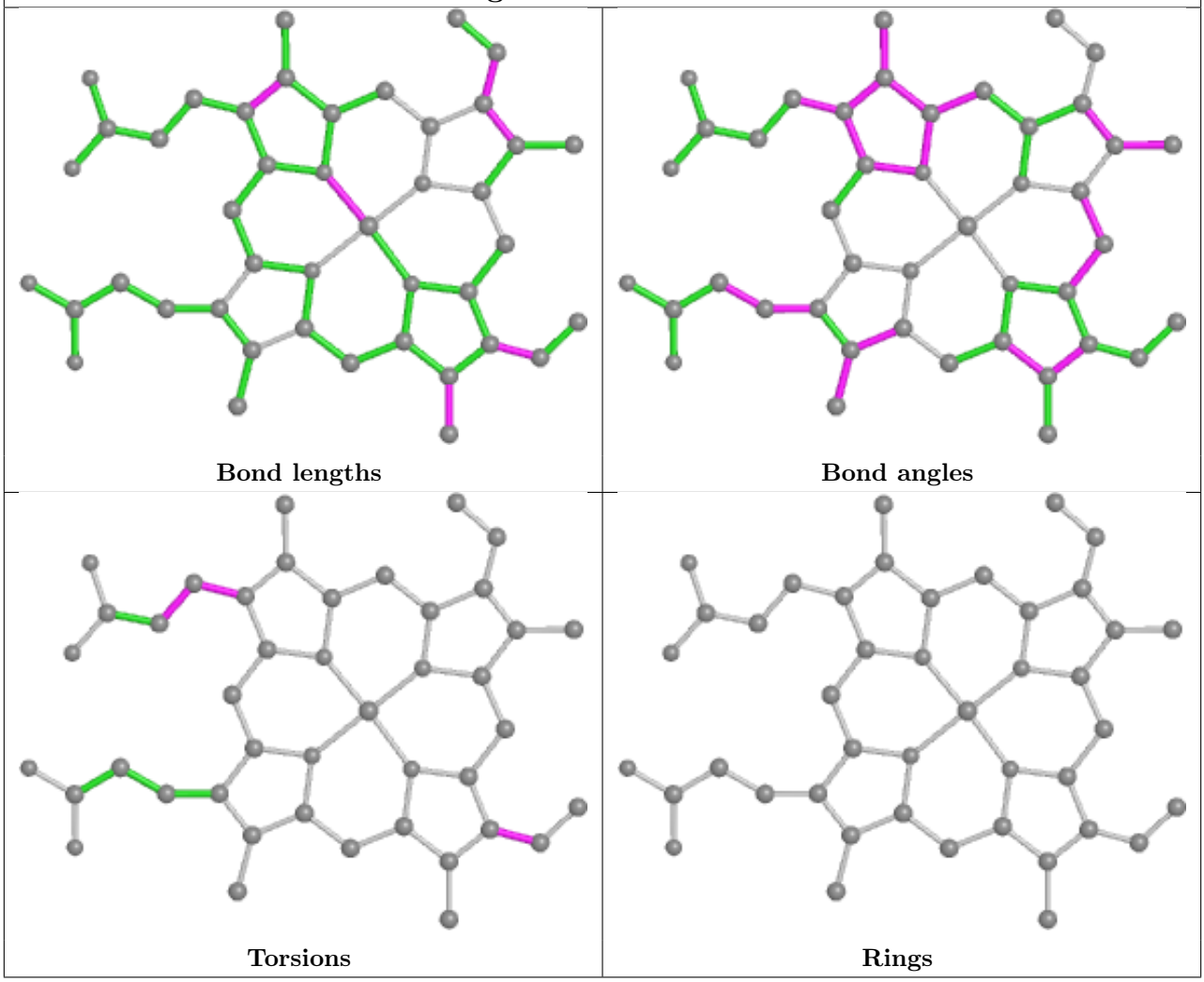


Torsions



Rings

Ligand HEM A 801



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	415/421 (98%)	0.37	34 (8%)	11	13	32, 50, 82, 132	0
1	B	409/421 (97%)	0.75	61 (14%)	2	2	34, 58, 103, 126	0
All	All	824/842 (97%)	0.56	95 (11%)	4	5	32, 53, 96, 132	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	721	TRP	7.2
1	B	720	VAL	6.7
1	B	357	ASP	5.6
1	B	716	TRP	5.4
1	A	624	ARG	5.0
1	B	360	PHE	5.0
1	B	683	TRP	4.9
1	B	493	PRO	4.7
1	A	353	VAL	4.5
1	B	719	HIS	4.4
1	A	351	GLU	4.4
1	A	305	PHE	4.3
1	B	715	PRO	4.2
1	B	686	PRO	4.0
1	B	396	THR	3.9
1	B	682	VAL	3.9
1	B	690	GLY	3.9
1	B	624	ARG	3.8
1	A	684	ILE	3.7
1	A	696	PHE	3.7
1	B	511	ILE	3.7
1	A	682	VAL	3.7
1	A	350	PRO	3.6
1	A	352	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	717	ASN	3.6
1	B	557	GLU	3.5
1	B	474	LYS	3.5
1	B	497	THR	3.5
1	B	687	PRO	3.4
1	B	496	SER	3.4
1	B	510	CYS	3.4
1	A	692	ILE	3.4
1	B	498	LEU	3.4
1	A	686	PRO	3.3
1	B	589	PHE	3.3
1	B	304	ARG	3.3
1	A	685	VAL	3.3
1	A	681	TRP	3.2
1	B	326	THR	3.1
1	A	355	THR	3.0
1	B	305	PHE	3.0
1	B	689	SER	3.0
1	B	358	GLN	3.0
1	A	689	SER	3.0
1	B	596	THR	3.0
1	B	492	GLN	2.9
1	B	621	LEU	2.9
1	A	690	GLY	2.9
1	B	490	TYR	2.9
1	B	508	GLU	2.8
1	A	395	THR	2.8
1	B	718	THR	2.8
1	B	572	VAL	2.8
1	A	687	PRO	2.7
1	B	688	MET	2.7
1	B	672	ARG	2.7
1	B	395	THR	2.7
1	B	685	VAL	2.7
1	A	327	LEU	2.6
1	B	512	GLN	2.6
1	B	504	VAL	2.6
1	B	354	ALA	2.5
1	B	374	ILE	2.5
1	B	397	SER	2.5
1	B	571	ALA	2.5
1	B	673	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	635	LEU	2.5
1	A	572	VAL	2.5
1	B	320	THR	2.4
1	A	304	ARG	2.4
1	B	394	ASP	2.4
1	A	356	LYS	2.4
1	A	620	ASN	2.4
1	B	494	ASP	2.3
1	A	683	TRP	2.3
1	A	700	MET	2.2
1	B	356	LYS	2.2
1	B	684	ILE	2.2
1	A	302	CYS	2.2
1	A	357	ASP	2.2
1	B	709	PHE	2.2
1	B	420	CYS	2.2
1	B	495	GLY	2.2
1	B	375	LYS	2.1
1	B	359	LEU	2.1
1	A	360	PHE	2.1
1	A	589	PHE	2.1
1	A	396	THR	2.1
1	A	498	LEU	2.1
1	B	380	LYS	2.1
1	A	596	THR	2.0
1	B	393	ILE	2.0
1	B	516	LYS	2.0
1	A	688	MET	2.0
1	A	420	CYS	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)

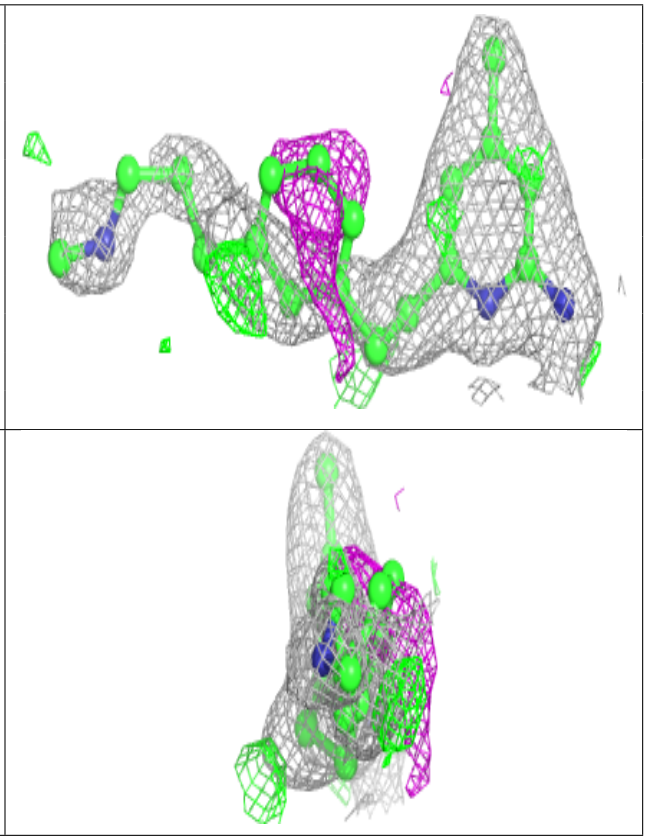
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	804	6/6	0.66	0.23	82,92,95,96	0
6	GOL	B	805	6/6	0.74	0.20	59,70,73,74	0
6	GOL	A	805	6/6	0.81	0.16	78,79,81,84	0
6	GOL	A	806	6/6	0.90	0.16	62,72,80,81	0
5	BYJ	A	804	21/21	0.91	0.28	34,68,95,101	0
5	BYJ	B	803	21/21	0.95	0.28	31,67,105,110	0
3	H4B	A	802	17/17	0.97	0.16	36,41,48,48	0
3	H4B	B	802	17/17	0.97	0.17	38,42,56,61	0
2	HEM	A	801	43/43	0.98	0.18	27,38,53,61	0
2	HEM	B	801	43/43	0.98	0.21	33,44,61,70	0
4	ZN	A	803	1/1	1.00	0.10	42,42,42,42	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.

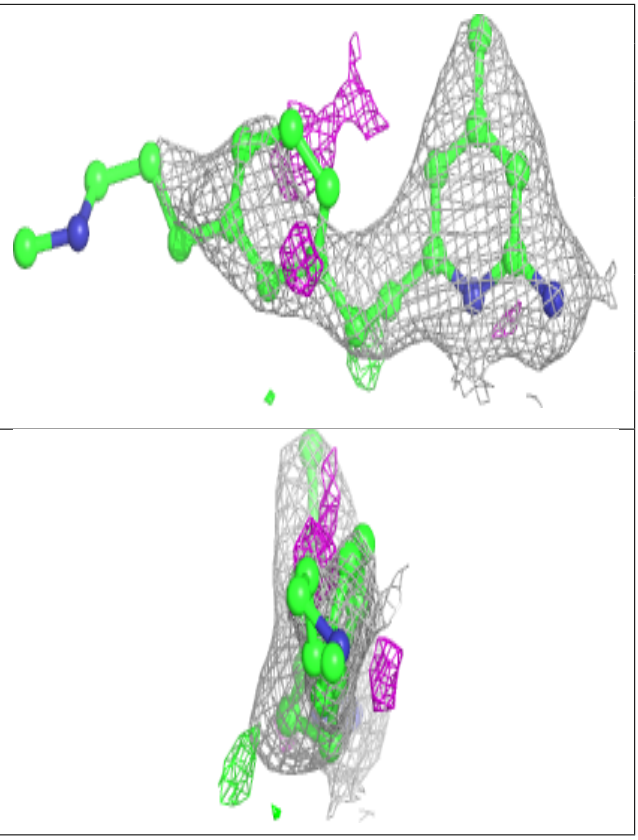
Electron density around BYJ A 804:

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



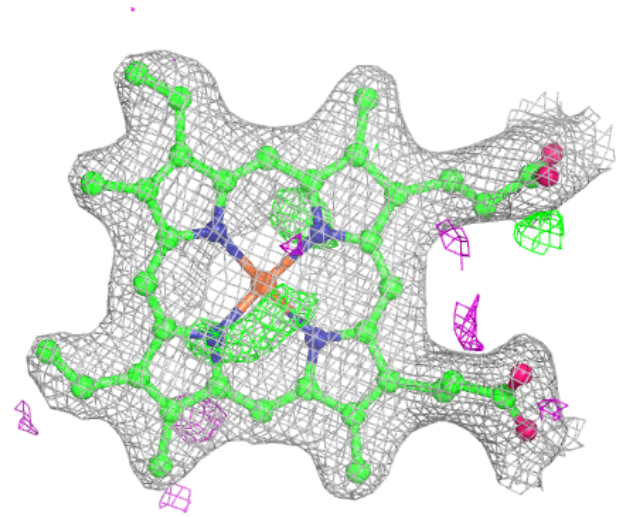
Electron density around BYJ B 803:

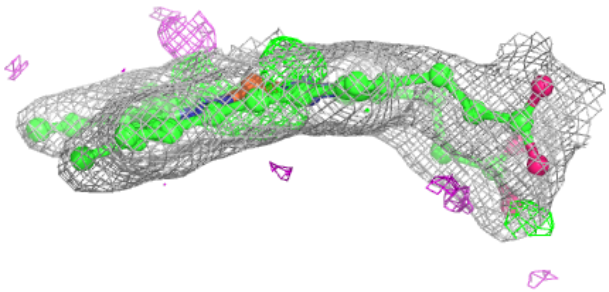
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

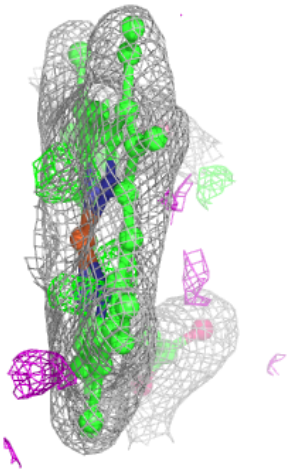


Electron density around HEM A 801:

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

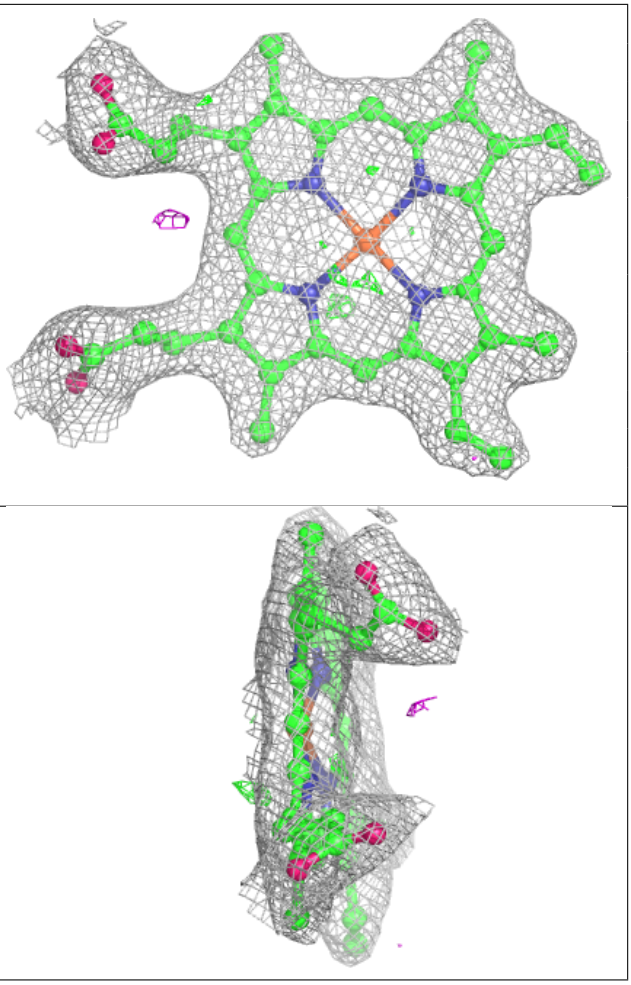






Electron density around HEM B 801:

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.