



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:42 pm BST

PDB ID : 4JSJ
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(((5-(((3-fluorophenethyl)amino)methyl)pyridin-3-yl)oxy)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-03-22
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

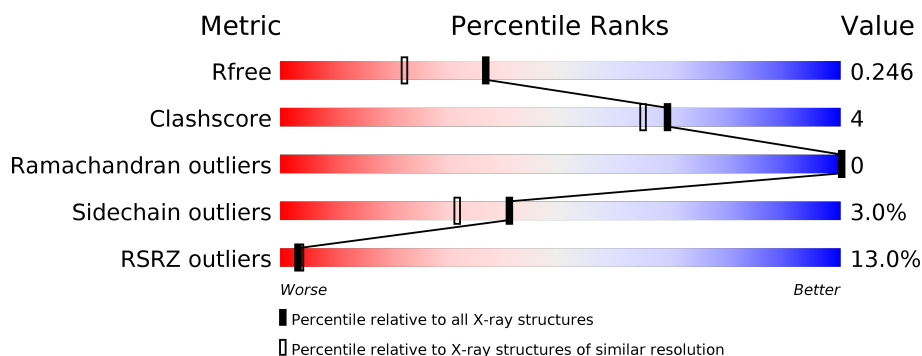
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>15%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>••</div> </div> </div>
1	B	422	<div> <div>10%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7237 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
1	A	407	Total	C	N	O	S	0	3	0
			3328	2131	567	609	21			
1	B	411	Total	C	N	O	S	3	4	0
			3360	2150	574	614	22			

- 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
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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- [illegible]

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

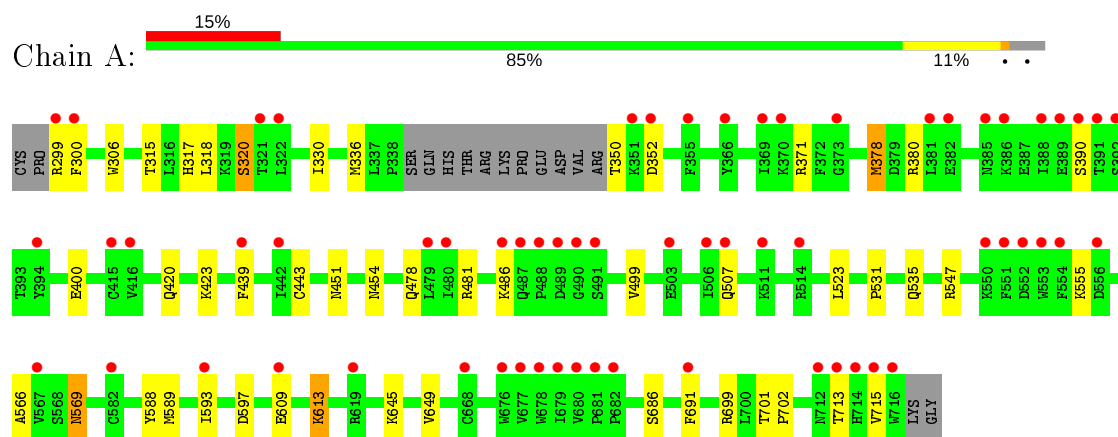
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	149	Total O 149 149	0	0
7	B	217	Total O 217 217	0	0

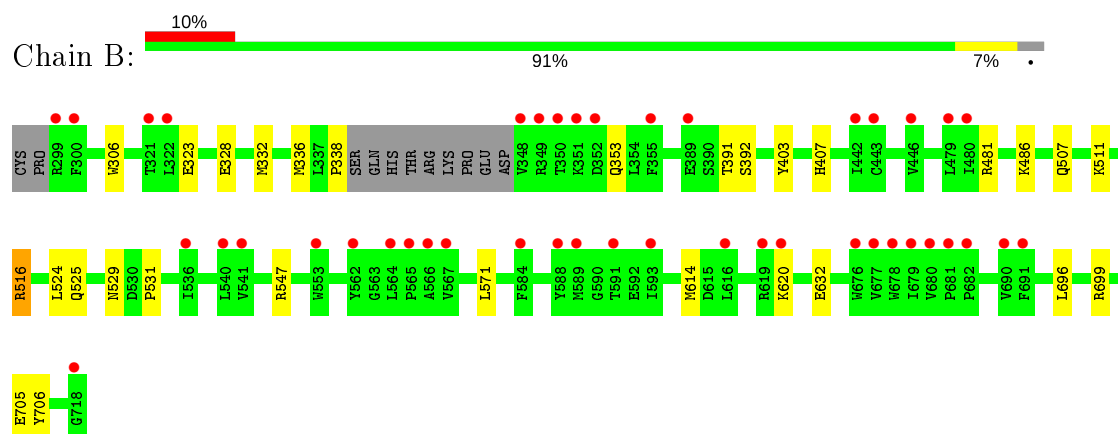
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: Nitric oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.77Å 111.28Å 164.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.80 – 1.92 43.80 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.80-1.92) 99.0 (43.80-1.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.225 0.211 , 0.246	Depositor DCC
R_{free} test set	3626 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.844	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7237	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, QJ7, H4B, ACT

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	0.65	0/3430	0.69	0/4655
1	B	0.76	0/3465	0.71	0/4697
All	All	0.71	0/6895	0.70	0/9352

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 ⓘ

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	3328	0	3240	28	0
1	B	3360	0	3280	17	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	27	0	23	2	0
5	B	27	0	23	3	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	149	0	0	3	0
7	B	217	0	0	2	0
All	All	7237	0	6662	50	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 (50) 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:HMC2	2:A:801:HEM:HBC2	1.60	0.82
1:A:701[B]:THR:HG22	7:A:920:HOH:O	1.81	0.78
1:B:332:MET:CE	1:B:338:PRO:HB3	2.18	0.74
1:A:535:GLN:HG2	7:A:1039:HOH:O	1.88	0.74
1:A:317:HIS:O	1:A:320:SER:HB3	1.88	0.73
1:B:699:ARG:NH2	1:B:705:GLU:OE1	2.22	0.73
1:A:300:PHE:HD2	1:A:315:THR:HG22	1.61	0.65
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.33	0.64
1:A:380:ARG:HD3	1:A:400:GLU:OE1	1.99	0.62
1:B:516:ARG:HD2	7:B:949:HOH:O	1.98	0.62
1:B:332:MET:HE3	1:B:338:PRO:HB3	1.80	0.62
1:A:378:MET:CE	1:A:378:MET:HA	2.33	0.59
1:A:486:LYS:HE2	1:A:499:VAL:HG11	1.84	0.58
1:B:511:LYS:HE2	7:B:1090:HOH:O	2.04	0.56
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.88	0.54
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.89	0.54
2:B:801:HEM:CBA	5:B:803:QJ7:H17	2.39	0.52
1:A:378:MET:HA	1:A:378:MET:HE2	1.91	0.52
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.92	0.51
1:A:609:GLU:O	1:A:613:LYS:HG2	2.10	0.51
1:A:701[B]:THR:HG23	1:A:702:PRO:HA	1.93	0.51
1:B:391:THR:O	1:B:392:SER:HB2	2.12	0.50
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.94	0.48
2:A:801:HEM:CMC	2:A:801:HEM:HBC2	2.36	0.48
2:B:801:HEM:HBA2	5:B:803:QJ7:H17	1.95	0.48
2:A:801:HEM:CBA	5:A:804:QJ7:H17	2.43	0.48
1:B:328:GLU:H	1:B:328:GLU:CD	2.18	0.47
1:B:525:GLN:HG3	1:B:529:ASN:O	2.15	0.46
2:B:801:HEM:HBC2	2:B:801:HEM:CMC	2.46	0.45
1:A:306:TRP:NE1	1:B:336:MET:HG3	2.32	0.44
1:A:451:ASN:HB3	1:A:454:ASN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:ILE:HA	1:A:597:ASP:HB2	2.00	0.44
2:A:801:HEM:HBA1	5:A:804:QJ7:H17	2.00	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.06	0.43
1:A:589:MET:HA	1:A:649:VAL:O	2.18	0.42
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.54	0.42
1:B:332:MET:HE2	1:B:338:PRO:HB3	1.97	0.42
1:B:614:MET:CE	1:B:632:GLU:HG3	2.50	0.42
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.85	0.42
1:B:706:TYR:OH	2:B:801:HEM:O1D	2.24	0.41
1:A:420:GLN:OE1	1:A:423:LYS:HE2	2.21	0.41
1:A:701[B]:THR:HG21	7:A:952:HOH:O	2.18	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.55	0.41
1:B:571:LEU:HD23	1:B:571:LEU:C	2.41	0.41
1:B:524:LEU:O	1:B:531:PRO:HA	2.21	0.40
1:A:478:GLN:HA	1:A:566:ALA:O	2.22	0.40
2:B:801:HEM:C1C	5:B:803:QJ7:H24	2.56	0.40
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.37	0.40
1:A:569:ASN:H	1:A:569:ASN:HD22	1.70	0.40
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.15	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	406/422 (96%)	393 (97%)	13 (3%)	0	100	100
1	B	411/422 (97%)	402 (98%)	9 (2%)	0	100	100
All	All	817/844 (97%)	795 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/377 (97%)	352 (96%)	14 (4%)	33	22
1	B	370/377 (98%)	362 (98%)	8 (2%)	52	45
All	All	736/754 (98%)	714 (97%)	22 (3%)	41	31

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	SER
1	A	350	THR
1	A	352	ASP
1	A	378	MET
1	A	390	SER
1	A	507	GLN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	613	LYS
1	A	645	LYS
1	A	699	ARG
1	A	713	THR
1	A	715	VAL
1	B	323	GLU
1	B	353	GLN
1	B	481	ARG
1	B	486	LYS
1	B	507	GLN
1	B	516	ARG
1	B	547	ARG
1	B	620	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
2	HEM	A	801	1	27,50,50	2.18	7 (25%)	17,82,82	2.34	6 (35%)
2	HEM	B	801	1	27,50,50	2.10	9 (33%)	17,82,82	2.51	6 (35%)
5	QJ7	B	803	-	29,29,29	0.99	1 (3%)	37,38,38	1.88	9 (24%)
4	ACT	A	803	-	1,3,3	1.49	0	0,3,3	0.00	-
3	H4B	B	802	-	16,18,18	1.20	2 (12%)	11,26,26	2.66	3 (27%)
3	H4B	A	802	-	16,18,18	0.97	2 (12%)	11,26,26	3.06	7 (63%)
4	ACT	B	804	-	1,3,3	1.80	0	0,3,3	0.00	-
5	QJ7	A	804	-	29,29,29	0.94	1 (3%)	37,38,38	1.56	4 (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
2	HEM	A	801	1	-	0/6/54/54	-
2	HEM	B	801	1	-	0/6/54/54	-
5	QJ7	B	803	-	-	1/12/12/12	0/3/3/3
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
5	QJ7	A	804	-	-	1/12/12/12	0/3/3/3
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C2B	-5.40	1.32	1.40
2	A	801	HEM	C3D-C2D	4.74	1.51	1.37
2	B	801	HEM	C3D-C2D	4.58	1.51	1.37
2	B	801	HEM	C3C-C2C	-4.32	1.34	1.40
2	B	801	HEM	C3B-C2B	-4.02	1.34	1.40
2	A	801	HEM	C3C-CAC	3.65	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.63	1.35	1.40
2	B	801	HEM	C3C-CAC	3.45	1.54	1.47
2	A	801	HEM	C3B-CAB	3.37	1.54	1.47
5	B	803	QJ7	C12-C13	3.05	1.42	1.38
3	B	802	H4B	C7-N8	2.62	1.49	1.44
5	A	804	QJ7	C12-C13	2.59	1.41	1.38
2	B	801	HEM	CMD-C2D	2.47	1.56	1.51
2	A	801	HEM	C1D-ND	2.44	1.41	1.36
2	B	801	HEM	C3B-CAB	2.39	1.52	1.47
3	B	802	H4B	C7-C6	2.37	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1D-ND	2.31	1.40	1.36
2	B	801	HEM	C4A-CHB	-2.18	1.34	1.41
3	A	802	H4B	C4A-N5	-2.14	1.33	1.38
3	A	802	H4B	C2-N2	2.11	1.38	1.33
2	A	801	HEM	CMD-C2D	2.01	1.55	1.51
2	B	801	HEM	CAD-C3D	2.00	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	H4B	C4-C4A-C8A	7.19	120.96	114.57
2	B	801	HEM	CBA-CAA-C2A	-6.99	99.60	112.49
5	B	803	QJ7	C02-N01-C06	5.85	122.53	118.10
3	A	802	H4B	C4-C4A-C8A	5.69	119.62	114.57
2	A	801	HEM	CBA-CAA-C2A	-5.68	102.02	112.49
5	B	803	QJ7	C14-C15-C16	5.06	121.59	116.71
3	A	802	H4B	C4-C4A-N5	4.54	122.94	119.12
2	A	801	HEM	CBD-CAD-C3D	-4.38	104.41	112.48
5	A	804	QJ7	C02-N01-C06	4.24	121.31	118.10
2	B	801	HEM	CBD-CAD-C3D	-4.14	104.85	112.48
3	A	802	H4B	C4-N3-C2	3.75	121.88	115.93
2	B	801	HEM	C1D-C2D-C3D	-3.62	104.48	107.00
3	B	802	H4B	C4-N3-C2	3.51	121.50	115.93
5	A	804	QJ7	C24-C23-C22	-3.40	118.87	123.29
3	A	802	H4B	N2-C2-N3	3.30	122.39	117.25
5	A	804	QJ7	C14-C15-C16	3.29	119.88	116.71
3	A	802	H4B	N3-C2-N1	-3.20	120.40	125.42
2	A	801	HEM	C1D-C2D-C3D	-2.93	104.96	107.00
3	A	802	H4B	C2-N1-C8A	2.92	121.08	114.54
2	A	801	HEM	CMC-C2C-C3C	2.86	130.02	124.68
5	B	803	QJ7	C05-C06-N01	-2.84	119.89	122.90
5	A	804	QJ7	C05-C06-N01	-2.81	119.92	122.90
5	B	803	QJ7	C24-C23-C22	-2.71	119.77	123.29
2	B	801	HEM	C4C-C3C-C2C	2.69	108.78	106.90
2	A	801	HEM	CAD-CBD-CGD	-2.52	108.44	112.67
5	B	803	QJ7	C13-C14-C15	-2.48	117.00	119.73
5	B	803	QJ7	C19-C20-C21	-2.46	107.16	112.87
5	B	803	QJ7	O09-C08-C06	2.45	116.02	109.42
3	B	802	H4B	C4A-C4-N3	-2.41	117.17	124.01
2	B	801	HEM	CMA-C3A-C4A	-2.37	124.83	128.46
2	B	801	HEM	CMB-C2B-C3B	2.31	128.99	124.68
2	A	801	HEM	C4C-C3C-C2C	2.29	108.50	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	C4A-C4-N3	-2.27	117.55	124.01
5	B	803	QJ7	F23-C23-C22	2.12	121.29	118.25
5	B	803	QJ7	C15-C17-N18	-2.12	107.30	112.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

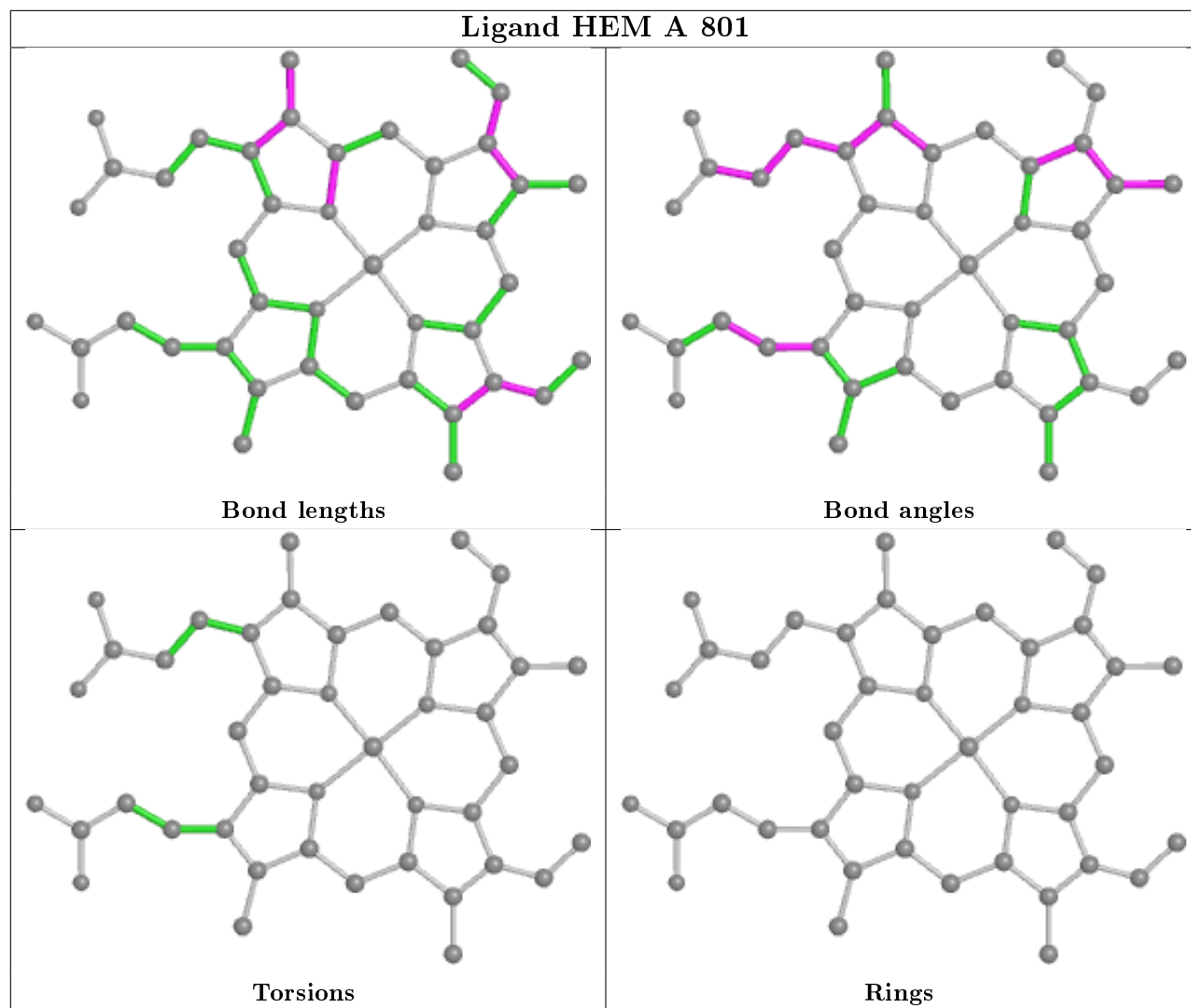
Mol	Chain	Res	Type	Atoms
5	B	803	QJ7	C15-C17-N18-C19
5	A	804	QJ7	C14-C13-O09-C08

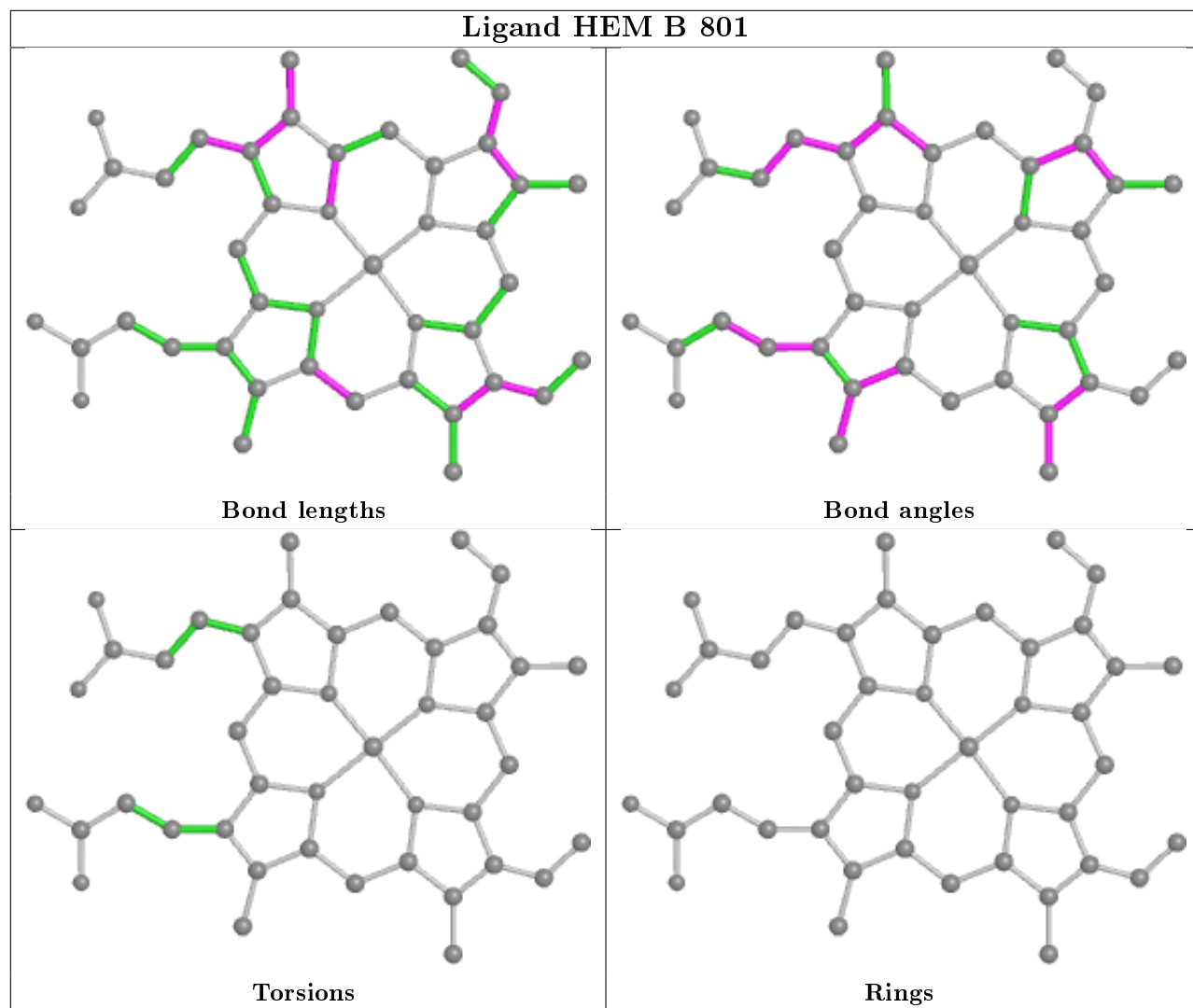
There are no ring outliers.

4 monomers are involved in 9 short contacts:

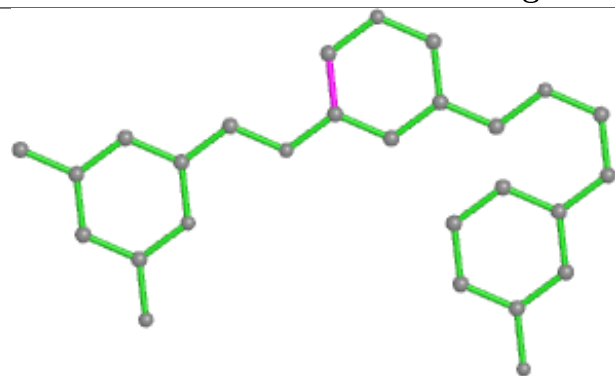
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	4	0
2	B	801	HEM	5	0
5	B	803	QJ7	3	0
5	A	804	QJ7	2	0

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

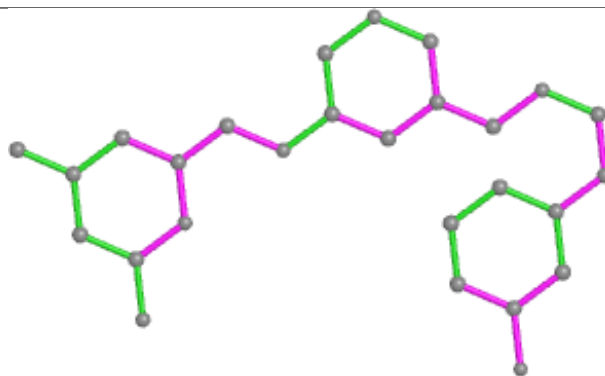




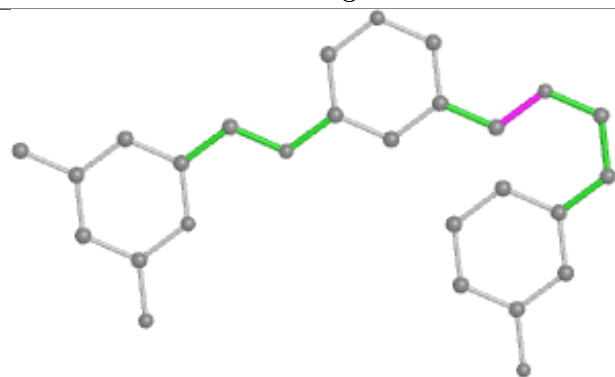
Ligand QJ7 B 803



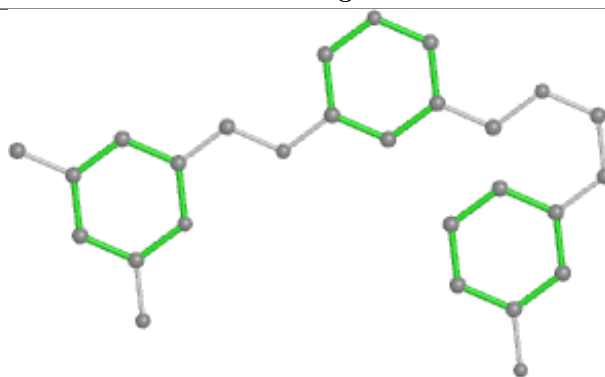
Bond lengths



Bond angles

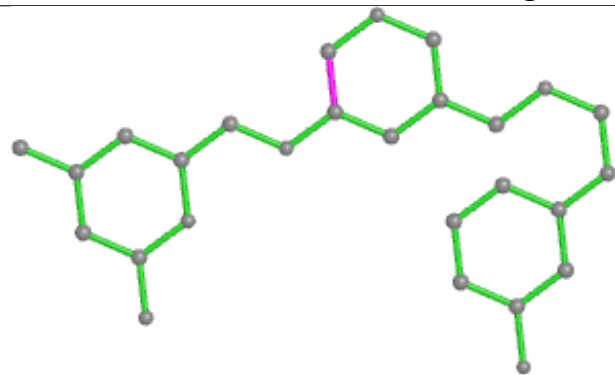


Torsions

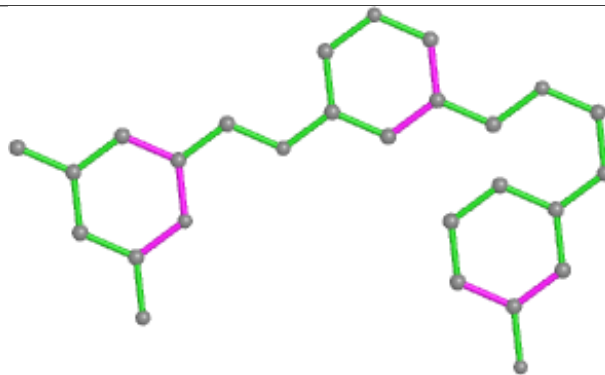


Rings

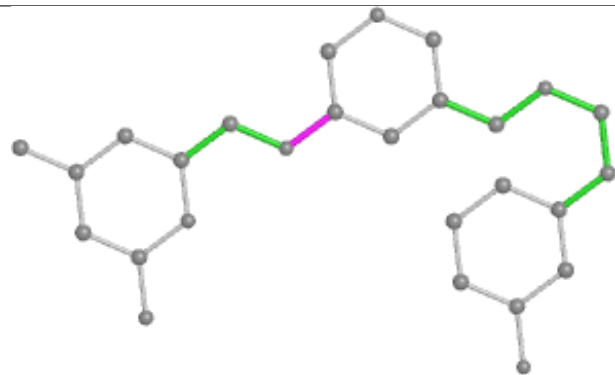
Ligand QJ7 A 804



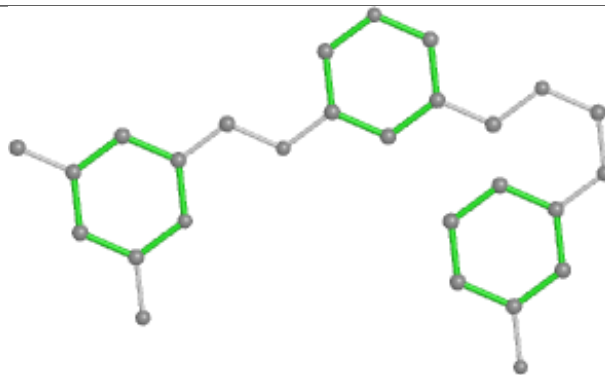
Bond lengths



Bond angles



Torsions



Rings

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, 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	407/422 (96%)	0.91	63 (15%) 2 2	27, 49, 86, 112	0
1	B	411/422 (97%)	0.62	43 (10%) 6 7	26, 39, 62, 90	0
All	All	818/844 (96%)	0.77	106 (12%) 3 3	26, 43, 82, 112	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.7
1	A	716	TRP	7.7
1	B	348	VAL	7.3
1	A	300	PHE	6.9
1	A	488	PRO	6.3
1	A	352	ASP	5.8
1	A	715	VAL	5.5
1	B	352	ASP	5.4
1	A	355	PHE	5.2
1	B	350	THR	5.1
1	B	718	GLY	5.0
1	B	619	ARG	4.8
1	A	351	LYS	4.8
1	A	322	LEU	4.5
1	A	713	THR	4.4
1	A	486	LYS	4.3
1	B	479	LEU	4.1
1	A	507	GLN	3.9
1	B	677	VAL	3.9
1	A	714	HIS	3.8
1	A	373	GLY	3.8
1	B	321	THR	3.6
1	B	567	VAL	3.6
1	A	385	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	321	THR	3.6
1	B	351	LYS	3.4
1	A	490	GLY	3.4
1	B	566	ALA	3.3
1	B	442	ILE	3.3
1	B	679	ILE	3.3
1	B	680	VAL	3.3
1	B	322	LEU	3.3
1	A	619	ARG	3.3
1	A	491	SER	3.2
1	A	678	TRP	3.2
1	A	487	GLN	3.2
1	B	443	CYS	3.2
1	A	489	ASP	3.1
1	A	386	LYS	3.1
1	B	678	TRP	3.0
1	B	564	LEU	3.0
1	A	554	PHE	3.0
1	A	567	VAL	2.9
1	B	480	ILE	2.9
1	A	299	ARG	2.9
1	B	591	THR	2.9
1	A	503	GLU	2.8
1	A	680	VAL	2.8
1	A	388	ILE	2.8
1	A	390	SER	2.8
1	A	677	VAL	2.8
1	A	391	THR	2.8
1	B	676	TRP	2.8
1	B	536	ILE	2.7
1	A	479	LEU	2.7
1	A	712	ASN	2.6
1	A	389	GLU	2.6
1	A	392	SER	2.6
1	B	349	ARG	2.6
1	A	369	ILE	2.6
1	B	446	VAL	2.6
1	A	691	PHE	2.5
1	A	668	CYS	2.5
1	A	553	TRP	2.5
1	A	609	GLU	2.4
1	B	588	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	442	ILE	2.4
1	B	620	LYS	2.4
1	B	355	PHE	2.4
1	B	682	PRO	2.4
1	A	681	PRO	2.4
1	B	540	LEU	2.4
1	A	676	TRP	2.4
1	B	691	PHE	2.3
1	B	553	TRP	2.3
1	B	616	LEU	2.3
1	B	565	PRO	2.3
1	B	681	PRO	2.3
1	A	382	GLU	2.3
1	A	682	PRO	2.3
1	B	593	ILE	2.3
1	A	415	CYS	2.3
1	B	690	VAL	2.2
1	A	366	TYR	2.2
1	A	551	PHE	2.2
1	A	381	LEU	2.1
1	A	514	ARG	2.1
1	A	556	ASP	2.1
1	B	389	GLU	2.1
1	B	299	ARG	2.1
1	B	589	MET	2.1
1	A	679	ILE	2.1
1	B	584	PHE	2.1
1	A	416	VAL	2.1
1	A	480	ILE	2.1
1	A	394	TYR	2.1
1	B	541	VAL	2.1
1	A	550	LYS	2.1
1	A	552	ASP	2.1
1	A	582	CYS	2.1
1	A	439	PHE	2.0
1	A	370	LYS	2.0
1	A	511	LYS	2.0
1	A	506	ILE	2.0
1	B	562	TYR	2.0
1	A	593	ILE	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

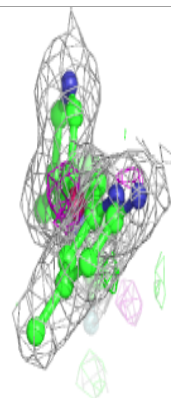
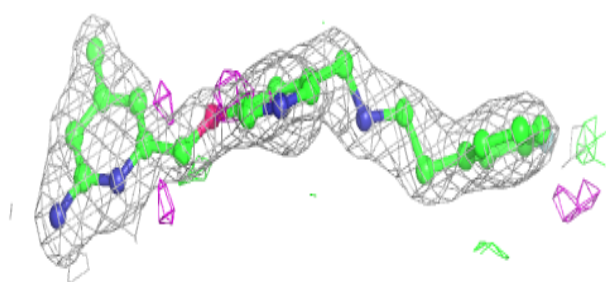
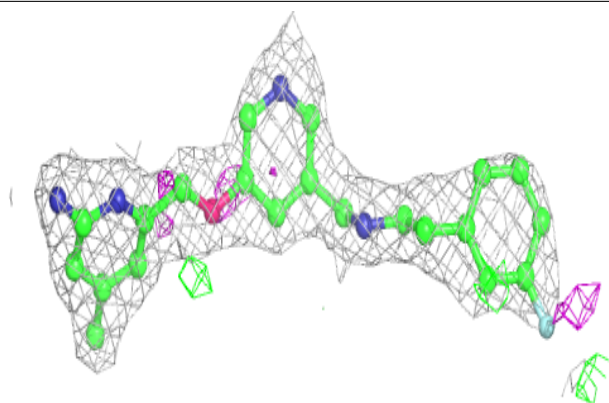
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	QJ7	B	803	27/27	0.88	0.21	31,47,63,67	0
5	QJ7	A	804	27/27	0.89	0.19	28,47,69,70	0
4	ACT	A	803	4/4	0.93	0.13	50,52,53,54	0
3	H4B	A	802	17/17	0.95	0.20	28,31,38,39	0
3	H4B	B	802	17/17	0.96	0.21	27,31,36,39	0
4	ACT	B	804	4/4	0.97	0.12	43,44,45,46	0
2	HEM	B	801	43/43	0.97	0.19	25,30,39,42	0
2	HEM	A	801	43/43	0.98	0.16	27,33,40,43	0
6	ZN	A	805	1/1	0.99	0.08	36,36,36,36	0

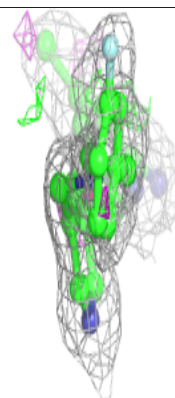
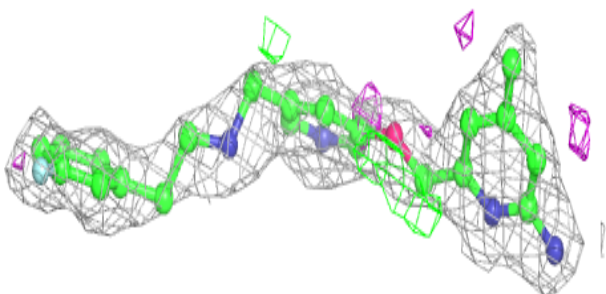
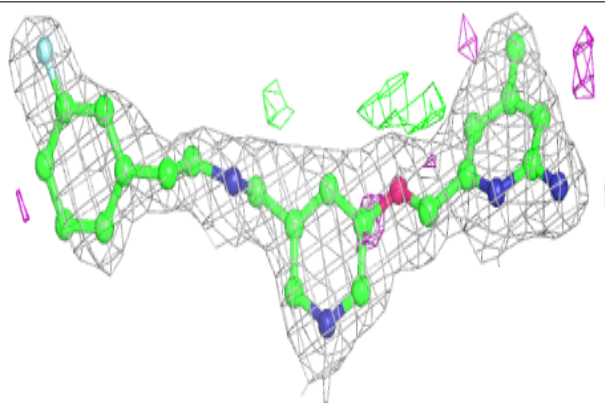
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QJ7 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)

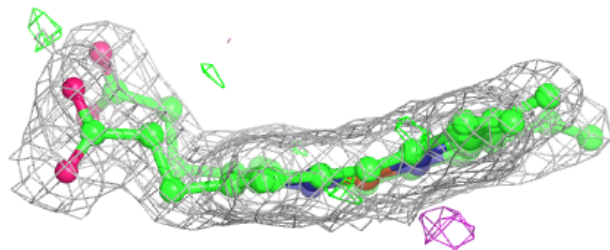
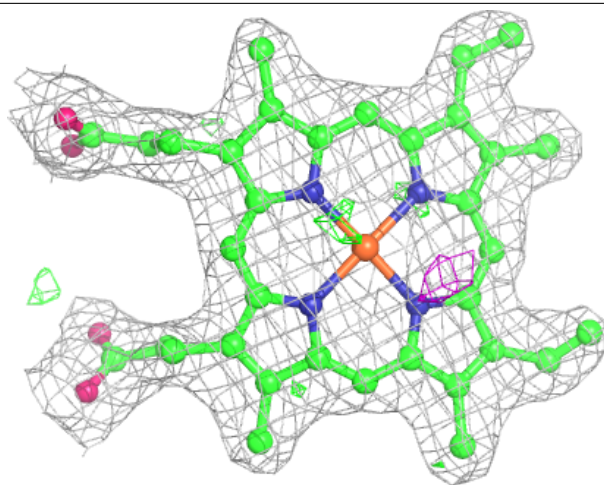
**Electron density around QJ7 A 804:**

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



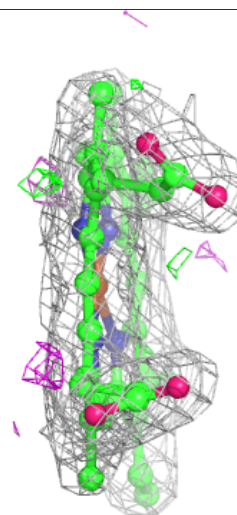
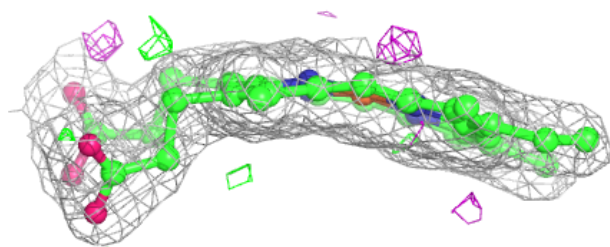
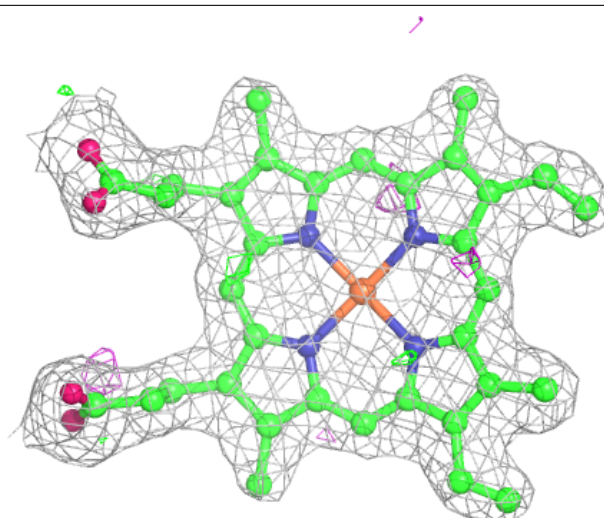
Electron density around HEM B 801:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.