



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:21 am BST

PDB ID : 4LUX
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-((((3R,5S)-5-(((6-amino-4-methylpyridin-2-yl)methoxy)methyl)pyrrolidin-3-yl)oxy)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-07-25
Resolution : 1.86 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

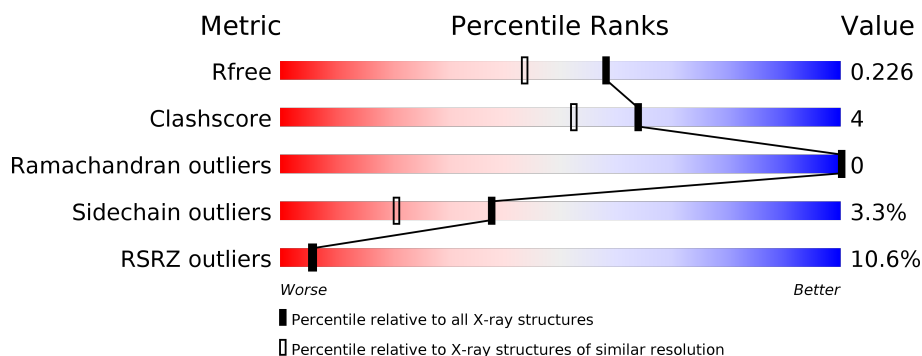
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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>14%</div> <div>87%</div> <div>7%</div> <div>• •</div> </div>
1	B	422	<div> <div>6%</div> <div>91%</div> <div>7%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7325 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	2	0
			3321	2126	567	606	22			
1	B	411	Total	C	N	O	S	0	4	0
			3360	2150	574	614	22			

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



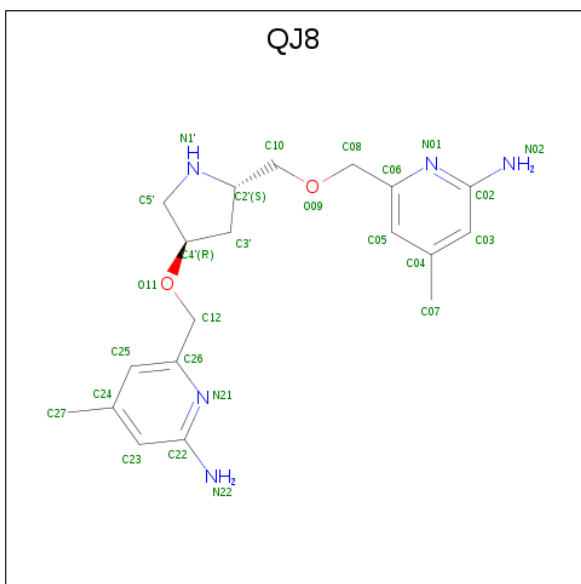
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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
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 6-({[(3R,5S)-5-{{(6-amino-4-methylpyridin-2-yl)methoxy}methyl}pyrrolidin-3-yl]oxy}methyl)-4-methylpyridin-2-amine (three-letter code: QJ8) (formula: C₁₉H₂₇N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	19	5	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			26	19	5	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

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

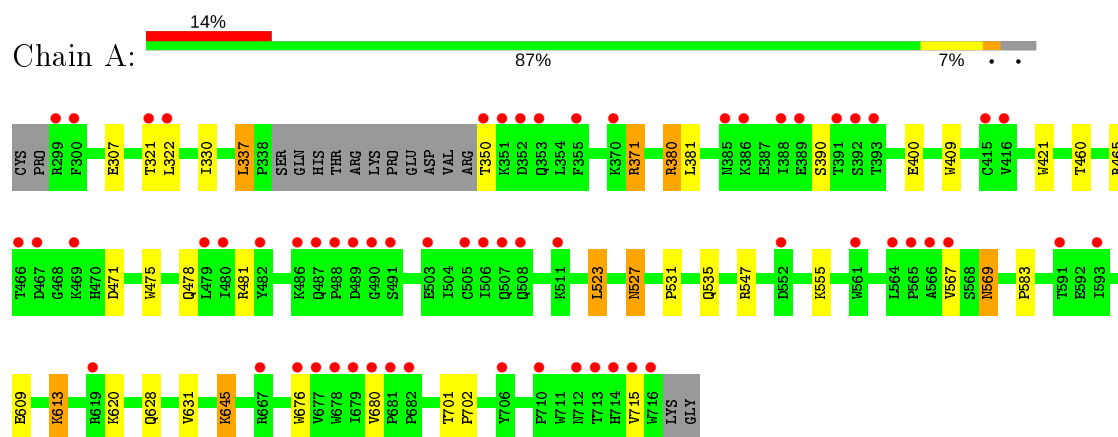
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	197	Total	O	0	0
			197	197		
7	B	266	Total	O	0	0
			266	266		

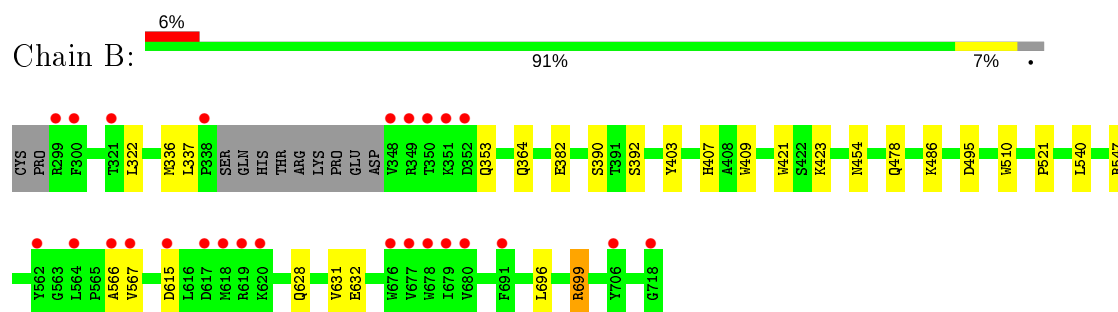
3 Residue-property plots [i](#)

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	51.84Å 110.89Å 164.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 1.86 39.01 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.01-1.86) 99.2 (39.01-1.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.212 0.195 , 0.226	Depositor DCC
R_{free} test set	3970 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	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	0.96	EDS
Total number of atoms	7325	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QJ8, HEM, ZN, 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	0.64	0/3420	0.66	0/4640
1	B	0.70	0/3465	0.68	1/4697 (0.0%)
All	All	0.67	0/6885	0.67	1/9337 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	495	ASP	CB-CG-OD1	5.05	122.84	118.30

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	3321	0	3232	30	0
1	B	3360	0	3280	18	0
2	A	43	0	30	9	0
2	B	43	0	30	6	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	26	0	27	8	0
4	B	26	0	27	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	3	1	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	197	0	0	2	0
7	B	266	0	0	5	0
All	All	7325	0	6662	57	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 (57) 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:O2A	4:A:803:QJ8:H12	1.46	1.13
1:A:535:GLN:HG2	7:A:1013:HOH:O	1.73	0.87
2:B:801:HEM:HBA2	4:B:803:QJ8:H9	1.61	0.83
1:A:567:VAL:HG22	4:A:803:QJ8:H18	1.67	0.75
2:B:801:HEM:CBA	4:B:803:QJ8:H9	2.18	0.73
2:A:801:HEM:O2A	4:A:803:QJ8:C5'	2.34	0.69
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.76	0.68
1:A:609:GLU:O	1:A:613:LYS:HG2	1.96	0.65
1:A:307:GLU:HG3	7:B:921:HOH:O	2.00	0.61
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.02	0.59
1:A:465:ARG:HD3	1:A:471:ASP:OD1	2.03	0.59
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.84	0.59
1:A:567:VAL:CG2	4:A:803:QJ8:H18	2.32	0.59
1:A:609:GLU:HG3	7:A:916:HOH:O	2.02	0.59
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.86	0.57
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.87	0.57
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.18	0.56
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.89	0.54
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.92	0.52
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.24	0.51
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.92	0.51
1:A:569:ASN:H	1:A:569:ASN:HD22	1.57	0.50
1:B:699:ARG:NH2	7:B:1152:HOH:O	2.43	0.50
2:A:801:HEM:CMC	2:A:801:HEM:HBC2	2.42	0.50
2:A:801:HEM:HMC1	2:A:801:HEM:HBC2	1.95	0.47
1:B:337:LEU:HD21	4:B:803:QJ8:H24	1.95	0.47
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.50	0.47
2:B:801:HEM:O2A	4:B:803:QJ8:H17	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.50	0.46
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.76	0.46
2:A:801:HEM:HBA1	4:A:803:QJ8:H21	1.97	0.45
2:B:801:HEM:CMC	2:B:801:HEM:HBC2	2.46	0.45
2:A:801:HEM:CBA	4:A:803:QJ8:H21	2.47	0.45
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.52	0.45
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.97	0.45
1:A:460:THR:O	1:A:583:PRO:HD2	2.16	0.44
2:B:801:HEM:HBA1	4:B:803:QJ8:H9	1.98	0.44
1:A:321:THR:HG23	1:A:322:LEU:HG	2.00	0.44
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.05	0.44
1:A:330:ILE:HD11	1:B:696:LEU:HD22	2.00	0.44
1:A:527:ASN:HA	1:A:527:ASN:HD22	1.68	0.43
1:A:337:LEU:HD21	4:A:803:QJ8:H3	2.01	0.43
2:A:801:HEM:O2D	4:A:803:QJ8:H10	2.17	0.43
1:B:322:LEU:HG	7:B:1135:HOH:O	2.18	0.43
1:A:645:LYS:HB2	1:A:645:LYS:HE3	1.47	0.43
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.52	0.42
1:B:336:MET:HE2	1:B:336:MET:HB2	2.00	0.42
1:A:631:VAL:CG1	1:B:628:GLN:HG3	2.48	0.42
1:B:382[B]:GLU:OE1	1:B:382[B]:GLU:HA	2.20	0.41
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.55	0.41
1:B:478:GLN:HA	1:B:566:ALA:O	2.20	0.41
2:A:801:HEM:HMB3	5:A:804:ACT:H2	2.01	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.41	0.41
1:B:615:ASP:HA	7:B:980:HOH:O	2.20	0.41
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.56	0.40
1:B:364:GLN:NE2	7:B:979:HOH:O	2.54	0.40
1:B:567:VAL:CG2	4:B:803:QJ8:H10	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/422 (96%)	396 (98%)	9 (2%)	0	100	100
1	B	411/422 (97%)	406 (99%)	5 (1%)	0	100	100
All	All	816/844 (97%)	802 (98%)	14 (2%)	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	365/377 (97%)	350 (96%)	15 (4%)	30	13
1	B	370/377 (98%)	361 (98%)	9 (2%)	49	33
All	All	735/754 (98%)	711 (97%)	24 (3%)	38	21

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	LEU
1	A	350	THR
1	A	371	ARG
1	A	380	ARG
1	A	381	LEU
1	A	390	SER
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	613	LYS
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	353	GLN
1	B	390	SER
1	B	392	SER

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Mol	Chain	Res	Type
1	B	423	LYS
1	B	454	ASN
1	B	486	LYS
1	B	540	LEU
1	B	547	ARG
1	B	699	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	454	ASN
1	B	507	GLN
1	B	601	ASN
1	B	605	ASN
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

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
3	H4B	A	802	-	16,18,18	0.97	1 (6%)	11,26,26	2.88	6 (54%)
5	ACT	B	804	-	1,3,3	1.69	0	0,3,3	0.00	-
5	ACT	A	804	-	1,3,3	1.47	0	0,3,3	0.00	-
4	QJ8	B	803	-	26,28,28	0.90	2 (7%)	33,38,38	2.62	15 (45%)
4	QJ8	A	803	-	26,28,28	0.84	0	33,38,38	2.06	9 (27%)
2	HEM	B	801	1	27,50,50	2.17	7 (25%)	17,82,82	2.04	4 (23%)
3	H4B	B	802	-	16,18,18	1.20	2 (12%)	11,26,26	2.54	5 (45%)
2	HEM	A	801	1	27,50,50	2.24	8 (29%)	17,82,82	2.18	7 (41%)

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
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	QJ8	B	803	-	-	7/11/20/20	0/3/3/3
4	QJ8	A	803	-	-	3/11/20/20	0/3/3/3
2	HEM	B	801	1	-	0/6/54/54	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
2	HEM	A	801	1	-	0/6/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C2B	-5.73	1.32	1.40
2	A	801	HEM	C3D-C2D	4.88	1.52	1.37
2	B	801	HEM	C3C-C2C	-4.44	1.34	1.40
2	B	801	HEM	C3C-CAC	4.40	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3D-C2D	4.37	1.50	1.37
2	B	801	HEM	C3B-C2B	-4.14	1.34	1.40
2	A	801	HEM	C3C-C2C	-4.14	1.34	1.40
2	A	801	HEM	C3C-CAC	3.64	1.55	1.47
2	B	801	HEM	CAD-C3D	3.20	1.57	1.52
2	A	801	HEM	C3B-CAB	3.13	1.54	1.47
2	B	801	HEM	C3B-CAB	2.94	1.53	1.47
2	B	801	HEM	CMD-C2D	2.90	1.57	1.51
3	B	802	H4B	C7-C6	2.68	1.54	1.52
2	A	801	HEM	CMB-C2B	2.17	1.56	1.51
3	A	802	H4B	C2-N2	2.14	1.38	1.33
2	A	801	HEM	CMA-C3A	2.10	1.56	1.51
4	B	803	QJ8	C26-N21	2.10	1.38	1.34
2	A	801	HEM	CMD-C2D	2.05	1.55	1.51
4	B	803	QJ8	C06-N01	2.02	1.38	1.34
3	B	802	H4B	C4-N3	2.02	1.36	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	QJ8	C22-N21-C26	7.00	123.41	118.10
2	B	801	HEM	CBA-CAA-C2A	-5.77	101.85	112.49
3	B	802	H4B	C4-C4A-C8A	5.65	119.59	114.57
4	B	803	QJ8	C02-N01-C06	5.55	122.31	118.10
4	B	803	QJ8	C12-C26-N21	5.03	125.90	115.71
2	A	801	HEM	CBA-CAA-C2A	-4.84	103.56	112.49
3	A	802	H4B	C4-C4A-C8A	4.62	118.67	114.57
3	A	802	H4B	C4-C4A-N5	4.43	122.84	119.12
4	B	803	QJ8	C22-N21-C26	4.40	121.44	118.10
4	B	803	QJ8	C25-C26-N21	-4.24	118.40	122.90
4	A	803	QJ8	C02-N01-C06	4.11	121.21	118.10
4	B	803	QJ8	C12-O11-C4'	3.95	120.92	113.78
4	B	803	QJ8	O11-C4'-C5'	-3.89	99.41	111.32
4	B	803	QJ8	C12-C26-C25	-3.87	115.70	121.08
3	B	802	H4B	C4-N3-C2	3.84	122.04	115.93
2	A	801	HEM	CBD-CAD-C3D	-3.83	105.42	112.48
3	A	802	H4B	N3-C2-N1	-3.79	119.47	125.42
3	A	802	H4B	C2-N1-C8A	3.55	122.50	114.54
4	B	803	QJ8	C08-C06-N01	3.51	122.83	115.71
4	A	803	QJ8	C08-O09-C10	-3.33	105.08	112.67
4	B	803	QJ8	N02-C02-N01	3.31	121.73	116.49
4	B	803	QJ8	O11-C4'-C3'	3.28	119.75	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CBD-CAD-C3D	-3.23	106.52	112.48
3	A	802	H4B	C4-N3-C2	3.16	120.95	115.93
3	B	802	H4B	N3-C2-N1	-2.90	120.87	125.42
2	A	801	HEM	CMC-C2C-C3C	2.82	129.96	124.68
4	B	803	QJ8	C08-C06-C05	-2.82	117.16	121.08
2	A	801	HEM	CAD-CBD-CGD	-2.81	107.96	112.67
4	B	803	QJ8	C05-C06-N01	-2.73	120.00	122.90
4	B	803	QJ8	N22-C22-N21	2.72	120.79	116.49
4	A	803	QJ8	C10-C2'-N1'	-2.69	106.83	111.58
4	A	803	QJ8	C25-C26-N21	-2.69	120.05	122.90
2	B	801	HEM	C1D-C2D-C3D	-2.65	105.15	107.00
4	A	803	QJ8	C3'-C4'-C5'	2.61	105.99	103.65
3	A	802	H4B	N2-C2-N3	2.57	121.24	117.25
2	A	801	HEM	C1D-C2D-C3D	-2.52	105.24	107.00
4	A	803	QJ8	C24-C25-C26	-2.49	118.69	120.32
4	A	803	QJ8	C05-C06-N01	-2.41	120.34	122.90
2	A	801	HEM	CMA-C3A-C4A	-2.34	124.87	128.46
2	B	801	HEM	CMA-C3A-C4A	-2.19	125.10	128.46
3	B	802	H4B	C4A-C4-N3	-2.17	117.85	124.01
4	B	803	QJ8	C27-C24-C25	-2.16	117.74	120.94
2	A	801	HEM	C4C-C3C-C2C	2.14	108.39	106.90
4	B	803	QJ8	C24-C25-C26	2.12	121.71	120.32
3	B	802	H4B	C2-N1-C8A	2.09	119.23	114.54
4	A	803	QJ8	N22-C22-N21	2.03	119.70	116.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

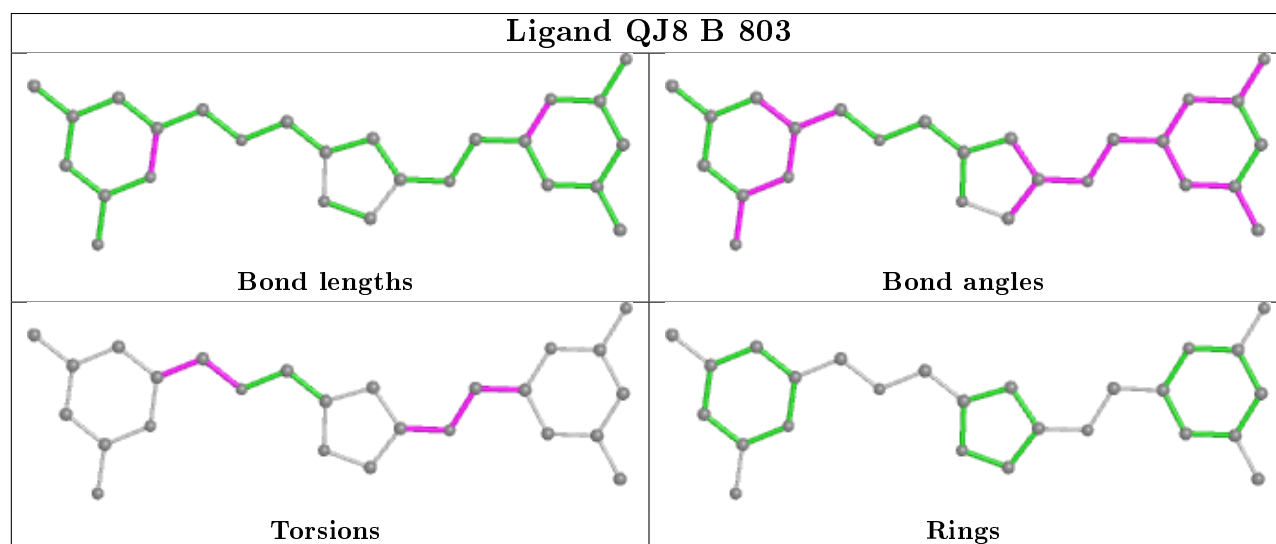
Mol	Chain	Res	Type	Atoms
4	B	803	QJ8	C3'-C4'-O11-C12
4	A	803	QJ8	C2'-C10-O09-C08
4	B	803	QJ8	C06-C08-O09-C10
4	A	803	QJ8	C26-C12-O11-C4'
4	B	803	QJ8	C26-C12-O11-C4'
4	A	803	QJ8	C06-C08-O09-C10
4	B	803	QJ8	N01-C06-C08-O09
4	B	803	QJ8	C05-C06-C08-O09
4	B	803	QJ8	O11-C12-C26-C25
4	B	803	QJ8	O11-C12-C26-N21

There are no ring outliers.

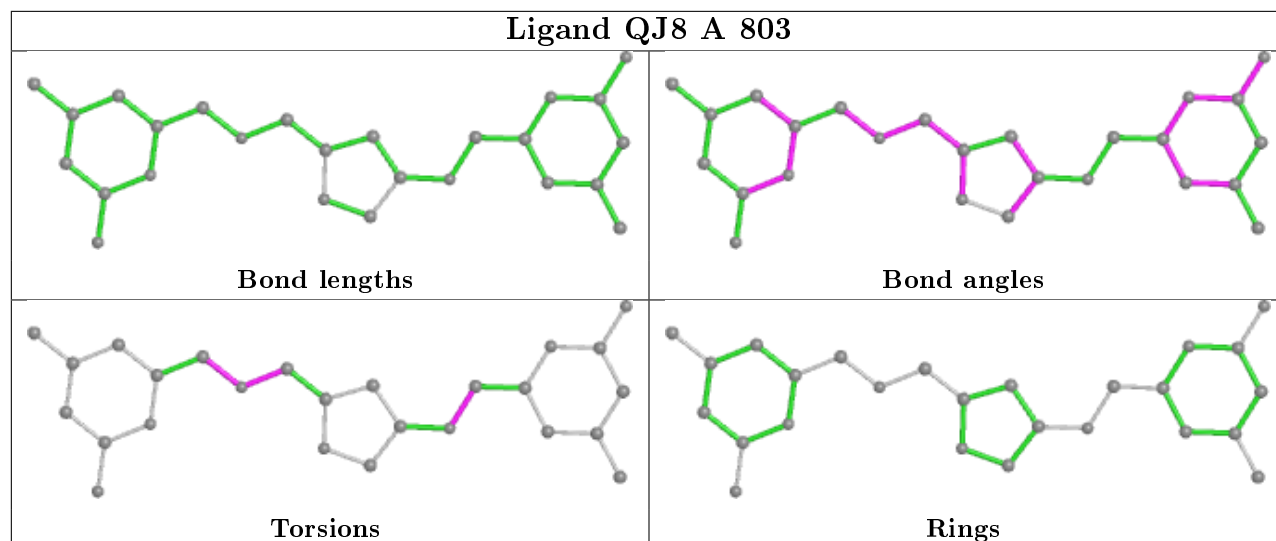
5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	ACT	1	0
4	B	803	QJ8	6	0
4	A	803	QJ8	8	0
2	B	801	HEM	6	0
2	A	801	HEM	9	0

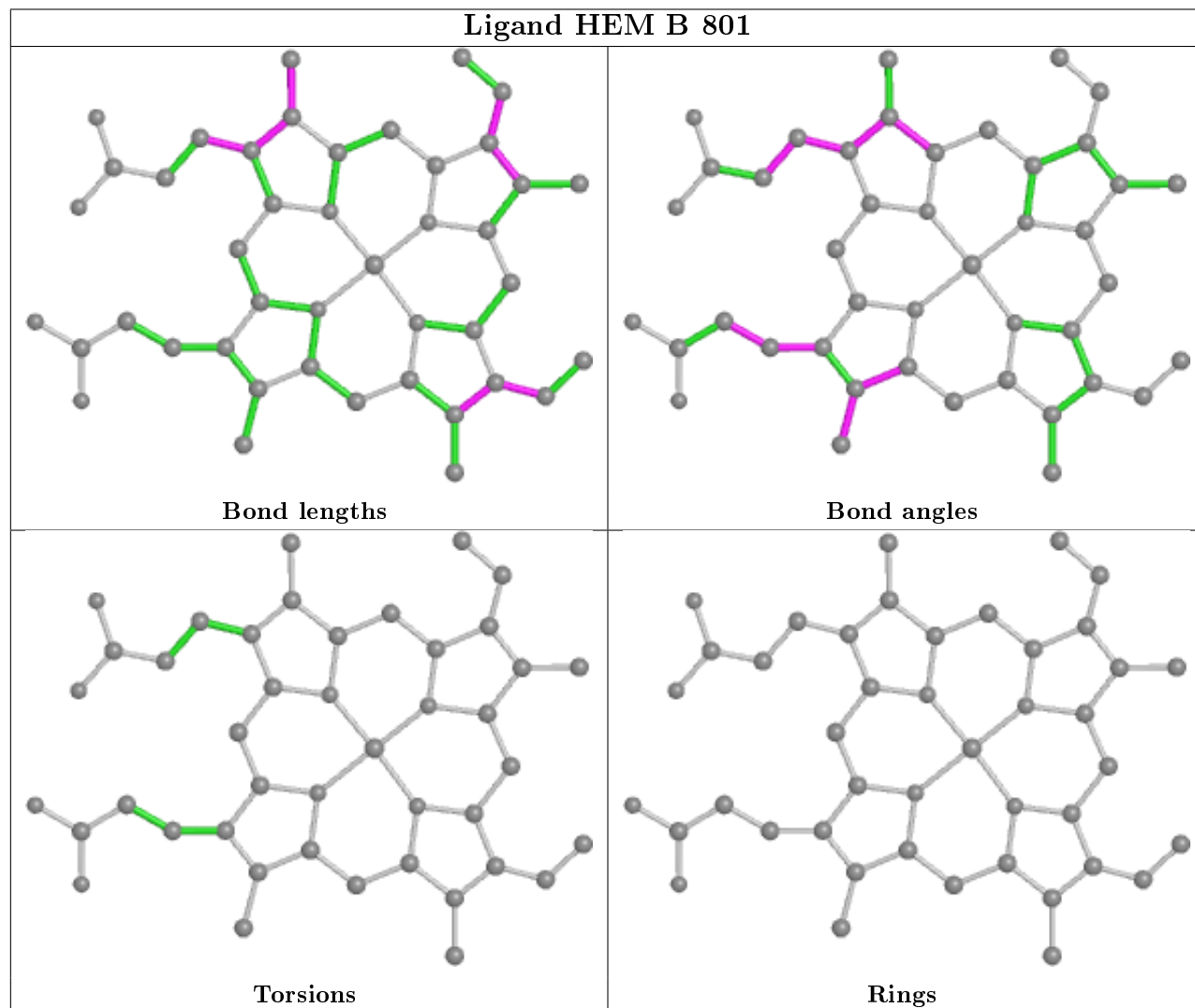
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

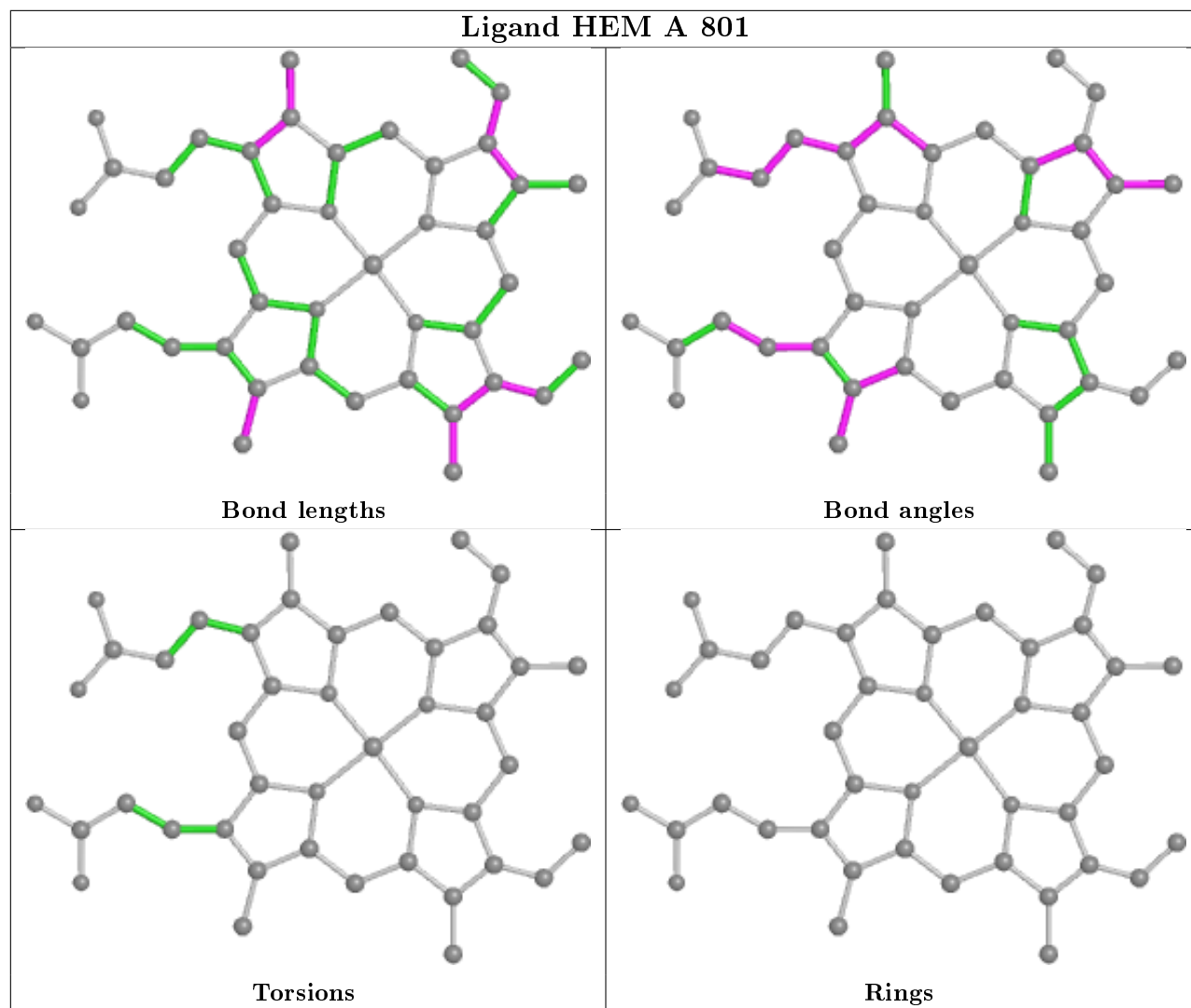


Ligand QJ8 A 803



Ligand HEM B 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 ⓘ

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%)	0.72	61 (14%) 2 2	22, 42, 75, 94	0
1	B	411/422 (97%)	0.25	26 (6%) 20 19	22, 33, 55, 84	0
All	All	818/844 (96%)	0.48	87 (10%) 6 6	22, 37, 70, 94	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	7.9
1	A	488	PRO	7.7
1	B	348	VAL	7.0
1	B	718	GLY	7.0
1	A	715	VAL	6.9
1	B	300	PHE	6.7
1	B	350	THR	6.1
1	A	350	THR	6.1
1	A	351	LYS	5.9
1	A	352	ASP	5.4
1	A	355	PHE	5.1
1	A	486	LYS	4.6
1	A	490	GLY	4.6
1	A	300	PHE	4.3
1	B	619	ARG	4.1
1	A	489	ASP	3.9
1	A	507	GLN	3.8
1	A	299	ARG	3.7
1	A	392	SER	3.6
1	A	491	SER	3.6
1	B	620	LYS	3.4
1	A	680	VAL	3.4
1	A	678	TRP	3.4
1	B	352	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	714	HIS	3.3
1	A	321	THR	3.3
1	A	679	ILE	3.2
1	B	677	VAL	3.2
1	A	676	TRP	3.2
1	A	706	TYR	3.2
1	A	480	ILE	3.2
1	A	503	GLU	3.1
1	A	322	LEU	3.1
1	A	619	ARG	3.1
1	A	469	LYS	3.1
1	B	321	THR	3.1
1	A	386	LYS	3.1
1	A	487	GLN	3.0
1	A	567	VAL	3.0
1	A	677	VAL	3.0
1	A	712	ASN	2.9
1	A	561	TRP	2.9
1	A	388	ILE	2.9
1	A	479	LEU	2.8
1	A	370	LYS	2.8
1	A	353	GLN	2.8
1	A	713	THR	2.8
1	B	349	ARG	2.8
1	A	593	ILE	2.8
1	B	680	VAL	2.7
1	B	676	TRP	2.6
1	A	393	THR	2.6
1	A	391	THR	2.6
1	A	508	GLN	2.6
1	A	389	GLU	2.6
1	B	567	VAL	2.6
1	B	678	TRP	2.5
1	B	566	ALA	2.5
1	A	511	LYS	2.5
1	B	679	ILE	2.5
1	A	467	ASP	2.4
1	A	681	PRO	2.4
1	A	667	ARG	2.3
1	B	562	TYR	2.3
1	A	710	PRO	2.3
1	B	615	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	566	ALA	2.3
1	A	385	ASN	2.3
1	A	564	LEU	2.3
1	A	415	CYS	2.3
1	B	617	ASP	2.2
1	A	565	PRO	2.2
1	A	682	PRO	2.2
1	B	691	PHE	2.2
1	A	466	THR	2.2
1	B	618	MET	2.1
1	A	552	ASP	2.1
1	B	706	TYR	2.1
1	A	416	VAL	2.1
1	B	338	PRO	2.1
1	B	299	ARG	2.1
1	B	351	LYS	2.1
1	A	482	TYR	2.0
1	B	564	LEU	2.0
1	A	591	THR	2.0
1	A	506	ILE	2.0
1	A	505	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 carbohydrates 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(\AA^2)	Q<0.9
4	QJ8	A	803	26/26	0.86	0.24	25,49,60,62	0
4	QJ8	B	803	26/26	0.87	0.22	26,51,55,57	0

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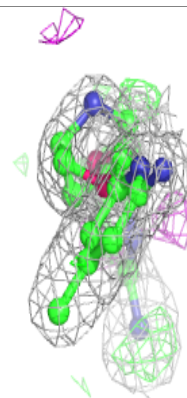
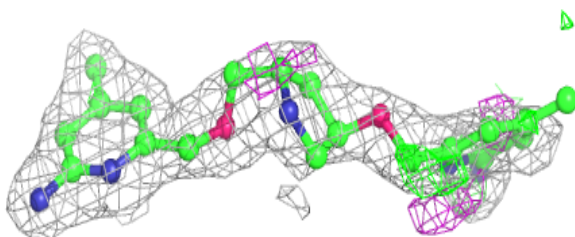
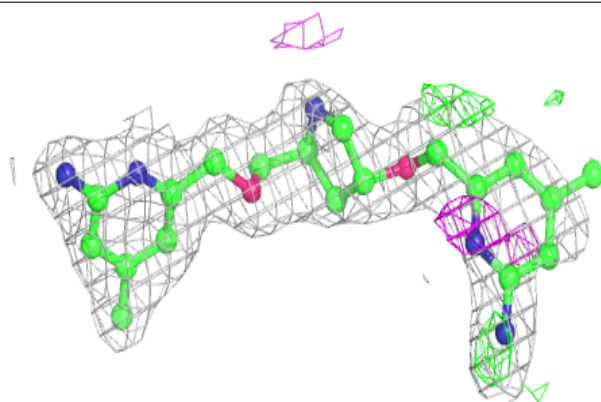
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ACT	A	804	4/4	0.96	0.11	43,45,46,47	0
3	H4B	A	802	17/17	0.96	0.15	24,26,31,33	0
5	ACT	B	804	4/4	0.96	0.10	35,36,37,38	0
3	H4B	B	802	17/17	0.96	0.18	23,27,32,33	0
2	HEM	A	801	43/43	0.97	0.20	24,27,32,34	0
2	HEM	B	801	43/43	0.98	0.18	20,24,33,35	0
6	ZN	A	805	1/1	0.99	0.09	31,31,31,31	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.

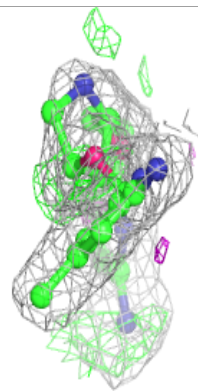
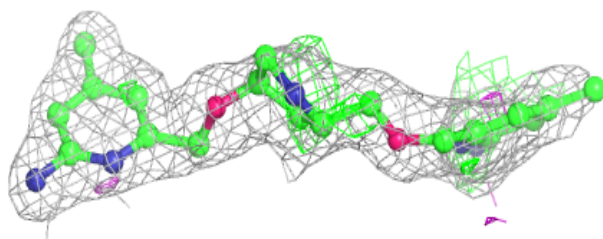
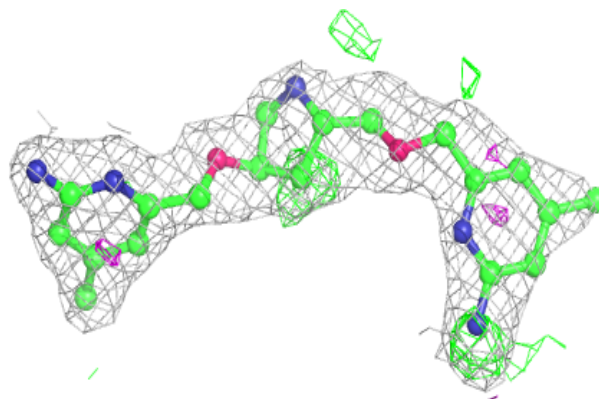
Electron density around QJ8 A 803:

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

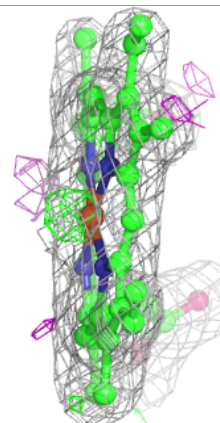
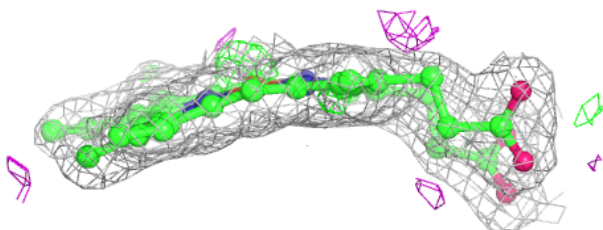
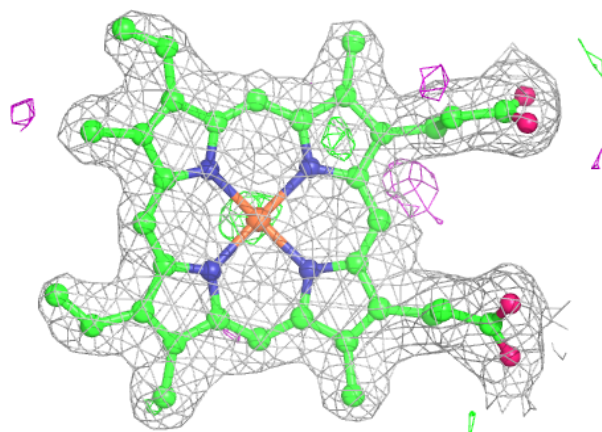


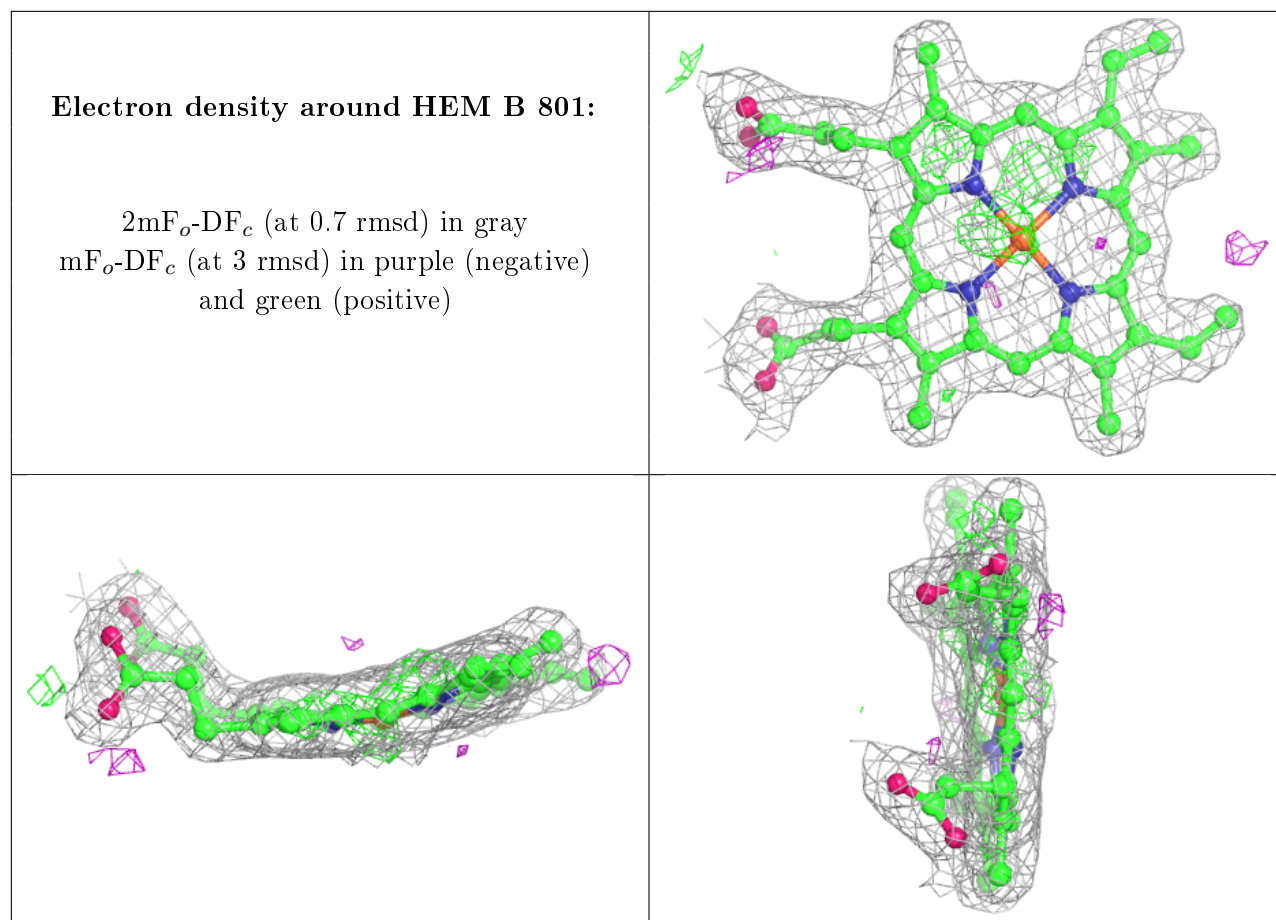
Electron density around QJ8 B 803:

$2mF_o-DF_c$ (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)





6.5 Other polymers ⓘ

There are no such residues in this entry.