



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:28 AM BST

PDB ID : 6PN5
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 7-(3-(Aminomethyl)-4-(pyridin-2-ylmethoxy)phenyl)-4-methylquinolin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2019-07-02
Resolution : 1.70 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 : 2.14.6
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) : 2.14.6

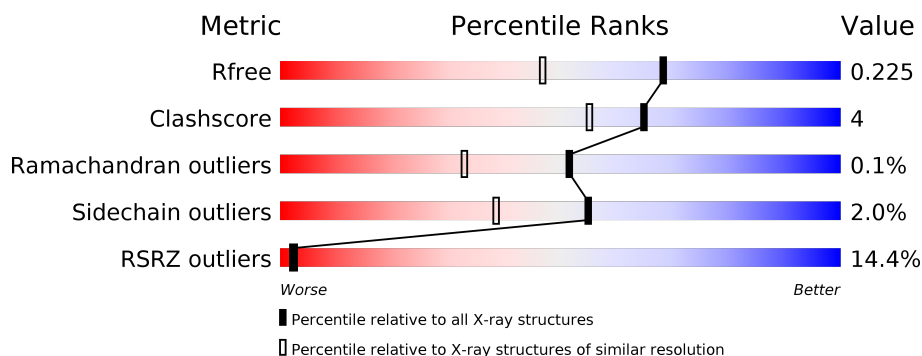
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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>20%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>
1	B	422	<div> <div>8%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	807	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7332 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	411	Total	C	N	O	S	0	3	0
			3352	2144	573	613	22			
1	B	411	Total	C	N	O	S	0	3	0
			3354	2146	574	612	22			

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



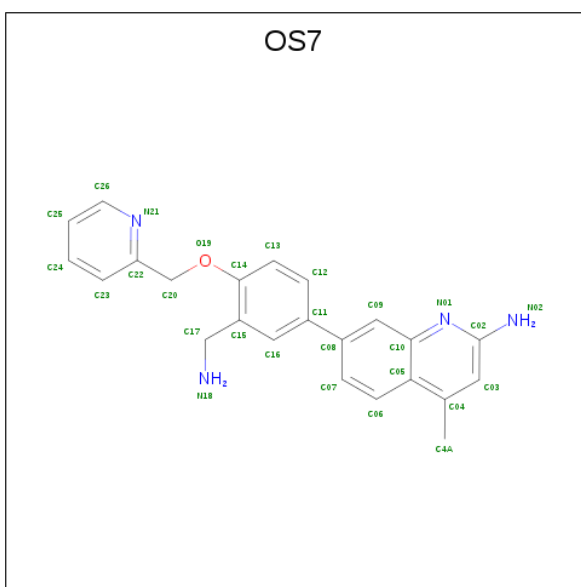
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 7-{3-(aminomethyl)-4-[(pyridin-2-yl)methoxy]phenyl}-4-methylquinolin-2-amine (three-letter code: OS7) (formula: C₂₃H₂₂N₄O) (labeled as "Ligand of Interest" by author).



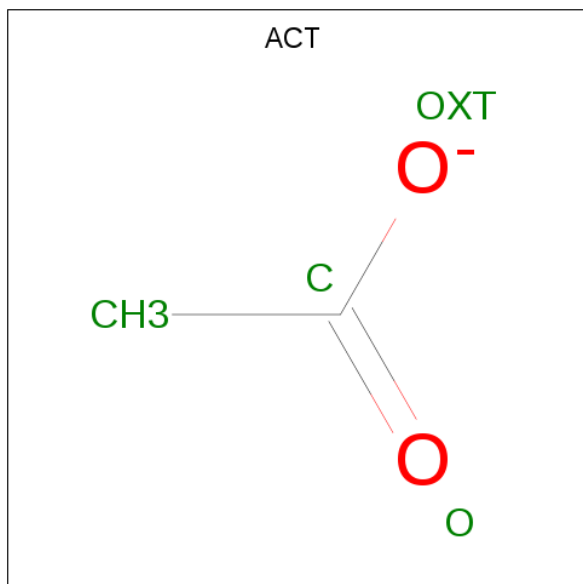
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	23	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			28	23	4	1		

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



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		

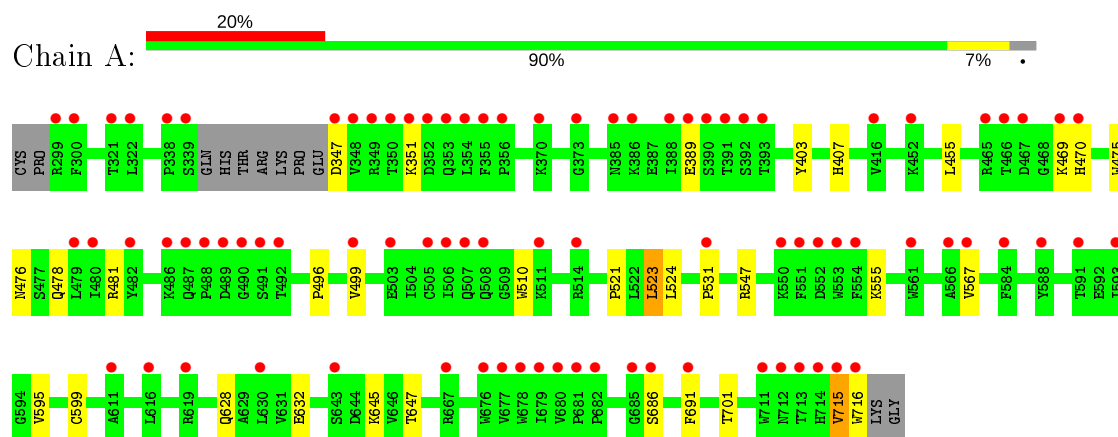
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	173	Total	O	0	0
			173	173		
8	B	250	Total	O	0	0
			250	250		

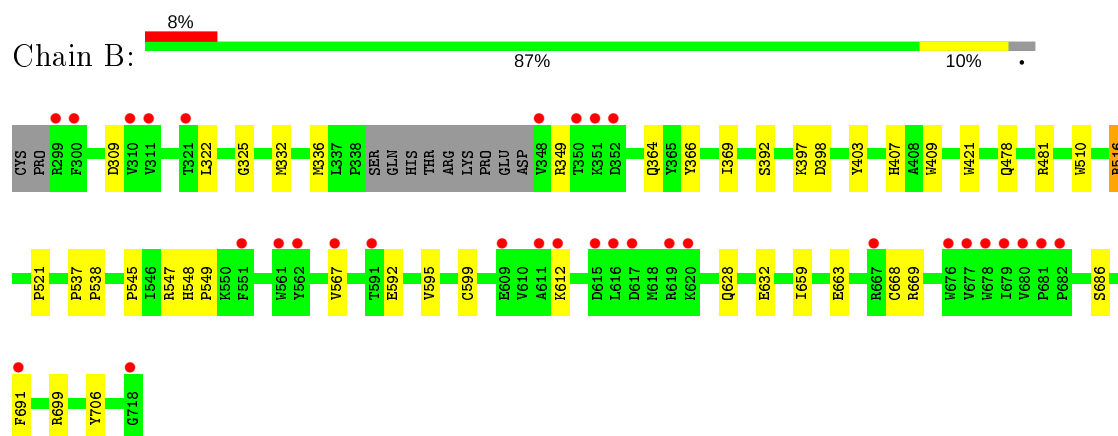
3 Residue-property plots [i](#)

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



- 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	52.10Å 111.16Å 164.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 1.70 39.04 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (39.04-1.70) 93.6 (39.04-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1496: ???)	Depositor
R, R_{free}	0.191 , 0.227 0.191 , 0.225	Depositor DCC
R_{free} test set	4947 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7332	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: GOL, ZN, H4B, OS7, ACT, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/3451	0.50	0/4683
1	B	0.38	0/3456	0.51	0/4685
All	All	0.36	0/6907	0.51	0/9368

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	3352	0	3264	19	0
1	B	3354	0	3272	29	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	28	0	0	2	0
4	B	28	0	0	4	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	18	0	24	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	173	0	0	3	0
8	B	250	0	0	3	0
All	All	7332	0	6656	55	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 (55) 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:523:LEU:HD22	1:A:531:PRO:HB2	1.60	0.82
1:B:706:TYR:OH	2:B:801:HEM:O2D	1.98	0.81
1:B:668[B]:CYS:SG	8:B:1138:HOH:O	2.45	0.74
1:B:516:ARG:HD2	6:B:805:GOL:H32	1.70	0.73
1:B:669:ARG:HH21	6:B:806:GOL:H11	1.55	0.70
2:B:801:HEM:HBC2	2:B:801:HEM:HMC2	1.74	0.70
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.74	0.69
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.75	0.69
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.75	0.68
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.77	0.67
1:B:398:ASP:H	6:B:807:GOL:H12	1.60	0.66
2:B:801:HEM:HBD1	4:B:803:OS7:C12	2.26	0.65
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.82	0.62
1:A:531:PRO:HD2	1:A:716:TRP:CZ3	2.35	0.62
1:A:351:LYS:NZ	1:A:389:GLU:O	2.37	0.58
1:A:567:VAL:HG21	4:A:803:OS7:C07	2.34	0.57
2:A:801:HEM:HBD1	2:A:801:HEM:HMD1	1.86	0.57
1:B:567:VAL:HG21	4:B:803:OS7:C07	2.35	0.56
2:A:801:HEM:HAD2	4:A:803:OS7:C12	2.36	0.55
1:B:516:ARG:NE	8:B:903:HOH:O	2.38	0.54
1:B:322:LEU:HB3	1:B:699:ARG:HH21	1.72	0.53
2:A:801:HEM:HBD2	8:A:1034:HOH:O	2.09	0.53
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.93	0.51
1:B:595:VAL:O	1:B:599:CYS:HB2	2.11	0.51
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.44	0.51
1:A:455:LEU:HD12	1:A:647:THR:HB	1.92	0.50
1:A:555:LYS:N	8:A:907:HOH:O	2.42	0.49
1:B:325:GLY:O	1:B:332:MET:HG3	2.13	0.48
1:B:398:ASP:HB2	6:B:807:GOL:H31	1.94	0.48
1:B:516:ARG:HD2	6:B:805:GOL:C3	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LYS:HB3	6:B:807:GOL:H32	1.94	0.48
1:B:592:GLU:OE2	4:B:803:OS7:N02	2.48	0.47
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.96	0.47
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.50	0.47
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.03	0.46
1:B:336:MET:HG2	4:B:803:OS7:C25	2.45	0.46
1:B:398:ASP:H	6:B:807:GOL:H32	1.80	0.45
1:A:531:PRO:HD2	1:A:716:TRP:HZ3	1.81	0.45
1:A:701[B]:THR:HG22	8:A:1022:HOH:O	2.16	0.44
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.48	0.44
1:A:595:VAL:O	1:A:599:CYS:HB2	2.18	0.44
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.53	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.43
1:A:524:LEU:O	1:A:531:PRO:HA	2.18	0.43
1:A:475:TRP:CE2	1:A:531:PRO:HG3	2.55	0.41
1:B:366:TYR:HA	1:B:369:ILE:HG12	2.02	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.55	0.41
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.55	0.41
1:B:364:GLN:OE1	8:B:901:HOH:O	2.22	0.41
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.56	0.41
1:B:398:ASP:H	6:B:807:GOL:C3	2.34	0.41
1:B:686:SER:HA	1:B:691:PHE:CG	2.56	0.40
2:A:801:HEM:HBD1	2:A:801:HEM:CMD	2.49	0.40
1:B:537:PRO:HA	1:B:538:PRO:HD3	1.99	0.40
1:B:659:ILE:O	1:B:663:GLU:HG3	2.22	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	409/422 (97%)	395 (97%)	13 (3%)	1 (0%)	47	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	410/422 (97%)	400 (98%)	10 (2%)	0	100	100
All	All	819/844 (97%)	795 (97%)	23 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	715	VAL

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	369/377 (98%)	361 (98%)	8 (2%)	52	34
1	B	369/377 (98%)	362 (98%)	7 (2%)	57	41
All	All	738/754 (98%)	723 (98%)	15 (2%)	55	38

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	ASP
1	A	469	LYS
1	A	470	HIS
1	A	476	ASN
1	A	523	LEU
1	A	547	ARG
1	A	645	LYS
1	A	715	VAL
1	B	309	ASP
1	B	349	ARG
1	B	392	SER
1	B	516	ARG
1	B	545	PRO
1	B	547	ARG
1	B	612	LYS

Some 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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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
4	OS7	A	803	-	31,31,31	0.83	1 (3%)	42,43,43	2.13	14 (33%)
6	GOL	B	805	-	5,5,5	0.37	0	5,5,5	0.65	0
3	H4B	B	802	-	16,18,18	0.83	0	11,26,26	2.44	5 (45%)
3	H4B	A	802	-	16,18,18	0.86	0	11,26,26	2.68	6 (54%)
2	HEM	A	801	1	27,50,50	1.90	5 (18%)	17,82,82	1.94	6 (35%)
2	HEM	B	801	1	27,50,50	1.95	4 (14%)	17,82,82	1.85	5 (29%)
6	GOL	B	806	-	5,5,5	0.37	0	5,5,5	0.23	0
6	GOL	B	807	-	5,5,5	0.35	0	5,5,5	0.57	0
5	ACT	A	804	-	1,3,3	1.45	0	0,3,3	0.00	-
5	ACT	B	804	-	1,3,3	1.23	0	0,3,3	0.00	-
4	OS7	B	803	-	31,31,31	0.89	1 (3%)	42,43,43	1.96	9 (21%)

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
4	OS7	A	803	-	-	5/11/11/11	0/4/4/4
6	GOL	B	805	-	-	4/4/4/4	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
2	HEM	A	801	1	-	3/6/54/54	-
2	HEM	B	801	1	-	1/6/54/54	-
6	GOL	B	806	-	-	4/4/4/4	-
6	GOL	B	807	-	-	2/4/4/4	-
4	OS7	B	803	-	-	3/11/11/11	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-5.24	1.33	1.40
2	A	801	HEM	C3B-C2B	-4.52	1.34	1.40
2	B	801	HEM	C3C-C2C	-3.86	1.35	1.40
2	A	801	HEM	C3C-C2C	-3.61	1.35	1.40
2	A	801	HEM	C3B-CAB	3.61	1.55	1.47
2	A	801	HEM	C3C-CAC	3.52	1.55	1.47
2	B	801	HEM	C3C-CAC	3.41	1.54	1.47
2	B	801	HEM	C3B-CAB	3.30	1.54	1.47
2	A	801	HEM	CAD-C3D	2.46	1.56	1.52
4	A	803	OS7	C02-N01	2.24	1.36	1.33
4	B	803	OS7	C05-C10	-2.10	1.39	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	OS7	O19-C14-C15	7.21	125.20	115.78
4	A	803	OS7	O19-C14-C15	6.15	123.82	115.78
4	A	803	OS7	C20-O19-C14	5.38	128.35	117.76
3	B	802	H4B	C4-C4A-C8A	5.17	119.16	114.57
3	A	802	H4B	C4-C4A-C8A	4.95	118.97	114.57
4	B	803	OS7	C20-O19-C14	4.93	127.47	117.76
2	A	801	HEM	CMD-C2D-C1D	-4.19	122.02	128.46
4	A	803	OS7	C04-C05-C10	4.07	120.21	118.01
2	B	801	HEM	CBA-CAA-C2A	-3.71	105.64	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	OS7	C16-C11-C08	-3.65	114.83	120.86
3	A	802	H4B	C4-C4A-N5	3.50	122.06	119.12
3	A	802	H4B	N3-C2-N1	-3.42	120.06	125.42
2	B	801	HEM	CAD-CBD-CGD	-3.34	107.07	112.67
3	A	802	H4B	C4-N3-C2	3.31	121.19	115.93
4	B	803	OS7	O19-C14-C13	-3.20	117.04	123.97
2	A	801	HEM	CBA-CAA-C2A	-3.17	106.64	112.49
4	A	803	OS7	O19-C14-C13	-3.13	117.20	123.97
4	B	803	OS7	C26-N21-C22	3.12	121.69	117.42
4	A	803	OS7	C05-C10-N01	-3.02	119.61	122.81
4	B	803	OS7	C04-C05-C10	2.93	119.60	118.01
3	B	802	H4B	C4-N3-C2	2.83	120.42	115.93
3	A	802	H4B	C2-N1-C8A	2.79	120.79	114.54
3	B	802	H4B	N3-C2-N1	-2.78	121.06	125.42
4	A	803	OS7	C12-C11-C08	2.71	126.04	121.36
2	B	801	HEM	CMA-C3A-C4A	-2.70	124.31	128.46
4	A	803	OS7	C26-N21-C22	2.61	121.00	117.42
4	B	803	OS7	C25-C26-N21	-2.51	119.32	123.43
2	B	801	HEM	CBD-CAD-C3D	2.51	117.10	112.48
3	B	802	H4B	C4-C4A-N5	2.51	121.22	119.12
3	B	802	H4B	C2-N1-C8A	2.49	120.11	114.54
2	A	801	HEM	CMD-C2D-C3D	2.47	129.60	124.94
4	B	803	OS7	C16-C11-C08	-2.38	116.93	120.86
2	A	801	HEM	CMC-C2C-C3C	2.33	129.03	124.68
2	A	801	HEM	CBD-CAD-C3D	2.31	116.73	112.48
4	A	803	OS7	C06-C05-C04	-2.31	119.25	123.66
4	A	803	OS7	C17-C15-C14	2.27	124.55	120.12
4	A	803	OS7	N02-C02-N01	2.26	120.12	118.26
4	A	803	OS7	C17-C15-C16	-2.23	116.40	120.38
4	B	803	OS7	C17-C15-C16	-2.20	116.47	120.38
4	A	803	OS7	C07-C08-C11	-2.15	117.62	121.36
2	B	801	HEM	CMD-C2D-C1D	-2.08	125.27	128.46
2	A	801	HEM	CMA-C3A-C4A	-2.06	125.31	128.46
4	B	803	OS7	C17-C15-C14	2.04	124.10	120.12
4	A	803	OS7	C03-C04-C05	2.03	119.78	117.78
3	A	802	H4B	N2-C2-N3	2.03	120.40	117.25

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C2D-C3D-CAD-CBD
2	A	801	HEM	C4D-C3D-CAD-CBD
6	B	805	GOL	C1-C2-C3-O3
6	B	806	GOL	C1-C2-C3-O3
6	B	807	GOL	O1-C1-C2-C3
4	B	803	OS7	C15-C14-O19-C20
6	B	805	GOL	O2-C2-C3-O3
4	A	803	OS7	C15-C14-O19-C20
6	B	805	GOL	O1-C1-C2-C3
6	B	806	GOL	O1-C1-C2-C3
4	B	803	OS7	C13-C14-O19-C20
6	B	806	GOL	O1-C1-C2-O2
6	B	807	GOL	O1-C1-C2-O2
6	B	805	GOL	O1-C1-C2-O2
4	A	803	OS7	C13-C14-O19-C20
4	B	803	OS7	C14-C15-C17-N18
4	A	803	OS7	C07-C08-C11-C16
6	B	806	GOL	O2-C2-C3-O3
2	B	801	HEM	C2A-CAA-CBA-CGA
4	A	803	OS7	C09-C08-C11-C16
4	A	803	OS7	C07-C08-C11-C12

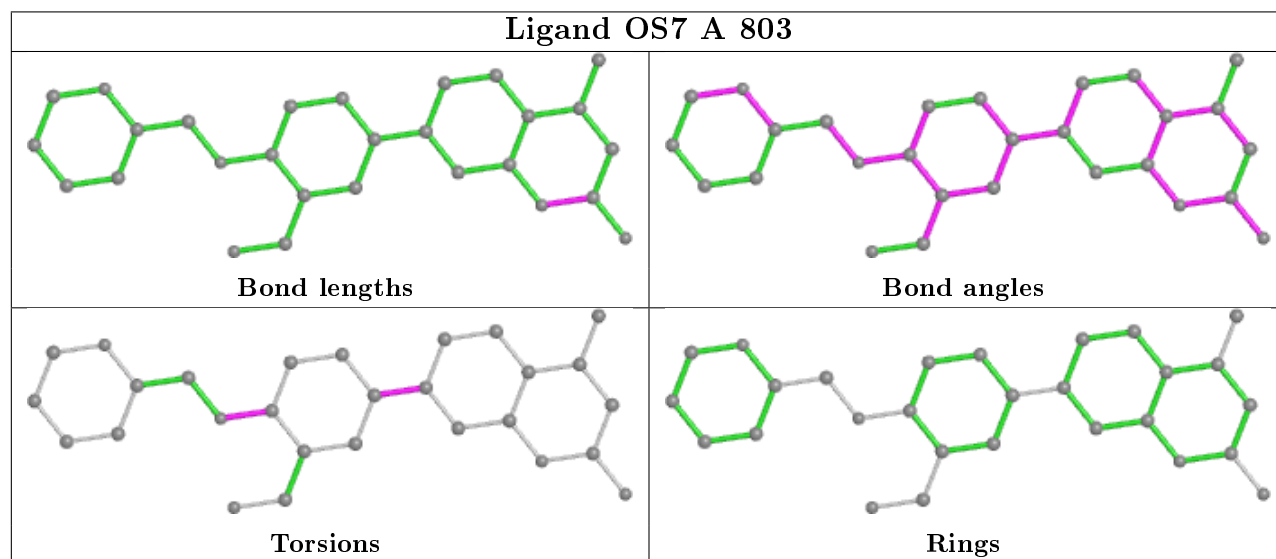
There are no ring outliers.

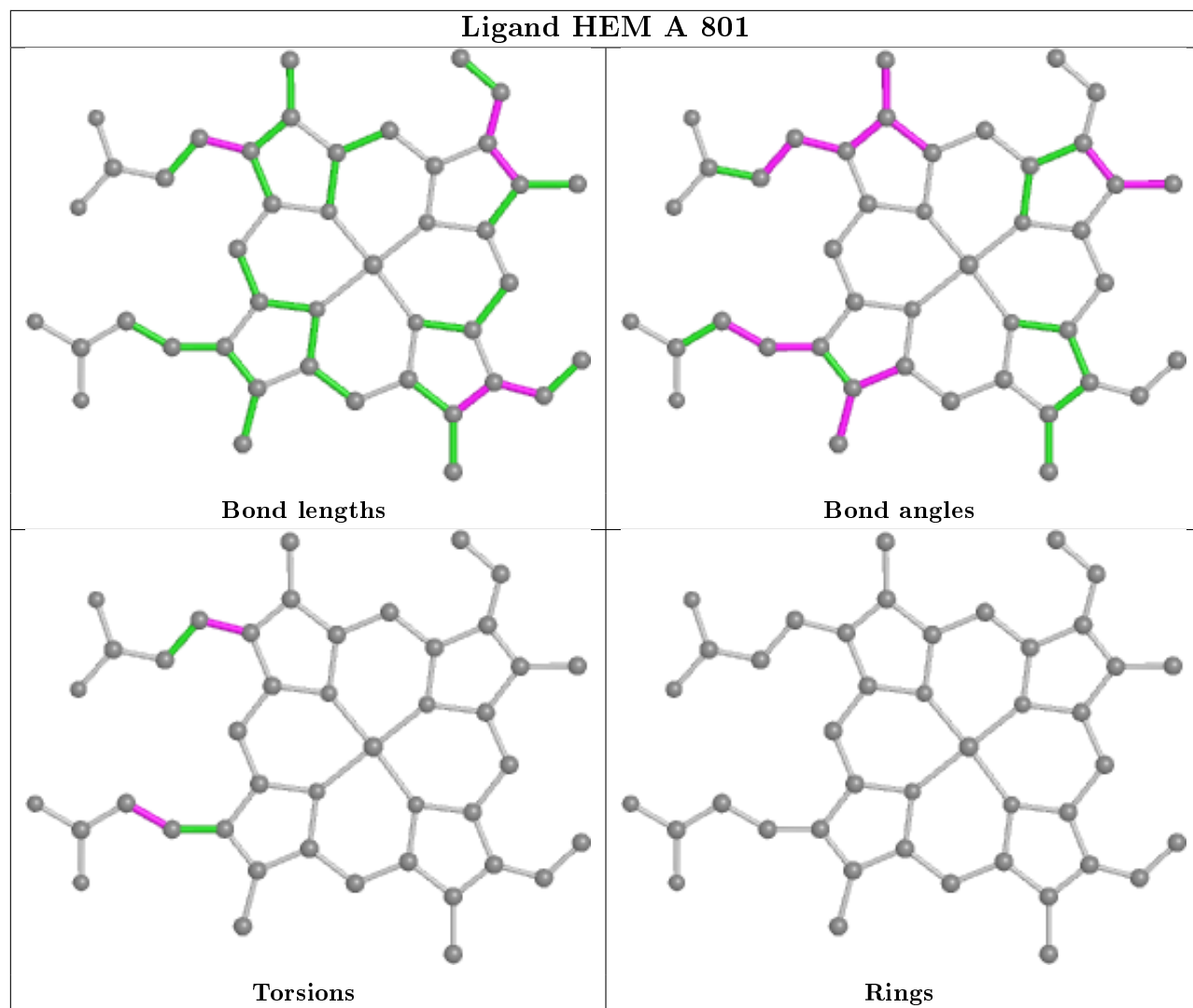
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	OS7	2	0
6	B	805	GOL	2	0
2	A	801	HEM	6	0
2	B	801	HEM	4	0
6	B	806	GOL	1	0
6	B	807	GOL	5	0
4	B	803	OS7	4	0

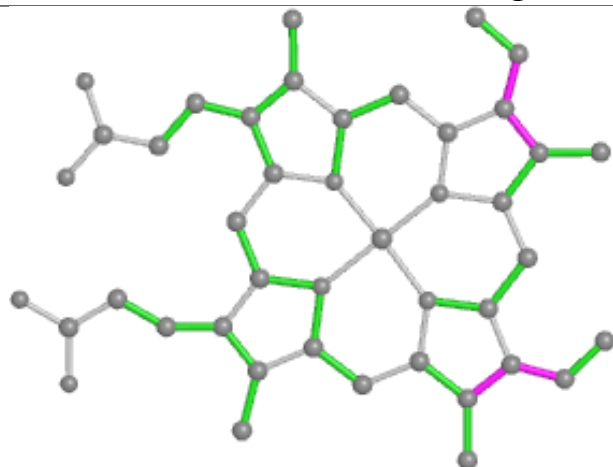
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

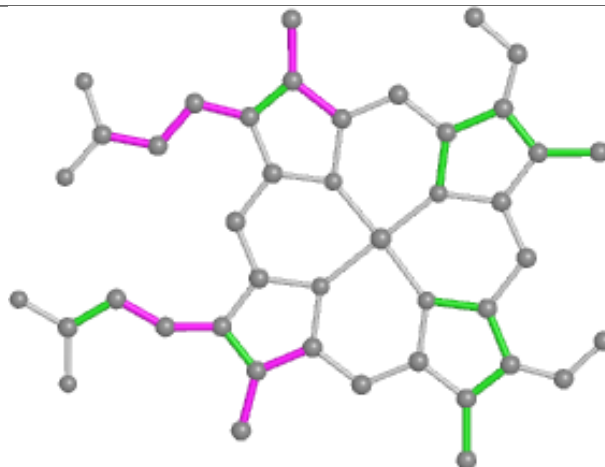




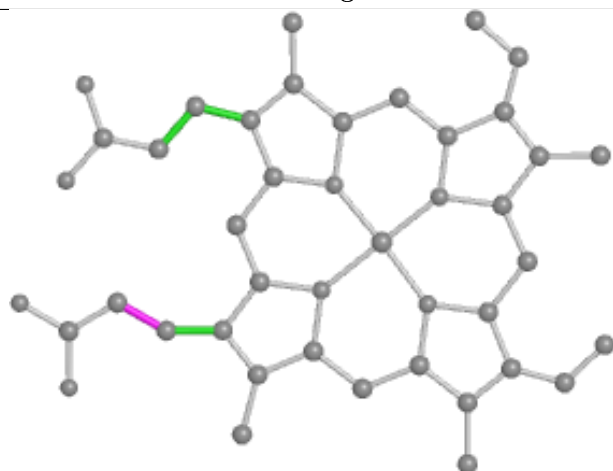
Ligand HEM B 801



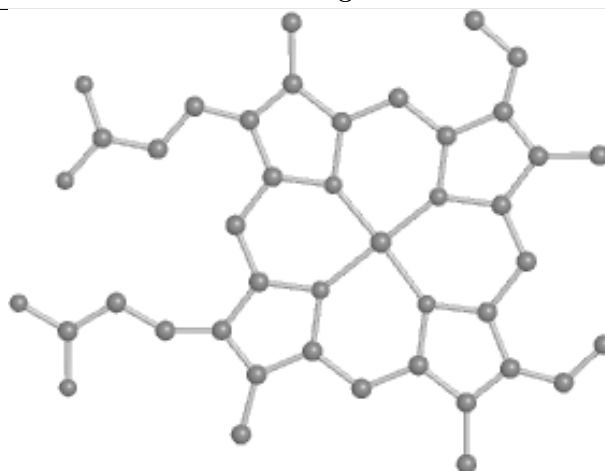
Bond lengths



Bond angles

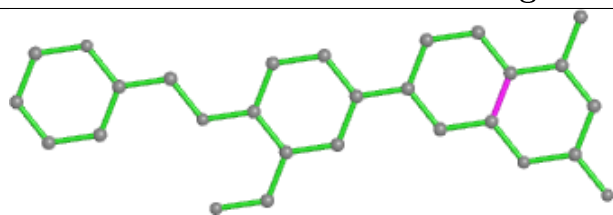


Torsions

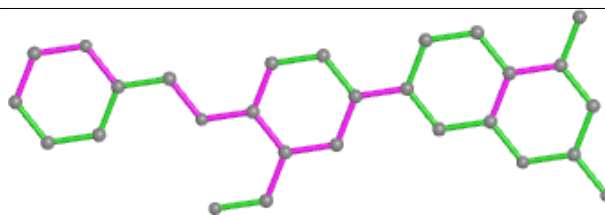


Rings

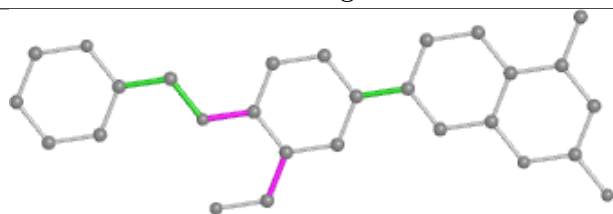
Ligand OS7 B 803



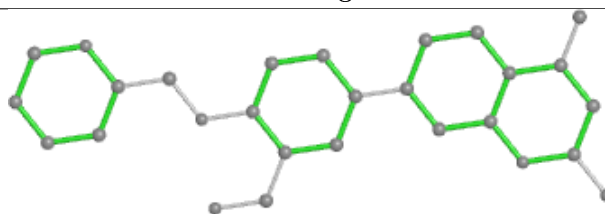
Bond lengths



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	411/422 (97%)	1.12	86 (20%) 1 0	30, 57, 110, 142	0
1	B	411/422 (97%)	0.43	32 (7%) 13 15	28, 45, 79, 110	1 (0%)
All	All	822/844 (97%)	0.78	118 (14%) 2 2	28, 49, 101, 142	1 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	VAL	10.6
1	A	715	VAL	10.5
1	A	716	TRP	9.0
1	B	300	PHE	9.0
1	A	506	ILE	6.9
1	A	488	PRO	6.9
1	B	348	VAL	6.2
1	B	350	THR	6.2
1	B	718	GLY	6.1
1	A	352	ASP	5.8
1	A	299	ARG	5.6
1	A	347	ASP	5.5
1	A	349	ARG	5.3
1	A	355	PHE	5.2
1	A	678	TRP	5.0
1	A	486	LYS	5.0
1	A	712	ASN	5.0
1	B	677	VAL	4.9
1	A	490	GLY	4.8
1	A	388	ILE	4.7
1	A	391	THR	4.7
1	A	551	PHE	4.7
1	A	677	VAL	4.6
1	A	713	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	507	GLN	4.4
1	A	679	ILE	4.3
1	A	386	LYS	4.3
1	B	619	ARG	4.2
1	A	491	SER	4.1
1	A	392	SER	4.1
1	A	711	TRP	4.1
1	A	351	LYS	4.1
1	A	390	SER	4.1
1	A	676	TRP	3.9
1	B	679	ILE	3.9
1	B	616	LEU	3.8
1	A	714	HIS	3.8
1	A	489	ASP	3.8
1	A	350	THR	3.8
1	A	300	PHE	3.7
1	B	299	ARG	3.7
1	A	322	LEU	3.7
1	A	373	GLY	3.7
1	A	619	ARG	3.6
1	A	389	GLU	3.6
1	B	611	ALA	3.5
1	A	480	ILE	3.5
1	A	487	GLN	3.5
1	B	676	TRP	3.4
1	B	680	VAL	3.4
1	B	620	LYS	3.4
1	A	584	PHE	3.3
1	B	310	VAL	3.3
1	B	678	TRP	3.2
1	A	416	VAL	3.1
1	A	680	VAL	3.1
1	A	553	TRP	3.1
1	A	321	THR	3.0
1	B	321	THR	3.0
1	A	567	VAL	3.0
1	A	370	LYS	2.9
1	A	470	HIS	2.9
1	A	469	LYS	2.9
1	A	681	PRO	2.9
1	A	588	TYR	2.9
1	B	352	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	503	GLU	2.8
1	A	393	THR	2.8
1	A	593	ILE	2.8
1	A	561	TRP	2.7
1	B	561	TRP	2.7
1	A	354	LEU	2.7
1	A	385	ASN	2.7
1	A	611	ALA	2.7
1	A	467	ASP	2.7
1	B	615	ASP	2.7
1	A	643	SER	2.7
1	A	339	SER	2.6
1	A	566	ALA	2.6
1	B	617	ASP	2.6
1	A	514	ARG	2.5
1	A	554	PHE	2.5
1	A	691	PHE	2.5
1	A	682	PRO	2.5
1	A	499	VAL	2.5
1	B	682	PRO	2.5
1	A	479	LEU	2.5
1	A	685	GLY	2.5
1	A	667	ARG	2.4
1	A	452	LYS	2.4
1	B	667	ARG	2.4
1	A	508	GLN	2.4
1	A	505	CYS	2.4
1	B	311	VAL	2.3
1	B	681	PRO	2.3
1	A	353	GLN	2.3
1	A	630	LEU	2.3
1	B	612	LYS	2.3
1	B	551	PHE	2.3
1	A	550	LYS	2.3
1	A	511	LYS	2.2
1	B	567	VAL	2.2
1	A	465	ARG	2.2
1	A	466	THR	2.2
1	B	609	GLU	2.2
1	A	531	PRO	2.2
1	B	562	TYR	2.1
1	A	492	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	2.1
1	B	691	PHE	2.1
1	B	351	LYS	2.1
1	A	591	THR	2.1
1	A	356	PRO	2.1
1	A	552	ASP	2.1
1	A	686	SER	2.1
1	A	482	TYR	2.0
1	A	616	LEU	2.0
1	B	591	THR	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 monosaccharides in this entry.

6.4 Ligands ⓘ

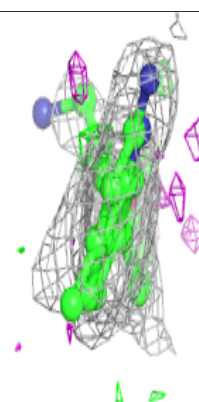
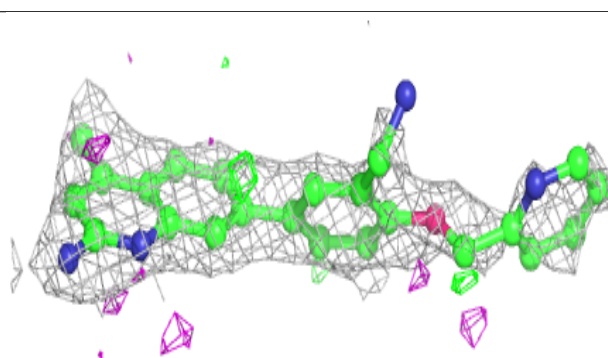
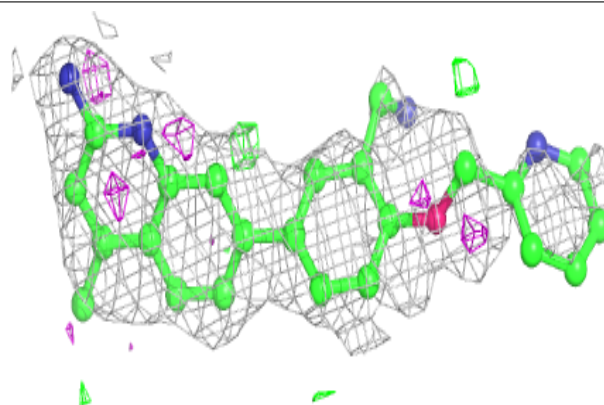
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	B	805	6/6	0.52	0.21	75,83,88,89	0
6	GOL	B	807	6/6	0.67	0.27	75,81,84,88	0
6	GOL	B	806	6/6	0.84	0.19	69,73,74,74	0
4	OS7	A	803	28/28	0.87	0.26	41,75,107,107	0
4	OS7	B	803	28/28	0.89	0.19	37,65,97,100	0
5	ACT	A	804	4/4	0.91	0.14	64,66,66,67	0
3	H4B	B	802	17/17	0.92	0.16	32,35,40,43	0
3	H4B	A	802	17/17	0.92	0.18	31,40,45,46	0
5	ACT	B	804	4/4	0.96	0.12	50,56,63,69	0
2	HEM	A	801	43/43	0.97	0.18	29,37,64,70	0
2	HEM	B	801	43/43	0.97	0.16	27,35,58,73	0
7	ZN	B	808	1/1	0.99	0.07	37,37,37,37	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.

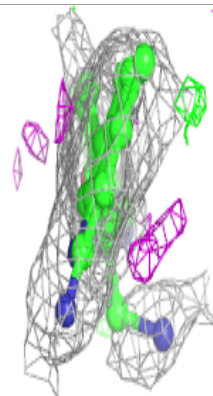
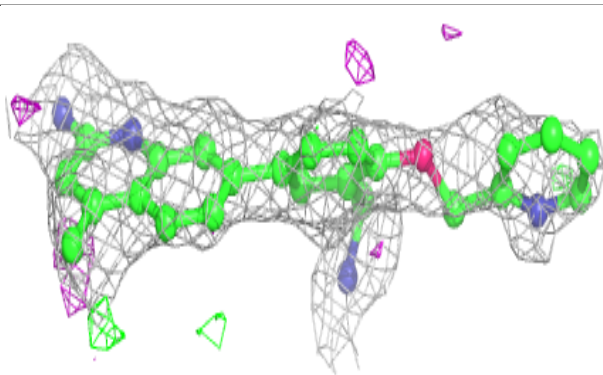
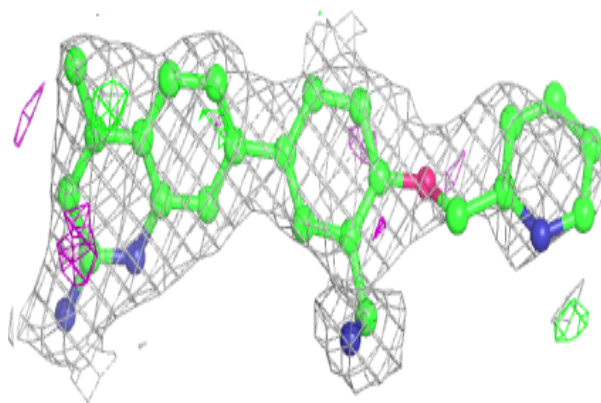
Electron density around OS7 A 803:

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



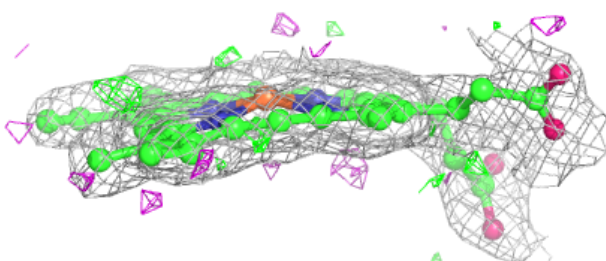
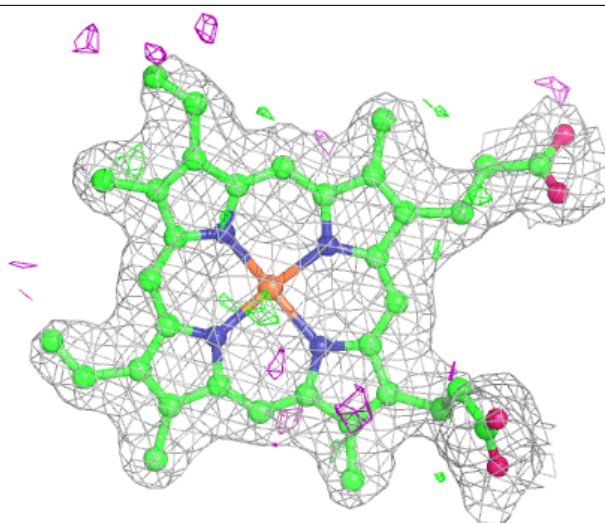
Electron density around OS7 B 803:

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



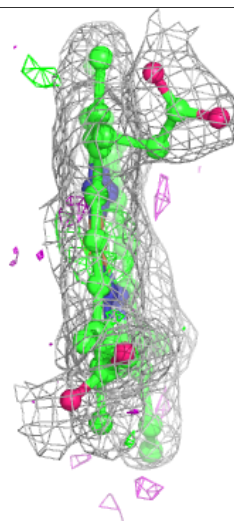
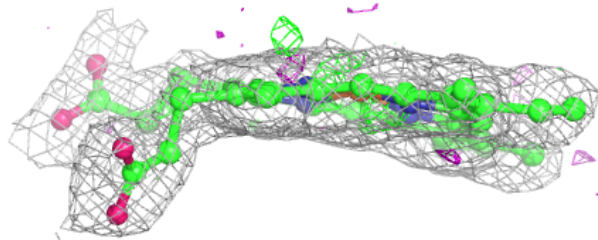
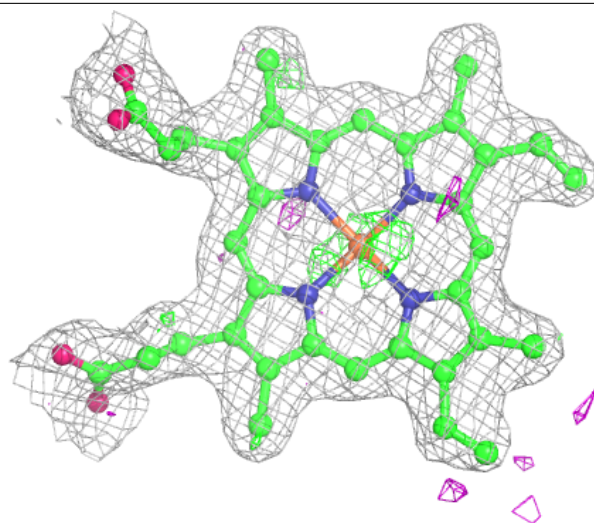
Electron density around HEM A 801:

$2mF_o-DF_c$ (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.