



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2022 – 02:05 PM EDT

PDB ID : 7S3Z
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with N2-(((3-((2-aminoquinolin-7-yl)methoxy)phenoxy)methyl)pyridine-2,6-diamine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2021-09-08
Resolution : 1.73 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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.29
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) : 2.29

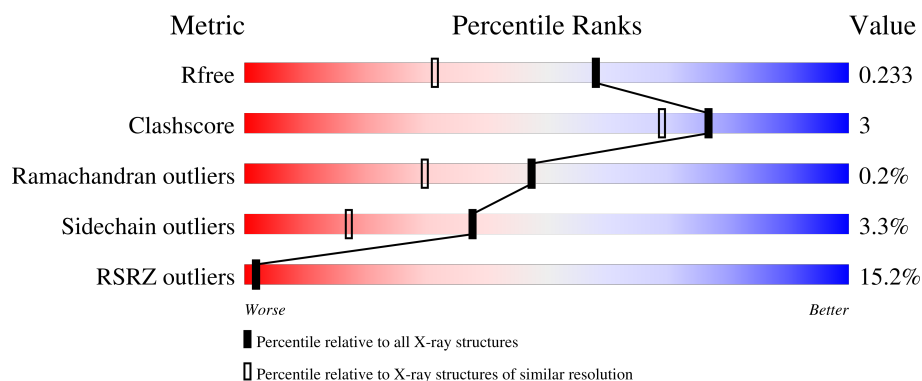
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 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 $\leq 5\%$. 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>21%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	B	422	<div> <div>9%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>

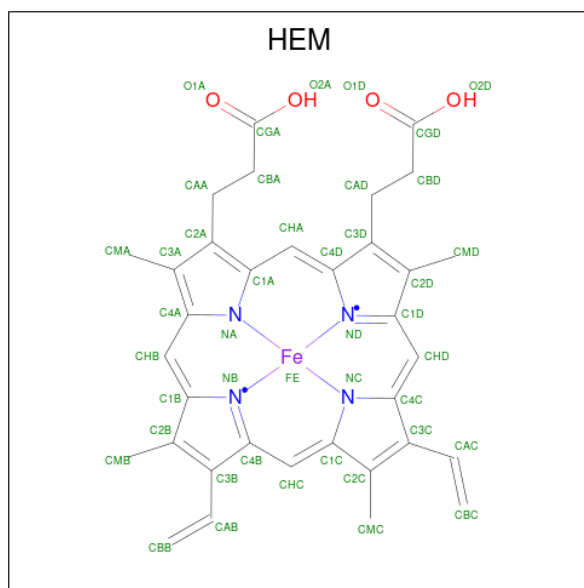
i

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 3348	C 2141	N 573	O 612	S 22	0	2	0
1	B	411	Total 3353	C 2145	N 574	O 612	S 22	0	3	0

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



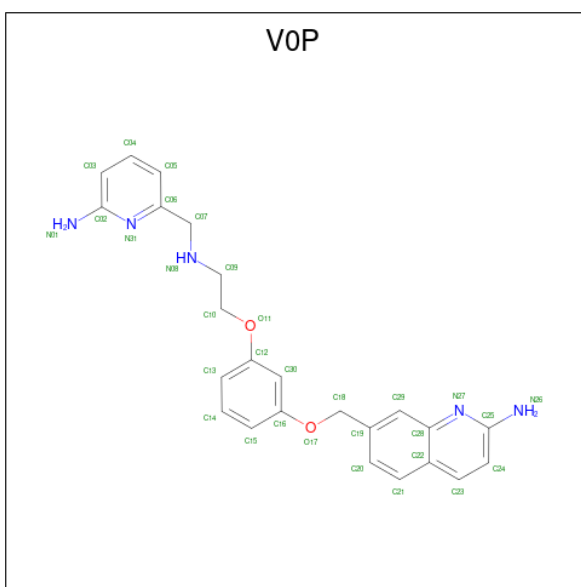
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



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-(2-[[[(6-aminopyridin-2-yl)methyl]amino]ethoxy]phenoxy]methyl}quinolin-2-amine (three-letter code: V0P) (formula: C₂₄H₂₅N₅O₂) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			31	24	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		

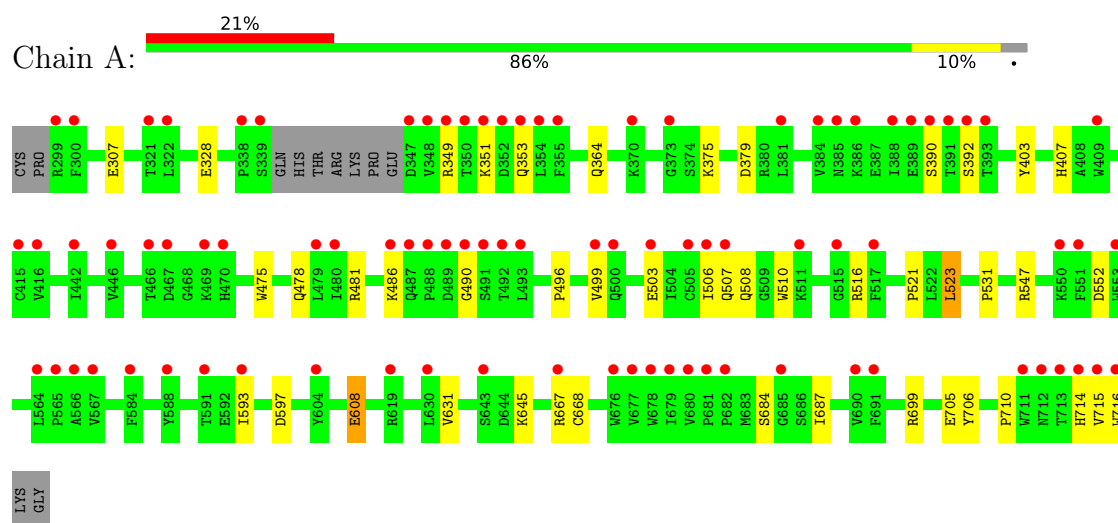
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	186	Total	O	0	0
			186	186		
7	B	294	Total	O	0	0
			294	294		

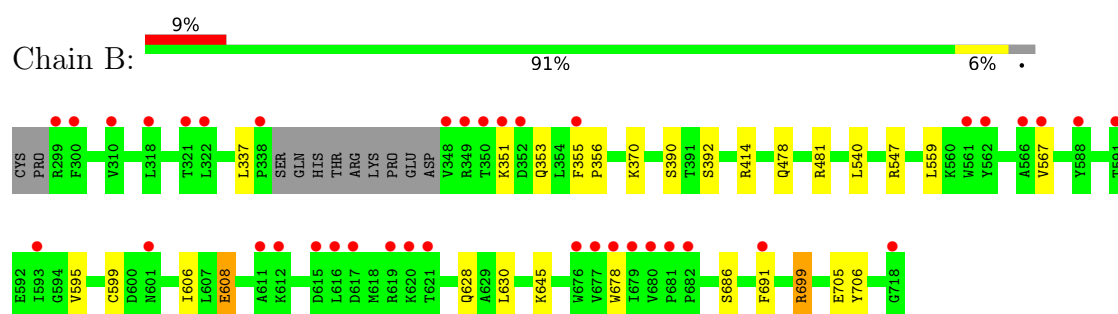
3 Residue-property plots [i](#)

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	52.17Å 111.89Å 164.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.19 – 1.73 39.19 – 1.73	Depositor EDS
% Data completeness (in resolution range)	94.5 (39.19-1.73) 95.3 (39.19-1.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, R_{free}	0.196 , 0.235 0.196 , 0.233	Depositor DCC
R_{free} test set	4816 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	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	0.97	EDS
Total number of atoms	7372	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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: ZN, ACT, VOP, HEM, H4B

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	0.36	0/3444	0.51	0/4672
1	B	0.39	0/3456	0.52	0/4685
All	All	0.38	0/6900	0.52	0/9357

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	3348	0	3257	21	0
1	B	3353	0	3270	15	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	31	0	0	0	0
4	B	31	0	0	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	186	0	0	2	1
7	B	294	0	0	3	1
All	All	7372	0	6623	40	1

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 (40) 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	1.62	0.80
1:A:706:TYR:OH	2:A:801:HEM:O2D	2.03	0.75
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.69	0.73
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.76	0.68
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.76	0.67
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.78	0.65
2:B:801:HEM:O1D	7:B:901:HOH:O	2.16	0.60
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.85	0.58
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.84	0.58
1:A:699:ARG:NH2	1:A:705:GLU:OE2	2.36	0.58
1:A:667:ARG:NH1	1:A:668[A]:CYS:SG	2.78	0.56
1:B:706:TYR:OH	2:B:801:HEM:O2D	2.15	0.56
1:A:506:ILE:C	1:A:508:GLN:H	2.09	0.55
1:A:716:TRP:O	7:A:901:HOH:O	2.18	0.54
1:B:567:VAL:HG21	4:B:803:VOP:C20	2.40	0.52
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.93	0.50
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.46	0.50
1:B:608:GLU:HG2	7:B:907:HOH:O	2.11	0.50
1:B:595:VAL:O	1:B:599:CYS:HB2	2.11	0.49
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.95	0.49
1:B:481:ARG:NE	7:B:913:HOH:O	2.44	0.49
1:A:516:ARG:N	7:A:908:HOH:O	2.46	0.48
1:B:355:PHE:N	1:B:356:PRO:HD2	2.30	0.45
1:B:608:GLU:HG2	1:B:608:GLU:H	1.50	0.45
1:A:508:GLN:NE2	1:A:716:TRP:HH2	2.15	0.44
1:B:699:ARG:NH2	1:B:705:GLU:OE1	2.51	0.44
1:A:375:LYS:NZ	1:A:379:ASP:OD1	2.50	0.43
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.52	0.43
1:A:608:GLU:H	1:A:608:GLU:HG2	1.39	0.43
1:B:559:LEU:HD11	1:B:606:ILE:HD13	2.01	0.43
1:B:595:VAL:HG13	1:B:630:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.07	0.42
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.02	0.41
1:B:370:LYS:HD3	1:B:370:LYS:HA	1.73	0.41
1:B:686:SER:HA	1:B:691:PHE:CG	2.56	0.41
1:A:593:ILE:HA	1:A:597:ASP:HB2	2.03	0.41
1:A:714:HIS:HD2	1:A:716:TRP:HE3	1.69	0.41
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.55	0.41
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.03	0.41
1:A:684:SER:HB3	1:A:687:ILE:HD11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1081:HOH:O	7:B:1164:HOH:O[3_545]	2.18	0.02

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	408/422 (97%)	396 (97%)	10 (2%)	2 (0%)	29	13
1	B	410/422 (97%)	402 (98%)	8 (2%)	0	100	100
All	All	818/844 (97%)	798 (98%)	18 (2%)	2 (0%)	47	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	GLY
1	A	507	GLN

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	368/377 (98%)	354 (96%)	14 (4%)	33	13
1	B	369/377 (98%)	359 (97%)	10 (3%)	44	25
All	All	737/754 (98%)	713 (97%)	24 (3%)	38	17

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

Mol	Chain	Res	Type
1	A	307	GLU
1	A	328	GLU
1	A	349	ARG
1	A	353	GLN
1	A	364	GLN
1	A	390	SER
1	A	486	LYS
1	A	503	GLU
1	A	523	LEU
1	A	547	ARG
1	A	552	ASP
1	A	608	GLU
1	A	645	LYS
1	A	715	VAL
1	B	337	LEU
1	B	351	LYS
1	B	353	GLN
1	B	390	SER
1	B	392	SER
1	B	540	LEU
1	B	547	ARG
1	B	608	GLU
1	B	645	LYS
1	B	699	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides 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
2	HEM	B	801	1	41,50,50	1.45	5 (12%)	45,82,82	1.83	7 (15%)
3	H4B	A	802	-	16,18,18	1.03	1 (6%)	11,26,26	2.44	5 (45%)
4	V0P	B	803	-	34,34,34	0.79	1 (2%)	44,45,45	1.32	5 (11%)
4	V0P	A	803	-	34,34,34	0.80	0	44,45,45	1.62	10 (22%)
5	ACT	B	804	-	3,3,3	0.79	0	3,3,3	0.73	0
5	ACT	A	804	-	3,3,3	0.73	0	3,3,3	0.80	0
2	HEM	A	801	1	41,50,50	1.46	6 (14%)	45,82,82	1.61	9 (20%)
3	H4B	B	802	-	16,18,18	0.92	1 (6%)	11,26,26	2.50	4 (36%)

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	B	801	1	-	3/12/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	V0P	B	803	-	-	3/13/13/13	0/4/4/4
4	V0P	A	803	-	-	7/13/13/13	0/4/4/4
2	HEM	A	801	1	-	4/12/54/54	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3C-C2C	-4.15	1.34	1.40
2	B	801	HEM	C3C-CAC	3.67	1.55	1.47
2	A	801	HEM	C3C-CAC	3.59	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.37	1.35	1.40
2	A	801	HEM	CAB-C3B	2.97	1.55	1.47
2	B	801	HEM	CAB-C3B	2.86	1.55	1.47
2	A	801	HEM	CMD-C2D	2.63	1.56	1.50
3	A	802	H4B	C4A-C4	-2.27	1.38	1.41
2	A	801	HEM	FE-NB	2.19	2.07	1.96
3	B	802	H4B	C4A-C4	-2.11	1.38	1.41
2	B	801	HEM	CMD-C2D	2.03	1.55	1.50
4	B	803	V0P	C22-C28	-2.03	1.39	1.42
2	B	801	HEM	CMB-C2B	2.00	1.55	1.50
2	A	801	HEM	CMC-C2C	2.00	1.56	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CBA-CAA-C2A	-7.52	99.79	112.62
3	B	802	H4B	C8A-C4A-C4	5.76	119.69	114.57
4	A	803	V0P	C02-N31-C06	5.46	122.24	118.10
3	A	802	H4B	C8A-C4A-C4	5.30	119.27	114.57
2	A	801	HEM	CBA-CAA-C2A	-4.04	105.72	112.62
4	B	803	V0P	C02-N31-C06	3.99	121.12	118.10
2	A	801	HEM	C4B-CHC-C1C	3.83	127.61	122.56
2	B	801	HEM	C4B-CHC-C1C	3.51	127.19	122.56
3	A	802	H4B	N1-C2-N3	-3.21	120.38	125.42
2	A	801	HEM	CAD-CBD-CGD	-3.11	106.91	113.60
3	A	802	H4B	C2-N3-C4	3.02	120.73	115.93
4	A	803	V0P	C19-C29-C28	-2.98	118.46	121.08
3	B	802	H4B	C2-N3-C4	2.94	120.60	115.93
3	B	802	H4B	N1-C2-N3	-2.94	120.81	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	V0P	C22-C28-N27	-2.85	118.02	122.26
2	B	801	HEM	CHD-C1D-ND	2.85	127.53	124.43
2	A	801	HEM	CHD-C1D-ND	2.81	127.48	124.43
4	A	803	V0P	N26-C25-N27	2.80	120.58	118.26
4	B	803	V0P	C07-C06-N31	2.57	121.12	116.61
2	A	801	HEM	CMC-C2C-C3C	2.55	129.45	124.68
4	B	803	V0P	N26-C25-N27	2.53	120.35	118.26
2	A	801	HEM	C3B-C2B-C1B	2.51	108.35	106.49
2	B	801	HEM	C4D-ND-C1D	2.50	107.66	105.07
2	A	801	HEM	C3D-C4D-ND	-2.42	107.47	110.17
3	A	802	H4B	C2-N1-C8A	2.40	119.92	114.54
3	B	802	H4B	C2-N1-C8A	2.38	119.88	114.54
2	B	801	HEM	CAD-C3D-C2D	-2.35	123.50	127.88
4	B	803	V0P	N01-C02-N31	2.35	120.20	116.49
4	A	803	V0P	C07-C06-N31	2.28	120.61	116.61
4	A	803	V0P	C05-C06-N31	-2.24	119.56	122.41
2	B	801	HEM	CMA-C3A-C4A	-2.24	125.03	128.46
2	A	801	HEM	CHA-C4D-ND	2.21	127.11	124.38
4	B	803	V0P	C24-C25-N27	-2.18	119.46	122.08
4	A	803	V0P	C23-C22-C28	2.14	121.48	118.45
2	B	801	HEM	CAD-C3D-C4D	2.13	128.39	124.66
3	A	802	H4B	N2-C2-N3	2.12	120.55	117.25
4	A	803	V0P	C23-C22-C21	-2.10	118.27	123.19
4	A	803	V0P	C18-C19-C20	-2.10	115.73	120.66
4	A	803	V0P	C10-O11-C12	2.03	123.24	117.93
2	A	801	HEM	C4D-ND-C1D	2.01	107.15	105.07

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	V0P	C10-C09-N08-C07
4	A	803	V0P	C30-C16-O17-C18
4	B	803	V0P	C30-C16-O17-C18
4	A	803	V0P	N08-C09-C10-O11
4	A	803	V0P	C15-C16-O17-C18
4	B	803	V0P	C15-C16-O17-C18
4	B	803	V0P	C09-C10-O11-C12
2	A	801	HEM	C2A-CAA-CBA-CGA
4	A	803	V0P	C30-C12-O11-C10
4	A	803	V0P	C09-C10-O11-C12
4	A	803	V0P	C13-C12-O11-C10

Continued on next page...

Continued from previous page...

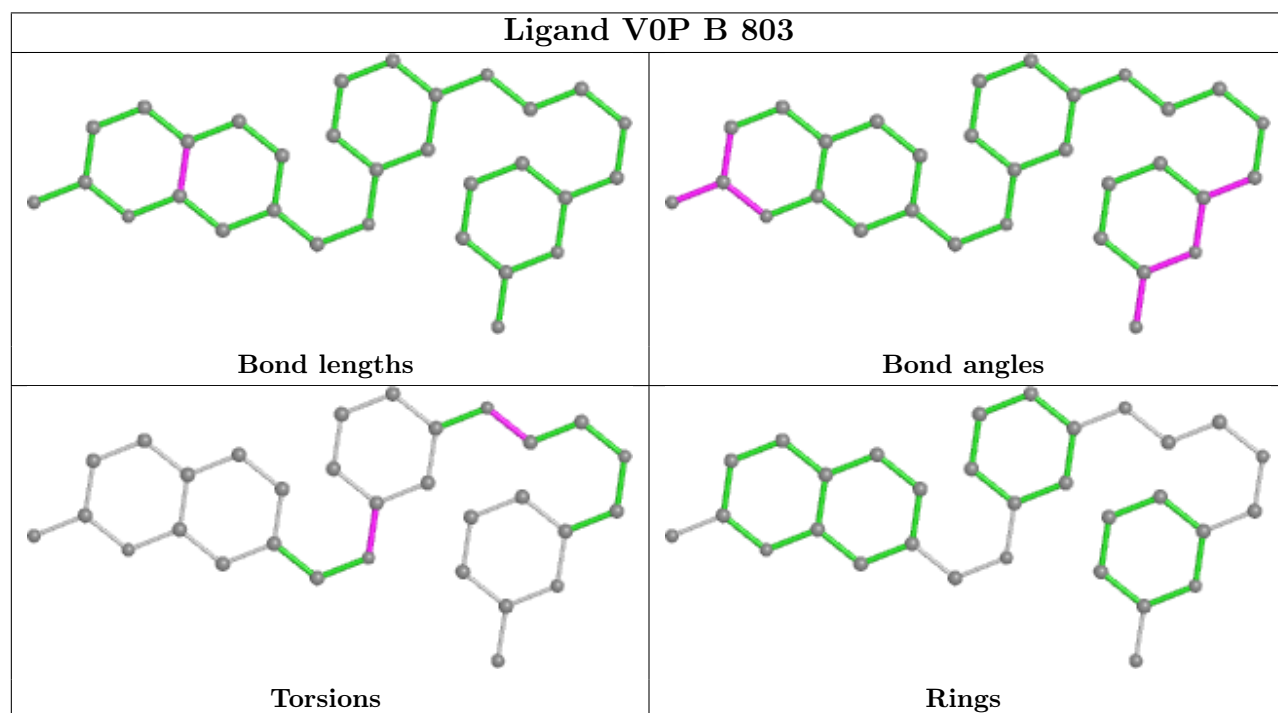
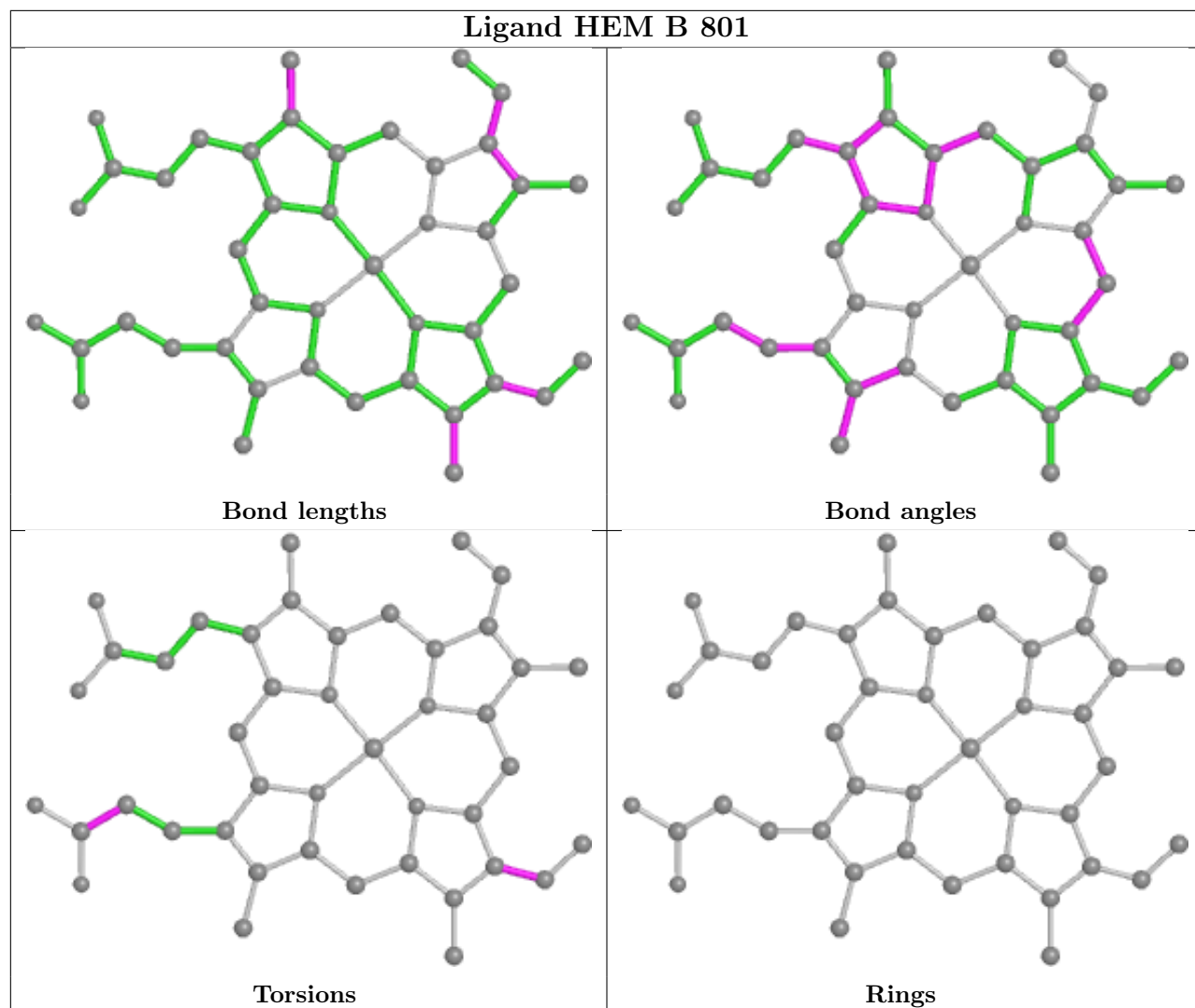
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
2	A	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

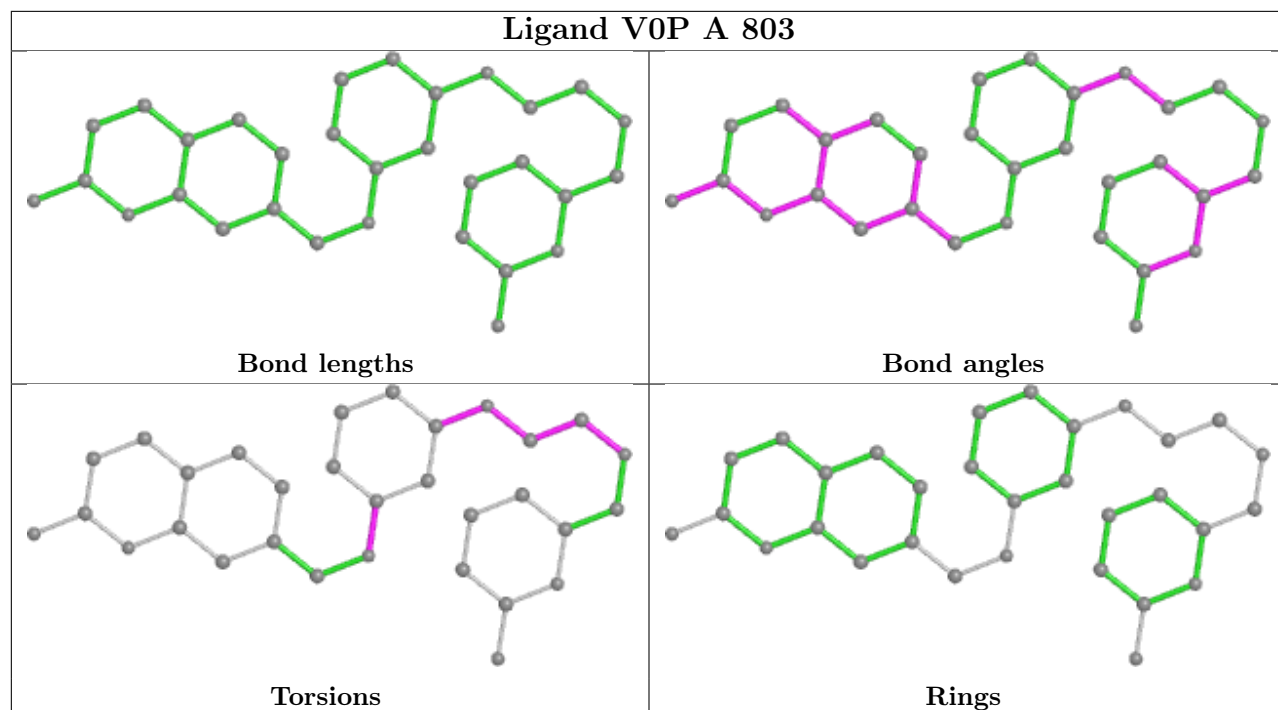
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	4	0
4	B	803	V0P	1	0
2	A	801	HEM	3	0

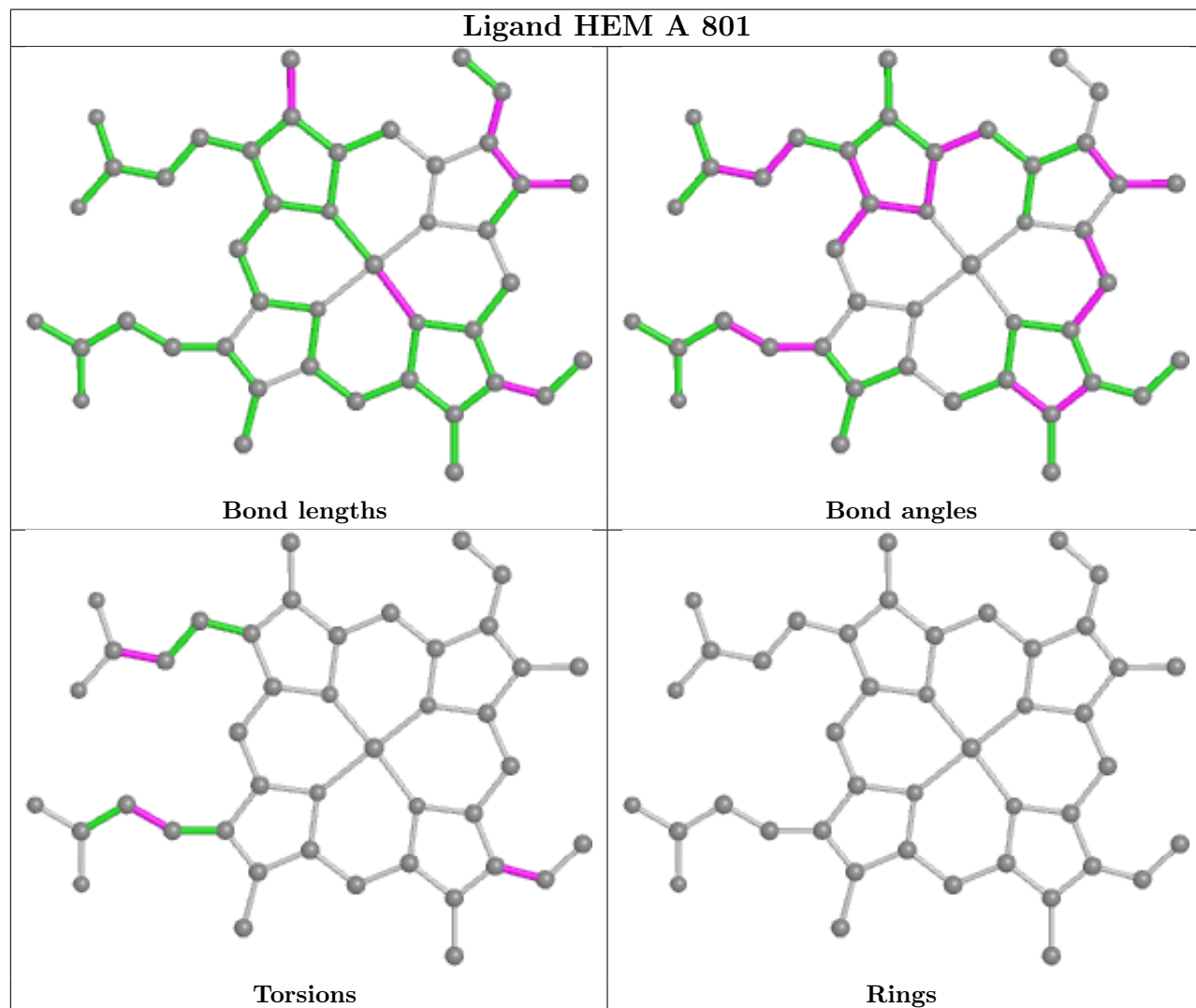
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 VOP A 803



Ligand HEM A 801



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%)	1.14	87 (21%) 0 0	32, 57, 108, 150	0
1	B	411/422 (97%)	0.49	38 (9%) 9 10	30, 46, 81, 111	0
All	All	822/844 (97%)	0.81	125 (15%) 2 2	30, 51, 100, 150	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	VAL	14.1
1	A	488	PRO	9.7
1	B	300	PHE	8.3
1	A	716	TRP	8.1
1	A	347	ASP	7.1
1	B	348	VAL	7.0
1	A	506	ILE	6.5
1	A	339	SER	6.4
1	A	715	VAL	6.1
1	A	490	GLY	6.0
1	B	350	THR	5.9
1	A	349	ARG	5.5
1	A	489	ASP	5.4
1	A	486	LYS	5.4
1	A	388	ILE	5.3
1	A	507	GLN	5.1
1	A	352	ASP	5.0
1	A	678	TRP	4.9
1	A	355	PHE	4.8
1	A	390	SER	4.8
1	B	299	ARG	4.8
1	A	677	VAL	4.8
1	A	350	THR	4.7
1	A	679	ILE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	373	GLY	4.6
1	A	391	THR	4.5
1	B	718	GLY	4.4
1	A	551	PHE	4.3
1	A	386	LYS	4.3
1	B	619	ARG	4.3
1	A	300	PHE	4.3
1	A	351	LYS	4.0
1	A	553	TRP	3.9
1	B	680	VAL	3.8
1	A	469	LYS	3.8
1	B	677	VAL	3.8
1	A	676	TRP	3.7
1	A	491	SER	3.6
1	A	567	VAL	3.6
1	A	322	LEU	3.5
1	A	691	PHE	3.5
1	B	679	ILE	3.4
1	A	393	THR	3.4
1	A	619	ARG	3.4
1	A	503	GLU	3.4
1	A	389	GLU	3.4
1	A	712	ASN	3.4
1	A	566	ALA	3.3
1	A	713	THR	3.3
1	A	353	GLN	3.3
1	B	318	LEU	3.2
1	A	480	ILE	3.2
1	A	487	GLN	3.2
1	B	616	LEU	3.2
1	A	584	PHE	3.1
1	A	479	LEU	3.1
1	A	354	LEU	3.0
1	A	681	PRO	3.0
1	A	667	ARG	2.9
1	B	310	VAL	2.9
1	A	415	CYS	2.9
1	B	567	VAL	2.9
1	A	511	LYS	2.8
1	B	322	LEU	2.8
1	A	714	HIS	2.8
1	A	321	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	492	THR	2.8
1	A	499	VAL	2.8
1	B	691	PHE	2.8
1	B	621	THR	2.8
1	A	643	SER	2.8
1	B	620	LYS	2.8
1	A	466	THR	2.7
1	B	617	ASP	2.7
1	A	517	PHE	2.7
1	B	351	LYS	2.7
1	B	562	TYR	2.7
1	B	566	ALA	2.7
1	B	611	ALA	2.7
1	A	392	SER	2.7
1	A	470	HIS	2.7
1	A	299	ARG	2.7
1	B	678	TRP	2.6
1	A	385	ASN	2.6
1	B	561	TRP	2.6
1	B	676	TRP	2.6
1	A	338	PRO	2.6
1	A	593	ILE	2.6
1	B	352	ASP	2.5
1	B	681	PRO	2.5
1	A	680	VAL	2.5
1	A	500	GLN	2.5
1	A	682	PRO	2.5
1	A	711	TRP	2.5
1	B	593	ILE	2.4
1	A	381	LEU	2.3
1	B	682	PRO	2.3
1	A	565	PRO	2.3
1	A	493	LEU	2.3
1	B	355	PHE	2.3
1	B	338	PRO	2.3
1	A	604	TYR	2.3
1	A	446	VAL	2.3
1	A	564	LEU	2.3
1	A	370	LYS	2.3
1	B	349	ARG	2.2
1	B	612	LYS	2.3
1	A	515	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	685	GLY	2.2
1	B	601	ASN	2.2
1	A	588	TYR	2.2
1	A	442	ILE	2.2
1	A	591	THR	2.2
1	A	416	VAL	2.2
1	B	321	THR	2.2
1	A	467	ASP	2.1
1	A	550	LYS	2.1
1	B	588	TYR	2.1
1	A	384	VAL	2.1
1	A	690	VAL	2.1
1	B	615	ASP	2.1
1	A	630	LEU	2.0
1	A	505	CYS	2.0
1	B	591	THR	2.0
1	A	409	TRP	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(\AA^2)	Q<0.9
5	ACT	A	804	4/4	0.79	0.21	68,72,77,79	0
4	V0P	A	803	31/31	0.84	0.31	36,103,116,119	0
4	V0P	B	803	31/31	0.89	0.27	36,101,116,116	0
3	H4B	A	802	17/17	0.92	0.15	38,46,60,61	0
5	ACT	B	804	4/4	0.93	0.15	57,67,72,81	0
3	H4B	B	802	17/17	0.94	0.13	39,47,59,60	0

Continued on next page...

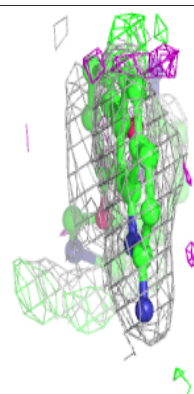
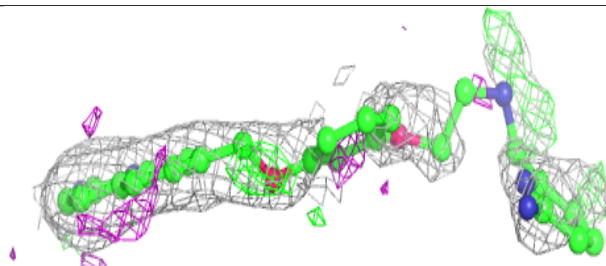
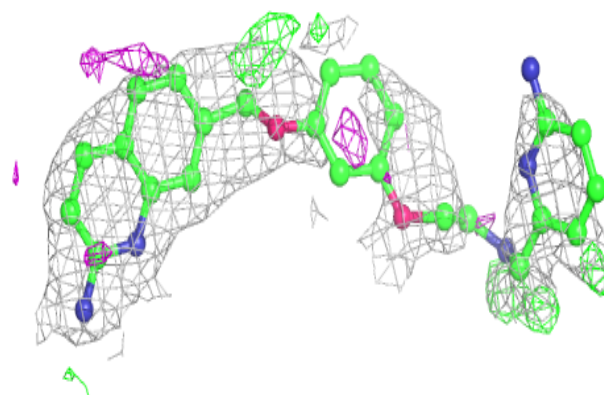
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	801	43/43	0.97	0.18	28,38,66,72	0
2	HEM	B	801	43/43	0.97	0.16	28,37,57,70	0
6	ZN	A	805	1/1	0.99	0.07	41,41,41,41	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.

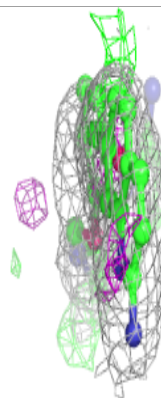
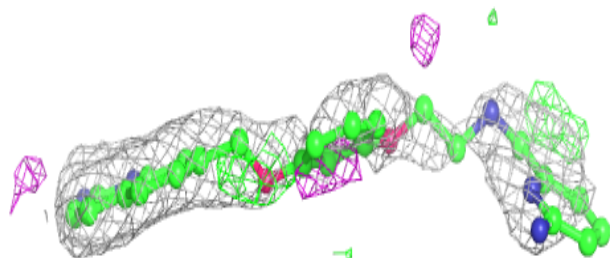
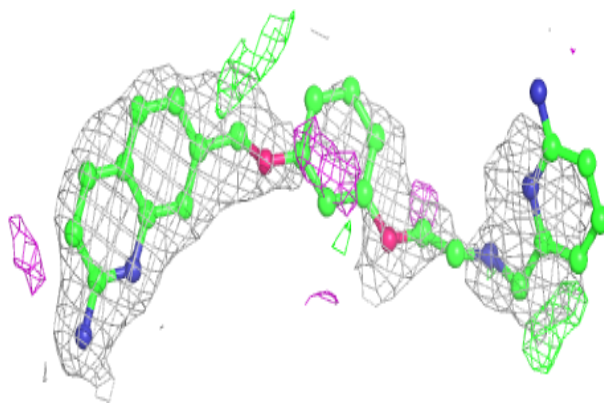
Electron density around V0P A 803:

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

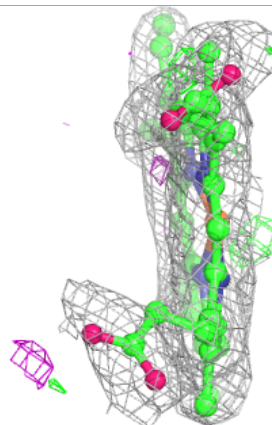
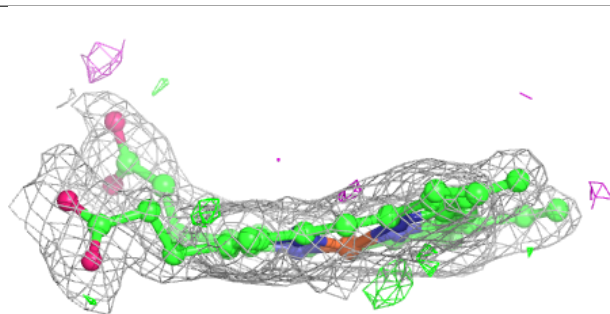
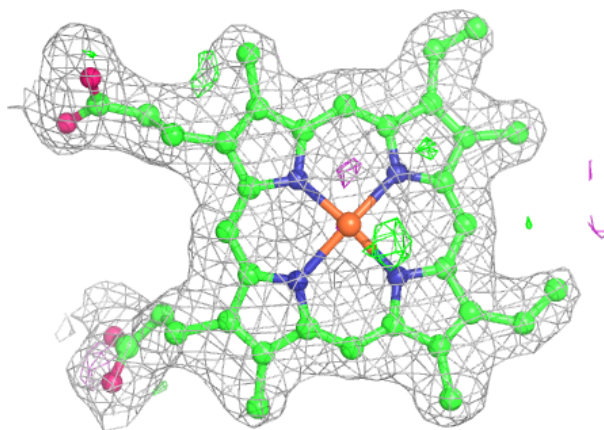


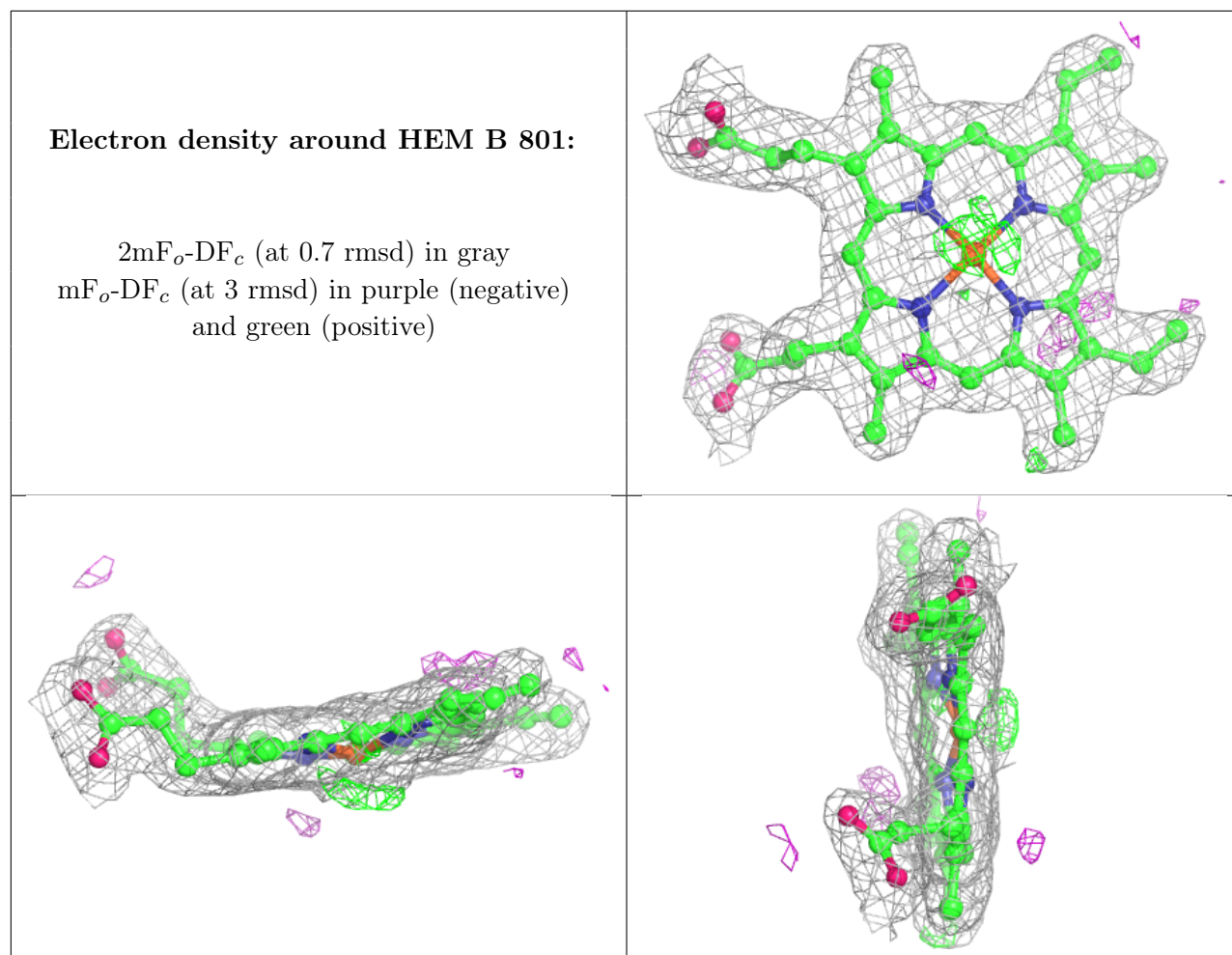
Electron density around V0P B 803:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.