



Full wwPDB X-ray Structure Validation Report i

Oct 6, 2023 – 01:45 AM EDT

PDB ID : 8FGF

Title : Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with 6-(5-(2-(dimethylamino)ethyl)-2,3-difluorophenethyl)pyridin-2-amine

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Deposited on : 2022-12-12

Resolution : 1.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the i symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

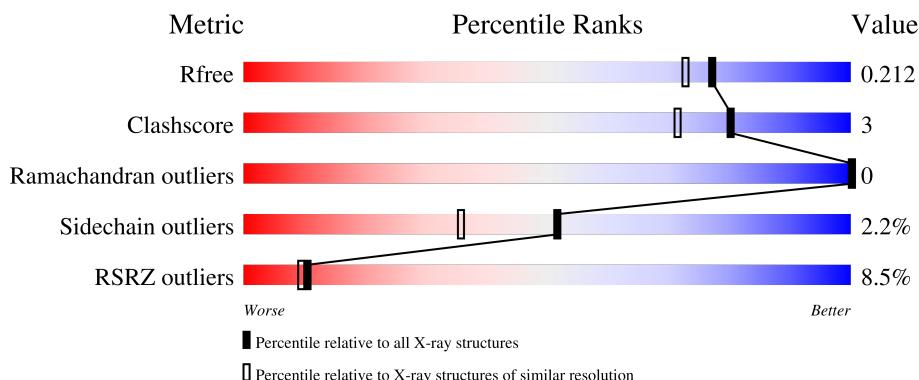
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

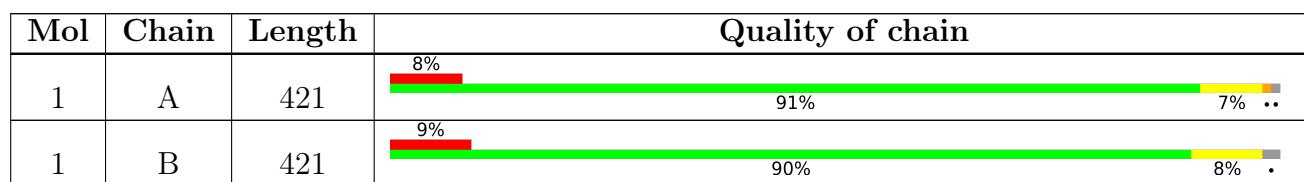
The reported resolution of this entry is 1.83 Å.

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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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.



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7701 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.

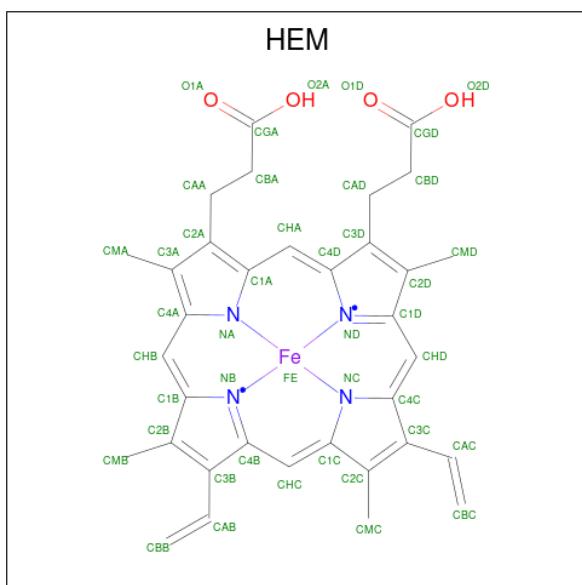
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	417	Total	C 3411	N 2183	O 581	S 624			
							23	0	4	0
1	B	411	Total	C 3367	N 2157	O 573	S 616			
							21	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

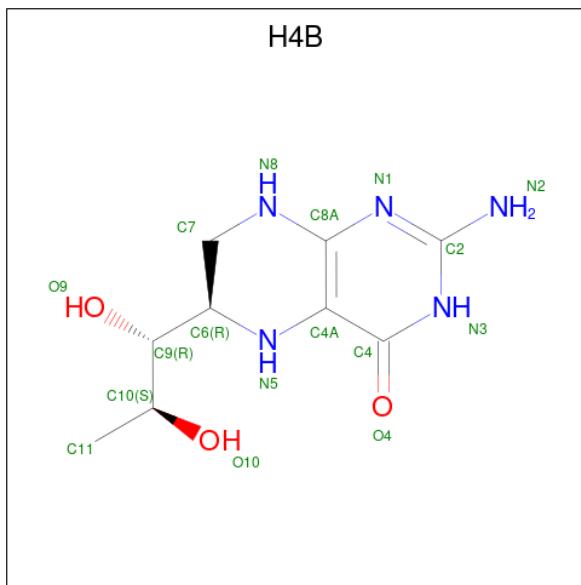
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



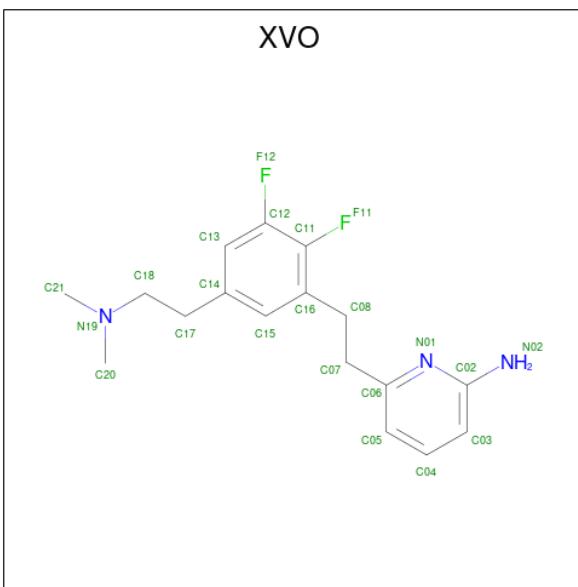
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total C Fe N O					0	0
2	B	1	Total C Fe N O					0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C₉H₁₅N₅O₃).



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

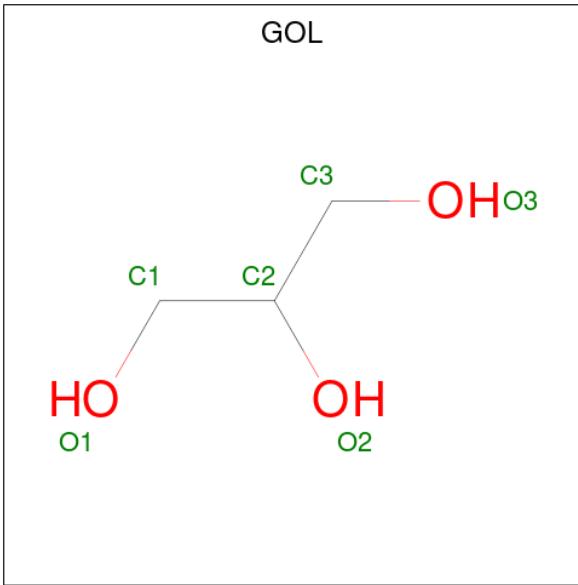
- Molecule 4 is 6-(2-{5-[2-(dimethylamino)ethyl]-2,3-difluorophenyl}ethyl)pyridin-2-amine (three-letter code: XVO) (formula: C₁₇H₂₁F₂N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	F	N	
			22	17	2	3	0

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	F	N	
			44	34	4	6	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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

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

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

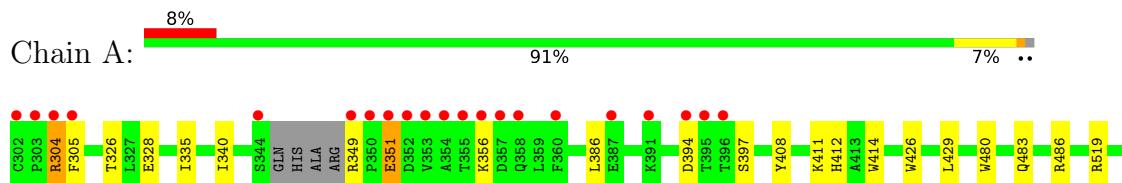
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	409	Total O 409 409	0	0
7	B	309	Total O 309 309	0	0

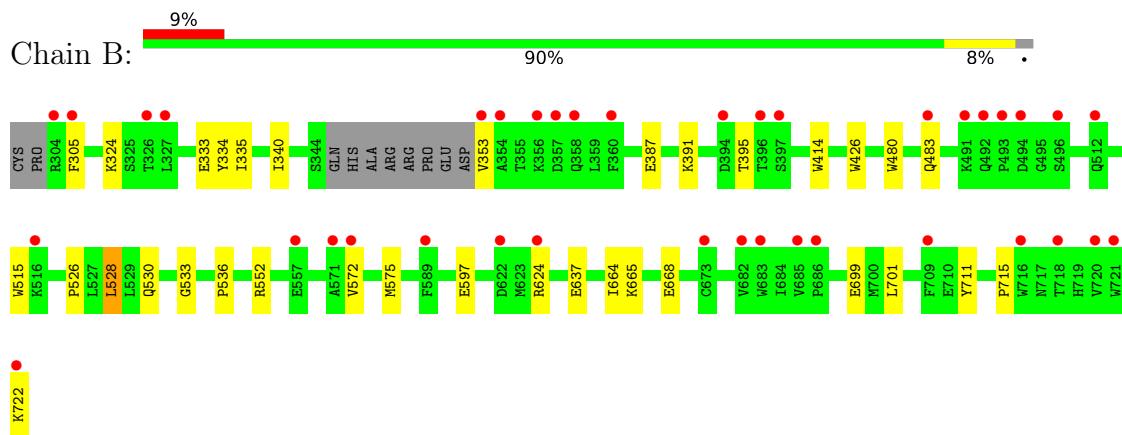
3 Residue-property plots

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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.40 Å 121.94 Å 164.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.93 – 1.83 38.63 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.93-1.83) 99.9 (38.63-1.83)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.18 (at 1.83 Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R , R_{free}	0.176 , 0.213 0.175 , 0.212	Depositor DCC
R_{free} test set	4634 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.1	EDS
L-test for twinning ²	$< L > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7701	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0/3520	0.53	0/4777
1	B	0.35	0/3475	0.50	0/4713
All	All	0.35	0/6995	0.52	0/9490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3411	0	3325	20	0
1	B	3367	0	3281	19	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	22	0	0	0	0
4	B	44	0	0	5	0
5	A	12	0	16	2	0
5	B	6	0	8	0	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	409	0	0	1	0
7	B	309	0	0	0	0
All	All	7701	0	6720	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (37) 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:528:LEU:HD22	1:A:536:PRO:HB2	1.64	0.78
1:A:349:ARG:HG2	1:A:351:GLU:H	1.58	0.69
1:A:519:ARG:NH1	7:A:901:HOH:O	2.24	0.69
1:B:664:ILE:O	1:B:668[B]:GLU:HG2	1.95	0.67
1:A:613:GLU:HG3	1:A:623:MET:HE1	1.77	0.65
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.79	0.65
1:A:429:LEU:O	5:A:805:GOL:H12	1.98	0.63
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.80	0.62
1:A:633:GLN:NE2	1:B:637:GLU:OE2	2.34	0.60
1:B:711:TYR:OH	2:B:801:HEM:O2D	2.19	0.57
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.87	0.56
1:B:575:MET:SD	4:B:803[A]:XVO:F12	2.56	0.53
1:A:711:TYR:OH	2:A:801:HEM:O1D	2.25	0.50
1:A:691:SER:HA	1:A:696:PHE:CG	2.50	0.47
1:A:411:LYS:NZ	5:A:805:GOL:H11	2.29	0.47
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.50	0.46
1:A:699:GLU:HB3	1:B:340:ILE:HD13	1.98	0.46
1:B:515:TRP:CE2	1:B:526:PRO:HD3	2.51	0.46
1:A:326:THR:HG21	1:A:706[A]:THR:HG22	1.98	0.45
1:A:408:TYR:CE1	1:A:412:HIS:CE1	3.04	0.45
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.51	0.45
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.52	0.45
1:A:483:GLN:HB2	1:A:486:ARG:HG2	1.99	0.44
1:A:356:LYS:HE2	1:A:397:SER:OG	2.18	0.43
1:B:334:TYR:C	1:B:335:ILE:HG13	2.39	0.43
1:A:340:ILE:HD13	1:B:699:GLU:HB3	2.00	0.42
1:B:480:TRP:HB2	1:B:528:LEU:HB3	2.00	0.42
1:B:483[B]:GLN:HG2	4:B:803[B]:XVO:C12	2.50	0.42
1:A:335:ILE:HD11	1:B:701:LEU:HB3	2.02	0.42
1:A:480:TRP:HB2	1:A:528:LEU:HB3	2.02	0.42
1:B:530:GLN:HE21	1:B:533:GLY:HA2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:VAL:HG21	4:B:803[A]:XVO:C11	2.50	0.41
1:B:387:GLU:OE2	1:B:391:LYS:NZ	2.46	0.41
2:B:801:HEM:HBD1	4:B:803[A]:XVO:C11	2.51	0.41
1:B:597:GLU:OE2	4:B:803[A]:XVO:N02	2.54	0.41
1:A:328:GLU:OE1	1:B:333:GLU:HB3	2.22	0.40
1:A:304:ARG:HD3	1:A:305:PHE:CE1	2.57	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	417/421 (99%)	411 (99%)	6 (1%)	0	100 100
1	B	411/421 (98%)	405 (98%)	6 (2%)	0	100 100
All	All	828/842 (98%)	816 (99%)	12 (1%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	377/376 (100%)	369 (98%)	8 (2%)	53 38
1	B	371/376 (99%)	362 (98%)	9 (2%)	49 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	748/752 (100%)	731 (98%)	17 (2%)	52 34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ARG
1	A	351	GLU
1	A	386	LEU
1	A	394	ASP
1	A	528	LEU
1	A	552	ARG
1	A	673[A]	CYS
1	A	673[B]	CYS
1	B	305	PHE
1	B	324	LYS
1	B	353	VAL
1	B	395	THR
1	B	528	LEU
1	B	552	ARG
1	B	624	ARG
1	B	665	LYS
1	B	722	LYS

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

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	XVO	A	803	-	23,23,23	0.41	0	30,31,31	2.62	8 (26%)
3	H4B	B	802	-	16,18,18	0.89	0	11,26,26	2.72	6 (54%)
2	HEM	B	801	1	41,50,50	1.52	6 (14%)	45,82,82	1.82	11 (24%)
4	XVO	B	803[A]	-	23,23,23	0.36	0	30,31,31	1.88	6 (20%)
2	HEM	A	801	1	41,50,50	1.42	3 (7%)	45,82,82	1.60	5 (11%)
5	GOL	A	804	-	5,5,5	0.38	0	5,5,5	0.21	0
4	XVO	B	803[B]	-	23,23,23	0.37	0	30,31,31	2.05	6 (20%)
5	GOL	B	804	-	5,5,5	0.36	0	5,5,5	0.26	0
5	GOL	A	805	-	5,5,5	0.42	0	5,5,5	0.55	0
3	H4B	A	802	-	16,18,18	0.82	1 (6%)	11,26,26	2.66	5 (45%)

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	XVO	A	803	-	-	4/10/10/10	0/2/2/2
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
2	HEM	B	801	1	-	2/12/54/54	-
4	XVO	B	803[A]	-	-	8/10/10/10	0/2/2/2
2	HEM	A	801	1	-	0/12/54/54	-
5	GOL	A	804	-	-	2/4/4/4	-
4	XVO	B	803[B]	-	-	4/10/10/10	0/2/2/2
5	GOL	B	804	-	-	2/4/4/4	-
5	GOL	A	805	-	-	4/4/4/4	-
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3C-C2C	-3.96	1.34	1.40
2	A	801	HEM	C3C-C2C	-3.67	1.35	1.40
2	A	801	HEM	C3C-CAC	3.53	1.55	1.47
2	B	801	HEM	C3C-CAC	3.49	1.55	1.47
2	A	801	HEM	CAB-C3B	3.07	1.55	1.47
2	B	801	HEM	CAB-C3B	2.80	1.55	1.47
2	B	801	HEM	CAA-C2A	2.20	1.55	1.52
2	B	801	HEM	CMC-C2C	2.13	1.56	1.51
2	B	801	HEM	CMB-C2B	2.11	1.55	1.50
3	A	802	H4B	C4A-C4	-2.09	1.38	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	XVO	C08-C07-C06	-7.59	95.98	112.99
2	A	801	HEM	CBA-CAA-C2A	-6.67	101.24	112.62
4	A	803	XVO	C02-N01-C06	5.98	122.63	118.10
4	A	803	XVO	C08-C16-C11	-5.83	116.05	120.73
2	B	801	HEM	C4B-CHC-C1C	5.67	130.04	122.56
3	B	802	H4B	C8A-C4A-C4	5.52	119.47	114.57
4	B	803[A]	XVO	C08-C16-C11	-4.99	116.72	120.73
4	B	803[A]	XVO	C02-N01-C06	4.91	121.82	118.10
4	A	803	XVO	C07-C08-C16	4.91	120.75	112.81
4	B	803[B]	XVO	C02-N01-C06	4.86	121.79	118.10
4	B	803[B]	XVO	C08-C16-C11	-4.86	116.83	120.73
3	A	802	H4B	C8A-C4A-C4	4.82	118.85	114.57
4	B	803[B]	XVO	C08-C07-C06	-4.78	102.27	112.99
2	B	801	HEM	CBA-CAA-C2A	-4.29	105.30	112.62
3	A	802	H4B	C2-N3-C4	4.12	122.48	115.93
4	B	803[A]	XVO	C15-C16-C11	3.65	120.10	116.76
4	B	803[B]	XVO	C15-C16-C11	3.63	120.08	116.76
4	A	803	XVO	C15-C16-C11	3.48	119.94	116.76
3	B	802	H4B	C2-N3-C4	3.47	121.44	115.93
3	A	802	H4B	N1-C2-N3	-3.34	120.18	125.42
3	B	802	H4B	C4-C4A-N5	3.31	121.90	119.12
2	A	801	HEM	CBD-CAD-C3D	-3.16	103.86	112.63
4	B	803[A]	XVO	C08-C07-C06	-3.11	106.01	112.99
2	B	801	HEM	CMA-C3A-C4A	-3.03	123.81	128.46
3	B	802	H4B	N1-C2-N3	-3.00	120.71	125.42
3	A	802	H4B	C4-C4A-N5	3.00	121.64	119.12
4	B	803[A]	XVO	C07-C06-N01	2.75	120.04	115.95
4	B	803[B]	XVO	C07-C08-C16	2.69	117.16	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CMC-C2C-C3C	2.65	129.64	124.68
2	B	801	HEM	CAD-C3D-C2D	-2.58	123.08	127.88
2	B	801	HEM	CHD-C1D-ND	2.44	127.09	124.43
3	B	802	H4B	C2-N1-C8A	2.42	119.96	114.54
2	B	801	HEM	C3D-C4D-ND	-2.41	107.48	110.17
2	A	801	HEM	C3B-C2B-C1B	2.40	108.27	106.49
2	B	801	HEM	C4D-ND-C1D	2.37	107.52	105.07
4	A	803	XVO	C05-C06-N01	-2.36	119.41	122.41
2	A	801	HEM	C4B-CHC-C1C	2.36	125.67	122.56
2	B	801	HEM	C3B-C2B-C1B	2.29	108.18	106.49
4	A	803	XVO	C08-C16-C15	2.28	124.01	119.41
2	B	801	HEM	C1B-NB-C4B	2.28	107.43	105.07
3	A	802	H4B	C2-N1-C8A	2.25	119.58	114.54
4	B	803[A]	XVO	C05-C06-N01	-2.18	119.65	122.41
3	B	802	H4B	N2-C2-N3	2.13	120.56	117.25
2	B	801	HEM	CHA-C4D-ND	2.07	126.94	124.38
2	B	801	HEM	C4A-C3A-C2A	2.06	108.43	107.00
4	A	803	XVO	C18-C17-C14	-2.06	106.28	112.16
4	B	803[B]	XVO	N02-C02-N01	2.02	119.69	116.49

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803[A]	XVO	C07-C08-C16-C11
4	B	803[B]	XVO	C07-C08-C16-C11
5	A	804	GOL	O1-C1-C2-O2
5	A	804	GOL	O1-C1-C2-C3
5	A	805	GOL	O1-C1-C2-O2
5	A	805	GOL	O1-C1-C2-C3
5	A	805	GOL	C1-C2-C3-O3
5	B	804	GOL	O1-C1-C2-C3
4	B	803[A]	XVO	C17-C18-N19-C20
4	B	803[A]	XVO	C17-C18-N19-C21
5	B	804	GOL	O1-C1-C2-O2
4	A	803	XVO	C14-C17-C18-N19
5	A	805	GOL	O2-C2-C3-O3
4	A	803	XVO	C17-C18-N19-C20
4	B	803[A]	XVO	C07-C08-C16-C15
2	B	801	HEM	C4B-C3B-CAB-CBB
4	A	803	XVO	C07-C08-C16-C11
2	B	801	HEM	C2A-CAA-CBA-CGA

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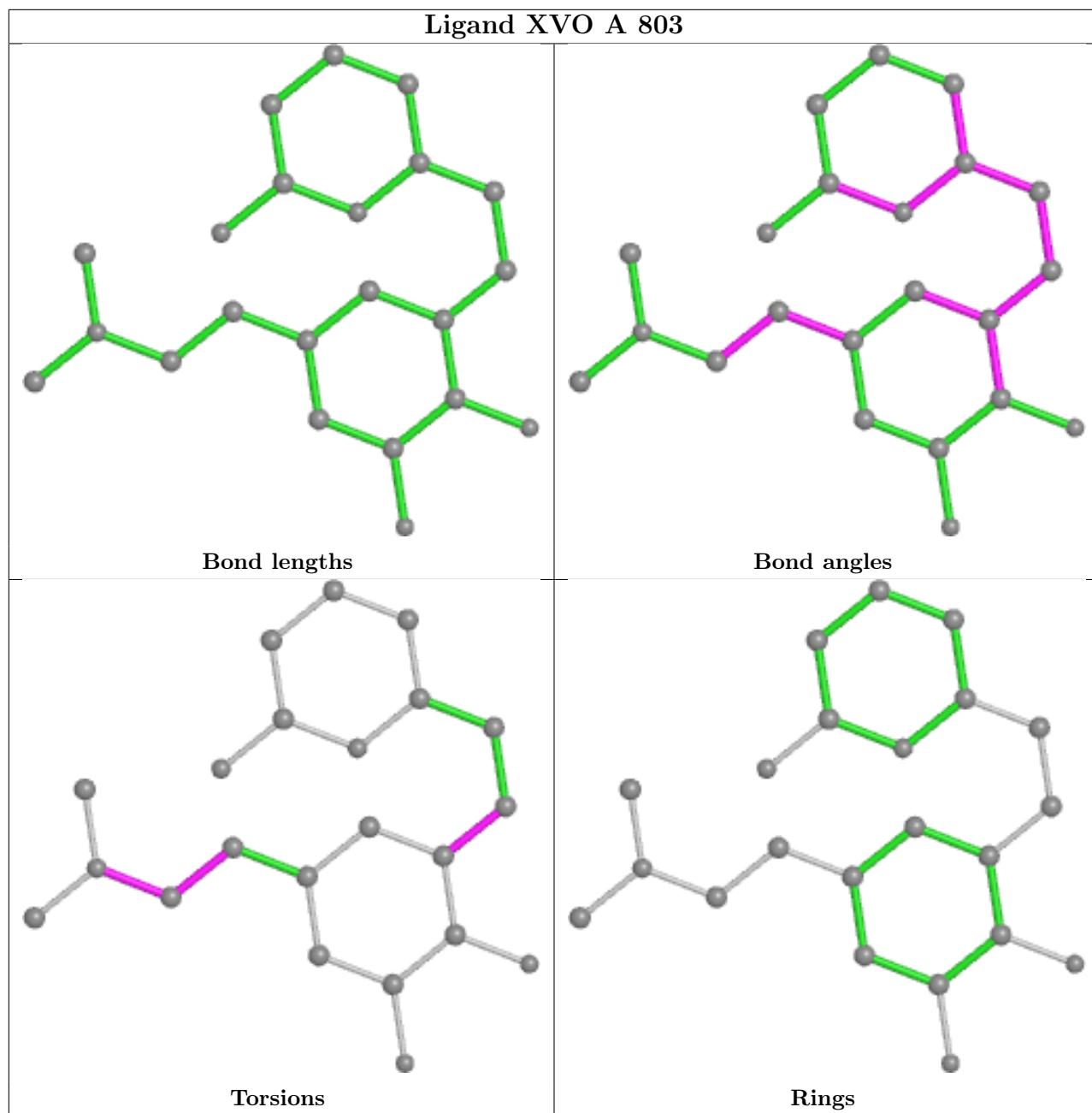
Mol	Chain	Res	Type	Atoms
4	B	803[A]	XVO	C13-C14-C17-C18
4	B	803[A]	XVO	C15-C14-C17-C18
4	B	803[B]	XVO	C15-C14-C17-C18
4	B	803[B]	XVO	C13-C14-C17-C18
4	A	803	XVO	C17-C18-N19-C21
4	B	803[A]	XVO	C05-C06-C07-C08
4	B	803[A]	XVO	N01-C06-C07-C08
4	B	803[B]	XVO	C07-C08-C16-C15

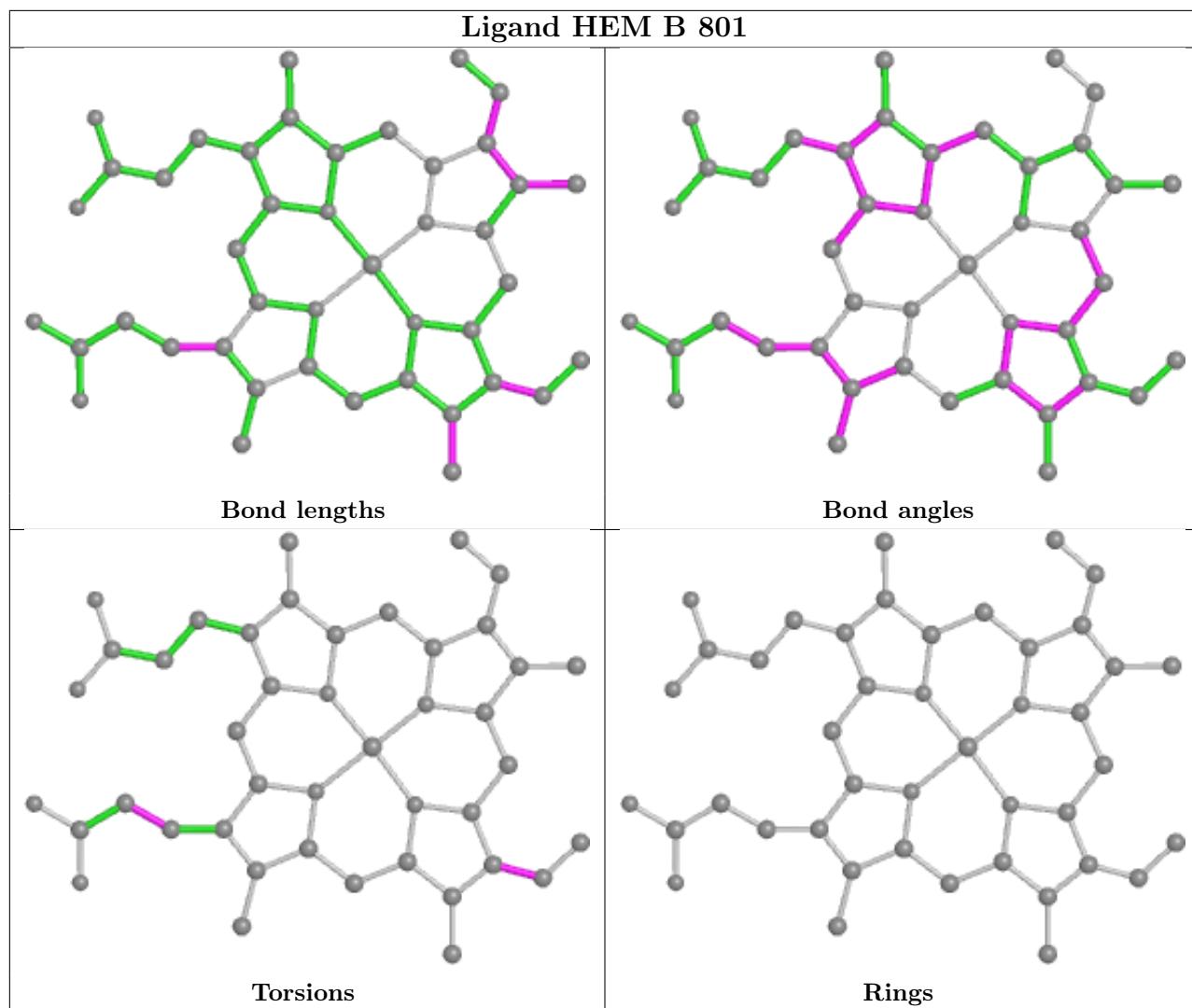
There are no ring outliers.

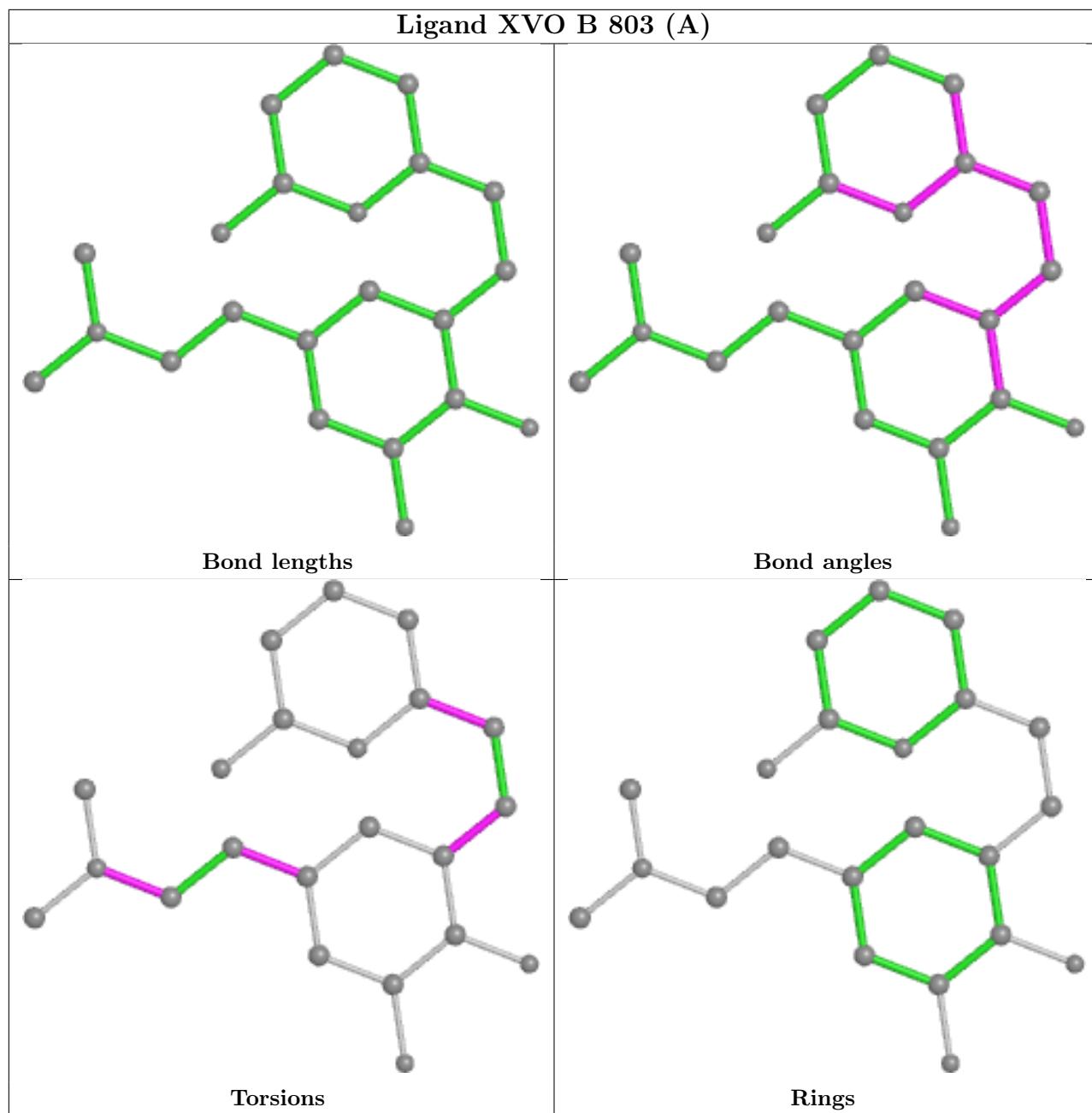
5 monomers are involved in 11 short contacts:

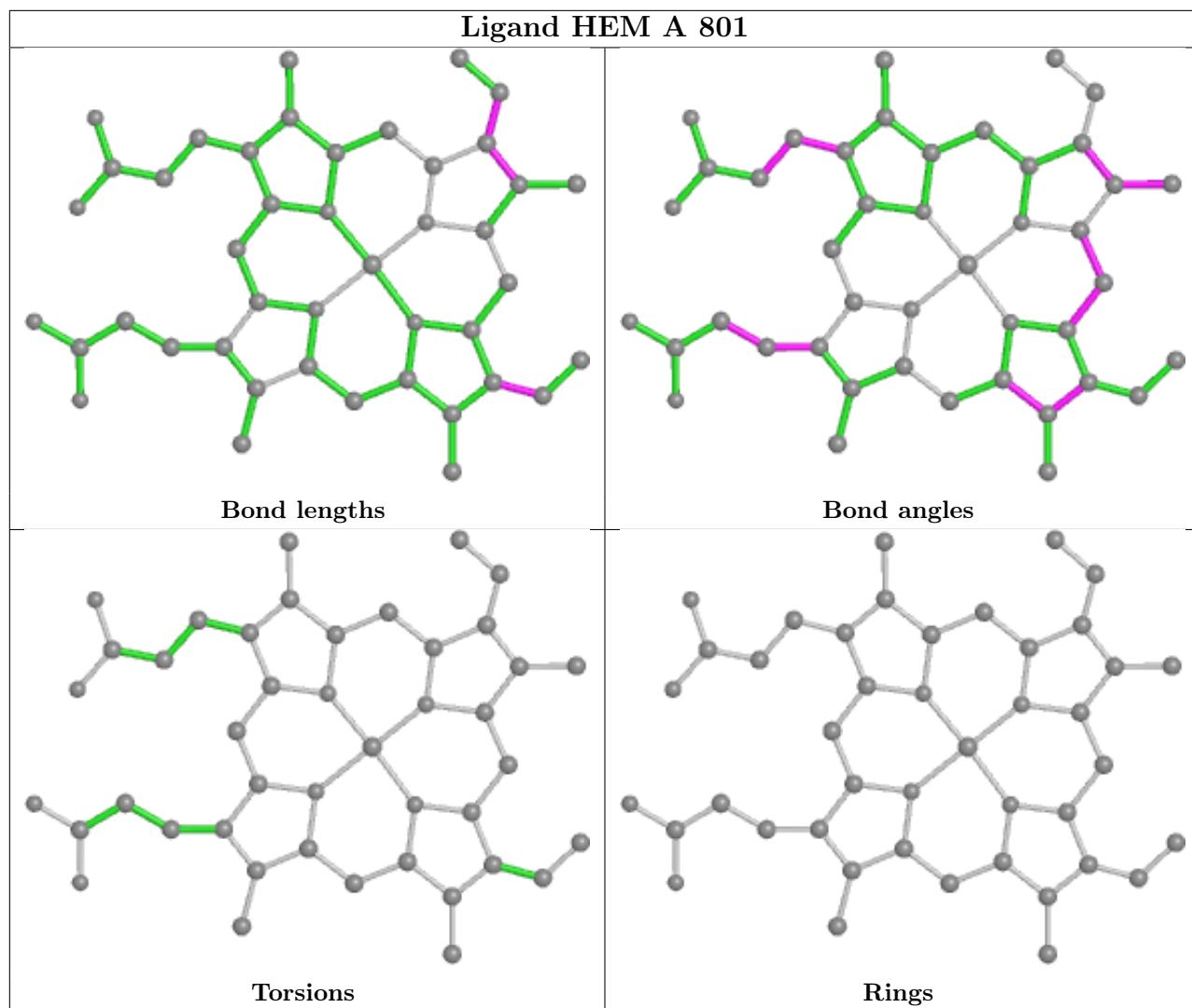
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	3	0
4	B	803[A]	XVO	4	0
2	A	801	HEM	2	0
4	B	803[B]	XVO	1	0
5	A	805	GOL	2	0

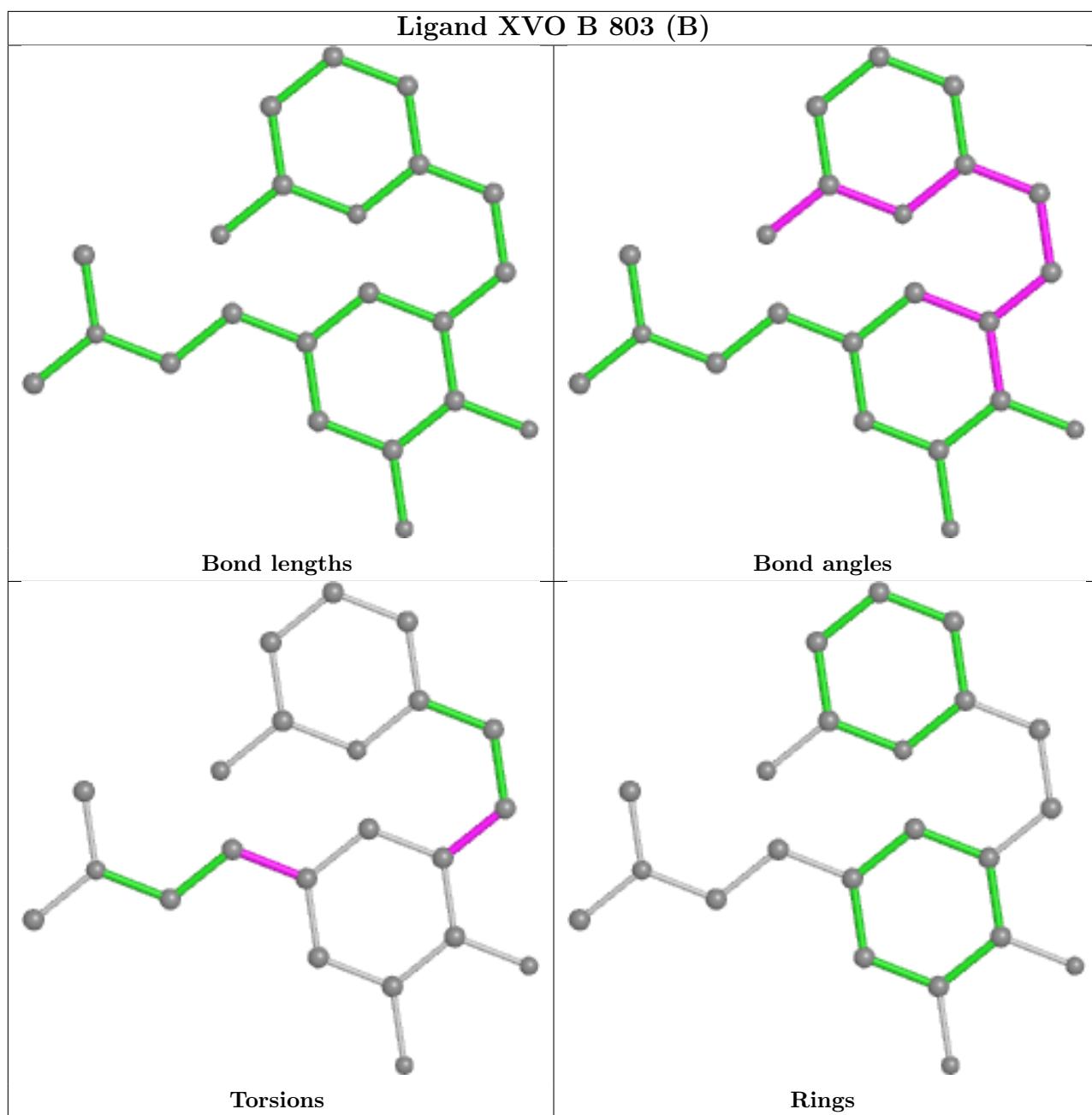
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/421 (99%)	0.20	32 (7%) 13 12	22, 35, 68, 125	0
1	B	411/421 (97%)	0.42	38 (9%) 9 7	24, 40, 77, 115	0
All	All	828/842 (98%)	0.31	70 (8%) 10 9	22, 38, 74, 125	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	PRO	9.0
1	B	721	TRP	6.7
1	B	720	VAL	6.2
1	B	326	THR	5.9
1	B	357	ASP	5.7
1	A	353	VAL	5.5
1	B	353	VAL	5.3
1	B	304	ARG	4.6
1	A	303	PRO	4.3
1	B	305	PHE	4.2
1	B	396	THR	4.2
1	A	302	CYS	4.0
1	A	344	SER	3.9
1	A	305	PHE	3.8
1	B	493	PRO	3.8
1	B	624	ARG	3.8
1	B	683	TRP	3.7
1	B	360	PHE	3.7
1	A	351	GLU	3.6
1	A	352	ASP	3.5
1	B	718	THR	3.3
1	B	572	VAL	3.2
1	A	395	THR	3.2
1	B	358	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	496	SER	3.1
1	A	355	THR	3.1
1	B	354	ALA	3.1
1	B	685	VAL	3.0
1	A	624	ARG	3.0
1	A	304	ARG	3.0
1	A	354	ALA	3.0
1	B	571	ALA	3.0
1	A	349	ARG	2.9
1	B	557	GLU	2.9
1	B	622	ASP	2.8
1	A	360	PHE	2.8
1	B	589	PHE	2.8
1	B	716	TRP	2.7
1	A	356	LYS	2.7
1	A	572	VAL	2.7
1	A	684	ILE	2.7
1	A	358	GLN	2.6
1	B	356	LYS	2.6
1	B	722	LYS	2.6
1	A	685	VAL	2.6
1	B	494	ASP	2.6
1	A	589	PHE	2.5
1	A	357	ASP	2.5
1	A	696	PHE	2.5
1	A	391	LYS	2.4
1	A	620	ASN	2.4
1	B	682	VAL	2.4
1	B	491	LYS	2.4
1	A	394	ASP	2.3
1	B	709	PHE	2.3
1	B	512	GLN	2.2
1	A	396	THR	2.2
1	B	394	ASP	2.2
1	B	673	CYS	2.2
1	A	692	ILE	2.2
1	A	683	TRP	2.2
1	B	492	GLN	2.2
1	B	397	SER	2.1
1	A	682	VAL	2.1
1	B	327	LEU	2.1
1	B	686	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	483[A]	GLN	2.1
1	A	681	TRP	2.1
1	B	516	LYS	2.1
1	A	387	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

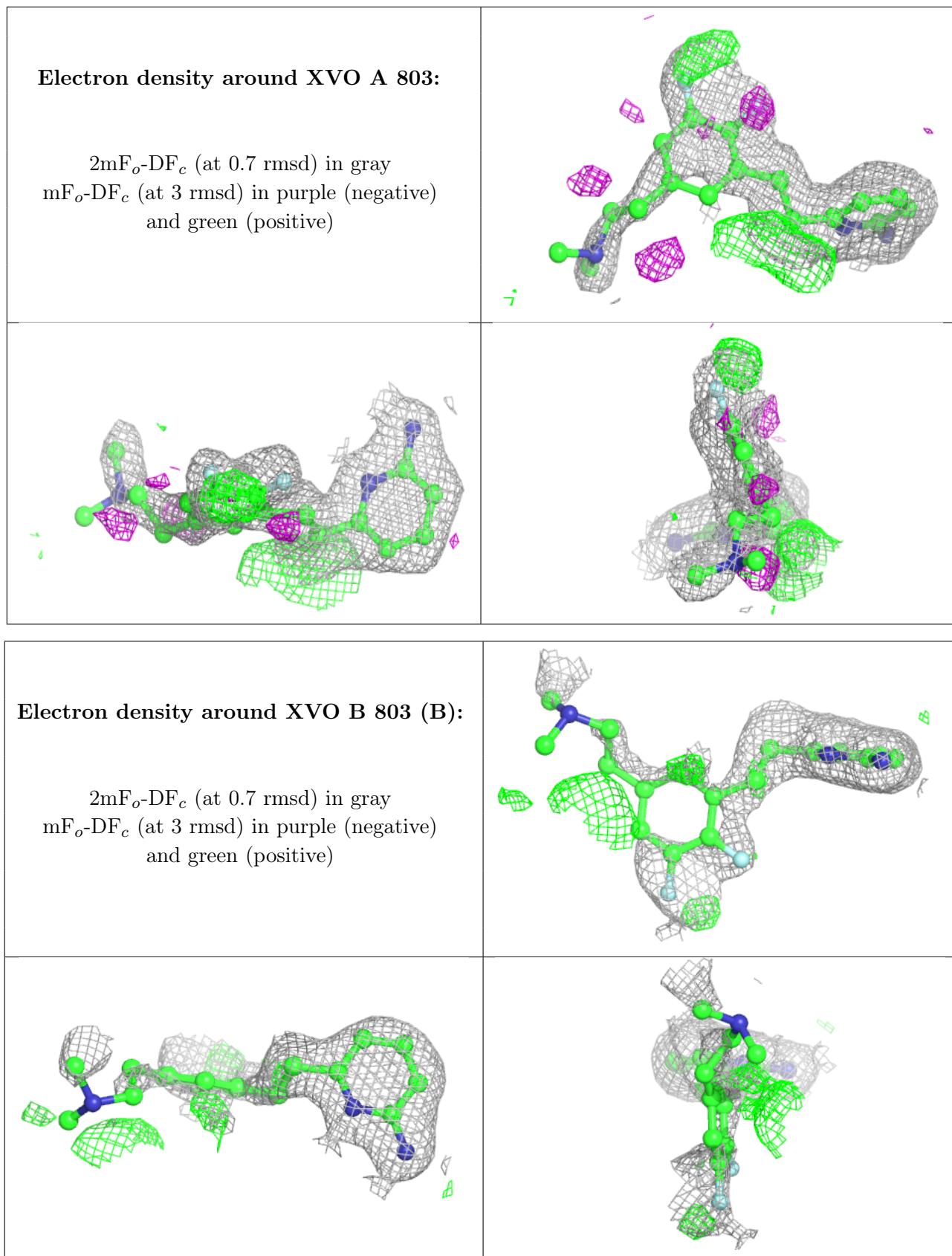
There are no monosaccharides in this entry.

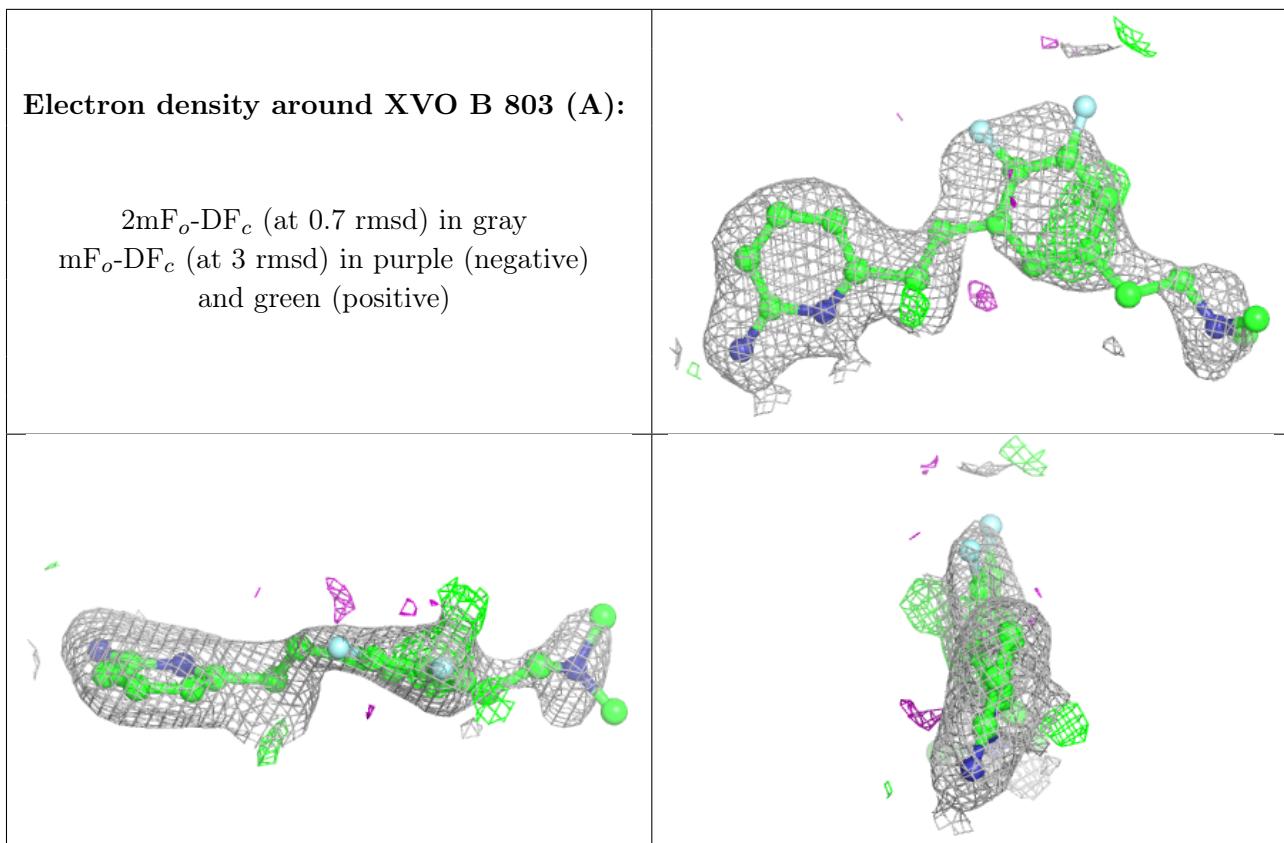
6.4 Ligands [\(i\)](#)

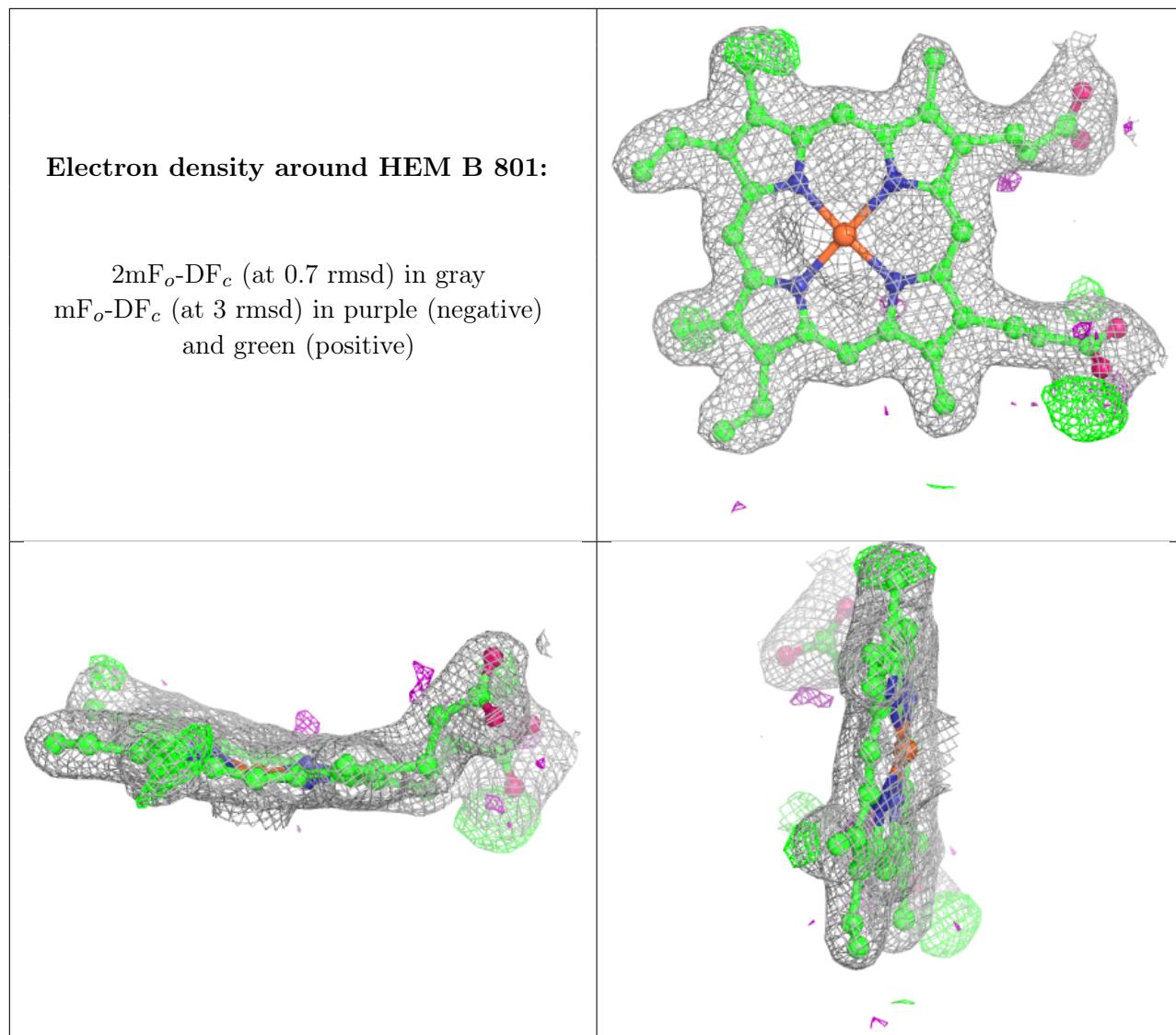
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

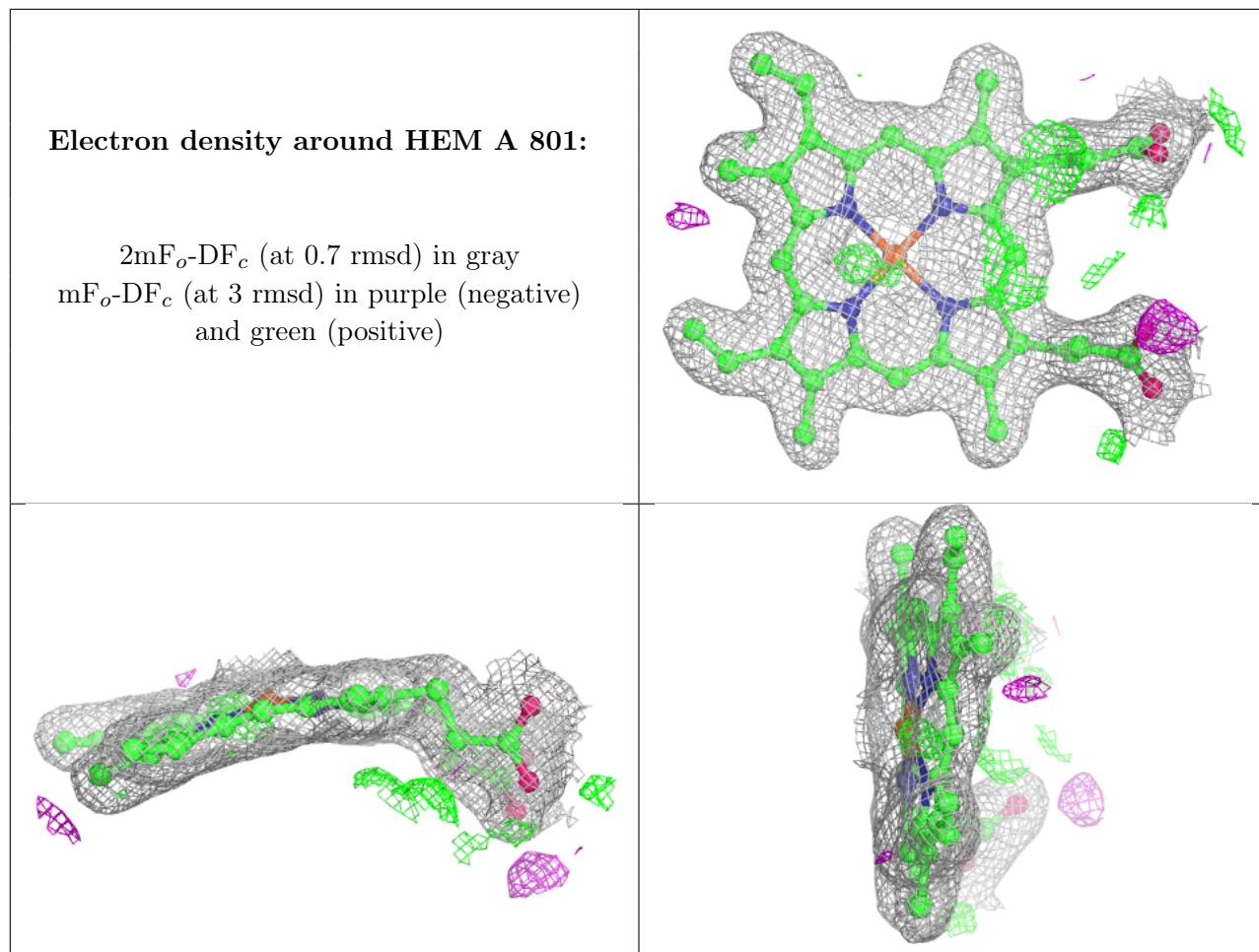
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	804	6/6	0.53	0.25	69,71,79,81	0
5	GOL	A	804	6/6	0.78	0.21	59,61,65,67	0
5	GOL	A	805	6/6	0.84	0.18	48,63,70,79	0
4	XVO	A	803	22/22	0.88	0.31	27,81,91,95	0
4	XVO	B	803[B]	22/22	0.90	0.63	27,58,64,67	22
4	XVO	B	803[A]	22/22	0.90	0.63	26,55,67,72	22
3	H4B	B	802	17/17	0.94	0.16	26,30,35,35	0
3	H4B	A	802	17/17	0.95	0.12	25,31,38,40	0
2	HEM	B	801	43/43	0.97	0.17	19,29,42,56	0
2	HEM	A	801	43/43	0.98	0.19	20,26,38,39	0
6	ZN	A	806	1/1	1.00	0.07	28,28,28,28	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.









6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.