



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 02:00 PM EDT

PDB ID : 5UNX
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-(2-(methylamino)ethyl)benzotrile
Authors : Li, H.; Poulos, T.L.
Deposited on : 2017-01-31
Resolution : 2.03 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)
Xtrriage (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

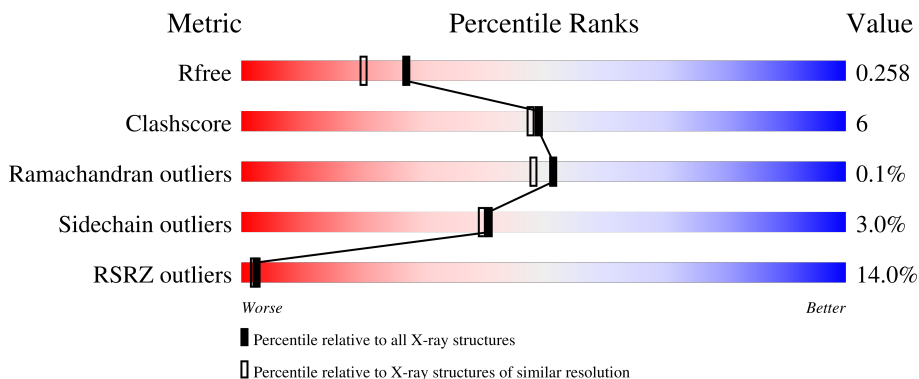
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	
1	B	422	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7065 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
			Total	C	N	O	S			
1	A	409	Total	C	N	O	S	0	2	0
			3334	2134	571	607	22			
1	B	411	Total	C	N	O	S	0	2	0
			3351	2144	574	612	21			

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



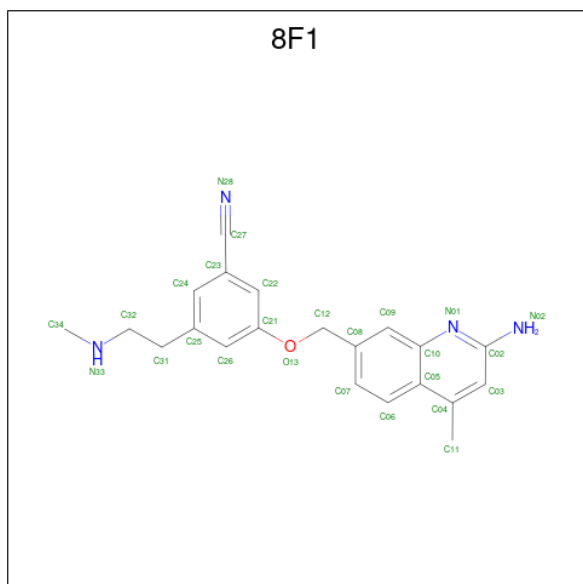
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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
			Total	C	N	O		
3	A	1	17	9	5	3	0	0
3	B	1	17	9	5	3	0	0

- Molecule 4 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[2-(methylamino)ethyl]benzonitrile (three-letter code: 8F1) (formula: C₂₁H₂₂N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	26	21	4	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	26	21	4	1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

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

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

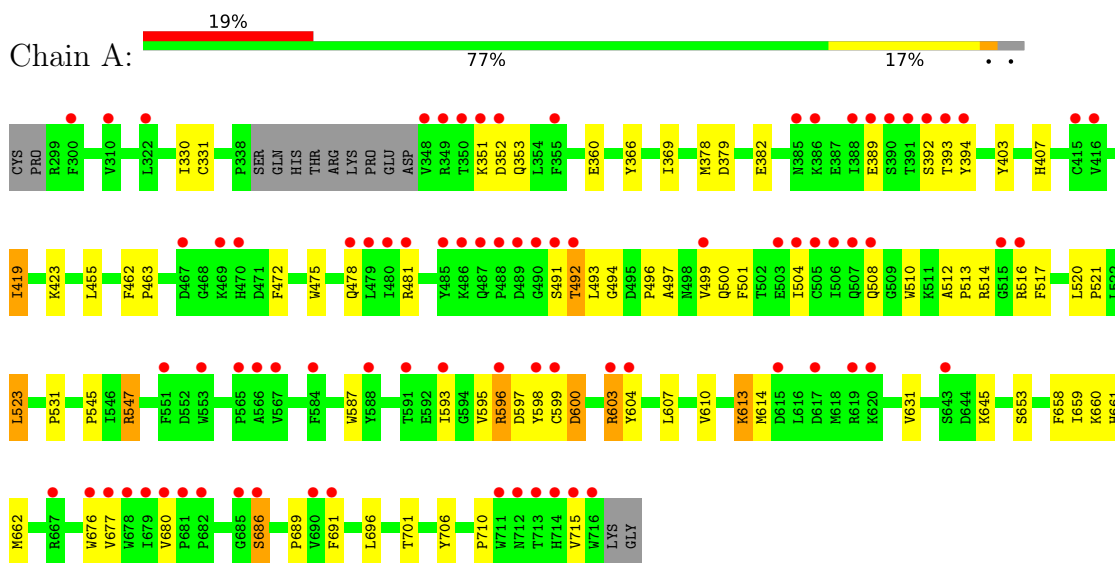
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	85	85	85	0	0
7	B	114	114	114	0	0

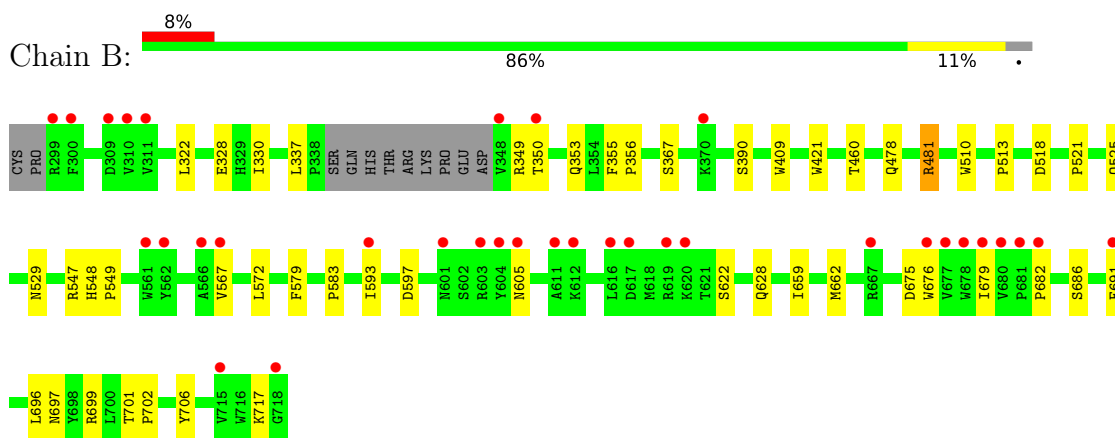
3 Residue-property plots [i](#)

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	51.63Å 111.72Å 164.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.13 – 2.03 39.13 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.13-2.03) 95.0 (39.13-1.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.205 , 0.258 0.207 , 0.258	Depositor DCC
R_{free} test set	3147 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtrriage
Anisotropy	0.643	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7065	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: ACT, H4B, 8F1, ZN, 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	0.39	0/3430	0.52	0/4653
1	B	0.41	0/3450	0.51	0/4677
All	All	0.40	0/6880	0.52	0/9330

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	613	LYS	Peptide

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	3334	0	3248	52	0
1	B	3351	0	3269	30	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	26	0	0	0	0
4	B	26	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
7	A	85	0	0	2	0
7	B	114	0	0	3	0
All	All	7065	0	6613	80	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 6.

All (80) 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	0.83
1:B:706:TYR:OH	2:B:801:HEM:O2D	2.01	0.77
1:A:706:TYR:OH	2:A:801:HEM:O2D	2.04	0.75
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.72	0.72
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.54	0.72
1:A:597:ASP:OD1	1:A:603:ARG:NH2	2.22	0.72
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.73	0.69
1:A:497:ALA:HB2	1:A:603:ARG:HD2	1.76	0.68
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.76	0.67
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.80	0.63
1:A:508:GLN:HE22	1:A:531:PRO:HD2	1.65	0.62
1:A:599:CYS:HB2	1:A:607:LEU:HG	1.80	0.62
1:A:596:ARG:O	1:A:600:ASP:HB2	2.00	0.61
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.82	0.60
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.85	0.59
1:A:419:ILE:HG13	1:A:661:HIS:HB2	1.86	0.56
1:A:379:ASP:O	1:A:382:GLU:HG3	2.06	0.55
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.88	0.54
1:B:605:ASN:O	7:B:901:HOH:O	2.18	0.54
1:A:686:SER:HB3	1:B:682:PRO:HB2	1.89	0.53
1:A:494:GLY:HA2	1:A:516:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.90	0.52
1:A:492:THR:OG1	1:A:496:PRO:HG3	2.09	0.52
1:B:593:ILE:HA	1:B:597:ASP:HB2	1.92	0.51
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.46	0.51
1:B:525:GLN:HG3	1:B:529:ASN:O	2.10	0.50
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.93	0.50
1:A:658:PHE:CE2	1:A:662:MET:HE2	2.47	0.49
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.48	0.49
1:A:593:ILE:HA	1:A:597:ASP:HB2	1.93	0.49
1:A:393:THR:OG1	1:A:394:TYR:N	2.46	0.48
1:A:516:ARG:HG3	1:A:517:PHE:CD1	2.49	0.48
1:B:593:ILE:O	1:B:597:ASP:HB2	2.14	0.48
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.96	0.48
1:B:350:THR:OG1	1:B:353:GLN:OE1	2.25	0.47
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.50	0.46
2:B:801:HEM:O1A	7:B:902:HOH:O	2.21	0.46
1:B:686:SER:HA	1:B:691:PHE:CG	2.50	0.46
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.31	0.46
1:A:659:ILE:HG13	1:A:689:PRO:HB2	1.97	0.46
1:B:717:LYS:NZ	7:B:910:HOH:O	2.49	0.45
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.38	0.45
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.52	0.44
1:A:352:ASP:OD1	1:A:353:GLN:N	2.51	0.44
1:A:595:VAL:HG12	1:B:686:SER:OG	2.18	0.44
1:A:686:SER:HA	1:A:691:PHE:CG	2.52	0.44
1:A:677:VAL:HG13	1:B:676:TRP:CZ3	2.53	0.44
1:A:500:GLN:O	1:A:504:ILE:HG13	2.18	0.43
1:B:572:LEU:HB3	1:B:579:PHE:HB2	2.00	0.43
1:A:645:LYS:HB2	1:A:645:LYS:HE3	1.75	0.43
1:A:331:CYS:HB3	1:B:697:ASN:HB3	2.00	0.43
1:A:423:LYS:HA	1:A:423:LYS:HD3	1.62	0.43
1:B:328:GLU:H	1:B:328:GLU:CD	2.22	0.43
1:B:662:MET:HB3	1:B:662:MET:HE2	1.67	0.43
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.00	0.43
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.54	0.43
1:B:567:VAL:HG21	4:B:803:8F1:C07	2.49	0.43
1:B:659:ILE:HD13	1:B:659:ILE:HA	1.81	0.42
2:A:801:HEM:CGA	3:A:802:H4B:HN3	2.32	0.42
1:B:460:THR:O	1:B:583:PRO:HD2	2.19	0.42
1:A:366:TYR:HA	1:A:369:ILE:HG12	2.01	0.42
1:A:696:LEU:HD22	1:B:330:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.92	0.42
1:A:491:SER:OG	1:A:492:THR:N	2.53	0.41
1:B:675:ASP:O	1:B:679:ILE:HG12	2.19	0.41
1:A:463:PRO:HG2	1:A:472:PHE:CZ	2.55	0.41
1:A:598:TYR:HA	1:A:604:TYR:HB2	2.01	0.41
1:A:603:ARG:HB3	1:A:604:TYR:H	1.56	0.41
1:A:378:MET:O	1:A:382:GLU:HG2	2.20	0.41
1:A:701:THR:HG22	7:A:951:HOH:O	2.20	0.41
1:A:610:VAL:O	1:A:614:MET:HG3	2.20	0.41
1:B:355:PHE:N	1:B:356:PRO:HD2	2.36	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.51	0.41
1:A:462:PHE:HB3	1:A:463:PRO:HD2	2.03	0.41
1:A:596:ARG:HG3	7:A:976:HOH:O	2.21	0.40
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.85	0.40
1:A:501:PHE:HA	1:A:504:ILE:HD12	2.03	0.40
1:A:510:TRP:CE2	1:A:521:PRO:HD3	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	406/422 (96%)	383 (94%)	22 (5%)	1 (0%)	47	43
1	B	409/422 (97%)	395 (97%)	14 (3%)	0	100	100
All	All	815/844 (97%)	778 (96%)	36 (4%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ARG

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	366/377 (97%)	351 (96%)	15 (4%)	30	27
1	B	368/377 (98%)	361 (98%)	7 (2%)	57	59
All	All	734/754 (97%)	712 (97%)	22 (3%)	41	40

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

Mol	Chain	Res	Type
1	A	360	GLU
1	A	389	GLU
1	A	419	ILE
1	A	492	THR
1	A	493	LEU
1	A	523	LEU
1	A	547	ARG
1	A	596	ARG
1	A	600	ASP
1	A	603	ARG
1	A	613	LYS
1	A	653	SER
1	A	660	LYS
1	A	686	SER
1	A	715	VAL
1	B	337	LEU
1	B	349	ARG
1	B	367	SER
1	B	390	SER
1	B	481	ARG
1	B	547	ARG
1	B	622	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	GLN

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	801	1	41,50,50	1.97	7 (17%)	45,82,82	1.94	11 (24%)
4	8F1	A	803	-	28,28,28	1.54	1 (3%)	37,38,38	1.18	4 (10%)
3	H4B	B	802	-	16,18,18	0.88	0	11,26,26	2.52	5 (45%)
4	8F1	B	803	-	28,28,28	1.59	1 (3%)	37,38,38	1.13	4 (10%)
5	ACT	A	804	-	3,3,3	0.77	0	3,3,3	0.73	0
2	HEM	B	801	1	41,50,50	2.01	8 (19%)	45,82,82	1.91	12 (26%)
5	ACT	B	804	-	3,3,3	0.78	0	3,3,3	0.63	0
3	H4B	A	802	-	16,18,18	0.91	1 (6%)	11,26,26	2.50	6 (54%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	801	1	-	8/12/54/54	-
4	8F1	A	803	-	-	1/11/11/11	0/3/3/3
3	H4B	B	802	-	-	3/8/17/17	0/2/2/2
4	8F1	B	803	-	-	3/11/11/11	0/3/3/3
2	HEM	B	801	1	-	2/12/54/54	-
3	H4B	A	802	-	-	4/8/17/17	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3D-C2D	8.02	1.53	1.36
2	B	801	HEM	C3D-C2D	7.96	1.53	1.36
4	B	803	8F1	C23-C27	-7.16	1.28	1.44
4	A	803	8F1	C23-C27	-6.91	1.29	1.44
2	B	801	HEM	C3C-C2C	-4.02	1.34	1.40
2	A	801	HEM	C3C-C2C	-3.79	1.35	1.40
2	B	801	HEM	C3C-CAC	3.47	1.54	1.47
2	A	801	HEM	C3C-CAC	3.32	1.54	1.47
2	B	801	HEM	FE-ND	3.09	2.12	1.96
2	A	801	HEM	CAB-C3B	2.94	1.55	1.47
2	B	801	HEM	CAB-C3B	2.89	1.55	1.47
2	A	801	HEM	FE-NB	2.86	2.11	1.96
2	B	801	HEM	FE-NB	2.85	2.11	1.96
2	B	801	HEM	CMD-C2D	2.26	1.55	1.50
2	A	801	HEM	CAA-C2A	2.24	1.55	1.52
3	A	802	H4B	C4A-C4	-2.08	1.38	1.41
2	A	801	HEM	CMD-C2D	2.05	1.55	1.50
2	B	801	HEM	CMB-C2B	2.01	1.55	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C4D-ND-C1D	6.34	111.62	105.07
2	A	801	HEM	C4D-ND-C1D	5.51	110.76	105.07
3	B	802	H4B	C8A-C4A-C4	4.91	118.93	114.57
3	A	802	H4B	C8A-C4A-C4	4.73	118.77	114.57
2	A	801	HEM	C4C-CHD-C1D	4.15	128.04	122.56
2	A	801	HEM	CAD-CBD-CGD	-4.01	104.97	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	8F1	C04-C05-C10	3.49	119.90	118.01
2	B	801	HEM	C4C-CHD-C1D	3.47	127.13	122.56
2	A	801	HEM	C4B-CHC-C1C	3.46	127.13	122.56
3	A	802	H4B	N1-C2-N3	-3.37	120.13	125.42
3	B	802	H4B	N1-C2-N3	-3.33	120.20	125.42
2	B	801	HEM	CAD-C3D-C4D	3.28	130.38	124.66
4	A	803	8F1	C04-C05-C10	3.19	119.74	118.01
2	B	801	HEM	C4B-CHC-C1C	3.16	126.72	122.56
3	A	802	H4B	C2-N3-C4	3.07	120.81	115.93
2	A	801	HEM	C3B-C2B-C1B	3.07	108.76	106.49
3	B	802	H4B	C2-N1-C8A	2.96	121.18	114.54
2	A	801	HEM	CHD-C1D-ND	2.91	127.59	124.43
2	B	801	HEM	C1B-NB-C4B	2.89	108.06	105.07
3	B	802	H4B	C4-C4A-N5	2.84	121.50	119.12
3	B	802	H4B	C2-N3-C4	2.81	120.39	115.93
2	A	801	HEM	C1B-NB-C4B	2.71	107.88	105.07
4	A	803	8F1	C05-C10-N01	-2.70	119.94	122.81
3	A	802	H4B	C2-N1-C8A	2.69	120.58	114.54
4	A	803	8F1	C12-O13-C21	2.69	124.28	117.65
2	A	801	HEM	CHA-C4D-ND	2.68	127.70	124.38
2	B	801	HEM	CAD-CBD-CGD	-2.68	107.84	113.60
2	B	801	HEM	C3B-C2B-C1B	2.62	108.43	106.49
4	B	803	8F1	C08-C09-C10	-2.59	118.80	121.08
2	A	801	HEM	CMD-C2D-C1D	2.58	128.96	125.04
2	B	801	HEM	CHD-C1D-ND	2.47	127.12	124.43
2	B	801	HEM	CAD-C3D-C2D	-2.47	123.28	127.88
3	A	802	H4B	C4-C4A-N5	2.46	121.19	119.12
4	A	803	8F1	C08-C09-C10	-2.44	118.94	121.08
2	A	801	HEM	C4A-C3A-C2A	2.43	108.69	107.00
3	A	802	H4B	N2-C2-N3	2.43	121.03	117.25
4	B	803	8F1	C05-C10-N01	-2.28	120.40	122.81
2	B	801	HEM	C3D-C4D-ND	-2.23	107.68	110.17
2	A	801	HEM	C3C-C4C-NC	-2.11	106.96	110.94
2	B	801	HEM	CBA-CAA-C2A	-2.02	109.17	112.62
2	B	801	HEM	CMD-C2D-C1D	2.01	128.10	125.04
4	B	803	8F1	C06-C05-C04	-2.01	119.83	123.66

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C1A-C2A-CAA-CBA

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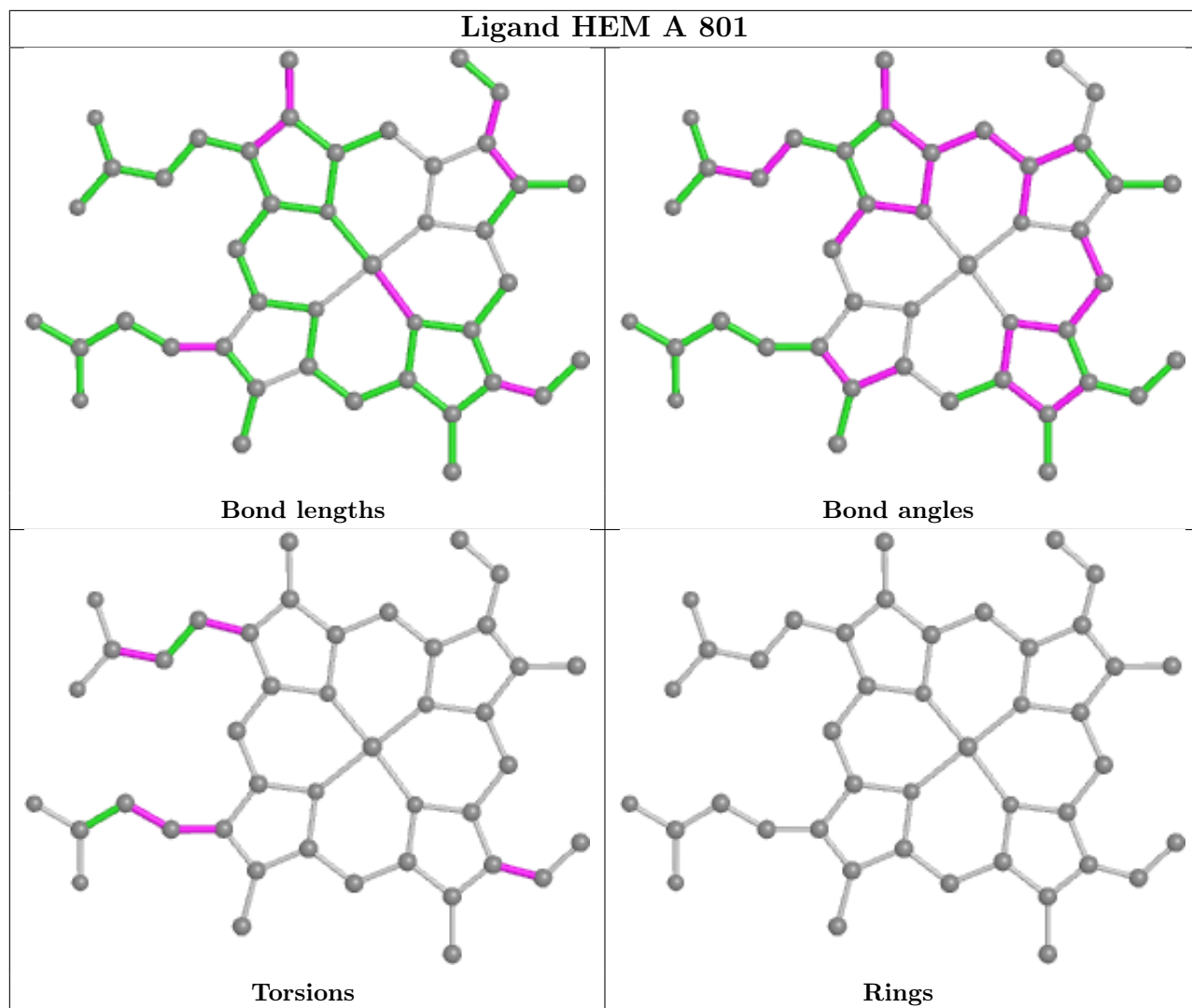
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C3A-C2A-CAA-CBA
2	A	801	HEM	C2A-CAA-CBA-CGA
3	A	802	H4B	N5-C6-C9-O9
3	A	802	H4B	C7-C6-C9-O9
3	A	802	H4B	C7-C6-C9-C10
3	B	802	H4B	C7-C6-C9-O9
3	B	802	H4B	C7-C6-C9-C10
4	A	803	8F1	C25-C31-C32-N33
4	B	803	8F1	C25-C31-C32-N33
4	B	803	8F1	C22-C21-O13-C12
4	B	803	8F1	C26-C21-O13-C12
2	B	801	HEM	C2A-CAA-CBA-CGA
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
3	B	802	H4B	N5-C6-C9-O9
2	A	801	HEM	C4D-C3D-CAD-CBD
3	A	802	H4B	N5-C6-C9-C10
2	A	801	HEM	C2D-C3D-CAD-CBD
2	A	801	HEM	CAD-CBD-CGD-O2D
2	A	801	HEM	CAD-CBD-CGD-O1D

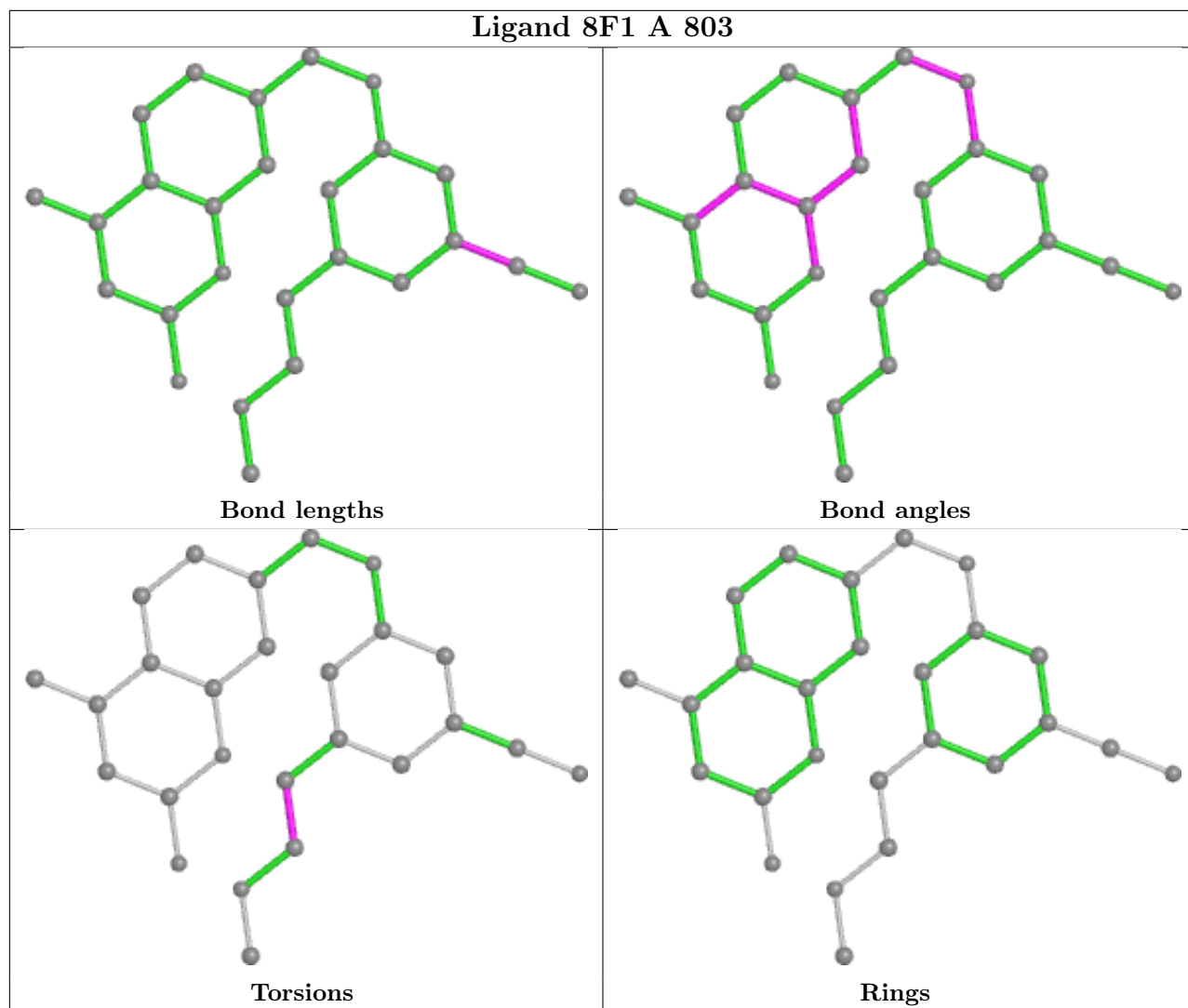
There are no ring outliers.

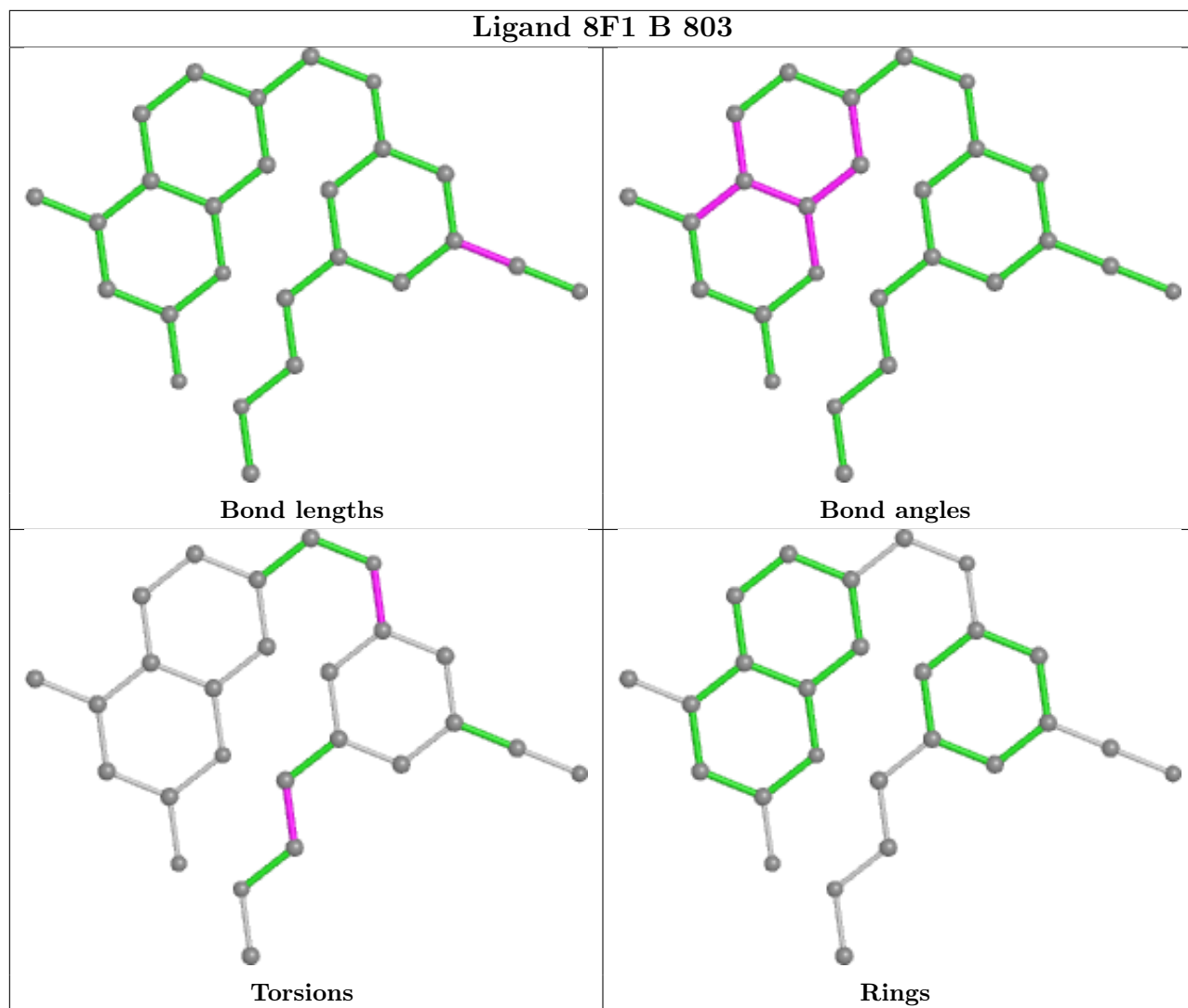
4 monomers are involved in 8 short contacts:

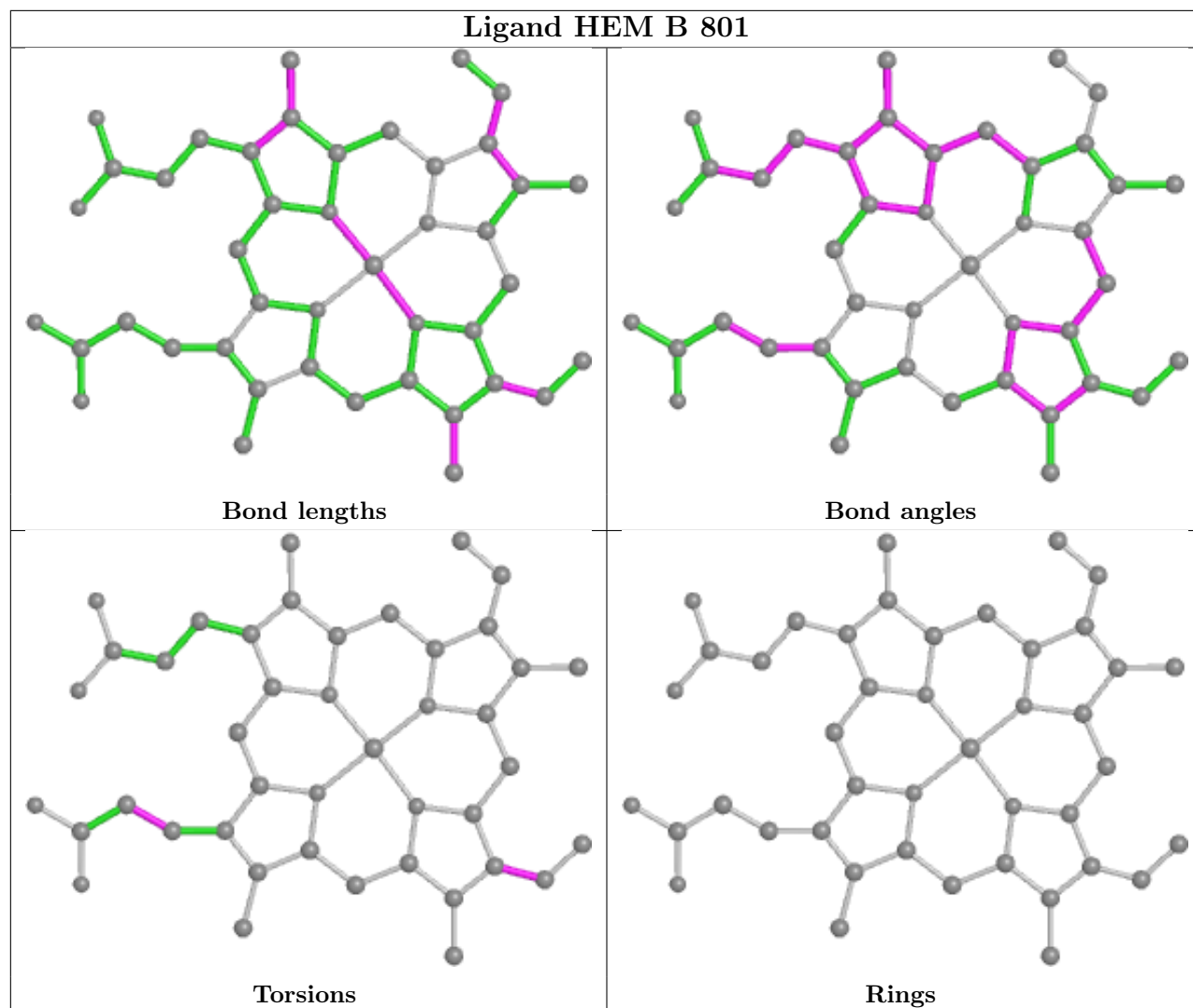
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	3	0
4	B	803	8F1	1	0
2	B	801	HEM	4	0
3	A	802	H4B	1	0

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

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	409/422 (96%)	0.95	81 (19%) 1 0	35, 68, 124, 164	0
1	B	411/422 (97%)	0.43	34 (8%) 11 10	35, 58, 97, 138	0
All	All	820/844 (97%)	0.69	115 (14%) 2 2	35, 63, 115, 164	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	9.3
1	A	716	TRP	7.2
1	A	352	ASP	5.8
1	A	348	VAL	4.7
1	A	490	GLY	4.6
1	B	300	PHE	4.6
1	A	488	PRO	4.5
1	B	619	ARG	4.5
1	B	348	VAL	4.4
1	A	508	GLN	4.4
1	A	713	THR	4.3
1	A	487	GLN	4.1
1	B	603	ARG	4.1
1	A	678	TRP	3.9
1	B	677	VAL	3.9
1	A	489	ASP	3.8
1	A	355	PHE	3.8
1	A	390	SER	3.8
1	B	299	ARG	3.7
1	A	507	GLN	3.7
1	A	677	VAL	3.6
1	A	679	ILE	3.5
1	A	470	HIS	3.5
1	A	349	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	599	CYS	3.5
1	A	603	ARG	3.5
1	A	388	ILE	3.5
1	A	567	VAL	3.4
1	A	499	VAL	3.4
1	A	503	GLU	3.3
1	A	712	ASN	3.3
1	A	566	ALA	3.3
1	A	551	PHE	3.3
1	A	506	ILE	3.3
1	A	714	HIS	3.3
1	A	492	THR	3.3
1	B	680	VAL	3.2
1	B	350	THR	3.2
1	A	584	PHE	3.1
1	A	486	LYS	3.1
1	B	310	VAL	3.1
1	A	667	ARG	3.1
1	B	620	LYS	3.0
1	A	322	LEU	3.0
1	A	479	LEU	3.0
1	A	391	THR	3.0
1	A	676	TRP	2.9
1	A	615	ASP	2.9
1	A	505	CYS	2.9
1	A	392	SER	2.9
1	A	351	LYS	2.9
1	A	389	GLU	2.9
1	A	681	PRO	2.9
1	A	491	SER	2.9
1	A	516	ARG	2.9
1	B	612	LYS	2.9
1	B	718	GLY	2.9
1	A	480	ILE	2.8
1	A	504	ILE	2.8
1	B	566	ALA	2.7
1	A	386	LYS	2.7
1	B	678	TRP	2.7
1	A	682	PRO	2.7
1	A	604	TYR	2.7
1	B	605	ASN	2.7
1	A	415	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	350	THR	2.7
1	A	588	TYR	2.6
1	A	643	SER	2.6
1	A	685	GLY	2.5
1	B	604	TYR	2.5
1	B	679	ILE	2.5
1	A	691	PHE	2.5
1	B	616	LEU	2.5
1	A	565	PRO	2.4
1	B	691	PHE	2.4
1	A	680	VAL	2.4
1	B	715	VAL	2.4
1	A	619	ARG	2.4
1	B	593	ILE	2.4
1	A	310	VAL	2.4
1	A	596	ARG	2.4
1	A	593	ILE	2.4
1	A	300	PHE	2.3
1	A	385	ASN	2.3
1	A	690	VAL	2.3
1	A	711	TRP	2.3
1	A	393	THR	2.3
1	B	309	ASP	2.3
1	B	682	PRO	2.3
1	B	611	ALA	2.3
1	A	617	ASP	2.3
1	B	676	TRP	2.3
1	A	553	TRP	2.2
1	A	416	VAL	2.2
1	A	478	GLN	2.2
1	B	370	LYS	2.2
1	B	601	ASN	2.2
1	B	617	ASP	2.2
1	A	469	LYS	2.2
1	A	686	SER	2.2
1	B	567	VAL	2.1
1	A	620	LYS	2.1
1	A	481	ARG	2.1
1	A	598	TYR	2.1
1	B	681	PRO	2.1
1	B	561	TRP	2.1
1	A	467	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	485	TYR	2.1
1	B	562	TYR	2.1
1	B	667	ARG	2.0
1	A	591	THR	2.0
1	A	515	GLY	2.0
1	A	394	TYR	2.0
1	B	311	VAL	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](#)

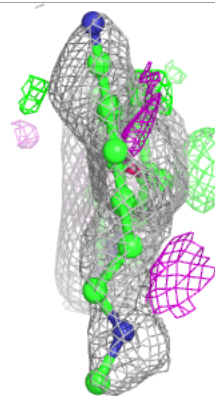
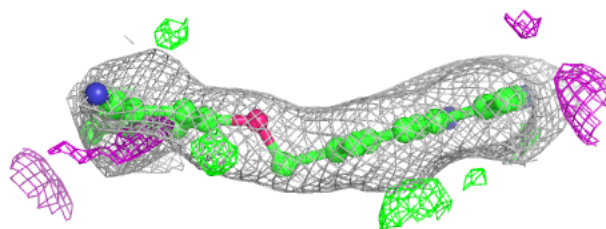
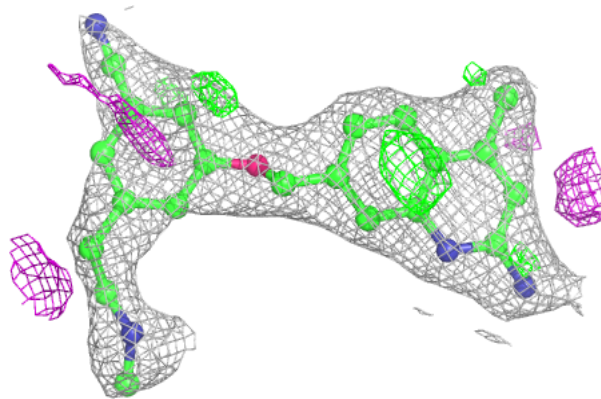
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	A	804	4/4	0.83	0.20	72,73,76,77	0
3	H4B	B	802	17/17	0.86	0.28	59,70,86,89	0
4	8F1	B	803	26/26	0.89	0.27	43,61,89,95	0
3	H4B	A	802	17/17	0.89	0.28	51,74,102,105	0
4	8F1	A	803	26/26	0.91	0.30	36,56,93,97	0
5	ACT	B	804	4/4	0.91	0.18	66,71,73,80	0
2	HEM	B	801	43/43	0.97	0.18	26,49,61,81	0
2	HEM	A	801	43/43	0.98	0.24	27,45,77,89	0
6	ZN	A	805	1/1	1.00	0.10	50,50,50,50	0

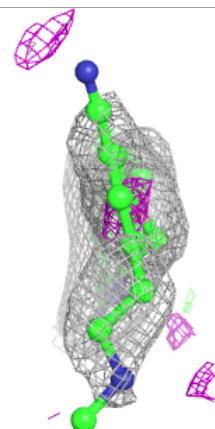
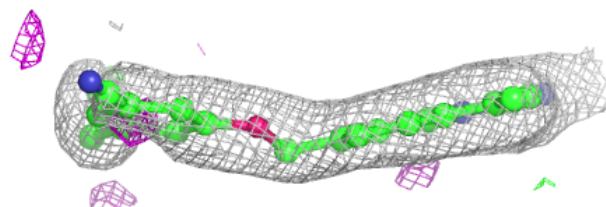
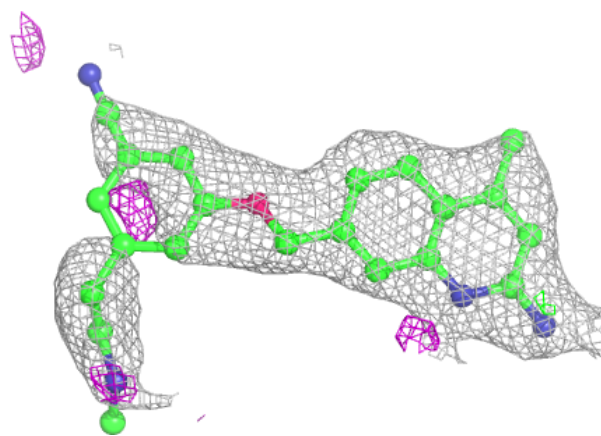
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8F1 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)

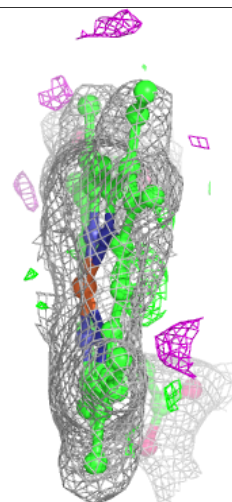
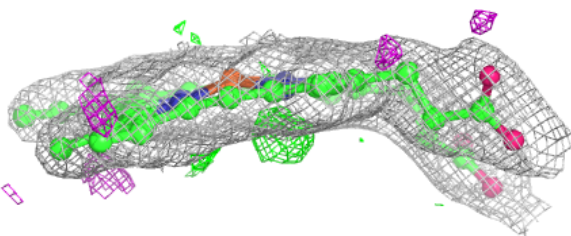
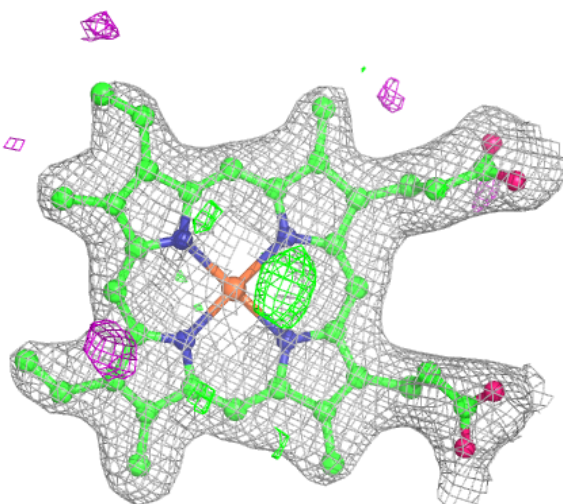
**Electron density around 8F1 A 803:**

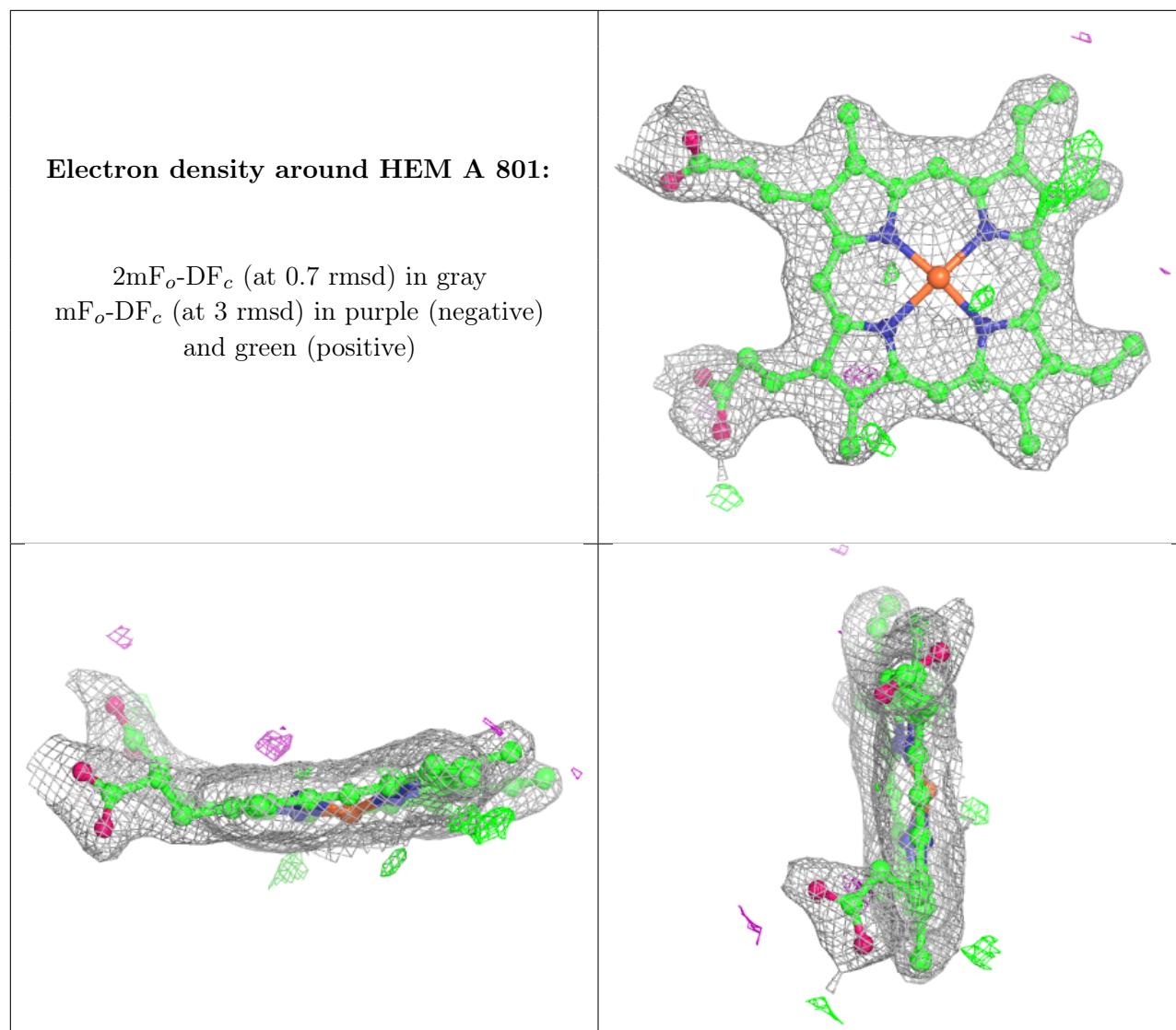
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.