WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 04:28 AM EDT

PDB ID	:	6PND
Title	:	Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with 7-(3-(2-Aminoethyl)phenyl)-4-methylquinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2019-07-02
Resolution	:	2.40 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:

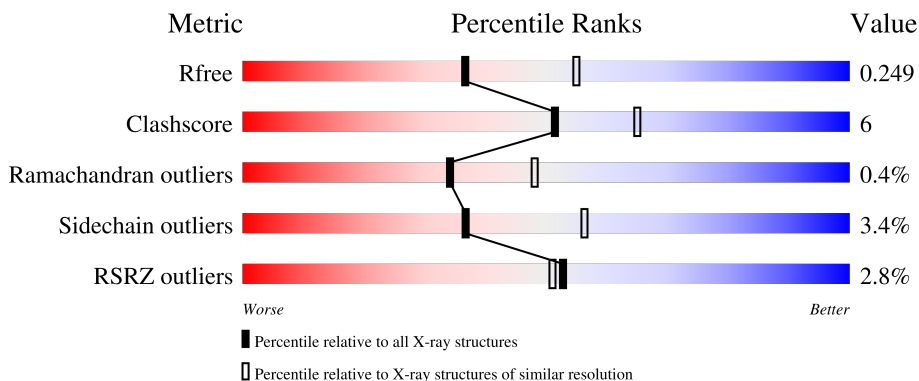|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.40 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	Percentile Ranks	Value
Rfree		0.249
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		3.4%
RSRZ outliers		2.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	421	83% 15%
1	B	421	82% 14%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7088 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	414	Total 3380	C 2164	N 575	O 619	S 22	0	2	0
1	B	409	Total 3343	C 2142	N 570	O 610	S 21	0	2	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: $C_{34}H_{32}FeN_4O_4$).

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: $C_9H_{15}N_5O_3$).
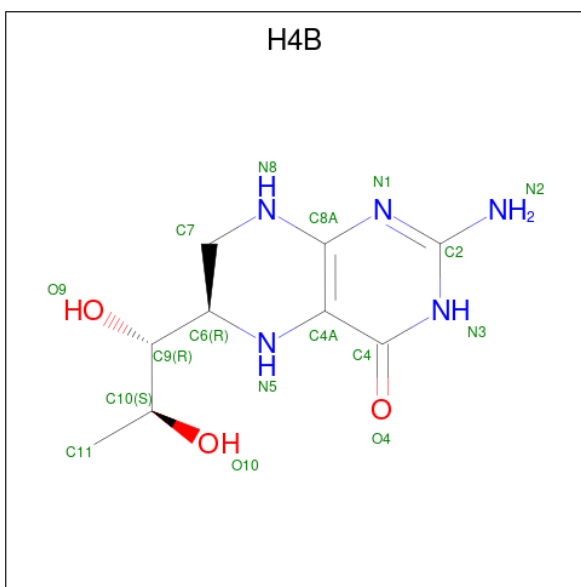
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-[3-(2-aminoethyl)phenyl]-4-methylquinolin-2-amine (three-letter code: OT4) (formula: $C_{18}H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).
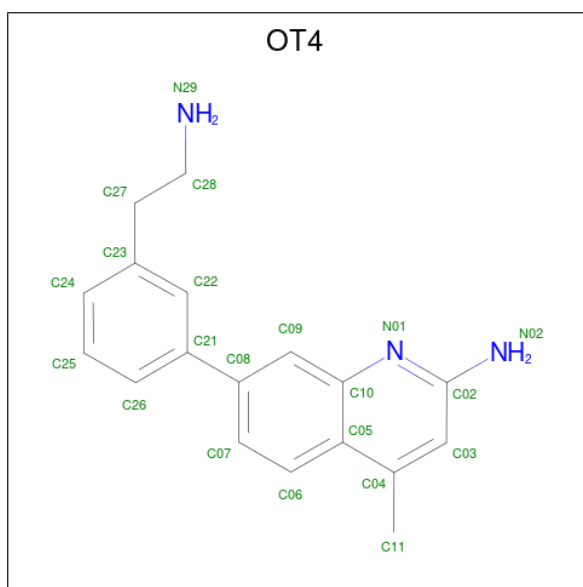
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 21	C 18	N 3	0	0
4	B	1	Total 21	C 18	N 3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total 111	O 111	0	0
6	B	91	Total 91	O 91	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

Chain A:

• Molecule 1: Nitric oxide synthase, brain

Chain B:
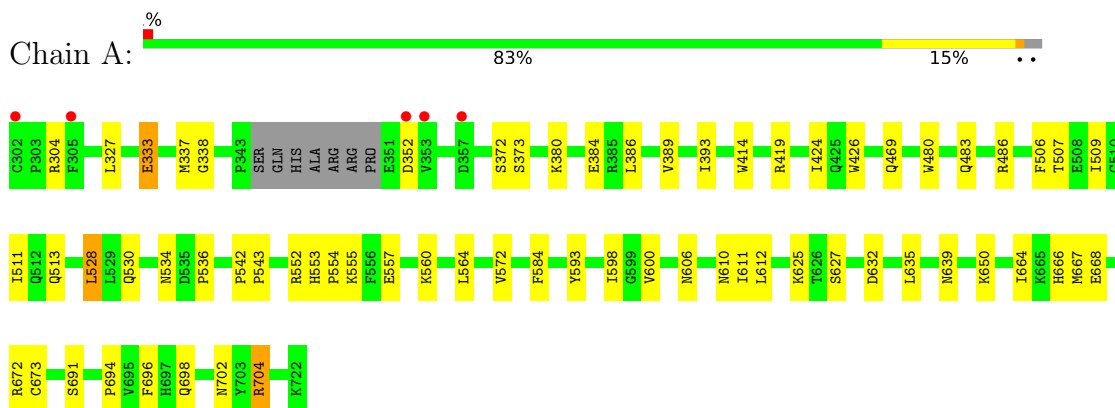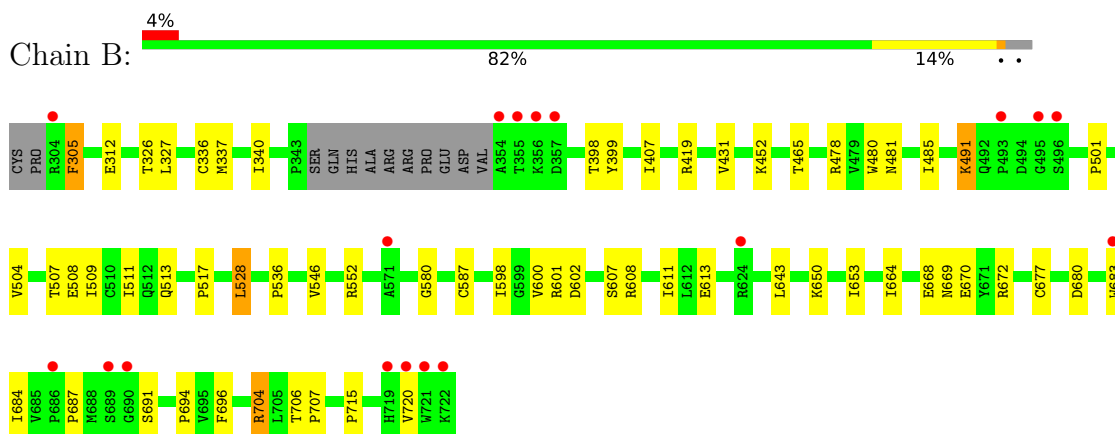
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.23Å 122.30Å 165.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.15 – 2.40 39.15 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.15-2.40) 98.7 (39.15-2.40)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.187 , 0.249 0.189 , 0.249	Depositor DCC
R_{free} test set	2047 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	1.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.5	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7088	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OT4, 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	0.38	0/3482	0.52	0/4724
1	B	0.37	0/3444	0.52	0/4671
All	All	0.38	0/6926	0.52	0/9395

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	3380	0	3288	36	0
1	B	3343	0	3257	38	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	1	0
4	A	21	0	0	1	0
4	B	21	0	0	0	0
5	A	1	0	0	0	0
6	A	111	0	0	2	1
6	B	91	0	0	3	1
All	All	7088	0	6635	75	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 6.

All (75) 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:B:491:LYS:HE3	1:B:491:LYS:H	1.43	0.82
1:A:419:ARG:HB2	2:A:801:HEM:HBD2	1.62	0.78
1:A:610:ASN:O	6:A:901:HOH:O	2.01	0.77
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.67	0.76
1:B:668:GLU:OE1	6:B:901:HOH:O	2.06	0.73
1:B:419:ARG:HB2	2:B:801:HEM:HBD2	1.71	0.72
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.72	0.71
1:A:664:ILE:HG13	1:A:694:PRO:HB2	1.74	0.70
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.74	0.69
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.78	0.65
1:B:485:ILE:HD13	1:B:546:VAL:HG13	1.80	0.64
1:A:327:LEU:HB2	1:A:704:ARG:NH1	2.14	0.63
1:A:600:VAL:HG13	1:A:635:LEU:HD11	1.79	0.62
1:A:667:MET:HE1	1:A:698:GLN:HG2	1.81	0.61
1:B:600:VAL:HG12	1:B:601:ARG:HD2	1.83	0.61
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.82	0.60
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.84	0.59
1:B:643:LEU:HD23	1:B:653:ILE:HD13	1.86	0.56
1:B:509:ILE:O	1:B:513:GLN:HG2	2.05	0.56
1:A:572:VAL:HG21	4:A:803:OT4:C07	2.37	0.55
1:A:691:SER:HB3	1:B:687:PRO:HB2	1.89	0.55
1:A:509:ILE:O	1:A:513:GLN:HG2	2.06	0.55
1:A:557:GLU:OE2	1:A:560:LYS:NZ	2.40	0.54
1:B:511:ILE:HG12	1:B:517:PRO:HG3	1.90	0.53
1:A:564:LEU:HD11	1:A:611:ILE:HD13	1.91	0.52
1:A:593:TYR:CD1	1:A:598:ILE:HD11	2.44	0.52
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.91	0.52
1:A:606:ASN:ND2	1:B:312:GLU:OE2	2.40	0.51
1:B:337:MET:HB3	1:B:340:ILE:HG13	1.92	0.50
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.46	0.50
1:B:305:PHE:HD1	1:B:305:PHE:N	2.10	0.50
1:A:380:LYS:NZ	1:A:384:GLU:OE2	2.44	0.49
1:A:668:GLU:O	1:A:672:ARG:HG2	2.11	0.49
1:B:305:PHE:N	1:B:305:PHE:CD1	2.80	0.49
1:A:389:VAL:O	1:A:393:ILE:HG13	2.13	0.48
1:A:507:THR:O	1:A:511:ILE:HG13	2.14	0.48
1:A:304:ARG:CZ	1:A:304:ARG:HB3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:SER:HA	1:A:696:PHE:CG	2.49	0.47
1:B:491:LYS:H	1:B:491:LYS:CE	2.22	0.47
1:B:507:THR:O	1:B:511:ILE:HG13	2.15	0.46
1:A:600:VAL:HG22	1:A:639:ASN:HD21	1.80	0.46
1:A:704:ARG:NH1	1:A:704:ARG:HB3	2.31	0.46
1:A:506:PHE:HA	1:A:509:ILE:HD12	1.98	0.46
1:B:664:ILE:HG13	1:B:694:PRO:HB2	1.97	0.46
1:A:333:GLU:HB2	6:B:938:HOH:O	2.16	0.45
1:B:419:ARG:HB2	2:B:801:HEM:CBD	2.45	0.45
1:A:555:LYS:HD3	1:A:555:LYS:HA	1.76	0.45
1:B:398:THR:OG1	1:B:399:TYR:N	2.50	0.45
1:A:542:PRO:HA	1:A:543:PRO:HD3	1.79	0.45
2:B:801:HEM:HHC	2:B:801:HEM:CBB	2.47	0.45
1:B:419:ARG:HD3	1:B:683:TRP:CD2	2.52	0.44
1:B:598:ILE:HA	1:B:602:ASP:HB2	1.98	0.44
1:B:407:ILE:HG12	1:B:431:VAL:HB	1.99	0.44
1:B:601:ARG:HH12	3:B:802:H4B:C4	2.31	0.44
1:B:670:GLU:HB2	1:B:677:CYS:HB2	2.01	0.43
1:A:530:GLN:HG3	1:A:534:ASN:O	2.19	0.43
1:B:327:LEU:HB2	1:B:704:ARG:HB3	2.00	0.43
1:B:669:ASN:OD1	1:B:672:ARG:NH2	2.51	0.43
1:B:501:PRO:HA	1:B:504:VAL:HG23	2.00	0.43
1:A:528:LEU:HD23	1:A:528:LEU:HA	1.85	0.42
1:A:424:ILE:HG13	1:A:666:HIS:HB2	2.01	0.42
1:B:452:LYS:NZ	6:B:913:HOH:O	2.52	0.42
1:B:680:ASP:O	1:B:684:ILE:HG12	2.20	0.42
1:A:469:GLN:HB3	1:A:584:PHE:CE2	2.54	0.42
1:B:528:LEU:HD23	1:B:528:LEU:HA	1.88	0.41
1:B:465:THR:O	1:B:587:CYS:HA	2.20	0.41
1:A:553:HIS:CG	1:A:554:PRO:HD2	2.55	0.41
1:A:513:GLN:NE2	6:A:905:HOH:O	2.54	0.41
1:B:691:SER:HA	1:B:696:PHE:CG	2.55	0.41
1:A:483:GLN:HB2	1:A:486:ARG:CG	2.50	0.41
1:A:702:ASN:HB3	1:B:336:CYS:HB3	2.02	0.41
1:B:504:VAL:O	1:B:508:GLU:HG3	2.20	0.41
1:B:607:SER:O	1:B:608:ARG:HD2	2.21	0.41
1:B:706:THR:HA	1:B:707:PRO:C	2.41	0.41
1:B:478:ARG:CZ	1:B:715:PRO:HG3	2.52	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)
6:A:943:HOH:O	6:B:975:HOH:O[2_995]	2.11	0.09

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	412/421 (98%)	394 (96%)	16 (4%)	2 (0%)	29	41
1	B	407/421 (97%)	387 (95%)	19 (5%)	1 (0%)	47	62
All	All	819/842 (97%)	781 (95%)	35 (4%)	3 (0%)	34	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	650	LYS
1	A	338	GLY
1	B	580	GLY

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	372/376 (99%)	358 (96%)	14 (4%)	33	51
1	B	367/376 (98%)	356 (97%)	11 (3%)	41	61
All	All	739/752 (98%)	714 (97%)	25 (3%)	37	56

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	GLU
1	A	337	MET
1	A	352	ASP
1	A	372	SER
1	A	373	SER
1	A	386	LEU
1	A	528	LEU
1	A	552	ARG
1	A	612	LEU
1	A	625	LYS
1	A	627	SER
1	A	632	ASP
1	A	673	CYS
1	A	704	ARG
1	B	305	PHE
1	B	326	THR
1	B	481	ASN
1	B	491	LYS
1	B	528	LEU
1	B	552	ARG
1	B	611	ILE
1	B	613	GLU
1	B	650	LYS
1	B	704	ARG
1	B	720	VAL

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	OT4	A	803	-	22,23,23	1.94	3 (13%)	30,32,32	1.29	3 (10%)
3	H4B	B	802	-	16,18,18	0.96	0	11,26,26	2.65	7 (63%)
2	HEM	A	801	1	41,50,50	1.91	5 (12%)	45,82,82	1.72	8 (17%)
3	H4B	A	802	-	16,18,18	0.92	0	11,26,26	2.64	7 (63%)
4	OT4	B	803	-	22,23,23	2.04	3 (13%)	30,32,32	1.62	6 (20%)
2	HEM	B	801	1	41,50,50	1.98	6 (14%)	45,82,82	1.91	10 (22%)

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	OT4	A	803	-	-	3/7/7/7	0/3/3/3
3	H4B	B	802	-	-	3/8/17/17	0/2/2/2
2	HEM	A	801	1	-	5/12/54/54	-
3	H4B	A	802	-	-	5/8/17/17	0/2/2/2
4	OT4	B	803	-	-	2/7/7/7	0/3/3/3
2	HEM	B	801	1	-	1/12/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3D-C2D	8.10	1.54	1.36
2	A	801	HEM	C3D-C2D	8.01	1.53	1.36
4	B	803	OT4	C22-C21	-5.98	1.29	1.39
4	B	803	OT4	C22-C23	-5.85	1.29	1.39
4	A	803	OT4	C22-C21	-5.66	1.30	1.39
4	A	803	OT4	C22-C23	-5.59	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3C-C2C	-4.55	1.34	1.40
2	A	801	HEM	C3C-C2C	-4.28	1.34	1.40
2	A	801	HEM	C3C-CAC	3.46	1.54	1.47
2	B	801	HEM	C3C-CAC	3.09	1.54	1.47
2	B	801	HEM	CAB-C3B	2.79	1.55	1.47
2	A	801	HEM	CAB-C3B	2.79	1.55	1.47
2	A	801	HEM	FE-ND	2.49	2.09	1.96
2	B	801	HEM	FE-ND	2.36	2.08	1.96
4	A	803	OT4	C02-N01	2.29	1.36	1.33
4	B	803	OT4	C02-N01	2.29	1.36	1.33
2	B	801	HEM	CMD-C2D	2.16	1.55	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C4D-ND-C1D	6.32	111.60	105.07
2	A	801	HEM	C4B-CHC-C1C	5.04	129.22	122.56
2	A	801	HEM	C4D-ND-C1D	4.94	110.18	105.07
3	A	802	H4B	C8A-C4A-C4	4.91	118.94	114.57
3	B	802	H4B	C8A-C4A-C4	4.85	118.88	114.57
2	B	801	HEM	C4B-CHC-C1C	4.83	128.93	122.56
4	B	803	OT4	C04-C05-C10	4.06	120.21	118.01
2	A	801	HEM	CHA-C4D-ND	3.69	128.94	124.38
3	A	802	H4B	C2-N3-C4	3.60	121.65	115.93
2	A	801	HEM	CBA-CAA-C2A	-3.56	106.55	112.62
3	A	802	H4B	N1-C2-N3	-3.55	119.86	125.42
3	B	802	H4B	N1-C2-N3	-3.54	119.86	125.42
2	B	801	HEM	CBD-CAD-C3D	-3.33	103.36	112.63
4	B	803	OT4	C05-C10-N01	-3.32	119.29	122.81
2	B	801	HEM	CAD-C3D-C4D	3.21	130.26	124.66
3	B	802	H4B	C2-N3-C4	3.12	120.88	115.93
4	A	803	OT4	C04-C05-C10	2.96	119.61	118.01
4	A	803	OT4	C05-C10-N01	-2.86	119.77	122.81
3	B	802	H4B	C4-C4A-N5	2.85	121.52	119.12
3	B	802	H4B	C2-N1-C8A	2.85	120.93	114.54
2	B	801	HEM	C3B-C2B-C1B	2.74	108.52	106.49
3	A	802	H4B	C2-N1-C8A	2.61	120.40	114.54
2	A	801	HEM	CAD-CBD-CGD	-2.51	108.19	113.60
2	A	801	HEM	C3B-C2B-C1B	2.51	108.35	106.49
2	B	801	HEM	CHD-C1D-ND	2.48	127.12	124.43
3	B	802	H4B	C4A-N5-C6	-2.40	114.63	121.16
4	B	803	OT4	C22-C21-C08	-2.38	116.92	120.86

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	C4-C4A-N5	2.37	121.11	119.12
2	B	801	HEM	C1B-NB-C4B	2.34	107.49	105.07
4	B	803	OT4	N02-C02-N01	2.32	120.18	118.26
3	A	802	H4B	N2-C2-N1	2.29	120.81	117.25
3	B	802	H4B	N2-C2-N3	2.18	120.64	117.25
3	A	802	H4B	C4A-N5-C6	-2.17	115.24	121.16
2	B	801	HEM	C4C-CHD-C1D	2.15	125.39	122.56
4	B	803	OT4	C08-C09-C10	-2.14	119.56	121.44
4	B	803	OT4	C06-C05-C04	-2.14	119.57	123.66
2	B	801	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
2	A	801	HEM	CMA-C3A-C4A	-2.11	125.23	128.46
4	A	803	OT4	N02-C02-N01	2.09	119.98	118.26
2	B	801	HEM	CAD-C3D-C2D	-2.08	124.01	127.88
2	A	801	HEM	CMC-C2C-C3C	2.03	128.47	124.68

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C2A-CAA-CBA-CGA
2	A	801	HEM	C2D-C3D-CAD-CBD
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	OT4	C23-C27-C28-N29
2	A	801	HEM	C4D-C3D-CAD-CBD
2	B	801	HEM	C2A-CAA-CBA-CGA
4	A	803	OT4	C24-C23-C27-C28
4	B	803	OT4	C24-C23-C27-C28
4	A	803	OT4	C22-C23-C27-C28
4	B	803	OT4	C22-C23-C27-C28
2	A	801	HEM	C4B-C3B-CAB-CBB
3	B	802	H4B	N5-C6-C9-O9
3	A	802	H4B	N5-C6-C9-C10
3	A	802	H4B	C11-C10-C9-O9
2	A	801	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.
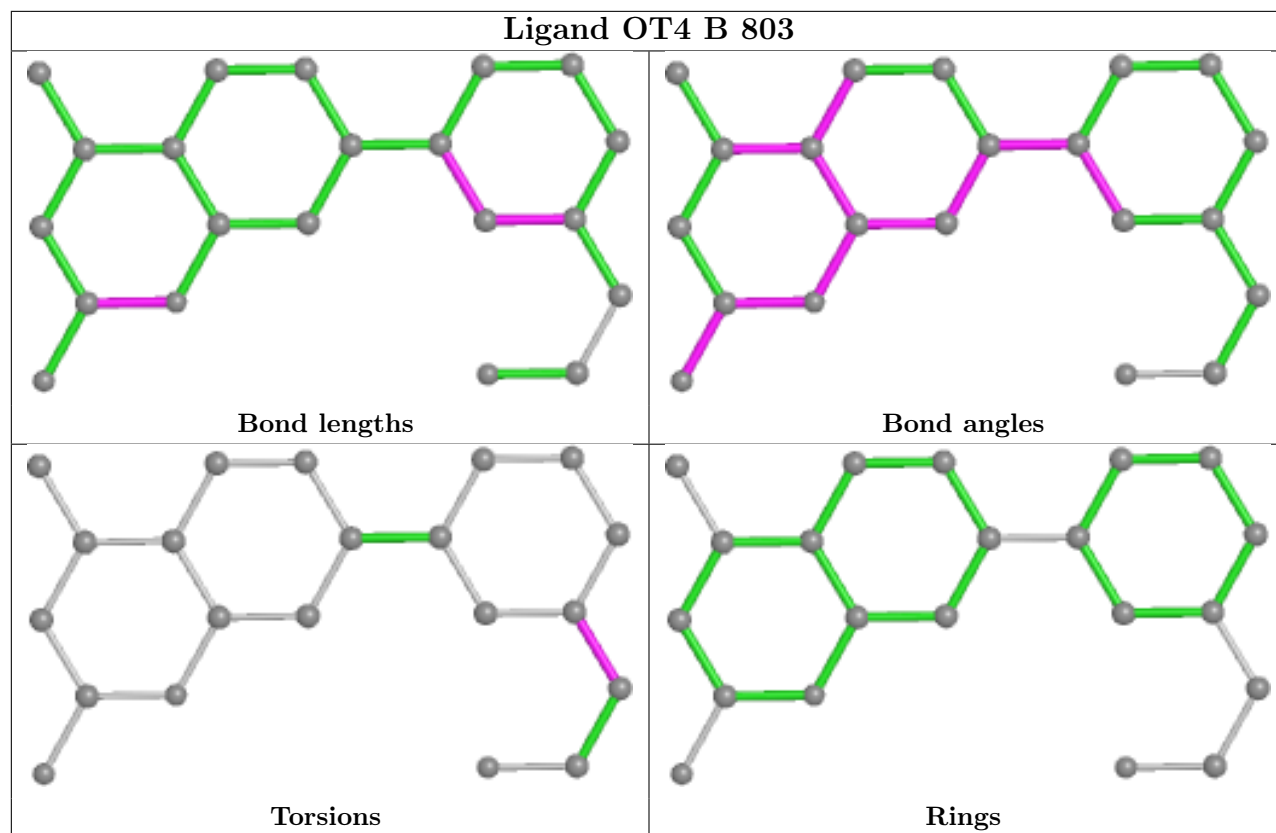
4 monomers are involved in 9 short contacts:

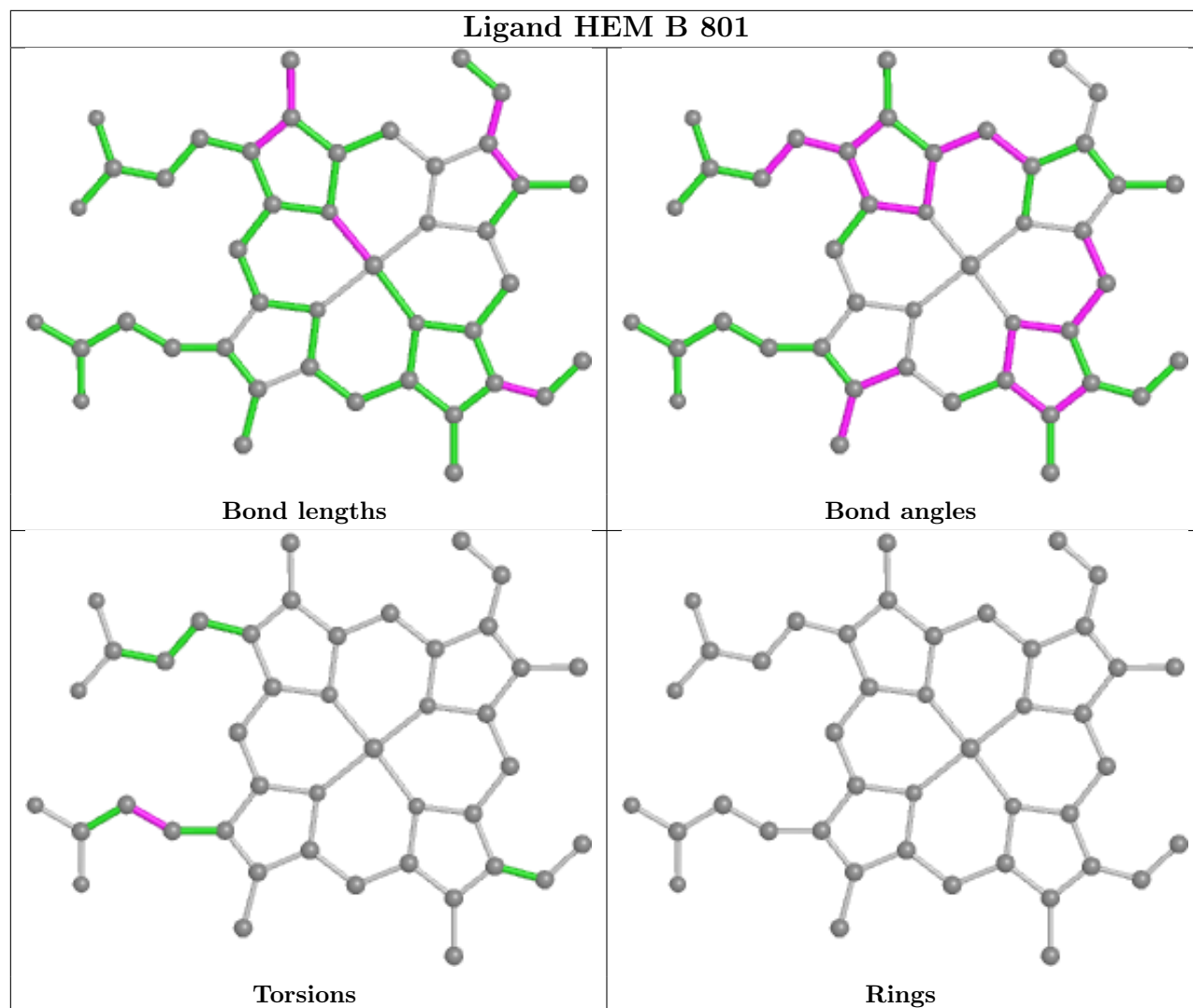| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	OT4	1	0
3	B	802	H4B	1	0
2	A	801	HEM	3	0
2	B	801	HEM	4	0

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 then 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 OT4 A 803

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand OT4 B 803

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 801

Bond lengths

Bond angles

Torsions

Rings
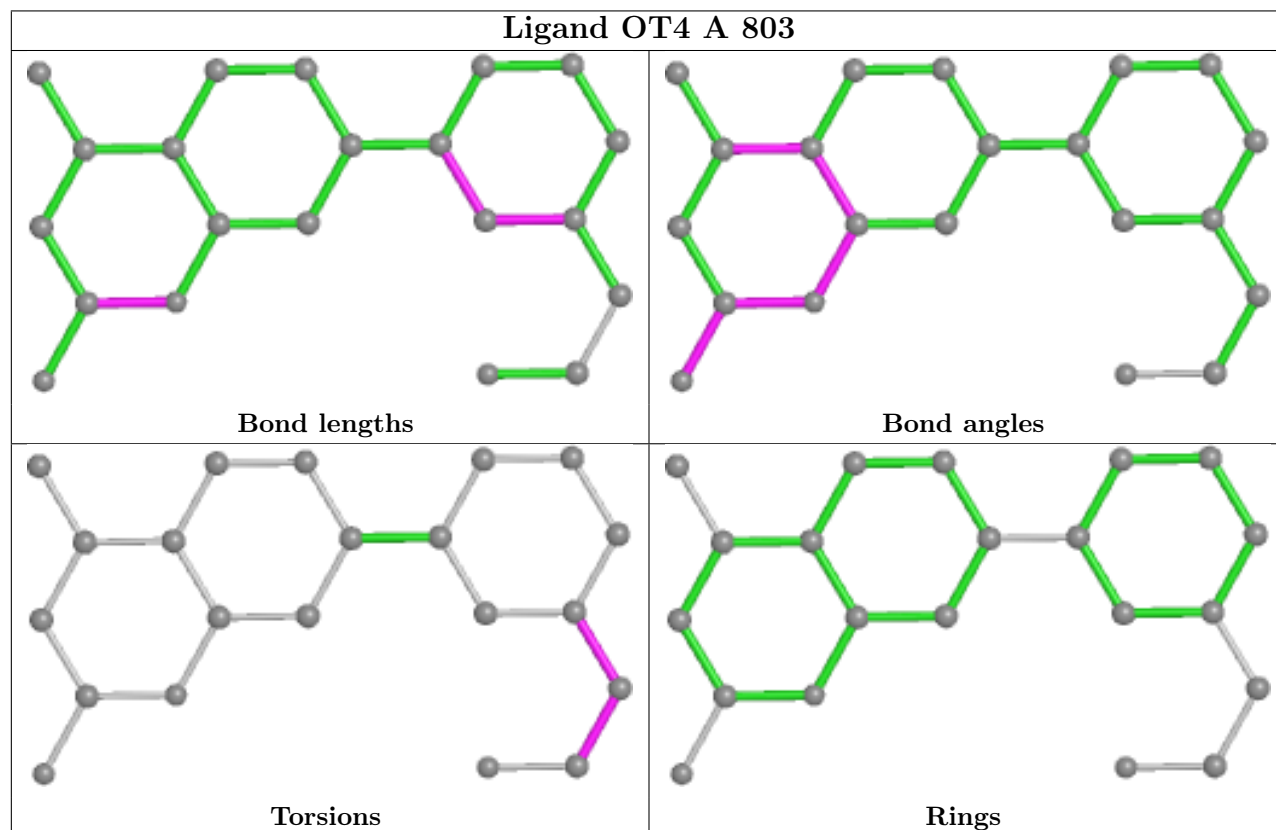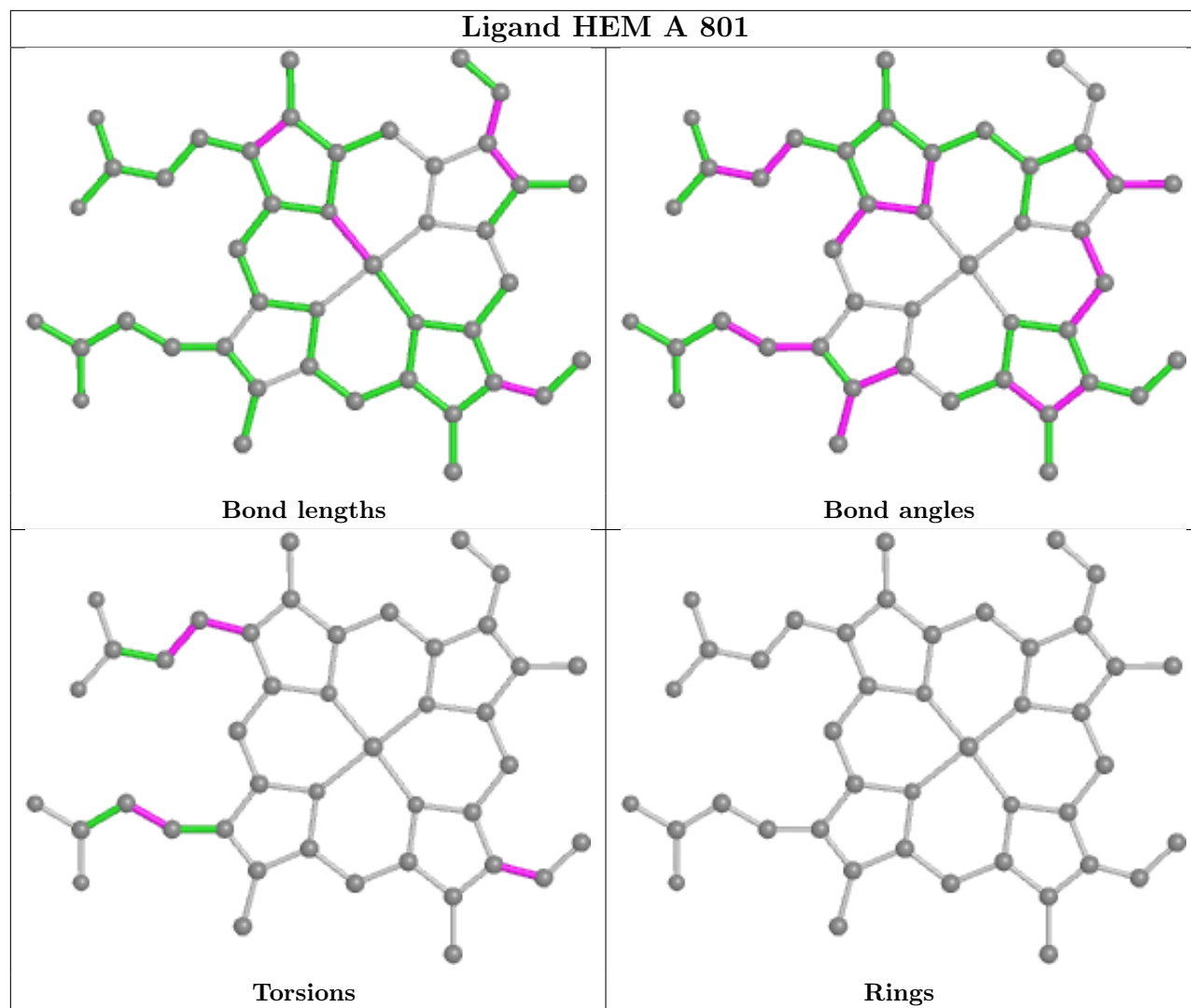
5.7 Other polymers ⓘ

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 (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	414/421 (98%)	-0.09	5 (1%)	79	77	32, 51, 86, 126	0
1	B	409/421 (97%)	0.12	18 (4%)	34	33	36, 58, 95, 119	0
All	All	823/842 (97%)	0.01	23 (2%)	53	51	32, 53, 91, 126	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	ASP	3.4
1	B	496	SER	3.3
1	B	624	ARG	3.3
1	B	721	TRP	3.2
1	B	720	VAL	3.2
1	B	304	ARG	3.2
1	B	357	ASP	3.1
1	A	305	PHE	3.1
1	B	495	GLY	3.0
1	B	493	PRO	2.8
1	A	357	ASP	2.5
1	B	690	GLY	2.5
1	B	683	TRP	2.4
1	A	353	VAL	2.4
1	B	571	ALA	2.4
1	B	354	ALA	2.4
1	B	355	THR	2.3
1	B	686	PRO	2.2
1	B	722	LYS	2.1
1	A	302	CYS	2.1
1	B	356	LYS	2.0
1	B	719	HIS	2.0
1	B	689	SER	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
3	H4B	B	802	17/17	0.91	0.28	62,77,88,89	0
3	H4B	A	802	17/17	0.92	0.20	46,60,78,79	0
4	OT4	B	803	21/21	0.93	0.34	46,59,85,88	0
4	OT4	A	803	21/21	0.94	0.22	43,55,78,81	0
2	HEM	A	801	43/43	0.97	0.20	22,35,65,81	0
2	HEM	B	801	43/43	0.97	0.23	36,47,62,65	0
5	ZN	A	804	1/1	0.99	0.14	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 OT4 B 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
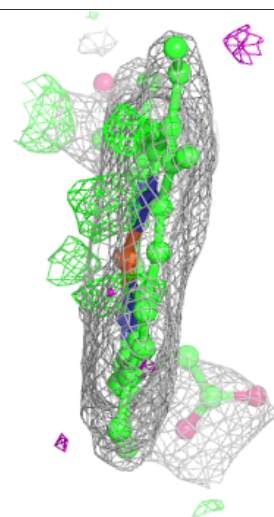mF_o-DF_c (at 3 rmsd) in purple (negative)
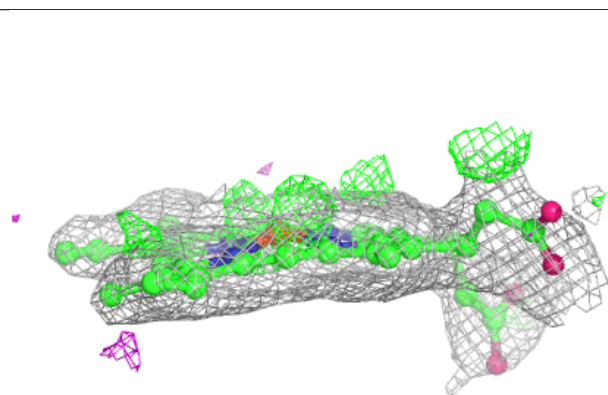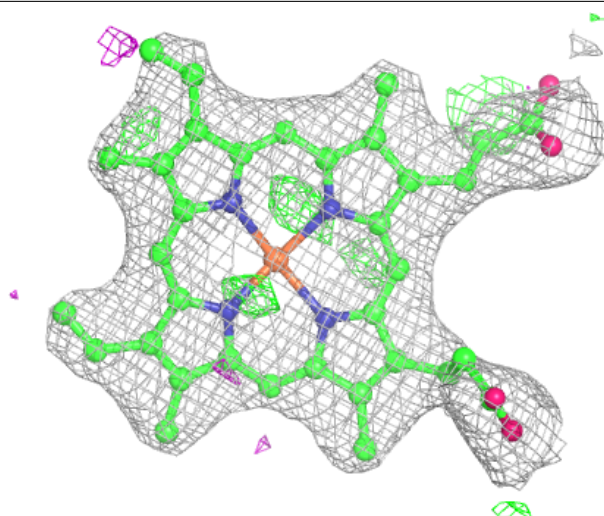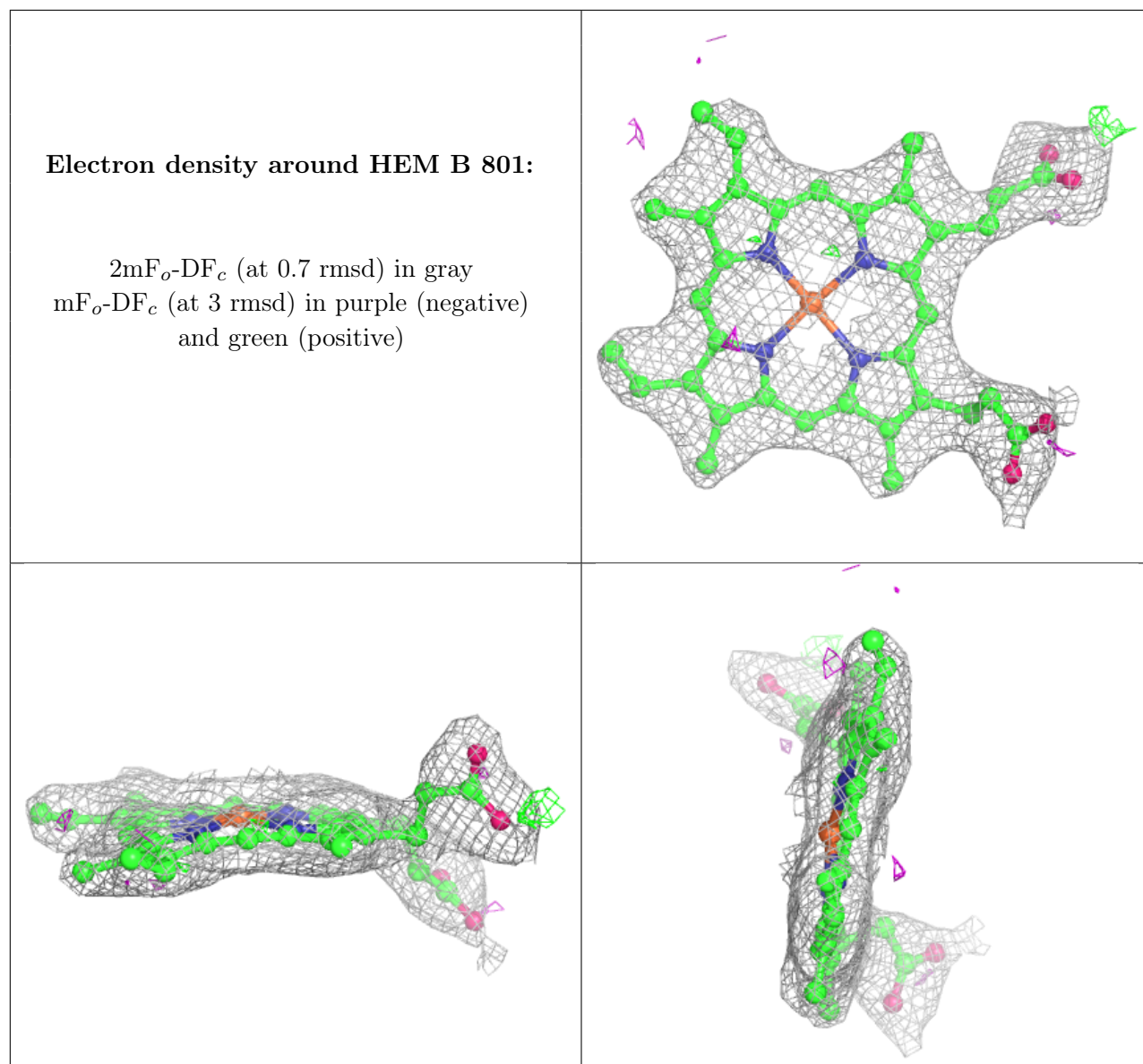and green (positive)
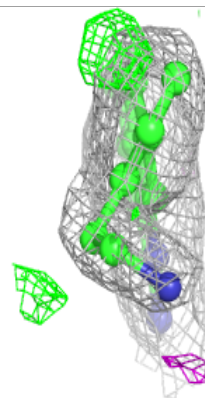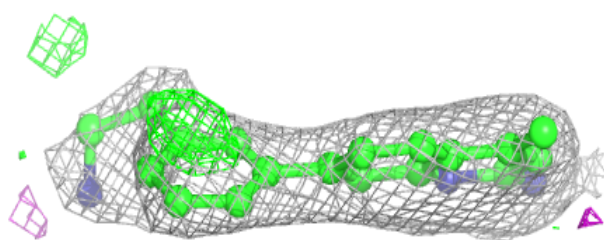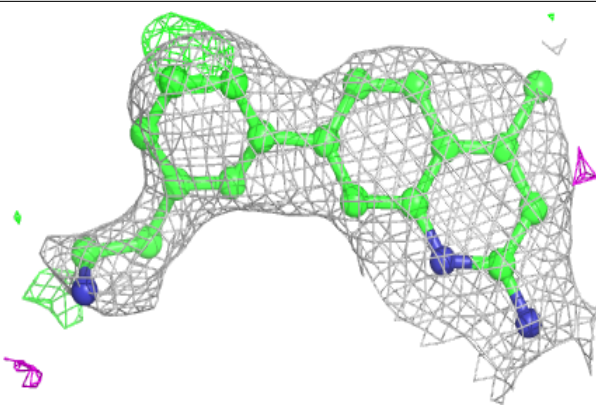
Electron density around OT4 A 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
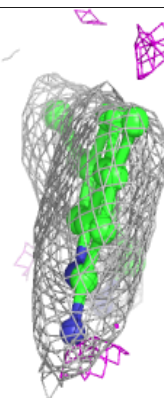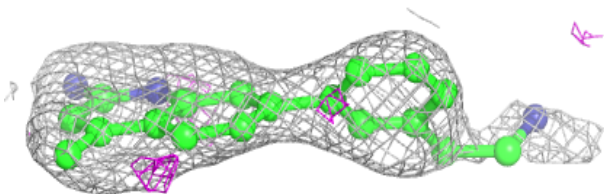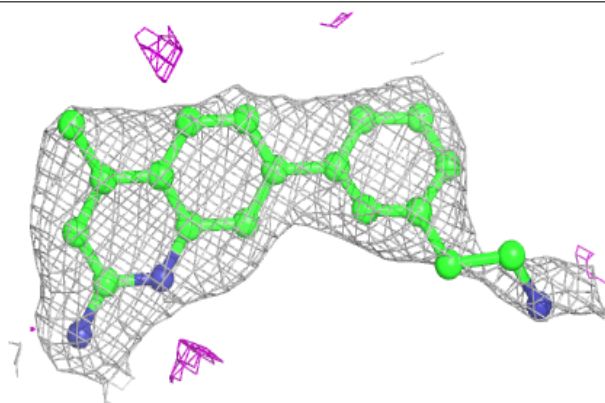
Electron density around HEM A 801:

$2mF_o$-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 ⓘ

There are no such residues in this entry.