



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 01:51 PM EDT

PDB ID : 7TSF
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(3-(4,4-difluoropiperidin-1-yl)prop-1-yn-1-yl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2022-01-31
Resolution : 1.78 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

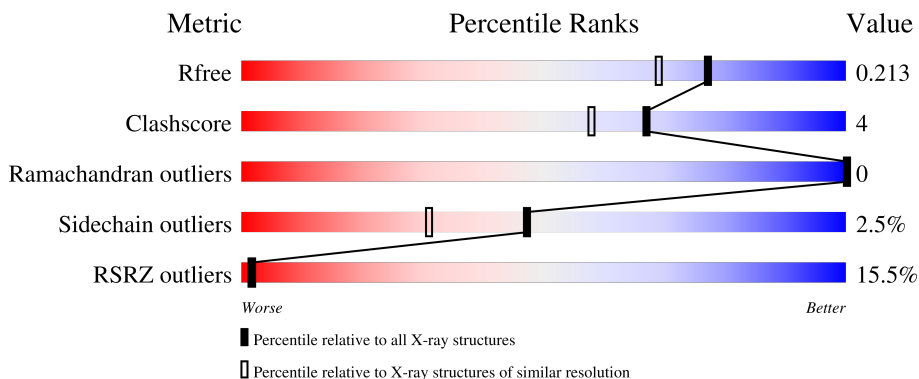
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

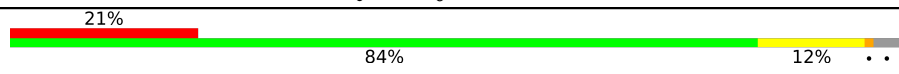

The reported resolution of this entry is 1.78 Å.

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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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](#)

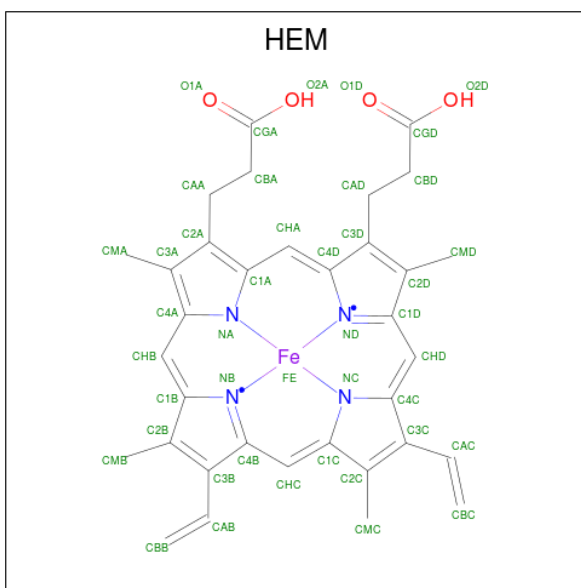
There are 7 unique types of molecules in this entry. The entry contains 7353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

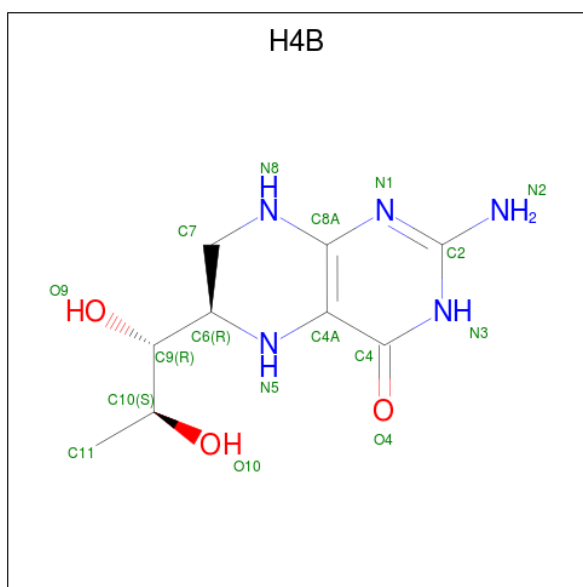
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	Total 3350	C 2144	N 572	O 612	S 22	0	4	0
1	B	411	Total 3353	C 2145	N 574	O 612	S 22	0	3	0

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



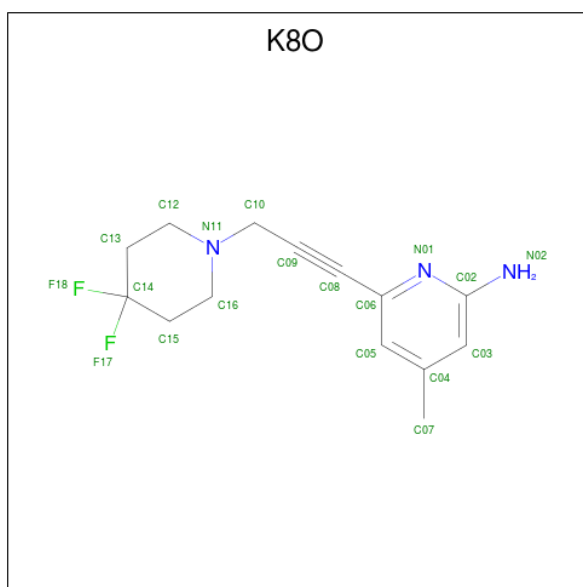
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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 6-[3-(4,4-difluoropiperidin-1-yl)prop-1-yn-1-yl]-4-methylpyridin-2-amine (three-letter code: K8O) (formula: $C_{14}H_{17}F_2N_3$) (labeled as "Ligand of Interest" by depositor).



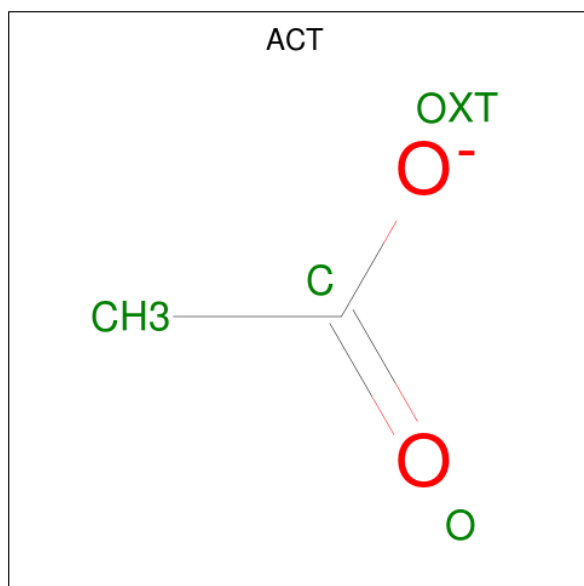
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
4	A	1	19	14	2	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
4	B	1	19	14	2	3	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

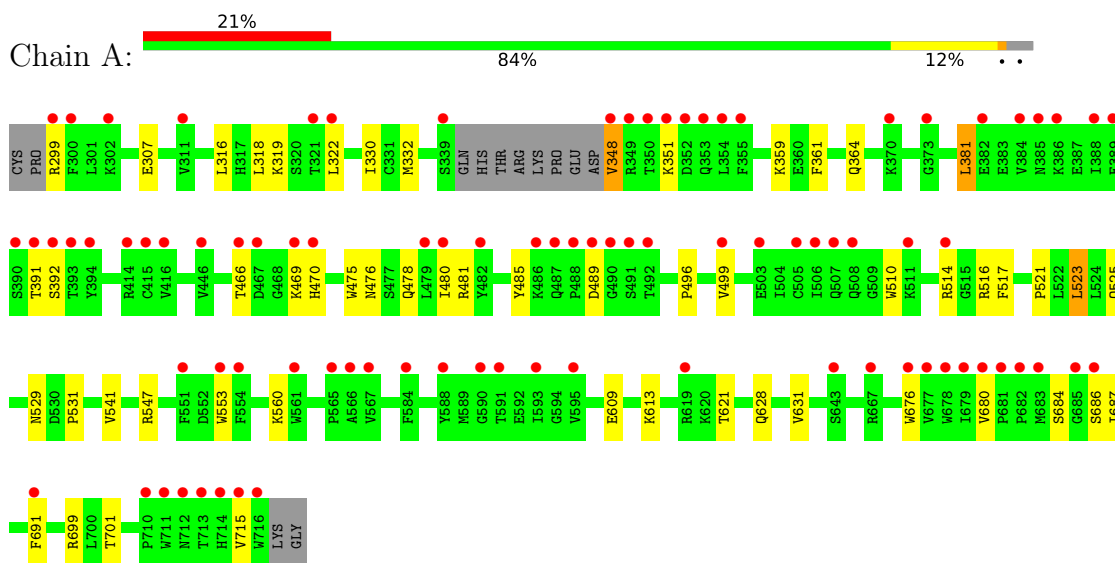
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	209	209	209	0	0
7	B	274	274	274	0	0

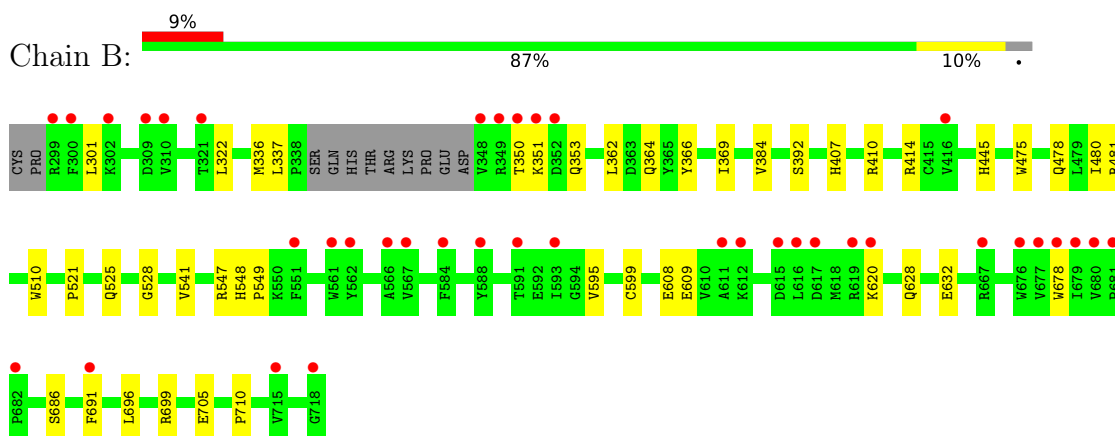
3 Residue-property plots i

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	52.07Å 110.96Å 164.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.07 – 1.78 39.06 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.07-1.78) 99.5 (39.06-1.78)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.77Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.181 , 0.214 0.180 , 0.213	Depositor DCC
R_{free} test set	4606 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtrriage
Anisotropy	0.934	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7353	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: H4B, K8O, ACT, 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	0.36	0/3455	0.52	0/4688
1	B	0.38	0/3456	0.52	0/4685
All	All	0.37	0/6911	0.52	0/9373

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	3350	0	3270	30	0
1	B	3353	0	3270	22	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	19	0	0	0	0
4	B	19	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	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	209	0	0	4	0
7	B	274	0	0	3	0
All	All	7353	0	6636	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (52) 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	1.70	0.72
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.72	0.71
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.71	0.71
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.74	0.69
1:B:364:GLN:OE1	7:B:901:HOH:O	2.10	0.67
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.80	0.64
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.80	0.63
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.65	0.61
1:B:699:ARG:NH2	1:B:705:GLU:OE1	2.35	0.59
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.86	0.57
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.86	0.57
1:A:359:LYS:HG3	1:A:381:LEU:HD21	1.88	0.54
1:A:701[B]:THR:HG22	7:A:1013:HOH:O	2.07	0.53
1:B:608:GLU:HG2	7:B:937:HOH:O	2.09	0.53
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.91	0.51
1:A:316:LEU:HD12	1:A:319:LYS:HE2	1.92	0.51
1:B:595:VAL:O	1:B:599:CYS:HB2	2.10	0.51
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.93	0.50
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.44	0.50
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.94	0.49
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.95	0.49
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.95	0.48
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.49	0.47
1:B:525:GLN:HE21	1:B:528:GLY:HA2	1.80	0.47
1:A:621:THR:HG22	7:A:1073:HOH:O	2.15	0.46
1:A:517:PHE:HB2	1:A:560:LYS:HE3	1.98	0.46
1:A:351:LYS:O	7:A:901:HOH:O	2.21	0.45
1:A:701[B]:THR:HG21	7:A:902:HOH:O	2.16	0.45
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.52	0.45
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.53	0.44
1:A:361:PHE:O	1:A:364:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.00	0.43
1:A:307:GLU:HG3	7:B:1070:HOH:O	2.18	0.43
1:B:480:ILE:HD13	1:B:541:VAL:HG13	2.00	0.43
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.54	0.43
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.99	0.43
1:A:553:TRP:CE3	1:A:613:LYS:HD2	2.54	0.42
1:B:350:THR:OG1	1:B:353:GLN:OE1	2.35	0.42
1:A:348:VAL:HG21	1:A:466:THR:O	2.20	0.42
1:A:391:THR:O	1:A:392:SER:OG	2.34	0.42
1:A:480:ILE:HD13	1:A:541:VAL:HG13	2.02	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.55	0.41
1:B:407:HIS:CE1	1:B:410:ARG:HH11	2.38	0.41
1:A:525:GLN:HG3	1:A:529:ASN:O	2.21	0.41
1:B:475:TRP:CE2	1:B:710:PRO:HB2	2.54	0.41
1:A:299:ARG:HG2	1:A:318:LEU:HD21	2.03	0.40
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.57	0.40
1:B:366:TYR:HA	1:B:369:ILE:HG12	2.03	0.40
1:B:445:HIS:CD2	1:B:445:HIS:C	2.95	0.40
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.56	0.40
1:B:686:SER:HA	1:B:691:PHE:CG	2.56	0.40
1:A:684:SER:HB3	1:A:687:ILE:HD11	2.03	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	410/422 (97%)	394 (96%)	16 (4%)	0	100	100
1	B	410/422 (97%)	399 (97%)	11 (3%)	0	100	100
All	All	820/844 (97%)	793 (97%)	27 (3%)	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	370/377 (98%)	359 (97%)	11 (3%)	41	24
1	B	369/377 (98%)	362 (98%)	7 (2%)	57	43
All	All	739/754 (98%)	721 (98%)	18 (2%)	47	33

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	VAL
1	A	381	LEU
1	A	469	LYS
1	A	470	HIS
1	A	476	ASN
1	A	489	ASP
1	A	516	ARG
1	A	523	LEU
1	A	547	ARG
1	A	609	GLU
1	A	715	VAL
1	B	336	MET
1	B	337	LEU
1	B	351	LYS
1	B	392	SER
1	B	547	ARG
1	B	609	GLU
1	B	620	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 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
5	ACT	B	804	-	3,3,3	0.82	0	3,3,3	0.51	0
2	HEM	A	801	1	41,50,50	1.48	5 (12%)	45,82,82	1.77	9 (20%)
3	H4B	A	802	-	16,18,18	0.91	1 (6%)	11,26,26	2.62	6 (54%)
4	K8O	A	803	-	20,20,20	2.66	6 (30%)	26,28,28	1.99	8 (30%)
5	ACT	A	804	-	3,3,3	0.74	0	3,3,3	0.83	0
3	H4B	B	802	-	16,18,18	0.97	1 (6%)	11,26,26	2.52	6 (54%)
2	HEM	B	801	1	41,50,50	1.52	6 (14%)	45,82,82	1.50	6 (13%)
4	K8O	B	803	-	20,20,20	2.47	5 (25%)	26,28,28	2.08	8 (30%)

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	A	801	1	-	1/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	K8O	A	803	-	-	5/5/18/18	0/2/2/2
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
2	HEM	B	801	1	-	0/12/54/54	-
4	K8O	B	803	-	-	3/5/18/18	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	K8O	C06-C08	-9.35	1.28	1.44
4	B	803	K8O	C06-C08	-8.97	1.29	1.44
2	B	801	HEM	C3C-C2C	-4.05	1.34	1.40
2	A	801	HEM	C3C-CAC	3.89	1.55	1.47
4	B	803	K8O	F18-C14	-3.69	1.31	1.38
4	A	803	K8O	F18-C14	-3.63	1.31	1.38
2	B	801	HEM	C3C-CAC	3.54	1.55	1.47
4	A	803	K8O	C10-N11	3.53	1.50	1.46
4	B	803	K8O	C15-C14	3.37	1.53	1.50
4	A	803	K8O	F17-C14	-3.34	1.32	1.38
4	B	803	K8O	F17-C14	-3.34	1.32	1.38
2	A	801	HEM	C3C-C2C	-2.98	1.36	1.40
2	A	801	HEM	CAB-C3B	2.78	1.55	1.47
4	A	803	K8O	C13-C14	2.72	1.52	1.50
2	B	801	HEM	CAB-C3B	2.70	1.54	1.47
2	A	801	HEM	FE-NB	2.38	2.08	1.96
3	B	802	H4B	C7-C6	2.33	1.54	1.52
2	B	801	HEM	CMB-C2B	2.18	1.55	1.50
2	A	801	HEM	CMC-C2C	2.10	1.56	1.51
3	A	802	H4B	C4A-C4	-2.06	1.38	1.41
4	A	803	K8O	C15-C14	2.06	1.52	1.50
2	B	801	HEM	CMC-C2C	2.04	1.56	1.51
2	B	801	HEM	CMD-C2D	2.02	1.55	1.50
4	B	803	K8O	C13-C14	2.01	1.52	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	C8A-C4A-C4	5.73	119.66	114.57
2	A	801	HEM	CBA-CAA-C2A	-5.52	103.21	112.62
3	B	802	H4B	C8A-C4A-C4	4.79	118.83	114.57
4	B	803	K8O	C10-N11-C12	-4.65	106.30	111.71
4	A	803	K8O	C13-C12-N11	-4.41	106.88	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CBA-CAA-C2A	-4.35	105.19	112.62
4	B	803	K8O	C05-C06-N01	-4.10	119.41	123.61
2	B	801	HEM	C4B-CHC-C1C	4.04	127.89	122.56
3	B	802	H4B	C2-N3-C4	3.82	122.00	115.93
4	A	803	K8O	C10-N11-C16	-3.78	107.31	111.71
4	A	803	K8O	C06-C08-C09	-3.70	168.62	176.18
4	B	803	K8O	C12-C13-C14	-3.67	107.50	111.43
4	A	803	K8O	C10-N11-C12	-3.38	107.78	111.71
2	A	801	HEM	C4B-CHC-C1C	3.26	126.86	122.56
4	B	803	K8O	C06-N01-C02	3.19	122.09	116.90
4	A	803	K8O	C16-C15-C14	-3.16	108.05	111.43
4	B	803	K8O	C13-C12-N11	-3.14	108.13	111.23
3	A	802	H4B	C2-N3-C4	3.09	120.83	115.93
4	B	803	K8O	C08-C06-N01	3.08	121.53	116.55
4	B	803	K8O	C15-C16-N11	-3.02	108.25	111.23
3	A	802	H4B	N1-C2-N3	-3.02	120.68	125.42
3	B	802	H4B	N1-C2-N3	-2.91	120.85	125.42
4	A	803	K8O	C05-C06-N01	-2.87	120.67	123.61
2	A	801	HEM	C2C-C3C-C4C	2.79	108.85	106.90
3	B	802	H4B	C4-C4A-N5	2.66	121.35	119.12
2	A	801	HEM	CBD-CAD-C3D	-2.59	105.43	112.63
2	A	801	HEM	C4D-ND-C1D	2.58	107.73	105.07
3	A	802	H4B	C2-N1-C8A	2.57	120.29	114.54
4	B	803	K8O	F17-C14-C13	-2.51	107.73	109.37
2	A	801	HEM	CMC-C2C-C3C	2.50	129.35	124.68
2	B	801	HEM	CBD-CAD-C3D	-2.48	105.74	112.63
2	A	801	HEM	CMB-C2B-C1B	2.37	128.64	125.04
4	A	803	K8O	C15-C16-N11	-2.34	108.92	111.23
2	A	801	HEM	C3C-C4C-NC	-2.32	106.57	110.94
3	B	802	H4B	N2-C2-N1	2.28	120.80	117.25
3	A	802	H4B	C4-C4A-N5	2.21	120.97	119.12
3	A	802	H4B	N2-C2-N3	2.20	120.68	117.25
2	B	801	HEM	CMC-C2C-C3C	2.18	128.75	124.68
2	B	801	HEM	CMA-C3A-C4A	-2.18	125.12	128.46
3	B	802	H4B	C2-N1-C8A	2.16	119.38	114.54
2	A	801	HEM	CAB-C3B-C2B	-2.14	121.54	128.60
4	A	803	K8O	C09-C10-N11	-2.08	109.66	113.89
2	B	801	HEM	C3C-C4C-NC	-2.04	107.08	110.94

There are no chirality outliers.

All (9) torsion outliers are listed below:

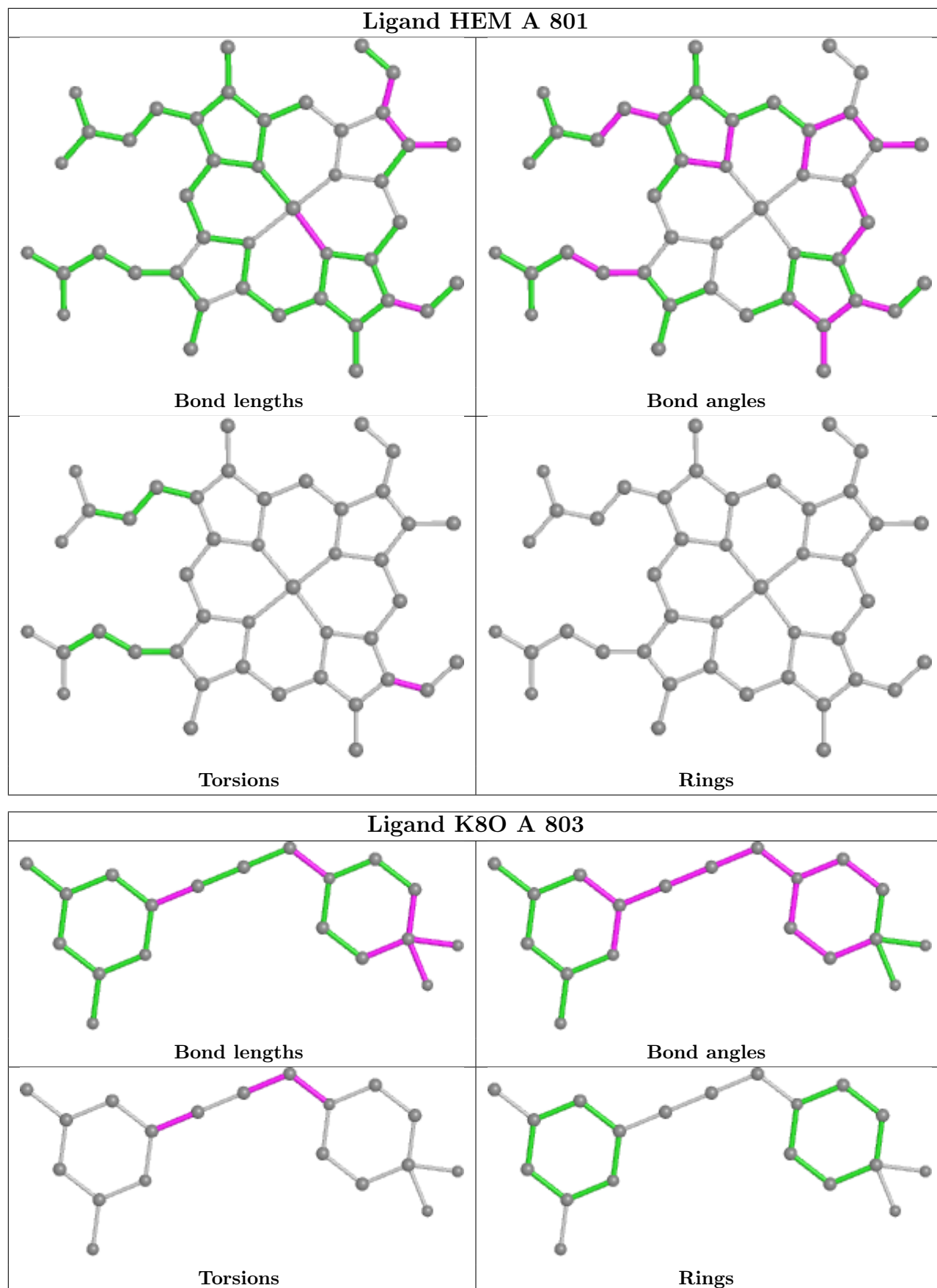
Mol	Chain	Res	Type	Atoms
4	A	803	K8O	C09-C10-N11-C16
4	A	803	K8O	C09-C10-N11-C12
4	A	803	K8O	N01-C06-C08-C09
4	B	803	K8O	C09-C10-N11-C16
4	B	803	K8O	C09-C10-N11-C12
2	A	801	HEM	C4B-C3B-CAB-CBB
4	A	803	K8O	C08-C09-C10-N11
4	A	803	K8O	C05-C06-C08-C09
4	B	803	K8O	N01-C06-C08-C09

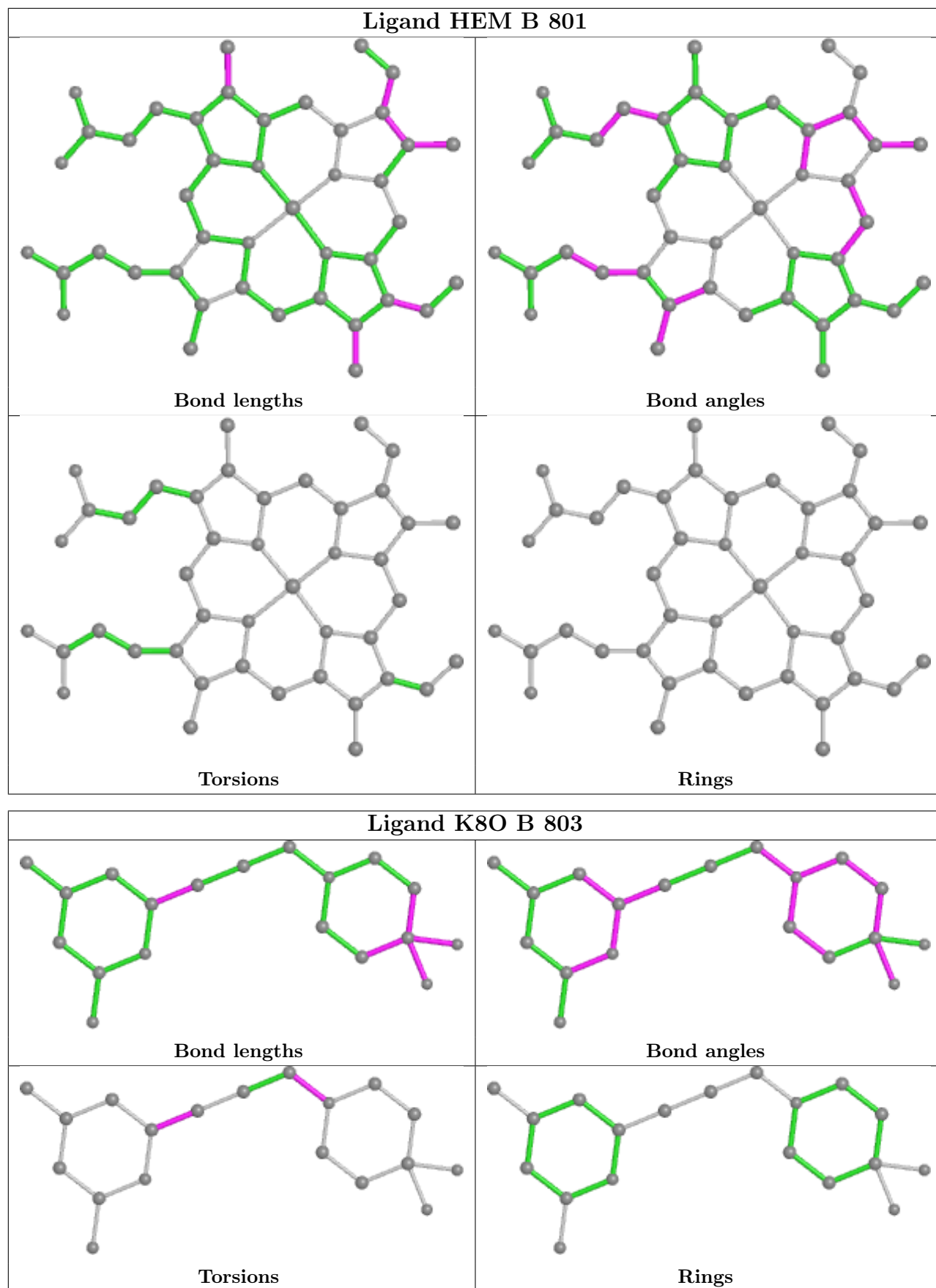
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	2	0
2	B	801	HEM	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

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	410/422 (97%)	1.14	88 (21%) 0 0	34, 61, 111, 157	0
1	B	411/422 (97%)	0.50	39 (9%) 8 8	33, 50, 86, 118	0
All	All	821/844 (97%)	0.82	127 (15%) 2 2	33, 54, 105, 157	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.8
1	A	716	TRP	8.5
1	A	715	VAL	8.0
1	B	348	VAL	7.9
1	A	348	VAL	7.7
1	A	355	PHE	7.1
1	A	339	SER	6.9
1	A	488	PRO	6.7
1	A	388	ILE	6.1
1	B	718	GLY	6.1
1	A	349	ARG	5.8
1	A	299	ARG	5.8
1	B	350	THR	5.6
1	A	506	ILE	5.2
1	B	677	VAL	5.1
1	A	679	ILE	4.9
1	A	678	TRP	4.9
1	A	300	PHE	4.9
1	A	551	PHE	4.8
1	A	350	THR	4.6
1	A	713	THR	4.6
1	A	352	ASP	4.6
1	A	351	LYS	4.5
1	A	676	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	393	THR	4.5
1	B	299	ARG	4.5
1	A	567	VAL	4.4
1	A	508	GLN	4.3
1	A	677	VAL	4.3
1	A	390	SER	4.3
1	B	680	VAL	4.3
1	A	711	TRP	4.2
1	B	611	ALA	4.2
1	A	712	ASN	4.1
1	A	553	TRP	4.1
1	A	507	GLN	4.1
1	A	593	ILE	3.9
1	A	479	LEU	3.9
1	A	480	ILE	3.9
1	A	392	SER	3.8
1	A	391	THR	3.8
1	B	676	TRP	3.8
1	A	503	GLU	3.8
1	B	679	ILE	3.7
1	A	489	ASP	3.7
1	A	619	ARG	3.7
1	A	470	HIS	3.7
1	A	566	ALA	3.6
1	B	619	ARG	3.6
1	A	389	GLU	3.6
1	B	351	LYS	3.6
1	A	491	SER	3.5
1	A	415	CYS	3.5
1	A	416	VAL	3.5
1	B	620	LYS	3.4
1	B	617	ASP	3.4
1	A	584	PHE	3.4
1	A	505	CYS	3.3
1	A	588	TYR	3.2
1	A	714	HIS	3.2
1	A	487	GLN	3.2
1	A	681	PRO	3.2
1	B	691	PHE	3.2
1	A	386	LYS	3.2
1	B	616	LEU	3.2
1	A	643	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	680	VAL	3.2
1	B	593	ILE	3.1
1	A	373	GLY	3.1
1	A	667	ARG	3.1
1	B	715	VAL	3.1
1	A	467	ASP	3.1
1	B	562	TYR	3.0
1	A	322	LEU	3.0
1	B	678	TRP	3.0
1	B	302	LYS	2.9
1	B	567	VAL	2.9
1	A	685	GLY	2.9
1	A	682	PRO	2.9
1	A	469	LYS	2.9
1	A	710	PRO	2.9
1	B	681	PRO	2.8
1	A	561	TRP	2.8
1	A	353	GLN	2.8
1	A	394	TYR	2.8
1	A	370	LYS	2.8
1	A	486	LYS	2.8
1	A	591	THR	2.7
1	B	349	ARG	2.7
1	B	682	PRO	2.7
1	B	566	ALA	2.6
1	B	551	PHE	2.6
1	A	499	VAL	2.6
1	B	612	LYS	2.6
1	A	311	VAL	2.6
1	A	691	PHE	2.5
1	B	352	ASP	2.5
1	A	511	LYS	2.5
1	A	554	PHE	2.5
1	A	490	GLY	2.5
1	A	382	GLU	2.4
1	A	354	LEU	2.4
1	B	588	TYR	2.4
1	A	446	VAL	2.4
1	B	667	ARG	2.4
1	A	385	ASN	2.4
1	A	321	THR	2.4
1	A	384	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	310	VAL	2.3
1	B	615	ASP	2.3
1	A	565	PRO	2.3
1	B	561	TRP	2.3
1	A	590	GLY	2.3
1	B	584	PHE	2.3
1	A	595	VAL	2.3
1	B	309	ASP	2.2
1	A	482	TYR	2.2
1	A	492	THR	2.2
1	A	514	ARG	2.2
1	B	321	THR	2.2
1	B	591	THR	2.2
1	B	416	VAL	2.2
1	A	686	SER	2.1
1	A	466	THR	2.1
1	A	414	ARG	2.1
1	A	683	MET	2.0
1	A	302	LYS	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.

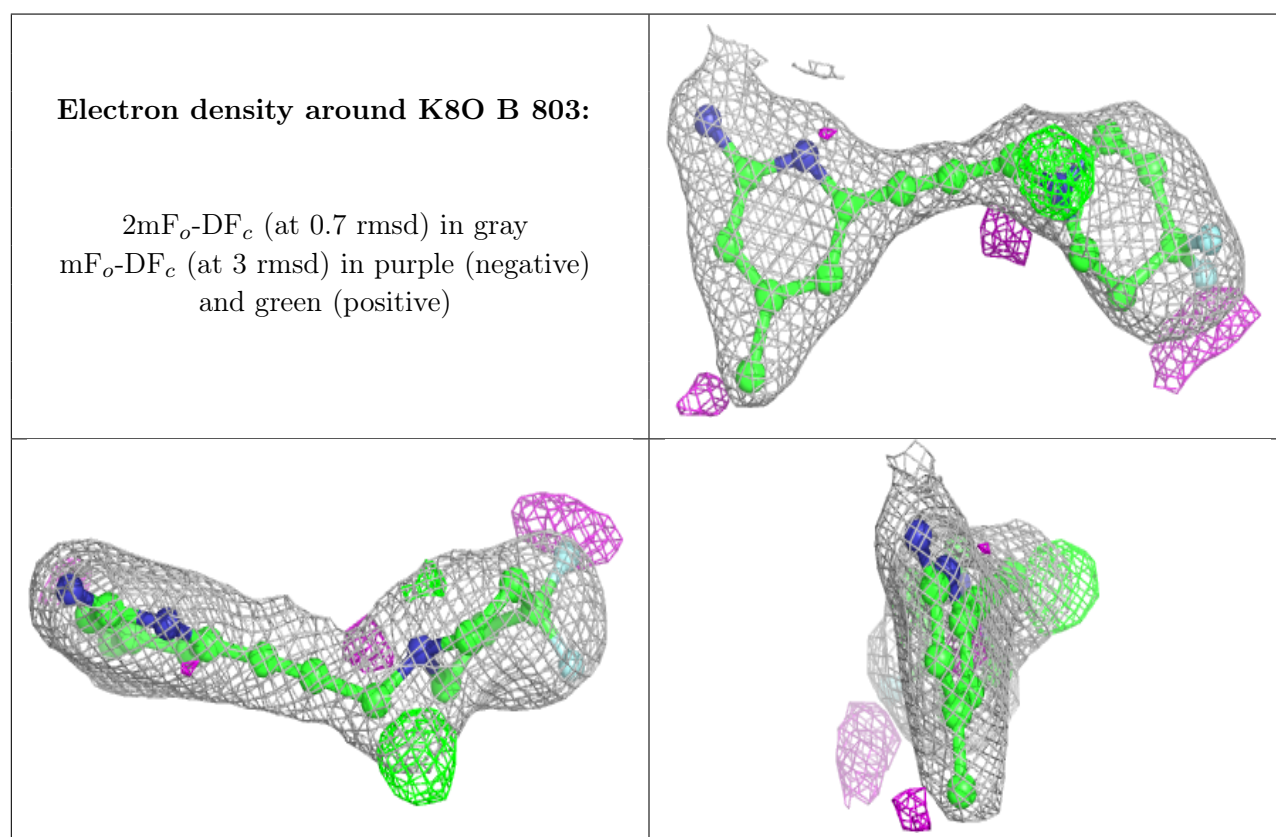
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K8O	B	803	19/19	0.93	0.21	37,57,88,94	0
4	K8O	A	803	19/19	0.94	0.30	39,67,103,104	0
3	H4B	A	802	17/17	0.96	0.16	39,42,46,48	0
5	ACT	A	804	4/4	0.96	0.13	73,74,74,76	0

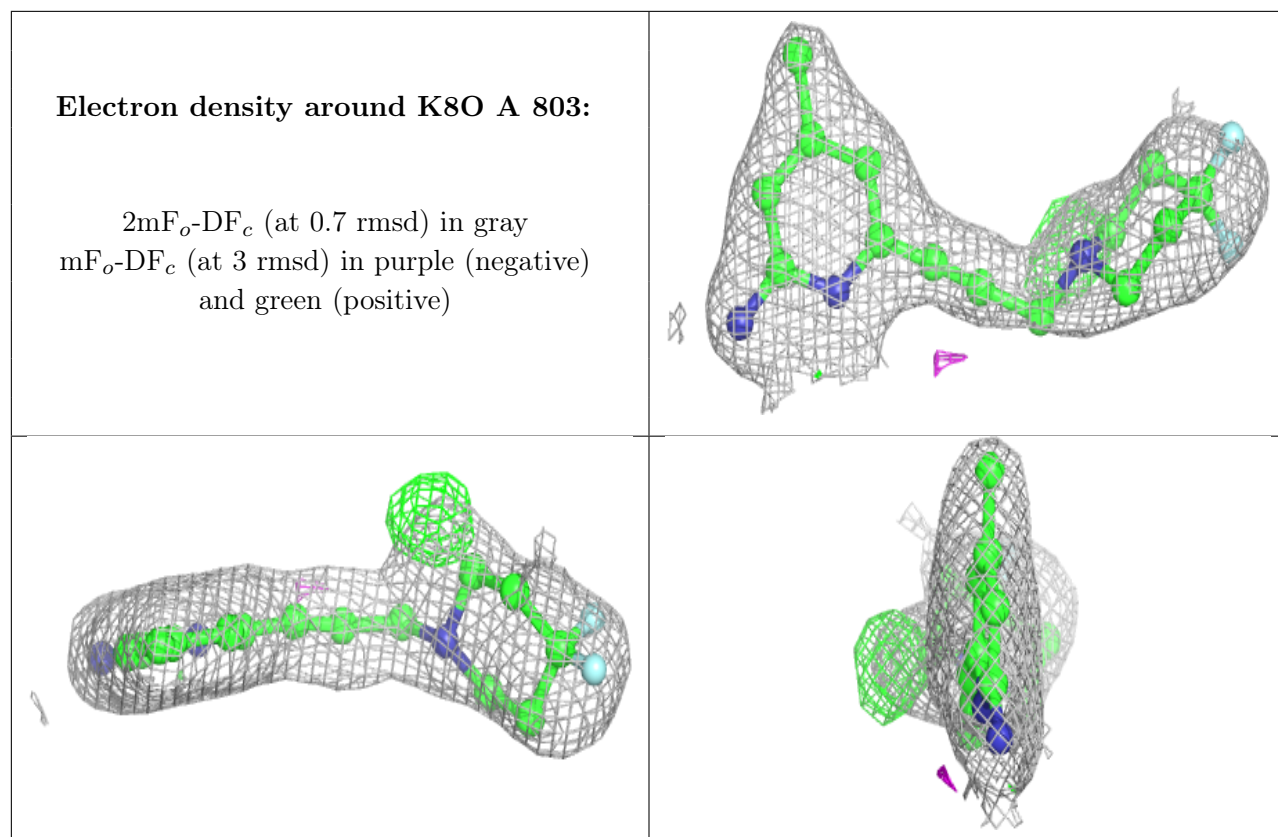
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ACT	B	804	4/4	0.96	0.15	68,70,78,86	0
3	H4B	B	802	17/17	0.97	0.18	36,40,44,45	0
2	HEM	A	801	43/43	0.98	0.20	30,39,55,65	0
2	HEM	B	801	43/43	0.98	0.16	29,39,49,56	0
6	ZN	A	805	1/1	0.99	0.07	44,44,44,44	0

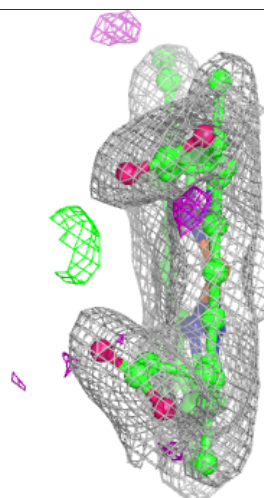
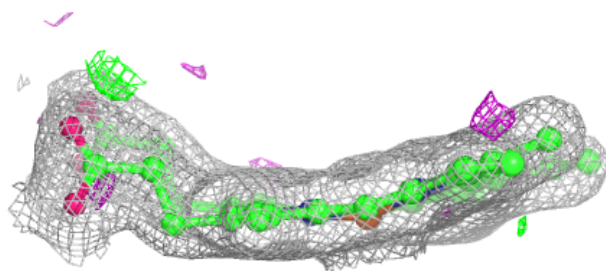
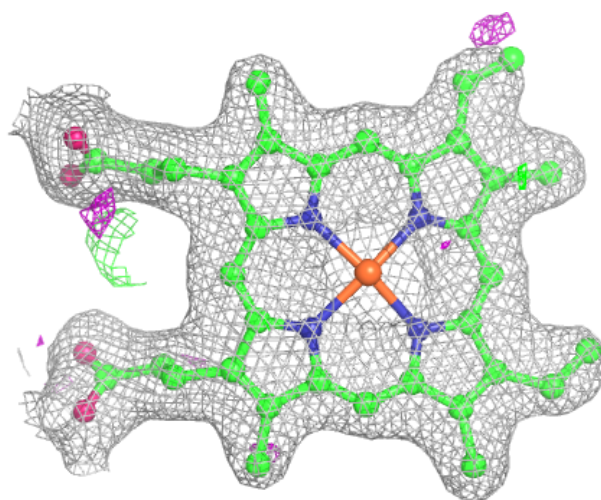
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

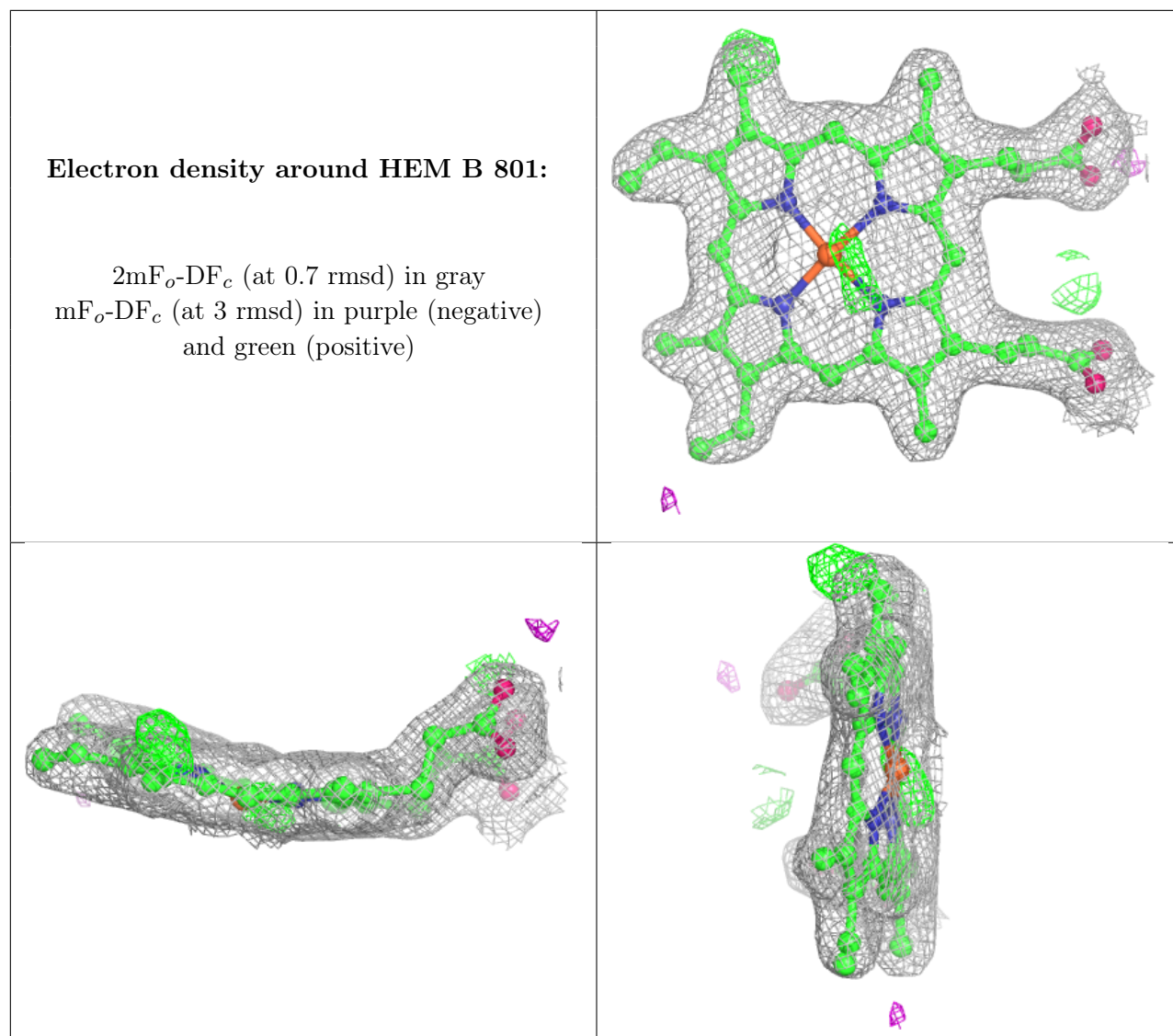




Electron density around HEM A 801:

$2mF_o-DF_c$ (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.