



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:27 AM UTC

PDB ID : 4JSE / pdb_00004jse
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with
6,6'-(pentane-1,5-diyl)bis(4-methylpyridin-2-amine)
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-03-22
Resolution : 1.97 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

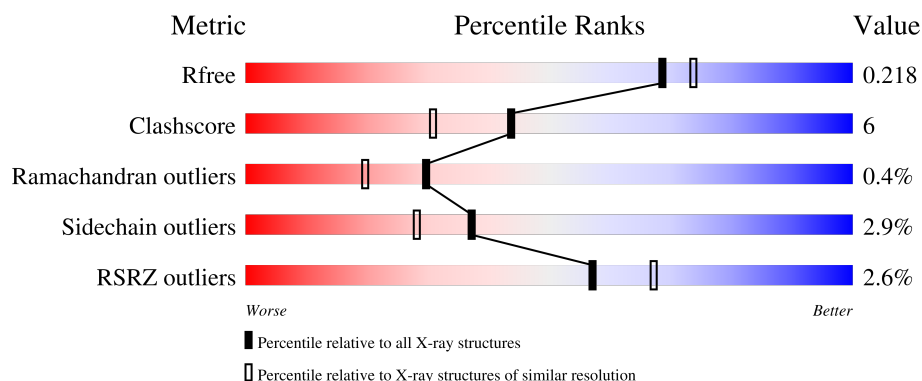
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

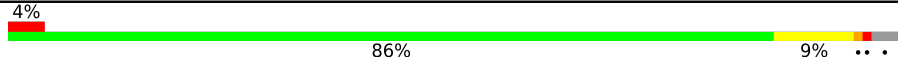
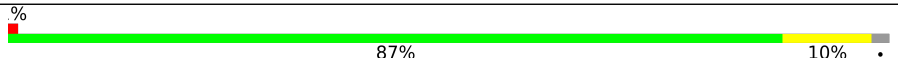
The reported resolution of this entry is 1.97 Å.

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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 8 unique types of molecules in this entry. The entry contains 7377 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	408	Total	C	N	O	S	0	6	0
			3348	2144	570	611	23			
1	B	412	Total	C	N	O	S	0	6	0
			3379	2162	578	616	23			

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



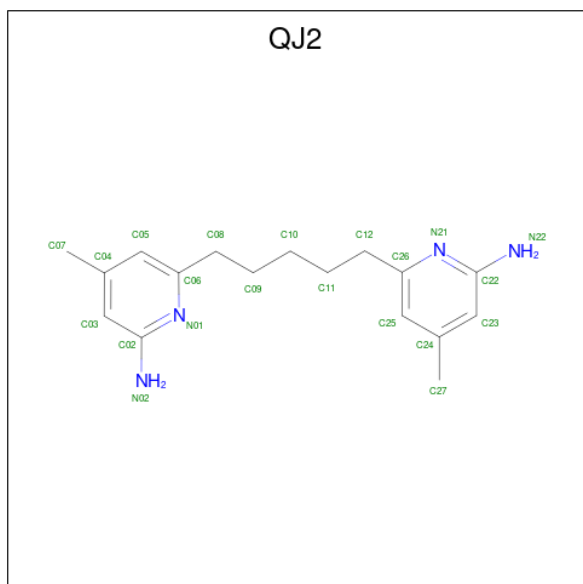
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is 6,6'-pentane-1,5-diylbis(4-methylpyridin-2-amine) (CCD ID: QJ2) (formula: $C_{17}H_{24}N_4$).



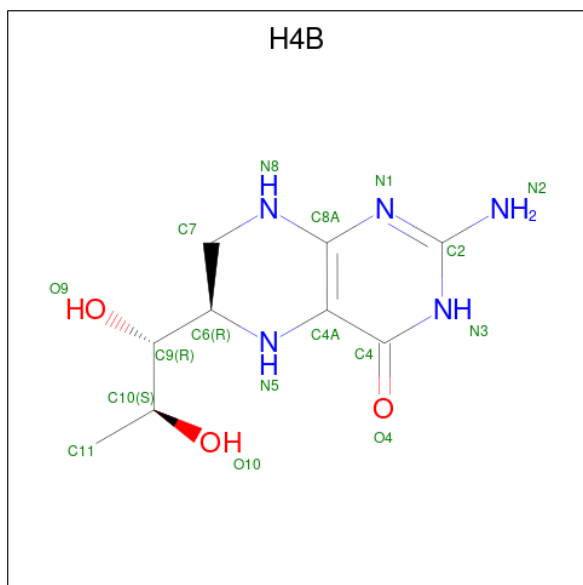
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			21	17	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			21	17	4		
4	B	1	Total	C	N	0	0
			21	17	4		
4	B	1	Total	C	N	0	0
			21	17	4		

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	5	3		
5	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Zn	0	1
			2	2		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	Cl 2	0	2
7	B	2	Total 2	Cl 2	0	0

- Molecule 8 is water.

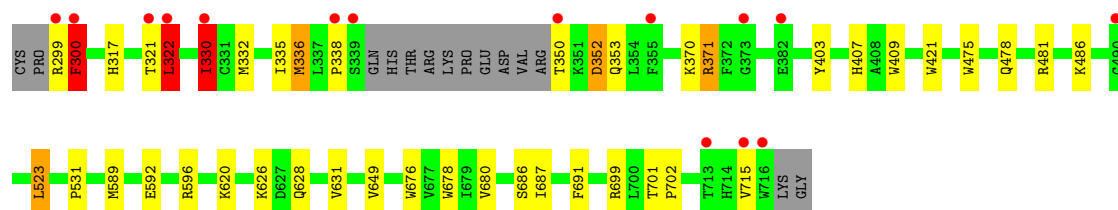
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	178	Total 178	O 178	0	0
8	B	253	Total 253	O 253	0	0

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.

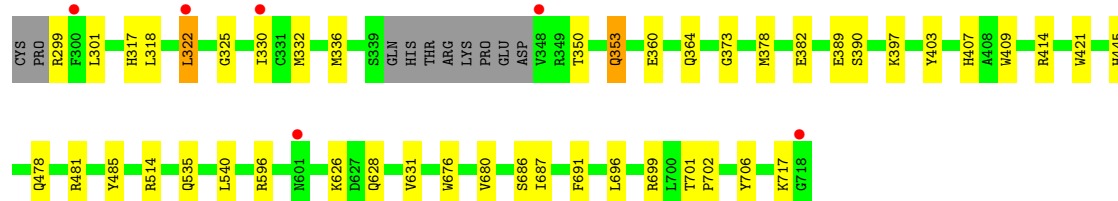
- Molecule 1: Nitric oxide synthase, brain

Chain A: 4% 86% 9% ...



- Molecule 1: Nitric oxide synthase, brain

Chain B: 0% 87% 10% ...



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.74Å 110.25Å 163.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 1.97 49.34 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.34-1.97) 98.8 (49.34-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.205 0.183 , 0.218	Depositor DCC
R_{free} test set	3286 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: QJ2, CL, HEM, H4B, ZN, ACT

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	0.77	0/3459	0.87	1/4692 (0.0%)
1	B	0.83	0/3490	0.87	0/4729
All	All	0.80	0/6949	0.87	1/9421 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ILE	N-CA-C	6.29	117.35	108.17

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	3348	0	3271	42	0
1	B	3379	0	3307	34	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	42	0	48	4	0
4	B	42	0	48	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	17	0	15	6	0
5	B	17	0	15	6	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	178	0	0	4	0
8	B	253	0	0	5	0
All	All	7377	0	6770	83	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 (83) 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:336[A]:MET:HA	1:A:336[A]:MET:HE3	1.47	0.94
1:A:336[A]:MET:HA	1:A:336[A]:MET:CE	1.97	0.94
1:A:371:ARG:HG2	1:A:371:ARG:HH21	1.33	0.93
1:A:371:ARG:HH21	1:A:371:ARG:CG	1.92	0.82
1:A:371:ARG:HG2	1:A:371:ARG:NH2	1.91	0.82
1:A:336[A]:MET:HE3	1:A:336[A]:MET:CA	2.11	0.80
1:B:336[A]:MET:HA	1:B:336[A]:MET:HE2	1.65	0.77
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.70	0.74
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.70	0.73
1:A:701[A]:THR:HG22	1:A:702:PRO:HA	1.70	0.73
2:B:801:HEM:O1A	5:B:802:H4B:N2	2.23	0.72
5:B:802:H4B:O10	5:B:802:H4B:H71	1.89	0.72
1:A:299:ARG:N	1:A:317:HIS:NE2	2.39	0.70
2:A:801:HEM:O1A	5:A:804:H4B:N3	2.27	0.66
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.77	0.64
1:A:336[A]:MET:SD	5:A:804:H4B:H6	2.38	0.63
1:B:336[A]:MET:SD	5:B:802:H4B:H6	2.38	0.62
1:A:321:THR:HG23	1:A:699:ARG:HH11	1.63	0.62
2:B:801:HEM:O1A	5:B:802:H4B:N3	2.36	0.59
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.85	0.58
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.86	0.58
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.86	0.58
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.87	0.57
1:B:299:ARG:HG2	1:B:317:HIS:NE2	2.21	0.56
1:A:336[A]:MET:SD	5:A:804:H4B:H9	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.87	0.55
1:B:364:GLN:NE2	8:B:967:HOH:O	2.39	0.55
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.91	0.53
2:A:801:HEM:O1A	5:A:804:H4B:N2	2.39	0.53
1:A:336[A]:MET:CE	1:A:678:TRP:HE1	2.22	0.52
1:A:321:THR:HG23	1:A:322:LEU:N	2.23	0.52
1:B:373:GLY:HA2	1:B:378:MET:HE3	1.92	0.51
1:A:596[B]:ARG:HG3	8:A:906:HOH:O	2.10	0.50
1:B:299:ARG:HD2	1:B:317:HIS:NE2	2.27	0.49
1:B:701:THR:HA	1:B:702:PRO:C	2.38	0.48
1:B:350:THR:O	1:B:353:GLN:HG2	2.13	0.47
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.50	0.47
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.97	0.47
1:B:596[B]:ARG:HG3	8:B:976:HOH:O	2.14	0.47
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.02	0.47
1:B:325:GLY:O	1:B:332:MET:HG3	2.15	0.47
1:B:445:HIS:C	1:B:445:HIS:CD2	2.94	0.46
1:A:478:GLN:HE21	4:A:805:QJ2:H6	1.80	0.46
2:B:801:HEM:HBA2	4:B:805:QJ2:H14	1.96	0.46
1:B:596[A]:ARG:NE	8:B:1098:HOH:O	2.49	0.46
4:A:803:QJ2:H20	8:A:1006:HOH:O	2.16	0.46
2:B:801:HEM:O1A	5:B:802:H4B:C2	2.64	0.45
1:A:336[A]:MET:HE2	1:A:678:TRP:HE1	1.81	0.45
1:A:336[A]:MET:HA	1:A:336[A]:MET:HE2	1.94	0.45
1:B:336[A]:MET:SD	5:B:802:H4B:H9	2.56	0.45
1:A:701[A]:THR:HG22	8:A:923:HOH:O	2.17	0.45
5:A:804:H4B:O10	5:A:804:H4B:H71	2.16	0.44
1:A:687:ILE:HD12	1:B:626:LYS:HB3	2.00	0.44
1:B:322:LEU:HB2	1:B:699:ARG:HD3	1.99	0.44
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.52	0.44
1:A:699:ARG:HD2	4:A:803:QJ2:H15	2.00	0.44
1:B:336[A]:MET:HE2	1:B:336[A]:MET:CA	2.41	0.44
1:A:352:ASP:OD2	1:A:352:ASP:N	2.51	0.44
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.99	0.44
1:A:686:SER:HA	1:A:691:PHE:CG	2.52	0.44
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.52	0.44
1:A:589:MET:HA	1:A:649:VAL:O	2.18	0.43
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.43
1:A:701[A]:THR:CG2	1:A:702:PRO:HA	2.42	0.43
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.54	0.42
1:A:592:GLU:OE1	4:A:805:QJ2:N01	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:801:HEM:O1A	5:A:804:H4B:C2	2.67	0.42
1:B:478:GLN:HE21	4:B:805:QJ2:H6	1.84	0.42
1:B:717:LYS:N	1:B:717:LYS:HD2	2.35	0.42
1:B:414:ARG:NH1	1:B:706:TYR:OH	2.52	0.42
1:B:596[A]:ARG:NH1	8:B:1119:HOH:O	2.52	0.41
1:A:626:LYS:HB3	1:B:687:ILE:HD12	2.03	0.41
1:A:335:ILE:C	1:A:336[A]:MET:HE3	2.45	0.41
1:A:631:VAL:HG11	1:B:628:GLN:HG2	2.02	0.41
1:A:300:PHE:HB3	8:A:1059:HOH:O	2.20	0.41
1:A:321:THR:HG23	1:A:699:ARG:NH1	2.30	0.41
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.08	0.41
1:B:676:TRP:CE2	1:B:680:VAL:HG21	2.56	0.40
1:B:535:GLN:HG3	8:B:1117:HOH:O	2.21	0.40
1:B:397:LYS:HD2	1:B:397:LYS:HA	1.79	0.40
1:A:322:LEU:HB2	1:A:699:ARG:NH1	2.37	0.40
1:B:686:SER:HA	1:B:691:PHE:CG	2.57	0.40

There are no symmetry-related clashes.

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	410/422 (97%)	398 (97%)	9 (2%)	3 (1%)	18	9
1	B	414/422 (98%)	407 (98%)	7 (2%)	0	100	100
All	All	824/844 (98%)	805 (98%)	16 (2%)	3 (0%)	30	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	300	PHE

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Mol	Chain	Res	Type
1	A	338	PRO

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	370/377 (98%)	356 (96%)	14 (4%)	29	19
1	B	373/377 (99%)	365 (98%)	8 (2%)	47	40
All	All	743/754 (98%)	721 (97%)	22 (3%)	37	27

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

Mol	Chain	Res	Type
1	A	300	PHE
1	A	322	LEU
1	A	330	ILE
1	A	336[A]	MET
1	A	336[B]	MET
1	A	350	THR
1	A	352	ASP
1	A	353	GLN
1	A	370	LYS
1	A	371	ARG
1	A	486	LYS
1	A	523	LEU
1	A	620	LYS
1	A	715	VAL
1	B	322	LEU
1	B	330	ILE
1	B	353	GLN
1	B	360	GLU
1	B	382	GLU
1	B	389	GLU
1	B	390	SER
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	A	425	GLN
1	A	454	ASN
1	A	478	GLN
1	A	508	GLN
1	A	527	ASN
1	A	535	GLN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	454	ASN
1	B	478	GLN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	628	GLN
1	B	697	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 7 are 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	$\# Z > 2$
2	HEM	B	801	1	50,50,50	1.83	13 (26%)	67,82,82	1.22	6 (8%)
4	QJ2	A	803	-	22,22,22	0.80	0	27,29,29	1.95	8 (29%)
5	H4B	B	802	-	17,18,18	0.93	0	14,26,26	1.88	5 (35%)
2	HEM	A	801	1	50,50,50	1.90	11 (22%)	67,82,82	1.48	12 (17%)
5	H4B	A	804	-	17,18,18	0.96	0	14,26,26	2.27	6 (42%)
3	ACT	B	804	-	3,3,3	0.92	0	3,3,3	0.45	0
4	QJ2	A	805	-	22,22,22	0.67	0	27,29,29	1.87	4 (14%)
4	QJ2	B	805	-	22,22,22	0.78	0	27,29,29	2.19	8 (29%)
3	ACT	A	802	-	3,3,3	0.83	0	3,3,3	0.75	0
4	QJ2	B	803	-	22,22,22	0.94	0	27,29,29	2.21	5 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	801	1	-	0/14/54/54	-
4	QJ2	A	803	-	-	4/8/8/8	0/2/2/2
5	H4B	B	802	-	-	3/8/17/17	0/2/2/2
2	HEM	A	801	1	-	1/14/54/54	-
5	H4B	A	804	-	-	3/8/17/17	0/2/2/2
4	QJ2	A	805	-	-	3/8/8/8	0/2/2/2
4	QJ2	B	805	-	-	1/8/8/8	0/2/2/2
4	QJ2	B	803	-	-	4/8/8/8	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3D-C2D	6.69	1.51	1.36
2	B	801	HEM	C3D-C2D	6.49	1.50	1.36
2	A	801	HEM	FE-ND	4.64	2.09	1.94
2	A	801	HEM	FE-NB	4.03	2.07	1.94
2	B	801	HEM	FE-ND	3.86	2.06	1.94
2	A	801	HEM	FE-NA	3.64	2.07	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	FE-NA	3.37	2.06	1.95
2	B	801	HEM	FE-NC	3.32	2.06	1.95
2	A	801	HEM	CMC-C2C	3.27	1.57	1.50
2	B	801	HEM	FE-NB	3.14	2.04	1.94
2	B	801	HEM	CMB-C2B	3.04	1.57	1.50
2	A	801	HEM	FE-NC	2.86	2.04	1.95
2	A	801	HEM	CMA-C3A	2.84	1.56	1.50
2	B	801	HEM	CAB-C3B	2.76	1.54	1.47
2	B	801	HEM	CAC-C3C	2.73	1.54	1.47
2	A	801	HEM	CAC-C3C	2.72	1.54	1.47
2	A	801	HEM	CAB-C3B	2.70	1.54	1.47
2	B	801	HEM	CMA-C3A	2.58	1.56	1.50
2	A	801	HEM	CMB-C2B	2.38	1.55	1.50
2	B	801	HEM	CMC-C2C	2.35	1.55	1.50
2	B	801	HEM	CMD-C2D	2.34	1.55	1.50
2	A	801	HEM	CMD-C2D	2.19	1.55	1.50
2	B	801	HEM	CAD-C3D	2.05	1.56	1.51
2	B	801	HEM	CAA-C2A	2.01	1.56	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	QJ2	C22-N21-C26	6.42	122.87	118.07
4	B	805	QJ2	C22-N21-C26	5.89	122.48	118.07
4	A	803	QJ2	C02-N01-C06	5.64	122.29	118.07
4	B	803	QJ2	C02-N01-C06	5.47	122.16	118.07
4	B	805	QJ2	C02-N01-C06	5.28	122.02	118.07
4	A	805	QJ2	C22-N21-C26	5.08	121.87	118.07
5	A	804	H4B	C2-N1-C8A	4.91	122.02	113.36
2	A	801	HEM	C4D-ND-C1D	4.90	111.01	105.21
4	A	805	QJ2	C02-N01-C06	4.75	121.62	118.07
4	A	803	QJ2	C22-N21-C26	4.66	121.56	118.07
2	A	801	HEM	CBA-CAA-C2A	-4.08	101.24	112.53
2	B	801	HEM	C4D-ND-C1D	4.06	110.01	105.21
5	B	802	H4B	C2-N1-C8A	3.99	120.41	113.36
4	B	805	QJ2	C05-C06-N01	-3.92	118.26	122.73
4	A	805	QJ2	C05-C06-N01	-3.83	118.36	122.73
2	B	801	HEM	C3B-C4B-NB	-3.48	106.97	109.47
2	A	801	HEM	CHA-C4D-ND	3.45	128.63	124.37
4	B	803	QJ2	C25-C26-N21	-3.34	118.92	122.73
4	B	803	QJ2	C08-C06-N01	3.30	121.06	116.06
4	B	803	QJ2	C05-C06-N01	-3.23	119.05	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	QJ2	C27-C24-C25	-3.17	116.63	120.92
2	A	801	HEM	CMD-C2D-C1D	3.10	129.87	125.03
5	A	804	H4B	C4-C4A-N5	3.06	124.60	116.27
2	A	801	HEM	CBD-CAD-C3D	-3.04	104.14	112.53
4	A	803	QJ2	C12-C26-N21	2.75	120.22	116.06
5	A	804	H4B	O10-C10-C9	-2.73	105.25	109.77
5	A	804	H4B	N3-C2-N1	-2.73	118.32	123.32
5	A	804	H4B	C4A-C4-N3	2.73	119.63	112.13
4	A	803	QJ2	C25-C26-N21	-2.71	119.64	122.73
4	B	805	QJ2	C11-C12-C26	-2.70	105.10	113.09
5	B	802	H4B	C4A-C4-N3	2.67	119.45	112.13
4	A	803	QJ2	C05-C06-N01	-2.54	119.84	122.73
4	A	803	QJ2	N22-C22-N21	2.49	120.60	116.59
4	B	805	QJ2	C08-C06-N01	2.38	119.67	116.06
4	A	805	QJ2	C11-C12-C26	-2.36	106.11	113.09
2	A	801	HEM	C3D-C4D-ND	-2.35	107.59	110.17
4	A	803	QJ2	C08-C06-N01	2.35	119.62	116.06
2	B	801	HEM	CBD-CAD-C3D	-2.35	106.04	112.53
5	B	802	H4B	N3-C2-N1	-2.34	119.03	123.32
2	B	801	HEM	C4B-C3B-C2B	2.33	109.42	107.28
2	B	801	HEM	CAD-C3D-C4D	2.32	128.74	124.70
2	A	801	HEM	C1D-C2D-C3D	-2.32	104.54	106.98
4	A	803	QJ2	N02-C02-N01	2.32	120.31	116.59
5	B	802	H4B	C4-C4A-N5	2.29	122.51	116.27
2	A	801	HEM	C4C-C3C-C2C	2.26	108.78	106.81
2	B	801	HEM	CBA-CAA-C2A	-2.23	106.37	112.53
2	A	801	HEM	CHC-C1C-NC	2.22	126.87	124.45
2	A	801	HEM	C3B-C4B-NB	-2.21	107.88	109.47
4	B	805	QJ2	C25-C26-N21	-2.21	120.21	122.73
5	B	802	H4B	O4-C4-C4A	-2.21	121.94	127.26
5	A	804	H4B	O4-C4-N3	-2.21	115.97	120.11
4	B	805	QJ2	C12-C26-N21	2.18	119.37	116.06
2	A	801	HEM	CAD-CBD-CGD	-2.13	108.00	113.67
2	A	801	HEM	CHD-C4C-NC	2.12	126.77	124.45

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	H4B	C7-C6-C9-O9
5	A	804	H4B	C7-C6-C9-C10
5	B	802	H4B	C7-C6-C9-O9

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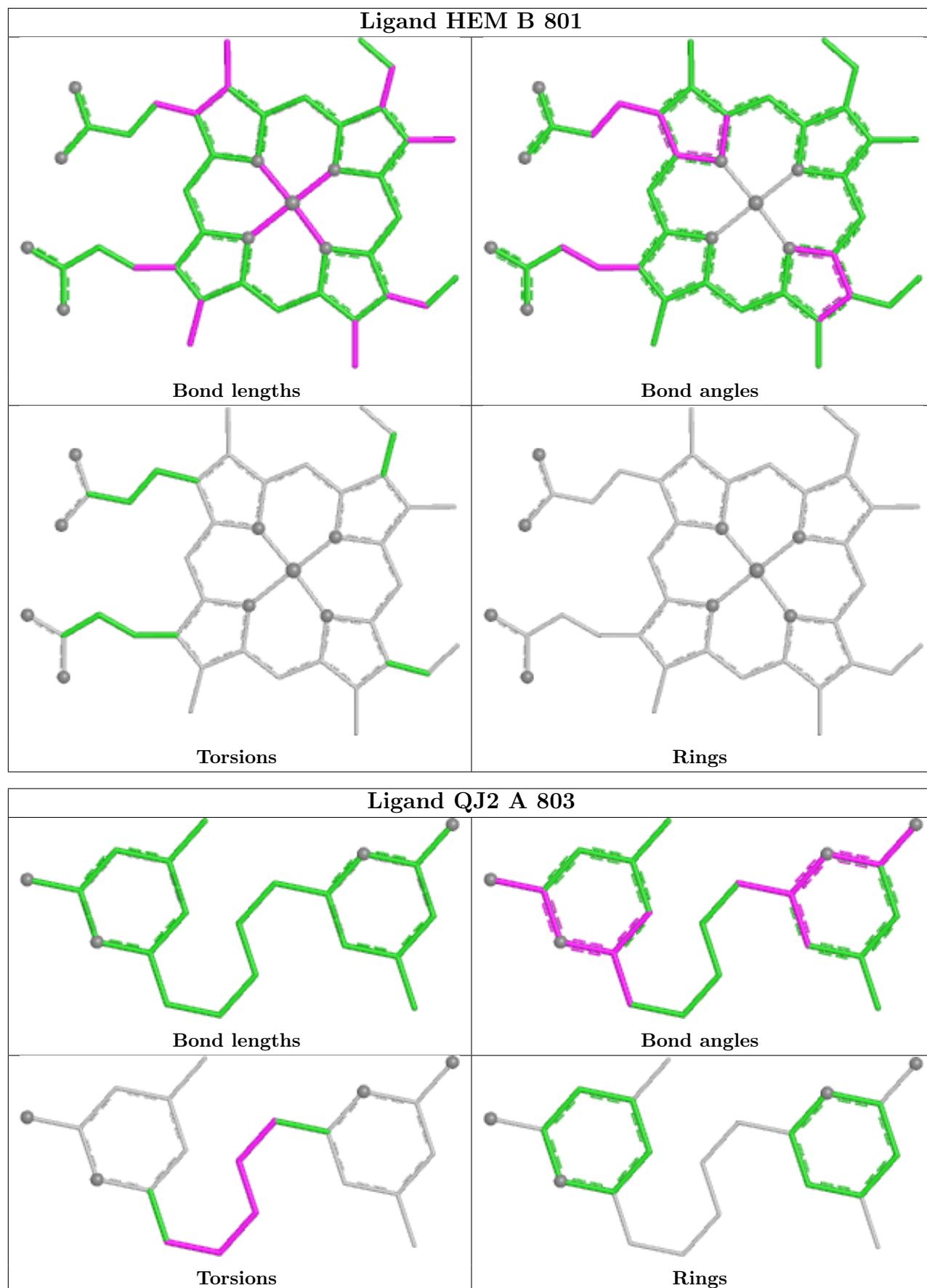
Mol	Chain	Res	Type	Atoms
5	B	802	H4B	C7-C6-C9-C10
4	A	803	QJ2	C10-C11-C12-C26
4	A	803	QJ2	C06-C08-C09-C10
4	B	803	QJ2	C10-C11-C12-C26
4	A	803	QJ2	C08-C09-C10-C11
2	A	801	HEM	C4B-C3B-CAB-CBB
4	A	805	QJ2	C08-C09-C10-C11
5	A	804	H4B	N5-C6-C9-O9
5	B	802	H4B	N5-C6-C9-O9
4	B	803	QJ2	C09-C10-C11-C12
4	B	805	QJ2	C08-C09-C10-C11
4	A	805	QJ2	N01-C06-C08-C09
4	B	803	QJ2	C11-C12-C26-C25
4	A	803	QJ2	C09-C10-C11-C12
4	B	803	QJ2	C11-C12-C26-N21
4	A	805	QJ2	C05-C06-C08-C09

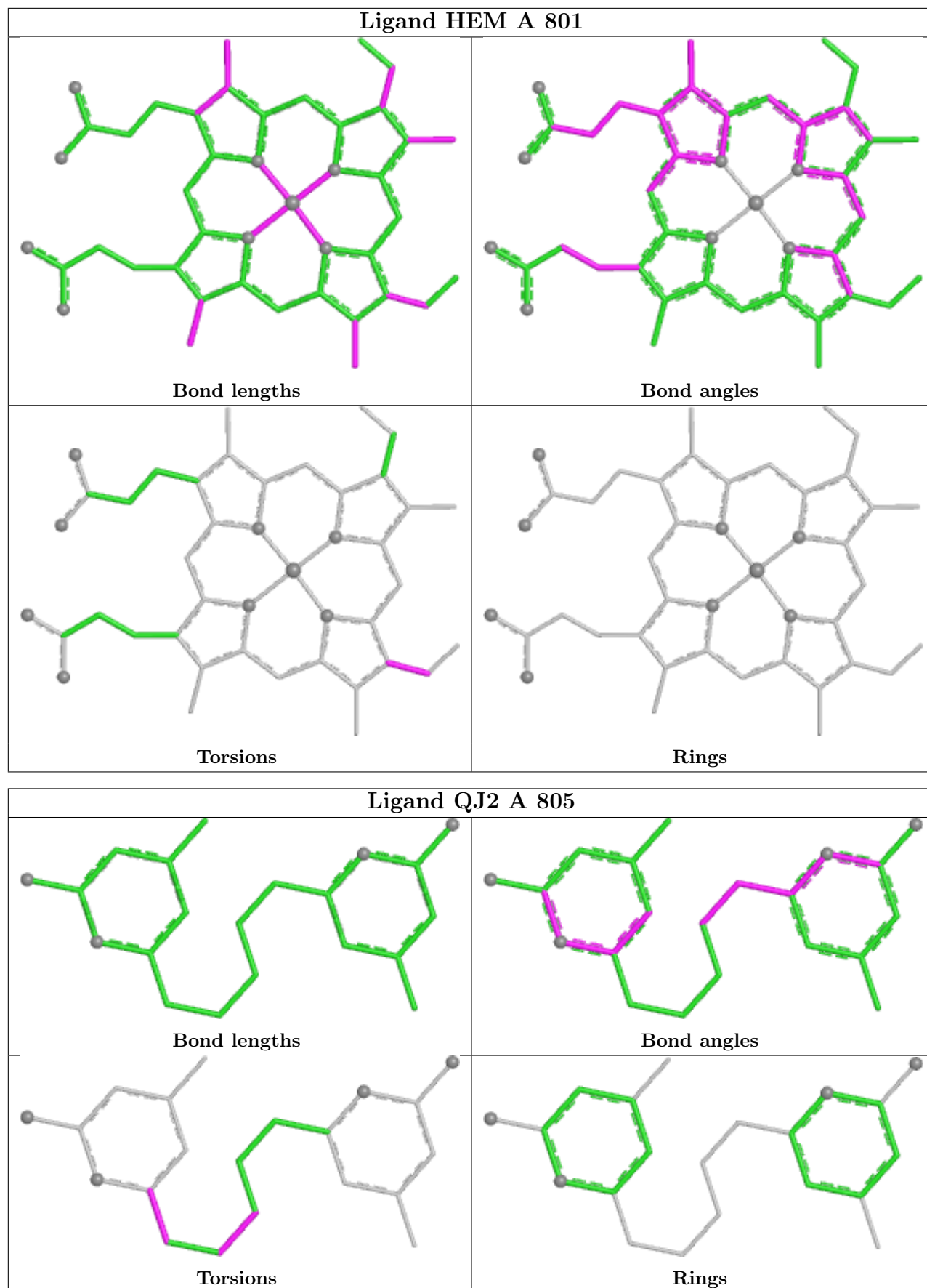
There are no ring outliers.

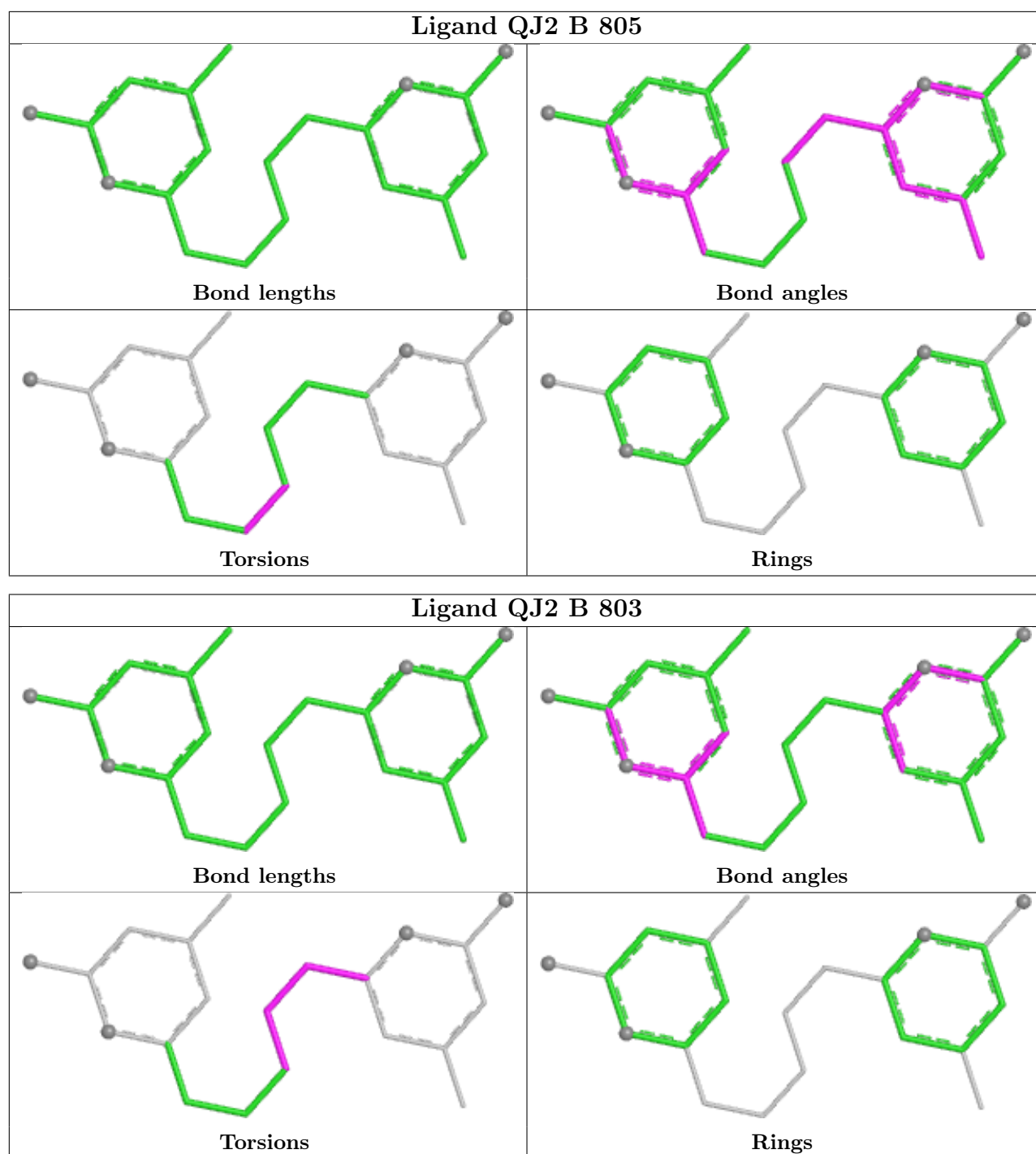
7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	5	0
4	A	803	QJ2	2	0
5	B	802	H4B	6	0
2	A	801	HEM	5	0
5	A	804	H4B	6	0
4	A	805	QJ2	2	0
4	B	805	QJ2	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	408/422 (96%)	0.21	15 (3%) 45 55	20, 38, 63, 85	6 (1%)
1	B	412/422 (97%)	-0.06	6 (1%) 72 80	19, 33, 54, 80	6 (1%)
All	All	820/844 (97%)	0.08	21 (2%) 57 67	19, 35, 61, 85	12 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	6.6
1	B	322	LEU	5.9
1	A	300	PHE	4.5
1	B	348	VAL	4.5
1	A	716	TRP	3.8
1	B	300	PHE	3.7
1	A	715	VAL	3.4
1	A	299	ARG	3.1
1	A	350	THR	2.7
1	A	713	THR	2.4
1	A	338	PRO	2.4
1	A	339	SER	2.4
1	B	330	ILE	2.4
1	A	321	THR	2.3
1	A	373	GLY	2.3
1	B	718	GLY	2.2
1	A	355	PHE	2.2
1	A	330	ILE	2.2
1	A	490	GLY	2.2
1	A	382	GLU	2.1
1	B	601	ASN	2.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

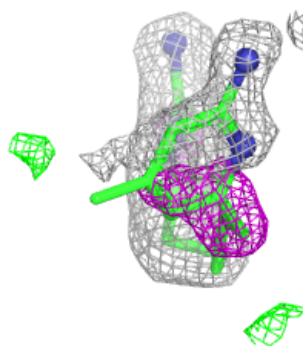
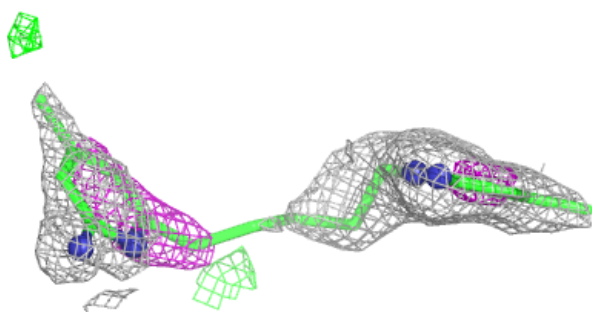
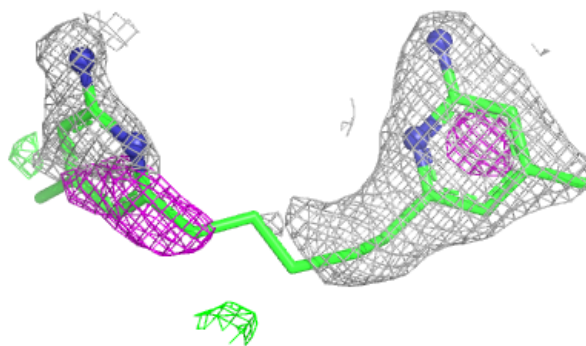
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QJ2	A	803	21/21	0.74	0.17	37,54,72,72	0
5	H4B	A	804	17/17	0.83	0.12	37,43,48,49	0
4	QJ2	B	803	21/21	0.84	0.15	35,50,71,73	0
4	QJ2	B	805	21/21	0.87	0.12	20,36,48,48	0
4	QJ2	A	805	21/21	0.89	0.10	21,35,45,46	0
5	H4B	B	802	17/17	0.90	0.13	44,51,55,56	0
3	ACT	A	802	4/4	0.94	0.10	41,42,42,43	0
7	CL	A	808[A]	1/1	0.95	0.07	40,40,40,40	1
7	CL	A	807[A]	1/1	0.96	0.07	35,35,35,35	1
3	ACT	B	804	4/4	0.96	0.06	37,38,39,40	0
2	HEM	A	801	43/43	0.97	0.07	25,29,41,50	0
7	CL	B	807	1/1	0.97	0.08	45,45,45,45	1
7	CL	B	808	1/1	0.97	0.06	42,42,42,42	1
2	HEM	B	801	43/43	0.98	0.07	22,25,38,48	0
6	ZN	A	809	1/1	0.99	0.02	32,32,32,32	0
6	ZN	B	806	1/1	0.99	0.04	36,36,36,36	1
6	ZN	A	806[A]	1/1	0.99	0.03	31,31,31,31	1

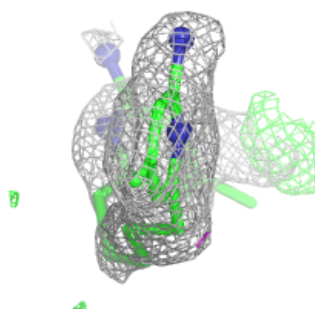
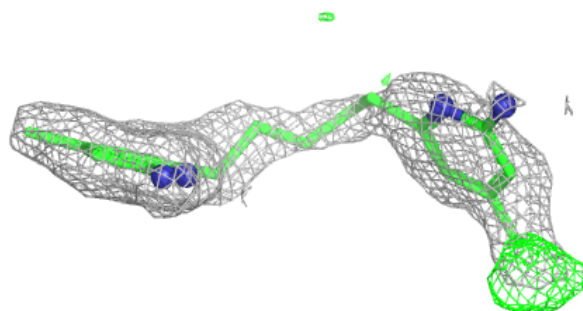
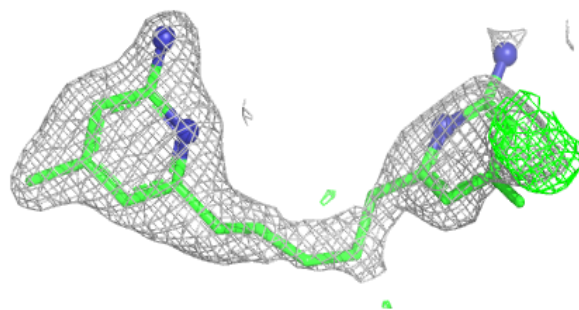
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QJ2 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)

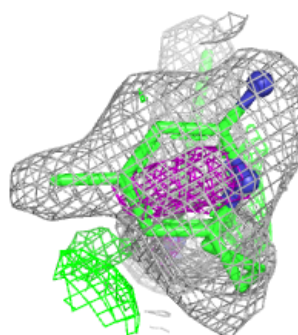
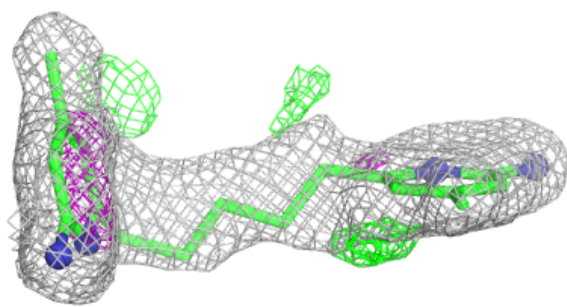
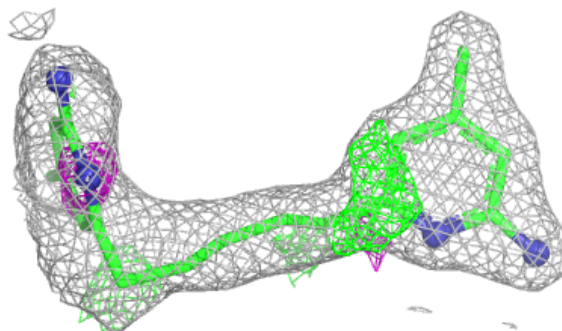
**Electron density around QJ2 B 803:**

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

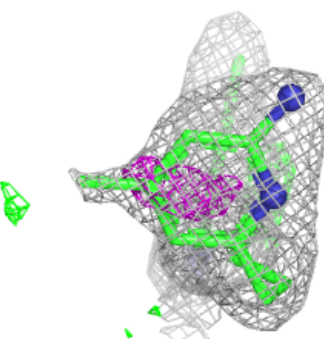
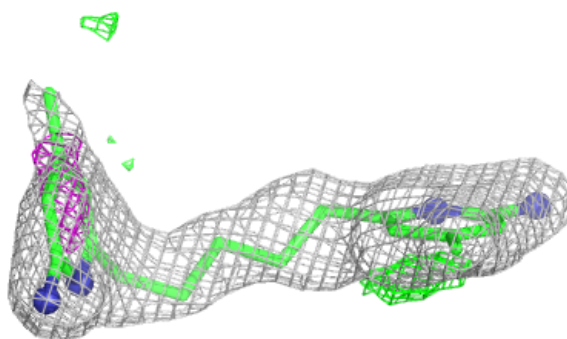
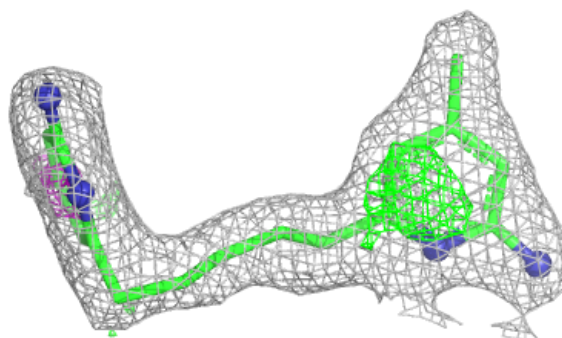


Electron density around QJ2 B 805:

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

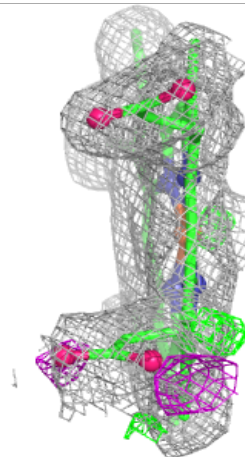
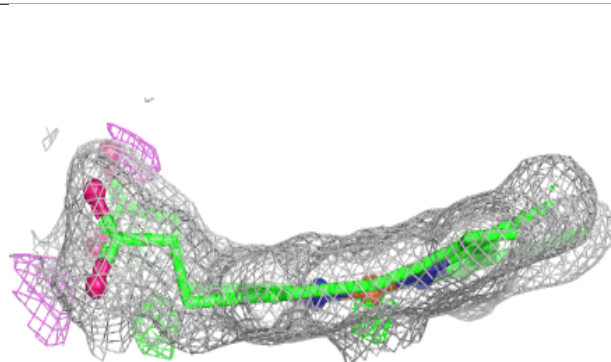
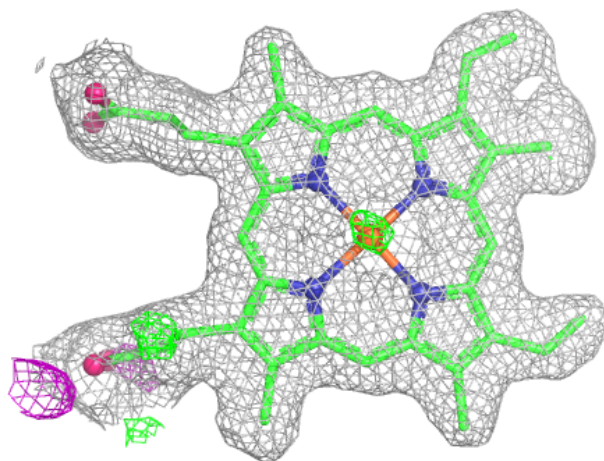
**Electron density around QJ2 A 805:**

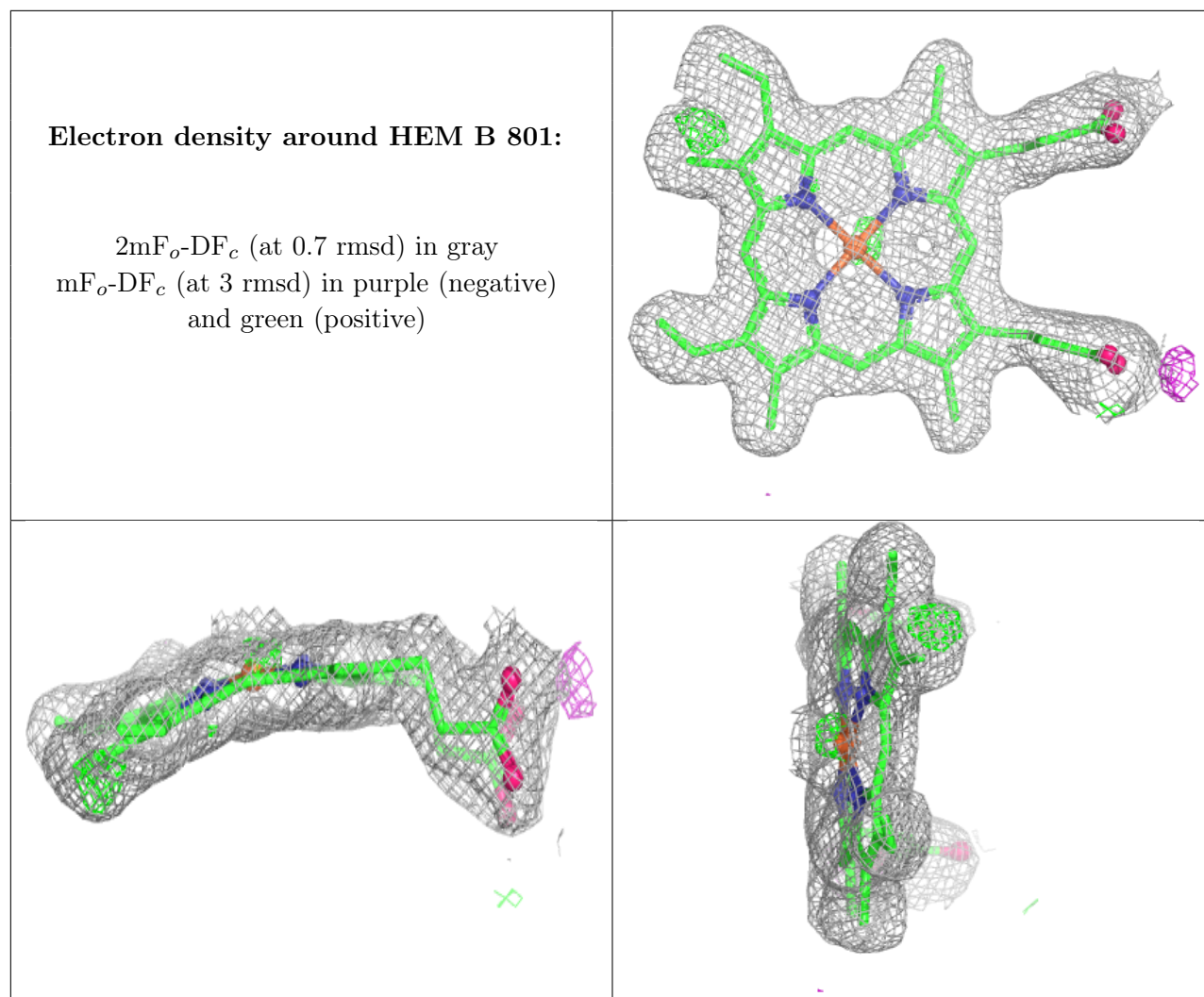
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 801:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.