



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 02:57 AM EDT

PDB ID : 3JX3
Title : Structure of rat neuronal nitric oxide synthase D597N/M336V mutant heme domain in complex with N1-[(3'R,4'R)-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl]-N2-(3'-fluorophenethyl)ethane-1,2-diamine
Authors : Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on : 2009-09-18
Resolution : 1.95 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 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 : 2.23.2
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) : 2.23.2

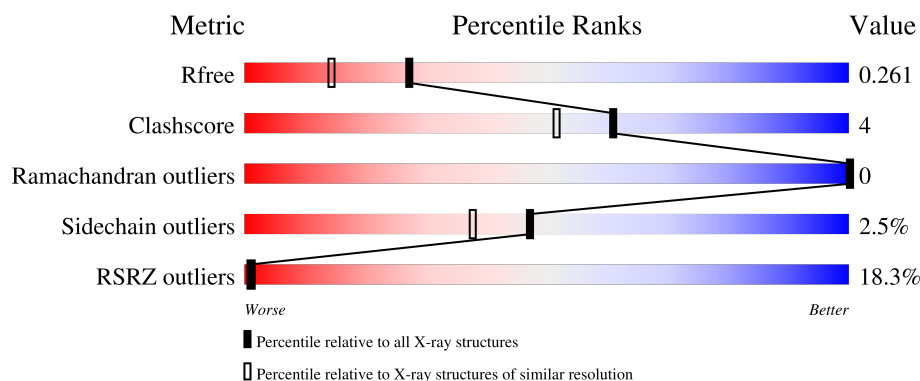
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 7144 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	407	Total	C	N	O	S	0	0	0
			3312	2121	567	604	20			
1	B	411	Total	C	N	O	S	0	0	0
			3344	2140	575	609	20			

There are 4 discrepancies between the modelled and reference sequences:

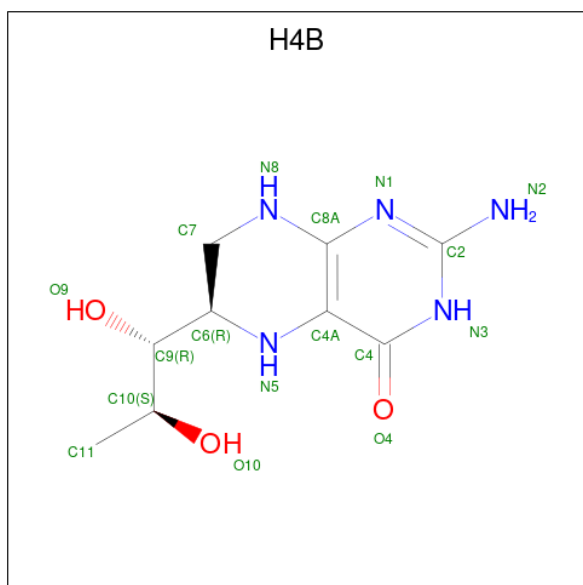
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	engineered mutation	UNP P29476
A	597	ASN	ASP	engineered mutation	UNP P29476
B	336	VAL	MET	engineered mutation	UNP P29476
B	597	ASN	ASP	engineered mutation	UNP P29476

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



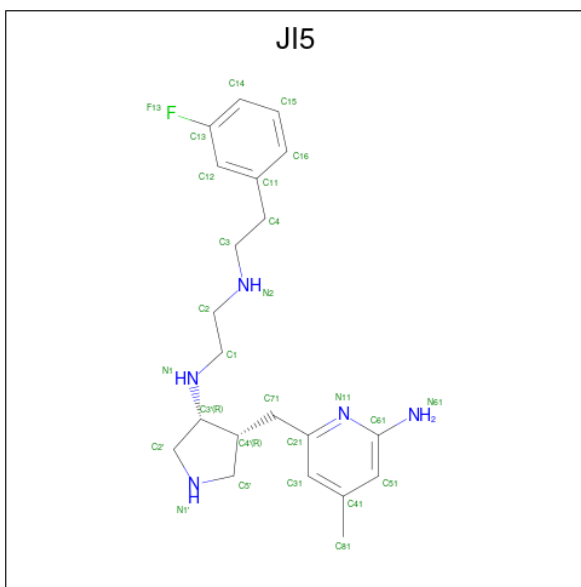
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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
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 N-[(3R,4R)-4-[(6-amino-4-methylpyridin-2-yl)methyl]pyrrolidin-3-yl]-N'-[2-(3-fluorophenyl)ethyl]ethane-1,2-diamine (three-letter code: JI5) (formula: $C_{21}H_{30}FN_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			27	21	1	5		
4	B	1	Total	C	F	N	0	0
			27	21	1	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

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

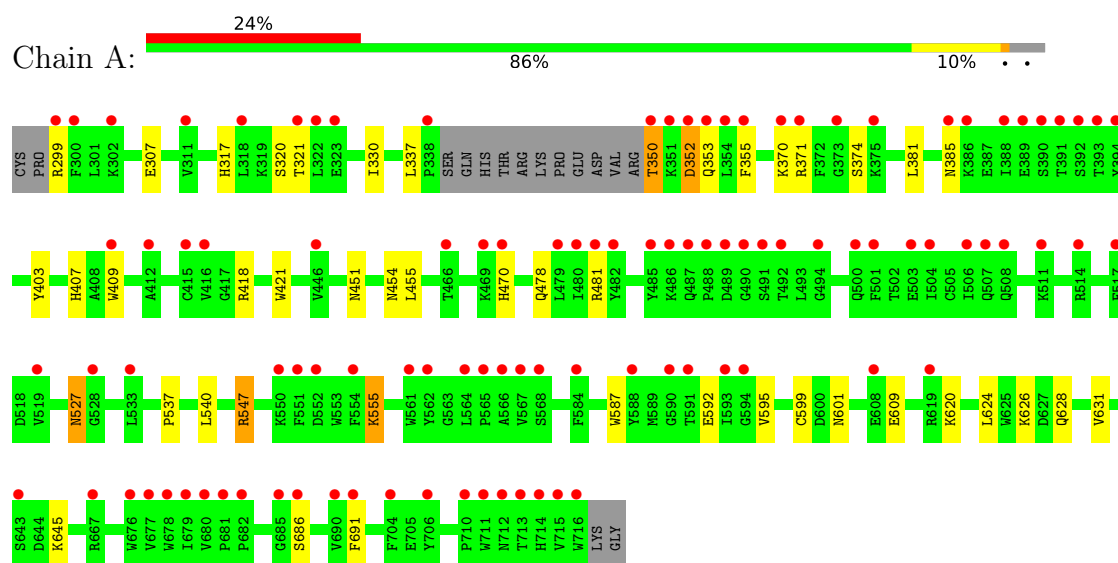
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	130	Total 130	O 130	0	0
7	B	175	Total 175	O 175	0	0

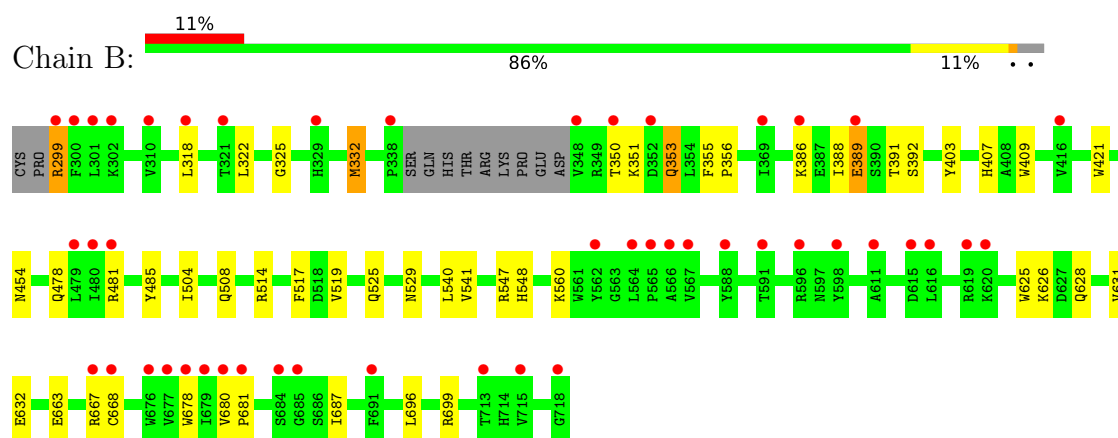
3 Residue-property plots [i](#)

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	51.84Å 110.90Å 164.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.95 – 1.95 38.94 – 1.95	Depositor EDS
% Data completeness (in resolution range)	89.5 (38.95-1.95) 89.5 (38.94-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.182 , 0.223 0.227 , 0.261	Depositor DCC
R_{free} test set	3080 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7144	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: HEM, ZN, JI5, ACT, H4B

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	0.82	2/3405 (0.1%)	0.73	3/4621 (0.1%)
1	B	0.76	0/3437	0.72	0/4661
All	All	0.79	2/6842 (0.0%)	0.72	3/9282 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	SER	CB-OG	6.00	1.50	1.42
1	A	609	GLU	C-O	5.16	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	A	547	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	418	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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	3312	0	3223	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3344	0	3261	28	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	30	4	0
4	B	27	0	30	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	130	0	0	2	0
7	B	175	0	0	2	0
All	All	7144	0	6640	60	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 (60) 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)
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.63	0.81
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.71	0.72
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.71	0.72
1:A:307:GLU:HG3	7:B:1021:HOH:O	1.91	0.70
1:B:668:CYS:HB3	7:B:1125:HOH:O	1.90	0.70
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.79	0.65
2:B:750:HEM:HBA2	4:B:800:JI5:H4	1.79	0.64
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.83	0.60
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.84	0.59
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.69	0.56
1:A:592:GLU:OE1	4:A:800:JI5:H16	2.06	0.56
1:B:391:THR:O	1:B:392:SER:HB2	2.06	0.55
1:A:317:HIS:O	1:A:320:SER:HB3	2.06	0.55
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.89	0.55
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.38	0.54
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.92	0.52
1:A:555:LYS:NZ	1:A:555:LYS:HB3	2.26	0.50
4:A:800:JI5:H2A	7:A:1030:HOH:O	2.10	0.50
1:B:519:VAL:HG21	1:B:541:VAL:HG11	1.91	0.50
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.40	0.50
2:B:750:HEM:HBB2	2:B:750:HEM:CHC	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:O	1:A:317:HIS:CE1	2.65	0.49
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.48	0.49
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.95	0.48
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.03	0.47
4:A:800:JI5:H1	7:A:1012:HOH:O	2.13	0.47
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.02	0.47
1:B:386:LYS:O	1:B:389:GLU:HG3	2.15	0.46
1:B:663:GLU:O	1:B:667:ARG:HD2	2.16	0.46
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.48	0.46
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.51	0.45
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.99	0.45
1:B:525:GLN:HG3	1:B:529:ASN:O	2.16	0.45
1:A:350:THR:N	1:A:353:GLN:HE21	2.15	0.44
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.47	0.44
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.52	0.44
1:A:337:LEU:HD21	4:A:800:JI5:H51	1.99	0.44
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.31	0.44
1:B:325:GLY:O	1:B:332:MET:HG3	2.17	0.44
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.86	0.44
1:A:595:VAL:O	1:A:599:CYS:HB2	2.19	0.43
1:A:624:LEU:HD23	1:A:624:LEU:N	2.33	0.43
1:A:527:ASN:HD22	1:A:527:ASN:HA	1.66	0.43
1:A:352:ASP:OD2	1:A:352:ASP:N	2.52	0.42
1:A:686:SER:HA	1:A:691:PHE:CG	2.54	0.42
1:B:388:ILE:O	1:B:392:SER:N	2.48	0.42
1:B:353:GLN:HE21	1:B:353:GLN:HB3	1.61	0.42
1:B:351:LYS:HE2	1:B:392:SER:OG	2.20	0.42
1:B:504:ILE:O	1:B:508:GLN:HG2	2.20	0.42
1:B:625:TRP:CZ3	1:B:626:LYS:HG2	2.55	0.42
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.42	0.41
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.55	0.41
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.56	0.41
1:B:517:PHE:CB	1:B:560:LYS:HE3	2.51	0.40
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.37	0.40
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.86	0.40
1:A:451:ASN:HB3	1:A:454:ASN:O	2.21	0.40
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.03	0.40
1:B:355:PHE:N	1:B:356:PRO:HD2	2.36	0.40
1:B:678:TRP:CH2	4:B:800:JI5:H5'A	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	403/422 (96%)	386 (96%)	17 (4%)	0	100	100
1	B	407/422 (96%)	399 (98%)	8 (2%)	0	100	100
All	All	810/844 (96%)	785 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	363/377 (96%)	353 (97%)	10 (3%)	43	33
1	B	366/377 (97%)	358 (98%)	8 (2%)	52	44
All	All	729/754 (97%)	711 (98%)	18 (2%)	47	38

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

Mol	Chain	Res	Type
1	A	321	THR
1	A	350	THR
1	A	352	ASP
1	A	371	ARG
1	A	381	LEU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS

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Mol	Chain	Res	Type
1	A	601	ASN
1	A	645	LYS
1	B	299	ARG
1	B	332	MET
1	B	350	THR
1	B	353	GLN
1	B	389	GLU
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	527	ASN
1	A	605	ASN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	601	ASN
1	B	605	ASN
1	B	642	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 monosaccharides in this entry.

5.6 Ligand geometry

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	750	1	27,50,50	2.11	8 (29%)	17,82,82	3.25	6 (35%)
4	JI5	B	800	-	27,29,29	0.87	0	30,38,38	1.91	6 (20%)
3	H4B	A	760	-	16,18,18	0.95	0	11,26,26	3.10	6 (54%)
5	ACT	A	860	-	1,3,3	2.10	1 (100%)	0,3,3	-	-
2	HEM	B	750	1	27,50,50	2.12	7 (25%)	17,82,82	3.02	5 (29%)
4	JI5	A	800	-	27,29,29	0.92	0	30,38,38	1.92	9 (30%)
5	ACT	B	860	-	1,3,3	1.71	0	0,3,3	-	-
3	H4B	B	760	-	16,18,18	1.23	2 (12%)	11,26,26	2.74	5 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	750	1	-	0/6/54/54	-
4	JI5	B	800	-	-	4/13/23/23	0/3/3/3
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1	-	0/6/54/54	-
4	JI5	A	800	-	-	1/13/23/23	0/3/3/3
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3C-C2C	-4.92	1.33	1.40
2	A	750	HEM	C3B-C2B	-4.92	1.33	1.40
2	A	750	HEM	C3D-C2D	4.60	1.51	1.37
2	B	750	HEM	C3B-C2B	-4.53	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	4.24	1.50	1.37
2	A	750	HEM	C3C-C2C	-3.88	1.35	1.40
2	A	750	HEM	C3B-CAB	3.43	1.54	1.47
2	B	750	HEM	C3C-CAC	3.41	1.54	1.47
2	B	750	HEM	C3B-CAB	3.32	1.54	1.47
2	A	750	HEM	C3C-CAC	3.30	1.54	1.47
3	B	760	H4B	C7-C6	3.17	1.55	1.52
2	A	750	HEM	C1D-ND	2.50	1.41	1.36
3	B	760	H4B	C4-N3	2.27	1.37	1.33
2	B	750	HEM	CMD-C2D	2.16	1.56	1.51
2	A	750	HEM	CMD-C2D	2.16	1.56	1.51
2	A	750	HEM	CMC-C2C	2.12	1.56	1.51
5	A	860	ACT	CH3-C	2.10	1.51	1.48
2	B	750	HEM	CMC-C2C	2.03	1.56	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-8.93	96.02	112.49
2	A	750	HEM	CBA-CAA-C2A	-8.49	96.83	112.49
2	A	750	HEM	CBD-CAD-C3D	-7.89	97.94	112.48
4	B	800	JI5	C1-N1-C3'	5.97	122.64	114.20
2	B	750	HEM	CBD-CAD-C3D	-5.72	101.95	112.48
4	A	800	JI5	C61-N11-C21	5.23	122.06	118.10
3	A	760	H4B	C4-C4A-N5	5.12	123.42	119.12
4	B	800	JI5	C61-N11-C21	5.04	121.92	118.10
3	A	760	H4B	C4-C4A-C8A	4.76	118.80	114.57
3	B	760	H4B	C4-C4A-C8A	4.66	118.71	114.57
2	B	750	HEM	C1D-C2D-C3D	-4.18	104.09	107.00
3	A	760	H4B	N3-C2-N1	-3.85	119.38	125.42
3	A	760	H4B	C4-N3-C2	3.77	121.92	115.93
3	B	760	H4B	N3-C2-N1	-3.62	119.74	125.42
3	B	760	H4B	C4-C4A-N5	3.57	122.11	119.12
3	B	760	H4B	C2-N1-C8A	3.55	122.50	114.54
2	A	750	HEM	CMC-C2C-C3C	3.45	131.13	124.68
3	A	760	H4B	C2-N1-C8A	3.41	122.17	114.54
4	A	800	JI5	C3-C4-C11	-3.30	105.22	112.87
2	A	750	HEM	C1D-C2D-C3D	-3.09	104.85	107.00
3	B	760	H4B	C4-N3-C2	3.07	120.81	115.93
4	A	800	JI5	C5'-N1'-C2'	2.97	112.44	105.42
4	B	800	JI5	C5'-N1'-C2'	2.96	112.41	105.42
2	B	750	HEM	CMA-C3A-C4A	-2.93	123.97	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	JI5	C2'-C3'-N1	-2.81	108.73	113.73
2	A	750	HEM	C4C-C3C-C2C	2.60	108.72	106.90
2	A	750	HEM	CMA-C3A-C4A	-2.54	124.56	128.46
4	B	800	JI5	C31-C21-N11	-2.50	120.25	122.90
4	A	800	JI5	C31-C21-N11	-2.48	120.28	122.90
4	A	800	JI5	C1-N1-C3'	2.45	117.67	114.20
4	B	800	JI5	C11-C12-C13	2.38	120.97	118.81
4	B	800	JI5	C14-C13-C12	-2.33	120.26	123.29
4	A	800	JI5	C16-C15-C14	-2.31	116.97	120.25
4	A	800	JI5	C4-C11-C12	-2.21	116.91	120.54
2	B	750	HEM	CMA-C3A-C2A	2.13	128.96	124.94
3	A	760	H4B	N2-C2-N3	2.10	120.52	117.25
4	A	800	JI5	N61-C61-N11	2.01	119.67	116.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	800	JI5	C2'-C3'-N1-C1
4	B	800	JI5	C4'-C3'-N1-C1
4	B	800	JI5	N1-C1-C2-N2
4	A	800	JI5	C2-C1-N1-C3'
4	B	800	JI5	C1-C2-N2-C3

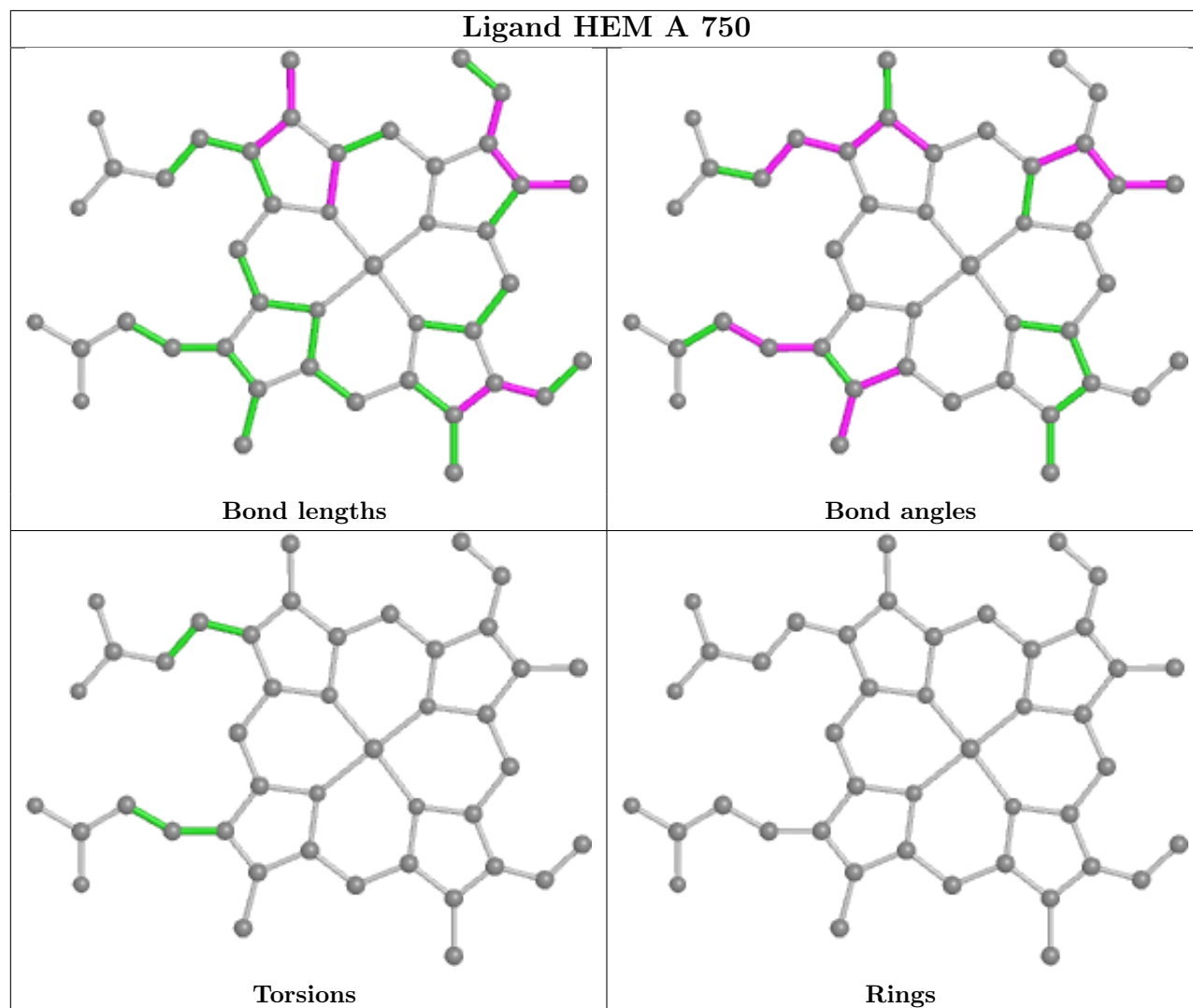
There are no ring outliers.

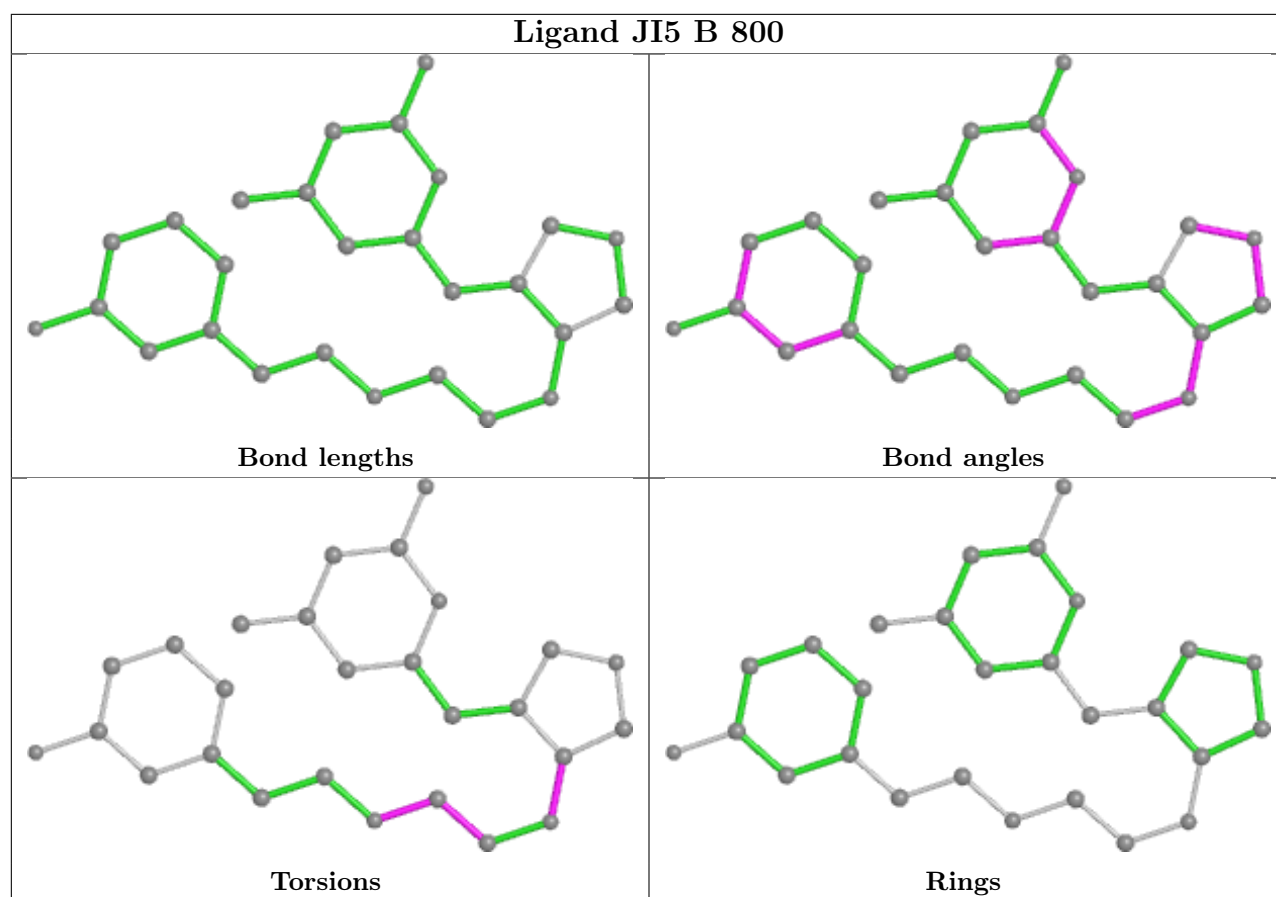
4 monomers are involved in 12 short contacts:

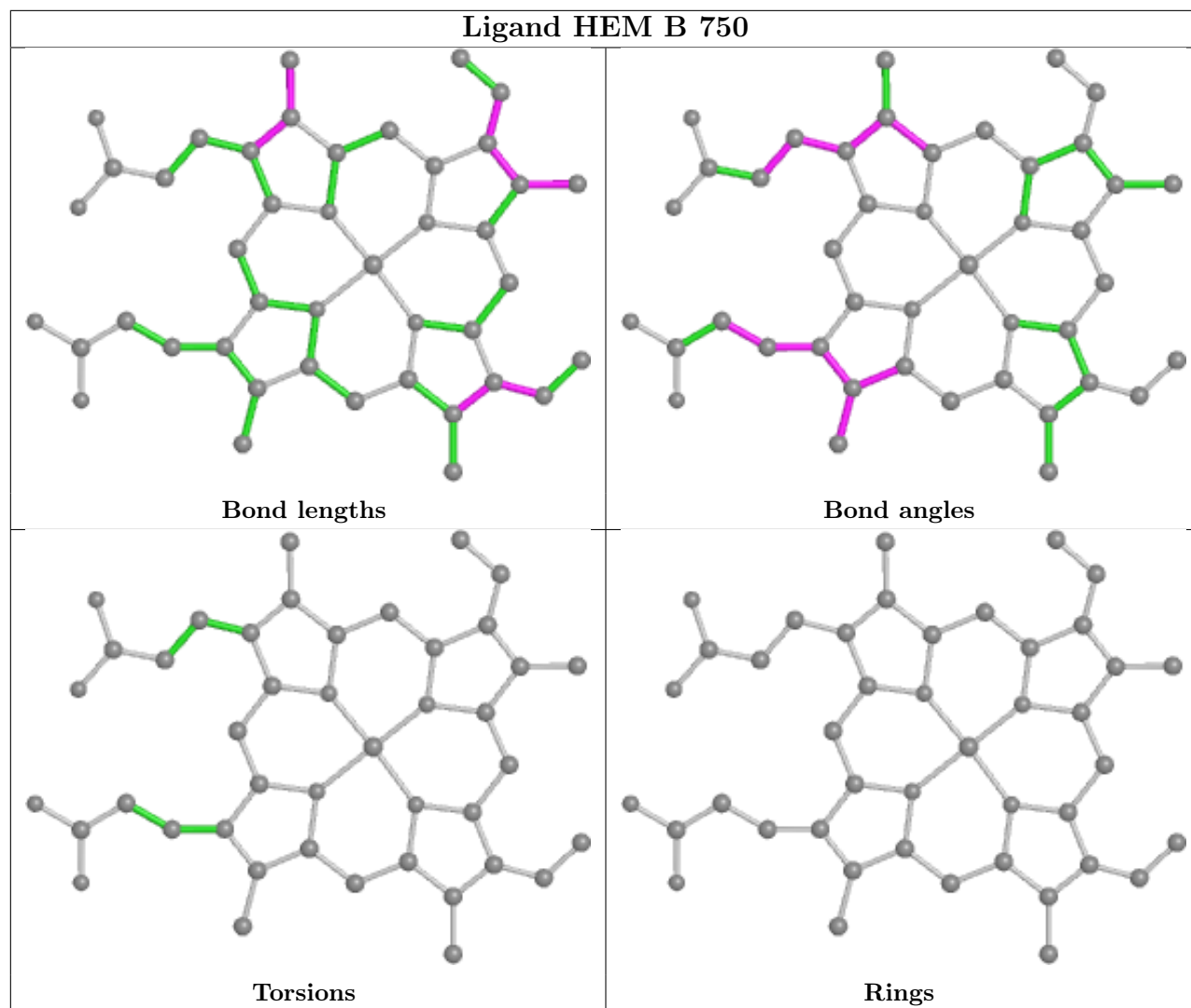
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	2	0
4	B	800	JI5	2	0
2	B	750	HEM	5	0
4	A	800	JI5	4	0

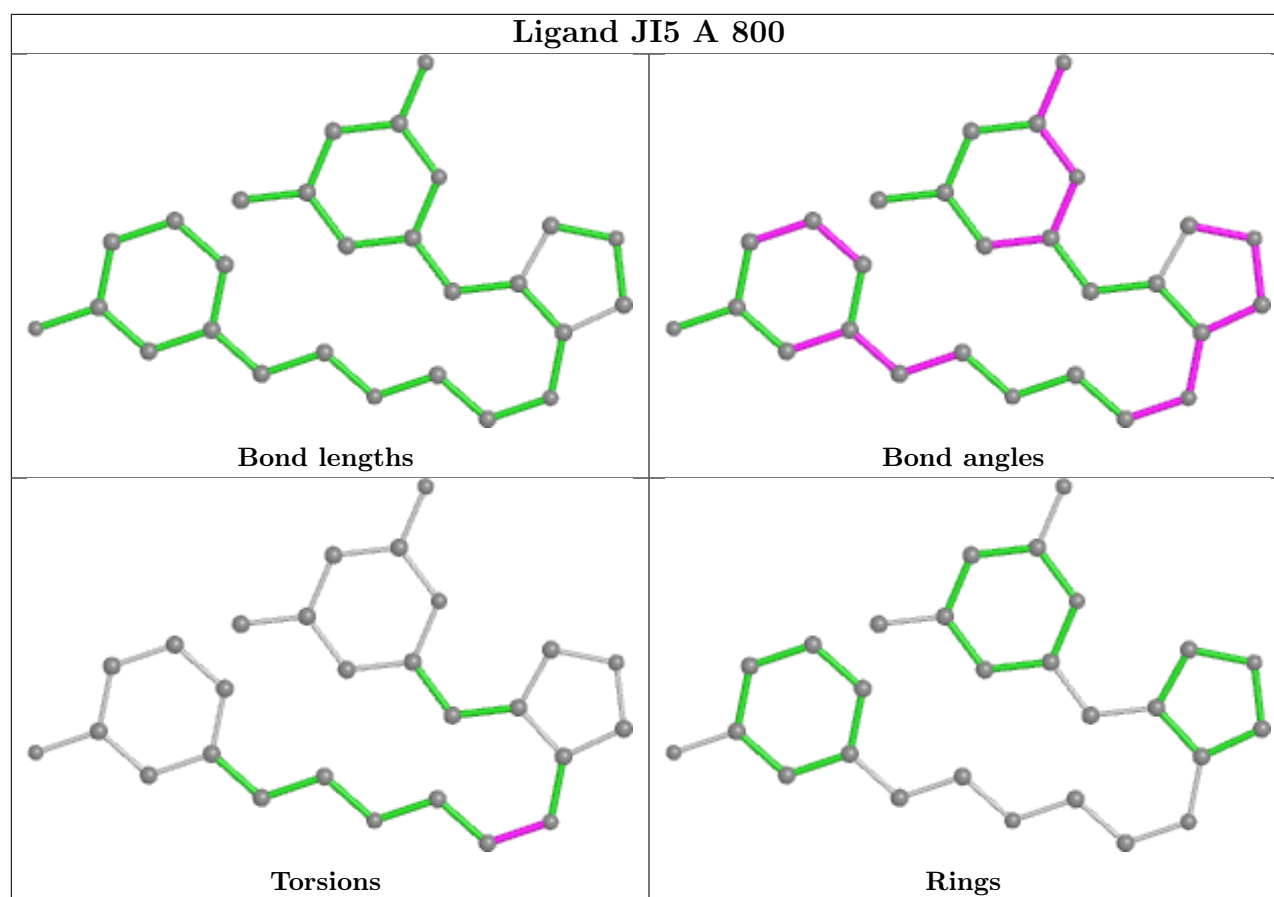
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	407/422 (96%)	1.35	103 (25%) 0 0	31, 57, 105, 131	1 (0%)
1	B	411/422 (97%)	0.78	47 (11%) 5 8	30, 46, 74, 99	1 (0%)
All	All	818/844 (96%)	1.06	150 (18%) 1 1	30, 51, 98, 131	2 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.2
1	A	716	TRP	8.9
1	A	300	PHE	6.7
1	B	352	ASP	6.6
1	A	352	ASP	6.4
1	B	348	VAL	6.0
1	A	488	PRO	5.9
1	A	486	LYS	5.6
1	A	715	VAL	5.6
1	A	481	ARG	5.6
1	B	619	ARG	5.5
1	A	355	PHE	5.3
1	A	551	PHE	5.1
1	B	481	ARG	4.9
1	A	678	TRP	4.6
1	A	469	LYS	4.4
1	A	680	VAL	4.4
1	A	713	THR	4.3
1	A	507	GLN	4.3
1	A	506	ILE	4.2
1	A	350	THR	4.1
1	A	619	ARG	4.0
1	A	714	HIS	4.0
1	A	351	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	567	VAL	4.0
1	A	593	ILE	3.9
1	A	712	ASN	3.9
1	A	591	THR	3.9
1	B	310	VAL	3.9
1	B	567	VAL	3.9
1	A	514	ARG	3.8
1	A	338	PRO	3.8
1	B	620	LYS	3.8
1	A	390	SER	3.7
1	A	388	ILE	3.7
1	A	676	TRP	3.7
1	A	517	PHE	3.7
1	B	680	VAL	3.6
1	B	301	LEU	3.6
1	A	677	VAL	3.6
1	B	611	ALA	3.6
1	A	706	TYR	3.6
1	A	511	LYS	3.6
1	A	415	CYS	3.5
1	B	350	THR	3.5
1	A	322	LEU	3.5
1	B	691	PHE	3.5
1	A	386	LYS	3.4
1	A	491	SER	3.4
1	B	677	VAL	3.4
1	A	480	ILE	3.4
1	A	588	TYR	3.4
1	B	718	GLY	3.3
1	B	616	LEU	3.3
1	B	715	VAL	3.3
1	A	503	GLU	3.3
1	A	416	VAL	3.3
1	A	299	ARG	3.3
1	A	504	ILE	3.2
1	B	678	TRP	3.2
1	B	321	THR	3.2
1	B	591	THR	3.1
1	A	371	ARG	3.1
1	A	561	TRP	3.1
1	A	353	GLN	3.1
1	A	679	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	691	PHE	3.0
1	B	615	ASP	3.0
1	A	682	PRO	3.0
1	B	676	TRP	3.0
1	A	482	TYR	3.0
1	A	562	TYR	2.9
1	B	338	PRO	2.9
1	A	564	LEU	2.9
1	A	394	TYR	2.9
1	B	566	ALA	2.9
1	A	710	PRO	2.9
1	B	299	ARG	2.8
1	A	470	HIS	2.8
1	B	302	LYS	2.8
1	A	487	GLN	2.8
1	B	588	TYR	2.7
1	B	667	ARG	2.7
1	A	508	GLN	2.7
1	A	554	PHE	2.7
1	A	584	PHE	2.7
1	A	492	THR	2.7
1	A	479	LEU	2.7
1	A	370	LYS	2.7
1	B	389	GLU	2.7
1	A	565	PRO	2.7
1	A	681	PRO	2.7
1	B	318	LEU	2.6
1	A	391	THR	2.6
1	A	392	SER	2.6
1	A	566	ALA	2.6
1	A	500	GLN	2.6
1	A	685	GLY	2.6
1	A	302	LYS	2.6
1	A	373	GLY	2.6
1	A	318	LEU	2.6
1	A	528	GLY	2.6
1	A	590	GLY	2.6
1	A	393	THR	2.5
1	A	711	TRP	2.5
1	B	713	THR	2.5
1	B	679	ILE	2.5
1	A	466	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	681	PRO	2.4
1	A	667	ARG	2.4
1	B	562	TYR	2.4
1	A	354	LEU	2.4
1	A	533	LEU	2.4
1	B	480	ILE	2.4
1	A	490	GLY	2.4
1	A	519	VAL	2.4
1	B	479	LEU	2.4
1	A	485	TYR	2.4
1	A	686	SER	2.4
1	A	489	ASP	2.3
1	B	565	PRO	2.3
1	A	311	VAL	2.3
1	A	608	GLU	2.3
1	B	598	TYR	2.3
1	A	501	PHE	2.3
1	A	704	PHE	2.3
1	A	446	VAL	2.3
1	B	564	LEU	2.3
1	A	321	THR	2.2
1	B	416	VAL	2.2
1	B	668	CYS	2.2
1	A	389	GLU	2.2
1	A	494	GLY	2.2
1	A	550	LYS	2.2
1	A	409	TRP	2.2
1	A	385	ASN	2.1
1	A	412	ALA	2.1
1	B	369	ILE	2.1
1	A	568	SER	2.1
1	B	684	SER	2.1
1	B	685	GLY	2.1
1	A	643	SER	2.1
1	A	323	GLU	2.1
1	A	594	GLY	2.1
1	A	690	VAL	2.1
1	B	596	ARG	2.0
1	A	552	ASP	2.0
1	B	329	HIS	2.0
1	A	375	LYS	2.0
1	B	386	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](#)

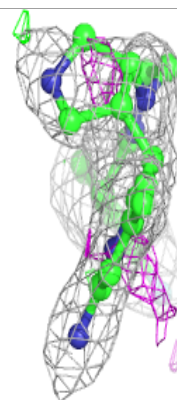
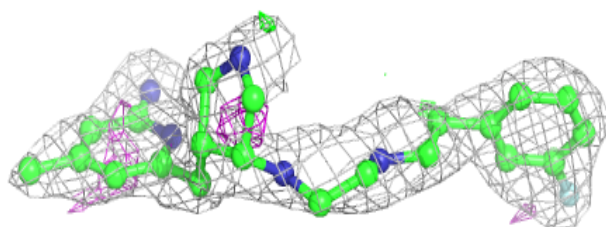
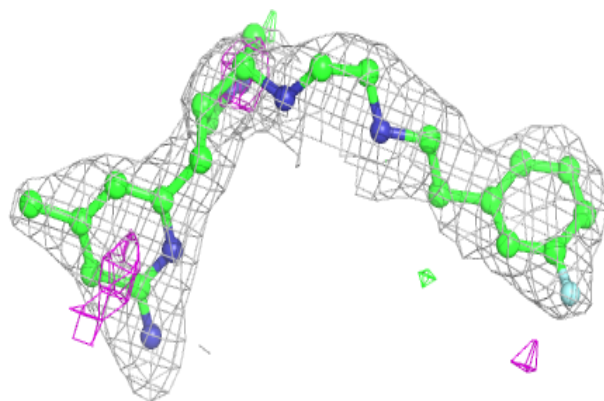
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	JI5	A	800	27/27	0.76	0.29	53,57,64,64	0
4	JI5	B	800	27/27	0.82	0.23	41,50,54,54	0
5	ACT	B	860	4/4	0.87	0.26	83,85,85,86	0
5	ACT	A	860	4/4	0.94	0.19	75,76,76,76	0
3	H4B	A	760	17/17	0.95	0.20	34,38,43,46	0
3	H4B	B	760	17/17	0.95	0.24	35,37,40,44	0
2	HEM	A	750	43/43	0.97	0.22	30,36,50,53	0
2	HEM	B	750	43/43	0.97	0.19	31,36,47,53	0
6	ZN	A	900	1/1	0.99	0.09	39,39,39,39	0

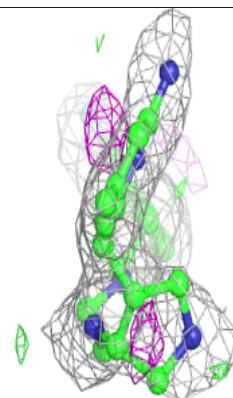
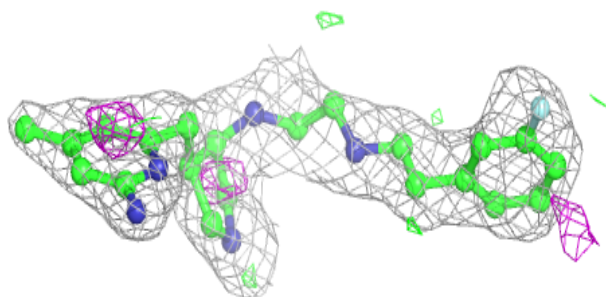
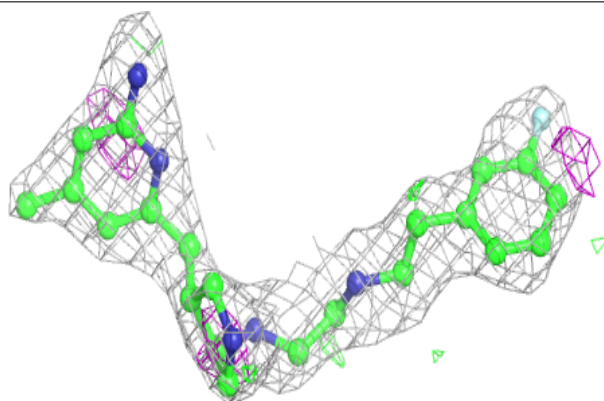
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JI5 A 800:

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

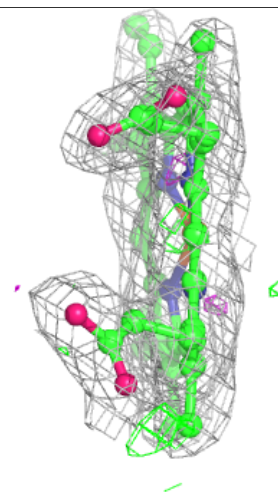
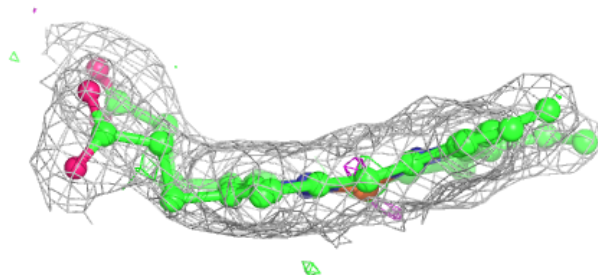
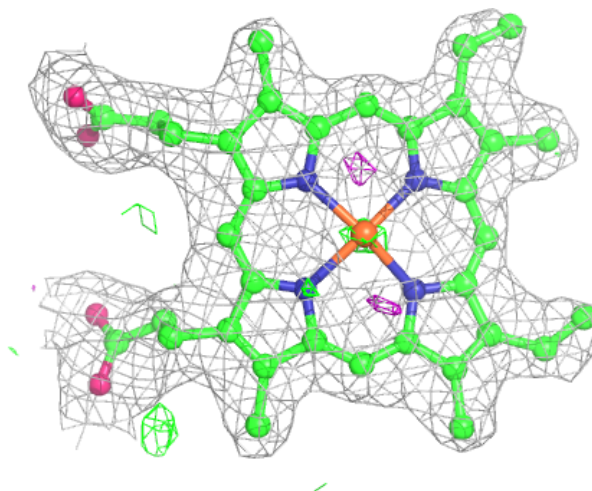
**Electron density around JI5 B 800:**

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



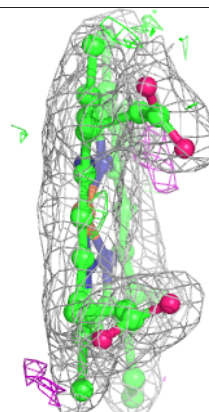
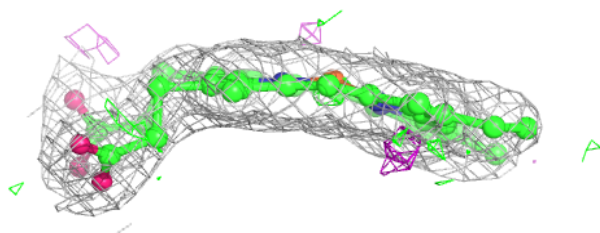
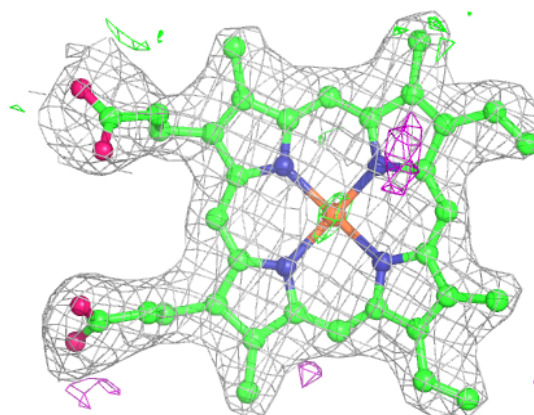
Electron density around HEM A 750:

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



Electron density around HEM B 750:

$2mF_o-DF_c$ (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.