Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 02:18 AM EST

PDB ID	:	3NLJ
Title	:	Structure of neuronal nitric oxide synthase D597N/M336V/Y706A triple mutant heme domain complexed with 6-{{(3'R,4'R)-3'-[2"-(3'''-fluorophenethylamino)ethoxy] pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine
Authors	:	Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on	:	2010-06-21
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

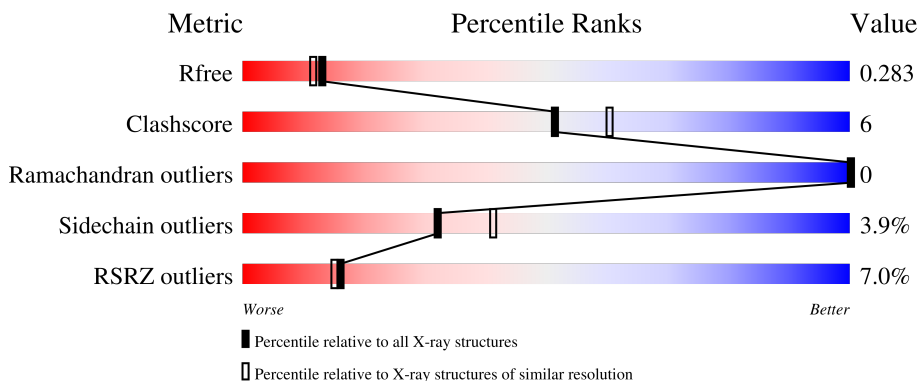|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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		0.283
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		3.9%
RSRZ outliers		7.0%

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	422	11% / 78% / 17% · ·
1	B	422	3% / 83% / 14% ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7050 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 3305	C 2115	N 567	O 603	S 20	0	0	0
1	B	411	Total 3337	C 2134	N 575	O 608	S 20	0	0	0

There are 6 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
A	706	ALA	TYR	engineered mutation	UNP P29476
B	336	VAL	MET	engineered mutation	UNP P29476
B	597	ASN	ASP	engineered mutation	UNP P29476
B	706	ALA	TYR	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	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 6-{[(3R,4R)-4-(2-{[2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: JRR) (formula: $C_{21}H_{29}FN_4O$).
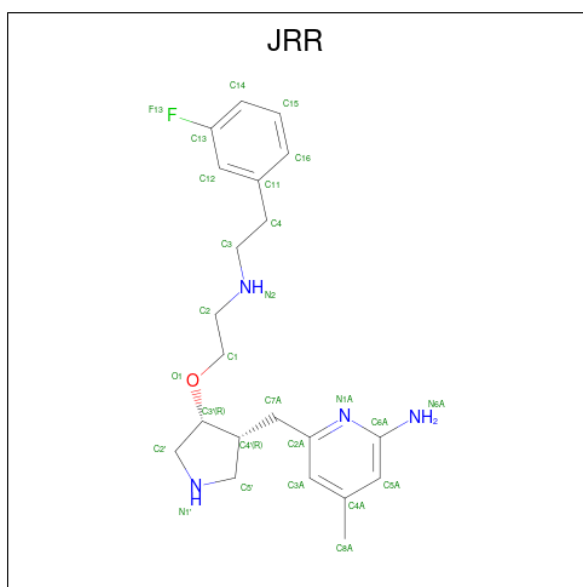
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

- 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 water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	89	Total O 89　89	0	0
6	B	137	Total O 137　137	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
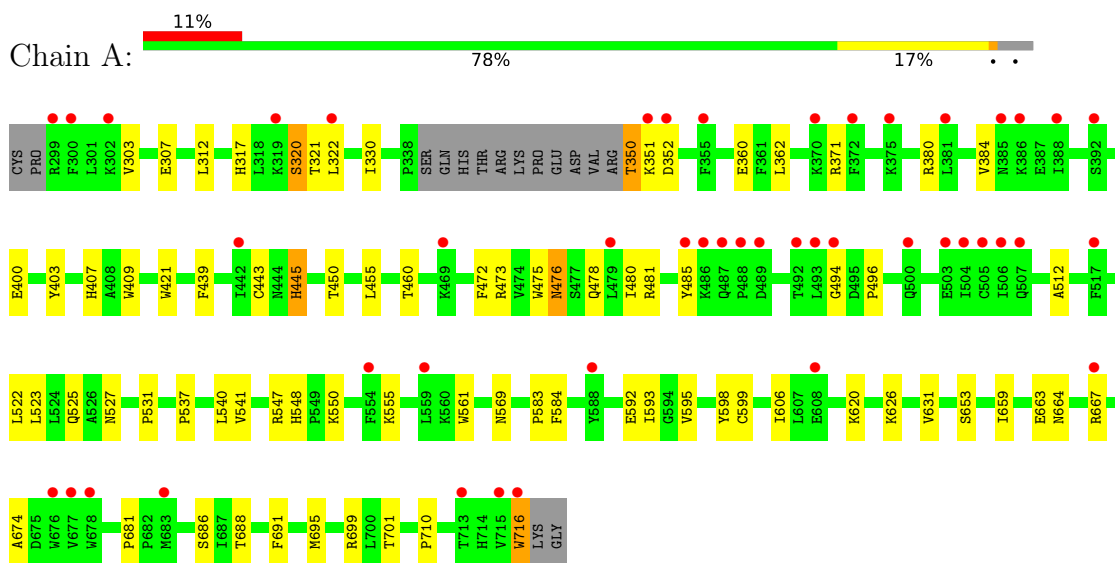
- Molecule 1: Nitric oxide synthase, brain
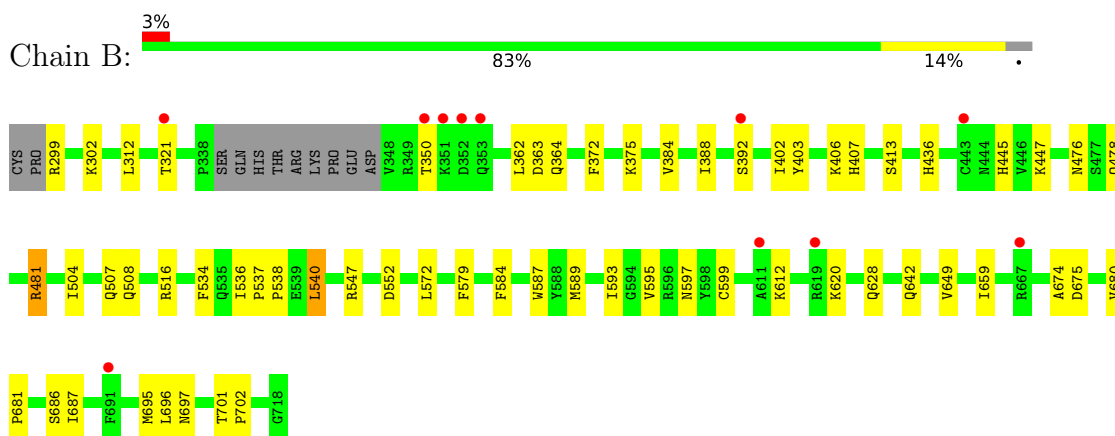
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.80Å 111.10Å 163.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.97 – 2.20 40.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.97-2.20) 98.6 (40.97-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.201 , 0.268 0.233 , 0.283	Depositor DCC
R_{free} test set	2423 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7050	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: JRR, H4B, HEM, 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	0.61	0/3397	0.67	0/4610
1	B	0.73	0/3429	0.74	1/4650 (0.0%)
All	All	0.67	0/6826	0.71	1/9260 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	675	ASP	CB-CG-OD1	5.22	123.00	118.30

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	3305	0	3221	40	0
1	B	3337	0	3259	32	0
2	A	43	0	30	7	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	29	1	0
4	B	27	0	29	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	89	0	0	1	0
6	B	137	0	0	7	0
All	All	7050	0	6634	75	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 (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:299:ARG:HB3	6:B:1131:HOH:O	1.65	0.96
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.72	0.72
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.69	0.72
1:B:504:ILE:O	1:B:508:GLN:HG2	1.94	0.67
1:B:536:ILE:HG13	6:B:1031:HOH:O	1.95	0.66
1:A:317:HIS:O	1:A:320:SER:HB3	1.96	0.65
1:B:388:ILE:O	1:B:392:SER:HA	1.98	0.64
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.82	0.60
1:A:592:GLU:OE1	4:A:800:JRR:H16	2.03	0.59
1:B:572:LEU:HB3	1:B:579:PHE:HB2	1.84	0.58
1:A:701:THR:HG23	6:A:1079:HOH:O	2.04	0.57
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.06	0.56
1:A:659:ILE:O	1:A:663:GLU:HG3	2.07	0.55
1:B:447:LYS:HE2	6:B:1137:HOH:O	2.05	0.55
1:A:595:VAL:O	1:A:599:CYS:HB2	2.08	0.54
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.88	0.54
1:B:589:MET:HA	1:B:649:VAL:O	2.07	0.54
1:A:664:ASN:OD1	1:A:667:ARG:NH2	2.39	0.53
1:B:447:LYS:HD2	1:B:540:LEU:HD11	1.91	0.52
1:B:363:ASP:HB3	1:B:372:PHE:HE1	1.74	0.52
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.36	0.52
1:B:321:THR:N	6:B:1132:HOH:O	2.38	0.52
1:B:701:THR:HA	1:B:702:PRO:C	2.29	0.52
1:A:476:ASN:HD21	1:A:522:LEU:HA	1.75	0.52
1:A:681:PRO:HG2	1:A:688:THR:HG21	1.92	0.51
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.46	0.51
1:B:436:HIS:CD2	1:B:534:PHE:HE2	2.29	0.50
1:A:686:SER:HA	1:A:691:PHE:CG	2.46	0.50
1:A:716:TRP:N	1:A:716:TRP:CD1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:HG3	6:B:1004:HOH:O	2.11	0.50
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.46	0.50
1:B:587:TRP:H	2:B:750:HEM:HAB	1.77	0.49
1:B:642:GLN:HA	6:B:1129:HOH:O	2.12	0.49
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.93	0.49
1:A:460:THR:O	1:A:583:PRO:HD2	2.12	0.49
1:A:439:PHE:HZ	1:A:537:PRO:HD3	1.78	0.48
1:A:548:HIS:CE1	1:A:550:LYS:HB2	2.48	0.48
1:B:445:HIS:C	1:B:445:HIS:CD2	2.87	0.48
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.95	0.48
1:A:494:GLY:O	1:A:496:PRO:HD3	2.14	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.02	0.47
1:B:364:GLN:NE2	6:B:1090:HOH:O	2.47	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.16	0.46
1:A:445:HIS:C	1:A:445:HIS:CD2	2.89	0.46
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.98	0.46
1:A:561:TRP:CD1	1:A:593:ILE:HG12	2.50	0.46
1:B:593:ILE:HA	1:B:597:ASN:HB2	1.98	0.45
1:A:450:THR:HA	1:A:455:LEU:HD22	1.96	0.45
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.52	0.45
1:A:303:VAL:HG23	1:A:312:LEU:HB2	1.98	0.45
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.82	0.45
1:B:413:SER:OG	1:B:697:ASN:ND2	2.50	0.45
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.98	0.45
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.84	0.45
1:A:322:LEU:HB2	1:A:699:ARG:HB2	2.00	0.45
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.98	0.45
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.10	0.44
1:B:674:ALA:HB3	1:B:695:MET:HB3	1.99	0.43
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.07	0.43
2:A:750:HEM:HHA	2:A:750:HEM:HBA1	2.01	0.43
1:B:537:PRO:HA	1:B:538:PRO:HD3	1.92	0.43
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.02	0.42
1:A:350:THR:HG22	1:A:351:LYS:H	1.84	0.42
1:A:478:GLN:HB2	1:A:481:ARG:HG3	2.02	0.42
1:A:472:PHE:HA	1:A:525:GLN:O	2.20	0.42
1:A:598:TYR:O	1:A:606:ILE:HG12	2.19	0.42
1:B:302:LYS:HA	1:B:312:LEU:O	2.20	0.42
1:A:626:LYS:HB3	1:B:687:ILE:HD12	2.02	0.41
2:A:750:HEM:HBA1	2:A:750:HEM:CHA	2.50	0.41
1:B:584:PHE:CD1	2:B:750:HEM:CAC	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:PHE:CD1	2:A:750:HEM:CAC	3.04	0.41
2:A:750:HEM:HHA	2:A:750:HEM:CBA	2.51	0.40
1:B:402:ILE:O	1:B:406:LYS:HG3	2.21	0.40
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.04	0.40
1:A:473:ARG:CZ	1:A:710:PRO:HG3	2.52	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%)	391 (97%)	12 (3%)	0	100	100
1	B	407/422 (96%)	394 (97%)	13 (3%)	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	362/376 (96%)	347 (96%)	15 (4%)	30	39
1	B	365/376 (97%)	352 (96%)	13 (4%)	35	45
All	All	727/752 (97%)	699 (96%)	28 (4%)	32	41

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	SER
1	A	321	THR
1	A	350	THR
1	A	352	ASP
1	A	360	GLU
1	A	371	ARG
1	A	445	HIS
1	A	476	ASN
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	653	SER
1	A	716	TRP
1	B	350	THR
1	B	375	LYS
1	B	476	ASN
1	B	481	ARG
1	B	507	GLN
1	B	516	ARG
1	B	540	LEU
1	B	547	ARG
1	B	552	ASP
1	B	612	LYS
1	B	620	LYS
1	B	659	ILE
1	B	686	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	487	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	329	HIS
1	B	364	GLN

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Mol	Chain	Res	Type
1	B	385	ASN
1	B	407	HIS
1	B	425	GLN
1	B	436	HIS
1	B	454	ASN
1	B	508	GLN
1	B	527	ASN
1	B	535	GLN
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 ⓘ

8 ligands are modelled in this entry.

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	JRR	A	800	-	28,29,29	0.58	0	31,38,38	1.62	5 (16%)
5	ACT	B	861	-	3,3,3	0.74	0	3,3,3	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	HEM	B	750	1	41,50,50	1.99	7 (17%)	45,82,82	1.63	6 (13%)
3	H4B	A	760	-	16,18,18	0.89	0	11,26,26	3.45	7 (63%)
5	ACT	A	860	-	3,3,3	0.76	0	3,3,3	0.70	0
2	HEM	A	750	1	41,50,50	1.97	8 (19%)	45,82,82	1.57	7 (15%)
3	H4B	B	761	-	16,18,18	1.33	2 (12%)	11,26,26	2.74	6 (54%)
4	JRR	B	800	-	28,29,29	0.59	0	31,38,38	1.79	5 (16%)

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	JRR	A	800	-	-	4/13/23/23	0/3/3/3
2	HEM	B	750	1	-	7/12/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	HEM	A	750	1	-	4/12/54/54	-
3	H4B	B	761	-	-	0/8/17/17	0/2/2/2
4	JRR	B	800	-	-	5/13/23/23	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	7.34	1.52	1.36
2	B	750	HEM	C3D-C2D	7.14	1.51	1.36
2	B	750	HEM	C3C-C2C	-6.25	1.31	1.40
2	A	750	HEM	C3C-C2C	-4.54	1.34	1.40
2	A	750	HEM	C3C-CAC	3.56	1.55	1.47
2	A	750	HEM	FE-NB	3.00	2.11	1.96
2	B	750	HEM	C3C-CAC	2.93	1.53	1.47
2	B	750	HEM	CMB-C2B	2.93	1.57	1.50
2	A	750	HEM	CAB-C3B	2.85	1.55	1.47
3	B	761	H4B	C7-N8	2.82	1.49	1.44
2	A	750	HEM	CMB-C2B	2.80	1.56	1.50
3	B	761	H4B	C4-N3	2.61	1.37	1.33
2	B	750	HEM	CMA-C3A	2.60	1.57	1.51
2	A	750	HEM	CMA-C3A	2.21	1.56	1.51
2	B	750	HEM	CAB-C3B	2.21	1.53	1.47
2	B	750	HEM	FE-ND	2.14	2.07	1.96
2	A	750	HEM	CMD-C2D	2.10	1.55	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	760	H4B	C4-C4A-N5	7.97	125.81	119.12
4	B	800	JRR	C6A-N1A-C2A	6.03	122.67	118.10
3	B	761	H4B	C8A-C4A-C4	5.82	119.74	114.57
2	B	750	HEM	C4D-ND-C1D	5.04	110.28	105.07
2	B	750	HEM	CBA-CAA-C2A	-4.94	104.19	112.62
4	A	800	JRR	C6A-N1A-C2A	4.67	121.64	118.10
2	A	750	HEM	C4D-ND-C1D	4.17	109.38	105.07
3	A	760	H4B	N1-C2-N3	-3.97	119.19	125.42
4	A	800	JRR	C3-C4-C11	-3.83	103.99	112.87
3	A	760	H4B	C2-N1-C8A	3.72	122.88	114.54
3	A	760	H4B	C2-N3-C4	3.72	121.83	115.93
2	B	750	HEM	CBD-CAD-C3D	-3.64	102.51	112.63
4	A	800	JRR	C5'-N1'-C2'	3.28	113.18	105.42
3	B	761	H4B	C2-N3-C4	3.22	121.05	115.93
3	B	761	H4B	C4-C4A-N5	3.12	121.74	119.12
4	B	800	JRR	C3A-C2A-N1A	-3.11	119.61	122.90
2	A	750	HEM	CHC-C4B-C3B	3.07	129.27	124.57
3	B	761	H4B	N1-C2-N3	-3.05	120.63	125.42
4	B	800	JRR	O1-C3'-C2'	-2.86	103.77	111.42
2	B	750	HEM	CHC-C4B-NB	2.86	127.54	124.43
2	A	750	HEM	CAA-CBA-CGA	-2.80	105.90	113.76
3	B	761	H4B	C2-N1-C8A	2.73	120.65	114.54
4	A	800	JRR	C3A-C2A-N1A	-2.71	120.03	122.90
4	B	800	JRR	C3-C4-C11	-2.69	106.64	112.87
3	A	760	H4B	C8A-C4A-C4	2.67	116.95	114.57
4	B	800	JRR	C5'-N1'-C2'	2.39	111.07	105.42
2	A	750	HEM	C1B-NB-C4B	2.28	107.43	105.07
4	A	800	JRR	N6A-C6A-N1A	2.27	120.07	116.49
2	A	750	HEM	CBD-CAD-C3D	-2.26	106.34	112.63
2	A	750	HEM	C4B-C3B-C2B	2.24	108.89	107.11
2	B	750	HEM	CMA-C3A-C4A	-2.18	125.12	128.46
2	B	750	HEM	CMC-C2C-C3C	2.12	128.64	124.68
3	A	760	H4B	C4A-N5-C6	-2.11	115.43	121.16
2	A	750	HEM	CMD-C2D-C1D	2.07	128.19	125.04
3	A	760	H4B	N2-C2-N1	2.07	120.47	117.25
3	B	761	H4B	N2-C2-N3	2.05	120.45	117.25

There are no chirality outliers.
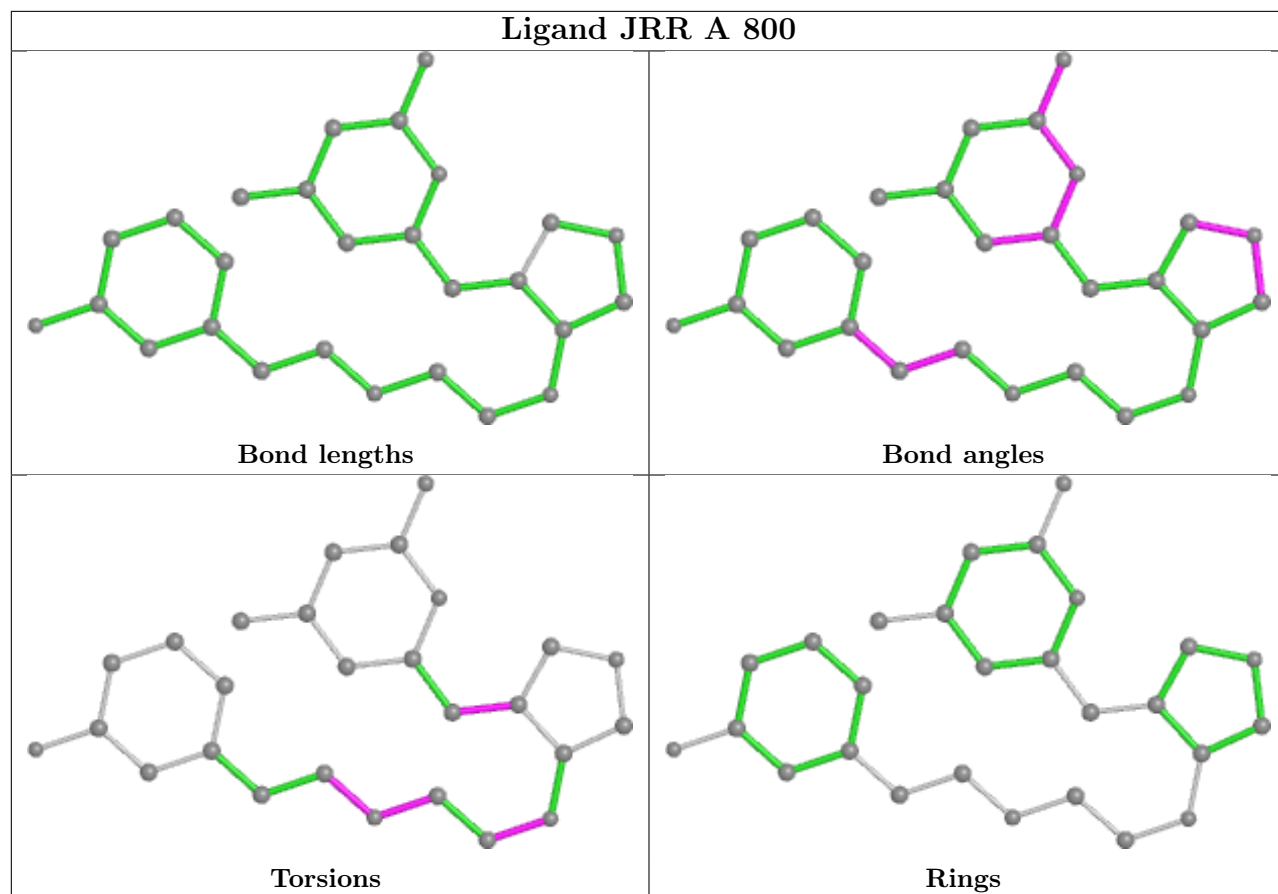
All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	750	HEM	C1A-C2A-CAA-CBA
2	A	750	HEM	C3A-C2A-CAA-CBA
2	B	750	HEM	C1A-C2A-CAA-CBA
2	B	750	HEM	C3A-C2A-CAA-CBA
2	B	750	HEM	C2B-C3B-CAB-CBB
2	B	750	HEM	C4B-C3B-CAB-CBB
4	A	800	JRR	C1-C2-N2-C3
4	B	800	JRR	C2'-C3'-O1-C1
4	B	800	JRR	N1A-C2A-C7A-C4'
2	A	750	HEM	C2A-CAA-CBA-CGA
2	B	750	HEM	C2A-CAA-CBA-CGA
4	B	800	JRR	C4-C3-N2-C2
2	A	750	HEM	C4B-C3B-CAB-CBB
4	B	800	JRR	C4'-C3'-O1-C1
4	A	800	JRR	C5'-C4'-C7A-C2A
4	A	800	JRR	C4-C3-N2-C2
4	B	800	JRR	C1-C2-N2-C3
4	A	800	JRR	C2-C1-O1-C3'
2	B	750	HEM	CAA-CBA-CGA-O2A
2	B	750	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

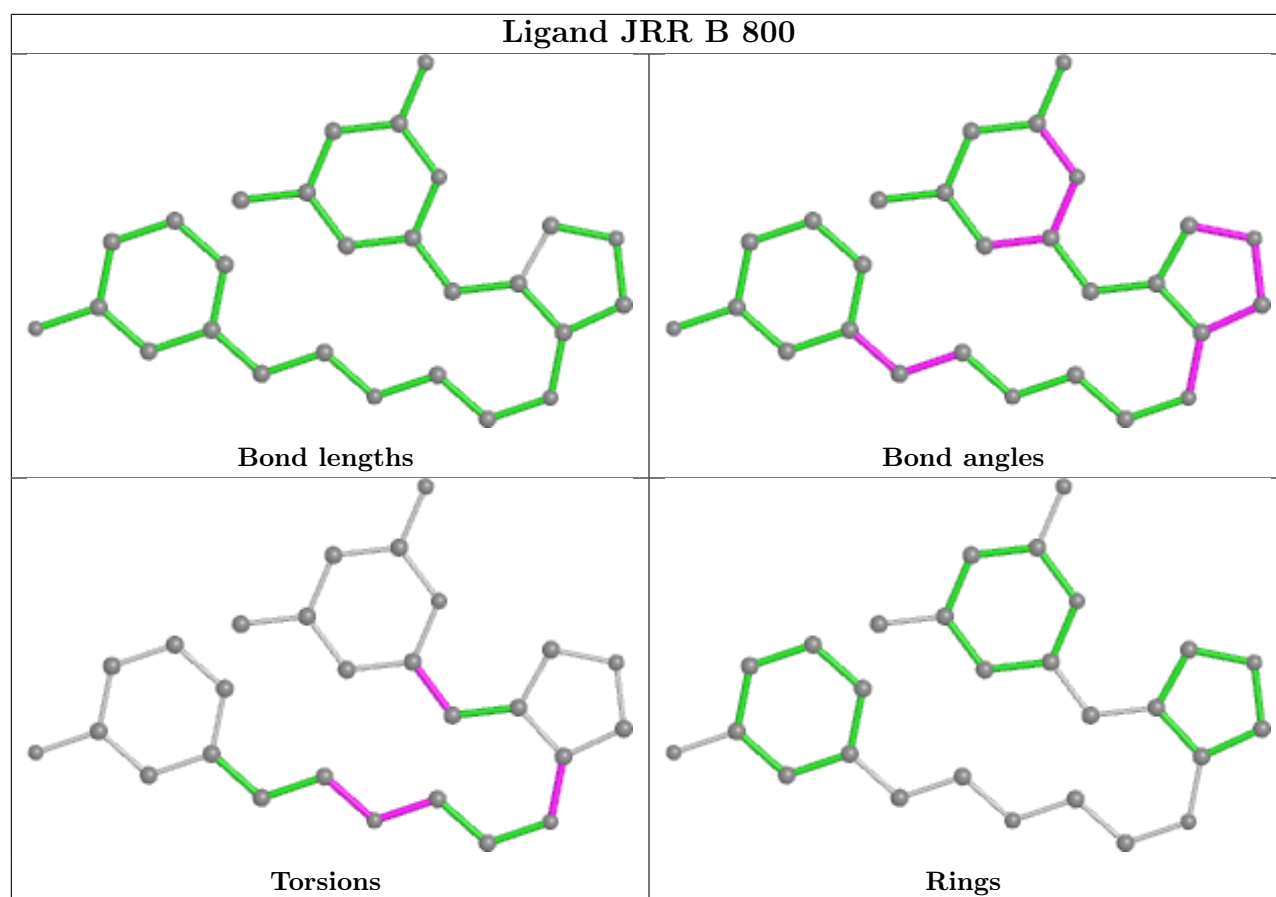3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	JRR	1	0
2	B	750	HEM	3	0
2	A	750	HEM	7	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 JRR A 800

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 750

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 750

Bond lengths

Bond angles

Torsions

Rings

Ligand JRR B 800

Bond lengths

Bond angles

Torsions

Rings
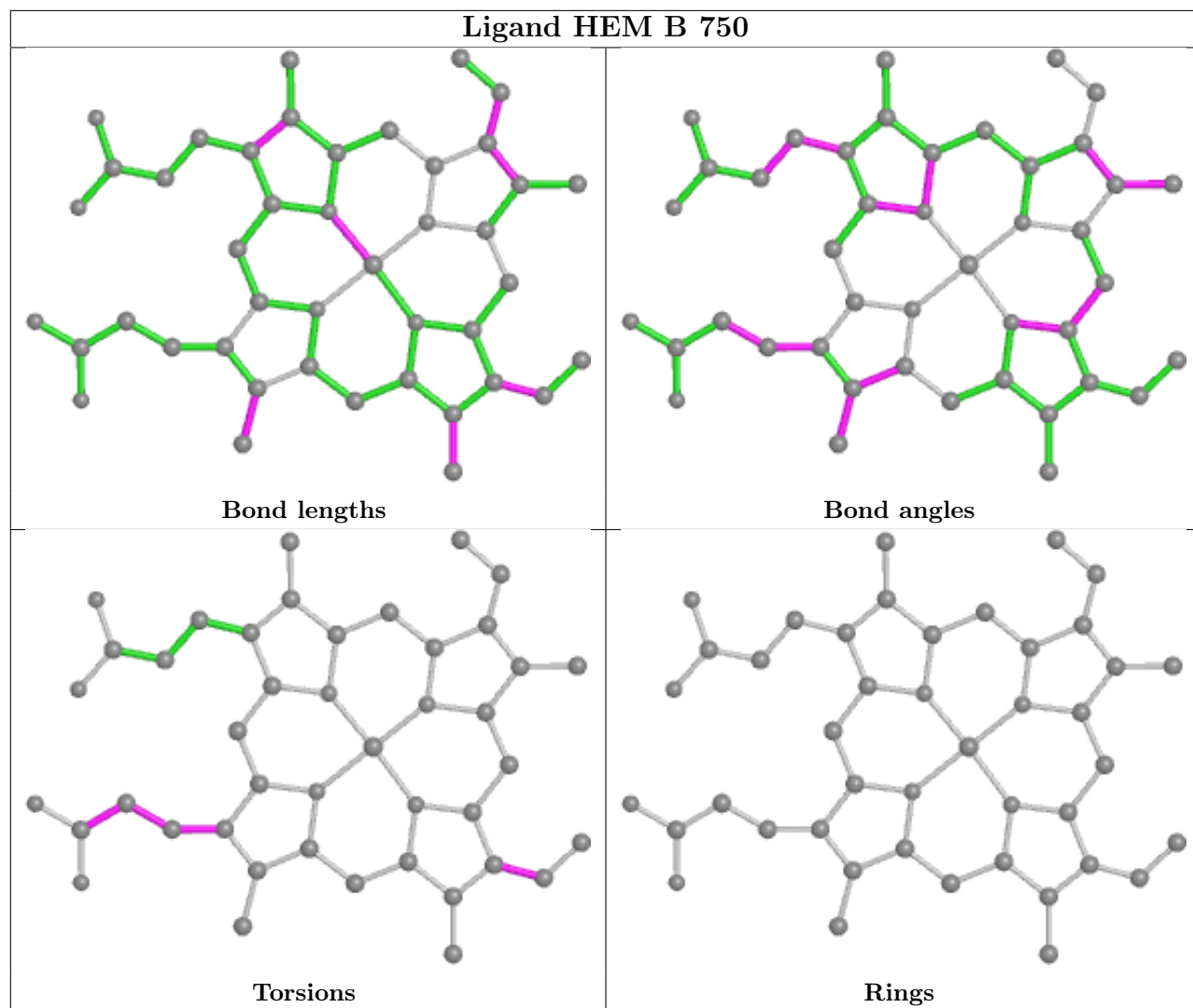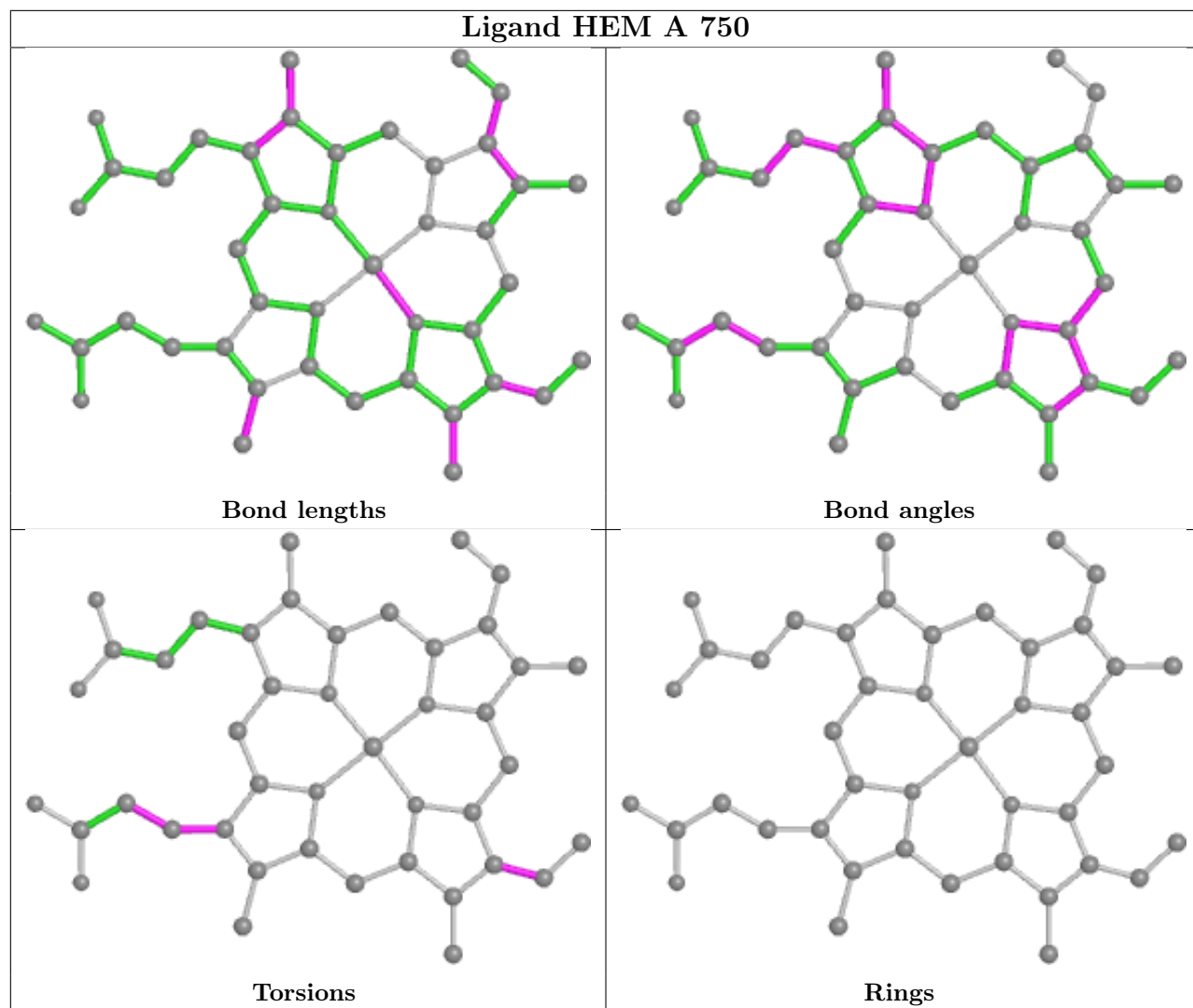
5.7 Other polymers ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	407/422 (96%)	0.67	46 (11%)	5	4	26, 54, 96, 122	0
1	B	411/422 (97%)	0.13	11 (2%)	54	52	24, 41, 67, 81	0
All	All	818/844 (96%)	0.40	57 (6%)	16	15	24, 46, 87, 122	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	6.4
1	A	715	VAL	5.2
1	A	300	PHE	5.0
1	A	375	LYS	4.6
1	A	716	TRP	4.5
1	B	321	THR	4.5
1	A	713	THR	4.3
1	A	352	ASP	3.8
1	A	494	GLY	3.6
1	B	352	ASP	3.5
1	A	355	PHE	3.3
1	A	503	GLU	3.3
1	A	507	GLN	3.2
1	A	469	LYS	3.2
1	A	386	LYS	3.1
1	A	299	ARG	3.1
1	B	351	LYS	3.1
1	A	351	LYS	3.0
1	B	619	ARG	2.9
1	A	487	GLN	2.9
1	A	319	LYS	2.9
1	A	492	THR	2.9
1	A	322	LEU	2.9
1	A	486	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	350	THR	2.8
1	A	485	TYR	2.7
1	A	678	TRP	2.7
1	A	381	LEU	2.5
1	A	667	ARG	2.5
1	B	667	ARG	2.5
1	A	372	PHE	2.5
1	A	506	ILE	2.5
1	A	493	LEU	2.5
1	B	392	SER	2.4
1	A	554	PHE	2.4
1	A	517	PHE	2.4
1	B	353	GLN	2.4
1	A	302	LYS	2.4
1	A	588	TYR	2.4
1	A	370	LYS	2.3
1	A	608	GLU	2.3
1	A	559	LEU	2.3
1	A	683	MET	2.3
1	A	385	ASN	2.3
1	A	676	TRP	2.2
1	A	677	VAL	2.2
1	A	392	SER	2.2
1	A	505	CYS	2.1
1	A	388	ILE	2.1
1	A	504	ILE	2.1
1	B	443	CYS	2.1
1	A	489	ASP	2.1
1	B	611	ALA	2.1
1	A	442	ILE	2.1
1	B	691	PHE	2.1
1	A	500	GLN	2.0
1	A	479	LEU	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
4	JRR	A	800	27/27	0.83	0.27	51,67,73,76	0
4	JRR	B	800	27/27	0.90	0.22	49,56,61,62	0
3	H4B	A	760	17/17	0.91	0.20	32,35,45,46	0
5	ACT	A	860	4/4	0.91	0.23	86,87,87,87	0
5	ACT	B	861	4/4	0.93	0.21	76,76,76,76	0
3	H4B	B	761	17/17	0.95	0.16	23,29,36,37	0
2	HEM	A	750	43/43	0.96	0.20	21,37,48,52	0
2	HEM	B	750	43/43	0.97	0.14	25,32,41,44	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 JRR A 800:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
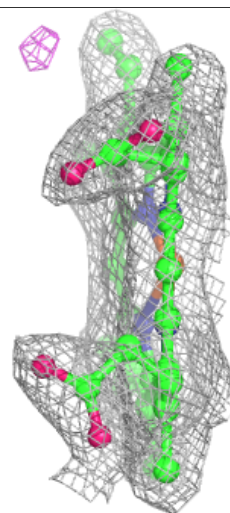mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
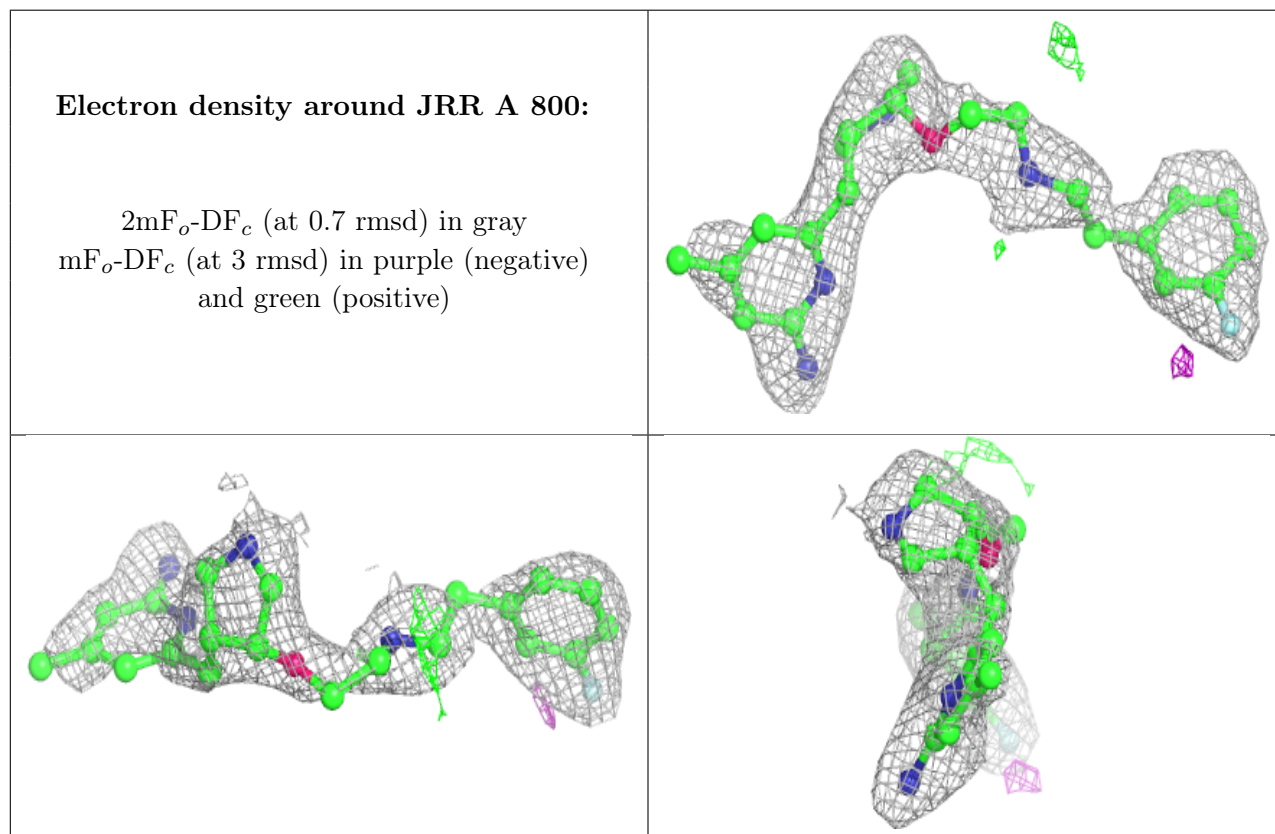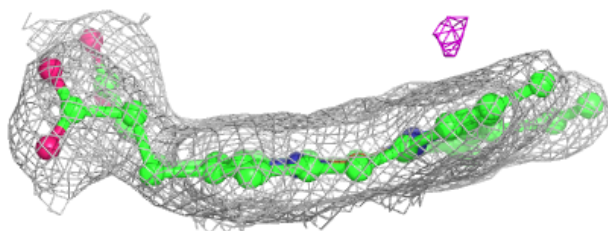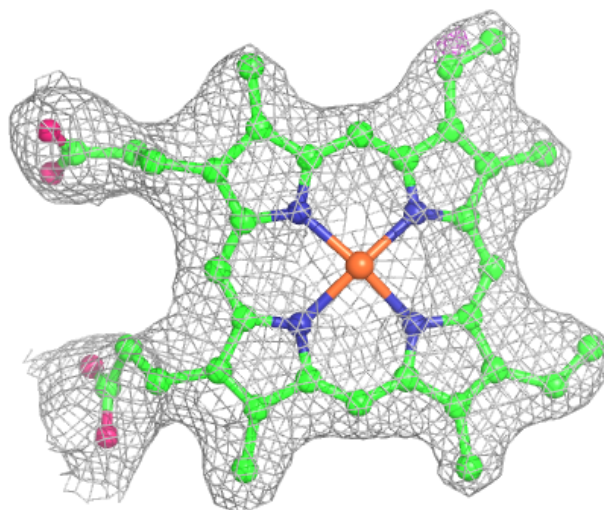
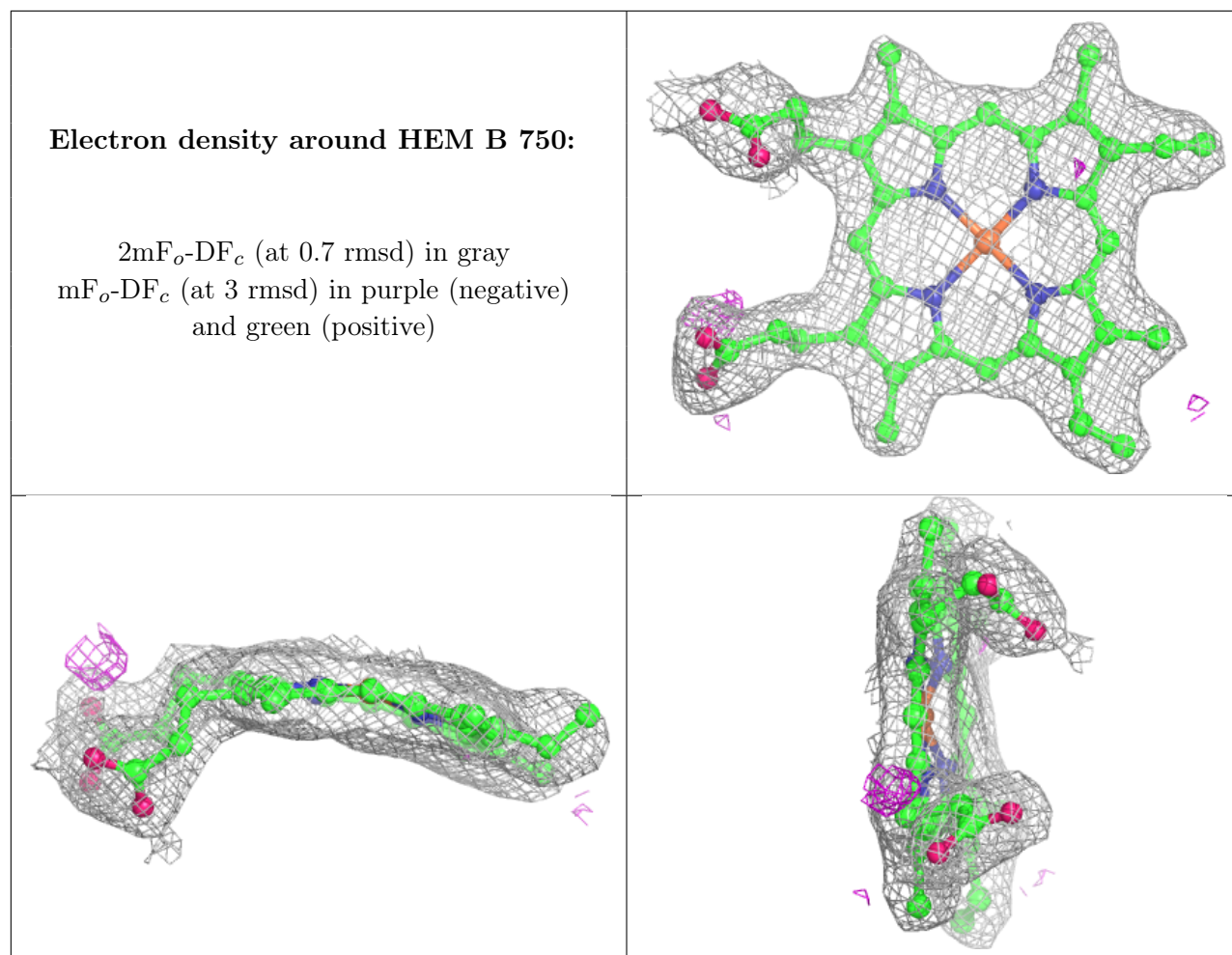**Electron density around JRR B 800:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
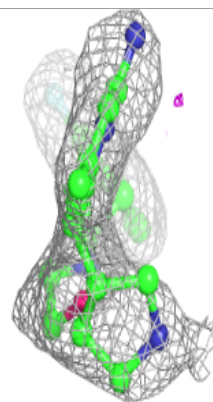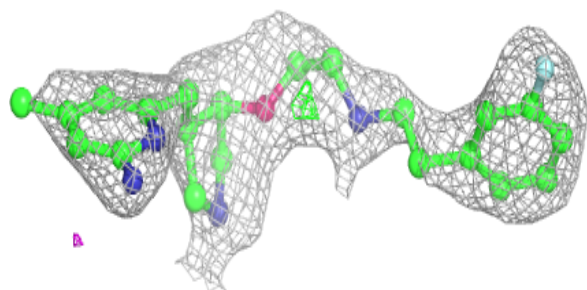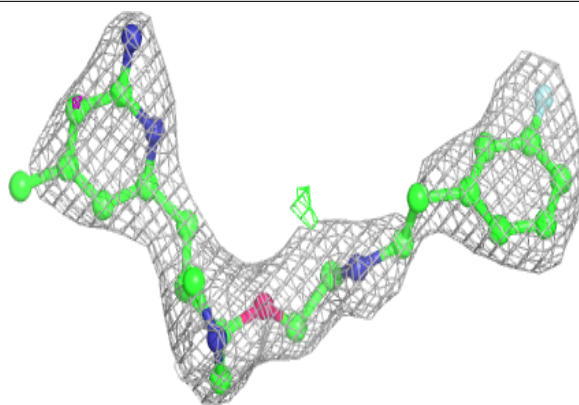
Electron density around HEM A 750:

$2mF_o-DF_c$ (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.