



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:11 am BST

PDB ID : 3N62
Title : Structure of neuronal nitric oxide synthase D597N mutant heme domain in complex with 6,6'-(2,2'-(pyridine-3,5-diyl)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)
Authors : Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on : 2010-05-25
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 : 2.11
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) : 2.11

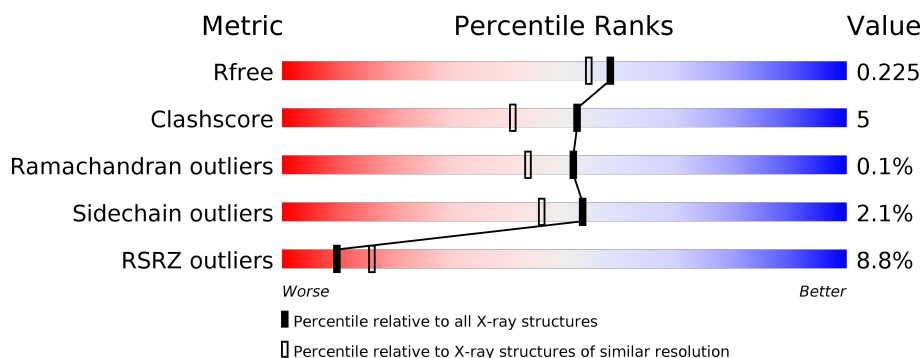
1 Overall quality at a glance

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 on 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	<div> <div>12%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>••</div> </div> </div>
1	B	422	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	H4B	A	760[B]	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7372 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	7	0
			3342	2142	570	608	22			
1	B	411	Total	C	N	O	S	0	3	0
			3357	2148	575	612	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476
B	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476

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



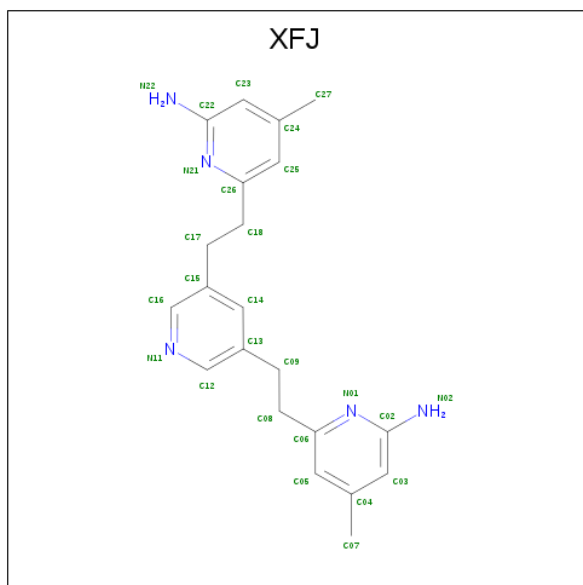
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			48	37	1	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			48	37	1	4	6	
							0	1

- Molecule 3 is 6,6'-(pyridine-3,5-diyl)bis(2,1-diyl)bis(4-methylpyridin-2-amine) (three-letter code: XFJ) (formula: C₂₁H₂₅N₅).



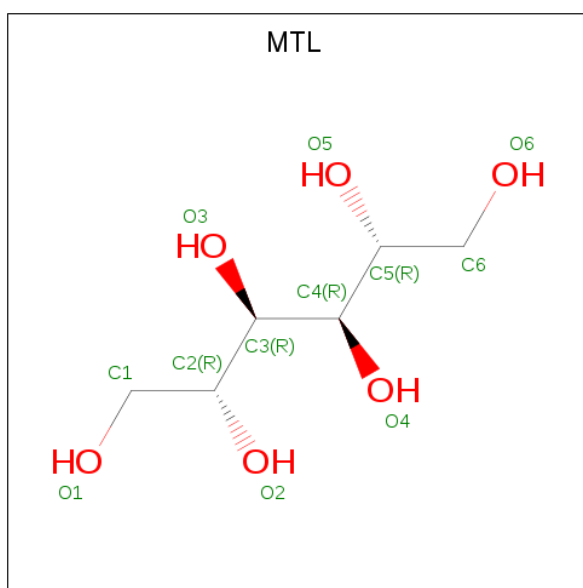
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N		
			26	21	5	0	0
3	B	1	Total	C	N		
			26	21	5	0	1
3	B	1	Total	C	N		
			26	21	5	0	0
3	B	1	Total	C	N		
			26	21	5	0	1

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 5 is D-MANNITOL (three-letter code: MTL) (formula: $C_6H_{14}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		
5	B	1	Total	C	O	0	0
			12	6	6		

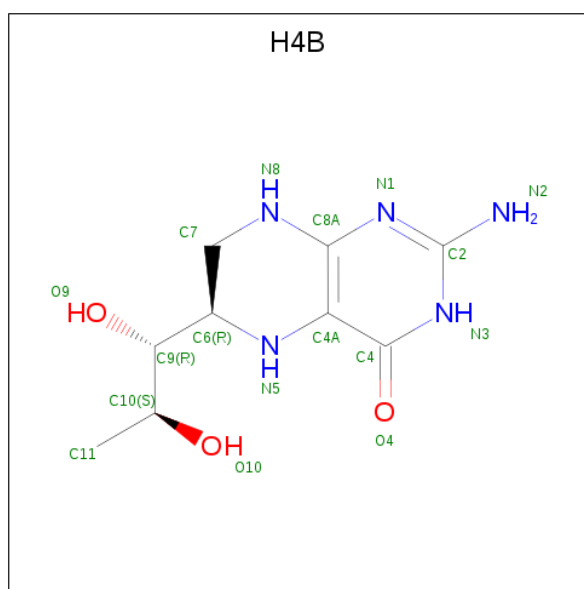
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total Zn 3 3	0	0

- Molecule 8 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C₉H₁₅N₅O₃).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	169	Total O 169 169	0	2

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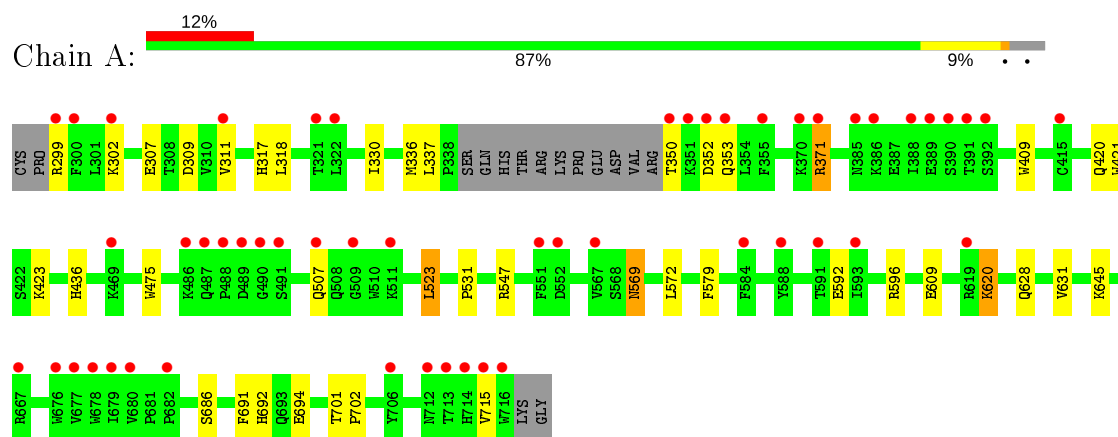
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	233	Total 233	O 233	0	2

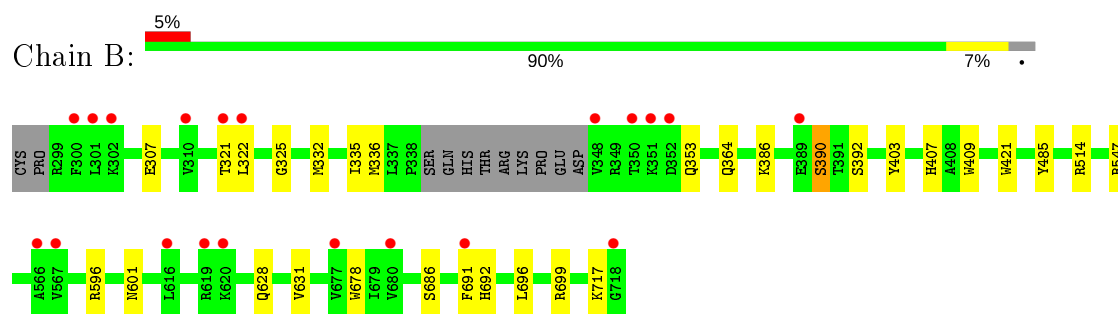
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: Nitric oxide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.81Å 110.39Å 164.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.95 38.46 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.64-1.95) 99.6 (38.46-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.173 , 0.208 0.187 , 0.225	Depositor DCC
R_{free} test set	3453 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.3	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	0.96	EDS
Total number of atoms	7372	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, XFJ, H4B, CL, MTL, ACT, 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	0.60	0/3456	0.61	0/4689
1	B	0.65	0/3459	0.65	0/4689
All	All	0.63	0/6915	0.63	0/9378

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3342	0	3274	34	0
1	B	3357	0	3277	24	0
2	A	48	0	8	7	0
2	B	48	0	8	9	0
3	A	26	0	25	2	0
3	B	78	0	70	10	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	12	0	14	3	0
5	B	12	0	14	0	0
6	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	1	0
7	A	3	0	0	0	0
8	A	17	0	11	7	0
8	B	17	0	13	6	0
9	A	169	0	0	3	0
9	B	233	0	0	2	0
All	All	7372	0	6720	71	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 5.

All (71) 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)
8:A:760[B]:H4B:N2	2:B:750[B]:HEM:O1A	1.61	1.30
2:A:750[B]:HEM:O1A	8:B:760[B]:H4B:N2	1.64	1.30
8:A:760[B]:H4B:N2	2:B:750[B]:HEM:CGA	2.11	1.13
8:A:760[B]:H4B:C2	2:B:750[B]:HEM:O1A	1.97	1.12
2:A:750[B]:HEM:O1A	8:B:760[B]:H4B:C2	1.97	1.11
2:A:750[B]:HEM:O1A	8:B:760[B]:H4B:N3	1.87	1.07
2:A:750[B]:HEM:CGA	8:B:760[B]:H4B:N2	2.21	1.02
8:A:760[B]:H4B:N3	2:B:750[B]:HEM:O1A	1.92	1.01
2:B:750[A]:HEM:O2A	3:B:719[A]:XFJ:H09	1.81	0.80
1:A:701[A]:THR:HG22	1:A:702:PRO:HA	1.65	0.77
1:A:299:ARG:HD2	1:A:318:LEU:CD2	2.19	0.72
1:A:299:ARG:O	1:A:317:HIS:CE1	2.44	0.70
1:A:299:ARG:O	1:A:317:HIS:HE1	1.78	0.67
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.06	0.67
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.77	0.66
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.60	0.66
1:A:596:ARG:NH1	2:A:750[B]:HEM:O2A	2.30	0.64
1:A:302:LYS:HE3	1:A:311:VAL:HG11	1.80	0.64
1:A:436:HIS:CE1	9:A:1163:HOH:O	2.51	0.63
1:B:325:GLY:O	1:B:332:MET:HG3	2.00	0.62
8:A:760[B]:H4B:H9	1:B:336:MET:HE2	1.82	0.61
1:A:299:ARG:HD2	1:A:318:LEU:HD21	1.85	0.58
1:A:299:ARG:HD2	1:A:318:LEU:HD22	1.83	0.58
1:A:336:MET:HE2	8:B:760[B]:H4B:H9	1.87	0.57
1:B:596:ARG:NH1	2:B:750[B]:HEM:O2A	2.38	0.56
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.55
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.68	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:SER:HA	1:A:691:PHE:CG	2.43	0.53
2:A:750[A]:HEM:O2A	3:B:805[A]:XFJ:H09	2.09	0.53
1:B:678:TRP:CH2	3:B:719[A]:XFJ:H08	2.44	0.53
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.97	0.53
2:B:750[A]:HEM:O2A	3:B:719[A]:XFJ:C09	2.55	0.51
5:A:870:MTL:H12	3:B:805[A]:XFJ:H27	1.91	0.51
1:B:678:TRP:CZ3	3:B:719[A]:XFJ:H08	2.47	0.50
1:A:330[A]:ILE:HD11	1:B:696:LEU:HB3	1.93	0.50
1:B:596:ARG:HB2	6:B:910:CL:CL	2.49	0.49
1:A:609:GLU:HG3	9:A:1009:HOH:O	2.13	0.48
1:A:420:GLN:OE1	1:A:423:LYS:HE2	2.14	0.47
1:A:592:GLU:HB3	1:A:596:ARG:NH2	2.29	0.47
1:A:596:ARG:NH1	2:A:750[A]:HEM:O2A	2.48	0.47
1:B:686:SER:HA	1:B:691:PHE:CG	2.50	0.47
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.50	0.46
1:A:336:MET:CE	8:B:760[B]:H4B:H9	2.44	0.46
1:A:307:GLU:HG2	1:A:692:HIS:CG	2.50	0.46
1:B:364:GLN:NE2	9:B:1314:HOH:O	2.49	0.45
1:A:337:LEU:HD21	3:A:800:XFJ:H23	1.97	0.45
5:A:870:MTL:O3	3:B:805[A]:XFJ:H27B	2.17	0.44
1:A:701[A]:THR:CG2	1:A:702:PRO:HA	2.42	0.44
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.99	0.44
1:A:569:ASN:H	1:A:569:ASN:HD22	1.65	0.44
8:A:760[B]:H4B:H9	1:B:336:MET:CE	2.47	0.43
8:A:760[B]:H4B:N2	2:B:750[B]:HEM:O2A	2.45	0.43
1:B:386:LYS:O	1:B:390:SER:HB3	2.17	0.43
1:A:436:HIS:HE1	9:A:1163:HOH:O	1.91	0.43
1:A:620:LYS:HE3	1:A:620:LYS:HB2	1.81	0.43
1:B:307:GLU:HG2	1:B:692:HIS:CG	2.54	0.43
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.84	0.42
6:A:910:CL:CL	3:B:805[A]:XFJ:H12	2.56	0.42
1:B:601:ASN:HB2	9:B:1347:HOH:O	2.19	0.42
1:B:596:ARG:NH1	2:B:750[A]:HEM:O2A	2.54	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.03	0.41
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.56	0.41
1:B:321:THR:HG23	1:B:322:LEU:HG	2.02	0.41
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.56	0.41
1:A:572:LEU:HB3	1:A:579:PHE:HB2	2.03	0.41
1:B:353:GLN:HG2	1:B:353:GLN:H	1.78	0.41
5:A:870:MTL:O3	3:B:805[A]:XFJ:C27	2.69	0.41
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLN:CG	1:B:631:VAL:HG11	2.51	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%)	399 (97%)	10 (2%)	1 (0%)	47	38
1	B	410/422 (97%)	402 (98%)	8 (2%)	0	100	100
All	All	820/844 (97%)	801 (98%)	18 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	ASP

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	30
1	B	369/377 (98%)	365 (99%)	4 (1%)	73	71
All	All	739/754 (98%)	724 (98%)	15 (2%)	53	48

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	THR
1	A	352	ASP
1	A	353	GLN
1	A	371	ARG
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	390	SER
1	B	392	SER
1	B	547	ARG
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	A	436	HIS
1	A	454	ASN
1	A	487	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	B	364	GLN
1	B	425	GLN
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	605	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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[A]	-	27,50,50	2.17	7 (25%)	17,82,82	2.36	6 (35%)
2	HEM	B	750[A]	-	27,50,50	2.21	9 (33%)	17,82,82	2.12	6 (35%)
2	HEM	B	750[B]	-	27,50,50	2.18	8 (29%)	17,82,82	2.31	6 (35%)
5	MTL	B	870	-	11,11,11	0.76	0	14,14,14	0.67	0
4	ACT	A	860	-	1,3,3	1.36	0	0,3,3	0.00	-
3	XFJ	B	805[A]	7	28,28,28	0.35	0	38,38,38	1.87	13 (34%)
4	ACT	B	860	-	1,3,3	1.52	0	0,3,3	0.00	-
8	H4B	A	760[B]	-	16,18,18	1.07	1 (6%)	11,26,26	2.66	4 (36%)
8	H4B	B	760[B]	-	16,18,18	0.94	0	11,26,26	2.75	6 (54%)
3	XFJ	B	800	-	28,28,28	0.78	1 (3%)	38,38,38	2.00	11 (28%)
3	XFJ	A	800	-	28,28,28	0.72	0	38,38,38	2.02	12 (31%)
3	XFJ	B	719[A]	7	28,28,28	0.35	0	38,38,38	1.91	13 (34%)
5	MTL	A	870	-	11,11,11	0.46	0	14,14,14	0.86	0
2	HEM	A	750[B]	-	27,50,50	2.13	6 (22%)	17,82,82	2.75	7 (41%)

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[A]	-	-	2/6/54/54	-
2	HEM	B	750[A]	-	-	0/6/54/54	-
2	HEM	B	750[B]	-	-	0/6/54/54	-
5	MTL	B	870	-	-	0/16/16/16	-
3	XFJ	B	805[A]	7	-	0/10/10/10	0/3/3/3
8	H4B	A	760[B]	-	-	2/8/17/17	0/2/2/2
8	H4B	B	760[B]	-	-	4/8/17/17	0/2/2/2
3	XFJ	B	800	-	-	0/10/10/10	0/3/3/3
3	XFJ	A	800	-	-	0/10/10/10	0/3/3/3
3	XFJ	B	719[A]	7	-	0/10/10/10	0/3/3/3
5	MTL	A	870	-	-	0/16/16/16	-
2	HEM	A	750[B]	-	-	0/6/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750[A]	HEM	C3B-C2B	-4.84	1.33	1.40
2	A	750[B]	HEM	C3B-C2B	-4.84	1.33	1.40
2	A	750[A]	HEM	C3D-C2D	4.83	1.52	1.37
2	A	750[B]	HEM	C3D-C2D	4.83	1.52	1.37
2	B	750[A]	HEM	C3C-C2C	-4.65	1.33	1.40
2	B	750[B]	HEM	C3C-C2C	-4.65	1.33	1.40
2	B	750[A]	HEM	C3D-C2D	4.53	1.51	1.37
2	B	750[B]	HEM	C3D-C2D	4.53	1.51	1.37
2	B	750[A]	HEM	C3B-C2B	-4.29	1.34	1.40
2	B	750[B]	HEM	C3B-C2B	-4.29	1.34	1.40
2	A	750[A]	HEM	C3C-C2C	-4.00	1.34	1.40
2	A	750[B]	HEM	C3C-C2C	-4.00	1.34	1.40
2	B	750[A]	HEM	C3B-CAB	3.93	1.55	1.47
2	B	750[B]	HEM	C3B-CAB	3.93	1.55	1.47
2	B	750[A]	HEM	C3C-CAC	3.73	1.55	1.47
2	B	750[B]	HEM	C3C-CAC	3.73	1.55	1.47
2	A	750[A]	HEM	C3B-CAB	3.56	1.55	1.47
2	A	750[B]	HEM	C3B-CAB	3.56	1.55	1.47
2	A	750[A]	HEM	C3C-CAC	3.13	1.54	1.47
2	A	750[B]	HEM	C3C-CAC	3.13	1.54	1.47
2	A	750[A]	HEM	CAA-C2A	2.67	1.56	1.52
2	B	750[A]	HEM	CAA-C2A	2.64	1.55	1.52
8	A	760[B]	H4B	C4-C4A	-2.58	1.38	1.41
2	B	750[A]	HEM	CAD-C3D	2.41	1.56	1.52
2	B	750[B]	HEM	CAD-C3D	2.41	1.56	1.52
2	A	750[A]	HEM	CMA-C3A	2.19	1.56	1.51
2	A	750[B]	HEM	CMA-C3A	2.19	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	XFJ	C06-N01	2.18	1.38	1.34
2	B	750[A]	HEM	CMB-C2B	2.09	1.56	1.51
2	B	750[B]	HEM	CMB-C2B	2.09	1.56	1.51
2	B	750[A]	HEM	CMD-C2D	2.06	1.55	1.51
2	B	750[B]	HEM	CMD-C2D	2.06	1.55	1.51

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750[A]	HEM	CBD-CAD-C3D	-6.82	99.92	112.48
2	A	750[B]	HEM	CBD-CAD-C3D	-6.82	99.92	112.48
2	B	750[A]	HEM	CBD-CAD-C3D	-6.10	101.23	112.48
2	B	750[B]	HEM	CBD-CAD-C3D	-6.10	101.23	112.48
8	A	760[B]	H4B	C4-C4A-C8A	5.95	119.86	114.57
2	A	750[B]	HEM	CAA-CBA-CGA	-5.85	102.85	112.67
8	B	760[B]	H4B	C4-C4A-C8A	5.74	119.67	114.57
3	A	800	XFJ	C22-N21-C26	5.14	122.00	118.10
3	B	800	XFJ	C02-N01-C06	4.59	121.58	118.10
3	B	805[A]	XFJ	C02-N01-C06	4.59	121.58	118.10
3	B	719[A]	XFJ	C02-N01-C06	4.52	121.53	118.10
3	B	800	XFJ	C22-N21-C26	4.46	121.48	118.10
2	B	750[B]	HEM	CAA-CBA-CGA	-4.37	105.34	112.67
3	A	800	XFJ	C02-N01-C06	4.33	121.38	118.10
3	B	719[A]	XFJ	C22-N21-C26	3.81	120.99	118.10
3	B	800	XFJ	C05-C06-N01	-3.77	118.90	122.90
3	A	800	XFJ	C05-C06-N01	-3.62	119.06	122.90
3	B	800	XFJ	C14-C15-C16	3.61	120.20	116.71
3	B	719[A]	XFJ	C14-C13-C12	3.47	120.06	116.71
3	A	800	XFJ	C14-C15-C16	3.43	120.02	116.71
3	B	719[A]	XFJ	C16-N11-C12	3.42	122.14	117.48
3	B	800	XFJ	C08-C06-N01	3.37	120.97	115.95
8	A	760[B]	H4B	C4-N3-C2	3.35	121.25	115.93
2	A	750[A]	HEM	C1D-C2D-C3D	-3.33	104.68	107.00
2	A	750[B]	HEM	C1D-C2D-C3D	-3.33	104.68	107.00
8	B	760[B]	H4B	C4-C4A-N5	3.27	121.87	119.12
2	B	750[A]	HEM	CMA-C3A-C4A	-3.24	123.48	128.46
2	B	750[B]	HEM	CMA-C3A-C4A	-3.24	123.48	128.46
8	B	760[B]	H4B	N3-C2-N1	-3.19	120.41	125.42
2	A	750[A]	HEM	CMA-C3A-C4A	-3.18	123.58	128.46
2	A	750[B]	HEM	CMA-C3A-C4A	-3.18	123.58	128.46
8	A	760[B]	H4B	N3-C2-N1	-3.14	120.50	125.42
3	B	719[A]	XFJ	C08-C06-N01	3.12	120.60	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	805[A]	XFJ	C14-C15-C16	3.09	119.70	116.71
3	A	800	XFJ	C15-C14-C13	-3.05	117.48	121.23
3	B	805[A]	XFJ	C08-C06-N01	2.92	120.30	115.95
8	B	760[B]	H4B	C4-N3-C2	2.92	120.57	115.93
3	B	805[A]	XFJ	C17-C18-C26	-2.87	106.56	112.99
8	B	760[B]	H4B	C2-N1-C8A	2.84	120.91	114.54
3	A	800	XFJ	C18-C26-N21	2.83	120.17	115.95
3	A	800	XFJ	C16-N11-C12	2.79	121.29	117.48
3	B	805[A]	XFJ	C22-N21-C26	2.79	120.21	118.10
3	B	805[A]	XFJ	C05-C06-N01	-2.76	119.97	122.90
3	B	805[A]	XFJ	C14-C13-C12	2.76	119.37	116.71
3	B	805[A]	XFJ	C16-N11-C12	2.71	121.18	117.48
3	B	800	XFJ	C17-C15-C16	-2.71	117.47	121.83
3	A	800	XFJ	C08-C06-N01	2.70	119.97	115.95
3	B	800	XFJ	C15-C14-C13	-2.70	117.91	121.23
3	B	800	XFJ	C09-C13-C12	-2.66	117.54	121.83
3	A	800	XFJ	C14-C13-C12	2.64	119.26	116.71
2	B	750[A]	HEM	C1D-C2D-C3D	-2.63	105.16	107.00
2	B	750[B]	HEM	C1D-C2D-C3D	-2.63	105.16	107.00
3	B	805[A]	XFJ	N22-C22-N21	2.60	120.60	116.49
2	A	750[A]	HEM	CMC-C2C-C3C	2.59	129.52	124.68
2	A	750[B]	HEM	CMC-C2C-C3C	2.59	129.52	124.68
3	B	800	XFJ	C25-C26-N21	-2.57	120.17	122.90
3	B	805[A]	XFJ	N02-C02-N01	2.57	120.55	116.49
3	A	800	XFJ	C24-C25-C26	-2.53	118.66	120.32
2	B	750[A]	HEM	CAA-CBA-CGA	-2.52	108.45	112.67
3	B	719[A]	XFJ	C18-C26-N21	2.51	119.68	115.95
3	B	800	XFJ	C16-N11-C12	2.50	120.89	117.48
3	B	719[A]	XFJ	C05-C06-N01	-2.44	120.31	122.90
8	A	760[B]	H4B	C2-N1-C8A	2.36	119.84	114.54
3	A	800	XFJ	C09-C13-C12	-2.33	118.08	121.83
3	B	719[A]	XFJ	C24-C25-C26	-2.31	118.80	120.32
3	B	719[A]	XFJ	C13-C12-N11	-2.26	119.30	123.72
3	B	719[A]	XFJ	N22-C22-N21	2.23	120.01	116.49
3	A	800	XFJ	N22-C22-N21	2.19	119.95	116.49
2	B	750[A]	HEM	CMA-C3A-C2A	2.19	129.07	124.94
2	B	750[B]	HEM	CMA-C3A-C2A	2.19	129.07	124.94
3	B	719[A]	XFJ	C17-C18-C26	-2.17	108.13	112.99
2	A	750[A]	HEM	C4C-C3C-C2C	2.17	108.41	106.90
2	A	750[B]	HEM	C4C-C3C-C2C	2.17	108.41	106.90
3	B	719[A]	XFJ	C14-C15-C16	2.15	118.79	116.71
3	B	805[A]	XFJ	C18-C26-N21	2.14	119.14	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	805[A]	XFJ	C15-C14-C13	-2.14	118.60	121.23
3	B	719[A]	XFJ	N02-C02-N01	2.11	119.83	116.49
3	B	805[A]	XFJ	C25-C26-N21	-2.11	120.66	122.90
2	A	750[A]	HEM	CMA-C3A-C2A	2.05	128.81	124.94
2	A	750[B]	HEM	CMA-C3A-C2A	2.05	128.81	124.94
3	B	800	XFJ	C14-C13-C12	2.05	118.69	116.71
8	B	760[B]	H4B	C4A-N5-C6	-2.05	115.59	121.16
2	B	750[A]	HEM	CMB-C2B-C3B	2.01	128.45	124.68
2	B	750[B]	HEM	CMB-C2B-C3B	2.01	128.45	124.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	750[A]	HEM	C1A-C2A-CAA-CBA
2	A	750[A]	HEM	C3A-C2A-CAA-CBA
8	B	760[B]	H4B	O10-C10-C9-C6
8	B	760[B]	H4B	O10-C10-C9-O9
8	B	760[B]	H4B	C11-C10-C9-O9
8	B	760[B]	H4B	C11-C10-C9-C6
8	A	760[B]	H4B	C11-C10-C9-O9
8	A	760[B]	H4B	O10-C10-C9-O9

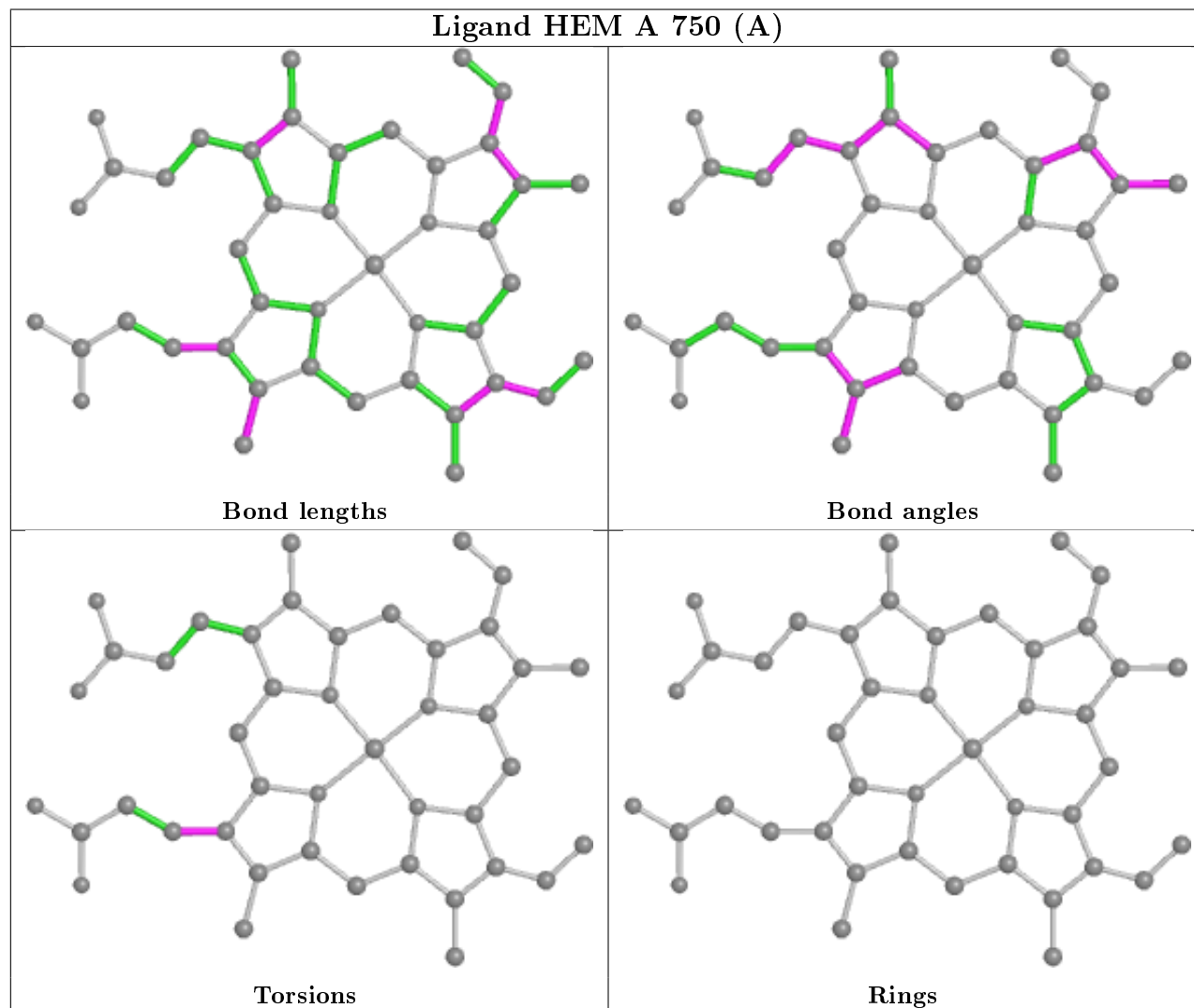
There are no ring outliers.

11 monomers are involved in 29 short contacts:

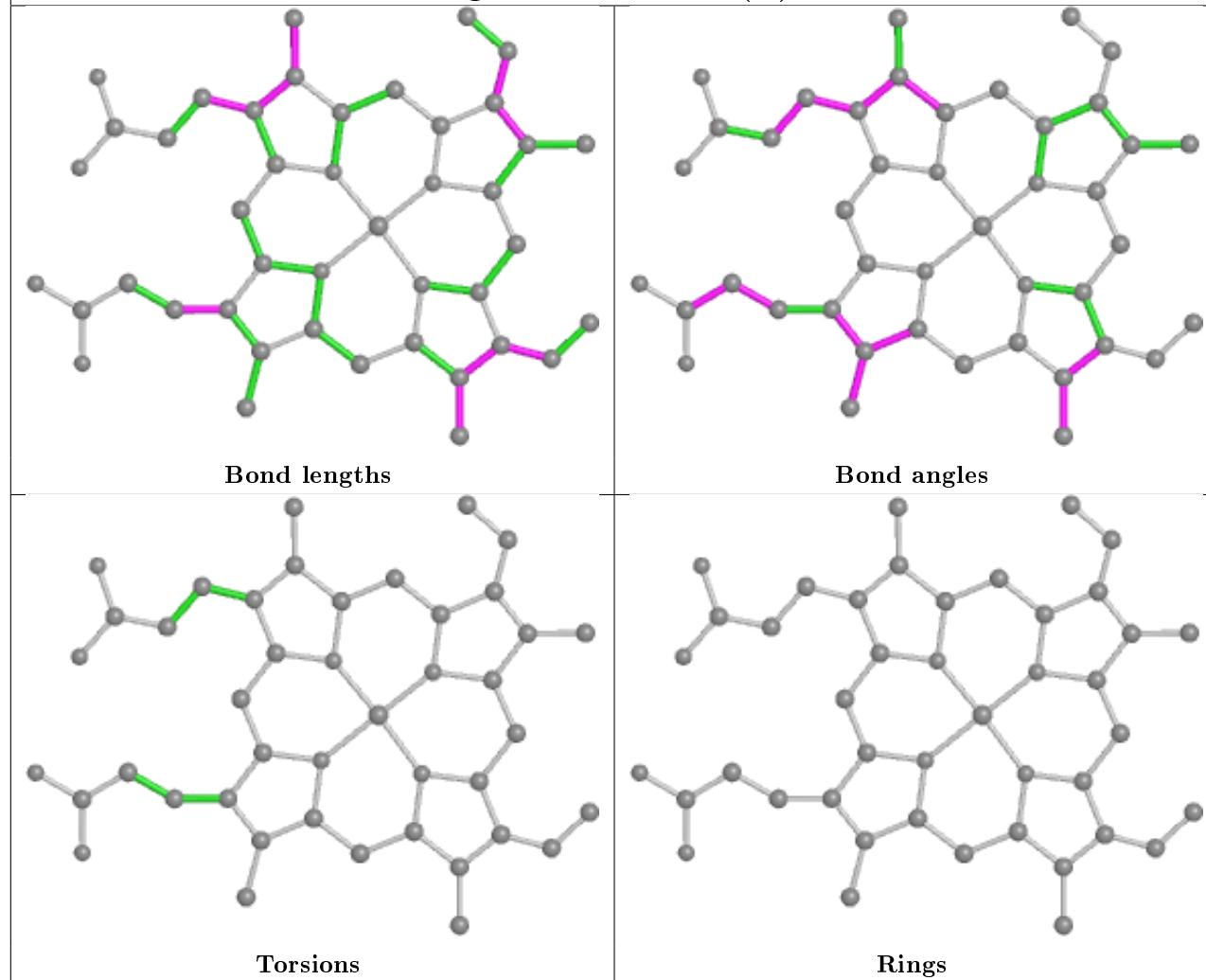
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750[A]	HEM	2	0
2	B	750[A]	HEM	3	0
2	B	750[B]	HEM	6	0
3	B	805[A]	XFJ	5	0
8	A	760[B]	H4B	7	0
8	B	760[B]	H4B	6	0
3	B	800	XFJ	1	0
3	A	800	XFJ	2	0
3	B	719[A]	XFJ	4	0
5	A	870	MTL	3	0
2	A	750[B]	HEM	5	0

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

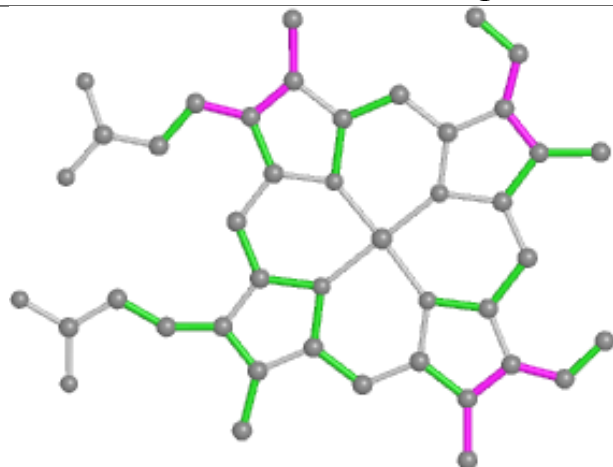
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



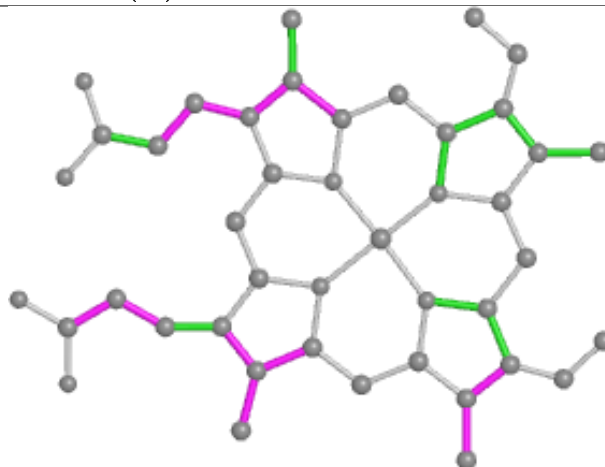
Ligand HEM B 750 (A)



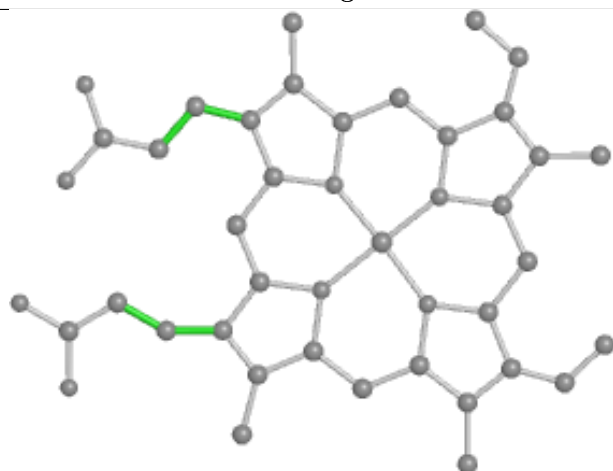
Ligand HEM B 750 (B)



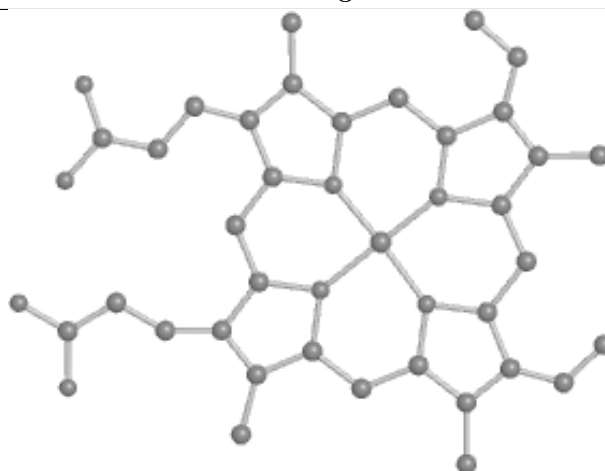
Bond lengths



Bond angles

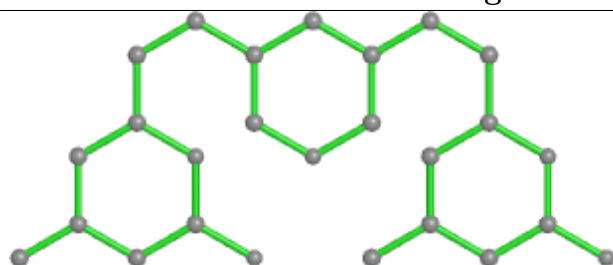


Torsions

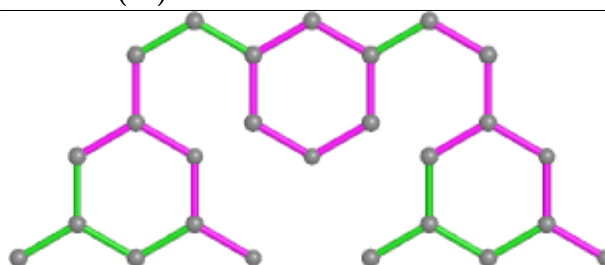


Rings

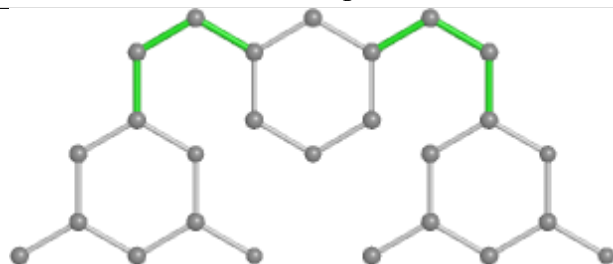
Ligand XFJ B 805 (A)



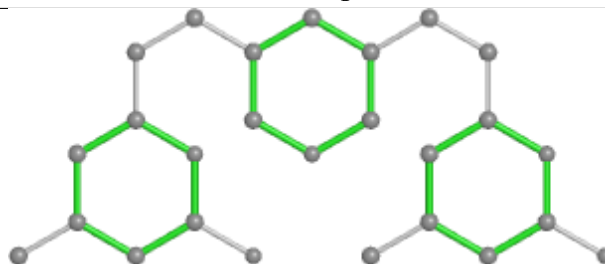
Bond lengths



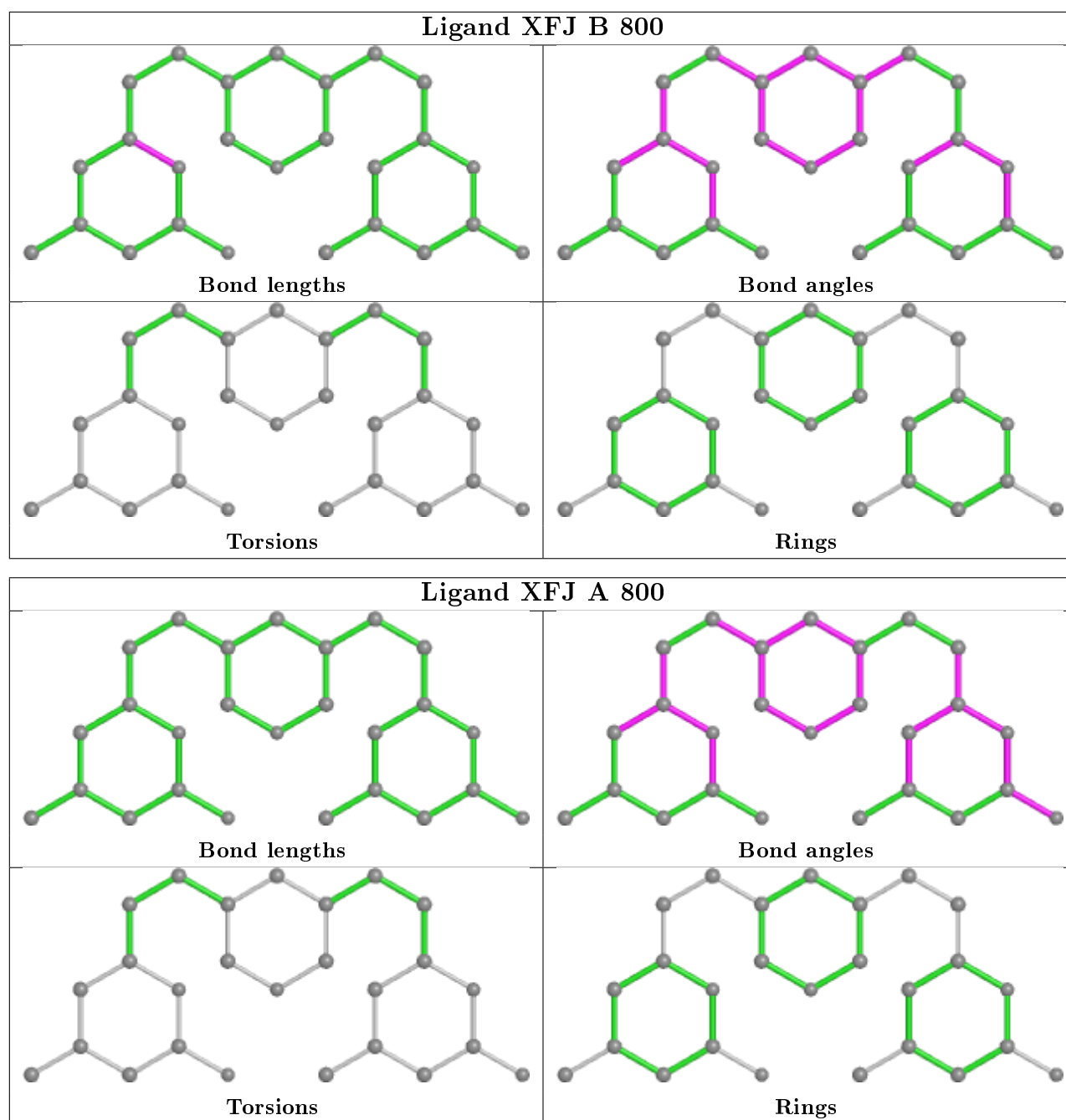
Bond angles



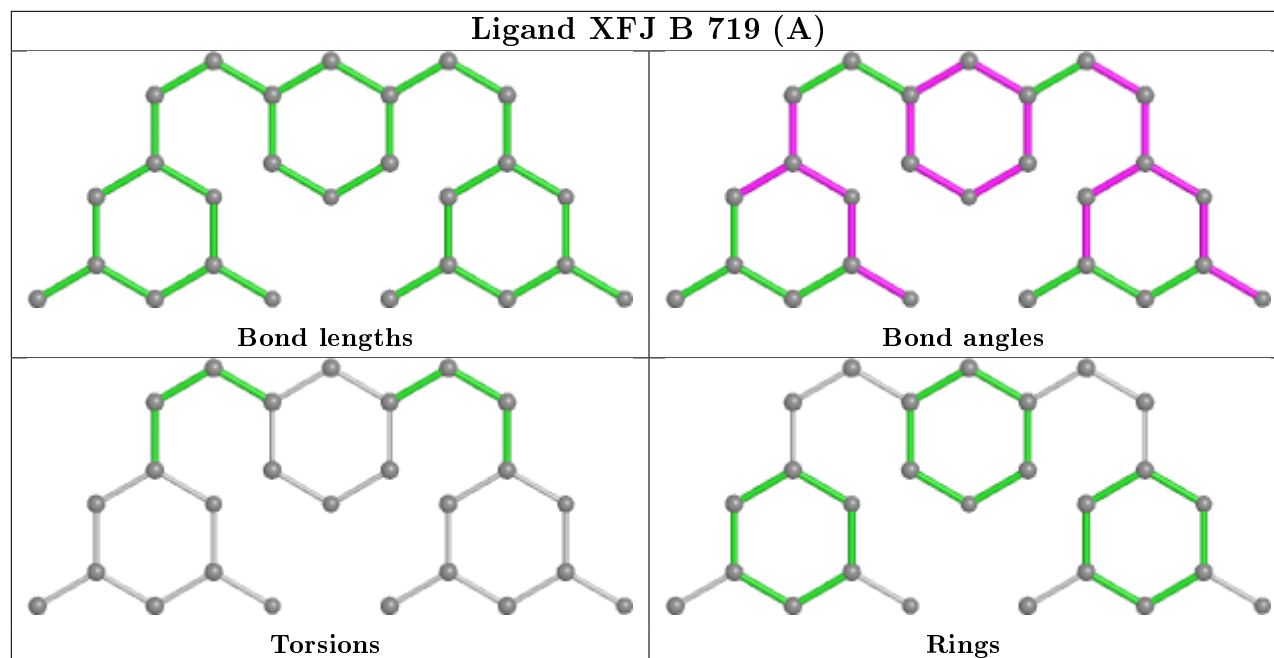
Torsions



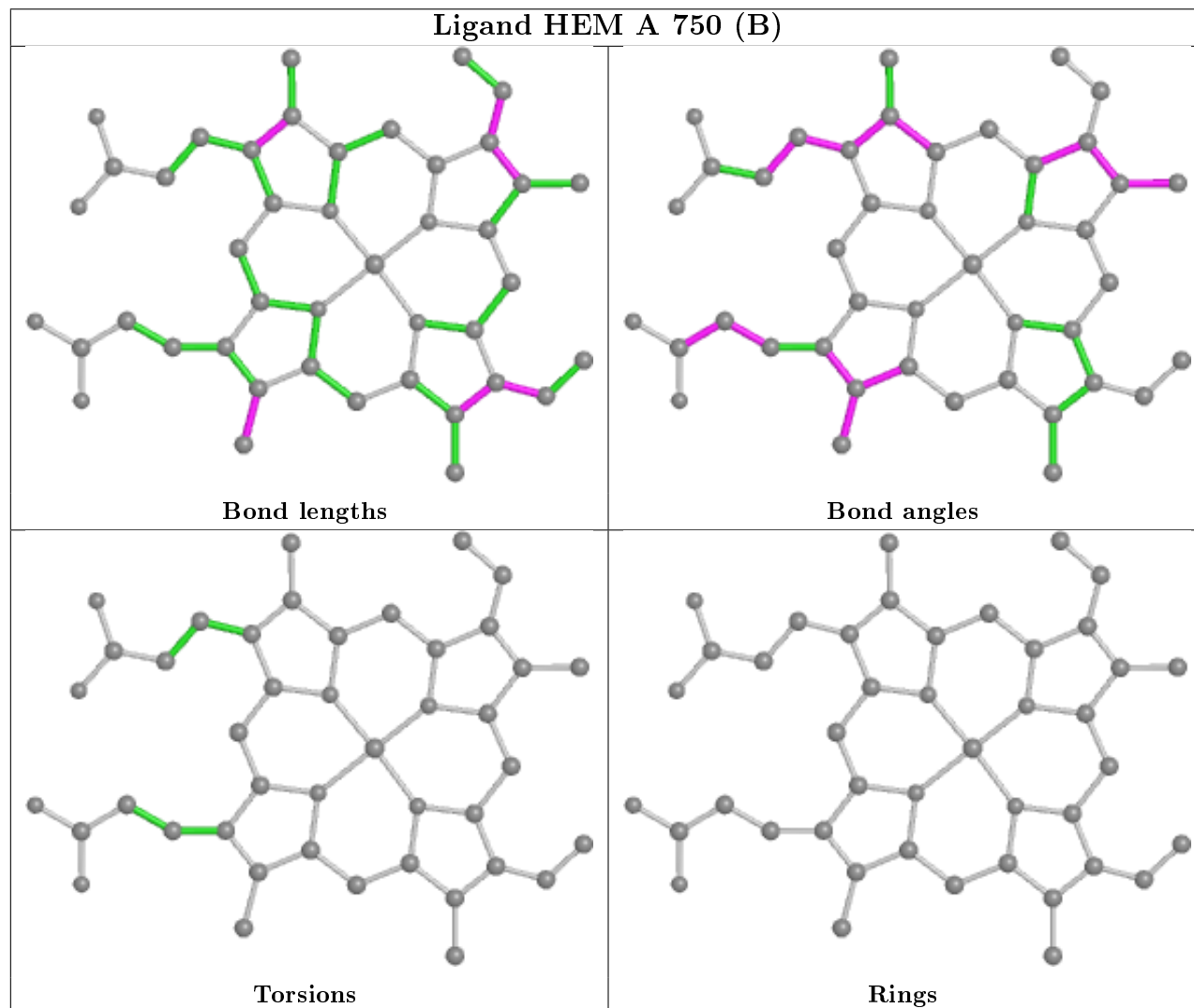
Rings



Ligand XFJ B 719 (A)



Ligand HEM A 750 (B)



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(Å ²)	Q<0.9
1	A	407/422 (96%)	0.69	52 (12%) 3 6	20, 38, 68, 86	0
1	B	411/422 (97%)	0.28	20 (4%) 29 39	19, 30, 52, 79	0
All	All	818/844 (96%)	0.48	72 (8%) 10 16	19, 34, 63, 86	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	ARG	7.3
1	B	348	VAL	6.5
1	B	350	THR	6.5
1	A	716	TRP	6.4
1	A	300	PHE	6.4
1	B	300	PHE	6.3
1	A	352	ASP	5.9
1	B	718	GLY	5.7
1	A	715	VAL	5.7
1	A	350	THR	5.7
1	A	351	LYS	5.0
1	A	488	PRO	4.9
1	A	486	LYS	4.7
1	A	355	PHE	4.5
1	A	321	THR	4.5
1	B	619	ARG	4.2
1	A	392	SER	4.2
1	B	352	ASP	4.2
1	A	489	ASP	3.7
1	A	713	THR	3.6
1	B	351	LYS	3.6
1	A	385	ASN	3.3
1	A	712	ASN	3.3
1	B	567	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	3.2
1	A	511	LYS	3.1
1	A	680	VAL	3.1
1	B	322	LEU	3.1
1	A	509	GLY	3.0
1	A	390	SER	3.0
1	A	678	TRP	2.9
1	A	386	LYS	2.8
1	A	551	PHE	2.8
1	A	469	LYS	2.8
1	A	388	ILE	2.8
1	A	593	ILE	2.8
1	A	567	VAL	2.8
1	A	491	SER	2.7
1	A	353	GLN	2.6
1	A	415	CYS	2.6
1	B	691	PHE	2.6
1	A	667[A]	ARG	2.6
1	B	566	ALA	2.6
1	A	487	GLN	2.6
1	A	490	GLY	2.6
1	A	584	PHE	2.5
1	A	389	GLU	2.5
1	A	619	ARG	2.5
1	B	680	VAL	2.5
1	A	371	ARG	2.4
1	A	677	VAL	2.4
1	A	507	GLN	2.4
1	A	591	THR	2.4
1	B	677	VAL	2.4
1	B	616	LEU	2.4
1	A	676	TRP	2.4
1	A	311	VAL	2.4
1	A	682	PRO	2.3
1	A	370	LYS	2.3
1	A	679	ILE	2.3
1	B	321	THR	2.3
1	B	302	LYS	2.3
1	A	714	HIS	2.3
1	A	302	LYS	2.2
1	B	301	LEU	2.2
1	B	620	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	706	TYR	2.1
1	A	552	ASP	2.1
1	B	310	VAL	2.1
1	A	588	TYR	2.1
1	B	389	GLU	2.1
1	A	391	THR	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 carbohydrates 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
5	MTL	A	870	12/12	0.78	0.39	20,30,33,34	12
8	H4B	A	760[B]	17/17	0.89	0.25	32,33,35,35	17
5	MTL	B	870	12/12	0.89	0.14	31,39,40,42	0
3	XFJ	A	800	26/26	0.90	0.23	23,34,39,41	0
8	H4B	B	760[B]	17/17	0.90	0.26	38,40,42,43	17
3	XFJ	B	719[A]	26/26	0.92	0.28	25,27,32,35	26
3	XFJ	B	805[A]	26/26	0.93	0.29	22,27,38,41	26
3	XFJ	B	800	26/26	0.94	0.18	22,31,35,36	0
4	ACT	A	860	4/4	0.94	0.18	48,48,49,49	0
4	ACT	B	860	4/4	0.96	0.10	35,37,38,38	0
6	CL	A	910	1/1	0.98	0.15	33,33,33,33	0
2	HEM	B	750[B]	43/43	0.98	0.17	18,21,34,39	5
2	HEM	A	750[A]	43/43	0.98	0.20	20,24,34,37	5
6	CL	B	910	1/1	0.98	0.13	32,32,32,32	0
2	HEM	B	750[A]	43/43	0.98	0.17	18,21,33,36	5
2	HEM	A	750[B]	43/43	0.98	0.20	20,24,35,39	5
7	ZN	A	900	1/1	0.99	0.06	28,28,28,28	0

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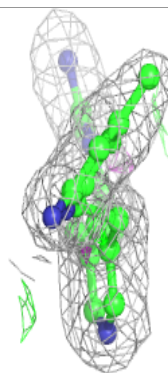
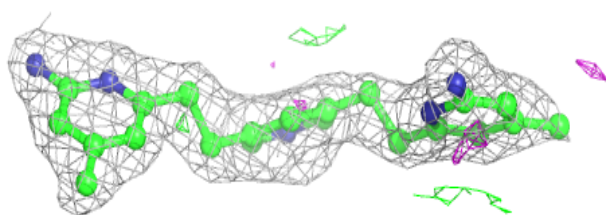
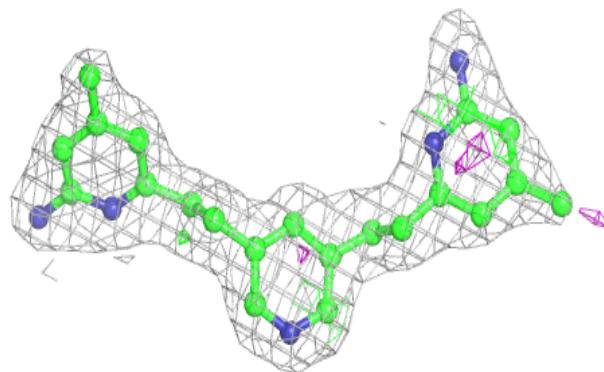
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ZN	A	901	1/1	0.99	0.12	24,24,24,24	1
7	ZN	A	719	1/1	0.99	0.11	24,24,24,24	1

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.

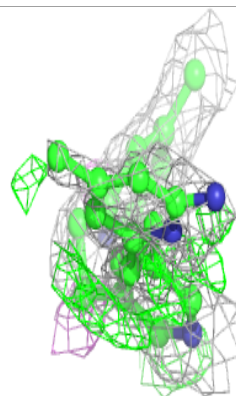
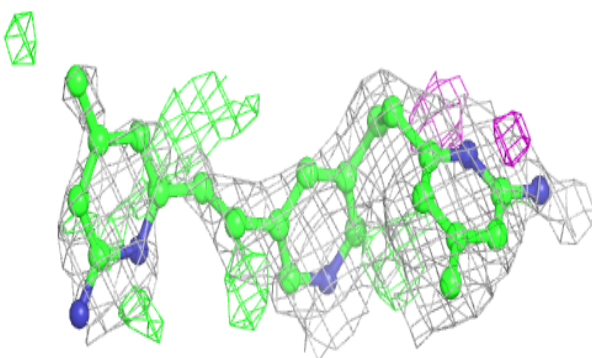
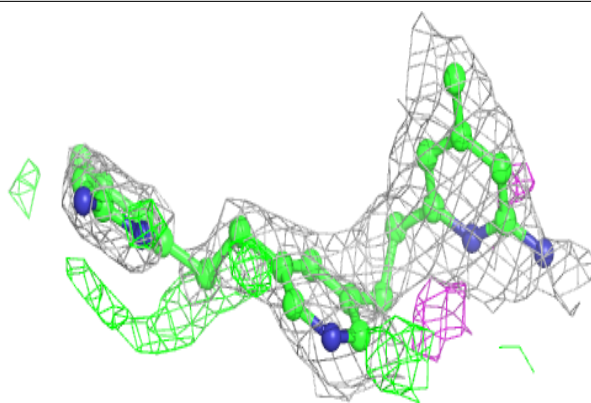
Electron density around XFJ A 800:

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

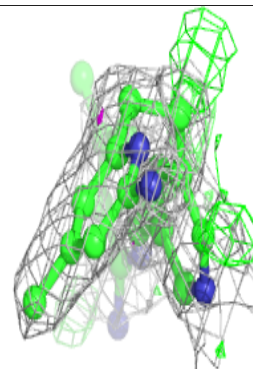
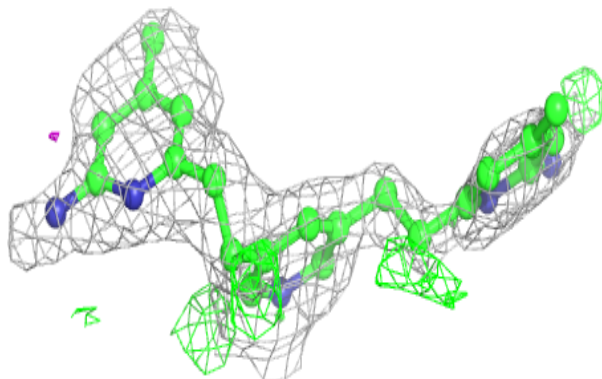
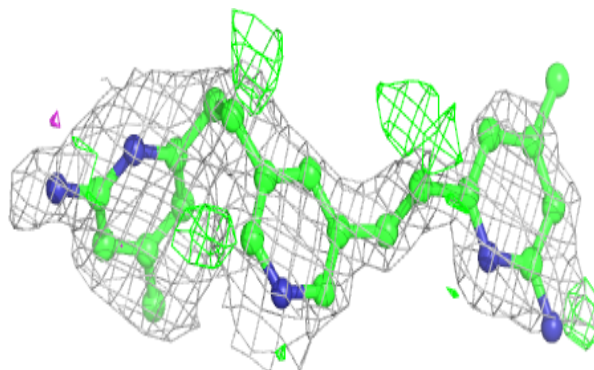


Electron density around XFJ B 719 (A):

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

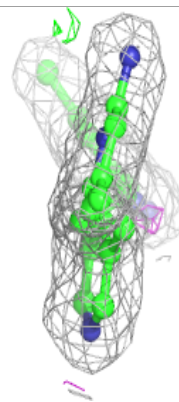
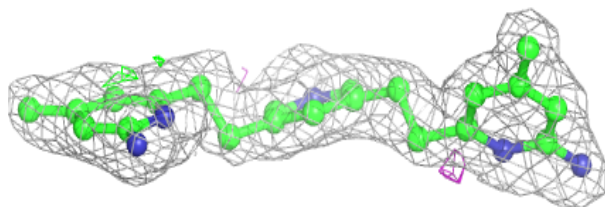
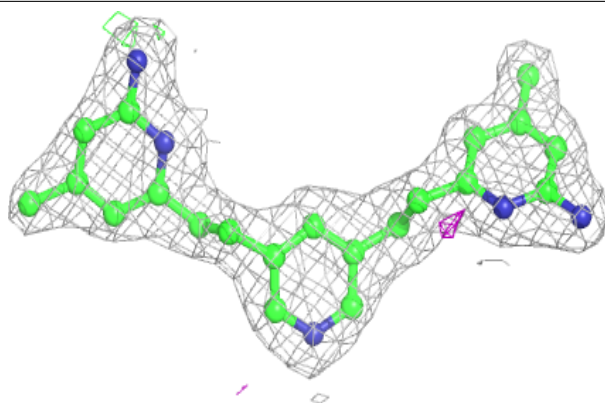
**Electron density around XFJ B 805 (A):**

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



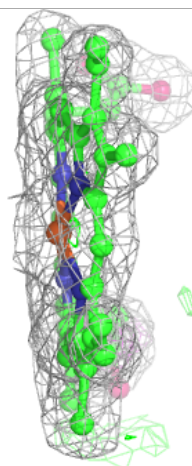
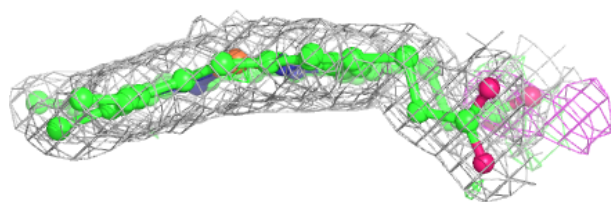
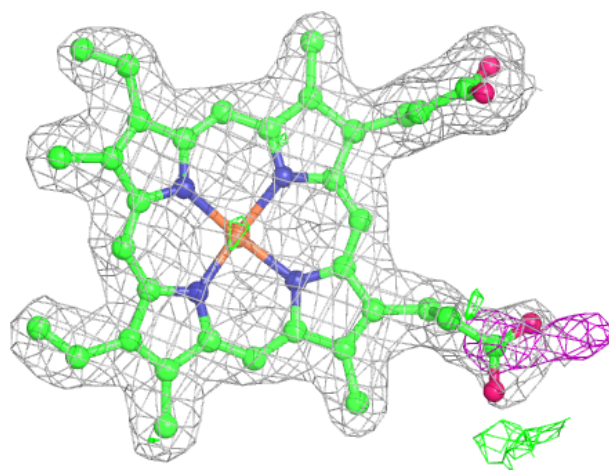
Electron density around XFJ B 800:

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



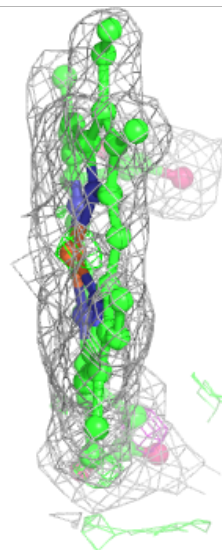
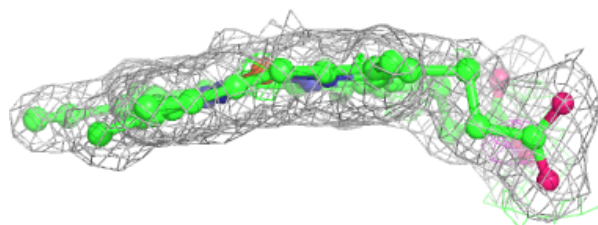
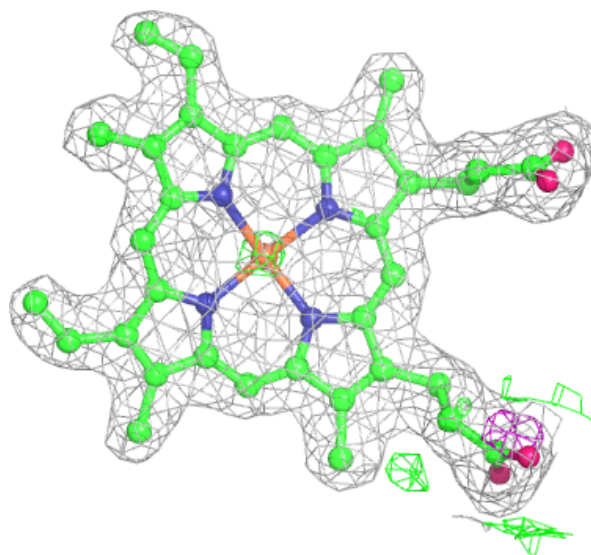
Electron density around HEM B 750 (B):

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



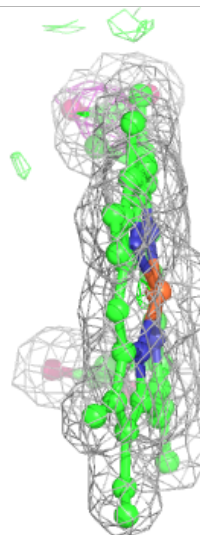
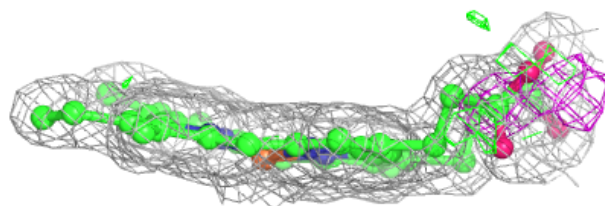
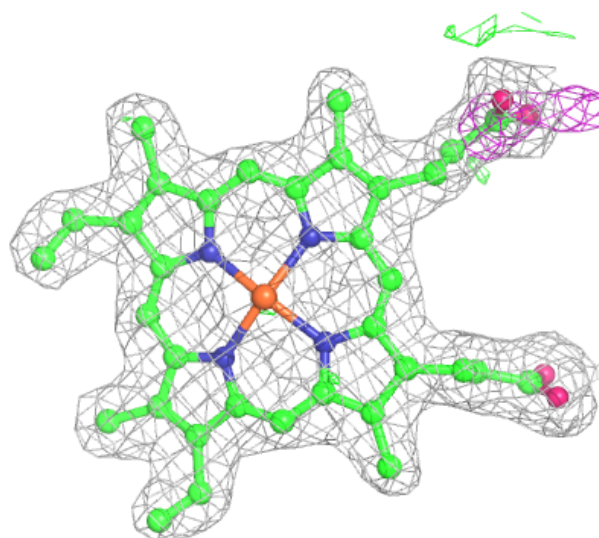
Electron density around HEM A 750 (A):

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



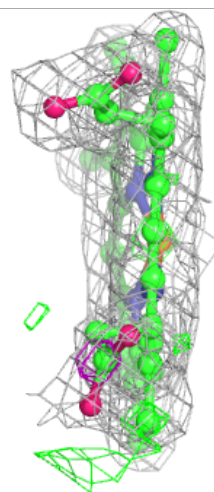
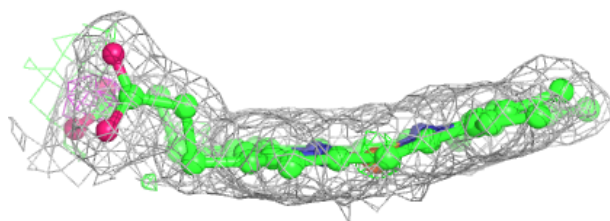
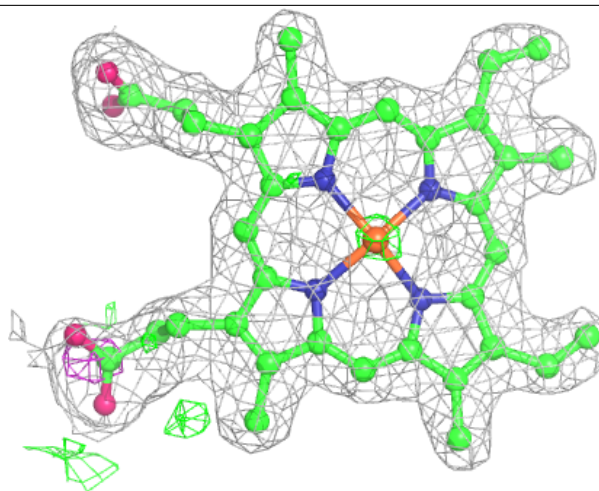
Electron density around HEM B 750 (A):

$2mF_o-DF_c$ (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 (B):

$2mF_o-DF_c$ (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.