



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:01 PM UTC

PDB ID : 3N65 / pdb_00003n65
Title : Structure of neuronal nitric oxide synthase S602H 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 : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

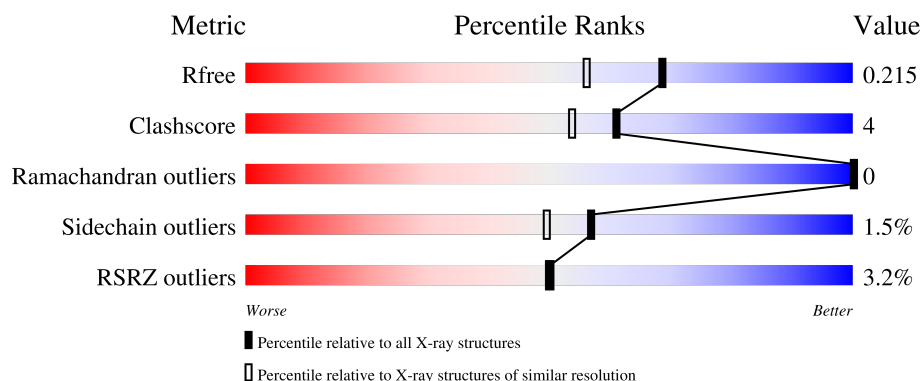
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

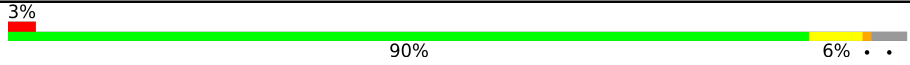
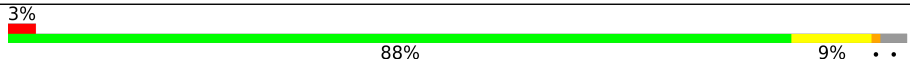
The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 9 unique types of molecules in this entry. The entry contains 7671 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.

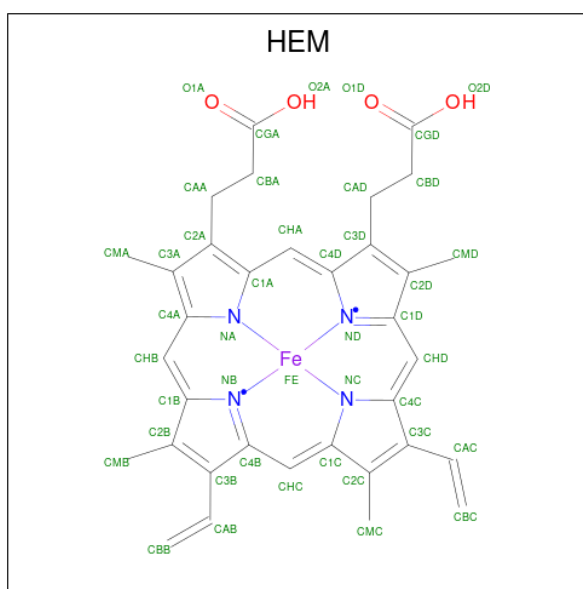
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	5	0
			3344	2144	571	607	22			
1	B	411	Total	C	N	O	S	0	11	0
			3401	2180	580	618	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	602	HIS	SER	engineered mutation	UNP P29476
B	602	HIS	SER	engineered mutation	UNP P29476

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



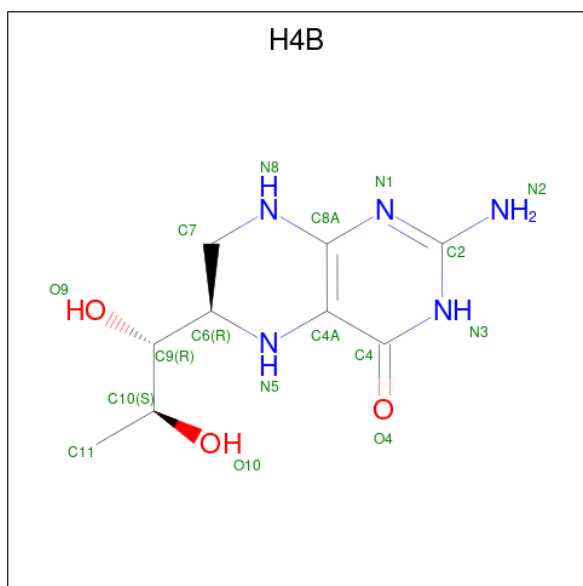
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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



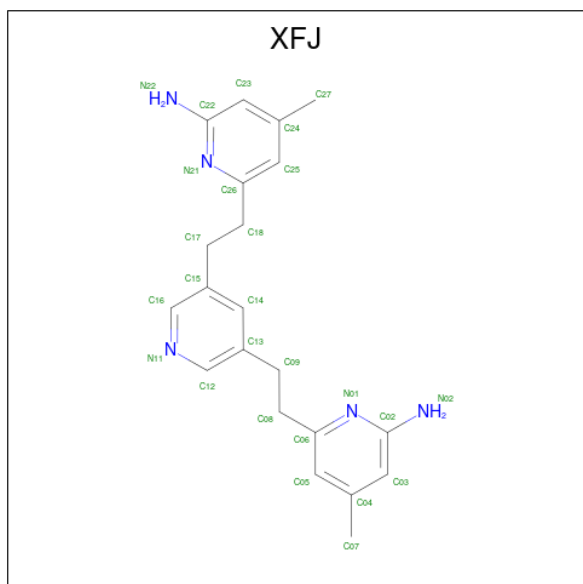
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			17	9	5	3		
3	B	1	Total	C	N	O	0	1
			17	9	5	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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 6,6'-(pyridine-3,5-diyl)diethane-2,1-diylbis(4-methylpyridin-2-amine) (CCD ID: XFJ) (formula: C₂₁H₂₅N₅).



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

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

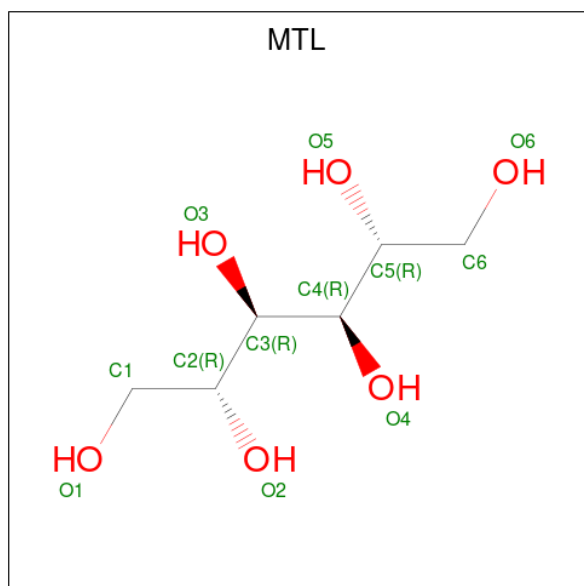
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is D-MANNITOL (CCD ID: MTL) (formula: C₆H₁₄O₆).



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

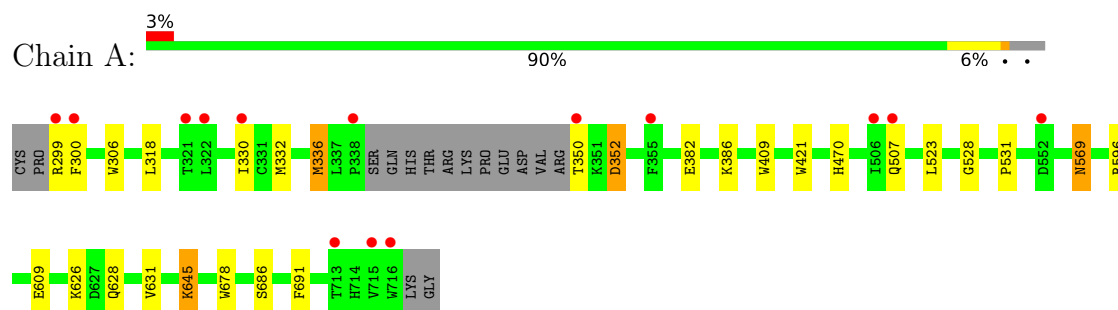
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	292	Total 292	O 292	0	0
9	B	385	Total 385	O 385	0	0

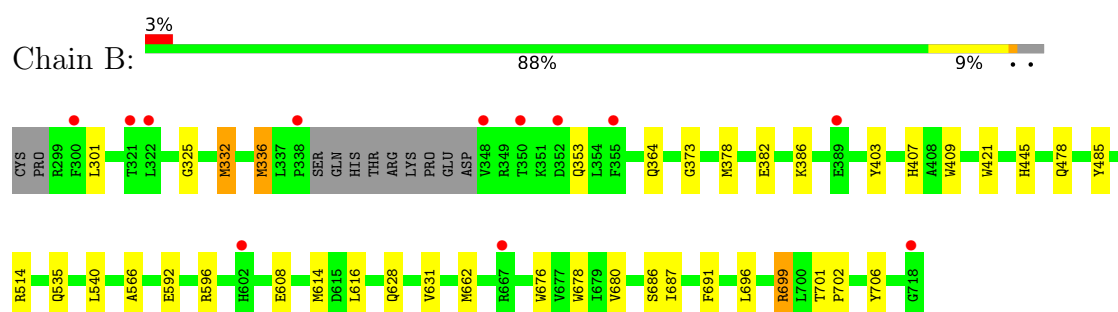
3 Residue-property plots [i](#)

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



• 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	51.98Å 110.58Å 164.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.36 – 1.80 47.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.36-1.80) 99.4 (47.36-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.194 0.189 , 0.215	Depositor DCC
R_{free} test set	4396 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: ACT, CL, H4B, XFJ, ZN, MTL, 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	0.73	0/3455	0.82	0/4688
1	B	0.77	0/3530	0.82	0/4785
All	All	0.75	0/6985	0.82	0/9473

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	3344	0	3255	23	0
1	B	3401	0	3329	31	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	17	0	7	2	0
3	B	17	0	15	3	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	26	0	25	0	0
5	B	78	0	68	4	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	3	0	0	0	0
8	B	12	0	14	2	0
9	A	292	0	0	2	0
9	B	385	0	0	4	0
All	All	7671	0	6779	58	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 (58) 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:O1A	3:B:760[B]:H4B:N2	1.64	1.27
2:A:750:HEM:O1A	3:A:760[B]:H4B:N2	1.89	1.05
2:B:750:HEM:HMC2	2:B:750:HEM:HBC2	1.60	0.81
1:A:336:MET:HE3	1:A:678:TRP:HZ2	1.46	0.79
1:A:596:ARG:NH2	9:A:1013:HOH:O	2.20	0.73
2:B:750:HEM:O1A	3:B:760[B]:H4B:C2	2.42	0.66
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.78	0.64
1:B:596:ARG:NH2	9:B:1296:HOH:O	2.30	0.64
1:A:609:GLU:HG3	9:A:1010:HOH:O	1.96	0.63
8:B:870:MTL:O3	5:B:719[A]:XFJ:H27	2.00	0.60
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.84	0.59
1:A:569:ASN:HD22	1:A:569:ASN:H	1.55	0.54
1:B:706[B]:TYR:OH	8:B:870:MTL:H11	2.07	0.54
1:A:686:SER:HA	1:A:691:PHE:CG	2.44	0.53
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.91	0.52
1:B:373:GLY:HA2	1:B:378:MET:HE3	1.91	0.52
1:A:336:MET:HE3	1:A:678:TRP:CZ2	2.36	0.52
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.92	0.51
1:B:382[B]:GLU:OE2	1:B:386:LYS:HE3	2.11	0.50
1:A:299:ARG:HG2	1:A:318:LEU:HD21	1.93	0.49
1:B:325:GLY:O	1:B:332:MET:HG3	2.13	0.49
1:A:306:TRP:CE2	1:B:336[A]:MET:HE3	2.48	0.49
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.95	0.48
1:B:686:SER:HA	1:B:691:PHE:CG	2.49	0.47
1:B:364:GLN:NE2	9:B:1560:HOH:O	2.47	0.47
1:B:699:ARG:HG3	1:B:699:ARG:NH1	2.29	0.47
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.97	0.46
1:A:382:GLU:OE2	1:A:386:LYS:HE3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:HIS:HA	1:A:528:GLY:HA3	1.99	0.45
1:B:592:GLU:HB3	1:B:596:ARG:NH2	2.31	0.45
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.99	0.45
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.05	0.44
1:B:678:TRP:CZ3	5:B:719[A]:XFJ:H08	2.52	0.44
1:B:676:TRP:CE2	1:B:680:VAL:HG21	2.53	0.44
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.43
1:B:699:ARG:HG3	1:B:699:ARG:HH11	1.84	0.43
1:B:535:GLN:HG3	9:B:1663:HOH:O	2.18	0.42
3:B:760[B]:H4B:H71	3:B:760[B]:H4B:H10	1.67	0.42
1:A:352:ASP:OD2	1:A:352:ASP:N	2.52	0.42
1:B:336[A]:MET:HE2	1:B:336[A]:MET:HB2	1.76	0.42
1:A:645:LYS:HE3	1:A:645:LYS:HB2	1.82	0.42
1:A:306:TRP:CD2	1:B:336[A]:MET:HE3	2.55	0.42
1:B:445:HIS:CD2	1:B:445:HIS:C	2.98	0.42
1:A:300:PHE:CD1	1:A:300:PHE:N	2.88	0.42
1:A:569:ASN:HD22	1:A:569:ASN:N	2.16	0.42
1:B:678:TRP:CH2	5:B:719[A]:XFJ:H08	2.54	0.42
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.55	0.41
1:A:631:VAL:HG11	1:B:628:GLN:HG2	2.00	0.41
1:B:614:MET:HE2	1:B:616:LEU:HD21	2.01	0.41
1:A:626:LYS:HB3	1:B:687:ILE:HD12	2.02	0.41
1:B:478:GLN:HA	1:B:566:ALA:O	2.21	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.46	0.41
1:A:300:PHE:N	1:A:300:PHE:HD1	2.18	0.40
1:B:608:GLU:HG3	9:B:1643:HOH:O	2.21	0.40
1:B:662:MET:HE2	1:B:662:MET:HB3	1.94	0.40
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.56	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	408/422 (97%)	397 (97%)	11 (3%)	0	100	100
1	B	418/422 (99%)	411 (98%)	7 (2%)	0	100	100
All	All	826/844 (98%)	808 (98%)	18 (2%)	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	368/377 (98%)	362 (98%)	6 (2%)	55	47
1	B	377/377 (100%)	371 (98%)	6 (2%)	55	47
All	All	745/754 (99%)	733 (98%)	12 (2%)	57	47

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	MET
1	A	350	THR
1	A	352	ASP
1	A	507	GLN
1	A	569	ASN
1	A	645	LYS
1	B	332	MET
1	B	336[A]	MET
1	B	336[B]	MET
1	B	353	GLN
1	B	540	LEU
1	B	699	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN

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Mol	Chain	Res	Type
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	395	GLN
1	B	425	GLN
1	B	507	GLN
1	B	535	GLN
1	B	605	ASN
1	B	628	GLN
1	B	642	GLN
1	B	697	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	XFJ	B	719[A]	7	28,28,28	0.51	0	36,38,38	1.75	9 (25%)
5	XFJ	B	805[A]	7	28,28,28	0.61	0	36,38,38	2.06	14 (38%)
4	ACT	A	860	-	3,3,3	0.77	0	3,3,3	0.85	0
2	HEM	A	750	1	50,50,50	1.94	11 (22%)	67,82,82	1.47	6 (8%)
3	H4B	B	760[B]	-	17,18,18	1.09	0	14,26,26	1.76	4 (28%)
2	HEM	B	750	1	50,50,50	1.86	10 (20%)	67,82,82	1.30	5 (7%)
5	XFJ	A	800	-	28,28,28	0.71	0	36,38,38	2.26	12 (33%)
8	MTL	B	870	-	11,11,11	0.71	0	14,14,14	0.65	0
4	ACT	B	860	-	3,3,3	0.74	0	3,3,3	1.03	0
5	XFJ	B	800	-	28,28,28	0.89	1 (3%)	36,38,38	2.22	13 (36%)

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
5	XFJ	B	719[A]	7	-	0/10/10/10	0/3/3/3
5	XFJ	B	805[A]	7	-	0/10/10/10	0/3/3/3
2	HEM	A	750	1	-	2/14/54/54	-
3	H4B	B	760[B]	-	-	4/8/17/17	0/2/2/2
2	HEM	B	750	1	-	1/14/54/54	-
5	XFJ	A	800	-	-	0/10/10/10	0/3/3/3
8	MTL	B	870	-	-	2/16/16/16	-
5	XFJ	B	800	-	-	0/10/10/10	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	6.47	1.50	1.36
2	B	750	HEM	C3D-C2D	6.07	1.49	1.36
2	A	750	HEM	FE-NB	5.29	2.11	1.94
2	A	750	HEM	FE-ND	4.89	2.10	1.94
2	B	750	HEM	FE-NB	4.28	2.08	1.94
2	B	750	HEM	FE-ND	4.03	2.07	1.94
2	A	750	HEM	FE-NC	3.96	2.08	1.95
2	B	750	HEM	FE-NA	3.64	2.07	1.95
2	B	750	HEM	FE-NC	3.37	2.06	1.95
2	A	750	HEM	CAC-C3C	3.23	1.56	1.47
2	B	750	HEM	CAC-C3C	3.13	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	CAB-C3B	3.11	1.55	1.47
2	A	750	HEM	CMC-C2C	2.79	1.56	1.50
2	A	750	HEM	CAB-C3B	2.69	1.54	1.47
2	B	750	HEM	CMD-C2D	2.64	1.56	1.50
2	B	750	HEM	CMC-C2C	2.62	1.56	1.50
2	A	750	HEM	CMA-C3A	2.46	1.55	1.50
2	A	750	HEM	FE-NA	2.45	2.03	1.95
2	B	750	HEM	CMB-C2B	2.41	1.55	1.50
2	A	750	HEM	CMB-C2B	2.32	1.55	1.50
2	A	750	HEM	CMD-C2D	2.24	1.55	1.50
5	B	800	XFJ	C14-C15	2.23	1.43	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	XFJ	C22-N21-C26	6.47	122.91	118.07
5	B	800	XFJ	C02-N01-C06	6.19	122.70	118.07
5	A	800	XFJ	C02-N01-C06	5.76	122.38	118.07
2	A	750	HEM	C4D-ND-C1D	5.05	111.18	105.21
5	B	805[A]	XFJ	C02-N01-C06	4.70	121.59	118.07
5	B	800	XFJ	C22-N21-C26	4.64	121.54	118.07
2	A	750	HEM	CBD-CAD-C3D	-4.57	99.91	112.53
2	B	750	HEM	C4D-ND-C1D	4.43	110.45	105.21
2	B	750	HEM	CBD-CAD-C3D	-4.17	101.01	112.53
5	B	805[A]	XFJ	C08-C06-N01	4.01	122.13	116.06
5	B	800	XFJ	C14-C15-C16	3.82	120.44	116.90
5	B	719[A]	XFJ	C02-N01-C06	3.67	120.81	118.07
5	B	719[A]	XFJ	C22-N21-C26	3.67	120.81	118.07
5	B	805[A]	XFJ	C22-N21-C26	3.64	120.80	118.07
5	A	800	XFJ	C05-C06-N01	-3.52	118.72	122.73
5	A	800	XFJ	C14-C15-C16	3.46	120.10	116.90
5	B	800	XFJ	C05-C06-N01	-3.42	118.83	122.73
5	B	719[A]	XFJ	C08-C06-N01	3.25	120.98	116.06
3	B	760[B]	H4B	C2-N1-C8A	3.25	119.09	113.36
5	B	719[A]	XFJ	C14-C15-C16	3.13	119.80	116.90
5	B	800	XFJ	C08-C06-N01	3.12	120.78	116.06
5	B	800	XFJ	C17-C15-C16	-3.09	116.23	121.73
3	B	760[B]	H4B	O4-C4-C4A	-3.05	119.92	127.26
5	B	805[A]	XFJ	C08-C06-C05	-3.04	117.25	121.65
5	A	800	XFJ	C08-C06-N01	3.01	120.63	116.06
5	B	805[A]	XFJ	N02-C02-N01	2.97	121.37	116.59
5	A	800	XFJ	C16-N11-C12	2.94	121.51	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	805[A]	XFJ	C14-C15-C16	2.87	119.56	116.90
2	A	750	HEM	C3B-C4B-NB	-2.82	107.44	109.47
5	A	800	XFJ	C15-C14-C13	-2.81	117.71	121.20
2	B	750	HEM	C1B-NB-C4B	2.77	108.49	105.21
5	B	800	XFJ	C05-C04-C03	2.77	121.19	118.11
5	B	719[A]	XFJ	C08-C06-C05	-2.77	117.64	121.65
5	A	800	XFJ	C17-C15-C16	-2.72	116.90	121.73
5	B	805[A]	XFJ	C05-C04-C03	2.71	121.12	118.11
5	B	800	XFJ	C15-C14-C13	-2.70	117.84	121.20
5	B	800	XFJ	C16-N11-C12	2.69	121.17	117.51
5	B	719[A]	XFJ	C14-C13-C12	2.68	119.39	116.90
2	A	750	HEM	CHC-C1C-NC	2.68	127.37	124.45
2	B	750	HEM	C3B-C4B-NB	-2.66	107.55	109.47
5	B	805[A]	XFJ	C14-C13-C12	2.59	119.30	116.90
5	B	805[A]	XFJ	C15-C14-C13	-2.55	118.02	121.20
5	B	800	XFJ	C09-C08-C06	-2.50	107.44	113.01
3	B	760[B]	H4B	C2-N3-C4	-2.45	120.67	125.11
5	B	805[A]	XFJ	C16-N11-C12	2.44	120.83	117.51
5	A	800	XFJ	C18-C26-N21	2.44	119.75	116.06
5	B	800	XFJ	C09-C13-C12	-2.38	117.49	121.73
5	A	800	XFJ	C14-C13-C12	2.35	119.07	116.90
5	B	800	XFJ	C17-C18-C26	-2.29	107.91	113.01
5	B	800	XFJ	C09-C13-C14	2.27	124.35	120.54
5	B	805[A]	XFJ	C09-C13-C12	-2.25	117.73	121.73
5	B	719[A]	XFJ	N02-C02-N01	2.25	120.20	116.59
5	B	805[A]	XFJ	C25-C26-N21	-2.24	120.17	122.73
5	B	805[A]	XFJ	N22-C22-N21	2.22	120.16	116.59
5	A	800	XFJ	C09-C13-C12	-2.19	117.83	121.73
5	B	719[A]	XFJ	C18-C26-N21	2.17	119.36	116.06
2	B	750	HEM	C4C-C3C-C2C	2.17	108.70	106.81
3	B	760[B]	H4B	C4A-C4-N3	2.12	117.94	112.13
2	A	750	HEM	O2A-CGA-CBA	2.11	120.68	114.00
5	A	800	XFJ	N22-C22-N21	2.11	119.98	116.59
5	B	719[A]	XFJ	C15-C14-C13	-2.09	118.59	121.20
5	B	805[A]	XFJ	C17-C15-C16	-2.07	118.05	121.73
2	A	750	HEM	C1B-NB-C4B	2.07	107.65	105.21

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	760[B]	H4B	O10-C10-C9-C6

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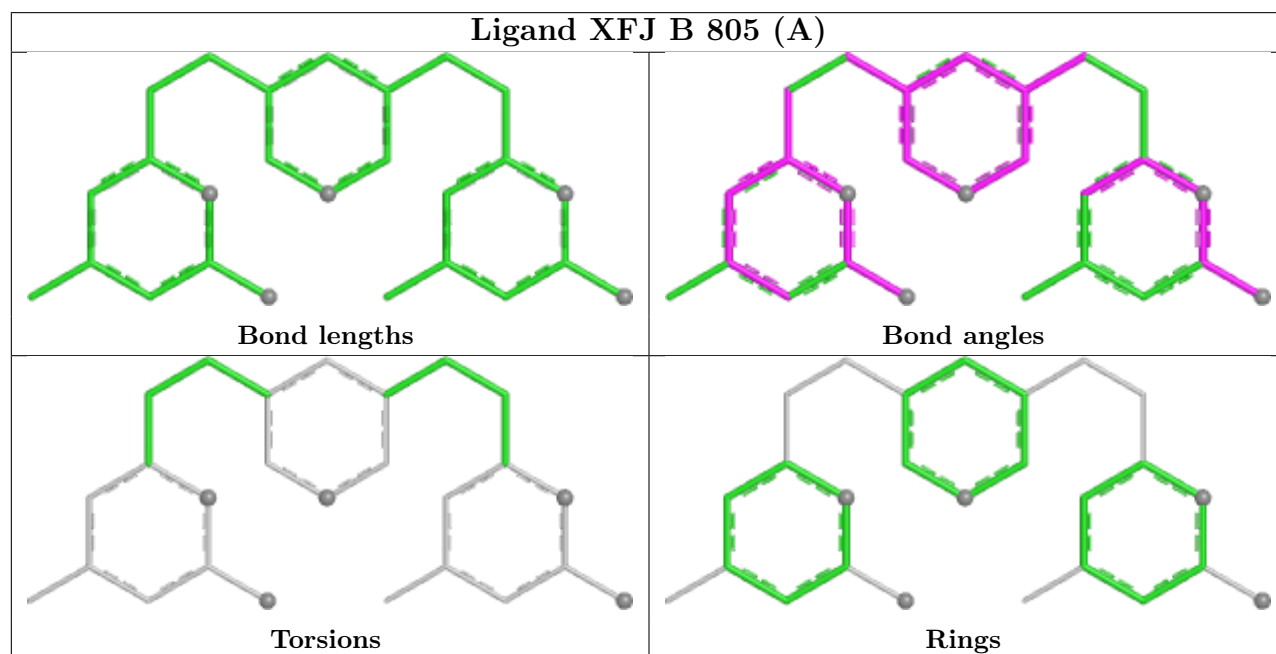
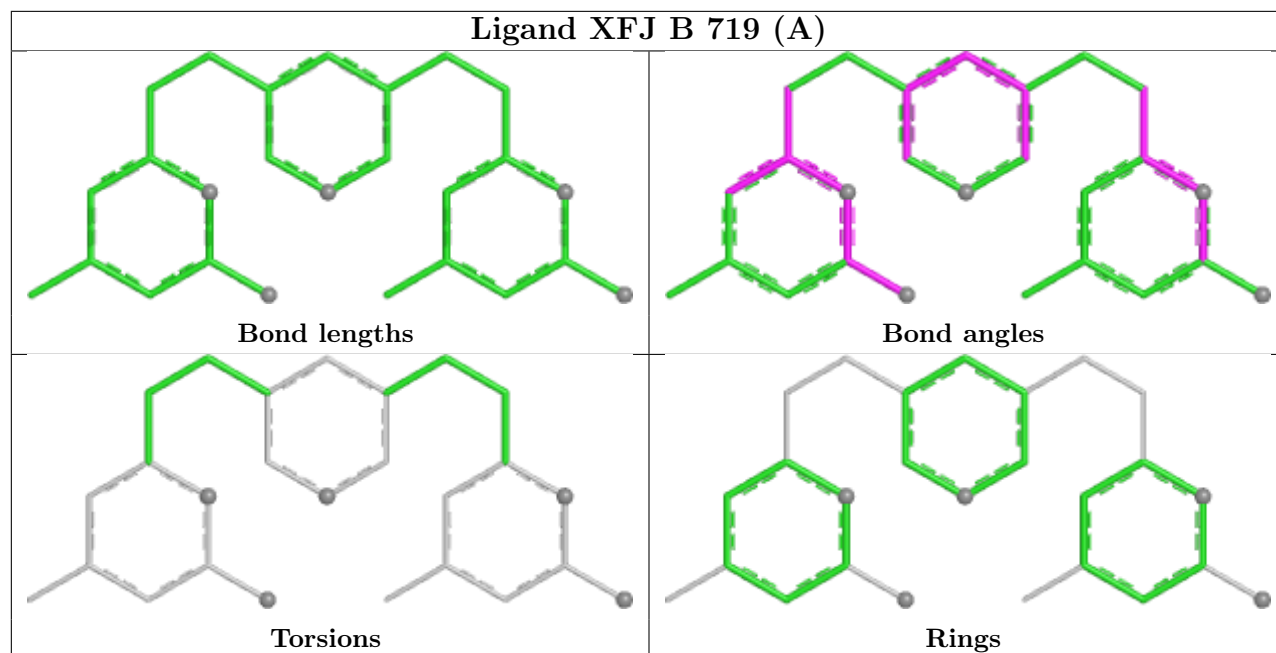
Mol	Chain	Res	Type	Atoms
2	A	750	HEM	C4B-C3B-CAB-CBB
3	B	760[B]	H4B	O10-C10-C9-O9
3	B	760[B]	H4B	C11-C10-C9-O9
3	B	760[B]	H4B	C11-C10-C9-C6
2	B	750	HEM	C2A-CAA-CBA-CGA
2	A	750	HEM	C2A-CAA-CBA-CGA
8	B	870	MTL	O1-C1-C2-C3
8	B	870	MTL	O1-C1-C2-O2

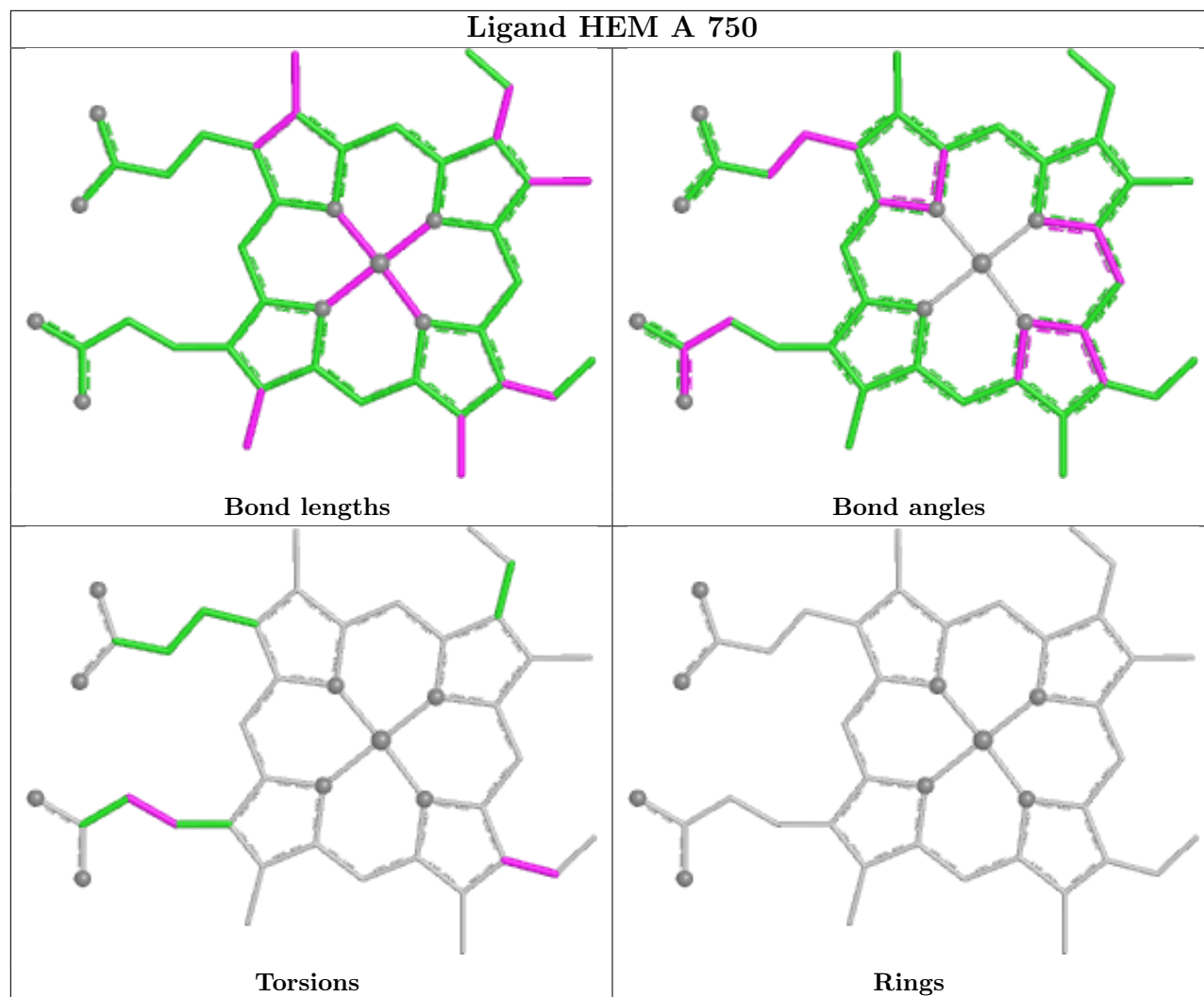
There are no ring outliers.

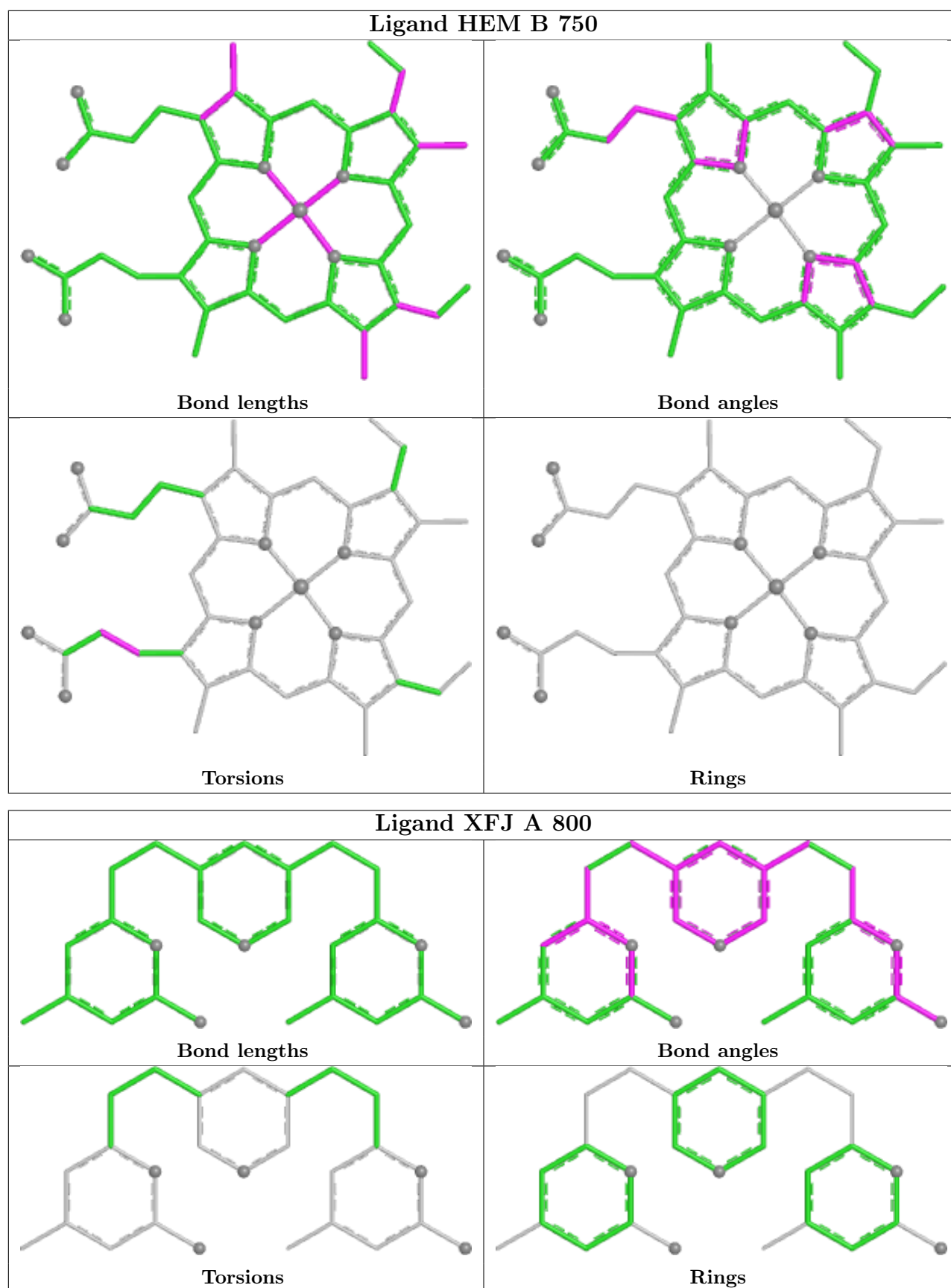
6 monomers are involved in 13 short contacts:

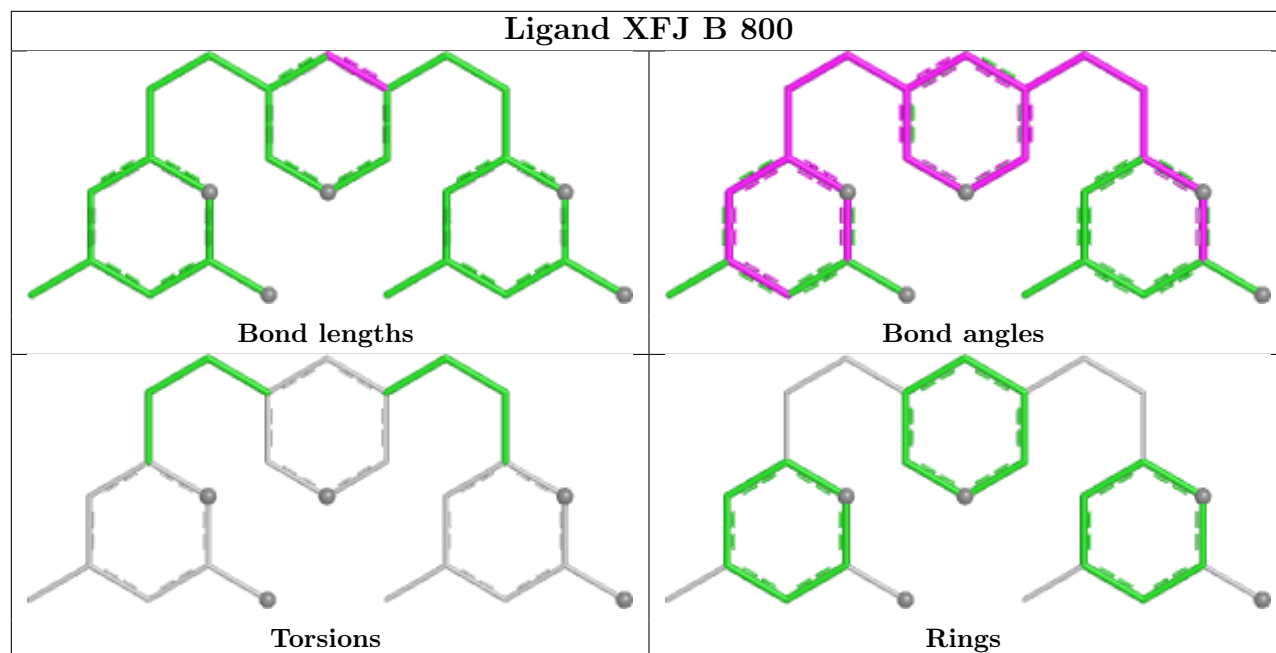
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	719[A]	XFJ	3	0
5	B	805[A]	XFJ	1	0
2	A	750	HEM	3	0
3	B	760[B]	H4B	3	0
2	B	750	HEM	4	0
8	B	870	MTL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	407/422 (96%)	0.32	14 (3%)	48 48	16, 33, 61, 77	5 (1%)
1	B	411/422 (97%)	-0.03	12 (2%)	53 53	12, 25, 47, 66	11 (2%)
All	All	818/844 (96%)	0.14	26 (3%)	50 50	12, 29, 57, 77	16 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	6.4
1	A	322	LEU	4.5
1	A	716	TRP	4.4
1	A	715	VAL	4.3
1	B	322	LEU	4.2
1	B	321	THR	4.2
1	A	338	PRO	4.0
1	A	300	PHE	3.9
1	A	713	THR	3.7
1	A	321	THR	3.7
1	A	355	PHE	3.4
1	B	350	THR	3.4
1	A	350	THR	3.3
1	B	338	PRO	3.2
1	B	718	GLY	3.2
1	B	352	ASP	3.1
1	A	299	ARG	2.9
1	B	389	GLU	2.8
1	B	300	PHE	2.7
1	A	552	ASP	2.6
1	A	330	ILE	2.5
1	A	506	ILE	2.4
1	B	355	PHE	2.3
1	B	602[A]	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	667	ARG	2.2
1	A	507	GLN	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

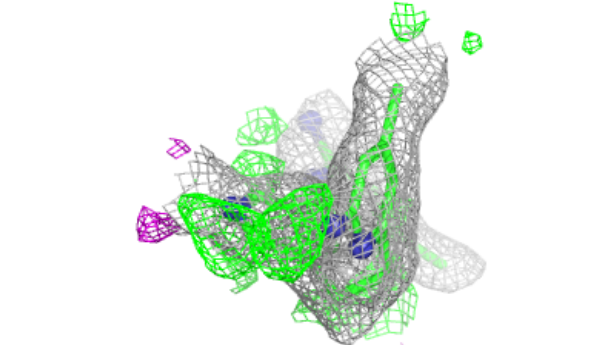
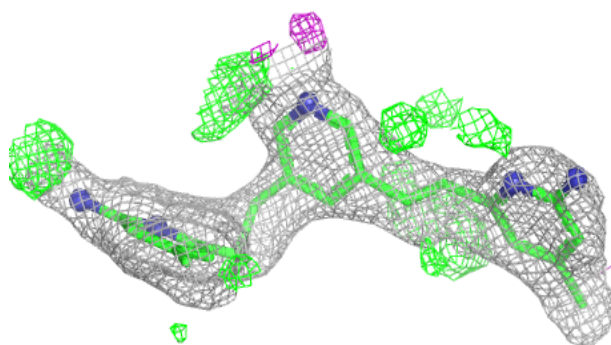
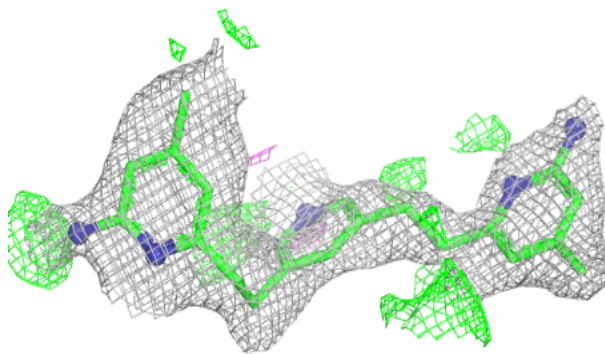
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	H4B	B	760[B]	17/17	0.63	0.19	17,19,21,23	17
3	H4B	A	760[B]	17/17	0.80	0.20	43,45,51,52	12
5	XFJ	B	719[A]	26/26	0.83	0.12	14,25,32,33	26
8	MTL	B	870	12/12	0.86	0.11	25,34,36,36	0
5	XFJ	B	805[A]	26/26	0.89	0.09	7,19,28,28	26
4	ACT	B	860	4/4	0.92	0.11	28,32,33,34	0
6	CL	B	910	1/1	0.94	0.09	31,31,31,31	0
5	XFJ	B	800	26/26	0.94	0.06	12,18,21,25	0
5	XFJ	A	800	26/26	0.95	0.06	13,18,22,23	0
4	ACT	A	860	4/4	0.96	0.09	38,39,40,41	0
7	ZN	A	900	1/1	0.97	0.04	25,25,25,25	0
7	ZN	A	901	1/1	0.97	0.04	22,22,22,22	1
7	ZN	A	719	1/1	0.97	0.04	23,23,23,23	1
6	CL	A	910	1/1	0.97	0.05	29,29,29,29	0
2	HEM	A	750	43/43	0.98	0.07	18,21,32,39	0
2	HEM	B	750	43/43	0.98	0.06	14,18,32,40	0

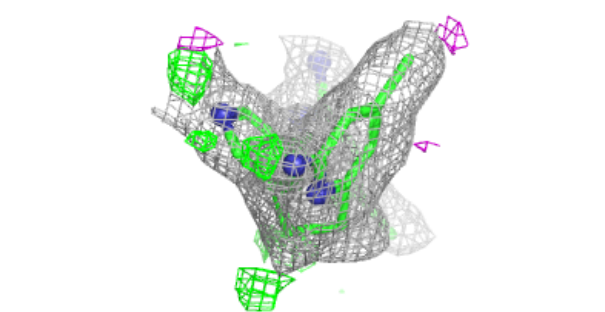
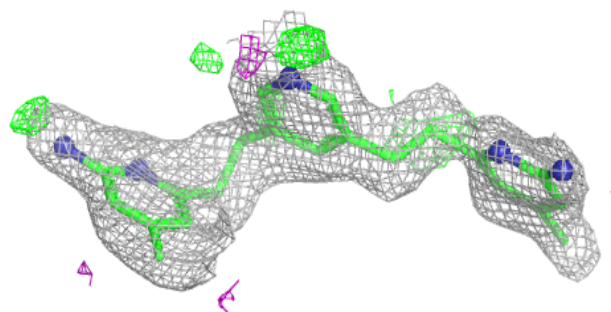
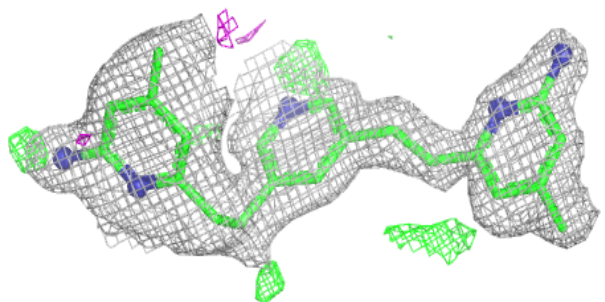
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

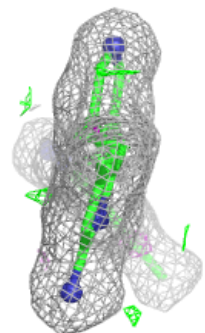
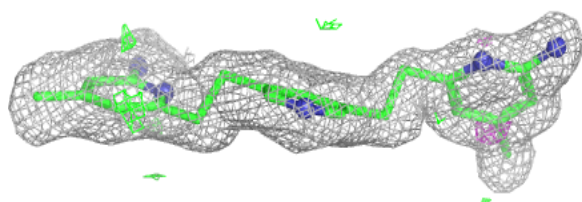
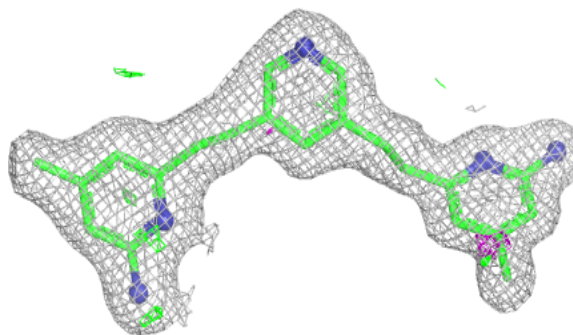
**Electron density around XFJ B 805 (A):**

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

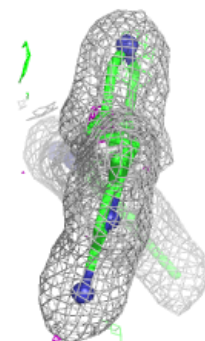
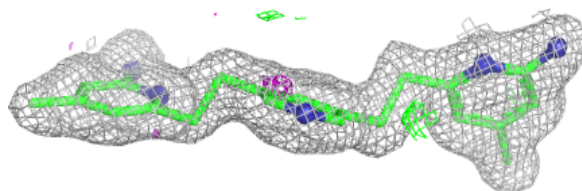
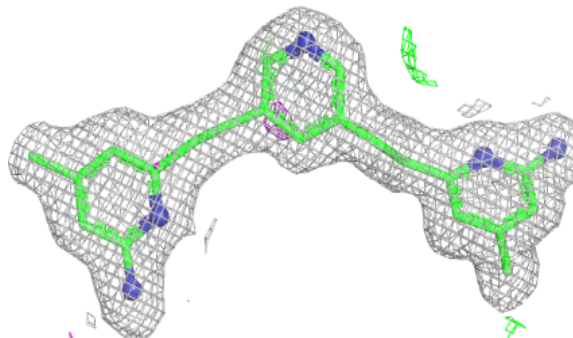


Electron density around XFJ B 800:

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

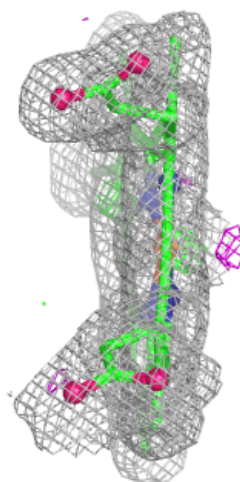
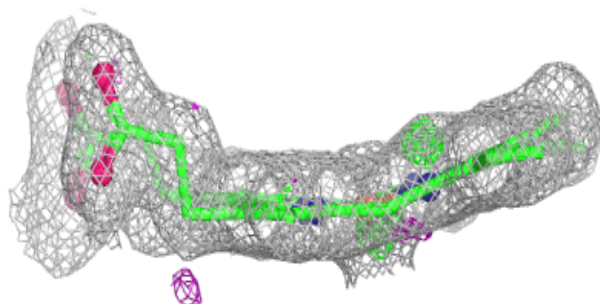
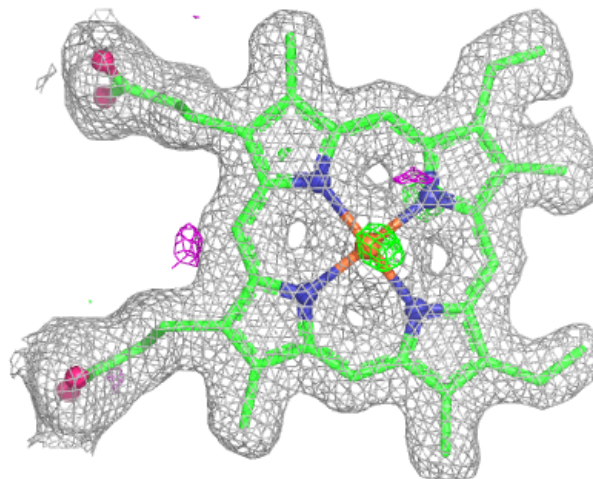
**Electron density around XFJ A 800:**

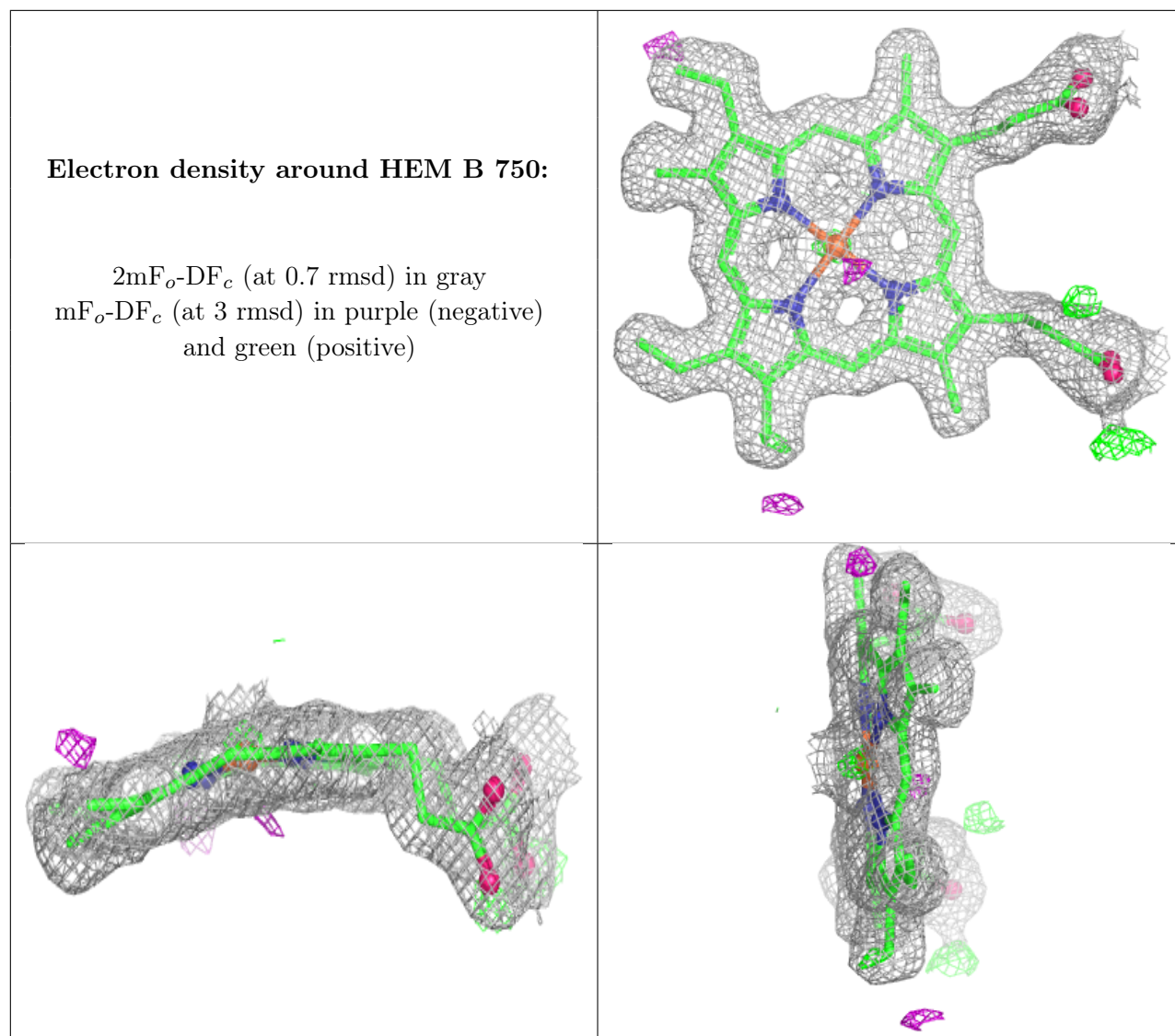
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.