



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:47 am BST

PDB ID : 3N60
Title : Structure of neuronal nitric oxide synthase heme domain in complex with 6,6'-(2,2'-(5-amino-1,3-phenylene)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 : 1.98 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

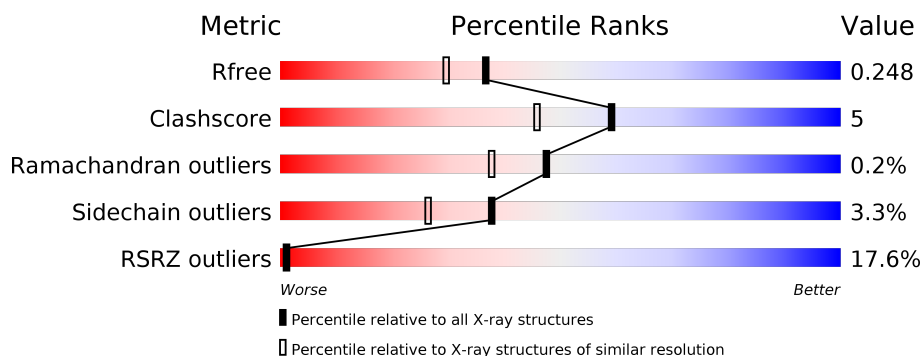
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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>23%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• •</div> </div> </div>
1	B	422	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7150 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.

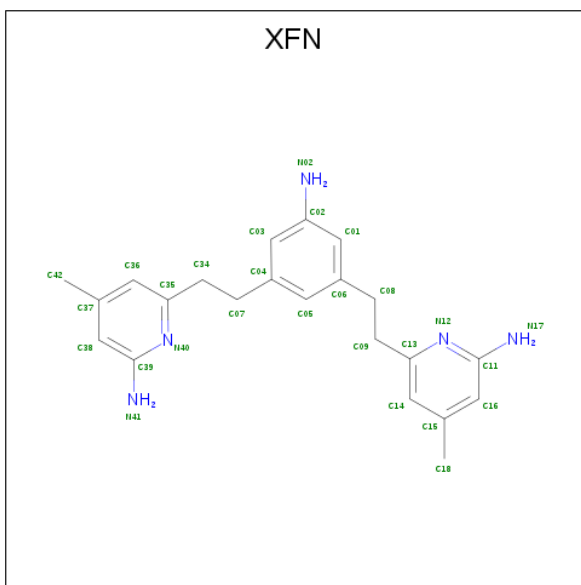
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	574	610	21			

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



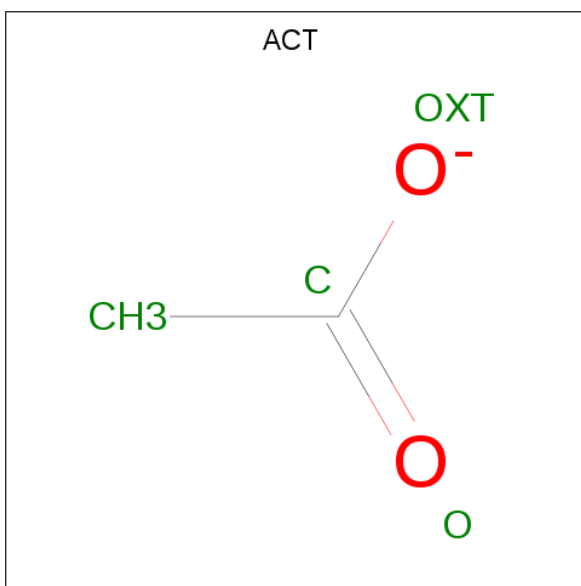
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6,6'-[(5-aminobenzene-1,3-diyl)diethane-2,1-diyl]bis(4-methylpyridin-2-amine) (three-letter code: XFN) (formula: $C_{22}H_{27}N_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 27 22 5	0	0
3	B	1	Total C N 27 22 5	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

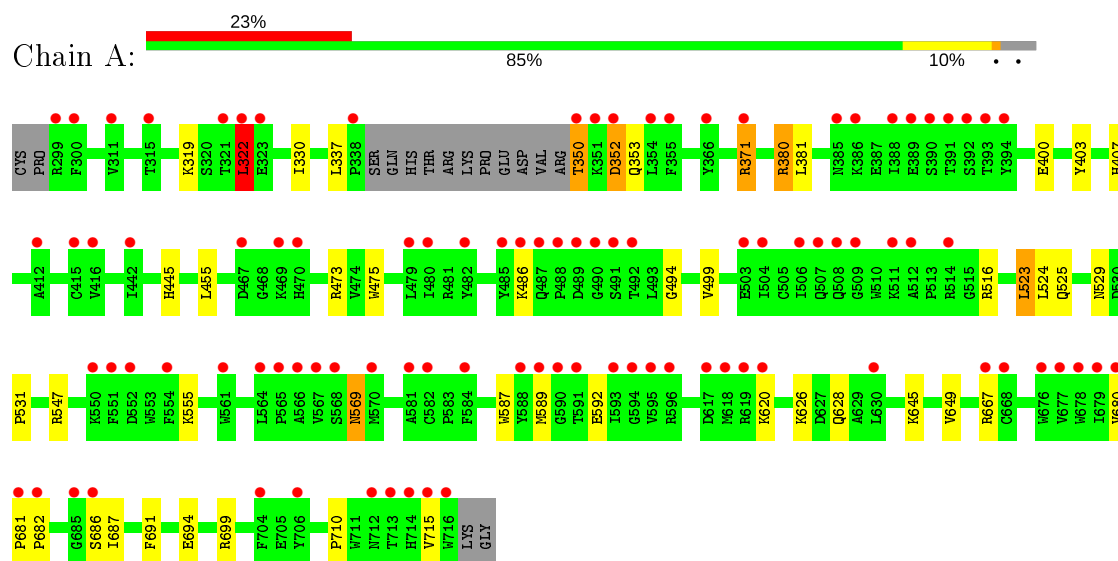
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	139	Total 139	O 139	0	0
7	B	198	Total 198	O 198	0	0

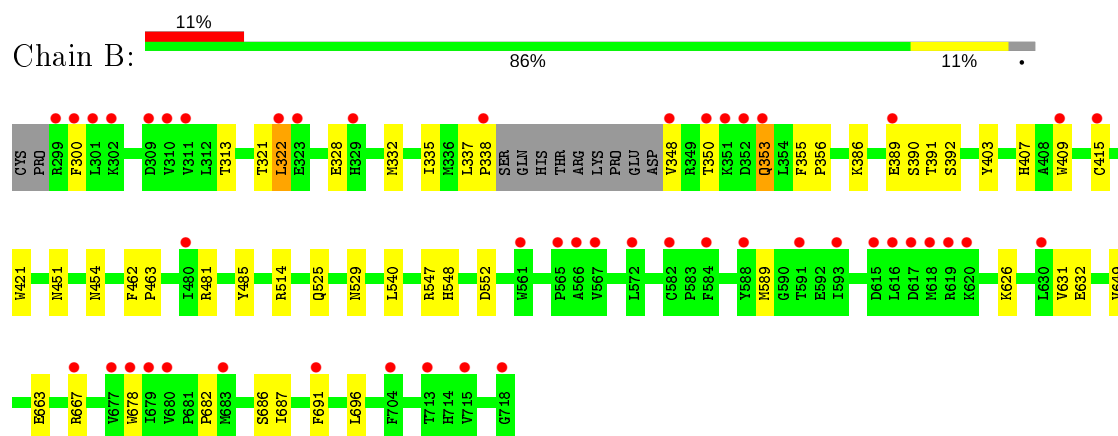
3 Residue-property plots [i](#)

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	51.86Å 111.17Å 164.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.63 – 1.98 36.94 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.63-1.98) 99.8 (36.94-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.191 , 0.232 0.207 , 0.248	Depositor DCC
R_{free} test set	3286 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7150	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, HEM, ZN, CL, XFN

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	0.68	0/3406	0.70	0/4621
1	B	0.74	0/3438	0.72	0/4661
All	All	0.71	0/6844	0.71	0/9282

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	3313	0	3221	36	0
1	B	3345	0	3259	32	0
2	A	43	0	30	1	0
2	B	43	0	30	4	0
3	A	27	0	27	1	0
3	B	27	0	27	1	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	3	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	139	0	0	1	0
7	B	198	0	0	1	0
All	All	7150	0	6600	63	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 (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.25	1.00
1:A:371:ARG:CG	1:A:371:ARG:HH21	1.83	0.90
1:A:371:ARG:HG2	1:A:371:ARG:NH2	1.88	0.85
1:A:350:THR:N	1:A:353:GLN:HE21	1.77	0.83
1:B:332:MET:HE3	1:B:338:PRO:HB3	1.74	0.69
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.13	0.64
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.52	0.63
1:B:332:MET:CE	1:B:338:PRO:HB3	2.28	0.62
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.81	0.62
1:A:486:LYS:HE2	1:A:499:VAL:HG11	1.82	0.61
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.83	0.60
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.82	0.60
1:A:322:LEU:HD12	1:A:699:ARG:HB3	1.88	0.56
1:B:328:GLU:H	1:B:328:GLU:CD	2.09	0.56
1:A:682:PRO:HB2	1:B:686:SER:HB2	1.87	0.56
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.55
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.37	0.54
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.90	0.53
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.91	0.53
1:A:525:GLN:HG3	1:A:529:ASN:O	2.10	0.52
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.92	0.51
1:A:352:ASP:N	1:A:352:ASP:OD2	2.43	0.51
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.92	0.50
2:B:750:HEM:CGA	2:B:750:HEM:HMA2	2.41	0.50
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.27	0.50
1:B:386:LYS:O	1:B:389:GLU:HG2	2.12	0.49
1:A:686:SER:HB2	1:B:682:PRO:HB2	1.93	0.49
1:A:589:MET:HA	1:A:649:VAL:O	2.12	0.49
1:A:686:SER:HA	1:A:691:PHE:CG	2.49	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.02	0.47
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.45	0.47
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.50	0.47
1:B:589:MET:HA	1:B:649:VAL:O	2.15	0.47
1:A:569:ASN:H	1:A:569:ASN:HD22	1.63	0.46
1:B:415:CYS:HB2	2:B:750:HEM:ND	2.31	0.45
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.81	0.45
1:B:678:TRP:CZ3	3:B:800:XFN:H08	2.51	0.45
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.17	0.45
1:B:451:ASN:HB3	1:B:454:ASN:O	2.17	0.45
1:A:524:LEU:O	1:A:531:PRO:HA	2.17	0.44
1:A:699:ARG:HD2	7:A:1105:HOH:O	2.17	0.44
1:A:350:THR:N	1:A:353:GLN:NE2	2.57	0.44
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.00	0.43
1:B:389:GLU:HG3	1:B:390:SER:N	2.32	0.43
1:B:525:GLN:HG3	1:B:529:ASN:O	2.18	0.43
1:A:494:GLY:HA2	1:A:516:ARG:O	2.18	0.43
1:B:391:THR:O	1:B:392:SER:HB2	2.19	0.43
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.50	0.42
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.53	0.42
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.92	0.41
1:A:687:ILE:HD12	1:B:626:LYS:HB3	2.02	0.41
1:A:592:GLU:OE1	3:A:800:XFN:N40	2.53	0.41
1:B:686:SER:HA	1:B:691:PHE:CG	2.55	0.41
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.51	0.41
1:B:454:ASN:ND2	7:B:1301:HOH:O	2.54	0.41
2:B:750:HEM:HBA2	2:B:750:HEM:CMA	2.50	0.41
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	0.41
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.56	0.40
1:B:300:PHE:HB3	1:B:313:THR:CG2	2.51	0.40
1:B:321:THR:O	1:B:322:LEU:O	2.39	0.40
1:B:353:GLN:HG2	1:B:353:GLN:H	1.66	0.40
1:B:355:PHE:N	1:B:356:PRO:HD2	2.37	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%)	390 (97%)	12 (3%)	1 (0%)	47	38
1	B	407/422 (96%)	396 (97%)	10 (2%)	1 (0%)	47	38
All	All	810/844 (96%)	786 (97%)	22 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	LEU
1	A	322	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/377 (96%)	347 (96%)	16 (4%)	28	16
1	B	366/377 (97%)	358 (98%)	8 (2%)	52	46
All	All	729/754 (97%)	705 (97%)	24 (3%)	38	26

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	322	LEU
1	A	337	LEU
1	A	350	THR
1	A	352	ASP
1	A	371	ARG
1	A	380	ARG
1	A	381	LEU
1	A	523	LEU
1	A	547	ARG

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Mol	Chain	Res	Type
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	667	ARG
1	A	715	VAL
1	B	337	LEU
1	B	348	VAL
1	B	350	THR
1	B	353	GLN
1	B	481	ARG
1	B	540	LEU
1	B	547	ARG
1	B	552	ASP

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

Mol	Chain	Res	Type
1	A	395	GLN
1	A	454	ASN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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
3	XFN	A	800	-	29,29,29	1.01	1 (3%)	38,40,40	2.36	12 (31%)
3	XFN	B	800	-	29,29,29	0.95	0	38,40,40	2.08	10 (26%)
2	HEM	A	750	1	27,50,50	2.00	9 (33%)	17,82,82	2.40	8 (47%)
2	HEM	B	750	1	27,50,50	2.18	9 (33%)	17,82,82	1.46	3 (17%)
4	ACT	B	860	-	1,3,3	1.89	0	0,3,3	0.00	-
4	ACT	A	860	-	1,3,3	1.62	0	0,3,3	0.00	-

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
3	XFN	A	800	-	-	4/10/10/10	0/3/3/3
2	HEM	A	750	1	-	2/6/54/54	-
3	XFN	B	800	-	-	4/10/10/10	0/3/3/3
2	HEM	B	750	1	-	3/6/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	4.60	1.51	1.37
2	B	750	HEM	C3B-C2B	-4.56	1.34	1.40
2	A	750	HEM	C3D-C2D	4.47	1.50	1.37
2	B	750	HEM	C3C-C2C	-4.46	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-CAB	3.77	1.55	1.47
2	B	750	HEM	C3C-CAC	3.34	1.54	1.47
2	A	750	HEM	C3B-C2B	-3.30	1.35	1.40
2	B	750	HEM	C3B-CAB	3.23	1.54	1.47
2	A	750	HEM	C3C-C2C	-3.15	1.36	1.40
2	A	750	HEM	C3C-CAC	3.09	1.54	1.47
2	A	750	HEM	CAA-C2A	2.91	1.56	1.52
3	A	800	XFN	C05-C04	2.79	1.44	1.39
2	B	750	HEM	CMA-C3A	2.75	1.57	1.51
2	B	750	HEM	CAD-C3D	2.60	1.56	1.52
2	B	750	HEM	CAA-C2A	2.54	1.55	1.52
2	A	750	HEM	CMA-C3A	2.28	1.56	1.51
2	B	750	HEM	CMD-C2D	2.20	1.56	1.51
2	A	750	HEM	CMC-C2C	2.08	1.56	1.51
2	A	750	HEM	CMD-C2D	2.07	1.55	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	XFN	C11-N12-C13	7.59	123.85	118.10
3	B	800	XFN	C11-N12-C13	7.15	123.52	118.10
3	A	800	XFN	C39-N40-C35	4.86	121.78	118.10
3	B	800	XFN	C39-N40-C35	4.83	121.76	118.10
3	A	800	XFN	C15-C14-C13	-4.58	117.32	120.32
2	A	750	HEM	CBD-CAD-C3D	-3.98	105.15	112.48
3	A	800	XFN	C36-C35-N40	-3.87	118.80	122.90
2	A	750	HEM	CMA-C3A-C4A	-3.79	122.64	128.46
3	A	800	XFN	C09-C13-C14	3.74	126.16	121.22
2	A	750	HEM	CMC-C2C-C3C	3.68	131.56	124.68
3	A	800	XFN	C34-C35-N40	3.45	121.09	115.95
3	B	800	XFN	C36-C35-N40	-3.43	119.27	122.90
3	A	800	XFN	C14-C13-N12	-3.35	119.35	122.90
2	A	750	HEM	CBA-CAA-C2A	3.25	118.47	112.49
3	A	800	XFN	C07-C04-C03	-3.24	115.23	120.54
2	A	750	HEM	C4C-C3C-C2C	3.19	109.12	106.90
3	A	800	XFN	C07-C04-C05	3.15	125.71	120.54
2	A	750	HEM	C1D-C2D-C3D	-3.11	104.83	107.00
3	B	800	XFN	C34-C35-N40	2.97	120.37	115.95
2	B	750	HEM	CMA-C3A-C4A	-2.95	123.93	128.46
3	B	800	XFN	C14-C13-N12	-2.90	119.82	122.90
3	B	800	XFN	C15-C14-C13	-2.87	118.44	120.32
2	B	750	HEM	CMA-C3A-C2A	2.77	130.17	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	XFN	C16-C15-C14	2.77	121.39	118.09
3	A	800	XFN	N41-C39-N40	2.68	120.73	116.49
3	A	800	XFN	C18-C15-C16	-2.63	117.04	120.94
2	B	750	HEM	CBD-CAD-C3D	-2.52	107.83	112.48
3	B	800	XFN	C09-C13-C14	2.47	124.49	121.22
3	B	800	XFN	N41-C39-N40	2.40	120.28	116.49
3	B	800	XFN	C07-C04-C05	2.22	124.17	120.54
2	A	750	HEM	CMA-C3A-C2A	2.12	128.95	124.94
2	A	750	HEM	C4A-C3A-C2A	2.04	108.41	107.00
3	B	800	XFN	N17-C11-N12	2.01	119.67	116.49

There are no chirality outliers.

All (13) 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	C2A-CAA-CBA-CGA
3	A	800	XFN	C01-C06-C08-C09
3	A	800	XFN	C05-C06-C08-C09
3	B	800	XFN	C05-C04-C07-C34
3	B	800	XFN	C01-C06-C08-C09
3	B	800	XFN	C03-C04-C07-C34
3	B	800	XFN	C05-C06-C08-C09
3	A	800	XFN	C05-C04-C07-C34
3	A	800	XFN	C03-C04-C07-C34

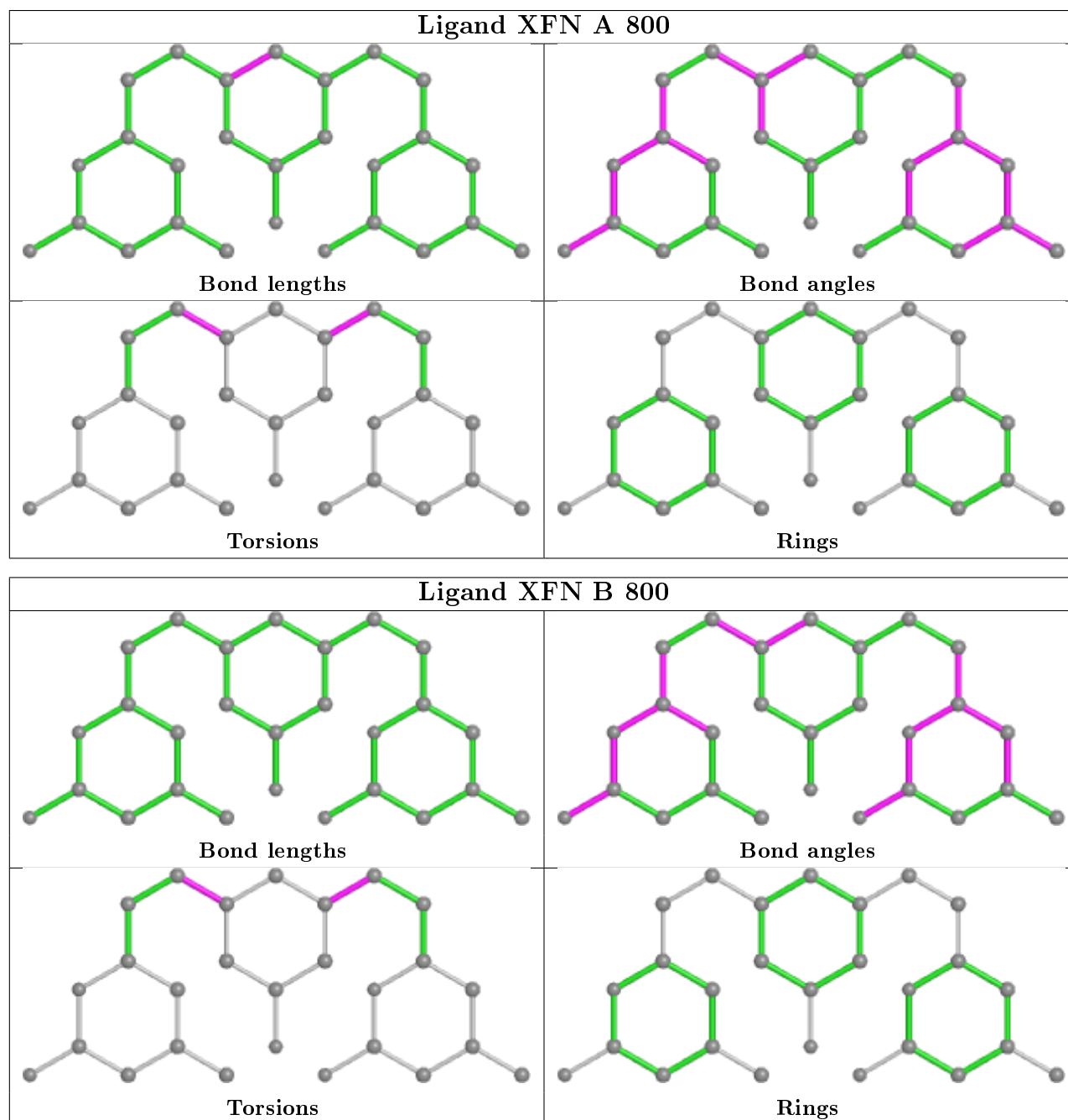
There are no ring outliers.

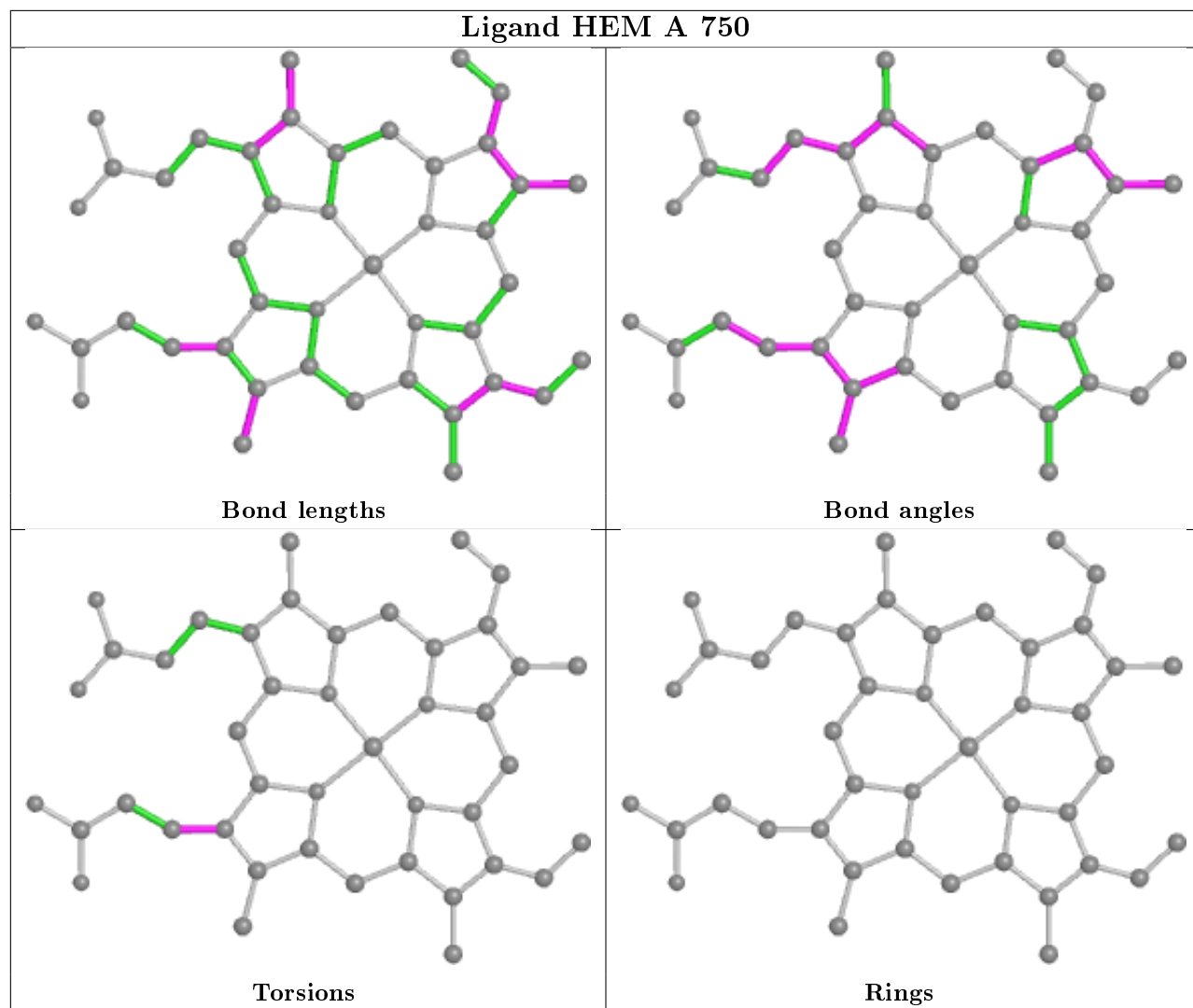
4 monomers are involved in 7 short contacts:

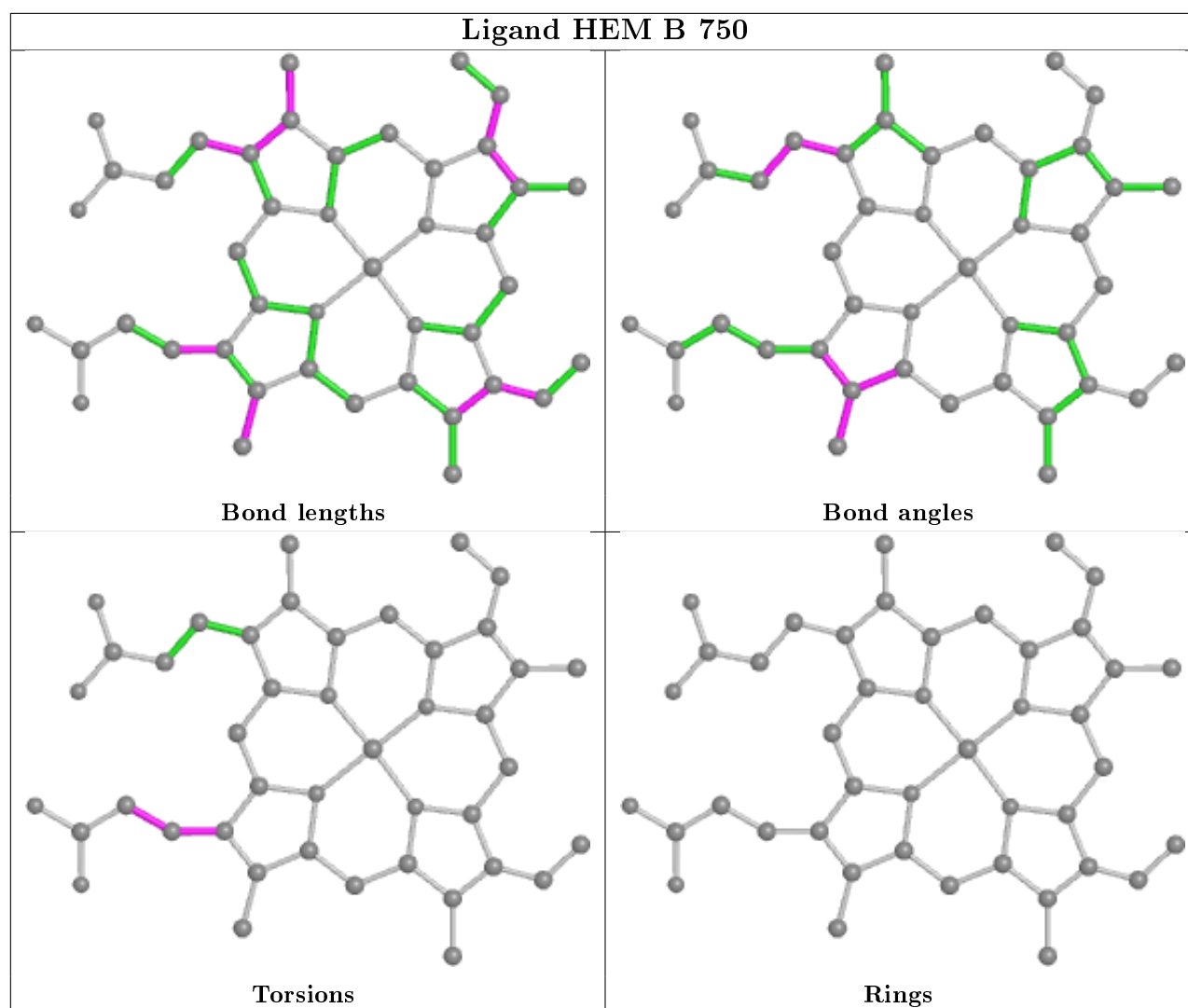
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	XFN	1	0
3	B	800	XFN	1	0
2	A	750	HEM	1	0
2	B	750	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/422 (96%)	1.17	96 (23%) 0 0	31, 56, 96, 124	0
1	B	411/422 (97%)	0.68	48 (11%) 4 5	31, 45, 71, 87	0
All	All	818/844 (96%)	0.92	144 (17%) 1 1	31, 50, 89, 124	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.3
1	A	716	TRP	8.5
1	B	348	VAL	6.4
1	A	300	PHE	6.2
1	B	718	GLY	5.9
1	A	715	VAL	5.8
1	A	355	PHE	5.8
1	A	488	PRO	5.8
1	A	322	LEU	5.0
1	B	619	ARG	4.9
1	A	567	VAL	4.6
1	A	479	LEU	4.5
1	A	352	ASP	4.4
1	A	338	PRO	4.4
1	A	489	ASP	4.4
1	A	351	LYS	4.2
1	A	486	LYS	4.2
1	A	593	ILE	4.2
1	A	491	SER	4.0
1	A	485	TYR	4.0
1	A	678	TRP	4.0
1	A	490	GLY	4.0
1	A	591	THR	4.0
1	B	616	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	554	PHE	3.8
1	A	311	VAL	3.8
1	A	712	ASN	3.7
1	A	713	THR	3.7
1	A	619	ARG	3.7
1	A	584	PHE	3.7
1	B	338	PRO	3.7
1	A	415	CYS	3.6
1	A	667	ARG	3.6
1	B	567	VAL	3.6
1	A	507	GLN	3.6
1	A	679	ILE	3.5
1	A	514	ARG	3.5
1	A	390	SER	3.5
1	B	620	LYS	3.4
1	A	487	GLN	3.4
1	A	677	VAL	3.4
1	B	310	VAL	3.3
1	A	680	VAL	3.3
1	B	350	THR	3.2
1	A	389	GLU	3.2
1	A	566	ALA	3.2
1	A	676	TRP	3.2
1	A	508	GLN	3.2
1	A	388	ILE	3.2
1	A	511	LYS	3.2
1	A	714	HIS	3.1
1	A	681	PRO	3.1
1	A	299	ARG	3.1
1	A	685	GLY	3.1
1	B	351	LYS	3.1
1	A	321	THR	3.1
1	B	299	ARG	3.0
1	B	667	ARG	3.0
1	A	492	THR	3.0
1	A	565	PRO	3.0
1	A	682	PRO	3.0
1	B	680	VAL	3.0
1	A	354	LEU	2.9
1	A	350	THR	2.9
1	A	704	PHE	2.9
1	A	503	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	551	PHE	2.9
1	A	392	SER	2.9
1	B	591	THR	2.9
1	B	311	VAL	2.9
1	B	715	VAL	2.9
1	B	677	VAL	2.8
1	A	594	GLY	2.8
1	A	393	THR	2.8
1	A	588	TYR	2.8
1	B	566	ALA	2.7
1	A	385	ASN	2.7
1	A	506	ILE	2.7
1	A	416	VAL	2.7
1	A	509	GLY	2.6
1	B	691	PHE	2.6
1	B	322	LEU	2.6
1	A	596	ARG	2.6
1	A	595	VAL	2.6
1	B	309	ASP	2.6
1	B	561	TRP	2.6
1	A	686	SER	2.6
1	A	391	THR	2.6
1	B	679	ILE	2.5
1	B	352	ASP	2.5
1	B	678	TRP	2.5
1	B	301	LEU	2.5
1	B	617	ASP	2.5
1	B	409	TRP	2.5
1	B	584	PHE	2.5
1	B	565	PRO	2.4
1	A	480	ILE	2.4
1	A	467	ASP	2.4
1	B	704	PHE	2.4
1	A	568	SER	2.4
1	A	706	TYR	2.4
1	A	668	CYS	2.4
1	B	593	ILE	2.4
1	A	366	TYR	2.4
1	A	323	GLU	2.4
1	A	590	GLY	2.4
1	B	582	CYS	2.4
1	B	630	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	550	LYS	2.3
1	B	713	THR	2.3
1	A	442	ILE	2.3
1	B	615	ASP	2.3
1	B	588	TYR	2.3
1	A	561	TRP	2.2
1	A	630	LEU	2.2
1	A	589	MET	2.2
1	B	618	MET	2.2
1	B	572	LEU	2.2
1	B	323	GLU	2.2
1	A	581	ALA	2.2
1	A	564	LEU	2.1
1	A	386	LYS	2.1
1	A	582	CYS	2.1
1	A	371	ARG	2.1
1	A	482	TYR	2.1
1	B	389	GLU	2.1
1	A	315	THR	2.1
1	A	469	LYS	2.1
1	A	412	ALA	2.1
1	B	415	CYS	2.1
1	B	329	HIS	2.1
1	A	512	ALA	2.1
1	A	504	ILE	2.1
1	B	480	ILE	2.1
1	A	570	MET	2.0
1	A	618	MET	2.0
1	A	552	ASP	2.0
1	A	620	LYS	2.0
1	A	617	ASP	2.0
1	B	353	GLN	2.0
1	B	683	MET	2.0
1	A	470	HIS	2.0
1	A	394	TYR	2.0
1	B	302	LYS	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 carbohydrates in this entry.

6.4 Ligands ⓘ

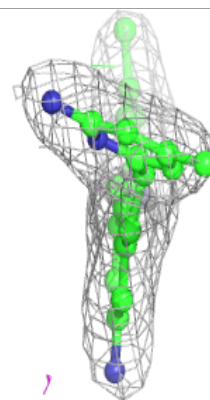
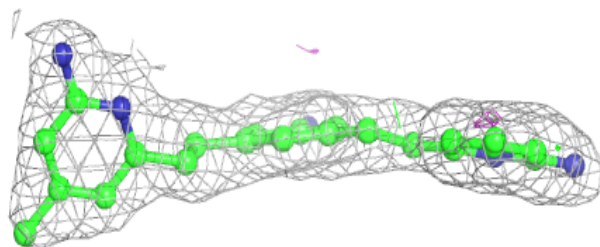
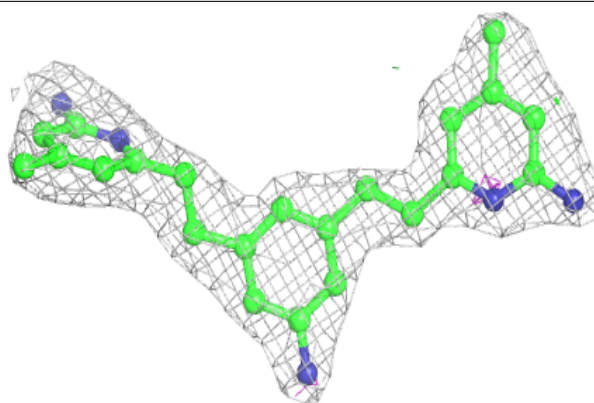
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	A	860	4/4	0.86	0.40	75,77,77,77	0
4	ACT	B	860	4/4	0.87	0.27	64,67,67,67	0
3	XFN	A	800	27/27	0.90	0.28	36,42,47,47	0
3	XFN	B	800	27/27	0.92	0.23	35,41,44,45	0
2	HEM	A	750	43/43	0.97	0.21	29,33,47,54	0
6	CL	B	930	1/1	0.97	0.28	50,50,50,50	0
2	HEM	B	750	43/43	0.98	0.18	28,35,47,51	0
6	CL	B	910	1/1	0.98	0.13	45,45,45,45	0
6	CL	A	930	1/1	0.98	0.24	49,49,49,49	0
5	ZN	A	719	1/1	0.99	0.13	35,35,35,35	1
6	CL	A	910	1/1	0.99	0.12	45,45,45,45	0
5	ZN	A	901	1/1	0.99	0.12	35,35,35,35	1
5	ZN	A	900	1/1	0.99	0.07	40,40,40,40	0

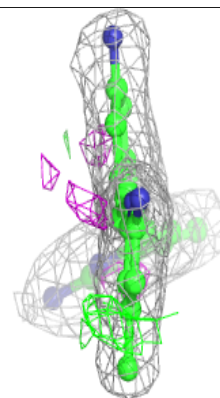
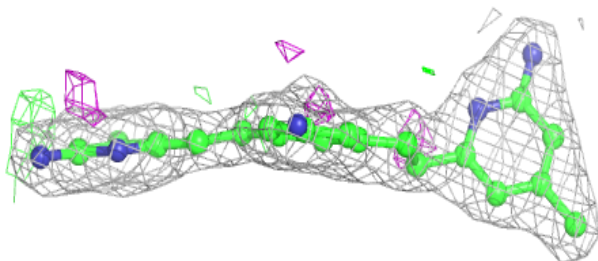
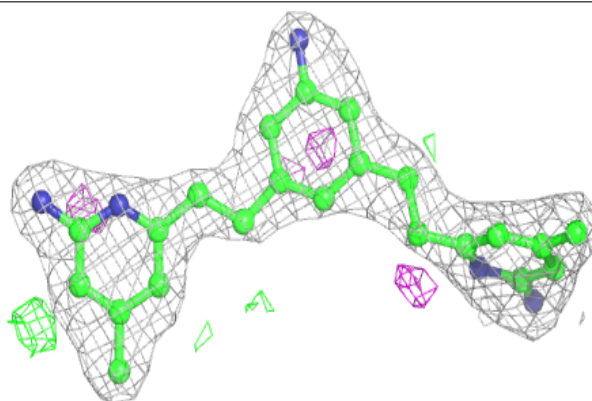
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XFN 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)

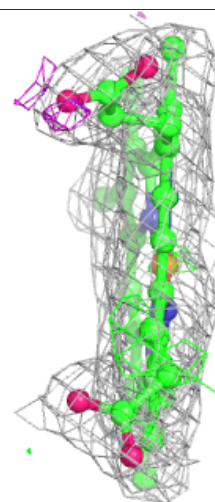
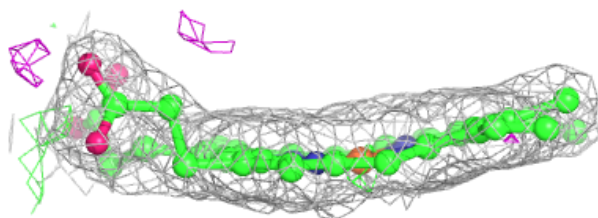
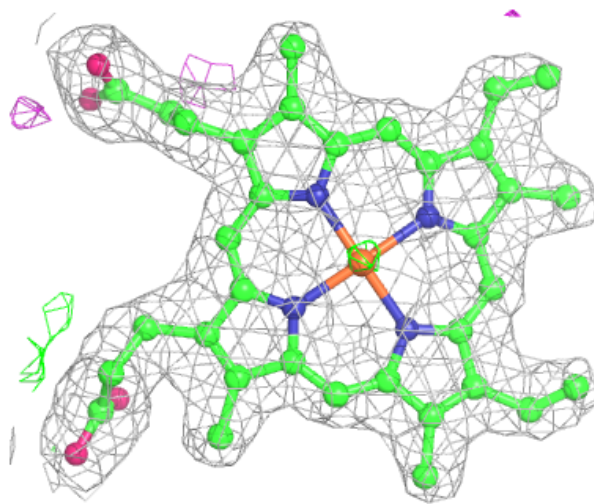
**Electron density around XFN B 800:**

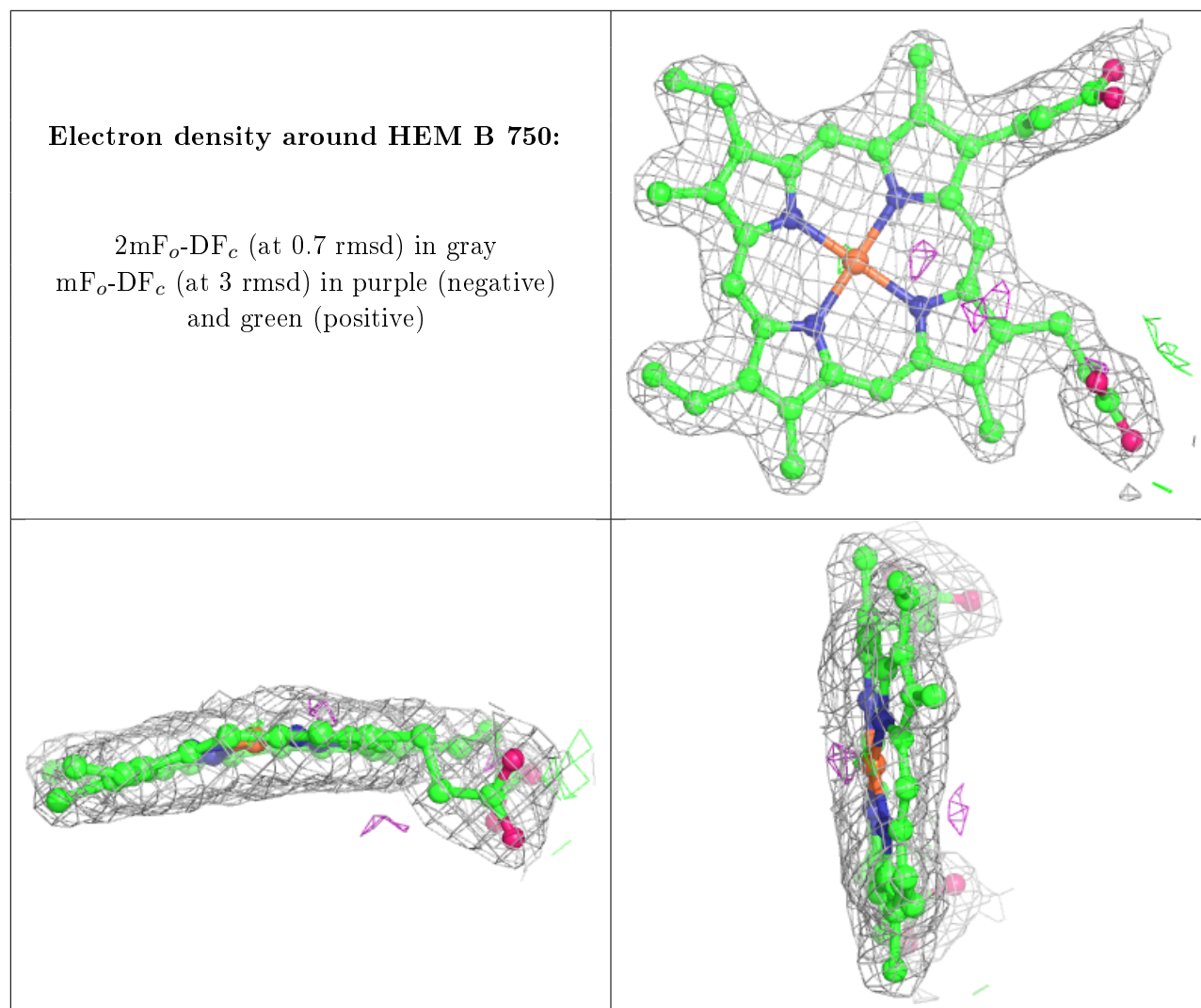
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.