



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:13 PM UTC

PDB ID : 5ADE / pdb_00005ade
Title : Structure of rat neuronal nitric oxide synthase M336V D597N mutant heme domain in complex with 7-((4-Chloro-3-((methylamino)methyl) phenoxy)methyl)quinolin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2015-08-20
Resolution : 2.10 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

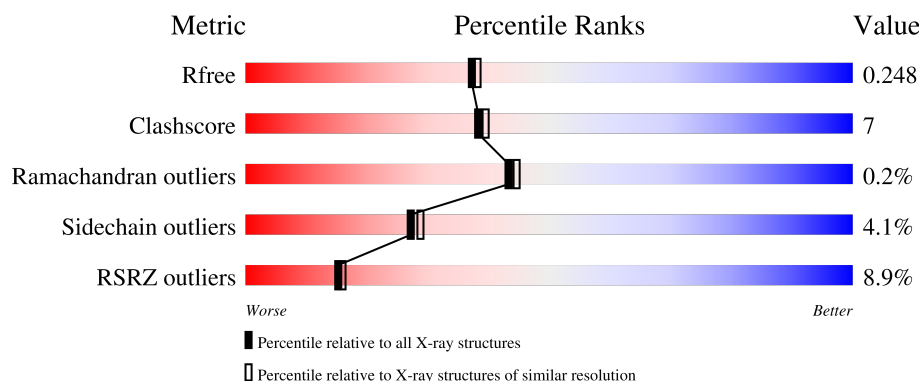
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	11% 73% 22% ..
1	B	422	7% 82% 15% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7089 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

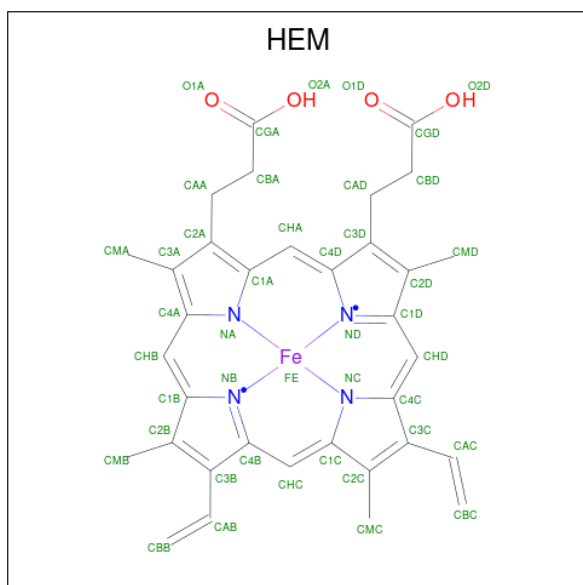
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, BRAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	2	1
			3322	2127	568	606	21			
1	B	411	Total	C	N	O	S	0	3	0
			3356	2148	575	613	20			

There are 4 discrepancies between the modelled and reference sequences:

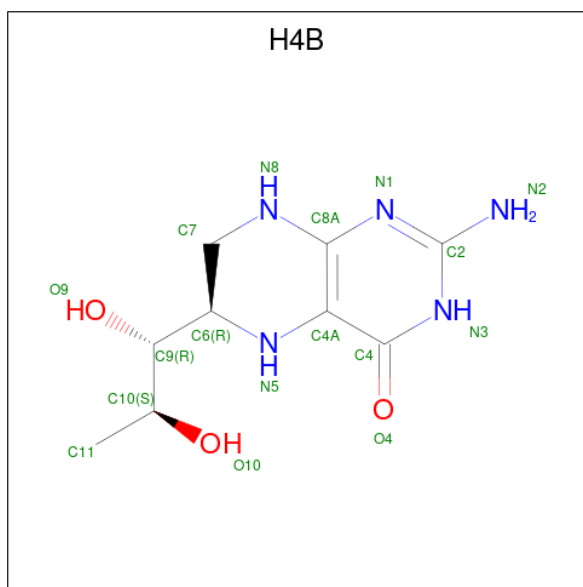
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	engineered mutation	UNP P29476
A	597	ASN	ASP	engineered mutation	UNP P29476
B	336	VAL	MET	engineered mutation	UNP P29476
B	597	ASN	ASP	engineered mutation	UNP P29476

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



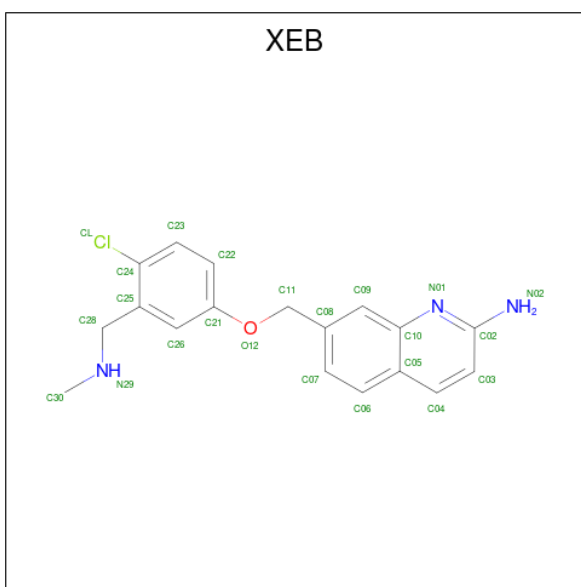
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



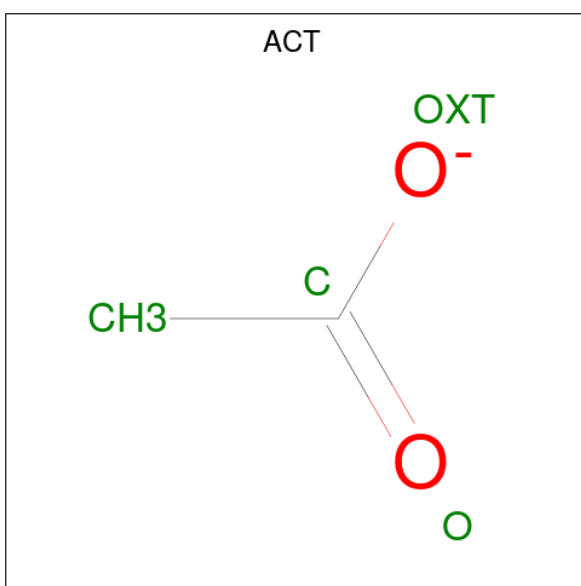
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-[[4-chloranyl-3-(methylaminomethyl)phenoxy]methyl]quinolin-2-amine (CCD ID: XEB) (formula: $C_{18}H_{18}ClN_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0
			23	18	1	3	1	
4	B	1	Total	C	Cl	N	O	0
			23	18	1	3	1	

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

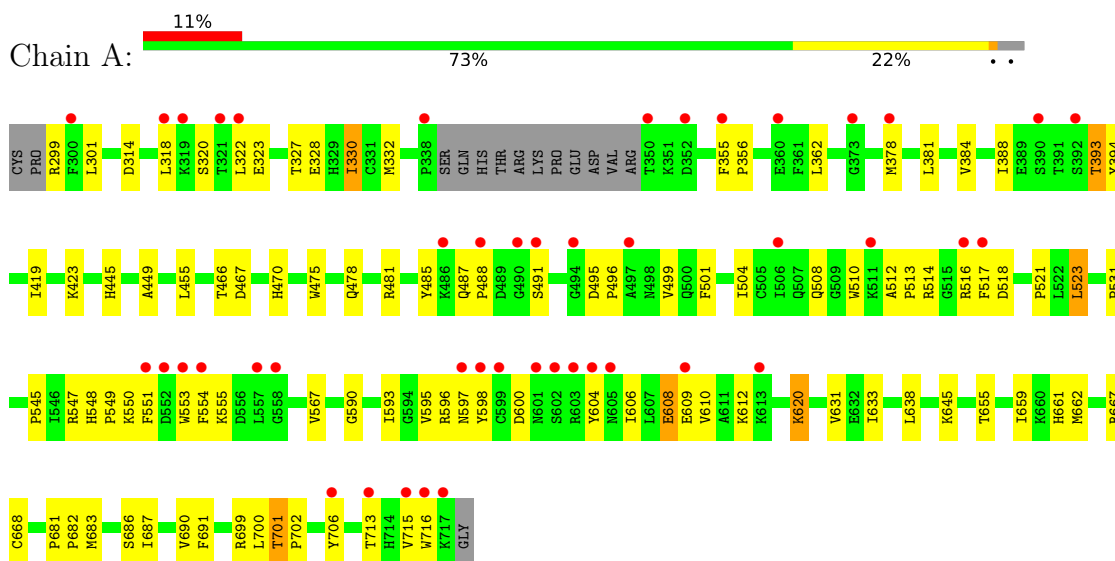
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	113	Total 113	O 113	0	0
7	B	123	Total 123	O 123	0	0

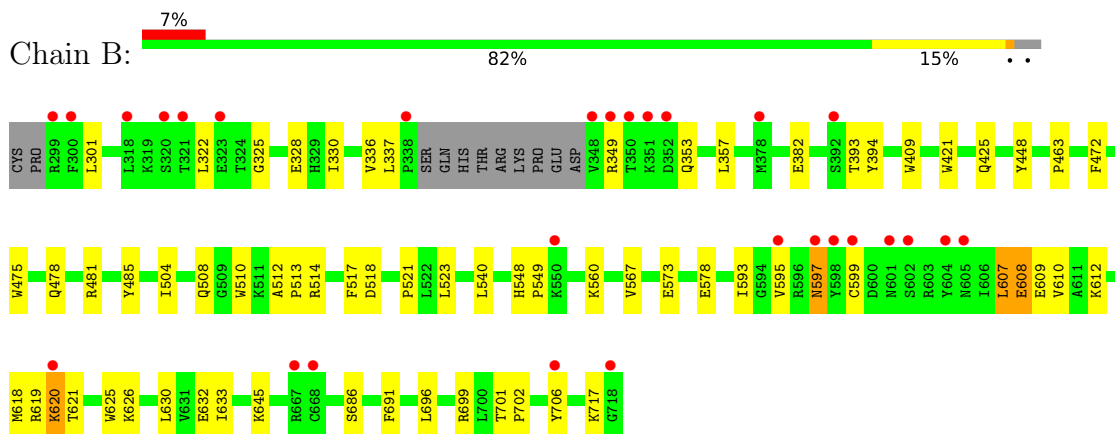
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN



• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.56Å 111.56Å 164.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.78 – 2.10 55.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	64.0 (55.78-2.10) 64.0 (55.78-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.248 0.183 , 0.248	Depositor DCC
R_{free} test set	1796 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7089	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 5.53% 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: H4B, ZN, XEB, 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	0.47	1/3421 (0.0%)	0.86	4/4643 (0.1%)
1	B	0.49	0/3458	0.85	3/4689 (0.1%)
All	All	0.48	1/6879 (0.0%)	0.85	7/9332 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	716	TRP	C-N	-6.78	1.23	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	597	ASN	N-CA-C	5.75	119.39	112.38
1	B	325	GLY	N-CA-C	-5.47	108.18	114.69
1	A	681	PRO	CA-C-N	5.33	126.36	120.45
1	A	681	PRO	C-N-CA	5.33	126.36	120.45
1	B	336	VAL	N-CA-C	5.29	116.06	110.72
1	A	495	ASP	CA-C-N	5.21	125.51	119.47
1	A	495	ASP	C-N-CA	5.21	125.51	119.47

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	3322	0	3234	51	0
1	B	3356	0	3277	38	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	23	0	18	3	0
4	B	23	0	18	5	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	113	0	0	1	0
7	B	123	0	0	0	0
All	All	7089	0	6643	93	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 7.

All (93) 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)
4:B:800:XEB:CL	4:B:800:XEB:N29	2.47	0.83
4:A:800:XEB:CL	4:A:800:XEB:N29	2.53	0.78
1:B:593:ILE:HA	1:B:597:ASN:HB2	1.68	0.76
2:B:750:HEM:HMC2	2:B:750:HEM:HBC2	1.69	0.73
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.70	0.71
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.79	0.65
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.79	0.64
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.82	0.62
1:A:393:THR:OG1	1:A:394:TYR:N	2.31	0.61
1:A:501:PHE:HA	1:A:504:ILE:HD12	1.84	0.59
1:A:598:TYR:HA	1:A:604:TYR:HB2	1.84	0.58
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.86	0.58
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.70	0.57
1:B:607:LEU:HD13	1:B:626:LYS:HG2	1.86	0.56
1:A:596:ARG:NH2	1:A:600:ASP:OD2	2.34	0.55
1:B:567:VAL:HG21	4:B:800:XEB:C07	2.36	0.55
1:A:554:PHE:HB3	7:A:2074:HOH:O	2.08	0.54
1:A:567:VAL:HG21	4:A:800:XEB:C07	2.39	0.53
1:B:393:THR:OG1	1:B:394:TYR:N	2.39	0.53
1:B:593:ILE:HA	1:B:597:ASN:HD22	1.75	0.52
2:B:750:HEM:O1D	4:B:800:XEB:H26	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:750:HEM:HBA2	4:A:800:XEB:H11	1.92	0.52
1:B:595:VAL:HG13	1:B:630:LEU:HD11	1.92	0.52
1:B:620:LYS:HD3	1:B:621:THR:H	1.74	0.52
1:A:299:ARG:HG2	1:A:318:LEU:HD11	1.92	0.51
1:B:504:ILE:O	1:B:508:GLN:HG2	2.10	0.51
1:B:706:TYR:OH	2:B:750:HEM:O1D	2.27	0.51
1:A:631:VAL:HG22	1:A:683:MET:HE1	1.94	0.50
1:A:320:SER:HA	1:A:700:LEU:HD23	1.94	0.50
1:B:463:PRO:HG2	1:B:472:PHE:CZ	2.48	0.49
1:A:513:PRO:HG2	1:A:518:ASP:CG	2.38	0.49
1:A:485:TYR:OH	1:A:518:ASP:OD2	2.24	0.49
1:A:659:ILE:HD11	1:A:690:VAL:HA	1.94	0.49
1:A:667:ARG:NH1	1:A:668[A]:CYS:SG	2.86	0.48
2:B:750:HEM:CBA	4:B:800:XEB:H11	2.44	0.47
1:A:419:ILE:HG13	1:A:661:HIS:HB2	1.96	0.47
1:A:449:ALA:O	1:A:455:LEU:HA	2.15	0.47
1:A:548:HIS:CG	1:A:549:PRO:HD2	2.49	0.47
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.97	0.47
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.96	0.47
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.29	0.46
1:A:595:VAL:HG11	1:A:682:PRO:HB2	1.97	0.46
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	0.45
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.98	0.45
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.51	0.45
1:A:686:SER:HA	1:A:691:PHE:CG	2.51	0.45
1:A:301:LEU:O	1:A:314:ASP:N	2.40	0.45
1:B:608:GLU:H	1:B:608:GLU:HG2	1.34	0.45
1:B:425:GLN:HG2	1:B:448:TYR:CZ	2.51	0.45
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.51	0.45
1:B:701:THR:HA	1:B:702:PRO:C	2.42	0.44
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.52	0.44
1:A:466:THR:OG1	1:A:467:ASP:N	2.50	0.44
1:B:686:SER:HA	1:B:691:PHE:CG	2.53	0.44
1:A:487:GLN:HB3	1:A:488:PRO:HD2	2.00	0.44
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.33	0.44
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.53	0.43
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.32	0.43
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.00	0.43
1:B:517:PHE:CB	1:B:560:LYS:HE2	2.49	0.43
1:A:701:THR:HG23	1:A:702:PRO:HA	2.01	0.43
1:B:517:PHE:HB3	1:B:560:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLU:HG2	1:B:328:GLU:HB3	2.00	0.43
1:A:512:ALA:C	1:A:514:ARG:H	2.26	0.43
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.44	0.42
1:A:322:LEU:HB3	1:A:699:ARG:HE	1.84	0.42
1:A:504:ILE:O	1:A:508:GLN:HG2	2.20	0.42
1:A:687:ILE:HD12	1:B:626:LYS:HB3	2.01	0.42
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.54	0.42
1:A:355:PHE:N	1:A:356:PRO:HD2	2.35	0.42
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.85	0.41
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.91	0.41
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.42	0.41
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.35	0.41
1:B:620:LYS:HD3	1:B:621:THR:N	2.35	0.41
1:B:512:ALA:HA	1:B:513:PRO:HD2	1.90	0.41
1:A:516:ARG:HB3	1:A:517:PHE:CD1	2.55	0.41
1:B:357:LEU:HD23	1:B:357:LEU:HA	1.93	0.41
1:B:478:GLN:HB2	1:B:481:ARG:HG3	2.03	0.41
1:A:593:ILE:O	1:A:597:ASN:HB2	2.21	0.41
1:B:599:CYS:SG	1:B:633:ILE:HD13	2.61	0.41
1:A:332:MET:HE1	1:B:301:LEU:HD22	2.03	0.41
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.02	0.41
1:A:590:GLY:HA3	1:A:638:LEU:HD21	2.03	0.41
1:B:337:LEU:HD21	4:B:800:XEB:H30B	2.03	0.41
1:A:606:ILE:HA	1:A:609:GLU:OE1	2.21	0.41
1:A:655:THR:O	1:A:659:ILE:HG12	2.21	0.41
1:B:349:ARG:HH12	1:B:578:GLU:CD	2.29	0.40
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.03	0.40
1:A:608:GLU:H	1:A:608:GLU:HG2	1.30	0.40
1:B:485:TYR:CE2	1:B:514:ARG:HA	2.56	0.40
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.57	0.40
1:B:618:MET:HA	1:B:625:TRP:CD1	2.56	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	406/422 (96%)	383 (94%)	22 (5%)	1 (0%)	43	44
1	B	410/422 (97%)	393 (96%)	16 (4%)	1 (0%)	43	44
All	All	816/844 (97%)	776 (95%)	38 (5%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	SER
1	B	619	ARG

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	365/377 (97%)	347 (95%)	18 (5%)	22	22
1	B	369/377 (98%)	357 (97%)	12 (3%)	33	37
All	All	734/754 (97%)	704 (96%)	30 (4%)	27	29

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	THR
1	A	328	GLU
1	A	330	ILE
1	A	378	MET
1	A	393	THR
1	A	423	LYS
1	A	470	HIS
1	A	523	LEU
1	A	550	LYS
1	A	555	LYS
1	A	608	GLU

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Mol	Chain	Res	Type
1	A	612	LYS
1	A	620	LYS
1	A	645	LYS
1	A	662	MET
1	A	701	THR
1	A	713	THR
1	A	715	VAL
1	B	330	ILE
1	B	353	GLN
1	B	382	GLU
1	B	540	LEU
1	B	573	GLU
1	B	607	LEU
1	B	608	GLU
1	B	609	GLU
1	B	612	LYS
1	B	620	LYS
1	B	645	LYS
1	B	717	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	436	HIS
1	B	329	HIS
1	B	436	HIS
1	B	451	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	B	860	-	3,3,3	0.81	0	3,3,3	0.67	0
4	XEB	A	800	-	25,25,25	1.20	2 (8%)	32,34,34	1.39	6 (18%)
3	H4B	B	760	-	17,18,18	0.86	0	14,26,26	2.02	5 (35%)
5	ACT	A	860	-	3,3,3	0.79	0	3,3,3	0.76	0
2	HEM	B	750	1	50,50,50	2.01	11 (22%)	67,82,82	1.50	9 (13%)
3	H4B	A	760	-	17,18,18	0.82	0	14,26,26	2.23	7 (50%)
2	HEM	A	750	1	50,50,50	2.26	9 (18%)	67,82,82	1.71	12 (17%)
4	XEB	B	800	-	25,25,25	1.10	2 (8%)	32,34,34	1.22	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XEB	A	800	-	-	3/8/8/8	0/3/3/3
3	H4B	B	760	-	-	3/8/17/17	0/2/2/2
2	HEM	B	750	1	-	4/14/54/54	-
3	H4B	A	760	-	-	3/8/17/17	0/2/2/2
2	HEM	A	750	1	-	6/14/54/54	-
4	XEB	B	800	-	-	5/8/8/8	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	7.97	1.54	1.36
2	B	750	HEM	C3D-C2D	7.85	1.53	1.36
2	A	750	HEM	FE-NA	7.18	2.18	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	FE-NB	7.13	2.16	1.94
2	B	750	HEM	FE-NB	6.81	2.15	1.94
2	A	750	HEM	FE-NC	4.27	2.09	1.95
2	B	750	HEM	FE-NA	4.07	2.08	1.95
2	B	750	HEM	FE-NC	3.80	2.07	1.95
2	A	750	HEM	FE-ND	3.49	2.05	1.94
4	B	800	XEB	C24-CL	3.32	1.81	1.73
4	A	800	XEB	C24-CL	3.24	1.81	1.73
2	A	750	HEM	CAB-C3B	3.02	1.55	1.47
2	B	750	HEM	CAB-C3B	2.90	1.55	1.47
2	B	750	HEM	CAC-C3C	2.87	1.55	1.47
2	A	750	HEM	CAC-C3C	2.83	1.54	1.47
2	B	750	HEM	CMC-C2C	2.43	1.55	1.50
2	B	750	HEM	C2A-C3A	-2.41	1.32	1.38
2	A	750	HEM	CMC-C2C	2.40	1.55	1.50
4	A	800	XEB	C05-C10	-2.28	1.38	1.42
2	B	750	HEM	FE-ND	2.20	2.01	1.94
2	A	750	HEM	C2A-C3A	-2.16	1.33	1.38
2	B	750	HEM	CMD-C2D	2.04	1.55	1.50
4	B	800	XEB	C06-C07	2.03	1.41	1.36
2	B	750	HEM	CMB-C2B	2.00	1.54	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	C4D-ND-C1D	6.09	112.41	105.21
2	B	750	HEM	C4D-ND-C1D	5.88	112.18	105.21
2	A	750	HEM	CAD-CBD-CGD	-4.45	101.86	113.67
3	A	760	H4B	C2-N1-C8A	4.40	121.13	113.36
2	B	750	HEM	CAD-CBD-CGD	-4.35	102.12	113.67
4	A	800	XEB	O12-C11-C08	4.29	121.77	109.16
3	B	760	H4B	C2-N1-C8A	4.04	120.49	113.36
2	A	750	HEM	C3B-C2B-C1B	3.75	109.23	106.41
2	A	750	HEM	CHA-C4D-ND	3.37	128.53	124.37
2	A	750	HEM	CBA-CAA-C2A	-3.35	103.27	112.53
4	B	800	XEB	O12-C11-C08	3.15	118.40	109.16
3	A	760	H4B	O4-C4-C4A	-3.09	119.81	127.26
2	A	750	HEM	C3B-C4B-NB	-3.05	107.28	109.47
3	A	760	H4B	C4A-C4-N3	2.89	120.08	112.13
3	B	760	H4B	O4-C4-C4A	-2.83	120.43	127.26
2	A	750	HEM	C1B-NB-C4B	2.76	108.48	105.21
3	B	760	H4B	C4A-C4-N3	2.74	119.67	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C2A-C1A-NA	-2.71	107.14	110.15
3	A	760	H4B	C2-N3-C4	-2.70	120.21	125.11
2	B	750	HEM	C3D-C4D-ND	-2.69	107.22	110.17
2	B	750	HEM	CHA-C4D-ND	2.68	127.69	124.37
2	A	750	HEM	CHB-C1B-NB	2.55	127.52	124.37
2	B	750	HEM	CAA-C2A-C1A	2.54	129.90	124.94
2	B	750	HEM	CAA-C2A-C3A	-2.48	121.50	127.07
4	B	800	XEB	C11-C08-C09	-2.42	115.84	121.23
2	A	750	HEM	CHD-C1D-ND	2.39	127.00	124.42
3	B	760	H4B	C2-N3-C4	-2.39	120.78	125.11
2	B	750	HEM	CHD-C1D-ND	2.35	126.95	124.42
2	A	750	HEM	C3D-C4D-ND	-2.35	107.60	110.17
3	A	760	H4B	C4-C4A-N5	2.30	122.53	116.27
4	B	800	XEB	C23-C24-C25	-2.28	118.63	122.19
3	A	760	H4B	N2-C2-N3	2.27	121.56	116.76
2	B	750	HEM	C1D-C2D-C3D	-2.22	104.64	106.98
4	A	800	XEB	C11-C08-C09	-2.21	116.31	121.23
4	A	800	XEB	C23-C24-C25	-2.16	118.81	122.19
4	A	800	XEB	C03-C02-N01	-2.11	119.57	122.09
3	A	760	H4B	O9-C9-C6	-2.10	104.24	109.28
4	B	800	XEB	C03-C02-N01	-2.09	119.58	122.09
3	B	760	H4B	C4-C4A-N5	2.08	121.93	116.27
4	A	800	XEB	C22-C21-C26	-2.08	117.71	120.50
2	A	750	HEM	C1D-C2D-C3D	-2.05	104.82	106.98
2	A	750	HEM	C2B-C1B-NB	-2.05	107.49	109.84
4	A	800	XEB	C11-C08-C07	2.00	125.26	120.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	760	H4B	C7-C6-C9-O9
3	B	760	H4B	C7-C6-C9-C10
4	A	800	XEB	C24-C25-C28-N29
4	A	800	XEB	C25-C28-N29-C30
4	B	800	XEB	C24-C25-C28-N29
4	B	800	XEB	C25-C28-N29-C30
4	B	800	XEB	C26-C25-C28-N29
4	A	800	XEB	C26-C25-C28-N29
2	A	750	HEM	C4D-C3D-CAD-CBD
2	A	750	HEM	C2D-C3D-CAD-CBD
2	A	750	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	B	750	HEM	C1A-C2A-CAA-CBA
4	B	800	XEB	C26-C21-O12-C11
2	A	750	HEM	C4B-C3B-CAB-CBB
2	B	750	HEM	C4B-C3B-CAB-CBB
3	B	760	H4B	N5-C6-C9-O9
4	B	800	XEB	C22-C21-O12-C11
3	A	760	H4B	C7-C6-C9-C10
2	A	750	HEM	CAD-CBD-CGD-O2D
2	A	750	HEM	CAD-CBD-CGD-O1D
3	A	760	H4B	C7-C6-C9-O9
2	B	750	HEM	C2A-CAA-CBA-CGA
2	B	750	HEM	C3A-C2A-CAA-CBA
3	A	760	H4B	N5-C6-C9-O9

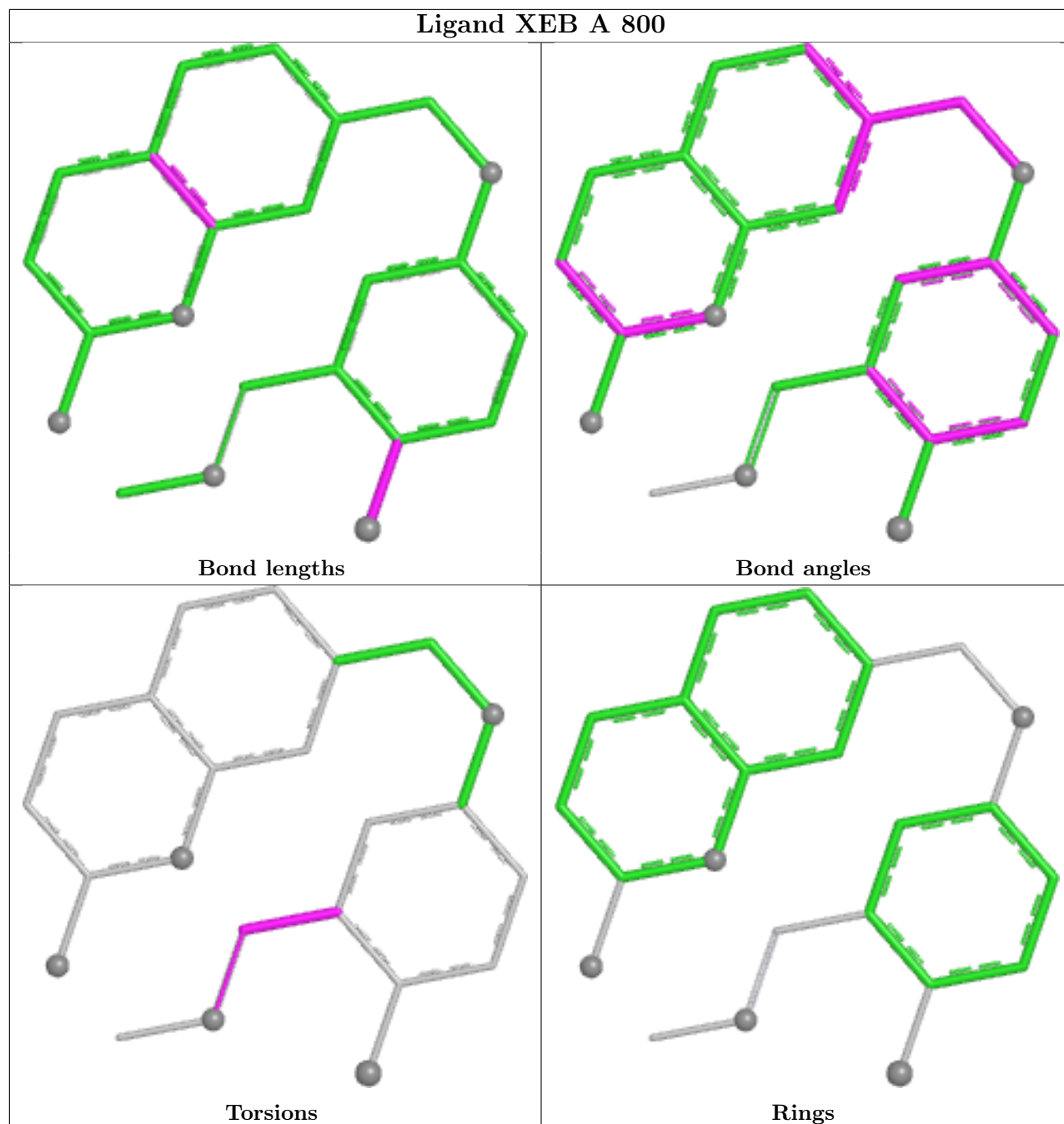
There are no ring outliers.

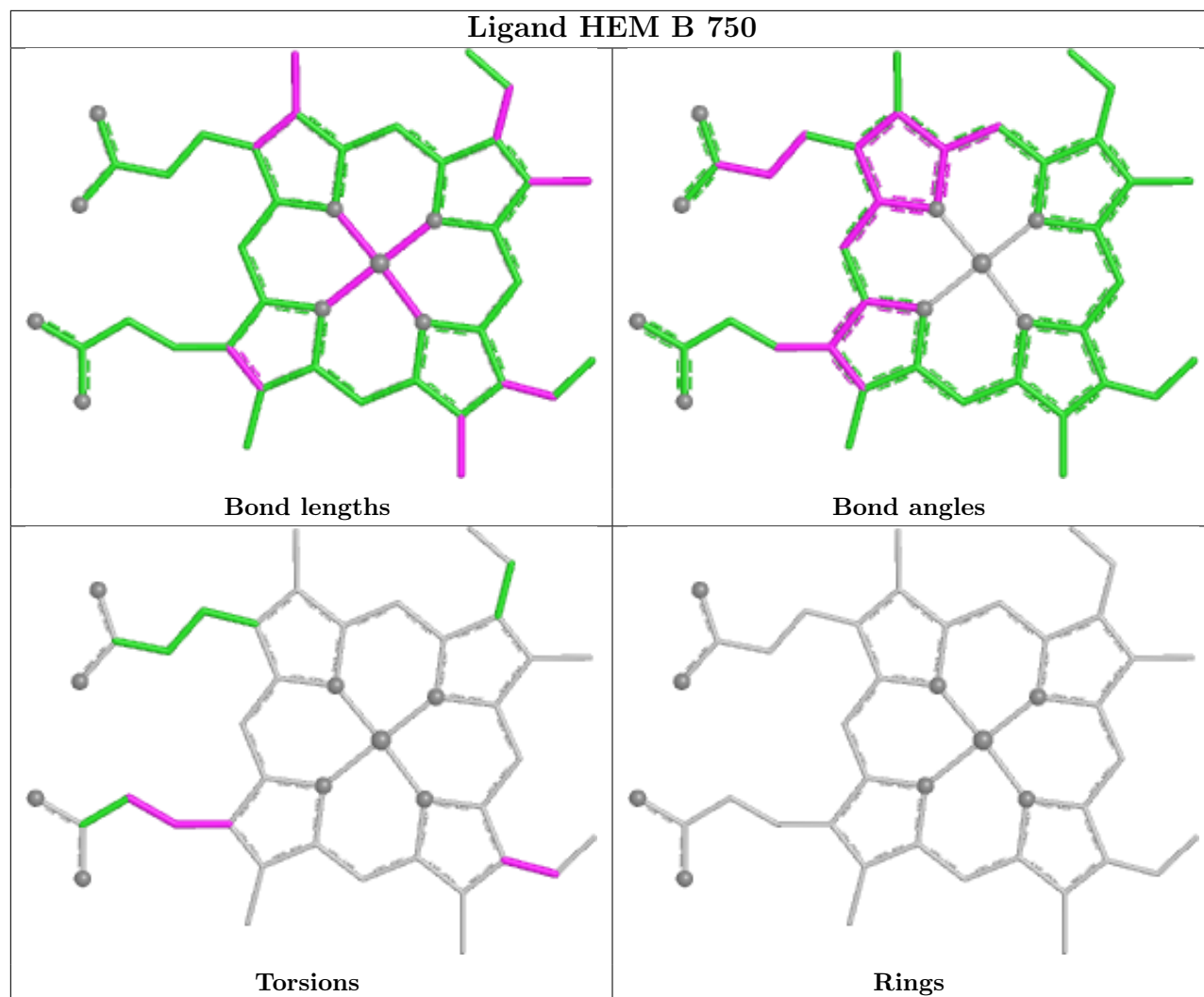
4 monomers are involved in 13 short contacts:

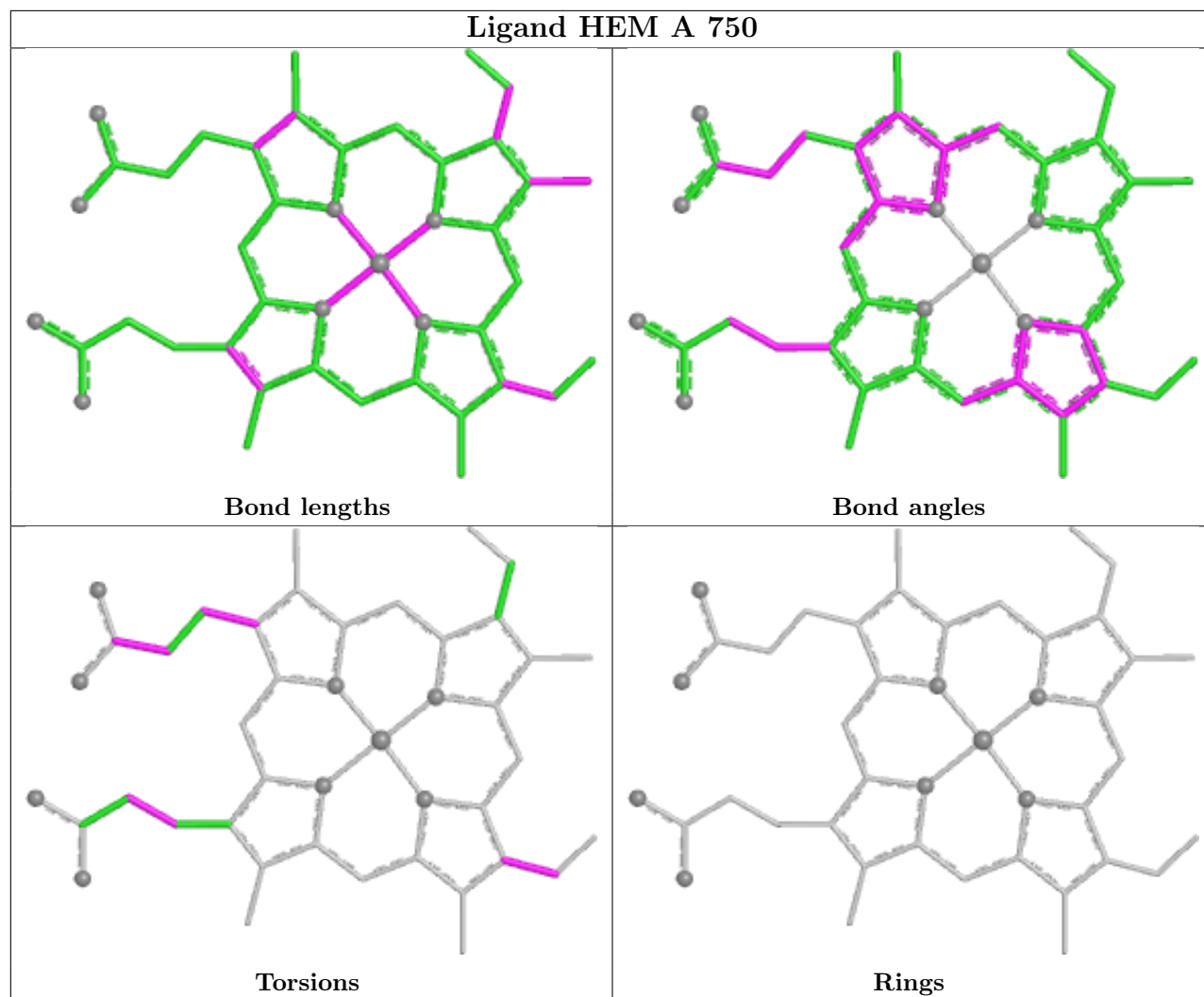
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	XEB	3	0
2	B	750	HEM	5	0
2	A	750	HEM	3	0
4	B	800	XEB	5	0

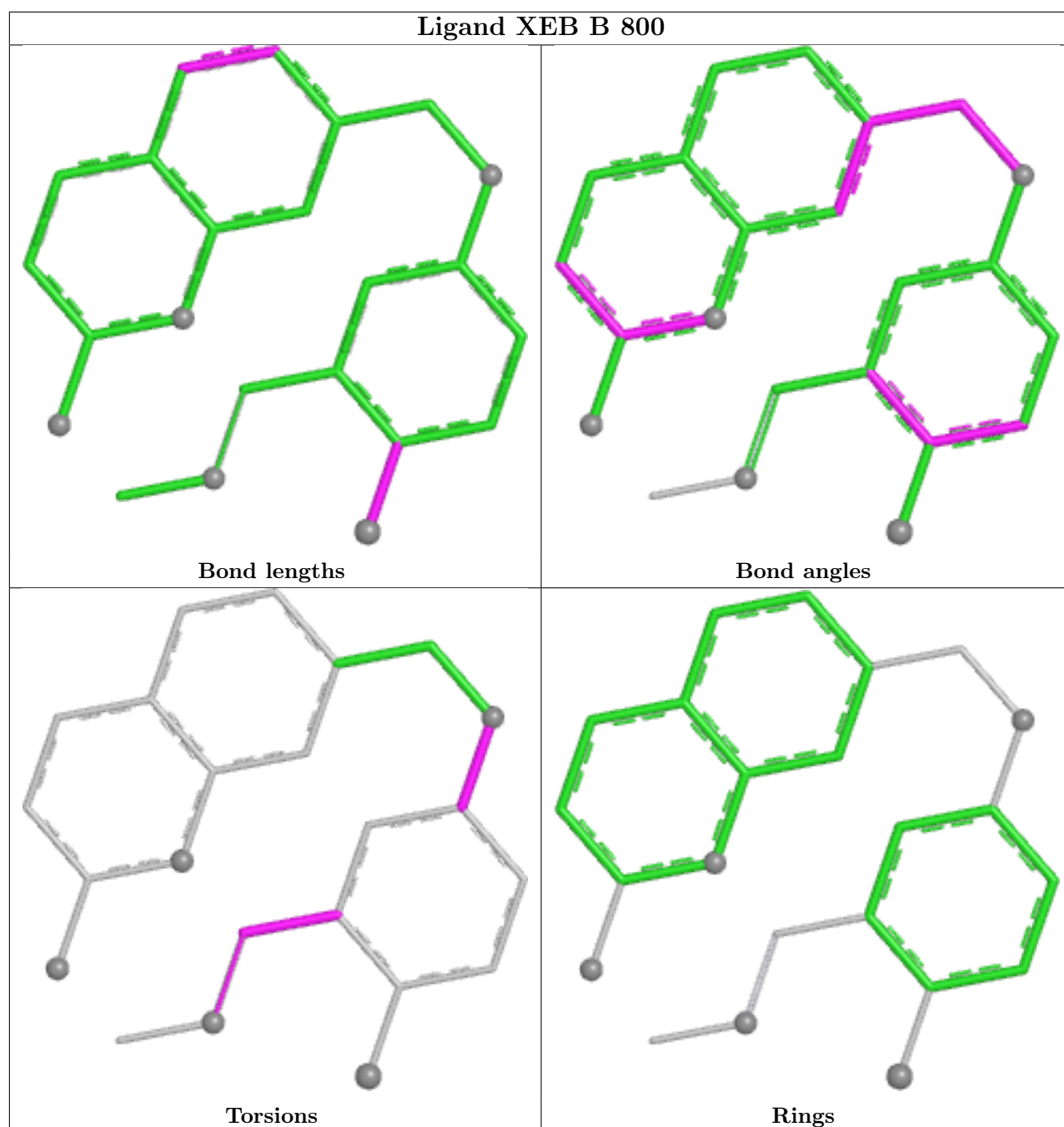
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 XEB A 800









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	408/422 (96%)	0.62	45 (11%)	10 11	21, 51, 100, 143	2 (0%)
1	B	411/422 (97%)	0.28	28 (6%)	23 25	19, 45, 84, 131	3 (0%)
All	All	819/844 (97%)	0.45	73 (8%)	15 16	19, 47, 98, 143	5 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	599	CYS	5.0
1	A	300	PHE	4.8
1	B	348	VAL	4.6
1	B	599	CYS	4.5
1	B	350	THR	4.3
1	B	300	PHE	4.3
1	B	338	PRO	4.2
1	A	604	TYR	4.1
1	B	351	LYS	3.9
1	A	597	ASN	3.8
1	A	322	LEU	3.7
1	A	338	PRO	3.6
1	A	318	LEU	3.5
1	A	553	TRP	3.5
1	A	716	TRP	3.3
1	B	604	TYR	3.3
1	A	551	PHE	3.3
1	B	321	THR	3.1
1	A	491	SER	3.1
1	A	706	TYR	3.0
1	A	558	GLY	3.0
1	A	609	GLU	3.0
1	B	595	VAL	3.0
1	A	355	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	603	ARG	2.8
1	A	715	VAL	2.8
1	A	488	PRO	2.8
1	A	321	THR	2.7
1	A	378	MET	2.7
1	B	392	SER	2.7
1	A	554	PHE	2.7
1	A	598	TYR	2.6
1	B	299	ARG	2.6
1	B	349	ARG	2.6
1	A	713	THR	2.6
1	A	490	GLY	2.6
1	B	352	ASP	2.6
1	B	602[A]	SER	2.6
1	A	373	GLY	2.5
1	A	557	LEU	2.5
1	A	601	ASN	2.5
1	A	602	SER	2.4
1	A	486	LYS	2.4
1	A	506	ILE	2.4
1	B	718	GLY	2.4
1	B	597	ASN	2.4
1	A	360	GLU	2.3
1	A	516	ARG	2.3
1	B	605	ASN	2.3
1	B	598	TYR	2.3
1	B	706	TYR	2.2
1	B	667	ARG	2.2
1	B	601	ASN	2.2
1	A	350	THR	2.2
1	A	494	GLY	2.2
1	A	319	LYS	2.2
1	A	552	ASP	2.2
1	A	497	ALA	2.1
1	A	605	ASN	2.1
1	A	517	PHE	2.1
1	A	613	LYS	2.1
1	A	717	LYS	2.1
1	B	318	LEU	2.1
1	B	620	LYS	2.1
1	A	352	ASP	2.1
1	B	320	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	511	LYS	2.1
1	B	378	MET	2.0
1	B	668	CYS	2.0
1	B	323	GLU	2.0
1	A	390	SER	2.0
1	A	392	SER	2.0
1	B	550	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

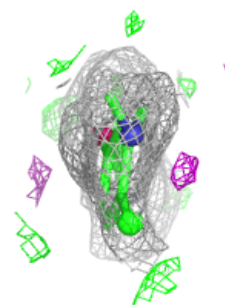
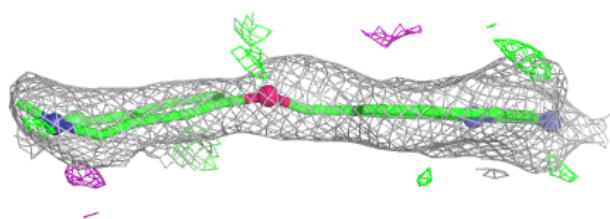
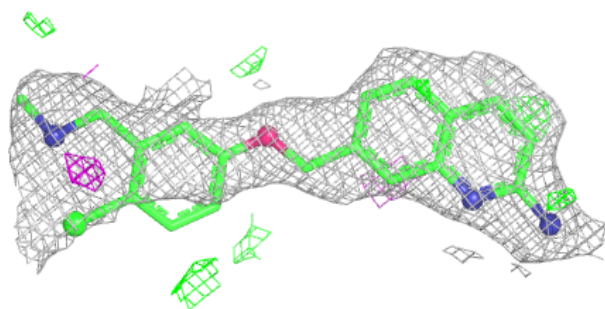
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	A	860	4/4	0.80	0.20	58,72,75,76	0
4	XEB	B	800	23/23	0.85	0.17	49,66,102,139	0
3	H4B	B	760	17/17	0.90	0.14	31,49,67,74	0
5	ACT	B	860	4/4	0.90	0.16	58,65,69,77	0
4	XEB	A	800	23/23	0.91	0.14	29,56,107,137	0
3	H4B	A	760	17/17	0.92	0.14	24,50,70,83	0
2	HEM	A	750	43/43	0.97	0.07	17,35,55,69	0
2	HEM	B	750	43/43	0.98	0.07	15,33,51,57	0
6	ZN	A	1717	1/1	0.98	0.04	42,42,42,42	0

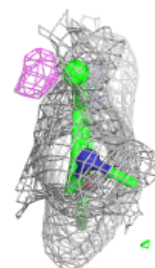
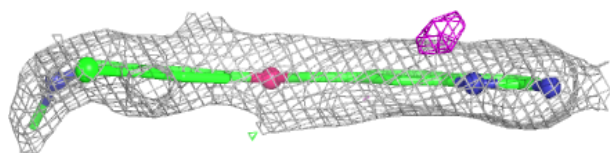
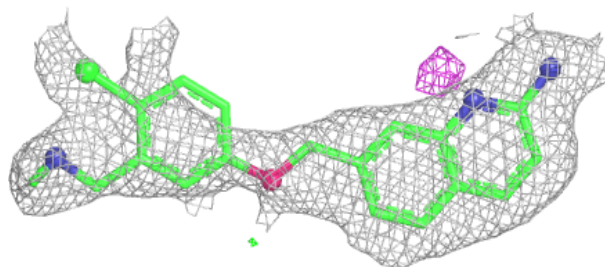
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XEB 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)

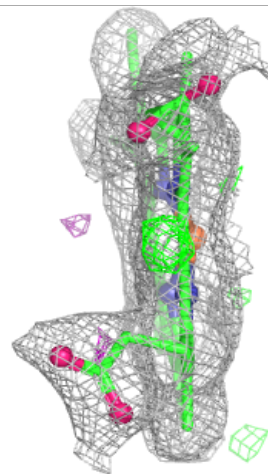
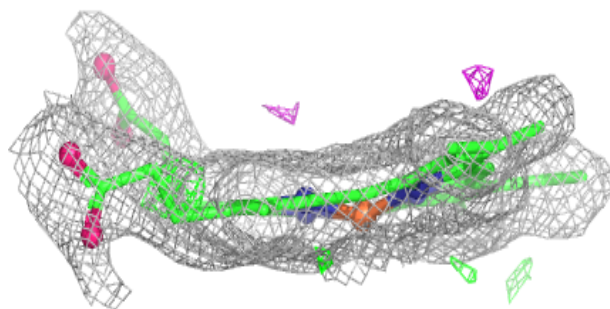
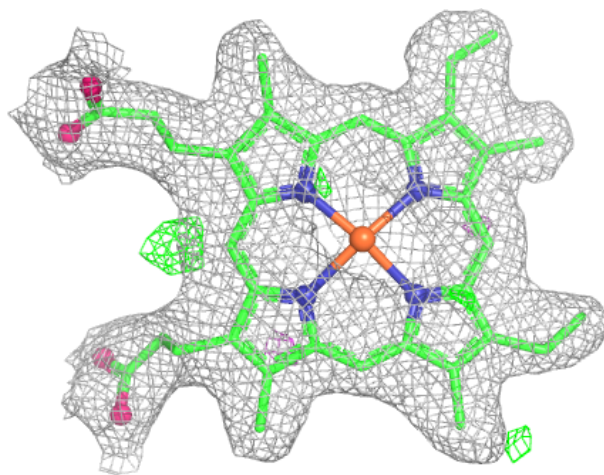
**Electron density around XEB A 800:**

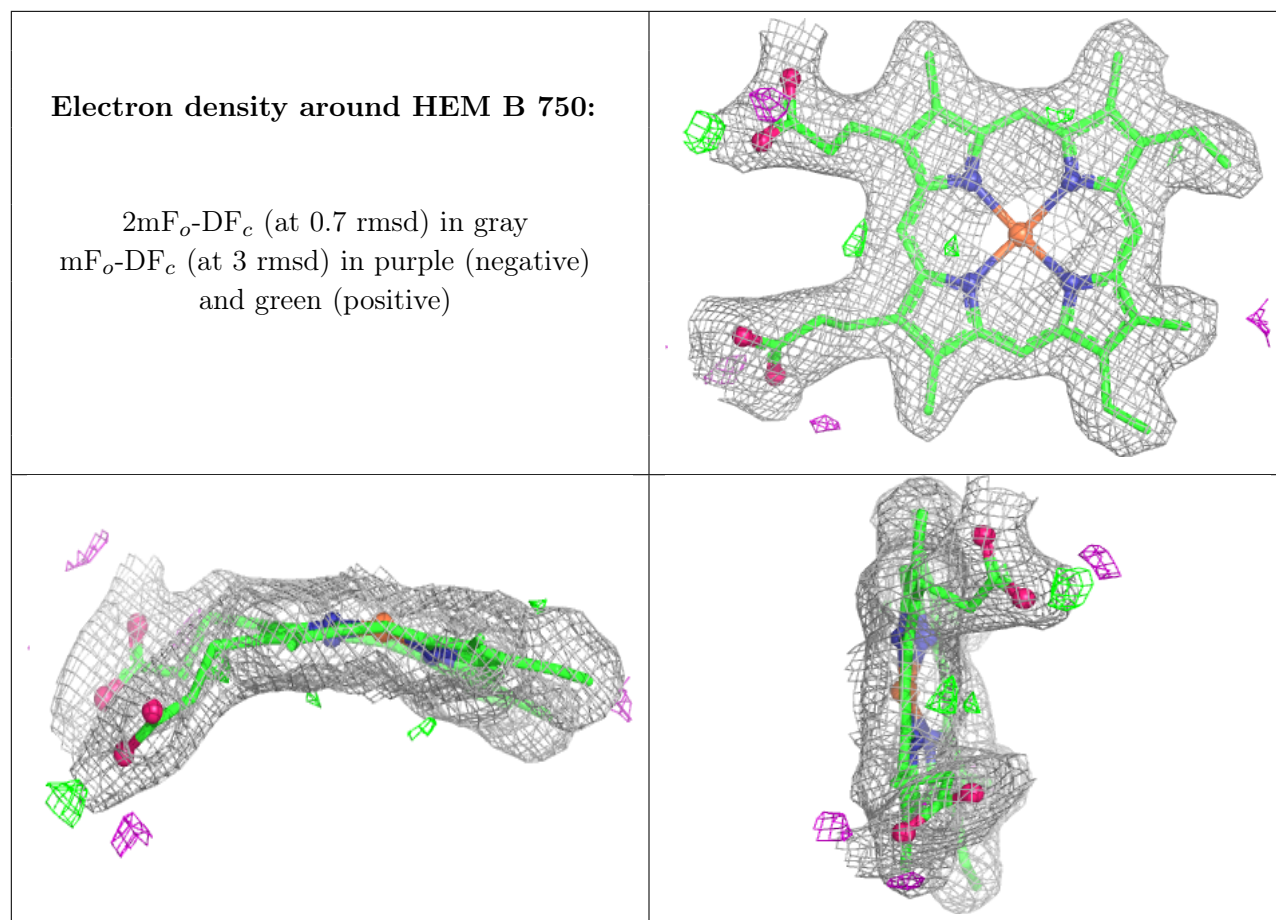
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.