



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:44 AM UTC

PDB ID : 3JT8 / pdb_00003jt8
Title : Structure of neuronal nitric oxide synthase heme domain complexed with N 5
-{3-[(1-methylethyl)sulfanyl]propanimidoyl}-L-ornithine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2009-09-11
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 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

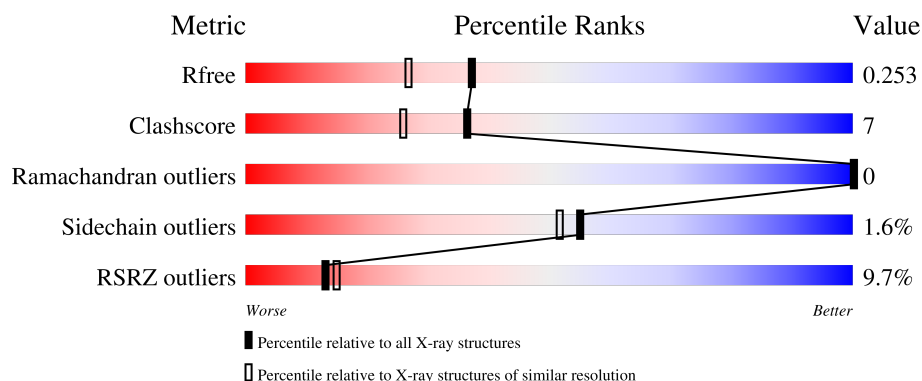
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 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	15% 87% 9% ••
1	B	422	4% 90% 8% •

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
4	JM4	A	800[A]	-	-	X	-
4	JM4	A	800[B]	-	-	X	-
4	JM4	B	800[A]	-	-	X	-
4	JM4	B	800[B]	-	-	X	-

2 Entry composition [i](#)

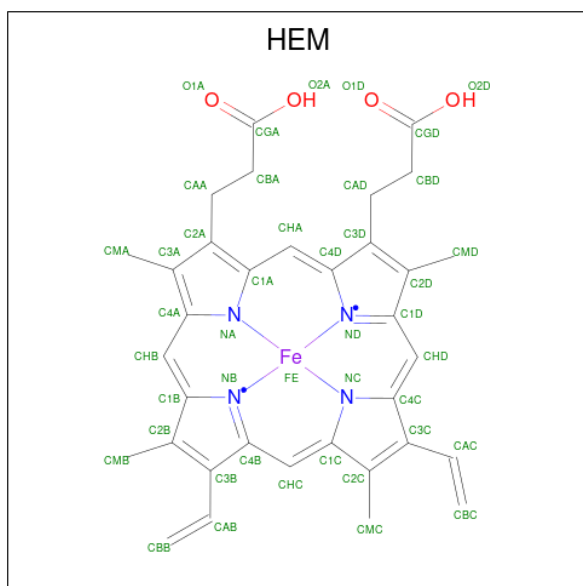
There are 7 unique types of molecules in this entry. The entry contains 7241 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	2	0
			3319	2125	566	606	22			
1	B	411	Total	C	N	O	S	0	3	0
			3354	2146	574	612	22			

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



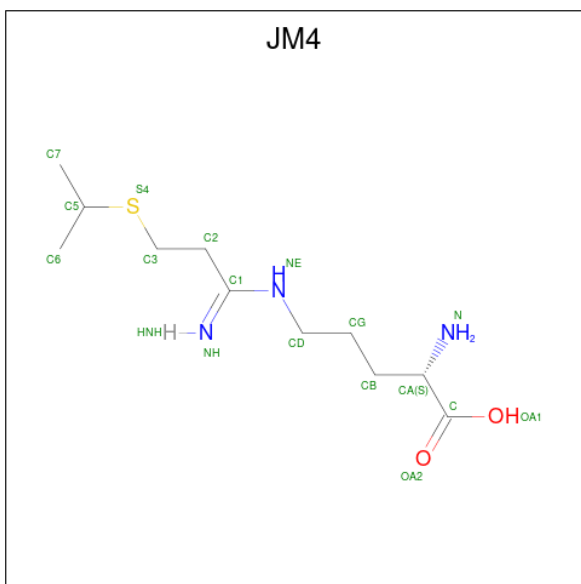
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N 5 -{3-[(1-methylethyl)sulfanyl]propanimidoyl}-L-ornithine (CCD ID: JM4) (formula: $C_{11}H_{23}N_3O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			29	20	5	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	1
			29	20	5	2	2		

- 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	Zn	0	0
			1	1		

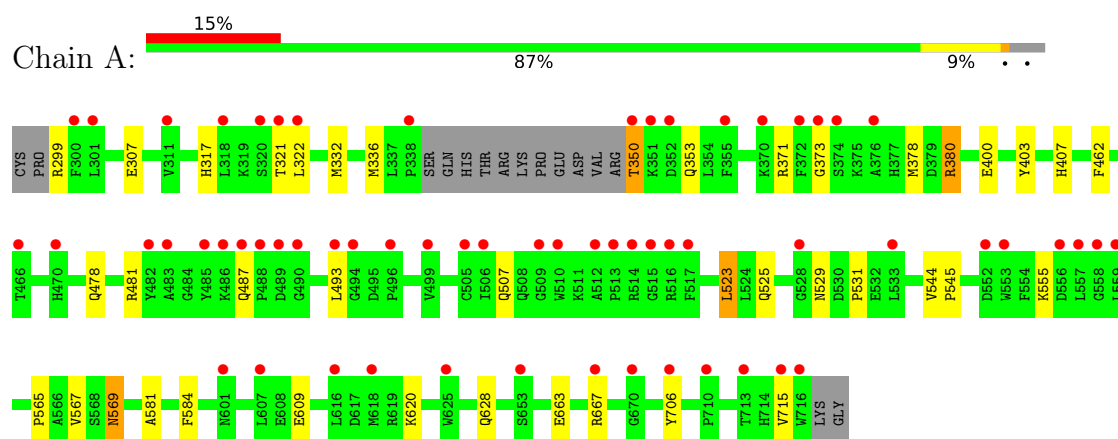
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	151	Total	O	0	0
			151	151		
7	B	230	Total	O	0	0
			230	230		

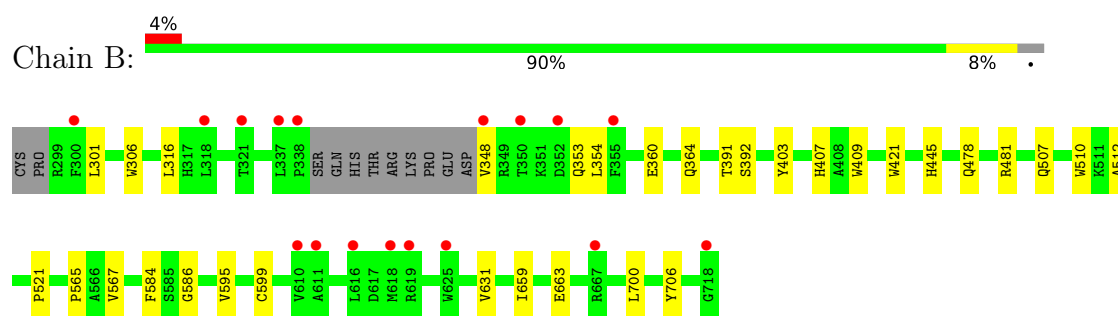
3 Residue-property plots

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

- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.19Å 111.37Å 164.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.11 – 1.95 38.11 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.11-1.95) 99.0 (38.11-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.187 , 0.222 0.223 , 0.253	Depositor DCC
R_{free} test set	3484 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7241	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H4B, HEM, ACT, JM4, ZN

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	0.66	0/3418	0.84	0/4637
1	B	0.74	0/3456	0.85	3/4685 (0.1%)
All	All	0.70	0/6874	0.84	3/9322 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ALA	CA-C-N	5.43	125.25	119.28
1	B	512	ALA	C-N-CA	5.43	125.25	119.28
1	B	354	LEU	N-CA-C	5.41	116.98	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3319	0	3231	32	0
1	B	3354	0	3274	30	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	29	0	38	33	0
4	B	29	0	38	27	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	151	0	0	2	0
7	B	230	0	0	4	0
All	All	7241	0	6677	98	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 (98) 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[B]:JM4:NE	4:B:800[B]:JM4:H6B	1.39	1.32
4:A:800[B]:JM4:H6B	4:A:800[B]:JM4:C1	1.70	1.21
4:A:800[B]:JM4:H6B	4:A:800[B]:JM4:C2	1.75	1.17
4:B:800[B]:JM4:NE	4:B:800[B]:JM4:C6	2.08	1.16
1:A:565:PRO:HB2	4:A:800[B]:JM4:H2A	1.28	1.10
4:B:800[B]:JM4:H6B	4:B:800[B]:JM4:CD	1.81	1.10
4:B:800[B]:JM4:H6A	4:B:800[B]:JM4:C1	1.80	1.10
4:A:800[B]:JM4:C2	4:A:800[B]:JM4:C6	2.34	1.03
4:A:800[B]:JM4:C1	4:A:800[B]:JM4:C6	2.35	1.02
4:B:800[B]:JM4:C6	4:B:800[B]:JM4:C1	2.38	1.01
4:A:800[B]:JM4:H6B	4:A:800[B]:JM4:H2	1.42	1.01
1:B:584:PHE:CE1	4:B:800[B]:JM4:H7B	2.01	0.96
1:B:584:PHE:HE1	4:B:800[B]:JM4:H7B	1.34	0.86
4:B:800[B]:JM4:H6B	4:B:800[B]:JM4:HDA	1.60	0.83
4:A:800[B]:JM4:H6B	4:A:800[B]:JM4:CD	2.08	0.82
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.63	0.81
1:B:586:GLY:H	4:B:800[B]:JM4:H3	1.49	0.77
4:A:800[B]:JM4:H6B	4:A:800[B]:JM4:HD	1.66	0.77
4:A:800[B]:JM4:H6B	4:A:800[B]:JM4:NE	1.99	0.76
1:A:567:VAL:HG21	4:A:800[A]:JM4:H6	1.69	0.73
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.71	0.71
1:A:584:PHE:CE1	4:A:800[B]:JM4:H7B	2.26	0.71
1:B:565:PRO:HB2	4:B:800[B]:JM4:H2	1.73	0.69
1:A:350:THR:N	1:A:353:GLN:HE21	1.93	0.66
1:A:584:PHE:HE1	4:A:800[B]:JM4:H7B	1.58	0.65
4:A:800[A]:JM4:HDA	4:A:800[A]:JM4:H6B	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:HG3	7:B:1069:HOH:O	1.98	0.63
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.80	0.62
4:A:800[B]:JM4:C1	4:A:800[B]:JM4:H6A	2.25	0.62
4:B:800[B]:JM4:H6B	4:B:800[B]:JM4:HNE	1.56	0.62
1:B:565:PRO:HG2	4:B:800[B]:JM4:H2A	1.83	0.61
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.82	0.61
1:B:584:PHE:HE1	4:B:800[A]:JM4:H5	1.65	0.61
1:A:565:PRO:CB	4:A:800[B]:JM4:H2A	2.19	0.61
1:B:584:PHE:HE1	4:B:800[B]:JM4:C7	2.11	0.61
2:B:750:HEM:C4D	4:B:800[A]:JM4:H6A	2.36	0.60
4:A:800[A]:JM4:CD	4:A:800[A]:JM4:H7A	2.31	0.60
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.86	0.57
1:A:663:GLU:O	1:A:667:ARG:HG2	2.04	0.56
2:B:750:HEM:C4B	4:B:800[A]:JM4:H3A	2.40	0.56
1:A:584:PHE:HE1	4:A:800[A]:JM4:H5	1.70	0.56
1:B:565:PRO:HG2	4:B:800[B]:JM4:C2	2.35	0.56
2:A:750:HEM:C4B	4:A:800[A]:JM4:H3A	2.41	0.55
4:B:800[A]:JM4:H6B	4:B:800[A]:JM4:HDA	1.88	0.55
1:A:567:VAL:HG21	4:A:800[B]:JM4:H7A	1.88	0.55
1:A:565:PRO:HG2	4:A:800[A]:JM4:H2A	1.89	0.54
1:A:567:VAL:HG21	4:A:800[A]:JM4:C6	2.37	0.54
1:B:567:VAL:HG21	4:B:800[A]:JM4:H6	1.88	0.53
4:A:800[A]:JM4:H7A	4:A:800[A]:JM4:H2	1.90	0.53
4:B:800[B]:JM4:C6	4:B:800[B]:JM4:HNE	2.17	0.53
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.10	0.52
1:B:445:HIS:C	1:B:445:HIS:CD2	2.88	0.52
1:A:299:ARG:O	1:A:317:HIS:CE1	2.63	0.52
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.93	0.51
4:A:800[A]:JM4:HDA	4:A:800[A]:JM4:H7A	1.91	0.51
4:A:800[A]:JM4:H7A	4:A:800[A]:JM4:HD	1.93	0.50
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.26	0.50
1:A:567:VAL:CG2	4:A:800[B]:JM4:H7A	2.43	0.49
1:B:364:GLN:NE2	7:B:1218:HOH:O	2.26	0.49
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.94	0.49
2:A:750:HEM:C4D	4:A:800[A]:JM4:H6A	2.47	0.49
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.49
1:B:391:THR:O	1:B:392:SER:HB2	2.13	0.48
1:B:567:VAL:HG21	4:B:800[A]:JM4:C6	2.43	0.48
1:B:507:GLN:NE2	7:B:1079:HOH:O	2.46	0.48
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.29	0.47
4:A:800[B]:JM4:HD	4:A:800[B]:JM4:H7A	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:VAL:O	1:B:599:CYS:HB2	2.16	0.46
1:B:706:TYR:OH	2:B:750:HEM:O1D	2.22	0.46
1:A:569:ASN:HD22	1:A:569:ASN:H	1.63	0.46
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.41	0.46
1:A:609:GLU:HG3	7:A:1148:HOH:O	2.16	0.45
4:A:800[A]:JM4:H3	4:A:800[A]:JM4:H7B	1.80	0.45
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.52	0.45
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.05	0.45
1:A:493:LEU:HA	7:A:1103:HOH:O	2.17	0.45
4:A:800[B]:JM4:H2	4:A:800[B]:JM4:HD	1.76	0.45
1:B:586:GLY:N	4:B:800[B]:JM4:H3	2.25	0.44
4:B:800[A]:JM4:H7B	4:B:800[A]:JM4:H3	1.68	0.44
1:A:321:THR:HG23	1:A:322:LEU:HG	2.00	0.44
4:A:800[B]:JM4:HNE	4:A:800[B]:JM4:HBA	1.61	0.44
4:A:800[A]:JM4:H2	4:A:800[A]:JM4:C7	2.48	0.43
1:B:565:PRO:HG2	4:B:800[A]:JM4:H2A	2.01	0.43
1:B:567:VAL:HG21	4:B:800[B]:JM4:H7A	2.00	0.43
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.53	0.43
1:A:373:GLY:HA2	1:A:378:MET:HE3	2.01	0.43
1:B:348:VAL:HG12	7:B:1168:HOH:O	2.19	0.43
1:A:628:GLN:HG2	1:B:631:VAL:HG11	2.00	0.43
1:B:316:LEU:HD21	1:B:700:LEU:HD11	2.01	0.42
1:B:567:VAL:CG2	4:B:800[B]:JM4:H7A	2.50	0.42
1:A:525:GLN:HG3	1:A:529:ASN:O	2.19	0.42
1:A:350:THR:N	1:A:353:GLN:NE2	2.66	0.41
1:A:567:VAL:CG2	4:A:800[A]:JM4:H6	2.43	0.41
1:A:462:PHE:HB2	1:A:581:ALA:HB3	2.03	0.41
4:B:800[A]:JM4:HDA	4:B:800[A]:JM4:H7A	2.03	0.40
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.93	0.40
4:A:800[B]:JM4:H6A	4:A:800[B]:JM4:NH	2.37	0.40
1:B:659:ILE:O	1:B:663:GLU:HG3	2.22	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	405/422 (96%)	396 (98%)	9 (2%)	0	100	100
1	B	410/422 (97%)	402 (98%)	8 (2%)	0	100	100
All	All	815/844 (97%)	798 (98%)	17 (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	365/377 (97%)	355 (97%)	10 (3%)	39	32
1	B	369/377 (98%)	367 (100%)	2 (0%)	81	82
All	All	734/754 (97%)	722 (98%)	12 (2%)	55	52

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

Mol	Chain	Res	Type
1	A	350	THR
1	A	371	ARG
1	A	380	ARG
1	A	487	GLN
1	A	507	GLN
1	A	523	LEU
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	715	VAL
1	B	353	GLN
1	B	360	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	385	ASN
1	A	436	HIS
1	A	454	ASN
1	A	507	GLN
1	A	508	GLN
1	A	569	ASN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	A	714	HIS
1	B	407	HIS
1	B	440	ASN
1	B	454	ASN
1	B	487	GLN
1	B	507	GLN
1	B	535	GLN
1	B	601	ASN
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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
4	JM4	A	800[B]	-	15,16,16	4.69	3 (20%)	11,19,19	0.91	0
5	ACT	B	860	-	3,3,3	0.70	0	3,3,3	1.06	0
5	ACT	A	860	-	3,3,3	0.83	0	3,3,3	0.77	0
4	JM4	B	800[A]	-	15,16,16	4.48	3 (20%)	11,19,19	0.94	1 (9%)
3	H4B	B	760	-	17,18,18	1.10	3 (17%)	14,26,26	1.91	4 (28%)
2	HEM	A	750	1	50,50,50	1.93	11 (22%)	67,82,82	1.42	6 (8%)
2	HEM	B	750	1	50,50,50	1.80	12 (24%)	67,82,82	1.24	7 (10%)
4	JM4	B	800[B]	-	15,16,16	4.64	3 (20%)	11,19,19	0.91	1 (9%)
4	JM4	A	800[A]	-	15,16,16	4.61	3 (20%)	11,19,19	0.92	1 (9%)
3	H4B	A	760	-	17,18,18	0.82	0	14,26,26	2.00	6 (42%)

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	JM4	A	800[B]	-	-	7/16/17/17	-
4	JM4	B	800[A]	-	-	4/16/17/17	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	A	750	1	-	1/14/54/54	-
2	HEM	B	750	1	-	0/14/54/54	-
4	JM4	B	800[B]	-	-	3/16/17/17	-
4	JM4	A	800[A]	-	-	4/16/17/17	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800[B]	JM4	C2-C1	-17.22	1.34	1.50
4	B	800[B]	JM4	C2-C1	-17.16	1.34	1.50
4	A	800[A]	JM4	C2-C1	-16.93	1.34	1.50
4	B	800[A]	JM4	C2-C1	-16.61	1.34	1.50
2	A	750	HEM	C3D-C2D	7.49	1.52	1.36
2	B	750	HEM	C3D-C2D	6.66	1.51	1.36
2	A	750	HEM	FE-NB	4.45	2.08	1.94
2	A	750	HEM	FE-NA	4.20	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800[B]	JM4	C3-S4	-3.92	1.75	1.81
4	A	800[A]	JM4	C3-S4	-3.91	1.75	1.81
2	B	750	HEM	FE-ND	3.87	2.06	1.94
2	B	750	HEM	FE-NA	3.82	2.07	1.95
2	A	750	HEM	FE-ND	3.79	2.06	1.94
4	B	800[B]	JM4	C3-S4	-3.68	1.76	1.81
2	A	750	HEM	FE-NC	3.56	2.06	1.95
4	A	800[B]	JM4	C1-NH	3.20	1.34	1.27
4	B	800[A]	JM4	C3-S4	-3.14	1.77	1.81
2	B	750	HEM	FE-NB	3.02	2.04	1.94
2	A	750	HEM	CAB-C3B	2.82	1.54	1.47
2	B	750	HEM	CAC-C3C	2.82	1.54	1.47
4	B	800[A]	JM4	C1-NH	2.80	1.33	1.27
2	B	750	HEM	FE-NC	2.73	2.04	1.95
4	B	800[B]	JM4	C1-NH	2.72	1.33	1.27
2	B	750	HEM	CAB-C3B	2.71	1.54	1.47
4	A	800[A]	JM4	C1-NH	2.61	1.33	1.27
2	B	750	HEM	CMC-C2C	2.61	1.56	1.50
2	B	750	HEM	CMD-C2D	2.50	1.55	1.50
2	B	750	HEM	CMB-C2B	2.48	1.55	1.50
2	A	750	HEM	CAC-C3C	2.46	1.54	1.47
2	B	750	HEM	C2A-C3A	-2.43	1.32	1.38
2	A	750	HEM	CMC-C2C	2.39	1.55	1.50
2	A	750	HEM	CMD-C2D	2.34	1.55	1.50
3	B	760	H4B	C7-C6	2.33	1.54	1.52
2	B	750	HEM	CMA-C3A	2.31	1.55	1.50
2	A	750	HEM	CMA-C3A	2.24	1.55	1.50
3	B	760	H4B	C7-N8	2.10	1.48	1.46
2	A	750	HEM	CMB-C2B	2.04	1.55	1.50
3	B	760	H4B	O4-C4	2.01	1.27	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	C4D-ND-C1D	5.78	112.05	105.21
3	A	760	H4B	C2-N1-C8A	4.75	121.74	113.36
2	B	750	HEM	CBA-CAA-C2A	-4.15	101.06	112.53
2	B	750	HEM	C4D-ND-C1D	4.11	110.07	105.21
3	B	760	H4B	C2-N1-C8A	4.06	120.52	113.36
2	A	750	HEM	CBA-CAA-C2A	-3.53	102.78	112.53
2	A	750	HEM	CBD-CAD-C3D	-3.09	103.99	112.53
2	B	750	HEM	CBD-CAD-C3D	-3.02	104.19	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	760	H4B	O4-C4-C4A	-2.97	120.10	127.26
3	A	760	H4B	C4A-C4-N3	2.61	119.28	112.13
3	B	760	H4B	C4A-C4-N3	2.59	119.23	112.13
3	A	760	H4B	O4-C4-C4A	-2.58	121.04	127.26
2	A	750	HEM	C3B-C2B-C1B	2.50	108.29	106.41
2	B	750	HEM	C2A-C1A-NA	-2.41	107.47	110.15
2	A	750	HEM	C4C-C3C-C2C	2.33	108.83	106.81
2	B	750	HEM	CAD-C3D-C4D	2.32	128.74	124.70
4	B	800[A]	JM4	OA1-C-OA2	-2.24	118.99	124.08
4	B	800[B]	JM4	OA1-C-OA2	-2.24	118.99	124.08
3	A	760	H4B	C2-N3-C4	-2.15	121.21	125.11
3	A	760	H4B	C4-C4A-N5	2.15	122.13	116.27
2	A	750	HEM	CHD-C1D-ND	2.15	126.73	124.42
3	A	760	H4B	N2-C2-N3	2.11	121.21	116.76
2	B	750	HEM	CHA-C4D-ND	2.06	126.92	124.37
2	B	750	HEM	CMD-C2D-C1D	2.03	128.21	125.03
4	A	800[A]	JM4	CG-CD-NE	-2.01	106.55	112.20
3	B	760	H4B	C4-C4A-N5	2.01	121.75	116.27

There are no chirality outliers.

All (19) torsion outliers are listed below:

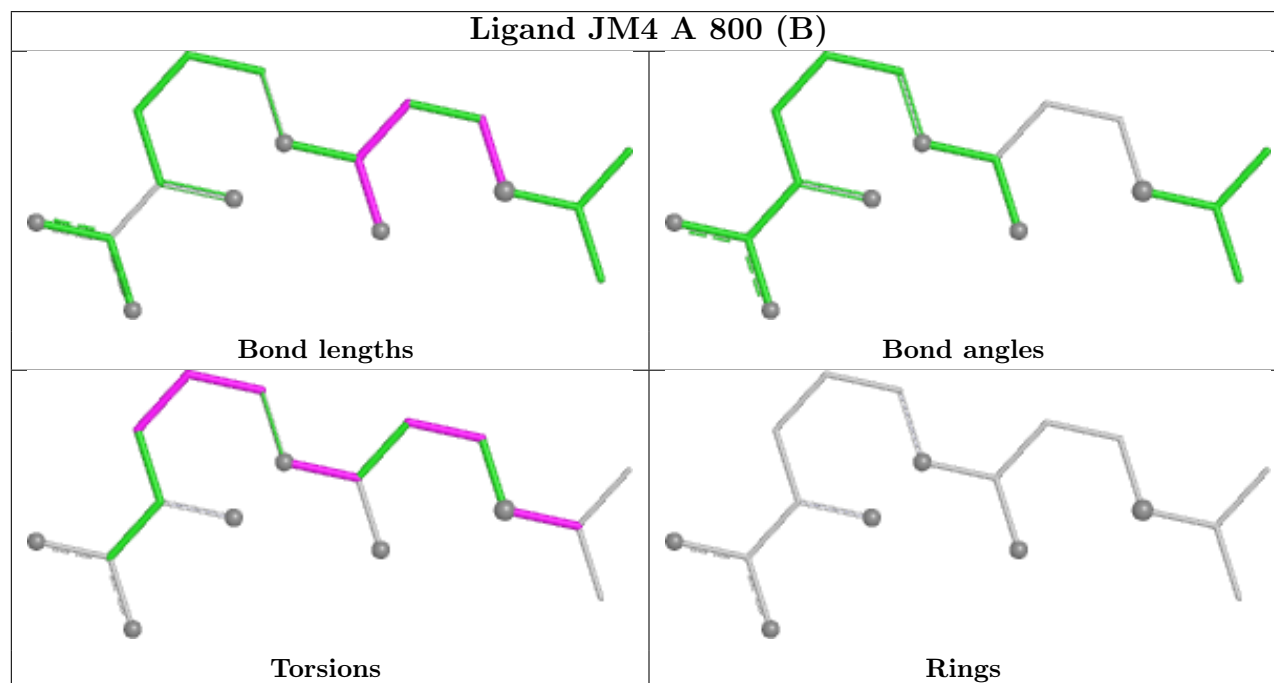
Mol	Chain	Res	Type	Atoms
4	A	800[A]	JM4	C7-C5-S4-C3
4	A	800[B]	JM4	NH-C1-NE-CD
4	A	800[B]	JM4	C1-C2-C3-S4
4	A	800[B]	JM4	C6-C5-S4-C3
4	A	800[B]	JM4	C7-C5-S4-C3
4	B	800[A]	JM4	C1-C2-C3-S4
4	B	800[A]	JM4	C7-C5-S4-C3
4	A	800[B]	JM4	C2-C1-NE-CD
4	A	800[A]	JM4	C2-C1-NE-CD
4	B	800[B]	JM4	C2-C1-NE-CD
4	A	800[B]	JM4	NE-CD-CG-CB
4	B	800[B]	JM4	NE-CD-CG-CB
4	A	800[B]	JM4	CA-CB-CG-CD
4	B	800[A]	JM4	C2-C1-NE-CD
4	B	800[A]	JM4	C6-C5-S4-C3
2	A	750	HEM	C4B-C3B-CAB-CBB
4	A	800[A]	JM4	NE-C1-C2-C3
4	A	800[A]	JM4	NH-C1-NE-CD
4	B	800[B]	JM4	NH-C1-NE-CD

There are no ring outliers.

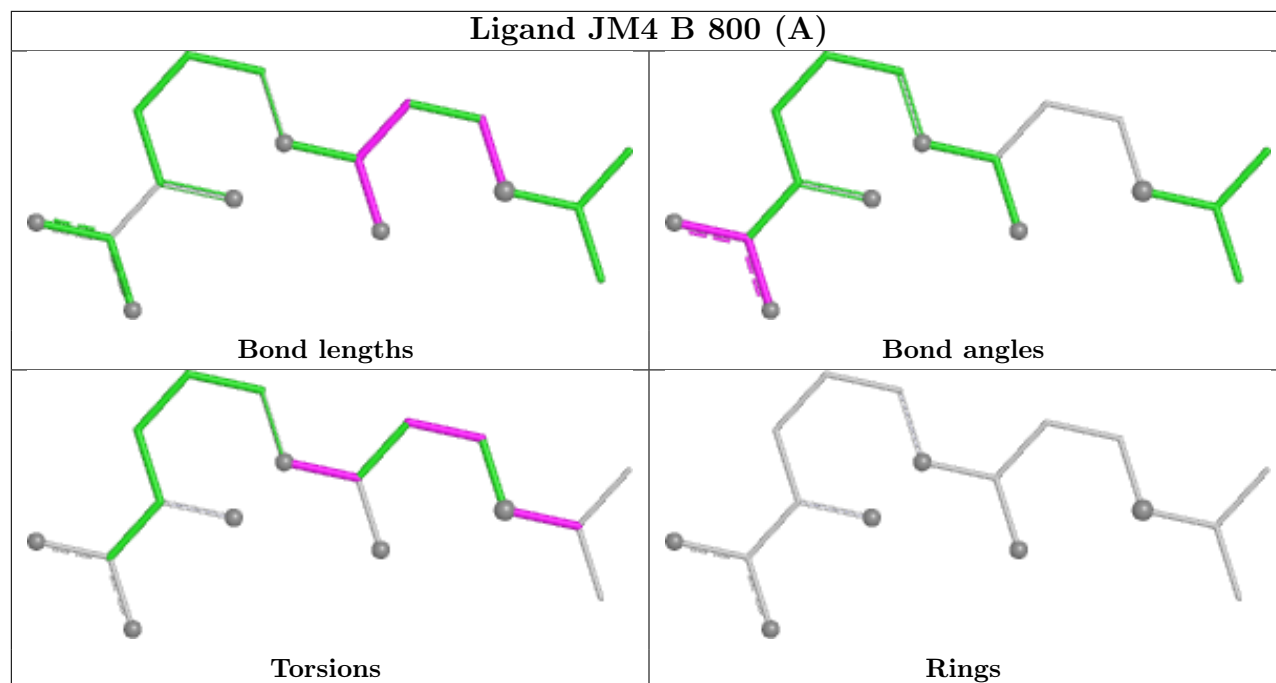
6 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800[B]	JM4	19	0
4	B	800[A]	JM4	9	0
2	A	750	HEM	6	0
2	B	750	HEM	4	0
4	B	800[B]	JM4	18	0
4	A	800[A]	JM4	14	0

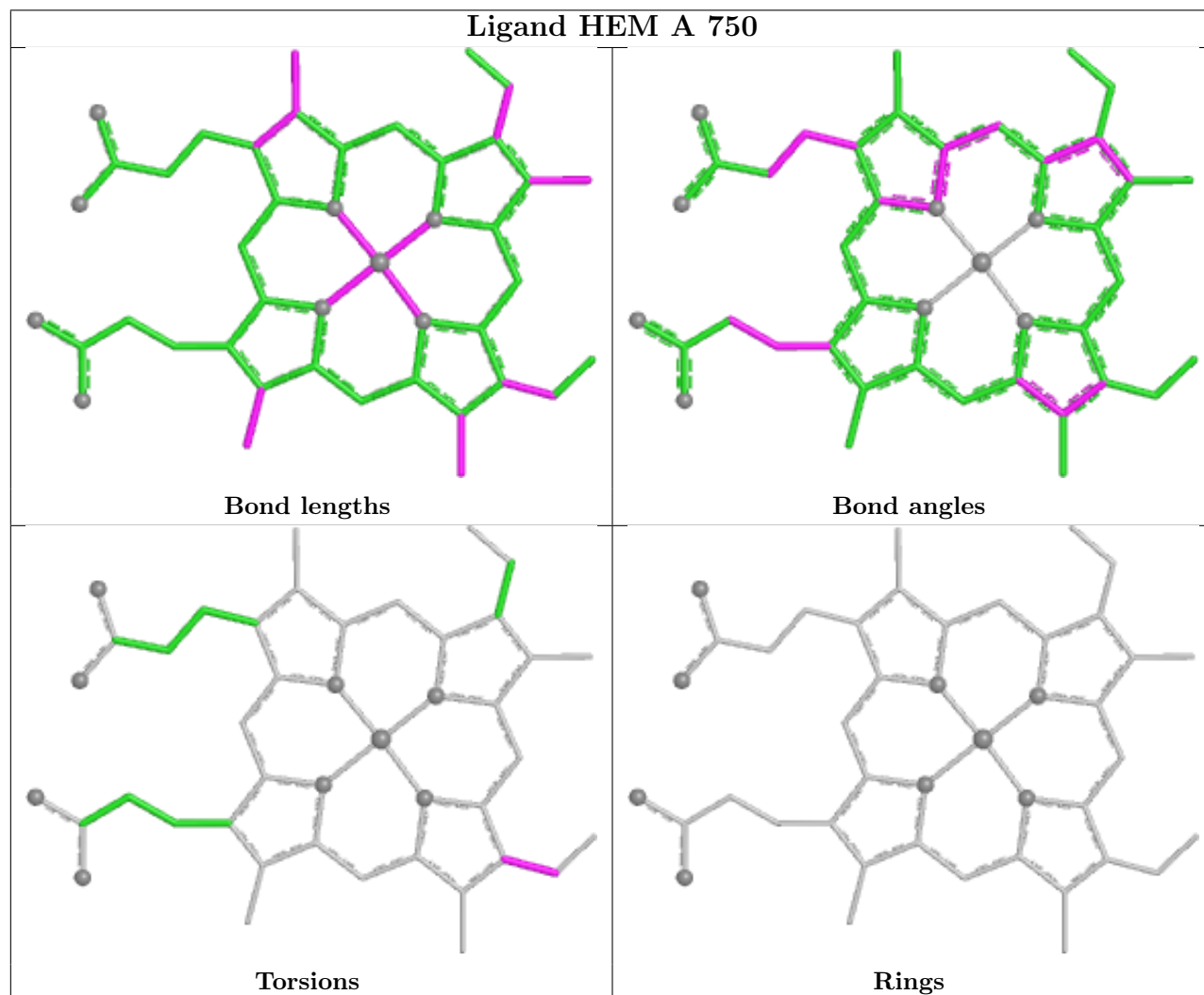
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

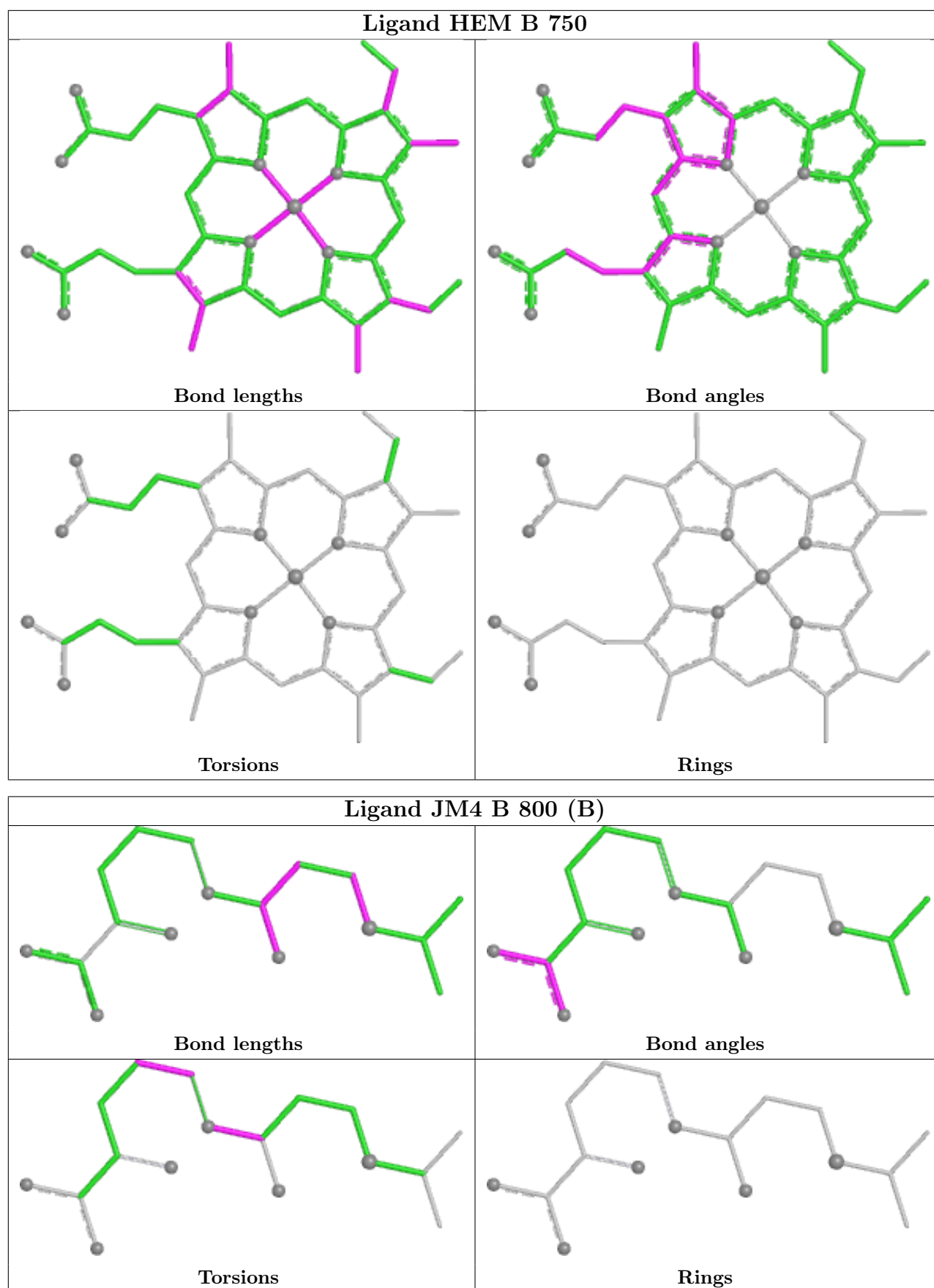


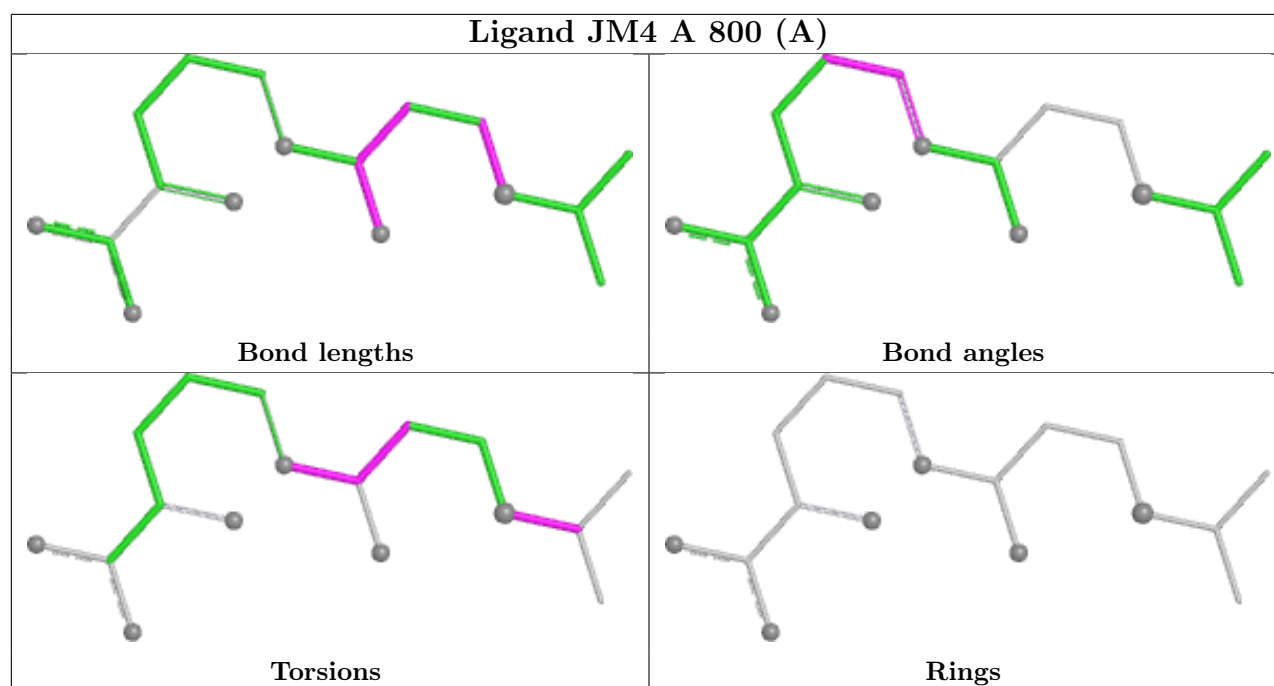
Ligand JM4 B 800 (A)



Ligand HEM A 750







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%)	0.95	62 (15%) 5 6	25, 52, 94, 123	2 (0%)
1	B	411/422 (97%)	0.38	17 (4%) 41 48	23, 39, 63, 81	3 (0%)
All	All	818/844 (96%)	0.66	79 (9%) 13 15	23, 45, 88, 123	5 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	5.4
1	A	494	GLY	4.6
1	B	338	PRO	4.5
1	A	493	LEU	4.3
1	A	512	ALA	4.3
1	A	300	PHE	4.2
1	A	338	PRO	4.0
1	A	513	PRO	4.0
1	B	355	PHE	4.0
1	A	715	VAL	3.9
1	A	510	TRP	3.8
1	A	485	TYR	3.7
1	A	488	PRO	3.7
1	B	611	ALA	3.7
1	A	483	ALA	3.6
1	A	514	ARG	3.6
1	A	517	PHE	3.5
1	A	618	MET	3.4
1	A	528	GLY	3.4
1	B	300	PHE	3.4
1	A	509	GLY	3.3
1	A	506	ILE	3.3
1	B	348	VAL	3.3
1	A	350	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	616	LEU	3.2
1	A	321	THR	3.1
1	A	376	ALA	3.1
1	A	311	VAL	3.1
1	A	355	PHE	3.1
1	B	618	MET	3.1
1	A	553	TRP	3.1
1	A	322	LEU	3.0
1	B	350	THR	3.0
1	A	670	GLY	3.0
1	A	466	THR	2.9
1	A	515	GLY	2.9
1	A	552	ASP	2.9
1	A	499	VAL	2.9
1	A	470	HIS	2.8
1	A	372	PHE	2.8
1	A	713	THR	2.8
1	A	487	GLN	2.8
1	B	352	ASP	2.8
1	A	351	LYS	2.8
1	A	505	CYS	2.7
1	A	616	LEU	2.7
1	A	625	TRP	2.6
1	A	667	ARG	2.6
1	A	490	GLY	2.6
1	B	321	THR	2.6
1	A	601	ASN	2.6
1	A	373	GLY	2.6
1	A	556	ASP	2.6
1	A	482	TYR	2.6
1	A	706	TYR	2.5
1	A	374	SER	2.5
1	A	533	LEU	2.5
1	B	625	TRP	2.4
1	A	496	PRO	2.4
1	A	653	SER	2.4
1	A	352	ASP	2.4
1	A	557	LEU	2.4
1	A	486	LYS	2.4
1	A	318	LEU	2.3
1	A	516	ARG	2.3
1	A	558	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	619	ARG	2.3
1	B	718	GLY	2.3
1	B	337	LEU	2.2
1	B	610	VAL	2.2
1	A	301	LEU	2.2
1	A	607	LEU	2.2
1	B	318	LEU	2.2
1	A	320	SER	2.2
1	A	489	ASP	2.1
1	A	559	LEU	2.1
1	A	370	LYS	2.1
1	B	667	ARG	2.1
1	A	710	PRO	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($\text{\AA}^2$)	Q<0.9
4	JM4	A	800[A]	17/17	0.88	0.15	42,47,51,53	12
4	JM4	A	800[B]	17/17	0.88	0.15	48,49,51,53	12
4	JM4	B	800[A]	17/17	0.88	0.15	43,47,49,50	12
4	JM4	B	800[B]	17/17	0.88	0.15	47,51,62,63	12
5	ACT	A	860	4/4	0.89	0.12	65,67,67,68	0
3	H4B	B	760	17/17	0.94	0.07	27,30,34,34	0
3	H4B	A	760	17/17	0.95	0.06	27,29,35,36	0
5	ACT	B	860	4/4	0.95	0.10	50,50,51,51	0
2	HEM	A	750	43/43	0.98	0.07	26,30,35,37	0
2	HEM	B	750	43/43	0.98	0.07	24,29,35,37	0

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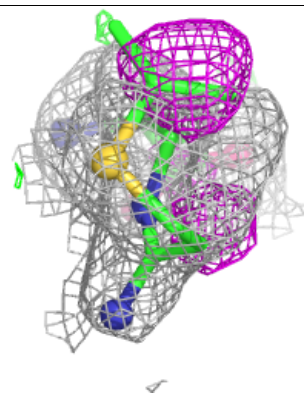
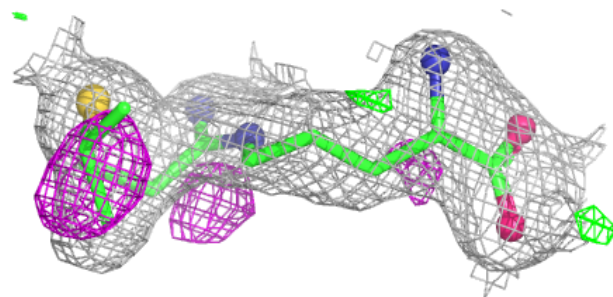
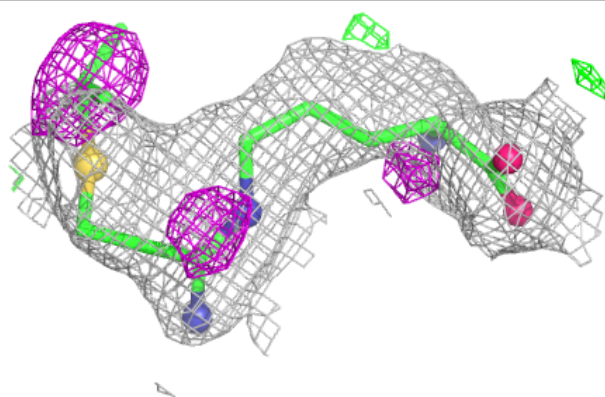
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ZN	A	900	1/1	0.99	0.02	34,34,34,34	0

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.

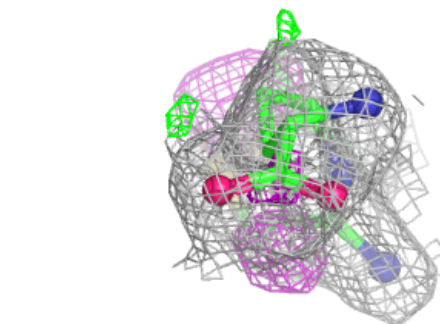
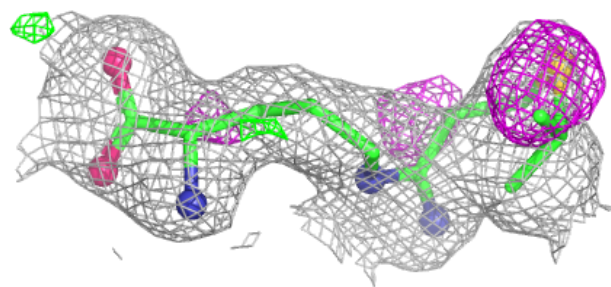
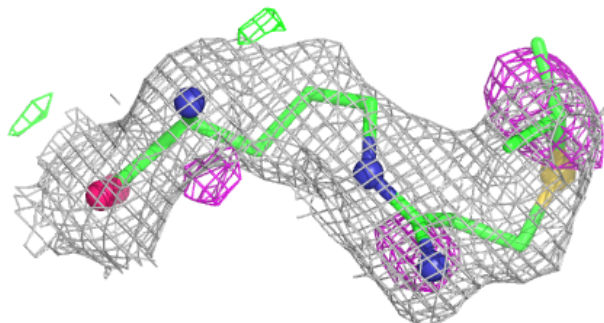
Electron density around JM4 A 800 (A):

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

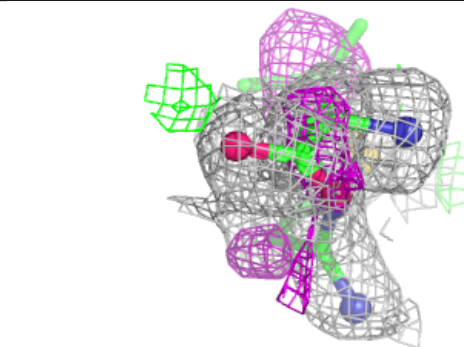
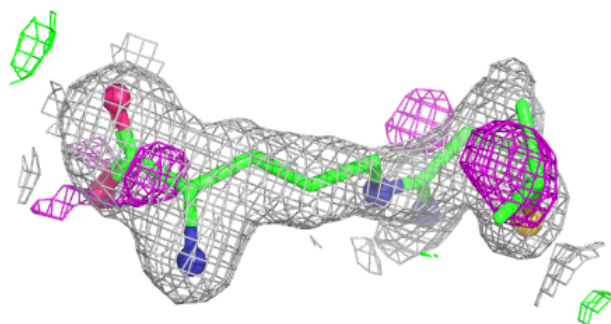
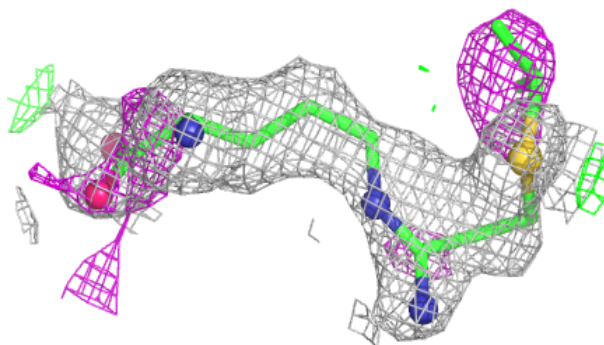


Electron density around JM4 A 800 (B):

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

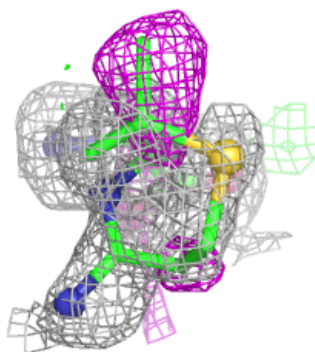
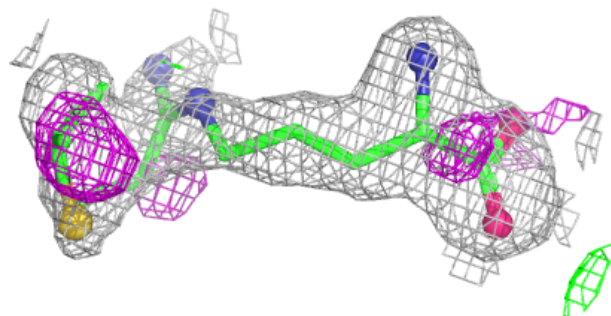
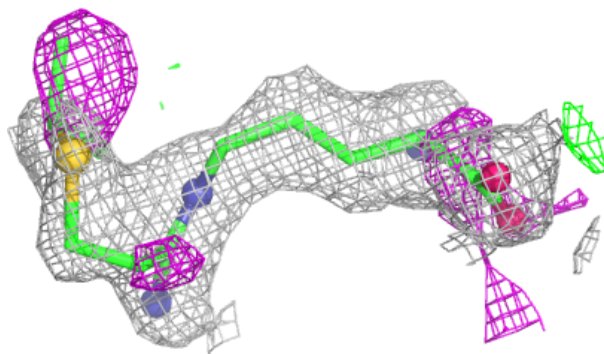
**Electron density around JM4 B 800 (A):**

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



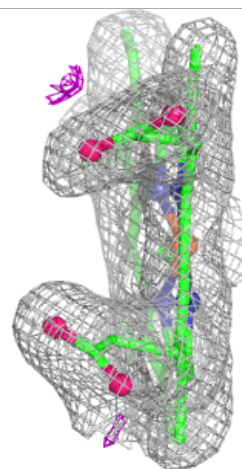
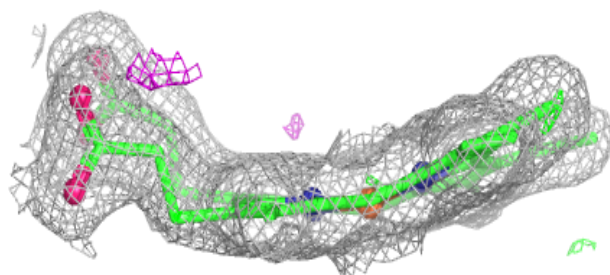
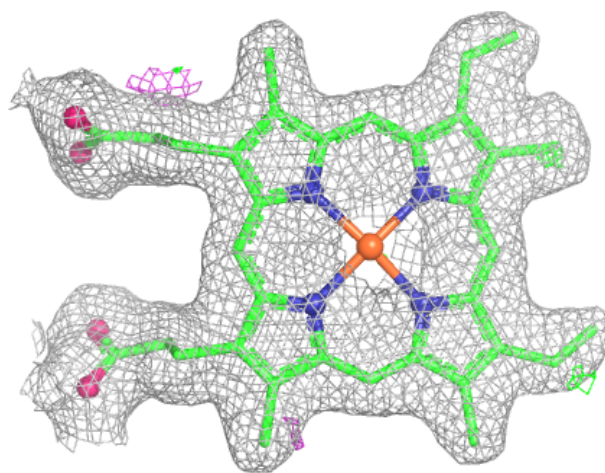
Electron density around JM4 B 800 (B):

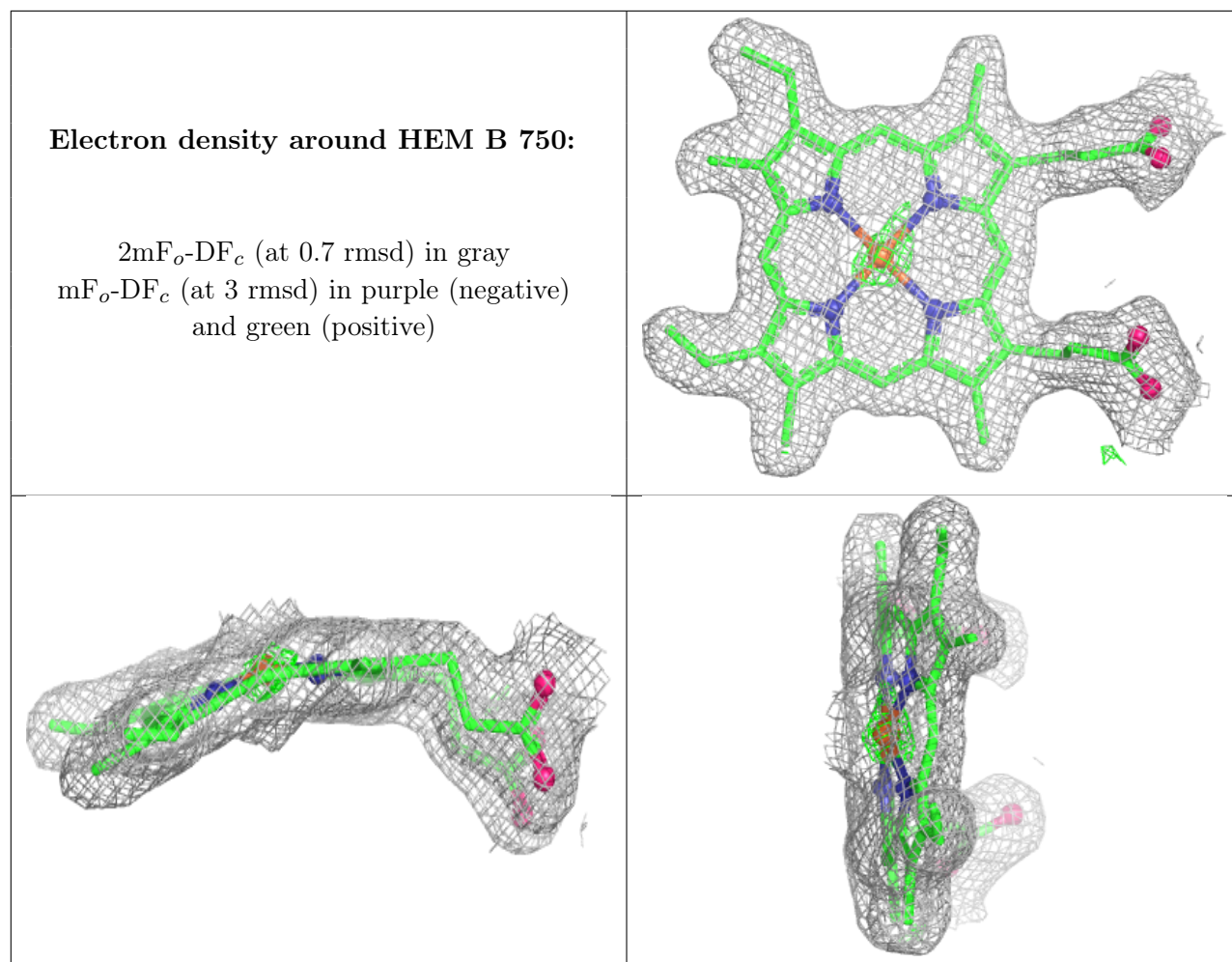
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 750:

$2mF_o-DF_c$ (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.