



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2024 – 08:28 pm BST

PDB ID : 5AGO
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with
(S)-2-Amino-5-(2-mercaptoacetimidamido)pentanoic acid
Authors : Li, H.; Poulos, T.L.
Deposited on : 2015-02-02
Resolution : 1.90 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

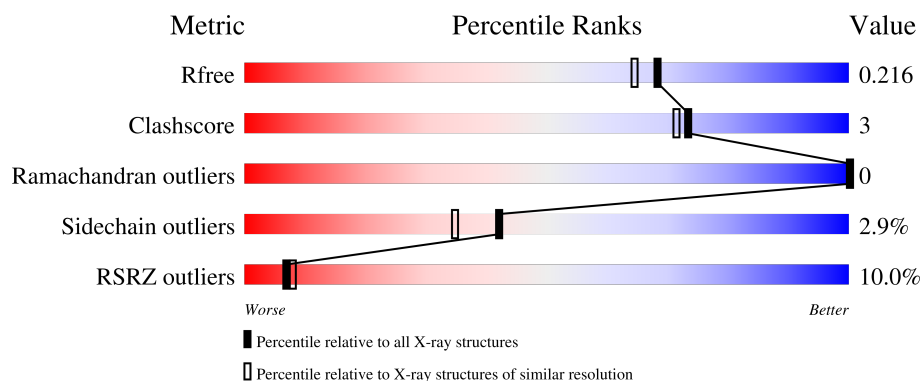
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	<div> <div>14%</div> <div>87%</div> <div>9%</div> <div>••</div> </div>
1	B	422	<div> <div>6%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7426 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.

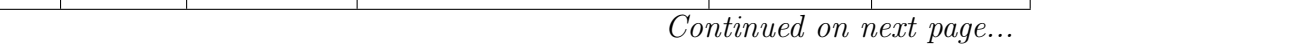
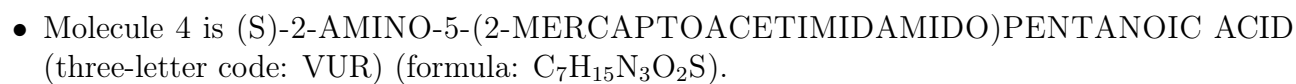
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	4	1
			3329	2131	567	609	22			
1	B	411	Total	C	N	O	S	0	4	0
			3360	2150	574	614	22			

- 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 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			17	9	4	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	1
			17	9	4	2	2		

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

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

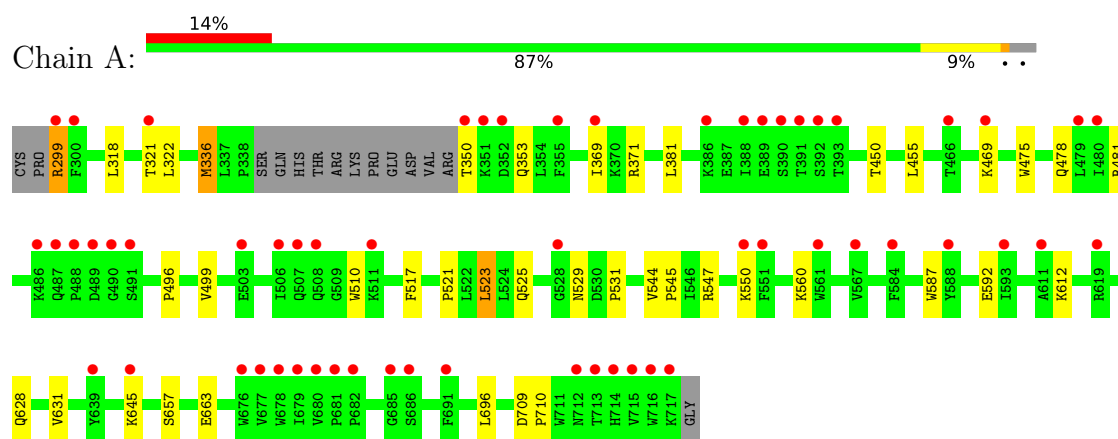
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	267	Total	O	0	0
			267	267		
7	B	307	Total	O	0	0
			307	307		

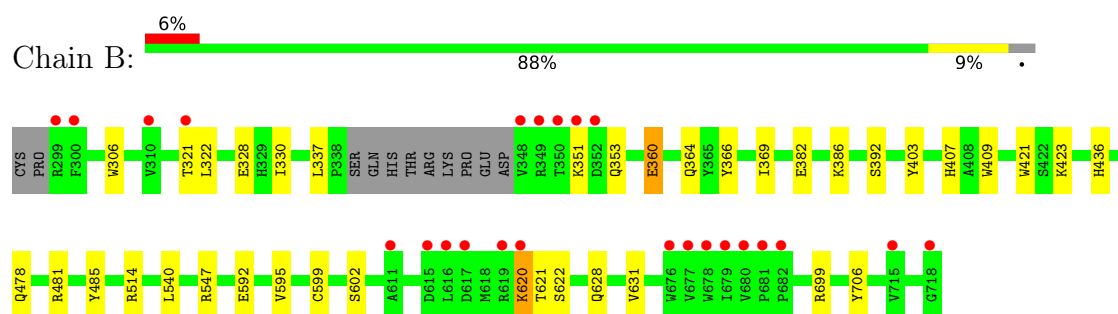
3 Residue-property plots [i](#)

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	51.95Å 110.66Å 164.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.95 – 1.90 38.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.95-1.90) 99.1 (38.95-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.176 , 0.215 0.178 , 0.216	Depositor DCC
R_{free} test set	3723 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7426	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 4.43% 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: HEM, H4B, ACT, VUR, 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	0.35	0/3434	0.50	0/4659
1	B	0.37	0/3465	0.50	0/4697
All	All	0.36	0/6899	0.50	0/9356

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	3329	0	3242	23	0
1	B	3360	0	3280	21	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	17	0	8	0	0
4	B	17	0	8	0	0
5	A	4	0	3	0	0
5	B	4	0	3	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	267	0	0	2	0
7	B	307	0	0	3	0
All	All	7426	0	6634	45	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 3.

All (45) 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:523:LEU:HD22	1:A:531:PRO:HB2	1.70	0.73
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.74	0.69
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.74	0.68
2:B:750:HEM:HMC2	2:B:750:HEM:HBC2	1.77	0.66
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.78	0.66
7:A:2008:HOH:O	1:B:602[B]:SER:OG	2.14	0.65
1:A:369:ILE:HG13	1:A:371:ARG:HG3	1.77	0.64
1:A:657[B]:SER:OG	7:A:2068:HOH:O	2.14	0.64
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.63	0.64
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.81	0.63
1:B:620:LYS:HD3	1:B:622:SER:H	1.68	0.58
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.86	0.58
1:A:350:THR:N	1:A:353:GLN:OE1	2.38	0.57
1:B:360:GLU:OE1	1:B:364:GLN:NE2	2.38	0.56
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.89	0.55
1:B:706:TYR:OH	2:B:750:HEM:O2D	2.17	0.53
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.94	0.49
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.97	0.47
1:B:620:LYS:HD3	1:B:621:THR:N	2.30	0.46
1:A:525:GLN:HG3	1:A:529:ASN:O	2.17	0.45
1:B:485:TYR:CE2	1:B:514:ARG:HA	2.51	0.45
1:B:366:TYR:HA	1:B:369:ILE:HG12	1.99	0.45
1:A:321:THR:HG23	1:A:322:LEU:HD12	1.99	0.44
1:B:595:VAL:O	1:B:599:CYS:HB2	2.18	0.44
1:A:299:ARG:HD2	1:A:318:LEU:HD21	1.99	0.44
1:B:382:GLU:O	1:B:386:LYS:HG3	2.18	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.43
1:A:336:MET:HE2	1:A:336:MET:HB3	1.96	0.43
1:A:517:PHE:HB2	1:A:560:LYS:HE3	2.01	0.42
1:B:436:HIS:HB2	7:B:2104:HOH:O	2.19	0.42
1:A:696:LEU:HB3	1:B:330:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:HA	1:A:455:LEU:HD22	2.01	0.41
5:B:860:ACT:H1	7:B:2088:HOH:O	2.20	0.41
1:B:386:LYS:NZ	7:B:2051:HOH:O	2.53	0.41
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.55	0.41
1:A:709:ASP:HA	1:A:710:PRO:HD3	1.91	0.41
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.32	0.41
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.36	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.02	0.41
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.56	0.41
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.97	0.40
1:A:628:GLN:HG2	1:B:631:VAL:HG11	2.03	0.40
1:A:475:TRP:CE2	1:A:710:PRO:HB2	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	411/422 (97%)	404 (98%)	7 (2%)	0	100	100
All	All	819/844 (97%)	801 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/377 (97%)	357 (97%)	10 (3%)	44	38
1	B	370/377 (98%)	359 (97%)	11 (3%)	41	33
All	All	737/754 (98%)	716 (97%)	21 (3%)	42	36

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ARG
1	A	336	MET
1	A	381	LEU
1	A	469	LYS
1	A	523	LEU
1	A	547	ARG
1	A	550	LYS
1	A	612	LYS
1	A	645	LYS
1	A	663	GLU
1	B	321	THR
1	B	328	GLU
1	B	337	LEU
1	B	351	LYS
1	B	353	GLN
1	B	360	GLU
1	B	392	SER
1	B	423	LYS
1	B	540	LEU
1	B	547	ARG
1	B	620	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	VUR	A	800[B]	-	8,12,12	3.17	2 (25%)	10,14,14	1.32	1 (10%)
3	H4B	A	760	-	16,18,18	0.91	0	11,26,26	2.51	4 (36%)
5	ACT	A	860	-	3,3,3	0.78	0	3,3,3	0.72	0
2	HEM	B	750	1	41,50,50	1.89	7 (17%)	45,82,82	2.02	9 (20%)
2	HEM	A	750	1	41,50,50	1.90	6 (14%)	45,82,82	2.05	9 (20%)
3	H4B	B	760	-	16,18,18	0.91	0	11,26,26	2.43	5 (45%)
4	VUR	B	800[B]	-	8,12,12	3.16	2 (25%)	10,14,14	1.33	1 (10%)
5	ACT	B	860	-	3,3,3	0.68	0	3,3,3	0.86	0
4	VUR	A	800[A]	-	8,12,12	3.19	2 (25%)	10,14,14	1.35	1 (10%)
4	VUR	B	800[A]	-	8,12,12	3.18	2 (25%)	10,14,14	1.34	1 (10%)

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	VUR	A	800[B]	-	-	4/11/13/13	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1	-	1/12/54/54	-
2	HEM	A	750	1	-	1/12/54/54	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	VUR	B	800[B]	-	-	3/11/13/13	-
4	VUR	A	800[A]	-	-	4/11/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	VUR	B	800[A]	-	-	3/11/13/13	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800[A]	VUR	CD-NE	-8.47	1.26	1.46
4	A	800[B]	VUR	CD-NE	-8.47	1.26	1.46
4	B	800[A]	VUR	CD-NE	-8.44	1.26	1.46
4	B	800[B]	VUR	CD-NE	-8.44	1.26	1.46
2	A	750	HEM	C3D-C2D	7.69	1.53	1.36
2	B	750	HEM	C3D-C2D	7.60	1.52	1.36
2	B	750	HEM	C3C-C2C	-3.77	1.35	1.40
2	A	750	HEM	C3C-CAC	3.77	1.55	1.47
2	B	750	HEM	C3C-CAC	3.66	1.55	1.47
2	A	750	HEM	C3C-C2C	-3.41	1.35	1.40
2	A	750	HEM	CAB-C3B	3.03	1.55	1.47
2	B	750	HEM	CAB-C3B	2.83	1.55	1.47
2	A	750	HEM	FE-NB	2.60	2.09	1.96
4	B	800[A]	VUR	C1-NH	2.54	1.34	1.27
4	A	800[A]	VUR	C1-NH	2.48	1.34	1.27
4	B	800[B]	VUR	C1-NH	2.32	1.33	1.27
4	A	800[B]	VUR	C1-NH	2.31	1.33	1.27
2	A	750	HEM	CMD-C2D	2.25	1.55	1.50
2	B	750	HEM	CMD-C2D	2.20	1.55	1.50
2	B	750	HEM	CMB-C2B	2.19	1.55	1.50
2	B	750	HEM	C3B-C2B	-2.00	1.33	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-7.29	100.18	112.62
2	A	750	HEM	CBA-CAA-C2A	-7.07	100.56	112.62
2	A	750	HEM	C4D-ND-C1D	6.17	111.45	105.07
3	A	760	H4B	C8A-C4A-C4	5.66	119.59	114.57
2	B	750	HEM	C4D-ND-C1D	5.34	110.59	105.07
3	B	760	H4B	C8A-C4A-C4	4.87	118.89	114.57
2	B	750	HEM	C4B-CHC-C1C	4.26	128.17	122.56
2	A	750	HEM	C4B-CHC-C1C	3.79	127.56	122.56
2	A	750	HEM	CBD-CAD-C3D	-3.44	103.07	112.63
3	B	760	H4B	C2-N3-C4	3.34	121.24	115.93
3	B	760	H4B	N1-C2-N3	-3.14	120.50	125.42
4	B	800[A]	VUR	CG-CD-NE	3.11	121.11	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800[B]	VUR	CG-CD-NE	3.11	121.11	112.21
2	B	750	HEM	CBD-CAD-C3D	-3.06	104.12	112.63
3	A	760	H4B	N1-C2-N3	-3.02	120.68	125.42
2	B	750	HEM	CMD-C2D-C1D	2.99	129.59	125.04
3	A	760	H4B	C2-N1-C8A	2.86	120.95	114.54
4	A	800[A]	VUR	CG-CD-NE	2.83	120.31	112.21
4	A	800[B]	VUR	CG-CD-NE	2.83	120.31	112.21
3	B	760	H4B	N2-C2-N1	2.58	121.27	117.25
2	A	750	HEM	CMC-C2C-C3C	2.55	129.46	124.68
3	A	760	H4B	C2-N3-C4	2.53	119.95	115.93
2	B	750	HEM	CAD-C3D-C4D	2.47	128.97	124.66
3	B	760	H4B	C2-N1-C8A	2.40	119.93	114.54
2	A	750	HEM	CMD-C2D-C1D	2.40	128.69	125.04
2	A	750	HEM	C4C-CHD-C1D	2.34	125.64	122.56
2	A	750	HEM	C3B-C2B-C1B	2.30	108.19	106.49
2	B	750	HEM	C3B-C2B-C1B	2.12	108.06	106.49
2	B	750	HEM	C1D-C2D-C3D	-2.10	104.75	106.96
2	A	750	HEM	C1B-NB-C4B	2.09	107.23	105.07
2	B	750	HEM	C4C-CHD-C1D	2.05	125.26	122.56

There are no chirality outliers.

All (16) torsion outliers are listed below:

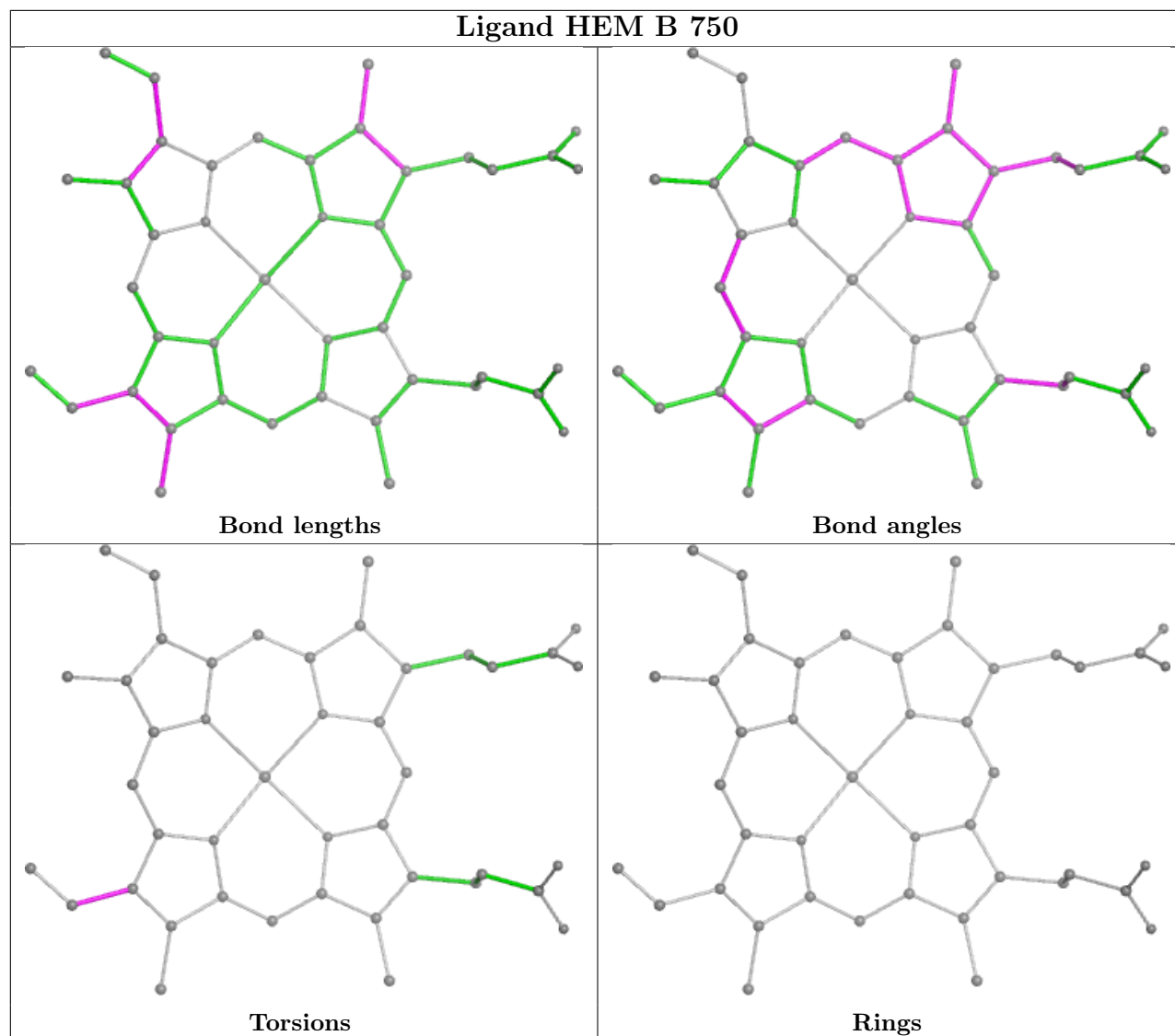
Mol	Chain	Res	Type	Atoms
4	A	800[A]	VUR	C2-C1-NE-CD
4	A	800[A]	VUR	NH-C1-NE-CD
4	A	800[B]	VUR	C2-C1-NE-CD
4	A	800[B]	VUR	NH-C1-NE-CD
4	B	800[A]	VUR	C2-C1-NE-CD
4	B	800[A]	VUR	NH-C1-NE-CD
4	B	800[B]	VUR	C2-C1-NE-CD
4	B	800[B]	VUR	NH-C1-NE-CD
4	A	800[A]	VUR	CA-CB-CG-CD
4	A	800[B]	VUR	CA-CB-CG-CD
4	B	800[A]	VUR	CA-CB-CG-CD
4	B	800[B]	VUR	CA-CB-CG-CD
2	A	750	HEM	C4B-C3B-CAB-CBB
2	B	750	HEM	C4B-C3B-CAB-CBB
4	A	800[A]	VUR	NE-CD-CG-CB
4	A	800[B]	VUR	NE-CD-CG-CB

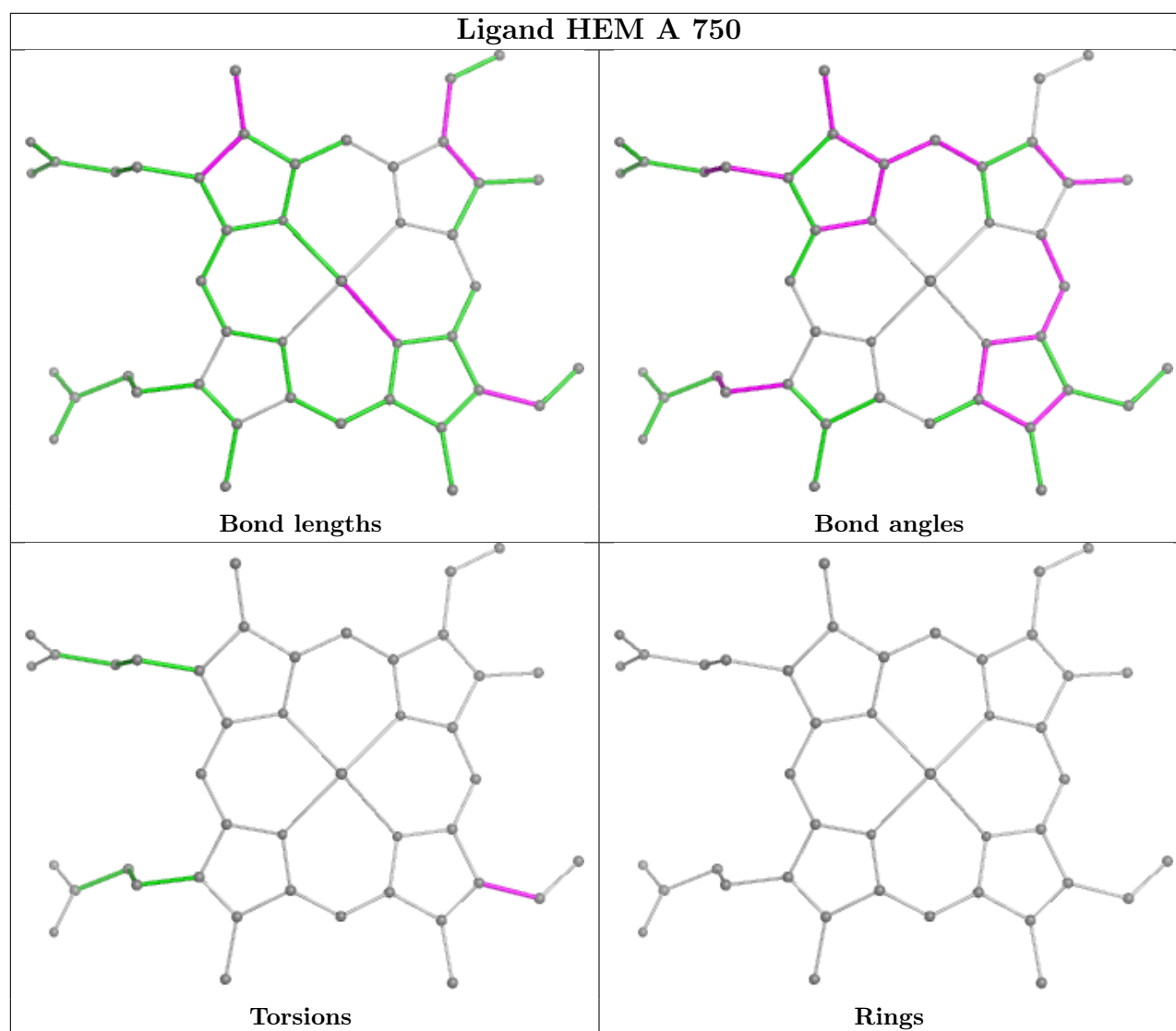
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	3	0
2	A	750	HEM	2	0
5	B	860	ACT	1	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	408/422 (96%)	0.61	58 (14%) 2 2	13, 31, 65, 99	0
1	B	411/422 (97%)	0.13	24 (5%) 23 25	11, 24, 53, 94	0
All	All	819/844 (97%)	0.37	82 (10%) 7 8	11, 27, 63, 99	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	9.0
1	A	299	ARG	7.6
1	A	715	VAL	7.4
1	B	300	PHE	7.3
1	A	716	TRP	7.1
1	A	717	LYS	6.5
1	B	350	THR	6.0
1	A	506	ILE	5.4
1	A	488	PRO	4.9
1	A	351	LYS	4.9
1	A	352	ASP	4.9
1	A	300	PHE	4.8
1	B	352	ASP	4.5
1	B	718	GLY	4.2
1	A	489	ASP	4.0
1	B	351	LYS	3.8
1	A	350	THR	3.7
1	A	551	PHE	3.7
1	B	619	ARG	3.7
1	A	713	THR	3.7
1	A	677	VAL	3.6
1	B	677	VAL	3.6
1	A	389	GLU	3.6
1	B	611	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	550	LYS	3.4
1	B	616	LEU	3.4
1	B	615	ASP	3.4
1	A	676	TRP	3.3
1	A	678	TRP	3.2
1	A	511	LYS	3.2
1	A	388	ILE	3.2
1	A	507	GLN	3.2
1	A	712	ASN	3.2
1	A	321	THR	3.1
1	B	321	THR	2.9
1	A	567	VAL	2.9
1	A	393	THR	2.8
1	A	390	SER	2.8
1	A	593	ILE	2.8
1	A	685	GLY	2.7
1	B	299	ARG	2.7
1	B	715	VAL	2.7
1	A	679	ILE	2.7
1	A	508	GLN	2.6
1	A	619	ARG	2.6
1	A	714	HIS	2.6
1	A	480	ILE	2.6
1	A	491	SER	2.6
1	B	678	TRP	2.6
1	B	620	LYS	2.6
1	A	487	GLN	2.6
1	A	391	THR	2.5
1	A	469	LYS	2.5
1	B	349	ARG	2.5
1	A	680	VAL	2.5
1	A	392	SER	2.4
1	A	611	ALA	2.4
1	A	490	GLY	2.4
1	A	355	PHE	2.4
1	A	588	TYR	2.4
1	A	682	PRO	2.4
1	A	503	GLU	2.3
1	B	617	ASP	2.3
1	B	682	PRO	2.3
1	A	645	LYS	2.3
1	A	584	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	681	PRO	2.2
1	B	310	VAL	2.2
1	A	479	LEU	2.2
1	A	528	GLY	2.2
1	A	681	PRO	2.2
1	A	691	PHE	2.2
1	A	466	THR	2.1
1	A	486	LYS	2.1
1	B	676	TRP	2.1
1	A	369	ILE	2.1
1	B	680	VAL	2.1
1	A	386	LYS	2.0
1	B	679	ILE	2.0
1	A	686	SER	2.0
1	A	639	TYR	2.0
1	A	561	TRP	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 monosaccharides 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.

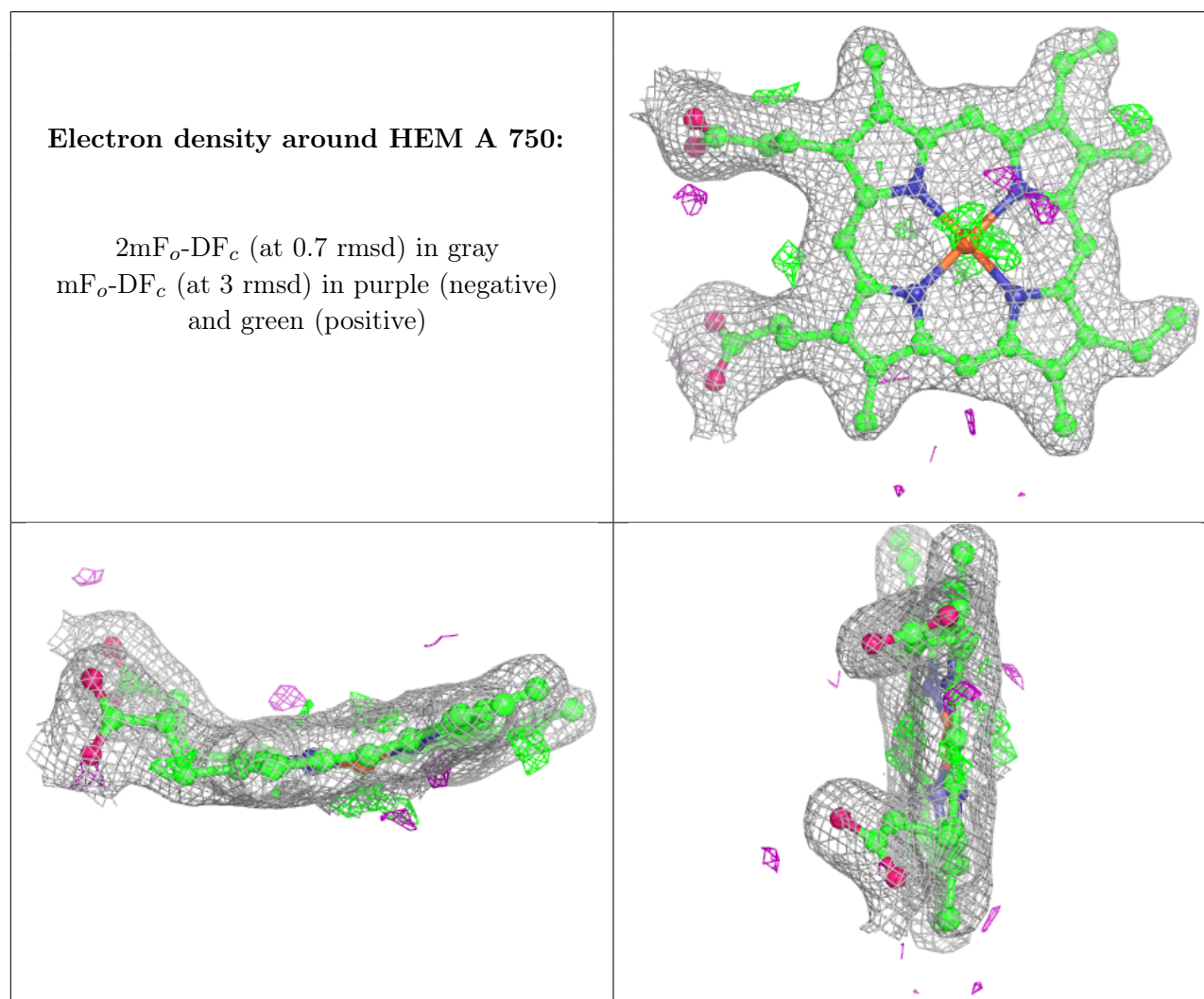
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	VUR	B	800[A]	13/13	0.78	0.27	30,45,54,61	4
4	VUR	B	800[B]	13/13	0.78	0.27	30,44,50,54	4
4	VUR	A	800[A]	13/13	0.82	0.40	36,46,58,66	4
4	VUR	A	800[B]	13/13	0.82	0.40	29,46,58,66	4
5	ACT	B	860	4/4	0.92	0.16	31,33,37,38	0
3	H4B	B	760	17/17	0.96	0.17	11,13,19,20	0
5	ACT	A	860	4/4	0.96	0.20	40,45,49,52	0

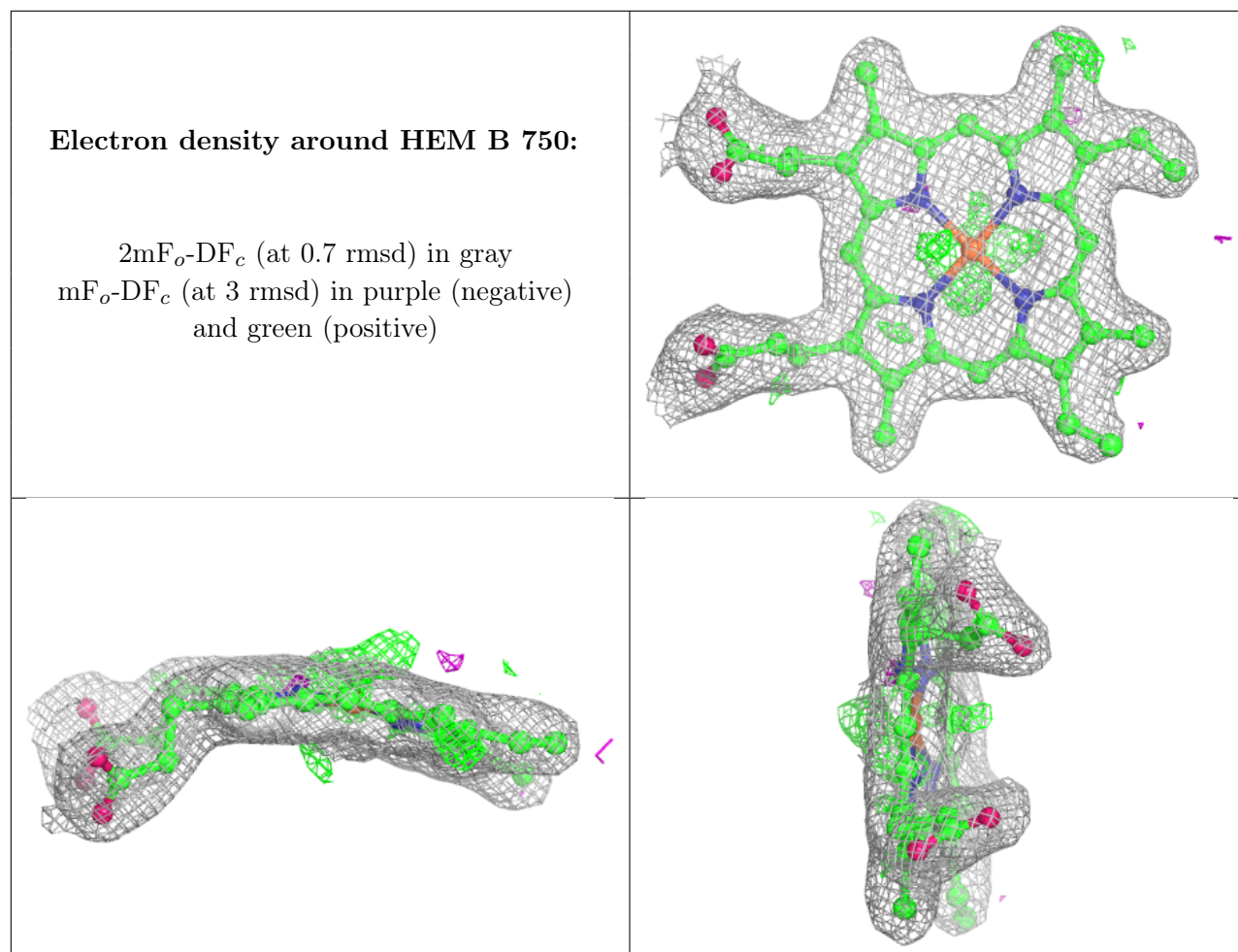
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	H4B	A	760	17/17	0.96	0.19	13,18,20,23	0
2	HEM	A	750	43/43	0.97	0.18	11,18,27,42	0
2	HEM	B	750	43/43	0.97	0.16	8,17,27,32	0
6	ZN	A	1717	1/1	0.99	0.07	18,18,18,18	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.