



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:30 pm BST

PDB ID : 5AD8
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with
7-((3-Aminomethyl)phenoxy)methyl)quinolin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2015-08-20
Resolution : 1.91 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

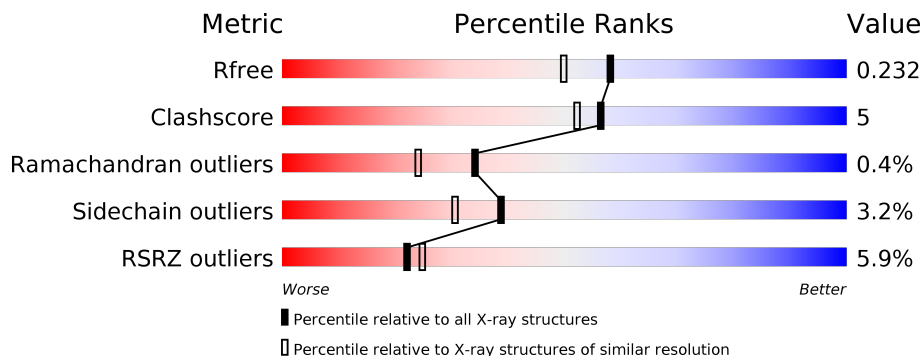
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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 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	 9% 80% 16%
1	B	422	 2% 89% 8%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7140 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
			Total	C	N	O	S			
1	A	408	Total 3317	C 2123	N 567	O 605	S 22	0	1	1
1	B	411	Total 3351	C 2144	N 574	O 612	S 21	0	2	0

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



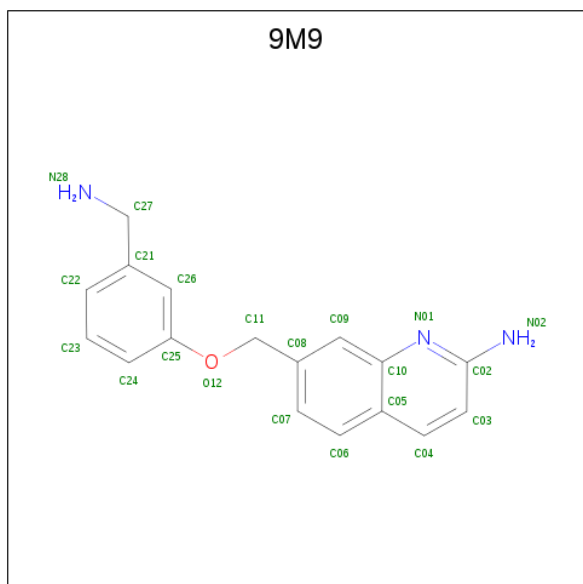
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 4 is 7-[[3-(aminomethyl)phenoxy]methyl]quinolin-2-amine (three-letter code: 9M9) (formula: $C_{17}H_{17}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	21	17	3	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	21	17	3	1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	128	128	128	0	0
7	B	173	173	173	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.93Å 111.86Å 164.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.13 – 1.91 47.10 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.13-1.91) 97.5 (47.10-1.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.91Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.232 0.190 , 0.232	Depositor DCC
R_{free} test set	3673 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtrriage
Anisotropy	0.897	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7140	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 9M9, HEM, ZN, H4B, ACT

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	0.36	0/3413	0.51	0/4631
1	B	0.37	0/3450	0.52	0/4677
All	All	0.37	0/6863	0.51	0/9308

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 [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	3317	0	3226	47	0
1	B	3351	0	3269	20	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	21	0	17	1	0
4	B	21	0	17	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	128	0	0	1	0
7	B	173	0	0	0	0
All	All	7140	0	6625	67	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 (67) 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	1.63	0.81
1:A:549:PRO:O	1:A:550:LYS:NZ	2.19	0.75
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.68	0.73
1:A:414:ARG:NH1	1:A:706:TYR:OH	2.25	0.70
2:B:750:HEM:HBC2	2:B:750:HEM:HMC2	1.74	0.70
1:B:350:THR:OG1	1:B:353:GLN:NE2	2.27	0.69
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.76	0.68
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.77	0.67
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.80	0.64
1:A:351:LYS:NZ	1:A:389:GLU:O	2.32	0.62
1:A:350:THR:N	1:A:353:GLN:OE1	2.35	0.60
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.69	0.58
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.85	0.58
1:B:414:ARG:NH1	1:B:706:TYR:OH	2.38	0.57
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.91	0.53
1:A:485:TYR:HE1	1:A:515:GLY:O	1.92	0.53
1:A:464:GLN:HB3	1:A:579:PHE:CE1	2.44	0.52
1:B:567:VAL:HG21	4:B:800:9M9:C07	2.39	0.52
1:A:513:PRO:O	1:A:515:GLY:N	2.43	0.51
1:A:393:THR:OG1	1:A:394:TYR:N	2.44	0.50
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.78	0.48
1:A:555:LYS:N	7:A:2084:HOH:O	2.45	0.48
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.95	0.48
1:A:517:PHE:HE1	1:A:604:TYR:CE1	2.31	0.48
1:B:596:ARG:O	1:B:600:ASP:HB2	2.13	0.48
1:A:517:PHE:HE2	1:A:559:LEU:HA	1.79	0.48
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.96	0.47
1:A:596:ARG:O	1:A:600:ASP:HB2	2.15	0.47
1:A:510:TRP:HB2	1:A:533:LEU:HD13	1.96	0.46
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.29	0.46
1:A:567:VAL:HG21	4:A:800:9M9:C07	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.31	0.46
1:A:465:ARG:NH1	1:A:578:GLU:OE1	2.44	0.45
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.31	0.45
1:B:351:LYS:HE2	1:B:389:GLU:HA	1.97	0.45
1:A:601:ASN:HB2	1:B:307:GLU:OE2	2.17	0.45
1:A:522:LEU:O	1:A:533:LEU:HA	2.17	0.44
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.53	0.44
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.06	0.44
1:A:511:LYS:HB3	1:A:511:LYS:HE2	1.70	0.44
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.00	0.43
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.43	0.43
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.82	0.43
1:B:322:LEU:HB2	1:B:699:ARG:HB2	2.01	0.43
1:B:317:HIS:O	1:B:320:SER:HB3	2.18	0.43
1:A:517:PHE:HE1	1:A:604:TYR:CZ	2.37	0.43
1:A:604:TYR:O	1:A:606:ILE:HG23	2.19	0.43
1:A:610:VAL:HG21	1:A:633:ILE:HD11	2.00	0.43
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.47	0.43
1:B:302:LYS:HB2	1:B:302:LYS:HE3	1.71	0.42
1:B:351:LYS:HB3	1:B:351:LYS:HE3	1.89	0.42
1:B:595:VAL:O	1:B:599:CYS:HB2	2.18	0.42
1:B:353:GLN:N	1:B:353:GLN:HE21	2.16	0.42
1:B:480:ILE:HD13	1:B:541:VAL:HG13	2.01	0.42
1:A:635:ILE:HG13	1:B:624:LEU:HD12	2.02	0.42
1:A:485:TYR:CZ	1:A:514:ARG:HA	2.55	0.41
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.01	0.41
1:A:709:ASP:HA	1:A:710:PRO:HD3	1.86	0.41
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.03	0.41
1:A:391:THR:O	1:A:392:SER:OG	2.31	0.41
1:A:451:ASN:HB3	1:A:454:ASN:O	2.21	0.41
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.56	0.41
1:A:486:LYS:HG3	1:A:499:VAL:HG11	2.03	0.40
1:B:501:PHE:HD2	1:B:520:LEU:HD13	1.86	0.40
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.50	0.40
1:A:494:GLY:O	1:A:496:PRO:HD3	2.21	0.40
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.49	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	405/422 (96%)	386 (95%)	16 (4%)	3 (1%)	22	12
1	B	409/422 (97%)	399 (98%)	10 (2%)	0	100	100
All	All	814/844 (96%)	785 (96%)	26 (3%)	3 (0%)	34	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ARG
1	A	491	SER
1	A	550	LYS

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	364/377 (97%)	353 (97%)	11 (3%)	41	33
1	B	368/377 (98%)	356 (97%)	12 (3%)	38	29
All	All	732/754 (97%)	709 (97%)	23 (3%)	39	32

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	THR
1	A	386	LYS
1	A	487	GLN

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Mol	Chain	Res	Type
1	A	523	LEU
1	A	547	ARG
1	A	550	LYS
1	A	552	ASP
1	A	555	LYS
1	A	601	ASN
1	A	612	LYS
1	A	645	LYS
1	B	320	SER
1	B	321	THR
1	B	337	LEU
1	B	351	LYS
1	B	353	GLN
1	B	382	GLU
1	B	392	SER
1	B	423	LYS
1	B	516	ARG
1	B	540	LEU
1	B	547	ARG
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	GLN
1	B	353	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry i

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
3	H4B	B	760	-	16,18,18	1.03	1 (6%)	11,26,26	2.43	5 (45%)
4	9M9	B	800	-	23,23,23	0.93	0	30,31,31	1.02	2 (6%)
2	HEM	B	750	1	27,50,50	2.16	5 (18%)	17,82,82	1.82	5 (29%)
3	H4B	A	760	-	16,18,18	0.85	0	11,26,26	2.54	5 (45%)
5	ACT	A	860	-	1,3,3	1.28	0	0,3,3	0.00	-
5	ACT	B	860	-	1,3,3	1.24	0	0,3,3	0.00	-
2	HEM	A	750	1	27,50,50	2.07	5 (18%)	17,82,82	2.12	5 (29%)
4	9M9	A	800	-	23,23,23	0.96	0	30,31,31	0.89	0

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	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	9M9	B	800	-	-	1/7/7/7	0/3/3/3
2	HEM	B	750	1	-	0/6/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	HEM	A	750	1	-	0/6/54/54	-
4	9M9	A	800	-	-	2/7/7/7	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	5.13	1.52	1.37
2	A	750	HEM	C3D-C2D	5.11	1.52	1.37
2	B	750	HEM	C3B-C2B	-4.24	1.34	1.40
2	A	750	HEM	C3B-C2B	-4.22	1.34	1.40
2	B	750	HEM	C3C-CAC	3.92	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3C-C2C	-3.91	1.34	1.40
2	A	750	HEM	C3C-C2C	-3.83	1.35	1.40
2	A	750	HEM	C3B-CAB	3.78	1.55	1.47
2	B	750	HEM	C3B-CAB	3.44	1.55	1.47
2	A	750	HEM	C3C-CAC	3.43	1.54	1.47
3	B	760	H4B	C4-C4A	-2.11	1.38	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-5.63	102.10	112.49
3	B	760	H4B	C4-C4A-C8A	5.04	119.05	114.57
3	A	760	H4B	C4-C4A-C8A	4.86	118.89	114.57
2	A	750	HEM	CAD-CBD-CGD	-4.08	105.82	112.67
2	B	750	HEM	CBA-CAA-C2A	-3.90	105.30	112.49
2	B	750	HEM	C1D-C2D-C3D	-3.58	104.51	107.00
3	A	760	H4B	N3-C2-N1	-3.50	119.94	125.42
3	A	760	H4B	C4-N3-C2	3.29	121.16	115.93
3	B	760	H4B	N3-C2-N1	-3.23	120.36	125.42
3	B	760	H4B	C4-N3-C2	2.81	120.39	115.93
3	A	760	H4B	C2-N1-C8A	2.77	120.75	114.54
2	A	750	HEM	C1D-C2D-C3D	-2.71	105.11	107.00
2	B	750	HEM	CAD-CBD-CGD	-2.70	108.14	112.67
3	B	760	H4B	C2-N1-C8A	2.62	120.41	114.54
4	B	800	9M9	C11-O12-C25	2.59	124.06	117.65
2	B	750	HEM	CMA-C3A-C4A	-2.43	124.72	128.46
2	B	750	HEM	CBD-CAD-C3D	-2.27	108.29	112.48
2	A	750	HEM	CMC-C2C-C3C	2.26	128.91	124.68
3	A	760	H4B	C4-C4A-N5	2.22	120.98	119.12
3	B	760	H4B	N2-C2-N3	2.14	120.58	117.25
4	B	800	9M9	C03-C02-N01	-2.13	119.52	122.08
2	A	750	HEM	C4C-C3C-C2C	2.04	108.32	106.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

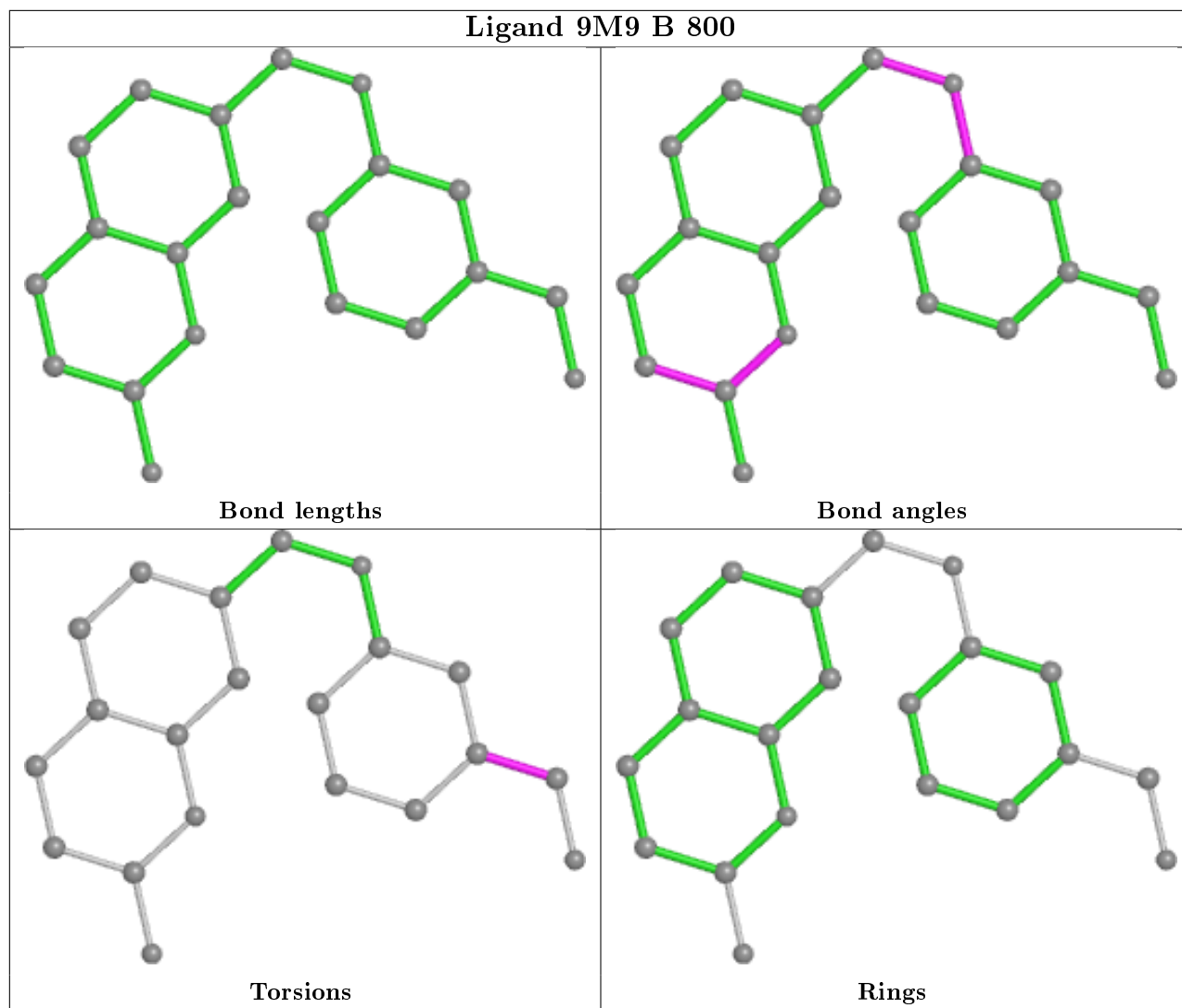
Mol	Chain	Res	Type	Atoms
4	A	800	9M9	C24-C25-O12-C11
4	A	800	9M9	C26-C25-O12-C11
4	B	800	9M9	C22-C21-C27-N28

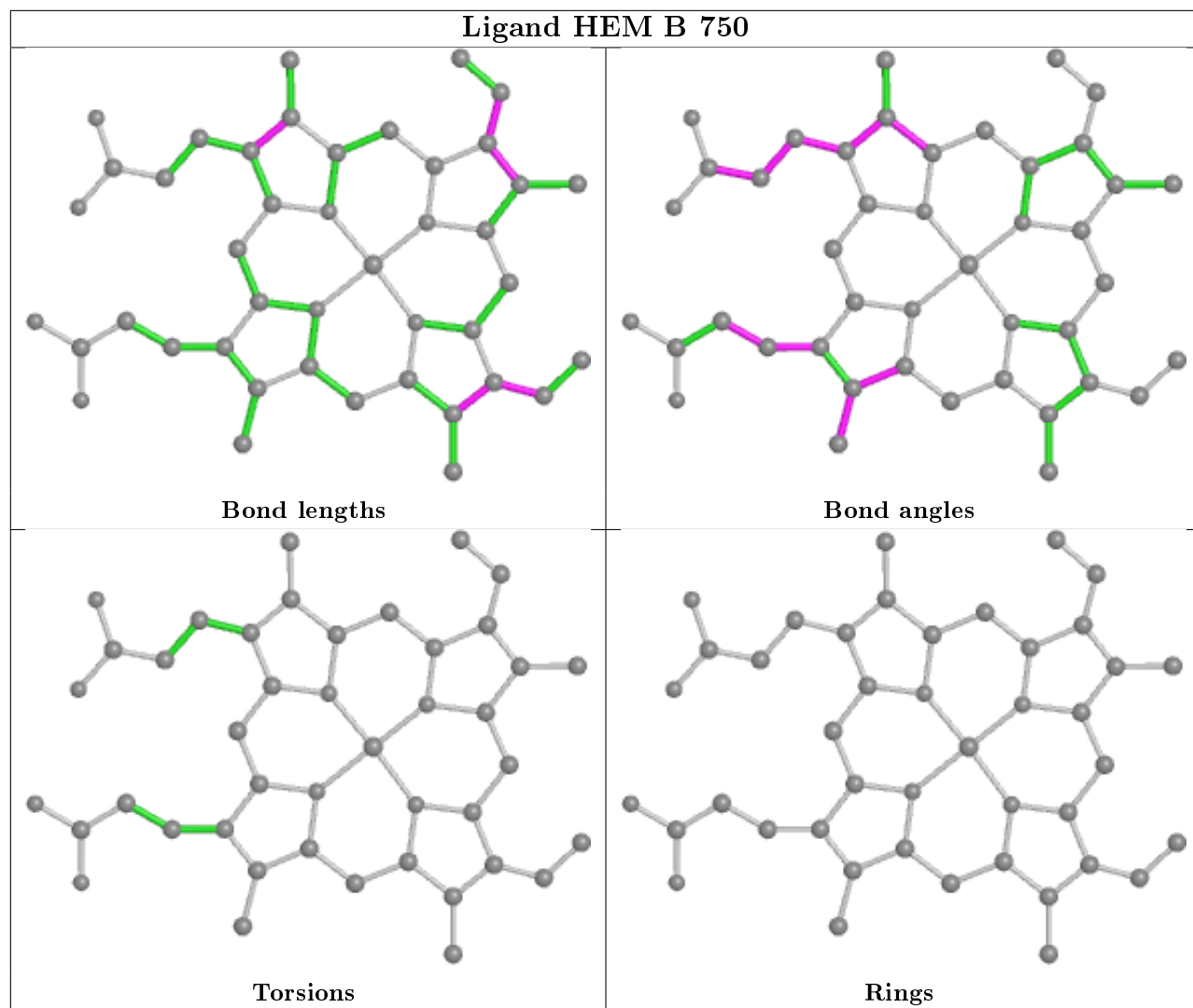
There are no ring outliers.

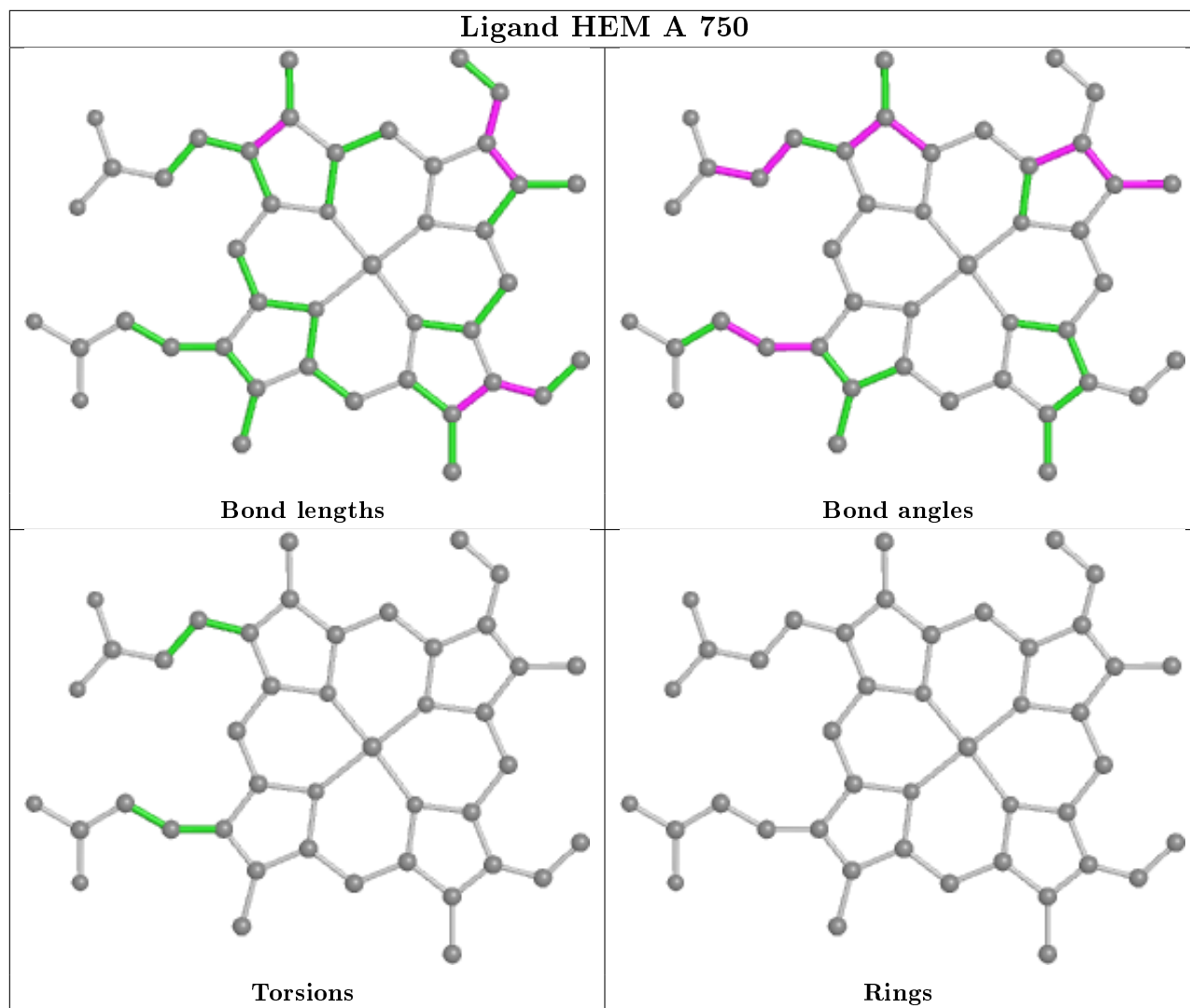
4 monomers are involved in 7 short contacts:

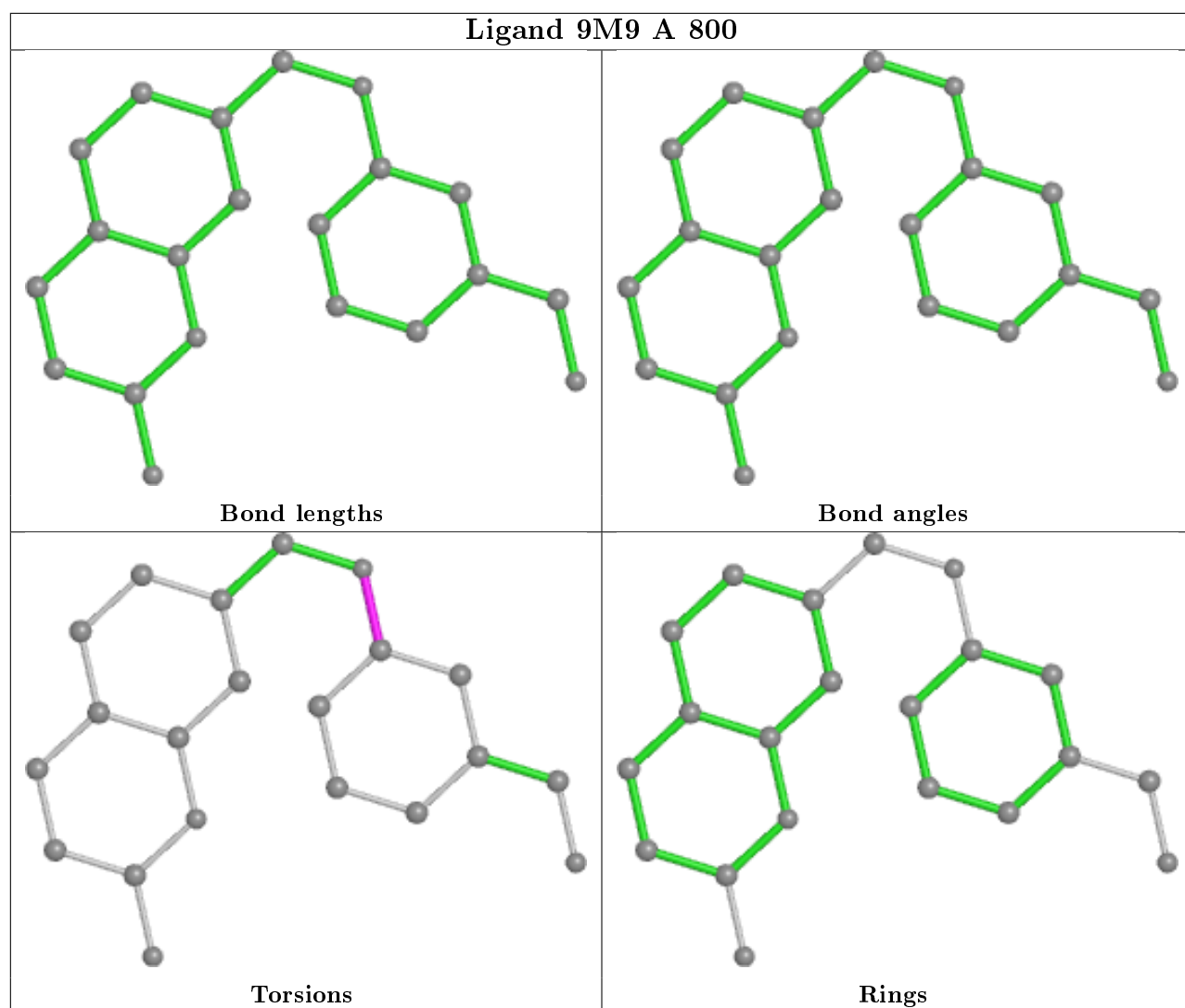
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	9M9	1	0
2	B	750	HEM	2	0
2	A	750	HEM	3	0
4	A	800	9M9	1	0

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%)	0.71	38 (9%) 8 10	19, 49, 100, 145	0
1	B	411/422 (97%)	0.36	10 (2%) 59 62	18, 39, 72, 103	0
All	All	819/844 (97%)	0.53	48 (5%) 22 25	18, 43, 92, 145	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	12.3
1	A	715	VAL	7.5
1	A	322	LEU	4.9
1	A	551	PHE	4.8
1	A	355	PHE	4.6
1	B	348	VAL	3.9
1	A	552	ASP	3.9
1	A	554	PHE	3.7
1	B	352	ASP	3.6
1	A	488	PRO	3.5
1	A	716	TRP	3.4
1	B	594	GLY	3.3
1	A	352	ASP	3.3
1	A	558	GLY	3.2
1	A	506	ILE	3.2
1	A	557	LEU	3.2
1	B	321	THR	3.2
1	A	599	CYS	3.2
1	A	493	LEU	3.1
1	A	494	GLY	3.1
1	B	718	GLY	3.0
1	A	386	LYS	2.9
1	B	350	THR	2.9
1	A	597	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	559	LEU	2.9
1	A	604	TYR	2.8
1	A	321	THR	2.8
1	A	388	ILE	2.8
1	B	355	PHE	2.8
1	A	553	TRP	2.7
1	A	389	GLU	2.7
1	B	337	LEU	2.6
1	A	351	LYS	2.5
1	A	470	HIS	2.5
1	A	598	TYR	2.5
1	A	300	PHE	2.4
1	A	609	GLU	2.4
1	B	389	GLU	2.4
1	A	556	ASP	2.4
1	A	606	ILE	2.3
1	A	381	LEU	2.3
1	A	619	ARG	2.2
1	A	328	GLU	2.2
1	A	354	LEU	2.2
1	A	486	LYS	2.1
1	B	300	PHE	2.1
1	A	373	GLY	2.0
1	A	608	GLU	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](#)

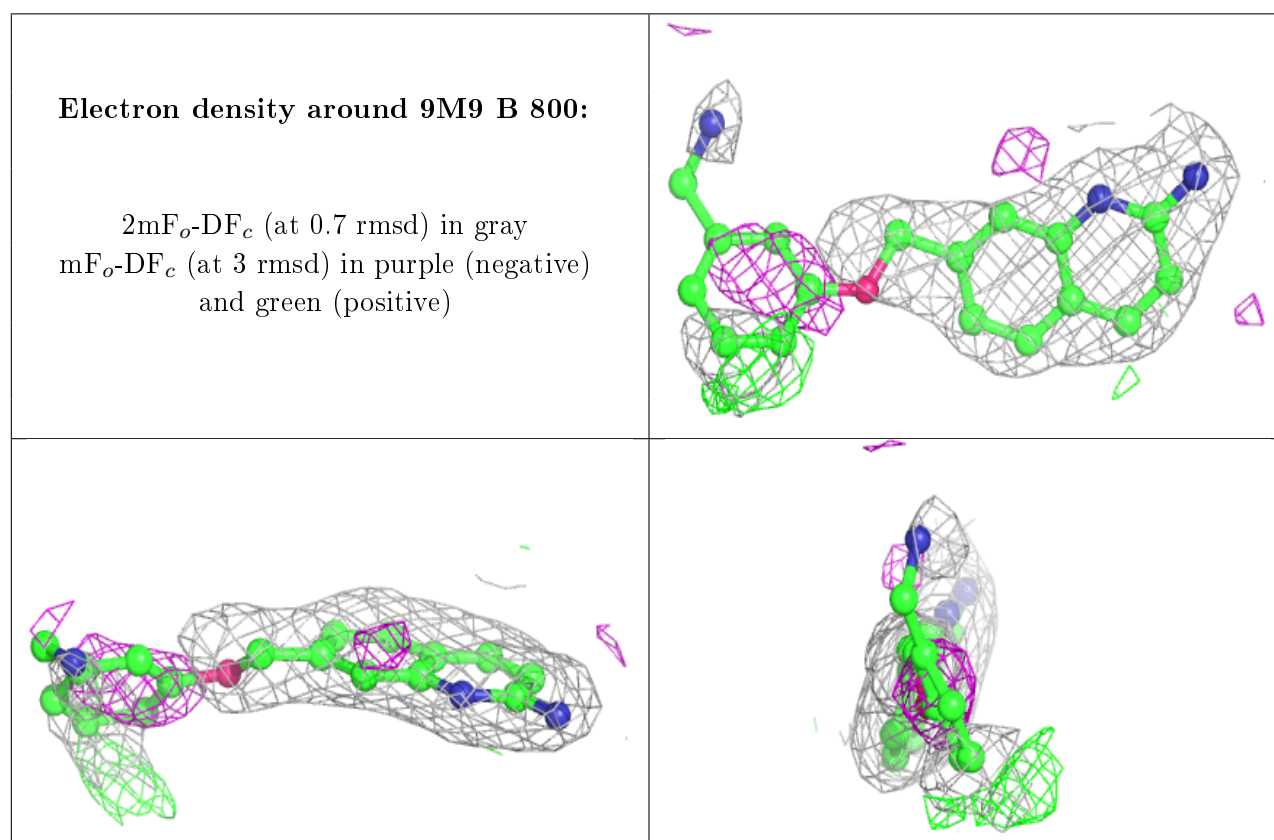
There are no carbohydrates in this entry.

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.

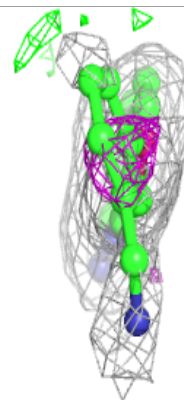
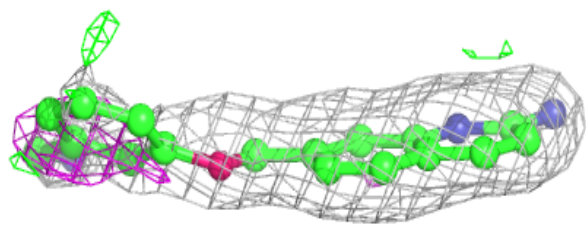
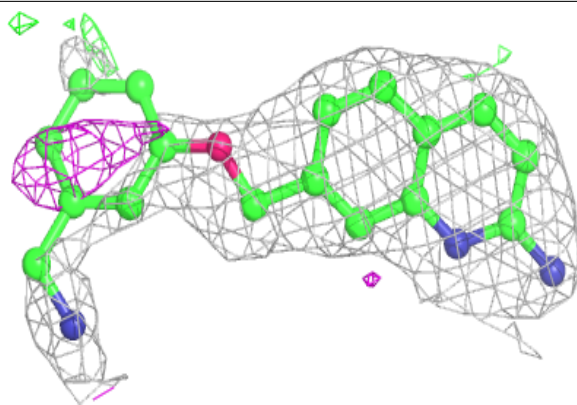
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	9M9	B	800	21/21	0.83	0.22	31,42,89,89	0
4	9M9	A	800	21/21	0.90	0.18	24,34,81,84	0
3	H4B	A	760	17/17	0.91	0.14	23,37,49,54	0
5	ACT	B	860	4/4	0.93	0.15	47,50,51,53	0
3	H4B	B	760	17/17	0.93	0.12	28,34,45,53	0
5	ACT	A	860	4/4	0.94	0.29	39,48,49,53	0
2	HEM	A	750	43/43	0.98	0.12	16,27,51,56	0
2	HEM	B	750	43/43	0.98	0.16	18,26,49,61	0
6	ZN	B	900	1/1	0.99	0.09	32,32,32,32	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.



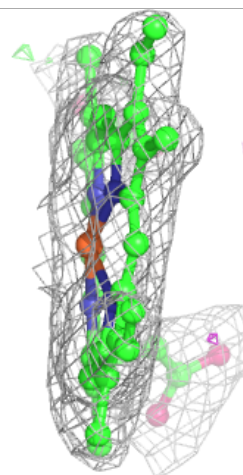
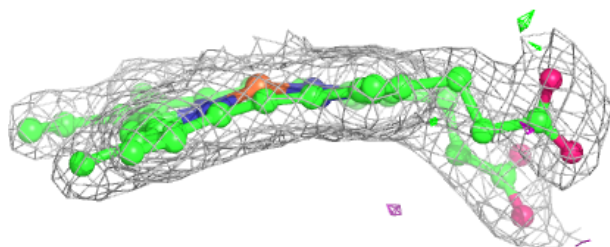
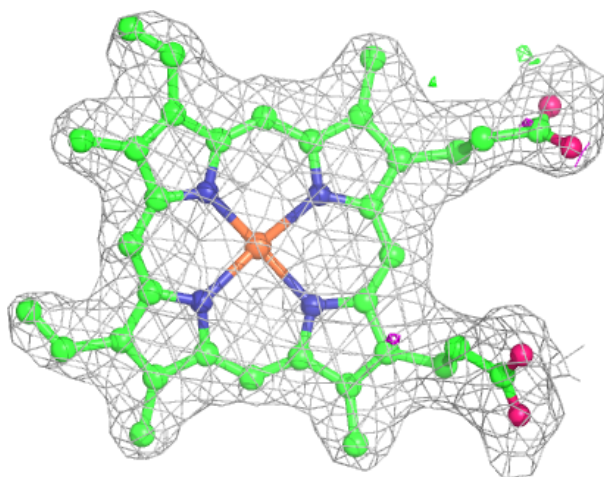
Electron density around 9M9 A 800:

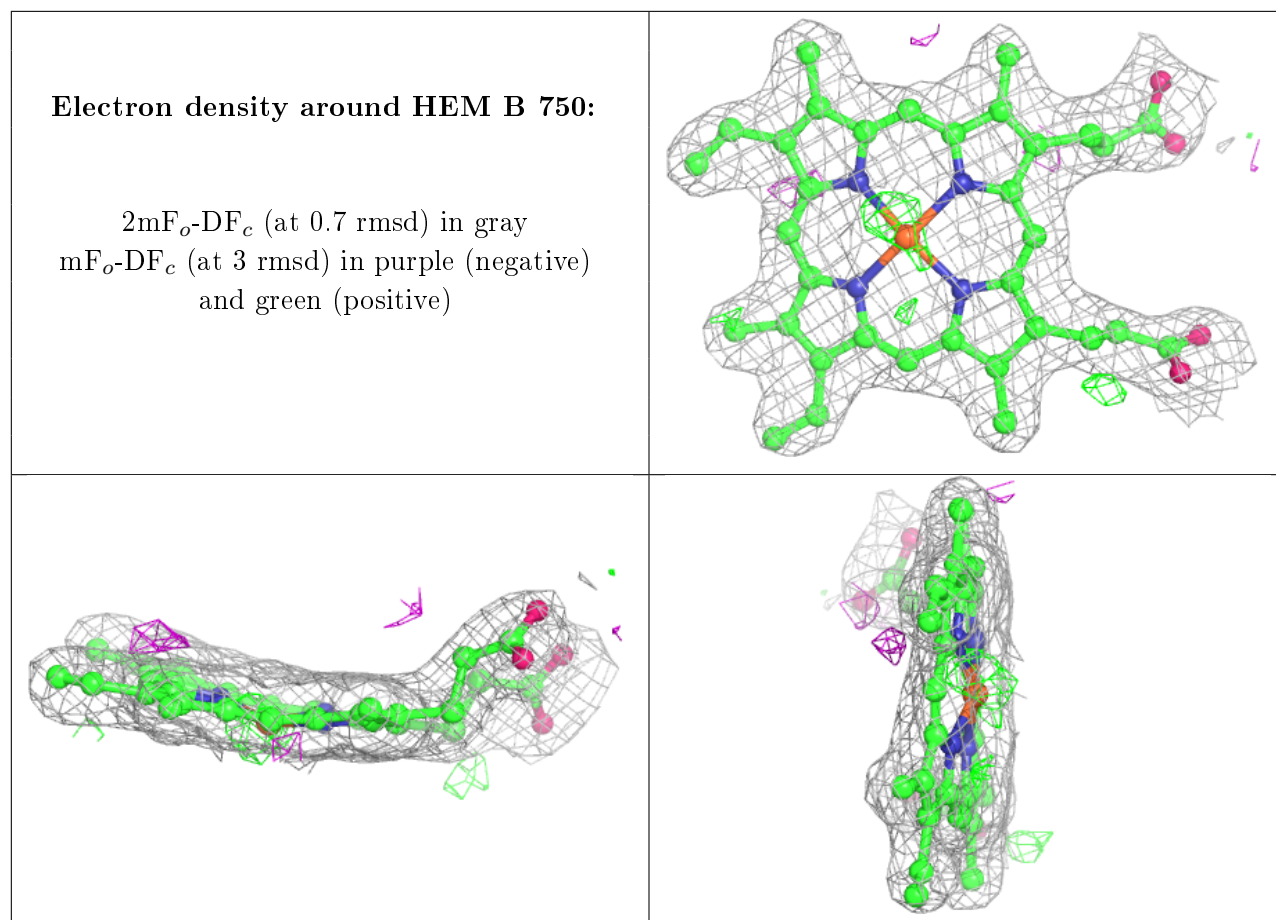
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 750:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.