



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:55 pm BST

PDB ID : 3PNG
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-((2-fluoro-2-(3-fluorophenyl)ethyl)amino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.; Poulos, T.L.
Deposited on : 2010-11-18
Resolution : 1.88 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

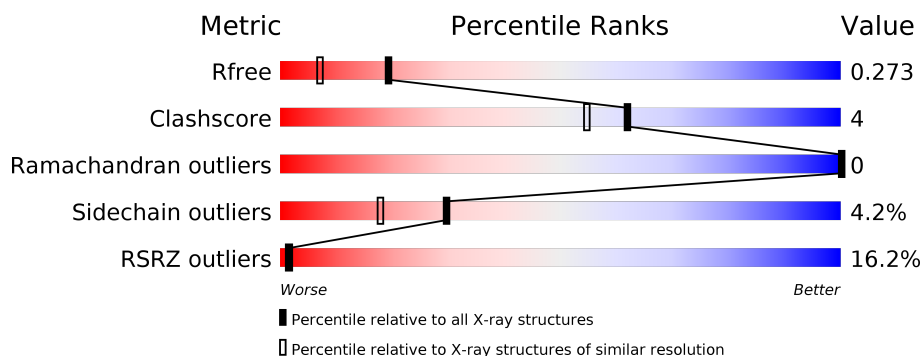
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	
1	B	422	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7240 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	409	Total	C	N	O	S	0	2	0
			3340	2138	571	609	22			
1	B	411	Total	C	N	O	S	0	2	0
			3357	2147	575	613	22			

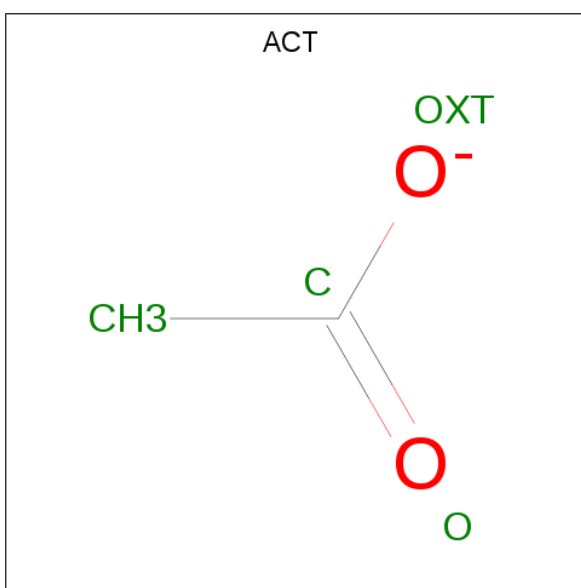
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





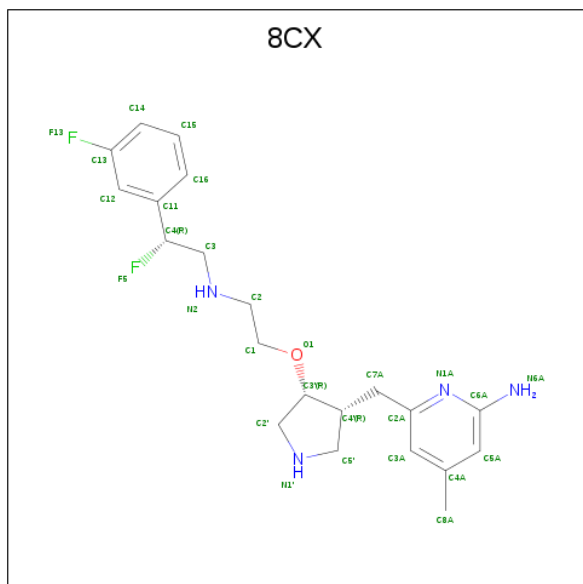
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 6-{[(3R,4R)-4-(2-{[(2R)-2-fluoro-2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: 8CX) (formula: $C_{21}H_{28}F_2N_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			28	21	2	4	1		
5	B	1	Total	C	F	N	O	0	0
			28	21	2	4	1		

- 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		

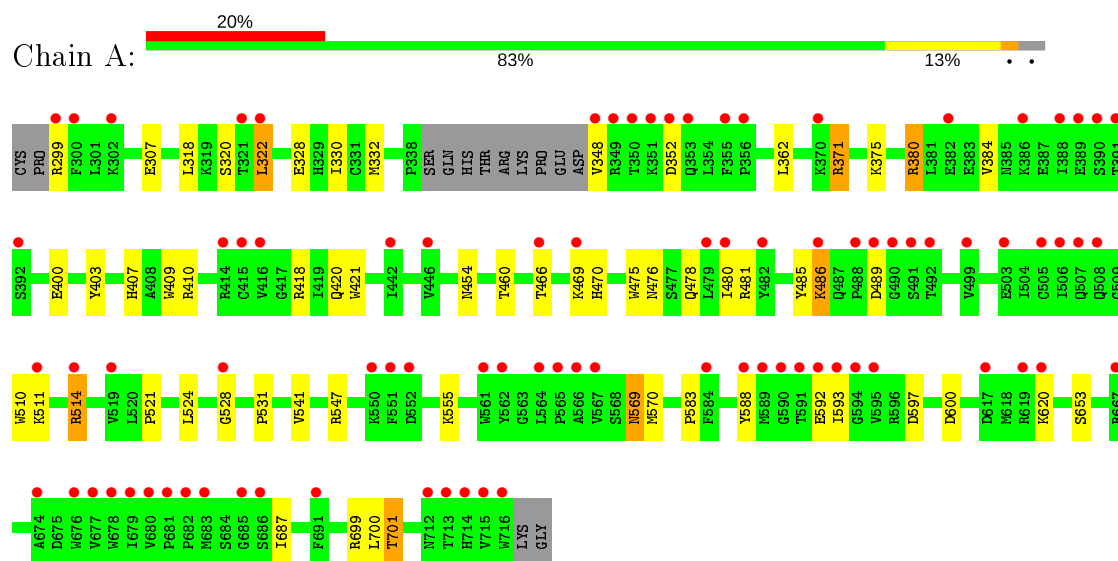
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	151	Total	O	0	0
			151	151		
7	B	207	Total	O	0	0
			207	207		

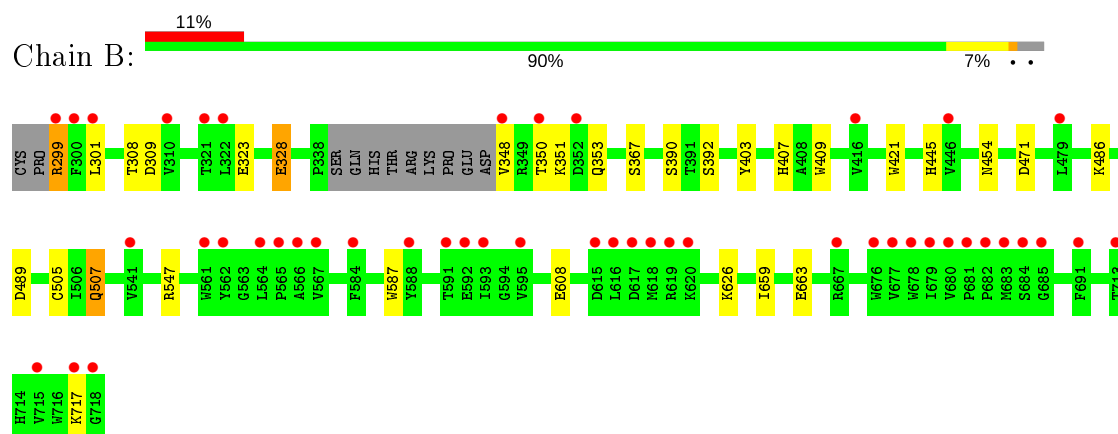
3 Residue-property plots [i](#)

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

- Molecule 1: Nitric oxide synthase, 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	51.81Å 110.75Å 163.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.89 – 1.88 38.89 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.89-1.88) 99.8 (38.89-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.235 0.233 , 0.273	Depositor DCC
R_{free} test set	3840 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7240	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 5.01% 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: 8CX, 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	0.73	0/3439	0.75	4/4665 (0.1%)
1	B	0.81	0/3453	0.82	5/4681 (0.1%)
All	All	0.77	0/6892	0.78	9/9346 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ASP	CB-CG-OD2	9.08	126.47	118.30
1	B	471	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	A	570	MET	CA-CB-CG	-6.57	102.13	113.30
1	A	600	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	471	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	505	CYS	CA-CB-SG	-5.96	103.28	114.00
1	A	570	MET	CG-SD-CE	5.55	109.08	100.20
1	A	410	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	489	ASP	CB-CG-OD1	-5.24	113.58	118.30

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	3340	0	3254	41	0
1	B	3357	0	3269	17	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	28	0	28	3	0
5	B	28	0	28	2	0
6	A	1	0	0	0	0
7	A	151	0	0	1	0
7	B	207	0	0	3	0
All	All	7240	0	6675	59	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 4.

All (59) 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:307:GLU:HG3	7:B:11:HOH:O	1.83	0.77
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.66	0.77
1:B:299:ARG:HG3	1:B:299:ARG:HH11	1.51	0.76
1:A:380:ARG:HD3	1:A:400:GLU:OE1	1.87	0.74
1:A:687:ILE:HD12	1:B:626:LYS:HB3	1.77	0.66
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.79	0.65
2:A:750:HEM:HBA1	5:A:800:8CX:H4	1.79	0.64
1:A:469:LYS:O	1:A:470:HIS:HD2	1.82	0.63
1:B:299:ARG:HH11	1:B:299:ARG:CG	2.12	0.62
1:A:514:ARG:HG3	1:A:514:ARG:HH21	1.65	0.60
1:A:332:MET:CE	1:B:301:LEU:HD22	2.32	0.59
1:A:514:ARG:HH21	1:A:514:ARG:CG	2.16	0.58
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.85	0.58
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.16	0.56
1:B:507:GLN:NE2	7:B:95:HOH:O	2.38	0.56
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.20	0.55
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.88	0.55
1:A:701:THR:HG23	7:A:228:HOH:O	2.07	0.53
1:A:569:ASN:H	1:A:569:ASN:HD22	1.54	0.53
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.90	0.52
1:A:322:LEU:HD12	1:A:699:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.92	0.50
1:B:328:GLU:CD	1:B:328:GLU:H	2.15	0.50
1:B:308:THR:O	1:B:309:ASP:HB2	2.11	0.49
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.77	0.49
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.01	0.49
1:A:332:MET:HE2	1:B:301:LEU:HD22	1.95	0.48
1:B:608:GLU:HG3	7:B:41:HOH:O	2.13	0.48
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.48	0.47
1:A:469:LYS:O	1:A:470:HIS:CD2	2.65	0.47
1:A:592[A]:GLU:OE1	5:A:800:8CX:H16	2.15	0.47
1:A:330:ILE:CG2	1:A:330:ILE:O	2.63	0.46
1:B:299:ARG:CG	1:B:299:ARG:NH1	2.74	0.46
2:A:750:HEM:CBA	5:A:800:8CX:H4	2.45	0.45
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.04	0.45
1:A:330:ILE:HG23	1:A:330:ILE:O	2.16	0.45
1:A:514:ARG:NH2	1:A:514:ARG:CG	2.78	0.45
1:A:299:ARG:HG3	1:A:318:LEU:CD2	2.47	0.45
1:B:659:ILE:O	1:B:663:GLU:HG3	2.17	0.45
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.52	0.44
1:A:460:THR:O	1:A:583:PRO:HD2	2.17	0.44
1:A:328:GLU:HB3	1:B:323:GLU:HG2	1.99	0.44
1:A:348:VAL:HG21	1:A:466:THR:O	2.18	0.43
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.39	0.42
1:A:470:HIS:HA	1:A:528:GLY:HA3	2.00	0.42
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.50	0.42
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.55	0.42
1:B:587:TRP:O	5:B:800:8CX:H15	2.20	0.42
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.54	0.42
1:A:510:TRP:CD1	1:A:521:PRO:HG3	2.55	0.42
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.35	0.41
2:B:750:HEM:CBA	5:B:800:8CX:H4	2.50	0.41
1:A:418:ARG:C	1:A:420:GLN:N	2.73	0.41
1:A:320:SER:HA	1:A:700:LEU:HD23	2.01	0.41
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.03	0.41
1:A:524:LEU:O	1:A:531:PRO:HA	2.20	0.41
1:A:593:ILE:HA	1:A:597:ASP:OD2	2.21	0.41
1:A:486:LYS:HG2	1:A:486:LYS:H	1.69	0.40
1:B:445:HIS:C	1:B:445:HIS:CD2	2.94	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	407/422 (96%)	396 (97%)	11 (3%)	0	100	100
1	B	409/422 (97%)	402 (98%)	7 (2%)	0	100	100
All	All	816/844 (97%)	798 (98%)	18 (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	367/377 (97%)	350 (95%)	17 (5%)	27	15
1	B	368/377 (98%)	354 (96%)	14 (4%)	33	21
All	All	735/754 (98%)	704 (96%)	31 (4%)	30	18

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	352	ASP
1	A	371	ARG
1	A	375	LYS
1	A	380	ARG
1	A	454	ASN
1	A	476	ASN
1	A	485	TYR

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Mol	Chain	Res	Type
1	A	486	LYS
1	A	489	ASP
1	A	511	LYS
1	A	514	ARG
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	653	SER
1	A	701	THR
1	B	299	ARG
1	B	328	GLU
1	B	348	VAL
1	B	350	THR
1	B	351	LYS
1	B	353	GLN
1	B	367	SER
1	B	390	SER
1	B	392	SER
1	B	454	ASN
1	B	486	LYS
1	B	507	GLN
1	B	547	ARG
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	470	HIS
1	A	527	ASN
1	A	569	ASN
1	A	601	ASN
1	A	605	ASN
1	A	697	ASN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN

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Mol	Chain	Res	Type
1	B	697	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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$
3	H4B	A	760	-	16,18,18	1.50	3 (18%)	11,26,26	3.29	7 (63%)
4	ACT	B	860	-	1,3,3	1.91	0	0,3,3	0.00	-
4	ACT	A	860	-	1,3,3	2.04	1 (100%)	0,3,3	0.00	-
5	8CX	B	800	-	27,30,30	0.89	2 (7%)	30,40,40	1.89	7 (23%)
5	8CX	A	800	-	27,30,30	1.02	2 (7%)	30,40,40	2.41	8 (26%)
2	HEM	A	750	1	27,50,50	2.05	7 (25%)	17,82,82	2.92	9 (52%)
2	HEM	B	750	1	27,50,50	2.01	5 (18%)	17,82,82	2.76	4 (23%)
3	H4B	B	760	-	16,18,18	1.24	1 (6%)	11,26,26	2.70	2 (18%)

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	A	760	-	-	0/8/17/17	0/2/2/2
5	8CX	B	800	-	-	4/16/26/26	0/3/3/3
5	8CX	A	800	-	-	5/16/26/26	0/3/3/3
2	HEM	A	750	1	-	0/6/54/54	-
2	HEM	B	750	1	-	0/6/54/54	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	5.19	1.53	1.37
2	B	750	HEM	C3C-C2C	-4.55	1.34	1.40
2	A	750	HEM	C3B-C2B	-4.18	1.34	1.40
2	B	750	HEM	C3D-C2D	4.16	1.50	1.37
2	B	750	HEM	C3B-C2B	-4.06	1.34	1.40
3	A	760	H4B	C2-N2	3.68	1.41	1.33
2	B	750	HEM	C3C-CAC	3.65	1.55	1.47
2	A	750	HEM	C3C-CAC	3.63	1.55	1.47
2	A	750	HEM	C3C-C2C	-3.31	1.35	1.40
2	A	750	HEM	C3B-CAB	3.11	1.54	1.47
2	B	750	HEM	C3B-CAB	2.97	1.54	1.47
5	A	800	8CX	C5A-C4A	2.69	1.43	1.39
5	B	800	8CX	C3-C4	2.49	1.54	1.51
2	A	750	HEM	CMD-C2D	2.43	1.56	1.51
3	A	760	H4B	C8A-N1	2.38	1.39	1.34
3	B	760	H4B	C7-N8	2.32	1.48	1.44
2	A	750	HEM	CMC-C2C	2.27	1.57	1.51
3	A	760	H4B	C4A-C8A	-2.19	1.37	1.41
5	A	800	8CX	C6A-N6A	2.09	1.41	1.35
4	A	860	ACT	CH3-C	2.04	1.51	1.48
5	B	800	8CX	C3-N2	-2.00	1.43	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-8.27	97.24	112.49
3	B	760	H4B	C4-C4A-C8A	7.79	121.49	114.57
2	A	750	HEM	CBA-CAA-C2A	-7.27	99.08	112.49
5	A	800	8CX	C4A-C3A-C2A	-7.24	115.58	120.32
5	A	800	8CX	C6A-N1A-C2A	6.95	123.37	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBD-CAD-C3D	-6.19	101.08	112.48
5	B	800	8CX	C6A-N1A-C2A	6.14	122.75	118.10
3	A	760	H4B	C4-C4A-N5	5.82	124.01	119.12
2	B	750	HEM	CBD-CAD-C3D	-4.98	103.31	112.48
3	A	760	H4B	N3-C2-N1	-4.43	118.46	125.42
3	A	760	H4B	C4-N3-C2	4.36	122.85	115.93
2	A	750	HEM	C1D-C2D-C3D	-3.79	104.36	107.00
2	B	750	HEM	C4A-C3A-C2A	-3.66	104.45	107.00
3	A	760	H4B	C4-C4A-C8A	3.57	117.75	114.57
5	A	800	8CX	C5'-N1'-C2'	3.39	113.42	105.42
3	A	760	H4B	C4A-N5-C6	-3.35	112.04	121.16
2	A	750	HEM	C4C-C3C-C2C	3.33	109.23	106.90
5	B	800	8CX	C3A-C2A-N1A	-3.22	119.48	122.90
2	A	750	HEM	CMD-C2D-C3D	2.92	130.44	124.94
5	B	800	8CX	C5'-N1'-C2'	2.87	112.19	105.42
5	A	800	8CX	C16-C11-C12	2.87	122.06	118.76
3	A	760	H4B	N2-C2-N3	2.75	121.53	117.25
5	B	800	8CX	F13-C13-C14	2.73	123.17	118.54
2	B	750	HEM	CMC-C2C-C3C	2.65	129.65	124.68
5	B	800	8CX	N6A-C6A-N1A	2.63	120.65	116.49
5	A	800	8CX	C5A-C6A-N1A	-2.60	116.17	121.75
5	A	800	8CX	C14-C13-C12	-2.59	119.93	123.29
3	B	760	H4B	C4-N3-C2	2.54	119.96	115.93
3	A	760	H4B	C2-N1-C8A	2.51	120.16	114.54
5	A	800	8CX	N6A-C6A-N1A	2.48	120.40	116.49
5	A	800	8CX	F13-C13-C14	2.46	122.72	118.54
5	B	800	8CX	C14-C13-C12	-2.27	120.35	123.29
2	A	750	HEM	CMB-C2B-C3B	2.14	128.68	124.68
2	A	750	HEM	CMD-C2D-C1D	-2.13	125.19	128.46
2	A	750	HEM	CMC-C2C-C3C	2.09	128.59	124.68
2	A	750	HEM	C3C-C4C-NC	-2.08	107.02	110.94
5	B	800	8CX	C11-C12-C13	2.04	120.86	118.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	800	8CX	C2'-C3'-O1-C1
5	B	800	8CX	N1A-C2A-C7A-C4'
5	A	800	8CX	C1-C2-N2-C3
5	B	800	8CX	C1-C2-N2-C3
5	A	800	8CX	O1-C1-C2-N2

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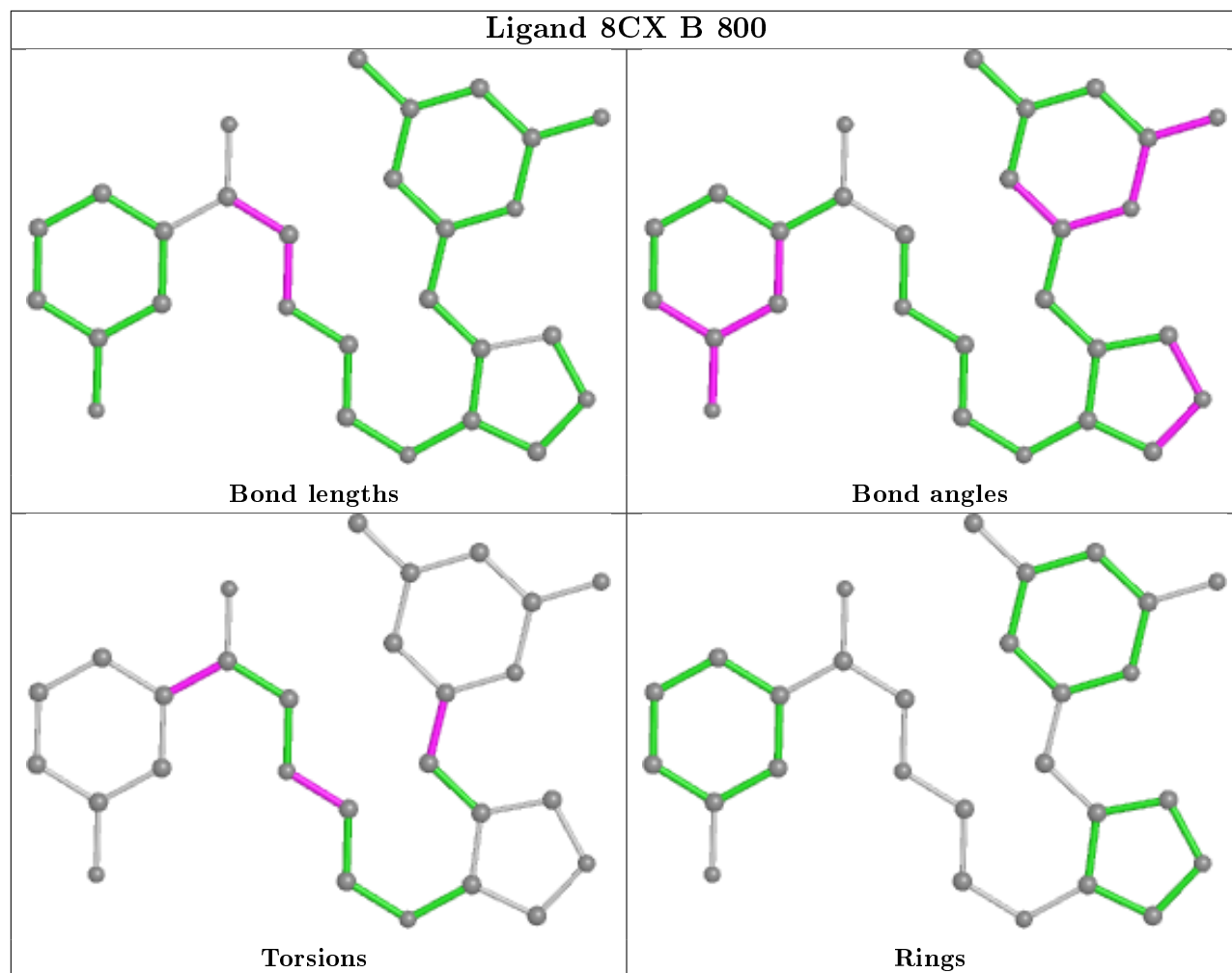
Mol	Chain	Res	Type	Atoms
5	A	800	8CX	C16-C11-C4-C3
5	A	800	8CX	C12-C11-C4-C3
5	B	800	8CX	C16-C11-C4-C3
5	B	800	8CX	C12-C11-C4-C3

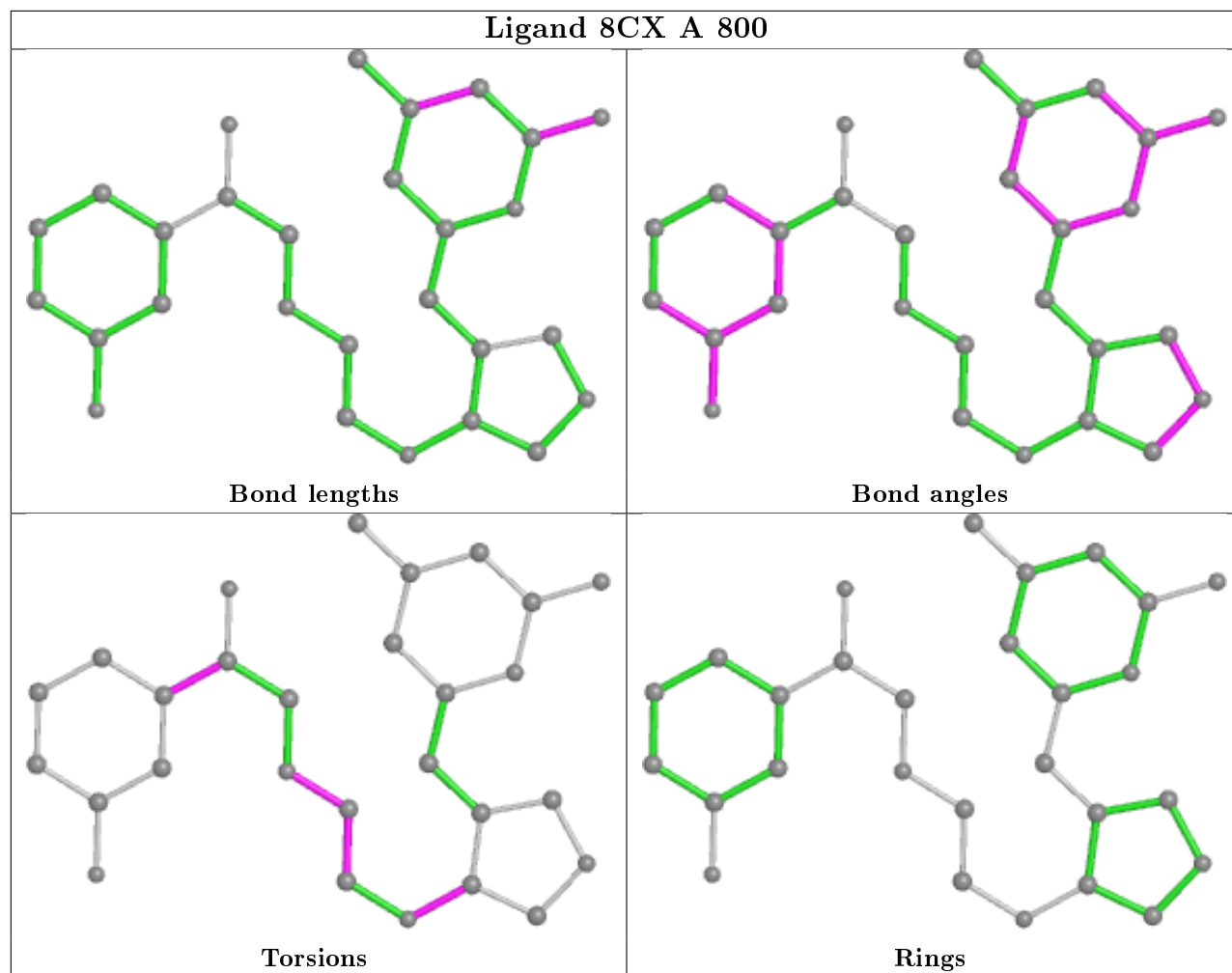
There are no ring outliers.

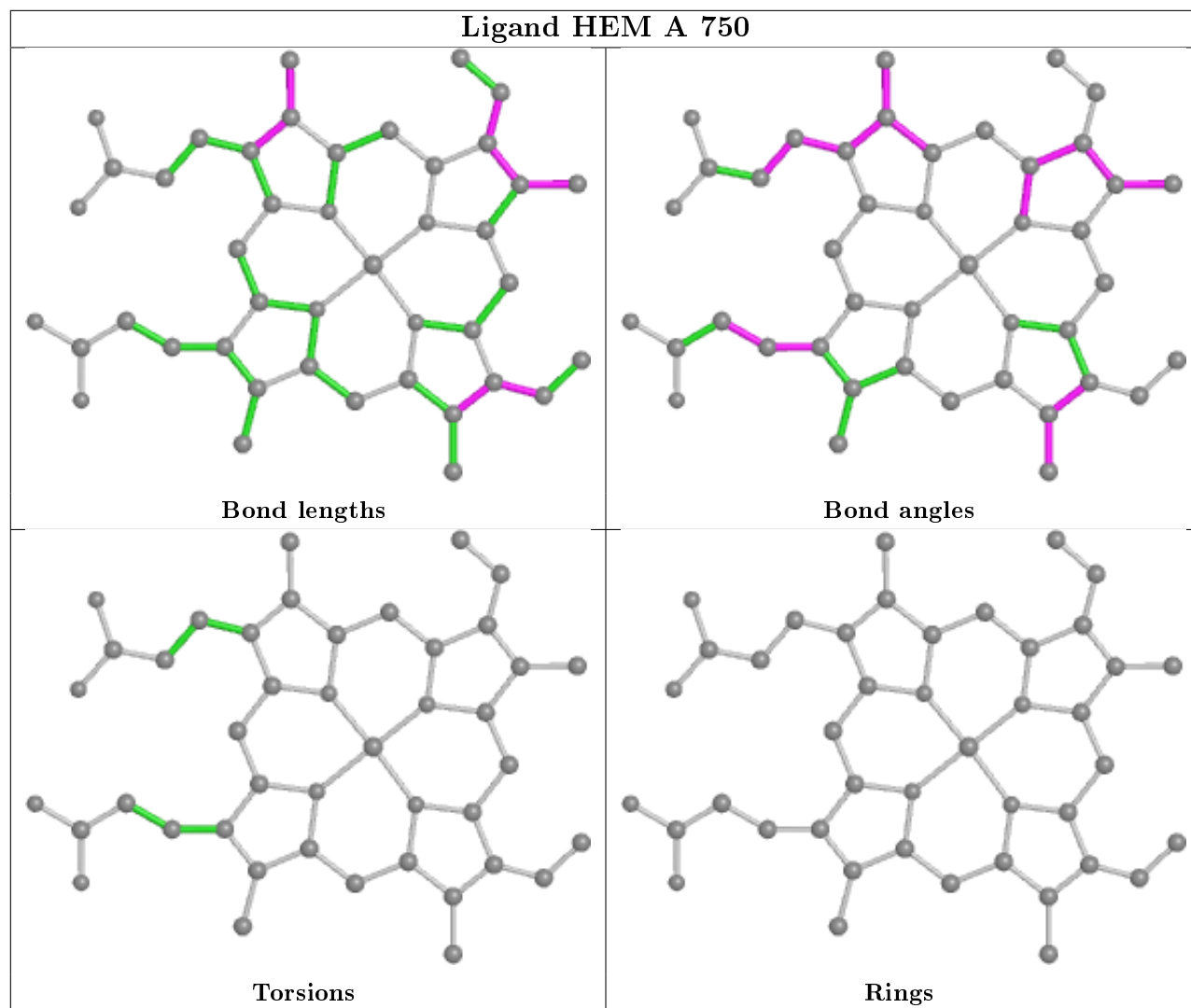
4 monomers are involved in 8 short contacts:

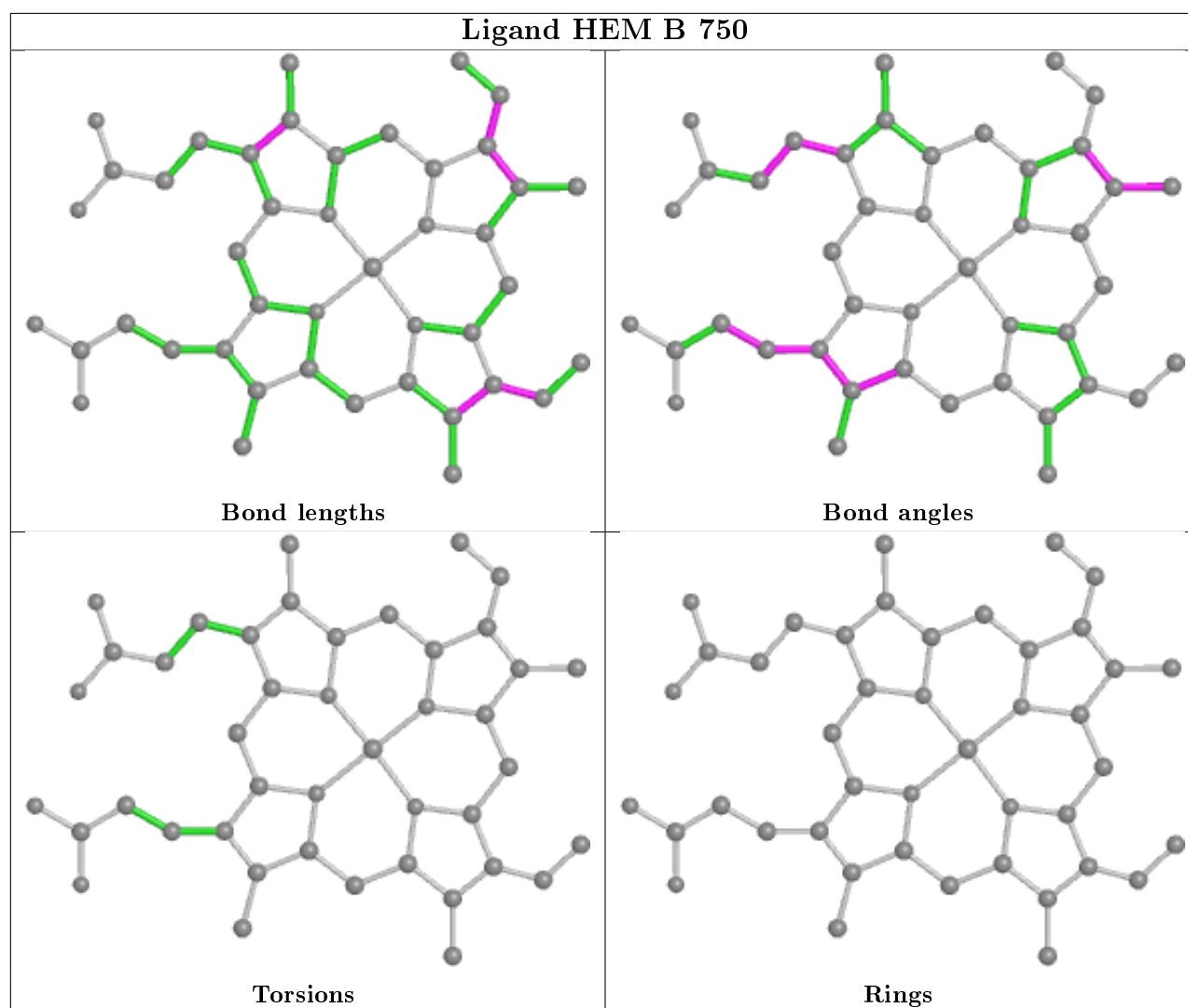
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	800	8CX	2	0
5	A	800	8CX	3	0
2	A	750	HEM	4	0
2	B	750	HEM	2	0

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	409/422 (96%)	1.15	86 (21%) 1 0	27, 52, 87, 115	0
1	B	411/422 (97%)	0.60	47 (11%) 5 5	28, 41, 66, 81	0
All	All	820/844 (97%)	0.88	133 (16%) 1 1	27, 46, 82, 115	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.8
1	A	488	PRO	8.0
1	A	713	THR	7.3
1	A	716	TRP	6.7
1	A	351	LYS	6.6
1	A	348	VAL	6.3
1	A	300	PHE	6.0
1	A	352	ASP	5.7
1	A	355	PHE	5.7
1	A	715	VAL	5.1
1	A	592[A]	GLU	5.0
1	B	677	VAL	4.9
1	A	322	LEU	4.7
1	B	619	ARG	4.7
1	A	486	LYS	4.6
1	A	677	VAL	4.4
1	B	616	LEU	4.3
1	A	678	TRP	4.3
1	A	619	ARG	4.2
1	A	593	ILE	4.2
1	A	506	ILE	4.2
1	A	567	VAL	4.2
1	A	321	THR	4.1
1	B	561	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	679	ILE	4.0
1	A	469	LYS	4.0
1	B	680	VAL	4.0
1	B	667	ARG	3.9
1	A	507	GLN	3.9
1	B	348	VAL	3.8
1	A	299	ARG	3.8
1	A	386	LYS	3.8
1	B	592[A]	GLU	3.8
1	A	551	PHE	3.7
1	A	561	TRP	3.6
1	B	679	ILE	3.6
1	A	479	LEU	3.6
1	A	388	ILE	3.6
1	A	415	CYS	3.6
1	B	350	THR	3.6
1	A	676	TRP	3.6
1	A	588	TYR	3.5
1	B	676	TRP	3.4
1	A	591	THR	3.4
1	A	491	SER	3.4
1	A	680	VAL	3.4
1	B	299	ARG	3.3
1	A	389	GLU	3.3
1	A	416	VAL	3.3
1	A	519	VAL	3.3
1	B	620	LYS	3.3
1	A	682	PRO	3.3
1	A	390	SER	3.2
1	A	566	ALA	3.2
1	A	349	ARG	3.2
1	A	565	PRO	3.2
1	B	718	GLY	3.2
1	B	691	PHE	3.1
1	A	490	GLY	3.0
1	A	356	PRO	3.0
1	A	714	HIS	3.0
1	B	566	ALA	3.0
1	B	310	VAL	2.9
1	A	391	THR	2.9
1	A	508	GLN	2.9
1	B	715	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	480	ILE	2.9
1	A	667	ARG	2.9
1	B	615	ASP	2.8
1	A	683	MET	2.8
1	A	595	VAL	2.8
1	A	564	LEU	2.8
1	B	322	LEU	2.8
1	B	681	PRO	2.7
1	A	528	GLY	2.7
1	A	712	ASN	2.7
1	A	681	PRO	2.7
1	A	511	LYS	2.7
1	A	562	TYR	2.7
1	A	503	GLU	2.7
1	A	482	TYR	2.7
1	B	567	VAL	2.7
1	A	446	VAL	2.6
1	B	682	PRO	2.6
1	A	674	ALA	2.6
1	A	489	ASP	2.6
1	B	617	ASP	2.6
1	B	588	TYR	2.6
1	B	416	VAL	2.6
1	A	514	ARG	2.5
1	B	591	THR	2.5
1	A	589	MET	2.5
1	A	685	GLY	2.5
1	A	353	GLN	2.5
1	B	618	MET	2.5
1	A	550	LYS	2.5
1	A	392	SER	2.4
1	A	584	PHE	2.4
1	B	479	LEU	2.4
1	B	562	TYR	2.4
1	A	691	PHE	2.4
1	B	352	ASP	2.4
1	A	382	GLU	2.4
1	A	350	THR	2.3
1	A	590	GLY	2.3
1	A	594	GLY	2.3
1	A	499	VAL	2.3
1	A	492	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	505	CYS	2.3
1	B	565	PRO	2.3
1	B	685	GLY	2.3
1	A	617	ASP	2.3
1	B	321	THR	2.2
1	A	442	ILE	2.2
1	B	564	LEU	2.2
1	A	370	LYS	2.2
1	B	717	LYS	2.2
1	B	593	ILE	2.2
1	A	686	SER	2.2
1	B	678	TRP	2.2
1	B	713	THR	2.2
1	B	684	SER	2.1
1	A	466	THR	2.1
1	A	302	LYS	2.1
1	B	683	MET	2.1
1	B	301	LEU	2.1
1	B	584	PHE	2.1
1	A	414	ARG	2.1
1	B	541	VAL	2.1
1	A	552	ASP	2.0
1	B	595	VAL	2.0
1	A	620	LYS	2.0
1	B	446	VAL	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](#)

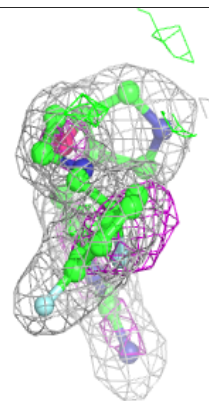
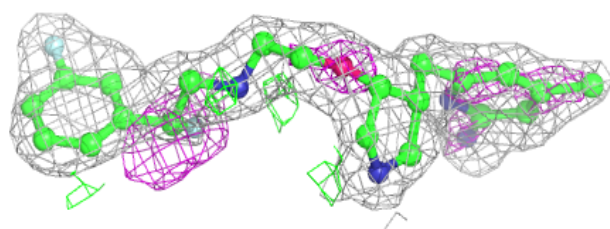
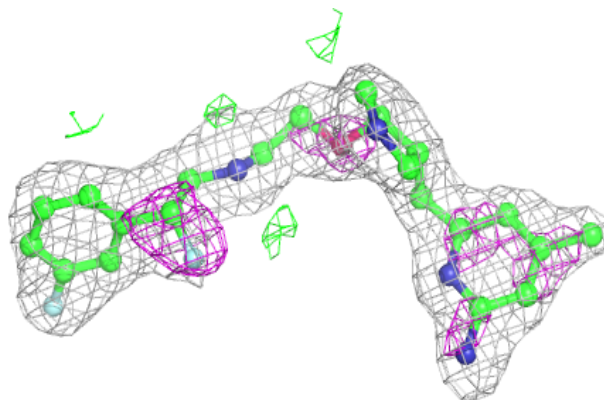
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	8CX	A	800	28/28	0.88	0.15	13,24,38,41	0
5	8CX	B	800	28/28	0.91	0.12	15,26,33,34	0
3	H4B	B	760	17/17	0.95	0.19	28,32,36,38	0
3	H4B	A	760	17/17	0.96	0.20	27,31,38,40	0
2	HEM	A	750	43/43	0.96	0.23	27,33,41,43	0
4	ACT	B	860	4/4	0.96	0.13	43,46,47,48	0
2	HEM	B	750	43/43	0.97	0.19	25,32,42,49	0
4	ACT	A	860	4/4	0.97	0.36	57,57,59,61	0
6	ZN	A	900	1/1	0.99	0.09	40,40,40,40	0

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

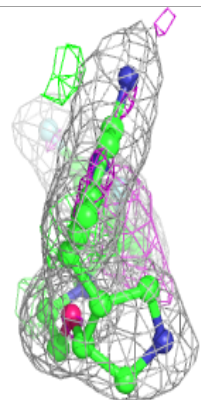
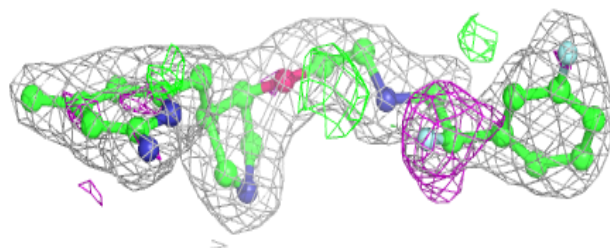
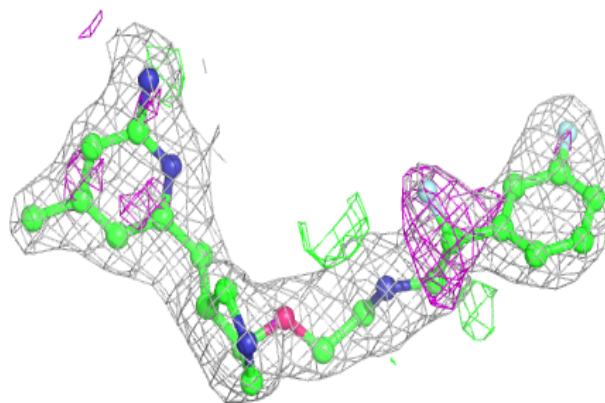
Electron density around 8CX A 800:

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



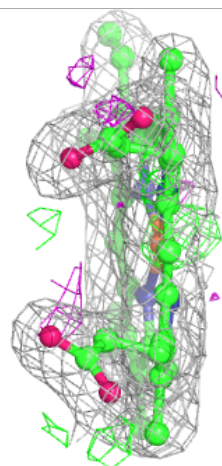
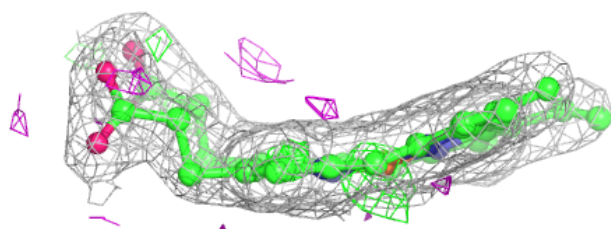
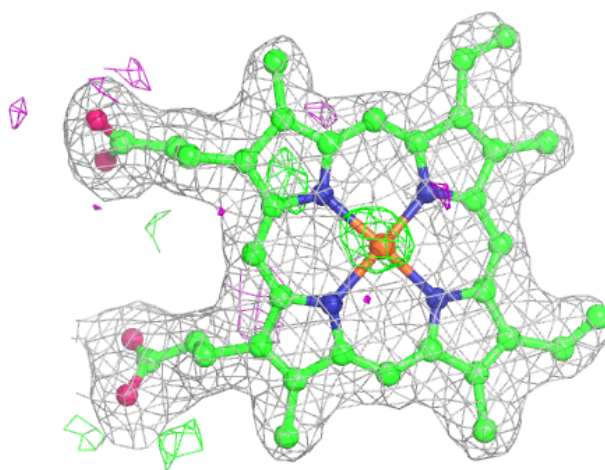
Electron density around 8CX B 800:

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



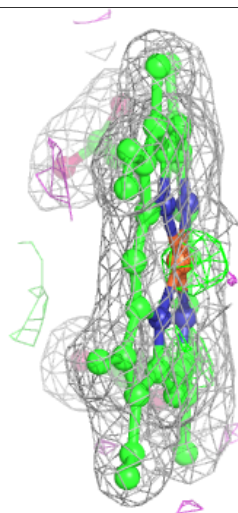
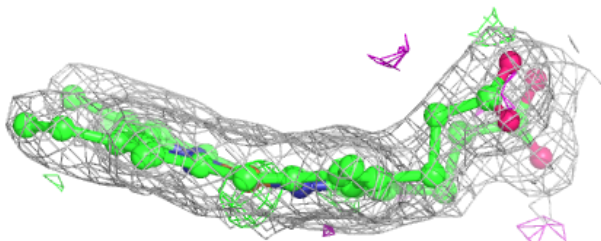
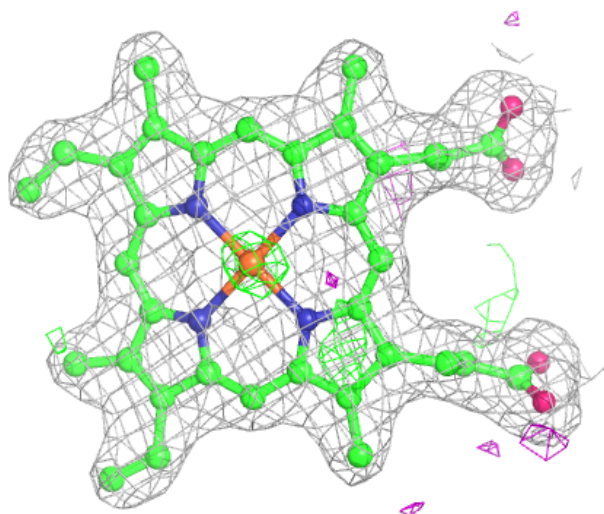
Electron density around HEM A 750:

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



Electron density around HEM B 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.