Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 07:35 pm BST

PDB ID	:	4UH4
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 3-(2-(6-Amino-4-methylpyridin-2-yl)ethyl)-5-(methyl(2-(methylamino)ethyl)amino)benzonitrile
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2015-03-23
Resolution	:	1.95 Å(reported)

The following versions of software and data (see references (i)) 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 1.95 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.
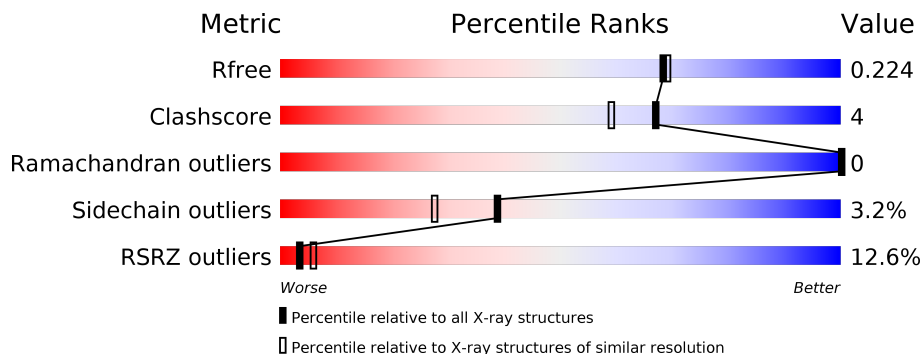
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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 <=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 7122 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 3317	C 2123	N 567	O 606	S 21	0	1	1
1	B	411	Total 3348	C 2142	N 574	O 611	S 21	0	1	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
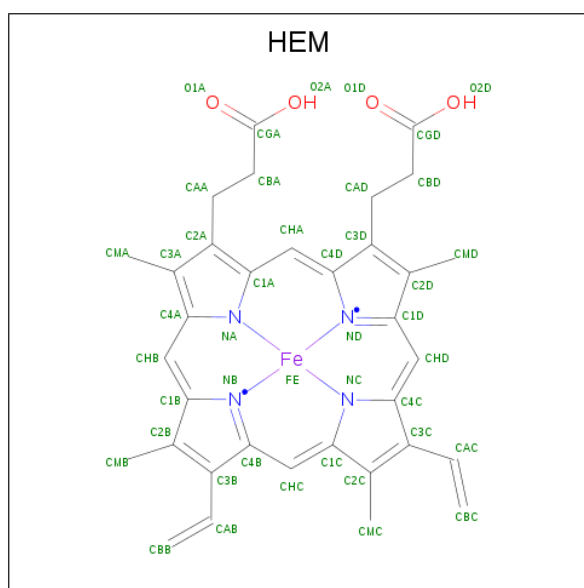
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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
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 3-(2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL)-5-(METHYL(2-(M ETHYLAMINO)ETHYL)AMINO)BENZONITRILE (three-letter code: Q1T) (formula: $C_{19}H_{25}N_5$).
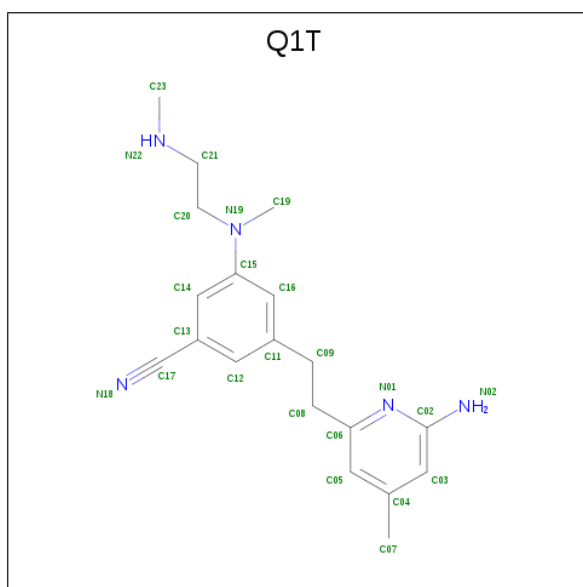
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			24	19	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 24	C 19	N 5	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	119	Total 119	O 119	0	0
7	B	161	Total 161	O 161	0	0

3 Residue-property plots ⓘ

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
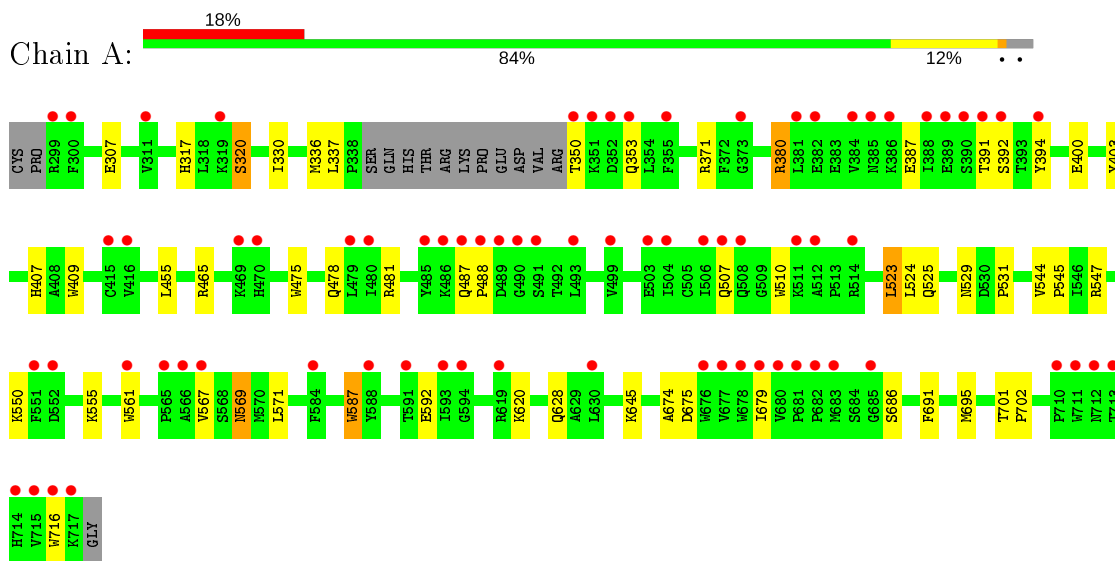
- Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN
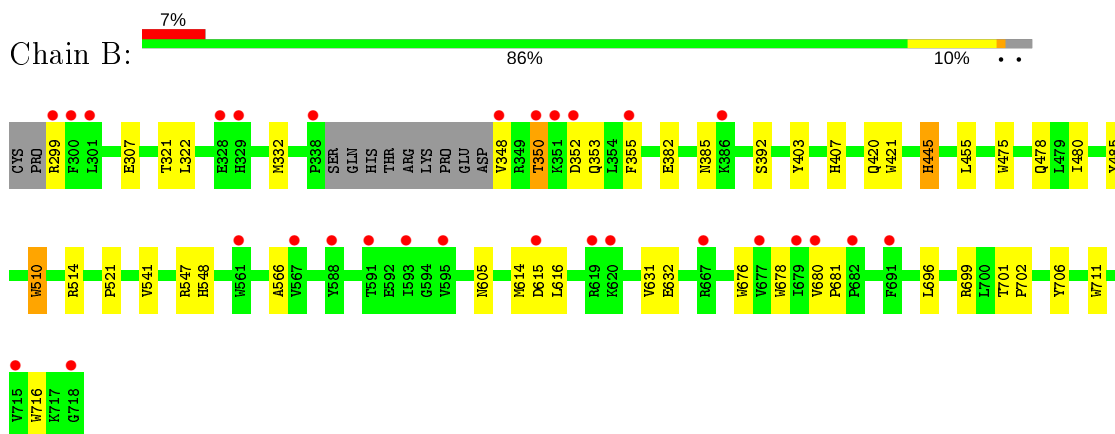
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.90Å 110.79Å 164.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.19 – 1.95 37.67 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.3 (92.19-1.95) 95.1 (37.67-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.191 , 0.224 0.194 , 0.224	Depositor DCC
R_{free} test set	2890 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.9	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7122	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 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: Q1T, ZN, H4B, HEM, 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	0.66	6/3413 (0.2%)	0.65	0/4631
1	B	0.72	7/3444 (0.2%)	0.70	0/4669
All	All	0.69	13/6857 (0.2%)	0.67	0/9300

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	711	TRP	CD2-CE2	5.47	1.48	1.41
1	A	716	TRP	CD2-CE2	5.40	1.47	1.41
1	B	716	TRP	CD2-CE2	5.40	1.47	1.41
1	A	587	TRP	CD2-CE2	5.36	1.47	1.41
1	B	676	TRP	CD2-CE2	5.20	1.47	1.41
1	A	475	TRP	CD2-CE2	5.19	1.47	1.41
1	B	421	TRP	CD2-CE2	5.18	1.47	1.41
1	B	475	TRP	CD2-CE2	5.17	1.47	1.41
1	A	409	TRP	CD2-CE2	5.15	1.47	1.41
1	B	510	TRP	CD2-CE2	5.09	1.47	1.41
1	A	561	TRP	CD2-CE2	5.08	1.47	1.41
1	B	678	TRP	CD2-CE2	5.05	1.47	1.41
1	A	510	TRP	CD2-CE2	5.00	1.47	1.41

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	3317	0	3226	25	0
1	B	3348	0	3264	21	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	24	0	25	3	0
4	B	24	0	25	2	0
5	A	4	0	3	0	0
5	B	4	0	3	1	0
6	A	1	0	0	0	0
7	A	119	0	0	1	0
7	B	161	0	0	3	0
All	All	7122	0	6636	52	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 (52) 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:B:615:ASP:HA	7:B:2136:HOH:O	1.84	0.76
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.66	0.76
1:A:307:GLU:HG3	7:B:2133:HOH:O	1.96	0.66
1:A:350:THR:HB	1:A:353:GLN:NE2	2.15	0.62
2:B:750:HEM:C1C	4:B:800:Q1T:H073	2.35	0.61
1:A:317:HIS:O	1:A:320:SER:HB3	2.01	0.60
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.84	0.59
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.03	0.58
1:B:605:ASN:ND2	7:B:2131:HOH:O	2.25	0.56
1:B:420:GLN:HE21	5:B:860:ACT:H2	1.71	0.56
1:A:525:GLN:HG3	1:A:529:ASN:O	2.07	0.55
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.89	0.54
1:B:706:TYR:OH	2:B:750:HEM:O2D	2.16	0.54
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.37	0.53
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.91	0.52
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.92	0.52
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.98	0.52
2:A:750:HEM:C1C	4:A:800:Q1T:H073	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.13	0.49
1:A:686:SER:HA	1:A:691:PHE:CG	2.48	0.49
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.96	0.48
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.48	0.48
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.45	0.46
1:B:485:TYR:CE2	1:B:514:ARG:HA	2.50	0.46
1:A:569:ASN:H	1:A:569:ASN:HD22	1.63	0.46
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.98	0.45
1:B:614:MET:HE2	1:B:616:LEU:HD21	1.99	0.45
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.51	0.45
1:A:465:ARG:HH12	1:A:571:LEU:HD11	1.81	0.45
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.33	0.44
1:A:391:THR:O	1:A:392:SER:OG	2.24	0.44
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.48	0.43
1:A:524:LEU:O	1:A:531:PRO:HA	2.18	0.43
1:B:322:LEU:HD12	1:B:699:ARG:HB3	2.01	0.43
1:A:674:ALA:HB3	1:A:695:MET:HB3	2.00	0.43
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.43
1:B:478:GLN:HA	1:B:566:ALA:O	2.19	0.43
1:A:567:VAL:HG23	4:A:800:Q1T:H05	2.01	0.42
1:B:350:THR:HB	1:B:352:ASP:HB2	2.00	0.42
1:A:675:ASP:O	1:A:679:ILE:HG12	2.20	0.42
1:A:592:GLU:OE2	4:A:800:Q1T:N01	2.52	0.42
7:A:2091:HOH:O	1:B:307:GLU:HG3	2.20	0.41
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.94	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.40	0.41
1:B:480:ILE:HD13	1:B:541:VAL:HG13	2.01	0.41
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.54	0.41
4:B:800:Q1T:H14	4:B:800:Q1T:H202	1.92	0.41
1:A:403:TYR:CE2	1:A:407:HIS:CE1	3.10	0.40
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.03	0.40
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.52	0.40
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.40
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.93	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%)	391 (96%)	14 (4%)	0	100	100
1	B	408/422 (97%)	399 (98%)	9 (2%)	0	100	100
All	All	813/844 (96%)	790 (97%)	23 (3%)	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	364/377 (97%)	351 (96%)	13 (4%)	35	23
1	B	367/377 (97%)	357 (97%)	10 (3%)	44	34
All	All	731/754 (97%)	708 (97%)	23 (3%)	39	28

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

Mol	Chain	Res	Type
1	A	320	SER
1	A	336	MET
1	A	337	LEU
1	A	371	ARG
1	A	380	ARG
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG

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Mol	Chain	Res	Type
1	A	550	LYS
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	B	321	THR
1	B	332	MET
1	B	348	VAL
1	B	350	THR
1	B	353	GLN
1	B	382	GLU
1	B	392	SER
1	B	445	HIS
1	B	455	LEU
1	B	547	ARG

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

Mol	Chain	Res	Type
1	A	353	GLN
1	A	425	GLN
1	A	454	ASN
1	A	478	GLN
1	A	507	GLN
1	A	527	ASN
1	A	535	GLN
1	A	569	ASN
1	A	628	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	420	GLN
1	B	425	GLN
1	B	454	ASN
1	B	478	GLN
1	B	601	ASN
1	B	642	GLN
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 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	1.30	3 (18%)	11,26,26	2.53	5 (45%)
5	ACT	B	860	-	1,3,3	2.80	1 (100%)	0,3,3	0.00	-
5	ACT	A	860	-	1,3,3	1.97	0	0,3,3	0.00	-
2	HEM	B	750	1	27,50,50	2.20	9 (33%)	17,82,82	3.36	8 (47%)
3	H4B	A	760	-	16,18,18	0.98	1 (6%)	11,26,26	2.80	6 (54%)
4	Q1T	B	800	-	25,25,25	1.58	1 (4%)	33,33,33	1.63	7 (21%)
2	HEM	A	750	1	27,50,50	2.28	10 (37%)	17,82,82	3.57	9 (52%)
4	Q1T	A	800	-	25,25,25	1.54	1 (4%)	33,33,33	1.91	7 (21%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	750	1	-	0/6/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	Q1T	B	800	-	-	1/15/15/15	0/2/2/2
2	HEM	A	750	1	-	0/6/54/54	-
4	Q1T	A	800	-	-	0/15/15/15	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	Q1T	C13-C17	-6.71	1.29	1.44
4	B	800	Q1T	C13-C17	-6.55	1.30	1.44
2	A	750	HEM	C3C-C2C	5.51	1.48	1.40
2	B	750	HEM	C4A-NA	4.85	1.46	1.36
2	B	750	HEM	C3C-C2C	4.70	1.46	1.40
2	A	750	HEM	C4A-NA	4.69	1.45	1.36
2	A	750	HEM	C1A-NA	4.54	1.45	1.36
2	B	750	HEM	C3B-C2B	4.38	1.46	1.40
2	B	750	HEM	C1A-NA	4.05	1.44	1.36
2	A	750	HEM	C2A-C3A	3.47	1.48	1.37
2	B	750	HEM	C2A-C3A	3.47	1.47	1.37
2	A	750	HEM	C3B-C2B	3.27	1.44	1.40
2	A	750	HEM	C1C-C2C	3.07	1.49	1.42
2	A	750	HEM	C3D-C2D	2.91	1.46	1.37
5	B	860	ACT	CH3-C	2.80	1.52	1.48
3	B	760	H4B	C7-C6	2.70	1.54	1.52
2	B	750	HEM	C4D-C3D	2.56	1.48	1.42
2	B	750	HEM	C1C-C2C	2.54	1.48	1.42
3	B	760	H4B	C4-N3	2.44	1.37	1.33
3	B	760	H4B	C7-N8	2.36	1.48	1.44
2	A	750	HEM	C1B-C2B	2.35	1.47	1.42
2	B	750	HEM	C3D-C2D	2.31	1.44	1.37
3	A	760	H4B	C4-N3	2.31	1.37	1.33
2	B	750	HEM	C1B-C2B	2.21	1.47	1.42
2	A	750	HEM	C4B-CHC	2.16	1.47	1.41
2	A	750	HEM	C4A-CHB	2.10	1.46	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	750	HEM	C1D-C2D-C3D	-8.74	100.91	107.00
2	B	750	HEM	C1D-C2D-C3D	-8.48	101.09	107.00
2	A	750	HEM	CBA-CAA-C2A	-6.84	99.86	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	750	HEM	CBA-CAA-C2A	-6.43	100.63	112.49
3	A	760	H4B	C4-C4A-N5	5.11	123.41	119.12
4	A	800	Q1T	C02-N01-C06	5.04	121.92	118.10
2	A	750	HEM	CAD-CBD-CGD	-5.01	104.26	112.67
2	A	750	HEM	C3B-C4B-NB	4.76	115.37	109.21
3	B	760	H4B	C4-C4A-C8A	4.68	118.73	114.57
4	A	800	Q1T	C09-C08-C06	-4.59	102.70	112.99
4	B	800	Q1T	C02-N01-C06	4.43	121.46	118.10
2	B	750	HEM	C3B-C4B-NB	4.29	114.75	109.21
2	B	750	HEM	CMB-C2B-C3B	3.93	132.04	124.68
3	A	760	H4B	N3-C2-N1	-3.90	119.31	125.42
2	A	750	HEM	CBD-CAD-C3D	-3.63	105.79	112.48
2	B	750	HEM	C4A-C3A-C2A	-3.52	104.55	107.00
4	B	800	Q1T	C05-C06-N01	-3.50	119.18	122.90
3	B	760	H4B	C4-C4A-N5	3.50	122.06	119.12
4	A	800	Q1T	C23-N22-C21	3.50	122.06	111.95
3	A	760	H4B	C4-N3-C2	3.42	121.36	115.93
4	A	800	Q1T	C05-C06-N01	-3.41	119.28	122.90
3	A	760	H4B	C2-N1-C8A	3.29	121.92	114.54
3	B	760	H4B	N3-C2-N1	-3.23	120.35	125.42
3	B	760	H4B	C4-N3-C2	3.20	121.02	115.93
2	A	750	HEM	CMC-C2C-C3C	3.18	130.63	124.68
4	B	800	Q1T	C08-C06-N01	3.17	120.68	115.95
4	A	800	Q1T	C08-C06-N01	3.17	120.67	115.95
4	A	800	Q1T	C14-C13-C17	2.99	123.52	119.54
3	A	760	H4B	C4-C4A-C8A	2.80	117.05	114.57
4	B	800	Q1T	C23-N22-C21	2.73	119.84	111.95
2	B	750	HEM	CBD-CAD-C3D	-2.66	107.58	112.48
2	A	750	HEM	CMB-C2B-C3B	2.61	129.55	124.68
3	B	760	H4B	C2-N1-C8A	2.56	120.28	114.54
4	A	800	Q1T	C12-C13-C17	-2.56	116.14	119.54
2	B	750	HEM	CAD-CBD-CGD	-2.54	108.41	112.67
4	B	800	Q1T	C16-C15-N19	-2.52	118.42	121.33
2	B	750	HEM	CMC-C2C-C3C	2.47	129.29	124.68
3	A	760	H4B	N2-C2-N3	2.47	121.09	117.25
4	B	800	Q1T	C09-C08-C06	-2.44	107.52	112.99
2	A	750	HEM	C4A-C3A-C2A	-2.41	105.32	107.00
2	A	750	HEM	CMD-C2D-C3D	2.22	129.13	124.94
4	B	800	Q1T	C14-C13-C17	2.15	122.40	119.54

There are no chirality outliers.
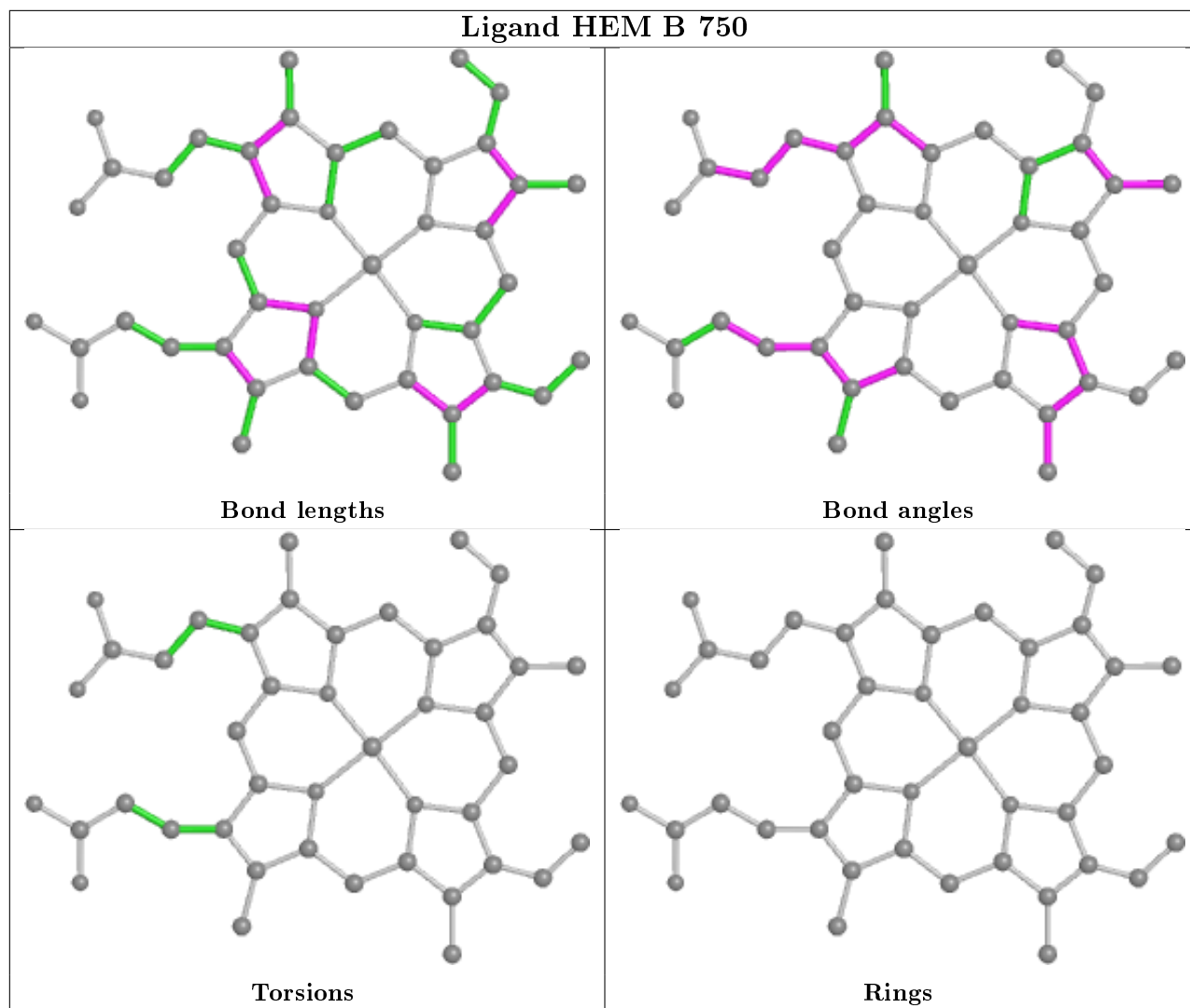
All (1) torsion outliers are listed below:
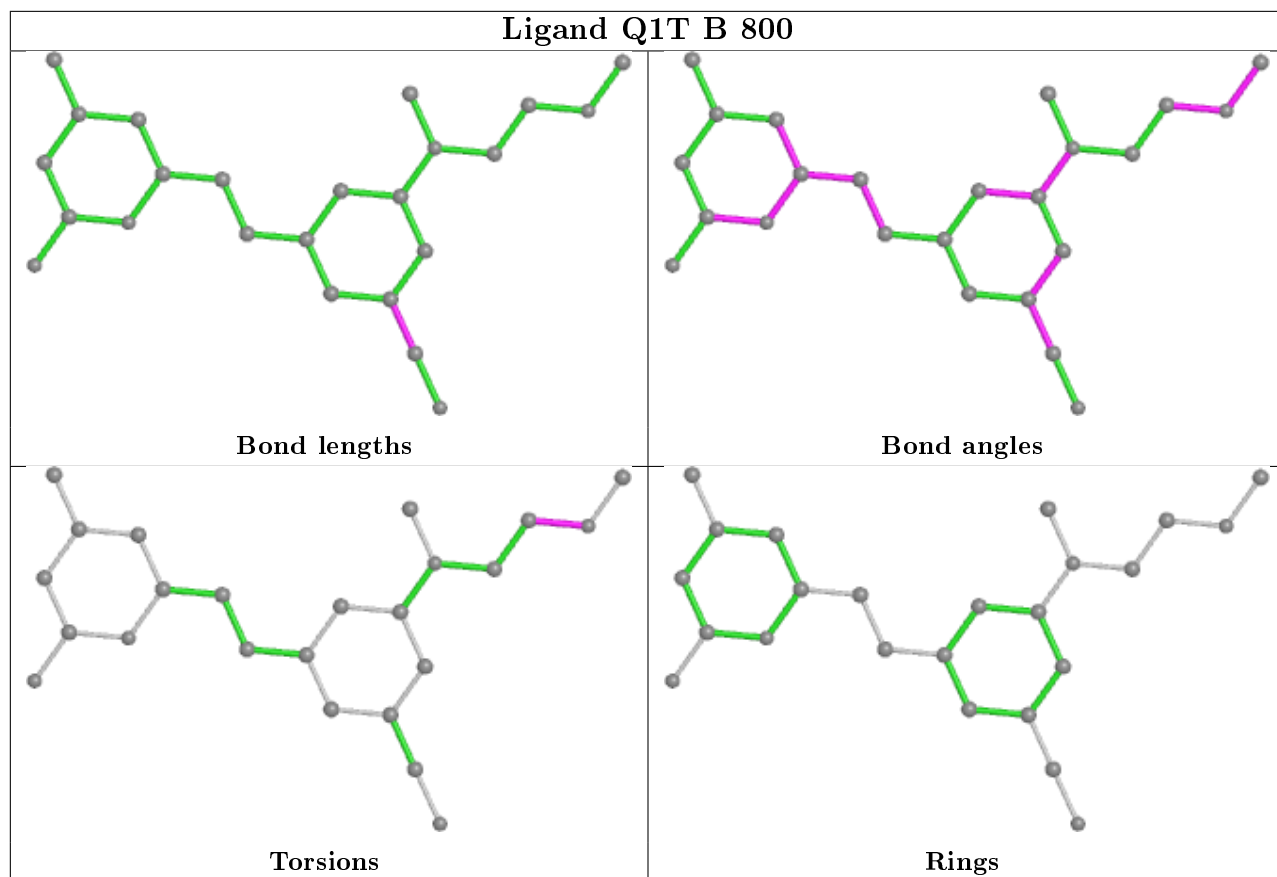
Mol	Chain	Res	Type	Atoms
4	B	800	Q1T	C20-C21-N22-C23

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	860	ACT	1	0
2	B	750	HEM	5	0
4	B	800	Q1T	2	0
2	A	750	HEM	3	0
4	A	800	Q1T	3	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 then 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 HEM B 750

Bond lengths

Bond angles

Torsions

Rings

Ligand Q1T B 800

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 750

Bond lengths

Bond angles

Torsions

Rings

Ligand Q1T A 800

Bond lengths

Bond angles

Torsions

Rings
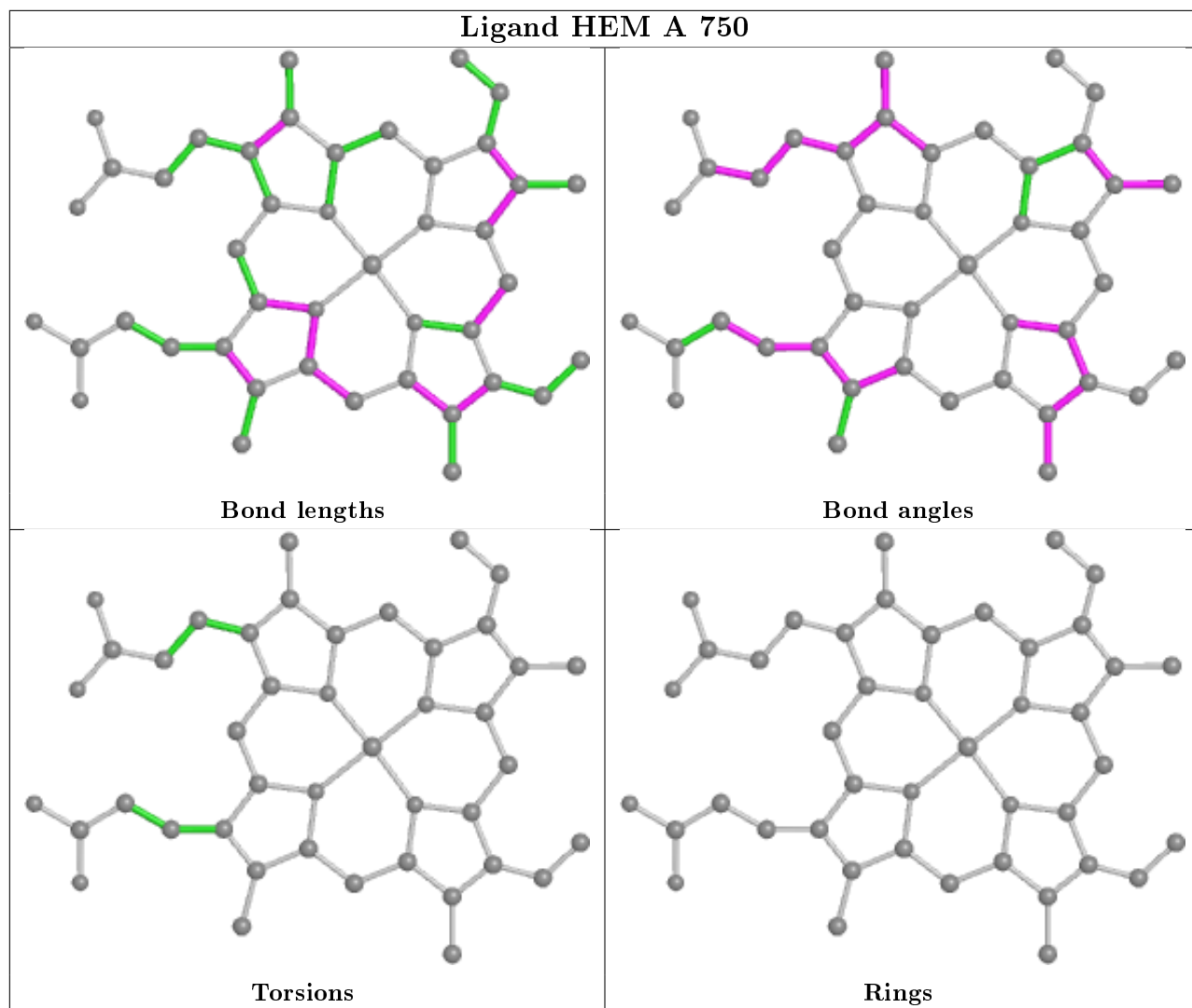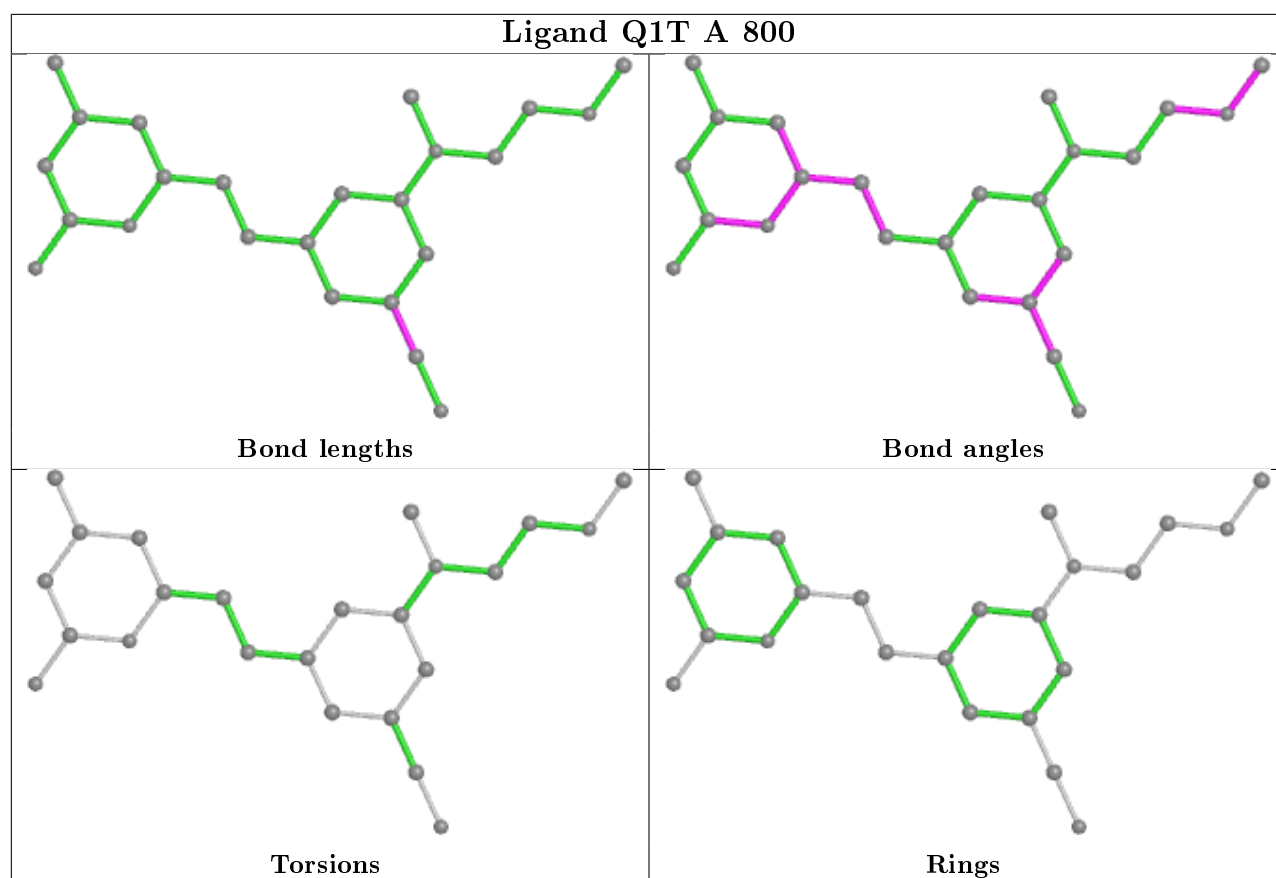
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.85	74 (18%)	1	1	25, 51, 94, 130	0
1	B	411/422 (97%)	0.35	29 (7%)	16	24	23, 39, 66, 87	0
All	All	819/844 (97%)	0.59	103 (12%)	3	6	23, 44, 86, 130	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	9.1
1	B	300	PHE	8.8
1	B	348	VAL	7.6
1	A	355	PHE	7.5
1	A	716	TRP	7.4
1	A	488	PRO	5.9
1	A	352	ASP	5.5
1	A	486	LYS	5.3
1	A	351	LYS	5.3
1	B	619	ARG	5.2
1	A	506	ILE	5.1
1	A	300	PHE	4.9
1	A	713	THR	4.6
1	A	388	ILE	4.4
1	A	715	VAL	4.4
1	A	619	ARG	4.3
1	A	299	ARG	4.1
1	B	667	ARG	4.0
1	A	350	THR	3.7
1	A	503	GLU	3.7
1	A	390	SER	3.6
1	A	508	GLN	3.6
1	B	301	LEU	3.6
1	A	507	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	338	PRO	3.5
1	A	389	GLU	3.4
1	B	351	LYS	3.3
1	A	391	THR	3.3
1	A	551	PHE	3.2
1	A	714	HIS	3.2
1	A	511	LYS	3.2
1	A	487	GLN	3.2
1	A	678	TRP	3.2
1	A	567	VAL	3.2
1	A	480	ILE	3.1
1	A	682	PRO	3.1
1	A	392	SER	3.0
1	B	350	THR	3.0
1	B	567	VAL	3.0
1	B	299	ARG	3.0
1	B	620	LYS	3.0
1	A	386	LYS	2.9
1	A	712	ASN	2.9
1	B	591	THR	2.9
1	B	718	GLY	2.9
1	A	469	LYS	2.8
1	A	479	LEU	2.8
1	A	710	PRO	2.8
1	B	680	VAL	2.8
1	B	691	PHE	2.7
1	A	311	VAL	2.7
1	A	514	ARG	2.7
1	A	504	ILE	2.6
1	B	677	VAL	2.6
1	A	489	ASP	2.6
1	A	491	SER	2.6
1	A	591	THR	2.6
1	A	680	VAL	2.6
1	A	470	HIS	2.5
1	A	493	LEU	2.5
1	A	385	ASN	2.5
1	B	328	GLU	2.5
1	A	373	GLY	2.5
1	A	685	GLY	2.5
1	A	683	MET	2.4
1	A	677	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	355	PHE	2.4
1	B	595	VAL	2.4
1	A	394	TYR	2.4
1	A	416	VAL	2.4
1	A	584	PHE	2.4
1	A	415	CYS	2.3
1	B	561	TRP	2.3
1	A	593	ILE	2.3
1	B	615	ASP	2.3
1	A	382	GLU	2.2
1	A	499	VAL	2.2
1	A	512	ALA	2.2
1	A	588	TYR	2.2
1	A	681	PRO	2.2
1	A	676	TRP	2.2
1	A	319	LYS	2.2
1	A	485	TYR	2.2
1	A	594	GLY	2.2
1	A	552	ASP	2.2
1	A	565	PRO	2.2
1	A	566	ALA	2.2
1	B	715	VAL	2.2
1	B	593	ILE	2.1
1	B	679	ILE	2.1
1	A	490	GLY	2.1
1	B	352	ASP	2.1
1	B	386	LYS	2.1
1	B	588	TYR	2.1
1	A	679	ILE	2.1
1	A	381	LEU	2.1
1	A	630	LEU	2.1
1	A	353	GLN	2.0
1	B	682	PRO	2.0
1	B	329	HIS	2.0
1	A	384	VAL	2.0
1	A	561	TRP	2.0
1	A	711	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 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($Å^2$)	Q<0.9
5	ACT	B	860	4/4	0.79	0.18	57,57,57,60	0
4	Q1T	A	800	24/24	0.89	0.20	18,39,44,47	0
4	Q1T	B	800	24/24	0.92	0.20	29,47,50,50	0
5	ACT	A	860	4/4	0.92	0.31	71,73,75,76	0
3	H4B	A	760	17/17	0.96	0.20	30,32,35,37	0
2	HEM	B	750	43/43	0.97	0.19	26,29,36,40	0
2	HEM	A	750	43/43	0.97	0.22	27,30,35,38	0
3	H4B	B	760	17/17	0.97	0.16	29,31,33,34	0
6	ZN	A	900	1/1	0.99	0.09	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.
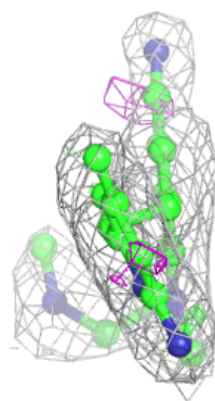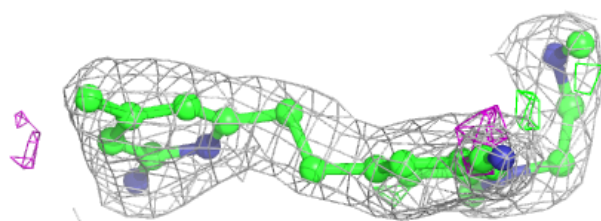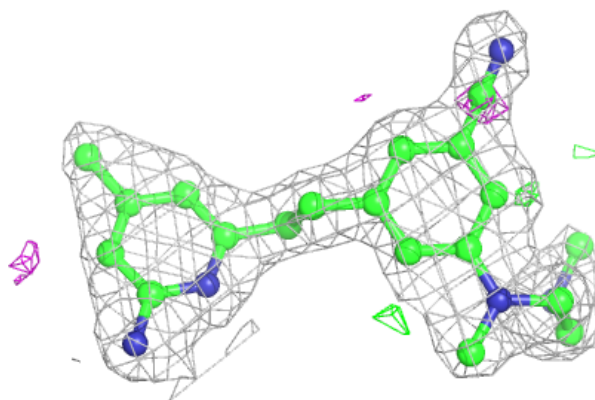
Electron density around Q1T A 800:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
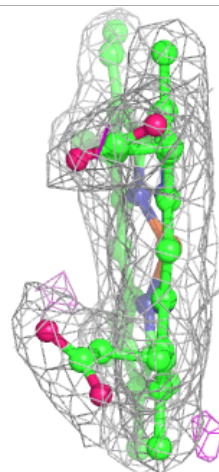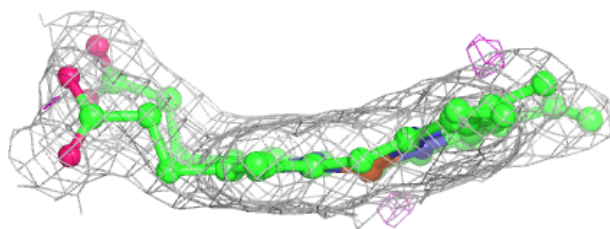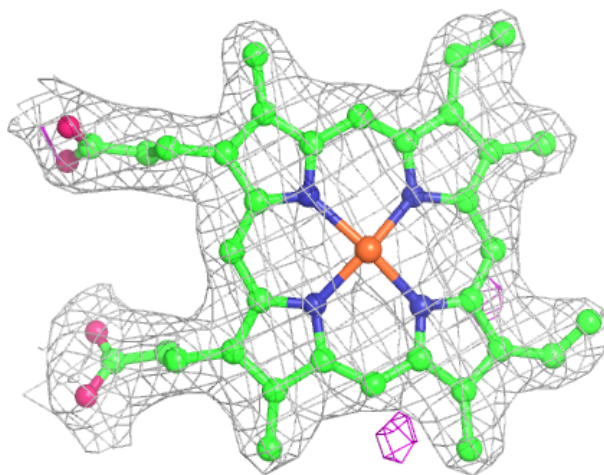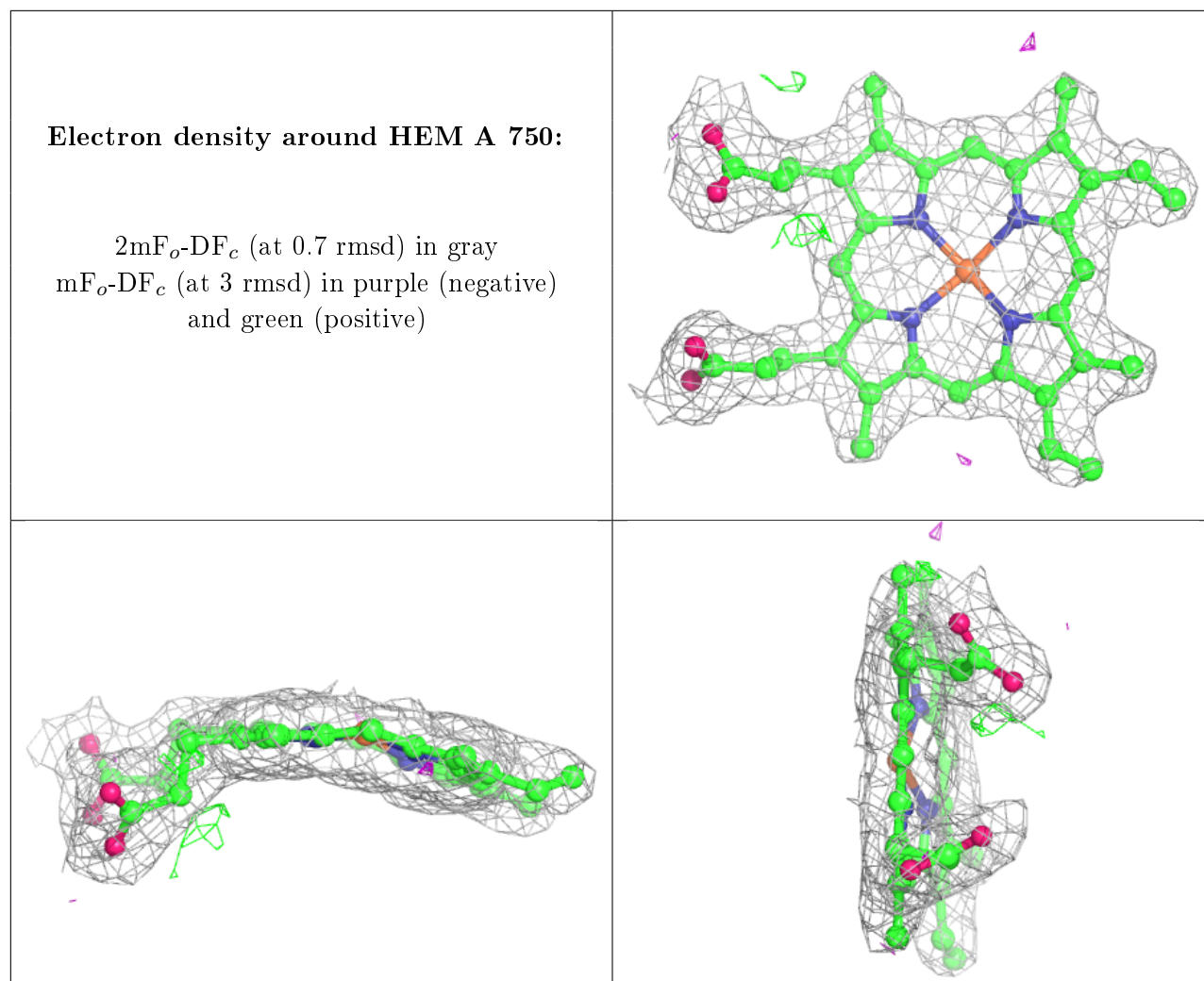and green (positive)
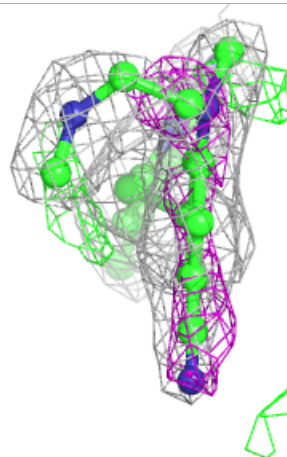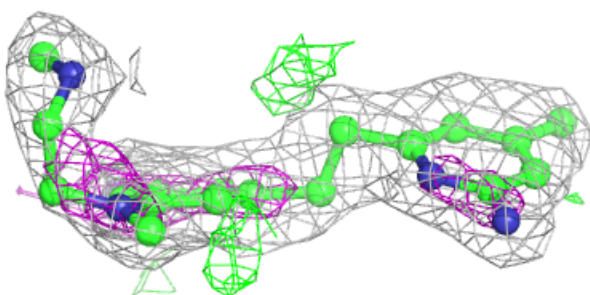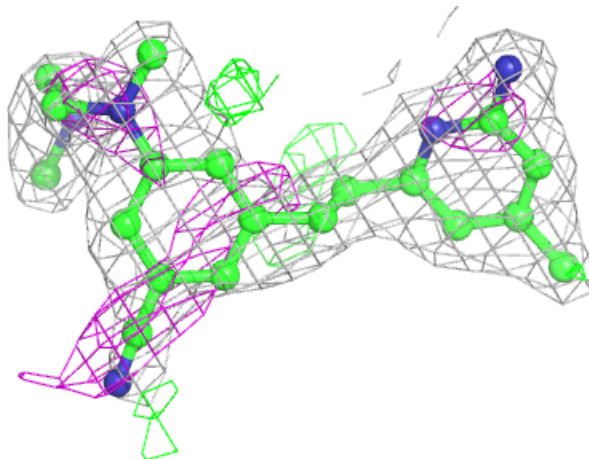
Electron density around Q1T B 800:

$2mF_o$-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 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)

Electron density around HEM A 750:

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

6.5 Other polymers (i)

There are no such residues in this entry.