



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:38 am BST

PDB ID : 4D2Y
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with (1R,2R)-2-(3-fluorobenzyl)-N-{2-[2-(1H-imidazol-1-yl)pyrimidin-4-yl]ethyl}cy clopropanamine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-10-20
Resolution : 1.98 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

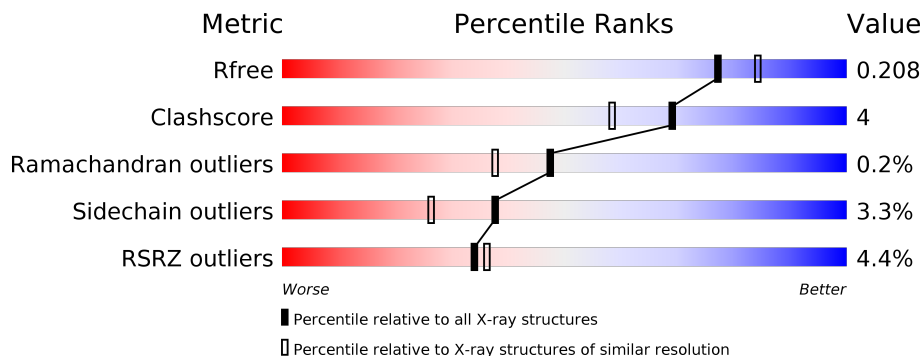
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

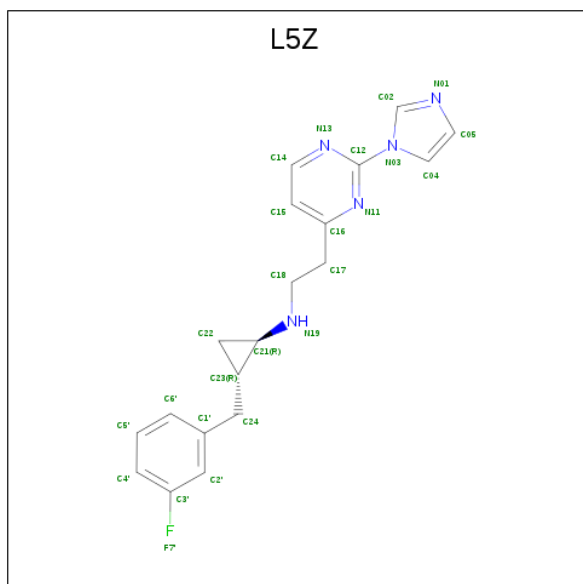
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	



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 (1R,2R)-2-(3-fluorobenzyl)-N-{2-[2-(1H-imidazol-1-yl)pyrimidin-4-yl]ethyl}cyclopropanamine (three-letter code: L5Z) (formula: C₁₉H₂₀FN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
4	A	1	25	19	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
4	B	1	25	19	1	5	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	A	1	1	1	0	0

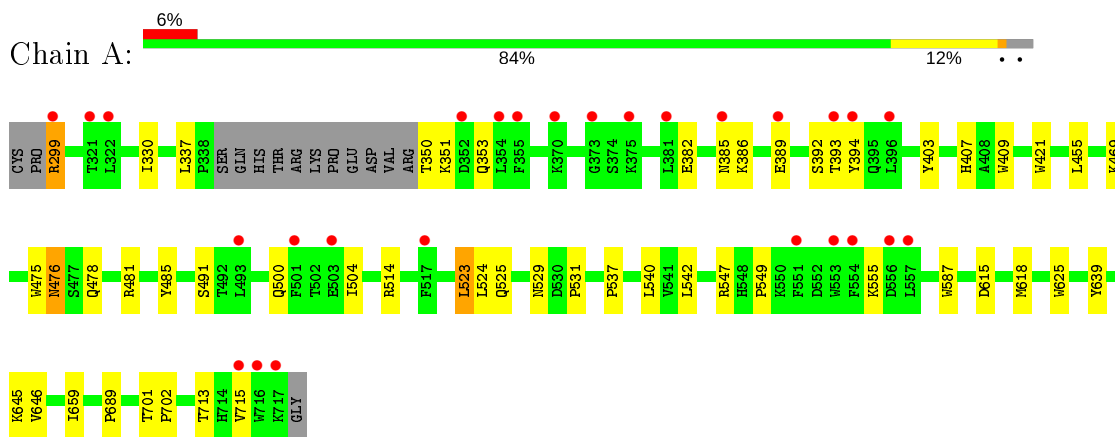
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	132	132	132	0	0
7	B	176	176	176	0	0

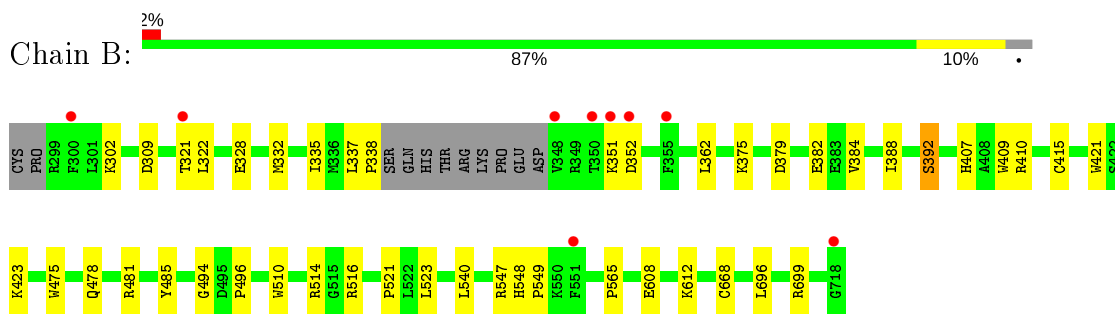
3 Residue-property plots [i](#)

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	51.85Å 110.47Å 164.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.84 – 1.98 49.45 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.84-1.98) 97.8 (49.45-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.98Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.171 , 0.208 0.171 , 0.208	Depositor DCC
R_{free} test set	3217 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.702	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7164	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: L5Z, 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	0.39	0/3422	0.53	0/4643
1	B	0.40	0/3453	0.53	0/4681
All	All	0.39	0/6875	0.53	0/9324

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	3323	0	3232	26	0
1	B	3354	0	3270	19	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	25	0	20	2	0
4	B	25	0	20	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	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	132	0	0	1	0
7	B	176	0	0	0	0
All	All	7164	0	6638	50	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 (50) 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	1.69	0.74
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.80	0.64
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.82	0.62
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.86	0.58
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.85	0.57
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.86	0.56
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.87	0.56
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.87	0.56
1:A:350:THR:N	1:A:353:GLN:OE1	2.40	0.53
1:B:608:GLU:O	1:B:612:LYS:HG3	2.09	0.52
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.92	0.52
1:A:299:ARG:N	7:A:2001:HOH:O	2.43	0.51
1:A:351:LYS:NZ	1:A:389:GLU:O	2.44	0.50
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.94	0.50
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.46	0.50
1:A:618:MET:HA	1:A:625:TRP:CD1	2.50	0.46
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.96	0.46
1:B:375:LYS:NZ	1:B:379:ASP:OD2	2.47	0.46
4:B:800:L5Z:H2'	4:B:800:L5Z:H23	1.77	0.46
1:A:525:GLN:HG3	1:A:529:ASN:O	2.17	0.45
1:A:659:ILE:HG13	1:A:689:PRO:HB2	1.99	0.45
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.99	0.45
1:B:302:LYS:HE3	1:B:302:LYS:HB2	1.77	0.45
1:B:388:ILE:O	1:B:392:SER:N	2.43	0.45
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.80	0.44
1:B:335:ILE:HB	1:B:338:PRO:HG3	1.99	0.43
1:B:565:PRO:HB2	4:B:800:L5Z:N13	2.33	0.43
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.07	0.43
1:B:494:GLY:O	1:B:496:PRO:HD3	2.18	0.43
1:A:500:GLN:O	1:A:504:ILE:HG13	2.19	0.43
1:A:393:THR:OG1	1:A:394:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.42
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.01	0.42
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.54	0.42
2:A:750:HEM:O2A	4:A:800:L5Z:H17	2.19	0.42
1:A:618:MET:HG2	1:A:625:TRP:CD2	2.55	0.42
1:B:407:HIS:CE1	1:B:410:ARG:HH11	2.37	0.42
1:B:415:CYS:HB2	2:B:750:HEM:ND	2.35	0.42
1:A:382:GLU:OE2	1:A:386:LYS:HE3	2.21	0.41
1:A:476:ASN:OD1	1:A:476:ASN:N	2.53	0.41
1:A:485:TYR:CE2	1:A:514:ARG:HA	2.56	0.41
1:A:524:LEU:O	1:A:531:PRO:HA	2.19	0.41
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.55	0.41
1:A:542:LEU:HD21	1:A:646:VAL:HG22	2.02	0.41
1:A:549:PRO:HB3	1:A:639:TYR:CE1	2.55	0.41
1:B:328:GLU:OE1	1:B:328:GLU:N	2.50	0.41
1:B:322:LEU:HB3	1:B:699:ARG:CZ	2.50	0.41
4:A:800:L5Z:H2'	4:A:800:L5Z:H23	1.87	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.42	0.40
1:B:548:HIS:CG	1:B:549:PRO:HD2	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	406/422 (96%)	387 (95%)	18 (4%)	1 (0%)	47	38
1	B	409/422 (97%)	402 (98%)	6 (2%)	1 (0%)	47	38
All	All	815/844 (97%)	789 (97%)	24 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	ASP
1	A	491	SER

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	365/377 (97%)	353 (97%)	12 (3%)	38	26
1	B	368/377 (98%)	356 (97%)	12 (3%)	38	26
All	All	733/754 (97%)	709 (97%)	24 (3%)	38	26

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ARG
1	A	337	LEU
1	A	385	ASN
1	A	469	LYS
1	A	476	ASN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	615	ASP
1	A	645	LYS
1	A	713	THR
1	A	715	VAL
1	B	309	ASP
1	B	321	THR
1	B	332	MET
1	B	337	LEU
1	B	351	LYS
1	B	382	GLU
1	B	392	SER
1	B	423	LYS
1	B	516	ARG
1	B	540	LEU

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Mol	Chain	Res	Type
1	B	547	ARG
1	B	668	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	407	HIS

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
5	ACT	B	860	-	1,3,3	1.25	0	0,3,3	0.00	-
3	H4B	B	760	-	16,18,18	0.90	0	11,26,26	2.65	5 (45%)
2	HEM	B	750	1,4	27,50,50	2.23	7 (25%)	17,82,82	1.74	3 (17%)
2	HEM	A	750	1,4	27,50,50	2.04	6 (22%)	17,82,82	1.90	3 (17%)
3	H4B	A	760	-	16,18,18	0.87	0	11,26,26	2.79	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	860	-	1,3,3	1.22	0	0,3,3	0.00	-
4	L5Z	A	800	2	27,28,28	1.30	5 (18%)	33,38,38	2.55	16 (48%)
4	L5Z	B	800	2	27,28,28	1.36	4 (14%)	33,38,38	2.40	16 (48%)

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
2	HEM	B	750	1,4	-	0/6/54/54	-
2	HEM	A	750	1,4	-	0/6/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	L5Z	A	800	2	-	2/8/19/19	0/4/4/4
4	L5Z	B	800	2	-	3/8/19/19	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3B-C2B	-5.06	1.33	1.40
2	A	750	HEM	C3D-C2D	5.05	1.52	1.37
2	B	750	HEM	C3D-C2D	5.05	1.52	1.37
2	B	750	HEM	C3C-C2C	-4.10	1.34	1.40
2	A	750	HEM	C3B-C2B	-4.07	1.34	1.40
2	A	750	HEM	C3B-CAB	3.82	1.55	1.47
2	A	750	HEM	C3C-CAC	3.69	1.55	1.47
2	B	750	HEM	C3C-CAC	3.64	1.55	1.47
2	B	750	HEM	C3B-CAB	3.63	1.55	1.47
2	A	750	HEM	C3C-C2C	-3.57	1.35	1.40
4	A	800	L5Z	C04-N03	-3.50	1.34	1.39
4	B	800	L5Z	C04-N03	-3.49	1.34	1.39
4	B	800	L5Z	C12-N11	3.12	1.36	1.32
4	B	800	L5Z	C22-C21	2.81	1.53	1.49
4	B	800	L5Z	C12-N13	2.74	1.35	1.31
4	A	800	L5Z	C22-C21	2.73	1.53	1.49
4	A	800	L5Z	C12-N13	2.60	1.35	1.31
4	A	800	L5Z	C12-N11	2.60	1.36	1.32
4	A	800	L5Z	C02-N03	-2.43	1.34	1.36
2	B	750	HEM	CMD-C2D	2.21	1.56	1.51
2	B	750	HEM	CAA-C2A	2.03	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	CMC-C2C	2.00	1.56	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	760	H4B	C4-C4A-C8A	6.26	120.13	114.57
3	A	760	H4B	C4-C4A-C8A	6.20	120.08	114.57
4	A	800	L5Z	C14-N13-C12	5.27	121.02	114.04
2	A	750	HEM	CBA-CAA-C2A	-4.97	103.32	112.49
4	A	800	L5Z	C22-C23-C24	-4.87	108.89	120.08
4	B	800	L5Z	C22-C23-C24	-4.66	109.37	120.08
4	B	800	L5Z	C14-N13-C12	4.44	119.92	114.04
4	A	800	L5Z	C22-C21-N19	-4.35	109.03	117.50
4	B	800	L5Z	C04-N03-C02	4.22	116.16	108.50
4	A	800	L5Z	C04-N03-C02	4.16	116.05	108.50
4	B	800	L5Z	N13-C12-N11	-4.06	121.48	126.08
4	A	800	L5Z	C15-C14-N13	-4.00	118.99	123.96
4	B	800	L5Z	C22-C21-N19	-3.99	109.73	117.50
4	A	800	L5Z	N13-C12-N11	-3.98	121.56	126.08
2	B	750	HEM	C1D-C2D-C3D	-3.96	104.24	107.00
2	B	750	HEM	CBA-CAA-C2A	-3.85	105.38	112.49
2	A	750	HEM	CBD-CAD-C3D	-3.85	105.39	112.48
4	B	800	L5Z	N13-C12-N03	3.79	120.69	114.81
3	A	760	H4B	C4-N3-C2	3.64	121.71	115.93
3	B	760	H4B	C4-N3-C2	3.45	121.41	115.93
4	B	800	L5Z	C14-C15-C16	3.38	119.79	116.62
4	B	800	L5Z	C15-C14-N13	-3.34	119.81	123.96
4	A	800	L5Z	N13-C12-N03	3.15	119.69	114.81
3	A	760	H4B	N3-C2-N1	-3.15	120.47	125.42
4	A	800	L5Z	C18-N19-C21	-3.11	109.81	114.20
4	A	800	L5Z	N11-C12-N03	3.02	118.69	114.78
4	A	800	L5Z	C1'-C24-C23	-2.99	108.74	113.65
4	A	800	L5Z	C14-C15-C16	2.97	119.41	116.62
4	B	800	L5Z	C15-C16-N11	-2.91	118.72	122.41
4	B	800	L5Z	C17-C16-N11	2.89	120.26	115.95
3	B	760	H4B	N3-C2-N1	-2.85	120.95	125.42
4	B	800	L5Z	C02-N03-C12	-2.76	120.60	126.02
4	A	800	L5Z	C4'-C3'-C2'	-2.74	119.73	123.29
4	A	800	L5Z	C02-N03-C12	-2.62	120.88	126.02
4	B	800	L5Z	C1'-C24-C23	-2.60	109.38	113.65
3	A	760	H4B	C2-N1-C8A	2.56	120.28	114.54
4	A	800	L5Z	C17-C16-N11	2.53	119.72	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	L5Z	C4'-C3'-C2'	-2.40	120.18	123.29
2	A	750	HEM	CMC-C2C-C3C	2.38	129.12	124.68
4	B	800	L5Z	N11-C12-N03	2.33	117.79	114.78
3	B	760	H4B	C2-N1-C8A	2.32	119.73	114.54
3	A	760	H4B	C4A-N5-C6	-2.24	115.05	121.16
4	A	800	L5Z	C05-C04-N03	-2.23	102.56	106.50
4	A	800	L5Z	C04-N03-C12	-2.21	123.01	125.50
4	B	800	L5Z	C05-C04-N03	-2.17	102.67	106.50
4	B	800	L5Z	C04-N03-C12	-2.07	123.16	125.50
3	B	760	H4B	N2-C2-N1	2.03	120.41	117.25
2	B	750	HEM	CBD-CAD-C3D	-2.03	108.73	112.48

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	800	L5Z	C2'-C1'-C24-C23
4	B	800	L5Z	C6'-C1'-C24-C23
4	A	800	L5Z	C17-C18-N19-C21
4	B	800	L5Z	C17-C18-N19-C21
4	A	800	L5Z	C2'-C1'-C24-C23

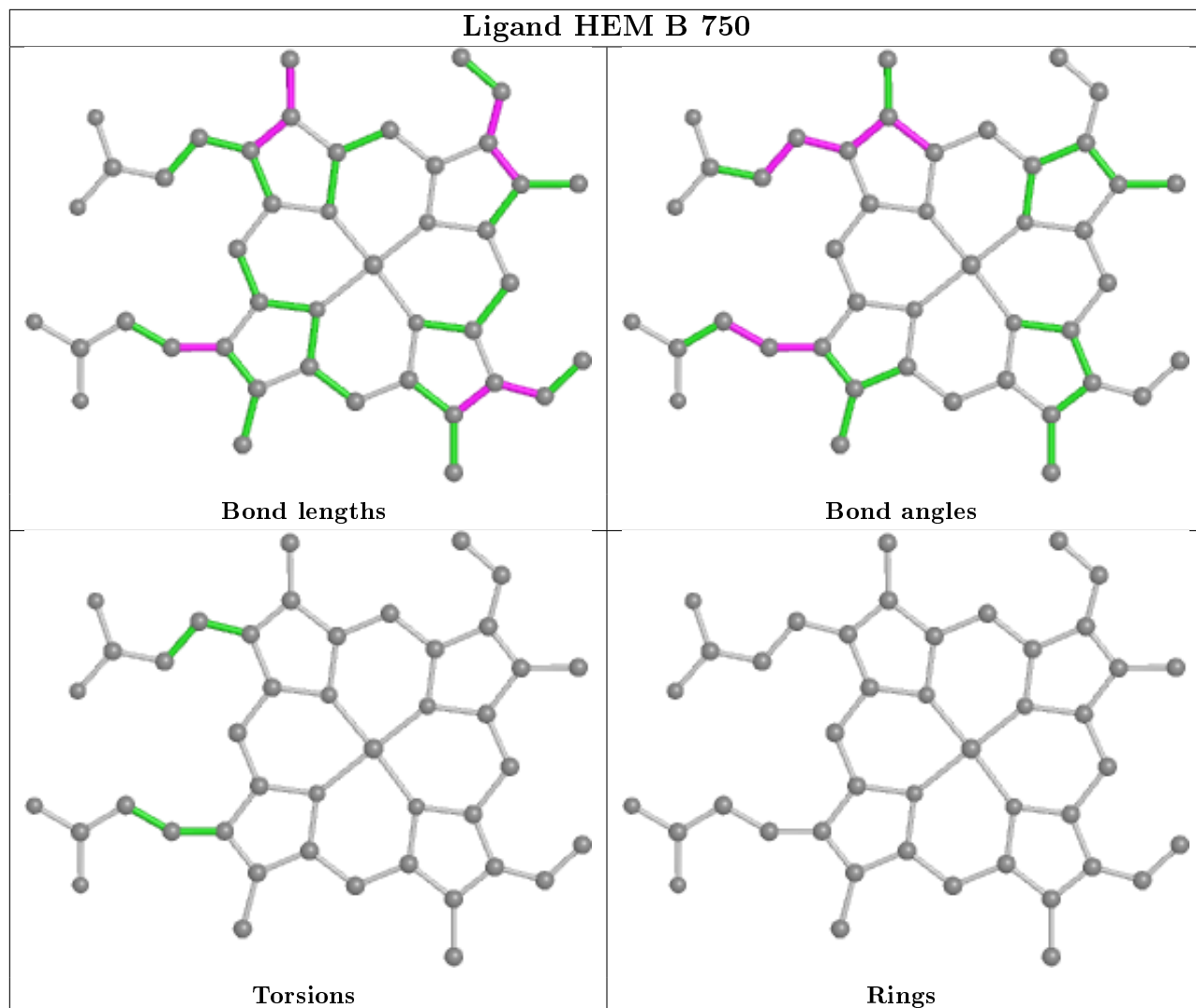
There are no ring outliers.

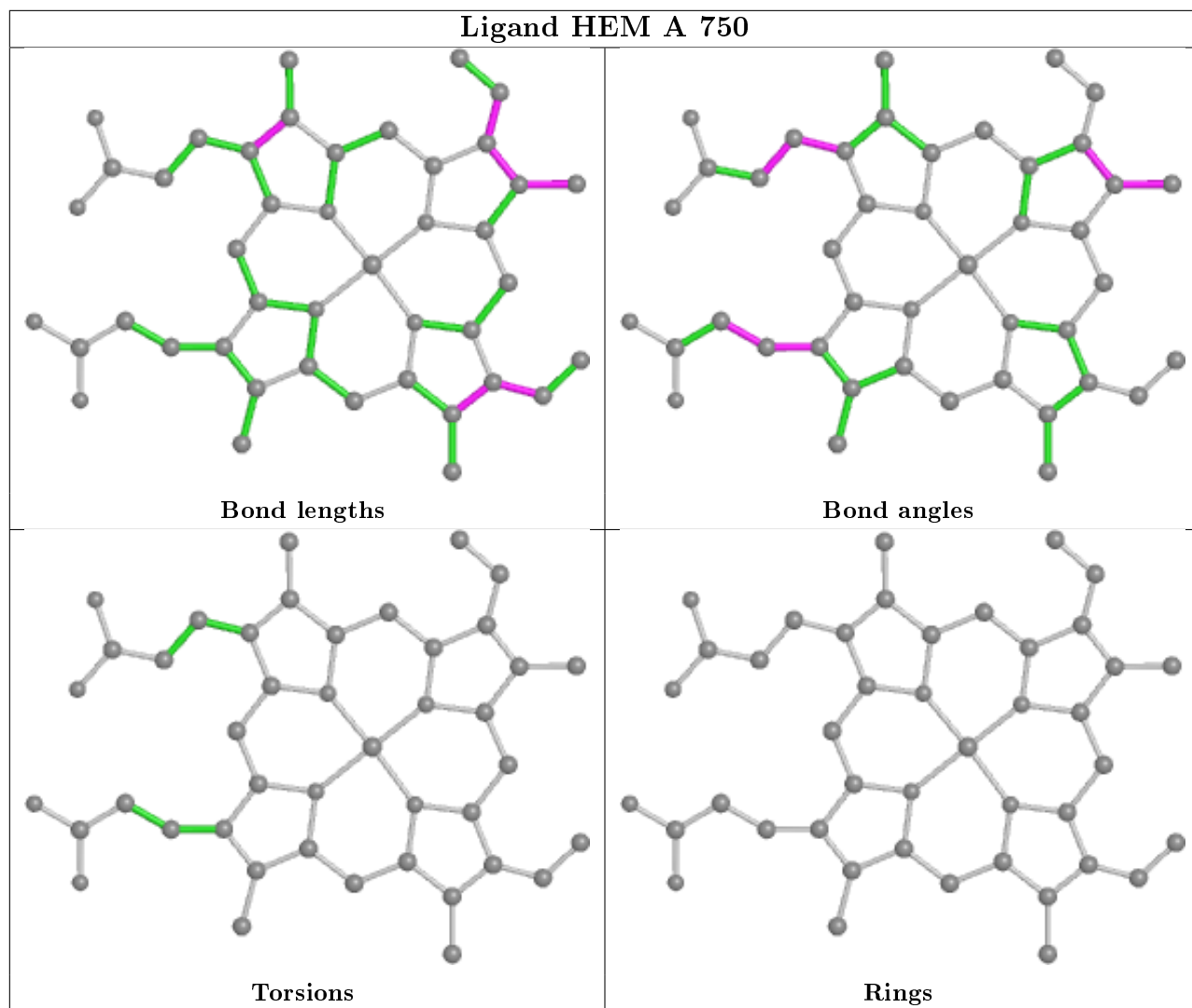
4 monomers are involved in 8 short contacts:

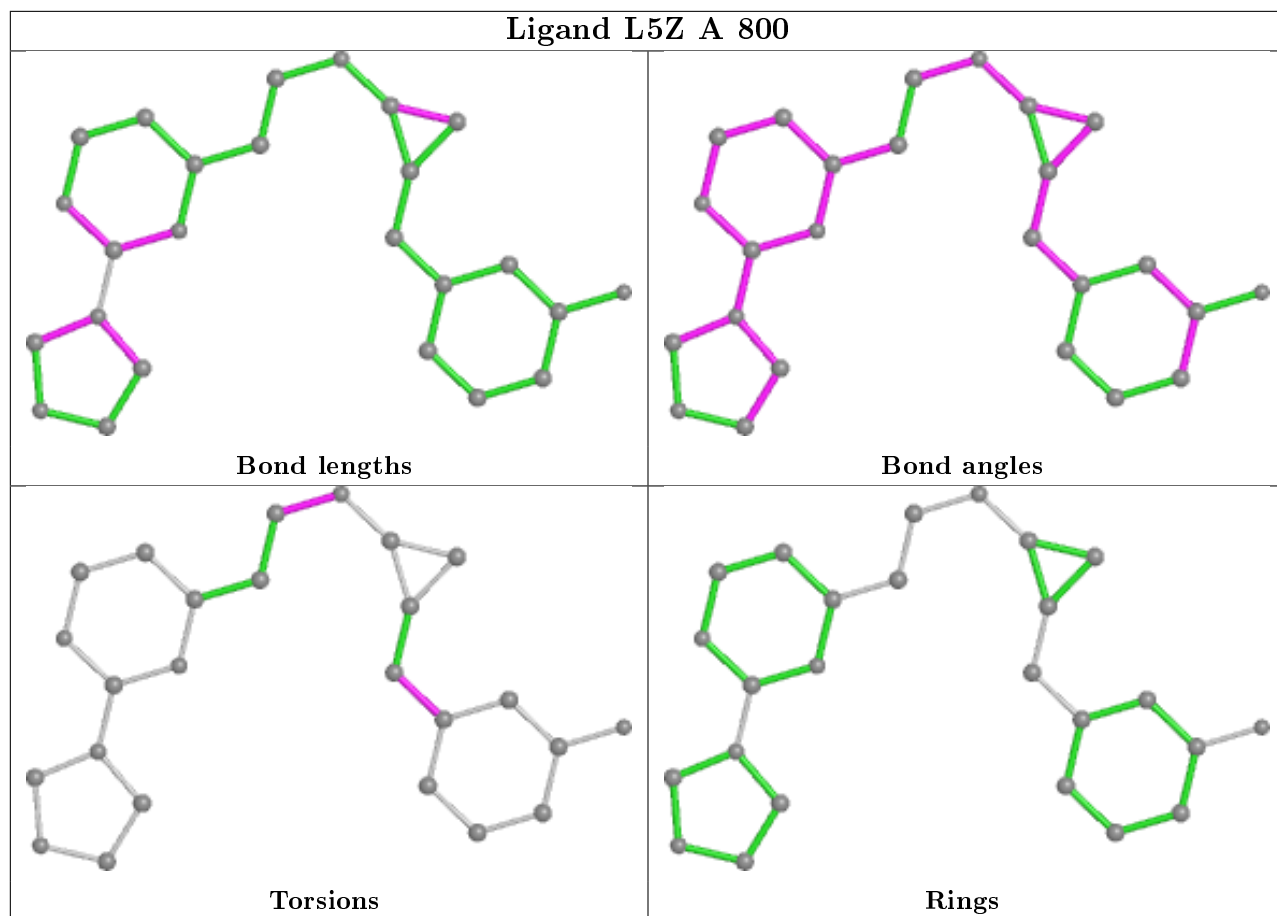
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	2	0
2	A	750	HEM	3	0
4	A	800	L5Z	2	0
4	B	800	L5Z	2	0

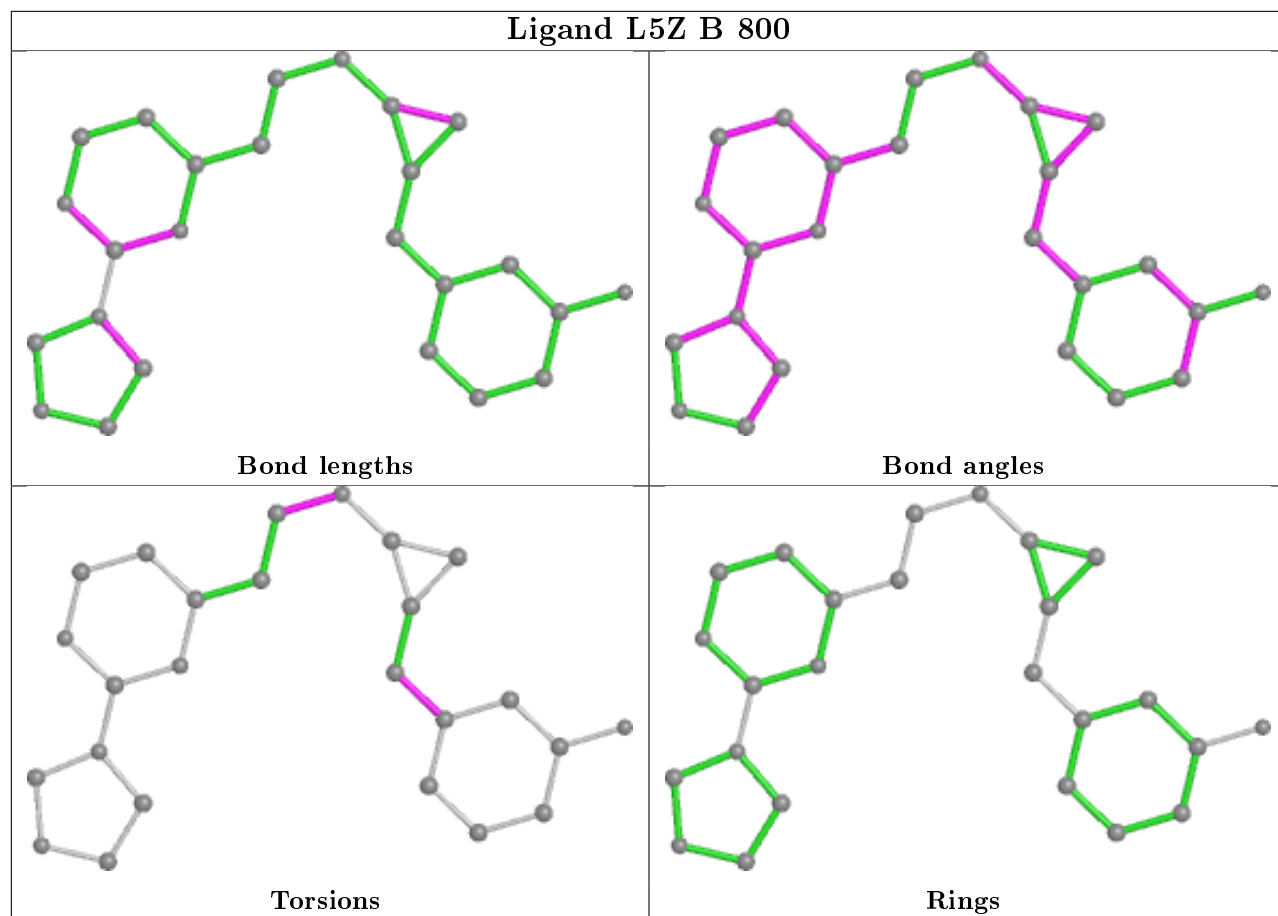
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	408/422 (96%)	0.62	27 (6%) 18 20	26, 55, 101, 148	0
1	B	411/422 (97%)	0.31	9 (2%) 62 63	24, 43, 77, 109	0
All	All	819/844 (97%)	0.47	36 (4%) 34 36	24, 48, 94, 148	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	13.6
1	A	355	PHE	5.9
1	A	321	THR	5.0
1	B	348	VAL	5.0
1	A	554	PHE	4.0
1	A	322	LEU	3.6
1	A	381	LEU	3.5
1	B	350	THR	3.5
1	A	503	GLU	3.5
1	A	715	VAL	3.4
1	B	321	THR	3.2
1	A	352	ASP	3.0
1	A	551	PHE	3.0
1	A	370	LYS	2.8
1	A	389	GLU	2.8
1	A	553	TRP	2.7
1	A	493	LEU	2.7
1	A	354	LEU	2.6
1	B	352	ASP	2.6
1	A	373	GLY	2.5
1	B	351	LYS	2.5
1	A	375	LYS	2.4
1	B	300	PHE	2.4
1	A	393	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	718	GLY	2.4
1	A	716	TRP	2.3
1	B	355	PHE	2.3
1	A	557	LEU	2.3
1	B	551	PHE	2.3
1	A	385	ASN	2.2
1	A	517	PHE	2.2
1	A	396	LEU	2.1
1	A	501	PHE	2.1
1	A	394	TYR	2.1
1	A	299	ARG	2.1
1	A	556	ASP	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.

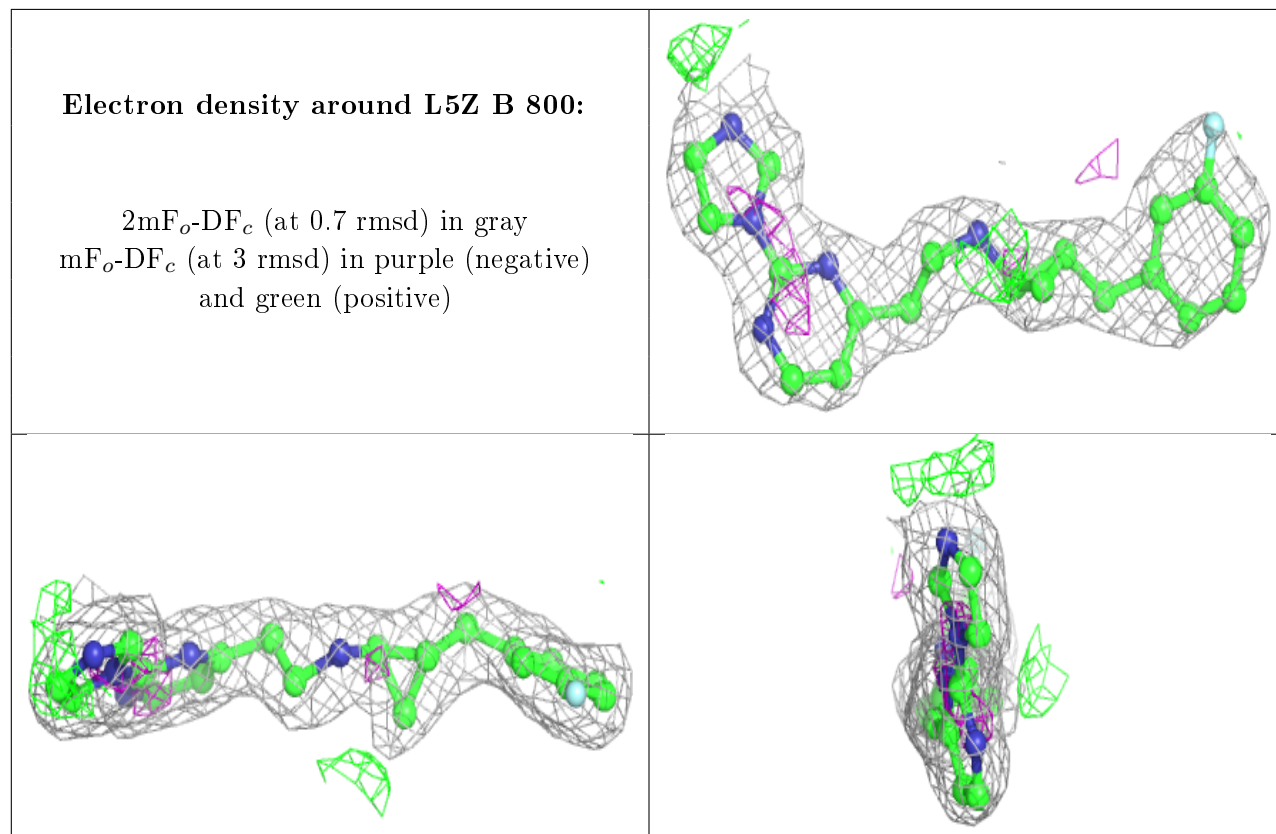
6.4 Ligands [i](#)

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
4	L5Z	B	800	25/25	0.94	0.13	27,38,69,83	0
5	ACT	A	860	4/4	0.95	0.28	68,73,74,75	0
5	ACT	B	860	4/4	0.96	0.17	48,52,60,65	0
3	H4B	A	760	17/17	0.96	0.11	25,33,37,39	0
4	L5Z	A	800	25/25	0.97	0.13	31,41,70,74	0
3	H4B	B	760	17/17	0.97	0.12	27,34,38,39	0
2	HEM	B	750	43/43	0.98	0.16	19,28,37,41	0
2	HEM	A	750	43/43	0.98	0.12	22,33,41,45	0
6	ZN	A	1717	1/1	1.00	0.09	38,38,38,38	0

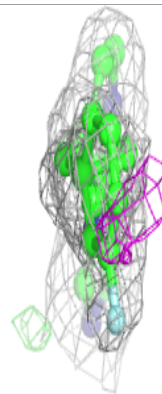
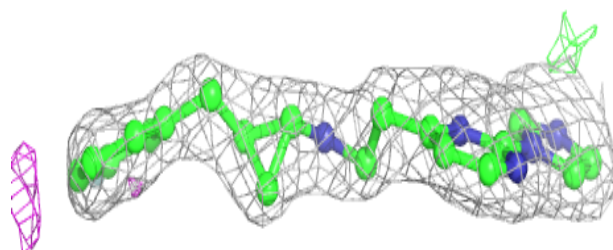
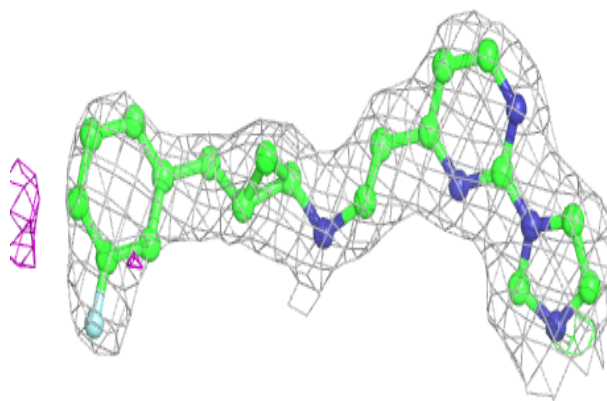
The following is a graphical depiction of the model fit to experimental electron density of all

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.



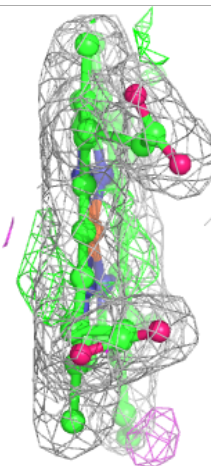
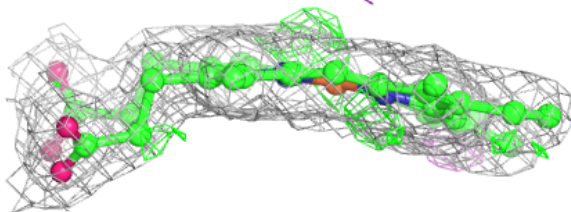
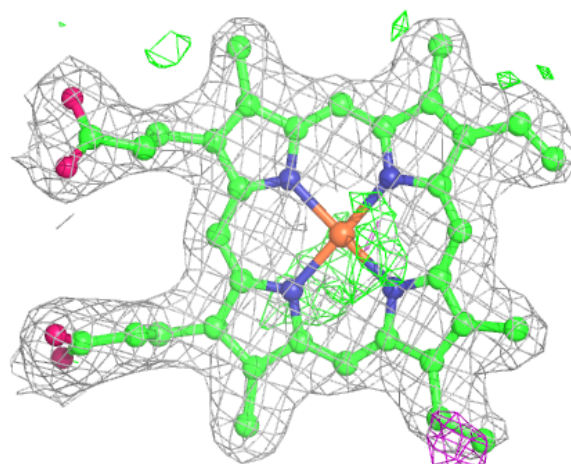
Electron density around L5Z A 800:

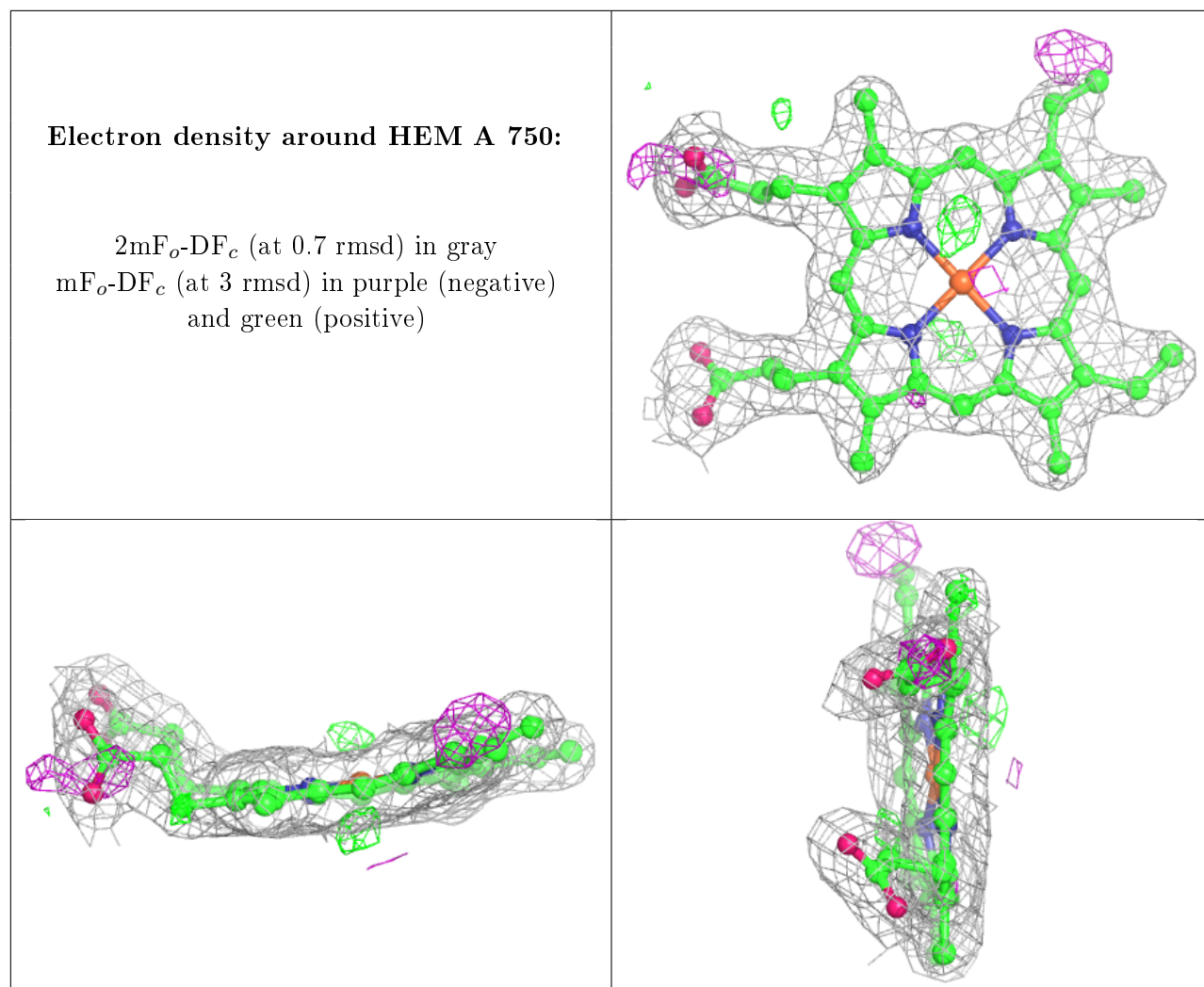
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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.