

wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 – 09:30 am BST

PDB ID : 4D34

Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex

with 2-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)-N-(3- fluorophenethyl)ethan-1-a

mine

Authors: Chreifi, G.; Li, H.; Poulos, T.L.

Deposited on : 2014-10-20

Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at $\frac{\text{https://www.wwpdb.org/validation/2017/XrayValidationReportHelp}}{\text{with specific help available everywhere you see the } \widehat{\textbf{1}} \text{ symbol.}$

The following versions of software and data (see references (1)) 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)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

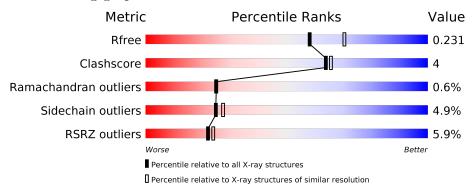
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	443	82%	8%	•	9%
1	В	443	79%	11%		9%



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6818 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.

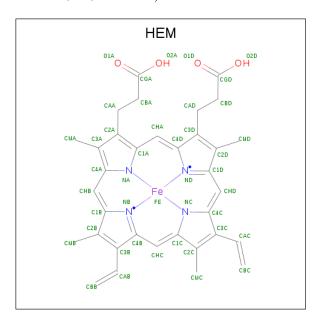
• Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues		${f Atoms}$					ZeroOcc	AltConf	Trace
1	A	405	Total 3229	As 1	C 2053	N 568	O 591	S 16	0	1	0
1	В	405	Total 3229	As 1	C 2054	N 569	O 589	S 16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
В	100	ARG	CYS	conflict	UNP P29473

• Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

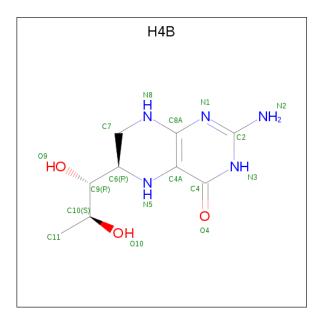
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Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf		
9	D	1	Total	С	Fe	N	О	0	0
	Б	1	43	34	1	4	4	U	U

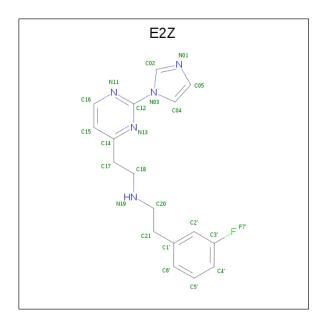
• Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

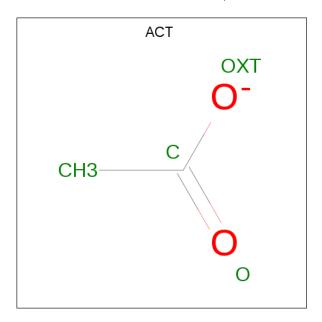
• Molecule 4 is 2-(3-fluorophenyl)-N-{2-[2-(1H-imidazol-1-yl)pyrimidin-4-yl]ethyl}ethanamine (three-letter code: E2Z) (formula: $C_{17}H_{18}FN_5$).





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	
4	Λ	Λ 1	Total	С	F	N	0	0	
4	A	1	23	17	1	5	0		
4	D	1	Total	С	F	N	0	0	
4	D	1	23	17	1	5	0	U	

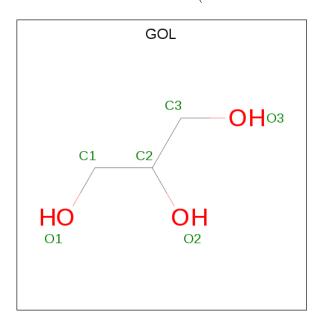
 \bullet Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$



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



• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	В	1	Total C O 6 3 3	0	0

• Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0

• Molecule 8 is water.

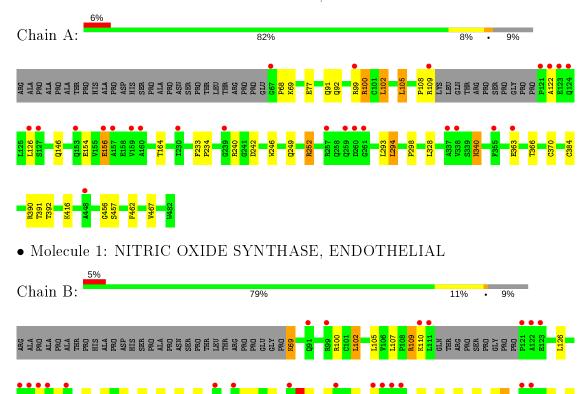
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
8	A	93	Total O 93 93	0	0
8	В	80	Total O 80 80	0	0



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, ENDOTHELIAL





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	58.16Å 106.63Å 156.64Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 - 2.25	Depositor
Resolution (A)	39.30 - 2.25	EDS
% Data completeness	98.8 (40.00-2.25)	Depositor
(in resolution range)	98.7 (39.30-2.25)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.36 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
D D.	0.176 , 0.231	Depositor
R, R_{free}	0.184 , 0.231	DCC
R_{free} test set	2320 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35 \; , 39.5$	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6818	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: GOL, ZN, H4B, CAS, E2Z, ACT, HEM

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		Boı	nd lengths	Bond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	0.74	$2/3312 \ (0.1\%)$	0.86	4/4509 (0.1%)
1	В	0.69	1/3308 (0.0%)	0.80	3/4502 (0.1%)
All	All	0.72	3/6620 (0.0%)	0.83	7/9011 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(exttt{A})$
1	В	363	GLU	CG-CD	9.61	1.66	1.51
1	A	363[A]	GLU	CG-CD	7.69	1.63	1.51
1	A	363[B]	GLU	CG-CD	7.69	1.63	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	363[A]	GLU	OE1-CD-OE2	-7.50	114.30	123.30
1	A	363[B]	GLU	OE1-CD-OE2	-7.50	114.30	123.30
1	A	252	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	В	363	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	В	240	ARG	NE-CZ-NH1	5.93	123.27	120.30

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	Α	3229	0	3133	22	0
1	В	3229	0	3141	28	0
2	A	43	0	30	5	0
2	В	43	0	30	5	0
3	A	17	0	15	0	0
3	В	17	0	15	1	0
4	A	23	0	18	1	0
4	В	23	0	18	3	0
5	A	4	0	3	0	0
5	В	4	0	3	0	0
6	A	6	0	8	0	0
6	В	6	0	8	0	0
7	A	1	0	0	0	0
8	A	93	0	0	2	0
8	В	80	0	0	0	0
All	All	6818	0	6422	55	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.

The worst 5 of 55 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{array}{c} \operatorname{Clash} \ \operatorname{overlap}\ (ext{\AA}) \end{array}$
1:B:384:CAS:AS	1:B:384:CAS:SG	2.49	1.30
1:A:384:CAS:AS	1:A:384:CAS:SG	2.59	1.21
2:A:500:HEM:HMC2	2:A:500:HEM:HBC2	1.68	0.74
2:B:500:HEM:HBC2	2:B:500:HEM:HMC2	1.71	0.73
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.75	0.68

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	Percent	iles
1	A	401/443 (90%)	380 (95%)	18 (4%)	3 (1%)	22 2	1
1	В	400/443 (90%)	384 (96%)	14 (4%)	2 (0%)	29 2	9
All	All	801/886 (90%)	764 (95%)	32 (4%)	5 (1%)	25 2	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	110	LYS
1	A	122	ALA
1	A	456	GLY
1	A	108	PRO
1	В	145	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	344/375 (92%)	327 (95%)	17 (5%)	25 27
1	В	344/375 (92%)	327 (95%)	17 (5%)	25 27
All	All	688/750 (92%)	654 (95%)	34 (5%)	25 27

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	THR
1	В	102	LEU
1	В	378	LEU
1	В	69	LYS
1	A	105	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	468	ASN
1	В	340	ASN
1	A	340	ASN
1	В	225	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\operatorname{Res} \left \operatorname{Link} \right $	Bond lengths			E	ond ang	gles	
MIOI	Type Chain Res L	25 LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
1	CAS	В	384	1	5,8,9	1.48	2 (40%)	1,9,11	0.54	0
1	CAS	A	384	1	5,8,9	1.44	1 (20%)	1,9,11	0.14	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	\mathbf{Res}	Link	Chirals	Torsions	Rings
1	CAS	В	384	1	-	0/0/7/9	-
1	CAS	A	384	1	_	0/0/7/9	_

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	384	CAS	AS-CE1	2.81	2.03	1.96
1	В	384	CAS	AS-CE1	2.14	2.01	1.96
1	В	384	CAS	AS-CE2	2.10	2.01	1.96



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	384	CAS	2	0
1	A	384	CAS	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Trans	Chain	Res	Link	В	ond leng	$\overline{ ext{gths}}$	Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	HEM	A	500	1,4	27,50,50	1.01	0	17,82,82	1.65	4 (23%)
2	HEM	В	500	1,4	27,50,50	1.10	3 (11%)	17,82,82	1.94	3 (17%)
4	E2Z	В	800	2	24,25,25	1.39	4 (16%)	28,32,32	2.54	11 (39%)
3	H4B	В	600	-	16,18,18	1.06	1 (6%)	11,26,26	2.40	5 (45%)
6	GOL	A	880	_	5,5,5	0.26	0	5,5,5	0.87	0
5	ACT	В	861	_	1,3,3	2.64	1 (100%)	0,3,3	0.00	=
6	GOL	В	880	_	5,5,5	0.34	0	5,5,5	0.77	0
4	E2Z	A	800	2	24,25,25	1.78	4 (16%)	28,32,32	2.39	6 (21%)
3	H4B	A	600	-	16,18,18	1.10	0	11,26,26	3.01	7 (63%)
5	ACT	A	860	-	1,3,3	1.69	0	0,3,3	0.00	-

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	s columns.
'-' means no outliers of that kind	were identified.			

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1,4	-	1/6/54/54	-
2	HEM	В	500	1,4	-	0/6/54/54	-
4	E2Z	В	800	2	-	2/8/12/12	0/3/3/3
3	H4B	В	600	-	-	0/8/17/17	0/2/2/2
6	GOL	A	880	_	-	2/4/4/4	-
6	GOL	В	880	_	-	2/4/4/4	-
4	E2Z	A	800	2	-	1/8/12/12	0/3/3/3
3	H4B	A	600	_	-	0/8/17/17	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	${f Observed(\AA)}$	$\mathbf{Ideal}(\mathbf{\AA})$
4	A	800	E2Z	C04-N03	-4.67	1.32	1.39
4	A	800	E2Z	C02-N03	-4.32	1.31	1.36
4	A	800	E2Z	C12-N11	4.09	1.38	1.31
4	В	800	E2Z	C04-N03	-3.85	1.33	1.39
4	В	800	E2Z	C02-N03	-3.31	1.33	1.36

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
4	A	800	E2Z	N11-C12-N13	-6.71	118.47	126.08
4	A	800	E2Z	C16-N11-C12	6.41	122.53	114.04
4	В	800	E2Z	N11-C12-N13	-5.94	119.34	126.08
2	В	500	HEM	CBA-CAA-C2A	-5.86	101.67	112.49
4	В	800	E2Z	C16-N11-C12	5.78	121.69	114.04

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	${f Res}$	Type	${f Atoms}$
2	A	500	HEM	C2A-CAA-CBA-CGA
4	A	800	E2Z	C17-C18-N19-C20
4	В	800	E2Z	N19-C20-C21-C1'
6	В	880	GOL	O1-C1-C2-C3
6	В	880	GOL	O1-C1-C2-O2

There are no ring outliers.

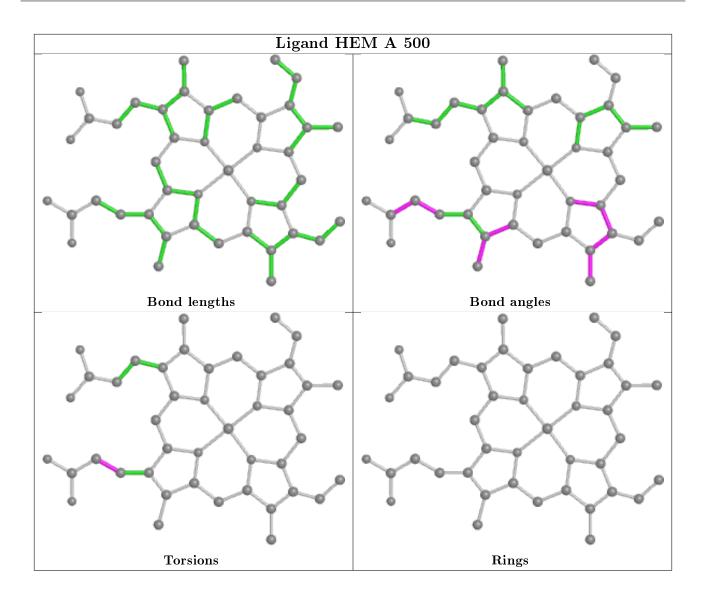
5 monomers are involved in 12 short contacts:



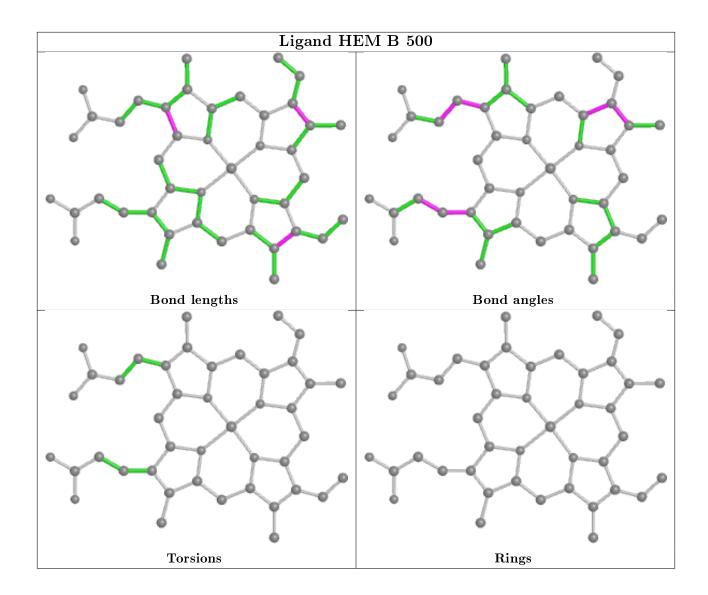
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	5	0
2	В	500	HEM	5	0
4	В	800	E2Z	3	0
3	В	600	H4B	1	0
4	A	800	E2Z	1	0

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 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.

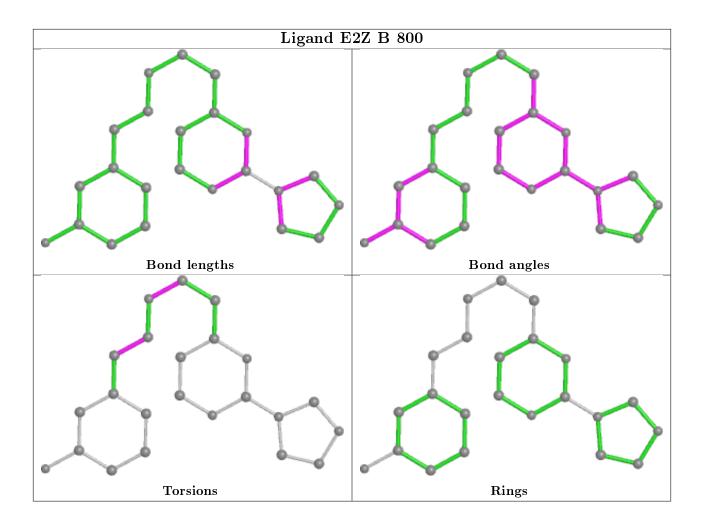




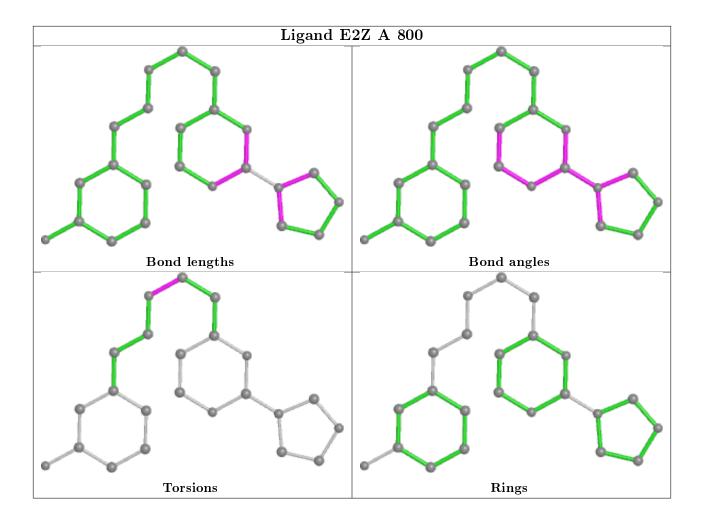












5.7 Other polymers (i)

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, 95^{th} 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 $>$	$\# \mathbf{RSRZ} >$	-2	$OWAB(A^2)$	Q<0.9
1	A	404/443 (91%)	0.12	25 (6%) 20	22	38, 50, 79, 120	0
1	В	404/443 (91%)	0.11	23 (5%) 23	25	37, 55, 86, 115	0
All	All	808/886 (91%)	0.11	48 (5%) 22	24	37, 52, 82, 120	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	GLU	5.4
1	В	259	GLN	5.3
1	A	259	GLN	5.0
1	В	141	LYS	4.7
1	A	160	ALA	4.2

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
1	CAS	A	384	9/10	0.94	0.11	47,49,79,88	0
1	CAS	В	384	9/10	0.96	0.13	63,67,104,112	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

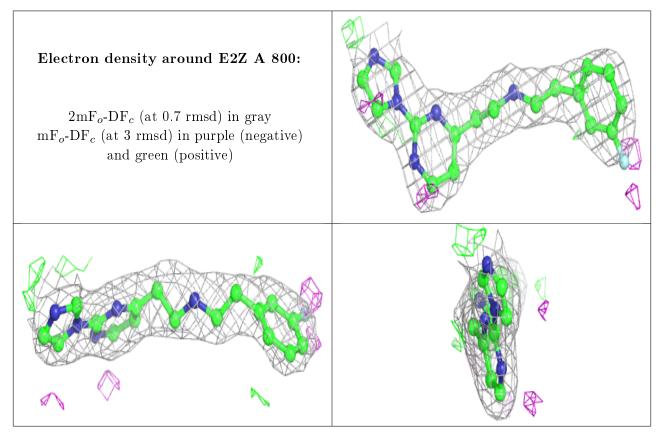


6.4 Ligands (i)

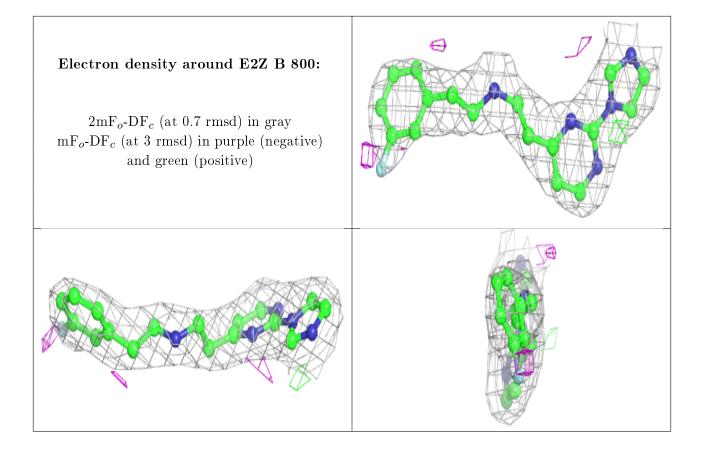
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
6	GOL	A	880	6/6	0.91	0.38	70,73,78,90	0
5	ACT	В	861	4/4	0.93	0.29	53,64,64,65	0
6	GOL	В	880	6/6	0.93	0.24	59,63,68,71	0
3	H4B	В	600	17/17	0.94	0.18	49,52,56,57	0
4	E2Z	A	800	23/23	0.95	0.23	41,46,68,77	0
5	ACT	A	860	4/4	0.96	0.10	53,60,60,62	0
3	H4B	A	600	17/17	0.97	0.16	45,50,54,55	0
4	E2Z	В	800	23/23	0.97	0.21	37,46,70,77	0
2	HEM	A	500	43/43	0.98	0.20	33,38,62,68	0
2	HEM	В	500	43/43	0.98	0.14	39,45,59,80	0
7	ZN	A	900	1/1	1.00	0.07	51,51,51,51	0

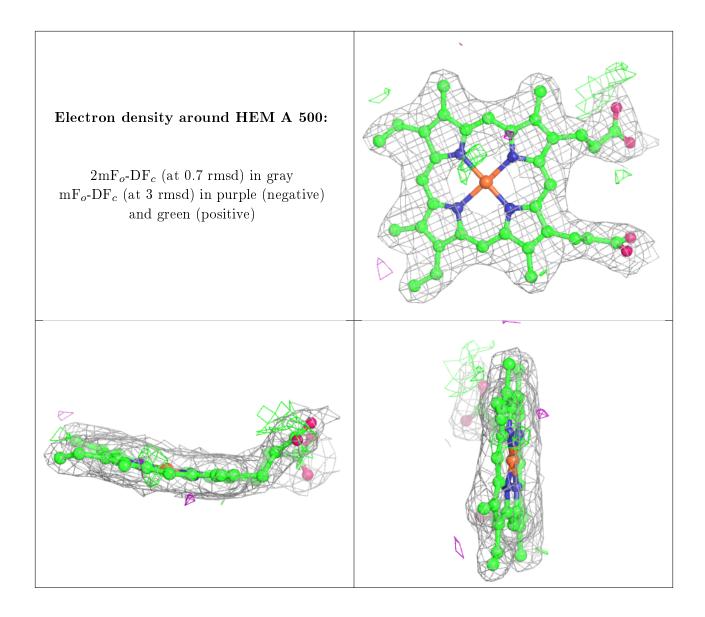
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



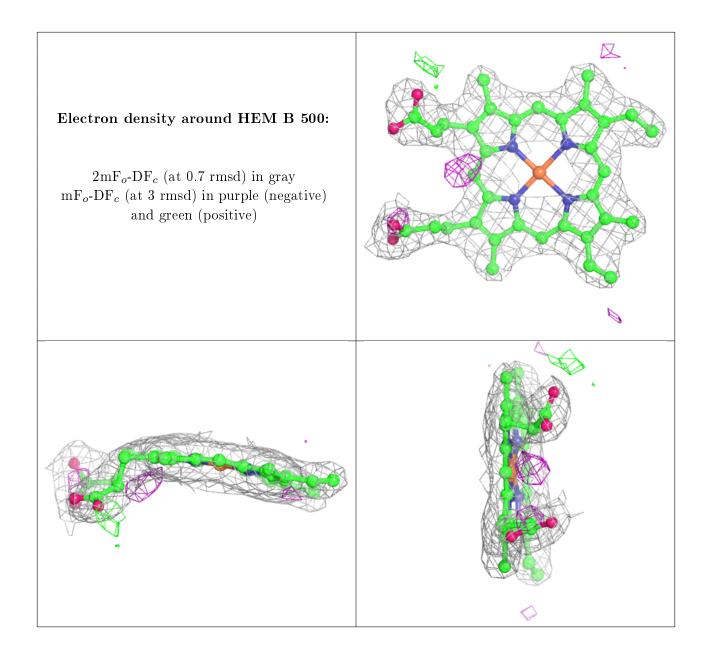












6.5 Other polymers (i)

There are no such residues in this entry.

