



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:27 am BST

PDB ID : 3RQP  
Title : Structure of the endothelial nitric oxide synthase heme domain in complex with 6-{{[(3R,4R)-4-(2-{{[(2R/2S)-1-(3-fluorophenyl)propan-2-yl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine  
Authors : Li, H.; Delker, S.L.; Poulos, T.L.  
Deposited on : 2011-04-28  
Resolution : 2.35 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](mailto: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.

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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

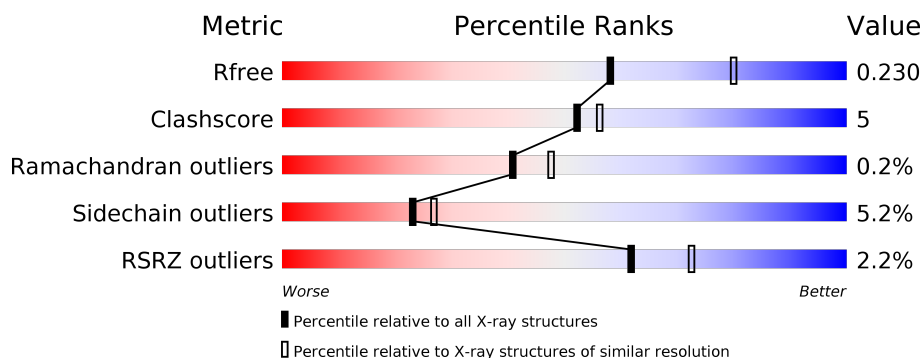
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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	443	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>9%</div> </div> </div>
1	B	443	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>9%</div> </div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6920 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	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	3	0
			3244	2061	572	595	16			
1	B	403	Total	C	N	O	S	0	2	0
			3218	2045	567	590	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		

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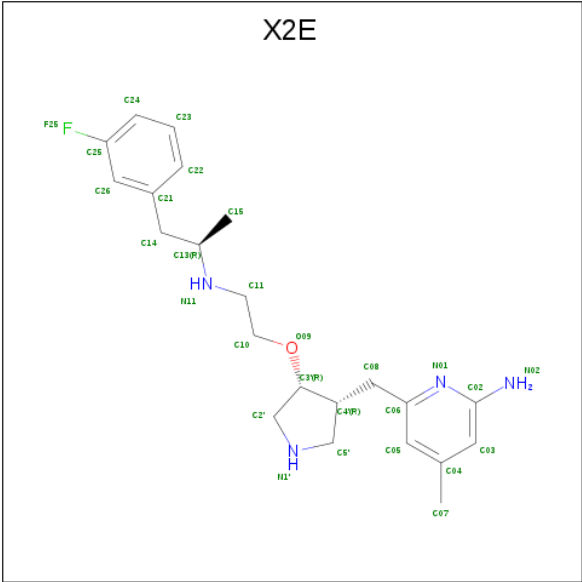
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



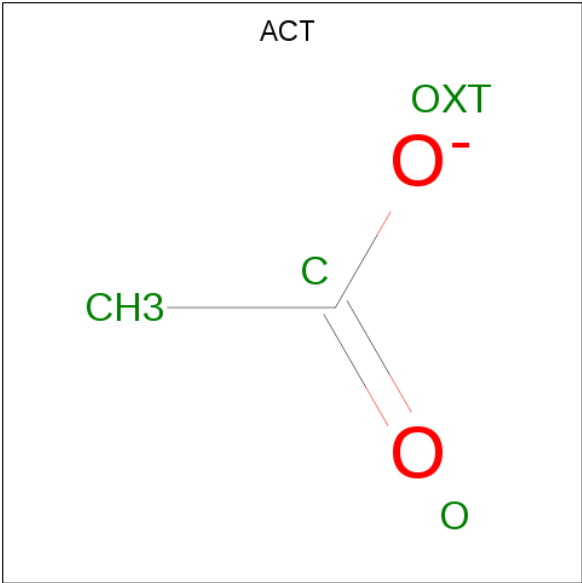
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[(3R,4R)-4-(2-[(2R)-1-(3-fluorophenyl)propan-2-yl]amino)ethoxy]pyrrolidin-3-ylmethyl]-4-methylpyridin-2-amine (three-letter code: X2E) (formula:  $C_{22}H_{31}FN_4O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			28	22	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			28	22	1	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



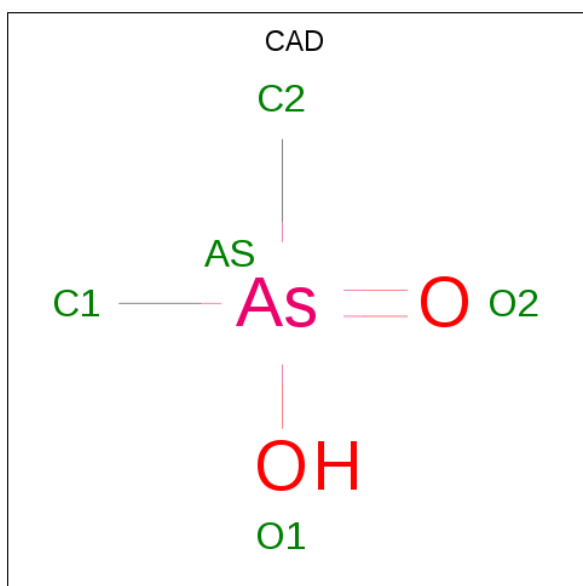
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is CACODYLIC ACID (three-letter code: CAD) (formula:  $C_2H_7AsO_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	As	C	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 3	As 1	C 2	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

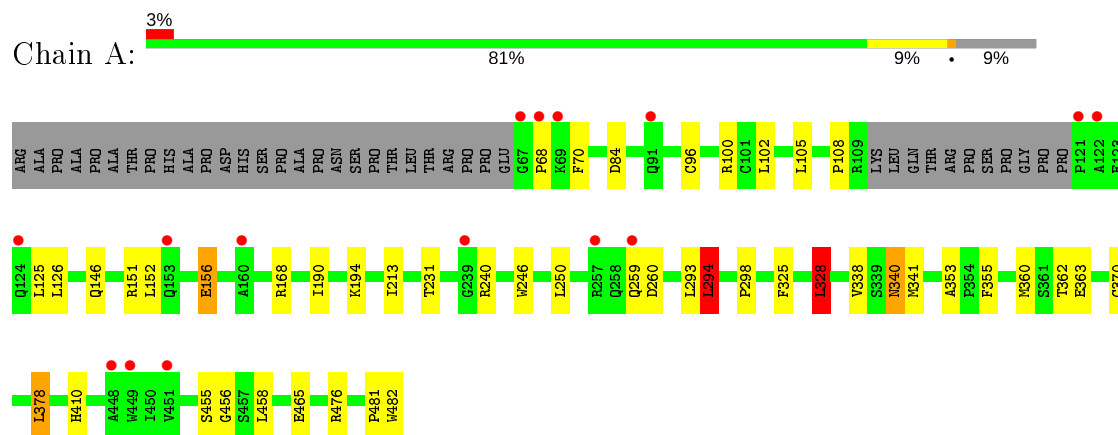
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	128	Total 128	O 128	0	0
9	B	127	Total 127	O 127	0	0

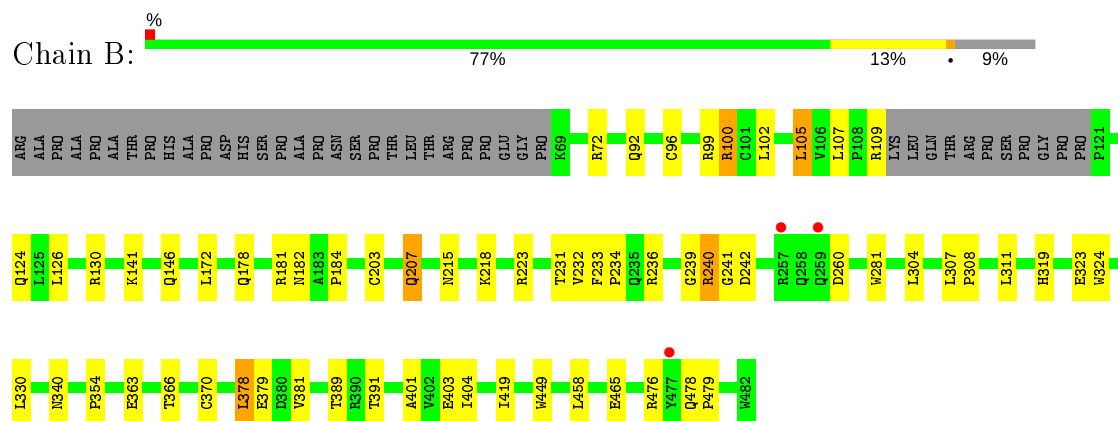
### 3 Residue-property plots [i](#)

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



- Molecule 1: Nitric oxide synthase, endothelial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.95Å 106.63Å 156.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.35 48.43 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.43-2.35) 99.4 (48.43-2.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.178 , 0.228 0.180 , 0.230	Depositor DCC
$R_{free}$ test set	2070 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, X2E, ACT, HEM, CAD

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	0.69	0/3338	0.72	2/4546 (0.0%)
1	B	0.73	1/3307 (0.0%)	0.72	0/4503
All	All	0.71	1/6645 (0.0%)	0.72	2/9049 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	CYS	CB-SG	-6.68	1.70	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	328	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	GLY	Peptide

## 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	3244	0	3142	34	0
1	B	3218	0	3121	36	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
4	A	28	0	31	3	0
4	B	28	0	31	6	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	3	0	0	0	0
7	B	3	0	0	1	0
8	A	1	0	0	0	0
9	A	128	0	0	2	0
9	B	127	0	0	4	0
All	All	6920	0	6437	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (72) 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:281:TRP:HB2	1:B:304:LEU:HD21	1.58	0.85
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.38	0.70
1:B:236:ARG:HD3	1:B:242:ASP:CG	2.13	0.69
1:A:410[B]:HIS:CE1	9:A:1123:HOH:O	2.45	0.69
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.74	0.69
1:A:340:ASN:HD22	1:A:340:ASN:H	1.40	0.68
1:B:236:ARG:HD3	1:B:242:ASP:OD1	1.94	0.68
1:B:231:THR:O	1:B:354:PRO:HD2	1.95	0.66
1:B:236:ARG:CD	1:B:242:ASP:OD1	2.46	0.64
1:B:478:GLN:HB2	1:B:479:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HB2	9:A:1006:HOH:O	1.97	0.63
1:A:363[A]:GLU:OE1	4:A:805:X2E:H22	2.00	0.61
1:B:378:LEU:HB2	9:B:1009:HOH:O	2.02	0.60
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.65	0.59
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.86	0.58
1:B:363[B]:GLU:OE2	4:B:805:X2E:H15B	2.04	0.58
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.86	0.57
1:A:68:PRO:O	1:B:109:ARG:NH2	2.38	0.56
1:B:449:TRP:HA	3:B:600:H4B:N1	2.21	0.56
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.88	0.56
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.46	0.55
1:B:366:THR:O	1:B:370:CYS:HB2	2.06	0.55
1:A:152:LEU:O	1:A:156:GLU:HG2	2.06	0.55
1:A:105:LEU:N	1:A:105:LEU:HD23	2.22	0.54
2:B:500:HEM:HBA2	4:B:805:X2E:H14	1.90	0.54
1:A:231:THR:O	1:A:353:ALA:HA	2.09	0.53
1:A:340:ASN:ND2	1:A:340:ASN:H	2.05	0.53
1:A:340:ASN:N	1:A:340:ASN:HD22	2.05	0.52
1:B:72:ARG:NH1	9:B:1124:HOH:O	2.42	0.52
1:B:107:LEU:HD21	4:B:805:X2E:H03	1.92	0.52
1:B:324:TRP:HB2	7:B:950:CAD:C1	2.40	0.51
1:A:151:ARG:HD3	1:A:168:ARG:NH2	2.26	0.51
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.39	0.51
1:A:458:LEU:HD21	1:B:401:ALA:HB2	1.93	0.49
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.94	0.49
1:B:363[A]:GLU:OE1	4:B:805:X2E:H22	2.13	0.49
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.93	0.49
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.95	0.49
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.94	0.49
1:B:236:ARG:HD3	1:B:242:ASP:OD2	2.13	0.49
1:A:481:PRO:HD2	1:A:482:TRP:CE3	2.48	0.48
1:B:207:GLN:HB2	9:B:1020:HOH:O	2.13	0.48
1:A:476:ARG:HH11	1:A:476:ARG:CG	2.26	0.48
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.96	0.48
2:B:500:HEM:CBB	2:B:500:HEM:HHC	2.43	0.47
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.95	0.47
1:B:240:ARG:HD2	1:B:241:GLY:O	2.15	0.47
1:A:360:MET:CE	1:A:362:THR:OG1	2.63	0.47
1:B:182:ASN:O	1:B:184:PRO:HD3	2.15	0.46
2:A:500:HEM:CBB	2:A:500:HEM:HHC	2.46	0.46
1:A:363[B]:GLU:OE2	4:A:805:X2E:N11	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ARG:HD2	9:B:1018:HOH:O	2.15	0.45
1:A:355:PHE:CD1	2:A:500:HEM:HAC	2.51	0.45
1:B:107:LEU:CD2	4:B:805:X2E:H03	2.47	0.44
4:B:805:X2E:H10A	4:B:805:X2E:H2'A	1.67	0.44
1:A:213:ILE:HG23	1:A:250:LEU:HD13	2.00	0.43
1:A:455:SER:O	1:A:458:LEU:HB2	2.17	0.43
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.58	0.43
1:A:246:TRP:CD1	1:A:481:PRO:HG2	2.53	0.43
1:A:126:LEU:HD11	1:A:156:GLU:HA	2.01	0.43
1:B:172:LEU:HD11	1:B:232:VAL:HG11	2.01	0.43
1:B:319:HIS:NE2	1:B:403:GLU:OE1	2.46	0.42
1:A:355:PHE:CD1	2:A:500:HEM:CAC	3.03	0.42
1:A:458:LEU:HD21	1:B:401:ALA:CB	2.49	0.42
1:A:325:PHE:HA	1:A:328:LEU:HD22	2.02	0.41
1:A:360:MET:HE2	1:A:362:THR:OG1	2.21	0.41
1:B:126:LEU:O	1:B:130:ARG:HG3	2.20	0.41
1:B:307:LEU:HA	1:B:308:PRO:HD3	1.96	0.41
1:A:70:PHE:HB3	1:A:84:ASP:O	2.20	0.41
1:A:338:VAL:CG1	1:A:341:MET:HG3	2.51	0.41
2:B:500:HEM:HBB2	2:B:500:HEM:CHC	2.47	0.40
2:A:500:HEM:O2A	4:A:805:X2E:N1'	2.54	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	404/443 (91%)	392 (97%)	10 (2%)	2 (0%)	29	32
1	B	400/443 (90%)	389 (97%)	11 (3%)	0	100	100
All	All	804/886 (91%)	781 (97%)	21 (3%)	2 (0%)	41	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	GLY
1	A	108	PRO

### 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	347/376 (92%)	333 (96%)	14 (4%)	31	39
1	B	344/376 (92%)	322 (94%)	22 (6%)	17	18
All	All	691/752 (92%)	655 (95%)	36 (5%)	23	27

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	102	LEU
1	A	125	LEU
1	A	146	GLN
1	A	156	GLU
1	A	190	ILE
1	A	194	LYS
1	A	259	GLN
1	A	260	ASP
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	B	92	GLN
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	124	GLN
1	B	141	LYS
1	B	146	GLN

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Mol	Chain	Res	Type
1	B	207	GLN
1	B	215	ASN
1	B	218	LYS
1	B	223	ARG
1	B	240	ARG
1	B	260	ASP
1	B	323	GLU
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	379	GLU
1	B	389	THR
1	B	391	THR
1	B	419	ILE
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	146	GLN
1	A	191	GLN
1	A	259	GLN
1	A	278	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	146	GLN
1	B	178	GLN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

### 5.3.3 RNA ⓘ

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	A	860	-	1,3,3	1.21	0	0,3,3	0.00	-
2	HEM	A	500	1	27,50,50	2.06	7 (25%)	17,82,82	1.83	3 (17%)
7	CAD	A	950	-	0,2,4	0.00	-	0,1,6	0.00	-
3	H4B	A	600	-	16,18,18	1.06	0	11,26,26	2.81	6 (54%)
3	H4B	B	600	-	16,18,18	1.30	2 (12%)	11,26,26	2.30	5 (45%)
5	ACT	B	860	-	1,3,3	1.48	0	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.37	0	5,5,5	1.06	0
7	CAD	B	950	-	0,2,4	0.00	-	0,1,6	0.00	-
4	X2E	B	805	-	29,30,30	1.10	2 (6%)	34,40,40	1.90	7 (20%)
6	GOL	A	880	-	5,5,5	0.37	0	5,5,5	0.58	0
4	X2E	A	805	-	29,30,30	1.05	2 (6%)	34,40,40	1.78	8 (23%)
2	HEM	B	500	1	27,50,50	2.20	6 (22%)	17,82,82	2.22	3 (17%)

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
2	HEM	A	500	1	-	0/6/54/54	-
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
6	GOL	B	880	-	-	1/4/4/4	-
4	X2E	B	805	-	-	6/15/25/25	0/3/3/3
6	GOL	A	880	-	-	1/4/4/4	-
4	X2E	A	805	-	-	4/15/25/25	0/3/3/3
2	HEM	B	500	1	-	0/6/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C2D	5.24	1.53	1.37
2	B	500	HEM	C3C-C2C	-4.91	1.33	1.40
2	B	500	HEM	C3B-C2B	-4.57	1.34	1.40
2	A	500	HEM	C3D-C2D	4.49	1.51	1.37
2	A	500	HEM	C3B-C2B	-4.43	1.34	1.40
2	A	500	HEM	C3C-C2C	-4.22	1.34	1.40
4	B	805	X2E	C13-N11	-4.07	1.42	1.48
2	B	500	HEM	C3B-CAB	3.95	1.56	1.47
2	A	500	HEM	C3B-CAB	3.50	1.55	1.47
3	B	600	H4B	C4-C4A	-3.43	1.36	1.41
2	A	500	HEM	C3C-CAC	3.32	1.54	1.47
2	B	500	HEM	C3C-CAC	3.23	1.54	1.47
4	A	805	X2E	C13-N11	-3.12	1.44	1.48
2	B	500	HEM	C1D-ND	2.42	1.41	1.36
3	B	600	H4B	C7-C6	2.23	1.54	1.52
4	A	805	X2E	C26-C25	2.15	1.41	1.37
4	B	805	X2E	C11-N11	-2.07	1.42	1.47
2	A	500	HEM	CMD-C2D	2.06	1.55	1.51
2	A	500	HEM	CAA-C2A	2.00	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CBA-CAA-C2A	-6.90	99.75	112.49
4	B	805	X2E	C02-N01-C06	5.78	122.48	118.10
2	A	500	HEM	CBA-CAA-C2A	-5.28	102.75	112.49
3	A	600	H4B	C4-C4A-N5	4.22	122.66	119.12
3	B	600	H4B	C4-C4A-C8A	4.10	118.21	114.57
3	A	600	H4B	C4-C4A-C8A	4.04	118.16	114.57
4	B	805	X2E	C04-C05-C06	-3.86	117.79	120.32
4	A	805	X2E	C02-N01-C06	3.85	121.02	118.10
3	A	600	H4B	N3-C2-N1	-3.72	119.58	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	X2E	C5'-N1'-C2'	3.72	114.20	105.42
3	A	600	H4B	C4-N3-C2	3.60	121.64	115.93
3	B	600	H4B	N3-C2-N1	-3.47	119.98	125.42
2	B	500	HEM	C1D-C2D-C3D	-3.46	104.59	107.00
4	A	805	X2E	C24-C25-C26	-3.43	118.83	123.29
2	A	500	HEM	CBD-CAD-C3D	-3.31	106.38	112.48
4	A	805	X2E	C5'-N1'-C2'	3.29	113.18	105.42
2	B	500	HEM	CBD-CAD-C3D	-3.16	106.66	112.48
4	A	805	X2E	C04-C05-C06	-3.11	118.28	120.32
3	A	600	H4B	C2-N1-C8A	3.11	121.50	114.54
3	B	600	H4B	N2-C2-N1	2.95	121.84	117.25
4	A	805	X2E	C10-O09-C3'	2.93	120.66	113.87
3	B	600	H4B	C2-N1-C8A	2.77	120.75	114.54
4	A	805	X2E	O09-C10-C11	-2.68	100.58	109.33
4	B	805	X2E	N02-C02-N01	2.62	120.62	116.49
3	B	600	H4B	C4-N3-C2	2.45	119.82	115.93
4	B	805	X2E	C06-C08-C4'	-2.42	107.59	115.55
4	A	805	X2E	C06-C08-C4'	-2.35	107.82	115.55
4	A	805	X2E	C15-C13-C14	2.32	116.68	111.91
4	B	805	X2E	C03-C02-N01	-2.27	116.89	121.75
4	B	805	X2E	O09-C10-C11	-2.23	102.05	109.33
2	A	500	HEM	C1D-C2D-C3D	-2.13	105.52	107.00
3	A	600	H4B	N2-C2-N3	2.09	120.50	117.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

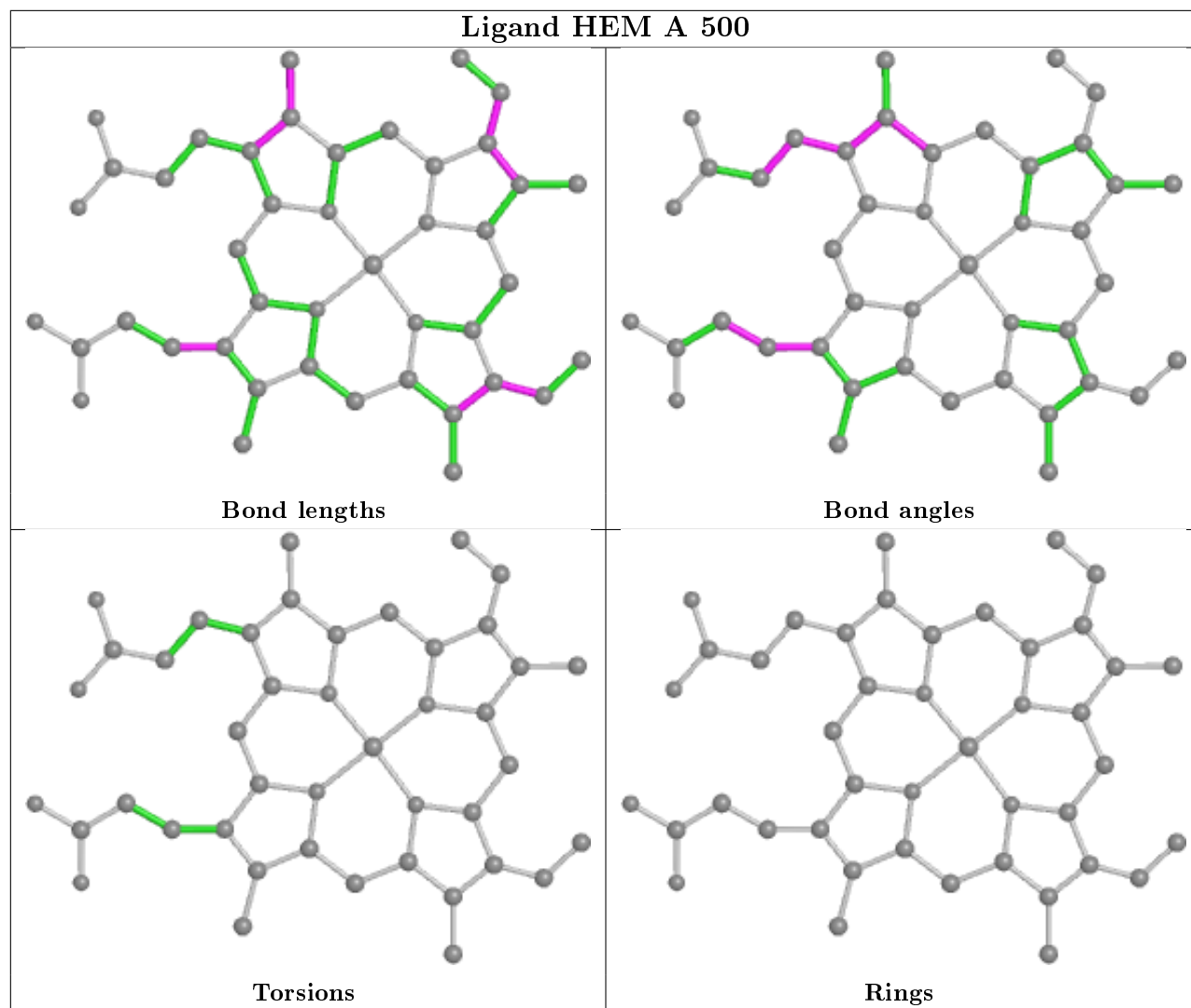
Mol	Chain	Res	Type	Atoms
4	B	805	X2E	C2'-C3'-O09-C10
4	B	805	X2E	C14-C13-N11-C11
4	B	805	X2E	C15-C13-N11-C11
4	A	805	X2E	C14-C13-N11-C11
4	A	805	X2E	C15-C13-N11-C11
4	B	805	X2E	O09-C10-C11-N11
4	A	805	X2E	O09-C10-C11-N11
6	A	880	GOL	O1-C1-C2-C3
4	B	805	X2E	C10-C11-N11-C13
4	A	805	X2E	C10-C11-N11-C13
4	B	805	X2E	C4'-C3'-O09-C10
6	B	880	GOL	C1-C2-C3-O3

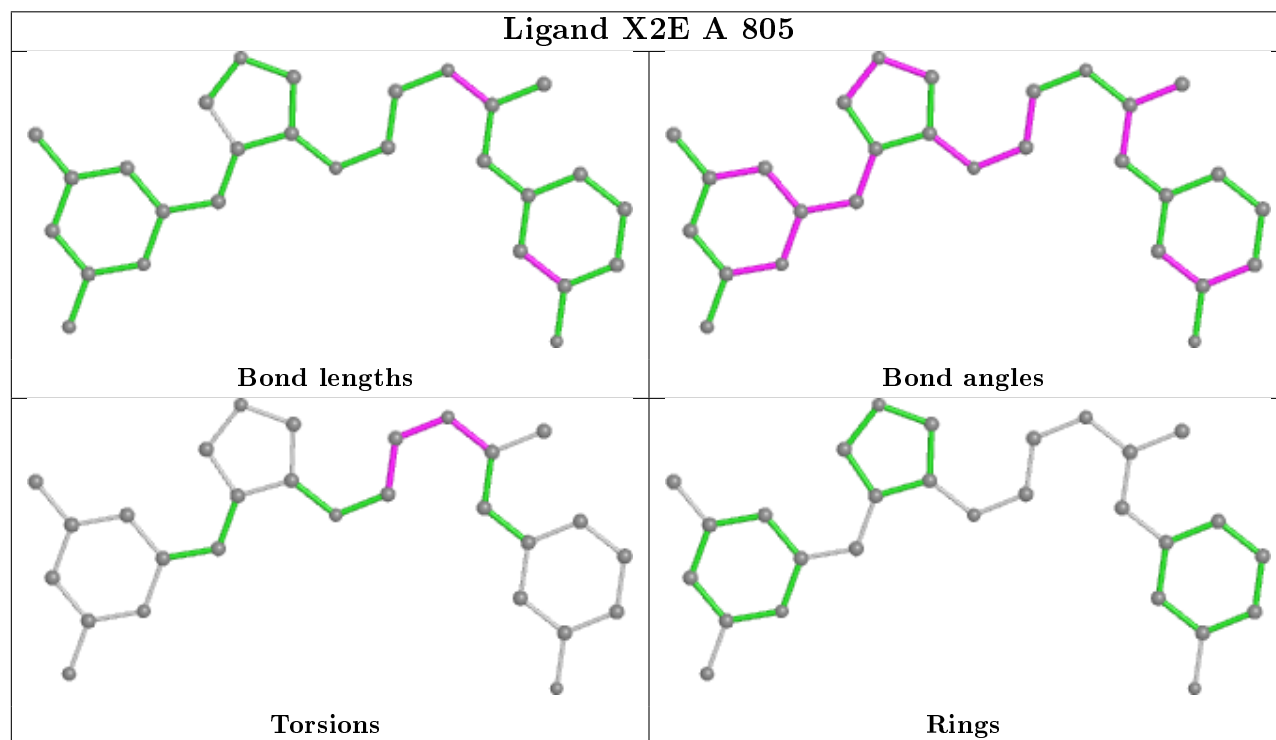
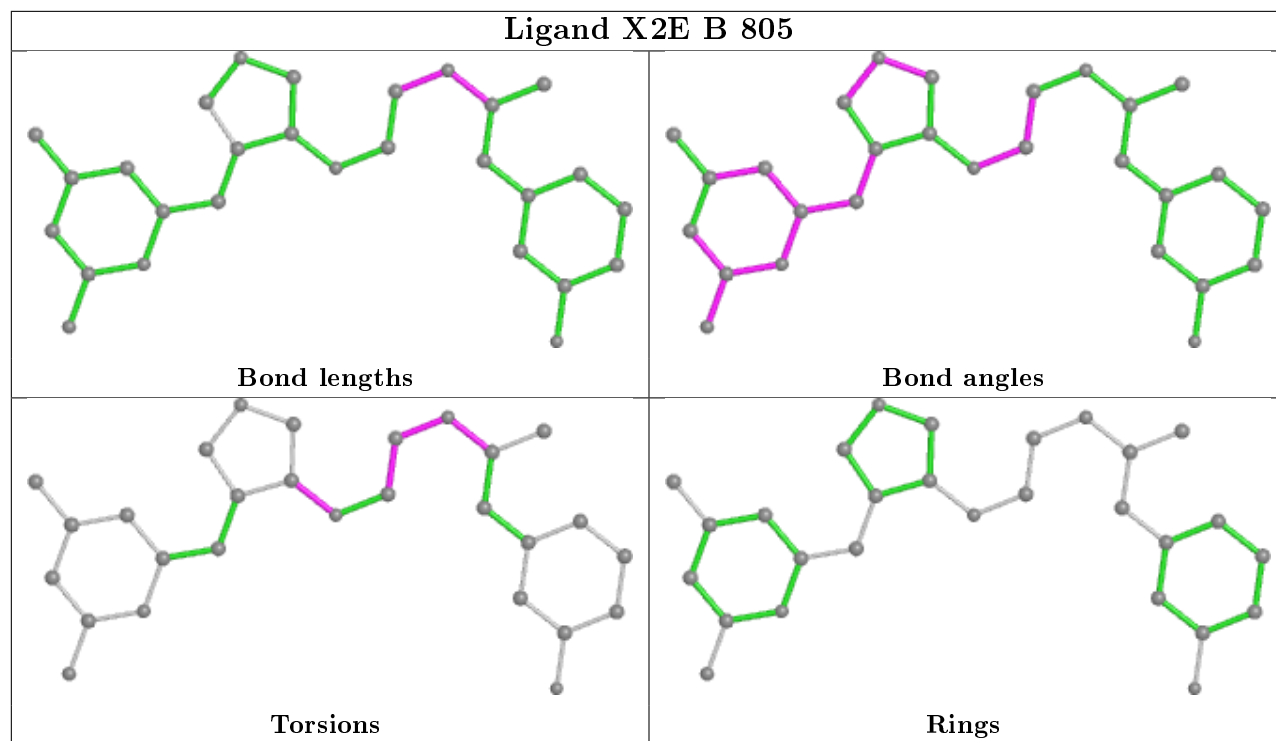
There are no ring outliers.

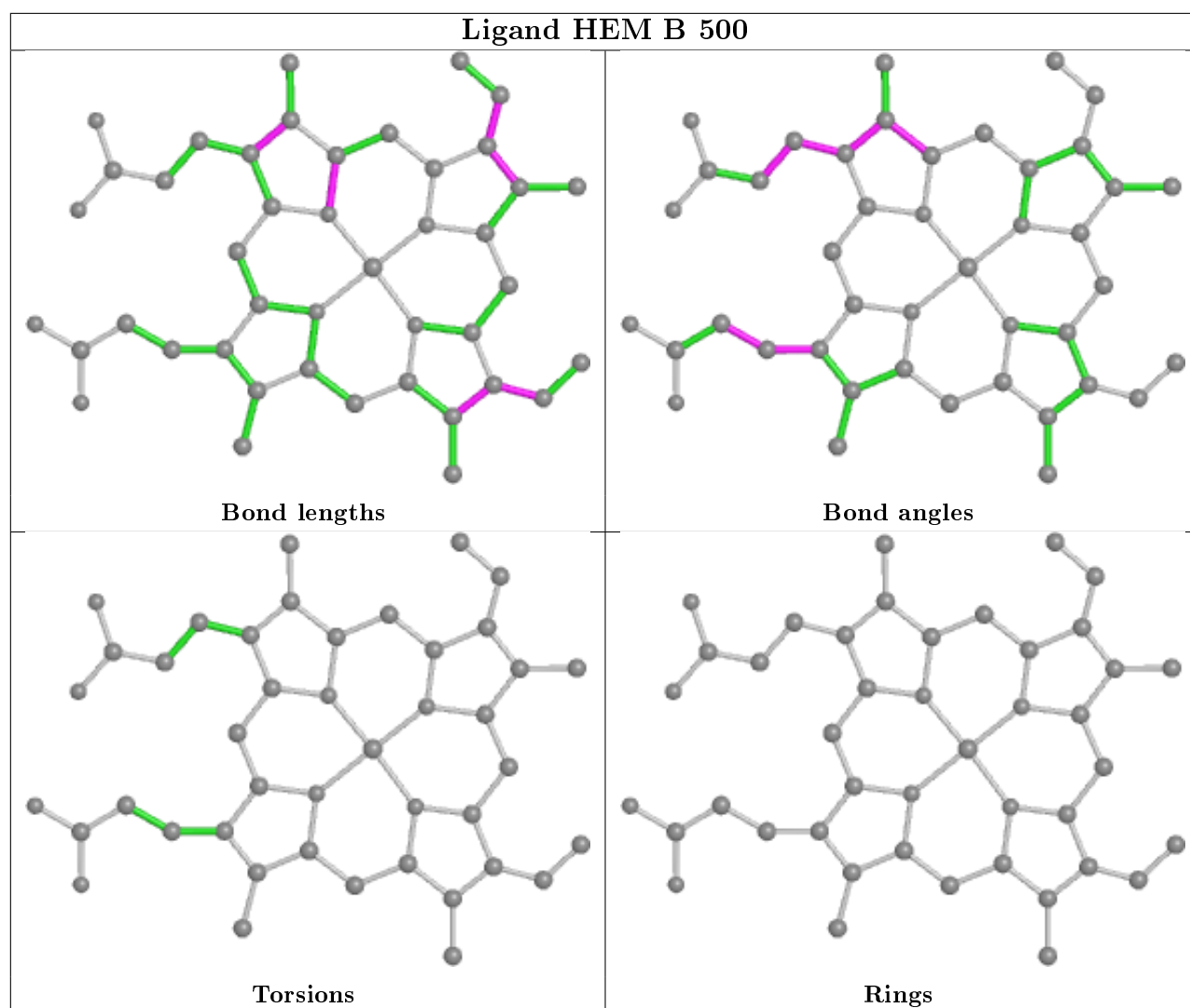
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	5	0
3	B	600	H4B	1	0
7	B	950	CAD	1	0
4	B	805	X2E	6	0
4	A	805	X2E	3	0
2	B	500	HEM	4	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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	405/443 (91%)	0.03	15 (3%) 41 54	23, 36, 62, 81	0
1	B	403/443 (90%)	-0.18	3 (0%) 87 92	23, 38, 63, 86	0
All	All	808/886 (91%)	-0.08	18 (2%) 62 72	23, 37, 63, 86	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLN	4.9
1	A	69	LYS	4.7
1	A	67	GLY	3.9
1	A	239	GLY	3.2
1	B	477[A]	TYR	3.1
1	B	259	GLN	2.7
1	A	153	GLN	2.5
1	A	91	GLN	2.5
1	A	121	PRO	2.4
1	A	257	ARG	2.4
1	B	257	ARG	2.4
1	A	448	ALA	2.2
1	A	449	TRP	2.2
1	A	124	GLN	2.2
1	A	451	VAL	2.1
1	A	160	ALA	2.1
1	A	68	PRO	2.1
1	A	122	ALA	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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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<sup>th</sup> 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.

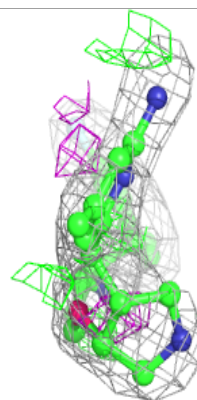
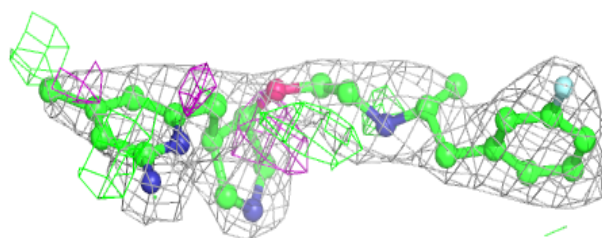
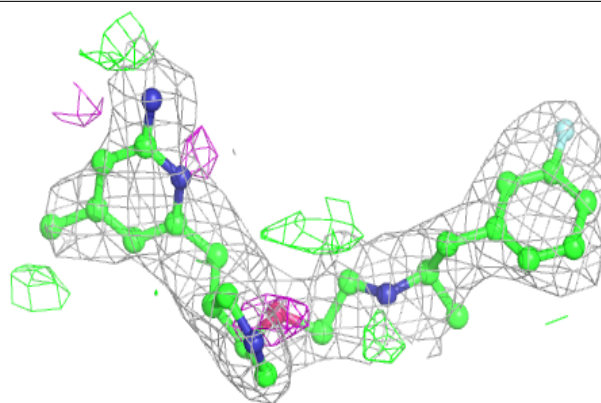
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	X2E	B	805	28/28	0.89	0.20	43,54,56,57	0
4	X2E	A	805	28/28	0.89	0.20	35,52,55,56	0
6	GOL	A	880	6/6	0.90	0.22	51,54,54,58	0
6	GOL	B	880	6/6	0.95	0.14	49,52,52,53	0
5	ACT	A	860	4/4	0.97	0.16	48,49,50,52	0
5	ACT	B	860	4/4	0.97	0.12	48,49,50,51	0
7	CAD	A	950	3/5	0.98	0.12	66,66,67,68	0
3	H4B	A	600	17/17	0.98	0.16	21,26,29,30	0
3	H4B	B	600	17/17	0.98	0.16	28,30,31,31	0
2	HEM	A	500	43/43	0.98	0.18	22,28,38,44	0
2	HEM	B	500	43/43	0.98	0.13	23,28,36,43	0
7	CAD	B	950	3/5	0.99	0.07	56,56,59,60	0
8	ZN	A	900	1/1	1.00	0.15	31,31,31,31	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.

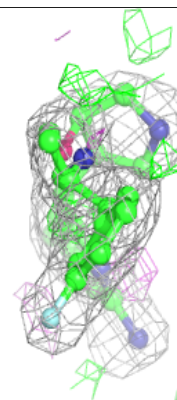
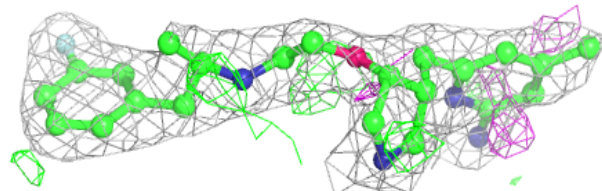
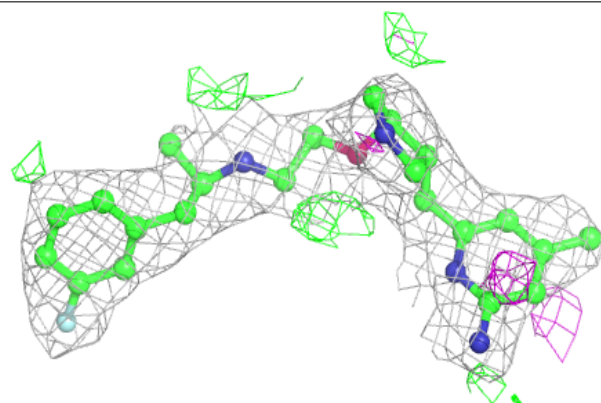


**Electron density around X2E B 805:**

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

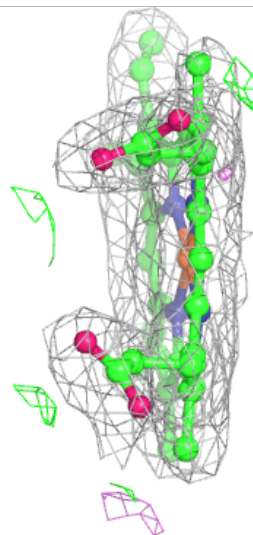
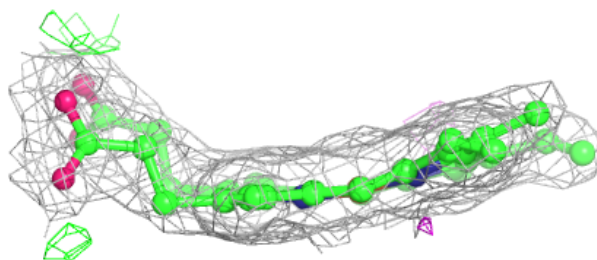
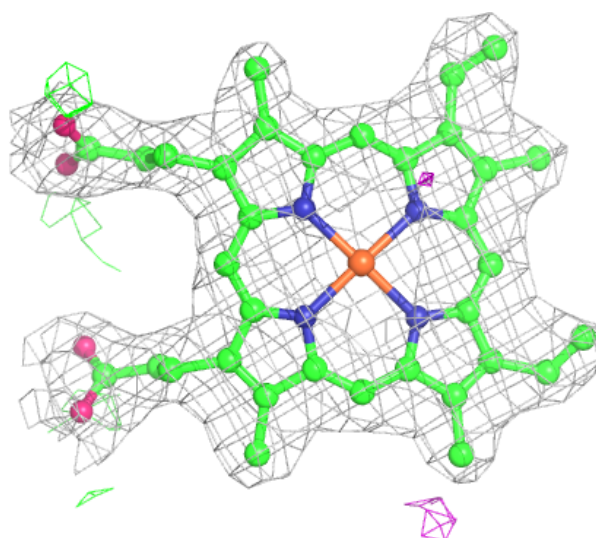
**Electron density around X2E A 805:**

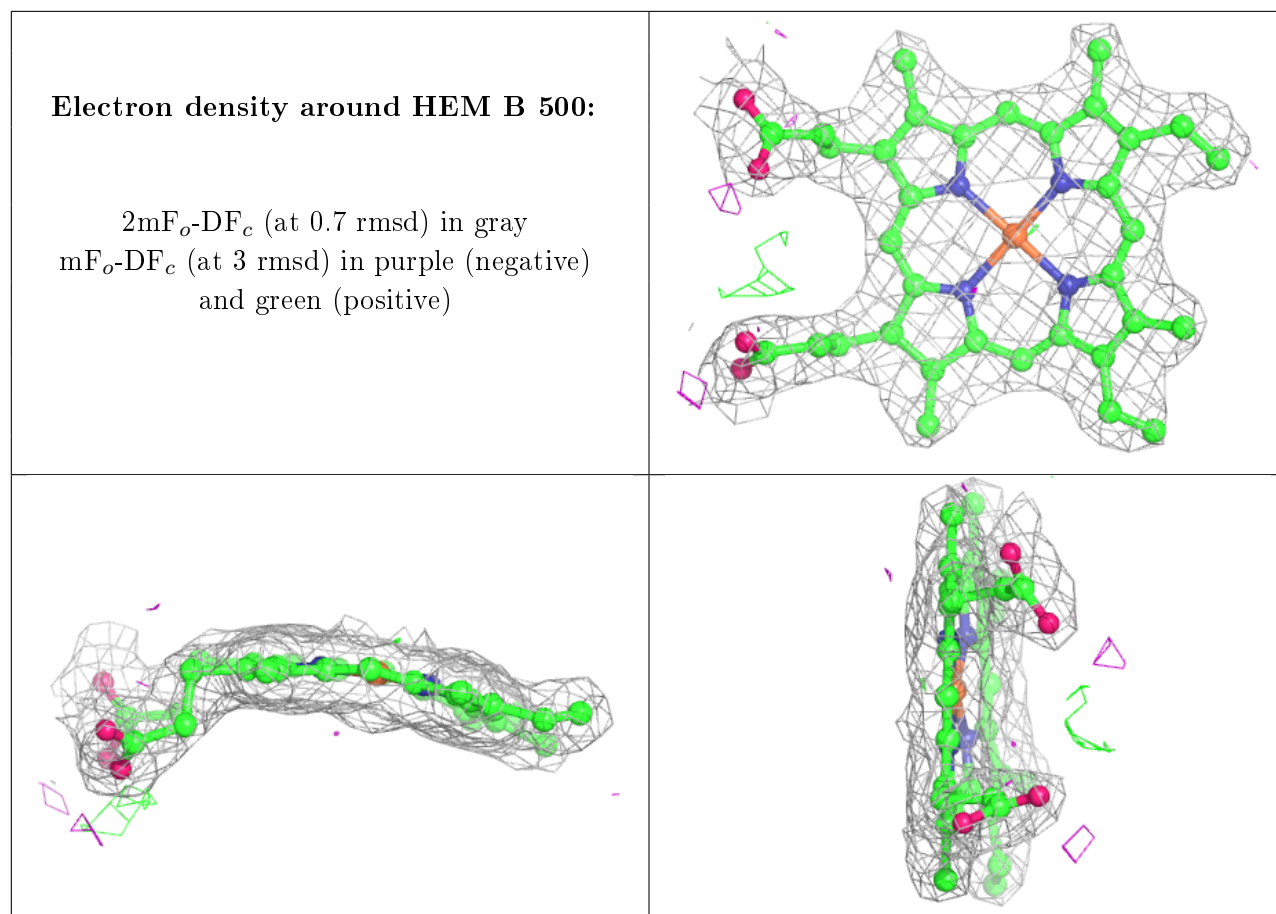
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 500:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.