



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 04:23 AM EDT

PDB ID : 4LUW  
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 6-((((3R,5S)-5-(((6-amino-4-methylpyridin-2-yl)methoxy)methyl)pyrrolidin-3-yl)oxy)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2013-07-25  
Resolution : 2.25 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

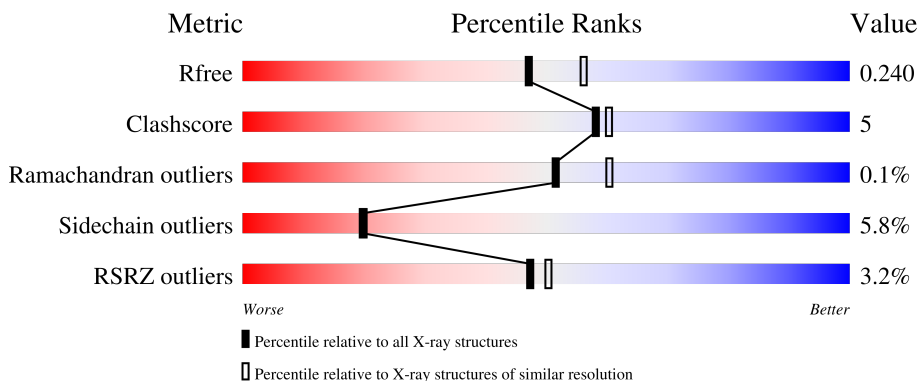
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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 of 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	442	 4% 83% 8% • 8%
1	B	442	 2% 79% 11% • 9%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 6941 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.

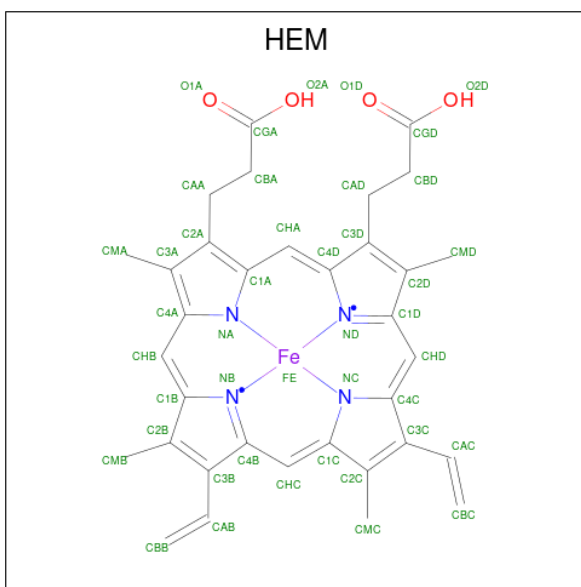
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
1	A	405	Total 3223	As 1	C 2049	N 568	O 589	S 16	0	0	0
1	B	404	Total 3221	As 1	C 2048	N 568	O 588	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
B	100	ARG	CYS	conflict	UNP P29473

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



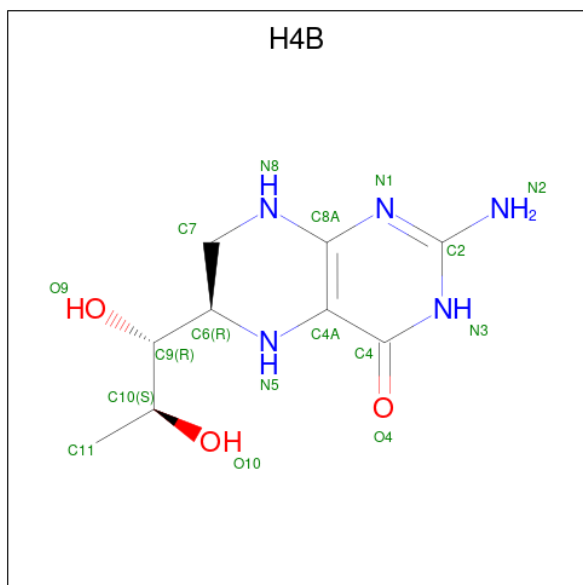
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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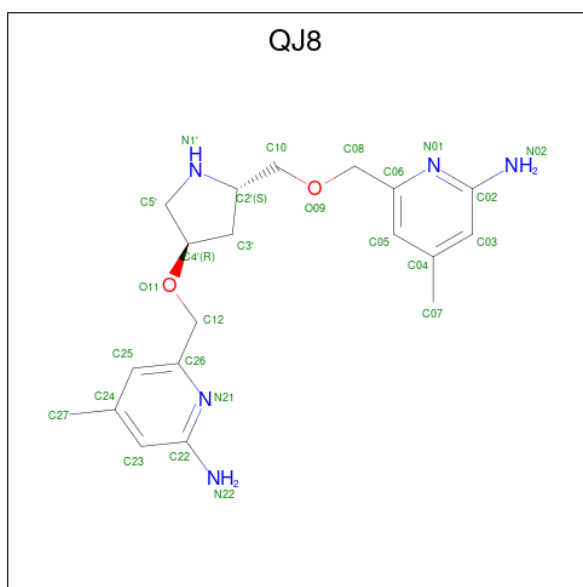
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	B	1	43	34	1	4	4	0	0

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



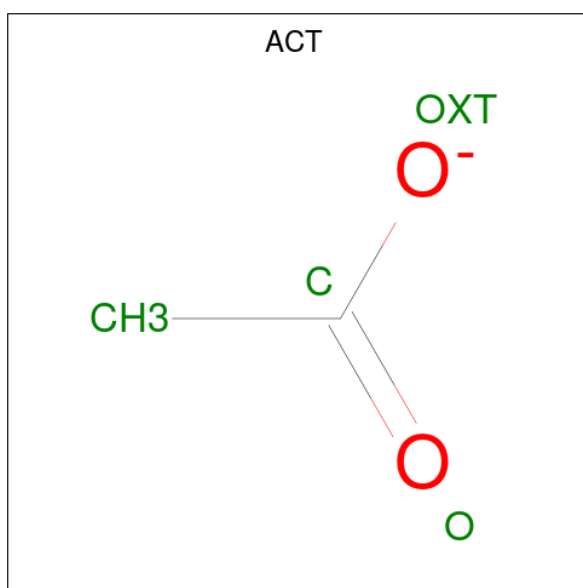
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	9	5	3	0	0
3	B	1	17	9	5	3	0	0

- Molecule 4 is 6-({[(3R,5S)-5-{{(6-amino-4-methylpyridin-2-yl)methoxy}methyl}pyrrolidin-3-yl]oxy}methyl)-4-methylpyridin-2-amine (three-letter code: QJ8) (formula:  $C_{19}H_{27}N_5O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	26	19	5	2	0	0
4	B	1	26	19	5	2	0	0

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



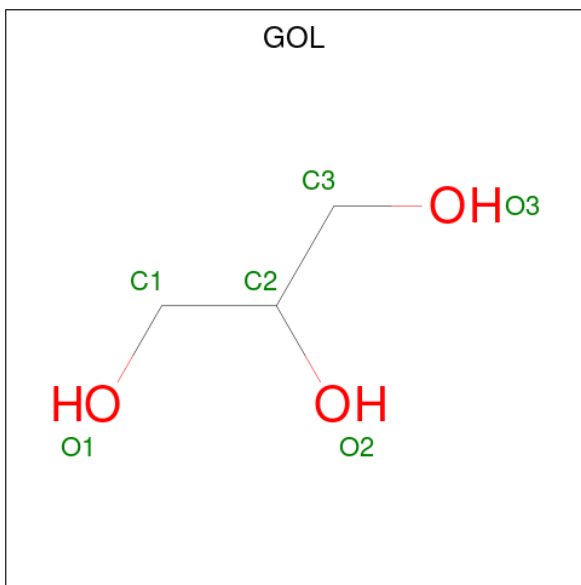
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

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

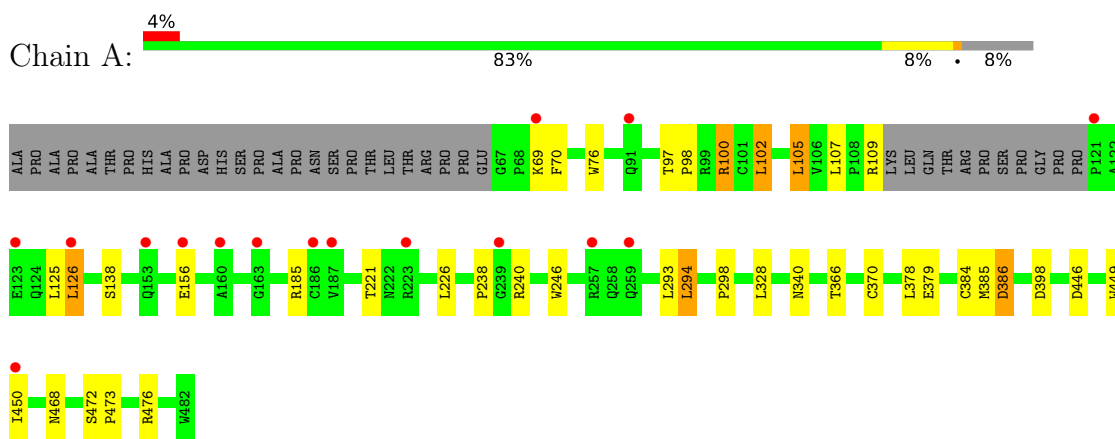
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	149	Total O 149 149	0	0
8	B	147	Total O 147 147	0	0

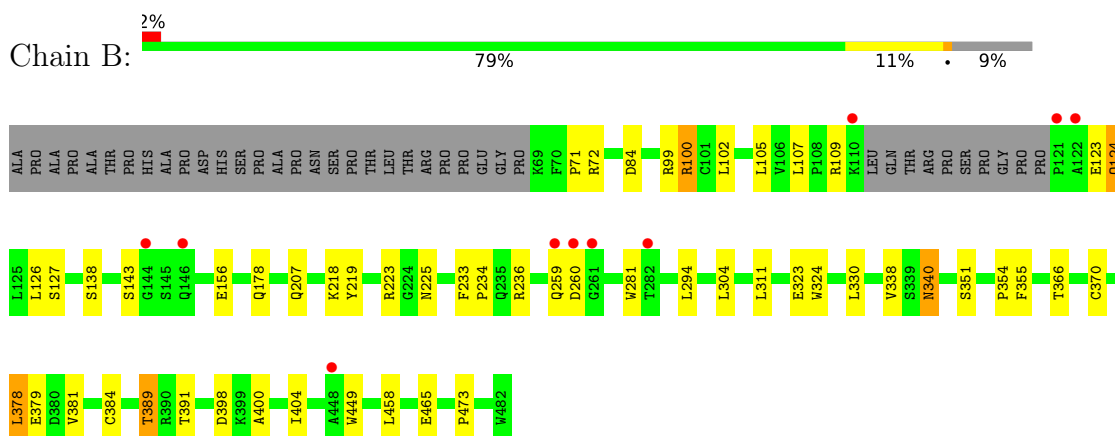
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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, $\alpha$ , $\beta$ , $\gamma$	58.11Å 106.56Å 156.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 2.25 44.07 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.07-2.25) 98.9 (44.07-2.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.24Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.185 , 0.233 0.191 , 0.240	Depositor DCC
$R_{free}$ test set	2323 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtrriage
Anisotropy	0.591	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, QJ8, ZN, H4B, HEM, GOL, CAS

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	0.70	0/3303	0.70	0/4497
1	B	0.68	0/3300	0.72	0/4491
All	All	0.69	0/6603	0.71	0/8988

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	3223	0	3127	20	0
1	B	3221	0	3130	27	0
2	A	43	0	30	7	0
2	B	43	0	30	10	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	26	0	27	5	0
4	B	26	0	27	8	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	149	0	0	2	0
8	B	147	0	0	1	0
All	All	6941	0	6429	63	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 (63) 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:384:CAS:SG	1:A:384:CAS:AS	2.81	0.98
2:B:501:HEM:O2D	4:B:503:QJ8:H15	1.76	0.85
1:B:389:THR:HB	8:B:687:HOH:O	1.83	0.77
2:A:501:HEM:O2D	4:A:503:QJ8:H12	1.83	0.77
1:B:324:TRP:HB2	1:B:384:CAS:CE1	2.19	0.72
2:A:501:HEM:HBA2	4:A:503:QJ8:H21	1.72	0.71
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.76	0.67
1:B:107:LEU:HD11	4:B:503:QJ8:H6	1.78	0.66
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.79	0.64
1:B:107:LEU:HD21	4:B:503:QJ8:H4	1.79	0.64
1:B:178:GLN:HB3	1:B:473:PRO:HG2	1.79	0.63
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.82	0.61
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.31	0.60
2:B:501:HEM:CMC	2:B:501:HEM:HBC2	2.32	0.60
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.86	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.87	0.57
1:B:366:THR:O	1:B:370:CYS:HB2	2.05	0.57
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.87	0.56
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.86	0.56
1:A:378:LEU:HB2	8:A:605:HOH:O	2.06	0.55
2:B:501:HEM:O2D	4:B:503:QJ8:C3'	2.54	0.54
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.47	0.54
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.89	0.54
2:B:501:HEM:O2A	4:B:503:QJ8:H18	2.10	0.51
1:A:76:TRP:CH2	4:B:503:QJ8:H5	2.46	0.51
1:A:105:LEU:HD23	1:A:105:LEU:N	2.26	0.51
1:A:126:LEU:HD11	1:A:156:GLU:HB3	1.93	0.50
1:B:340:ASN:HD22	1:B:340:ASN:H	1.57	0.50
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASP:O	1:A:450:ILE:HG12	2.12	0.49
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.96	0.48
2:B:501:HEM:C1C	4:B:503:QJ8:H28	2.49	0.47
2:A:501:HEM:CBA	4:A:503:QJ8:H21	2.43	0.47
1:B:400:ALA:O	1:B:404:ILE:HG13	2.14	0.47
2:B:501:HEM:HMC1	2:B:501:HEM:CBC	2.44	0.47
4:A:503:QJ8:H11	8:A:749:HOH:O	2.14	0.47
1:A:100:ARG:NH1	1:A:102:LEU:HD22	2.30	0.46
1:A:449:TRP:HA	3:A:502:H4B:N1	2.31	0.46
2:B:501:HEM:HHC	2:B:501:HEM:CBB	2.46	0.45
1:A:366:THR:O	1:A:370:CYS:HB2	2.17	0.45
1:B:99:ARG:HG2	1:B:100:ARG:HD2	2.00	0.44
1:B:218:LYS:HD3	1:B:219:TYR:N	2.32	0.44
1:A:70:PHE:O	1:B:109:ARG:NH2	2.51	0.43
1:A:384:CAS:AS	1:A:384:CAS:CB	3.27	0.43
1:B:107:LEU:HD21	4:B:503:QJ8:C27	2.47	0.43
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.49	0.43
1:B:281:TRP:HB2	1:B:304:LEU:HD21	2.00	0.43
1:A:221:THR:O	1:A:226:LEU:HD12	2.18	0.42
1:A:472:SER:HA	1:A:473:PRO:C	2.40	0.42
1:B:338:VAL:O	1:B:354:PRO:HA	2.20	0.41
2:B:501:HEM:CMC	2:B:501:HEM:CBC	2.98	0.41
2:A:501:HEM:O2D	4:A:503:QJ8:C5'	2.60	0.41
1:B:449:TRP:HA	3:B:502:H4B:N1	2.34	0.41
2:A:501:HEM:CBB	2:A:501:HEM:HHC	2.51	0.41
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	2.02	0.41
1:B:338:VAL:HB	1:B:355:PHE:CZ	2.55	0.41
1:B:138:SER:HA	1:B:143:SER:HB2	2.03	0.41
1:A:385:MET:O	1:A:386:ASP:HB2	2.21	0.41
1:B:126:LEU:HD12	1:B:126:LEU:HA	1.86	0.41
1:A:97:THR:HB	1:A:98:PRO:HD2	2.03	0.40
1:B:123:GLU:HG2	1:B:124:GLN:N	2.36	0.40
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.02	0.40
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.57	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	400/442 (90%)	388 (97%)	12 (3%)	0	100	100
1	B	399/442 (90%)	381 (96%)	17 (4%)	1 (0%)	41	46
All	All	799/884 (90%)	769 (96%)	29 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	ASP

### 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	343/374 (92%)	324 (94%)	19 (6%)	21	21
1	B	343/374 (92%)	322 (94%)	21 (6%)	18	18
All	All	686/748 (92%)	646 (94%)	40 (6%)	20	20

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	107	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	109	ARG
1	A	125	LEU
1	A	126	LEU
1	A	138	SER
1	A	238	PRO
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	379	GLU
1	A	386	ASP
1	A	398	ASP
1	A	468	ASN
1	A	476	ARG
1	B	72	ARG
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	124	GLN
1	B	127	SER
1	B	207	GLN
1	B	223	ARG
1	B	225	ASN
1	B	259	GLN
1	B	294	LEU
1	B	311	LEU
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	398	ASP
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	153	GLN
1	A	166	HIS
1	A	191	GLN

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Mol	Chain	Res	Type
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CAS	B	384	1	5,8,9	1.05	0	1,9,11	0.42	0
1	CAS	A	384	1	5,8,9	1.09	0	1,9,11	0.51	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	Res	Link	Chirals	Torsions	Rings
1	CAS	B	384	1	-	0/0/7/9	-
1	CAS	A	384	1	-	0/0/7/9	-

There are no bond length outliers.

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 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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
6	GOL	B	506	-	5,5,5	0.45	0	5,5,5	0.74	0
5	ACT	A	504	-	3,3,3	0.87	0	3,3,3	0.40	0
2	HEM	B	501	1	41,50,50	1.85	6 (14%)	45,82,82	1.80	8 (17%)
5	ACT	B	504	-	3,3,3	0.85	0	3,3,3	0.71	0
5	ACT	B	505	-	3,3,3	0.89	0	3,3,3	0.83	0
3	H4B	B	502	-	16,18,18	0.88	0	11,26,26	2.85	6 (54%)
4	QJ8	A	503	-	26,28,28	1.03	2 (7%)	33,38,38	2.09	9 (27%)
2	HEM	A	501	1	41,50,50	1.92	9 (21%)	45,82,82	1.59	7 (15%)
6	GOL	A	506	-	5,5,5	0.32	0	5,5,5	0.75	0
4	QJ8	B	503	-	26,28,28	0.64	0	33,38,38	2.17	12 (36%)
5	ACT	A	505	-	3,3,3	1.10	0	3,3,3	0.59	0
3	H4B	A	502	-	16,18,18	1.09	1 (6%)	11,26,26	2.69	6 (54%)

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
6	GOL	B	506	-	-	2/4/4/4	-
2	HEM	B	501	1	-	0/12/54/54	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	QJ8	A	503	-	-	4/11/20/20	0/3/3/3
2	HEM	A	501	1	-	0/12/54/54	-
6	GOL	A	506	-	-	0/4/4/4	-
4	QJ8	B	503	-	-	7/11/20/20	0/3/3/3
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3D-C2D	6.92	1.51	1.36
2	A	501	HEM	C3D-C2D	6.83	1.51	1.36
2	A	501	HEM	C3C-C2C	-4.34	1.34	1.40
2	B	501	HEM	C3C-C2C	-4.01	1.34	1.40
2	B	501	HEM	C3C-CAC	3.35	1.54	1.47
2	B	501	HEM	CAB-C3B	3.17	1.56	1.47
2	A	501	HEM	C3C-CAC	2.96	1.53	1.47
2	A	501	HEM	C1B-NB	-2.73	1.35	1.40
2	A	501	HEM	CAA-C2A	2.56	1.55	1.52
2	A	501	HEM	CAB-C3B	2.54	1.54	1.47
4	A	503	QJ8	C06-N01	2.32	1.38	1.34
3	A	502	H4B	C4-N3	2.28	1.37	1.33
2	A	501	HEM	C3B-C2B	-2.14	1.32	1.37
2	A	501	HEM	C4A-NA	2.14	1.40	1.36
2	A	501	HEM	CMC-C2C	2.14	1.56	1.51
2	B	501	HEM	CMD-C2D	2.13	1.55	1.50
4	A	503	QJ8	C03-C04	2.08	1.42	1.39
2	B	501	HEM	FE-ND	2.08	2.07	1.96

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CBA-CAA-C2A	-6.60	101.35	112.62
3	B	502	H4B	C4-C4A-N5	6.46	124.54	119.12
4	B	503	QJ8	C02-N01-C06	5.60	122.34	118.10
4	A	503	QJ8	C02-N01-C06	5.55	122.31	118.10
2	A	501	HEM	C4D-ND-C1D	5.52	110.77	105.07
4	A	503	QJ8	C22-N21-C26	5.38	122.17	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	C8A-C4A-C4	4.82	118.85	114.57
4	B	503	QJ8	C22-N21-C26	4.60	121.58	118.10
2	B	501	HEM	C4D-ND-C1D	4.23	109.45	105.07
4	A	503	QJ8	C04-C05-C06	-4.16	117.59	120.32
4	B	503	QJ8	C24-C25-C26	-3.82	117.82	120.32
3	A	502	H4B	C4-C4A-N5	3.76	122.28	119.12
3	A	502	H4B	C2-N3-C4	3.70	121.81	115.93
2	B	501	HEM	CMD-C2D-C1D	3.56	130.45	125.04
3	B	502	H4B	C8A-C4A-C4	3.53	117.71	114.57
2	B	501	HEM	C3B-C2B-C1B	3.48	109.06	106.49
4	A	503	QJ8	C10-C2'-N1'	-3.39	105.60	111.58
4	A	503	QJ8	C25-C26-N21	-3.37	119.33	122.90
2	A	501	HEM	CHA-C4D-ND	3.36	128.53	124.38
4	B	503	QJ8	N22-C22-N21	3.31	121.73	116.49
3	B	502	H4B	N1-C2-N3	-3.31	120.23	125.42
4	B	503	QJ8	C3'-C4'-C5'	3.25	106.56	103.65
4	B	503	QJ8	C05-C06-N01	-3.13	119.58	122.90
4	B	503	QJ8	C25-C24-C23	3.12	121.81	118.09
3	A	502	H4B	N1-C2-N3	-3.10	120.55	125.42
3	B	502	H4B	C2-N1-C8A	2.90	121.05	114.54
2	B	501	HEM	CBD-CAD-C3D	-2.88	104.61	112.63
4	B	503	QJ8	C12-C26-N21	2.88	121.55	115.71
2	A	501	HEM	CBD-CAD-C3D	-2.81	104.81	112.63
2	B	501	HEM	C1D-C2D-C3D	-2.81	104.00	106.96
2	A	501	HEM	CMA-C3A-C4A	-2.62	124.44	128.46
3	A	502	H4B	C2-N1-C8A	2.55	120.25	114.54
2	B	501	HEM	CAD-C3D-C4D	2.46	128.96	124.66
2	A	501	HEM	C2C-C3C-C4C	2.44	108.60	106.90
4	A	503	QJ8	C05-C04-C03	2.44	121.00	118.09
4	B	503	QJ8	O09-C08-C06	2.42	117.84	110.94
3	B	502	H4B	C2-N3-C4	2.41	119.75	115.93
2	B	501	HEM	C4B-CHC-C1C	2.41	125.73	122.56
4	B	503	QJ8	C12-C26-C25	-2.38	117.77	121.08
4	A	503	QJ8	N22-C22-N21	2.27	120.08	116.49
4	B	503	QJ8	C08-C06-C05	2.21	124.15	121.08
2	A	501	HEM	CBA-CAA-C2A	-2.20	108.86	112.62
3	A	502	H4B	C4A-C4-N3	-2.16	117.88	124.01
4	A	503	QJ8	O11-C4'-C3'	2.15	116.30	109.77
4	B	503	QJ8	C25-C26-N21	-2.10	120.67	122.90
3	B	502	H4B	N2-C2-N3	2.05	120.44	117.25
2	A	501	HEM	CMA-C3A-C2A	2.03	128.78	124.94
4	A	503	QJ8	C12-O11-C4'	-2.02	110.14	113.78

There are no chirality outliers.

All (13) torsion outliers are listed below:

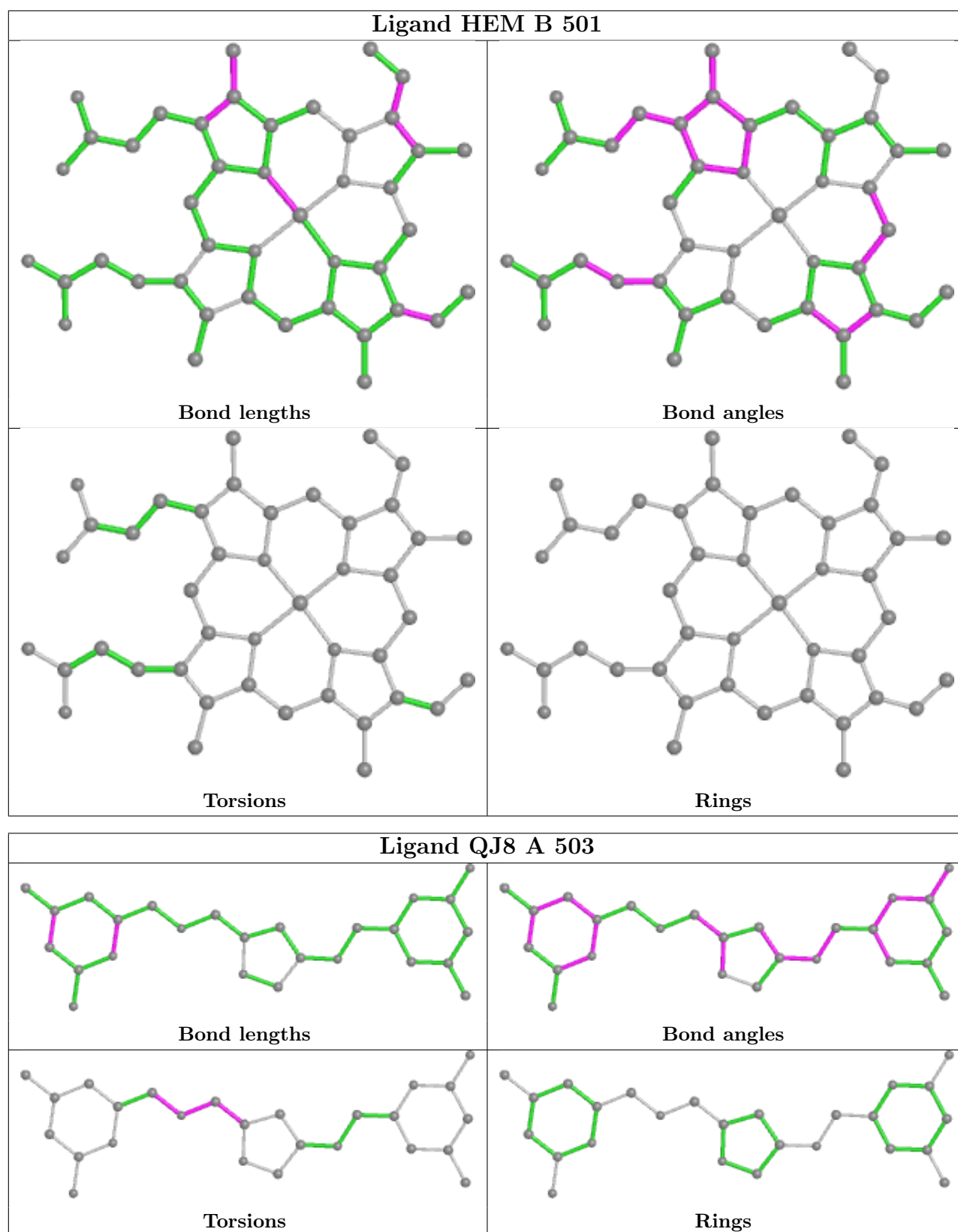
Mol	Chain	Res	Type	Atoms
4	A	503	QJ8	O09-C10-C2'-C3'
4	B	503	QJ8	O09-C10-C2'-N1'
4	B	503	QJ8	O09-C10-C2'-C3'
6	B	506	GOL	C1-C2-C3-O3
6	B	506	GOL	O2-C2-C3-O3
4	A	503	QJ8	C2'-C10-O09-C08
4	B	503	QJ8	C2'-C10-O09-C08
4	B	503	QJ8	C26-C12-O11-C4'
4	B	503	QJ8	C06-C08-O09-C10
4	A	503	QJ8	C06-C08-O09-C10
4	B	503	QJ8	C5'-C4'-O11-C12
4	B	503	QJ8	C3'-C4'-O11-C12
4	A	503	QJ8	O09-C10-C2'-N1'

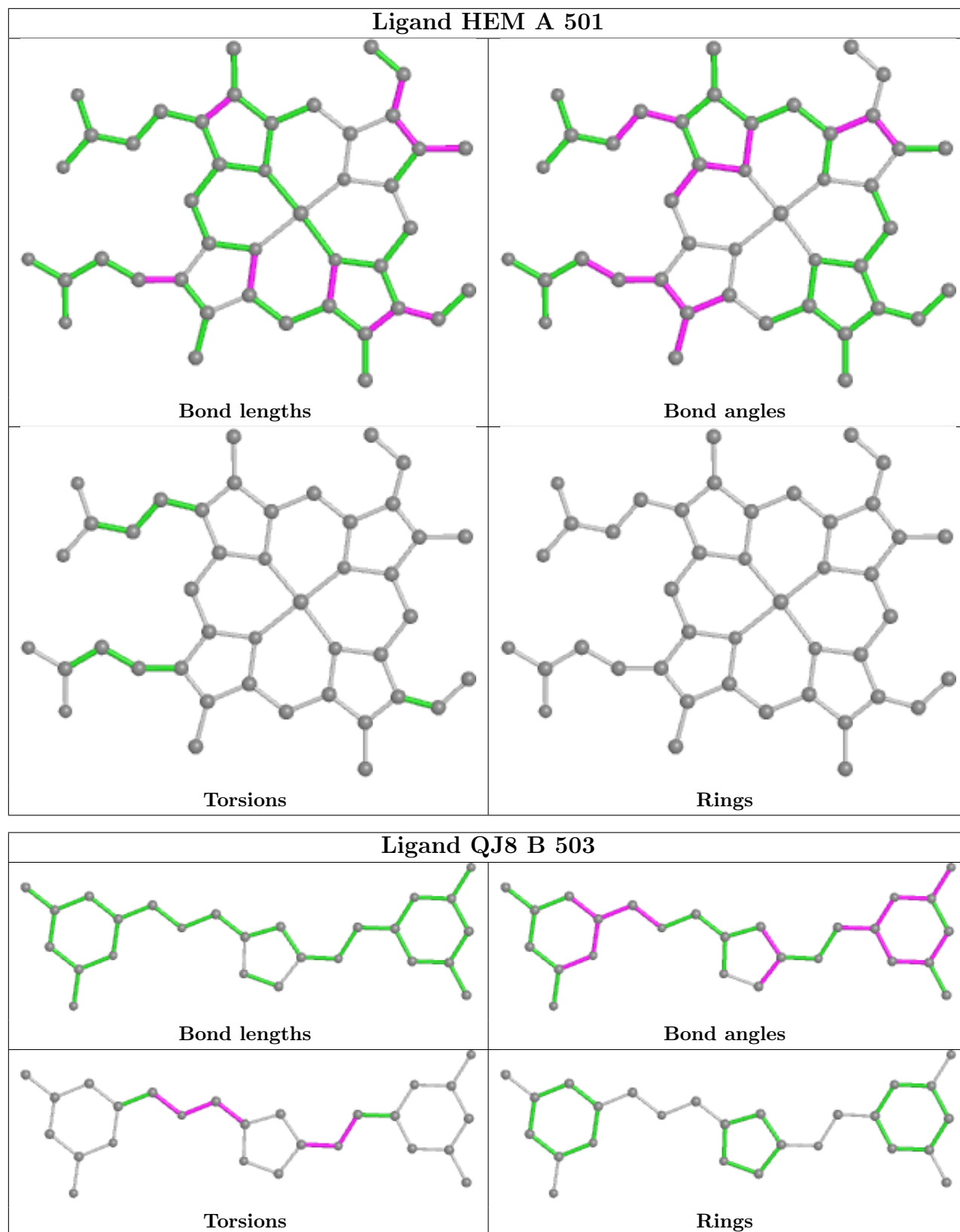
There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	10	0
3	B	502	H4B	1	0
4	A	503	QJ8	5	0
2	A	501	HEM	7	0
4	B	503	QJ8	8	0
3	A	502	H4B	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 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	404/442 (91%)	0.09	16 (3%) 38 40	27, 40, 64, 81	0
1	B	403/442 (91%)	-0.07	10 (2%) 57 60	27, 44, 69, 90	0
All	All	807/884 (91%)	0.01	26 (3%) 47 50	27, 41, 66, 90	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	5.0
1	A	123	GLU	3.8
1	A	239	GLY	3.8
1	A	259	GLN	3.7
1	B	282	THR	3.6
1	B	261	GLY	3.1
1	A	160	ALA	3.0
1	B	121	PRO	2.8
1	B	146	GLN	2.8
1	A	450	ILE	2.8
1	A	156	GLU	2.8
1	B	260	ASP	2.8
1	A	257	ARG	2.7
1	B	144	GLY	2.7
1	A	186	CYS	2.5
1	A	69	LYS	2.5
1	B	110	LYS	2.5
1	B	122	ALA	2.3
1	A	163	GLY	2.3
1	A	187	VAL	2.3
1	A	91	GLN	2.2
1	A	121	PRO	2.2
1	A	223	ARG	2.2
1	B	448	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	153	GLN	2.2
1	A	126	LEU	2.0

## 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<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
1	CAS	A	384	9/10	0.95	0.10	41,42,80,80	0
1	CAS	B	384	9/10	0.97	0.09	54,55,71,72	0

## 6.3 Carbohydrates [i](#)

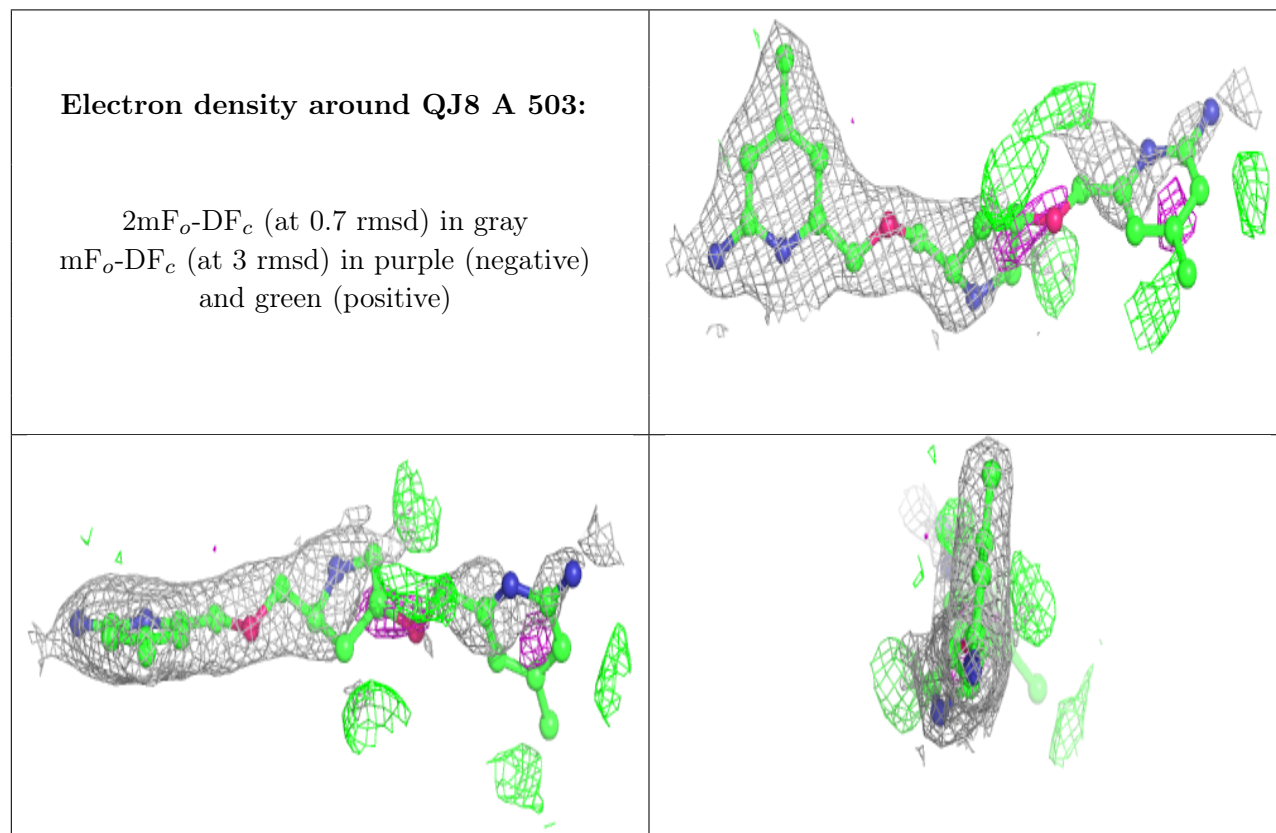
There are no monosaccharides in this entry.

## 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<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	QJ8	A	503	26/26	0.84	0.29	29,70,92,92	0
4	QJ8	B	503	26/26	0.84	0.32	28,78,97,98	0
6	GOL	A	506	6/6	0.89	0.20	57,57,58,61	0
5	ACT	A	504	4/4	0.93	0.12	36,37,41,44	0
5	ACT	B	505	4/4	0.95	0.13	41,43,45,45	0
6	GOL	B	506	6/6	0.95	0.30	54,54,55,55	0
5	ACT	A	505	4/4	0.96	0.13	33,35,36,40	0
3	H4B	A	502	17/17	0.97	0.17	30,34,37,38	0
5	ACT	B	504	4/4	0.98	0.22	55,58,58,61	0
2	HEM	A	501	43/43	0.98	0.20	22,28,40,43	0
3	H4B	B	502	17/17	0.98	0.21	28,32,33,37	0
2	HEM	B	501	43/43	0.98	0.15	27,31,38,42	0
7	ZN	A	507	1/1	0.99	0.11	38,38,38,38	0

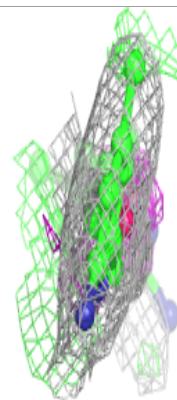
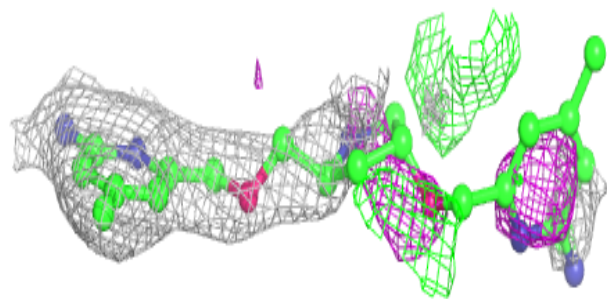
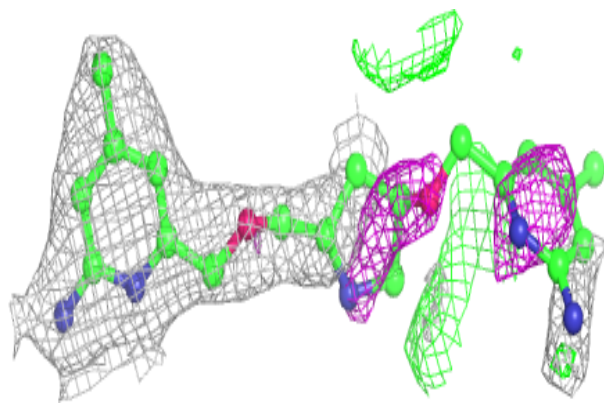
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





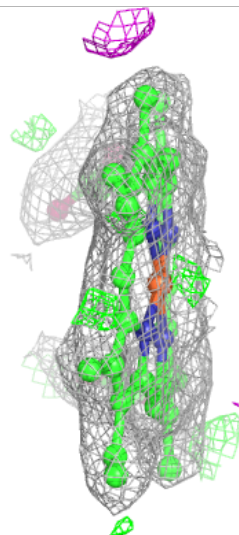
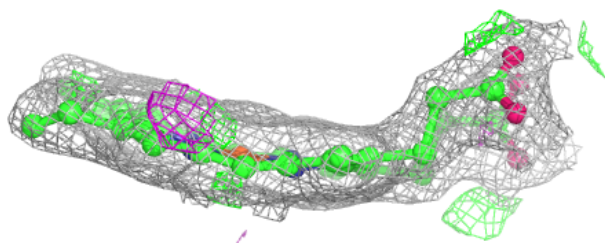
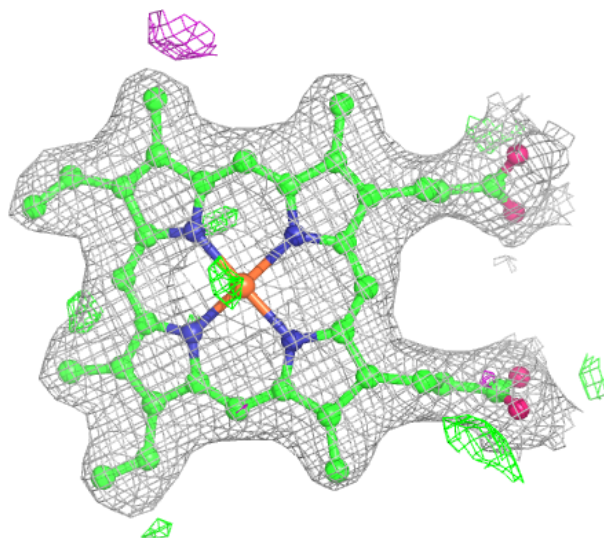
**Electron density around QJ8 B 503:**

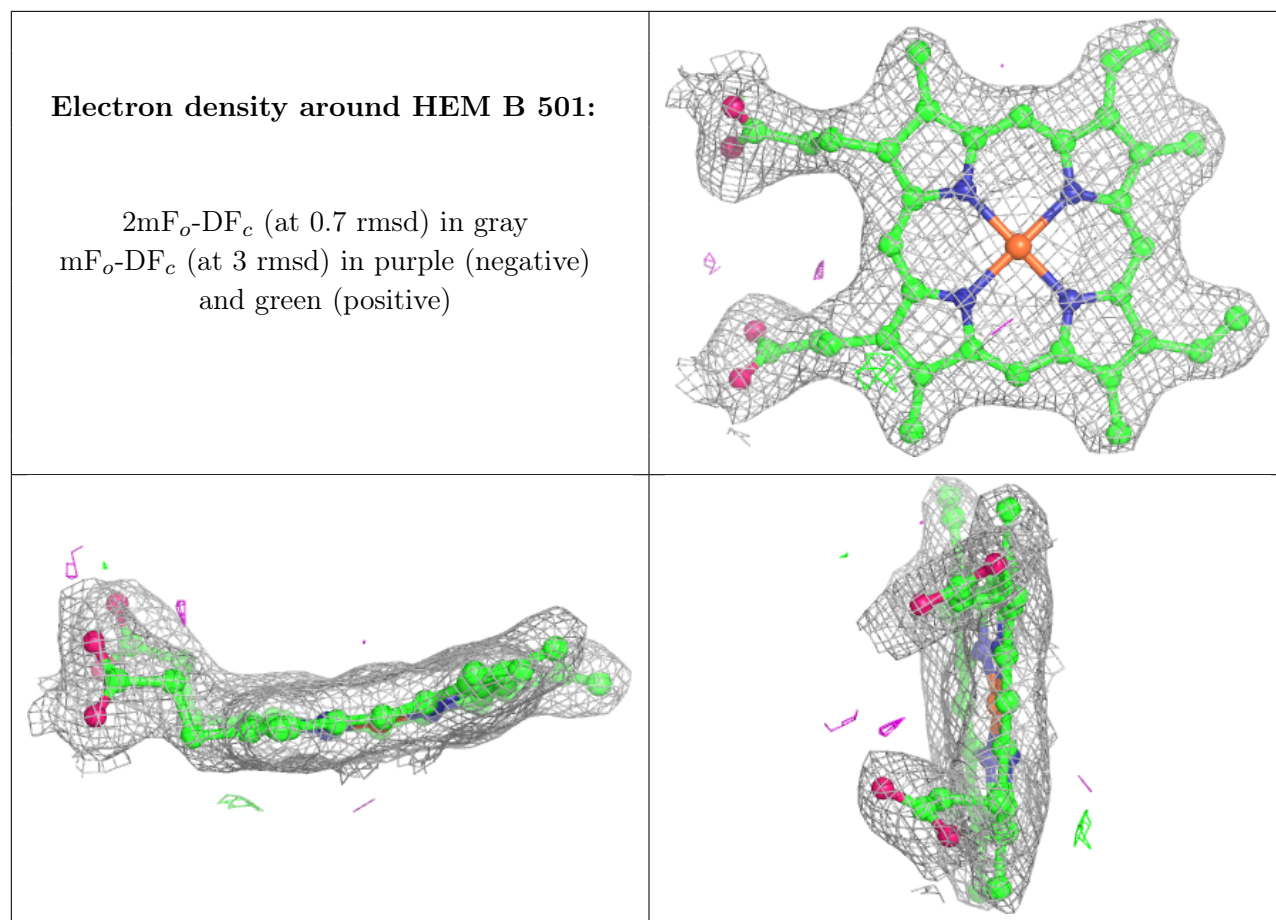
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 501:**

$2mF_o-DF_c$  (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.