



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:40 am BST

PDB ID : 4K5K  
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with ((2S, 3S)-1,3-bis((6-(2,5-dimethyl-1H-pyrrol-1-yl)-4-methylpyridin-2-yl)methoxy)-2-aminobutane  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2013-04-14  
Resolution : 2.00 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 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

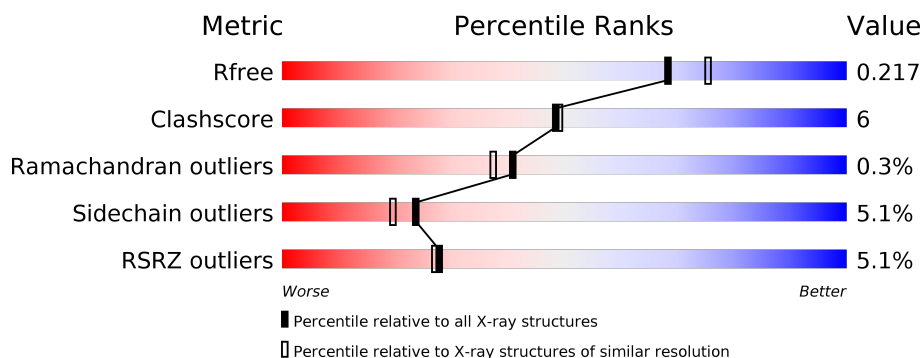
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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>5%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>9%</div> </div> </div>
1	B	443	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	Q13	B	503	-	-	X	-
5	ACT	A	505	-	-	X	-
5	ACT	B	505	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6984 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.

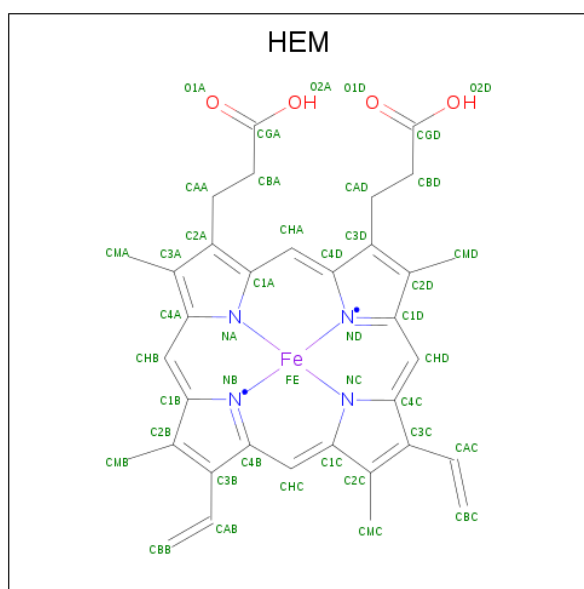
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			
1	B	404	Total	As	C	N	O	S	0	1	0
			3227	1	2052	569	589	16			

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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

*Continued on next page...*

Continued from previous page...

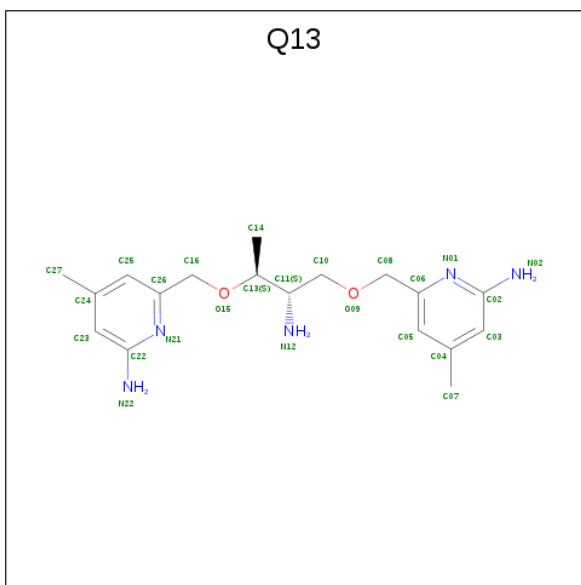
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



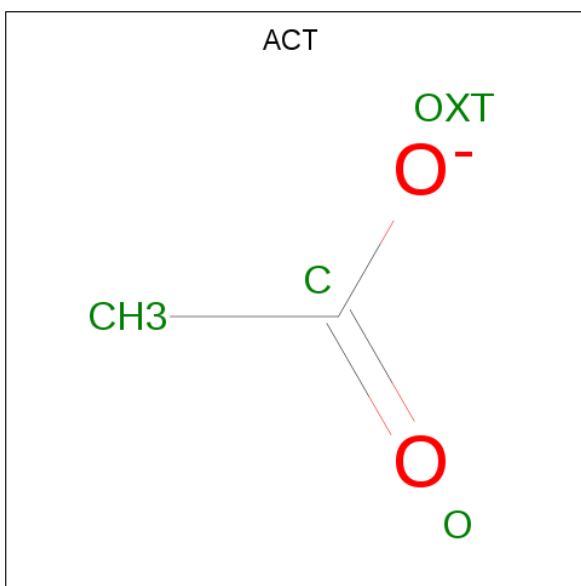
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6,6'-{[(2S,3S)-2-aminobutane-1,3-diyl]bis(oxymethanediyl)} bis(4-methylpyridine-2-amine) (three-letter code: Q13) (formula:  $C_{18}H_{27}N_5O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	18	5	2		
4	B	1	Total	C	N	O	0	0
			25	18	5	2		

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



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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

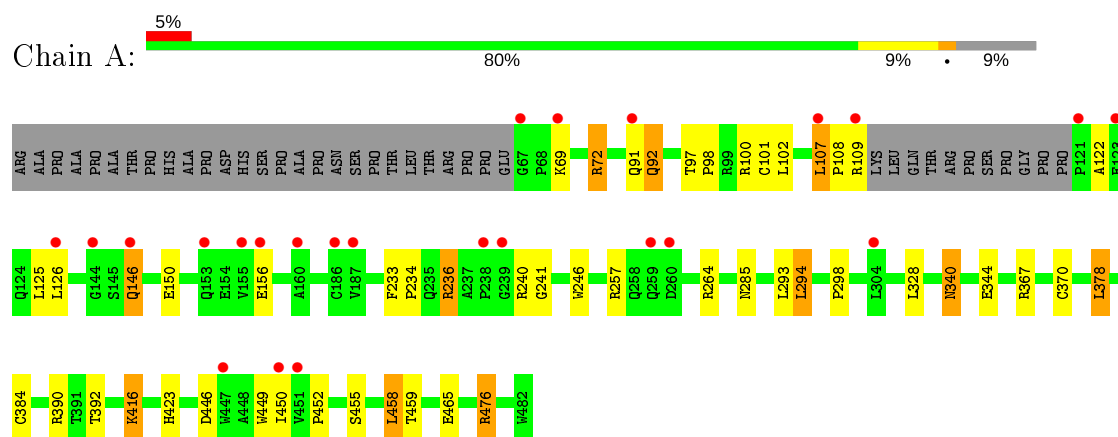
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	173	Total	O	0	0
			173	173		
8	B	162	Total	O	0	0
			162	162		

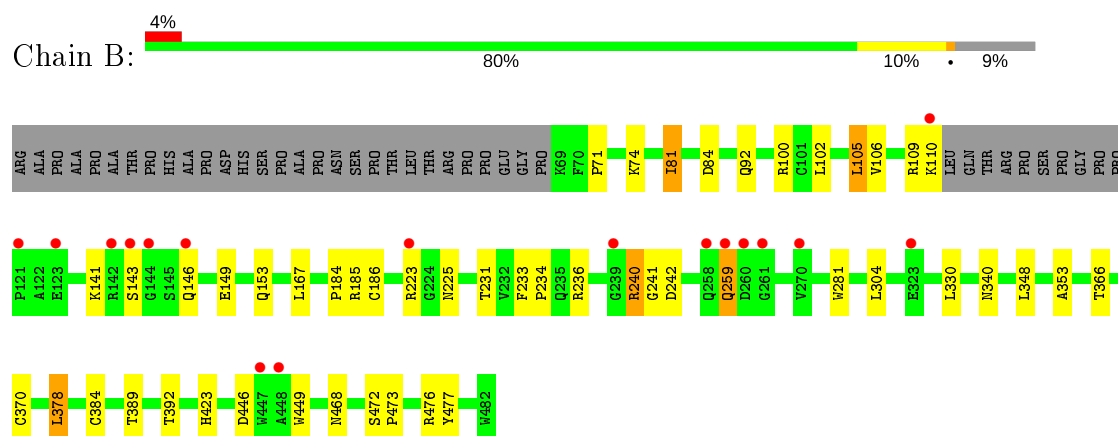
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	57.92Å 106.47Å 156.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.44 – 2.00 48.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.44-2.00) 99.4 (48.40-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.179 , 0.217 0.178 , 0.217	Depositor DCC
$R_{free}$ test set	3320 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: GOL, ZN, H4B, CAS, Q13, 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	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.67	0/3303	0.76	0/4497
1	B	0.72	0/3309	0.80	4/4503 (0.1%)
All	All	0.69	0/6612	0.78	4/9000 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	185	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	240	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	446	ASP	CB-CG-OD1	5.30	123.07	118.30

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	A	3223	0	3127	37	0
1	B	3227	0	3138	33	0
2	A	43	0	30	2	0
2	B	43	0	30	8	0
3	A	17	0	15	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
4	A	25	0	27	5	0
4	B	25	0	27	9	0
5	A	8	0	6	2	0
5	B	8	0	6	2	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	173	0	0	3	0
8	B	162	0	0	4	0
All	All	6984	0	6437	78	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 6.

All (78) 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:384:CAS:AS	1:B:384:CAS:SG	2.46	1.33
1:A:384:CAS:AS	1:A:384:CAS:SG	2.56	1.24
1:A:236:ARG:HB2	1:A:236:ARG:HH11	0.97	1.14
1:A:236:ARG:HB2	1:A:236:ARG:NH1	1.67	1.07
1:A:236:ARG:CB	1:A:236:ARG:HH11	1.71	1.03
1:B:236:ARG:HD3	1:B:242:ASP:OD1	1.88	0.72
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.72	0.72
4:B:503:Q13:H11	5:B:505:ACT:H3	1.73	0.70
1:A:378:LEU:HB2	8:A:615:HOH:O	1.92	0.68
1:A:72:ARG:HD3	8:A:709:HOH:O	1.95	0.65
1:B:236:ARG:HD3	1:B:242:ASP:CG	2.18	0.64
1:B:186:CYS:HB2	2:B:501:HEM:ND	2.14	0.63
4:A:503:Q13:H11	5:A:505:ACT:H1	1.83	0.61
1:B:236:ARG:CD	1:B:242:ASP:OD1	2.49	0.60
1:B:384:CAS:SG	1:B:384:CAS:CE1	2.91	0.58
1:B:106:VAL:HG12	4:B:503:Q13:H1	1.69	0.58
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.86	0.57
2:A:501:HEM:HBA2	4:A:503:Q13:H21	1.85	0.57
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.35	0.57
1:B:149:GLU:O	1:B:153:GLN:HG3	2.05	0.56
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.36	0.55
1:B:384:CAS:AS	1:B:384:CAS:CB	3.14	0.55
1:B:146:GLN:HA	1:B:146:GLN:OE1	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD21	4:A:503:Q13:H3	1.89	0.54
1:A:92:GLN:OE1	1:A:476:ARG:NH1	2.39	0.54
1:B:74:LYS:HD2	1:B:81:ILE:HD11	1.89	0.54
1:A:384:CAS:CB	1:A:384:CAS:AS	3.16	0.53
1:B:378:LEU:HB2	8:B:624:HOH:O	2.10	0.52
1:A:449:TRP:HA	3:A:502:H4B:N1	2.25	0.52
2:B:501:HEM:CBA	4:B:503:Q13:H21	2.40	0.52
4:A:503:Q13:H11	5:A:505:ACT:CH3	2.39	0.51
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.50	0.51
1:B:92[B]:GLN:NE2	8:B:736:HOH:O	2.43	0.51
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.41	0.51
1:A:240:ARG:HD2	1:A:241:GLY:O	2.11	0.51
1:A:344:GLU:OE1	1:A:476:ARG:NH2	2.44	0.50
4:B:503:Q13:C14	5:B:505:ACT:H3	2.42	0.50
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.94	0.50
2:B:501:HEM:C1C	4:B:503:Q13:H28	2.48	0.49
1:A:340:ASN:HD22	1:A:340:ASN:H	1.59	0.49
1:B:186:CYS:HB2	2:B:501:HEM:C4D	2.46	0.49
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.96	0.48
1:B:366:THR:O	1:B:370:CYS:HB2	2.13	0.48
2:B:501:HEM:HBA2	4:B:503:Q13:H21	1.95	0.47
1:A:452:PRO:HG2	1:A:459:THR:HG21	1.95	0.47
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.79	0.47
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.70	0.47
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.95	0.47
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.98	0.46
1:A:423:HIS:HB2	1:B:392:THR:HB	1.98	0.46
1:B:106:VAL:CG1	4:B:503:Q13:H1	2.28	0.46
1:A:264:ARG:HD3	1:A:285:ASN:O	2.17	0.45
1:B:106:VAL:CG1	4:B:503:Q13:N22	2.80	0.45
1:A:416:LYS:HA	1:A:416:LYS:HE3	1.98	0.45
2:A:501:HEM:C1C	4:A:503:Q13:H28	2.52	0.45
1:A:108:PRO:HG3	8:A:735:HOH:O	2.17	0.45
1:A:455:SER:O	1:A:458:LEU:HB2	2.17	0.44
1:B:449:TRP:HA	3:B:502:H4B:N1	2.32	0.44
1:A:240:ARG:CD	1:A:241:GLY:O	2.66	0.44
1:A:392:THR:HB	1:B:423:HIS:HB2	1.99	0.44
1:B:231:THR:O	1:B:353:ALA:HA	2.18	0.43
1:B:477:TYR:CZ	4:B:503:Q13:N22	2.87	0.43
1:A:390:ARG:HB2	1:A:390:ARG:HE	1.64	0.43
1:B:476:ARG:NH1	8:B:664:HOH:O	2.52	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:HH12	3:A:502:H4B:C4	2.32	0.42
1:A:97:THR:HB	1:A:98:PRO:HD2	2.01	0.42
1:A:101:CYS:HB3	1:B:468:ASN:HB3	2.02	0.42
1:A:465:GLU:HB3	1:B:105:LEU:HD22	2.01	0.41
1:A:236:ARG:NH1	1:A:236:ARG:CB	2.51	0.41
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.60	0.41
1:B:184:PRO:HD2	8:B:618:HOH:O	2.19	0.41
1:B:167:LEU:HG	1:B:348:LEU:HD12	2.02	0.41
1:A:146:GLN:HB3	1:A:146:GLN:HE21	1.62	0.41
1:A:233:PHE:HB3	1:A:234:PRO:CD	2.51	0.40
1:A:146:GLN:O	1:A:150:GLU:HG3	2.22	0.40
1:B:240:ARG:HD2	1:B:241:GLY:O	2.21	0.40
1:A:446:ASP:O	1:A:450:ILE:HG12	2.22	0.40
1:B:472:SER:HA	1:B:473:PRO:C	2.41	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	400/443 (90%)	388 (97%)	11 (3%)	1 (0%)	41	37
1	B	400/443 (90%)	387 (97%)	12 (3%)	1 (0%)	41	37
All	All	800/886 (90%)	775 (97%)	23 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	A	122	ALA

### 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	343/375 (92%)	323 (94%)	20 (6%)	20	15
1	B	344/375 (92%)	329 (96%)	15 (4%)	28	25
All	All	687/750 (92%)	652 (95%)	35 (5%)	24	19

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	72	ARG
1	A	91	GLN
1	A	92	GLN
1	A	100	ARG
1	A	102	LEU
1	A	107	LEU
1	A	109	ARG
1	A	125	LEU
1	A	146	GLN
1	A	156	GLU
1	A	236	ARG
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	416	LYS
1	A	458	LEU
1	A	476	ARG
1	B	81	ILE
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	110	LYS
1	B	141	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	143	SER
1	B	223	ARG
1	B	225	ASN
1	B	259	GLN
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	389	THR

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	91	GLN
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	259	GLN
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 ⓘ

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	1.33	1 (20%)	1,9,11	0.48	0
1	CAS	A	384	1	5,8,9	1.06	0	1,9,11	0.21	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	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE2	2.11	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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	384	CAS	3	0
1	A	384	CAS	2	0

## 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
3	H4B	A	502	-	16,18,18	0.94	0	11,26,26	3.24	6 (54%)
5	ACT	B	504	-	1,3,3	1.33	0	0,3,3	0.00	-
2	HEM	B	501	1	27,50,50	0.95	1 (3%)	17,82,82	1.54	1 (5%)
4	Q13	B	503	-	26,26,26	0.68	0	30,35,35	2.12	8 (26%)
4	Q13	A	503	-	26,26,26	0.98	0	30,35,35	1.93	6 (20%)
3	H4B	B	502	-	16,18,18	0.66	0	11,26,26	2.75	6 (54%)
5	ACT	A	504	-	1,3,3	1.39	0	0,3,3	0.00	-
2	HEM	A	501	1	27,50,50	1.11	2 (7%)	17,82,82	1.92	5 (29%)
6	GOL	B	506	-	5,5,5	0.29	0	5,5,5	0.68	0
5	ACT	A	505	-	1,3,3	2.11	1 (100%)	0,3,3	0.00	-
6	GOL	A	506	-	5,5,5	0.28	0	5,5,5	0.75	0
5	ACT	B	505	-	1,3,3	2.08	1 (100%)	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 columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
6	GOL	A	506	-	-	0/4/4/4	-
2	HEM	B	501	1	-	0/6/54/54	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	Q13	A	503	-	-	8/14/15/15	0/2/2/2
4	Q13	B	503	-	-	4/14/15/15	0/2/2/2
2	HEM	A	501	1	-	0/6/54/54	-
6	GOL	B	506	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C4D-C3D	3.41	1.50	1.42
2	B	501	HEM	C3B-C2B	-2.85	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C4A-NA	2.16	1.40	1.36
5	A	505	ACT	CH3-C	2.11	1.51	1.48
5	B	505	ACT	CH3-C	2.08	1.51	1.48

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	Q13	C02-N01-C06	7.38	123.69	118.10
3	A	502	H4B	C4-C4A-N5	6.55	124.62	119.12
3	B	502	H4B	C4-C4A-N5	5.34	123.60	119.12
4	A	503	Q13	C02-N01-C06	5.14	121.99	118.10
2	B	501	HEM	CBA-CAA-C2A	-4.76	103.70	112.49
3	A	502	H4B	C4-C4A-C8A	4.65	118.70	114.57
4	A	503	Q13	C05-C06-N01	-4.37	118.27	122.90
4	A	503	Q13	C08-C06-C05	4.27	127.01	121.08
4	B	503	Q13	C08-C06-C05	4.23	126.95	121.08
2	A	501	HEM	CAA-CBA-CGA	3.82	119.09	112.67
3	A	502	H4B	N3-C2-N1	-3.80	119.45	125.42
3	A	502	H4B	C4-N3-C2	3.69	121.80	115.93
3	B	502	H4B	C4-C4A-C8A	3.66	117.82	114.57
4	B	503	Q13	C05-C06-N01	-3.63	119.05	122.90
4	A	503	Q13	C22-N21-C26	3.46	120.72	118.10
3	B	502	H4B	N3-C2-N1	-3.42	120.06	125.42
2	A	501	HEM	C1D-C2D-C3D	-3.41	104.63	107.00
4	B	503	Q13	C22-N21-C26	3.39	120.67	118.10
2	A	501	HEM	CBA-CAA-C2A	-3.19	106.60	112.49
3	A	502	H4B	C2-N1-C8A	2.99	121.25	114.54
3	B	502	H4B	N2-C2-N3	2.97	121.88	117.25
4	A	503	Q13	O09-C08-C06	2.93	119.28	110.94
3	B	502	H4B	C4-N3-C2	2.93	120.58	115.93
3	B	502	H4B	C2-N1-C8A	2.76	120.72	114.54
3	A	502	H4B	N2-C2-N3	2.70	121.45	117.25
4	B	503	Q13	C07-C04-C03	-2.67	116.98	120.94
4	B	503	Q13	C04-C05-C06	-2.65	118.58	120.32
2	A	501	HEM	CMD-C2D-C3D	2.32	129.32	124.94
4	B	503	Q13	C25-C26-N21	-2.32	120.44	122.90
2	A	501	HEM	CMB-C2B-C3B	2.17	128.74	124.68
4	B	503	Q13	O09-C08-C06	2.13	116.99	110.94
4	A	503	Q13	C25-C26-N21	-2.12	120.66	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

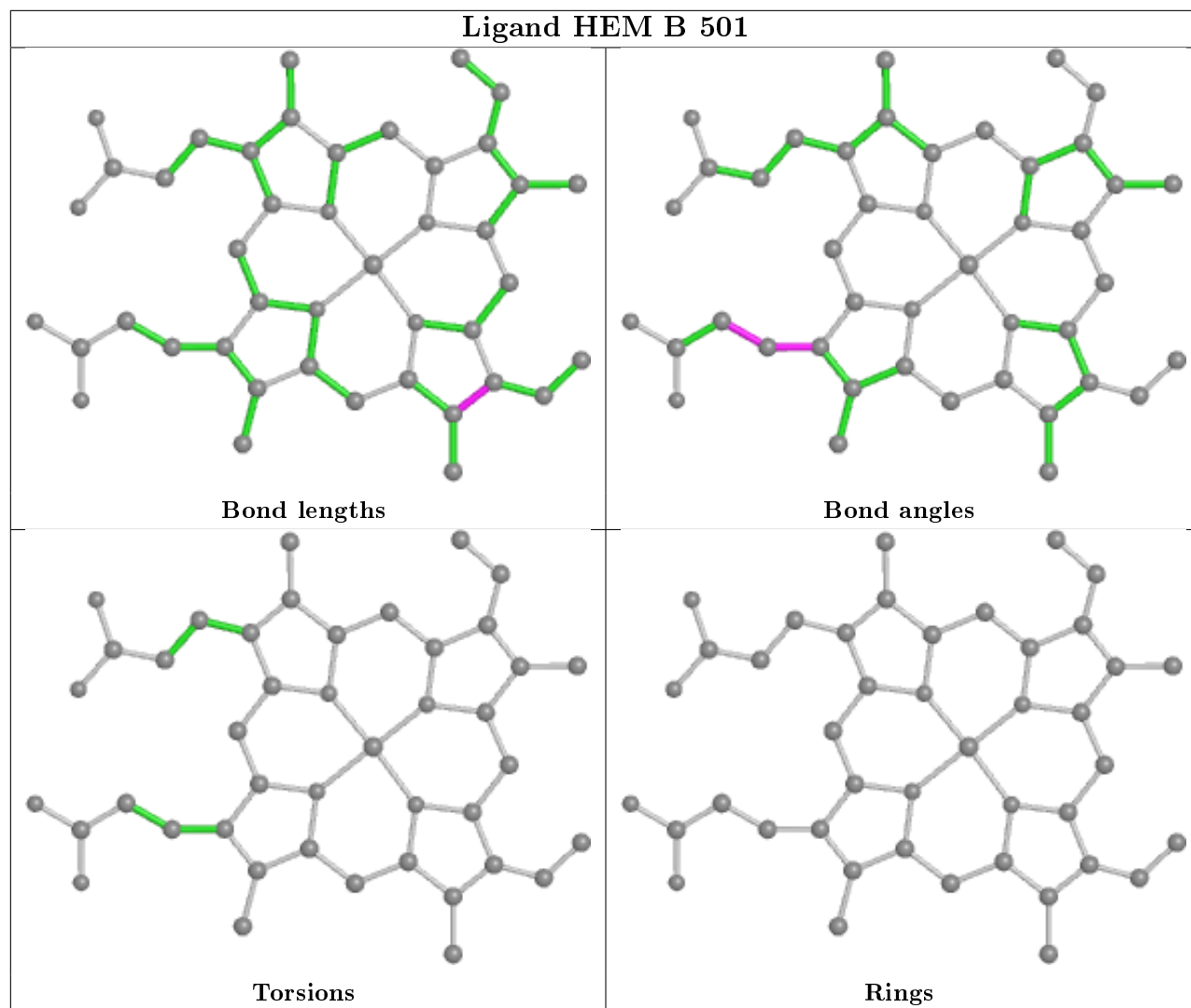
Mol	Chain	Res	Type	Atoms
4	B	503	Q13	C14-C13-O15-C16
4	A	503	Q13	C14-C13-O15-C16
4	A	503	Q13	C10-C11-C13-O15
4	A	503	Q13	N12-C11-C13-C14
4	A	503	Q13	C10-C11-C13-C14
4	B	503	Q13	C11-C10-O09-C08
4	A	503	Q13	C11-C10-O09-C08
4	A	503	Q13	C26-C16-O15-C13
4	A	503	Q13	O15-C16-C26-N21
4	A	503	Q13	O15-C16-C26-C25
4	B	503	Q13	O15-C16-C26-C25
4	B	503	Q13	O15-C16-C26-N21

There are no ring outliers.

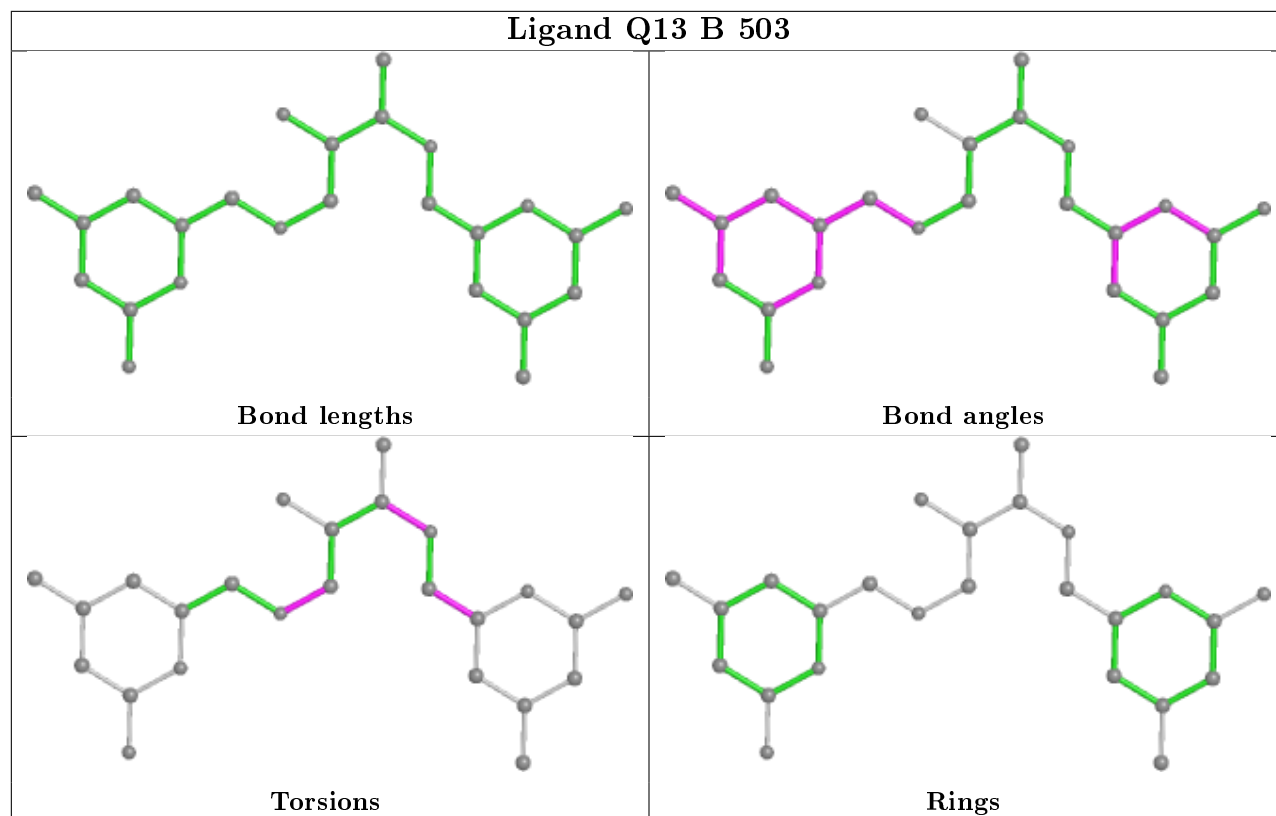
8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	H4B	2	0
2	B	501	HEM	8	0
4	B	503	Q13	9	0
4	A	503	Q13	5	0
3	B	502	H4B	1	0
2	A	501	HEM	2	0
5	A	505	ACT	2	0
5	B	505	ACT	2	0

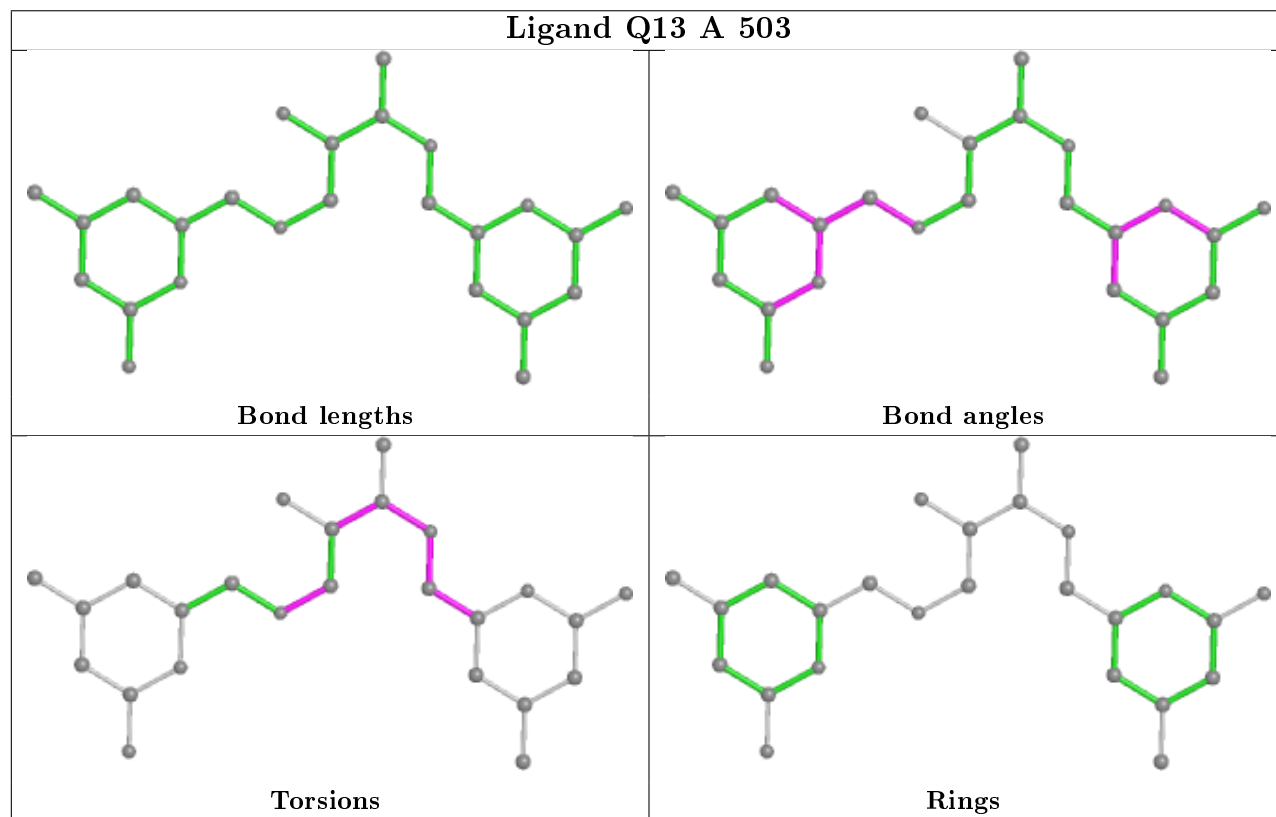
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

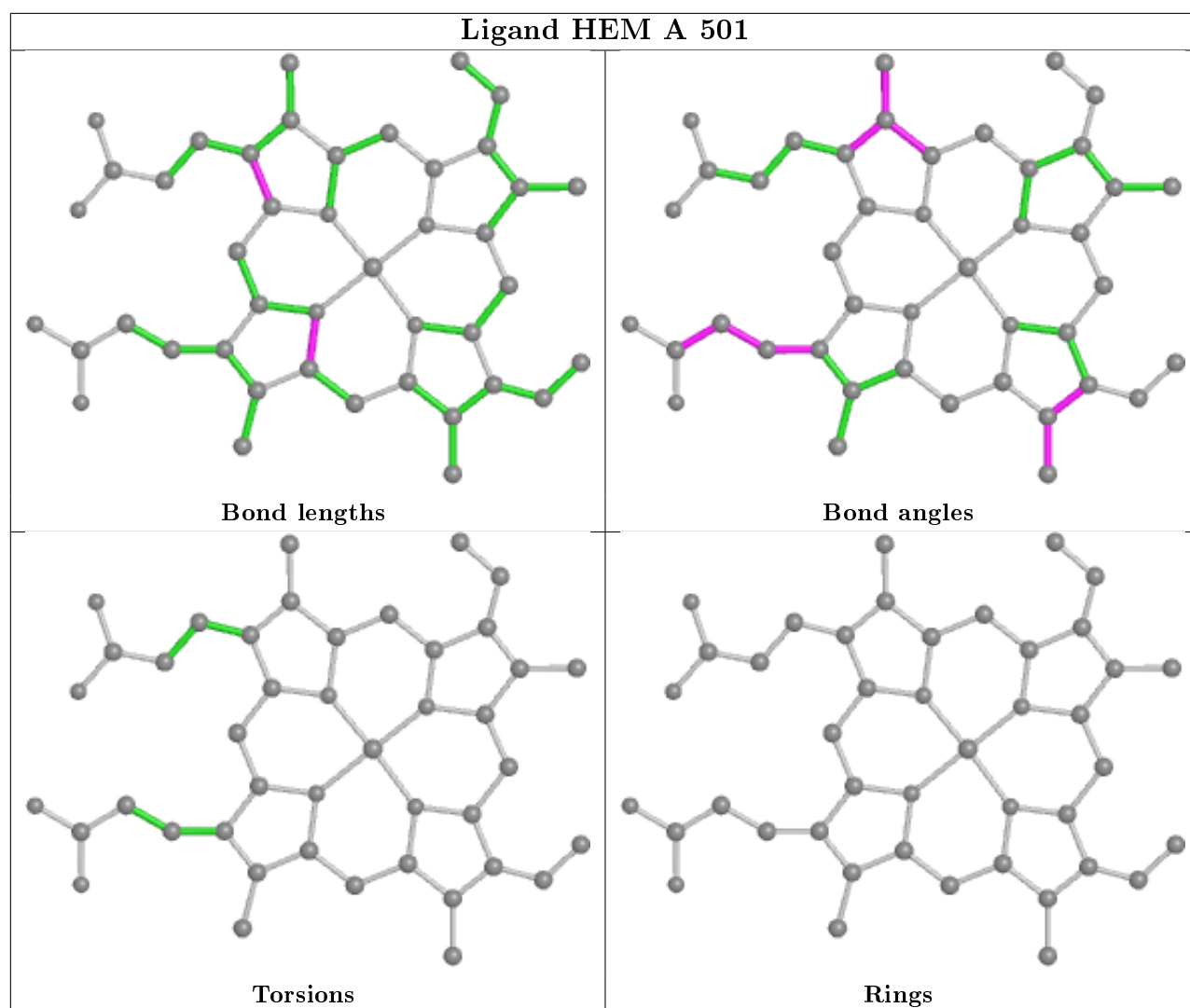


## Ligand Q13 B 503



## Ligand Q13 A 503





## 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, 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	404/443 (91%)	0.33	24 (5%) 22 21	30, 44, 72, 93	0
1	B	403/443 (90%)	0.11	17 (4%) 36 35	29, 46, 73, 110	0
All	All	807/886 (91%)	0.22	41 (5%) 28 27	29, 45, 73, 110	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	6.0
1	B	110	LYS	5.7
1	A	69	LYS	4.4
1	B	142	ARG	4.4
1	A	259	GLN	4.3
1	A	123	GLU	3.8
1	A	67	GLY	3.8
1	B	146	GLN	3.7
1	A	239	GLY	3.7
1	B	260	ASP	3.5
1	A	91	GLN	3.3
1	A	109	ARG	3.3
1	B	261	GLY	3.3
1	A	238	PRO	3.1
1	A	450	ILE	3.1
1	A	160	ALA	3.0
1	B	121	PRO	2.8
1	B	144	GLY	2.7
1	A	144	GLY	2.7
1	A	126	LEU	2.7
1	A	187	VAL	2.5
1	B	447	TRP	2.5
1	B	323	GLU	2.5
1	B	223	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	121	PRO	2.4
1	B	258	GLN	2.4
1	A	155	VAL	2.4
1	A	153	GLN	2.4
1	A	451	VAL	2.4
1	A	447	TRP	2.4
1	B	143	SER	2.4
1	A	186	CYS	2.3
1	B	270	VAL	2.3
1	B	448	ALA	2.3
1	A	156	GLU	2.2
1	A	146	GLN	2.2
1	B	123	GLU	2.1
1	A	304	LEU	2.1
1	B	239	GLY	2.1
1	A	107	LEU	2.0
1	A	260	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	B	384	9/10	0.96	0.10	52,53,70,77	0
1	CAS	A	384	9/10	0.98	0.08	42,45,74,74	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

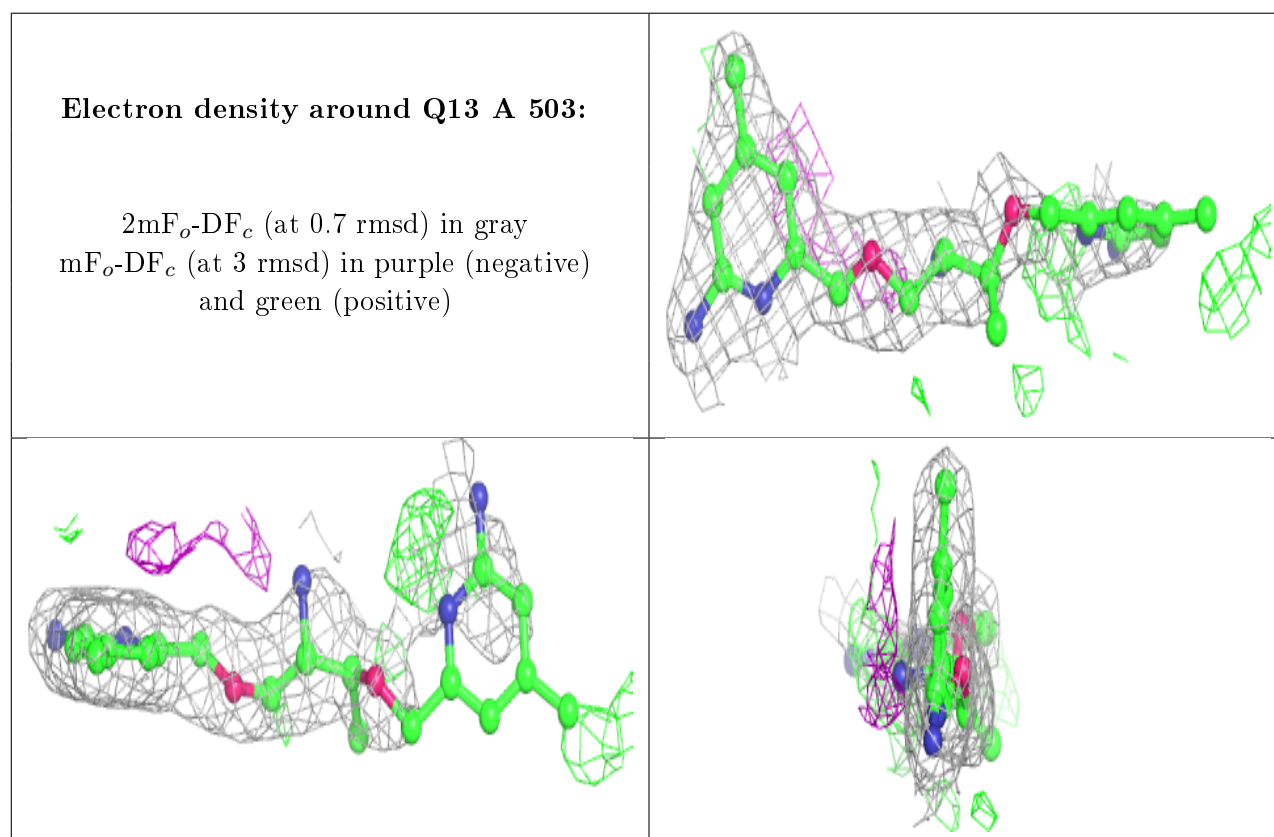
## 6.4 Ligands ⓘ

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.



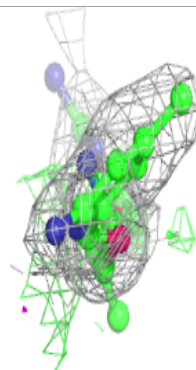
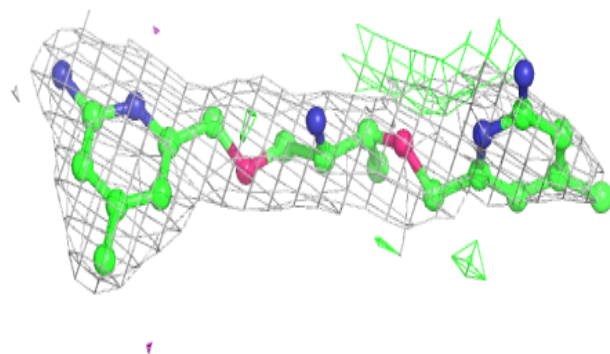
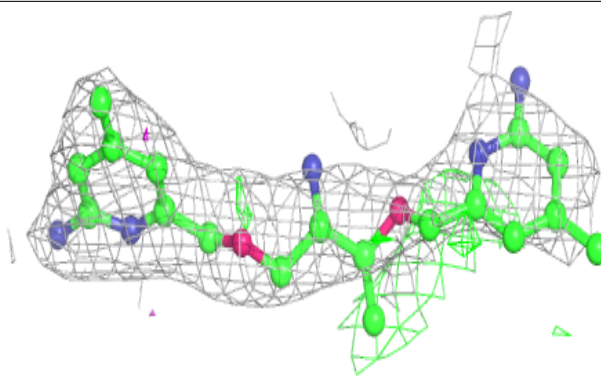
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	B	506	6/6	0.85	0.21	55,73,78,80	0
6	GOL	A	506	6/6	0.86	0.20	68,71,77,79	0
5	ACT	A	505	4/4	0.90	0.14	47,51,52,56	0
4	Q13	A	503	25/25	0.93	0.23	36,69,126,129	0
5	ACT	B	504	4/4	0.93	0.18	51,56,57,60	0
4	Q13	B	503	25/25	0.94	0.19	37,75,111,112	0
5	ACT	B	505	4/4	0.95	0.15	45,49,51,54	0
3	H4B	A	502	17/17	0.96	0.17	41,44,47,47	0
3	H4B	B	502	17/17	0.96	0.15	36,41,48,49	0
5	ACT	A	504	4/4	0.97	0.13	54,56,58,63	0
2	HEM	A	501	43/43	0.97	0.20	32,38,44,52	0
2	HEM	B	501	43/43	0.98	0.16	32,36,47,51	0
7	ZN	A	507	1/1	0.98	0.08	48,48,48,48	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.



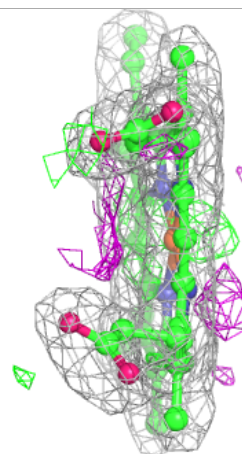
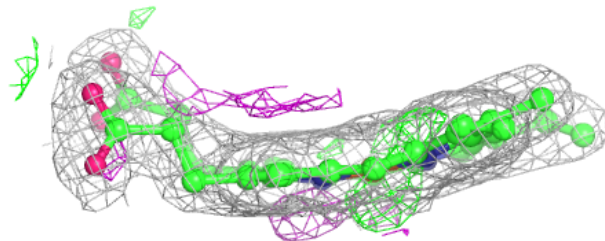
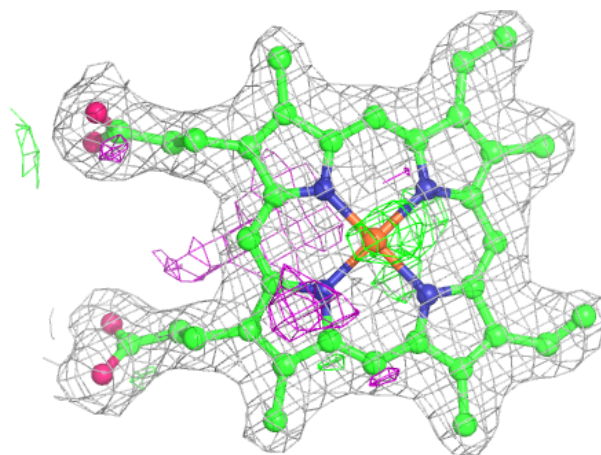
**Electron density around Q13 B 503:**

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



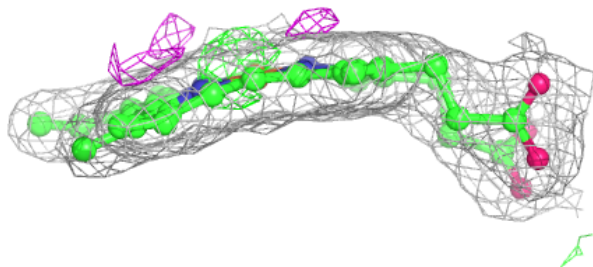
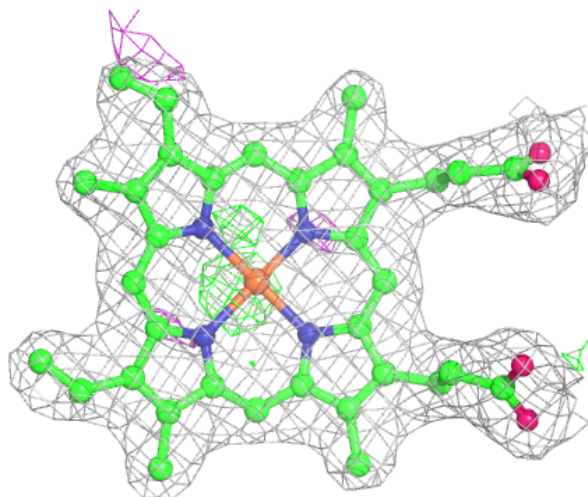
**Electron density around HEM A 501:**

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



**Electron density around HEM B 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 ⓘ

There are no such residues in this entry.