



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:51 am BST

PDB ID : 4CU1  
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 6-[(2S)-3-amino-2-{5-[2-(6-amino-4-methylpyridin-2-yl)ethyl]pyridin-3-yl}propyl]-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2014-03-15  
Resolution : 1.89 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

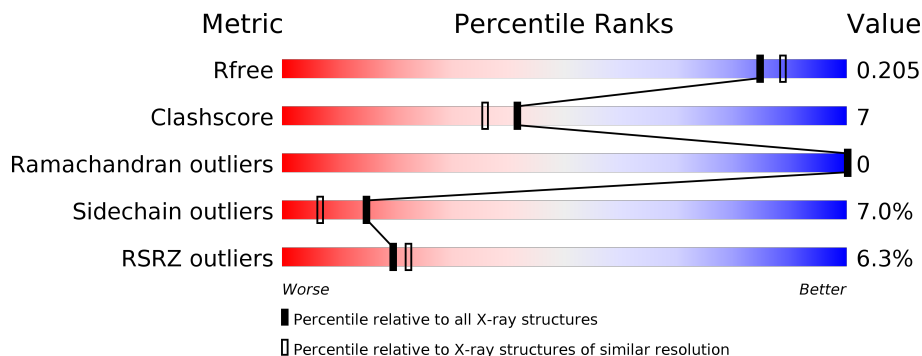
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	<p>7% (poor fit), 79% (0 outliers), 10% (1 outlier), 9% (2+ outliers)</p>
2	B	443	<p>5% (poor fit), 75% (0 outliers), 14% (1 outlier), 9% (2+ outliers)</p>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6933 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	3223	1	2049	568	589	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	404	3218	2046	568	588	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

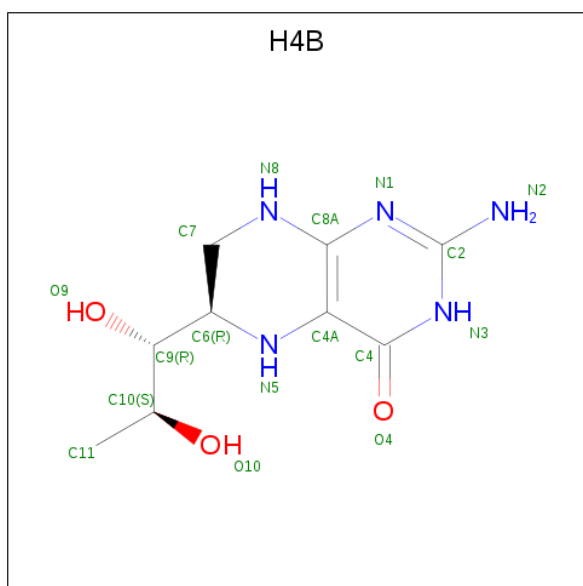
Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ARG	CYS	variant	UNP P29473

- Molecule 3 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
3	A	1	43	34	1	4	4	0	0
3	B	1	43	34	1	4	4	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



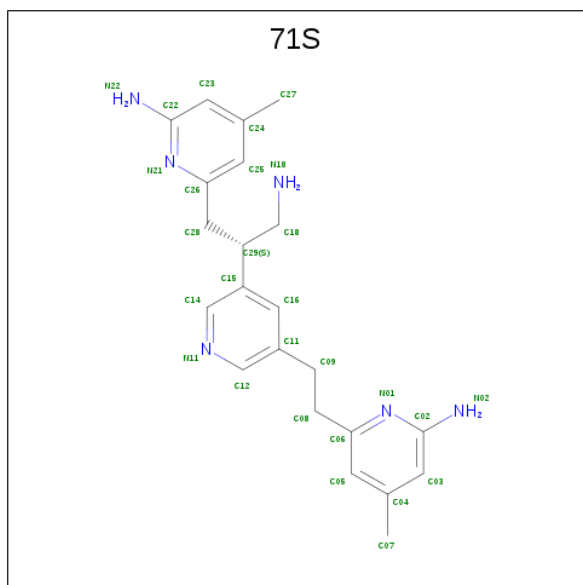
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	17	9	5	3	0	0

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

- Molecule 5 is 6-[(2S)-3-amino-2-{5-[2-(6-amino-4-methylpyridin-2-yl)ethyl]pyridin-3-yl}propyl]-4-methylpyridin-2-amine (three-letter code: 71S) (formula: C<sub>22</sub>H<sub>28</sub>N<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	A	1	28	22	6	0	0
5	B	1	28	22	6	0	0

- Molecule 6 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
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

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

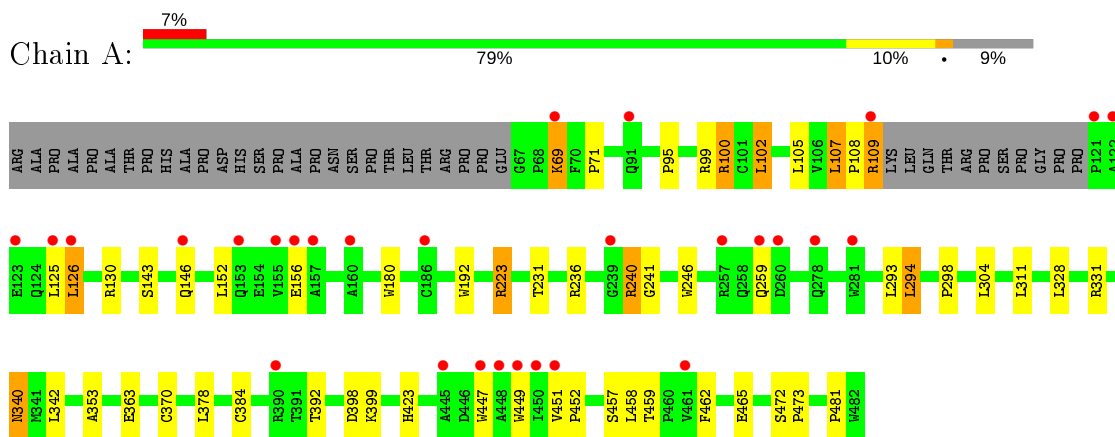
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	170	Total 170	O 170	0	0
9	B	125	Total 125	O 125	0	0

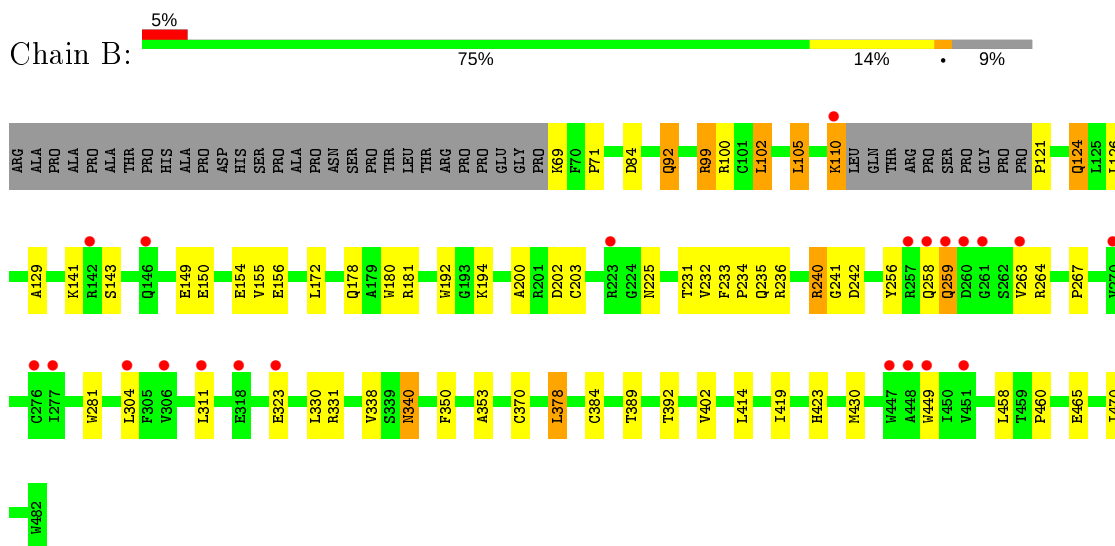
### 3 Residue-property plots [i](#)

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 2: NITRIC OXIDE SYNTHASE, ENDOTHELIAL





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.34Å 105.17Å 155.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.04 – 1.89 47.88 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (87.04-1.89) 98.6 (47.88-1.89)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.170 , 0.205 0.170 , 0.205	Depositor DCC
$R_{free}$ test set	3704 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtrriage
Anisotropy	0.323	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 71S, 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	0.59	0/3303	0.74	1/4497 (0.0%)
2	B	0.56	0/3307	0.72	0/4502
All	All	0.57	0/6610	0.73	1/8999 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3223	0	3127	46	0
2	B	3218	0	3131	41	0
3	A	43	0	30	6	0
3	B	43	0	30	4	0
4	A	17	0	15	2	0
4	B	17	0	15	1	0
5	A	28	0	28	8	0
5	B	28	0	28	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4	0	3	0	0
6	B	4	0	3	0	0
7	A	6	0	8	1	0
7	B	6	0	8	0	0
8	B	1	0	0	0	0
9	A	170	0	0	2	0
9	B	125	0	0	2	0
All	All	6933	0	6426	92	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 7.

All (92) 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:223:ARG:HH11	1:A:223:ARG:HG3	1.24	1.01
3:A:500:HEM:O1D	5:A:800:71S:H282	1.72	0.90
1:A:384:CAS:AS	1:A:384:CAS:SG	2.93	0.87
1:A:109:ARG:HH11	1:A:109:ARG:HA	1.47	0.79
2:B:384:CYS:SG	9:B:2096:HOH:O	2.39	0.79
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.68	0.76
1:A:384:CAS:CE2	1:A:384:CAS:SG	2.78	0.72
3:B:500:HEM:O1D	5:B:800:71S:H282	1.92	0.69
2:B:236:ARG:CD	2:B:242:ASP:OD1	2.40	0.69
2:B:178:GLN:HE22	2:B:181:ARG:HH11	1.42	0.67
2:B:236:ARG:HD2	2:B:242:ASP:OD1	1.94	0.66
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.05	0.65
1:A:109:ARG:NH1	1:A:109:ARG:HA	2.12	0.64
2:B:92:GLN:HG3	2:B:470:ILE:HG21	1.78	0.64
1:A:223:ARG:NH1	1:A:223:ARG:HG3	2.03	0.63
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.79	0.62
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.29	0.62
3:A:500:HEM:HBB2	3:A:500:HEM:HHC	1.82	0.62
2:B:449:TRP:CH2	5:B:800:71S:H182	2.35	0.61
1:A:107:LEU:HD21	5:A:800:71S:H273	1.83	0.60
1:A:105:LEU:HD22	2:B:465:GLU:HB3	1.83	0.59
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.83	0.59
3:B:500:HEM:HBB2	3:B:500:HEM:HHC	1.85	0.57
2:B:150:GLU:O	2:B:154:GLU:HG3	2.04	0.56
1:A:449:TRP:CH2	5:A:800:71S:H182	2.40	0.56
1:A:126:LEU:O	1:A:130:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:TRP:HA	4:A:600:H4B:N1	2.21	0.56
2:B:281:TRP:HB2	2:B:304:LEU:HD21	1.88	0.55
2:B:236:ARG:HD3	2:B:242:ASP:OD1	2.06	0.55
2:B:178:GLN:HE22	2:B:181:ARG:NH1	2.04	0.55
2:B:378:LEU:HB2	9:B:2094:HOH:O	2.06	0.54
2:B:338:VAL:CG2	5:B:800:71S:H092	2.39	0.53
2:B:240:ARG:HD2	2:B:241:GLY:O	2.09	0.53
2:B:121:PRO:HG2	2:B:124:GLN:HB2	1.92	0.52
2:B:129:ALA:HB1	2:B:155:VAL:HG11	1.92	0.52
2:B:92:GLN:HG3	2:B:470:ILE:CG2	2.39	0.52
2:B:340:ASN:OD1	5:B:800:71S:N22	2.43	0.52
2:B:236:ARG:HD3	2:B:242:ASP:CG	2.30	0.51
1:A:236:ARG:HB2	1:A:236:ARG:NH1	2.26	0.51
3:A:500:HEM:CBB	3:A:500:HEM:HHC	2.41	0.50
2:B:99:ARG:HB2	2:B:99:ARG:HH11	1.76	0.50
1:A:392:THR:HB	2:B:423:HIS:HB2	1.93	0.50
2:B:126:LEU:HD11	2:B:156:GLU:HA	1.94	0.49
2:B:231:THR:O	2:B:353:ALA:HA	2.11	0.49
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.51	0.49
2:B:110:LYS:O	2:B:110:LYS:HE2	2.12	0.49
2:B:338:VAL:HG23	5:B:800:71S:H05	1.94	0.49
2:B:370:CYS:SG	2:B:378:LEU:HD13	2.53	0.48
2:B:449:TRP:HA	4:B:600:H4B:N1	2.28	0.47
1:A:472:SER:HA	1:A:473:PRO:C	2.34	0.47
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.96	0.47
1:A:423:HIS:HB2	2:B:392:THR:HB	1.98	0.46
1:A:100:ARG:NH1	1:A:102:LEU:HD22	2.30	0.46
1:A:340:ASN:HD22	1:A:340:ASN:H	1.63	0.46
1:A:236:ARG:CB	1:A:236:ARG:HH11	2.28	0.46
2:B:256:TYR:O	2:B:258:GLN:NE2	2.49	0.45
1:A:236:ARG:HB2	1:A:236:ARG:HH11	1.81	0.45
1:A:363:GLU:OE1	5:A:800:71S:N01	2.49	0.45
1:A:378:LEU:HB2	9:A:2125:HOH:O	2.16	0.44
1:A:294:LEU:HD13	1:A:304:LEU:HD12	1.99	0.44
2:B:200:ALA:O	2:B:203:CYS:HB2	2.17	0.44
2:B:235:GLN:HB3	2:B:350:PHE:CE1	2.53	0.44
1:A:152:LEU:O	1:A:156:GLU:HG3	2.17	0.44
3:A:500:HEM:HBB2	3:A:500:HEM:CHC	2.47	0.44
2:B:259:GLN:HG3	2:B:259:GLN:H	1.64	0.44
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.53	0.43
1:A:457:SER:HA	1:A:462:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HD3	1:A:298:PRO:CG	2.47	0.43
3:A:500:HEM:C1C	5:A:800:71S:H073	2.53	0.43
3:B:500:HEM:O2A	5:B:800:71S:C16	2.65	0.43
1:A:447:TRP:CE2	1:A:451:VAL:HG21	2.53	0.43
1:A:95:PRO:HB3	1:A:108:PRO:CB	2.48	0.43
1:A:340:ASN:HD21	5:A:800:71S:H222	1.66	0.43
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.74	0.43
2:B:233:PHE:HB3	2:B:234:PRO:CD	2.48	0.43
1:A:240:ARG:HD2	1:A:241:GLY:O	2.18	0.42
2:B:430:MET:HG3	2:B:460:PRO:HB2	2.01	0.42
1:A:452:PRO:HG2	1:A:459:THR:HG21	2.01	0.42
5:A:800:71S:H181	7:A:880:GOL:H32	2.00	0.42
2:B:180:TRP:CE3	2:B:192:TRP:HA	2.54	0.42
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.42
2:B:263:VAL:HG11	2:B:267:PRO:HA	2.01	0.42
1:A:109:ARG:HD3	1:A:109:ARG:HA	1.81	0.42
1:A:465:GLU:HB3	2:B:105:LEU:HD22	2.01	0.41
2:B:71:PRO:HG2	2:B:84:ASP:HB3	2.02	0.41
1:A:143:SER:HB3	9:A:2031:HOH:O	2.20	0.41
3:B:500:HEM:CBB	3:B:500:HEM:HHC	2.49	0.41
1:A:71:PRO:HB3	2:B:102:LEU:HD11	2.02	0.41
2:B:172:LEU:HD11	2:B:232:VAL:HG11	2.02	0.41
3:A:500:HEM:O1A	4:A:600:H4B:N3	2.45	0.41
1:A:449:TRP:HH2	5:A:800:71S:H281	1.86	0.41
1:A:399:LYS:HG2	2:B:402:VAL:HG11	2.02	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%)	389 (97%)	11 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	400/443 (90%)	390 (98%)	10 (2%)	0	100	100
All	All	800/886 (90%)	779 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/375 (92%)	322 (94%)	21 (6%)	18	9
2	B	344/376 (92%)	317 (92%)	27 (8%)	12	5
All	All	687/751 (92%)	639 (93%)	48 (7%)	15	7

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	99	ARG
1	A	100	ARG
1	A	102	LEU
1	A	107	LEU
1	A	109	ARG
1	A	125	LEU
1	A	126	LEU
1	A	146	GLN
1	A	223	ARG
1	A	259	GLN
1	A	293	LEU
1	A	294	LEU
1	A	311	LEU
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	342	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	398	ASP
1	A	458	LEU
1	A	481	PRO
2	B	69	LYS
2	B	92	GLN
2	B	99	ARG
2	B	100	ARG
2	B	102	LEU
2	B	105	LEU
2	B	110	LYS
2	B	124	GLN
2	B	141	LYS
2	B	143	SER
2	B	149	GLU
2	B	194	LYS
2	B	202	ASP
2	B	225	ASN
2	B	240	ARG
2	B	259	GLN
2	B	264	ARG
2	B	311	LEU
2	B	323	GLU
2	B	330	LEU
2	B	331	ARG
2	B	340	ASN
2	B	378	LEU
2	B	389	THR
2	B	414	LEU
2	B	419	ILE
2	B	458	LEU

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	249	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
2	B	178	GLN

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Mol	Chain	Res	Type
2	B	191	GLN
2	B	207	GLN
2	B	222	ASN
2	B	225	ASN
2	B	258	GLN
2	B	376	ASN
2	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](#)

1 non-standard protein/DNA/RNA residue is 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	A	384	1	5,8,9	1.14	0	1,9,11	0.47	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	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.

1 monomer is involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	71S	B	800	-	29,30,30	0.90	2 (6%)	36,41,41	2.39	14 (38%)
7	GOL	B	880	-	5,5,5	0.31	0	5,5,5	0.85	0
4	H4B	A	600	-	16,18,18	1.00	1 (6%)	11,26,26	3.00	7 (63%)
6	ACT	B	860	-	1,3,3	1.61	0	0,3,3	0.00	-
6	ACT	A	860	-	1,3,3	1.36	0	0,3,3	0.00	-
3	HEM	A	500	1	27,50,50	0.89	1 (3%)	17,82,82	1.67	4 (23%)
3	HEM	B	500	2	27,50,50	0.93	1 (3%)	17,82,82	2.18	5 (29%)
4	H4B	B	600	-	16,18,18	1.17	2 (12%)	11,26,26	2.20	5 (45%)
7	GOL	A	880	-	5,5,5	0.21	0	5,5,5	0.73	0
5	71S	A	800	-	29,30,30	0.98	2 (6%)	36,41,41	2.28	15 (41%)

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
5	71S	B	800	-	-	5/15/15/15	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	880	-	-	0/4/4/4	-
4	H4B	A	600	-	-	0/8/17/17	0/2/2/2
3	HEM	A	500	1	-	0/6/54/54	-
3	HEM	B	500	2	-	0/6/54/54	-
4	H4B	B	600	-	-	0/8/17/17	0/2/2/2
7	GOL	A	880	-	-	0/4/4/4	-
5	71S	A	800	-	-	5/15/15/15	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	H4B	C4-C4A	-3.05	1.37	1.41
5	B	800	71S	C08-C09	-2.75	1.34	1.53
5	A	800	71S	C08-C09	-2.65	1.35	1.53
4	A	600	H4B	C7-C6	2.42	1.54	1.52
5	B	800	71S	C16-C15	2.37	1.42	1.39
3	A	500	HEM	C4D-C3D	2.28	1.47	1.42
5	A	800	71S	C16-C15	2.24	1.42	1.39
4	B	600	H4B	C7-C6	2.15	1.54	1.52
3	B	500	HEM	C4D-C3D	2.12	1.47	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	800	71S	C02-N01-C06	6.57	123.08	118.10
3	B	500	HEM	CBA-CAA-C2A	-5.75	101.89	112.49
5	A	800	71S	C02-N01-C06	5.70	122.42	118.10
5	A	800	71S	C09-C08-C06	5.33	124.94	112.99
5	B	800	71S	C09-C08-C06	5.02	124.25	112.99
5	B	800	71S	C05-C06-N01	-4.88	117.73	122.90
4	A	600	H4B	C4-N3-C2	4.74	123.47	115.93
4	A	600	H4B	C4-C4A-C8A	4.53	118.60	114.57
5	A	800	71S	C16-C15-C14	4.42	120.39	117.44
4	A	600	H4B	C4-C4A-N5	4.11	122.57	119.12
3	B	500	HEM	C1D-C2D-C3D	-4.05	104.18	107.00
5	A	800	71S	C09-C11-C12	-3.98	115.42	121.83
4	A	600	H4B	N3-C2-N1	-3.93	119.26	125.42
4	B	600	H4B	C4-C4A-C8A	3.89	118.02	114.57
5	B	800	71S	C22-N21-C26	3.82	120.99	118.10
5	B	800	71S	C09-C11-C12	-3.81	115.69	121.83
5	A	800	71S	C05-C06-N01	-3.80	118.87	122.90
5	B	800	71S	C08-C06-N01	3.75	121.54	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	HEM	CBA-CAA-C2A	-3.68	105.70	112.49
3	B	500	HEM	CBD-CAD-C3D	-3.34	106.31	112.48
5	A	800	71S	C22-N21-C26	3.13	120.47	118.10
5	B	800	71S	C09-C11-C16	3.00	125.47	120.54
5	A	800	71S	C15-C16-C11	-2.90	116.92	120.94
4	B	600	H4B	C4-N3-C2	2.82	120.42	115.93
5	A	800	71S	C09-C11-C16	2.82	125.17	120.54
5	A	800	71S	C14-C15-C29	-2.82	114.96	121.38
4	B	600	H4B	N3-C2-N1	-2.82	121.00	125.42
5	A	800	71S	C16-C11-C12	2.80	119.41	116.71
5	B	800	71S	C24-C25-C26	-2.78	118.50	120.32
4	A	600	H4B	N2-C2-N3	2.67	121.40	117.25
4	B	600	H4B	C4-C4A-N5	2.63	121.33	119.12
3	A	500	HEM	CAA-CBA-CGA	2.54	116.94	112.67
4	A	600	H4B	C2-N1-C8A	2.51	120.16	114.54
5	A	800	71S	C12-N11-C14	2.43	120.80	117.48
4	A	600	H4B	C4A-C4-N3	-2.37	117.29	124.01
3	A	500	HEM	C3B-C4B-NB	-2.37	106.15	109.21
4	B	600	H4B	C2-N1-C8A	2.33	119.75	114.54
5	B	800	71S	C16-C15-C14	2.32	118.99	117.44
5	B	800	71S	C14-C15-C29	-2.30	116.14	121.38
3	B	500	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
3	A	500	HEM	CBD-CAD-C3D	-2.29	108.26	112.48
5	A	800	71S	C24-C25-C26	-2.28	118.83	120.32
5	B	800	71S	C05-C04-C03	2.24	120.77	118.09
5	B	800	71S	C16-C11-C12	2.17	118.81	116.71
5	A	800	71S	C15-C14-N11	-2.14	120.77	124.14
5	B	800	71S	C16-C15-C29	2.14	124.87	120.73
3	B	500	HEM	CMD-C2D-C3D	2.12	128.94	124.94
5	B	800	71S	C12-N11-C14	2.12	120.37	117.48
5	A	800	71S	C08-C06-N01	2.11	119.10	115.95
5	A	800	71S	C16-C15-C29	2.03	124.65	120.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	800	71S	C26-C28-C29-C15
5	B	800	71S	C26-C28-C29-C18
5	A	800	71S	C26-C28-C29-C15
5	A	800	71S	C26-C28-C29-C18
5	A	800	71S	N18-C18-C29-C15

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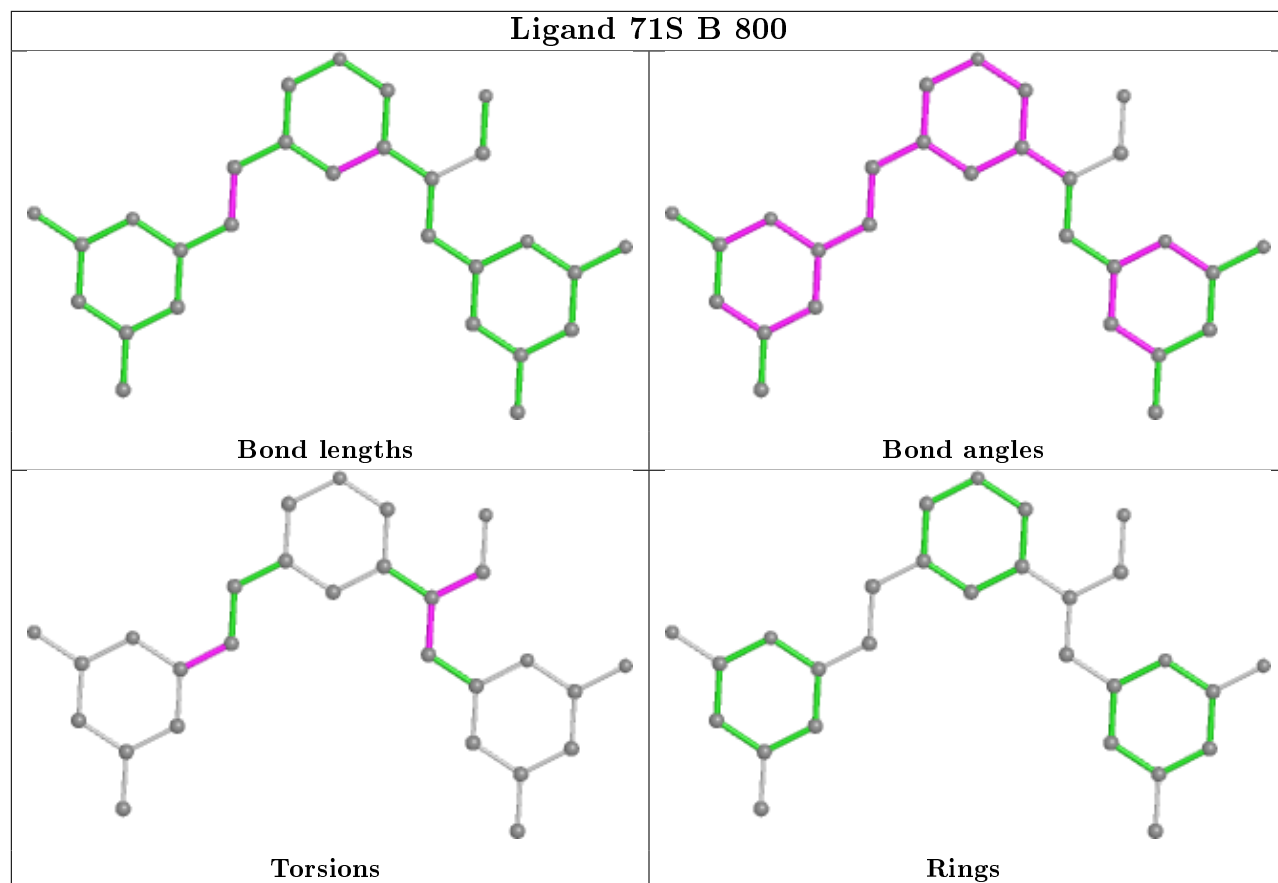
Mol	Chain	Res	Type	Atoms
5	A	800	71S	N01-C06-C08-C09
5	A	800	71S	C05-C06-C08-C09
5	B	800	71S	N18-C18-C29-C15
5	B	800	71S	N01-C06-C08-C09
5	B	800	71S	C05-C06-C08-C09

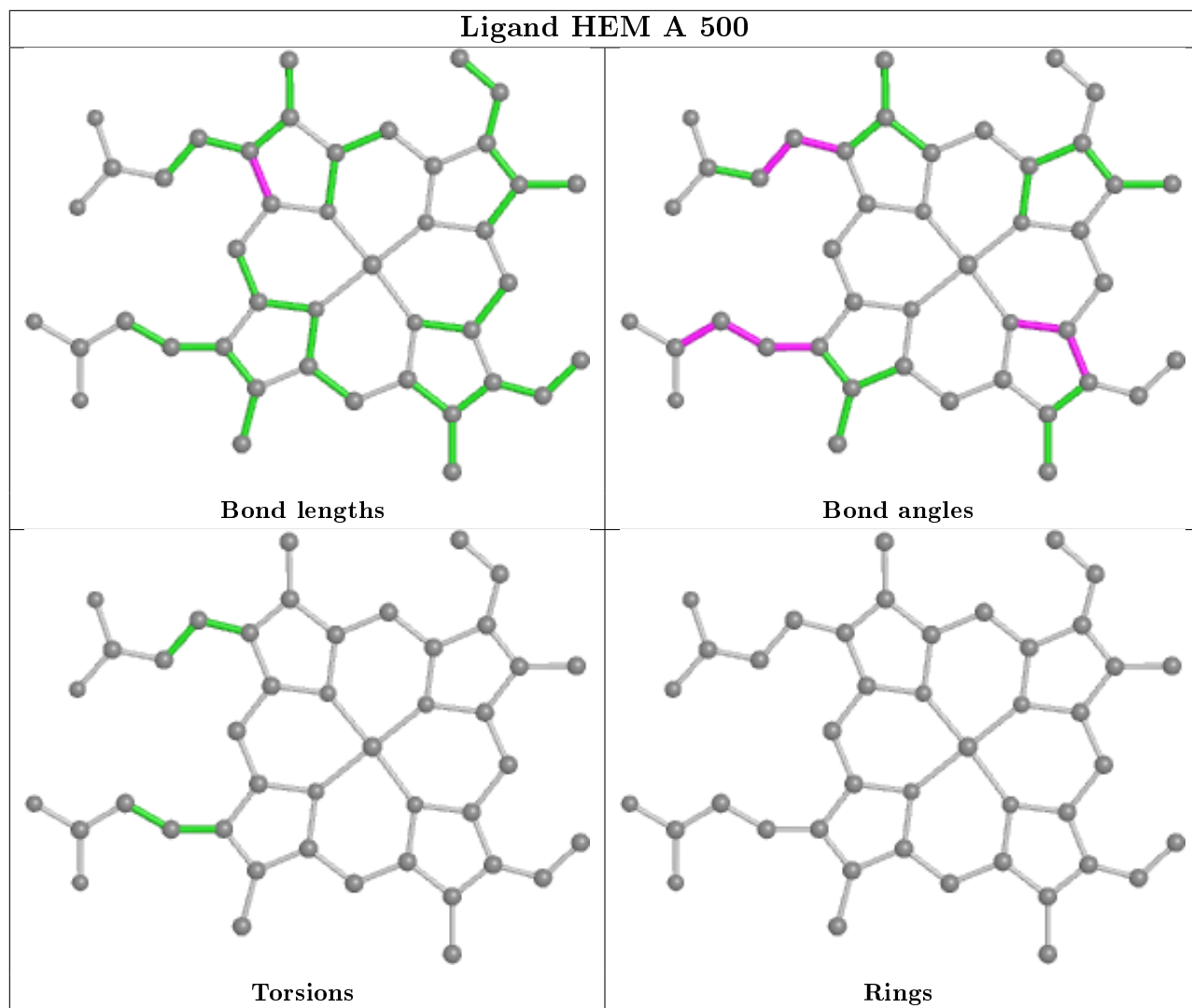
There are no ring outliers.

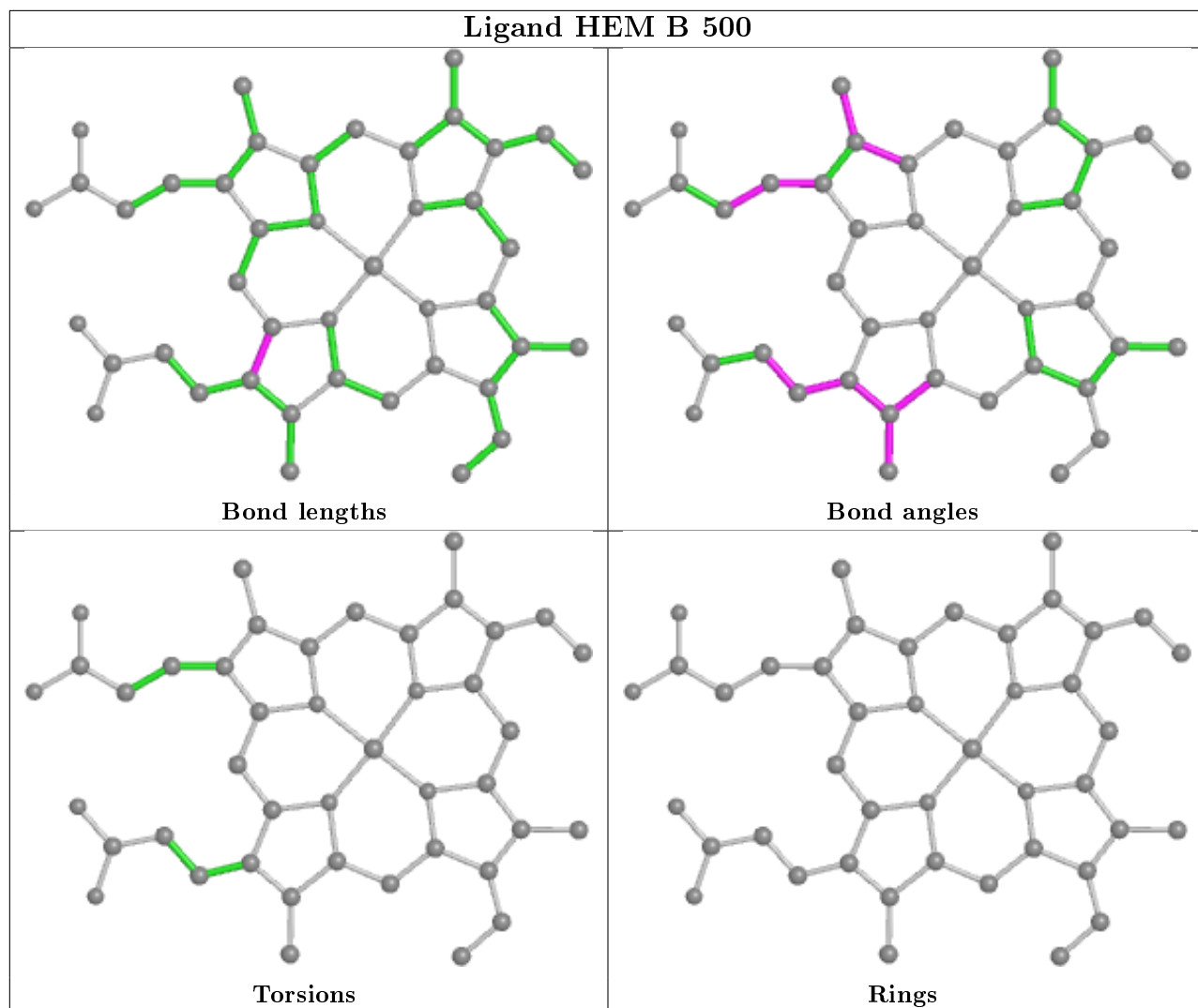
7 monomers are involved in 22 short contacts:

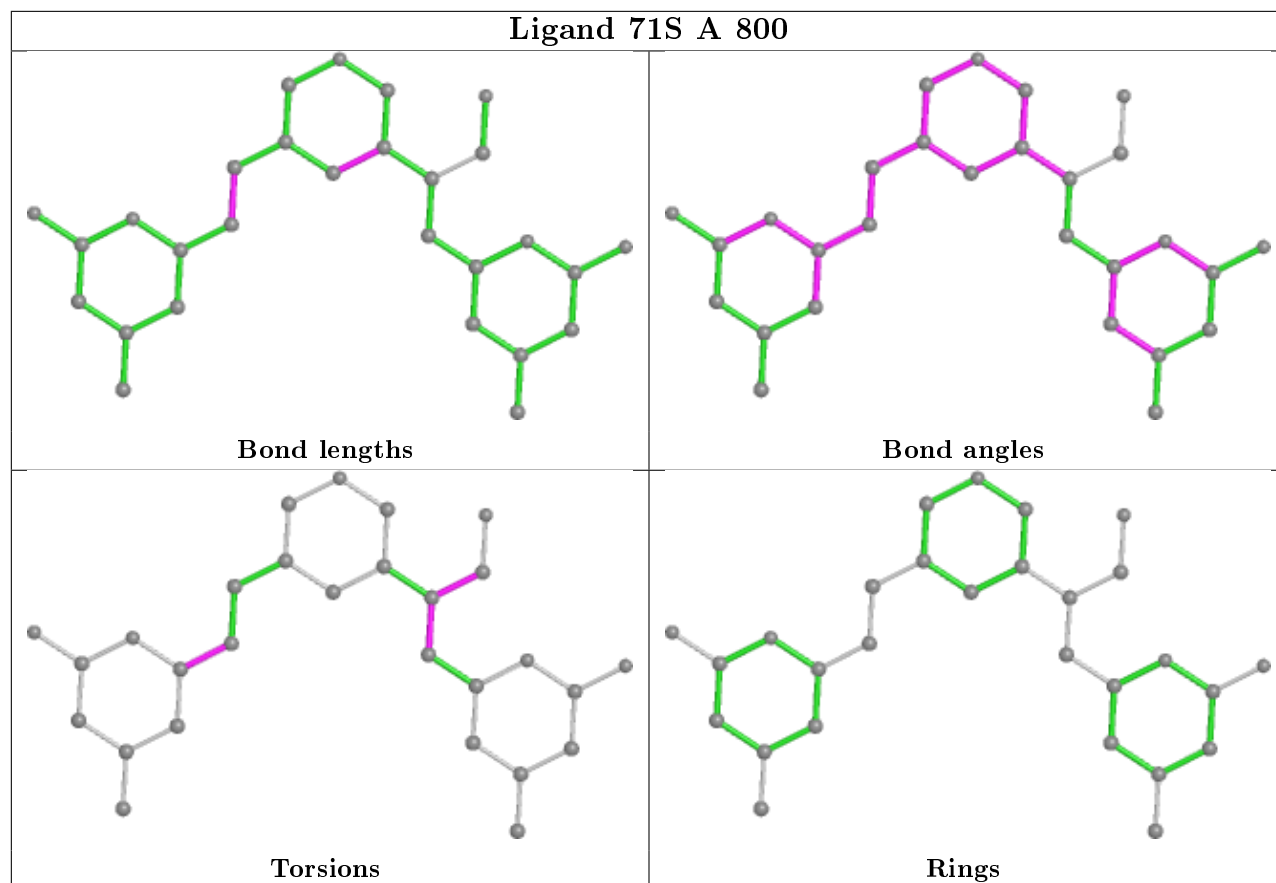
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	800	71S	6	0
4	A	600	H4B	2	0
3	A	500	HEM	6	0
3	B	500	HEM	4	0
4	B	600	H4B	1	0
7	A	880	GOL	1	0
5	A	800	71S	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.54	29 (7%) 15 17	27, 40, 69, 91	0
2	B	404/443 (91%)	0.39	22 (5%) 25 29	27, 45, 74, 110	0
All	All	808/886 (91%)	0.46	51 (6%) 20 22	27, 43, 72, 110	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	259	GLN	7.7
1	A	123	GLU	5.1
1	A	122	ALA	4.8
1	A	160	ALA	4.3
2	B	260	ASP	4.3
2	B	110	LYS	4.2
1	A	259	GLN	4.0
1	A	121	PRO	4.0
1	A	153	GLN	3.7
1	A	450	ILE	3.6
1	A	126	LEU	3.5
2	B	257	ARG	3.5
2	B	263	VAL	3.3
2	B	146	GLN	3.2
2	B	261	GLY	3.1
1	A	448	ALA	3.1
1	A	69	LYS	2.9
2	B	447	TRP	2.9
1	A	109	ARG	2.9
1	A	449	TRP	2.8
1	A	257	ARG	2.7
1	A	155	VAL	2.7
2	B	449	TRP	2.7
2	B	223	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	447	TRP	2.7
2	B	448	ALA	2.6
2	B	270	VAL	2.5
2	B	306	VAL	2.5
2	B	258	GLN	2.5
1	A	461	VAL	2.5
2	B	276	CYS	2.5
2	B	323	GLU	2.5
1	A	91	GLN	2.4
1	A	125	LEU	2.4
1	A	451	VAL	2.4
1	A	239	GLY	2.4
1	A	281	TRP	2.3
2	B	311	LEU	2.3
1	A	157	ALA	2.3
1	A	445	ALA	2.3
2	B	318	GLU	2.3
2	B	277	ILE	2.3
1	A	186	CYS	2.3
1	A	278	GLN	2.2
1	A	390	ARG	2.2
2	B	304	LEU	2.1
2	B	451	VAL	2.1
1	A	146	GLN	2.1
1	A	260	ASP	2.0
2	B	142	ARG	2.0
1	A	156	GLU	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	0.93	0.12	40,42,82,108	0

## 6.3 Carbohydrates [i](#)

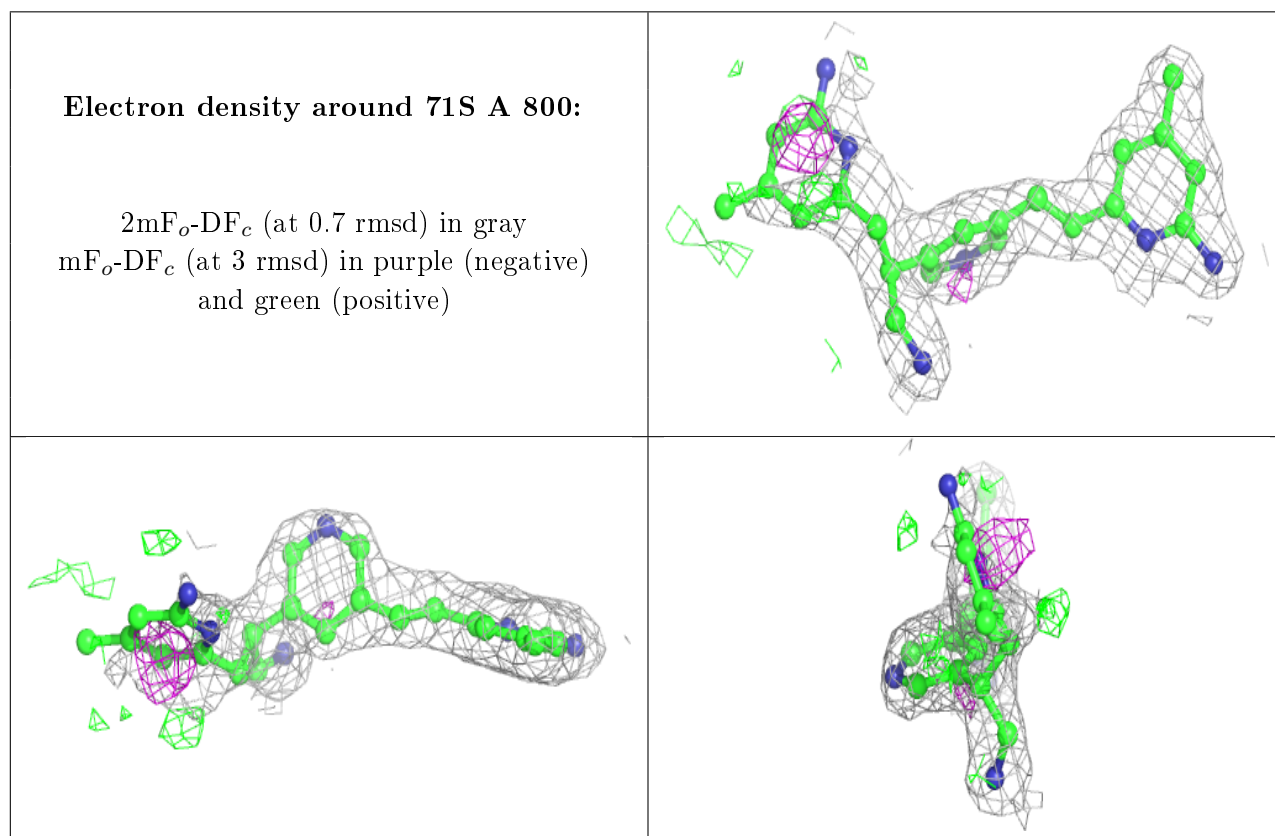
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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.

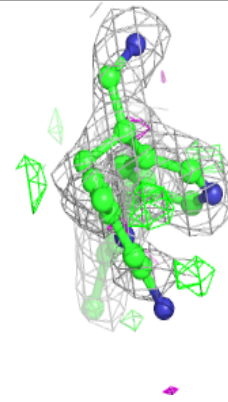
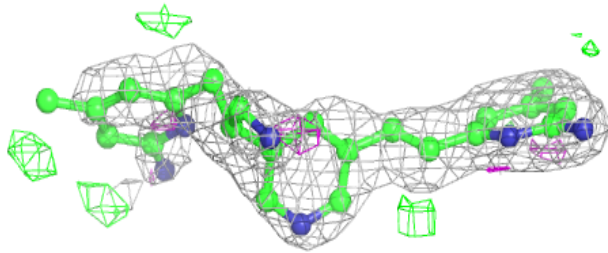
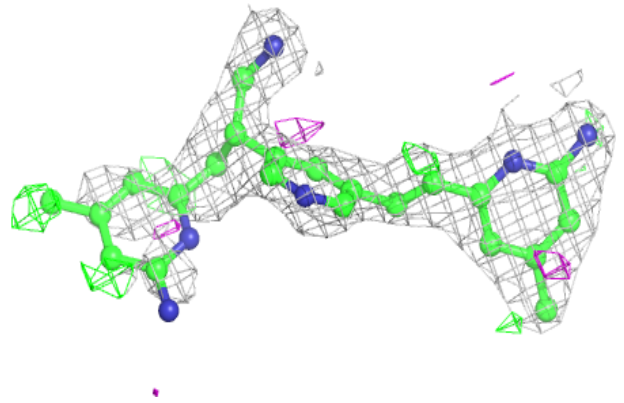
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	B	880	6/6	0.84	0.19	51,54,57,58	0
7	GOL	A	880	6/6	0.90	0.21	50,56,59,69	0
5	71S	A	800	28/28	0.92	0.19	31,56,106,112	0
5	71S	B	800	28/28	0.93	0.16	35,58,94,98	0
6	ACT	B	860	4/4	0.95	0.33	53,59,60,62	0
6	ACT	A	860	4/4	0.95	0.12	48,53,54,57	0
3	HEM	B	500	43/43	0.98	0.13	29,33,40,43	0
4	H4B	B	600	17/17	0.98	0.17	25,29,32,34	0
4	H4B	A	600	17/17	0.98	0.17	28,31,35,35	0
3	HEM	A	500	43/43	0.98	0.17	25,28,39,43	0
8	ZN	B	900	1/1	0.99	0.09	37,37,37,37	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.



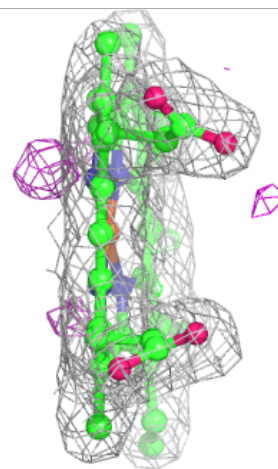
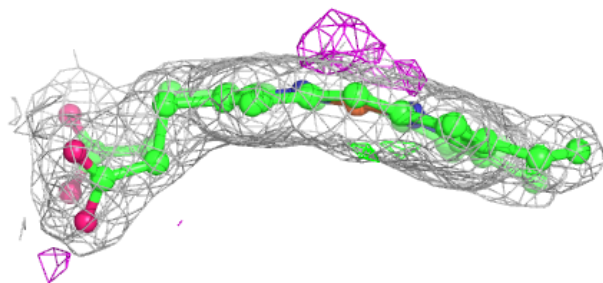
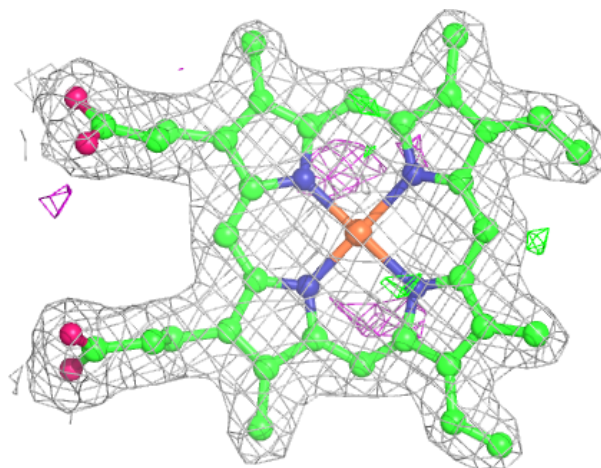
**Electron density around 71S B 800:**

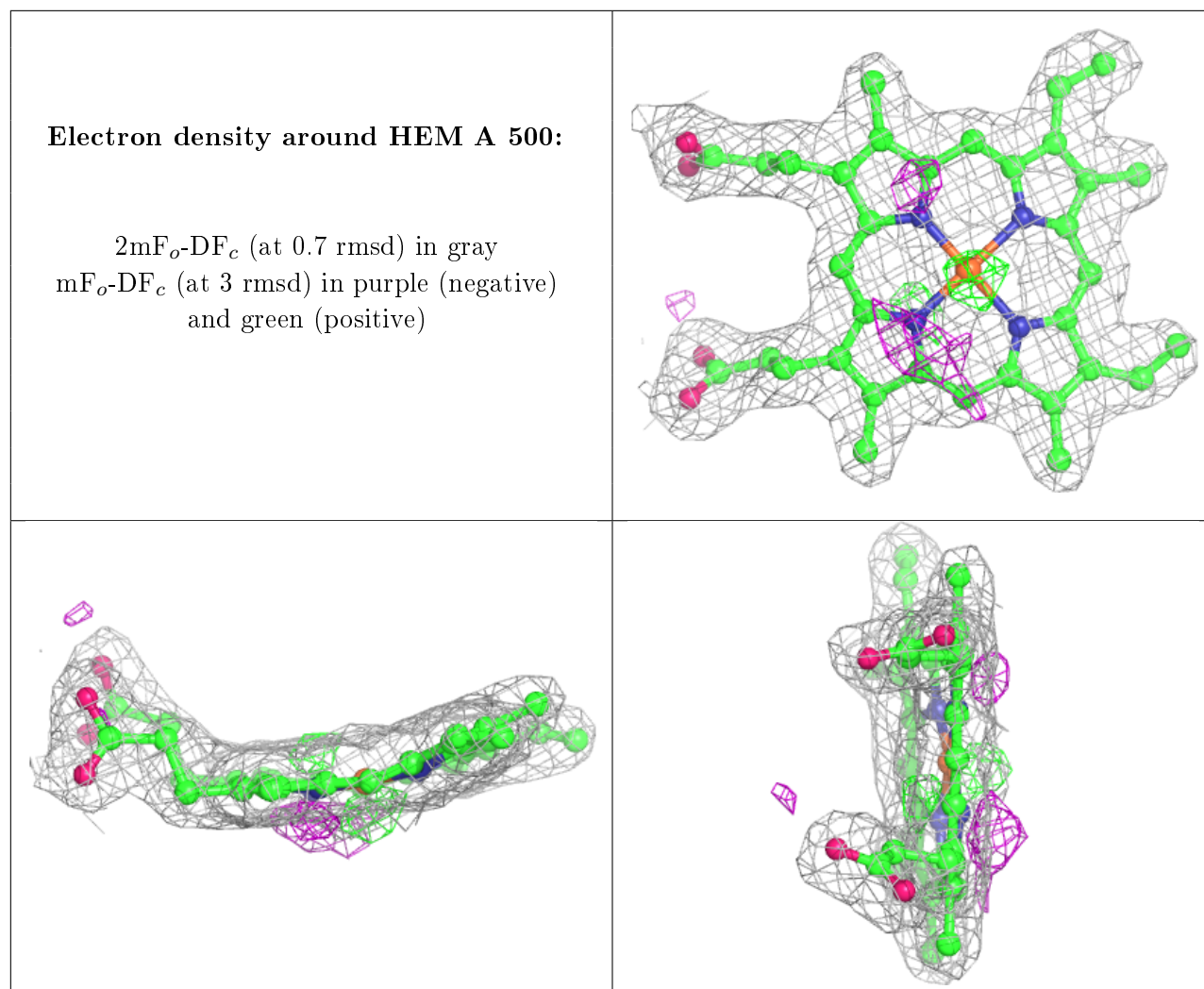
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM B 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.