



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2024 – 11:15 AM EST

PDB ID : 2HX2  
Title : Bovine eNOS heme domain complexed with (4S)-N-{4-Amino-5-[(2-aminoethyl)-hydroxyamino]-pentyl}-N'-nitroguanidine  
Authors : Igarashi, J.; Li, H.; Poulos, T.L.  
Deposited on : 2006-08-02  
Resolution : 1.95 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

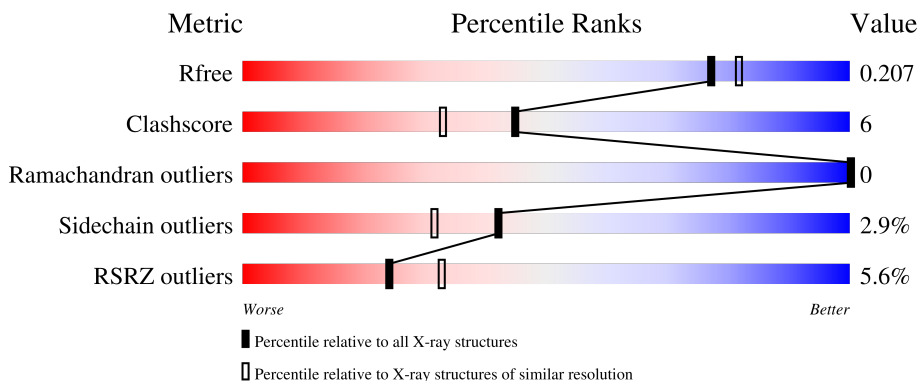
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

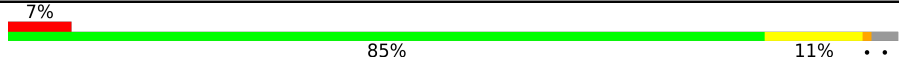
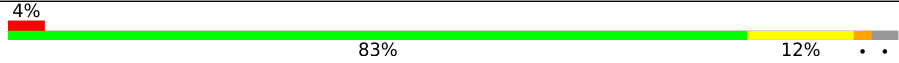
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	416	 7% 85% 11% ..
1	B	416	 4% 83% 12% ..

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7132 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.

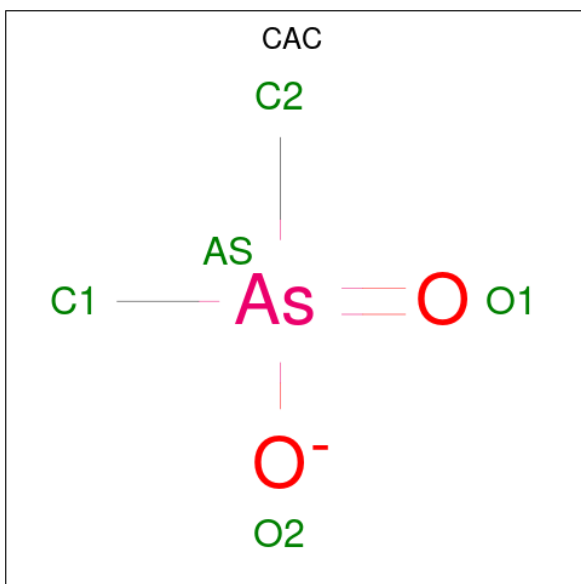
- Molecule 1 is a protein called Nitric-oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	3202	2036	563	587	16	0	0	0
1	B	402	3202	2035	565	586	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



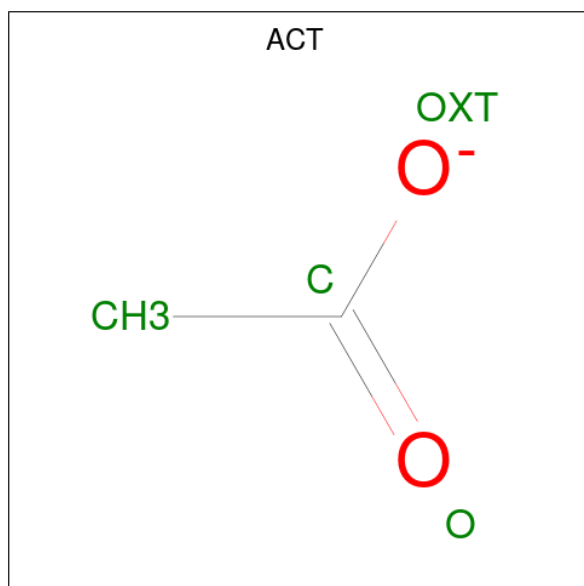
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	As C		
2	A	1	3	1 2	0	0

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

- Molecule 3 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
			Total	C	O		
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

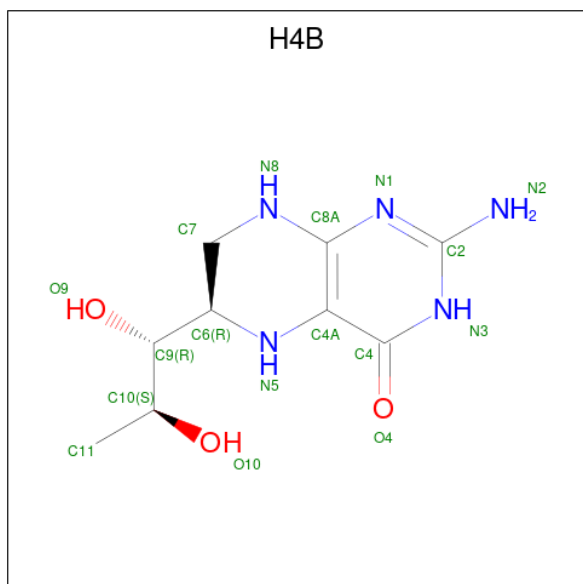
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

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



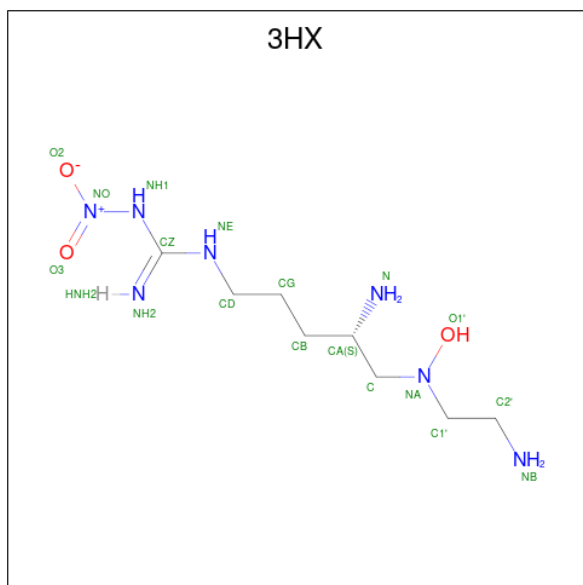
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
6	A	1	Total	9	5	3	0	0

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

- Molecule 7 is (4S)-N-{4-AMINO-5-[(2-AMINOETHYL)(HYDROXYAMINO)]-PENTYL}-N'-NITROGUANIDINE (three-letter code: 3HX) (formula: C<sub>8</sub>H<sub>21</sub>N<sub>7</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	18	8	7	3	0	0
7	B	1	18	8	7	3	0	0

- Molecule 8 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
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0

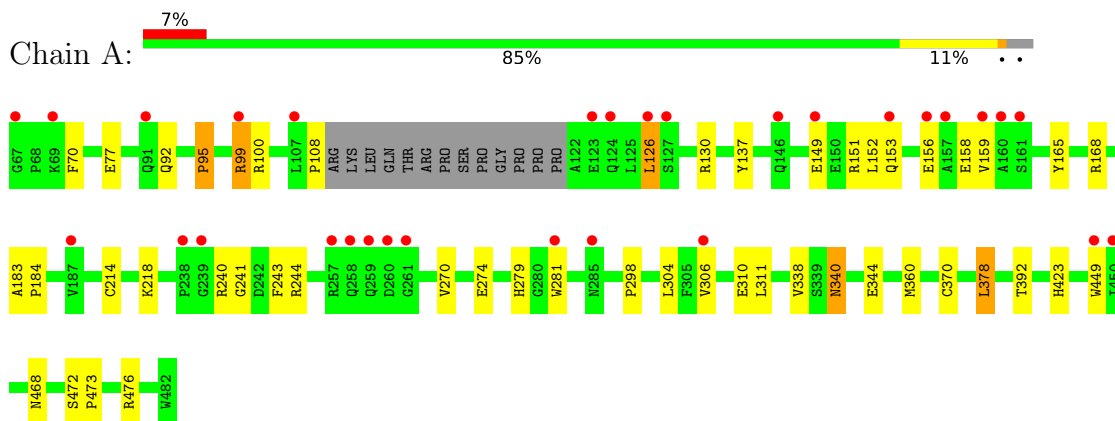
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	269	Total O 269 269	0	0
9	B	268	Total O 268 268	0	0

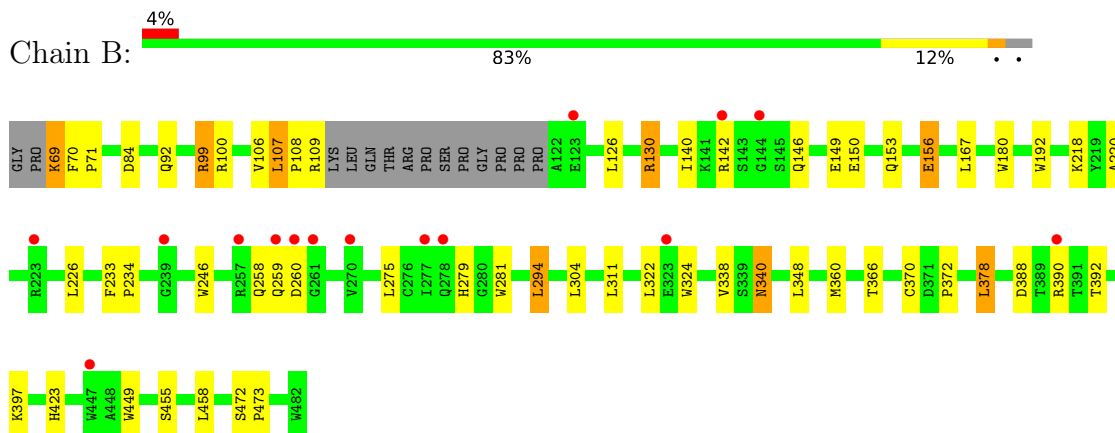
### 3 Residue-property plots [i](#)

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



- Molecule 1: Nitric-oxide synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.82Å 106.85Å 156.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 1.95 48.36 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.36-1.95) 98.3 (48.36-1.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 1.95Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.180 , 0.213 0.175 , 0.207	Depositor DCC
$R_{free}$ test set	3472 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: ZN, GOL, 3HX, H4B, ACT, CAC, 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	0.42	0/3291	0.65	1/4483 (0.0%)
1	B	0.42	0/3290	0.67	1/4480 (0.0%)
All	All	0.42	0/6581	0.66	2/8963 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	360	MET	N-CA-C	-5.79	95.37	111.00
1	A	360	MET	N-CA-C	-5.27	96.77	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain

### 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	3202	0	3106	41	0
1	B	3202	0	3109	44	0
2	A	3	0	0	0	0
2	B	3	0	0	1	0
3	A	8	0	6	0	0
3	B	8	0	6	0	0
4	A	1	0	0	0	0
5	A	43	0	30	1	0
5	B	43	0	30	1	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	18	0	21	4	0
7	B	18	0	21	3	0
8	A	6	0	8	1	0
8	B	6	0	8	0	0
9	A	269	0	0	6	0
9	B	268	0	0	2	0
All	All	7132	0	6375	84	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 (84) 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:126:LEU:HD11	1:A:156:GLU:HG2	1.49	0.93
1:A:92:GLN:HE22	1:A:476:ARG:HH22	0.97	0.90
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.57	0.85
1:A:92:GLN:NE2	1:A:476:ARG:HH22	1.76	0.83
1:B:130:ARG:HH11	1:B:130:ARG:HB3	1.42	0.82
1:B:69:LYS:HD2	1:B:70:PHE:H	1.48	0.78
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.49	0.77
1:B:338:VAL:HG22	7:B:793:3HX:H1	1.66	0.75
1:A:243:PHE:O	1:A:244:ARG:HG2	1.87	0.75
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.49	0.74
1:B:106:VAL:HG12	1:B:107:LEU:HD13	1.72	0.71
1:A:149:GLU:O	1:A:153:GLN:HG2	1.93	0.69
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.24	0.67
1:B:388:ASP:OD1	1:B:390:ARG:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.10	0.66
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.36	0.65
1:B:126:LEU:O	1:B:130:ARG:HG3	1.96	0.65
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.78	0.64
1:A:99:ARG:HB2	1:A:99:ARG:NH1	2.13	0.63
8:A:880:GOL:H2	9:A:906:HOH:O	1.98	0.62
1:B:126:LEU:HD21	1:B:156:GLU:OE2	2.00	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.43	0.59
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.85	0.59
1:A:152:LEU:O	1:A:156:GLU:HG3	2.05	0.56
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.86	0.56
1:B:338:VAL:CG2	7:B:793:3HX:H1	2.35	0.56
1:A:270:VAL:O	1:A:274:GLU:HG3	2.06	0.55
1:B:69:LYS:HD2	1:B:70:PHE:N	2.21	0.54
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.89	0.54
5:B:700:HEM:O2D	7:B:793:3HX:H1'2	2.08	0.54
1:A:126:LEU:HD12	1:A:130:ARG:CZ	2.39	0.53
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.91	0.52
1:B:146:GLN:O	1:B:150:GLU:HG3	2.10	0.52
1:A:240:ARG:HD2	1:A:241:GLY:O	2.09	0.52
1:B:149:GLU:O	1:B:153:GLN:HG3	2.10	0.51
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.92	0.51
1:B:246:TRP:HB2	1:B:294:LEU:HB3	1.93	0.51
1:B:340:ASN:HD22	1:B:340:ASN:H	1.58	0.50
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.95	0.49
5:A:700:HEM:O2D	7:A:793:3HX:H2	2.12	0.49
1:A:214:CYS:SG	9:A:1168:HOH:O	2.60	0.49
1:A:340:ASN:HD21	7:A:793:3HX:H2'1	1.78	0.49
1:A:240:ARG:NH2	9:A:1071:HOH:O	2.42	0.49
1:A:378:LEU:HB2	9:A:905:HOH:O	2.13	0.49
1:A:151:ARG:HD3	1:A:168:ARG:CZ	2.43	0.49
1:A:338:VAL:CG2	7:A:793:3HX:H1	2.43	0.49
1:B:69:LYS:HD2	1:B:69:LYS:N	2.28	0.48
1:A:310:GLU:HG2	9:A:1159:HOH:O	2.13	0.48
1:A:449:TRP:HA	6:A:760:H4B:N1	2.28	0.48
1:B:259:GLN:H	1:B:259:GLN:CD	2.17	0.48
1:B:449:TRP:HA	6:B:760:H4B:N1	2.29	0.47
1:B:378:LEU:HB2	9:B:1076:HOH:O	2.15	0.47
1:A:423:HIS:HB2	1:B:392:THR:HB	1.96	0.46
1:A:99:ARG:CZ	1:A:99:ARG:HA	2.46	0.45
1:A:70:PHE:O	1:B:109:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:HG22	7:A:793:3HX:H1	1.99	0.45
1:A:218:LYS:HE2	1:A:311:LEU:HD21	1.98	0.44
1:B:340:ASN:HD22	1:B:340:ASN:N	2.13	0.44
1:A:158:GLU:HG2	1:A:165:TYR:HA	2.00	0.43
1:A:279:HIS:HE1	9:A:1092:HOH:O	2.00	0.43
1:B:218:LYS:HE3	1:B:311:LEU:HD11	2.00	0.43
1:B:366:THR:O	1:B:370:CYS:HB2	2.19	0.43
1:A:126:LEU:HD23	1:A:159:VAL:HG11	2.01	0.43
1:A:99:ARG:NH1	1:A:99:ARG:CB	2.80	0.43
1:B:472:SER:HA	1:B:473:PRO:C	2.39	0.43
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.49	0.43
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.54	0.42
1:A:472:SER:HA	1:A:473:PRO:C	2.39	0.42
1:B:340:ASN:H	1:B:340:ASN:ND2	2.17	0.42
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.01	0.42
1:A:126:LEU:HD12	1:A:130:ARG:NH1	2.34	0.41
1:B:108:PRO:HA	9:B:1019:HOH:O	2.20	0.41
1:A:126:LEU:HD21	1:A:156:GLU:HA	2.02	0.41
1:A:344:GLU:OE1	1:A:476:ARG:NH2	2.53	0.41
1:B:259:GLN:NE2	1:B:260:ASP:OD1	2.54	0.41
1:B:130:ARG:HH11	1:B:130:ARG:CB	2.21	0.41
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.96	0.41
1:A:392:THR:HB	1:B:423:HIS:HB2	2.03	0.41
1:B:455:SER:HB3	1:B:458:LEU:HD12	2.01	0.41
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.56	0.41
1:B:99:ARG:HH11	1:B:99:ARG:CB	2.26	0.40
1:B:220:ALA:O	1:B:226:LEU:HA	2.22	0.40
1:B:324:TRP:HB2	2:B:850:CAC:C2	2.52	0.40
1:B:275:LEU:O	1:B:279:HIS:HD2	2.04	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	399/416 (96%)	392 (98%)	7 (2%)	0	100	100
1	B	398/416 (96%)	382 (96%)	16 (4%)	0	100	100
All	All	797/832 (96%)	774 (97%)	23 (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	342/354 (97%)	334 (98%)	8 (2%)	50	42
1	B	342/354 (97%)	330 (96%)	12 (4%)	36	24
All	All	684/708 (97%)	664 (97%)	20 (3%)	42	31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	PRO
1	A	99	ARG
1	A	100	ARG
1	A	126	LEU
1	A	306	VAL
1	A	340	ASN
1	A	378	LEU
1	A	468	ASN
1	B	69	LYS
1	B	92	GLN
1	B	99	ARG
1	B	100	ARG
1	B	107	LEU
1	B	130	ARG
1	B	156	GLU
1	B	258	GLN
1	B	294	LEU
1	B	340	ASN

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Mol	Chain	Res	Type
1	B	378	LEU
1	B	397	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	92	GLN
1	A	191	GLN
1	A	278	GLN
1	A	279	HIS
1	A	340	ASN
1	A	413	GLN
1	A	468	ASN
1	B	89	GLN
1	B	191	GLN
1	B	279	HIS
1	B	340	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	H4B	A	760	-	16,18,18	2.28	6 (37%)	11,26,26	4.14	7 (63%)
3	ACT	B	860	-	3,3,3	0.93	0	3,3,3	0.70	0
3	ACT	A	860	-	3,3,3	0.89	0	3,3,3	0.79	0
3	ACT	B	861	-	3,3,3	0.85	0	3,3,3	0.81	0
2	CAC	B	850	1	0,2,4	-	-	0,1,6	-	-
7	3HX	A	793	-	11,17,17	1.89	4 (36%)	11,20,20	0.95	0
5	HEM	A	700	1	41,50,50	1.21	4 (9%)	45,82,82	1.25	5 (11%)
7	3HX	B	793	-	11,17,17	2.08	4 (36%)	11,20,20	1.12	0
8	GOL	B	880	-	5,5,5	0.18	0	5,5,5	0.21	0
8	GOL	A	880	-	5,5,5	0.21	0	5,5,5	0.18	0
5	HEM	B	700	1	41,50,50	1.29	5 (12%)	45,82,82	1.52	5 (11%)
6	H4B	B	760	-	16,18,18	2.22	5 (31%)	11,26,26	4.26	8 (72%)
2	CAC	A	850	1	0,2,4	-	-	0,1,6	-	-
3	ACT	A	861	-	3,3,3	0.90	0	3,3,3	0.97	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2
7	3HX	A	793	-	-	5/14/18/18	-
5	HEM	A	700	1	-	0/12/54/54	-
7	3HX	B	793	-	-	9/14/18/18	-
8	GOL	B	880	-	-	2/4/4/4	-
8	GOL	A	880	-	-	0/4/4/4	-
5	HEM	B	700	1	-	0/12/54/54	-
6	H4B	B	760	-	-	0/8/17/17	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	760	H4B	C4-N3	5.42	1.42	1.33
6	B	760	H4B	C4-N3	5.15	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	760	H4B	C4A-N5	4.60	1.47	1.38
6	A	760	H4B	C6-N5	4.23	1.54	1.45
6	A	760	H4B	C4A-N5	4.23	1.46	1.38
6	B	760	H4B	C6-N5	4.10	1.54	1.45
7	B	793	3HX	CB-CA	4.06	1.59	1.53
7	A	793	3HX	CB-CA	3.20	1.57	1.53
5	A	700	HEM	C3C-CAC	-3.01	1.41	1.47
5	B	700	HEM	CHB-C1B	2.87	1.42	1.35
7	A	793	3HX	CZ-NH2	2.86	1.37	1.29
7	B	793	3HX	CD-NE	2.76	1.52	1.46
7	B	793	3HX	CZ-NH2	2.76	1.37	1.29
7	A	793	3HX	CD-NE	2.75	1.52	1.46
7	B	793	3HX	O1'-NA	-2.58	1.40	1.45
5	B	700	HEM	C1B-NB	-2.45	1.36	1.40
5	A	700	HEM	CAB-C3B	-2.41	1.40	1.47
5	A	700	HEM	C4A-NA	2.32	1.40	1.36
6	A	760	H4B	C7-N8	2.22	1.48	1.44
5	A	700	HEM	CAA-C2A	2.17	1.55	1.52
7	A	793	3HX	O1'-NA	-2.16	1.41	1.45
6	B	760	H4B	C8A-N1	2.16	1.38	1.34
6	A	760	H4B	C8A-N1	2.15	1.38	1.34
5	B	700	HEM	C4A-NA	2.13	1.40	1.36
5	B	700	HEM	C3C-C2C	-2.12	1.37	1.40
6	A	760	H4B	C7-C6	2.11	1.54	1.52
6	B	760	H4B	C7-N8	2.05	1.48	1.44
5	B	700	HEM	C3C-CAC	-2.05	1.43	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	760	H4B	C8A-C4A-C4	9.29	122.82	114.57
6	A	760	H4B	C8A-C4A-C4	8.62	122.23	114.57
5	B	700	HEM	CBA-CAA-C2A	-6.04	102.31	112.62
6	A	760	H4B	C2-N3-C4	5.81	125.17	115.93
6	B	760	H4B	C2-N3-C4	5.76	125.08	115.93
6	A	760	H4B	N1-C2-N3	-4.89	117.75	125.42
6	B	760	H4B	N1-C2-N3	-4.67	118.10	125.42
5	A	700	HEM	CBA-CAA-C2A	-4.18	105.49	112.62
5	B	700	HEM	C2C-C3C-C4C	-3.69	104.32	106.90
6	A	760	H4B	C2-N1-C8A	3.67	122.76	114.54
6	A	760	H4B	C4A-C4-N3	-3.67	113.59	124.01
6	B	760	H4B	C4A-C4-N3	-3.64	113.65	124.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	H4B	N2-C2-N1	3.42	122.57	117.25
6	B	760	H4B	N2-C2-N1	3.42	122.57	117.25
6	B	760	H4B	C2-N1-C8A	3.35	122.05	114.54
6	B	760	H4B	C4A-N5-C6	-3.21	112.44	121.16
6	A	760	H4B	C4A-N5-C6	-3.19	112.48	121.16
5	B	700	HEM	C4B-CHC-C1C	3.19	126.76	122.56
6	B	760	H4B	C4-C4A-N5	-3.06	116.56	119.12
5	A	700	HEM	C4B-CHC-C1C	2.42	125.76	122.56
5	B	700	HEM	C4B-C3B-C2B	-2.27	105.31	107.11
5	A	700	HEM	C4A-C3A-C2A	-2.25	105.43	107.00
5	A	700	HEM	C2C-C3C-C4C	-2.21	105.35	106.90
5	B	700	HEM	C3B-C2B-C1B	2.14	108.07	106.49
5	A	700	HEM	C4C-CHD-C1D	2.13	125.37	122.56

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	793	3HX	N-CA-CB-CG
7	A	793	3HX	C2'-C1'-NA-O1'
7	A	793	3HX	NA-C1'-C2'-NB
7	B	793	3HX	CZ-NH1-NO-O3
7	B	793	3HX	NA-C-CA-N
7	B	793	3HX	CA-CB-CG-CD
7	B	793	3HX	C2'-C1'-NA-O1'
7	B	793	3HX	NA-C1'-C2'-NB
7	B	793	3HX	NE-CD-CG-CB
8	B	880	GOL	O1-C1-C2-C3
7	A	793	3HX	C-CA-CB-CG
8	B	880	GOL	O1-C1-C2-O2
7	B	793	3HX	NA-C-CA-CB
7	A	793	3HX	CA-C-NA-C1'
7	B	793	3HX	CA-C-NA-C1'
7	B	793	3HX	CG-CD-NE-CZ

There are no ring outliers.

8 monomers are involved in 11 short contacts:

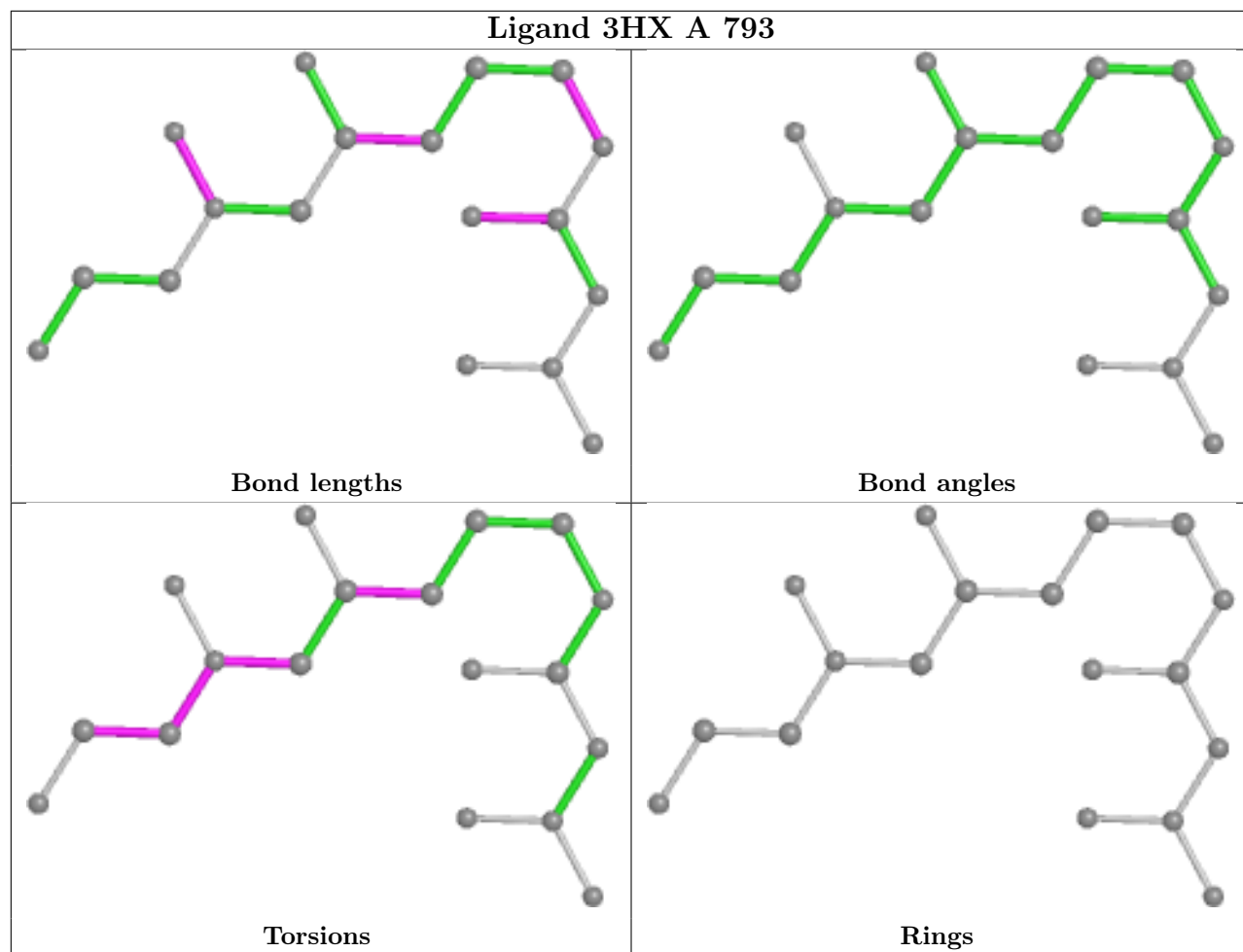
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	760	H4B	1	0
2	B	850	CAC	1	0

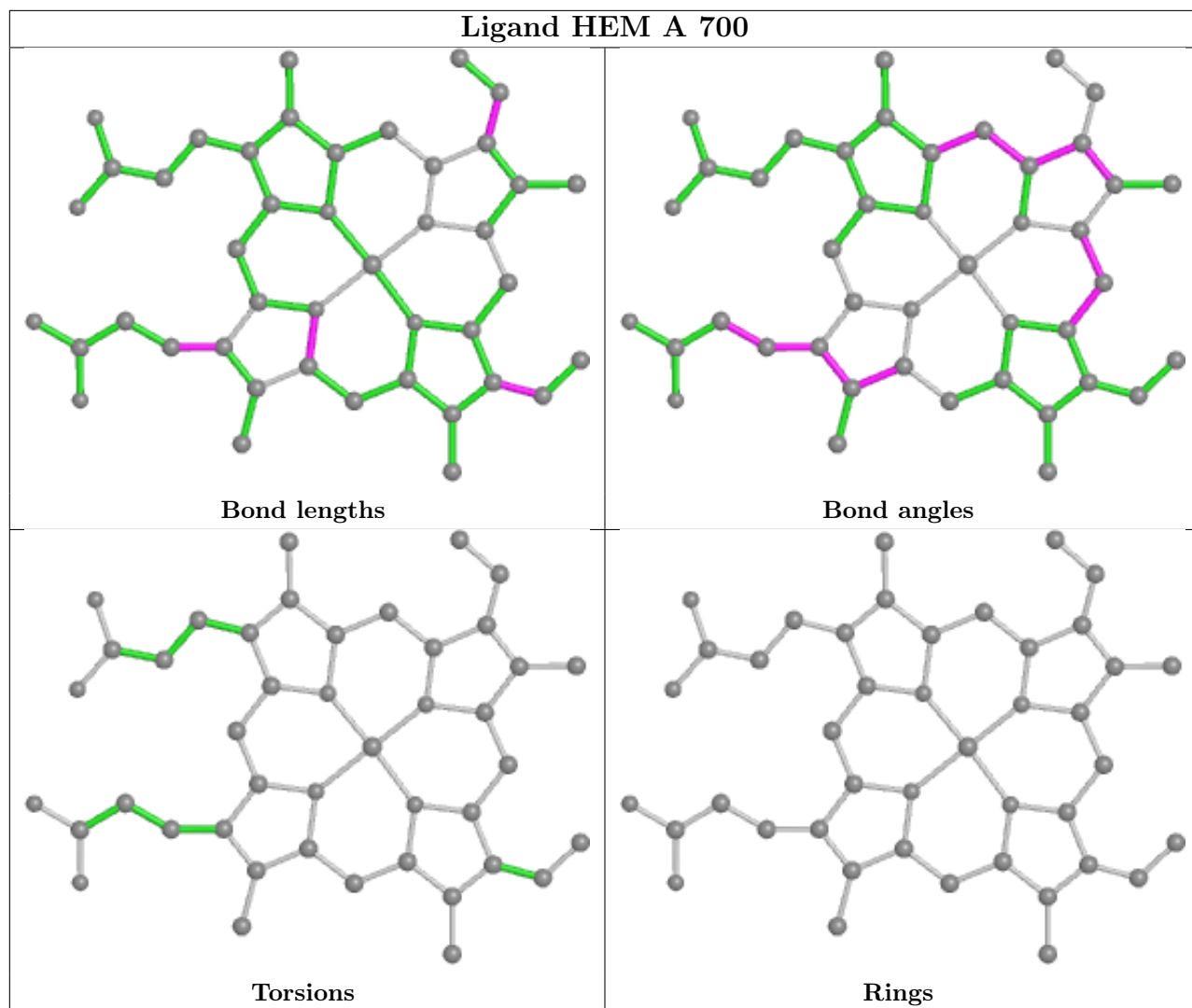
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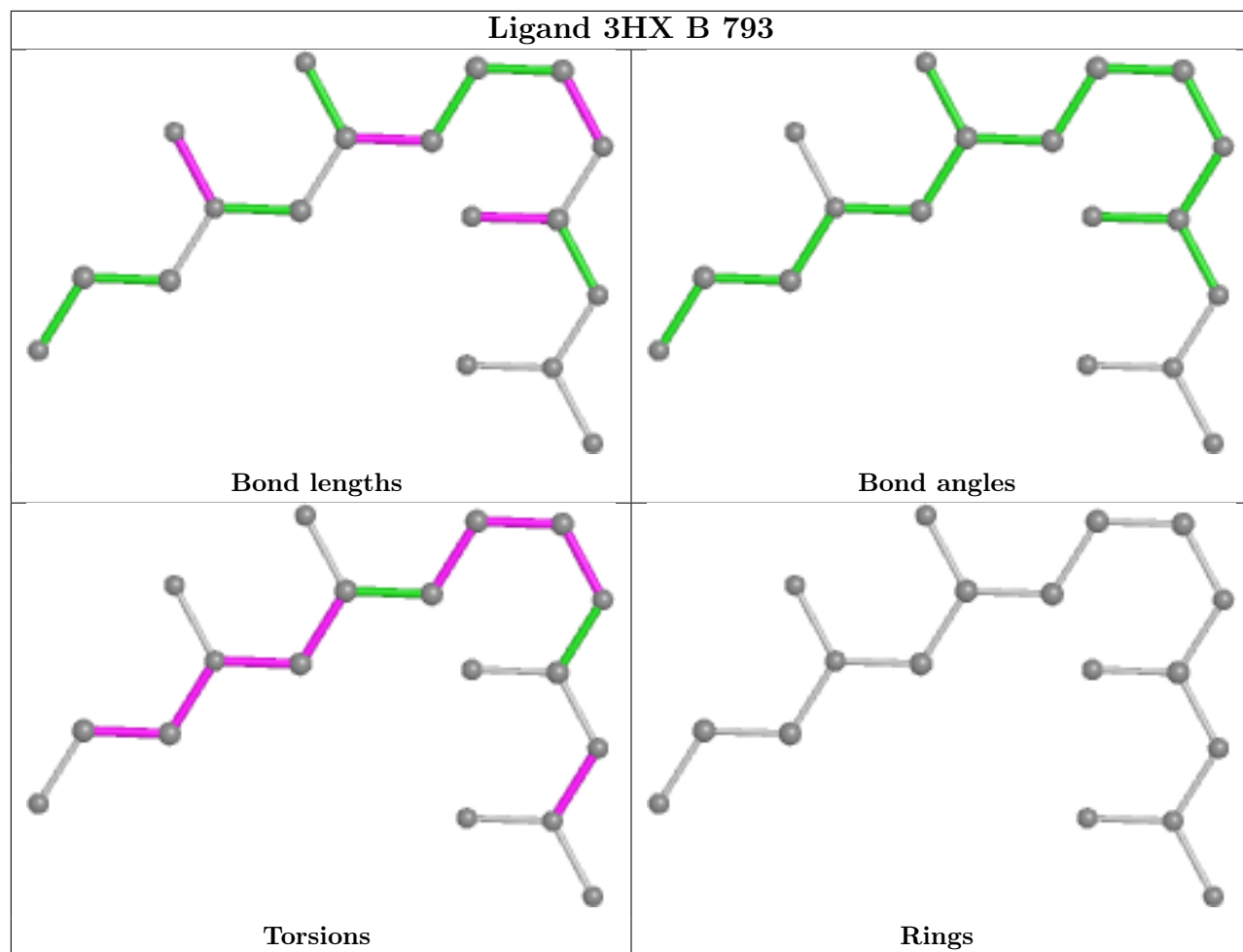
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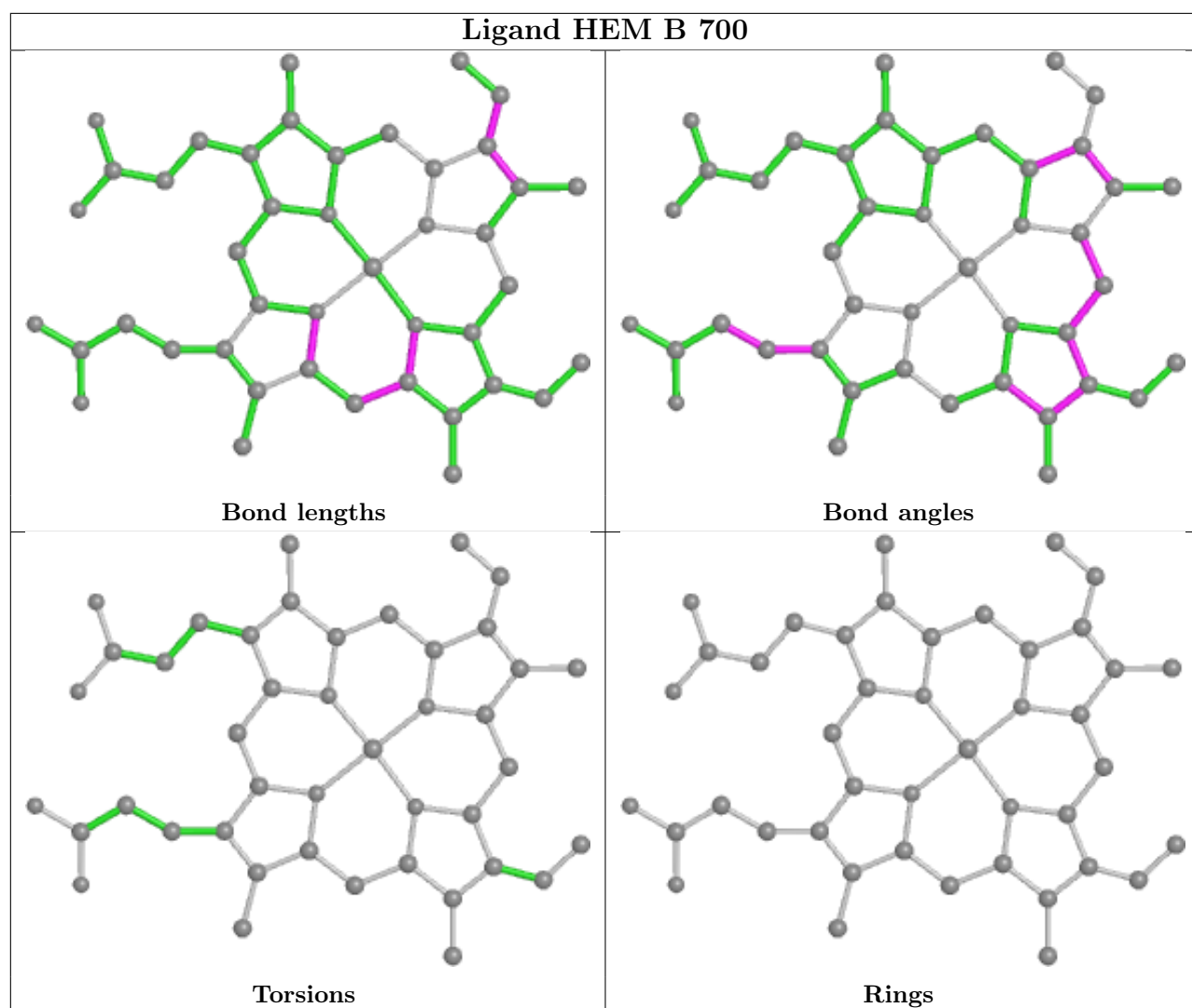
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	793	3HX	4	0
5	A	700	HEM	1	0
7	B	793	3HX	3	0
8	A	880	GOL	1	0
5	B	700	HEM	1	0
6	B	760	H4B	1	0

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

### 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	403/416 (96%)	0.34	30 (7%) 14 22	20, 30, 54, 73	0
1	B	402/416 (96%)	0.20	15 (3%) 41 51	21, 32, 53, 73	0
All	All	805/832 (96%)	0.27	45 (5%) 24 33	20, 31, 54, 73	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	GLY	5.0
1	A	259	GLN	5.0
1	A	123	GLU	5.0
1	B	259	GLN	4.6
1	A	126	LEU	4.4
1	B	390	ARG	3.7
1	A	160	ALA	3.6
1	B	239	GLY	3.5
1	A	238	PRO	3.4
1	A	67	GLY	3.4
1	A	153	GLN	3.2
1	A	69	LYS	3.1
1	B	323	GLU	3.0
1	B	123	GLU	2.8
1	A	261	GLY	2.8
1	B	260	ASP	2.8
1	A	99	ARG	2.7
1	B	257	ARG	2.7
1	B	223	ARG	2.7
1	A	91	GLN	2.7
1	A	124	GLN	2.7
1	A	161	SER	2.7
1	A	107	LEU	2.6
1	A	450	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	277	ILE	2.5
1	A	285	ASN	2.5
1	A	260	ASP	2.4
1	A	157	ALA	2.4
1	A	281	TRP	2.3
1	A	257	ARG	2.2
1	B	270	VAL	2.2
1	A	127	SER	2.2
1	A	306	VAL	2.2
1	A	258	GLN	2.2
1	B	278	GLN	2.1
1	A	187	VAL	2.1
1	A	449	TRP	2.1
1	A	159	VAL	2.1
1	B	142	ARG	2.1
1	B	144	GLY	2.1
1	A	156	GLU	2.1
1	B	261	GLY	2.1
1	B	447	TRP	2.0
1	A	149	GLU	2.0
1	A	146	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [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.

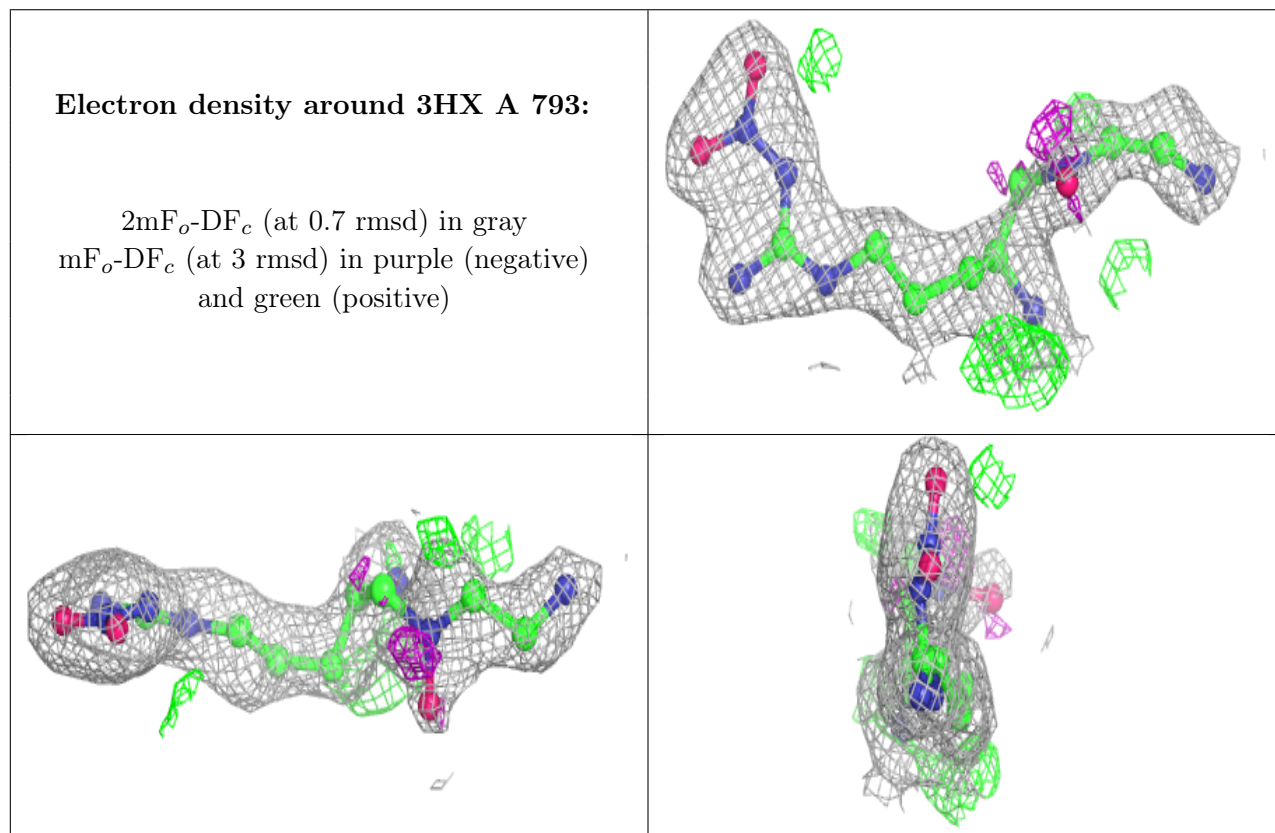
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	GOL	A	880	6/6	0.78	0.32	61,61,62,63	0
3	ACT	A	860	4/4	0.82	0.28	41,42,45,45	0

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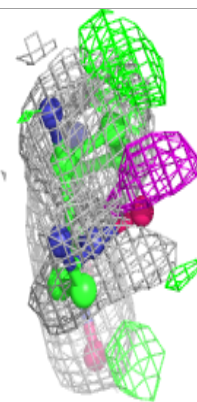
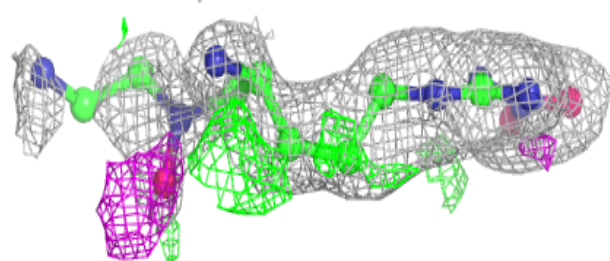
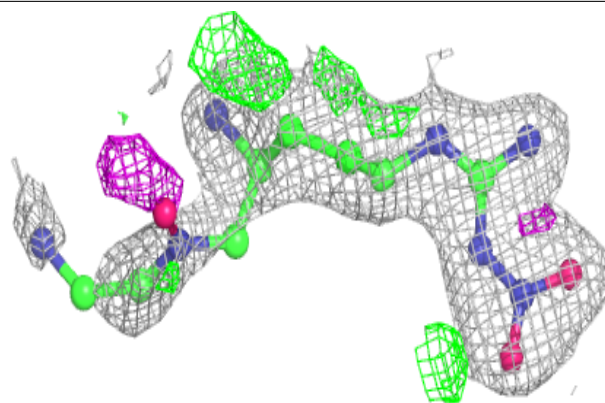
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	A	861	4/4	0.83	0.19	40,41,41,42	0
3	ACT	B	860	4/4	0.86	0.12	46,47,47,48	0
8	GOL	B	880	6/6	0.88	0.21	40,45,46,47	0
7	3HX	A	793	18/18	0.89	0.20	30,46,55,56	0
7	3HX	B	793	18/18	0.89	0.19	31,47,63,63	0
3	ACT	B	861	4/4	0.93	0.22	43,44,44,45	0
6	H4B	A	760	17/17	0.97	0.17	21,22,25,26	0
6	H4B	B	760	17/17	0.97	0.17	20,23,25,26	0
5	HEM	A	700	43/43	0.99	0.16	20,22,30,32	0
5	HEM	B	700	43/43	0.99	0.10	19,23,29,30	0
2	CAC	A	850	3/5	0.99	0.13	42,42,43,46	0
2	CAC	B	850	3/5	0.99	0.08	47,47,48,49	0
4	ZN	A	900	1/1	1.00	0.10	24,24,24,24	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.



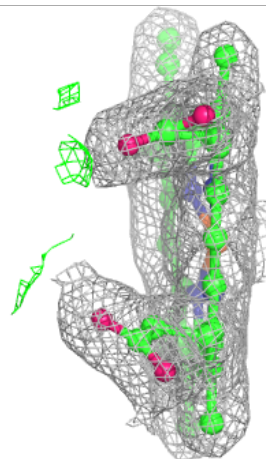
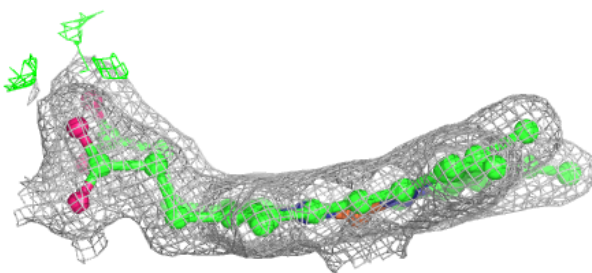
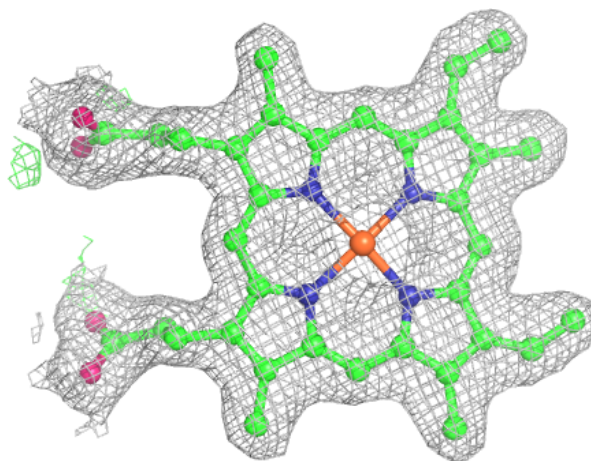
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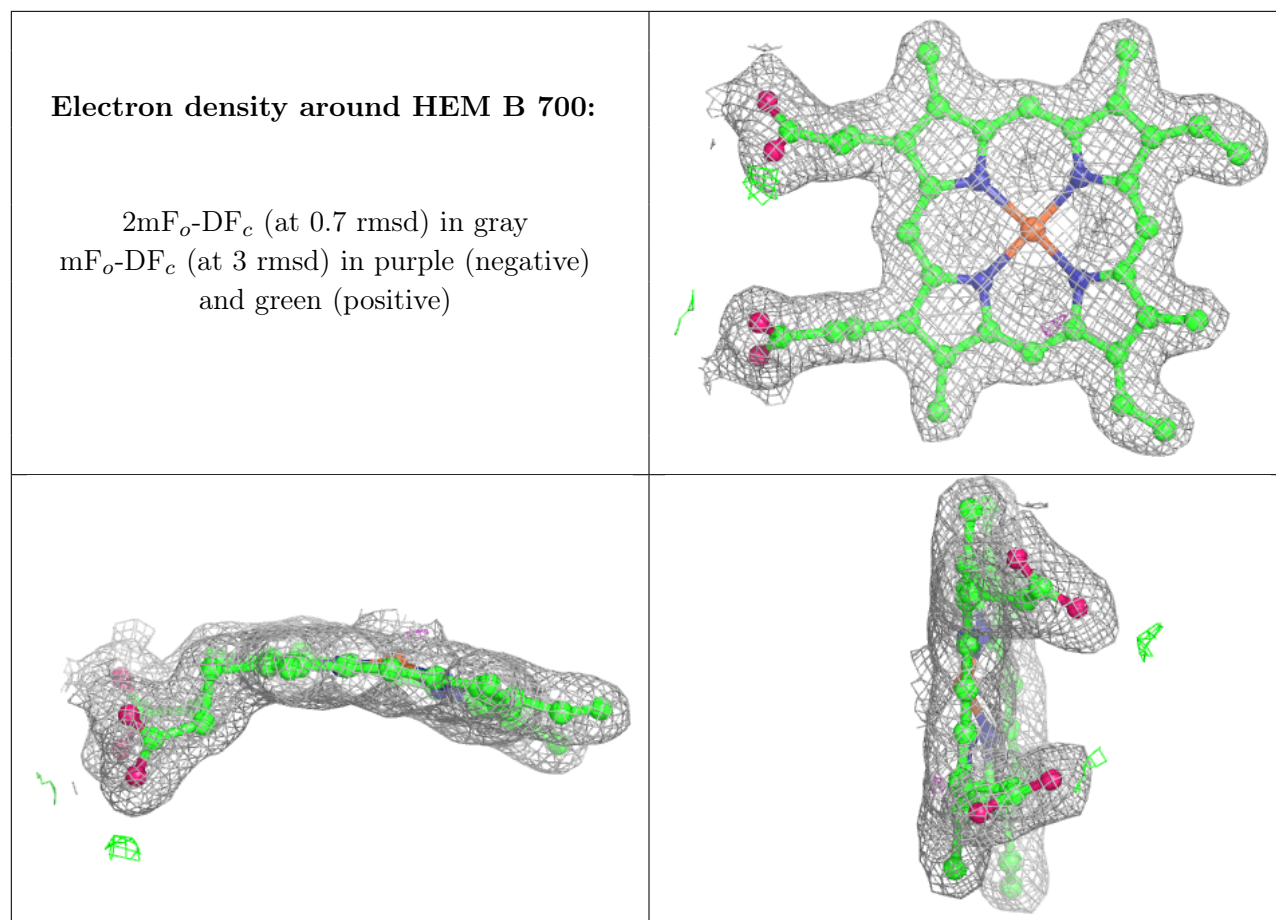
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 700:**

$2mF_o-DF_c$  (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.