



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:20 PM GMT

PDB ID : 1V4X  
Title : Crystal structure of bluefin tuna hemoglobin deoxy form at pH5.0  
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Deposited on : 2003-11-19  
Resolution : 1.60 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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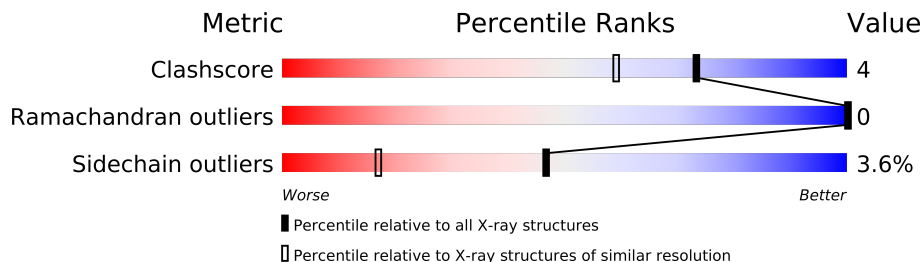
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.60 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))
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	144	
1	C	144	
2	B	146	
2	D	146	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4916 atoms, of which 0 are hydrogen and 0 are deuterium.

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 hemoglobin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1088	699	184	199	6			
1	C	144	Total	C	N	O	S	0	0	0
			1088	699	184	199	6			

- Molecule 2 is a protein called hemoglobin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1143	733	197	209	4			
2	D	146	Total	C	N	O	S	0	0	0
			1143	733	197	209	4			

- 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
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total 61	O 61	0	0
4	B	103	Total 103	O 103	0	0
4	C	72	Total 72	O 72	0	0
4	D	46	Total 46	O 46	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

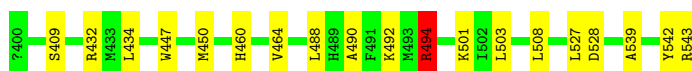
- Molecule 1: hemoglobin alpha chain

Chain A: 



- Molecule 1: hemoglobin alpha chain

Chain C: 



- Molecule 2: hemoglobin beta chain

Chain B: 



- Molecule 2: hemoglobin beta chain

Chain D: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.98Å 60.54Å 80.64Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	19.73 – 1.60	Depositor
% Data completeness (in resolution range)	100.0 (19.73-1.60)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.22	Depositor
R, $R_{free}$	0.204 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ACE

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	0.83	0/1110	0.91	4/1499 (0.3%)
1	C	0.86	0/1110	0.92	4/1499 (0.3%)
2	B	0.86	0/1168	0.94	6/1585 (0.4%)
2	D	0.83	0/1168	0.88	5/1585 (0.3%)
All	All	0.85	0/4556	0.91	19/6168 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ASP	CB-CG-OD2	8.07	125.56	118.30
1	A	49	ASP	CB-CG-OD2	7.37	124.93	118.30
2	B	272	ASP	CB-CG-OD2	7.27	124.85	118.30
2	B	294	ASP	CB-CG-OD2	7.16	124.74	118.30
1	C	494	ARG	NE-CZ-NH2	-7.06	116.77	120.30
2	B	306	LEU	CB-CG-CD2	6.91	122.75	111.00
2	D	652	ASP	CB-CG-OD2	6.39	124.05	118.30
2	D	708	ASP	CB-CG-OD2	6.28	123.96	118.30
2	B	301	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	528	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	488	LEU	CA-CB-CG	5.89	128.85	115.30
2	D	694	ASP	CB-CG-OD2	5.77	123.49	118.30
2	B	268	LEU	CB-CG-CD2	5.73	120.73	111.00
1	C	543	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	A	128	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	320	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	5	ASP	CB-CG-OD2	5.31	123.08	118.30
2	D	741	LEU	CB-CG-CD1	-5.30	101.98	111.00
2	D	743	ARG	NE-CZ-NH2	-5.21	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1088	0	1120	15	0
1	C	1088	0	1120	13	0
2	B	1143	0	1132	6	0
2	D	1143	0	1132	12	0
3	A	43	0	30	4	0
3	B	43	0	30	1	0
3	C	43	0	30	2	0
3	D	43	0	30	1	0
4	A	61	0	0	0	0
4	B	103	0	0	0	0
4	C	72	0	0	0	0
4	D	46	0	0	0	0
All	All	4916	0	4624	39	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (39) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:490:ALA:O	1:C:494:ARG:HD3	1.68	0.92
1:C:432:ARG:HH11	2:D:727:GLN:HE21	1.38	0.72
1:C:432:ARG:HD3	2:D:727:GLN:HE22	1.59	0.68
1:A:32:ARG:HH11	2:B:327:GLN:HE21	1.44	0.66
1:A:47:TRP:HH2	1:A:60:HIS:HB2	1.66	0.61
1:A:47:TRP:CH2	1:A:60:HIS:HB2	2.36	0.60
1:C:447:TRP:CD2	1:C:460:HIS:HE1	2.19	0.60
1:A:47:TRP:HH2	1:A:60:HIS:CB	2.16	0.58
1:C:432:ARG:HH11	2:D:727:GLN:NE2	2.03	0.55
1:A:60:HIS:CE1	3:A:144:HEM:C4D	2.94	0.55
2:D:603:TRP:CZ3	2:D:732:LYS:HD3	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:60:HIS:HE1	3:A:144:HEM:CHA	2.23	0.52
1:A:32:ARG:HH11	2:B:327:GLN:NE2	2.07	0.52
1:C:464:VAL:HG11	1:C:503:LEU:HD21	1.92	0.51
1:A:21:SER:O	1:A:25:ILE:HG13	2.11	0.51
1:A:26:GLY:CA	1:A:65:MET:HG2	2.41	0.50
1:C:490:ALA:O	1:C:494:ARG:CD	2.51	0.50
1:A:60:HIS:HE1	3:A:144:HEM:C4D	2.30	0.49
1:C:432:ARG:HD3	2:D:727:GLN:NE2	2.26	0.49
2:D:601:VAL:CG1	2:D:732:LYS:HE2	2.43	0.48
2:D:641:TYR:CE1	2:D:698:VAL:HA	2.49	0.48
1:A:8:LYS:HG2	1:A:75:ILE:HG12	1.97	0.47
1:A:85:LEU:HD21	3:A:144:HEM:HMA3	1.96	0.46
1:C:508:LEU:HD23	1:C:527:LEU:HD23	1.98	0.45
1:C:539:ALA:HA	1:C:542:TYR:CD1	2.53	0.44
2:D:732:LYS:O	2:D:736:VAL:HG23	2.18	0.44
2:D:663:HIS:HE1	3:D:747:HEM:C4D	2.36	0.43
1:C:447:TRP:CH2	3:C:544:HEM:HBD1	2.54	0.43
2:D:667:VAL:HG11	2:D:706:LEU:HD11	2.01	0.43
1:A:32:ARG:HD3	2:B:327:GLN:HE22	1.83	0.43
2:B:238:THR:HB	3:B:347:HEM:HBC1	2.00	0.43
2:B:273:ARG:HG2	2:B:285:TYR:OH	2.18	0.42
1:C:434:LEU:HD13	1:C:450:MET:HB3	2.02	0.42
2:D:601:VAL:HG11	2:D:732:LYS:HE2	2.01	0.41
2:D:674:ALA:HB2	2:D:685:TYR:CE1	2.56	0.41
3:C:544:HEM:CMC	3:C:544:HEM:HBC2	2.50	0.41
1:A:26:GLY:HA3	1:A:65:MET:HG2	2.03	0.40
2:B:237:TRP:HA	1:C:494:ARG:HD2	2.03	0.40
1:A:46:HIS:H	1:A:46:HIS:CD2	2.40	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	142/144 (99%)	140 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
2	B	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	D	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
All	All	572/580 (99%)	564 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	117/117 (100%)	113 (97%)	4 (3%)	49	19
1	C	117/117 (100%)	113 (97%)	4 (3%)	49	19
2	B	119/119 (100%)	115 (97%)	4 (3%)	49	19
2	D	119/119 (100%)	114 (96%)	5 (4%)	40	13
All	All	472/472 (100%)	455 (96%)	17 (4%)	47	17

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	46	HIS
1	A	113	LYS
1	A	141	ARG
2	B	268	LEU
2	B	277	ASN
2	B	286	SER
2	B	306	LEU
1	C	409	SER
1	C	492	LYS
1	C	494	ARG
1	C	501	LYS
2	D	601	VAL
2	D	659	LYS

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Mol	Chain	Res	Type
2	D	668	LEU
2	D	695	LYS
2	D	706	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	60	HIS
2	B	206	GLN
2	B	327	GLN
2	D	663	HIS
2	D	717	ASN
2	D	727	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands 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
3	HEM	A	144	1	49,50,50	2.70	20 (40%)	46,82,82	2.15	8 (17%)
3	HEM	B	347	2	49,50,50	2.60	17 (34%)	46,82,82	2.47	13 (28%)
3	HEM	C	544	1	49,50,50	2.55	16 (32%)	46,82,82	2.01	10 (21%)
3	HEM	D	747	2	49,50,50	2.65	17 (34%)	46,82,82	2.32	7 (15%)

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	HEM	A	144	1	-	0/14/114/114	0/0/8/8
3	HEM	B	347	2	-	0/14/114/114	0/0/8/8
3	HEM	C	544	1	-	0/14/114/114	0/0/8/8
3	HEM	D	747	2	-	0/14/114/114	0/0/8/8

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	347	HEM	C2B-C1B	7.98	1.46	1.44
3	A	144	HEM	C2D-C1D	7.93	1.46	1.44
3	D	747	HEM	C2D-C1D	7.81	1.46	1.44
3	C	544	HEM	C2D-C1D	6.45	1.46	1.44
3	D	747	HEM	C3B-C2B	-5.78	1.33	1.43
3	C	544	HEM	C3B-C2B	-5.64	1.33	1.43
3	B	347	HEM	C3C-C2C	-5.59	1.34	1.43
3	A	144	HEM	C4A-C3A	5.58	1.47	1.40
3	A	144	HEM	C3D-C2D	5.56	1.53	1.43
3	D	747	HEM	C3D-C2D	5.41	1.53	1.43
3	D	747	HEM	C3C-C2C	-5.35	1.34	1.43
3	A	144	HEM	C3B-C2B	-5.33	1.34	1.43
3	B	347	HEM	C4A-C3A	5.31	1.46	1.40
3	A	144	HEM	C3C-C2C	-5.29	1.34	1.43
3	C	544	HEM	C4A-C3A	5.14	1.46	1.40
3	D	747	HEM	FE-ND	5.12	2.16	1.97
3	C	544	HEM	C3C-C2C	-5.09	1.34	1.43
3	D	747	HEM	C4A-C3A	4.92	1.46	1.40
3	B	347	HEM	C3D-C2D	4.88	1.52	1.43
3	C	544	HEM	FE-NA	4.85	2.13	1.92
3	C	544	HEM	C3B-CAB	4.83	1.55	1.40
3	A	144	HEM	C3C-CAC	4.73	1.55	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	347	HEM	C3B-C2B	-4.72	1.35	1.43
3	C	544	HEM	C3D-C2D	4.70	1.52	1.43
3	B	347	HEM	C3C-CAC	4.58	1.54	1.40
3	C	544	HEM	C3C-CAC	4.45	1.54	1.40
3	D	747	HEM	C3C-CAC	4.41	1.54	1.40
3	A	144	HEM	FE-ND	4.38	2.13	1.97
3	A	144	HEM	FE-NA	4.23	2.10	1.92
3	A	144	HEM	C3B-CAB	4.18	1.53	1.40
3	D	747	HEM	C3B-CAB	4.13	1.53	1.40
3	B	347	HEM	C3B-CAB	4.12	1.53	1.40
3	D	747	HEM	FE-NC	3.91	2.12	1.97
3	B	347	HEM	FE-NB	3.83	2.11	1.97
3	A	144	HEM	FE-NB	3.79	2.11	1.97
3	B	347	HEM	FE-ND	3.38	2.10	1.97
3	B	347	HEM	FE-NA	3.38	2.06	1.92
3	C	544	HEM	C3D-C4D	3.36	1.45	1.44
3	D	747	HEM	FE-NA	3.34	2.06	1.92
3	B	347	HEM	C3D-C4D	3.23	1.45	1.44
3	A	144	HEM	C2B-C1B	3.17	1.45	1.44
3	B	347	HEM	CMB-C2B	3.12	1.57	1.47
3	C	544	HEM	FE-NC	3.11	2.09	1.97
3	D	747	HEM	CMC-C2C	3.02	1.56	1.47
3	C	544	HEM	CMB-C2B	2.99	1.56	1.47
3	B	347	HEM	FE-NC	2.98	2.09	1.97
3	C	544	HEM	CHA-C4D	2.94	1.40	1.35
3	C	544	HEM	C2B-C1B	2.89	1.45	1.44
3	C	544	HEM	CAA-C2A	2.80	1.56	1.52
3	D	747	HEM	CMB-C2B	2.79	1.56	1.47
3	C	544	HEM	CMD-C2D	2.70	1.55	1.47
3	D	747	HEM	FE-NB	2.65	2.07	1.97
3	D	747	HEM	CAA-C2A	2.61	1.56	1.52
3	B	347	HEM	CMD-C2D	2.59	1.55	1.47
3	A	144	HEM	CMC-C2C	2.52	1.55	1.47
3	D	747	HEM	CMD-C2D	2.52	1.55	1.47
3	A	144	HEM	CMD-C2D	2.50	1.55	1.47
3	A	144	HEM	C3D-C4D	2.44	1.45	1.44
3	A	144	HEM	CMB-C2B	2.41	1.54	1.47
3	B	347	HEM	CHA-C4D	2.37	1.39	1.35
3	A	144	HEM	CHB-C1B	2.37	1.39	1.35
3	D	747	HEM	CHA-C4D	2.36	1.39	1.35
3	B	347	HEM	C4C-NC	2.31	1.41	1.38
3	A	144	HEM	CHA-C4D	2.30	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	144	HEM	FE-NC	2.29	2.06	1.97
3	A	144	HEM	CAA-C2A	2.27	1.56	1.52
3	C	544	HEM	CMA-C3A	2.27	1.56	1.51
3	D	747	HEM	CMA-C3A	2.19	1.56	1.51
3	B	347	HEM	C2D-C1D	2.12	1.45	1.44
3	A	144	HEM	CMA-C3A	2.07	1.56	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	747	HEM	C3B-C4B-NB	-10.34	106.60	114.00
3	B	347	HEM	C3B-C4B-NB	-9.34	107.32	114.00
3	A	144	HEM	C3B-C4B-NB	-8.86	107.66	114.00
3	C	544	HEM	C3B-C4B-NB	-7.91	108.34	114.00
3	B	347	HEM	C4D-ND-C1D	7.31	112.64	105.16
3	D	747	HEM	C4D-ND-C1D	6.41	111.72	105.16
3	C	544	HEM	C4D-ND-C1D	5.81	111.10	105.16
3	A	144	HEM	CBD-CAD-C3D	-5.73	101.87	114.37
3	A	144	HEM	C4D-ND-C1D	5.49	110.78	105.16
3	B	347	HEM	CHD-C1D-ND	4.51	128.33	124.58
3	B	347	HEM	C2D-C1D-ND	-4.27	107.89	112.93
3	B	347	HEM	CBA-CAA-C2A	-4.26	105.19	112.69
3	A	144	HEM	CHD-C4C-NC	4.25	128.42	124.73
3	D	747	HEM	C2D-C1D-ND	-3.86	108.37	112.93
3	D	747	HEM	C1B-NB-C4B	3.66	108.91	105.16
3	D	747	HEM	CHC-C4B-NB	3.53	127.52	124.58
3	C	544	HEM	CHB-C1B-NB	3.27	128.79	124.31
3	C	544	HEM	CMA-C3A-C4A	-3.24	123.63	128.62
3	C	544	HEM	CHC-C4B-NB	3.21	127.25	124.58
3	C	544	HEM	C2D-C1D-ND	-3.20	109.16	112.93
3	D	747	HEM	CAD-CBD-CGD	-3.16	103.63	113.48
3	B	347	HEM	CHC-C4B-NB	2.96	127.05	124.58
3	A	144	HEM	C1B-NB-C4B	2.79	108.02	105.16
3	C	544	HEM	CHA-C4D-ND	2.74	128.07	124.31
3	C	544	HEM	CAD-C3D-C4D	2.65	129.29	124.53
3	B	347	HEM	CAD-C3D-C4D	2.63	129.26	124.53
3	B	347	HEM	CHA-C4D-ND	2.62	127.91	124.31
3	C	544	HEM	CMA-C3A-C2A	2.60	129.84	124.94
3	D	747	HEM	CBA-CAA-C2A	-2.55	108.20	112.69
3	B	347	HEM	C1B-NB-C4B	2.47	107.69	105.16
3	A	144	HEM	C2D-C1D-ND	-2.43	110.06	112.93
3	B	347	HEM	CBD-CAD-C3D	-2.39	109.15	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	347	HEM	CHB-C4A-NA	2.37	128.54	124.58
3	A	144	HEM	C4C-NC-C1C	2.34	107.97	105.53
3	A	144	HEM	C3A-C4A-NA	-2.27	107.70	109.41
3	B	347	HEM	C4C-NC-C1C	2.11	107.73	105.53
3	C	544	HEM	CBA-CAA-C2A	-2.05	109.08	112.69
3	B	347	HEM	C3A-C4A-NA	-2.00	107.90	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.