



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:44 am GMT

PDB ID : 4NOS  
Title : HUMAN INDUCIBLE NITRIC OXIDE SYNTHASE WITH INHIBITOR  
Authors : Fischmann, T.O.; Weber, P.C.  
Deposited on : 1999-02-03  
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

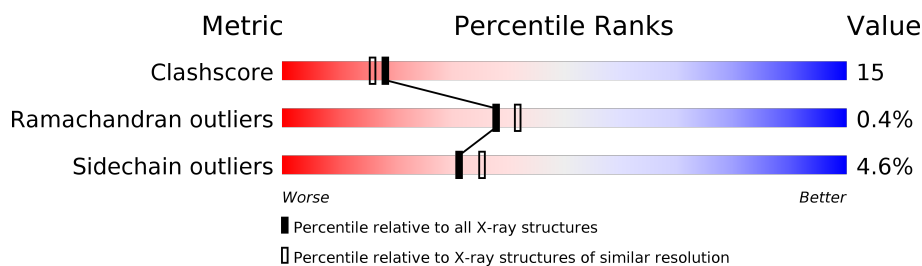
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	
1	C	427	
1	D	427	

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
5	ITU	B	1012	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15317 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 INDUCIBLE NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	1
			3420	2186	600	612	22			
1	B	421	Total	C	N	O	S	0	0	1
			3420	2186	600	612	22			
1	C	421	Total	C	N	O	S	0	0	1
			3420	2186	600	612	22			
1	D	421	Total	C	N	O	S	0	0	1
			3420	2186	600	612	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	ILE	LEU	CONFLICT	UNP P35228
B	423	ILE	LEU	CONFLICT	UNP P35228
C	423	ILE	LEU	CONFLICT	UNP P35228
D	423	ILE	LEU	CONFLICT	UNP P35228

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

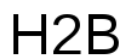
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



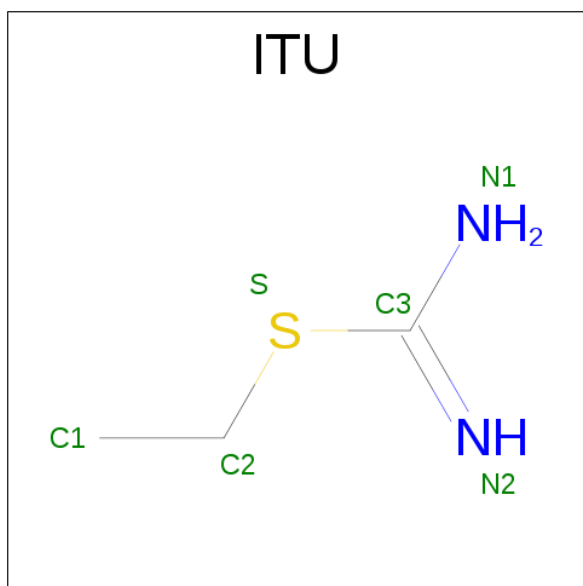
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 2-AMINO-6-(1,2-DIHYDROXY-PROPYL)-7,8-DIHYDRO-6H-PTERIDIN-4-ONE (three-letter code: H2B) (formula:  $\text{C}_9\text{H}_{13}\text{N}_5\text{O}_3$ ).



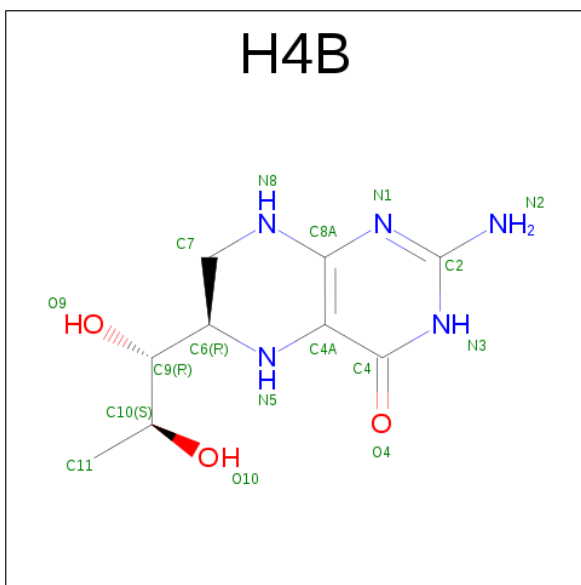
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is ETHYLISOTHIOUREA (three-letter code: ITU) (formula:  $C_3H_8N_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			6	3	2	1		
5	B	1	Total	C	N	S	0	0
			6	3	2	1		
5	C	1	Total	C	N	S	0	0
			6	3	2	1		
5	D	1	Total	C	N	S	0	0
			6	3	2	1		

- 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
6	B	1	Total	C	N	O	0	0
			17	9	5	3		
6	C	1	Total	C	N	O	0	0
			17	9	5	3		
6	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 7 is water.

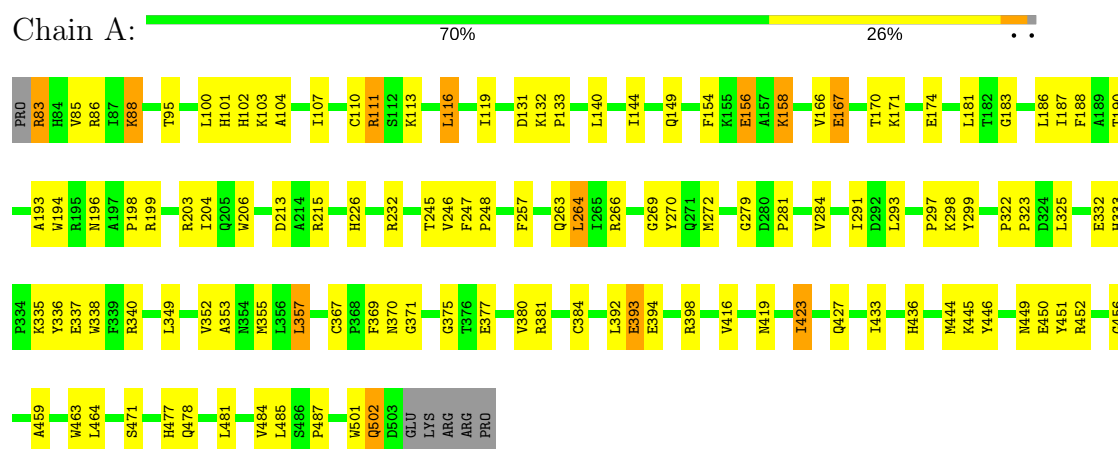
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	336	Total	O	0	0
			336	336		
7	B	335	Total	O	0	0
			335	335		
7	C	339	Total	O	0	0
			339	339		
7	D	361	Total	O	0	0
			361	361		

### 3 Residue-property plots

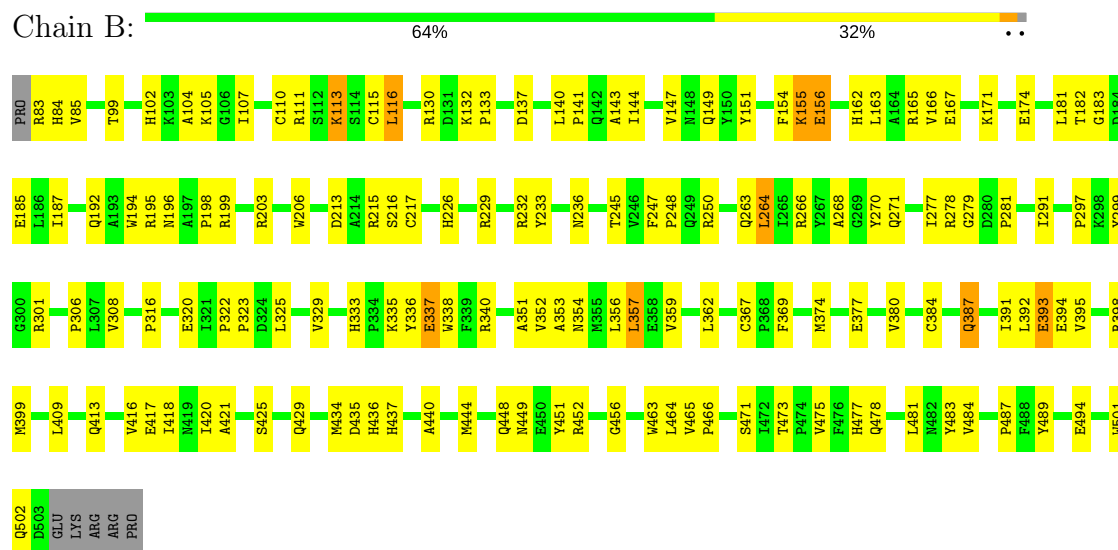
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: INDUCIBLE NITRIC OXIDE SYNTHASE



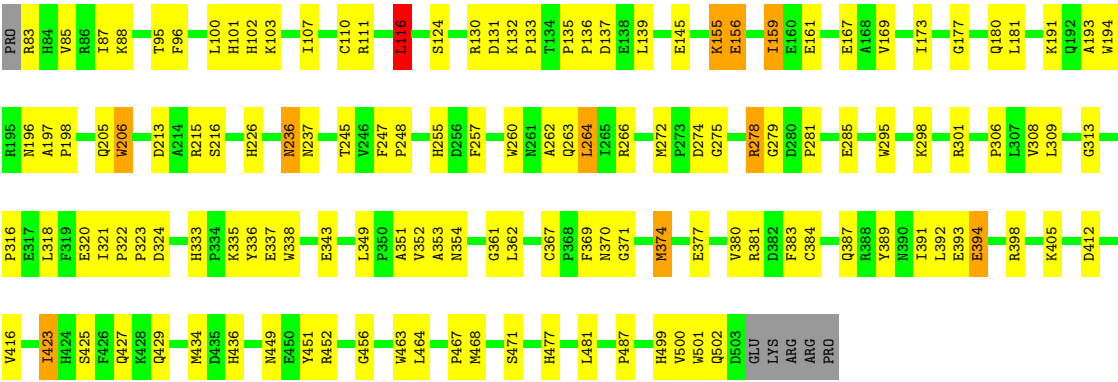
#### • Molecule 1: INDUCIBLE NITRIC OXIDE SYNTHASE



#### • Molecule 1: INDUCIBLE NITRIC OXIDE SYNTHASE







● Molecule 1: INDUCIBLE NITRIC OXIDE SYNTHASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.76Å 156.67Å 190.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.25	Depositor
% Data completeness (in resolution range)	88.7 (8.00-2.25)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.199 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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, ZN, ITU, H4B, H2B

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	0.51	0/3519	0.70	1/4776 (0.0%)
1	B	0.53	0/3519	0.71	1/4776 (0.0%)
1	C	0.53	0/3519	0.74	3/4776 (0.1%)
1	D	0.54	0/3519	0.75	4/4776 (0.1%)
All	All	0.53	0/14076	0.72	9/19104 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	D	221	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	371	GLY	N-CA-C	-5.91	98.32	113.10
1	C	371	GLY	N-CA-C	-5.68	98.89	113.10
1	C	374	MET	N-CA-C	-5.64	95.78	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	3420	0	3326	101	0
1	B	3420	0	3326	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3420	0	3326	100	1
1	D	3420	0	3326	89	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	43	0	30	9	0
3	B	43	0	30	4	0
3	C	43	0	30	8	0
3	D	43	0	30	9	0
4	A	17	0	13	0	0
5	A	6	0	7	2	0
5	B	6	0	7	4	0
5	C	6	0	7	3	0
5	D	6	0	7	2	0
6	B	17	0	15	1	0
6	C	17	0	15	2	0
6	D	17	0	15	1	0
7	A	336	0	0	10	0
7	B	335	0	0	15	1
7	C	339	0	0	16	0
7	D	361	0	0	9	0
All	All	15317	0	13510	412	1

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 15.

The worst 5 of 412 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:C:481:LEU:HD22	1:D:116:LEU:HD22	1.52	0.90
3:C:2010:HEM:HMC2	3:C:2010:HEM:HBC2	1.56	0.88
1:A:88:LYS:HB2	1:A:95:THR:HG22	1.57	0.84
3:D:3010:HEM:HBC2	3:D:3010:HEM:HMC2	1.61	0.82
1:D:217:CYS:SG	7:D:3344:HOH:O	2.28	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASP:O	7:B:1165:HOH:O[4_455]	2.19	0.01

## 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	419/427 (98%)	390 (93%)	28 (7%)	1 (0%)	51	60
1	B	419/427 (98%)	395 (94%)	24 (6%)	0	100	100
1	C	419/427 (98%)	390 (93%)	26 (6%)	3 (1%)	25	25
1	D	419/427 (98%)	398 (95%)	19 (4%)	2 (0%)	32	33
All	All	1676/1708 (98%)	1573 (94%)	97 (6%)	6 (0%)	38	42

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	236	ASN
1	D	206	TRP
1	C	206	TRP
1	A	203	ARG
1	D	236	ASN

### 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	366/373 (98%)	350 (96%)	16 (4%)	33	37
1	B	366/373 (98%)	351 (96%)	15 (4%)	35	42
1	C	366/373 (98%)	347 (95%)	19 (5%)	27	29
1	D	366/373 (98%)	348 (95%)	18 (5%)	29	32
All	All	1464/1492 (98%)	1396 (95%)	68 (5%)	31	35

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	502	GLN
1	C	264	LEU
1	D	266	ARG
1	C	116	LEU
1	C	156	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	387	GLN
1	B	477	HIS
1	D	436	HIS
1	B	436	HIS
1	C	97	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are 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	HEM	A	510	1	28,50,50	1.90	8 (28%)	17,82,82	2.07	9 (52%)
4	H2B	A	511	-	13,18,18	2.00	3 (23%)	11,26,26	2.65	6 (54%)
5	ITU	A	512	-	4,5,5	0.74	0	3,5,5	1.35	1 (33%)
3	HEM	B	1010	1	28,50,50	1.99	9 (32%)	17,82,82	2.05	7 (41%)
6	H4B	B	1011	-	14,18,18	1.89	4 (28%)	12,26,26	3.81	6 (50%)
5	ITU	B	1012	-	4,5,5	0.93	0	3,5,5	1.79	1 (33%)
3	HEM	C	2010	1	28,50,50	1.80	6 (21%)	17,82,82	1.99	6 (35%)
6	H4B	C	2011	-	14,18,18	1.80	2 (14%)	12,26,26	3.77	6 (50%)
5	ITU	C	2012	-	4,5,5	0.98	0	3,5,5	1.67	1 (33%)
3	HEM	D	3010	1	28,50,50	2.03	8 (28%)	17,82,82	1.73	5 (29%)
6	H4B	D	3011	-	14,18,18	1.99	4 (28%)	12,26,26	3.81	6 (50%)
5	ITU	D	3012	-	4,5,5	0.98	0	3,5,5	0.75	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
3	HEM	A	510	1	-	0/6/54/54	0/0/8/8
4	H2B	A	511	-	-	0/8/33/33	0/2/2/2
5	ITU	A	512	-	-	0/3/3/3	0/0/0/0
3	HEM	B	1010	1	-	0/6/54/54	0/0/8/8
6	H4B	B	1011	-	-	0/8/17/17	0/2/2/2
5	ITU	B	1012	-	-	0/3/3/3	0/0/0/0
3	HEM	C	2010	1	-	0/6/54/54	0/0/8/8
6	H4B	C	2011	-	-	0/8/17/17	0/2/2/2
5	ITU	C	2012	-	-	0/3/3/3	0/0/0/0
3	HEM	D	3010	1	-	0/6/54/54	0/0/8/8
6	H4B	D	3011	-	-	0/8/17/17	0/2/2/2
5	ITU	D	3012	-	-	0/3/3/3	0/0/0/0

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1010	HEM	C3C-C2C	-3.69	1.35	1.40
3	A	510	HEM	C3C-C2C	-3.52	1.35	1.40
3	C	2010	HEM	C3C-C2C	-3.52	1.35	1.40
3	D	3010	HEM	C3C-C2C	-3.52	1.35	1.40
3	D	3010	HEM	C3B-C2B	-3.37	1.35	1.40

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	2010	HEM	CBD-CAD-C3D	-4.52	103.85	112.47
3	B	1010	HEM	CBD-CAD-C3D	-4.50	103.88	112.47
4	A	511	H2B	N1-C2-N3	-4.15	120.05	126.41
3	A	510	HEM	CBD-CAD-C3D	-3.89	105.04	112.47
6	C	2011	H4B	N3-C2-N1	-3.70	119.44	125.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	510	HEM	9	0
5	A	512	ITU	2	0
3	B	1010	HEM	4	0
6	B	1011	H4B	1	0
5	B	1012	ITU	4	0
3	C	2010	HEM	8	0
6	C	2011	H4B	2	0
5	C	2012	ITU	3	0
3	D	3010	HEM	9	0
6	D	3011	H4B	1	0
5	D	3012	ITU	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.