



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 11:25 AM UTC

PDB ID : 5C6E / pdb_00005c6e
Title : Joint X-ray/neutron structure of equine cyanomet hemoglobin in R state
Authors : Dajnowicz, S.; Sean, S.; Hanson, B.L.; Fisher, S.Z.; Langan, P.; Kovalevsky, A.Y.; Mueser, T.C.
Deposited on : 2015-06-22
Resolution : 1.70 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

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>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 1.70 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5239 atoms, of which 2118 are hydrogens and 705 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	141	Total	C	D	H	N	O	S	0	102	0
			2294	684	224	1001	187	196	2			

- Molecule 2 is a protein called Hemoglobin subunit beta.

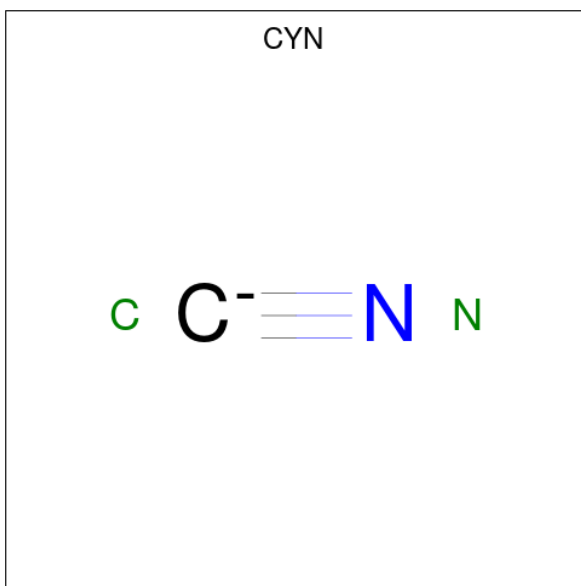
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	146	Total	C	D	H	N	O	S	0	107	0
			2426	728	235	1057	200	204	2			

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



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O		0	0
			73	34	1	30	4	4			
3	B	1	Total	C	Fe	H	N	O		0	0
			73	34	1	30	4	4			

- Molecule 4 is CYANIDE ION (CCD ID: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			2	1	1		
4	B	1	Total	C	N	0	0
			2	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	62	Total	D	O	0	0
			186	124	62		
5	B	61	Total	D	O	0	0
			183	122	61		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.86Å 63.16Å 54.71Å 90.00° 110.75° 90.00°	Depositor
Resolution (Å)	30.20 – 1.70	Depositor
% Data completeness (in resolution range)	88.8 (30.20-1.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.70Å)	Xtriage
Refinement program	nCNS 1.0.0	Depositor
R, R_{free}	0.210 , 0.233	Depositor
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.026	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5239	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

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
4	CYN	B	202	-	1,1,1	0.34	0	-		
3	HEM	A	201	1	50,50,50	1.31	9 (18%)	67,82,82	1.25	5 (7%)
4	CYN	A	202	-	1,1,1	0.41	0	-		
3	HEM	B	201	2	50,50,50	1.30	10 (20%)	67,82,82	1.19	6 (8%)

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	201	1	-	3/14/54/54	-
3	HEM	B	201	2	-	2/14/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	HEM	CAC-C3C	2.74	1.54	1.47
3	A	201	HEM	C3B-C2B	-2.59	1.31	1.37
3	B	201	HEM	CMC-C2C	2.50	1.55	1.50
3	A	201	HEM	CAC-C3C	2.45	1.53	1.47
3	B	201	HEM	CMB-C2B	2.45	1.55	1.50
3	A	201	HEM	CAB-C3B	2.41	1.53	1.47
3	B	201	HEM	CAB-C3B	2.37	1.53	1.47
3	A	201	HEM	CMA-C3A	2.37	1.55	1.50
3	A	201	HEM	CMB-C2B	2.36	1.55	1.50
3	A	201	HEM	FE-ND	2.34	2.02	1.94
3	B	201	HEM	FE-ND	2.20	2.01	1.94
3	A	201	HEM	C2A-C3A	-2.16	1.33	1.38
3	B	201	HEM	C3B-C2B	-2.11	1.32	1.37
3	A	201	HEM	CMD-C2D	2.06	1.55	1.50
3	B	201	HEM	C2A-C3A	-2.06	1.33	1.38
3	B	201	HEM	CMD-C2D	2.04	1.54	1.50
3	B	201	HEM	FE-NC	2.03	2.01	1.95
3	A	201	HEM	CMC-C2C	2.02	1.54	1.50
3	B	201	HEM	FE-NB	2.00	2.01	1.94

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	HEM	O2A-CGA-O1A	3.86	133.26	123.33
3	A	201	HEM	CMB-C2B-C1B	-3.34	119.82	125.03
3	B	201	HEM	CMB-C2B-C1B	-3.15	120.11	125.03
3	A	201	HEM	CHB-C4A-NA	3.12	129.51	123.86
3	B	201	HEM	O1A-CGA-CBA	-2.54	115.04	123.09
3	A	201	HEM	C4A-CHB-C1B	-2.53	120.29	126.25
3	B	201	HEM	CAB-C3B-C2B	2.50	136.54	128.43
3	B	201	HEM	O2A-CGA-O1A	2.49	129.74	123.33
3	A	201	HEM	O1A-CGA-CBA	-2.40	115.49	123.09
3	B	201	HEM	CHC-C4B-NB	2.32	126.92	124.42
3	B	201	HEM	CAC-C3C-C4C	-2.00	120.03	124.82

There are no chirality outliers.

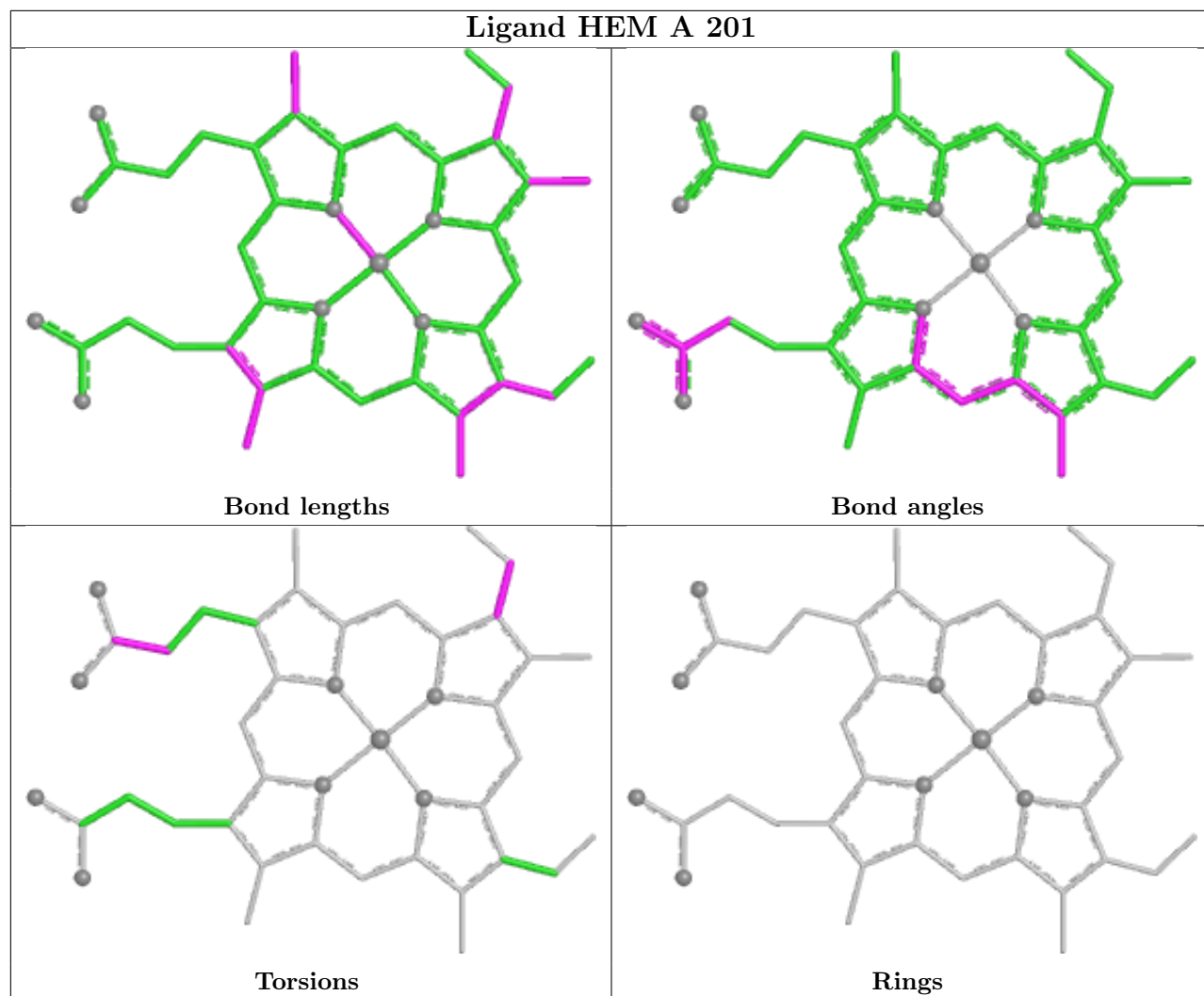
All (5) torsion outliers are listed below:

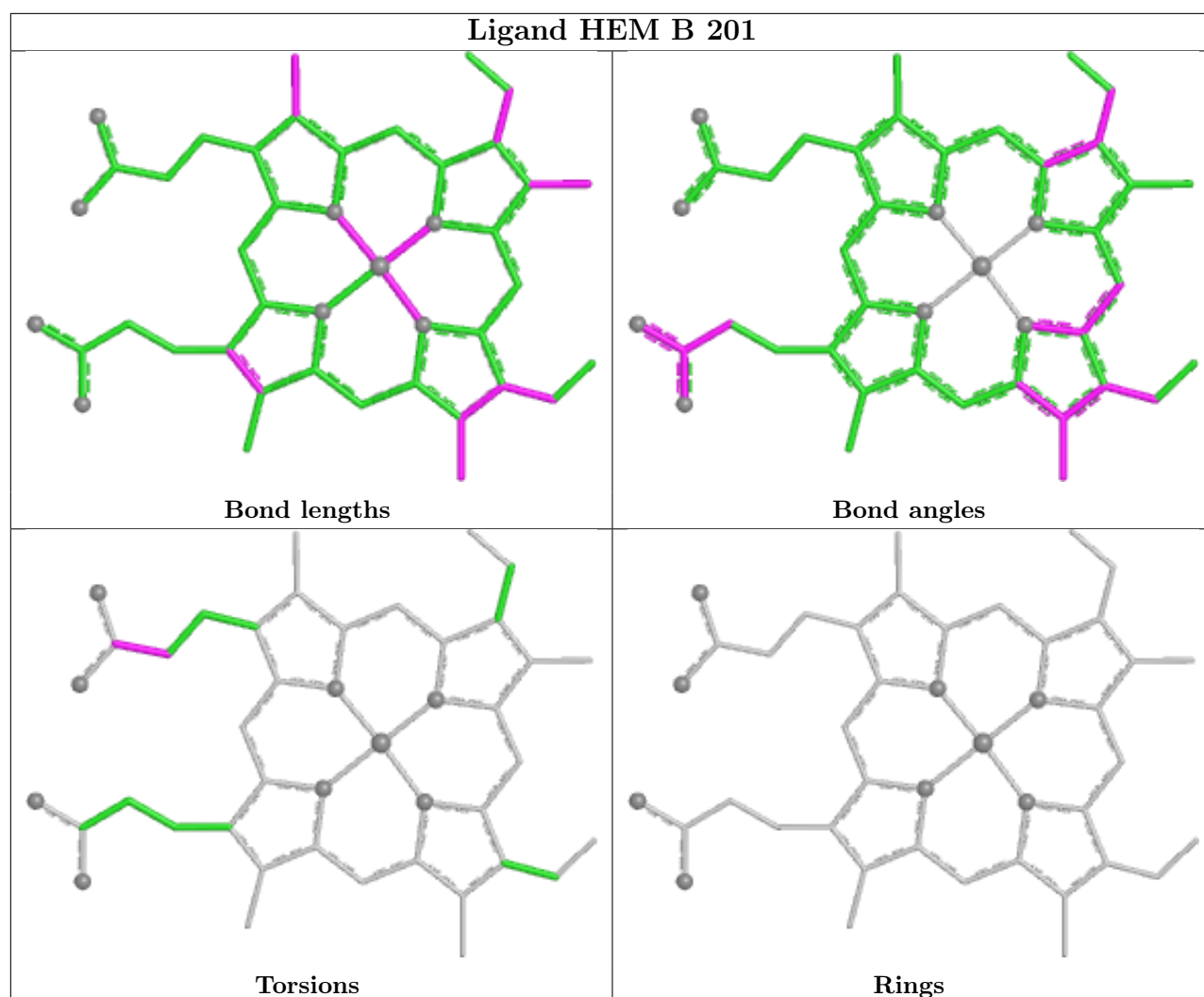
Mol	Chain	Res	Type	Atoms
3	A	201	HEM	CAD-CBD-CGD-O1D
3	A	201	HEM	CAD-CBD-CGD-O2D
3	A	201	HEM	C4C-C3C-CAC-CBC
3	B	201	HEM	CAD-CBD-CGD-O1D
3	B	201	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

No monomer is involved in short contacts.

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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.