



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2017 – 12:04 AM EDT

PDB ID : 1F4J
Title : STRUCTURE OF TETRAGONAL CRYSTALS OF HUMAN ERYTHROCYTE CATALASE
Authors : Safo, M.K.; Musayev, F.N.; Wu, S.H.; Abraham, D.J.; Ko, T.P.
Deposited on : unknown
Resolution : 2.40 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

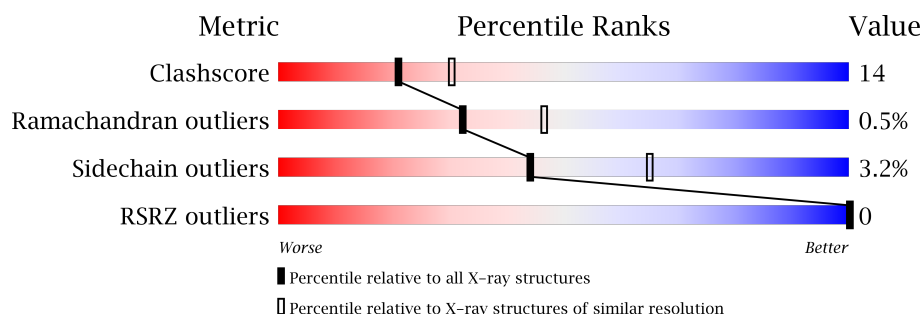
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	527	
1	B	527	
1	C	527	
1	D	527	

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
2	HEM	A	600	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16813 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 CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3845	2450	677	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3849	2452	677	708	12			
1	C	481	Total	C	N	O	S	0	0	0
			3863	2461	680	710	12			
1	D	479	Total	C	N	O	S	0	0	0
			3845	2450	677	706	12			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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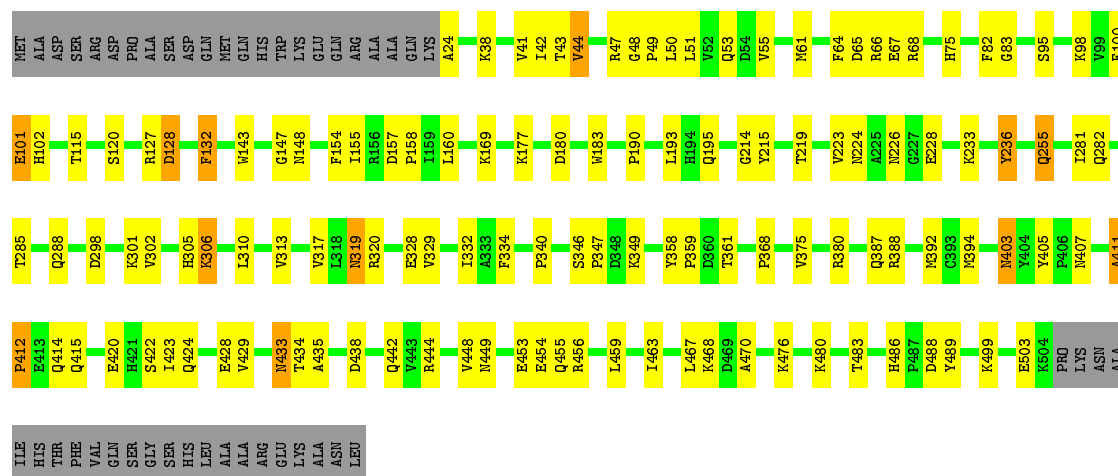
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

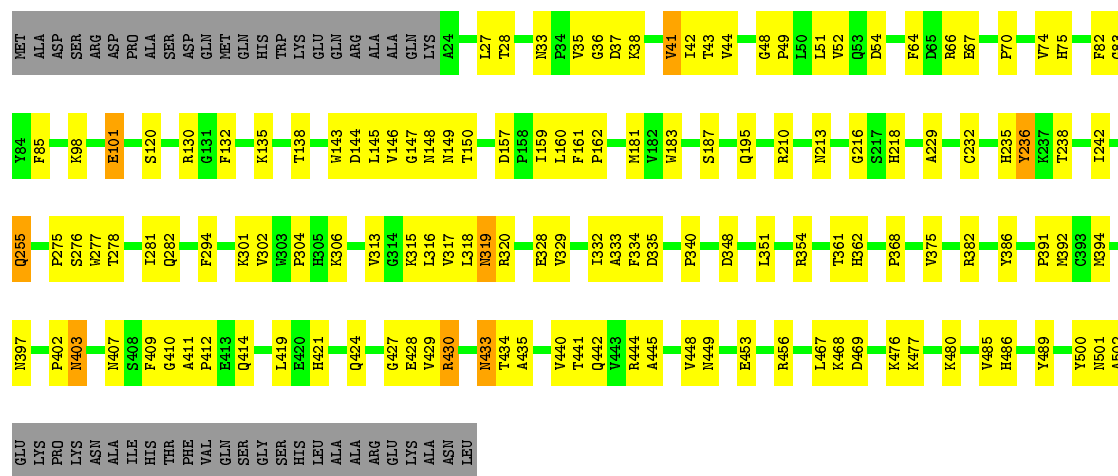
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	318	Total 318	O 318	0	0
3	B	312	Total 312	O 312	0	0
3	C	295	Total 295	O 295	0	0
3	D	314	Total 314	O 314	0	0

Chain C:  67% 22% 9%



• Molecule 1: CATALASE

Chain D:  65% 24% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	203.60 Å 203.60 Å 144.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	204.00 – 2.40 143.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.8 (204.00-2.40) 93.4 (143.97-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.40 Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.196 , 0.244 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16813	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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.

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: 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	0/3960	0.66	0/5384
1	B	0.42	0/3964	0.65	0/5389
1	C	0.42	0/3978	0.65	0/5407
1	D	0.43	0/3960	0.66	0/5384
All	All	0.42	0/15862	0.66	0/21564

There are no bond length outliers.

There are no bond angle outliers.

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	3845	0	3687	103	0
1	B	3849	0	3688	108	0
1	C	3863	0	3706	137	0
1	D	3845	0	3687	117	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
2	C	43	0	30	3	0
2	D	43	0	30	6	0
3	A	318	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	312	0	0	8	0
3	C	295	0	0	8	0
3	D	314	0	0	3	0
All	All	16813	0	14888	418	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 14.

The worst 5 of 418 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:306:LYS:HD2	1:A:306:LYS:H	1.25	1.01
1:B:306:LYS:H	1:B:306:LYS:HD2	1.22	1.00
1:A:414:GLN:NE2	1:C:38:LYS:H	1.63	0.97
1:D:306:LYS:H	1:D:306:LYS:HD2	1.27	0.97
1:A:302:VAL:H	1:A:442:GLN:HE22	1.22	0.86

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	477/527 (90%)	448 (94%)	28 (6%)	1 (0%)	51	67
1	B	477/527 (90%)	451 (94%)	25 (5%)	1 (0%)	51	67
1	C	479/527 (91%)	446 (93%)	28 (6%)	5 (1%)	18	26
1	D	477/527 (90%)	441 (92%)	33 (7%)	3 (1%)	28	41
All	All	1910/2108 (91%)	1786 (94%)	114 (6%)	10 (0%)	32	46

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	101	GLU
1	B	101	GLU
1	D	101	GLU
1	D	120	SER
1	A	120	SER

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	412/451 (91%)	396 (96%)	16 (4%)	37	56
1	B	413/451 (92%)	399 (97%)	14 (3%)	42	63
1	C	414/451 (92%)	402 (97%)	12 (3%)	48	68
1	D	412/451 (91%)	401 (97%)	11 (3%)	50	71
All	All	1651/1804 (92%)	1598 (97%)	53 (3%)	44	65

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	382	ARG
1	B	489	TYR
1	D	255	GLN
1	B	394	MET
1	B	417	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	471	GLN
1	C	321	ASN
1	D	442	GLN
1	C	226	ASN
1	C	403	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	$\# Z > 2$
2	HEM	A	600	1	28,50,50	2.21	8 (28%)	17,82,82	1.43	2 (11%)
2	HEM	B	600	1	28,50,50	1.68	8 (28%)	17,82,82	1.52	2 (11%)
2	HEM	C	600	1	28,50,50	1.96	12 (42%)	17,82,82	1.38	4 (23%)
2	HEM	D	600	1	28,50,50	2.06	9 (32%)	17,82,82	1.49	2 (11%)

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
2	HEM	A	600	1	-	0/6/54/54	0/0/8/8
2	HEM	B	600	1	-	0/6/54/54	0/0/8/8
2	HEM	C	600	1	-	0/6/54/54	0/0/8/8
2	HEM	D	600	1	-	0/6/54/54	0/0/8/8

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	C3B-CAB	-5.31	1.37	1.47
2	A	600	HEM	C3B-CAB	-5.08	1.37	1.47
2	D	600	HEM	C3B-C2B	-4.74	1.34	1.40
2	B	600	HEM	C3C-CAC	-3.99	1.39	1.47
2	C	600	HEM	C3B-CAB	-3.88	1.40	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	CBD-CAD-C3D	-4.58	103.73	112.47
2	D	600	HEM	CBD-CAD-C3D	-4.03	104.79	112.47
2	C	600	HEM	CAD-C3D-C2D	-2.57	121.67	129.00
2	D	600	HEM	CAD-C3D-C2D	-2.07	123.10	129.00
2	C	600	HEM	CBD-CAD-C3D	-2.06	108.53	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	1	0
2	C	600	HEM	3	0
2	D	600	HEM	6	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](#)

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, 95th 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 ²)	Q<0.9
1	A	479/527 (90%)	-0.23	0 100 100	23, 36, 53, 62	0
1	B	479/527 (90%)	-0.23	0 100 100	24, 35, 49, 67	0
1	C	481/527 (91%)	-0.20	0 100 100	24, 39, 55, 72	0
1	D	479/527 (90%)	-0.21	0 100 100	26, 36, 52, 62	0
All	All	1918/2108 (90%)	-0.22	0 100 100	23, 36, 53, 72	0

There are no RSRZ outliers to report.

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	HEM	A	600	43/43	0.96	0.17	2.08	32,37,44,47	0
2	HEM	D	600	43/43	0.97	0.18	1.67	25,36,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEM	C	600	43/43	0.97	0.17	1.28	31,36,40,42	0
2	HEM	B	600	43/43	0.97	0.17	1.09	29,36,41,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.