



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 10:01 PM GMT

PDB ID : 1HYN
Title : CRYSTAL STRUCTURE OF THE CYTOPLASMIC DOMAIN OF HUMAN
ERYTHROCYTE BAND-3 PROTEIN
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Deposited on : 2001-01-20
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

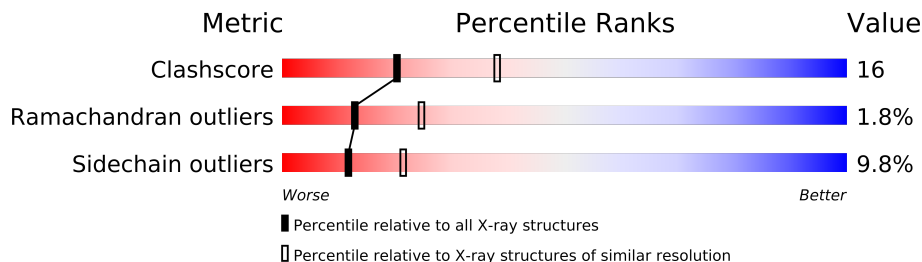
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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 ≥ 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	P	379	
1	Q	379	
1	R	379	
1	S	379	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9698 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 BAND 3 ANION TRANSPORT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	293	Total	C	N	O	S	0	0	0
			2318	1473	404	435	6			
1	Q	302	Total	C	N	O	S	0	0	0
			2382	1511	416	449	6			
1	R	300	Total	C	N	O	S	0	0	0
			2366	1502	412	446	6			
1	S	293	Total	C	N	O	S	0	0	0
			2318	1473	404	435	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	71	Total	O	0	0
			71	71		
2	Q	87	Total	O	0	0
			87	87		
2	R	87	Total	O	0	0
			87	87		
2	S	69	Total	O	0	0
			69	69		

[illegible]

Chain S:

LEU PHE	V293	L167	V65	MET
	R294	L170	M66	GLU
	R296		K69	LEU
		V173	N70	GLN
M300		A176	Q71	ASP
	L311		E72	ASP
L319		T179	R74	TYR
	V320	R180		GLU
L321		P184		ASP
P322		L195		MET
P323				MET
P324				GLU
S328		L199		LEU
	E329			LEU
L332		E202		GLN
	L333	Q203		GLU
S334		G204		GLU
	L335	D205		TYR
V338		G206		GLU
	Q339	G207		ASP
L343		T208		PRO
		E209		ASP
Y347		G210		ILE
	Q348	H211		PRO
SER		S212		GLU
	SER	P213		SER
PRO		I216		GLN
ALA		L217		GLU
LYS		A226		PRO
PRO		T227		ALA
ASP		L228		ALA
SER		V231		HIS
SER		G232		ASP
PHE		D235		THR
TYR		F236		GLU
LYS		L242		ALA
GLY				ALA
LEU		A255		THR
ASP		L258		ASP
LEU		I262		TYR
ASN		L269		HIS
GLY		Y278		THR
PRO		L288		THR
GLN		M289		SER
GLN		K160		HIS
THR				THR
GLY				THR
GLN				HIS
THR				K56
GLY				V57
GLN				E63
THR				L64
GLY				E63
GLN				L64

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.59Å 92.58Å 123.33Å 90.00° 131.86° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (8.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9698	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	P	0.41	0/2366	0.69	2/3213 (0.1%)
1	Q	0.40	0/2433	0.70	1/3305 (0.0%)
1	R	0.41	0/2416	0.70	1/3282 (0.0%)
1	S	0.42	0/2366	0.72	5/3213 (0.2%)
All	All	0.41	0/9581	0.70	9/13013 (0.1%)

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	P	332	LEU	CA-CB-CG	-6.49	100.38	115.30
1	S	56	LYS	N-CA-C	-6.08	94.60	111.00
1	R	82	VAL	N-CA-C	-6.00	94.81	111.00
1	S	332	LEU	CA-CB-CG	-5.92	101.68	115.30
1	S	71	GLN	O-C-N	5.74	131.89	122.70

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	P	2318	0	2320	97	0
1	Q	2382	0	2378	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2366	0	2366	80	0
1	S	2318	0	2320	82	0
2	P	71	0	0	3	0
2	Q	87	0	0	4	0
2	R	87	0	0	3	0
2	S	69	0	0	0	0
All	All	9698	0	9384	297	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 16.

The worst 5 of 297 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:73:LEU:HD13	1:S:184:PRO:HB3	1.29	1.11
1:R:73:LEU:HD13	1:R:184:PRO:HB3	1.30	1.08
1:Q:73:LEU:HD13	1:Q:184:PRO:HB3	1.36	1.07
1:S:87:ASN:HD21	1:S:98:HIS:HE1	1.12	0.98
1:P:73:LEU:O	1:P:159:LEU:HD13	1.66	0.95

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	P	291/379 (77%)	275 (94%)	14 (5%)	2 (1%)	30	58
1	Q	300/379 (79%)	279 (93%)	11 (4%)	10 (3%)	6	9
1	R	298/379 (79%)	280 (94%)	12 (4%)	6 (2%)	11	21
1	S	291/379 (77%)	275 (94%)	13 (4%)	3 (1%)	22	45
All	All	1180/1516 (78%)	1109 (94%)	50 (4%)	21 (2%)	13	25

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	327	PRO
1	Q	204	GLY
1	R	57	VAL
1	R	336	VAL
1	Q	56	LYS

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	P	251/327 (77%)	221 (88%)	30 (12%)	7	13
1	Q	259/327 (79%)	235 (91%)	24 (9%)	13	24
1	R	257/327 (79%)	232 (90%)	25 (10%)	12	22
1	S	251/327 (77%)	230 (92%)	21 (8%)	16	29
All	All	1018/1308 (78%)	918 (90%)	100 (10%)	12	21

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	228	LEU
1	R	69	LYS
1	S	212	SER
1	Q	252	GLU
1	Q	311	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	163	HIS
1	Q	203	GLN
1	S	163	HIS
1	Q	186	GLN
1	R	87	ASN

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 ⓘ

There are no ligands in this entry.

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.