



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 06:18 PM EDT

PDB ID : 3LBX
Title : Crystal Structure of the Erythrocyte Spectrin Tetramerization Domain Complex
Authors : Ipsaro, J.J.; Harper, S.L.; Messick, T.E.; Marmorstein, R.; Mondragon, A.; Speicher, D.W.
Deposited on : unknown
Resolution : 2.80 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

<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
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

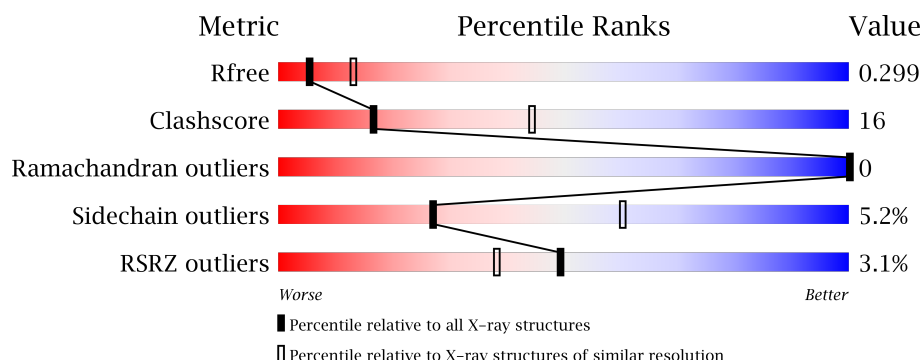
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	161	<div> <div>0.2%</div> <div>60%</div> <div>23%</div> <div>13%</div> </div>
2	B	185	<div> <div>4%</div> <div>70%</div> <div>26%</div> <div>0%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2673 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 Spectrin alpha chain, erythrocyte.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1176	730	211	232	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P02549
A	-1	SER	-	EXPRESSION TAG	UNP P02549
A	0	GLY	-	EXPRESSION TAG	UNP P02549

- Molecule 2 is a protein called Spectrin beta chain, erythrocyte.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1497	935	268	286	8			

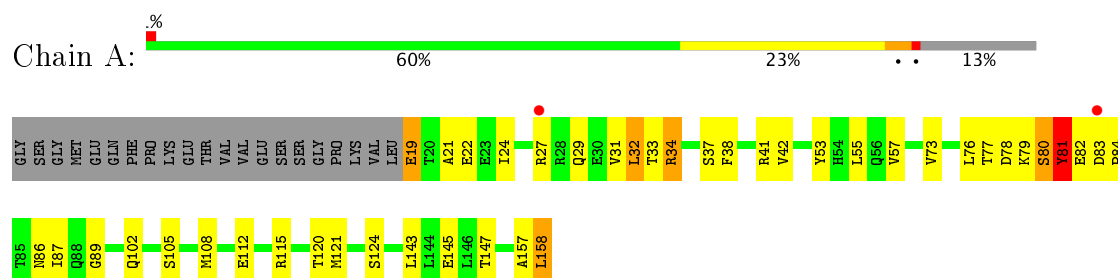
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1900	GLY	-	EXPRESSION TAG	UNP P11277
B	1901	SER	-	EXPRESSION TAG	UNP P11277

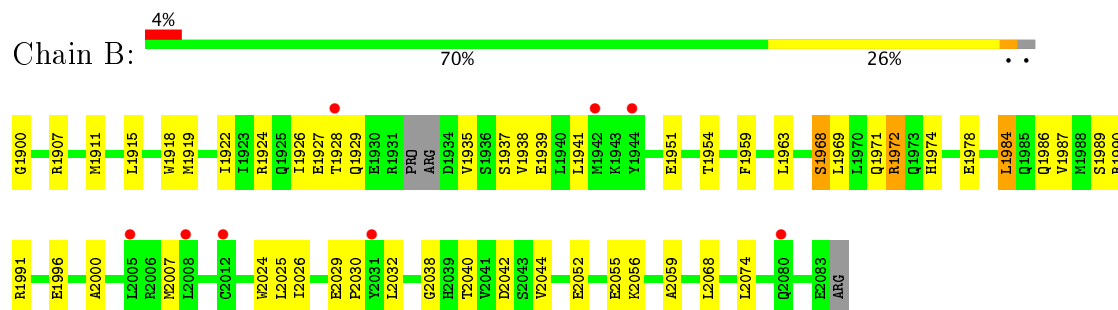
3 Residue-property plots [i](#)

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.

- Molecule 1: Spectrin alpha chain, erythrocyte



- Molecule 2: Spectrin beta chain, erythrocyte



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	213.90Å 213.90Å 31.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.80 36.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.00-2.80) 98.4 (36.68-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.268 , 0.299 0.272 , 0.299	Depositor DCC
R_{free} test set	922 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2673	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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

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	A	0.65	0/1193	0.72	0/1598
2	B	0.48	0/1521	0.59	0/2038
All	All	0.56	0/2714	0.65	0/3636

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	SER	Peptide
1	A	81	TYR	Peptide
2	B	1929	GLN	Peptide

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	1176	0	1159	44	1
2	B	1497	0	1475	44	1
All	All	2673	0	2634	84	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 16.

All (84) 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)
2:B:2052:GLU:HA	2:B:2055:GLU:OE2	1.61	1.00
1:A:29:GLN:O	1:A:32:LEU:HB3	1.78	0.82
1:A:143:LEU:O	1:A:147:THR:HG23	1.82	0.79
2:B:1919:MET:HE2	2:B:1991:ARG:HA	1.63	0.78
2:B:1968:SER:O	2:B:1972:ARG:HG2	1.83	0.78
1:A:76:LEU:HD11	1:A:147:THR:HG22	1.68	0.75
1:A:32:LEU:HD13	1:A:32:LEU:C	2.07	0.74
1:A:158:LEU:HD12	1:A:158:LEU:N	2.08	0.67
2:B:1969:LEU:O	2:B:1972:ARG:O	2.13	0.67
1:A:21:ALA:O	1:A:24:ILE:N	2.28	0.66
1:A:21:ALA:HB3	1:A:24:ILE:HB	1.77	0.65
1:A:87:ILE:CD1	1:A:157:ALA:HB1	2.27	0.65
1:A:32:LEU:HD22	1:A:32:LEU:O	1.98	0.64
1:A:32:LEU:HD13	1:A:33:THR:N	2.14	0.62
1:A:24:ILE:HG21	1:A:27:ARG:HH21	1.66	0.61
1:A:38:PHE:O	1:A:42:VAL:HG23	2.01	0.61
2:B:1951:GLU:O	2:B:1954:THR:OG1	2.19	0.59
1:A:87:ILE:HD13	1:A:157:ALA:CB	2.33	0.58
1:A:83:ASP:N	1:A:84:PRO:HD3	2.17	0.58
2:B:1919:MET:HE3	2:B:1959:PHE:CZ	2.38	0.58
1:A:21:ALA:CB	1:A:24:ILE:HB	2.34	0.58
2:B:1924:ARG:O	2:B:1928:THR:HG23	2.03	0.58
1:A:158:LEU:CD1	1:A:158:LEU:N	2.66	0.57
2:B:1911:MET:O	2:B:1915:LEU:HD13	2.04	0.57
2:B:1907:ARG:O	2:B:1911:MET:HE2	2.05	0.57
2:B:1935:VAL:HG21	2:B:1939:GLU:CB	2.37	0.55
1:A:19:GLU:O	1:A:22:GLU:OE2	2.25	0.55
1:A:87:ILE:HD13	1:A:157:ALA:HB1	1.88	0.55
2:B:1996:GLU:O	2:B:2000:ALA:HB2	2.07	0.55
1:A:120:THR:HG23	1:A:121:MET:O	2.07	0.55
2:B:2024:TRP:HE3	2:B:2025:LEU:HD23	1.71	0.54
1:A:34:ARG:HH21	2:B:2025:LEU:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1972:ARG:O	2:B:1974:HIS:N	2.38	0.54
1:A:83:ASP:N	1:A:84:PRO:CD	2.70	0.54
2:B:1971:GLN:HG2	2:B:1972:ARG:N	2.23	0.53
1:A:19:GLU:N	1:A:19:GLU:CD	2.62	0.53
1:A:27:ARG:O	1:A:31:VAL:HG23	2.09	0.53
2:B:1935:VAL:HG23	2:B:1941:LEU:HD22	1.90	0.53
2:B:2007:MET:SD	2:B:2074:LEU:HD23	2.48	0.52
1:A:86:ASN:ND2	1:A:89:GLY:H	2.07	0.52
1:A:102:GLN:O	1:A:105:SER:HB3	2.10	0.51
2:B:1935:VAL:HG11	2:B:1938:VAL:C	2.30	0.51
2:B:2032:LEU:HD23	2:B:2032:LEU:O	2.10	0.50
2:B:1918:TRP:CZ2	2:B:1922:ILE:HD12	2.48	0.49
1:A:32:LEU:CD1	1:A:32:LEU:C	2.78	0.49
2:B:1919:MET:CE	2:B:1991:ARG:HA	2.40	0.49
2:B:2040:THR:HG22	2:B:2042:ASP:H	1.76	0.49
1:A:73:VAL:O	1:A:77:THR:HG23	2.13	0.48
2:B:1919:MET:HE3	2:B:1959:PHE:HZ	1.78	0.48
1:A:29:GLN:NE2	2:B:2068:LEU:O	2.47	0.48
2:B:2052:GLU:O	2:B:2055:GLU:HG2	2.13	0.48
1:A:34:ARG:HH12	2:B:2026:ILE:CD1	2.26	0.48
1:A:53:TYR:O	1:A:57:VAL:HG23	2.14	0.48
1:A:82:GLU:HB3	1:A:84:PRO:HD3	1.94	0.47
2:B:1986:GLN:HG3	2:B:1990:ARG:NH1	2.30	0.47
2:B:1935:VAL:HG11	2:B:1938:VAL:O	2.15	0.46
2:B:1984:LEU:HA	2:B:1987:VAL:HG12	1.97	0.45
2:B:1935:VAL:HG21	2:B:1939:GLU:HB2	1.99	0.45
1:A:21:ALA:O	1:A:24:ILE:HB	2.16	0.45
2:B:1996:GLU:O	2:B:2000:ALA:CB	2.65	0.45
1:A:24:ILE:HG22	1:A:24:ILE:O	2.16	0.44
1:A:77:THR:C	1:A:79:LYS:H	2.21	0.44
2:B:1968:SER:O	2:B:1972:ARG:CG	2.62	0.44
1:A:19:GLU:C	1:A:22:GLU:OE2	2.56	0.44
2:B:1935:VAL:CG2	2:B:1941:LEU:HD13	2.48	0.44
1:A:87:ILE:HD13	1:A:157:ALA:HB3	2.00	0.43
2:B:1926:ILE:HG22	2:B:1927:GLU:N	2.32	0.43
1:A:76:LEU:CD1	1:A:147:THR:HG22	2.42	0.43
2:B:2040:THR:O	2:B:2044:VAL:HG23	2.19	0.42
2:B:2038:GLY:HA3	2:B:2044:VAL:HG22	2.01	0.42
2:B:2029:GLU:N	2:B:2030:PRO:HD2	2.34	0.42
2:B:1919:MET:HE3	2:B:1959:PHE:CE1	2.55	0.42
1:A:79:LYS:O	1:A:81:TYR:CD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1911:MET:O	2:B:1915:LEU:CD1	2.67	0.42
1:A:24:ILE:HG21	1:A:27:ARG:NH2	2.34	0.42
1:A:108:MET:O	1:A:112:GLU:HG3	2.20	0.41
1:A:55:LEU:HD12	1:A:55:LEU:O	2.20	0.41
2:B:1978:GLU:N	2:B:1978:GLU:OE1	2.47	0.41
1:A:41:ARG:NE	2:B:2032:LEU:HD21	2.35	0.41
1:A:157:ALA:C	1:A:158:LEU:CD1	2.89	0.41
2:B:1937:SER:OG	2:B:1938:VAL:N	2.53	0.41
2:B:1972:ARG:HG2	2:B:1972:ARG:H	1.66	0.40
1:A:19:GLU:CA	1:A:22:GLU:OE2	2.69	0.40
2:B:2056:LYS:O	2:B:2059:ALA:HB3	2.21	0.40

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:A:145:GLU:OE2	2:B:1900:GLY:N[3_546]	2.11	0.09

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	138/161 (86%)	132 (96%)	6 (4%)	0	100	100
2	B	178/185 (96%)	172 (97%)	6 (3%)	0	100	100
All	All	316/346 (91%)	304 (96%)	12 (4%)	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	128/146 (88%)	118 (92%)	10 (8%)	15	39
2	B	160/163 (98%)	155 (97%)	5 (3%)	45	79
All	All	288/309 (93%)	273 (95%)	15 (5%)	27	60

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	32	LEU
1	A	34	ARG
1	A	37	SER
1	A	78	ASP
1	A	80	SER
1	A	81	TYR
1	A	115	ARG
1	A	124	SER
1	A	158	LEU
2	B	1963	LEU
2	B	1968	SER
2	B	1972	ARG
2	B	1984	LEU
2	B	1989	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	86	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	140/161 (86%)	0.23	2 (1%) 75 69	2, 25, 52, 59	0
2	B	182/185 (98%)	0.36	8 (4%) 35 25	4, 35, 51, 55	0
All	All	322/346 (93%)	0.31	10 (3%) 49 38	2, 31, 52, 59	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2012	CYS	5.0
1	A	83	ASP	4.7
2	B	1944	TYR	4.4
2	B	2005	LEU	3.7
2	B	1928	THR	3.1
2	B	2008	LEU	2.3
2	B	2080	GLN	2.2
2	B	1942	MET	2.1
2	B	2031	TYR	2.1
1	A	27	ARG	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.