



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:04 pm BST

PDB ID : 6M3Q
Title : Crystal structure of AnkB/beta4-spectrin complex
Authors : Li, J.; Chen, K.; Zhu, R.; Zhang, M.
Deposited on : 2020-03-04
Resolution : 3.44 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

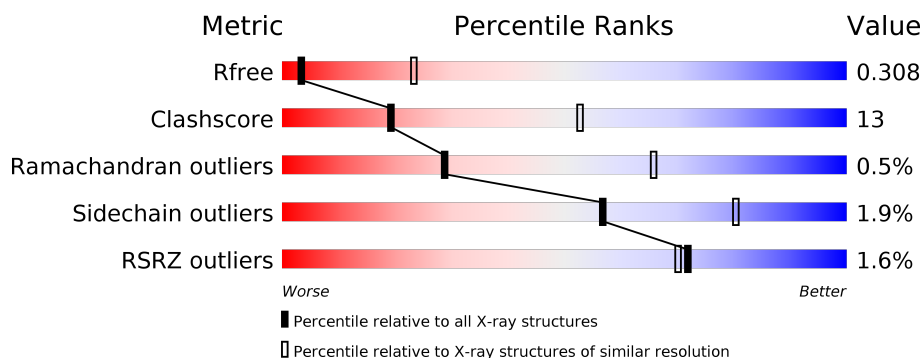
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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}	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)

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 respectively. 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	E	475	<div> <div> <div></div> <div>67%</div> <div>27%</div> <div>• 5%</div> </div> </div>
2	F	322	<div> <div> <div>2%</div> <div>67%</div> <div>26%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5445 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 Ankyrin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	453	Total	C	N	O	S	0	0	0
			3360	2139	581	616	24			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	PHE	deletion	UNP Q01484
E	?	-	LEU	deletion	UNP Q01484
E	?	-	GLY	deletion	UNP Q01484
E	?	-	LYS	deletion	UNP Q01484
E	?	-	LEU	deletion	UNP Q01484
E	?	-	HIS	deletion	UNP Q01484
E	?	-	LEU	deletion	UNP Q01484
E	?	-	PRO	deletion	UNP Q01484
E	?	-	THR	deletion	UNP Q01484
E	?	-	ALA	deletion	UNP Q01484
E	?	-	PRO	deletion	UNP Q01484
E	?	-	PRO	deletion	UNP Q01484
E	?	-	PRO	deletion	UNP Q01484
E	?	-	LEU	deletion	UNP Q01484
E	?	-	ASN	deletion	UNP Q01484
E	?	-	GLU	deletion	UNP Q01484
E	?	-	GLY	deletion	UNP Q01484
E	?	-	GLU	deletion	UNP Q01484
E	?	-	SER	deletion	UNP Q01484
E	?	-	LEU	deletion	UNP Q01484
E	?	-	VAL	deletion	UNP Q01484
E	?	-	SER	deletion	UNP Q01484
E	?	-	ARG	deletion	UNP Q01484
E	?	-	ILE	deletion	UNP Q01484
E	?	-	LEU	deletion	UNP Q01484
E	?	-	GLN	deletion	UNP Q01484
E	?	-	LEU	deletion	UNP Q01484

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLY	deletion	UNP Q01484
E	?	-	PRO	deletion	UNP Q01484
E	?	-	PRO	deletion	UNP Q01484
E	?	-	GLY	deletion	UNP Q01484
E	?	-	THR	deletion	UNP Q01484
E	?	-	LYS	deletion	UNP Q01484

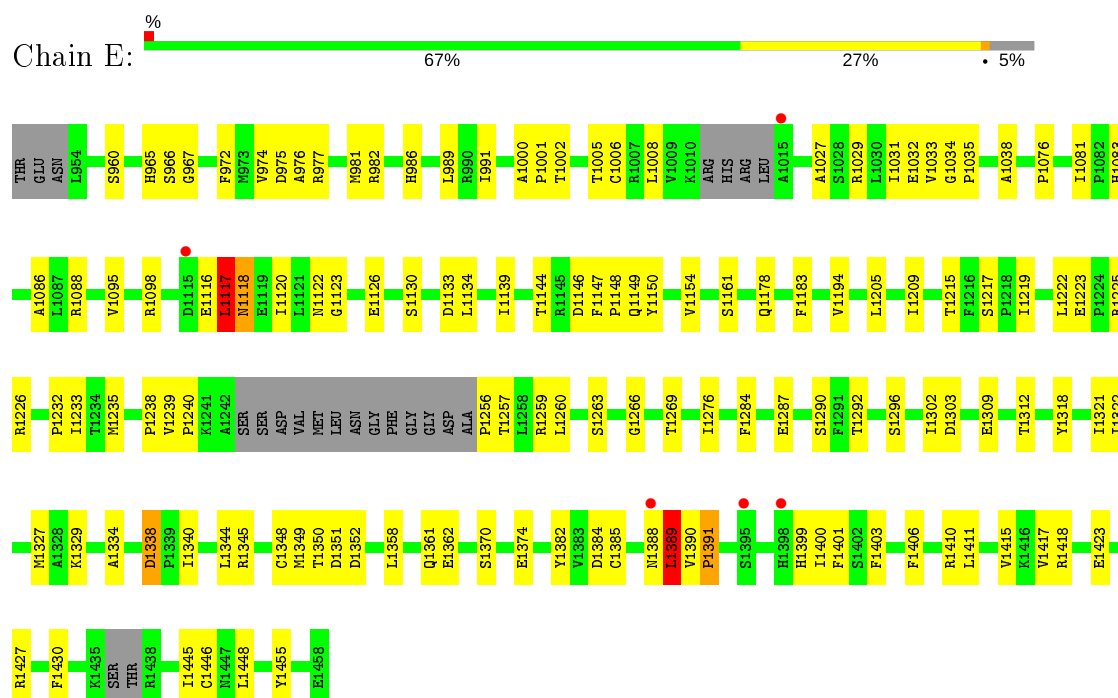
- Molecule 2 is a protein called Spectrin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	301	Total	C	N	O	S	0	0	0
			2085	1321	354	402	8			

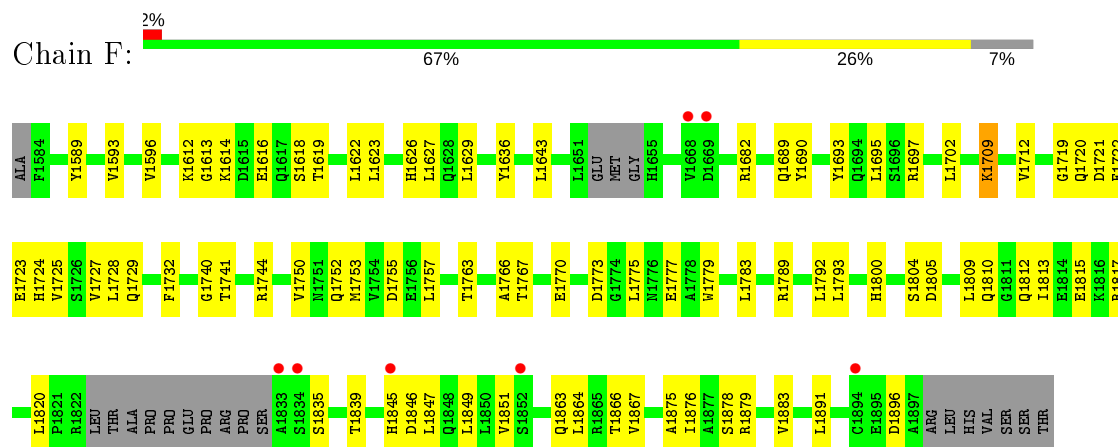
3 Residue-property plots

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.

• Molecule 1: Ankyrin-2



• Molecule 2: Spectrin beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.90Å 110.48Å 131.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.36 – 3.44 35.36 – 3.44	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.36-3.44) 98.0 (35.36-3.44)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.252 , 0.307 0.252 , 0.308	Depositor DCC
R_{free} test set	667 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5445	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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](#)

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	E	0.32	0/3433	0.64	2/4690 (0.0%)
2	F	0.30	0/2116	0.52	1/2893 (0.0%)
All	All	0.32	0/5549	0.60	3/7583 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1117	LEU	CA-CB-CG	7.84	133.33	115.30
1	E	1389	LEU	CA-CB-CG	6.69	130.68	115.30
2	F	1792	LEU	CA-CB-CG	5.11	127.06	115.30

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	E	3360	0	3218	85	1
2	F	2085	0	1821	55	1
All	All	5445	0	5039	135	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 13.

The worst 5 of 135 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:F:1616:GLU:OE1	2:F:1697:ARG:NH2	2.13	0.81
1:E:1005:THR:O	1:E:1033:VAL:HA	1.86	0.75
1:E:1038:ALA:HB3	1:E:1147:PHE:HB2	1.67	0.75
1:E:1098:ARG:NH2	1:E:1146:ASP:OD1	2.20	0.72
1:E:1382:TYR:HA	1:E:1400:ILE:HG22	1.72	0.72

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:E:1226:ARG:NH2	2:F:1896:ASP:OD1[3_654]	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	E	445/475 (94%)	421 (95%)	20 (4%)	4 (1%)	17	54
2	F	295/322 (92%)	288 (98%)	7 (2%)	0	100	100
All	All	740/797 (93%)	709 (96%)	27 (4%)	4 (0%)	29	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	976	ALA
1	E	1148	PRO
1	E	1232	PRO
1	E	1391	PRO

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	E	352/419 (84%)	345 (98%)	7 (2%)	55	79
2	F	174/272 (64%)	171 (98%)	3 (2%)	60	82
All	All	526/691 (76%)	516 (98%)	10 (2%)	57	80

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1389	LEU
1	E	1399	HIS
2	F	1682	ARG
1	E	1338	ASP
1	E	1446	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	986	HIS
1	E	1361	GLN
2	F	1724	HIS

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](#)

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	E	453/475 (95%)	-0.17	5 (1%) 80 77	24, 48, 100, 227	0
2	F	301/322 (93%)	0.02	7 (2%) 60 58	30, 75, 138, 156	0
All	All	754/797 (94%)	-0.09	12 (1%) 72 70	24, 58, 121, 227	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1115	ASP	5.6
1	E	1388	ASN	3.7
1	E	1398	HIS	3.1
2	F	1833	ALA	2.8
2	F	1834	SER	2.8

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.