



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 09:23 PM EDT

PDB ID : 6DC0
Title : Tribbles (TRIB1) pseudokinase fused to CCAAT-enhancer binding protein (C/EBPalpha) degron
Authors : Jamieson, S.A.; Brewster, J.L.; Mace, P.D.
Deposited on : 2018-05-03
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

<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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

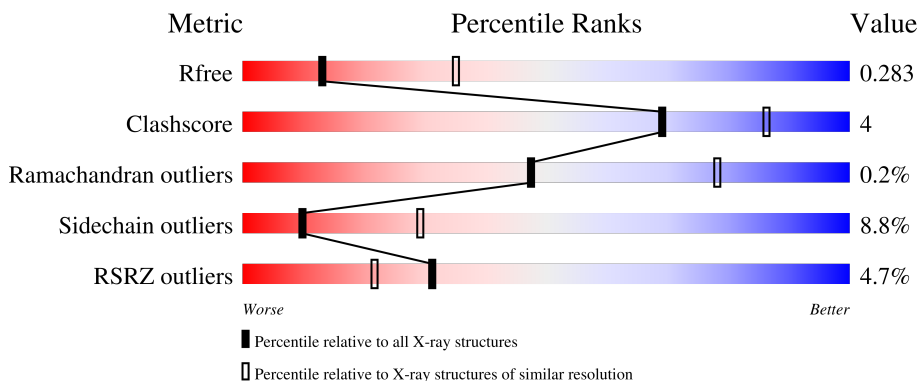
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of 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	A	292	 4% 76% 13% • 9%
1	B	292	 4% 76% 14% •• 8%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4357 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 Tribbles homolog 1,CCAAT/enhancer-binding protein alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2147	1367	382	389	9	0	1	0
1	B	270	2170	1384	382	394	10	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	SER	-	expression tag	UNP Q96RU8
A	85	ALA	-	expression tag	UNP Q96RU8
A	86	PRO	-	expression tag	UNP Q96RU8
A	87	GLY	-	expression tag	UNP Q96RU8
A	88	PRO	-	expression tag	UNP Q96RU8
A	89	SER	-	expression tag	UNP Q96RU8
A	486	GLY	-	linker	UNP Q96RU8
A	487	SER	-	linker	UNP Q96RU8
A	488	GLY	-	linker	UNP Q96RU8
A	489	SER	-	linker	UNP Q96RU8
A	490	SER	-	linker	UNP Q96RU8
A	491	GLY	-	linker	UNP Q96RU8
A	492	GLY	-	linker	UNP Q96RU8
A	494	GLY	LEU	conflict	UNP P49715
B	84	SER	-	expression tag	UNP Q96RU8
B	85	ALA	-	expression tag	UNP Q96RU8
B	86	PRO	-	expression tag	UNP Q96RU8
B	87	GLY	-	expression tag	UNP Q96RU8
B	88	PRO	-	expression tag	UNP Q96RU8
B	89	SER	-	expression tag	UNP Q96RU8
B	486	GLY	-	linker	UNP Q96RU8
B	487	SER	-	linker	UNP Q96RU8
B	488	GLY	-	linker	UNP Q96RU8
B	489	SER	-	linker	UNP Q96RU8
B	490	SER	-	linker	UNP Q96RU8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	491	GLY	-	linker	UNP Q96RU8
B	492	GLY	-	linker	UNP Q96RU8
B	494	GLY	LEU	conflict	UNP P49715

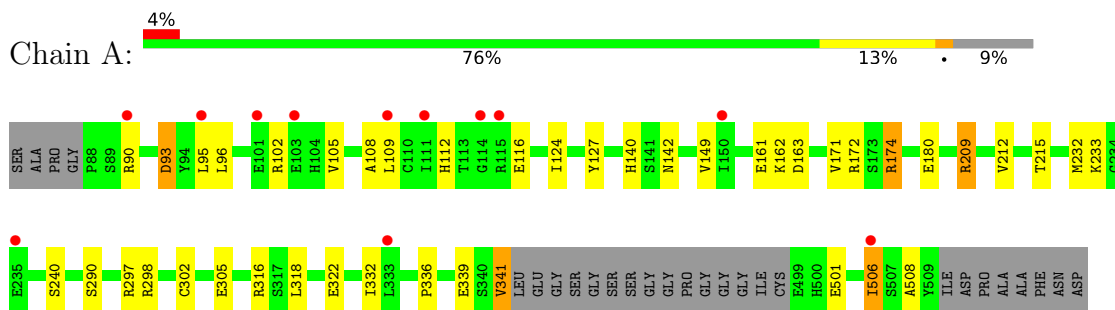
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	20	Total O 20 20	0	0

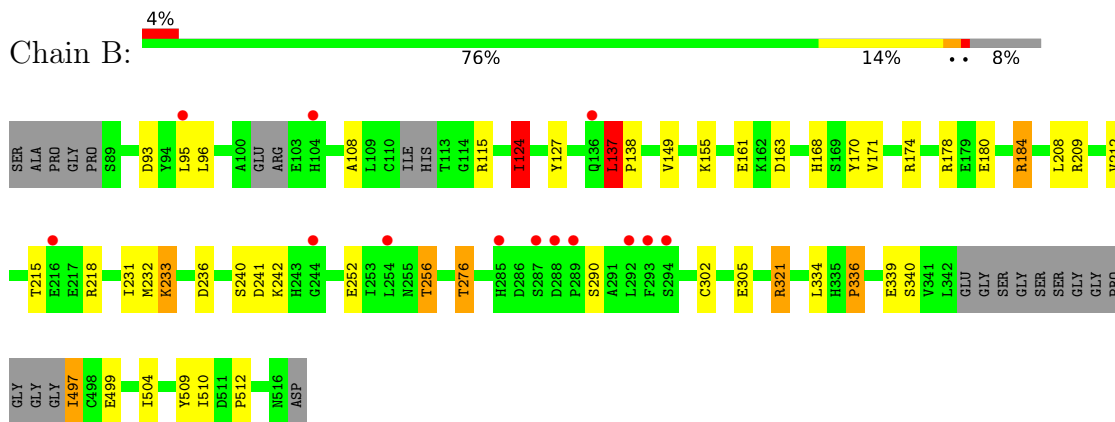
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Tribbles homolog 1,CCAAT/enhancer-binding protein alpha



- Molecule 1: Tribbles homolog 1,CCAAT/enhancer-binding protein alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.81Å 98.81Å 332.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.70 – 2.80 48.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.70-2.80) 99.8 (48.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.220 , 0.277 0.230 , 0.283	Depositor DCC
R_{free} test set	1222 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4357	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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	A	0.56	0/2200	0.86	3/2972 (0.1%)
1	B	0.56	0/2218	0.88	5/2996 (0.2%)
All	All	0.56	0/4418	0.87	8/5968 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	A	209	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	124	ILE	CB-CA-C	-5.97	99.66	111.60
1	A	316	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	241	ASP	CB-CG-OD1	5.49	123.25	118.30
1	A	298	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	184	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	137	LEU	CA-CB-CG	5.01	126.82	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	A	2147	0	2157	17	0
1	B	2170	0	2176	19	0
2	A	20	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	0	0	0
All	All	4357	0	4333	32	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 4.

All (32) 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:B:510:ILE:HG22	1:B:512:PRO:HD3	1.83	0.60
1:B:252:GLU:O	1:B:256:THR:HB	2.08	0.54
1:A:140:HIS:CD2	1:A:142:ASN:H	2.27	0.52
1:A:163:ASP:HB2	1:A:212:VAL:HB	1.90	0.52
1:B:170:TYR:OH	1:B:174:ARG:NH1	2.43	0.52
1:A:506:ILE:C	1:A:506:ILE:HD12	2.31	0.51
1:A:109:LEU:HD23	1:A:116:GLU:HA	1.93	0.51
1:B:163:ASP:HB2	1:B:212:VAL:HB	1.93	0.49
1:B:115:ARG:NH2	1:B:161:GLU:OE2	2.44	0.48
1:A:336:PRO:O	1:A:339:GLU:HG2	2.13	0.48
1:B:336:PRO:O	1:B:339:GLU:HG2	2.13	0.48
1:A:297:ARG:HB3	1:B:334:LEU:HD13	1.96	0.47
1:A:172:ARG:HG3	1:B:497:ILE:HD13	1.96	0.47
1:A:93:ASP:OD2	1:A:112:HIS:NE2	2.48	0.46
1:B:504:ILE:HD12	1:B:509:TYR:CE1	2.50	0.46
1:A:95:LEU:O	1:A:108:ALA:HA	2.16	0.46
1:A:501:GLU:HG3	1:B:168:HIS:CD2	2.50	0.46
1:B:137:LEU:HD22	1:B:138:PRO:HD2	1.97	0.46
1:B:233:LYS:NZ	1:B:236:ASP:OD2	2.49	0.44
1:A:171:VAL:O	1:A:174:ARG:O	2.35	0.44
1:A:162:LYS:HG2	1:A:163:ASP:N	2.33	0.44
1:B:95:LEU:O	1:B:108:ALA:HA	2.18	0.44
1:B:124:ILE:HD13	1:B:155:LYS:C	2.37	0.43
1:B:208:LEU:HD11	1:B:276:THR:CG2	2.48	0.43
1:A:102:ARG:HB3	1:A:105:VAL:HB	1.99	0.43
1:B:171:VAL:O	1:B:174:ARG:O	2.38	0.42
1:A:180:GLU:HA	1:A:341:VAL:HG23	2.01	0.41
1:B:321:ARG:CZ	1:B:321:ARG:HB3	2.51	0.41
1:A:318:LEU:HD21	1:A:332:ILE:HG12	2.03	0.41
1:B:178:ARG:CZ	1:B:180:GLU:HB2	2.51	0.41
1:A:180:GLU:HA	1:A:341:VAL:CG2	2.51	0.40
1:A:506:ILE:HG13	1:B:242:LYS:HB3	2.04	0.40

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	262/292 (90%)	240 (92%)	21 (8%)	1 (0%)	34	66
1	B	262/292 (90%)	249 (95%)	13 (5%)	0	100	100
All	All	524/584 (90%)	489 (93%)	34 (6%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	ALA

5.3.2 Protein sidechains [i](#)

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	237/252 (94%)	218 (92%)	19 (8%)	12	34
1	B	239/252 (95%)	216 (90%)	23 (10%)	8	24
All	All	476/504 (94%)	434 (91%)	42 (9%)	10	29

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	93	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	LEU
1	A	124	ILE
1	A	127	TYR
1	A	149	VAL
1	A	161	GLU
1	A	174	ARG
1	A	209	ARG
1	A	215	THR
1	A	232	MET
1	A	233	LYS
1	A	240	SER
1	A	290	SER
1	A	302	CYS
1	A	305	GLU
1	A	322	GLU
1	A	341	VAL
1	A	506	ILE
1	B	93	ASP
1	B	96	LEU
1	B	124	ILE
1	B	127	TYR
1	B	137	LEU
1	B	149	VAL
1	B	184	ARG
1	B	209	ARG
1	B	215	THR
1	B	231	ILE
1	B	232	MET
1	B	233	LYS
1	B	240	SER
1	B	256	THR
1	B	276	THR
1	B	290	SER
1	B	302	CYS
1	B	305	GLU
1	B	321	ARG
1	B	336	PRO
1	B	340	SER
1	B	497	ILE
1	B	499	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	140	HIS
1	A	335	HIS
1	B	168	HIS
1	B	516	ASN

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 monosaccharides 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

6.1 Protein, DNA and RNA chains

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	265/292 (90%)	0.27	12 (4%) 33 23	77, 104, 145, 176	0
1	B	270/292 (92%)	0.29	13 (4%) 30 21	86, 114, 153, 182	0
All	All	535/584 (91%)	0.28	25 (4%) 31 22	77, 109, 152, 182	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	ILE	4.7
1	A	333	LEU	3.7
1	B	293	PHE	3.7
1	A	506	ILE	3.6
1	B	292	LEU	3.5
1	A	114	GLY	3.4
1	A	109	LEU	3.3
1	B	287	SER	3.2
1	B	289	PRO	3.2
1	A	95	LEU	3.1
1	B	254	LEU	3.0
1	A	103	GLU	3.0
1	B	95	LEU	2.9
1	A	90	ARG	2.7
1	B	294	SER	2.5
1	B	136	GLN	2.5
1	B	244	GLY	2.5
1	A	101	GLU	2.5
1	B	104	HIS	2.3
1	A	115	ARG	2.3
1	B	288	ASP	2.1
1	B	285	HIS	2.1
1	A	150	ILE	2.1
1	A	235	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	216	GLU	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 monosaccharides 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.