



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 10:01 pm BST

PDB ID : 2IYB
Title : Structure of complex between the 3rd LIM domain of TES and the EVH1 domain of Mena
Authors : Briggs, D.C.; McDonald, N.Q.
Deposited on : 2006-07-14
Resolution : 2.35 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

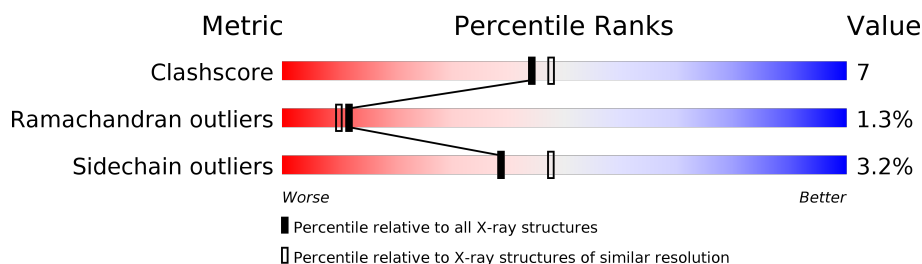
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	114	95% 5%
1	B	114	93% . . .
1	C	114	82% 11% 6% .
1	D	114	89% 9% . .
2	E	65	83% 12% . .
2	F	65	82% 9% 6% .
2	G	65	88% 11% .
2	H	65	78% 12% 5% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5780 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 PROTEIN ENABLED HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			878	550	161	161	6			
1	B	113	Total	C	N	O	S	0	0	0
			873	548	161	158	6			
1	C	112	Total	C	N	O	S	0	0	0
			856	540	156	155	5			
1	D	112	Total	C	N	O	S	0	0	0
			875	547	163	160	5			

- Molecule 2 is a protein called TESTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	64	Total	C	N	O	S	0	0	0
			480	302	82	84	12			
2	F	63	Total	C	N	O	S	0	0	0
			479	298	82	87	12			
2	G	64	Total	C	N	O	S	0	0	0
			469	293	82	82	12			
2	H	63	Total	C	N	O	S	0	0	0
			477	296	82	87	12			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	2	Total	Zn	0	0
			2	2		
3	G	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		
3	E	3	Total	Zn	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	66	Total O 66 66	0	0
4	B	72	Total O 72 72	0	0
4	C	44	Total O 44 44	0	0
4	D	60	Total O 60 60	0	0
4	E	42	Total O 42 42	0	0
4	F	38	Total O 38 38	0	0
4	G	32	Total O 32 32	0	0
4	H	30	Total O 30 30	0	0

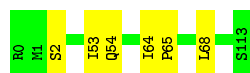
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: PROTEIN ENABLED HOMOLOG

Chain A: 




- Molecule 1: PROTEIN ENABLED HOMOLOG

Chain B: 




- Molecule 1: PROTEIN ENABLED HOMOLOG

Chain C: 




- Molecule 1: PROTEIN ENABLED HOMOLOG

Chain D: 




- Molecule 2: TESTIN

Chain E: 

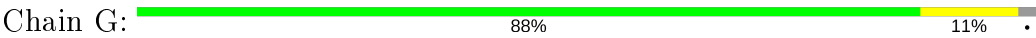


- Molecule 2: TESTIN

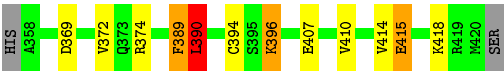
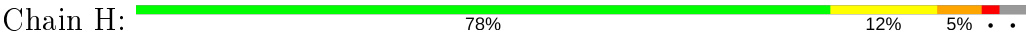
Chain F: 



● Molecule 2: TESTIN



● Molecule 2: TESTIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	66.55 Å 292.93 Å 37.13 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.96 – 2.35	Depositor
% Data completeness (in resolution range)	100.0 (64.96-2.35)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5780	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0/898	0.54	0/1217
1	B	0.41	0/893	0.53	0/1209
1	C	0.39	0/876	0.50	0/1189
1	D	0.40	0/895	0.51	0/1212
2	E	0.44	0/490	0.64	0/661
2	F	0.43	0/489	0.69	0/660
2	G	0.39	0/479	0.56	0/648
2	H	0.44	0/487	0.68	0/657
All	All	0.41	0/5507	0.57	0/7453

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	B	0	2
1	C	0	3
2	E	0	1
2	F	0	1
2	H	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	MET	Peptide
1	B	94	LYS	Peptide
1	C	55	ASP	Peptide
1	C	73	ALA	Peptide
1	C	83	ALA	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	878	0	825	4	0
1	B	873	0	830	12	0
1	C	856	0	796	20	0
1	D	875	0	828	4	0
2	E	480	0	441	8	0
2	F	479	0	443	10	0
2	G	469	0	421	3	0
2	H	477	0	436	11	0
3	E	3	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	66	0	0	0	0
4	B	72	0	0	2	0
4	C	44	0	0	1	0
4	D	60	0	0	0	0
4	E	42	0	0	0	0
4	F	38	0	0	0	0
4	G	32	0	0	0	0
4	H	30	0	0	1	0
All	All	5780	0	5020	69	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 7.

The worst 5 of 69 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:C:83:ALA:HB3	1:C:84:ARG:CB	1.80	1.09
2:F:419:ARG:HG2	2:F:419:ARG:HH11	1.02	1.08
1:C:74:THR:HG21	4:C:2032:HOH:O	1.63	0.98
1:C:83:ALA:CB	1:C:84:ARG:CB	2.42	0.96
1:B:1:MET:N	1:B:2:SER:HB3	1.80	0.95

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	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
1	B	111/114 (97%)	104 (94%)	6 (5%)	1 (1%)	17	17
1	C	110/114 (96%)	103 (94%)	4 (4%)	3 (3%)	5	2
1	D	110/114 (96%)	107 (97%)	2 (2%)	1 (1%)	17	17
2	E	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	9	8
2	F	61/65 (94%)	56 (92%)	4 (7%)	1 (2%)	9	8
2	G	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
2	H	61/65 (94%)	56 (92%)	3 (5%)	2 (3%)	4	2
All	All	689/716 (96%)	648 (94%)	32 (5%)	9 (1%)	12	10

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	HIS
1	C	74	THR
1	D	83	ALA
2	H	390	LEU
2	H	415	GLU

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	88/94 (94%)	87 (99%)	1 (1%)	73	84
1	B	88/94 (94%)	87 (99%)	1 (1%)	73	84
1	C	83/94 (88%)	82 (99%)	1 (1%)	71	82
1	D	89/94 (95%)	86 (97%)	3 (3%)	37	46
2	E	52/59 (88%)	50 (96%)	2 (4%)	33	41
2	F	55/59 (93%)	51 (93%)	4 (7%)	14	14
2	G	50/59 (85%)	48 (96%)	2 (4%)	31	39
2	H	54/59 (92%)	50 (93%)	4 (7%)	13	14
All	All	559/612 (91%)	541 (97%)	18 (3%)	39	47

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	374	ARG
2	F	379	ASN
2	H	374	ARG
2	E	373	GLN
2	E	374	ARG

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

Mol	Chain	Res	Type
1	D	20	ASN
2	E	362	GLN

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 ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.