wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 05:01 PM EDT

PDB ID	:	4ZEM
Title	:	Crystal structure of eIF2B beta from Chaetomium thermophilum
Authors	:	Kuhle, B.; Ficner, R.
Deposited on	:	2015-04-20
Resolution	:	2.55 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 (i) 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 (1)) were used in the production of this report:

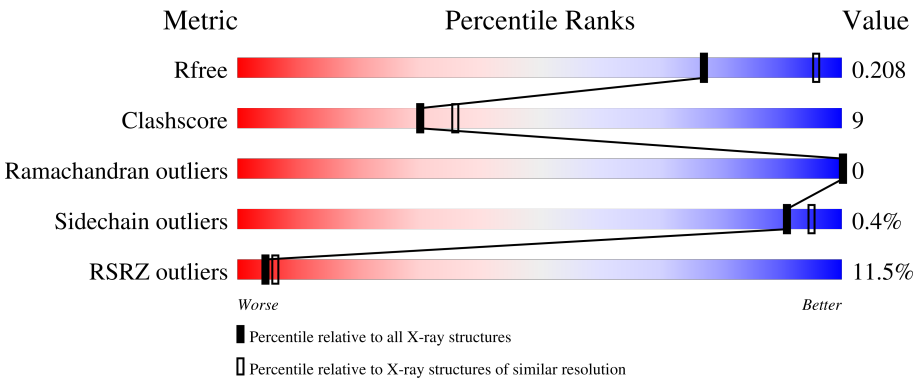
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	393	6% 73% 11% 17%
1	B	393	12% 57% 19% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4904 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 Translation initiation factor eIF2b-like protein,Translation initiation factor eIF2b-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2540	1608	447	477	8	0	2	0
			Total	C	N	O	S			
1	B	298	2304	1462	405	431	6	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	VAL	-	linker	UNP G0SEE6
A	94	ARG	-	linker	UNP G0SEE6
A	95	ARG	-	linker	UNP G0SEE6
A	96	VAL	-	linker	UNP G0SEE6
A	97	LEU	-	linker	UNP G0SEE6
A	98	GLY	-	linker	UNP G0SEE6
A	99	LEU	-	linker	UNP G0SEE6
A	100	ILE	-	linker	UNP G0SEE6
A	101	ARG	-	linker	UNP G0SEE6
A	102	ASP	-	linker	UNP G0SEE6
A	103	GLU	-	linker	UNP G0SEE6
A	104	ALA	-	linker	UNP G0SEE6
A	105	SER	-	linker	UNP G0SEE6
A	106	GLU	-	linker	UNP G0SEE6
A	107	ASN	-	linker	UNP G0SEE6
A	108	ARG	-	linker	UNP G0SEE6
A	109	ASN	-	linker	UNP G0SEE6
A	110	ALA	-	linker	UNP G0SEE6
A	111	ASP	-	linker	UNP G0SEE6
A	112	ASP	-	linker	UNP G0SEE6
A	113	ILE	-	linker	UNP G0SEE6
A	114	ALA	-	linker	UNP G0SEE6
A	115	SER	-	linker	UNP G0SEE6
A	116	ASP	-	linker	UNP G0SEE6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ALA	-	linker	UNP G0SEE6
A	118	ALA	-	linker	UNP G0SEE6
A	119	SER	-	linker	UNP G0SEE6
A	120	ASP	-	linker	UNP G0SEE6
A	121	ILE	-	linker	UNP G0SEE6
A	122	GLN	-	linker	UNP G0SEE6
B	93	VAL	-	linker	UNP G0SEE6
B	94	ARG	-	linker	UNP G0SEE6
B	95	ARG	-	linker	UNP G0SEE6
B	96	VAL	-	linker	UNP G0SEE6
B	97	LEU	-	linker	UNP G0SEE6
B	98	GLY	-	linker	UNP G0SEE6
B	99	LEU	-	linker	UNP G0SEE6
B	100	ILE	-	linker	UNP G0SEE6
B	101	ARG	-	linker	UNP G0SEE6
B	102	ASP	-	linker	UNP G0SEE6
B	103	GLU	-	linker	UNP G0SEE6
B	104	ALA	-	linker	UNP G0SEE6
B	105	SER	-	linker	UNP G0SEE6
B	132	GLU	-	linker	UNP G0SEE6
B	133	ASN	-	linker	UNP G0SEE6
B	134	ARG	-	linker	UNP G0SEE6
B	135	ASN	-	linker	UNP G0SEE6
B	136	ALA	-	linker	UNP G0SEE6
B	137	ASP	-	linker	UNP G0SEE6
B	138	ASP	-	linker	UNP G0SEE6
B	139	ILE	-	linker	UNP G0SEE6
B	140	ALA	-	linker	UNP G0SEE6
B	141	SER	-	linker	UNP G0SEE6
B	142	ASP	-	linker	UNP G0SEE6
B	143	ALA	-	linker	UNP G0SEE6
B	144	ALA	-	linker	UNP G0SEE6
B	145	SER	-	linker	UNP G0SEE6
B	146	ASP	-	linker	UNP G0SEE6
B	147	ILE	-	linker	UNP G0SEE6
B	148	GLN	-	linker	UNP G0SEE6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	34	34	34	0	0

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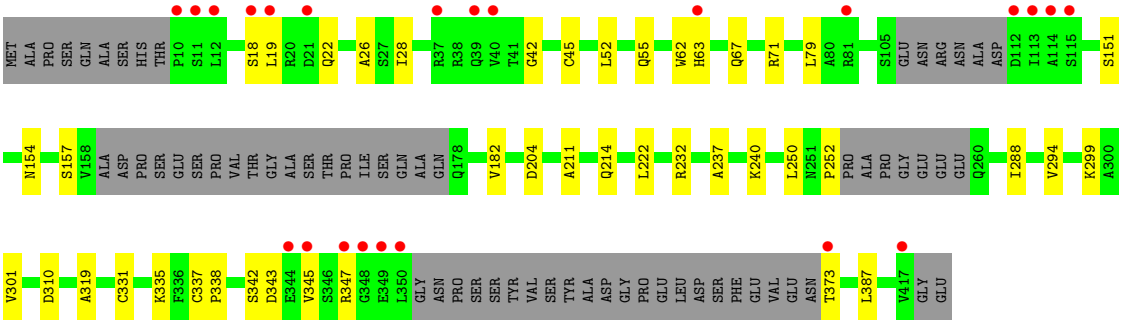
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	26	26	26	0	0

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.

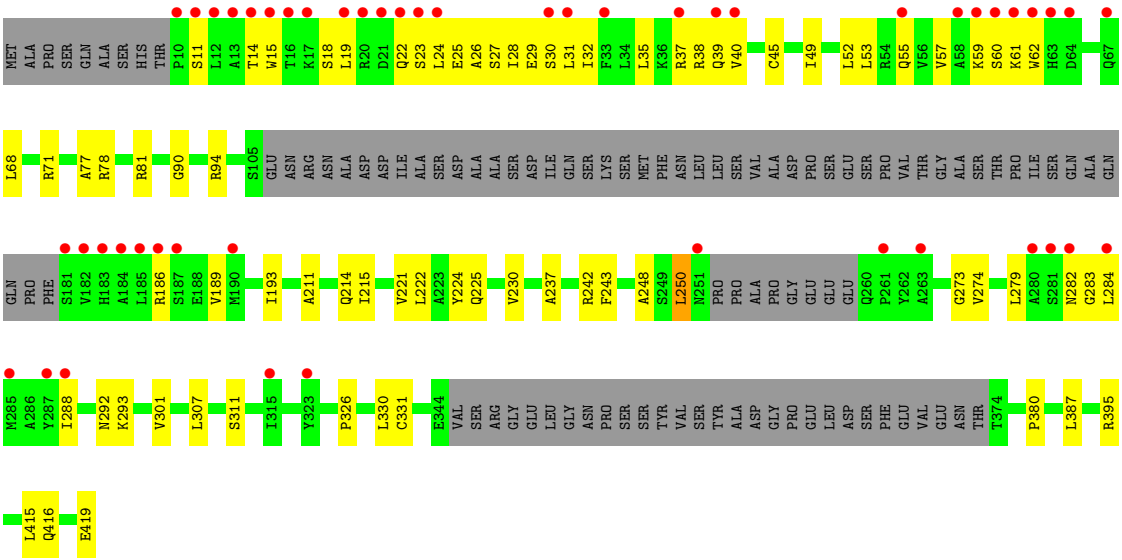
• Molecule 1: Translation initiation factor eIF2b-like protein,Translation initiation factor eIF2b-like protein

Chain A:



• Molecule 1: Translation initiation factor eIF2b-like protein,Translation initiation factor eIF2b-like protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	138.00Å 138.00Å 146.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.46 – 2.55 46.32 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.46-2.55) 99.9 (46.32-2.54)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.176 , 0.204 0.183 , 0.208	Depositor DCC
R_{free} test set	1728 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4904	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.31	0/2583	0.51	0/3501
1	B	0.30	0/2344	0.52	0/3178
All	All	0.31	0/4927	0.52	0/6679

There are no bond length outliers.

There are no bond angle outliers.

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	2540	0	2555	25	0
1	B	2304	0	2327	66	0
2	A	34	0	0	0	0
2	B	26	0	0	0	0
All	All	4904	0	4882	90	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 9.

The worst 5 of 90 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:25:GLU:O	1:B:29:GLU:HG3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLN:NE2	1:B:27:SER:OG	2.12	0.81
1:B:35:LEU:HD23	1:B:40:VAL:CG2	2.13	0.79
1:A:343:ASP:O	1:A:347:ARG:HG3	1.87	0.74
1:A:204:ASP:OD2	1:A:232[B]:ARG:NH2	2.20	0.74

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	320/393 (81%)	317 (99%)	3 (1%)	0	100	100
1	B	290/393 (74%)	287 (99%)	3 (1%)	0	100	100
All	All	610/786 (78%)	604 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	271/323 (84%)	271 (100%)	0	100	100
1	B	244/323 (76%)	242 (99%)	2 (1%)	81	88
All	All	515/646 (80%)	513 (100%)	2 (0%)	91	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39	GLN
1	B	250	LEU

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

Mol	Chain	Res	Type
1	B	22	GLN
1	B	39	GLN
1	B	55	GLN

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 (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	328/393 (83%)	0.50	23 (7%)	16	19	32, 61, 117, 150	0
1	B	298/393 (75%)	0.98	49 (16%)	1	1	36, 74, 143, 161	0
All	All	626/786 (79%)	0.73	72 (11%)	4	6	32, 66, 133, 161	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	ARG	7.1
1	B	10	PRO	6.8
1	B	63	HIS	5.8
1	A	349	GLU	5.5
1	B	184	ALA	5.5

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.