



wwPDB X-ray Structure Validation Summary Report

Feb 19, 2016 – 07:45 PM GMT

PDB ID : 4WPX
Title : Chaetomium thermophilum TREX2 CID domain complex
Authors : Valkov, E.; Stewart, M.
Deposited on : 2014-10-21
Resolution : 3.31 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
<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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

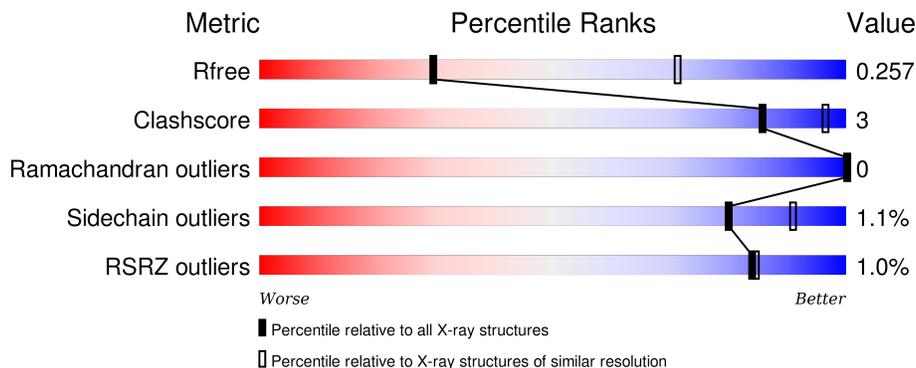
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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	177	 93%
1	D	177	 90% 7%
2	B	89	 79% 12% 9%
2	E	89	 84% 7% 9%
3	C	181	 52% 8% 40%

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Mol	Chain	Length	Quality of chain
3	F	181	 <p>A horizontal bar chart showing the quality of chain. The bar is divided into four segments: a small red segment (2%), a large green segment (56%), a small yellow segment (9%), and a large grey segment (35%).</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 11834 atoms, of which 5845 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 Cell division control protein 31-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	171	2749	873	1350	249	270	7	0	0	0
1	D	172	2773	879	1363	253	271	7	0	0	0

- Molecule 2 is a protein called Putative SAC3 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	81	1404	454	688	135	125	2	0	0	0
2	E	81	1404	454	688	135	125	2	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1082	GLY	-	expression tag	UNP G0SGL4
B	1083	HIS	-	expression tag	UNP G0SGL4
B	1084	MET	-	expression tag	UNP G0SGL4
E	1082	GLY	-	expression tag	UNP G0SGL4
E	1083	HIS	-	expression tag	UNP G0SGL4
E	1084	MET	-	expression tag	UNP G0SGL4

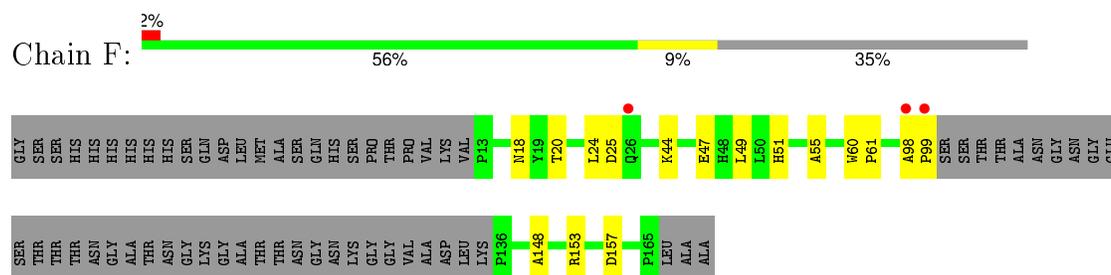
- Molecule 3 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	108	1686	526	846	155	158	1	0	0	0
3	F	117	1818	569	910	164	173	2	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	GLY	-	expression tag	UNP G0S6Y1
C	-11	SER	-	expression tag	UNP G0S6Y1
C	-10	SER	-	expression tag	UNP G0S6Y1
C	-9	HIS	-	expression tag	UNP G0S6Y1
C	-8	HIS	-	expression tag	UNP G0S6Y1
C	-7	HIS	-	expression tag	UNP G0S6Y1
C	-6	HIS	-	expression tag	UNP G0S6Y1
C	-5	HIS	-	expression tag	UNP G0S6Y1
C	-4	HIS	-	expression tag	UNP G0S6Y1
C	-3	SER	-	expression tag	UNP G0S6Y1
C	-2	GLN	-	expression tag	UNP G0S6Y1
C	-1	ASP	-	expression tag	UNP G0S6Y1
C	0	LEU	-	expression tag	UNP G0S6Y1
F	-12	GLY	-	expression tag	UNP G0S6Y1
F	-11	SER	-	expression tag	UNP G0S6Y1
F	-10	SER	-	expression tag	UNP G0S6Y1
F	-9	HIS	-	expression tag	UNP G0S6Y1
F	-8	HIS	-	expression tag	UNP G0S6Y1
F	-7	HIS	-	expression tag	UNP G0S6Y1
F	-6	HIS	-	expression tag	UNP G0S6Y1
F	-5	HIS	-	expression tag	UNP G0S6Y1
F	-4	HIS	-	expression tag	UNP G0S6Y1
F	-3	SER	-	expression tag	UNP G0S6Y1
F	-2	GLN	-	expression tag	UNP G0S6Y1
F	-1	ASP	-	expression tag	UNP G0S6Y1
F	0	LEU	-	expression tag	UNP G0S6Y1

- Molecule 3: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.53Å 168.29Å 69.22Å 90.00° 112.21° 90.00°	Depositor
Resolution (Å)	19.90 – 3.31 19.90 – 3.31	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.90-3.31) 89.4 (19.90-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.218 , 0.277 0.223 , 0.257	Depositor DCC
R_{free} test set	887 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.3	EDS
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 17466 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11834	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.24	0/1426	0.38	0/1921
1	D	0.24	0/1437	0.39	0/1935
2	B	0.29	0/735	0.40	0/987
2	E	0.29	0/735	0.43	0/987
3	C	0.26	0/856	0.48	0/1167
3	F	0.29	0/926	0.53	0/1264
All	All	0.26	0/6115	0.43	0/8261

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	1399	1350	1350	4	0
1	D	1410	1363	1363	7	0
2	B	716	688	688	7	0
2	E	716	688	688	3	0
3	C	840	846	846	7	0
3	F	908	910	910	9	0
All	All	5989	5845	5845	33	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 3.

The worst 5 of 33 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:D:84:CYS:SG	1:D:89:ARG:NH1	2.54	0.81
1:D:8:GLN:OE1	1:D:89:ARG:NH2	2.24	0.70
1:A:173:MET:O	2:B:1160:ARG:NH2	2.31	0.64
1:D:53:ARG:NH2	2:E:1137:GLU:OE2	2.33	0.61
1:A:8:GLN:OE1	1:A:89:ARG:NH2	2.33	0.60

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	169/177 (96%)	168 (99%)	1 (1%)	0	100	100
1	D	170/177 (96%)	169 (99%)	1 (1%)	0	100	100
2	B	79/89 (89%)	78 (99%)	1 (1%)	0	100	100
2	E	79/89 (89%)	77 (98%)	2 (2%)	0	100	100
3	C	104/181 (58%)	101 (97%)	3 (3%)	0	100	100
3	F	113/181 (62%)	110 (97%)	3 (3%)	0	100	100
All	All	714/894 (80%)	703 (98%)	11 (2%)	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	151/155 (97%)	150 (99%)	1 (1%)	88	95
1	D	152/155 (98%)	150 (99%)	2 (1%)	76	89
2	B	71/78 (91%)	71 (100%)	0	100	100
2	E	71/78 (91%)	70 (99%)	1 (1%)	74	89
3	C	94/150 (63%)	93 (99%)	1 (1%)	80	91
3	F	102/150 (68%)	100 (98%)	2 (2%)	63	85
All	All	641/766 (84%)	634 (99%)	7 (1%)	80	91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	172	LEU
3	F	49	LEU
2	E	1091	MET
3	C	18	ASN
3	F	18	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	A	171/177 (96%)	-0.12	0 100 100	45, 81, 121, 141	0
1	D	172/177 (97%)	-0.17	2 (1%) 81 81	42, 80, 122, 144	0
2	B	81/89 (91%)	-0.15	0 100 100	47, 74, 97, 118	0
2	E	81/89 (91%)	-0.23	0 100 100	51, 74, 99, 122	0
3	C	108/181 (59%)	0.00	2 (1%) 70 69	46, 82, 123, 139	0
3	F	117/181 (64%)	0.09	3 (2%) 59 58	51, 86, 127, 145	0
All	All	730/894 (81%)	-0.09	7 (0%) 84 84	42, 79, 121, 145	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	99	PRO	4.5
3	F	98	ALA	2.9
3	F	26	GLN	2.9
1	D	80	HIS	2.5
3	C	159	LEU	2.4

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

There are no such residues in this entry.