



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 7, 2018 – 11:06 PM EDT

PDB ID : 5F5U
Title : Crystal structure of the Snu23-Prp38-MFAP1(217-258) complex of Chaetomium thermophilum
Authors : Ulrich, A.K.C.; Seeger, M.; Bartlick, N.; Wahl, M.C.
Deposited on : 2015-12-04
Resolution : 2.75 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	:	rb-20031021
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

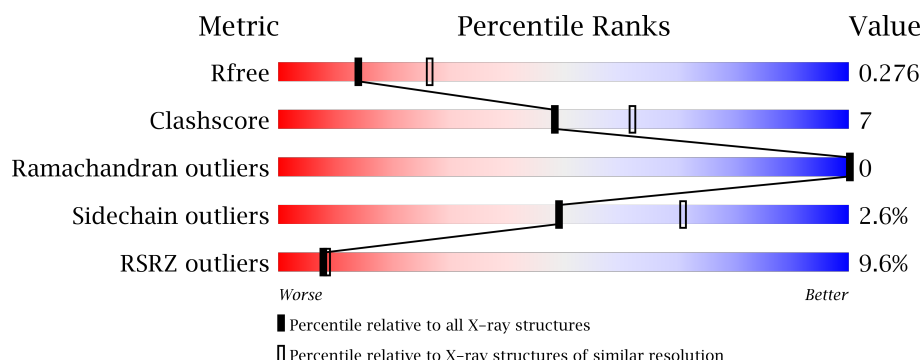
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	111664	1033 (2.76-2.72)
Clashscore	122126	1084 (2.76-2.72)
Ramachandran outliers	120053	1064 (2.76-2.72)
Sidechain outliers	120020	1065 (2.76-2.72)
RSRZ outliers	108989	1008 (2.76-2.72)

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	223	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>16%</div> </div> </div>
1	D	223	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>9%</div> </div> </div>
1	G	223	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	84	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>•</div> <div>46%</div> </div> </div>
2	E	84	<div> <div>4%</div> <div> <div></div> <div>38%</div> <div>7%</div> <div>55%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	84	<div><div></div><div>5%</div><div>43%</div><div>7%</div><div>50%</div></div>
3	C	36	<div><div></div><div>14%</div><div>72%</div><div>17%</div><div>11%</div></div>
3	F	36	<div><div></div><div>14%</div><div>58%</div><div>22%</div><div>19%</div></div>
3	I	36	<div><div></div><div>17%</div><div>72%</div><div>6%</div><div>22%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6676 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 Prp38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1530	984	260	280	6			
1	D	202	Total	C	N	O	S	0	0	0
			1636	1044	280	306	6			
1	G	194	Total	C	N	O	S	0	0	0
			1576	1011	268	291	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G0S1D3
A	-1	ALA	-	expression tag	UNP G0S1D3
A	0	MET	-	expression tag	UNP G0S1D3
A	1	GLY	-	expression tag	UNP G0S1D3
D	-2	GLY	-	expression tag	UNP G0S1D3
D	-1	ALA	-	expression tag	UNP G0S1D3
D	0	MET	-	expression tag	UNP G0S1D3
D	1	GLY	-	expression tag	UNP G0S1D3
G	-2	GLY	-	expression tag	UNP G0S1D3
G	-1	ALA	-	expression tag	UNP G0S1D3
G	0	MET	-	expression tag	UNP G0S1D3
G	1	GLY	-	expression tag	UNP G0S1D3

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	45	Total	C	N	O	S	0	0	0
			374	225	74	74	1			
2	E	38	Total	C	N	O		0	0	0
			334	203	70	61				
2	H	42	Total	C	N	O		0	0	0
			364	219	74	71				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	213	GLY	-	expression tag	UNP G0SHD7
B	214	ALA	-	expression tag	UNP G0SHD7
B	215	MET	-	expression tag	UNP G0SHD7
B	216	GLY	-	expression tag	UNP G0SHD7
E	213	GLY	-	expression tag	UNP G0SHD7
E	214	ALA	-	expression tag	UNP G0SHD7
E	215	MET	-	expression tag	UNP G0SHD7
E	216	GLY	-	expression tag	UNP G0SHD7
H	213	GLY	-	expression tag	UNP G0SHD7
H	214	ALA	-	expression tag	UNP G0SHD7
H	215	MET	-	expression tag	UNP G0SHD7
H	216	GLY	-	expression tag	UNP G0SHD7

- Molecule 3 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	32	Total	C	N	O	0	0	0
			268	168	49	51			
3	F	29	Total	C	N	O	0	0	0
			251	158	46	47			
3	I	28	Total	C	N	O	0	0	0
			242	153	45	44			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	129	GLY	-	expression tag	UNP G0S6R0
C	130	ALA	-	expression tag	UNP G0S6R0
F	129	GLY	-	expression tag	UNP G0S6R0
F	130	ALA	-	expression tag	UNP G0S6R0
I	129	GLY	-	expression tag	UNP G0S6R0
I	130	ALA	-	expression tag	UNP G0S6R0

- Molecule 4 is water.

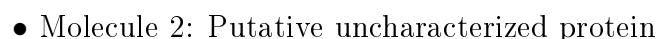
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	7	Total	O	0	0
			7	7		

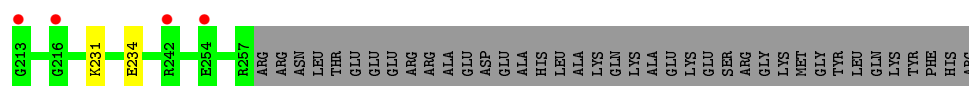
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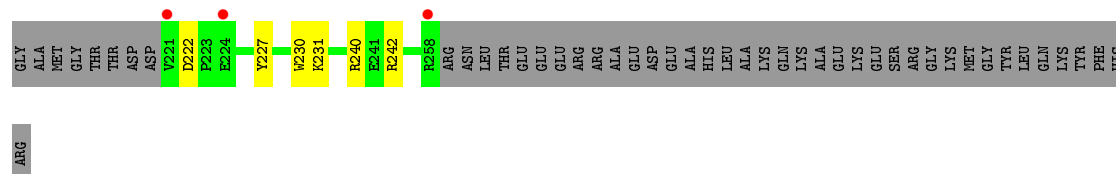
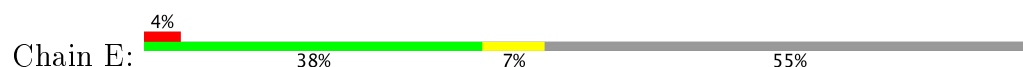
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	5	Total 5	O 5	0	0
4	D	27	Total 27	O 27	0	0
4	E	2	Total 2	O 2	0	0
4	F	3	Total 3	O 3	0	0
4	G	30	Total 30	O 30	0	0
4	H	5	Total 5	O 5	0	0
4	I	2	Total 2	O 2	0	0

- Molecule 1: Prp38

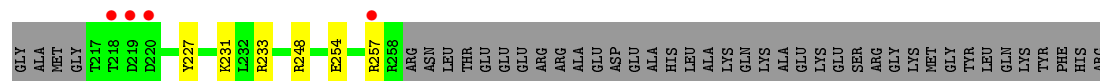
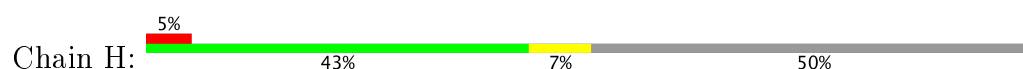




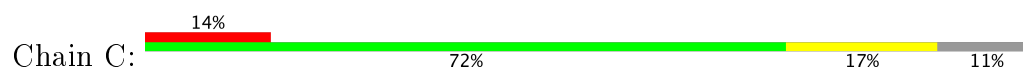
- Molecule 2: Putative uncharacterized protein



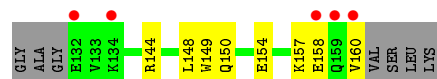
- Molecule 2: Putative uncharacterized protein



- Molecule 3: Zinc finger domain-containing protein



- Molecule 3: Zinc finger domain-containing protein



- Molecule 3: Zinc finger domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.96 Å 95.26 Å 133.96 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.75 19.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.93-2.75) 99.8 (19.93-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.75 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.275 0.231 , 0.276	Depositor DCC
R_{free} test set	1527 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6676	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.63% 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	0.26	0/1561	0.46	0/2107
1	D	0.26	0/1667	0.44	0/2248
1	G	0.26	0/1607	0.45	0/2168
2	B	0.24	0/377	0.44	0/504
2	E	0.23	0/337	0.42	0/449
2	H	0.25	0/367	0.45	0/491
3	C	0.25	0/271	0.37	0/360
3	F	0.26	0/254	0.46	0/337
3	I	0.27	0/245	0.42	0/325
All	All	0.25	0/6686	0.45	0/8989

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	1530	0	1555	16	0
1	D	1636	0	1651	26	0
1	G	1576	0	1598	36	0
2	B	374	0	364	2	0
2	E	334	0	335	5	0
2	H	364	0	357	5	0
3	C	268	0	270	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	251	0	253	6	0
3	I	242	0	247	2	0
4	A	20	0	0	0	0
4	B	7	0	0	0	0
4	C	5	0	0	1	0
4	D	27	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	30	0	0	0	0
4	H	5	0	0	0	0
4	I	2	0	0	0	0
All	All	6676	0	6630	86	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 86 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:109:GLY:HA3	1:D:116:LEU:HD23	1.76	0.67
1:G:161:ASP:OD2	2:H:233:ARG:NH1	2.27	0.67
1:G:150:LYS:HZ2	1:G:155:THR:HG23	1.60	0.66
1:G:65:VAL:O	1:G:69:VAL:HG22	1.99	0.63
1:G:35:MET:O	1:G:40:ARG:NH1	2.32	0.62

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	186/223 (83%)	186 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	200/223 (90%)	198 (99%)	2 (1%)	0	100	100
1	G	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
2	B	43/84 (51%)	43 (100%)	0	0	100	100
2	E	36/84 (43%)	36 (100%)	0	0	100	100
2	H	40/84 (48%)	40 (100%)	0	0	100	100
3	C	30/36 (83%)	30 (100%)	0	0	100	100
3	F	27/36 (75%)	27 (100%)	0	0	100	100
3	I	26/36 (72%)	26 (100%)	0	0	100	100
All	All	780/1029 (76%)	775 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	167/194 (86%)	164 (98%)	3 (2%)	62	79
1	D	178/194 (92%)	172 (97%)	6 (3%)	40	63
1	G	171/194 (88%)	164 (96%)	7 (4%)	33	56
2	B	36/69 (52%)	36 (100%)	0	100	100
2	E	32/69 (46%)	31 (97%)	1 (3%)	43	66
2	H	36/69 (52%)	36 (100%)	0	100	100
3	C	28/30 (93%)	28 (100%)	0	100	100
3	F	26/30 (87%)	25 (96%)	1 (4%)	36	59
3	I	25/30 (83%)	25 (100%)	0	100	100
All	All	699/879 (80%)	681 (97%)	18 (3%)	49	71

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

Mol	Chain	Res	Type
1	D	149	ARG
2	E	222	ASP
1	G	128	ARG
1	D	91	LYS
1	D	144	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	212	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 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	188/223 (84%)	0.03	7 (3%) 41 47	39, 67, 134, 182	0
1	D	202/223 (90%)	0.22	21 (10%) 6 6	43, 70, 193, 251	0
1	G	194/223 (86%)	0.50	22 (11%) 5 5	42, 101, 165, 186	0
2	B	45/84 (53%)	0.37	4 (8%) 9 11	66, 96, 150, 160	0
2	E	38/84 (45%)	0.35	3 (7%) 12 15	76, 98, 151, 178	0
2	H	42/84 (50%)	0.38	4 (9%) 8 9	62, 101, 145, 168	0
3	C	32/36 (88%)	0.78	5 (15%) 2 2	62, 87, 179, 213	0
3	F	29/36 (80%)	1.02	5 (17%) 1 1	74, 109, 175, 217	0
3	I	28/36 (77%)	1.12	6 (21%) 1 1	96, 120, 181, 217	0
All	All	798/1029 (77%)	0.35	77 (9%) 8 8	39, 85, 166, 251	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	155	THR	6.5
3	C	162	SER	6.5
3	I	160	VAL	5.7
3	I	159	GLN	5.6
3	F	160	VAL	5.0

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.