Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 09:38 AM EDT

PDB ID	:	5D60
Title	:	Structure of Chaetomium thermophilum Skn7 coiled-coil domain, crystal form III
Authors	:	Neudegger, T.; Verghese, J.; Hayer-Hartl, M.; Hartl, F.U.; Bracher, A.
Deposited on	:	2015-08-11
Resolution	:	1.90 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 (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:

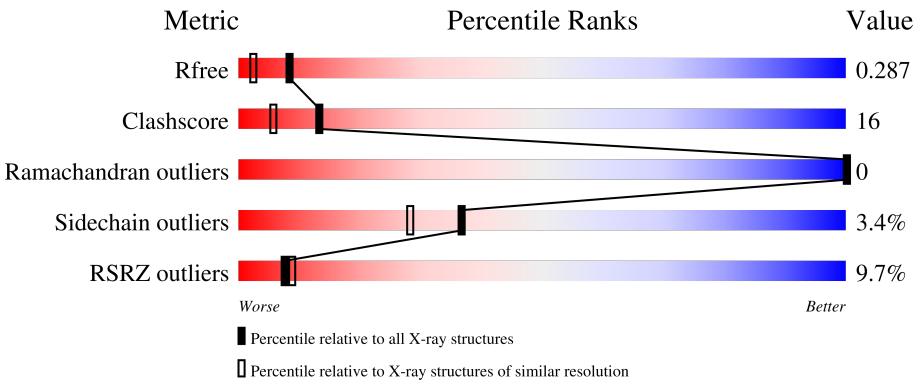
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	61	7%, 56%, 33%, •, 10%
1	B	61	10%, 74%, 20%, 7%
1	C	61	11%, 79%, 21%
1	D	61	10%, 74%, 25%, •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1927 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 Putative transcription factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	55	432	262	78	89	3	0	0	0
1	B	61	471	288	83	97	3	0	0	0
1	C	61	472	289	84	96	3	0	0	0
1	D	61	475	291	85	96	3	0	0	0

- Molecule 2 is water.

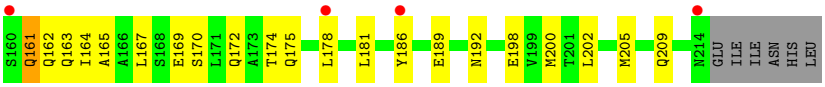
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	17	17	17	0	0
2	B	14	14	14	0	0
2	C	31	31	31	0	0
2	D	15	15	15	0	0

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: Putative transcription factor

Chain A:

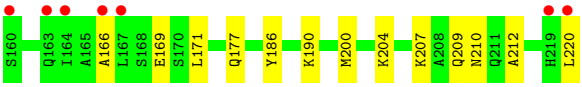


- Molecule 1: Putative transcription factor

Chain B:

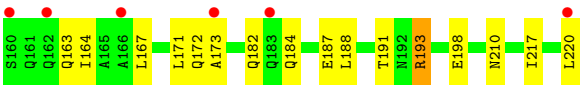
- Molecule 1: Putative transcription factor

Chain C:



- Molecule 1: Putative transcription factor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.73Å 40.20Å 52.78Å 90.00° 118.57° 90.00°	Depositor
Resolution (Å)	44.55 – 1.90 44.55 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (44.55-1.90) 98.8 (44.55-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.240 , 0.295 0.241 , 0.287	Depositor DCC
R_{free} test set	774 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.56$, $< L^2 > = 0.41$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.000 for h,-k,-h-l 0.000 for -h-l,-k,l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.923 for H, K, L 0.077 for -H, -K, H+L	Depositor
Outliers	4 of 14939 reflections (0.027%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	1927	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.14% 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	0.95	0/432	0.87	1/580 (0.2%)
1	B	0.84	0/471	0.85	0/633
1	C	0.99	0/473	0.89	0/636
1	D	0.92	0/476	0.97	3/640 (0.5%)
All	All	0.93	0/1852	0.90	4/2489 (0.2%)

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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	193	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	198	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	D	193	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	200	MET	CG-SD-CE	-5.06	92.10	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	160	SER	Peptide

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	432	0	439	22	0
1	B	471	0	474	25	0
1	C	472	0	473	29	0
1	D	475	0	476	21	0
2	A	17	0	0	2	0
2	B	14	0	0	1	0
2	C	31	0	0	10	0
2	D	15	0	0	3	0
All	All	1927	0	1862	60	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 16.

All (60) 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:169:GLU:HG3	2:C:315:HOH:O	1.62	1.00
1:B:198:GLU:HB3	1:C:200:MET:HE1	1.46	0.96
1:C:212:ALA:HB1	1:D:217:ILE:HD11	1.49	0.95
1:B:209:GLN:HG3	2:C:301:HOH:O	1.70	0.91
1:C:169:GLU:HB3	2:C:302:HOH:O	1.72	0.88
1:B:198:GLU:HG3	1:C:200:MET:HE3	1.59	0.82
1:C:209:GLN:NE2	1:D:210:ASN:OD1	2.12	0.82
1:C:177:GLN:HG3	1:D:182:GLN:HE21	1.56	0.69
1:B:198:GLU:HB3	1:C:200:MET:CE	2.21	0.68
1:C:166:ALA:HA	2:C:302:HOH:O	1.92	0.68
1:C:209:GLN:OE1	2:C:301:HOH:O	2.12	0.67
1:C:212:ALA:CB	1:D:217:ILE:HD11	2.25	0.66
1:A:186:TYR:CD1	1:D:184:GLN:NE2	2.64	0.65
1:C:177:GLN:HE21	1:D:182:GLN:HG3	1.60	0.65
1:A:162:GLN:NE2	2:A:301:HOH:O	2.31	0.63
1:A:174:THR:O	1:A:178:LEU:HD13	2.02	0.59
1:B:193:ARG:HD3	2:B:311:HOH:O	2.03	0.59
1:C:186:TYR:CZ	1:C:190:LYS:HD2	2.37	0.59
1:A:167:LEU:HD11	1:B:168:SER:OG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLU:HG3	1:C:200:MET:CE	2.30	0.57
1:B:198:GLU:CG	1:C:200:MET:HE3	2.34	0.56
1:B:198:GLU:CB	1:C:200:MET:HE1	2.29	0.56
1:A:164:ILE:HG21	1:D:163:GLN:HB3	1.89	0.54
1:D:171:LEU:O	1:D:171:LEU:HD23	2.07	0.54
1:D:187:GLU:HG2	2:D:314:HOH:O	2.06	0.54
1:B:198:GLU:CG	1:C:200:MET:CE	2.87	0.53
1:A:165:ALA:HB3	2:A:307:HOH:O	2.07	0.53
1:B:205:MET:HE1	1:C:207:LYS:HE2	1.91	0.53
1:B:198:GLU:CB	1:C:200:MET:CE	2.86	0.52
1:A:192:ASN:HB3	1:D:191:THR:HG22	1.91	0.51
1:A:164:ILE:CD1	1:D:164:ILE:HD11	2.41	0.50
1:C:220:LEU:HD22	1:D:220:LEU:HD11	1.92	0.49
1:A:169:GLU:O	1:A:172:GLN:HG3	2.11	0.49
1:A:170:SER:HB3	1:B:171:LEU:HD12	1.95	0.49
1:C:204:LYS:HE2	2:C:319:HOH:O	2.13	0.48
1:A:186:TYR:CE1	1:D:184:GLN:NE2	2.82	0.47
1:A:175:GLN:NE2	1:D:173:ALA:HB3	2.29	0.47
1:A:202:LEU:HD21	1:B:203:GLN:HA	1.96	0.46
1:D:172:GLN:HA	1:D:172:GLN:OE1	2.17	0.45
1:B:170:SER:HB3	1:C:171:LEU:HD23	1.99	0.45
1:B:205:MET:CE	1:C:207:LYS:HE2	2.47	0.44
1:C:166:ALA:HA	2:C:325:HOH:O	2.17	0.44
1:A:192:ASN:ND2	1:D:188:LEU:HD12	2.32	0.44
1:B:209:GLN:HG2	1:C:210:ASN:OD1	2.19	0.43
1:C:204:LYS:CE	2:C:319:HOH:O	2.65	0.43
1:A:167:LEU:CD1	1:B:168:SER:OG	2.66	0.43
1:B:160:SER:C	1:B:162:GLN:N	2.70	0.43
1:D:193:ARG:HD3	2:D:313:HOH:O	2.18	0.43
1:C:186:TYR:CE2	1:C:190:LYS:HD2	2.53	0.43
1:C:177:GLN:NE2	2:C:307:HOH:O	2.51	0.43
1:A:205:MET:HE2	1:B:206:VAL:HG12	2.01	0.42
1:C:220:LEU:HD22	1:D:220:LEU:CD1	2.49	0.41
1:B:209:GLN:CG	2:C:301:HOH:O	2.47	0.41
1:A:181:LEU:HD13	1:B:181:LEU:HD23	2.02	0.41
1:A:161:GLN:HG2	1:D:163:GLN:HE22	1.85	0.41
1:D:187:GLU:CG	2:D:314:HOH:O	2.66	0.41
1:A:174:THR:HG23	1:B:178:LEU:CD1	2.51	0.41
1:A:163:GLN:CD	1:B:164:ILE:HG22	2.41	0.41
1:A:167:LEU:HD23	1:D:167:LEU:HD13	2.04	0.40
1:A:198:GLU:HG3	1:B:200:MET:CE	2.52	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	53/61 (87%)	53 (100%)	0	0	100	100
1	B	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
1	C	59/61 (97%)	59 (100%)	0	0	100	100
1	D	59/61 (97%)	59 (100%)	0	0	100	100
All	All	230/244 (94%)	229 (100%)	1 (0%)	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	49/55 (89%)	46 (94%)	3 (6%)	18	9
1	B	52/55 (94%)	48 (92%)	4 (8%)	13	5
1	C	52/55 (94%)	52 (100%)	0	100	100
1	D	52/55 (94%)	52 (100%)	0	100	100
All	All	205/220 (93%)	198 (97%)	7 (3%)	37	28

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	189	GLU
1	A	209	GLN
1	B	171	LEU
1	B	176	GLN
1	B	193	ARG
1	B	209	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	192	ASN
1	B	175	GLN
1	B	177	GLN
1	B	182	GLN
1	C	177	GLN
1	C	183	GLN
1	C	184	GLN
1	C	211	GLN
1	D	176	GLN
1	D	182	GLN
1	D	184	GLN
1	D	203	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	55/61 (90%)	0.56	4 (7%) 15 16	24, 45, 70, 87	0
1	B	61/61 (100%)	0.50	6 (9%) 7 8	27, 47, 78, 83	0
1	C	61/61 (100%)	0.53	7 (11%) 4 5	23, 39, 79, 95	0
1	D	61/61 (100%)	0.56	6 (9%) 7 8	23, 43, 74, 84	0
All	All	238/244 (97%)	0.54	23 (9%) 7 9	23, 44, 79, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164	ILE	4.6
1	C	163	GLN	3.8
1	A	186	TYR	3.5
1	C	160	SER	3.5
1	B	220	LEU	3.4
1	D	166	ALA	3.4
1	D	173	ALA	3.3
1	C	166	ALA	3.3
1	C	219	HIS	3.0
1	B	168	SER	2.9
1	D	162	GLN	2.8
1	D	183	GLN	2.7
1	C	220	LEU	2.7
1	B	218	ASN	2.6
1	C	167	LEU	2.6
1	A	160	SER	2.5
1	D	160	SER	2.5
1	B	167	LEU	2.3
1	A	214	ASN	2.3
1	B	210	ASN	2.3
1	D	220	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	2.1
1	B	164	ILE	2.1

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.