

Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 09:57 pm BST

PDB ID	:	5HB5
Title	:	Crystal structure of Chaetomium thermophilum Nup145N APD
Authors	:	Lin, D.H.; Stuwe, T.; Hoelz, A.
Deposited on		
Resolution	:	1.50 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 following versions of software and data (see references (1)) were used in the production of this report:

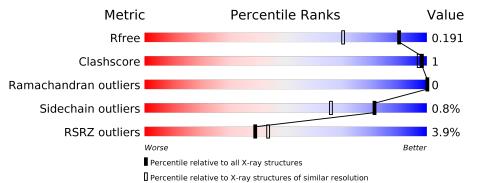
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries}, { m resolution\ range}({ m \AA}))$		
R_{free}	130704	2936 (1.50-1.50)		
Clashscore	141614	3144 (1.50-1.50)		
Ramachandran outliers	138981	3066 (1.50-1.50)		
Sidechain outliers	138945	3064 (1.50-1.50)		
RSRZ outliers	127900	2884 (1.50-1.50)		

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 <=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	А	140	97%	
1	В	140	97%	•



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5127 atoms, of which 2374 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 Nucleoporin NUP145.

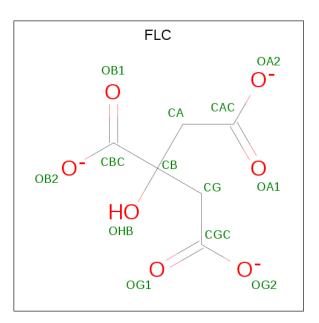
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	139	rotar	С		Ν	О	S	0	11	0
			2396	755	1203	218	215	5	U U		
1	В	140	Total	С	Η	Ν	Ο	\mathbf{S}	0	1	0
	D	140	2274	720	1136	207	206	5	0	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP G0SAK3
A	-2	PRO	-	expression tag	UNP G0SAK3
A	-1	HIS	-	expression tag	UNP G0SAK3
А	0	MET	-	expression tag	UNP G0SAK3
В	-3	GLY	-	expression tag	UNP G0SAK3
В	-2	PRO	-	expression tag	UNP G0SAK3
В	-1	HIS	-	expression tag	UNP G0SAK3
В	0	MET	-	expression tag	UNP G0SAK3

• Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
2	А	1	Total	С	Η	Ο	0	0
	11	L	18	6	5	7	0	0
2	A	1	Total	С	Η	Ο	0	0
		*	18	6	5	7	0	0
2	В	1	Total	С	Η	Ο	0	0
	D	*	18	6	5	7	0	0
2	В	1	Total	С	Η	Ο	0	1
	D	*	18	6	5	7	0	Ĩ
2	В	1	Total	С	Η	Ο	0	0
	D	*	18	6	5	7	0	
2	В	1	Total	С	Η	Ο	0	0
			18	6	5	7		
2	В	1	Total	С	Η	Ο	0	0
			18	6	5	7		3

• Molecule 3 is water.

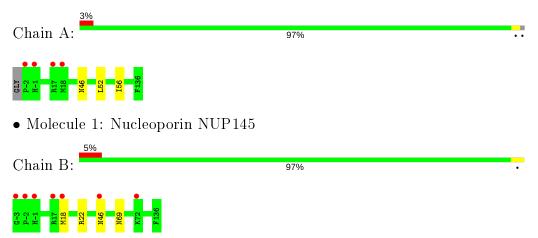
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	165	Total O 169 169	0	5
3	В	158	Total O 162 162	0	4



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 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: Nucleoporin NUP145





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	46.08Å 34.86Å 78.18Å	Depositor
a, b, c, α , β , γ	90.00° 99.37° 90.00°	Depositor
Resolution (Å)	27.66 - 1.50	Depositor
Resolution (A)	27.66 - 1.50	EDS
% Data completeness	97.2 (27.66-1.50)	Depositor
(in resolution range)	$97.3\ (27.66-1.50)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.05 (at 1.50 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
D D.	0.161 , 0.189	Depositor
R, R_{free}	0.163 , 0.191	DCC
R_{free} test set	2012 reflections $(5.20%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	14.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.42 , 48.2	EDS
L-test for twinning ²	$ \langle L \rangle = 0.56, \langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5127	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 53.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8979e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/1223	0.54	0/1654	
1	В	0.33	0/1168	0.54	0/1585	
All	All	0.32	0/2391	0.54	0/3239	

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	А	1193	1203	1194	1	0
1	В	1138	1136	1131	2	1
2	А	26	10	10	0	0
2	В	65	25	25	0	1
3	А	169	0	0	0	0
3	В	162	0	0	1	0
All	All	2753	2374	2360	3	1

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 1.

All (3) 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:69[B]:ASN:ND2	3:B:303:HOH:O	2.43	0.50
1:A:52[A]:LEU:HD12	1:A:56:ILE:HB	1.97	0.45
1:B:18:MET:O	1:B:22:ARG:NH2	2.53	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69[B]:ASN:ND2	2:B:201:FLC:OB1[2_646]	2.14	0.06

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	Perce	ntiles
1	А	148/140~(106%)	141 (95%)	7~(5%)	0	100	100
1	В	142/140~(101%)	137~(96%)	5~(4%)	0	100	100
All	All	290/280~(104%)	278~(96%)	12~(4%)	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	А	131/120~(109%)	130~(99%)	1 (1%)	81 66		
1	В	124/120~(103%)	123~(99%)	1 (1%)	81 66		
All	All	255/240~(106%)	253~(99%)	2(1%)	81 66		

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

Mol	Chain	Res	Type
1	А	46	ASN
1	В	46	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)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Tune	Chain	Dog	Link	B	ond leng	gths	В	ond ang	gles
	Type Chain Res Li		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
2	FLC	А	201	-	3,12,12	1.23	0	$3,\!17,\!17$	1.40	0



Mal	Mol Type Ch	Chain	Res	Link	B	ond leng	gths	B	ond ang	gles	
	туре	Cham	TIES	TIES		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FLC	В	201	-	$3,\!12,\!12$	1.23	0	$3,\!17,\!17$	1.48	1 (33%)	
2	FLC	В	205	-	3,12,12	1.22	0	$3,\!17,\!17$	1.25	1 (33%)	
2	FLC	В	203	-	$3,\!12,\!12$	1.18	0	$3,\!17,\!17$	0.64	0	
2	FLC	А	202	-	$3,\!12,\!12$	1.19	0	$3,\!17,\!17$	1.10	0	
2	FLC	В	204	-	3,12,12	1.21	0	$3,\!17,\!17$	1.35	1 (33%)	
2	FLC	В	202[A]	-	$3,\!12,\!12$	1.20	0	$3,\!17,\!17$	1.51	0	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	А	201	-	-	3/6/16/16	-
2	FLC	В	201	-	-	3/6/16/16	-
2	FLC	В	205	-	-	0/6/16/16	-
2	FLC	В	203	-	-	6/6/16/16	-
2	FLC	А	202	-	-	2/6/16/16	-
2	FLC	В	204	-	-	0/6/16/16	-
2	FLC	В	202[A]	-	-	3/6/16/16	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	205	FLC	CB-CG-CGC	-2.10	111.62	114.98
2	В	204	FLC	CB-CG-CGC	-2.06	111.69	114.98
2	В	201	FLC	CB-CG-CGC	-2.00	111.78	114.98

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	201	FLC	CAC-CA-CB-CG
2	В	201	FLC	CAC-CA-CB-CBC
2	В	203	FLC	CAC-CA-CB-CBC
2	В	203	FLC	CBC-CB-CG-CGC
2	В	203	FLC	CA-CB-CG-CGC
2	В	203	FLC	OHB-CB-CG-CGC

Continued on next page...



		-		
\mathbf{Mol}	Chain	\mathbf{Res}	\mathbf{Type}	Atoms
2	В	203	FLC	CAC-CA-CB-OHB
2	В	203	FLC	CAC-CA-CB-CG
2	В	202[A]	FLC	CAC-CA-CB-CG
2	В	202[A]	FLC	CAC-CA-CB-OHB
2	А	201	FLC	CAC-CA-CB-OHB
2	В	201	FLC	CAC-CA-CB-OHB
2	В	201	FLC	CAC-CA-CB-CG
2	А	201	FLC	CAC-CA-CB-CBC
2	А	202	FLC	CBC-CB-CG-CGC
2	В	202[A]	FLC	CAC-CA-CB-CBC
2	А	202	FLC	OHB-CB-CG-CGC

Continued from previous page...

There are no ring outliers.

1 monomer is involved in 1 short contact:

N	Лоl	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
	2	В	201	FLC	0	1

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, 95^{th} 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	А	139/140~(99%)	-0.24	4 (2%) 51 56	10, 16, 30, 62	0
1	В	140/140~(100%)	-0.22	7 (5%) 28 31	10, 16, 35, 52	0
All	All	279/280~(99%)	-0.23	11 (3%) 39 44	10, 16, 33, 62	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	-2	PRO	5.7
1	В	17	ARG	5.2
1	В	-3	GLY	5.0
1	А	-1	HIS	4.9
1	В	18	MET	4.1
1	А	17	ARG	3.9
1	А	18	MET	3.6
1	В	-1	HIS	3.4
1	В	46	ASN	2.7
1	В	-2	PRO	2.4
1	В	72	LYS	2.3

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$\mathbf{Q}{<}0.9$
2	FLC	В	204	13/13	0.38	0.24	62,76,88,88	0
2	FLC	А	202	13/13	0.40	0.28	$55,\!67,\!78,\!85$	0
2	FLC	В	203	13/13	0.43	0.34	$53,\!69,\!77,\!79$	0
2	FLC	А	201	13/13	0.55	0.34	55,70,77,91	18
2	FLC	В	201	13/13	0.62	0.20	46,61,68,68	0
2	FLC	В	205	13/13	0.65	0.25	$20,\!35,\!56,\!56$	18
2	FLC	В	202[A]	13/13	0.72	0.20	$55,\!67,\!78,\!80$	0

6.5 Other polymers (i)

There are no such residues in this entry.

