

wwPDB X-ray Structure Validation Summary Report (i)

Apr 30, 2024 – 02:46 PM JST

PDB ID : 8IYM

Title: Crystal structure of a protein acetyltransferase, HP0935

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Deposited on : 2023-04-05

Resolution : 2.00 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

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

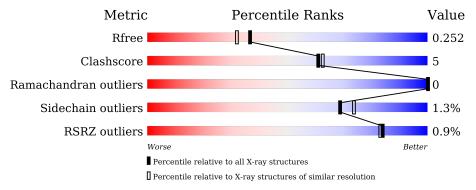
 $Validation\ Pipeline\ (wwPDB-VP) \quad : \quad 2.36.2$

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 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	163	85%	10%	• 5%
1	В	163	76%	17%	7%
1	С	163	82%	11%	7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SCN	В	204	-	-	X	-
4	SCN	В	205	-	-	X	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3955 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 N-acetyltransferase domain-containing protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	155	Total	С	N	О	S	0 1	1	0
1	A	155	1223	791	200	225	7	0	1	
1	D	151	Total	С	N	О	S	0	9	0
1	Б	101	1192	775	192	217	8	0	2	0
1	С	152	Total	С	N	О	S	0	2	0
1		102	1216	793	193	221	9		3	U

There are 9 discrepancies between the modelled and reference sequences:

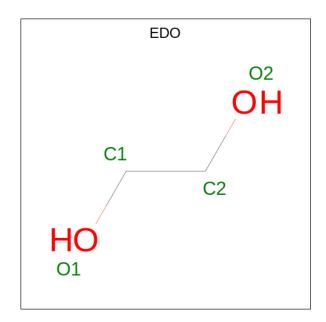
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP O25589
A	0	MET	-	expression tag	UNP O25589
A	1	VAL	MET	engineered mutation	UNP O25589
В	-1	SER	-	expression tag	UNP O25589
В	0	MET	-	expression tag	UNP O25589
В	1	VAL	MET	engineered mutation	UNP O25589
С	-1	SER	-	expression tag	UNP O25589
С	0	MET	-	expression tag	UNP O25589
С	1	VAL	MET	engineered mutation	UNP O25589

• Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mo	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
2		A	2	Total K 2 2	0	0
2		С	1	Total K 1 1	0	0

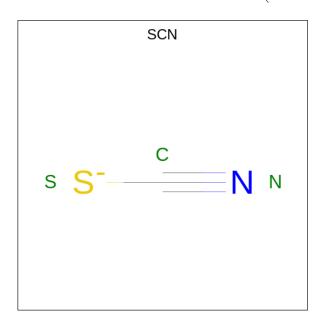
• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	В	1	Total C O 4 2 2	0	0
3	С	1	Total C O 4 2 2	0	0

• Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



N	Iol	Chain	Residues	Atoms				ZeroOcc	AltConf
	4	A	1	Total 3	C 1	N 1	S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 3 1 1 1	0	0
4	В	1	Total C N S 3 1 1 1	0	0
4	В	1	Total C N S 3 1 1 1	0	0
4	В	1	Total C N S 3 1 1 1	0	0
4	В	1	Total C N S 3 1 1 1	0	0
4	В	1	Total C N S 3 1 1 1	0	0
4	С	1	Total C N S 3 1 1 1	0	0
4	С	1	Total C N S 3 1 1 1	0	0

• Molecule 5 is water.

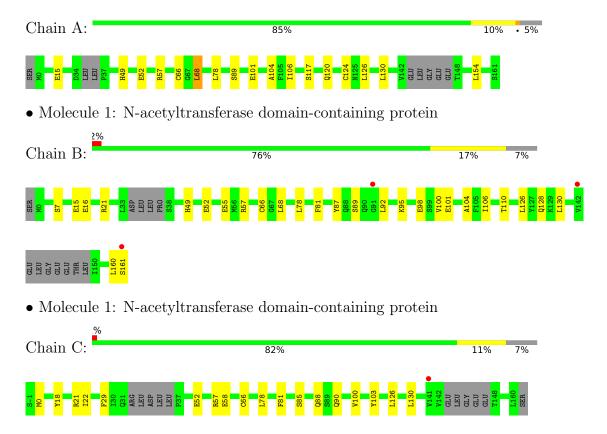
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	101	Total O 101 101	0	0
5	В	85	Total O 85 85	0	0
5	С	96	Total O 96 96	0	0



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: N-acetyltransferase domain-containing protein





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	117.86Å 66.17Å 70.90Å	Depositor	
a, b, c, α , β , γ	90.00° 91.42° 90.00°	Depositor	
Resolution (Å)	70.88 - 2.00	Depositor	
	70.88 - 2.00	EDS	
% Data completeness	99.8 (70.88-2.00)	Depositor	
(in resolution range)	99.8 (70.88-2.00)	EDS	
R_{merge}	0.12	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.61 (at 2.00Å)	Xtriage	
Refinement program	REFMAC 5.8.0405	Depositor	
D D.	0.215 , 0.246	Depositor	
R, R_{free}	0.222 , 0.252	DCC	
R_{free} test set	1880 reflections (5.09%)	wwPDB-VP	
Wilson B-factor (Å ²)	19.1	Xtriage	
Anisotropy	0.229	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.37\;,52.1$	EDS	
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage	
Estimated twinning fraction	0.009 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.007 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.108 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.095 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.017 for -h,-k,l	Xtriage	
Reported twinning fraction	0.900 for H, K, L 0.100 for $1/2\text{H-}3/2\text{K}, -1/2\text{H-}1/2\text{K}, -\text{L}$	Depositor	
Outliers	2 of 36942 reflections (0.005%)	Xtriage	
F_o, F_c correlation	0.92	EDS	
Total number of atoms	3955	wwPDB-VP	
Average B, all atoms (Å ²)	24.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.28% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: K, EDO, SCN

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).

Mal	Chain	Bo	nd lengths	Bond angles		
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.86	3/1248 (0.2%)	1.02	1/1675 (0.1%)	
1	В	0.79	4/1216 (0.3%)	0.95	2/1635 (0.1%)	
1	С	0.76	$2/1250 \ (0.2\%)$	0.99	3/1680 (0.2%)	
All	All	0.80	9/3714 (0.2%)	0.99	6/4990 (0.1%)	

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	A	0	1
1	В	0	1
1	С	0	1
All	All	0	3

The worst 5 of 9 bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}({ ext{ iny A}})$
1	A	15	GLU	CD-OE1	14.12	1.41	1.25
1	В	16	GLU	CD-OE2	-6.41	1.18	1.25
1	A	52	GLU	CD-OE2	-6.35	1.18	1.25
1	В	52	GLU	CD-OE2	-6.32	1.18	1.25
1	A	101	GLU	CD-OE1	-5.93	1.19	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	С	21	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	В	21	ARG	NE-CZ-NH1	6.25	123.42	120.30

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	С	21	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	С	29	PHE	CB-CG-CD1	5.20	124.44	120.80
1	В	49	HIS	CA-CB-CG	5.18	122.40	113.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	ARG	Sidechain
1	В	57	ARG	Sidechain
1	С	57	ARG	Sidechain

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	1223	0	1190	7	0
1	В	1192	0	1158	18	0
1	С	1216	0	1221	11	0
2	A	2	0	0	0	0
2	С	1	0	0	0	0
3	A	4	0	6	0	0
3	В	4	0	6	0	0
3	С	4	0	6	0	0
4	A	6	0	0	0	0
4	В	15	0	0	4	0
4	С	6	0	0	1	0
5	A	101	0	0	2	0
5	В	85	0	0	2	0
5	С	96	0	0	0	0
All	All	3955	0	3587	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 5.

The worst 5 of 33 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:C:66[A]:CYS:HG	1:C:81:PHE:HD2	0.94	0.94
1:B:66[A]:CYS:HG	1:B:81:PHE:HD2	0.93	0.87
1:B:7:SER:O	4:B:204:SCN:S	2.48	0.71
1:B:128:GLN:HG2	5:B:358:HOH:O	1.90	0.71
1:B:98:GLU:OE2	4:B:205:SCN:S	2.55	0.65

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	Perce	ntiles
1	A	150/163 (92%)	150 (100%)	0	0	100	100
1	В	147/163 (90%)	146 (99%)	1 (1%)	0	100	100
1	С	149/163 (91%)	147 (99%)	2 (1%)	0	100	100
All	All	446/489 (91%)	443 (99%)	3 (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	128/145 (88%)	127 (99%)	1 (1%)	81 86
1	В	124/145 (86%)	121 (98%)	3 (2%)	49 51
1	С	134/145 (92%)	133 (99%)	1 (1%)	84 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	386/435 (89%)	381 (99%)	5 (1%)	69 74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ILE
1	В	89	SER
1	В	95	LYS
1	В	106	ILE
1	С	90	GLN

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

Mol	Chain	Res	Type
1	A	31	GLN
1	A	128	GLN
1	В	120	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)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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 Type		Chain	Chain	Des	Res Link	Bond lengths			Bond angles		
Moi Type	Type	nes		Counts		RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	SCN	В	204	-	1,2,2	0.60	0	0,1,1	-	-	
4	SCN	В	205	-	1,2,2	0.62	0	0,1,1	-	-	
4	SCN	В	206	-	1,2,2	1.42	0	0,1,1	-	-	
3	EDO	С	202	-	3,3,3	0.18	0	2,2,2	0.41	0	
4	SCN	С	203	-	1,2,2	0.08	0	0,1,1	-	-	
4	SCN	С	204	-	1,2,2	0.39	0	0,1,1	-	-	
4	SCN	A	205	-	1,2,2	1.92	0	0,1,1	-	-	
4	SCN	В	202	-	1,2,2	0.24	0	0,1,1	-	-	
4	SCN	A	204	-	1,2,2	0.84	0	0,1,1	-	-	
4	SCN	В	203	-	1,2,2	0.27	0	0,1,1	-	-	
3	EDO	В	201	-	3,3,3	0.35	0	2,2,2	0.26	0	
3	EDO	A	203	-	3,3,3	0.27	0	2,2,2	0.10	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
3	EDO	В	201	-	-	0/1/1/1	-
3	EDO	С	202	-	-	0/1/1/1	-
3	EDO	A	203	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	203	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	204	SCN	2	0
4	В	205	SCN	2	0
4	С	204	SCN	1	0



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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	155/163~(95%)	-0.30	0 100 100	11, 22, 41, 51	1 (0%)
1	В	151/163 (92%)	-0.18	3 (1%) 65 63	11, 23, 40, 61	0
1	С	152/163 (93%)	-0.16	1 (0%) 87 87	11, 23, 46, 64	1 (0%)
All	All	458/489 (93%)	-0.21	4 (0%) 84 83	11, 23, 43, 64	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	141	VAL	2.8
1	В	161	SER	2.6
1	В	91	GLY	2.3
1	В	142	VAL	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)

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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
2	K	С	201	1/1	0.78	0.16	52,52,52,52	1
4	SCN	В	203	3/3	0.89	0.19	32,32,39,42	0
4	SCN	С	203	3/3	0.92	0.11	33,33,45,55	0
4	SCN	В	202	3/3	0.94	0.07	25,25,31,39	0
4	SCN	С	204	3/3	0.94	0.16	39,39,41,44	0
3	EDO	С	202	4/4	0.95	0.10	20,21,21,21	0
4	SCN	В	204	3/3	0.95	0.31	21,21,31,47	0
4	SCN	A	205	3/3	0.95	0.23	21,21,22,24	0
2	K	A	201	1/1	0.95	0.07	29,29,29,29	0
3	EDO	В	201	4/4	0.96	0.07	17,18,20,22	0
2	K	A	202	1/1	0.97	0.12	44,44,44,44	0
4	SCN	В	206	3/3	0.97	0.19	27,27,32,37	0
3	EDO	A	203	4/4	0.97	0.07	19,19,19,20	0
4	SCN	A	204	3/3	0.97	0.13	21,21,29,40	0
4	SCN	В	205	3/3	0.98	0.16	35,35,43,51	0

6.5 Other polymers (i)

There are no such residues in this entry.

