



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 11:39 AM EDT

PDB ID : 2OD7
Title : Crystal Structure of yHst2 bound to the intermediate analogue ADP-HPD,
and and aceylated H4 peptide
Authors : Marmorstein, R.Q.; Sanders, B.D.
Deposited on : unknown
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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

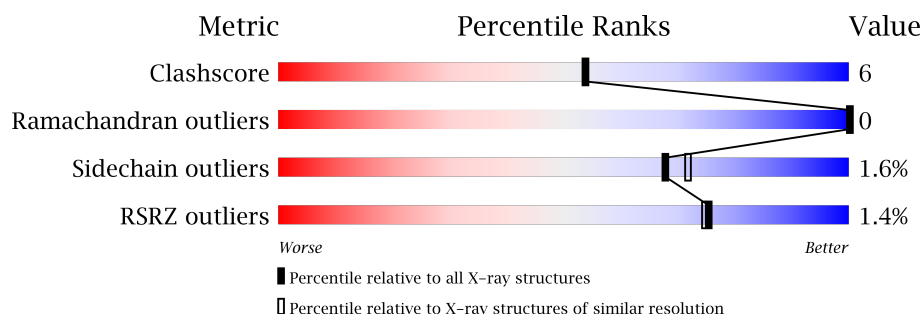
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 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	308	
2	B	14	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2515 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 NAD-dependent deacetylase HST2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2286	1478	377	419	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	INITIATING METHIONINE	UNP P53686
A	-12	ARG	-	CLONING ARTIFACT	UNP P53686
A	-11	GLY	-	CLONING ARTIFACT	UNP P53686
A	-10	SER	-	CLONING ARTIFACT	UNP P53686
A	-9	HIS	-	EXPRESSION TAG	UNP P53686
A	-8	HIS	-	EXPRESSION TAG	UNP P53686
A	-7	HIS	-	EXPRESSION TAG	UNP P53686
A	-6	HIS	-	EXPRESSION TAG	UNP P53686
A	-5	HIS	-	EXPRESSION TAG	UNP P53686
A	-4	HIS	-	EXPRESSION TAG	UNP P53686
A	-3	GLY	-	CLONING ARTIFACT	UNP P53686
A	-2	MET	-	CLONING ARTIFACT	UNP P53686
A	-1	ALA	-	CLONING ARTIFACT	UNP P53686
A	0	SER	-	CLONING ARTIFACT	UNP P53686

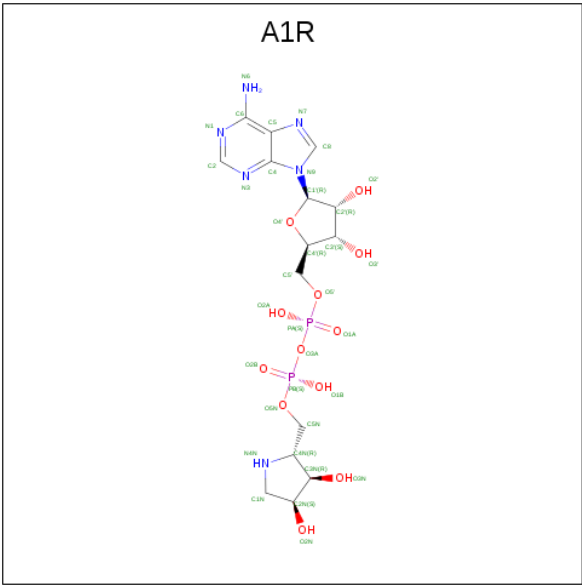
- Molecule 2 is a protein called Acetylated histone H4 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			60	36	15	9			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 5'-O-[(S)-{[(S)-{[(2R,3R,4S)-3,4-DIHYDROXYPYRROLIDIN-2-YL]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]ADENOSINE (three-letter code: A1R) (formula: C₁₅H₂₄N₆O₁₂P₂).

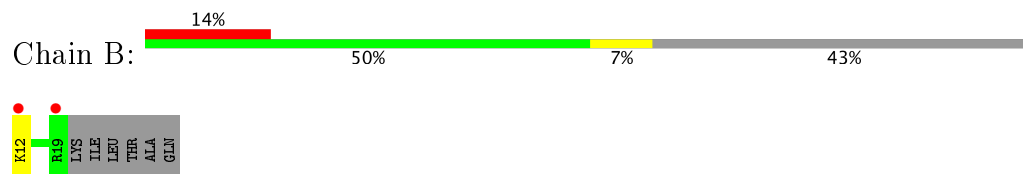


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	35	15	6	12	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	2	Total	O	0	0
			2	2		

- Molecule 1: NAD-dependent deacetylase HST2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.76 Å 106.76 Å 67.69 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.92 – 2.00 41.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.4 (41.92-2.00) 91.4 (41.91-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.34 (at 2.00 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.234 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2515	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A1R, ALY

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	1.79	33/2345 (1.4%)	1.39	25/3178 (0.8%)
2	B	0.34	0/47	0.57	0/58
All	All	1.77	33/2392 (1.4%)	1.38	25/3236 (0.8%)

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	TYR	CD1-CE1	-8.16	1.27	1.39
1	A	166	ASP	CB-CG	6.91	1.66	1.51
1	A	139	ALA	CA-CB	6.88	1.67	1.52
1	A	237	GLU	CD-OE1	6.55	1.32	1.25
1	A	154	VAL	CB-CG1	-6.51	1.39	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASP	CB-CG-OD2	13.40	130.36	118.30
1	A	92	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	A	57	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	A	43	ASP	CB-CG-OD1	9.42	126.78	118.30
1	A	187	ASP	CB-CG-OD2	8.90	126.31	118.30

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	2286	0	2263	29	0
2	B	60	0	58	5	0
3	A	1	0	0	0	0
4	A	35	0	22	0	0
5	A	131	0	0	1	0
5	B	2	0	0	0	0
All	All	2515	0	2343	29	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 6.

The worst 5 of 29 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:A:104:GLN:HE22	1:A:127:LYS:H	1.24	0.86
1:A:36:SER:HB3	1:A:41:ILE:HD12	1.58	0.84
1:A:158:LYS:NZ	1:A:165:LYS:O	2.14	0.80
1:A:27:VAL:HG11	1:A:220:ILE:HD12	1.77	0.67
1:A:158:LYS:CE	1:A:166:ASP:O	2.47	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	285/308 (92%)	277 (97%)	8 (3%)	0	100	100
2	B	5/14 (36%)	5 (100%)	0	0	100	100
All	All	290/322 (90%)	282 (97%)	8 (3%)	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	252/271 (93%)	248 (98%)	4 (2%)	68	72
2	B	3/9 (33%)	3 (100%)	0	100	100
All	All	255/280 (91%)	251 (98%)	4 (2%)	68	72

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	24	ASN
1	A	153	GLN
1	A	224	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	267	HIS
1	A	123	GLN
1	A	104	GLN
1	A	153	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ALY	B	16	2	11,11,12	1.51	3 (27%)	9,12,14	1.85	1 (11%)

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	ALY	B	16	2	-	0/8/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	ALY	CA-C	2.35	1.53	1.50
2	B	16	ALY	CH-NZ	2.78	1.41	1.34
2	B	16	ALY	OH-CH	3.05	1.30	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	ALY	CE-NZ-CH	-4.73	114.87	122.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	A1R	A	1001	-	32,38,38	2.83	9 (28%)	29,58,58	3.58	8 (27%)

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
4	A1R	A	1001	-	-	0/18/51/51	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	A1R	C2N-C3N	-5.52	1.44	1.53
4	A	1001	A1R	C5N-C4N	-5.30	1.41	1.52
4	A	1001	A1R	C2'-C1'	-3.80	1.47	1.53
4	A	1001	A1R	PB-O2B	-2.75	1.40	1.50
4	A	1001	A1R	O5N-C5N	-2.35	1.35	1.44

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	A1R	O2N-C2N-C1N	-8.38	90.68	110.86
4	A	1001	A1R	O2N-C2N-C3N	-8.00	96.06	111.28
4	A	1001	A1R	C5N-C4N-N4N	-7.96	93.96	111.52
4	A	1001	A1R	N3-C2-N1	-7.40	122.42	128.86
4	A	1001	A1R	C1'-N9-C4	-3.55	120.51	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	16:ALY	C	17:ARG	N	1.15

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	289/308 (93%)	-0.25	2 (0%) 87 87	17, 30, 56, 75	0
2	B	7/14 (50%)	1.39	2 (28%) 1 1	43, 52, 73, 109	0
All	All	296/322 (91%)	-0.21	4 (1%) 75 75	17, 31, 58, 109	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	ARG	3.2
1	A	24	ASN	2.4
2	B	12	LYS	2.4
1	A	21	SER	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	ALY	B	16	12/13	0.90	0.13	-	22,26,32,33	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
4	A1R	A	1001	35/35	0.88	0.16	1.35	35,39,52,58	0
3	ZN	A	701	1/1	0.99	0.11	1.21	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.