



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:07 am GMT

PDB ID : 3FHT
Title : Crystal structure of human Dbp5 in complex with AMPPNP and RNA
Authors : von Moeller, H.; Conti, E.
Deposited on : 2008-12-10
Resolution : 2.20 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 : trunk28620
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) : recalc28949

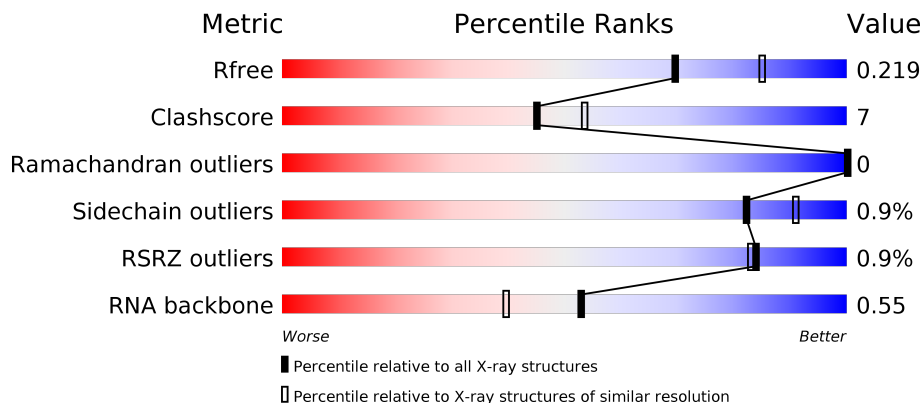
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)
RNA backbone	2435	1007 (2.74-1.66)

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	412	<div> <div></div> <div>82% 13% 5%</div> </div>
1	B	412	<div> <div></div> <div>81% 13% 6%</div> </div>
2	C	10	<div> <div></div> <div>30% 10% 20% 40%</div> </div>
2	D	10	<div> <div></div> <div>20% 30% 10% 40%</div> </div>

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	GOL	B	3732	-	-	-	X
4	GOL	B	3734	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6815 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 ATP-dependent RNA helicase DDX19B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	87	1	0
			3116	1975	546	575	20			
1	B	387	Total	C	N	O	S	41	1	0
			3074	1949	536	569	20			

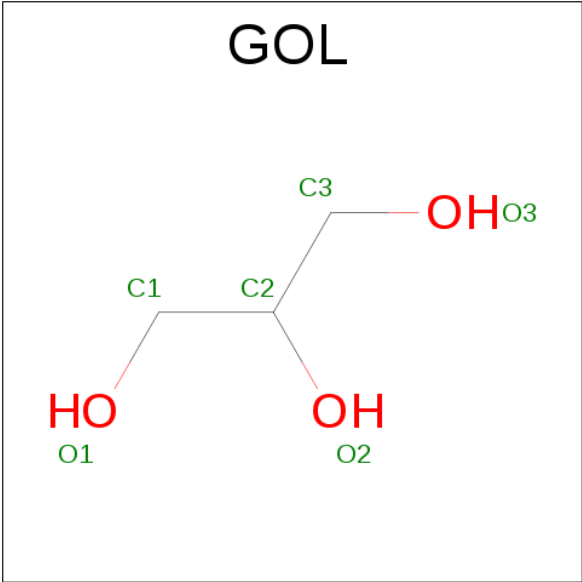
- Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			
2	D	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

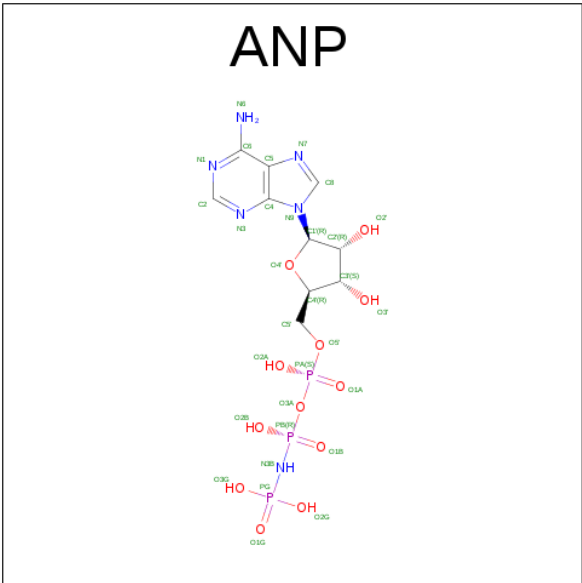
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total	O	0	0
			142	142		
6	B	147	Total	O	0	0
			147	147		
6	C	7	Total	O	0	0
			7	7		
6	D	4	Total	O	0	0
			4	4		

- Molecule 1: ATP-dependent RNA helicase DDX19B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.60Å 79.66Å 124.54Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	41.52 – 2.20 41.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.52-2.20) 99.4 (41.51-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.168 , 0.225 0.171 , 0.219	Depositor DCC
R_{free} test set	2061 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6815	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ANP

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	0.94	1/3170 (0.0%)	0.87	4/4277 (0.1%)
1	B	0.94	3/3127 (0.1%)	0.87	2/4220 (0.0%)
2	C	1.25	0/131	1.98	6/200 (3.0%)
2	D	1.61	0/128	2.28	8/196 (4.1%)
All	All	0.97	4/6556 (0.1%)	0.96	20/8893 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	400	GLU	CB-CG	5.33	1.62	1.52
1	B	461	LYS	CB-CG	5.32	1.67	1.52
1	A	339	PHE	CE1-CZ	5.08	1.47	1.37
1	B	433	PHE	CE2-CZ	5.08	1.47	1.37

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	U	N3-C2-O2	-8.99	115.91	122.20
2	C	5	U	N3-C4-O4	-8.60	113.38	119.40
2	D	6	U	N3-C2-O2	-7.96	116.63	122.20
2	C	5	U	N1-C2-O2	7.57	128.10	122.80
2	D	5	U	N3-C4-O4	-7.46	114.18	119.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3116	0	3187	46	0
1	B	3074	0	3136	45	0
2	C	120	0	61	3	0
2	D	117	0	62	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	2	0
4	B	18	0	24	2	0
5	A	31	0	13	2	0
5	B	31	0	13	1	0
6	A	142	0	0	5	0
6	B	147	0	0	2	0
6	C	7	0	0	0	0
6	D	4	0	0	0	0
All	All	6815	0	6504	94	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 94 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:334:ALA:HB3	1:B:403:SER:OG	1.32	1.22
1:B:227:LYS:HE2	2:D:6:U:O2'	1.57	1.02
1:B:334:ALA:CB	1:B:403:SER:OG	2.19	0.90
1:A:195:ALA:HB2	1:A:211:GLU:CG	2.07	0.83
1:B:361:ALA:HB2	1:B:384:GLU:HG2	1.61	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	391/412 (95%)	387 (99%)	4 (1%)	0	100	100
1	B	384/412 (93%)	380 (99%)	4 (1%)	0	100	100
All	All	775/824 (94%)	767 (99%)	8 (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	345/363 (95%)	340 (99%)	5 (1%)	71	84
1	B	341/363 (94%)	340 (100%)	1 (0%)	94	97
All	All	686/726 (94%)	680 (99%)	6 (1%)	82	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	B	429	ARG
1	A	414	LYS
1	A	129	GLU
1	A	429	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	HIS
1	B	358	HIS
1	B	155	GLN
1	A	401	GLN
1	B	121	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	5/10 (50%)	1 (20%)	0
2	D	5/10 (50%)	0	0
All	All	10/20 (50%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	6	U

There are no RNA pucker outliers to report.

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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	GOL	A	3731	-	5,5,5	0.34	0	5,5,5	1.25	1 (20%)
5	ANP	A	480	3	29,33,33	2.62	8 (27%)	28,52,52	2.95	7 (25%)
5	ANP	B	2	3	29,33,33	2.17	8 (27%)	28,52,52	3.24	9 (32%)
4	GOL	B	3732	-	5,5,5	0.26	0	5,5,5	1.16	0
4	GOL	B	3733	-	5,5,5	0.26	0	5,5,5	0.62	0
4	GOL	B	3734	-	5,5,5	0.17	0	5,5,5	0.97	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
4	GOL	A	3731	-	-	0/4/4/4	0/0/0/0
5	ANP	A	480	3	-	0/13/38/38	0/3/3/3
5	ANP	B	2	3	-	0/13/38/38	0/3/3/3
4	GOL	B	3732	-	-	0/4/4/4	0/0/0/0
4	GOL	B	3733	-	-	0/4/4/4	0/0/0/0
4	GOL	B	3734	-	-	0/4/4/4	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2	ANP	PB-O2B	-3.42	1.47	1.56
5	A	480	ANP	PB-O2B	-3.02	1.48	1.56
5	A	480	ANP	C2'-C1'	-2.73	1.49	1.53
5	B	2	ANP	PG-O3G	-2.57	1.49	1.56
5	A	480	ANP	PG-O2G	-2.43	1.50	1.56

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2	ANP	N3-C2-N1	-11.10	119.19	128.86
5	A	480	ANP	N3-C2-N1	-9.49	120.59	128.86
5	A	480	ANP	O1G-PG-N3B	-8.32	99.34	111.79
5	B	2	ANP	O1G-PG-N3B	-7.63	100.38	111.79
5	B	2	ANP	O3'-C3'-C4'	-3.37	101.24	111.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3731	GOL	2	0
5	A	480	ANP	2	0
5	B	2	ANP	1	0
4	B	3732	GOL	1	0
4	B	3733	GOL	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, 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	390/412 (94%)	-0.46	5 (1%) 77 75	8, 19, 34, 40	19 (4%)
1	B	387/412 (93%)	-0.50	2 (0%) 90 90	8, 19, 33, 42	10 (2%)
2	C	6/10 (60%)	-0.57	0 100 100	22, 25, 52, 55	0
2	D	6/10 (60%)	-0.66	0 100 100	23, 25, 41, 67	0
All	All	789/844 (93%)	-0.48	7 (0%) 84 83	8, 19, 34, 67	29 (3%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	ALA	6.3
1	A	334	ALA	3.8
1	A	205	ARG	3.5
1	A	228	LEU	2.2
1	B	200	GLY	2.2

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. 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	GOL	B	3732	6/6	0.87	0.19	3.71	43,46,48,51	0
4	GOL	B	3734	6/6	0.88	0.13	2.47	51,54,55,56	0
4	GOL	B	3733	6/6	0.93	0.10	1.16	36,41,43,44	0
5	ANP	B	2	31/31	0.99	0.08	-0.85	7,14,19,21	0
4	GOL	A	3731	6/6	0.96	0.09	-0.99	33,36,39,40	0
5	ANP	A	480	31/31	0.99	0.08	-1.38	7,14,17,20	0
3	MG	B	1	1/1	0.98	0.04	-2.55	16,16,16,16	0
3	MG	A	1	1/1	0.98	0.05	-	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.