

wwPDB EM Validation Summary Report (i)

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PDB ID	:	8HWD
EMDB ID	:	EMD-35054
Title	:	Cryo-EM Structure of D5 ADP form
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Deposited on	:	2022-12-29
Resolution	:	3.30 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp 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:

EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain				
1	А	785	26%	12% •	61%	I	
1	В	785	32%	15% •	52%	I	
1	С	785	32%	11% •	56%	I	
1	D	785	24%	13% •	62%	I	
1	Е	785	23%	9%	69%		
1	F	785	22%	10% •	67%	I	

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
2	ADP	D	1001	-	-	Х	-



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15029 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	Δ	308	Total	С	Ν	Ο	\mathbf{S}	0	0
L	Π	500	2505	1603	427	461	14	0	0
1	F	258	Total	С	Ν	Ο	\mathbf{S}	0	0
	Ľ	200	2092	1338	354	388	12	0	0
1	Л	200	Total	С	Ν	Ο	\mathbf{S}	0	0
	D	299	2427	1548	412	455	12	0	0
1	F	247	Total	С	Ν	0	\mathbf{S}	0	0
	Ľ	241	2012	1293	335	373	11	0	0
1	С	344	Total	С	Ν	0	\mathbf{S}	0	0
	U	044	2786	1772	478	522	14	0	0
1	B	378	Total	С	Ν	0	S	0	0
	D	510	3045	1939	518	572	16	0	0

• Molecule 1 is a protein called Primase D5.

• Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			AltConf
9	Δ	1	Total	С	Ν	Ο	Р	0
	A	1	27	10	5	10	2	0
2	F	1	Total	С	Ν	Ο	Р	0
2	Ľ	T	27	10	5	10	2	0
2	Л	1	Total	С	Ν	Ο	Р	0
2	D	1	27	10	5	10	2	0
2	E	1	Total	С	Ν	Ο	Р	0
2	Ľ	1	27	10	5	10	2	0
2	С	1	Total	С	Ν	Ο	Р	0
2	U	1	27	10	5	10	2	0
2	В	1	Total	\mathbf{C}	Ν	Ο	Р	0
	D	1	27	10	5	10	2	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. 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. 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: Primase D5

















4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	621428	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification		
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor



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: ADP

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	Mol Chain		lengths	Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/2550	0.50	0/3430
1	В	0.26	0/3108	0.52	0/4198
1	С	0.26	0/2839	0.52	0/3828
1	D	0.33	0/2472	0.55	0/3328
1	Е	0.24	0/2050	0.48	0/2757
1	F	0.26	0/2129	0.50	0/2863
All	All	0.27	0/15148	0.51	0/20404

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	2505	0	2541	72	0
1	В	3045	0	3055	83	0
1	С	2786	0	2803	64	0
1	D	2427	0	2438	114	0
1	Е	2012	0	2038	45	0
1	F	2092	0	2125	64	0
2	А	27	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	27	0	12	5	0
2	С	27	0	12	1	0
2	D	27	0	12	13	0
2	Е	27	0	12	4	0
2	F	27	0	12	1	0
All	All	15029	0	15072	422	0

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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 14.

The worst 5 of 422 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:D:655:LEU:HD22	2:D:1001:ADP:C2	1.45	1.48
1:D:655:LEU:HD22	2:D:1001:ADP:N3	1.67	1.08
1:D:655:LEU:CD2	2:D:1001:ADP:C2	2.41	1.03
1:D:655:LEU:CD2	2:D:1001:ADP:N3	2.36	0.87
1:D:507:THR:HG21	1:D:626:PHE:HB3	1.57	0.84

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 PDB entries followed by that with respect to all EM entries.

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	296/785~(38%)	275~(93%)	21 (7%)	0	100	100
1	В	376/785~(48%)	341 (91%)	35~(9%)	0	100	100
1	С	336/785~(43%)	309~(92%)	27~(8%)	0	100	100
1	D	289/785~(37%)	262 (91%)	26~(9%)	1 (0%)	41	71
1	Е	237/785~(30%)	219 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed Favoured Allowed		Outliers	Perce	ntiles	
1	F	248/785~(32%)	221 (89%)	27 (11%)	0	100	100
All	All	1782/4710~(38%)	1627 (91%)	154 (9%)	1 (0%)	54	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	457	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	Perce	entiles
1	А	283/725~(39%)	269~(95%)	14 (5%)	25	56
1	В	343/725~(47%)	322~(94%)	21 (6%)	18	48
1	С	314/725~(43%)	301~(96%)	13~(4%)	30	61
1	D	273/725~(38%)	260~(95%)	13~(5%)	25	56
1	Ε	228/725~(31%)	218~(96%)	10 (4%)	28	59
1	F	237/725~(33%)	229~(97%)	8~(3%)	37	65
All	All	1678/4350~(39%)	1599~(95%)	79(5%)	30	57

 $5~{\rm of}~79$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	С	670	TYR
1	В	534	ASP
1	В	380	SER
1	В	473	ASP
1	В	607	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such side chains are listed below:



Mol	Chain	Res	Type
1	С	358	ASN
1	С	466	ASN
1	С	573	ASN
1	С	475	ASN
1	D	466	ASN

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)

6 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).

Mal	Tuno	Chain	Chain Bos Link Bond lengths				ths	Bond angles		
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	D	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	В	1001	-	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
2	ADP	С	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	F	1001	-	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	А	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
2	ADP	Е	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



'-' mea	- means no outliers of that kind were identified.										
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings				
2	ADP	D	1001	-	-	3/12/32/32	0/3/3/3				
2	ADP	В	1001	-	-	3/12/32/32	0/3/3/3				
2	ADP	С	1001	-	-	3/12/32/32	0/3/3/3				
2	ADP	F	1001	-	-	4/12/32/32	0/3/3/3				
2	ADP	А	1001	-	-	2/12/32/32	0/3/3/3				
2	ADP	Е	1001	-	-	2/12/32/32	0/3/3/3				

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. , , ۰. . .

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

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1001	ADP	C5-C4	2.53	1.47	1.40
2	F	1001	ADP	C5-C4	2.50	1.47	1.40
2	D	1001	ADP	C5-C4	2.47	1.47	1.40
2	Ε	1001	ADP	C5-C4	2.46	1.47	1.40
2	С	1001	ADP	C5-C4	2.46	1.47	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	1001	ADP	PA-O3A-PB	-3.88	119.51	132.83
2	А	1001	ADP	PA-O3A-PB	-3.88	119.51	132.83
2	F	1001	ADP	PA-O3A-PB	-3.57	120.58	132.83
2	D	1001	ADP	PA-O3A-PB	-3.41	121.12	132.83
2	С	1001	ADP	C3'-C2'-C1'	3.40	106.10	100.98

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	А	1001	ADP	C5'-O5'-PA-O1A
2	А	1001	ADP	C5'-O5'-PA-O3A
2	D	1001	ADP	C5'-O5'-PA-O2A
2	D	1001	ADP	C5'-O5'-PA-O3A
2	Е	1001	ADP	PB-O3A-PA-O5'

There are no ring outliers.

6 monomers are involved in 29 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	ADP	13	0
2	В	1001	ADP	5	0
2	С	1001	ADP	1	0
2	F	1001	ADP	1	0
2	А	1001	ADP	5	0
2	Е	1001	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient must be highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.















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.

