



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:37 AM GMT

PDB ID : 3PJR
Title : HELICASE SUBSTRATE COMPLEX
Authors : Velankar, S.S.; Soultanas, P.; Dillingham, M.S.; Subramanya, H.S.; Wigley, D.B.
Deposited on : 1999-03-12
Resolution : 3.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

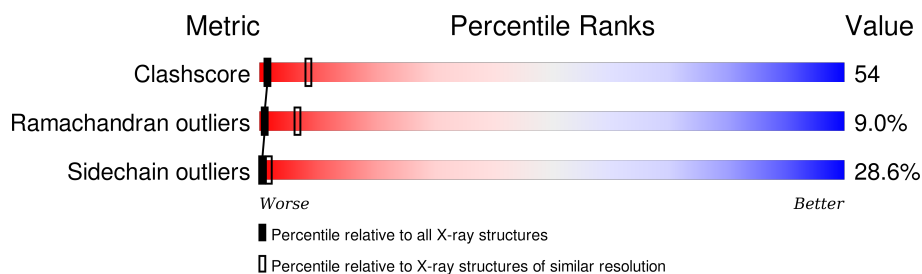
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	Y	15	
2	Z	10	
3	A	724	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5765 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 DNA chain called 5'-D(*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	15	Total	C	N	O	P	0	0	0
			303	147	48	94	14			

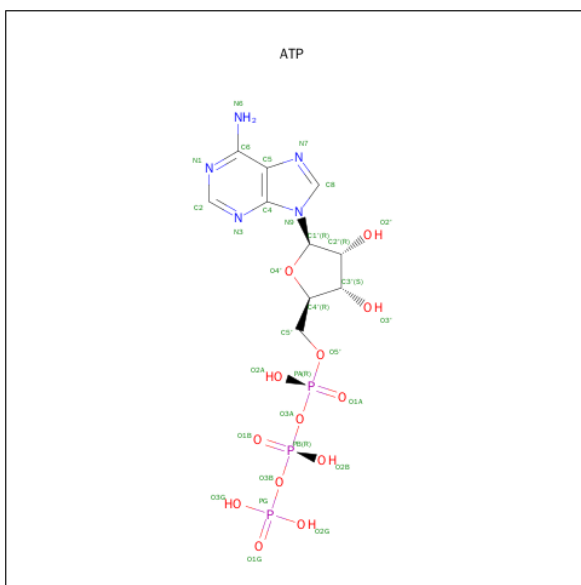
- Molecule 2 is a DNA chain called 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	10	Total	C	N	O	P	0	0	0
			201	96	39	57	9			

- Molecule 3 is a protein called HELICASE PCRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	646	Total	C	N	O	S	0	0	0
			5230	3304	916	991	19			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: 5'-D(*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*TP*TP*T)-3'

Chain Y: 




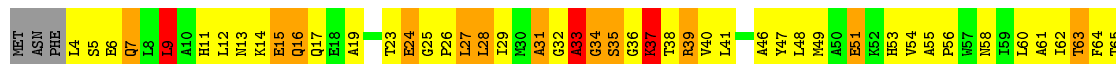
- Molecule 2: 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'

Chain Z: 

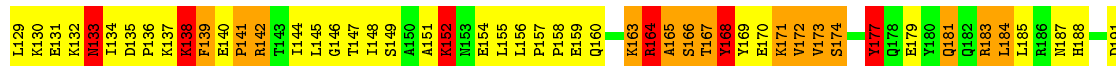


- Molecule 3: HELICASE PCRA

Chain A: 















PRO	T648	H587	E523	L483
ILE	A649	N588	N524	Q454
GLY	S650	R589		A455
ILE	R651	S590	D527	
LYS	R652	L591	D528	Q459
ARG	GLN	E592	K529	A460
LEU	ALA	D593	S530	L461
LEU	GLY	D594	L531	A462
ALA	ALA	E595	I532	A463
LYS	SER	E596	A533	F464
PHE	ARG	N597	F534	R465
ALA	PRO	E598	L535	S466
PRO	ALA	E599	T536	Q467
ILE	VAL	E600		L468
GLU	SER	R601	I540	E469
LYS	ARG	R602	I541	
VAL	PRO	L603	S542	T472
	GLN	A604	D543	Q473
	ALA	Y605	L544	L474
	SER	V606	D545	Q475
	GLY	G607	E546	Q476
	ALA	I608	LEU	Y477
	VAL	T609	ASP	Y478
	GLY	R610	GLY	
	SER	A611	T550	E482
	TRP	E612	E551	L483
	LYS	E613	Q552	Y484
	VAL	E614	A553	E485
	GLY	L615	A554	E486
	ASP	V616		V487
	ARG		D557	
	ALA	S619	A558	R490
	ASN	A620	V559	
	HIS	Q621	M560	Y493
	ARG	R622	L561	
	LYS	R623	M562	N496
	TRP	T624	T563	L497
	GLY	L625	L564	
	ILE	F626	H565	
	GLY	G627	A566	
	THR	R628	A567	
	VAL	L629	K568	
	VAL	Q630	G569	
	SER	R631	L570	
	VAL	D632	E571	
	ARG	P633	F572	
	GLY	P634	P573	R508
	GLY	S635	V574	L509
	GLY	R636	V575	E510
	ASP	F637	F576	O511
	ASP	L638	L577	L512
	GLN	R639	I578	D513
	GLU	E640	G579	E514
	LEU	I641	N580	F515
	ASP	P642	E581	L516
	ILE	A643	E582	S517
	ALA	R644	G583	V518
	PHE	L645	I584	T519
	PRO	L646	F585	H521
	SER	E647	P586	F522

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.12Å 105.12Å 380.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	92.0 (10.00-3.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5765	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

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: ATP

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	Y	1.56	4/337 (1.2%)	3.06	50/519 (9.6%)
2	Z	2.27	6/225 (2.7%)	3.84	39/345 (11.3%)
3	A	0.68	7/5319 (0.1%)	1.60	69/7184 (1.0%)
All	All	0.87	17/5881 (0.3%)	1.88	158/8048 (2.0%)

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
2	Z	1	0
3	A	0	63
All	All	1	63

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	28	DG	N9-C8	12.27	1.46	1.37
2	Z	28	DG	C2'-C1'	11.86	1.64	1.52
2	Z	28	DG	C8-N7	-11.06	1.24	1.30
1	Y	11	DT	C3'-O3'	-7.58	1.34	1.44
2	Z	27	DA	C2'-C1'	7.16	1.59	1.52

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	652	ARG	CD-NE-CZ	38.94	178.12	123.60
3	A	310	ARG	CD-NE-CZ	36.72	175.00	123.60
2	Z	28	DG	C4-N9-C1'	21.13	153.97	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	28	DG	C8-N9-C1'	-20.87	99.87	127.00
2	Z	28	DG	N3-C4-C5	-20.27	118.47	128.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	Z	33	DG	C3'

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	16	GLN	Mainchain
3	A	24	GLU	Mainchain
3	A	27	LEU	Mainchain
3	A	31	ALA	Mainchain
3	A	9	LEU	Mainchain

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	Y	303	0	174	56	0
2	Z	201	0	113	36	0
3	A	5230	0	5230	530	0
4	A	31	0	12	7	0
All	All	5765	0	5529	607	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 54.

The worst 5 of 607 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:Y:12:DT:H5''	1:Y:12:DT:C6	1.65	1.31
1:Y:12:DT:C5'	1:Y:12:DT:H6	1.47	1.27
1:Y:5:DT:H2'	1:Y:6:DG:C8	1.77	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:ALA:HB3	3:A:251:ASP:HB2	1.36	1.08
1:Y:12:DT:C6	1:Y:12:DT:C5'	2.31	1.00

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
3	A	642/724 (89%)	471 (73%)	113 (18%)	58 (9%)	1 6

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	33	ALA
3	A	35	SER
3	A	83	ALA
3	A	84	ALA
3	A	113	PHE

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
3	A	560/618 (91%)	400 (71%)	160 (29%)	0 1

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	329	GLU
3	A	375	ASN
3	A	599	GLU
3	A	339	ARG
3	A	352	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	187	ASN
3	A	245	ASN
3	A	511	ASN
3	A	214	GLN
3	A	232	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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
4	ATP	A	725	-	24,33,33	1.58	6 (25%)	31,52,52	1.83	9 (29%)

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	ATP	A	725	-	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	725	ATP	C8-N7	-3.22	1.28	1.34
4	A	725	ATP	O4'-C1'	-2.61	1.37	1.41
4	A	725	ATP	PG-O2G	-2.41	1.46	1.54
4	A	725	ATP	C5-N7	-2.27	1.31	1.39
4	A	725	ATP	PB-O2B	-2.17	1.45	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	725	ATP	PB-O3B-PG	-4.31	118.21	132.67
4	A	725	ATP	PA-O3A-PB	-3.78	122.12	132.73
4	A	725	ATP	O2'-C2'-C3'	-2.24	104.54	111.83
4	A	725	ATP	O2B-PB-O3A	2.13	114.76	105.09
4	A	725	ATP	C1'-N9-C4	2.23	130.31	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	725	ATP	7	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.