



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3PJR / pdb_00003pjr
Title : HELICASE SUBSTRATE COMPLEX
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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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

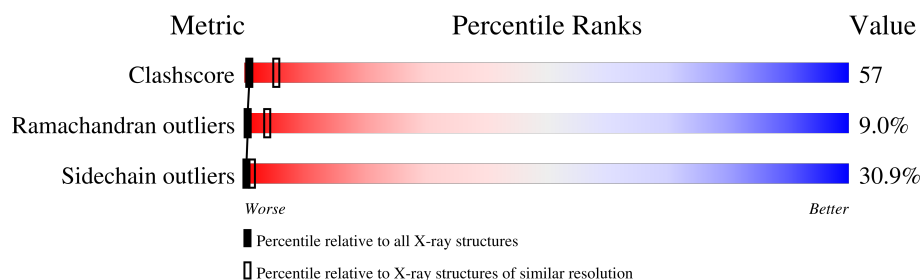
1 Overall quality at a glance

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	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	Y	15	7% 53% 40%
2	Z	10	10% 90%
3	A	724	19% 39% 23% 8% 11%

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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



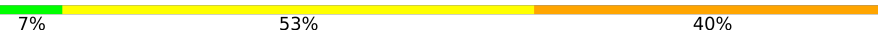
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

Note EDS was not executed.

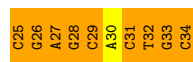
- Molecule 1: 5'-D(*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*TP*TP*T)-3'

Chain Y: 



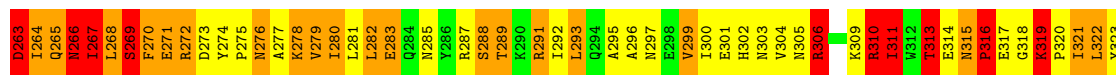
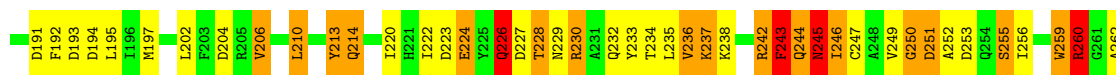
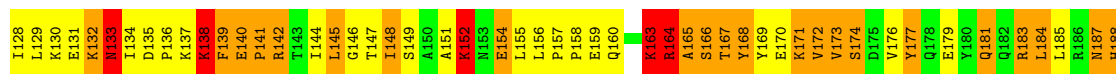
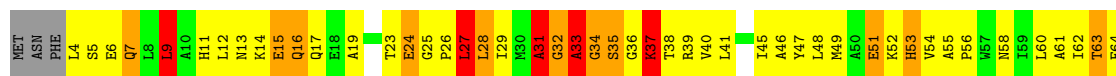
- Molecule 2: 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'

Chain Z: 



- Molecule 3: HELICASE PCRA

Chain A: 



GLY	P634	R573	N511	L445
GLY	S635	V574	L512	G446
GLY	R636	V575	D513	E447
ASP	F637	F576	E514	L448
ASP	L638	L577	F515	E449
GLN	M639	I578	L516	M450
GLU	E640	G579	S517	L451
LEU	I641	R580	V518	G452
ASP	P642	E581	T519	L453
ALA	A643	E582	R520	G454
ALA	H644	G583	R521	A455
PHE	L645	I584	F522	K456
PRO	L646	R585	F523	A457
SER	E647	F586	R524	A458
PRO	T648	H587		G459
PRO	A649	N588	D527	A460
GLY	S650	R589	D528	L461
ILE	R651	S590	K529	A462
ILE	R652	L591	S530	M463
LYS		E592	L531	F464
ARG	GLN	D593	T532	R465
LEU	ALA	D594	A533	S466
LEU	GLY	D595	F534	Q467
ALA	ALA	E596	L535	L468
LYS	SER	M597	T536	E469
PHE	ARG	E598	D537	
ALA	PRO	E599	L538	
ALA	ALA	E600	A539	T472
PRO	VAL	R601	L540	Q473
ILE	SER	ARG	T541	L474
GLU	GLY	PRO	S542	Q475
LYS	ARG	GLN	D543	E476
VAL	ALA	ALA	L544	Y477
	SER	GLY	D545	V478
	GLY	VAL	E546	
	ALA	ALA	LEU	E482
	VAL	VAL	ASP	L483
	GLY	GLY	GLY	V484
	SER	TRP	T550	E485
	TRP	LYS	E551	E486
	VAL	VAL	Q552	V487
	GLY	GLY	A553	L488
	ILE	GLY	A554	D489
	THR	THR		K490
	VAL	VAL	D557	
	VAL	VAL	A558	Y493
	SER	VAL	V559	
	VAL	VAL	M560	M496
	ARG	ARG	L561	L497
		LYS	M562	
		TRP	T563	E500
		GLY	L564	R501
		ILE	H565	T502
		GLY	A566	I503
		THR	R567	E504
		VAL	I629	A505
		VAL	R568	G506
		VAL	G569	S507
		SER	L570	R508
		VAL	D571	L509
		ARG	F572	E510

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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

5.1 Standard geometry

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	0.80	0/337	2.22	17/519 (3.3%)
2	Z	1.08	1/225 (0.4%)	2.85	25/345 (7.2%)
3	A	0.89	8/5319 (0.2%)	2.04	137/7184 (1.9%)
All	All	0.89	9/5881 (0.2%)	2.09	179/8048 (2.2%)

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 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	386	PHE	C-O	8.18	1.34	1.24
3	A	310	ARG	CD-NE	-7.40	1.35	1.46
3	A	383	GLY	N-CA	-6.60	1.37	1.45
3	A	652	ARG	NE-CZ	-6.33	1.26	1.33
3	A	652	ARG	CD-NE	-6.06	1.37	1.46

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	652	ARG	CD-NE-CZ	38.37	178.12	124.40
3	A	310	ARG	CD-NE-CZ	36.15	175.00	124.40
3	A	651	ARG	CA-C-N	24.40	165.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	651	ARG	C-N-CA	24.40	165.61	121.70
2	Z	28	DG	C8-N9-C1'	-18.09	99.87	127.00

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

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	35	0
3	A	5230	0	5232	568	0
4	A	31	0	12	7	0
All	All	5765	0	5531	644	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 57.

The worst 5 of 644 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:C6	1:Y:12:DT:H5''	1.65	1.31
1:Y:12:DT:H6	1:Y:12:DT:C5'	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%)	0 4

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%)	387 (69%)	173 (31%)	0 1

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	430	LEU
3	A	542	SER
3	A	453	LEU
3	A	504	GLU
3	A	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	303	ASN
3	A	467	GLN
3	A	524	ASN
3	A	475	GLN
3	A	375	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 oligosaccharides 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	-	32,33,33	1.65	5 (15%)	48,52,52	1.52	9 (18%)

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	-	-	12/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	725	ATP	PA-O3A	4.25	1.64	1.59
4	A	725	ATP	C5-N7	-4.04	1.31	1.39
4	A	725	ATP	C2-N1	2.41	1.38	1.33
4	A	725	ATP	PG-O2G	-2.35	1.46	1.54
4	A	725	ATP	PB-O2B	-2.09	1.45	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	725	ATP	C4-N9-C8	-4.06	101.48	105.74
4	A	725	ATP	O4'-C1'-N9	3.36	114.55	108.09
4	A	725	ATP	O2B-PB-O3B	3.00	115.38	107.27
4	A	725	ATP	C6-C5-N7	-2.97	126.36	132.09
4	A	725	ATP	N9-C8-N7	2.82	117.94	113.94

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

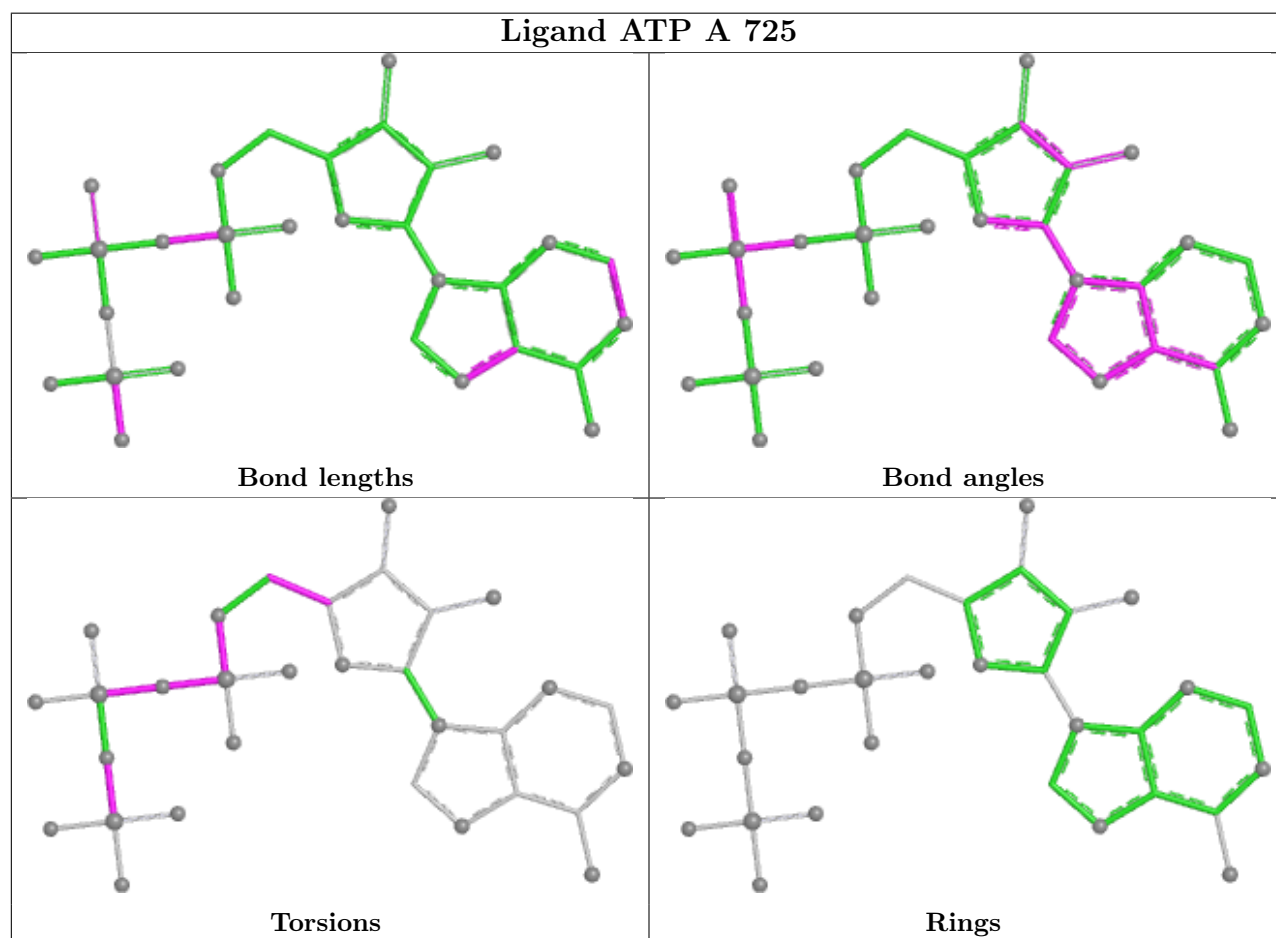
Mol	Chain	Res	Type	Atoms
4	A	725	ATP	PB-O3B-PG-O3G
4	A	725	ATP	C5'-O5'-PA-O1A
4	A	725	ATP	C5'-O5'-PA-O2A
4	A	725	ATP	C5'-O5'-PA-O3A
4	A	725	ATP	O4'-C4'-C5'-O5'

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

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 than 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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are 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 ⓘ

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.