



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:41 PM UTC

PDB ID : 8TCH / pdb_00008tch
Title : Initiation of replication protein with helicase activity encoded by Pathogenicity Island SaPIBov1
Authors : Mir-Sanchis, I.; Rice, P.
Deposited on : 2023-07-01
Resolution : 2.70 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

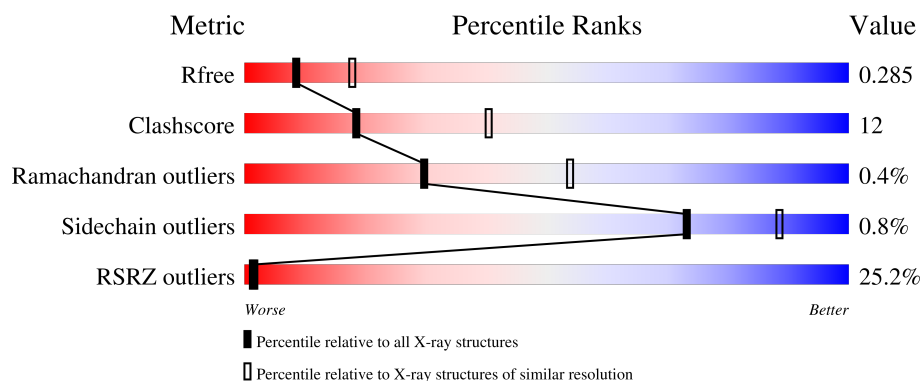
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	580	20% 63% 20% • 17%
1	B	580	23% 63% 21% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15038 atoms, of which 7135 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 Pathogenicity island protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	484	Total	C	H	N	O	S	0	0	0
			7511	2515	3589	656	740	11			
1	B	487	Total	C	H	N	O	S	0	0	0
			7489	2529	3546	658	746	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP A0A2X2JYA8
A	-9	HIS	-	expression tag	UNP A0A2X2JYA8
A	-8	HIS	-	expression tag	UNP A0A2X2JYA8
A	-7	HIS	-	expression tag	UNP A0A2X2JYA8
A	-6	HIS	-	expression tag	UNP A0A2X2JYA8
A	-5	HIS	-	expression tag	UNP A0A2X2JYA8
A	-4	HIS	-	expression tag	UNP A0A2X2JYA8
A	-3	GLY	-	expression tag	UNP A0A2X2JYA8
A	-2	ARG	-	expression tag	UNP A0A2X2JYA8
A	-1	GLY	-	expression tag	UNP A0A2X2JYA8
A	0	SER	-	expression tag	UNP A0A2X2JYA8
A	350	PRO	GLN	conflict	UNP A0A2X2JYA8
A	462	LEU	ILE	conflict	UNP A0A2X2JYA8
A	474	ALA	VAL	conflict	UNP A0A2X2JYA8
A	548	LYS	ARG	conflict	UNP A0A2X2JYA8
A	555	LEU	PHE	conflict	UNP A0A2X2JYA8
B	-10	MET	-	initiating methionine	UNP A0A2X2JYA8
B	-9	HIS	-	expression tag	UNP A0A2X2JYA8
B	-8	HIS	-	expression tag	UNP A0A2X2JYA8
B	-7	HIS	-	expression tag	UNP A0A2X2JYA8
B	-6	HIS	-	expression tag	UNP A0A2X2JYA8
B	-5	HIS	-	expression tag	UNP A0A2X2JYA8
B	-4	HIS	-	expression tag	UNP A0A2X2JYA8
B	-3	GLY	-	expression tag	UNP A0A2X2JYA8
B	-2	ARG	-	expression tag	UNP A0A2X2JYA8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A2X2JYA8
B	0	SER	-	expression tag	UNP A0A2X2JYA8
B	350	PRO	GLN	conflict	UNP A0A2X2JYA8
B	462	LEU	ILE	conflict	UNP A0A2X2JYA8
B	474	ALA	VAL	conflict	UNP A0A2X2JYA8
B	548	LYS	ARG	conflict	UNP A0A2X2JYA8
B	555	LEU	PHE	conflict	UNP A0A2X2JYA8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	23	Total	O	0	0
			23	23		



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	115.41Å 115.41Å 310.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.57 – 2.70 47.57 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.57-2.70) 99.8 (47.57-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.265 , 0.281 0.271 , 0.285	Depositor DCC
R_{free} test set	2077 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15038	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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](#)

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	0.16	0/3994	0.41	0/5372
1	B	0.16	0/4016	0.44	2/5401 (0.0%)
All	All	0.16	0/8010	0.43	2/10773 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ASN	CA-C-N	8.54	140.27	126.86
1	B	87	ASN	C-N-CA	8.54	140.27	126.86

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	3922	3589	3940	93	0
1	B	3943	3546	3959	98	0
2	A	15	0	0	2	0
2	B	23	0	0	0	0
All	All	7903	7135	7899	189	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 12.

The worst 5 of 189 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:210:TYR:HH	1:B:432:HIS:HE2	1.09	0.90
1:A:205:VAL:HG23	1:A:241:THR:HG23	1.54	0.90
1:B:230:ILE:HG22	1:B:347:LEU:HB2	1.56	0.88
1:A:199:ILE:HG23	1:A:202:LEU:HB2	1.56	0.87
1:B:185:LYS:HB3	1:B:369:TYR:CD2	2.13	0.82

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	468/580 (81%)	435 (93%)	30 (6%)	3 (1%)	21	44
1	B	469/580 (81%)	435 (93%)	33 (7%)	1 (0%)	43	68
All	All	937/1160 (81%)	870 (93%)	63 (7%)	4 (0%)	30	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	ASN
1	A	273	ASN
1	A	384	LYS
1	A	199	ILE

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	
1	A	439/522 (84%)	436 (99%)	3 (1%)	76	90
1	B	442/522 (85%)	438 (99%)	4 (1%)	70	87
All	All	881/1044 (84%)	874 (99%)	7 (1%)	73	88

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	132	LYS
1	B	227	ILE
1	B	513	ILE
1	B	437	ILE
1	A	513	ILE

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

Mol	Chain	Res	Type
1	A	189	GLN
1	A	464	GLN
1	B	472	ASN
1	B	273	ASN
1	A	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	484/580 (83%)	1.12	114 (23%)	2 1	40, 98, 180, 325	0
1	B	487/580 (83%)	1.29	131 (26%)	1 1	41, 109, 189, 250	0
All	All	971/1160 (83%)	1.21	245 (25%)	1 1	40, 103, 187, 325	0

The worst 5 of 245 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	567	SER	10.1
1	A	351	PRO	7.2
1	A	166	VAL	6.9
1	A	232	GLY	6.6
1	B	427	ILE	6.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.