

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	8IIC
Title	:	Crystal structure of Israeli acute paralysis virus RNA-dependent RNA poly-
		merase delta40 mutant (residues 41-546)
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Deposited on	:	2023-02-24
Resolution	:	3.25 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 (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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.25 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 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 <=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	А	524	% 5 5%	18%	27%		
1	В	524	59%	21%	• 19%		



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6070 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 Polymerase polyprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	383	Total 2931	C 1864	N 492	0 548	S 27	0	0	0
1	В	425	Total 3133	C 1987	N 530	O 586	S 30	0	0	0

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	4	Total O 4 4	0	0
2	В	2	Total O 2 2	0	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 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.



• Molecule 1: Polymerase polyprotein



N352 P353 A354 T356 T356 P357 P357 L358 L358 <mark>V391</mark> S392 <mark>M393</mark> V394 T416 I417 L327 M328 D329 V330 L367 R368 1380 K381 M382 T383 D386 F387 <mark>E410</mark> W411 Y412 N413 A306 7401 1402 1403 1403 5405 R328 E31 L432 LYS GLY VAL ASN GLY GLV C439 C440 K441 W442 R443 R443 R443 R443 E488 L492 E495 E495 M499 E500 L501 L501 S502 T511 N478 R540 F541 L542 M546 L528 D529



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants	167.93Å 167.93Å 218.32Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Bosolution(A)	23.78 - 3.25	Depositor
Resolution (A)	23.78 - 3.25	EDS
% Data completeness	95.1 (23.78-3.25)	Depositor
(in resolution range)	95.1 (23.78-3.25)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.16 (at 3.23 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
P. P.	0.211 , 0.246	Depositor
n, n_{free}	0.211 , 0.246	DCC
R_{free} test set	1401 reflections (5.05%)	wwPDB-VP
Wilson B-factor $(Å^2)$	62.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , 63.9	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6070	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	А	0.57	0/2989	0.71	0/4049	
1	В	0.46	0/3194	0.67	0/4339	
All	All	0.52	0/6183	0.69	0/8388	

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	2931	0	2666	66	0
1	В	3133	0	2717	85	0
2	А	4	0	0	0	0
2	В	2	0	0	0	0
All	All	6070	0	5383	151	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 13.

The worst 5 of 151 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:440:PRO:HG2	1:B:443:ARG:HH21	1.51	0.74



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:HD11	1:A:356:THR:HG22	1.71	0.73
1:B:520:TYR:HE1	1:B:526:ASP:HB3	1.55	0.72
1:B:382:MET:HE3	1:B:411:TRP:HZ2	1.56	0.70
1:A:244:TYR:CZ	1:A:323:ARG:HG3	2.26	0.70

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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	Perce	entiles
1	А	371/524~(71%)	347~(94%)	24~(6%)	0	100	100
1	В	415/524~(79%)	387~(93%)	27~(6%)	1 (0%)	47	77
All	All	786/1048~(75%)	734 (93%)	51 (6%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	63	HIS

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	А	283/463~(61%)	274~(97%)	9~(3%)	39 66

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	В	279/463~(60%)	272~(98%)	7~(2%)	47	71
All	All	562/926~(61%)	546~(97%)	16 (3%)	43	69

5 of 16 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	526	ASP
1	В	421	PHE
1	А	541	PHE
1	В	412	TYR
1	А	527	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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, 95^{th} 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	383/524~(73%)	-0.39	4 (1%) 82 82	17, 40, 79, 96	0
1	В	425/524 (81%)	-0.30	0 100 100	25, 60, 85, 105	1 (0%)
All	All	808/1048~(77%)	-0.34	4 (0%) 91 90	17, 53, 84, 105	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	138	CYS	2.6
1	А	350	SER	2.6
1	А	351	GLY	2.3
1	А	185	ASP	2.0

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 monosaccharides 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.

