



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2025 – 10:07 AM EDT

PDB ID : 9CA6 / pdb_00009ca6
Title : Rns Pocket Mutant - I14F/I17F
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Deposited on : 2024-06-17
Resolution : 3.00 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

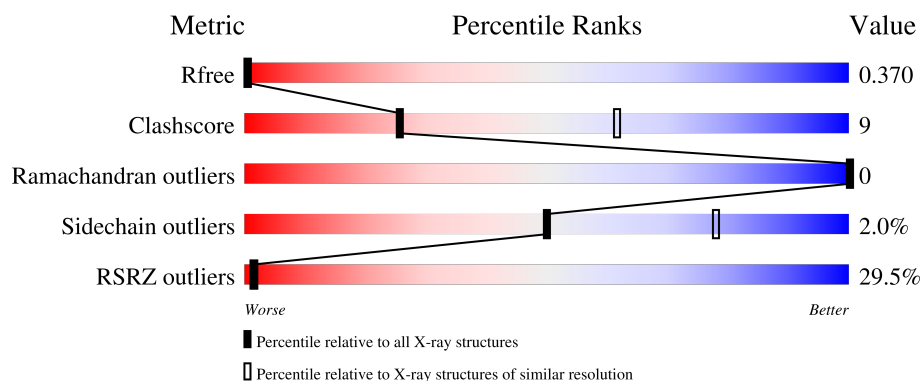
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	265	<div> <div>26%</div> <div>67%</div> <div>22%</div> <div>••</div> <div>9%</div> </div>
1	B	265	<div> <div>27%</div> <div>66%</div> <div>22%</div> <div>•</div> <div>9%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3941 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 Regulatory protein Rns.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1967	1264	330	361	12			
1	B	241	Total	C	N	O	S	0	0	0
			1974	1267	331	364	12			

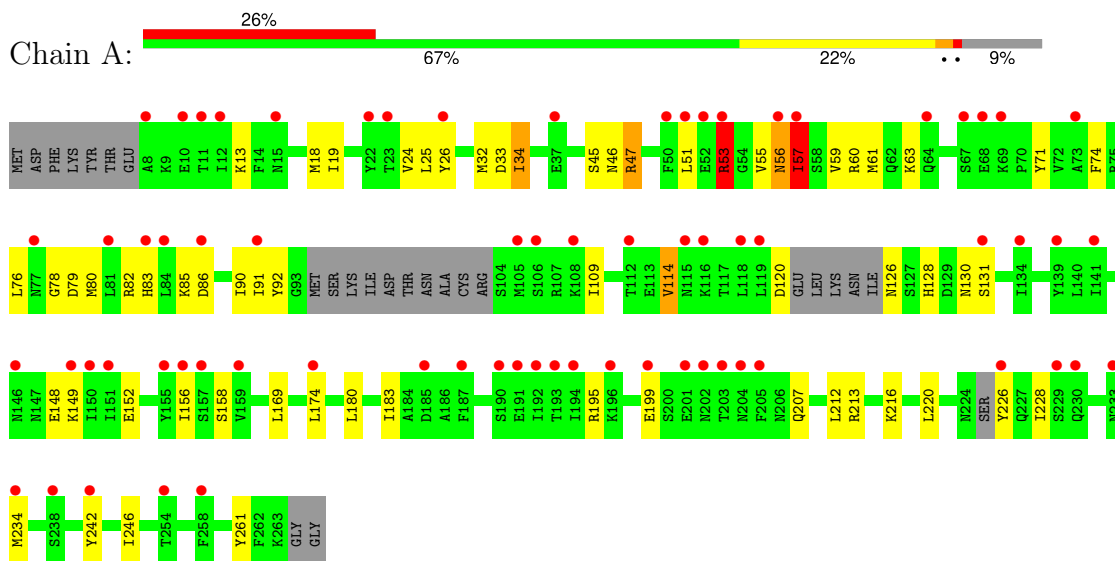
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	GLU	conflict	UNP P16114
A	14	PHE	ILE	engineered mutation	UNP P16114
A	17	PHE	ILE	engineered mutation	UNP P16114
B	8	ALA	GLU	conflict	UNP P16114
B	14	PHE	ILE	engineered mutation	UNP P16114
B	17	PHE	ILE	engineered mutation	UNP P16114

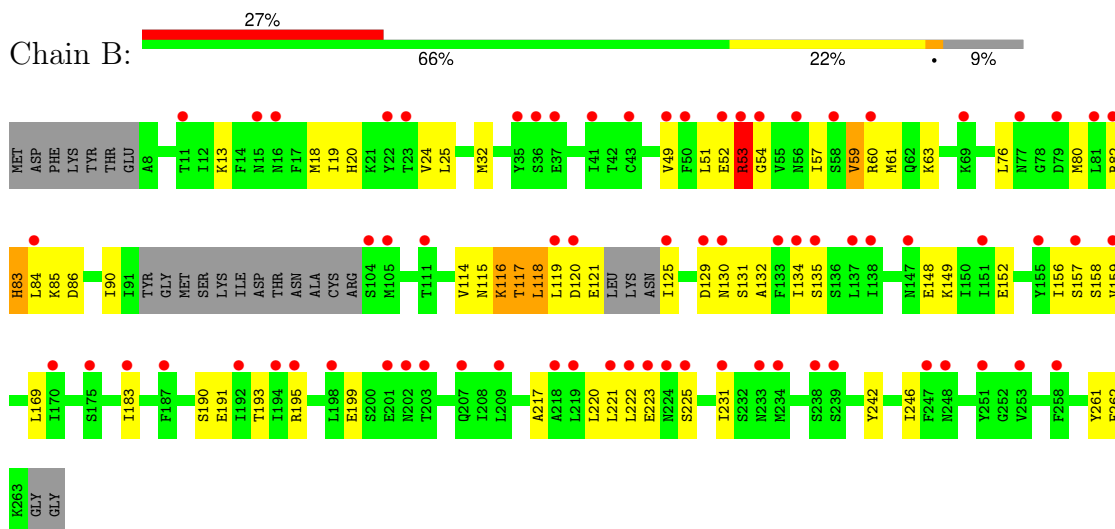
3 Residue-property plots [i](#)

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: Regulatory protein Rns



• Molecule 1: Regulatory protein Rns



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.81Å 96.68Å 138.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 3.00 29.20 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.20-3.00) 83.2 (29.20-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.352 , 0.369 0.353 , 0.370	Depositor DCC
R_{free} test set	11973 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	3941	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6057e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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	0.76	10/1997 (0.5%)	0.84	19/2677 (0.7%)
1	B	0.67	3/2004 (0.1%)	0.74	10/2688 (0.4%)
All	All	0.72	13/4001 (0.3%)	0.79	29/5365 (0.5%)

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
1	A	0	3
1	B	0	1
All	All	0	4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	SER	C-N	-18.88	1.07	1.33
1	B	83	HIS	C-N	-17.64	1.11	1.33
1	B	59	VAL	C-N	-13.37	1.14	1.33
1	A	57	ILE	C-N	-11.36	1.18	1.33
1	B	82	ARG	C-N	10.93	1.47	1.33

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	SER	O-C-N	-12.32	107.62	122.65
1	A	34	ILE	O-C-N	-10.45	111.44	123.03
1	B	59	VAL	O-C-N	9.73	133.57	123.07
1	B	82	ARG	CA-C-N	-9.64	107.91	120.44
1	B	82	ARG	C-N-CA	-9.64	107.91	120.44

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	A	53	ARG	Sidechain
1	A	57	ILE	Mainchain
1	B	53	ARG	Sidechain

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	A	1967	0	2011	38	1
1	B	1974	0	2022	41	1
All	All	3941	0	4033	75	1

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 9.

The worst 5 of 75 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:114:VAL:HG11	1:B:117:THR:CG2	1.94	0.95
1:B:114:VAL:HG11	1:B:117:THR:HG23	1.53	0.91
1:B:114:VAL:CG1	1:B:117:THR:HG23	2.07	0.84
1:A:34:ILE:HG23	1:A:57:ILE:HD12	1.69	0.75
1:B:114:VAL:HG11	1:B:117:THR:HG22	1.72	0.71

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:NE2	1:B:225:SER:O[2_455]	1.97	0.23

5.3 Torsion angles

5.3.1 Protein backbone

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	232/265 (88%)	225 (97%)	7 (3%)	0	100	100
1	B	235/265 (89%)	227 (97%)	8 (3%)	0	100	100
All	All	467/530 (88%)	452 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	224/246 (91%)	220 (98%)	4 (2%)	54	80
1	B	226/246 (92%)	221 (98%)	5 (2%)	47	76
All	All	450/492 (92%)	441 (98%)	9 (2%)	50	78

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	57	ILE
1	B	118	LEU
1	A	228	ILE
1	B	24	VAL
1	B	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	248	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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	57:ILE	C	58:SER	N	1.18
1	B	59:VAL	C	60:ARG	N	1.14
1	B	83:HIS	C	84:LEU	N	1.11
1	A	45:SER	C	46:ASN	N	1.07

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	240/265 (90%)	1.69	70 (29%) 1 1	60, 78, 98, 107	0
1	B	241/265 (90%)	1.62	72 (29%) 1 1	60, 76, 91, 112	0
All	All	481/530 (90%)	1.65	142 (29%) 1 1	60, 77, 96, 112	0

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	ASN	6.7
1	B	201	GLU	5.4
1	B	159	VAL	5.4
1	A	203	THR	5.2
1	A	156	ILE	4.9

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.