

wwPDB X-ray Structure Validation Summary Report (i)

Aug 18, 2021 – 06:02 am BST

PDB ID 7A33

> Title Crystal structure of the c-Src SH3 domain mutant S94A-T98D-V111L-N113S

> > -T114S at pH 3.0

: Camara-Artigas, A.; Plaza-Garrido, M.; Salinas-Garcia, M.C. Authors

Deposited on 2020-08-18

0.96 Å(reported) Resolution

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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 2.23.1EDS

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

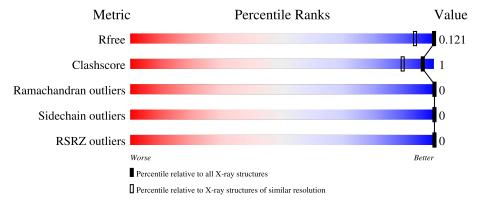
Validation Pipeline (wwPDB-VP) 2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 0.96 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1243 (1.06-0.86)
Clashscore	141614	1321 (1.06-0.86)
Ramachandran outliers	138981	1233 (1.06-0.86)
Sidechain outliers	138945	1235 (1.06-0.86)
RSRZ outliers	127900	1209 (1.06-0.86)

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	A	60	95%	-			
1	В	60	95%	-			



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2285 atoms, of which 1045 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 Proto-oncogene tyrosine-protein kinase Src.

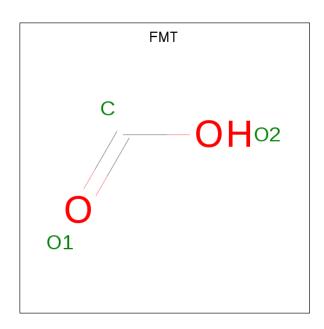
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	59	Total	С	Н	Ν	О	0	19	0
1	A	99	1018	331	498	86	103	0	10	U
1	D	58	Total	С	Н	N	О	0	22	0
1		30	1101	353	541	93	114	0	22	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	SER	engineered mutation	UNP P00523
A	98	ASP	THR	engineered mutation	UNP P00523
A	111	LEU	VAL	engineered mutation	UNP P00523
A	113	SER	ASN	engineered mutation	UNP P00523
A	114	SER	THR	engineered mutation	UNP P00523
В	94	ALA	SER	engineered mutation	UNP P00523
В	98	ASP	THR	engineered mutation	UNP P00523
В	111	LEU	VAL	engineered mutation	UNP P00523
В	113	SER	ASN	engineered mutation	UNP P00523
В	114	SER	THR	engineered mutation	UNP P00523

• Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 5				0	0
2	A	1	Total 5				0	0
2	В	1	Total 5		H 2	O 2	0	0

 \bullet Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Na 1 1	0	0

• Molecule 4 is water.

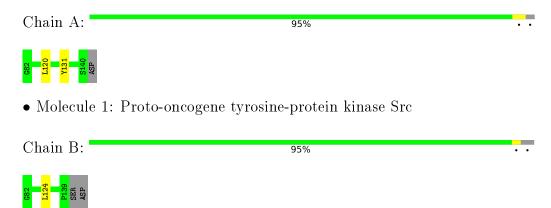
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	70	Total O 70 70	0	1
4	В	80	Total O 80 80	0	2



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: Proto-oncogene tyrosine-protein kinase Src





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	23.20Å 63.26Å 30.07Å	Depositor
a, b, c, α , β , γ	90.00° 95.65° 90.00°	Depositor
Resolution (Å)	19.22 - 0.96	Depositor
resolution (A)	19.22 - 0.96	EDS
% Data completeness	86.8 (19.22-0.96)	Depositor
(in resolution range)	94.4 (19.22-0.96)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.46 (at 0.96Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
P. P.	0.119 , 0.134	Depositor
R, R_{free}	0.119 , 0.121	DCC
R_{free} test set	2451 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	6.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41 , 44.2	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2285	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.26% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, FMT

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.44	0/582	0.73	0/794	
1	В	0.47	0/640	0.72	0/872	
All	All	0.46	0/1222	0.72	0/1666	

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	A	520	498	447	2	0
1	В	560	541	461	1	0
2	A	6	4	2	0	0
2	В	3	2	1	0	0
3	В	1	0	0	0	0
4	A	70	0	0	0	0
4	В	80	0	0	0	0
All	All	1240	1045	911	2	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 1.



All (2) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	1100111 1		Clash overlap (Å)
1:A:120[B]:LEU:HG	1:A:131:TYR:CE1	2.47	0.50
1:A:120[A]:LEU:HD21	1:B:124[A]:LEU:HD22	1.98	0.44

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 Outlier		Outliers	Perce	\mathbf{ntiles}
1	A	70/60 (117%)	70 (100%)	0	0	100	100
1	В	78/60 (130%)	78 (100%)	0	0	100	100
All	All	148/120 (123%)	148 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	59/51 (116%)	59 (100%)	0	100 100		
1	В	68/51 (133%)	68 (100%)	0	100 100		
All	All	127/102 (124%)	127 (100%)	0	100 100		



There are no protein residues with a non-rotameric sidechain to report.

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)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	Tuno	Chain	Res	Link	${\bf Bond\ lengths}$			Bond angles		
WIOI	Type				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMT	A	202	_	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	В	201	_	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	A	201	_	0,2,2	0.00	-	0,1,1	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q<0.9
1	A	59/60 (98%)	0.02	0 100	100	5, 7, 14, 17	0
1	В	58/60 (96%)	0.02	0 100	100	4, 7, 11, 14	0
All	All	117/120 (97%)	0.02	0 100	100	4, 7, 12, 17	0

There are no RSRZ outliers to report.

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	FMT	A	201	3/3	0.99	0.05	6,7,8,8	0
2	FMT	A	202	3/3	0.99	0.07	6,7,8,8	0
2	FMT	В	201	3/3	0.99	0.06	9,9,10,12	0
3	NA	В	202	1/1	1.00	0.08	6,6,6,6	0



6.5 Other polymers (i)

There are no such residues in this entry.

