

Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 02:38 pm GMT

PDB ID	:	7NYL
Title	:	Mutant H493A of SH3 domain of JNK-interacting Protein 1 (JIP1)
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Deposited on		
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

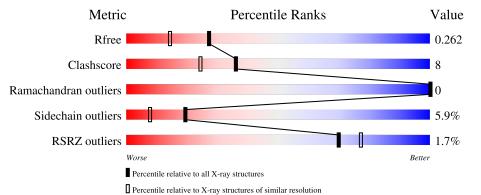
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	AAA	63	^{3%} 76%	16% 8%				
1	BBB	63	76%	19% ••				
2	С	2	50%	50%				



7NYL

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1087 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 SH3 domain of JNK-interacting Protein 1 (JIP1).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	1 AAA	58	Total	С	Ν	Ο	S	0	0	0
			486	313	79	93	1			
1	BBB	62	Total	С	Ν	Ο	S	0	0	0
	1 BBB	62	517	331	85	99	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	487	GLY	-	expression tag	UNP Q9UQF2
AAA	488	HIS	-	expression tag	UNP Q9UQF2
AAA	489	MET	-	expression tag	UNP Q9UQF2
AAA	493	ALA	HIS	engineered mutation	UNP Q9UQF2
BBB	487	GLY	-	expression tag	UNP Q9UQF2
BBB	488	HIS	-	expression tag	UNP Q9UQF2
BBB	489	MET	-	expression tag	UNP Q9UQF2
BBB	493	ALA	HIS	engineered mutation	UNP Q9UQF2

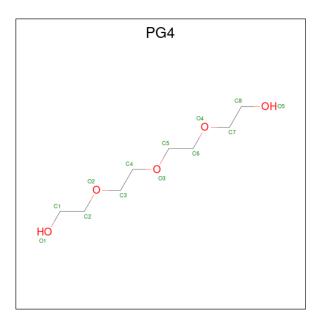
• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	At	\mathbf{oms}		ZeroOcc	AltConf	Trace
2	С	2	Total 23	C 12	0 11	0	0	0

• Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 13 8 5	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	26	TotalO2626	0	0
4	BBB	22	TotalO2222	0	0

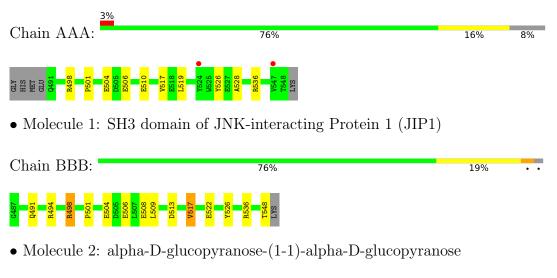


CTC CTC

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: SH3 domain of JNK-interacting Protein 1 (JIP1)



Chain C:	50%	50%

WORLDWIDE PROTEIN DATA BANK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	28.05Å 45.55 Å 46.01 Å	Depositor
a, b, c, α , β , γ	90.00° 104.27° 90.00°	Depositor
Resolution (Å)	44.59 - 1.95	Depositor
Resolution (A)	44.59 - 1.95	EDS
% Data completeness	99.8 (44.59-1.95)	Depositor
(in resolution range)	99.8 (44.59-1.95)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.44 (at 1.95 \text{\AA})$	Xtriage
Refinement program	REFMAC $7.0.078$	Depositor
B B.	0.205 , 0.255	Depositor
R, R_{free}	0.213 , 0.262	DCC
R_{free} test set	403 reflections $(4.85%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	28.1	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 44.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.51, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1087	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.52% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, GLC

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	Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AAA	0.73	1/499~(0.2%)	0.89	0/680	
1	BBB	0.68	0/531	0.97	0/722	
All	All	0.71	1/1030~(0.1%)	0.93	0/1402	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	AAA	504	GLU	CD-OE2	5.02	1.31	1.25

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	AAA	486	0	453	8	0
1	BBB	517	0	478	8	0
2	С	23	0	21	0	0
3	AAA	13	0	18	0	0
4	AAA	26	0	0	1	0
4	BBB	22	0	0	1	0
All	All	1087	0	970	16	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 8.

All (16) 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:AAA:528:ALA:O	1:AAA:536:ARG:HD2	1.81	0.81
1:BBB:491:GLN:HG3	1:BBB:548:THR:OG1	1.92	0.69
1:BBB:498:ARG:HG3	1:BBB:498:ARG:HH11	1.58	0.68
1:BBB:508:GLU:OE1	4:BBB:601:HOH:O	2.12	0.67
1:BBB:498:ARG:HG3	1:BBB:498:ARG:NH1	2.17	0.59
1:AAA:498:ARG:NH2	4:AAA:701:HOH:O	2.37	0.58
1:BBB:498:ARG:NH1	1:BBB:509:LEU:O	2.40	0.55
1:BBB:517:VAL:HG13	1:BBB:526:TYR:CD1	2.41	0.55
1:AAA:517:VAL:HG13	1:AAA:526:TYR:CD1	2.43	0.53
1:AAA:528:ALA:C	1:AAA:536:ARG:HH21	2.18	0.46
1:AAA:528:ALA:O	1:AAA:536:ARG:CD	2.58	0.45
1:AAA:501:PRO:HB3	1:AAA:506:GLU:HB2	1.97	0.45
1:AAA:517:VAL:HG13	1:AAA:526:TYR:CE1	2.52	0.44
1:BBB:501:PRO:HB3	1:BBB:506:GLU:HB2	2.00	0.43
1:AAA:498:ARG:NH1	1:AAA:510:GLU:OE2	2.50	0.42
1:BBB:494:ARG:HA	1:BBB:513:ASP:O	2.21	0.41

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	ntiles
1	AAA	56/63~(89%)	54 (96%)	2(4%)	0	100	100
1	BBB	60/63~(95%)	57~(95%)	3~(5%)	0	100	100
All	All	116/126~(92%)	111 (96%)	5 (4%)	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	AAA	49/53~(92%)	48 (98%)	1 (2%)	55 48
1	BBB	52/53~(98%)	47 (90%)	5 (10%)	8 2
All	All	101/106~(95%)	95~(94%)	6~(6%)	19 8

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	519	LEU
1	BBB	498	ARG
1	BBB	504	GLU
1	BBB	517	VAL
1	BBB	522	GLU
1	BBB	536	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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)

2 monosaccharides are 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

Bond lengths Bond angles										
RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).										
expected value. A bond length (or angle) with $ Z > 2$ is considered an outlier worth inspection.										

\mathbf{Mol}	Type	Chain	Res	Link		Dona lengths		Dolld angles		
IVIOI	туре	Onam	TICS		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	GLC	С	1	2	11,11,12	0.87	0	$15,\!15,\!17$	1.55	6 (40%)
2	GLC	С	2	2	12,12,12	0.93	0	17,17,17	0.89	0

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
2	GLC	С	1	2	-	0/2/19/22	0/1/1/1
2	GLC	С	2	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	1	GLC	O5-C5-C6	2.51	111.13	107.20
2	С	1	GLC	C1-C2-C3	2.50	112.74	109.67
2	С	1	GLC	C2-C3-C4	2.31	114.89	110.89
2	С	1	GLC	O2-C2-C1	-2.29	104.47	109.15
2	С	1	GLC	C1-O5-C5	2.19	115.16	112.19
2	С	1	GLC	O3-C3-C4	-2.08	105.55	110.35

There are no chirality outliers.

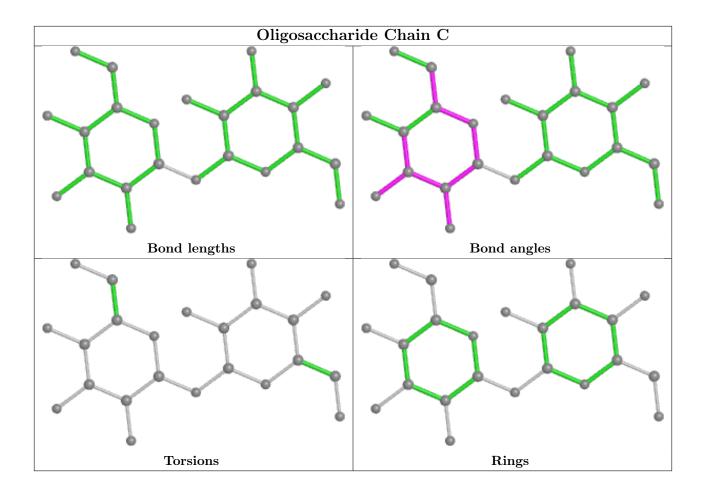
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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		s Link	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	PG4	AAA	601	-	$12,\!12,\!12$	0.26	0	11,11,11	0.25	0

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
3	PG4	AAA	601	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	601	PG4	O4-C7-C8-O5
3	AAA	601	PG4	C1-C2-O2-C3
3	AAA	601	PG4	C3-C4-O3-C5
3	AAA	601	PG4	O2-C3-C4-O3
3	AAA	601	PG4	C8-C7-O4-C6
3	AAA	601	PG4	O3-C5-C6-O4

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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	AAA	58/63~(92%)	-0.00	2 (3%) 45 55	20, 33, 52, 71	0
1	BBB	62/63~(98%)	-0.18	0 100 100	18, 29, 49, 66	0
All	All	120/126~(95%)	-0.10	2 (1%) 70 77	18, 31, 51, 71	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	524	TYR	3.4
1	AAA	547	VAL	2.5

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

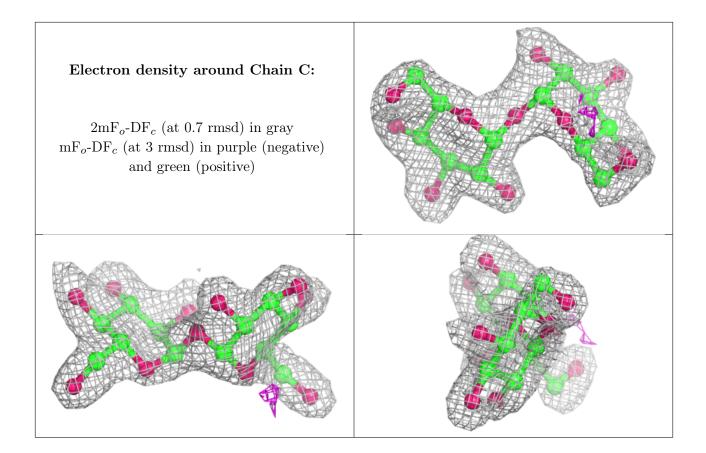
6.3 Carbohydrates (i)

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
2	GLC	С	1	11/12	0.82	0.19	37,46,49,52	0
2	GLC	С	2	12/12	0.90	0.17	$36,\!41,\!45,\!47$	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





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	$B-factors(Å^2)$	Q<0.9
3	PG4	AAA	601	13/13	0.90	0.13	$48,\!58,\!64,\!65$	0

6.5 Other polymers (i)

There are no such residues in this entry.

