



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 13, 2021 – 06:09 pm GMT

PDB ID : 7NYO
Title : Mutant A541L of SH3 domain of JNK-interacting Protein 1 (JIP1)
Authors : Perez, L.M.; Ielasi, F.S.; Palencia, A.; Jensen, M.R.
Deposited on : 2021-03-23
Resolution : 1.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

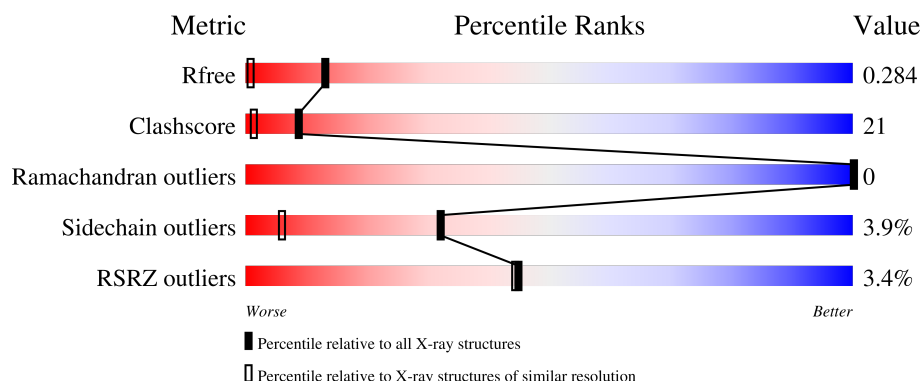
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	AAA	63	<div> <div>3%</div> <div>67%</div> <div>25%</div> <div>6%</div> </div>
1	BBB	63	<div> <div>2%</div> <div>71%</div> <div>21%</div> <div>6%</div> </div>
1	CCC	63	<div> <div>2%</div> <div>76%</div> <div>17%</div> <div>5%</div> </div>
1	DDD	63	<div> <div>6%</div> <div>63%</div> <div>30%</div> <div>6%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2638 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	AAA	59	Total	C	N	O	S	0	3	0
			523	338	83	101	1			
1	BBB	59	Total	C	N	O	S	0	3	0
			526	338	86	101	1			
1	CCC	60	Total	C	N	O	S	0	1	0
			520	334	84	100	2			
1	DDD	59	Total	C	N	O	S	0	0	0
			496	319	81	95	1			

There are 16 discrepancies between the modelled and reference sequences:

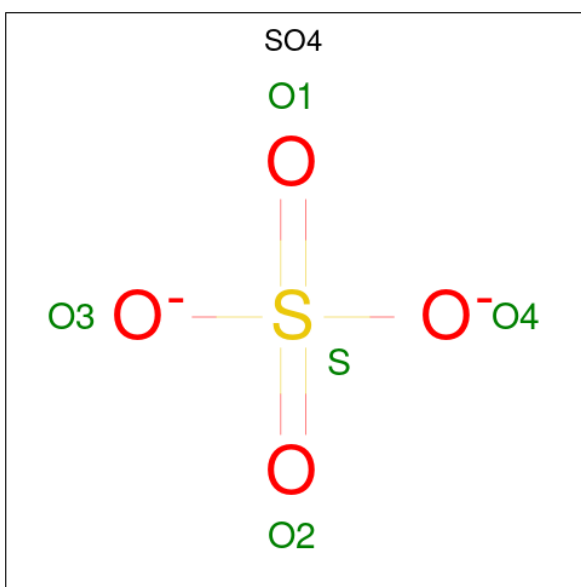
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	487	GLY	-	expression tag	UNP Q9UQF2
AAA	488	HIS	-	expression tag	UNP Q9UQF2
AAA	489	MET	-	expression tag	UNP Q9UQF2
AAA	541	LEU	ALA	engineered mutation	UNP Q9UQF2
BBB	487	GLY	-	expression tag	UNP Q9UQF2
BBB	488	HIS	-	expression tag	UNP Q9UQF2
BBB	489	MET	-	expression tag	UNP Q9UQF2
BBB	541	LEU	ALA	engineered mutation	UNP Q9UQF2
CCC	487	GLY	-	expression tag	UNP Q9UQF2
CCC	488	HIS	-	expression tag	UNP Q9UQF2
CCC	489	MET	-	expression tag	UNP Q9UQF2
CCC	541	LEU	ALA	engineered mutation	UNP Q9UQF2
DDD	487	GLY	-	expression tag	UNP Q9UQF2
DDD	488	HIS	-	expression tag	UNP Q9UQF2
DDD	489	MET	-	expression tag	UNP Q9UQF2
DDD	541	LEU	ALA	engineered mutation	UNP Q9UQF2

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	DDD	1	Total	C	O	0	0
			4	2	2		

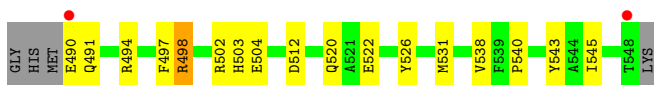
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	127	Total	O	0	0
			127	127		
5	BBB	149	Total	O	0	0
			149	149		
5	CCC	123	Total	O	0	0
			123	123		
5	DDD	126	Total	O	0	0
			126	126		

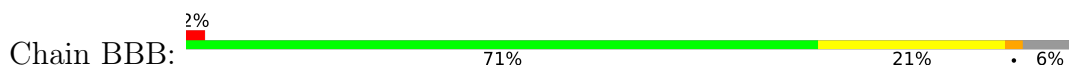
3 Residue-property plots [i](#)

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.

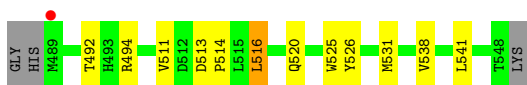
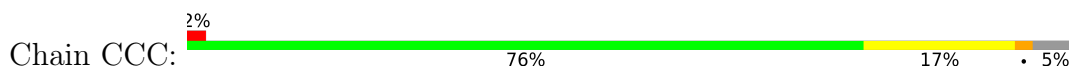
- Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.09Å 67.10Å 59.14Å 90.00° 126.70° 90.00°	Depositor
Resolution (Å)	47.42 – 1.40 47.42 – 1.40	Depositor EDS
% Data completeness (in resolution range)	70.4 (47.42-1.40) 70.4 (47.42-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.40Å)	Xtriage
Refinement program	REFMAC 7.0.078	Depositor
R, R_{free}	0.192 , 0.276 0.200 , 0.284	Depositor DCC
R_{free} test set	2116 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2638	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SO4, PG4

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	AAA	0.74	0/543	1.01	0/739
1	BBB	0.74	0/546	0.86	0/742
1	CCC	0.70	0/534	0.90	1/726 (0.1%)
1	DDD	0.77	0/510	0.93	0/695
All	All	0.74	0/2133	0.93	1/2902 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	494	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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	523	0	489	22	0
1	BBB	526	0	491	22	0
1	CCC	520	0	481	18	0
1	DDD	496	0	452	21	0
2	AAA	26	0	36	0	0
2	CCC	13	0	18	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	5	0	0	0	0
4	DDD	4	0	6	0	0
5	AAA	127	0	0	13	1
5	BBB	149	0	0	18	0
5	CCC	123	0	0	23	1
5	DDD	126	0	0	18	1
All	All	2638	0	1973	84	2

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 21.

The worst 5 of 84 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:DDD:494:ARG:HG3	5:DDD:701:HOH:O	1.46	1.14
1:BBB:525:TRP:HZ3	5:BBB:875:HOH:O	1.35	1.10
2:CCC:601:PG4:H52	5:CCC:725:HOH:O	1.53	1.07
1:CCC:513:ASP:HB2	5:CCC:709:HOH:O	1.64	0.95
1:CCC:511:VAL:HG21	5:CCC:790:HOH:O	1.71	0.90

All (2) 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)
5:CCC:817:HOH:O	5:DDD:734:HOH:O[2_555]	2.14	0.06
5:AAA:821:HOH:O	5:AAA:821:HOH:O[2_555]	2.17	0.03

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	AAA	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
1	BBB	60/63 (95%)	60 (100%)	0	0	100	100
1	CCC	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
1	DDD	57/63 (90%)	56 (98%)	1 (2%)	0	100	100
All	All	236/252 (94%)	233 (99%)	3 (1%)	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	AAA	55/55 (100%)	53 (96%)	2 (4%)	35	7
1	BBB	55/55 (100%)	53 (96%)	2 (4%)	35	7
1	CCC	54/55 (98%)	53 (98%)	1 (2%)	57	25
1	DDD	50/55 (91%)	47 (94%)	3 (6%)	19	2
All	All	214/220 (97%)	206 (96%)	8 (4%)	32	7

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	548	THR
1	DDD	523	ASP
1	CCC	516	LEU
1	BBB	548	THR
1	DDD	512	ASP

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

5.3.3 RNA ⓘ

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](#)

5 ligands 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 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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	BBB	701	-	4,4,4	0.29	0	6,6,6	0.20	0
4	EDO	DDD	601	-	3,3,3	0.77	0	2,2,2	0.46	0
2	PG4	AAA	602	-	12,12,12	0.27	0	11,11,11	0.14	0
2	PG4	AAA	601	-	12,12,12	0.14	0	11,11,11	0.24	0
2	PG4	CCC	601	-	12,12,12	0.11	0	11,11,11	0.32	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	PG4	CCC	601	-	-	5/10/10/10	-
2	PG4	AAA	601	-	-	2/10/10/10	-
2	PG4	AAA	602	-	-	5/10/10/10	-
4	EDO	DDD	601	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	602	PG4	O3-C5-C6-O4
2	CCC	601	PG4	O3-C5-C6-O4
2	CCC	601	PG4	O2-C3-C4-O3
2	AAA	602	PG4	O1-C1-C2-O2
2	AAA	602	PG4	O4-C7-C8-O5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	601	PG4	2	0

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	AAA	59/63 (93%)	0.19	2 (3%) 45 44	12, 19, 36, 62	0
1	BBB	59/63 (93%)	0.12	1 (1%) 70 69	13, 20, 40, 54	0
1	CCC	60/63 (95%)	0.15	1 (1%) 70 69	12, 18, 38, 62	0
1	DDD	59/63 (93%)	0.37	4 (6%) 17 15	15, 21, 56, 71	0
All	All	237/252 (94%)	0.21	8 (3%) 45 44	12, 20, 40, 71	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	548	THR	6.0
1	BBB	548	THR	4.4
1	DDD	520	GLN	4.3
1	DDD	519	LEU	4.1
1	CCC	489	MET	3.6

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, 95th 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(\AA^2)	Q<0.9
2	PG4	AAA	602	13/13	0.83	0.15	26,29,37,38	13
4	EDO	DDD	601	4/4	0.87	0.22	24,26,27,28	4
2	PG4	CCC	601	13/13	0.92	0.13	19,21,24,29	13
3	SO4	BBB	701	5/5	0.96	0.10	40,40,45,53	0
2	PG4	AAA	601	13/13	0.96	0.13	21,24,26,27	13

6.5 Other polymers [i](#)

There are no such residues in this entry.