



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:13 AM UTC

PDB ID : 9T2I / pdb_00009t2i
Title : SP100 nuclear antigen with crystallization epitope mutations N816D:T820R
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Deposited on : 2025-10-22
Resolution : 1.35 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 ⓘ 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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

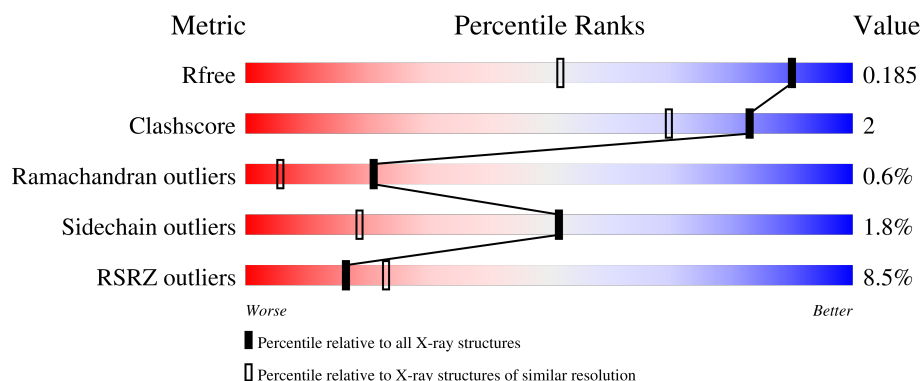
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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}	180053	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	178	<div> <div>7%</div> <div> <div></div> <div>93%</div> <div>...</div> </div> </div>
1	B	178	<div> <div>9%</div> <div> <div></div> <div>89%</div> <div>... 7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6088 atoms, of which 2815 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 Isoform Sp100-C of Nuclear autoantigen Sp-100.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	178	Total	C	H	N	O	S	0	16	0
			3021	975	1466	277	285	18			
1	B	165	Total	C	H	N	O	S	0	10	0
			2772	900	1349	252	253	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	816	ASP	ASN	engineered mutation	UNP P23497
A	820	ARG	THR	engineered mutation	UNP P23497
B	816	ASP	ASN	engineered mutation	UNP P23497
B	820	ARG	THR	engineered mutation	UNP P23497

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

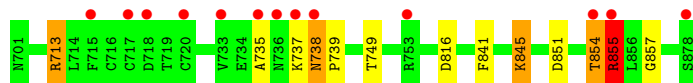
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total	O	0	0
			163	163		
3	B	127	Total	O	0	0
			127	127		

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.

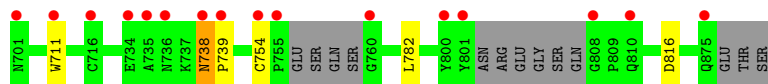
- Molecule 1: Isoform Sp100-C of Nuclear autoantigen Sp-100

Chain A: 7% 93%



- Molecule 1: Isoform Sp100-C of Nuclear autoantigen Sp-100

Chain B: 9% 89% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.09Å 45.73Å 83.95Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	56.19 – 1.35 56.19 – 1.35	Depositor EDS
% Data completeness (in resolution range)	95.5 (56.19-1.35) 95.5 (56.19-1.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.126)	Depositor
R, R_{free}	0.158 , 0.185 0.158 , 0.185	Depositor DCC
R_{free} test set	5030 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6088	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

5.1 Standard geometry

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

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	0.78	0/1664	1.03	5/2234 (0.2%)
1	B	0.82	0/1502	1.02	1/2015 (0.0%)
All	All	0.80	0/3166	1.03	6/4249 (0.1%)

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	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	854	THR	CA-CB-OG1	5.77	118.26	109.60
1	B	816	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	851	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	816	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	749	THR	CA-CB-OG1	-5.15	101.88	109.60
1	A	855	ARG	N-CA-CB	5.10	118.08	110.22

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	713	ARG	Sidechain
1	A	855	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	1555	1466	1428	9	0
1	B	1423	1349	1322	5	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	163	0	0	0	0
3	B	127	0	0	1	0
All	All	3273	2815	2750	14	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 2.

All (14) 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:A:841:PHE:O	1:A:845:LYS:HE3	1.93	0.69
1:A:738:ASN:HB3	1:A:739:PRO:HD2	1.76	0.68
1:A:845:LYS:HE2	1:A:857:GLY:HA3	1.77	0.67
1:B:754:CYS:N	3:B:1001:HOH:O	2.32	0.62
1:A:738:ASN:CB	1:A:739:PRO:HD2	2.32	0.59
1:A:738:ASN:HB3	1:A:739:PRO:CD	2.34	0.57
1:B:738:ASN:CB	1:B:739:PRO:HD3	2.35	0.56
1:A:845:LYS:HE2	1:A:857:GLY:C	2.29	0.56
1:A:845:LYS:HE2	1:A:857:GLY:CA	2.37	0.54
1:B:738:ASN:HB2	1:B:739:PRO:HD3	1.90	0.52
1:B:738:ASN:CB	1:B:739:PRO:CD	2.89	0.50
1:A:738:ASN:CB	1:A:739:PRO:CD	2.90	0.48
1:B:738:ASN:HB2	1:B:739:PRO:CD	2.43	0.48
1:A:735:ALA:HB3	1:A:737:LYS:HE3	1.99	0.44

There are no symmetry-related clashes.

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	192/178 (108%)	187 (97%)	4 (2%)	1 (0%)	24	7
1	B	169/178 (95%)	165 (98%)	3 (2%)	1 (1%)	21	6
All	All	361/356 (101%)	352 (98%)	7 (2%)	2 (1%)	21	6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	738	ASN
1	B	738	ASN

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	184/169 (109%)	180 (98%)	4 (2%)	45	14
1	B	166/169 (98%)	164 (99%)	2 (1%)	63	32
All	All	350/338 (104%)	344 (98%)	6 (2%)	51	20

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

Mol	Chain	Res	Type
1	A	713	ARG
1	A	845	LYS
1	A	854	THR
1	A	855	ARG

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Mol	Chain	Res	Type
1	B	711	TRP
1	B	782	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	ASN
1	A	709	ASN
1	B	701	ASN
1	B	738	ASN
1	B	770	GLN

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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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

6.1 Protein, DNA and RNA chains

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	178/178 (100%)	0.26	13 (7%)	21 29	10, 26, 51, 83	8 (4%)
1	B	165/178 (92%)	0.37	16 (9%)	13 19	12, 27, 51, 76	5 (3%)
All	All	343/356 (96%)	0.31	29 (8%)	16 23	10, 26, 51, 83	13 (3%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	ALA	6.4
1	B	800	TYR	6.2
1	B	754	CYS	5.2
1	A	736	ASN	4.4
1	B	735	ALA	4.3
1	B	738	ASN	3.8
1	B	808	GLY	3.6
1	B	755	PRO	3.4
1	B	711	TRP	3.4
1	B	739	PRO	3.3
1	A	717	CYS	3.2
1	A	737	LYS	3.2
1	B	801	TYR	3.1
1	B	760	GLY	3.1
1	A	878	SER	3.1
1	A	738	ASN	3.0
1	B	701	ASN	2.8
1	B	736	ASN	2.7
1	A	733	VAL	2.7
1	B	734	GLU	2.7
1	A	855	ARG	2.6
1	B	716	CYS	2.4
1	A	715	PHE	2.3
1	B	875	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	720	CYS	2.2
1	B	810	GLN	2.2
1	A	854	THR	2.2
1	A	718	ASP	2.1
1	A	753	ARG	2.1

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](#)

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	ZN	A	903	1/1	0.25	0.29	156,156,156,156	0
2	ZN	A	902	1/1	0.99	0.05	36,36,36,36	0
2	ZN	A	901	1/1	1.00	0.02	26,26,26,26	0
2	ZN	B	901	1/1	1.00	0.05	24,24,24,24	0
2	ZN	B	902	1/1	1.00	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.