

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 5M9O

Title : Crystal structure of human SND1 extended Tudor domain in complex with a

symmetrically dimethylated E2F peptide

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Deposited on : 2016-11-01

Resolution : 1.45 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 (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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

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

Xtriage (Phenix) : 1.13 EDS : 2.37.1

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)

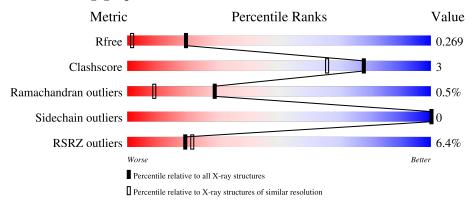
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

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 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	224	5%	91% 5% •				
2	В	9	11%	11%	11%	11%	56%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1921 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 Staphylococcal nuclease domain-containing protein 1.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	216	Total 1715	C 1086	N 294	O 329	S 6	0	1	0

• Molecule 2 is a protein called E2F peptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	4	Total 40	C 24	N 12	O 4	0	0	0

• Molecule 3 is water.

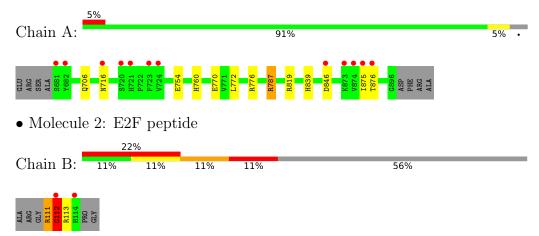
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	163	Total O 163 163	0	0
3	В	3	Total O 3 3	0	0



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: Staphylococcal nuclease domain-containing protein 1





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	36.24Å 80.63Å 39.29Å	Danagitan	
a, b, c, α , β , γ	90.00° 90.38° 90.00°	Depositor	
Resolution (Å)	28.14 - 1.45	Depositor	
Resolution (A)	28.14 - 1.45	EDS	
% Data completeness	95.8 (28.14-1.45)	Depositor	
(in resolution range)	95.9 (28.14-1.45)	EDS	
R_{merge}	0.04	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.70 (at 1.45Å)	Xtriage	
Refinement program	REFMAC 5.8.0131	Depositor	
D.D.	0.229 , 0.261	Depositor	
R, R_{free}	0.235 , 0.269	DCC	
R_{free} test set	1920 reflections (5.01%)	wwPDB-VP	
Wilson B-factor (Å ²)	17.3	Xtriage	
Anisotropy	0.023	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 35.2	EDS	
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	1921	wwPDB-VP	
Average B, all atoms (Å ²)	22.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.12% 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: 2MR

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).

Mal	Mol Chain		lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.52	0/1755	0.73	1/2384 (0.0%)	
2	В	0.65	0/13	0.85	0/14	
All	All	0.52	0/1768	0.73	1/2398 (0.0%)	

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
2	В	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	787	ARG	NE-CZ-NH1	5.32	122.96	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	112	GLY	Peptide

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1715	0	1672	8	1
2	В	40	0	41	2	0
3	A	163	0	0	5	0
3	В	3	0	0	0	0
All	All	1921	0	1713	10	1

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 3.

The worst 5 of 10 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:B:111:2MR:N	2:B:112:GLY:O	2.25	0.69
1:A:770:GLU:HG2	1:A:772:LEU:HG	1.81	0.62
1:A:776:ARG:NH1	3:A:1001:HOH:O	2.33	0.61
1:A:716:ASN:ND2	3:A:1003:HOH:O	2.38	0.55
1:A:706:GLN:NE2	3:A:1004:HOH:O	2.40	0.54

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)	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\begin{subarray}{c} \begin{subarray}{c} \begi$
1:A:787:ARG:NH2	1:A:846:ASP:OD1[1_554]	2.19	0.01

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	A	215/224 (96%)	212 (99%)	3 (1%)	0	100 100
2	В	1/9 (11%)	0	0	1 (100%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	216/233 (93%)	212 (98%)	3 (1%)	1 (0%)	29 9

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	112	GLY

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	186/193 (96%)	186 (100%)	0	100	100	
2	В	1/3 (33%)	1 (100%)	0	100	100	
All	All	187/196 (95%)	187 (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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	706	GLN
1	A	760	HIS
1	A	792	GLN
1	A	839	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	Tuno	Chain	Res	Dec	Dec	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
2	2MR	В	111	2	10,12,13	0.79	0	5,13,15	1.69	2 (40%)		
2	2MR	В	113	2	10,12,13	0.96	1 (10%)	5,13,15	1.08	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	2MR	В	111	2	-	3/10/13/15	-
2	2MR	В	113	2	-	0/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
2	В	113	2MR	CZ-NH2	-2.35	1.28	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	В	111	2MR	NE-CZ-NH2	-3.03	116.70	119.48
2	В	111	2MR	CD-NE-CZ	2.24	127.59	123.41

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	111	2MR	N-CA-CB-CG
2	В	111	2MR	C-CA-CB-CG
2	В	111	2MR	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	111	2MR	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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)

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	<RSRZ $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	216/224 (96%)	0.40	12 (5%) 24 26	10, 20, 34, 50	0
2	В	2/9~(22%)	4.96	2 (100%) 0 0	52, 52, 52, 56	0
All	All	218/233 (93%)	0.44	14 (6%) 19 21	10, 20, 37, 56	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	112	GLY	7.4
1	A	681	SER	4.5
1	A	724	VAL	3.7
1	A	846	ASP	3.6
1	A	876	THR	2.6

6.2 Non-standard residues in protein, DNA, RNA chains (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	2MR	В	111	13/14	0.52	0.34	60,62,63,64	0
2	2MR	В	113	13/14	0.83	0.15	17,22,46,47	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.

