



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2023 – 10:28 pm GMT

PDB ID : 8Q2M  
Title : 18mer DNA mimic Foldamer with an Aliphatic linker in complex with Sac7d V26A/M29A protein  
Authors : Deepak, D.; Corvaglia, V.; Wu, J.; Huc, I.  
Deposited on : 2023-08-02  
Resolution : 3.21 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](mailto: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>.

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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 : 2.36  
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

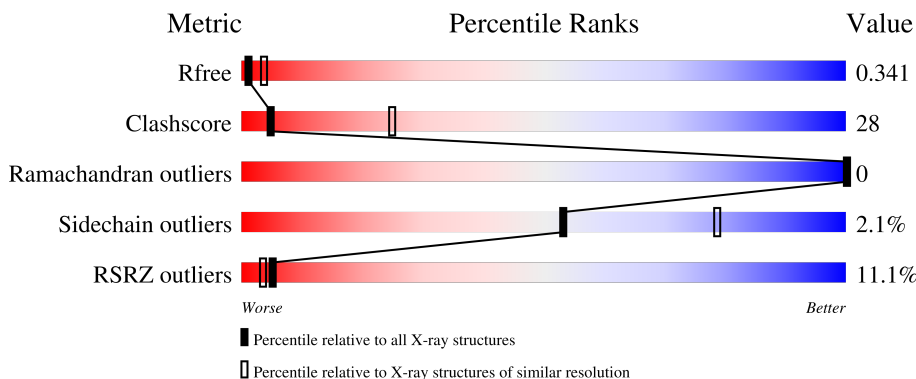
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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  $\geq 3$ , 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	AA	66	
2	A	10	
2	B	10	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	V4F	B	112	-	X	-	-
2	V4F	B	114	-	X	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 820 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 DNA-binding protein 7b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	63	474	294	86	92	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	26	ALA	VAL	conflict	UNP P13123
AA	29	ALA	MET	conflict	UNP P13123

- Molecule 2 is a protein called DNA mimic Foldamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	A	10	173	103	17	45	8	0	0	0
2	B	10	173	103	17	45	8	0	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: DNA-binding protein 7b

Chain AA: 



- Molecule 2: DNA mimic Foldamer

Chain A: 



- Molecule 2: DNA mimic Foldamer

Chain B: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.92Å 70.92Å 119.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.71 – 3.21 42.79 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.71-3.21) 100.0 (42.79-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.94 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.325 , 0.335 0.328 , 0.341	Depositor DCC
$R_{free}$ test set	323 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	113.9	Xtrriage
Anisotropy	0.447	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 113.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: V5F, V4F, V53, GOA

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	AA	0.89	0/477	1.11	1/633 (0.2%)

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	AA	0	1
2	B	0	5
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	22	LYS	CD-CE-NZ	6.15	125.85	111.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	61	ALA	Mainchain
2	B	112	V4F	Mainchain
2	B	114	V4F	Mainchain
2	B	116	V5F	Mainchain,Peptide
2	B	117	V4F	Mainchain

## 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	AA	474	0	480	26	1
2	A	173	0	0	4	2
2	B	173	0	0	8	3
All	All	820	0	480	36	5

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 28.

The worst 5 of 36 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:AA:15:VAL:HG23	1:AA:19:LYS:HE3	1.75	0.69
1:AA:52:LYS:NZ	1:AA:56:ASP:OD2	2.24	0.68
1:AA:61:ALA:O	1:AA:63:ARG:HD3	1.94	0.67
2:A:102:V4F:N	2:A:102:V4F:NAH	2.44	0.65
1:AA:3:LYS:HD3	1:AA:5:LYS:HE2	1.78	0.65

All (5) 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)
1:AA:5:LYS:NZ	2:A:108:V53:O1[11_555]	1.30	0.90
2:B:111:GOA:CA	2:B:111:GOA:O2[4_545]	1.42	0.78
2:A:101:GOA:CA	2:A:101:GOA:O2[7_555]	1.47	0.73
2:B:111:GOA:CA	2:B:111:GOA:CA[4_545]	1.85	0.35
2:B:112:V4F:O3	2:B:112:V4F:O3[4_545]	1.99	0.21

## 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	AA	61/66 (92%)	58 (95%)	3 (5%)	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	AA	47/55 (86%)	46 (98%)	1 (2%)	53	79

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	63	ARG

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](#)

18 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	V4F	A	102	2	21,21,22	2.76	6 (28%)	27,30,32	2.60	12 (44%)
2	V53	B	113	2	20,20,21	2.86	6 (30%)	25,29,31	3.01	9 (36%)
2	V53	A	105	2	20,20,21	2.56	3 (15%)	25,29,31	2.25	10 (40%)
2	V53	A	108	2	20,20,21	2.90	6 (30%)	25,29,31	2.49	15 (60%)
2	V53	B	115	2	20,20,21	2.86	8 (40%)	25,29,31	3.03	11 (44%)
2	V4F	B	117	2	21,21,22	2.61	8 (38%)	27,30,32	2.33	10 (37%)
2	V53	A	103	2	20,20,21	2.85	8 (40%)	25,29,31	2.62	9 (36%)
2	V53	A	110	2	21,21,21	3.26	7 (33%)	29,31,31	2.22	9 (31%)
2	V53	B	120	2	21,21,21	2.00	5 (23%)	29,31,31	3.10	14 (48%)
2	V4F	A	107	2	21,21,22	3.31	7 (33%)	27,30,32	2.50	8 (29%)
2	V4F	A	109	2	21,21,22	2.30	4 (19%)	27,30,32	3.04	10 (37%)
2	V4F	B	119	2	21,21,22	2.40	5 (23%)	27,30,32	3.42	15 (55%)
2	V53	B	118	2	20,20,21	2.06	4 (20%)	25,29,31	2.84	7 (28%)
2	V5F	A	106	2	11,12,13	1.23	1 (9%)	14,15,17	2.37	6 (42%)
2	V4F	A	104	2	21,21,22	2.30	5 (23%)	27,30,32	2.26	8 (29%)
2	V5F	B	116	2	11,12,13	1.28	1 (9%)	14,15,17	3.69	5 (35%)
2	V4F	B	112	2	21,21,22	3.08	7 (33%)	27,30,32	3.57	13 (48%)
2	V4F	B	114	2	21,21,22	2.78	6 (28%)	27,30,32	3.57	14 (51%)

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	V4F	A	102	2	-	5/10/10/12	0/2/2/2
2	V53	B	113	2	-	1/8/8/10	0/2/2/2
2	V53	A	105	2	-	1/8/8/10	0/2/2/2
2	V53	A	108	2	-	0/8/8/10	0/2/2/2
2	V53	B	115	2	-	4/8/8/10	0/2/2/2
2	V4F	B	117	2	-	6/10/10/12	0/2/2/2
2	V53	A	103	2	-	2/8/8/10	0/2/2/2
2	V53	A	110	2	-	0/10/10/10	0/2/2/2
2	V53	B	120	2	-	3/10/10/10	0/2/2/2
2	V4F	A	107	2	-	2/10/10/12	0/2/2/2
2	V4F	A	109	2	-	4/10/10/12	0/2/2/2
2	V4F	B	119	2	-	3/10/10/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	V53	B	118	2	-	3/8/8/10	0/2/2/2
2	V5F	A	106	2	-	1/4/6/8	0/1/1/1
2	V4F	A	104	2	-	1/10/10/12	0/2/2/2
2	V5F	B	116	2	-	1/4/6/8	0/1/1/1
2	V4F	B	112	2	-	8/10/10/12	0/2/2/2
2	V4F	B	114	2	-	6/10/10/12	0/2/2/2

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	107	V4F	CAE-C	-13.01	1.35	1.48
2	B	114	V4F	CAE-C	-10.05	1.38	1.48
2	A	108	V53	CAJ-C	-9.98	1.38	1.48
2	B	113	V53	CAJ-C	-9.86	1.38	1.48
2	B	115	V53	CAJ-C	-9.83	1.38	1.48

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	V4F	O-C-CAE	-10.86	113.93	124.22
2	B	116	V5F	O1-C6-CB	10.09	124.77	106.59
2	B	120	V53	O1-P-C01	-9.84	78.04	112.92
2	B	119	V4F	C-CAE-NAH	9.54	124.01	114.66
2	A	107	V4F	O-C-CAE	-9.05	115.64	124.22

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	102	V4F	N-CA-CAJ-CAM
2	A	102	V4F	O01-C01-P-O1
2	B	112	V4F	O-C-CAE-CAD
2	B	112	V4F	O-C-CAE-NAH
2	B	112	V4F	CAL-CAF-O01-C01

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	102	V4F	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	108	V53	0	1
2	B	115	V53	1	0
2	B	117	V4F	1	0
2	A	103	V53	1	0
2	B	119	V4F	2	0
2	B	116	V5F	1	0
2	B	112	V4F	2	1
2	B	114	V4F	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	63/66 (95%)	0.56	7 (11%) <b>5</b> <b>3</b>	109, 147, 171, 187	0
2	A	0/10	-	-	-	-
2	B	0/10	-	-	-	-
All	All	63/86 (73%)	0.56	7 (11%) <b>5</b> <b>3</b>	109, 147, 171, 187	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	5	LYS	4.1
1	AA	42	ARG	3.8
1	AA	44	ALA	3.1
1	AA	30	VAL	2.9
1	AA	3	LYS	2.9

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	V4F	B	112	20/21	0.68	0.35	103,124,156,159	0
2	V53	B	120	20/20	0.70	0.26	100,107,149,153	0
2	V53	B	118	19/20	0.72	0.25	99,113,165,168	0
2	V4F	A	104	20/21	0.74	0.27	87,103,133,134	0
2	V4F	A	102	20/21	0.81	0.22	93,105,135,139	0
2	V4F	B	114	20/21	0.82	0.34	92,115,163,171	0
2	V4F	A	109	20/21	0.82	0.42	93,104,142,152	0
2	V53	A	110	20/20	0.82	0.22	80,89,137,144	0
2	V5F	B	116	12/13	0.82	0.44	89,102,107,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	V53	B	113	19/20	0.87	0.37	86,95,140,150	0
2	V4F	B	119	20/21	0.88	0.14	91,108,114,126	0
2	V53	A	103	19/20	0.91	0.25	71,76,108,113	0
2	V4F	A	107	20/21	0.91	0.17	79,91,116,123	0
2	V4F	B	117	20/21	0.91	0.20	98,102,133,136	0
2	V53	B	115	19/20	0.91	0.26	91,100,144,147	0
2	V53	A	108	19/20	0.92	0.22	68,81,122,135	0
2	V53	A	105	19/20	0.92	0.19	67,82,132,138	0
2	V5F	A	106	12/13	0.94	0.34	64,80,91,92	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.