



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2024 – 04:22 pm BST

PDB ID : 8QHM  
Title : DNA mimic Foldamer with sticky ends  
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Deposited on : 2023-09-08  
Resolution : 3.00 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 : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

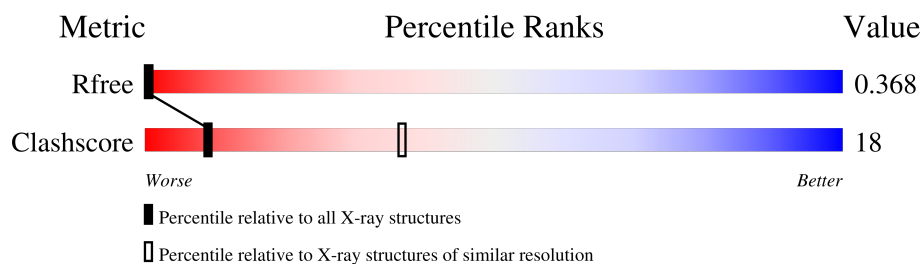
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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 <sub>free</sub>	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)

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	A	17	
1	F	17	

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
1	V4F	A	12	-	X	-	-
1	V53	A	13	-	X	-	-
1	V5F	A	14	-	X	-	-
1	VNW	A	15	-	X	-	-
1	9JV	A	16	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	V4F	A	2	-	X	-	-
1	V4F	A	4	-	X	-	-
1	V4F	F	12	-	X	-	-
1	VNW	F	15	-	X	-	-
1	V4F	F	2	-	X	-	-
1	V53	F	7	-	X	-	-
1	V4F	F	8	-	X	-	-

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 609 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 mimic Foldamer.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	17	Total	C	N	O	P	Se	0	0	0
			314	192	33	75	13	1			
1	F	16	Total	C	N	O	P	Se	0	0	0
			295	181	31	70	12	1			

### 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.

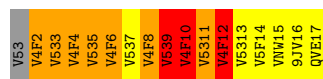
- Molecule 1: DNA mimic Foldamer

Chain A: 



- Molecule 1: DNA mimic Foldamer

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.15Å 74.15Å 83.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.00 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.97-3.00) 94.6 (19.97-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.347 , 0.381 0.348 , 0.368	Depositor DCC
$R_{free}$ test set	262 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 97.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.66	EDS
Total number of atoms	609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: VNW, V5F, QVE, V4F, V53, 9JV

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	11
1	F	0	12
All	All	0	23

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	V4F	Peptide
1	A	3	V53	Peptide
1	A	4	V4F	Peptide
1	A	5	V53	Peptide
1	A	6	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	A	314	0	0	8	0
1	F	295	0	0	3	0
All	All	609	0	0	11	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 18.

The worst 5 of 11 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:13:V53:N	1:A:15:VNW:CG	2.51	0.73
1:F:9:V53:O2	1:F:11:V53:O1	2.14	0.65
1:F:10:V4F:O2	1:F:12:V4F:O3	2.16	0.63
1:A:6:V4F:N	1:A:6:V4F:NAH	2.52	0.56
1:A:3:V53:O	1:A:6:V4F:N	2.40	0.54

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

33 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
1	V4F	F	10	1	21,21,22	2.32	6 (28%)	27,30,32	4.39	13 (48%)
1	V4F	A	12	1	21,21,22	2.67	11 (52%)	27,30,32	3.70	13 (48%)
1	V53	F	5	1	20,20,21	2.11	7 (35%)	25,29,31	2.87	12 (48%)
1	V4F	F	12	1	21,21,22	1.78	5 (23%)	27,30,32	5.06	18 (66%)
1	V53	F	7	1	20,20,21	1.81	9 (45%)	25,29,31	3.89	12 (48%)
1	V4F	A	6	1	21,21,22	1.71	4 (19%)	27,30,32	4.67	10 (37%)
1	VNW	A	15	1	16,16,17	1.86	4 (25%)	18,22,24	6.00	12 (66%)
1	V53	A	9	1	20,20,21	2.58	8 (40%)	25,29,31	4.67	13 (52%)
1	VNW	F	15	1	16,16,17	2.57	8 (50%)	18,22,24	5.89	10 (55%)
1	V4F	A	2	1	21,21,22	1.67	5 (23%)	27,30,32	6.83	15 (55%)
1	V4F	F	6	1	21,21,22	2.40	10 (47%)	27,30,32	5.24	12 (44%)
1	V4F	A	10	1	21,21,22	2.41	10 (47%)	27,30,32	4.35	10 (37%)
1	V5F	F	14	1	11,12,13	2.34	4 (36%)	14,15,17	3.13	6 (42%)
1	QVE	A	17	1	20,20,20	1.98	9 (45%)	27,28,28	2.82	12 (44%)
1	V53	A	5	1	20,20,21	1.70	3 (15%)	25,29,31	2.42	10 (40%)
1	9JV	A	16	1	16,16,17	2.48	7 (43%)	19,22,24	6.09	9 (47%)
1	V4F	F	2	1	21,21,22	2.27	8 (38%)	27,30,32	5.74	15 (55%)
1	V53	A	7	1	20,20,21	1.80	6 (30%)	25,29,31	3.73	8 (32%)
1	V53	F	11	1	20,20,21	1.79	5 (25%)	25,29,31	4.56	15 (60%)
1	V4F	A	8	1	21,21,22	2.43	7 (33%)	27,30,32	5.71	12 (44%)
1	V4F	A	4	1	21,21,22	2.57	8 (38%)	27,30,32	4.31	12 (44%)
1	V53	F	3	1	20,20,21	2.52	5 (25%)	25,29,31	4.52	10 (40%)
1	QVE	F	17	1	20,20,20	1.83	7 (35%)	27,28,28	3.16	11 (40%)
1	V53	F	9	1	20,20,21	1.66	4 (20%)	25,29,31	3.02	13 (52%)
1	V53	A	13	1	20,20,21	3.00	6 (30%)	25,29,31	5.16	14 (56%)
1	9JV	F	16	1	16,16,17	2.09	3 (18%)	19,22,24	5.59	6 (31%)
1	V53	A	3	1	20,20,21	2.32	4 (20%)	25,29,31	3.62	13 (52%)
1	V4F	F	8	1	21,21,22	2.70	8 (38%)	27,30,32	4.47	13 (48%)
1	V53	A	11	1	20,20,21	1.90	5 (25%)	25,29,31	4.18	10 (40%)
1	V4F	F	4	1	21,21,22	2.32	8 (38%)	27,30,32	4.67	10 (37%)
1	V5F	A	14	1	11,12,13	1.45	2 (18%)	14,15,17	4.52	12 (85%)
1	V53	F	13	1	20,20,21	1.73	7 (35%)	25,29,31	8.04	11 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	V53	A	1	1	20,20,21	2.72	8 (40%)	25,29,31	2.77	9 (36%)

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
1	V4F	F	10	1	-	3/10/10/12	0/2/2/2
1	V4F	A	12	1	-	5/10/10/12	0/2/2/2
1	V53	F	5	1	-	0/8/8/10	0/2/2/2
1	V4F	F	12	1	-	5/10/10/12	0/2/2/2
1	V53	F	7	1	-	6/8/8/10	0/2/2/2
1	V4F	A	6	1	-	6/10/10/12	0/2/2/2
1	VNW	A	15	1	-	2/4/4/6	0/2/2/2
1	V53	A	9	1	-	2/8/8/10	0/2/2/2
1	VNW	F	15	1	-	2/4/4/6	0/2/2/2
1	V4F	A	2	1	-	8/10/10/12	0/2/2/2
1	V4F	F	6	1	-	3/10/10/12	0/2/2/2
1	V4F	A	10	1	-	0/10/10/12	0/2/2/2
1	V5F	F	14	1	-	1/4/6/8	0/1/1/1
1	QVE	A	17	1	-	2/9/9/9	0/2/2/2
1	V53	A	5	1	-	5/8/8/10	0/2/2/2
1	9JV	A	16	1	-	3/4/4/6	0/2/2/2
1	V4F	F	2	1	-	8/10/10/12	0/2/2/2
1	V53	A	7	1	-	0/8/8/10	0/2/2/2
1	V53	F	11	1	-	3/8/8/10	0/2/2/2
1	V4F	A	8	1	-	6/10/10/12	0/2/2/2
1	V4F	A	4	1	-	6/10/10/12	0/2/2/2
1	V53	F	3	1	-	2/8/8/10	0/2/2/2
1	QVE	F	17	1	-	5/9/9/9	0/2/2/2
1	V53	F	9	1	-	0/8/8/10	0/2/2/2
1	V53	A	13	1	-	4/8/8/10	0/2/2/2
1	9JV	F	16	1	-	4/4/4/6	0/2/2/2
1	V53	A	3	1	-	3/8/8/10	0/2/2/2
1	V4F	F	8	1	-	9/10/10/12	0/2/2/2
1	V53	A	11	1	-	0/8/8/10	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	V4F	F	4	1	-	7/10/10/12	0/2/2/2
1	V5F	A	14	1	-	1/4/6/8	0/1/1/1
1	V53	F	13	1	-	2/8/8/10	0/2/2/2
1	V53	A	1	1	-	0/8/8/10	0/2/2/2

The worst 5 of 211 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	V53	CAJ-C	10.44	1.59	1.48
1	A	4	V4F	CAE-NAH	-8.82	1.23	1.33
1	F	3	V53	CAJ-C	8.20	1.57	1.48
1	A	1	V53	CAJ-C	8.03	1.57	1.48
1	A	8	V4F	CAE-C	7.98	1.57	1.48

The worst 5 of 381 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	V53	C-CAJ-NAH	24.82	138.98	114.66
1	F	13	V53	CAD-CAJ-C	-23.43	100.97	121.23
1	A	2	V4F	O-C-CAE	-20.08	105.19	124.22
1	A	2	V4F	CAD-CAE-C	-19.03	104.78	121.23
1	F	13	V53	O-C-CAJ	-18.76	106.44	124.22

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2	V4F	O-C-CAE-CAD
1	A	2	V4F	O-C-CAE-NAH
1	A	2	V4F	N-CA-CAJ-CAM
1	A	2	V4F	O01-C01-P-O3
1	A	2	V4F	O01-C01-P-O2

There are no ring outliers.

12 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	10	V4F	1	0
1	F	12	V4F	2	0
1	A	6	V4F	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	15	VNW	1	0
1	A	10	V4F	2	0
1	A	7	V53	2	0
1	F	11	V53	1	0
1	A	8	V4F	1	0
1	F	9	V53	1	0
1	A	13	V53	2	0
1	A	3	V53	2	0
1	A	11	V53	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

### 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, 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	A	0/17	-	-	-	-
1	F	0/17	-	-	-	-
All	All	0/34	-	-	-	-

There are no RSRZ outliers to report.

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

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
1	V53	A	9	19/20	0.87	0.19	12,23,32,38	0
1	V4F	A	2	20/21	0.88	0.15	6,15,25,31	0
1	9JV	A	16	15/16	0.88	0.18	12,17,30,38	0
1	V53	F	9	19/20	0.90	0.17	9,17,29,38	0
1	QVE	F	17	19/19	0.90	0.19	11,18,28,35	0
1	V53	A	7	19/20	0.91	0.15	14,19,34,45	0
1	V4F	F	10	20/21	0.91	0.15	12,22,41,52	0
1	V53	F	13	19/20	0.91	0.14	8,19,41,56	0
1	V4F	A	8	20/21	0.91	0.16	8,18,26,45	0
1	V4F	F	2	20/21	0.91	0.14	4,19,41,65	0
1	V53	A	5	19/20	0.92	0.13	4,11,29,63	0
1	V53	F	5	19/20	0.92	0.14	7,17,31,44	0
1	V4F	A	6	20/21	0.92	0.13	9,15,24,38	0
1	V53	F	11	19/20	0.92	0.15	11,16,37,41	0
1	V4F	A	12	20/21	0.92	0.14	10,17,32,47	0
1	V4F	F	6	20/21	0.92	0.13	12,21,52,64	0
1	V53	A	1	19/20	0.92	0.13	7,11,16,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	V4F	F	4	20/21	0.92	0.14	10,19,35,55	0
1	V4F	A	4	20/21	0.93	0.13	9,12,38,44	0
1	V53	A	3	19/20	0.93	0.12	5,10,30,33	0
1	V4F	F	12	20/21	0.93	0.13	10,24,55,65	0
1	V53	A	13	19/20	0.93	0.13	10,19,32,36	0
1	V4F	A	10	20/21	0.93	0.14	11,17,31,33	0
1	V5F	A	14	12/13	0.93	0.15	6,15,21,33	0
1	V4F	F	8	20/21	0.93	0.13	12,22,35,52	0
1	QVE	A	17	19/19	0.93	0.14	7,14,25,26	0
1	V53	A	11	19/20	0.93	0.13	10,18,41,49	0
1	VNW	F	15	15/16	0.94	0.14	0,17,27,48	0
1	V53	F	7	19/20	0.94	0.12	12,15,46,48	0
1	9JV	F	16	15/16	0.94	0.14	6,11,17,43	0
1	V53	F	3	19/20	0.94	0.14	8,13,30,36	0
1	V5F	F	14	12/13	0.94	0.12	7,13,15,21	0
1	VNW	A	15	15/16	0.96	0.12	8,12,21,45	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.