

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 8, 2020 – 08:16 PM BST

PDB ID : 6Q6X

Title: Structure of Fucosylated D-antimicrobial peptide SB6 in complex with the

Fucose-binding lectin PA-IIL at 1.525 Angstrom resolution

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Deposited on : 2018-12-12

Resolution : 1.52 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 following versions of software and data (see references (1)) 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 : 2.13.1

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)

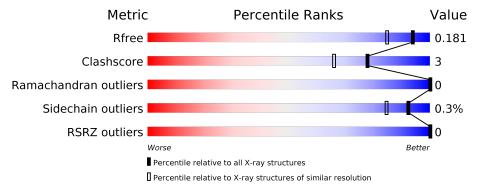
Validation Pipeline (wwPDB-VP) : 2.13.1

## 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 1.52 Å.

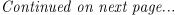
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 on 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	114	96%	•••
1	В	114	90%	10%
1	С	114	95%	5%
1	D	114	96%	•
2	Е	12	83%	17%
2	F	12	83%	17%





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Mo	Chain	Length	Quality of chain				
2	G	12	100%				
2	Н	12	100%				



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4275 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 Fucose-binding lectin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
1	A	114	Total	С	N	О	0	0	0
1	Λ	114	822	506	140	176	0	U	U
1	В	114	Total	С	N	О	0	0	0
1		114	822	506	140	176			
1	С	C 114	Total	С	N	О	0	0	0
1			822	506	140	176	U	U	U
1 D	114	Total	С	N	О	0	0	0	
		818	504	140	174	0	0	U	

• Molecule 2 is a protein (with D amino acids) called SB6.

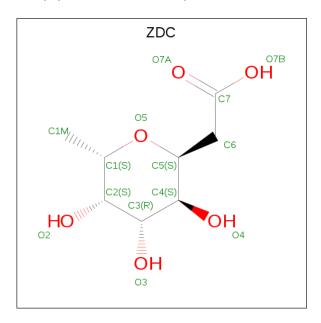
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	12	Total C N O	0	0	0
	Ľ	12	93 64 16 13	U	U	U
2	F	12	Total C N O	0	0	0
	Δ Γ	12	100 69 18 13	0		. 0
2	G	12	Total C N O	0	0	0
	G	12	96 66 17 13	0	U	0
2	Н	12	Total C N O	0	0	0
	11	12	100 69 18 13	0	U	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	3	Total Ca 3 3	0	0
3	A	3	Total Ca 3 3	0	0
3	D	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0



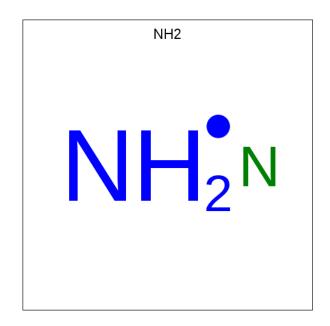
• Molecule 4 is 3,7-anhydro-2,8-dideoxy-L-glycero-D-gluco-octonic acid (three-letter code: ZDC) (formula:  $C_8H_{14}O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 13 8 5	0	0
4	F	1	Total C O 13 8 5	0	0
4	G	1	Total C O 13 8 5	0	0
4	Н	1	Total C O 13 8 5	0	0

• Molecule 5 is AMINO GROUP (three-letter code: NH2) (formula: H<sub>2</sub>N).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	1	Total N	0	0
)	نا	1	1 1	0	U
5	F	1	Total N	0	0
)	1'	1	1 1	0	U
5	G	1	Total N	0	0
)	G	1	1 1	0	U
5	Н	1	Total N	0	0
3	11	1	$\begin{vmatrix} 1 & 1 \end{vmatrix}$	0	U

#### • Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	118	Total O 118 118	0	0
6	Е	6	Total O 6 6	0	0
6	В	116	Total O 116 116	0	0
6	F	12	Total O 12 12	0	0
6	С	116	Total O 116 116	0	0
6	G	9	Total O 9 9	0	0
6	D	141	Total O 141 141	0	0
6	Н	20	Total O 20 20	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: Fucose-binding lectin





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• Molecule 2: SB6

Chain G:

There are no outlier residues recorded for this chain.

• Molecule 2: SB6

Chain H:

There are no outlier residues recorded for this chain.



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	52.47Å 59.42Å 72.06Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $106.12^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	47.51 - 1.52	Depositor
resolution (A)	47.51 - 1.53	EDS
% Data completeness	87.4 (47.51-1.52)	Depositor
(in resolution range)	96.7 (47.51-1.53)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$< I/\sigma(I) > 1$	1.15 (at 1.52Å)	Xtriage
Refinement program	PHENIX	Depositor
$R, R_{free}$	0.158 , $0.182$	Depositor
It, It free	0.157 , 0.181	DCC
$R_{free}$ test set	3140  reflections  (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.8	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39, 55.1	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o$ , $F_c$ correlation	0.96	EDS
Total number of atoms	4275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.45% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: DLE, DAL, CA, DTY, NH2, DLY, ZDC

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	
MIOI		RMSZ	# Z >5	RMSZ	# Z  > 5
1	A	0.34	0/832	0.57	0/1140
1	В	0.33	0/832	0.55	0/1140
1	С	0.34	0/832	0.57	0/1140
1	D	0.32	0/828	0.56	0/1135
All	All	0.33	0/3324	0.56	0/4555

There are no bond length outliers.

There are no bond angle outliers.

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	822	0	791	4	0
1	В	822	0	791	9	0
1	С	822	0	791	3	0
1	D	818	0	787	4	0
2	E	93	0	99	2	0
2	F	100	0	117	1	0
2	G	96	0	107	0	0
2	Н	100	0	117	0	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	3	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	Ε	13	0	9	0	0
4	F	13	0	9	0	0
4	G	13	0	9	0	0
4	Η	13	0	9	0	0
5	Ε	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	Η	1	0	0	0	0
6	A	118	0	0	2	1
6	В	116	0	0	3	2
6	С	116	0	0	0	3
6	D	141	0	0	0	2
6	Ε	6	0	0	2	0
6	F	12	0	0	0	0
6	G	9	0	0	0	0
6	Н	20	0	0	0	0
All	All	4275	0	3636	21	4

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 21 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll}  ext{Interatomic} \  ext{distance} & ( ext{Å}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap} & ( ext{Å}) \end{aligned}$
2:E:5:DLY:NZ	6:E:301:HOH:O	1.89	1.05
1:B:66:GLN:OE1	6:B:401:HOH:O	1.96	0.83
1:B:66:GLN:NE2	6:B:403:HOH:O	2.12	0.81
1:B:86:GLU:OE2	6:B:402:HOH:O	2.00	0.78
1:A:66:GLN:NE2	6:A:401:HOH:O	2.21	0.71

All (4) 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	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	Clash overlap (Å)
6:B:505:HOH:O	6:C:512:HOH:O[2_454]	2.04	0.16
6:B:410:HOH:O	6:C:416:HOH:O[1_455]	2.16	0.04
6:C:490:HOH:O	6:D:420:HOH:O[2_445]	2.17	0.03

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Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} & ( ext{Å}) \end{aligned}$	Clash overlap (Å)
6:A:479:HOH:O	6:D:524:HOH:O[2_445]	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	Perce	ntiles
1	A	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
1	В	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
1	С	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
1	D	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
All	All	448/456 (98%)	436 (97%)	12 (3%)	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	Percen	tiles
1	A	$92/93\ (99\%)$	91 (99%)	1 (1%)	73	52
1	В	$92/93\ (99\%)$	92 (100%)	0	100	100
1	С	$92/93\ (99\%)$	92 (100%)	0	100	100
1	D	91/93 (98%)	91 (100%)	0	100	100
All	All	367/372 (99%)	366 (100%)	1 (0%)	92	84



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

Mol	Chain	Res	Type
1	A	70	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	26	GLN
1	В	66	GLN
1	D	46	ASN
1	D	80	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)

48 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are modelled with single atom and 8 are monoatomic - leaving 4 for Mogul analysis.

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	Mol Type Chain		oin Bos	Res	Link	Bo	Bond lengths			Bond angles		
MIOI	Type	Chain	nes		nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ZDC	F	1	3,2	13,13,14	0.88	0	17,18,20	1.64	4 (23%)		
4	ZDC	G	1	3,2	13,13,14	0.90	0	17,18,20	1.74	2 (11%)		
4	ZDC	Е	1	3,2	13,13,14	0.96	0	17,18,20	1.47	2 (11%)		
4	ZDC	Н	1	3,2	13,13,14	0.93	0	17,18,20	1.64	3 (17%)		

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
4	ZDC	F	1	3,2	-	1/3/23/24	0/1/1/1
4	ZDC	G	1	3,2	-	1/3/23/24	0/1/1/1
4	ZDC	E	1	3,2	-	2/3/23/24	0/1/1/1
4	ZDC	Н	1	3,2	-	1/3/23/24	0/1/1/1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^o)$
4	G	1	ZDC	C3-C4-C5	-3.87	103.34	110.24
4	G	1	ZDC	O5-C5-C6	3.37	121.84	110.56
4	Н	1	ZDC	C3-C4-C5	-3.33	104.30	110.24
4	F	1	ZDC	C3-C4-C5	-3.14	104.64	110.24
4	F	1	ZDC	O5-C5-C6	2.99	120.56	110.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	ZDC	O5-C5-C6-C7
4	Е	1	ZDC	O5-C5-C6-C7
4	F	1	ZDC	C5-C6-C7-O7A
4	E	1	ZDC	C5-C6-C7-O7A
4	Н	1	ZDC	O5-C5-C6-C7



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 (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 $>$	# RSRZ > 2		Z>2	$OWAB(A^2)$	Q < 0.9
1	A	114/114 (100%)	-0.24	0	100	100	7, 9, 19, 48	0
1	В	114/114 (100%)	-0.18	0	100	100	7, 11, 25, 36	0
1	С	$114/114 \; (100\%)$	-0.30	0	100	100	7, 10, 19, 35	0
1	D	$114/114 \; (100\%)$	-0.29	0	100	100	8, 10, 22, 27	0
2	Е	0/12	-		-		_	-
2	F	0/12	-		-		-	-
2	G	0/12	-		-		_	-
2	Н	0/12	-		-		-	-
All	All	456/504~(90%)	-0.25	0	100	100	7, 10, 22, 48	0

There are no RSRZ outliers to report.

### 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	DLE	E	10	8/9	0.67	0.29	36,37,37,38	0
2	DLE	G	13	8/9	0.72	0.18	30,31,32,33	0
2	DLY	E	9	9/10	0.80	0.16	35,36,38,40	0
2	DLE	E	7	8/9	0.80	0.17	32,33,35,35	0
2	DLY	G	12	9/10	0.81	0.18	28,30,33,33	0
2	DLY	E	4	9/10	0.81	0.15	18,24,27,27	0
2	DLE	E	13	8/9	0.81	0.14	37,38,39,40	0
2	DLE	G	10	8/9	0.82	0.17	24,25,27,27	0
2	DLY	E	5	9/10	0.82	0.18	26,31,38,38	0
2	DAL	G	11	5/6	0.84	0.14	25,26,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	DLY	Е	8	5/10	0.84	0.21	37,38,38,39	0
2	DLY	G	9	5/10	0.87	0.11	25,25,26,26	0
2	DAL	Е	11	5/6	0.88	0.13	36,37,38,40	0
2	DAL	Е	6	5/6	0.89	0.16	30,31,31,32	0
2	DLY	G	8	9/10	0.89	0.21	25,29,38,39	0
2	DLE	G	7	8/9	0.89	0.10	17,21,23,24	0
2	DLY	Е	12	6/10	0.89	0.16	39,40,40,41	0
2	DTY	G	3	12/13	0.90	0.17	14,27,32,33	0
2	DTY	F	3	12/13	0.91	0.11	18,25,29,32	0
2	DAL	F	11	5/6	0.91	0.10	20,20,21,23	0
2	DLE	F	10	8/9	0.92	0.13	21,23,27,28	0
2	DLY	Н	12	9/10	0.93	0.11	15,20,24,26	0
2	DLY	Н	5	9/10	0.93	0.12	14,15,25,25	0
2	DLE	F	7	8/9	0.93	0.11	18,20,28,29	0
2	DLE	Н	13	8/9	0.93	0.11	23,24,25,28	0
2	DAL	G	6	5/6	0.93	0.08	16,17,18,18	0
2	DLY	F	9	9/10	0.93	0.12	21,23,32,33	0
2	DLY	F	8	9/10	0.93	0.18	21,24,38,39	0
2	DLY	Н	4	9/10	0.93	0.12	11,14,22,24	0
2	DLY	F	5	9/10	0.93	0.10	19,20,32,33	0
2	DLY	Н	2	9/10	0.94	0.12	11,13,26,28	0
2	DLY	G	5	9/10	0.94	0.12	21,22,31,33	0
2	DLY	F	12	9/10	0.94	0.13	18,19,33,35	0
2	DLY	G	4	9/10	0.94	0.10	19,21,22,24	0
2	DTY	Е	3	12/13	0.94	0.10	13,18,23,23	0
2	DLE	Н	10	8/9	0.94	0.13	16,17,22,22	0
2	DLY	F	4	9/10	0.94	0.15	20,21,32,32	0
2	DLY	Е	2	9/10	0.94	0.11	12,16,26,29	0
2	DLE	Н	7	8/9	0.94	0.10	14,15,22,23	0
2	DAL	Н	6	5/6	0.95	0.13	13,14,15,16	0
2	DLY	G	2	9/10	0.95	0.13	12,14,28,31	0
2	DLY	H	8	9/10	0.95	0.15	14,15,23,24	0
2	DTY	Н	3	12/13	0.95	0.08	11,12,13,13	0
2	DLY	F	2	9/10	0.95	0.14	13,18,33,35	0
2	DLY	H	9	9/10	0.95	0.10	15,16,28,29	0
2	DLE	F	13	8/9	0.95	0.09	18,20,23,23	0
2	DAL	F	6	5/6	0.96	0.10	18,18,19,20	0
2	DAL	Н	11	5/6	0.97	0.07	14,14,15,16	0

# 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,  $95^{th}$  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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
5	NH2	E	202	1/1	0.76	0.13	38,38,38,38	0
5	NH2	G	202	1/1	0.89	0.13	$33,\!33,\!33,\!33$	0
5	NH2	Н	202	1/1	0.93	0.08	26,26,26,26	0
4	ZDC	Н	1	13/14	0.97	0.08	8,10,11,13	0
4	ZDC	F	1	13/14	0.97	0.07	8,9,10,10	0
4	ZDC	E	1	13/14	0.97	0.09	6,8,11,11	0
4	ZDC	G	1	13/14	0.98	0.07	7,9,12,12	0
5	NH2	F	202	1/1	0.98	0.07	21,21,21,21	0
3	CA	A	301	1/1	1.00	0.07	8,8,8,8	0
3	CA	В	301	1/1	1.00	0.06	9,9,9,9	0
3	CA	A	303	1/1	1.00	0.07	7,7,7,7	0
3	CA	С	301	1/1	1.00	0.07	8,8,8,8	0
3	CA	В	302	1/1	1.00	0.06	9,9,9,9	0
3	CA	A	302	1/1	1.00	0.07	7,7,7,7	0
3	CA	В	303	1/1	1.00	0.06	9,9,9,9	0
3	CA	D	301	1/1	1.00	0.07	9,9,9,9	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

