



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 24, 2018 – 09:33 PM EST

PDB ID : 1QKC  
Title : ESCHERICHIA COLI FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) IN COMPLEX DELTA TWO-ALBOMYCIN  
Authors : Ferguson, A.D.; Braun, V.; Fiedler, H.-P.; Coulton, J.W.; Diederichs, K.; Welte, W.  
Deposited on : 1999-07-18  
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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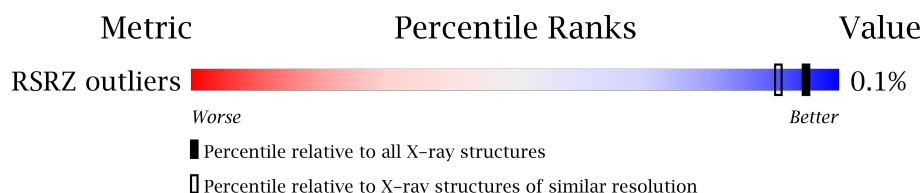
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	<b>FAILED</b>
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

**i**

## X-RAY DIFFRACTION

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))
RSRZ outliers	101464	1006 (3.12-3.08)

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
12	ALB	A	1022[A]	-	-	-	X
12	ALB	A	1022[B]	-	-	-	X
8	FTT	A	1002	-	-	-	X
8	FTT	A	1004	-	-	-	X
8	FTT	A	1005	-	-	-	X
8	FTT	A	1007	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 6195 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.

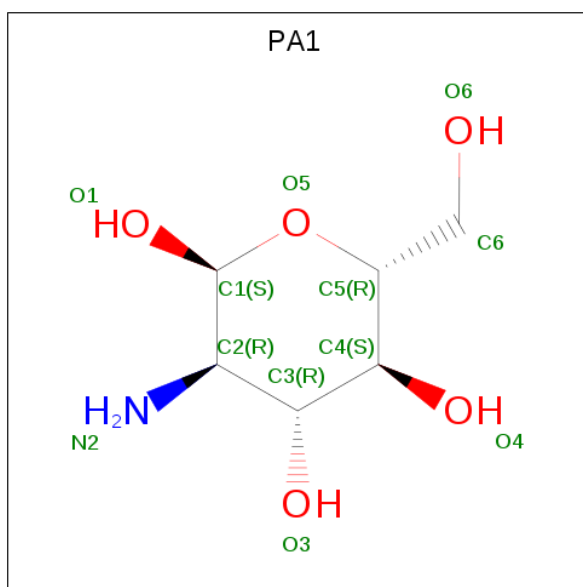
- Molecule 1 is a protein called FERRIC HYDROXAMATE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	0	0
			5523	3475	944	1090	14			

There are 11 discrepancies between the modelled and reference sequences:

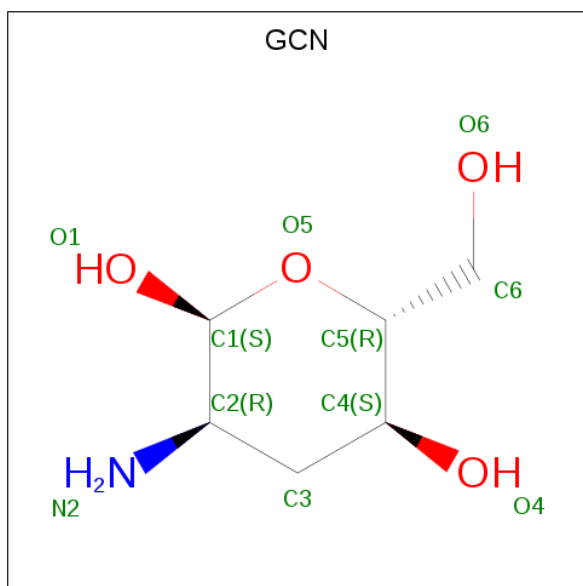
Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP P06971
A	407	SER	-	insertion	UNP P06971
A	408	HIS	-	insertion	UNP P06971
A	409	HIS	-	insertion	UNP P06971
A	410	HIS	-	insertion	UNP P06971
A	411	HIS	-	insertion	UNP P06971
A	412	HIS	-	insertion	UNP P06971
A	413	HIS	-	insertion	UNP P06971
A	414	GLY	-	insertion	UNP P06971
A	415	SER	-	insertion	UNP P06971
A	416	SER	-	insertion	UNP P06971

- Molecule 2 is 2-amino-2-deoxy-alpha-D-glucopyranose (three-letter code: PA1) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>5</sub>).



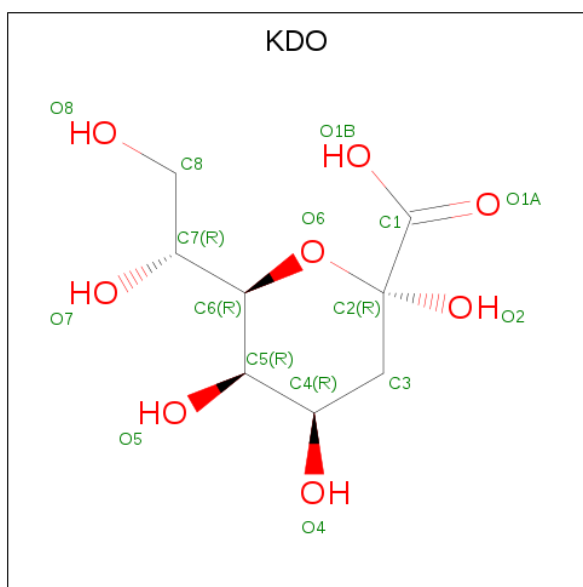
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 3 is 3-DEOXY-D-GLUCOSAMINE (three-letter code: GCN) (formula:  $C_6H_{13}NO_4$ ).



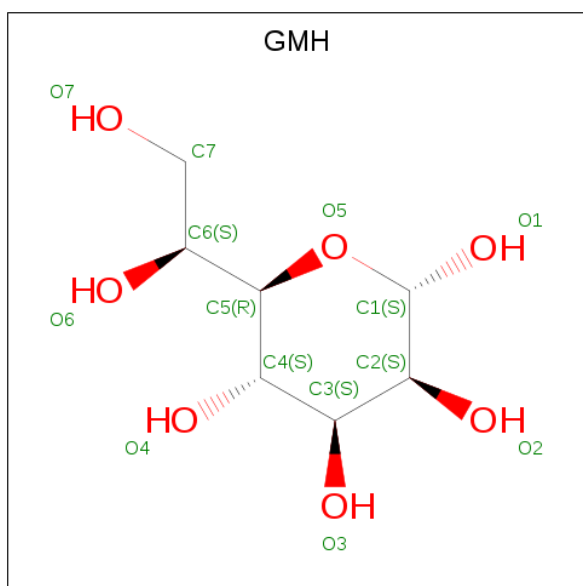
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 4 is 3-DEOXY-D-MANNO-OCT-2-ULOSONIC ACID (three-letter code: KDO) (formula:  $C_8H_{14}O_8$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			15	8	7		
4	A	1	Total	C	O	0	0
			15	8	7		

- Molecule 5 is L-GLYCERO-D-MANNO-HEPTOPYRANOSE (three-letter code: GMH) (formula:  $C_7H_{14}O_7$ ).



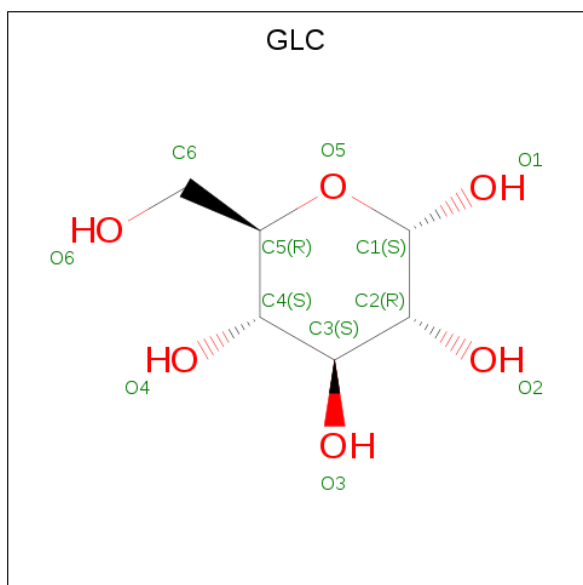
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	7	6		

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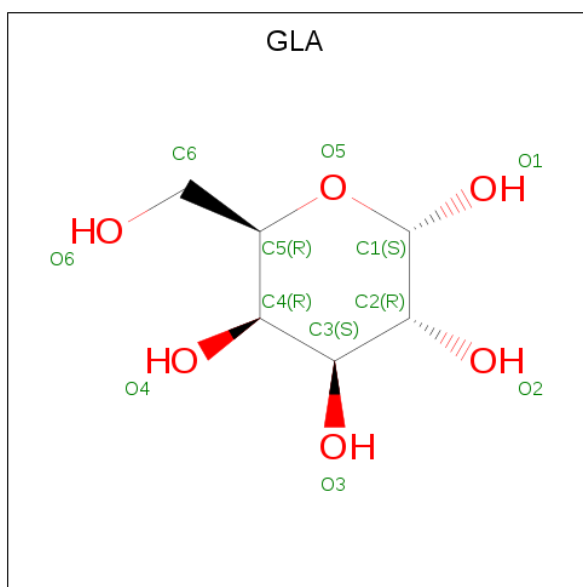
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	7	6		
5	A	1	Total	C	O	0	0
			13	7	6		

- Molecule 6 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula:  $C_6H_{12}O_6$ ).



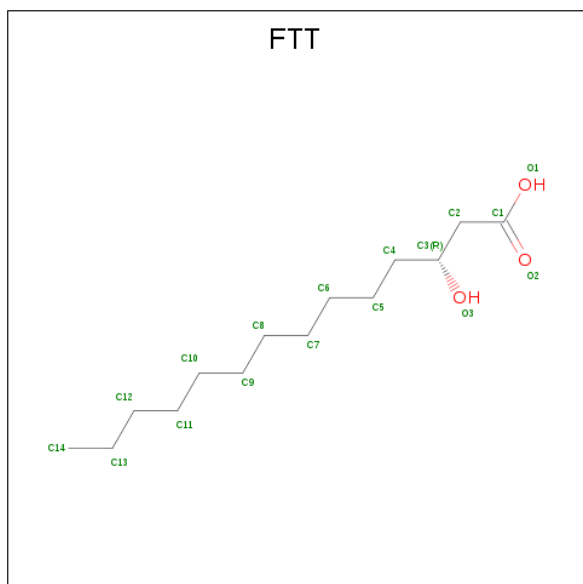
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA D-GALACTOSE (three-letter code: GLA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula:  $C_{14}H_{28}O_3$ ).



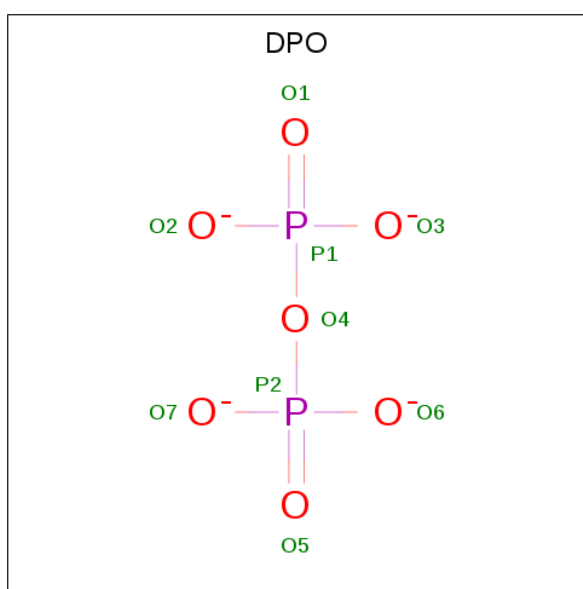
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			16	14	2		
8	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			16	14	2		
8	A	1	Total	C	O	0	0
			13	12	1		
8	A	1	Total	C	O	0	0
			17	14	3		
8	A	1	Total	C	O	0	0
			15	14	1		

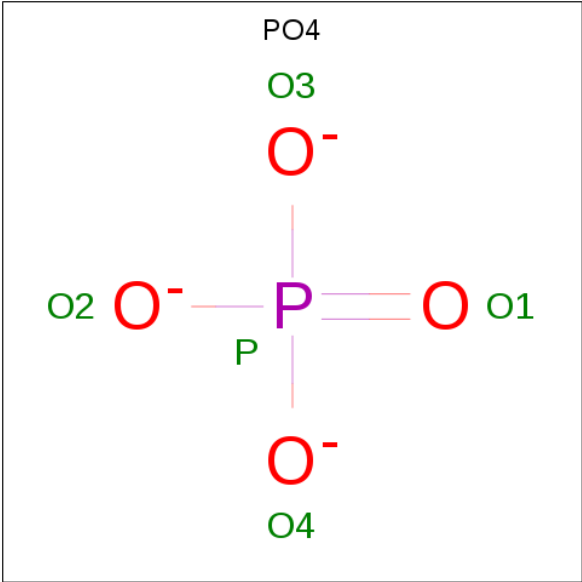
- Molecule 9 is DIPHOSPHATE (three-letter code: DPO) (formula:  $O_7P_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	P	0	0
			8	6	2		
9	A	1	Total	O	P	0	0
			8	6	2		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



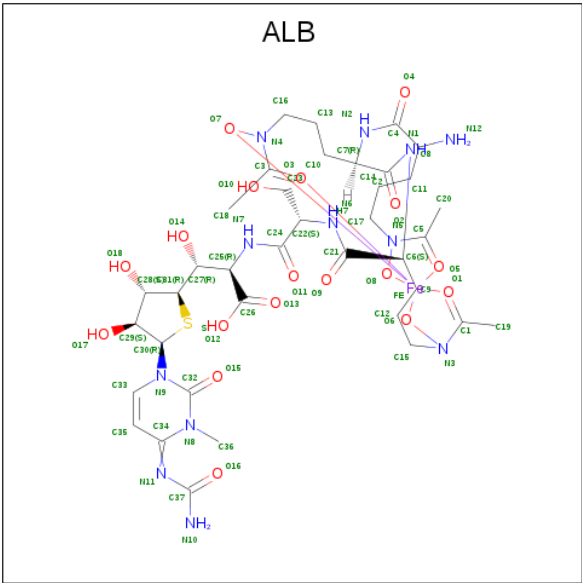


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	P	0	0
			4	3	1		
10	A	1	Total	O	P	0	0
			4	3	1		

- Molecule 11 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Ni	0	0
			1	1		

- Molecule 12 is DELTA-2-ALBOMYCIN A1 (three-letter code: ALB) (formula: C<sub>37</sub>H<sub>57</sub>FeN<sub>12</sub>O<sub>18</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	A	1	Total	C	Fe	N	O	S	0	1
			97	51	1	17	26	2		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	332	Total	O	0	0
			332	332		

MolProbity failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.80 Å 171.80 Å 86.35 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.10 47.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-3.10) 92.8 (47.12-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.69 Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.222 , 0.283 0.220 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

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

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

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#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

validation-pack failed to run properly - this section is therefore empty.

### 4.5 Carbohydrates [i](#)

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### 4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

### 4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 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	A	707/725 (97%)	-0.55	1 (0%) 95 90	44, 80, 113, 117	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	SER	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	FTT	A	1007	15/17	0.90	0.66	14.61	79,99,107,110	0
8	FTT	A	1005	13/17	0.91	0.43	7.58	77,80,89,90	0
8	FTT	A	1002	16/17	0.90	0.36	5.74	80,91,96,96	0
8	FTT	A	1004	16/17	0.93	0.32	4.43	70,73,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
12	ALB	A	1022[A]	69/69	0.93	0.35	2.67	69,88,114,120	28
12	ALB	A	1022[B]	69/69	0.93	0.35	2.67	69,87,115,120	28
5	GMH	A	1010	13/14	0.95	0.10	-2.53	72,78,83,87	0
4	KDO	A	1008	15/16	0.97	0.08	-2.99	67,74,78,84	0
6	GLC	A	1018	11/12	0.92	0.25	-	111,114,116,117	0
5	GMH	A	1011	13/14	0.94	0.10	-	89,98,111,116	0
10	PO4	A	1014	4/5	0.96	0.13	-	76,77,78,84	0
6	GLC	A	1017	11/12	0.93	0.17	-	93,101,110,113	0
7	GLA	A	1019	11/12	0.93	0.10	-	110,112,113,113	0
9	DPO	A	1015	8/9	0.96	0.09	-	86,89,93,94	4
8	FTT	A	1006	17/17	0.94	0.34	-	67,91,100,100	0
6	GLC	A	1020	11/12	0.80	0.40	-	116,116,117,118	0
8	FTT	A	1003	7/17	0.89	0.14	-	88,103,108,109	0
10	PO4	A	1016	4/5	0.96	0.07	-	112,113,114,114	0
3	GCN	A	1001	10/11	0.95	0.07	-	46,54,63,71	0
5	GMH	A	1012	13/14	0.82	0.19	-	115,116,117,118	0
2	PA1	A	1000	11/12	0.96	0.08	-	53,64,78,81	0
9	DPO	A	1013	8/9	0.97	0.10	-	84,86,90,92	4
4	KDO	A	1009	15/16	0.94	0.10	-	80,84,88,90	0
11	NI	A	1021	1/1	0.94	0.07	-	119,119,119,119	0

## 5.5 Other polymers ⓘ

There are no such residues in this entry.