



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:24 PM BST

PDB ID : 6WN8  
Title : 2.70 Angstrom Resolution Crystal Structure of Uracil Phosphoribosyl Transferase from *Klebsiella pneumoniae*  
Authors : Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Dubrovskaya, I.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2020-04-22  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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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	:	1.8.5 (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

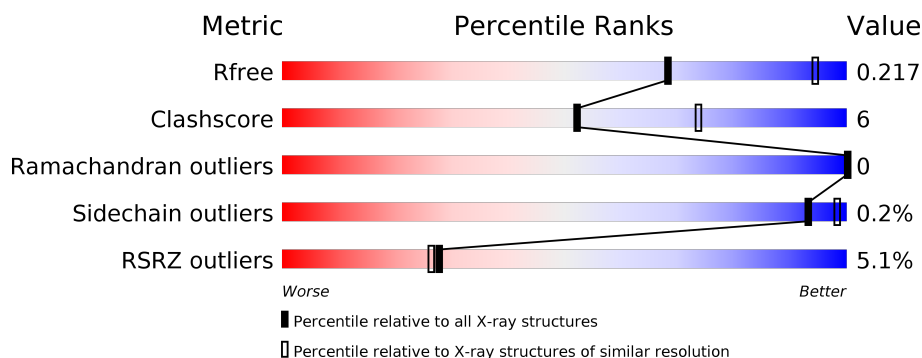
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



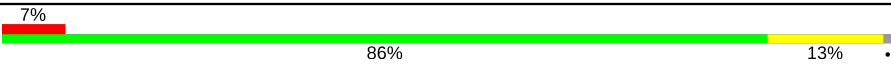


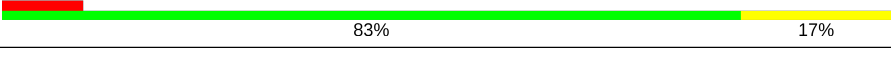
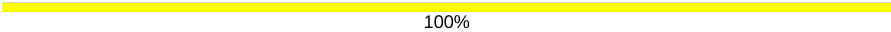
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	211	<div> <div>3%</div> <div>81% 18%</div> </div>
1	B	211	<div> <div>2%</div> <div>86% 11%</div> </div>
1	C	211	<div> <div>4%</div> <div>85% 14%</div> </div>
1	D	211	<div> <div>4%</div> <div>84% 13%</div> </div>
1	E	211	<div> <div>6%</div> <div>84% 15%</div> </div>
1	F	211	<div> <div>2%</div> <div>88% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	211	
1	H	211	
1	I	211	
1	J	211	
2	K	2	

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
4	SO4	A	309	-	-	-	X
4	SO4	A	310	-	-	-	X
4	SO4	C	309	-	-	-	X
4	SO4	F	310	-	-	-	X
4	SO4	G	308	-	-	-	X
4	SO4	H	306	-	-	-	X
4	SO4	H	307	-	-	-	X
4	SO4	H	310	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16930 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 Uracil phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1588	1013	266	301	8			
1	B	206	Total	C	N	O	S	0	0	0
			1563	997	264	294	8			
1	C	210	Total	C	N	O	S	0	1	0
			1604	1021	270	305	8			
1	D	205	Total	C	N	O	S	0	0	0
			1555	993	262	292	8			
1	E	210	Total	C	N	O	S	0	0	0
			1596	1017	268	303	8			
1	F	209	Total	C	N	O	S	0	2	0
			1605	1023	270	304	8			
1	G	209	Total	C	N	O	S	0	0	0
			1588	1013	266	301	8			
1	H	209	Total	C	N	O	S	0	1	0
			1596	1017	268	303	8			
1	I	210	Total	C	N	O	S	0	0	0
			1596	1017	268	303	8			
1	J	210	Total	C	N	O	S	0	1	0
			1605	1022	269	306	8			

There are 30 discrepancies between the modelled and reference sequences:

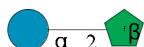
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A1Y0PUH0
A	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
A	0	ALA	-	expression tag	UNP A0A1Y0PUH0
B	-2	SER	-	expression tag	UNP A0A1Y0PUH0
B	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
B	0	ALA	-	expression tag	UNP A0A1Y0PUH0
C	-2	SER	-	expression tag	UNP A0A1Y0PUH0
C	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
C	0	ALA	-	expression tag	UNP A0A1Y0PUH0

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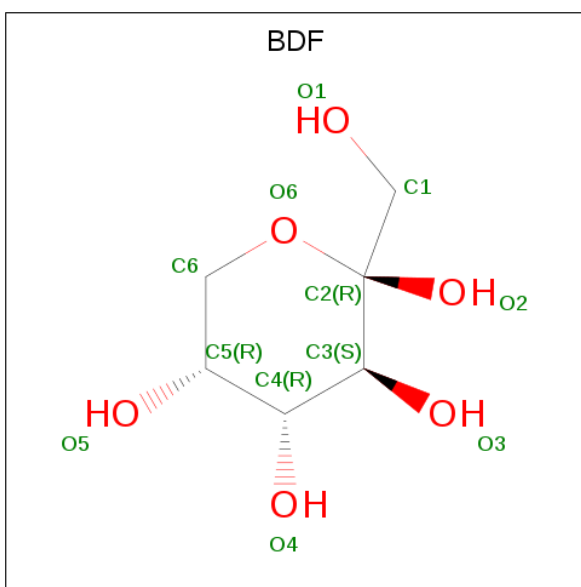
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP A0A1Y0PUH0
D	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
D	0	ALA	-	expression tag	UNP A0A1Y0PUH0
E	-2	SER	-	expression tag	UNP A0A1Y0PUH0
E	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
E	0	ALA	-	expression tag	UNP A0A1Y0PUH0
F	-2	SER	-	expression tag	UNP A0A1Y0PUH0
F	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
F	0	ALA	-	expression tag	UNP A0A1Y0PUH0
G	-2	SER	-	expression tag	UNP A0A1Y0PUH0
G	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
G	0	ALA	-	expression tag	UNP A0A1Y0PUH0
H	-2	SER	-	expression tag	UNP A0A1Y0PUH0
H	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
H	0	ALA	-	expression tag	UNP A0A1Y0PUH0
I	-2	SER	-	expression tag	UNP A0A1Y0PUH0
I	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
I	0	ALA	-	expression tag	UNP A0A1Y0PUH0
J	-2	SER	-	expression tag	UNP A0A1Y0PUH0
J	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
J	0	ALA	-	expression tag	UNP A0A1Y0PUH0

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



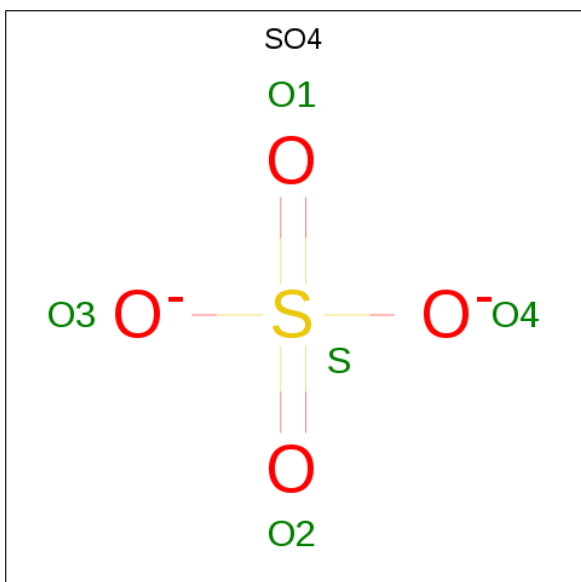
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is beta-D-fructopyranose (three-letter code: BDF) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	A	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Cl 1 1	0	0
5	J	5	Total Cl 5 5	0	0
5	D	1	Total Cl 1 1	0	0
5	E	3	Total Cl 3 3	0	0
5	B	2	Total Cl 2 2	0	0
5	I	2	Total Cl 2 2	0	0
5	C	1	Total Cl 1 1	0	0
5	A	4	Total Cl 4 4	0	0
5	F	4	Total Cl 4 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	31	Total O 31 31	0	0
6	B	53	Total O 53 53	0	0

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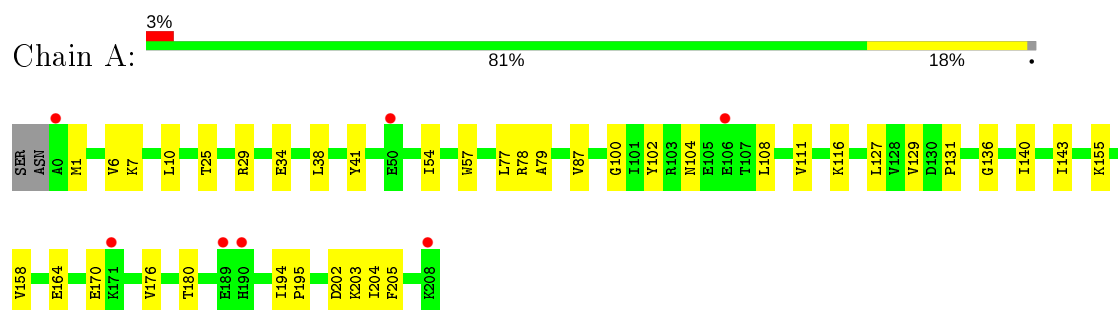
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	77	Total 77	O 77	0	0
6	D	52	Total 52	O 52	0	0
6	E	46	Total 46	O 46	0	0
6	F	68	Total 68	O 68	0	0
6	G	28	Total 28	O 28	0	0
6	H	30	Total 30	O 30	0	0
6	I	52	Total 52	O 52	0	0
6	J	36	Total 36	O 36	0	0

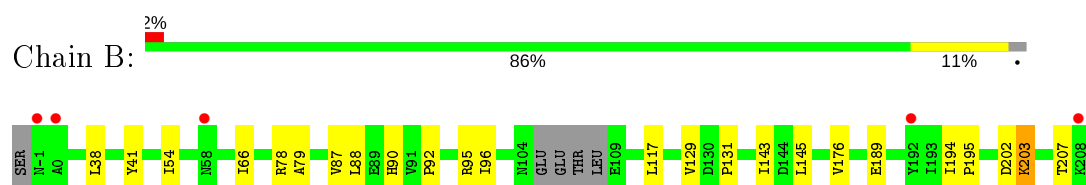
### 3 Residue-property plots [i](#)

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.

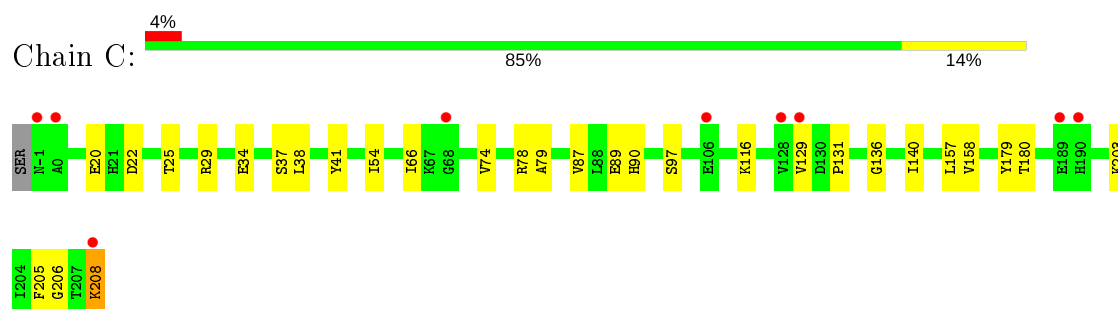
- Molecule 1: Uracil phosphoribosyltransferase



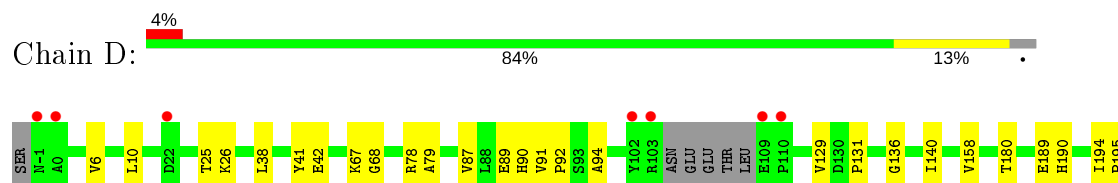
- Molecule 1: Uracil phosphoribosyltransferase



- Molecule 1: Uracil phosphoribosyltransferase

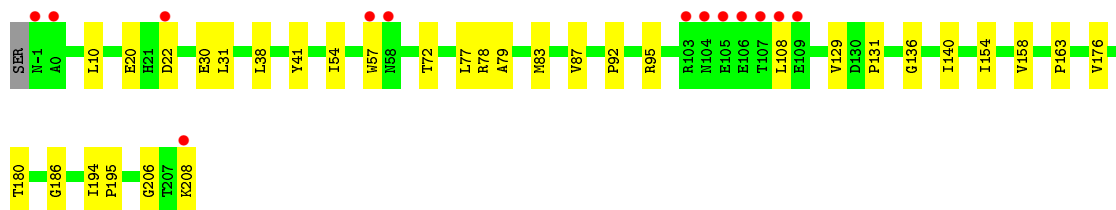
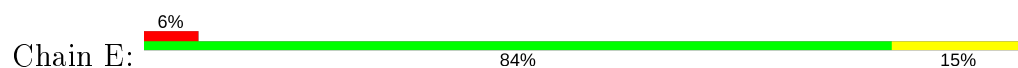


- Molecule 1: Uracil phosphoribosyltransferase

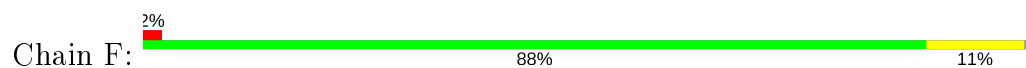




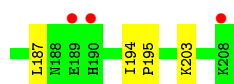
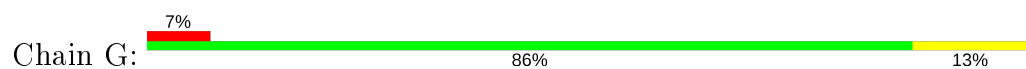
- Molecule 1: Uracil phosphoribosyltransferase



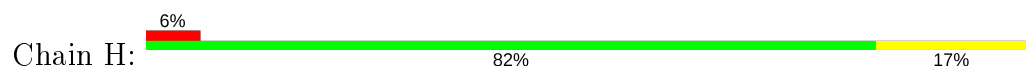
- Molecule 1: Uracil phosphoribosyltransferase



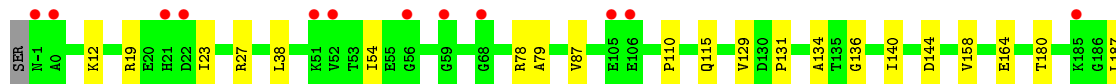
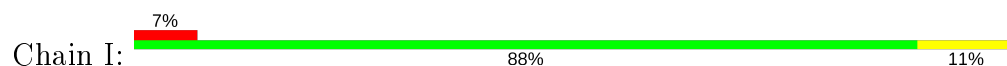
- Molecule 1: Uracil phosphoribosyltransferase

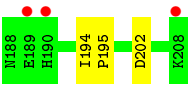


- Molecule 1: Uracil phosphoribosyltransferase

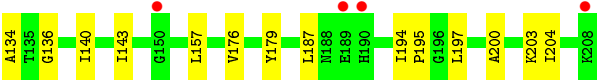
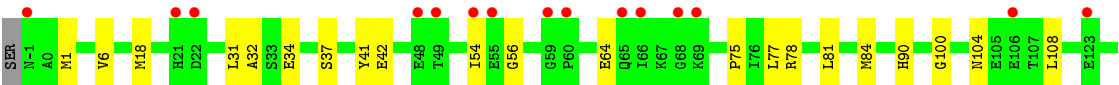
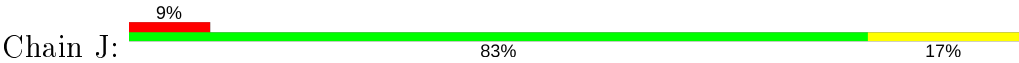


- Molecule 1: Uracil phosphoribosyltransferase

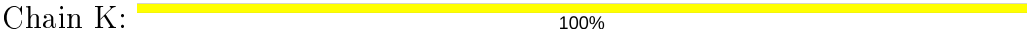




● Molecule 1: Uracil phosphoribosyltransferase



● Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.35Å 203.35Å 157.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 2.70 29.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.71-2.70) 100.0 (29.71-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.189 , 0.219 0.190 , 0.217	Depositor DCC
$R_{free}$ test set	5203 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, BDF, SO4, FRU, CL

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	A	0.66	0/1613	0.71	0/2182
1	B	0.65	0/1587	0.71	0/2145
1	C	0.66	0/1629	0.73	0/2204
1	D	0.66	0/1579	0.71	0/2134
1	E	0.66	0/1621	0.72	0/2193
1	F	0.66	0/1630	0.72	0/2204
1	G	0.67	0/1613	0.72	0/2182
1	H	0.67	0/1621	0.71	0/2193
1	I	0.67	0/1621	0.71	0/2193
1	J	0.67	0/1630	0.71	0/2205
All	All	0.66	0/16144	0.72	0/21835

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

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	1588	0	1652	29	0
1	B	1563	0	1627	22	0
1	C	1604	0	1663	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1555	0	1621	19	0
1	E	1596	0	1658	22	0
1	F	1605	0	1669	18	0
1	G	1588	0	1652	17	0
1	H	1596	0	1657	25	0
1	I	1596	0	1658	18	0
1	J	1605	0	1663	29	0
2	K	23	0	21	0	0
3	A	24	0	24	2	0
3	B	12	0	12	0	0
3	E	24	0	24	0	0
4	A	45	0	0	0	0
4	B	40	0	0	0	0
4	C	55	0	0	0	0
4	D	55	0	0	1	0
4	E	35	0	0	0	0
4	F	45	0	0	1	0
4	G	40	0	0	1	0
4	H	60	0	0	0	0
4	I	45	0	0	0	0
4	J	35	0	0	1	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	0	0
5	F	4	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0
5	J	5	0	0	0	0
6	A	31	0	0	0	0
6	B	53	0	0	0	0
6	C	77	0	0	0	0
6	D	52	0	0	1	0
6	E	46	0	0	0	0
6	F	68	0	0	0	0
6	G	28	0	0	0	0
6	H	30	0	0	0	0
6	I	52	0	0	0	0
6	J	36	0	0	0	0
All	All	16930	0	16601	182	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 6.

All (182) 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:J:81:LEU:HD23	1:J:84:MET:HE3	1.50	0.91
1:J:81:LEU:HD23	1:J:84:MET:CE	2.05	0.86
1:A:29:ARG:NH2	1:D:92:PRO:O	2.23	0.70
1:D:87:VAL:HG21	1:D:129:VAL:HG11	1.75	0.68
1:B:95:ARG:HD2	1:C:206:GLY:O	1.94	0.67
1:A:116:LYS:HE3	1:D:78:ARG:CZ	2.24	0.67
1:B:87:VAL:HG21	1:B:129:VAL:HG11	1.79	0.65
1:J:81:LEU:CD2	1:J:84:MET:HE3	2.24	0.64
1:A:29:ARG:HG2	1:A:204:ILE:HG23	1.81	0.63
1:G:78:ARG:HB2	4:G:306:SO4:O4	2.00	0.61
1:J:75:PRO:HG3	1:J:84:MET:HE2	1.83	0.61
1:A:57:TRP:HH2	1:B:203:LYS:HE2	1.66	0.61
1:B:92:PRO:O	1:C:29:ARG:NH1	2.35	0.60
1:H:20:GLU:OE1	1:H:22:ASP:N	2.34	0.60
1:D:194:ILE:HA	1:D:195:PRO:C	2.23	0.58
1:C:25:THR:HG23	1:C:203:LYS:O	2.04	0.58
1:I:12:LYS:HE2	1:J:64:GLU:OE1	2.04	0.58
1:J:81:LEU:CD2	1:J:84:MET:CE	2.81	0.58
1:A:87:VAL:HG21	1:A:129:VAL:HG11	1.87	0.57
1:G:134:ALA:O	1:G:187:LEU:HD11	2.05	0.56
1:I:194:ILE:HA	1:I:195:PRO:C	2.26	0.56
1:J:143:ILE:HD13	1:J:176:VAL:HG21	1.87	0.56
1:B:189:GLU:N	1:B:189:GLU:OE2	2.35	0.56
1:G:35:VAL:O	1:G:39:LEU:HD13	2.06	0.55
1:I:164:GLU:N	1:I:164:GLU:OE1	2.35	0.55
1:C:20:GLU:OE2	1:C:22:ASP:N	2.38	0.55
1:C:41:TYR:CD1	1:D:38:LEU:HD22	2.41	0.55
1:H:25:THR:HG23	1:H:203:LYS:O	2.07	0.55
1:A:78:ARG:NH2	1:A:202:ASP:OD1	2.39	0.55
1:B:203:LYS:HD3	1:B:203:LYS:O	2.07	0.54
1:C:87:VAL:HG21	1:C:129:VAL:HG11	1.90	0.54
1:B:202:ASP:HB3	1:B:207:THR:O	2.08	0.54
1:E:92:PRO:O	1:H:29:ARG:NH2	2.41	0.54
1:B:79:ALA:HB1	1:B:131:PRO:HG2	1.90	0.54
1:G:143:ILE:HD13	1:G:176:VAL:HG21	1.90	0.54
1:E:41:TYR:CD1	1:F:38:LEU:HD22	2.43	0.53
1:C:54:ILE:C	1:C:54:ILE:HD12	2.29	0.53
1:F:115:GLN:NE2	1:I:110:PRO:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:VAL:HG21	1:E:129:VAL:HG21	1.90	0.52
1:G:38:LEU:HD22	1:H:41:TYR:CD1	2.45	0.52
1:E:208:LYS:OXT	1:H:116:LYS:NZ	2.42	0.52
1:E:54:ILE:HD12	1:E:54:ILE:C	2.30	0.52
1:E:83:MET:HB2	1:E:129:VAL:CG1	2.39	0.52
1:E:20:GLU:OE2	1:E:22:ASP:N	2.41	0.52
1:F:23:ILE:HD11	1:F:27:ARG:HG2	1.92	0.52
1:F:194:ILE:HA	1:F:195:PRO:C	2.30	0.52
1:G:194:ILE:HA	1:G:195:PRO:C	2.30	0.52
1:G:54:ILE:HD12	1:G:54:ILE:C	2.30	0.51
1:E:79:ALA:HB1	1:E:131:PRO:HG2	1.90	0.51
1:J:6:VAL:HG22	1:J:42:GLU:HG2	1.93	0.51
1:G:90:HIS:ND1	1:H:38:LEU:HD21	2.26	0.51
1:G:104:ASN:O	1:G:108:LEU:N	2.42	0.51
1:J:54:ILE:HD12	1:J:54:ILE:C	2.32	0.51
1:A:78:ARG:HB3	1:A:205:PHE:CZ	2.46	0.51
1:D:91:VAL:HG12	1:D:94:ALA:HB2	1.92	0.50
1:B:54:ILE:HD12	1:B:54:ILE:C	2.32	0.50
1:F:109:GLU:HG2	1:I:115:GLN:HE21	1.76	0.50
1:I:23:ILE:HD11	1:I:27:ARG:HG2	1.93	0.50
1:H:54:ILE:HD12	1:H:54:ILE:C	2.31	0.50
1:H:6:VAL:HG22	1:H:42:GLU:HG2	1.94	0.50
1:J:136:GLY:O	1:J:140:ILE:HG13	2.12	0.50
1:D:25:THR:HG23	1:D:203:LYS:O	2.11	0.50
1:B:194:ILE:HA	1:B:195:PRO:C	2.31	0.50
1:A:194:ILE:HA	1:A:195:PRO:C	2.32	0.49
1:A:143:ILE:HD13	1:A:176:VAL:HG11	1.94	0.49
1:B:78:ARG:NH1	1:C:116:LYS:HG2	2.27	0.49
1:E:57:TRP:HH2	1:F:203:LYS:HE2	1.76	0.49
1:I:134:ALA:O	1:I:187:LEU:HD11	2.12	0.49
1:J:194:ILE:HA	1:J:195:PRO:C	2.34	0.49
1:A:41:TYR:CD1	1:B:38:LEU:HD22	2.49	0.48
1:A:38:LEU:HD22	1:B:41:TYR:CD1	2.48	0.48
1:E:30:GLU:HG3	1:E:31:LEU:N	2.28	0.48
1:J:134:ALA:O	1:J:187:LEU:HD11	2.13	0.48
1:H:194:ILE:HA	1:H:195:PRO:C	2.34	0.48
1:I:54:ILE:C	1:I:54:ILE:HD12	2.33	0.48
1:F:136:GLY:O	1:F:140:ILE:HG13	2.13	0.48
1:C:79:ALA:HB1	1:C:131:PRO:HG2	1.95	0.48
1:J:18:MET:HE2	1:J:32:ALA:N	2.28	0.48
1:H:83:MET:HB2	1:H:129:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:LEU:HD23	1:G:84:MET:HG3	1.96	0.47
1:J:1:MET:HG3	1:J:176:VAL:O	2.14	0.47
1:J:200:ALA:O	1:J:204:ILE:HG13	2.14	0.47
1:D:6:VAL:HG22	1:D:42:GLU:HG2	1.96	0.47
1:B:117:LEU:HD11	1:B:145:LEU:CD2	2.45	0.47
1:C:90:HIS:CE1	1:D:38:LEU:HD21	2.50	0.47
1:J:75:PRO:HG3	1:J:84:MET:CE	2.44	0.47
1:A:104:ASN:O	1:A:108:LEU:N	2.42	0.47
1:A:127:LEU:HD23	1:A:155:LYS:HB2	1.96	0.46
1:C:158:VAL:O	1:C:180:THR:HA	2.14	0.46
1:H:108:LEU:HD12	1:H:108:LEU:N	2.30	0.46
1:F:78:ARG:HB2	4:F:302:SO4:O2	2.15	0.46
1:B:145:LEU:C	1:B:145:LEU:HD23	2.36	0.46
1:H:79:ALA:HB1	1:H:131:PRO:HG2	1.97	0.46
1:F:54:ILE:HD12	1:F:54:ILE:C	2.36	0.46
1:H:157:LEU:HD23	1:H:179:TYR:HB2	1.97	0.46
1:A:79:ALA:HB1	1:A:131:PRO:HG2	1.98	0.46
1:H:164:GLU:OE1	1:H:164:GLU:N	2.42	0.46
1:C:38:LEU:HD22	1:D:41:TYR:CD1	2.51	0.46
1:E:136:GLY:O	1:E:140:ILE:HG13	2.16	0.45
1:A:54:ILE:C	1:A:54:ILE:HD12	2.37	0.45
1:C:66:ILE:HD11	1:D:10:LEU:HD23	1.99	0.45
1:A:116:LYS:NZ	4:D:303:SO4:O1	2.45	0.45
1:E:194:ILE:HA	1:E:195:PRO:C	2.37	0.45
1:A:38:LEU:HD21	1:B:90:HIS:ND1	2.31	0.45
1:D:189:GLU:HG3	1:D:190:HIS:CD2	2.52	0.45
1:E:108:LEU:HD12	1:E:108:LEU:N	2.32	0.45
1:H:78:ARG:NH2	1:H:202:ASP:OD1	2.50	0.45
1:C:37:SER:HB2	1:C:90:HIS:NE2	2.31	0.45
1:C:208:LYS:HD2	1:C:208:LYS:N	2.32	0.45
1:D:26:LYS:NZ	6:D:402:HOH:O	2.50	0.45
1:B:143:ILE:HD13	1:B:176:VAL:HG21	1.99	0.45
1:F:200:ALA:O	1:F:204:ILE:HG13	2.16	0.45
1:A:10:LEU:HD23	1:B:66:ILE:HD11	1.98	0.44
1:H:78:ARG:HB3	1:H:205:PHE:CZ	2.52	0.44
1:E:77:LEU:HA	1:E:78:ARG:HA	1.78	0.44
1:C:74:VAL:HG22	1:C:97:SER:HB2	1.99	0.44
1:I:38:LEU:HD21	1:J:90:HIS:ND1	2.32	0.44
1:J:157:LEU:HD23	1:J:179:TYR:HB2	2.00	0.44
1:C:136:GLY:O	1:C:140:ILE:HG13	2.17	0.44
1:J:104:ASN:O	1:J:108:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB2	1:A:170:GLU:HG3	1.99	0.43
1:E:154:ILE:HB	1:E:176:VAL:HG12	2.00	0.43
1:G:87:VAL:HG21	1:G:129:VAL:HG11	2.00	0.43
1:J:77:LEU:HB2	1:J:100:GLY:HA2	1.99	0.43
1:A:38:LEU:HD21	1:B:90:HIS:CE1	2.53	0.43
1:D:79:ALA:HB1	1:D:131:PRO:HG2	1.99	0.43
1:F:148[B]:ASN:ND2	1:I:144:ASP:OD2	2.47	0.43
1:J:78:ARG:HB2	4:J:304:SO4:O2	2.19	0.43
1:D:67:LYS:HG2	1:D:68:GLY:N	2.33	0.43
1:J:18:MET:HE2	1:J:31:LEU:C	2.39	0.43
1:G:136:GLY:O	1:G:140:ILE:HG13	2.19	0.43
1:J:34:GLU:O	1:J:37:SER:HB3	2.19	0.43
1:I:38:LEU:HD22	1:J:41:TYR:CD1	2.54	0.43
1:D:158:VAL:O	1:D:180:THR:HA	2.18	0.43
1:E:38:LEU:HD22	1:F:41:TYR:CD1	2.54	0.42
1:H:128:VAL:HG11	1:H:139:MET:SD	2.58	0.42
1:I:158:VAL:O	1:I:180:THR:HA	2.19	0.42
1:I:38:LEU:HD22	1:J:41:TYR:HD1	1.84	0.42
1:H:127:LEU:HD23	1:H:155:LYS:HB2	2.02	0.42
1:I:78:ARG:NH2	1:I:202:ASP:OD1	2.51	0.42
1:A:158:VAL:O	1:A:180:THR:HA	2.19	0.42
1:A:7:LYS:H	3:A:301:BDF:H12	1.84	0.42
1:I:87:VAL:HG21	1:I:129:VAL:HG11	2.01	0.42
1:G:25:THR:HG23	1:G:203:LYS:O	2.20	0.42
1:H:72:THR:HA	1:H:95:ARG:O	2.20	0.42
1:I:19:ARG:O	1:J:56:GLY:HA2	2.19	0.42
1:A:164:GLU:OE1	1:A:164:GLU:N	2.46	0.42
1:G:157:LEU:HD23	1:G:179:TYR:HB2	2.02	0.42
1:C:89:GLU:OE1	1:D:89:GLU:OE1	2.38	0.42
1:E:206:GLY:O	1:H:95:ARG:HD3	2.20	0.42
1:J:197:LEU:O	1:J:203:LYS:HE3	2.20	0.42
1:A:34:GLU:OE1	1:B:90:HIS:ND1	2.50	0.42
1:E:10:LEU:HD13	1:F:90:HIS:HB3	2.02	0.42
1:E:83:MET:HB2	1:E:129:VAL:HG11	2.02	0.41
1:H:158:VAL:O	1:H:180:THR:HA	2.20	0.41
1:A:136:GLY:O	1:A:140:ILE:HG13	2.21	0.41
1:D:136:GLY:O	1:D:140:ILE:HG13	2.19	0.41
1:F:157:LEU:N	1:F:157:LEU:HD12	2.35	0.41
1:C:34:GLU:OE2	1:D:90:HIS:HA	2.21	0.41
1:F:79:ALA:HB1	1:F:131:PRO:HG2	2.02	0.41
1:A:25:THR:HG23	1:A:203:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HB3	1:C:205:PHE:CZ	2.56	0.41
1:E:72:THR:HA	1:E:95:ARG:O	2.21	0.41
1:G:56:GLY:HA2	1:H:19:ARG:O	2.21	0.41
1:H:173:HIS:O	1:H:176:VAL:HG22	2.20	0.41
1:F:156:VAL:C	1:F:157:LEU:HD12	2.41	0.41
1:E:158:VAL:O	1:E:180:THR:HA	2.21	0.41
1:A:77:LEU:HB2	1:A:100:GLY:HA2	2.03	0.41
1:B:202:ASP:CB	1:B:207:THR:O	2.69	0.41
1:C:157:LEU:HD23	1:C:179:TYR:HB2	2.02	0.41
1:F:118:VAL:HG22	1:F:119:SER:N	2.36	0.41
1:I:79:ALA:HB1	1:I:131:PRO:HG2	2.03	0.41
1:I:136:GLY:O	1:I:140:ILE:HG13	2.22	0.40
1:J:18:MET:HE3	1:J:31:LEU:HB3	2.03	0.40
1:F:108:LEU:N	1:F:108:LEU:HD12	2.36	0.40
1:G:12:LYS:HD2	1:H:64:GLU:OE1	2.21	0.40
1:A:102:TYR:CZ	1:A:111:VAL:HG11	2.56	0.40
1:E:163:PRO:HD2	1:E:186:GLY:HA2	2.04	0.40
1:A:6:VAL:HA	3:A:301:BDF:H11	2.04	0.40
1:J:18:MET:CE	1:J:31:LEU:C	2.90	0.40
1:B:88:LEU:HD11	1:B:96:ILE:HD11	2.04	0.40
1:G:34:GLU:OE2	1:H:90:HIS:ND1	2.54	0.40

There are no symmetry-related clashes.

## 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	207/211 (98%)	199 (96%)	8 (4%)	0	100	100
1	B	202/211 (96%)	196 (97%)	6 (3%)	0	100	100
1	C	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
1	D	201/211 (95%)	192 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
1	F	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
1	G	207/211 (98%)	199 (96%)	8 (4%)	0	100	100
1	H	208/211 (99%)	193 (93%)	15 (7%)	0	100	100
1	I	208/211 (99%)	197 (95%)	11 (5%)	0	100	100
1	J	209/211 (99%)	197 (94%)	12 (6%)	0	100	100
All	All	2068/2110 (98%)	1971 (95%)	97 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	173/175 (99%)	173 (100%)	0	100	100
1	B	170/175 (97%)	169 (99%)	1 (1%)	86	95
1	C	175/175 (100%)	174 (99%)	1 (1%)	86	95
1	D	169/175 (97%)	169 (100%)	0	100	100
1	E	174/175 (99%)	174 (100%)	0	100	100
1	F	175/175 (100%)	174 (99%)	1 (1%)	86	95
1	G	173/175 (99%)	173 (100%)	0	100	100
1	H	174/175 (99%)	173 (99%)	1 (1%)	86	95
1	I	174/175 (99%)	174 (100%)	0	100	100
1	J	175/175 (100%)	175 (100%)	0	100	100
All	All	1732/1750 (99%)	1728 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	203	LYS

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Mol	Chain	Res	Type
1	C	208	LYS
1	F	203	LYS
1	H	203	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	104	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 monosaccharides 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	GLC	K	1	2	11,11,12	0.31	0	15,15,17	1.06	1 (6%)
2	FRU	K	2	2	11,12,12	0.73	1 (9%)	10,18,18	0.79	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	GLC	K	1	2	-	2/2/19/22	0/1/1/1
2	FRU	K	2	2	-	3/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	FRU	O2-C2	2.10	1.44	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	GLC	C1-O5-C5	3.09	116.38	112.19

There are no chirality outliers.

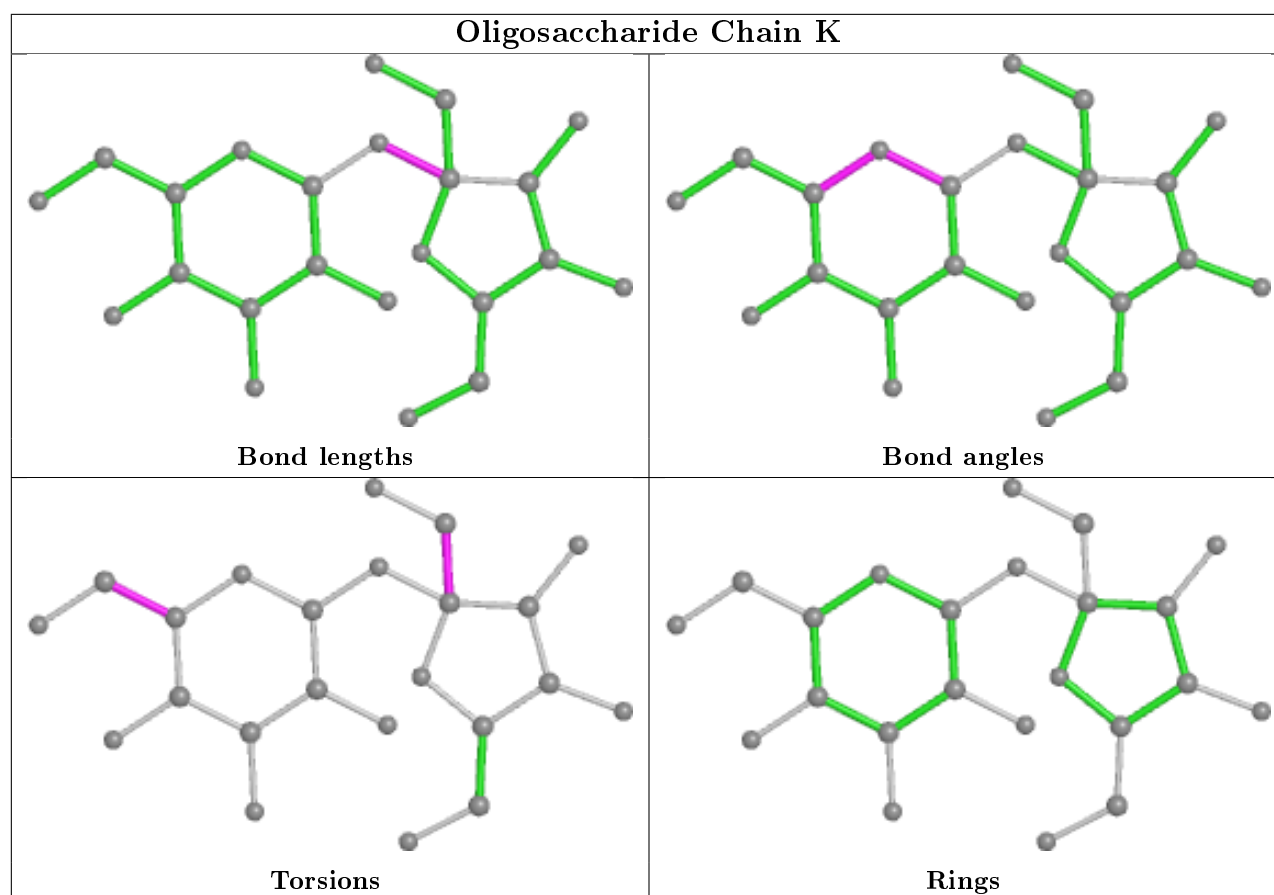
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	FRU	O1-C1-C2-O2
2	K	1	GLC	O5-C5-C6-O6
2	K	2	FRU	O1-C1-C2-C3
2	K	2	FRU	O1-C1-C2-O5
2	K	1	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

Of 119 ligands modelled in this entry, 23 are monoatomic - leaving 96 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	F	304	-	4,4,4	0.40	0	6,6,6	0.05	0
4	SO4	G	307	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	B	302	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	H	305	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	B	309	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	H	301	-	4,4,4	0.40	0	6,6,6	0.05	0
4	SO4	D	301	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	F	308	-	4,4,4	0.39	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	G	305	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	H	303	-	4,4,4	0.41	0	6,6,6	0.05	0
4	SO4	J	305	-	4,4,4	0.38	0	6,6,6	0.06	0
4	SO4	J	304	-	4,4,4	0.40	0	6,6,6	0.05	0
4	SO4	A	308	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	D	310	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	I	309	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	I	304	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	E	305	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	C	308	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	D	305	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	H	304	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	G	306	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	C	309	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	G	308	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	C	305	-	4,4,4	0.37	0	6,6,6	0.04	0
4	SO4	B	308	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	C	306	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	J	303	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	F	303	-	4,4,4	0.39	0	6,6,6	0.07	0
4	SO4	H	306	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	F	307	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	J	306	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	E	308	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	G	301	-	4,4,4	0.39	0	6,6,6	0.05	0
3	BDF	E	301	-	12,12,12	0.35	0	18,18,18	0.79	0
4	SO4	A	311	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	I	308	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	J	302	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	I	306	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	I	302	-	4,4,4	0.40	0	6,6,6	0.07	0
4	SO4	I	305	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	C	302	-	4,4,4	0.40	0	6,6,6	0.05	0
4	SO4	I	303	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	F	310	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	A	307	-	4,4,4	0.40	0	6,6,6	0.04	0
4	SO4	D	306	-	4,4,4	0.37	0	6,6,6	0.05	0
4	SO4	B	305	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	H	310	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	D	309	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	G	303	-	4,4,4	0.39	0	6,6,6	0.06	0
4	SO4	C	301	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	E	306	-	4,4,4	0.39	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	D	303	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	H	311	-	4,4,4	0.38	0	6,6,6	0.04	0
4	SO4	D	302	-	4,4,4	0.39	0	6,6,6	0.04	0
3	BDF	A	301	-	12,12,12	0.30	0	18,18,18	0.49	0
4	SO4	D	304	-	4,4,4	0.39	0	6,6,6	0.04	0
4	SO4	J	307	-	4,4,4	0.40	0	6,6,6	0.05	0
4	SO4	B	304	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	D	308	-	4,4,4	0.39	0	6,6,6	0.05	0
3	BDF	E	302	-	12,12,12	0.35	0	18,18,18	0.44	0
4	SO4	H	302	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	A	304	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	J	301	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	H	308	-	4,4,4	0.39	0	6,6,6	0.05	0
3	BDF	A	302	-	12,12,12	0.31	0	18,18,18	0.37	0
4	SO4	B	307	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	E	303	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	B	303	-	4,4,4	0.39	0	6,6,6	0.06	0
4	SO4	C	304	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	I	301	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	D	311	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	E	304	-	4,4,4	0.40	0	6,6,6	0.05	0
4	SO4	H	307	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	C	311	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	A	303	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	F	309	-	4,4,4	0.38	0	6,6,6	0.05	0
3	BDF	B	301	-	12,12,12	0.21	0	18,18,18	0.72	0
4	SO4	A	309	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	G	302	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	I	307	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	A	305	-	4,4,4	0.40	0	6,6,6	0.08	0
4	SO4	C	310	-	4,4,4	0.38	0	6,6,6	0.04	0
4	SO4	E	307	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	F	306	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	G	304	-	4,4,4	0.40	0	6,6,6	0.05	0
4	SO4	A	306	-	4,4,4	0.38	0	6,6,6	0.05	0
4	SO4	D	307	-	4,4,4	0.40	0	6,6,6	0.05	0
4	SO4	E	309	-	4,4,4	0.39	0	6,6,6	0.04	0
4	SO4	A	310	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	C	307	-	4,4,4	0.38	0	6,6,6	0.04	0
4	SO4	H	312	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	B	306	-	4,4,4	0.38	0	6,6,6	0.04	0
4	SO4	C	303	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	F	305	-	4,4,4	0.40	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	F	302	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	H	309	-	4,4,4	0.38	0	6,6,6	0.05	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
3	BDF	A	302	-	-	0/3/23/23	0/1/1/1
3	BDF	E	301	-	-	0/3/23/23	0/1/1/1
3	BDF	B	301	-	-	0/3/23/23	0/1/1/1
3	BDF	E	302	-	-	1/3/23/23	0/1/1/1
3	BDF	A	301	-	-	0/3/23/23	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	302	BDF	O1-C1-C2-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	304	SO4	1	0
4	G	306	SO4	1	0
4	D	303	SO4	1	0
3	A	301	BDF	2	0
4	F	302	SO4	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	209/211 (99%)	-0.02	7 (3%) 46 46	44, 56, 79, 90	0
1	B	206/211 (97%)	0.01	5 (2%) 59 60	36, 49, 75, 101	0
1	C	210/211 (99%)	0.05	9 (4%) 35 33	37, 49, 73, 94	0
1	D	205/211 (97%)	-0.01	8 (3%) 39 38	39, 53, 73, 122	0
1	E	210/211 (99%)	0.08	13 (6%) 20 19	38, 51, 79, 134	0
1	F	209/211 (99%)	-0.11	4 (1%) 66 69	36, 47, 67, 86	0
1	G	209/211 (99%)	0.12	14 (6%) 17 16	47, 64, 90, 109	0
1	H	209/211 (99%)	0.24	13 (6%) 20 19	45, 65, 92, 111	0
1	I	210/211 (99%)	0.03	15 (7%) 16 14	43, 60, 88, 108	0
1	J	210/211 (99%)	0.18	19 (9%) 9 7	45, 61, 91, 113	0
All	All	2087/2110 (98%)	0.06	107 (5%) 28 26	36, 56, 85, 134	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	-1	ASN	7.7
1	D	-1	ASN	6.1
1	G	190	HIS	5.8
1	C	-1	ASN	5.7
1	E	108	LEU	5.5
1	E	-1	ASN	4.8
1	G	208	LYS	4.7
1	B	-1	ASN	4.6
1	E	109	GLU	4.5
1	C	208	LYS	4.4
1	H	189	GLU	4.3
1	J	60	PRO	4.3
1	J	-1	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	105	GLU	4.1
1	I	189	GLU	4.0
1	A	189	GLU	4.0
1	B	208	LYS	4.0
1	E	107	THR	3.9
1	E	106	GLU	3.9
1	D	0	ALA	3.8
1	J	189	GLU	3.7
1	J	69	LYS	3.6
1	H	68	GLY	3.6
1	J	54	ILE	3.6
1	F	189	GLU	3.5
1	D	103	ARG	3.5
1	I	208	LYS	3.4
1	B	58	ASN	3.3
1	E	103	ARG	3.3
1	G	189	GLU	3.3
1	H	22	ASP	3.2
1	I	22	ASP	3.2
1	D	110	PRO	3.2
1	C	189	GLU	3.2
1	E	22	ASP	3.2
1	E	208	LYS	3.1
1	D	102	TYR	3.1
1	E	104	ASN	3.1
1	H	190	HIS	3.0
1	I	106	GLU	3.0
1	B	0	ALA	3.0
1	D	208	LYS	3.0
1	C	68	GLY	2.9
1	A	106	GLU	2.9
1	I	105	GLU	2.8
1	H	54	ILE	2.8
1	A	0	ALA	2.8
1	C	0	ALA	2.8
1	G	53	THR	2.7
1	H	171	LYS	2.7
1	J	22	ASP	2.7
1	H	48	GLU	2.7
1	H	208	LYS	2.7
1	J	59	GLY	2.7
1	F	208	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	129	VAL	2.7
1	I	190	HIS	2.7
1	H	2	LYS	2.6
1	J	49	THR	2.6
1	D	109	GLU	2.6
1	I	0	ALA	2.6
1	I	51	LYS	2.6
1	G	57	TRP	2.5
1	G	174	PRO	2.5
1	E	58	ASN	2.5
1	D	22	ASP	2.5
1	G	0	ALA	2.5
1	J	48	GLU	2.4
1	A	190	HIS	2.4
1	A	171	LYS	2.4
1	E	0	ALA	2.4
1	J	150	GLY	2.4
1	F	22	ASP	2.4
1	A	50	GLU	2.4
1	A	208	LYS	2.4
1	C	106	GLU	2.4
1	J	208	LYS	2.4
1	G	106	GLU	2.4
1	J	55	GLU	2.4
1	C	190	HIS	2.3
1	H	192	TYR	2.3
1	J	190	HIS	2.3
1	I	59	GLY	2.3
1	J	21	HIS	2.3
1	I	52	VAL	2.3
1	F	102	TYR	2.3
1	J	66	ILE	2.3
1	G	105	GLU	2.2
1	I	68	GLY	2.2
1	J	123	GLU	2.2
1	J	65	GLN	2.2
1	G	52	VAL	2.2
1	I	21	HIS	2.2
1	G	51	LYS	2.2
1	G	68	GLY	2.2
1	C	128	VAL	2.2
1	H	0	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	68	GLY	2.2
1	H	170	GLU	2.1
1	H	21	HIS	2.1
1	G	67	LYS	2.1
1	I	56	GLY	2.1
1	I	185	LYS	2.1
1	G	2	LYS	2.0
1	B	192	TYR	2.0
1	E	57	TRP	2.0
1	J	106	GLU	2.0

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

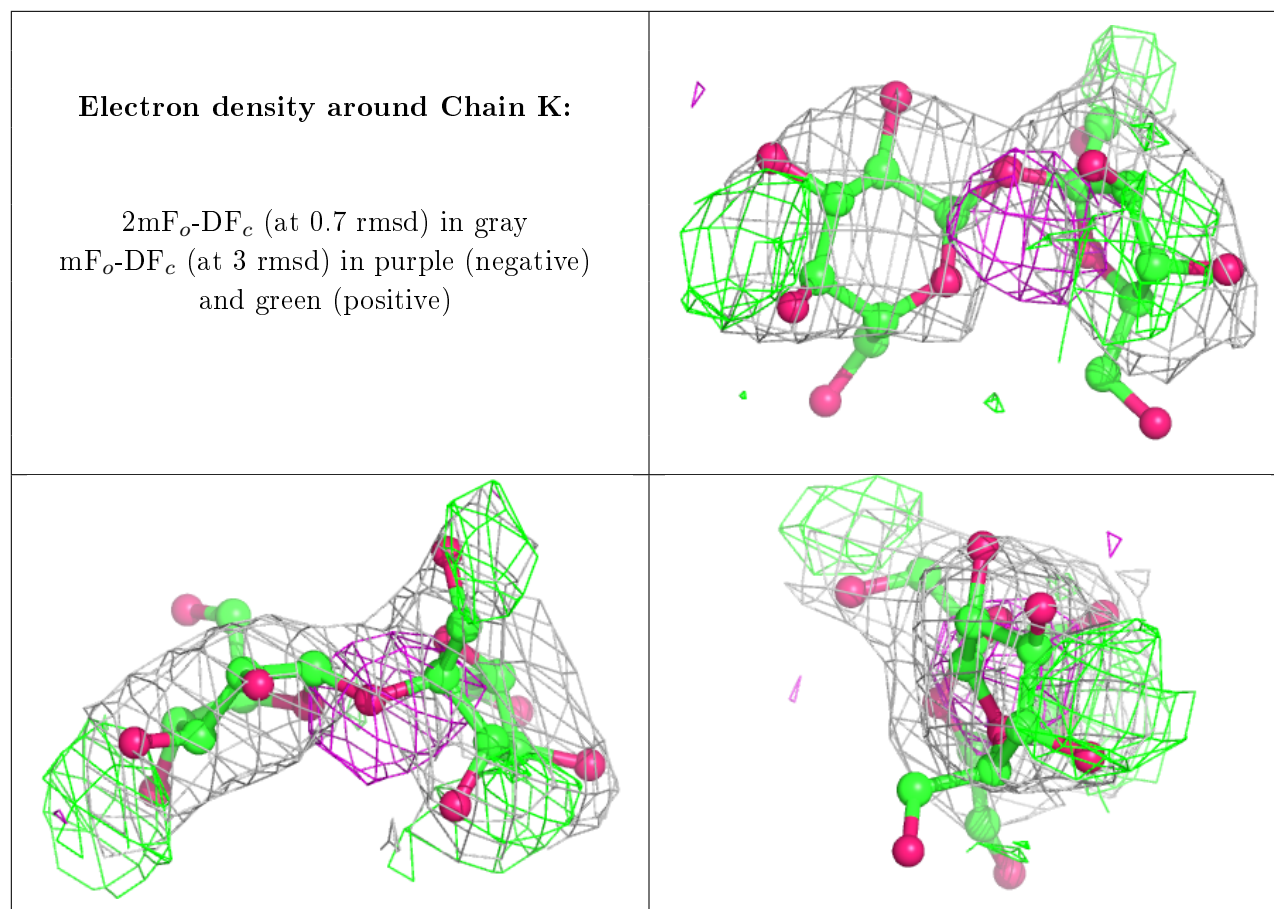
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [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( $\text{\AA}^2$ )	Q<0.9
2	FRU	K	2	12/12	0.61	0.36	92,97,106,111	0
2	GLC	K	1	11/12	0.80	0.36	93,100,112,113	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.4 Ligands ⓘ

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
4	SO4	H	310	5/5	0.47	0.47	151,151,155,156	0
4	SO4	H	306	5/5	0.60	0.51	147,149,152,157	0
4	SO4	H	311	5/5	0.62	0.36	131,132,141,143	0
4	SO4	G	308	5/5	0.64	0.44	136,141,144,145	0
4	SO4	C	305	5/5	0.74	0.17	79,85,87,94	0
4	SO4	C	309	5/5	0.74	0.42	113,120,124,125	0
4	SO4	H	309	5/5	0.75	0.23	122,126,128,130	0
4	SO4	D	308	5/5	0.76	0.27	126,126,127,131	0
4	SO4	H	307	5/5	0.76	0.45	143,143,145,147	0
4	SO4	F	308	5/5	0.76	0.34	113,115,117,118	0
4	SO4	F	310	5/5	0.78	0.57	129,133,135,135	0
4	SO4	D	309	5/5	0.78	0.20	92,96,100,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	310	5/5	0.79	0.46	112,116,121,124	0
4	SO4	A	309	5/5	0.79	0.44	114,117,121,121	0
4	SO4	I	309	5/5	0.80	0.29	122,122,125,129	0
5	CL	E	312	1/1	0.81	0.20	79,79,79,79	0
5	CL	J	312	1/1	0.81	0.20	79,79,79,79	0
4	SO4	J	303	5/5	0.81	0.31	122,129,130,130	0
4	SO4	D	311	5/5	0.81	0.19	106,107,113,118	0
4	SO4	D	310	5/5	0.82	0.54	134,136,137,139	0
4	SO4	F	309	5/5	0.82	0.41	111,113,119,121	0
4	SO4	D	304	5/5	0.82	0.32	85,96,99,102	0
4	SO4	I	307	5/5	0.82	0.23	114,118,121,124	0
4	SO4	G	307	5/5	0.82	0.26	107,108,113,114	0
4	SO4	B	306	5/5	0.82	0.17	98,100,101,108	0
4	SO4	A	311	5/5	0.82	0.53	124,126,127,127	0
5	CL	I	311	1/1	0.83	0.24	87,87,87,87	0
5	CL	C	312	1/1	0.83	0.22	86,86,86,86	0
5	CL	E	311	1/1	0.83	0.21	85,85,85,85	0
3	BDF	A	301	12/12	0.84	0.29	71,83,84,85	0
5	CL	G	309	1/1	0.84	0.08	90,90,90,90	0
4	SO4	C	310	5/5	0.85	0.15	98,106,112,114	0
3	BDF	B	301	12/12	0.86	0.22	71,79,84,86	0
4	SO4	B	309	5/5	0.87	0.52	118,122,123,123	0
5	CL	J	308	1/1	0.87	0.19	83,83,83,83	0
5	CL	A	314	1/1	0.87	0.10	90,90,90,90	0
4	SO4	C	311	5/5	0.88	0.44	109,112,115,115	0
5	CL	A	315	1/1	0.88	0.33	93,93,93,93	0
5	CL	J	311	1/1	0.88	0.39	85,85,85,85	0
4	SO4	H	305	5/5	0.88	0.41	121,121,127,129	0
5	CL	B	311	1/1	0.88	0.21	77,77,77,77	0
4	SO4	A	308	5/5	0.89	0.27	99,102,103,107	0
3	BDF	E	302	12/12	0.89	0.23	95,101,103,105	0
3	BDF	A	302	12/12	0.89	0.26	99,105,108,110	0
4	SO4	D	306	5/5	0.89	0.15	86,89,90,98	0
5	CL	F	313	1/1	0.90	0.16	72,72,72,72	0
4	SO4	E	308	5/5	0.90	0.21	94,100,102,104	0
4	SO4	B	305	5/5	0.90	0.12	98,105,109,112	0
5	CL	A	312	1/1	0.90	0.26	95,95,95,95	0
3	BDF	E	301	12/12	0.90	0.26	63,76,80,86	0
5	CL	J	310	1/1	0.90	0.13	90,90,90,90	0
5	CL	F	311	1/1	0.90	0.25	88,88,88,88	0
4	SO4	E	303	5/5	0.91	0.12	89,95,101,101	0
5	CL	J	309	1/1	0.91	0.07	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	308	5/5	0.91	0.12	101,102,108,111	0
5	CL	F	314	1/1	0.92	0.24	79,79,79,79	0
5	CL	B	310	1/1	0.92	0.10	84,84,84,84	0
4	SO4	C	307	5/5	0.92	0.30	98,99,105,106	0
4	SO4	H	308	5/5	0.92	0.33	120,123,125,127	0
4	SO4	F	306	5/5	0.92	0.14	99,100,103,106	0
5	CL	F	312	1/1	0.93	0.41	88,88,88,88	0
4	SO4	D	305	5/5	0.93	0.12	96,98,100,103	0
4	SO4	F	307	5/5	0.93	0.13	114,117,124,125	0
4	SO4	C	304	5/5	0.93	0.19	83,83,86,88	0
4	SO4	J	301	5/5	0.93	0.19	109,113,114,116	0
4	SO4	J	307	5/5	0.94	0.14	86,87,91,93	0
4	SO4	I	308	5/5	0.94	0.37	97,99,104,105	0
4	SO4	B	302	5/5	0.94	0.17	61,69,74,74	0
5	CL	E	310	1/1	0.94	0.16	85,85,85,85	0
4	SO4	D	302	5/5	0.95	0.15	61,66,70,74	0
4	SO4	H	302	5/5	0.95	0.14	88,88,92,93	0
5	CL	I	310	1/1	0.95	0.39	88,88,88,88	0
4	SO4	J	302	5/5	0.96	0.14	66,69,74,74	0
4	SO4	D	301	5/5	0.96	0.10	71,72,77,80	0
5	CL	A	313	1/1	0.96	0.36	88,88,88,88	0
4	SO4	G	304	5/5	0.96	0.19	66,68,71,77	0
4	SO4	A	306	5/5	0.96	0.22	79,79,83,85	0
4	SO4	H	304	5/5	0.96	0.20	76,80,85,85	0
4	SO4	E	309	5/5	0.96	0.28	93,95,95,97	0
4	SO4	E	306	5/5	0.96	0.11	67,70,73,75	0
4	SO4	G	306	5/5	0.96	0.13	63,67,70,70	0
4	SO4	J	306	5/5	0.96	0.20	101,102,106,107	0
4	SO4	C	303	5/5	0.96	0.19	70,71,73,74	0
5	CL	D	312	1/1	0.96	0.20	79,79,79,79	0
4	SO4	I	306	5/5	0.97	0.10	75,78,81,81	0
4	SO4	I	303	5/5	0.97	0.16	75,75,77,78	0
4	SO4	H	312	5/5	0.97	0.15	57,57,60,61	0
4	SO4	G	301	5/5	0.97	0.12	58,58,59,63	0
4	SO4	I	301	5/5	0.97	0.14	56,61,64,64	0
4	SO4	F	305	5/5	0.97	0.16	65,67,68,70	0
4	SO4	G	303	5/5	0.97	0.13	66,67,71,77	0
4	SO4	G	302	5/5	0.98	0.10	69,70,73,74	0
4	SO4	I	305	5/5	0.98	0.11	49,51,52,53	0
4	SO4	A	305	5/5	0.98	0.14	47,49,52,57	0
4	SO4	I	304	5/5	0.98	0.17	66,68,69,71	0
4	SO4	E	305	5/5	0.98	0.10	50,52,53,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	303	5/5	0.98	0.09	52,54,56,57	0
4	SO4	E	304	5/5	0.98	0.15	61,61,64,70	0
4	SO4	B	304	5/5	0.98	0.09	63,65,67,69	0
4	SO4	A	307	5/5	0.98	0.10	69,72,76,76	0
4	SO4	G	305	5/5	0.98	0.19	79,82,83,83	0
4	SO4	H	301	5/5	0.98	0.13	59,63,65,72	0
4	SO4	A	303	5/5	0.98	0.13	60,64,65,66	0
4	SO4	A	304	5/5	0.98	0.23	75,77,79,79	0
4	SO4	H	303	5/5	0.98	0.14	72,72,79,87	0
4	SO4	J	304	5/5	0.98	0.08	54,54,57,57	0
4	SO4	F	302	5/5	0.98	0.12	54,54,57,62	0
4	SO4	I	302	5/5	0.98	0.12	48,49,51,53	0
4	SO4	C	306	5/5	0.99	0.17	67,72,73,74	0
4	SO4	D	307	5/5	0.99	0.08	63,64,69,70	0
4	SO4	J	305	5/5	0.99	0.12	48,49,51,53	0
4	SO4	F	304	5/5	0.99	0.08	51,52,54,55	0
4	SO4	C	308	5/5	0.99	0.10	55,58,60,61	0
4	SO4	B	307	5/5	0.99	0.09	44,45,46,46	0
4	SO4	C	301	5/5	0.99	0.16	43,45,46,46	0
4	SO4	E	307	5/5	0.99	0.12	63,64,67,69	0
4	SO4	B	303	5/5	0.99	0.14	50,51,55,59	0
4	SO4	F	303	5/5	0.99	0.11	37,37,38,40	0
4	SO4	C	302	5/5	0.99	0.13	54,58,59,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.