



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:25 AM UTC

PDB ID : 6WN8 / pdb_00006wn8
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

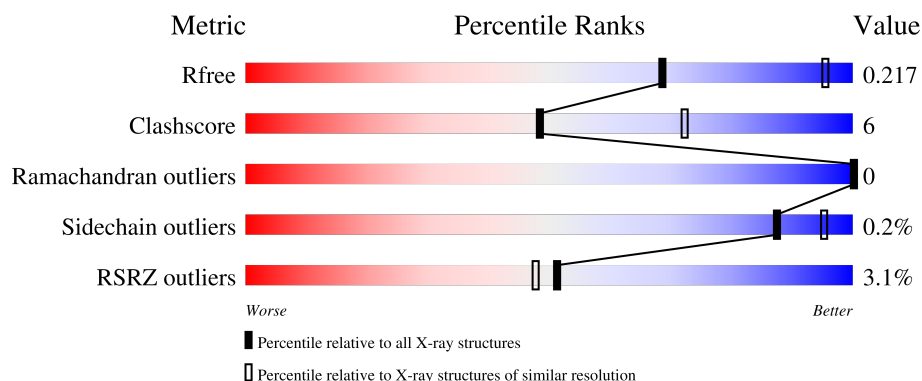
1 Overall quality at a glance

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.



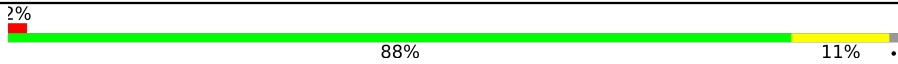
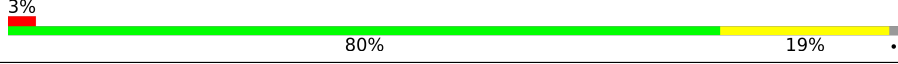
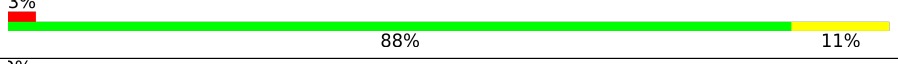
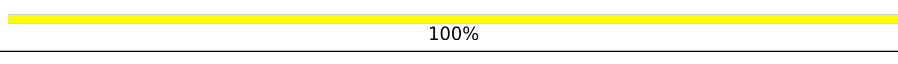
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 of 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 $\leq 5\%$. 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	2% 79% 20% .
1	B	211	4% 86% 11% .
1	C	211	% 84% 16% .
1	D	211	4% 83% 14% .
1	E	211	6% 84% 15% .

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Mol	Chain	Length	Quality of chain
1	F	211	 2% 88% 11%
1	G	211	 2% 86% 12%
1	H	211	 3% 80% 19%
1	I	211	 3% 88% 11%
1	J	211	 2% 83% 16%
2	K	2	 100%

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:

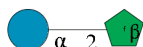
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A1Y0PUH0
A	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
A	0	ALA	-	expression tag	UNP A0A1Y0PUH0
B	-2	SER	-	expression tag	UNP A0A1Y0PUH0
B	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
B	0	ALA	-	expression tag	UNP A0A1Y0PUH0
C	-2	SER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

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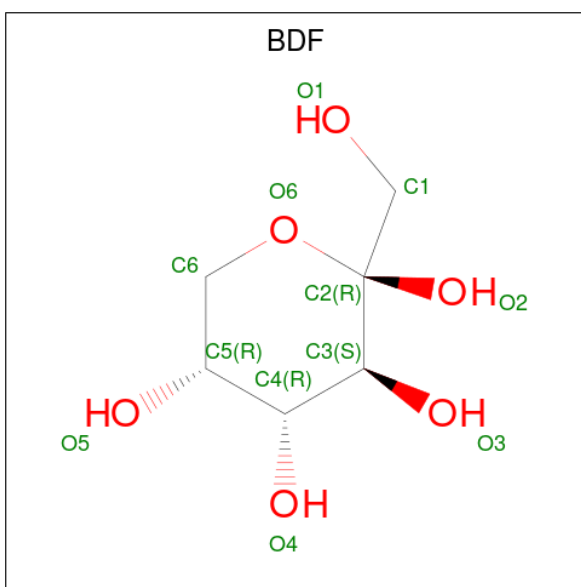
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP A0A1Y0PUH0
D	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
D	0	ALA	-	expression tag	UNP A0A1Y0PUH0
E	-2	SER	-	expression tag	UNP A0A1Y0PUH0
E	-1	ASN	-	expression tag	UNP A0A1Y0PUH0
E	0	ALA	-	expression tag	UNP A0A1Y0PUH0
F	-2	SER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



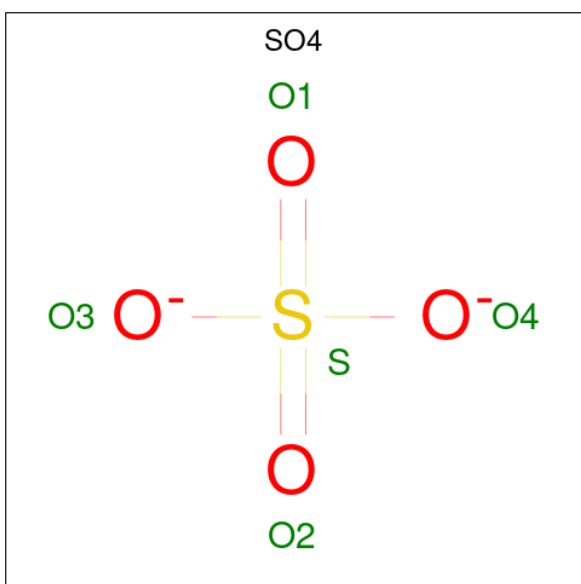
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is beta-D-fructopyranose (CCD ID: BDF) (formula: C₆H₁₂O₆).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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	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	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is water.

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

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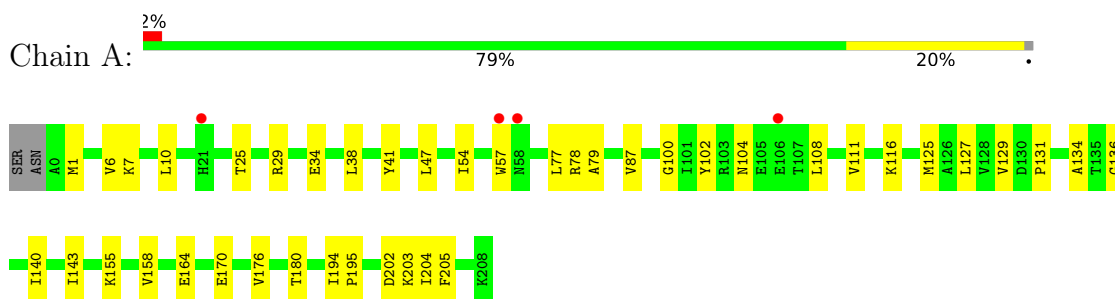
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	77	Total 77	O 77	0	0
6	D	52	Total 52	O 52	0	0
6	E	46	Total 46	O 46	0	0
6	F	68	Total 68	O 68	0	0
6	G	28	Total 28	O 28	0	0
6	H	30	Total 30	O 30	0	0
6	I	52	Total 52	O 52	0	0
6	J	36	Total 36	O 36	0	0

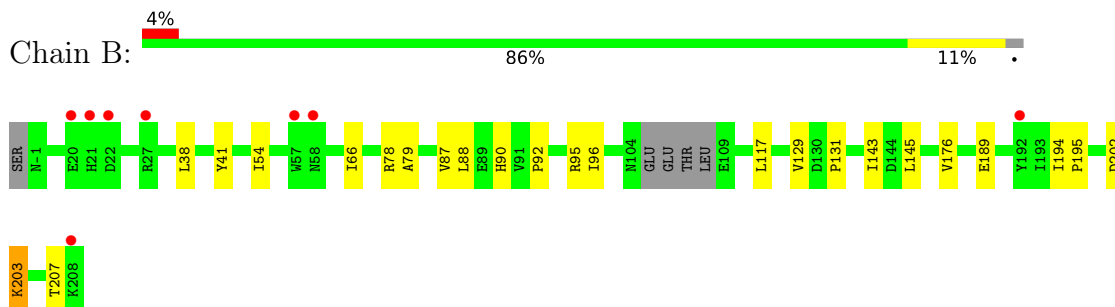
3 Residue-property plots [i](#)

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.

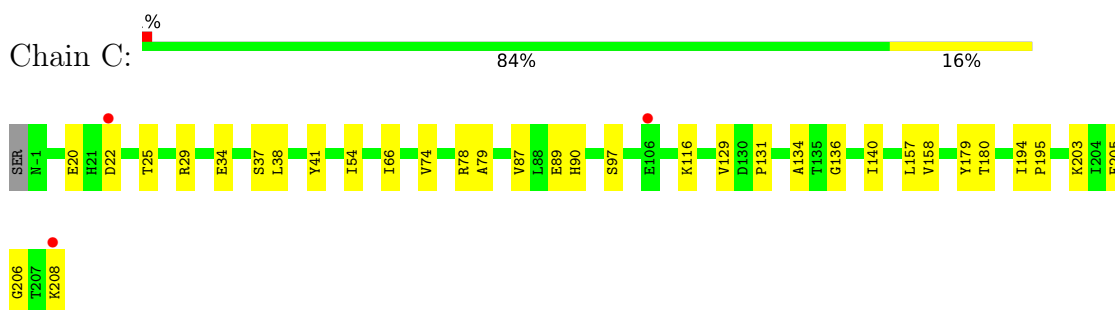
- Molecule 1: Uracil phosphoribosyltransferase



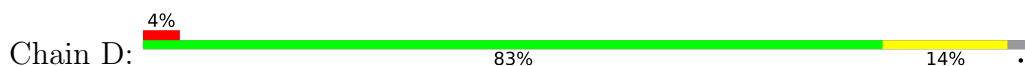
- Molecule 1: Uracil phosphoribosyltransferase

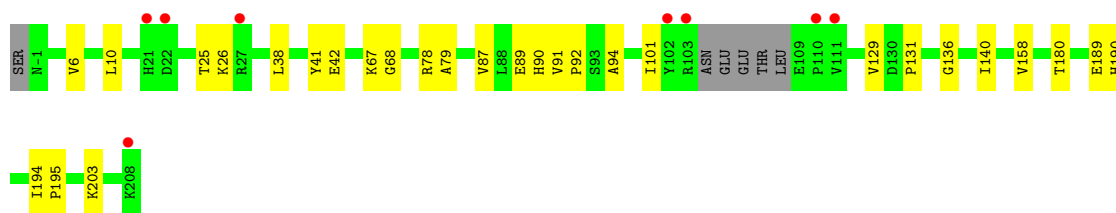


- Molecule 1: Uracil phosphoribosyltransferase

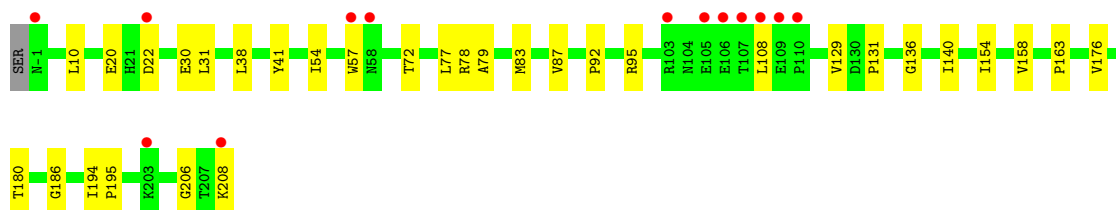
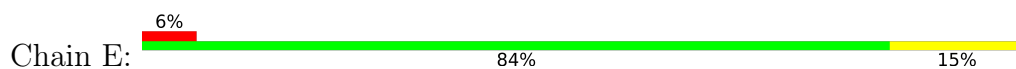


- Molecule 1: Uracil phosphoribosyltransferase

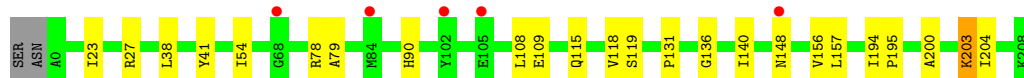
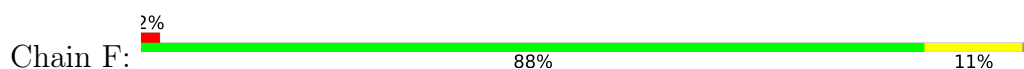




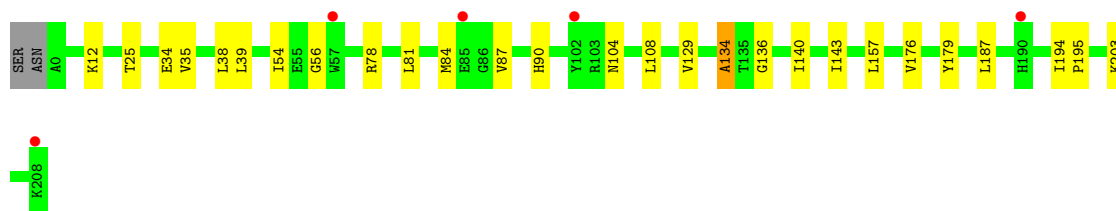
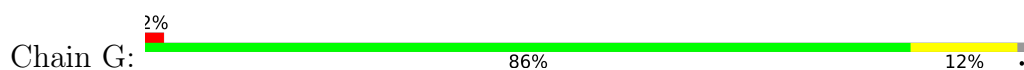
- Molecule 1: Uracil phosphoribosyltransferase



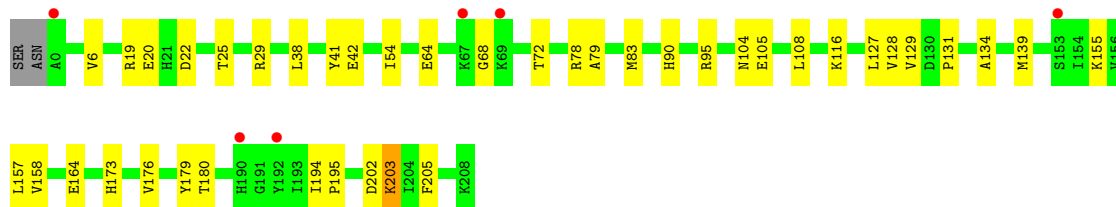
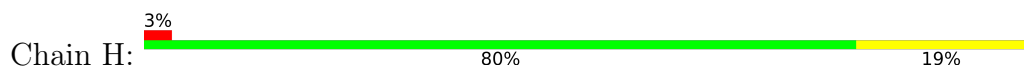
- Molecule 1: Uracil phosphoribosyltransferase



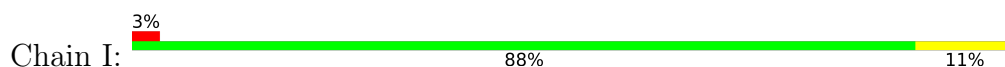
- Molecule 1: Uracil phosphoribosyltransferase

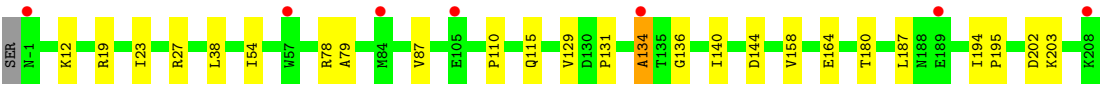


- Molecule 1: Uracil phosphoribosyltransferase

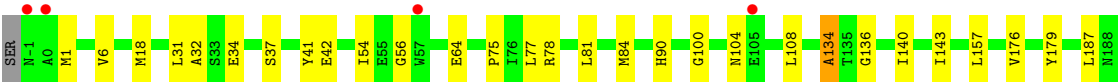
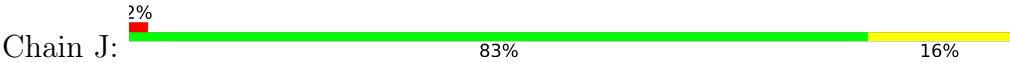


- Molecule 1: Uracil phosphoribosyltransferase

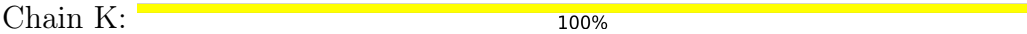




• Molecule 1: Uracil phosphoribosyltransferase



• 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, α , β , γ	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) 99.9 (29.71-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	55.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, SO4, FRU, BDF, 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	1.02	0/1613	1.23	1/2182 (0.0%)
1	B	1.00	0/1587	1.21	0/2145
1	C	1.02	0/1629	1.24	1/2204 (0.0%)
1	D	1.01	0/1579	1.22	1/2134 (0.0%)
1	E	1.02	0/1621	1.24	0/2193
1	F	1.02	0/1630	1.24	0/2204
1	G	1.03	0/1613	1.24	1/2182 (0.0%)
1	H	1.02	0/1621	1.23	4/2193 (0.2%)
1	I	1.04	0/1621	1.23	1/2193 (0.0%)
1	J	1.04	0/1630	1.25	1/2205 (0.0%)
All	All	1.02	0/16144	1.23	10/21835 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	134	ALA	N-CA-C	7.47	122.62	111.04
1	I	134	ALA	N-CA-C	7.20	122.20	111.04
1	H	104	ASN	N-CA-C	-7.10	99.53	110.10
1	H	105	GLU	N-CA-C	6.86	121.10	113.21
1	A	134	ALA	N-CA-C	6.67	121.39	111.04
1	C	134	ALA	N-CA-C	5.96	120.28	111.04
1	H	134	ALA	N-CA-C	5.84	120.09	111.04
1	J	134	ALA	N-CA-C	5.59	119.71	111.04
1	H	68	GLY	CA-C-O	-5.53	118.15	122.52
1	D	101	ILE	CB-CA-C	-5.03	103.88	110.98

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	30	0
1	B	1563	0	1627	22	0
1	C	1604	0	1663	22	0
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	28	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	183	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 (183) 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:CE	2.05	0.86
1:J:75:PRO:HG3	1:J:84:MET:HE2	1.57	0.85
1:J:81:LEU:HD23	1:J:84:MET:HE3	1.62	0.81
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:D:194:ILE:HA	1:D:195:PRO:C	2.23	0.63
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:A:57:TRP:HH2	1:B:203:LYS:HE2	1.66	0.61
1:I:194:ILE:HA	1:I:195:PRO:C	2.26	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: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:C:54:ILE:HD12	1:C:54:ILE:C	2.29	0.57
1:G:54:ILE:HD12	1:G:54:ILE:C	2.30	0.57
1:E:54:ILE:C	1:E:54:ILE:HD12	2.30	0.57
1:F:194:ILE:HA	1:F:195:PRO:C	2.30	0.57
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: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:H:54:ILE:C	1:H:54:ILE:HD12	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:VAL:O	1:G:39:LEU:HD13	2.06	0.55
1:G:194:ILE:HA	1:G:195:PRO:C	2.30	0.55
1:I:164:GLU:OE1	1:I:164:GLU:N	2.35	0.55
1:J:54:ILE:C	1:J:54:ILE:HD12	2.32	0.55
1:B:54:ILE:C	1:B:54:ILE:HD12	2.32	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:194:ILE:HA	1:B:195:PRO:C	2.31	0.54
1:B:203:LYS:O	1:B:203:LYS:HD3	2.07	0.54
1:C:87:VAL:HG21	1:C:129:VAL:HG11	1.90	0.54
1:J:81:LEU:CD2	1:J:84:MET:HE1	2.37	0.54
1:A:194:ILE:HA	1:A:195:PRO:C	2.32	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:H:194:ILE:HA	1:H:195:PRO:C	2.34	0.53
1:I:54:ILE:C	1:I:54:ILE:HD12	2.33	0.53
1:E:41:TYR:CD1	1:F:38:LEU:HD22	2.43	0.53
1:J:194:ILE:HA	1:J:195:PRO:C	2.34	0.53
1:F:115:GLN:NE2	1:I:110:PRO:O	2.42	0.53
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:20:GLU:OE2	1:E:22:ASP:N	2.41	0.52
1:E:83:MET:HB2	1:E:129:VAL:CG1	2.39	0.52
1:F:23:ILE:HD11	1:F:27:ARG:HG2	1.92	0.52
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:B:145:LEU:C	1:B:145:LEU:HD23	2.36	0.51
1:F:54:ILE:C	1:F:54:ILE:HD12	2.36	0.51
1:G:104:ASN:O	1:G:108:LEU:N	2.42	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: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:A:54:ILE:C	1:A:54:ILE:HD12	2.37	0.50
1:E:194:ILE:HA	1:E:195:PRO:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:38:LEU:HD22	1:B:41:TYR:CD1	2.48	0.48
1:A:41:TYR:CD1	1:B:38:LEU:HD22	2.49	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:F:136:GLY:O	1:F:140:ILE:HG13	2.13	0.48
1:J:18:MET:HE2	1:J:31:LEU:C	2.39	0.48
1:C:79:ALA:HB1	1:C:131:PRO:HG2	1.95	0.48
1:H:83:MET:HB2	1:H:129:VAL:CG1	2.43	0.48
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: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:J:75:PRO:CG	1:J:84:MET:HE2	2.39	0.46
1:F:78:ARG:HB2	4:F:302:SO4:O2	2.15	0.46
1:J:18:MET:HE2	1:J:32:ALA:N	2.30	0.46
1:H:79:ALA:HB1	1:H:131:PRO:HG2	1.97	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:F:156:VAL:C	1:F:157:LEU:HD12	2.41	0.45
1:E:136:GLY:O	1:E:140:ILE:HG13	2.16	0.45
1:A:116:LYS:NZ	4:D:303:SO4:O1	2.45	0.45
1:C:66:ILE:HD11	1:D:10:LEU:HD23	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:SER:HB2	1:C:90:HIS:NE2	2.31	0.45
1:C:208:LYS:N	1:C:208:LYS:HD2	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:J:18:MET:CE	1:J:31:LEU:C	2.90	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
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: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:C:194:ILE:HA	1:C:195:PRO:C	2.44	0.42
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:7:LYS:H	3:A:301:BDF:H12	1.84	0.42
1:A:158:VAL:O	1:A:180:THR:HA	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:F:157:LEU:N	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
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:E:158:VAL:O	1:E:180:THR:HA	2.21	0.41
1:A:47:LEU:HD21	1:A:125:MET:HE1	2.03	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: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: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

5.3.1 Protein backbone

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
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%)	78	91
1	C	175/175 (100%)	175 (100%)	0	100	100
1	D	169/175 (97%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	174/175 (99%)	174 (100%)	0	100	100
1	F	175/175 (100%)	174 (99%)	1 (1%)	78	91
1	G	173/175 (99%)	173 (100%)	0	100	100
1	H	174/175 (99%)	173 (99%)	1 (1%)	78	91
1	I	174/175 (99%)	173 (99%)	1 (1%)	78	91
1	J	175/175 (100%)	175 (100%)	0	100	100
All	All	1732/1750 (99%)	1728 (100%)	4 (0%)	87	95

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

Mol	Chain	Res	Type
1	B	203	LYS
1	F	203	LYS
1	H	203	LYS
1	I	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	B	120	ASN
1	D	190	HIS
1	E	190	HIS
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	0.99	1 (6%)
2	FRU	K	2	2	11,12,12	0.70	1 (9%)	10,18,18	0.81	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	2.09	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	3.13	116.38	112.19

There are no chirality outliers.

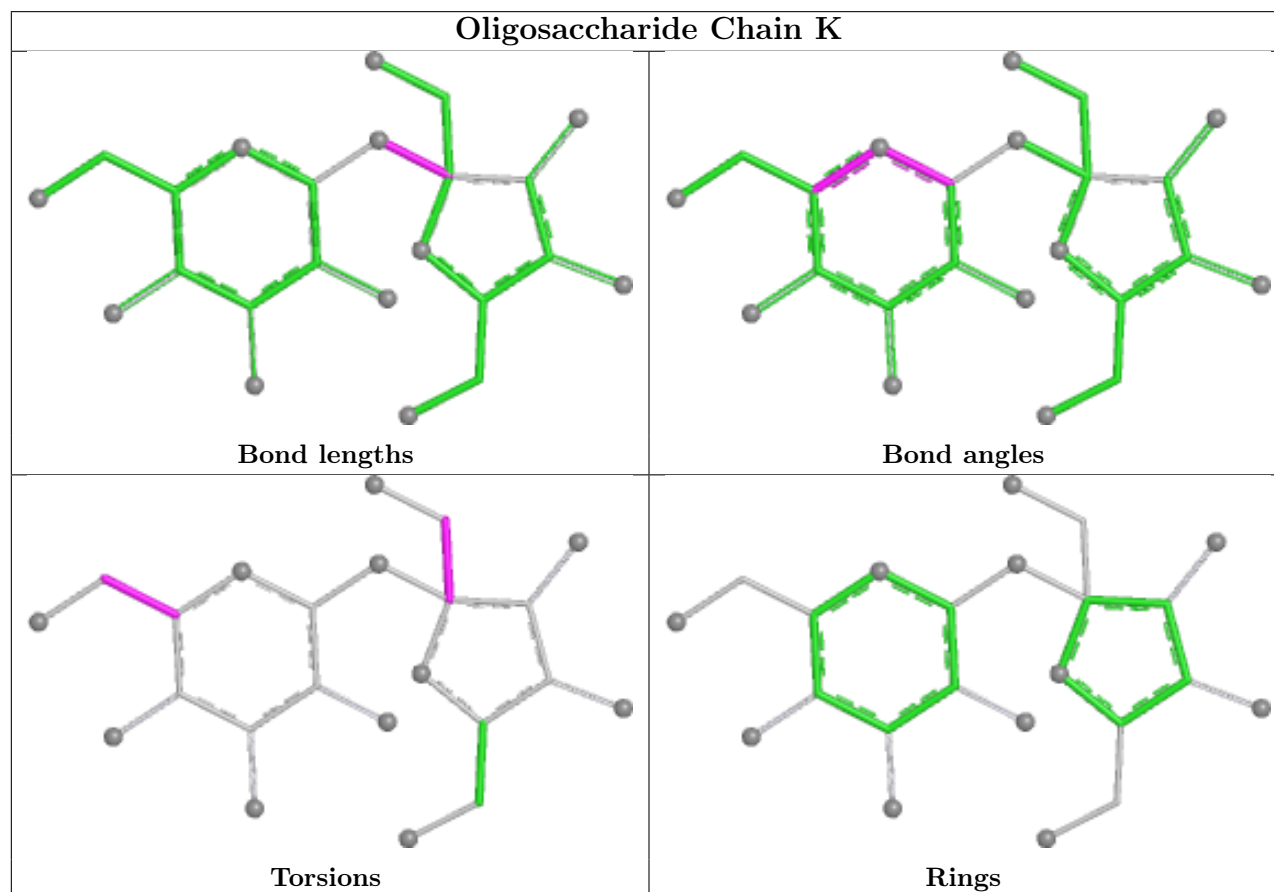
All (5) torsion outliers are listed below:

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	E	308	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	F	304	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	C	310	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	C	305	-	4,4,4	0.33	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	308	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	E	309	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	J	301	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	E	306	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	C	311	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	D	306	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	H	305	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	J	304	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	B	303	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	C	307	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	H	311	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	J	305	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	F	303	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	G	303	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	B	309	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	A	303	-	4,4,4	0.35	0	6,6,6	0.10	0
4	SO4	A	304	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	I	307	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	C	306	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	I	308	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	F	309	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	G	301	-	4,4,4	0.34	0	6,6,6	0.05	0
3	BDF	E	302	-	12,12,12	0.23	0	18,18,18	0.41	0
4	SO4	A	308	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	A	309	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	G	308	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	B	306	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	G	305	-	4,4,4	0.34	0	6,6,6	0.08	0
3	BDF	E	301	-	12,12,12	0.23	0	18,18,18	0.75	0
4	SO4	E	303	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	H	302	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	B	305	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	J	307	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	I	304	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	I	305	-	4,4,4	0.35	0	6,6,6	0.06	0
4	SO4	C	308	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	A	310	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	A	306	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	G	307	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	J	303	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	F	305	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	G	302	-	4,4,4	0.34	0	6,6,6	0.07	0
3	BDF	A	301	-	12,12,12	0.23	0	18,18,18	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	308	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	B	302	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	B	304	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	D	301	-	4,4,4	0.34	0	6,6,6	0.08	0
3	BDF	A	302	-	12,12,12	0.24	0	18,18,18	0.36	0
4	SO4	H	310	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	C	302	-	4,4,4	0.35	0	6,6,6	0.06	0
4	SO4	C	303	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	C	304	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	F	307	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	A	305	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	F	302	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	F	310	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	A	311	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	F	306	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	C	301	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	D	303	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	F	308	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	I	309	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	H	308	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	H	304	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	H	303	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	E	305	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	G	306	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	D	309	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	I	303	-	4,4,4	0.34	0	6,6,6	0.08	0
3	BDF	B	301	-	12,12,12	0.18	0	18,18,18	0.65	0
4	SO4	I	306	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	H	306	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	H	309	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	D	307	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	E	304	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	D	310	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	H	312	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	C	309	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	E	307	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	H	307	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	I	302	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	B	307	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	G	304	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	J	302	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	J	306	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	D	304	-	4,4,4	0.34	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	305	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	I	301	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	D	311	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	H	301	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	D	302	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	A	307	-	4,4,4	0.35	0	6,6,6	0.07	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	B	301	-	-	0/3/23/23	0/1/1/1
3	BDF	A	302	-	-	2/3/23/23	0/1/1/1
3	BDF	E	302	-	-	0/3/23/23	0/1/1/1
3	BDF	A	301	-	-	0/3/23/23	0/1/1/1
3	BDF	E	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 (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	BDF	O1-C1-C2-O6
3	A	302	BDF	O1-C1-C2-O2

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
3	A	301	BDF	2	0
4	F	302	SO4	1	0
4	D	303	SO4	1	0
4	G	306	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, 95th 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 ²)	Q<0.9
1	A	209/211 (99%)	0.05	4 (1%) 66 63	44, 56, 79, 90	0
1	B	206/211 (97%)	-0.00	8 (3%) 43 39	36, 49, 75, 101	0
1	C	210/211 (99%)	-0.11	3 (1%) 73 72	28, 49, 73, 94	1 (0%)
1	D	205/211 (97%)	0.02	8 (3%) 43 39	40, 53, 73, 122	0
1	E	210/211 (99%)	0.08	13 (6%) 26 23	38, 51, 79, 134	0
1	F	209/211 (99%)	-0.11	5 (2%) 59 56	22, 47, 67, 86	2 (0%)
1	G	209/211 (99%)	0.16	5 (2%) 59 56	47, 64, 90, 109	0
1	H	209/211 (99%)	0.24	6 (2%) 53 50	35, 65, 92, 111	1 (0%)
1	I	210/211 (99%)	0.06	7 (3%) 49 45	43, 60, 88, 108	0
1	J	210/211 (99%)	0.18	5 (2%) 59 56	32, 61, 91, 113	1 (0%)
All	All	2087/2110 (98%)	0.06	64 (3%) 51 48	22, 56, 85, 134	5 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	108	LEU	6.5
1	D	103	ARG	5.6
1	C	208	LYS	4.4
1	F	148[A]	ASN	4.3
1	E	110	PRO	4.2
1	H	0	ALA	4.0
1	D	111	VAL	4.0
1	G	208	LYS	3.9
1	E	103	ARG	3.8
1	I	105	GLU	3.3
1	E	-1	ASN	3.3
1	A	57	TRP	3.3
1	E	105	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	110	PRO	3.0
1	J	57	TRP	3.0
1	E	109	GLU	3.0
1	F	102	TYR	3.0
1	G	57	TRP	3.0
1	I	-1	ASN	3.0
1	I	84	MET	2.9
1	H	153	SER	2.9
1	D	22	ASP	2.8
1	J	0	ALA	2.8
1	G	102	TYR	2.7
1	E	57	TRP	2.7
1	B	58	ASN	2.7
1	I	208	LYS	2.7
1	I	57	TRP	2.7
1	J	-1	ASN	2.7
1	B	208	LYS	2.6
1	B	27	ARG	2.6
1	B	57	TRP	2.5
1	E	106	GLU	2.5
1	H	192	TYR	2.5
1	B	22	ASP	2.4
1	E	208	LYS	2.4
1	H	69	LYS	2.4
1	C	106	GLU	2.4
1	H	67	LYS	2.4
1	A	21	HIS	2.4
1	E	22	ASP	2.4
1	A	58	ASN	2.4
1	D	208	LYS	2.4
1	F	105	GLU	2.3
1	D	27	ARG	2.3
1	H	190	HIS	2.3
1	G	85	GLU	2.3
1	J	105	GLU	2.3
1	E	58	ASN	2.3
1	B	192	TYR	2.3
1	F	84	MET	2.2
1	D	102	TYR	2.2
1	F	68	GLY	2.2
1	B	20	GLU	2.1
1	J	189	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	22	ASP	2.1
1	A	106	GLU	2.1
1	E	107	THR	2.1
1	B	21	HIS	2.1
1	E	203	LYS	2.1
1	I	134	ALA	2.0
1	I	189	GLU	2.0
1	D	21	HIS	2.0
1	G	190	HIS	2.0

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

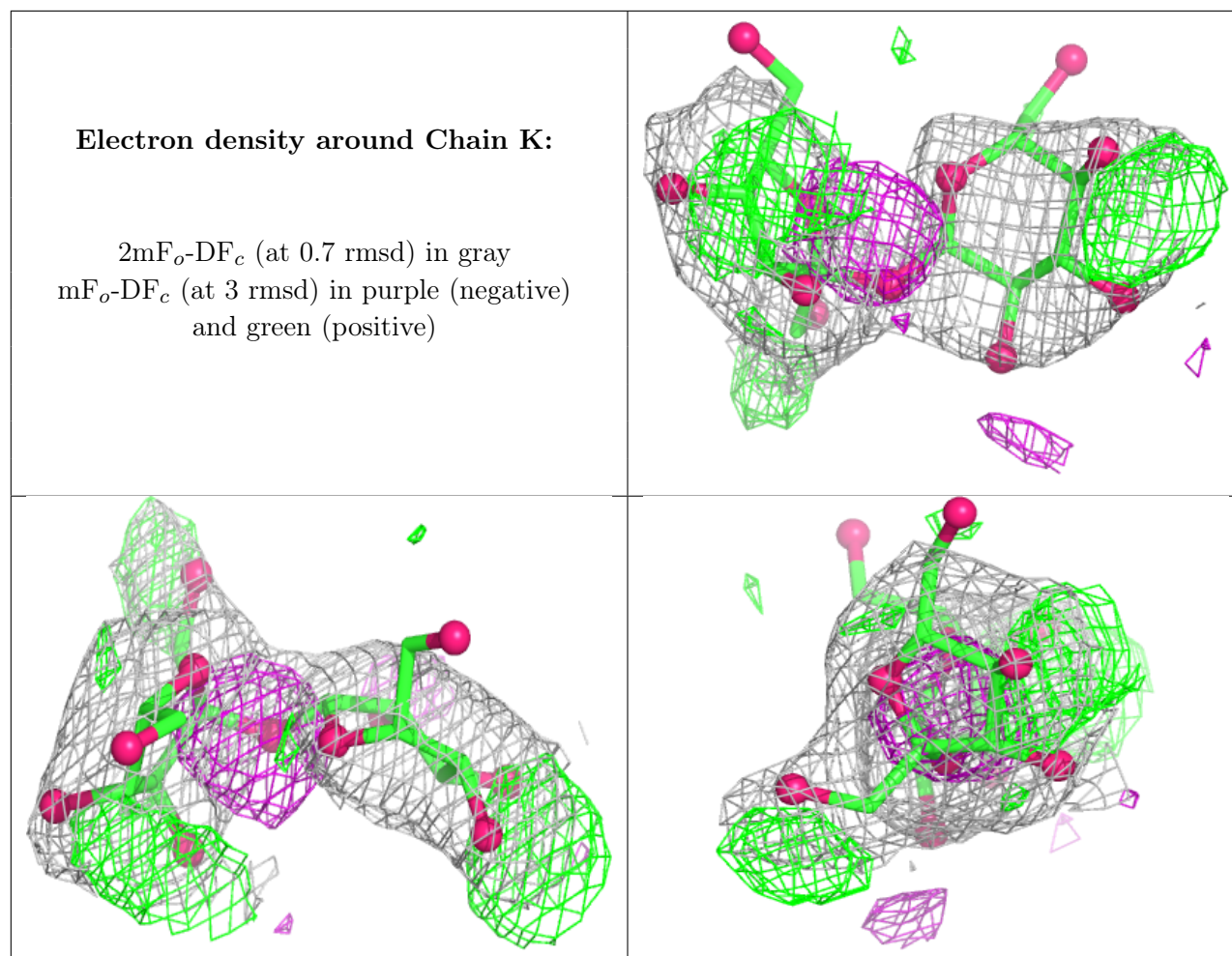
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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 ²)	Q<0.9
2	FRU	K	2	12/12	0.69	0.23	92,97,106,111	0
2	GLC	K	1	11/12	0.74	0.23	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 [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, 95th 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 ²)	Q<0.9
4	SO4	G	308	5/5	0.55	0.13	136,141,144,145	0
4	SO4	D	308	5/5	0.59	0.15	126,126,127,131	0
4	SO4	A	310	5/5	0.60	0.23	112,116,121,124	0
4	SO4	H	306	5/5	0.64	0.11	147,149,152,157	0
4	SO4	H	307	5/5	0.64	0.10	143,143,145,147	0
4	SO4	C	309	5/5	0.65	0.22	113,120,124,125	0
4	SO4	J	303	5/5	0.68	0.14	122,129,130,130	0
4	SO4	H	305	5/5	0.70	0.09	121,121,127,129	0
4	SO4	G	307	5/5	0.71	0.16	107,108,113,114	0
4	SO4	I	307	5/5	0.71	0.17	114,118,121,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	I	309	5/5	0.71	0.20	122,122,125,129	0
4	SO4	A	311	5/5	0.71	0.12	124,126,127,127	0
4	SO4	H	309	5/5	0.72	0.13	122,126,128,130	0
4	SO4	C	305	5/5	0.72	0.16	79,85,87,94	0
4	SO4	A	309	5/5	0.73	0.17	114,117,121,121	0
4	SO4	C	310	5/5	0.73	0.19	98,106,112,114	0
4	SO4	F	309	5/5	0.74	0.18	111,113,119,121	0
4	SO4	H	311	5/5	0.75	0.17	131,132,141,143	0
5	CL	E	311	1/1	0.75	0.10	85,85,85,85	0
4	SO4	J	301	5/5	0.76	0.15	109,113,114,116	0
4	SO4	D	306	5/5	0.78	0.13	86,89,90,98	0
4	SO4	B	309	5/5	0.78	0.23	118,122,123,123	0
4	SO4	D	310	5/5	0.78	0.11	134,136,137,139	0
4	SO4	B	305	5/5	0.78	0.15	98,105,109,112	0
4	SO4	H	308	5/5	0.79	0.11	120,123,125,127	0
5	CL	A	312	1/1	0.79	0.14	95,95,95,95	0
3	BDF	A	301	12/12	0.79	0.13	71,83,84,85	0
4	SO4	D	305	5/5	0.80	0.13	96,98,100,103	0
4	SO4	B	308	5/5	0.80	0.13	101,102,108,111	0
4	SO4	F	308	5/5	0.80	0.20	113,115,117,118	0
4	SO4	F	306	5/5	0.81	0.15	99,100,103,106	0
4	SO4	E	303	5/5	0.82	0.12	89,95,101,101	0
4	SO4	E	306	5/5	0.82	0.11	67,70,73,75	0
4	SO4	H	310	5/5	0.82	0.12	151,151,155,156	0
4	SO4	F	310	5/5	0.82	0.13	129,133,135,135	0
4	SO4	B	306	5/5	0.82	0.15	98,100,101,108	0
4	SO4	D	304	5/5	0.83	0.18	85,96,99,102	0
3	BDF	B	301	12/12	0.83	0.15	71,79,84,86	0
4	SO4	J	306	5/5	0.83	0.14	101,102,106,107	0
4	SO4	D	311	5/5	0.83	0.13	106,107,113,118	0
3	BDF	E	302	12/12	0.83	0.17	95,101,103,105	0
4	SO4	F	307	5/5	0.84	0.16	114,117,124,125	0
4	SO4	D	309	5/5	0.84	0.14	92,96,100,106	0
3	BDF	E	301	12/12	0.85	0.13	63,76,80,86	0
4	SO4	C	311	5/5	0.85	0.19	109,112,115,115	0
4	SO4	E	308	5/5	0.86	0.12	94,100,102,104	0
4	SO4	I	308	5/5	0.86	0.19	97,99,104,105	0
5	CL	I	310	1/1	0.86	0.11	88,88,88,88	0
4	SO4	A	308	5/5	0.87	0.16	99,102,103,107	0
5	CL	D	312	1/1	0.87	0.13	79,79,79,79	0
3	BDF	A	302	12/12	0.87	0.15	99,105,108,110	0
4	SO4	I	306	5/5	0.87	0.12	75,78,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	D	301	5/5	0.88	0.10	71,72,77,80	0
4	SO4	C	307	5/5	0.88	0.20	98,99,105,106	0
4	SO4	H	302	5/5	0.88	0.12	88,88,92,93	0
5	CL	J	311	1/1	0.88	0.12	85,85,85,85	0
4	SO4	J	307	5/5	0.89	0.10	86,87,91,93	0
4	SO4	E	309	5/5	0.89	0.12	93,95,95,97	0
4	SO4	B	302	5/5	0.90	0.09	61,69,74,74	0
5	CL	A	315	1/1	0.90	0.09	93,93,93,93	0
5	CL	B	311	1/1	0.90	0.09	77,77,77,77	0
5	CL	C	312	1/1	0.90	0.10	86,86,86,86	0
4	SO4	G	301	5/5	0.91	0.10	58,58,59,63	0
5	CL	F	311	1/1	0.91	0.09	88,88,88,88	0
5	CL	G	309	1/1	0.91	0.15	90,90,90,90	0
4	SO4	C	304	5/5	0.91	0.12	83,83,86,88	0
5	CL	E	310	1/1	0.91	0.12	85,85,85,85	0
5	CL	E	312	1/1	0.92	0.09	79,79,79,79	0
4	SO4	H	312	5/5	0.92	0.10	57,57,60,61	0
5	CL	F	312	1/1	0.92	0.10	88,88,88,88	0
5	CL	A	314	1/1	0.92	0.10	90,90,90,90	0
4	SO4	G	304	5/5	0.92	0.13	66,68,71,77	0
5	CL	I	311	1/1	0.92	0.10	87,87,87,87	0
5	CL	J	308	1/1	0.92	0.10	83,83,83,83	0
5	CL	J	310	1/1	0.92	0.13	90,90,90,90	0
4	SO4	G	306	5/5	0.92	0.10	63,67,70,70	0
4	SO4	A	304	5/5	0.93	0.13	75,77,79,79	0
5	CL	F	314	1/1	0.93	0.08	79,79,79,79	0
4	SO4	G	305	5/5	0.93	0.12	79,82,83,83	0
4	SO4	G	303	5/5	0.93	0.10	66,67,71,77	0
4	SO4	H	303	5/5	0.93	0.08	72,72,79,87	0
5	CL	A	313	1/1	0.93	0.08	88,88,88,88	0
4	SO4	I	302	5/5	0.93	0.09	48,49,51,53	0
4	SO4	J	302	5/5	0.93	0.12	66,69,74,74	0
5	CL	J	312	1/1	0.93	0.10	79,79,79,79	0
4	SO4	A	306	5/5	0.94	0.14	79,79,83,85	0
5	CL	B	310	1/1	0.94	0.08	84,84,84,84	0
4	SO4	H	301	5/5	0.94	0.08	59,63,65,72	0
4	SO4	E	304	5/5	0.94	0.10	61,61,64,70	0
4	SO4	D	302	5/5	0.94	0.10	61,66,70,74	0
4	SO4	C	303	5/5	0.94	0.15	70,71,73,74	0
4	SO4	A	307	5/5	0.95	0.07	69,72,76,76	0
4	SO4	A	305	5/5	0.95	0.07	47,49,52,57	0
4	SO4	C	302	5/5	0.95	0.08	54,58,59,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	H	304	5/5	0.95	0.11	76,80,85,85	0
4	SO4	D	307	5/5	0.95	0.08	63,64,69,70	0
5	CL	F	313	1/1	0.95	0.07	72,72,72,72	0
4	SO4	D	303	5/5	0.95	0.07	52,54,56,57	0
4	SO4	E	305	5/5	0.96	0.07	50,52,53,56	0
4	SO4	C	306	5/5	0.96	0.09	67,72,73,74	0
4	SO4	E	307	5/5	0.96	0.07	63,64,67,69	0
4	SO4	A	303	5/5	0.96	0.07	60,64,65,66	0
4	SO4	B	304	5/5	0.96	0.10	63,65,67,69	0
4	SO4	J	305	5/5	0.96	0.07	48,49,51,53	0
4	SO4	I	303	5/5	0.96	0.12	75,75,77,78	0
4	SO4	I	304	5/5	0.96	0.10	66,68,69,71	0
4	SO4	F	305	5/5	0.96	0.09	65,67,68,70	0
4	SO4	G	302	5/5	0.96	0.08	69,70,73,74	0
4	SO4	I	305	5/5	0.97	0.08	49,51,52,53	0
4	SO4	B	303	5/5	0.97	0.09	50,51,55,59	0
5	CL	J	309	1/1	0.97	0.07	78,78,78,78	0
4	SO4	F	302	5/5	0.97	0.06	54,54,57,62	0
4	SO4	I	301	5/5	0.97	0.06	56,61,64,64	0
4	SO4	J	304	5/5	0.97	0.10	54,54,57,57	0
4	SO4	C	308	5/5	0.98	0.06	55,58,60,61	0
4	SO4	F	303	5/5	0.98	0.05	37,37,38,40	0
4	SO4	F	304	5/5	0.98	0.06	51,52,54,55	0
4	SO4	C	301	5/5	0.98	0.05	43,45,46,46	0
4	SO4	B	307	5/5	0.99	0.04	44,45,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.