



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 07:48 am BST

PDB ID : 1RXU
Title : E. coli uridine phosphorylase: thymidine phosphate complex
Authors : Caradoc-Davies, T.T.; Cutfield, S.M.; Lamont, I.L.; Cutfield, J.F.
Deposited on : 2003-12-18
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

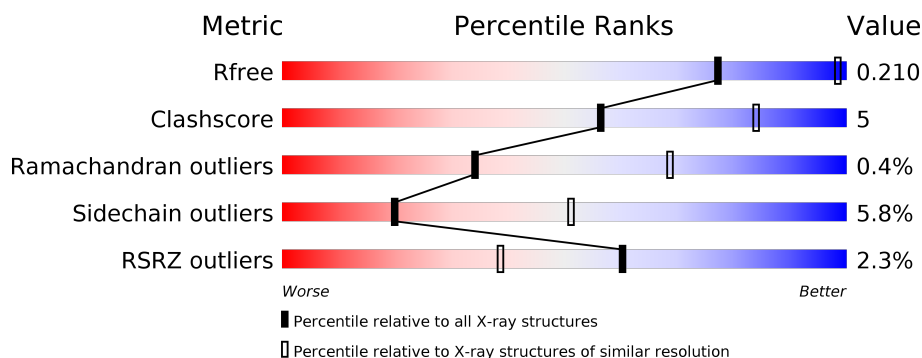
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	253	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
1	B	253	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	253	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
1	D	253	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	E	253	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>
1	F	253	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	253	
1	H	253	
1	I	253	
1	J	253	
1	K	253	
1	L	253	
1	M	253	
1	N	253	
1	O	253	
1	P	253	
1	Q	253	
1	R	253	

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
2	PO4	D	2041	-	-	X	-
2	PO4	E	2051	-	-	X	-
2	PO4	F	2061	-	-	X	-
2	PO4	K	2111	-	-	X	-
2	PO4	O	2151	-	-	X	-
4	THM	A	2012	X	-	-	-
4	THM	B	2022	X	-	-	-
4	THM	C	2032	X	-	-	-
4	THM	D	2042	X	-	-	-
4	THM	E	2052	X	-	-	-
4	THM	F	2062	X	-	-	-
4	THM	G	2072	X	-	-	-
4	THM	H	2082	X	-	-	-
4	THM	I	2092	X	-	-	-
4	THM	J	2102	X	-	-	-
4	THM	K	2112	X	-	-	-
4	THM	L	2122	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	THM	M	2132	X	-	-	-
4	THM	N	2142	X	-	-	-
4	THM	O	2152	X	-	-	-
4	THM	P	2162	X	-	-	-
4	THM	Q	2172	X	-	-	-
4	THM	R	2182	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35307 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	B	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	C	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	D	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	E	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	F	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	G	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	H	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	I	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	J	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	K	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	L	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	M	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	N	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	O	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	P	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	R	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		

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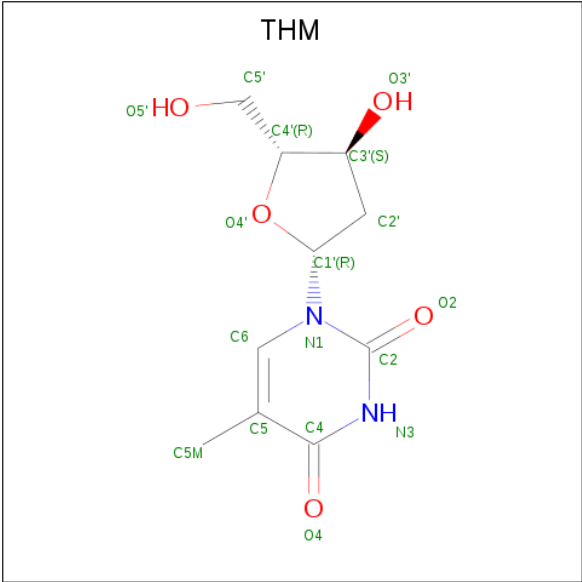
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		
2	O	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	K	0	0
			1	1		
3	Q	1	Total	K	0	0
			1	1		
3	K	1	Total	K	0	0
			1	1		
3	I	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	O	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		
3	M	1	Total	K	0	0
			1	1		

- Molecule 4 is THYMIDINE (three-letter code: THM) (formula: C₁₀H₁₄N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	10	2	5		
4	B	1	Total	C	N	O	0	0
			17	10	2	5		
4	C	1	Total	C	N	O	0	0
			17	10	2	5		
4	D	1	Total	C	N	O	0	0
			17	10	2	5		
4	E	1	Total	C	N	O	0	0
			17	10	2	5		
4	F	1	Total	C	N	O	0	0
			17	10	2	5		
4	G	1	Total	C	N	O	0	0
			17	10	2	5		
4	H	1	Total	C	N	O	0	0
			17	10	2	5		
4	I	1	Total	C	N	O	0	0
			17	10	2	5		
4	J	1	Total	C	N	O	0	0
			17	10	2	5		
4	K	1	Total	C	N	O	0	0
			17	10	2	5		
4	L	1	Total	C	N	O	0	0
			17	10	2	5		
4	M	1	Total	C	N	O	0	0
			17	10	2	5		
4	N	1	Total	C	N	O	0	0
			17	10	2	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	O	1	Total	C	N	O	0	0
			17	10	2	5		
4	P	1	Total	C	N	O	0	0
			17	10	2	5		
4	Q	1	Total	C	N	O	0	0
			17	10	2	5		
4	R	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	57	Total	O	0	0
			57	57		
5	C	62	Total	O	0	0
			62	62		
5	D	57	Total	O	0	0
			57	57		
5	E	59	Total	O	0	0
			59	59		
5	F	58	Total	O	0	0
			58	58		
5	G	59	Total	O	0	0
			59	59		
5	H	57	Total	O	0	0
			57	57		
5	I	60	Total	O	0	0
			60	60		
5	J	59	Total	O	0	0
			59	59		
5	K	58	Total	O	0	0
			58	58		
5	L	61	Total	O	0	0
			61	61		
5	M	60	Total	O	0	0
			60	60		
5	N	60	Total	O	0	0
			60	60		
5	O	58	Total	O	0	0
			58	58		

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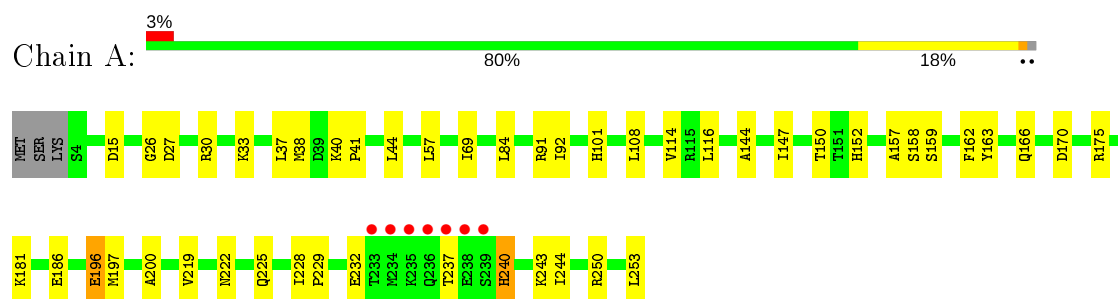
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	59	Total 59	O 59	0	0
5	Q	61	Total 61	O 61	0	0
5	R	58	Total 58	O 58	0	0

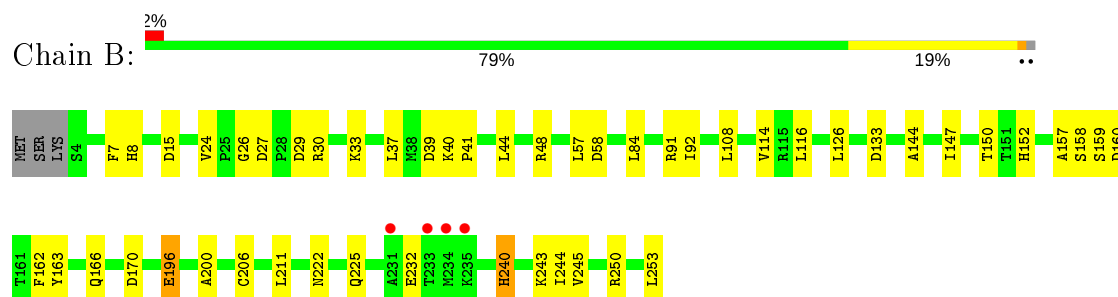
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

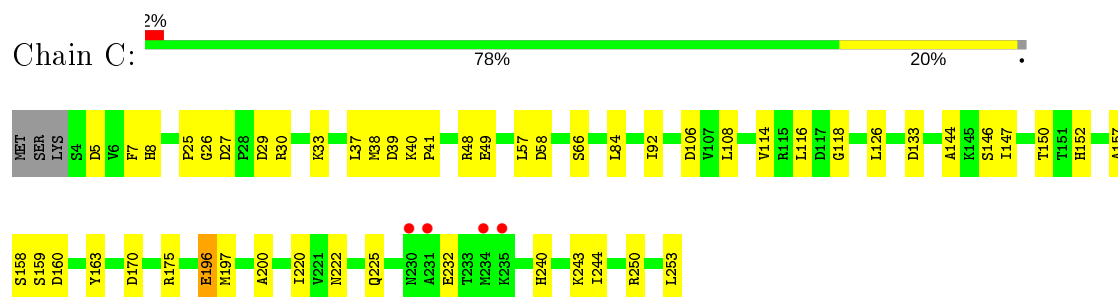
- Molecule 1: Uridine phosphorylase



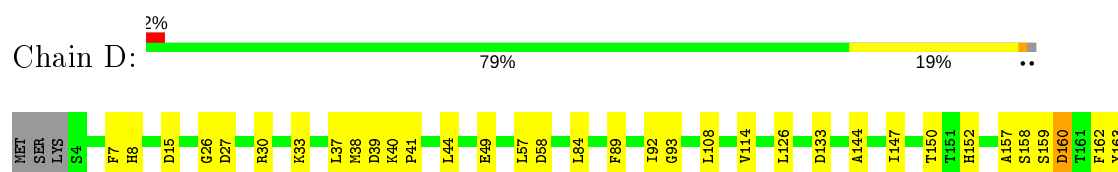
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

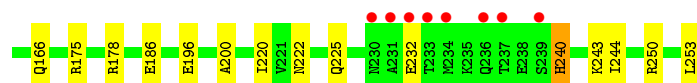
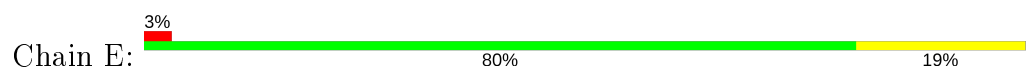


- Molecule 1: Uridine phosphorylase

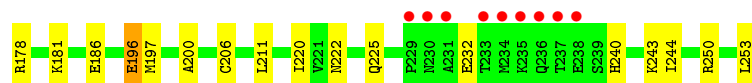
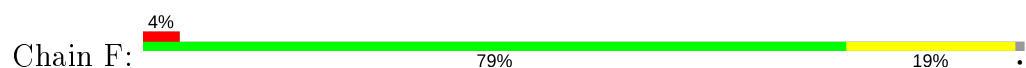




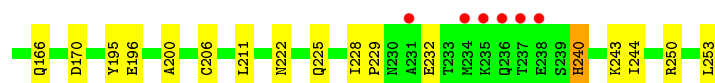
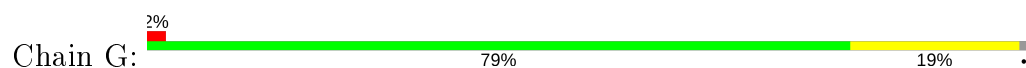
- Molecule 1: Uridine phosphorylase



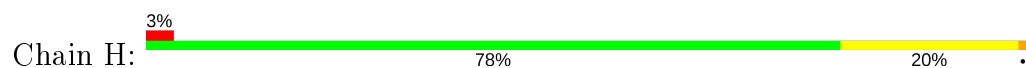
- Molecule 1: Uridine phosphorylase



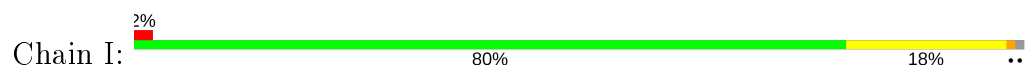
- Molecule 1: Uridine phosphorylase

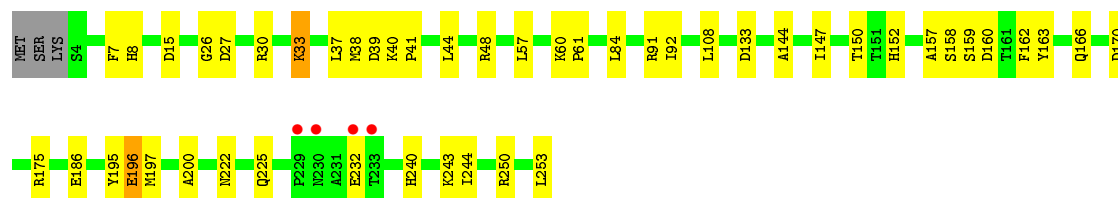


- Molecule 1: Uridine phosphorylase

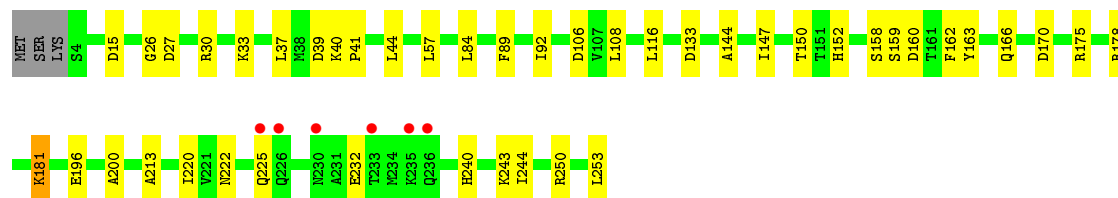
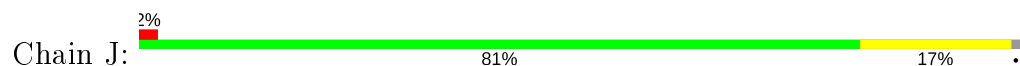


- Molecule 1: Uridine phosphorylase

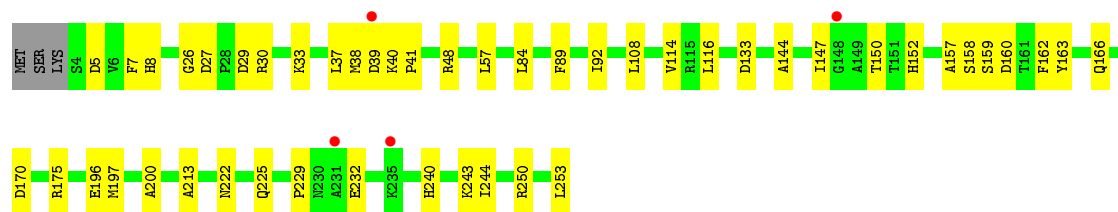
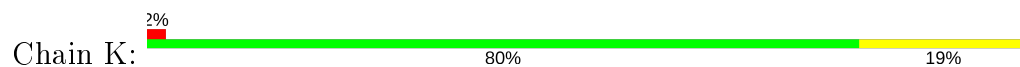




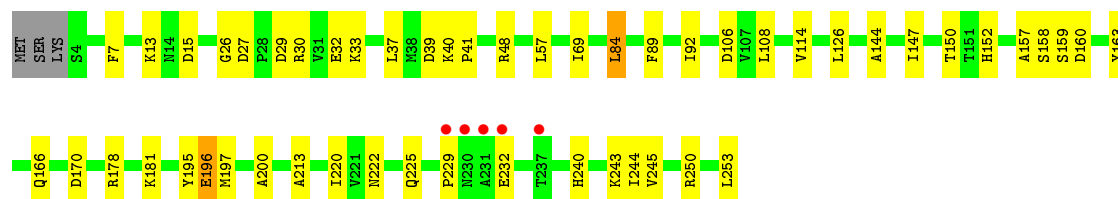
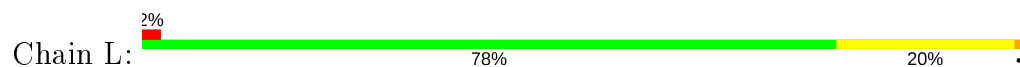
- Molecule 1: Uridine phosphorylase



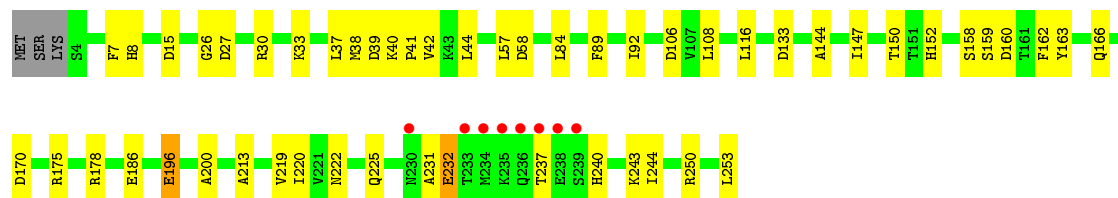
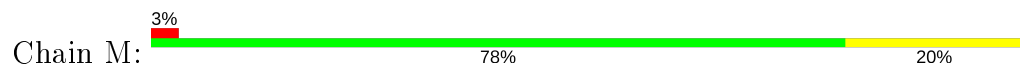
- Molecule 1: Uridine phosphorylase



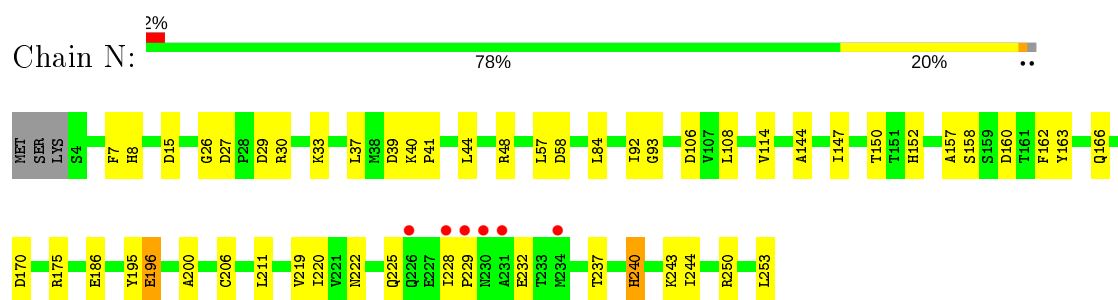
- Molecule 1: Uridine phosphorylase



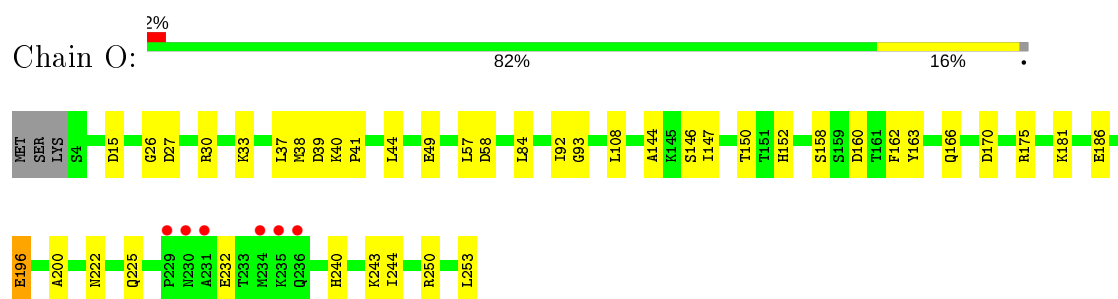
- Molecule 1: Uridine phosphorylase



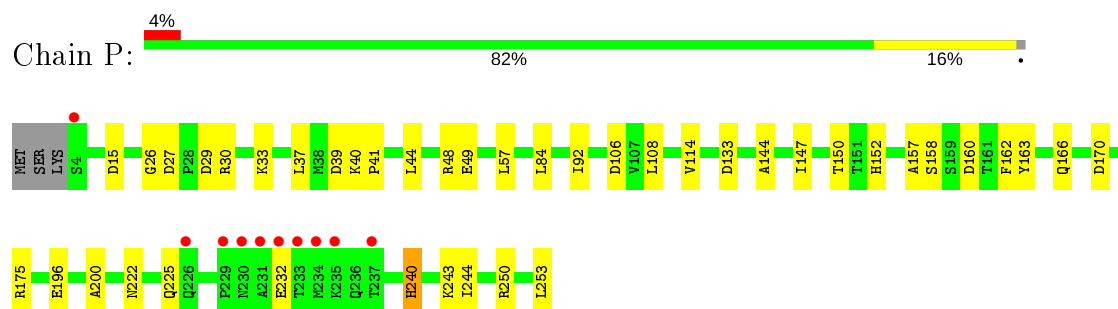
- Molecule 1: Uridine phosphorylase



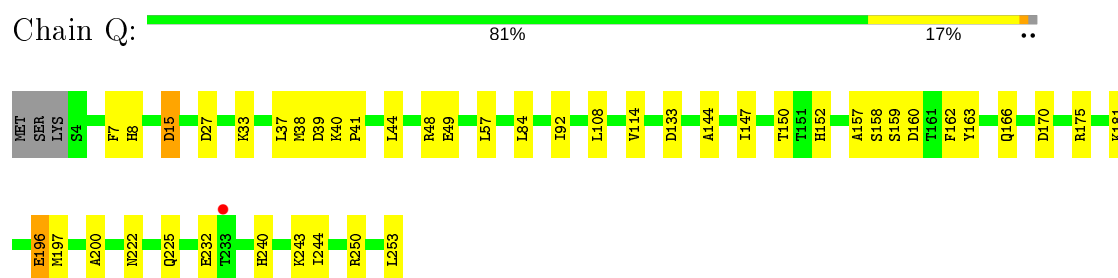
- Molecule 1: Uridine phosphorylase



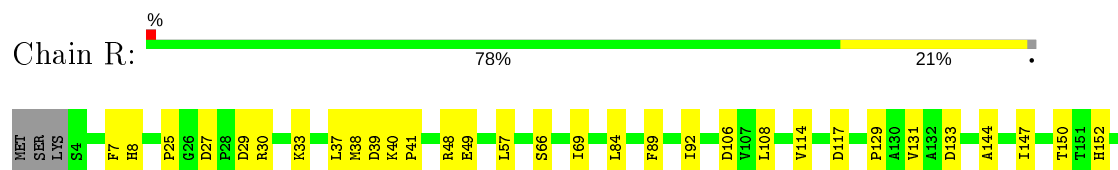
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	156.24Å 97.66Å 161.45Å 90.00° 118.23° 90.00°	Depositor
Resolution (Å)	25.00 – 3.10 24.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (25.00-3.10) 97.5 (24.92-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.212 , 0.229 0.193 , 0.210	Depositor DCC
R_{free} test set	3824 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.001 for -h-l,k,h 0.001 for l,k,-h-l 0.021 for h,-k,-h-l 0.006 for -h-l,-k,l 0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35307	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4850e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, THM

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	0.48	0/1912	0.74	3/2595 (0.1%)
1	B	0.51	0/1912	0.75	7/2595 (0.3%)
1	C	0.55	0/1912	0.77	8/2595 (0.3%)
1	D	0.49	0/1912	0.75	5/2595 (0.2%)
1	E	0.48	0/1912	0.74	6/2595 (0.2%)
1	F	0.45	0/1912	0.73	5/2595 (0.2%)
1	G	0.51	0/1912	0.75	7/2595 (0.3%)
1	H	0.51	0/1912	0.76	7/2595 (0.3%)
1	I	0.47	0/1912	0.74	6/2595 (0.2%)
1	J	0.48	0/1912	0.73	6/2595 (0.2%)
1	K	0.55	0/1912	0.75	6/2595 (0.2%)
1	L	0.56	0/1912	0.79	7/2595 (0.3%)
1	M	0.50	0/1912	0.75	6/2595 (0.2%)
1	N	0.49	0/1912	0.73	6/2595 (0.2%)
1	O	0.43	0/1912	0.72	4/2595 (0.2%)
1	P	0.42	0/1912	0.72	7/2595 (0.3%)
1	Q	0.47	0/1912	0.74	6/2595 (0.2%)
1	R	0.48	0/1912	0.76	8/2595 (0.3%)
All	All	0.49	0/34416	0.75	110/46710 (0.2%)

There are no bond length outliers.

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	27	ASP	CB-CG-OD2	9.17	126.55	118.30
1	L	27	ASP	CB-CG-OD2	8.77	126.19	118.30
1	O	27	ASP	CB-CG-OD2	8.64	126.07	118.30
1	I	27	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	27	ASP	CB-CG-OD2	8.38	125.84	118.30

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	1880	0	1884	22	2
1	B	1880	0	1884	21	0
1	C	1880	0	1884	22	1
1	D	1880	0	1884	23	1
1	E	1880	0	1884	19	0
1	F	1880	0	1884	28	0
1	G	1880	0	1884	20	1
1	H	1880	0	1884	19	9
1	I	1880	0	1884	19	0
1	J	1880	0	1884	16	0
1	K	1880	0	1884	23	0
1	L	1880	0	1885	21	9
1	M	1880	0	1884	24	1
1	N	1880	0	1884	22	0
1	O	1880	0	1884	23	0
1	P	1880	0	1884	14	0
1	Q	1880	0	1884	17	0
1	R	1880	0	1884	19	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	3	0
2	E	5	0	0	2	0
2	F	5	0	0	2	0
2	G	5	0	0	1	0
2	H	5	0	0	1	0
2	I	5	0	0	0	0
2	J	5	0	0	1	0
2	K	5	0	0	3	0
2	L	5	0	0	0	0
2	M	5	0	0	1	0
2	N	5	0	0	1	0
2	O	5	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
4	A	17	0	13	0	0
4	B	17	0	13	0	0
4	C	17	0	13	2	0
4	D	17	0	13	0	0
4	E	17	0	13	1	0
4	F	17	0	13	2	0
4	G	17	0	13	0	0
4	H	17	0	13	0	0
4	I	17	0	13	0	0
4	J	17	0	13	1	0
4	K	17	0	13	0	0
4	L	17	0	13	1	0
4	M	17	0	13	1	0
4	N	17	0	13	1	0
4	O	17	0	13	1	0
4	P	17	0	13	0	0
4	Q	17	0	13	1	0
4	R	17	0	13	0	0
5	A	59	0	0	0	0
5	B	57	0	0	0	0
5	C	62	0	0	0	1
5	D	57	0	0	0	0
5	E	59	0	0	0	0
5	F	58	0	0	0	1
5	G	59	0	0	0	0
5	H	57	0	0	0	0
5	I	60	0	0	1	0
5	J	59	0	0	0	0
5	K	58	0	0	0	0
5	L	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	60	0	0	1	0
5	N	60	0	0	1	2
5	O	58	0	0	0	0
5	P	59	0	0	0	0
5	Q	61	0	0	0	0
5	R	58	0	0	1	0
All	All	35307	0	34147	342	14

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 5.

The worst 5 of 342 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:K:39:ASP:OD2	1:M:42:VAL:CG1	1.76	1.34
1:F:32:GLU:OE2	1:O:146:SER:HA	1.25	1.33
1:F:32:GLU:OE2	1:O:146:SER:CA	1.78	1.32
1:F:32:GLU:OE2	1:O:146:SER:C	1.76	1.24
1:K:39:ASP:OD2	1:M:42:VAL:HG11	1.09	1.21

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232:GLU:CG	1:L:13:LYS:CE[2_657]	1.02	1.18
1:H:232:GLU:CG	1:L:13:LYS:NZ[2_657]	1.34	0.86
1:H:232:GLU:CB	1:L:13:LYS:CD[2_657]	1.35	0.85
1:H:232:GLU:CG	1:L:13:LYS:CD[2_657]	1.47	0.73
1:H:232:GLU:CB	1:L:13:LYS:CE[2_657]	1.68	0.52

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	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	34	69
1	B	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	34	69
1	C	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	34	69
1	D	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	34	69
1	E	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	34	69
1	F	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	34	69
1	G	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	34	69
1	H	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	34	69
1	I	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	34	69
1	J	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	34	69
1	K	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	34	69
1	L	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	34	69
1	M	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	34	69
1	N	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	34	69
1	O	248/253 (98%)	244 (98%)	3 (1%)	1 (0%)	34	69
1	P	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	34	69
1	Q	248/253 (98%)	244 (98%)	3 (1%)	1 (0%)	34	69
1	R	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	34	69
All	All	4464/4554 (98%)	4364 (98%)	82 (2%)	18 (0%)	34	69

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	TYR
1	L	163	TYR
1	A	163	TYR
1	C	163	TYR
1	D	163	TYR

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	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	B	201/204 (98%)	190 (94%)	11 (6%)	21	53
1	C	201/204 (98%)	190 (94%)	11 (6%)	21	53
1	D	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	E	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	F	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	G	201/204 (98%)	191 (95%)	10 (5%)	24	57
1	H	201/204 (98%)	188 (94%)	13 (6%)	17	47
1	I	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	J	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	K	201/204 (98%)	190 (94%)	11 (6%)	21	53
1	L	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	M	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	N	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	O	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	P	201/204 (98%)	190 (94%)	11 (6%)	21	53
1	Q	201/204 (98%)	189 (94%)	12 (6%)	19	49
1	R	201/204 (98%)	189 (94%)	12 (6%)	19	49
All	All	3618/3672 (98%)	3407 (94%)	211 (6%)	20	51

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	84	LEU
1	K	37	LEU
1	Q	196	GLU
1	I	150	THR
1	J	84	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	225	GLN
1	K	225	GLN
1	Q	226	GLN
1	I	226	GLN

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Mol	Chain	Res	Type
1	J	225	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 9 are monoatomic - leaving 36 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$
2	PO4	E	2051	-	4,4,4	0.80	0	6,6,6	0.58	0
2	PO4	M	2131	-	4,4,4	1.05	0	6,6,6	0.62	0
2	PO4	D	2041	-	4,4,4	1.08	0	6,6,6	0.44	0
4	THM	L	2122	-	15,18,18	2.16	3 (20%)	16,26,26	4.53	6 (37%)
4	THM	C	2032	-	15,18,18	2.41	3 (20%)	16,26,26	4.67	6 (37%)
4	THM	O	2152	-	15,18,18	2.23	3 (20%)	16,26,26	4.20	4 (25%)
4	THM	A	2012	-	15,18,18	2.26	3 (20%)	16,26,26	4.41	4 (25%)
2	PO4	B	2021	-	4,4,4	1.07	0	6,6,6	0.57	0
2	PO4	C	2031	-	4,4,4	0.84	0	6,6,6	0.59	0
4	THM	J	2102	-	15,18,18	2.56	3 (20%)	16,26,26	4.71	5 (31%)
4	THM	D	2042	-	15,18,18	2.36	3 (20%)	16,26,26	4.20	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	THM	G	2072	-	15,18,18	2.32	3 (20%)	16,26,26	4.19	5 (31%)
4	THM	N	2142	-	15,18,18	2.30	3 (20%)	16,26,26	4.27	6 (37%)
2	PO4	L	2121	-	4,4,4	0.88	0	6,6,6	0.54	0
4	THM	Q	2172	-	15,18,18	2.15	3 (20%)	16,26,26	4.49	5 (31%)
2	PO4	K	2111	-	4,4,4	1.00	0	6,6,6	0.60	0
4	THM	H	2082	-	15,18,18	2.35	3 (20%)	16,26,26	4.39	6 (37%)
2	PO4	I	2091	-	4,4,4	0.97	0	6,6,6	0.61	0
4	THM	P	2162	-	15,18,18	2.25	3 (20%)	16,26,26	4.37	6 (37%)
2	PO4	G	2071	-	4,4,4	0.88	0	6,6,6	0.61	0
2	PO4	R	2181	-	4,4,4	0.88	0	6,6,6	0.67	0
2	PO4	F	2061	-	4,4,4	1.00	0	6,6,6	0.78	0
4	THM	R	2182	-	15,18,18	2.34	3 (20%)	16,26,26	4.67	5 (31%)
2	PO4	A	2011	-	4,4,4	0.95	0	6,6,6	0.38	0
2	PO4	P	2161	-	4,4,4	0.87	0	6,6,6	0.44	0
2	PO4	J	2101	-	4,4,4	1.02	0	6,6,6	0.40	0
2	PO4	N	2141	-	4,4,4	0.83	0	6,6,6	0.59	0
4	THM	B	2022	-	15,18,18	2.15	3 (20%)	16,26,26	4.62	5 (31%)
4	THM	M	2132	-	15,18,18	2.30	3 (20%)	16,26,26	4.43	5 (31%)
4	THM	E	2052	-	15,18,18	2.17	3 (20%)	16,26,26	4.18	4 (25%)
4	THM	F	2062	-	15,18,18	2.13	3 (20%)	16,26,26	4.42	5 (31%)
4	THM	K	2112	-	15,18,18	2.29	3 (20%)	16,26,26	4.29	5 (31%)
2	PO4	Q	2171	-	4,4,4	0.95	0	6,6,6	0.50	0
4	THM	I	2092	-	15,18,18	2.56	3 (20%)	16,26,26	4.23	4 (25%)
2	PO4	H	2081	-	4,4,4	0.93	0	6,6,6	0.79	0
2	PO4	O	2151	-	4,4,4	1.01	0	6,6,6	0.49	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
4	THM	P	2162	-	1/1/3/3	1/3/18/18	0/2/2/2
4	THM	A	2012	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	J	2102	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	Q	2172	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	D	2042	-	1/1/3/3	1/3/18/18	0/2/2/2
4	THM	G	2072	-	1/1/3/3	0/3/18/18	0/2/2/2
4	THM	N	2142	-	1/1/3/3	2/3/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	THM	B	2022	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	O	2152	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	L	2122	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	C	2032	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	F	2062	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	K	2112	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	H	2082	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	R	2182	-	1/1/3/3	0/3/18/18	0/2/2/2
4	THM	I	2092	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	M	2132	-	1/1/3/3	2/3/18/18	0/2/2/2
4	THM	E	2052	-	1/1/3/3	2/3/18/18	0/2/2/2

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2102	THM	C4-N3	7.58	1.46	1.33
4	I	2092	THM	C4-N3	7.36	1.45	1.33
4	D	2042	THM	C4-N3	6.95	1.45	1.33
4	R	2182	THM	C4-N3	6.93	1.45	1.33
4	C	2032	THM	C4-N3	6.87	1.45	1.33

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	2182	THM	C2'-C1'-N1	15.17	149.27	114.27
4	J	2102	THM	C2'-C1'-N1	14.97	148.80	114.27
4	A	2012	THM	C2'-C1'-N1	14.71	148.19	114.27
4	L	2122	THM	C2'-C1'-N1	14.60	147.95	114.27
4	B	2022	THM	C2'-C1'-N1	14.60	147.94	114.27

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2022	THM	C1'
4	L	2122	THM	C1'
4	C	2032	THM	C1'
4	A	2012	THM	C1'
4	J	2102	THM	C1'

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	2172	THM	C3'-C4'-C5'-O5'
4	E	2052	THM	C3'-C4'-C5'-O5'
4	B	2022	THM	O4'-C4'-C5'-O5'
4	Q	2172	THM	O4'-C4'-C5'-O5'
4	E	2052	THM	O4'-C4'-C5'-O5'

There are no ring outliers.

23 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2051	PO4	2	0
2	M	2131	PO4	1	0
2	D	2041	PO4	3	0
4	L	2122	THM	1	0
4	C	2032	THM	2	0
4	O	2152	THM	1	0
2	B	2021	PO4	1	0
2	C	2031	PO4	1	0
4	J	2102	THM	1	0
4	N	2142	THM	1	0
4	Q	2172	THM	1	0
2	K	2111	PO4	3	0
2	G	2071	PO4	1	0
2	R	2181	PO4	1	0
2	F	2061	PO4	2	0
2	A	2011	PO4	1	0
2	J	2101	PO4	1	0
2	N	2141	PO4	1	0
4	M	2132	THM	1	0
4	E	2052	THM	1	0
4	F	2062	THM	2	0
2	H	2081	PO4	1	0
2	O	2151	PO4	3	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	250/253 (98%)	-0.40	7 (2%)	53	30	7, 22, 47, 73	0
1	B	250/253 (98%)	-0.53	4 (1%)	72	51	7, 22, 47, 73	0
1	C	250/253 (98%)	-0.46	4 (1%)	72	51	7, 22, 47, 73	0
1	D	250/253 (98%)	-0.46	6 (2%)	59	37	7, 22, 47, 73	0
1	E	250/253 (98%)	-0.38	8 (3%)	47	25	7, 22, 47, 73	0
1	F	250/253 (98%)	-0.32	9 (3%)	42	22	7, 22, 47, 73	0
1	G	250/253 (98%)	-0.47	6 (2%)	59	37	7, 22, 47, 73	0
1	H	250/253 (98%)	-0.47	7 (2%)	53	30	7, 22, 47, 73	0
1	I	250/253 (98%)	-0.41	4 (1%)	72	51	7, 22, 47, 73	0
1	J	250/253 (98%)	-0.33	6 (2%)	59	37	7, 22, 47, 73	0
1	K	250/253 (98%)	-0.56	4 (1%)	72	51	7, 22, 47, 73	0
1	L	250/253 (98%)	-0.49	5 (2%)	65	44	7, 22, 47, 73	0
1	M	250/253 (98%)	-0.35	8 (3%)	47	25	7, 22, 47, 73	0
1	N	250/253 (98%)	-0.35	6 (2%)	59	37	7, 22, 47, 73	0
1	O	250/253 (98%)	-0.29	6 (2%)	59	37	7, 22, 47, 73	0
1	P	250/253 (98%)	-0.22	10 (4%)	38	19	7, 22, 47, 73	0
1	Q	250/253 (98%)	-0.40	1 (0%)	92	84	7, 22, 47, 73	0
1	R	250/253 (98%)	-0.41	3 (1%)	79	61	7, 22, 47, 73	0
All	All	4500/4554 (98%)	-0.41	104 (2%)	60	39	7, 22, 48, 73	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	229	PRO	7.4
1	M	238	GLU	5.6
1	H	236	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	M	239	SER	5.2
1	N	231	ALA	5.1

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](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
2	PO4	P	2161	5/5	0.80	0.34	72,73,73,73	0
2	PO4	H	2081	5/5	0.82	0.33	76,76,77,77	0
3	K	Q	3008	1/1	0.83	0.14	70,70,70,70	0
2	PO4	E	2051	5/5	0.87	0.27	73,73,75,75	0
3	K	F	3003	1/1	0.89	0.07	54,54,54,54	0
3	K	O	3009	1/1	0.89	0.09	66,66,66,66	0
4	THM	C	2032	17/17	0.90	0.24	45,47,48,48	0
4	THM	P	2162	17/17	0.90	0.25	43,45,46,46	0
2	PO4	R	2181	5/5	0.90	0.24	69,70,70,71	0
4	THM	J	2102	17/17	0.91	0.24	37,43,44,45	0
2	PO4	N	2141	5/5	0.91	0.22	63,63,64,64	0
2	PO4	C	2031	5/5	0.91	0.27	74,74,74,75	0
4	THM	I	2092	17/17	0.92	0.22	45,46,48,48	0
2	PO4	J	2101	5/5	0.92	0.26	59,59,60,60	0
2	PO4	G	2071	5/5	0.92	0.26	77,77,77,77	0
4	THM	Q	2172	17/17	0.92	0.26	42,45,46,46	0
3	K	K	3006	1/1	0.93	0.05	28,28,28,28	0
4	THM	O	2152	17/17	0.93	0.26	44,47,48,50	0
3	K	C	3002	1/1	0.93	0.10	37,37,37,37	0
4	THM	M	2132	17/17	0.93	0.21	37,39,40,42	0
2	PO4	M	2131	5/5	0.93	0.29	77,77,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	THM	N	2142	17/17	0.93	0.22	53,54,54,55	0
2	PO4	O	2151	5/5	0.93	0.16	61,62,62,62	0
4	THM	F	2062	17/17	0.94	0.22	43,44,45,45	0
2	PO4	Q	2171	5/5	0.94	0.22	67,67,67,68	0
4	THM	L	2122	17/17	0.94	0.22	35,41,42,43	0
3	K	M	3007	1/1	0.94	0.08	50,50,50,50	0
4	THM	H	2082	17/17	0.94	0.20	40,42,44,45	0
4	THM	A	2012	17/17	0.95	0.23	41,42,43,45	0
4	THM	E	2052	17/17	0.95	0.23	38,40,44,45	0
4	THM	D	2042	17/17	0.95	0.16	44,46,49,51	0
4	THM	K	2112	17/17	0.95	0.21	36,43,44,45	0
3	K	I	3005	1/1	0.95	0.08	49,49,49,49	0
4	THM	G	2072	17/17	0.95	0.19	44,47,51,53	0
2	PO4	I	2091	5/5	0.95	0.15	48,48,48,48	0
3	K	G	3004	1/1	0.95	0.07	45,45,45,45	0
4	THM	R	2182	17/17	0.96	0.23	37,40,41,42	0
2	PO4	L	2121	5/5	0.96	0.14	61,61,61,61	0
4	THM	B	2022	17/17	0.96	0.16	42,44,45,45	0
2	PO4	F	2061	5/5	0.96	0.14	51,51,51,51	0
3	K	A	3001	1/1	0.97	0.05	40,40,40,40	0
2	PO4	B	2021	5/5	0.97	0.13	58,59,59,59	0
2	PO4	K	2111	5/5	0.97	0.15	65,65,65,65	0
2	PO4	D	2041	5/5	0.97	0.12	55,55,56,56	0
2	PO4	A	2011	5/5	0.97	0.13	69,69,69,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.