



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:05 PM GMT

PDB ID : 1RXC  
Title : E. COLI uridine phosphorylase: 5-fluorouracil ribose-1-phosphate complex  
Authors : Caradoc-Davies, T.T.; Cutfield, S.M.; Lamont, I.L.; Cutfield, J.F.  
Deposited on : 2003-12-18  
Resolution : 2.35 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

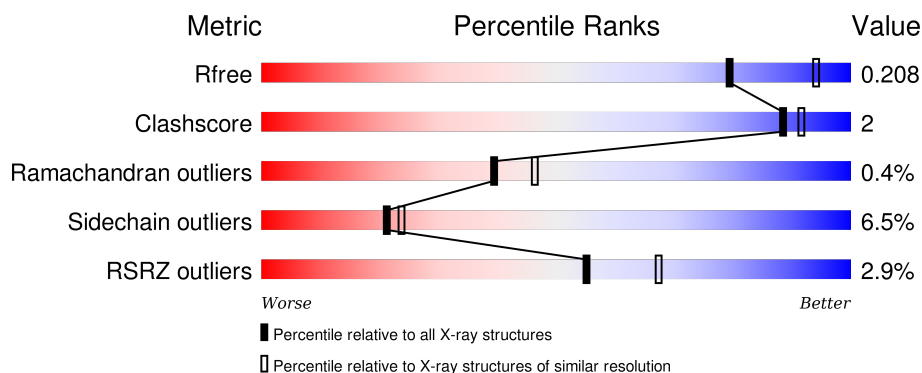
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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>4%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	B	253	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	C	253	<div> <div>4%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	D	253	<div> <div>4%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	E	253	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	253	
1	G	253	
1	H	253	
1	I	253	
1	J	253	
1	K	253	
1	L	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	R1P	B	2012	-	-	-	X
2	R1P	C	2082	-	-	-	X
2	R1P	D	2022	-	-	-	X
2	R1P	E	2032	-	-	-	X
2	R1P	F	2002	-	-	-	X
2	R1P	I	2042	-	-	-	X
2	R1P	K	2062	-	-	-	X
2	R1P	L	2072	-	-	-	X

## 2 Entry composition

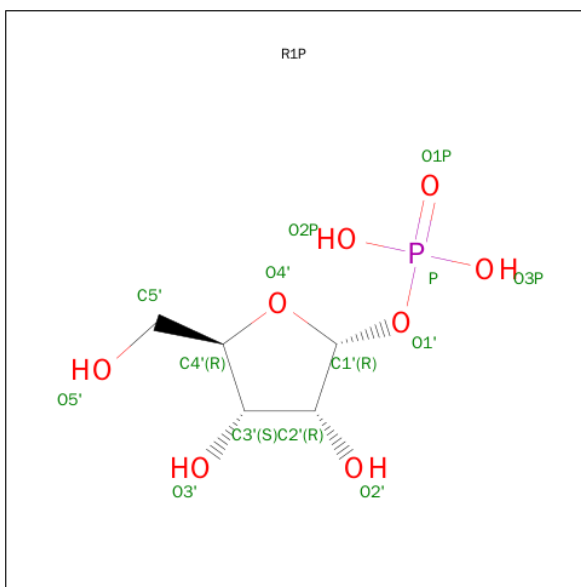
There are 7 unique types of molecules in this entry. The entry contains 23681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	246	Total	C	N	O	S	0	0	0
			1847	1158	323	356	10			
1	B	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	C	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	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	245	Total	C	N	O	S	0	0	0
			1839	1153	321	354	11			
1	H	240	Total	C	N	O	S	0	0	0
			1801	1130	315	346	10			
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	243	Total	C	N	O	S	0	0	0
			1822	1144	319	349	10			
1	L	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			

- Molecule 2 is SUGAR (ALPHA-D-RIBOSE-1-PHOSPHATE) (three-letter code: R1P) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	O	P	0	0
			14	5	8	1		
2	B	1	Total	C	O	P	0	0
			14	5	8	1		
2	D	1	Total	C	O	P	0	0
			14	5	8	1		
2	E	1	Total	C	O	P	0	0
			14	5	8	1		
2	I	1	Total	C	O	P	0	0
			14	5	8	1		
2	K	1	Total	C	O	P	0	0
			14	5	8	1		
2	L	1	Total	C	O	P	0	0
			14	5	8	1		
2	C	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

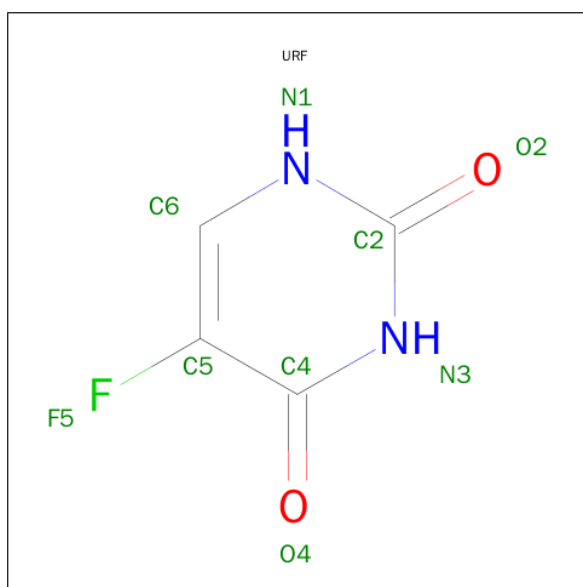


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

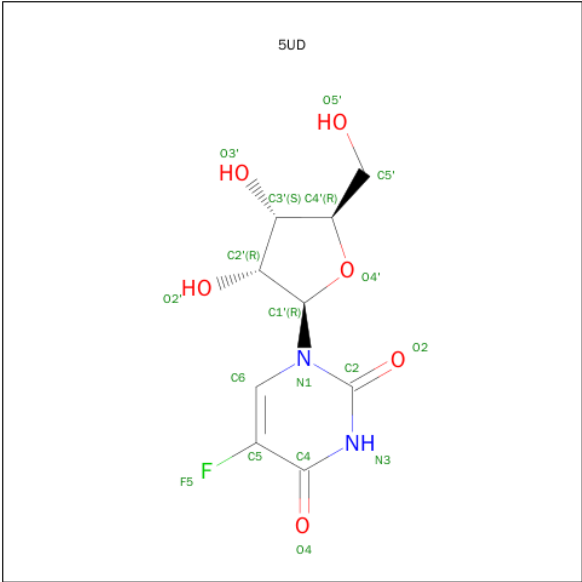
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	1	Total	K	0	0
			1	1		
4	I	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		

- Molecule 5 is 5-FLUOROURACIL (three-letter code: URF) (formula: C<sub>4</sub>H<sub>3</sub>FN<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
5	B	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
5	D	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
5	E	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
5	I	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
5	K	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
5	L	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
5	C	1	Total	C	F	N	O	0	0
			9	4	1	2	2		

- Molecule 6 is 5-FLUOROURIDINE (three-letter code: 5UD) (formula:  $C_9H_{11}FN_2O_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	J	1	Total	C	F	N	O	0	0
			18	9	1	2	6		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	90	Total	O	0	0
			90	90		
7	B	101	Total	O	0	0
			101	101		
7	C	85	Total	O	0	0
			85	85		
7	D	88	Total	O	0	0
			88	88		
7	E	98	Total	O	0	0
			98	98		
7	F	96	Total	O	0	0
			96	96		
7	G	89	Total	O	0	0
			89	89		
7	H	113	Total	O	0	0
			113	113		
7	I	95	Total	O	0	0
			95	95		
7	J	120	Total	O	0	0
			120	120		
7	K	90	Total	O	0	0
			90	90		

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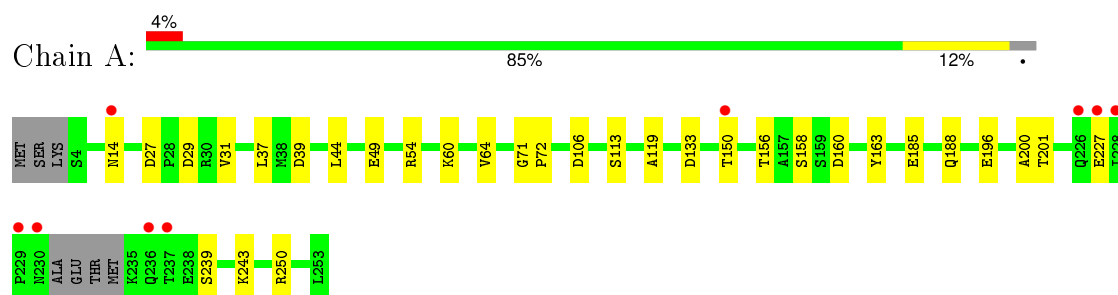
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	84	Total	O	0	0
			84	84		

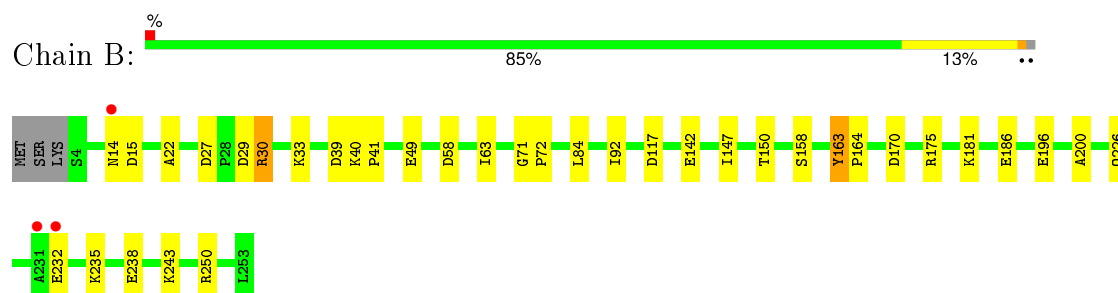
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

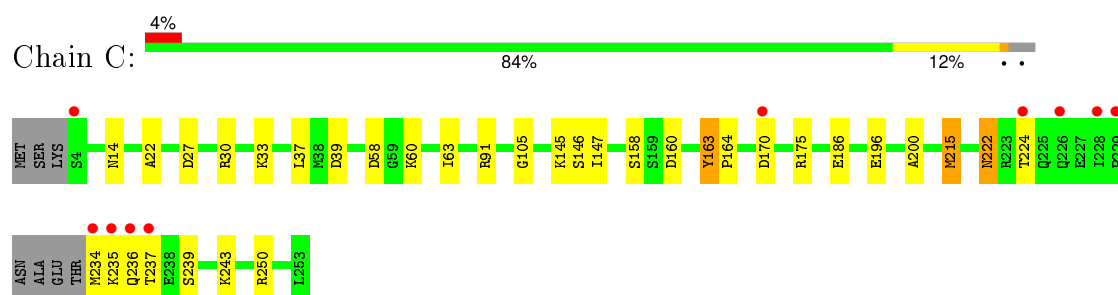
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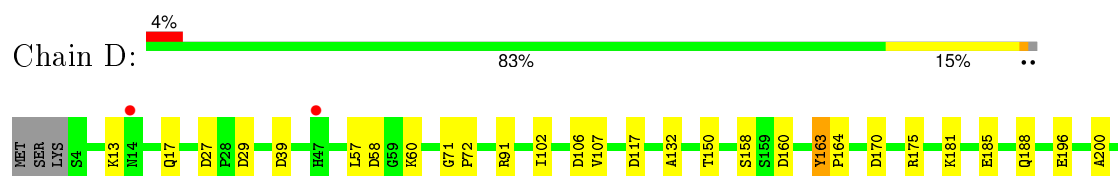
- Molecule 1: Uridine phosphorylase

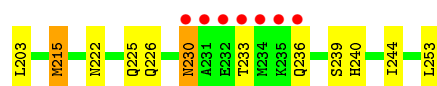


- Molecule 1: Uridine phosphorylase

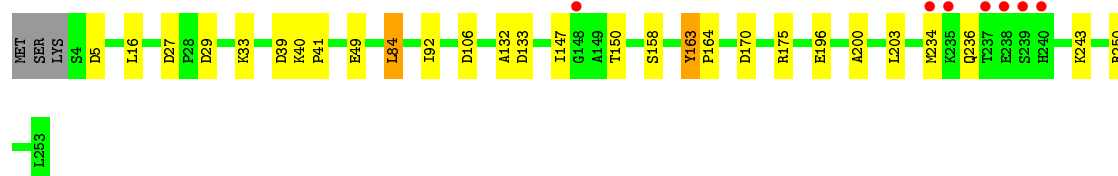
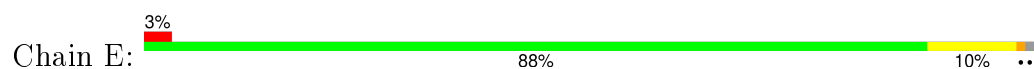


- Molecule 1: Uridine phosphorylase

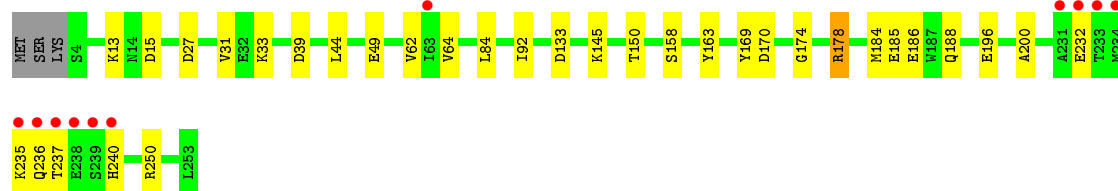
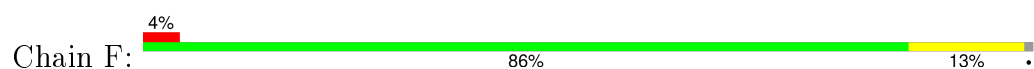




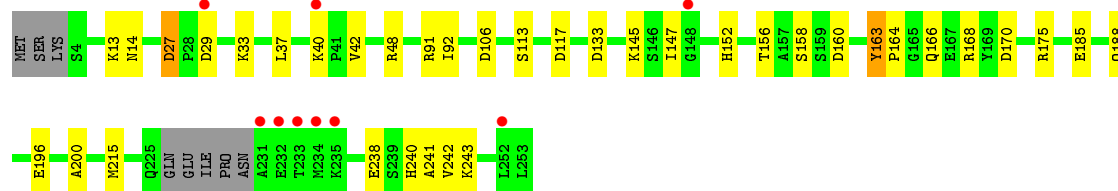
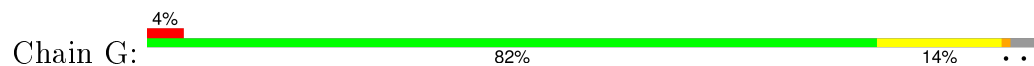
- Molecule 1: Uridine phosphorylase



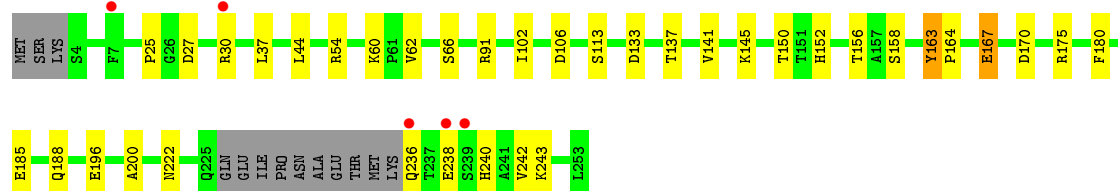
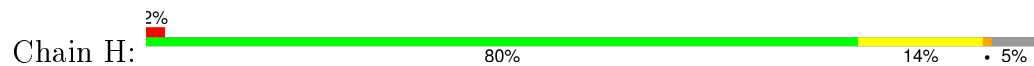
- Molecule 1: Uridine phosphorylase



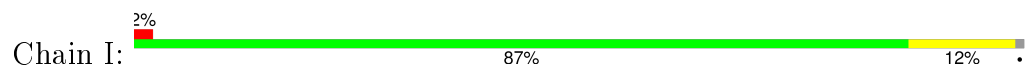
- Molecule 1: Uridine phosphorylase

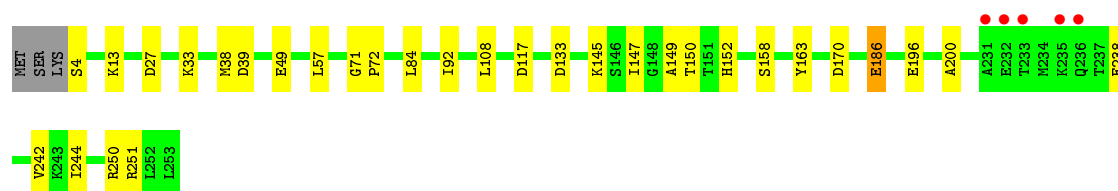


- Molecule 1: Uridine phosphorylase

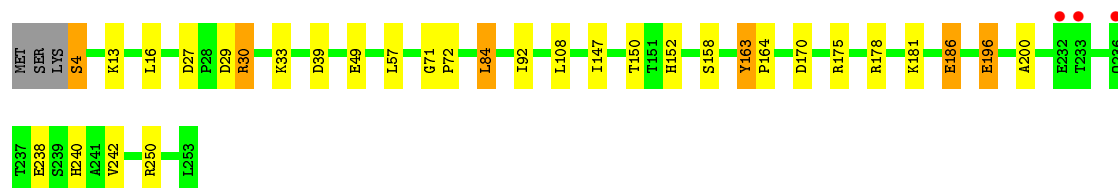
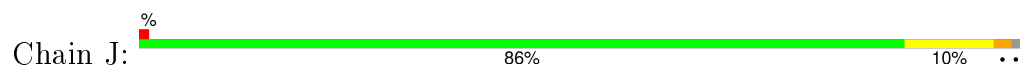


- Molecule 1: Uridine phosphorylase

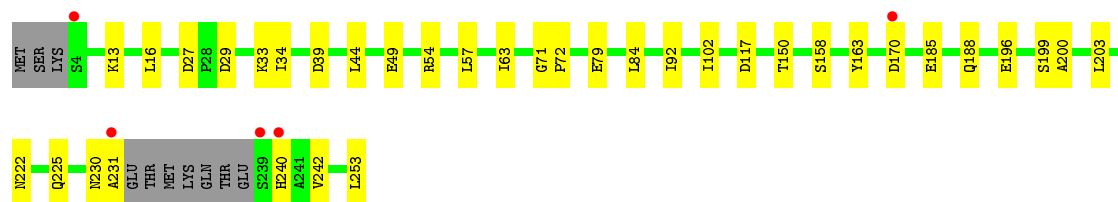
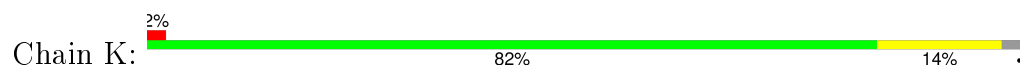




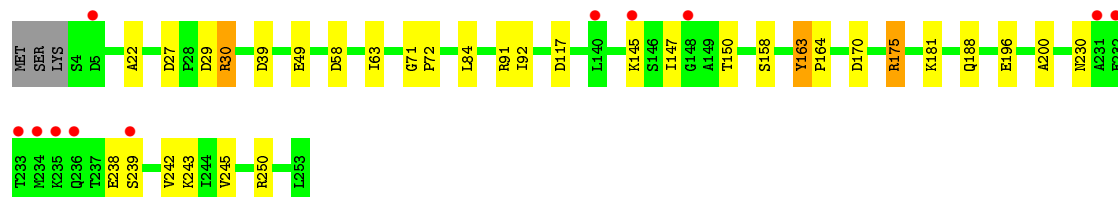
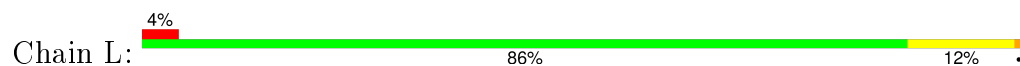
- Molecule 1: Uridine phosphorylase



- 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, $\alpha$ , $\beta$ , $\gamma$	90.19Å 191.70Å 91.91Å 90.00° 118.50° 90.00°	Depositor
Resolution (Å)	16.93 – 2.35 16.93 – 2.35	Depositor EDS
% Data completeness (in resolution range)	92.7 (16.93-2.35) 92.7 (16.93-2.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.150 , 0.203 0.161 , 0.208	Depositor DCC
$R_{free}$ test set	5294 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.8	EDS
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.015 for h,-k,-h-l 0.018 for -h-l,-k,l 0.019 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 105171 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: K, 5UD, URF, PO4, R1P

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	0.42	0/1878	0.74	6/2549 (0.2%)
1	B	0.43	0/1912	0.74	8/2595 (0.3%)
1	C	0.42	0/1882	0.73	4/2552 (0.2%)
1	D	0.42	0/1912	0.75	8/2595 (0.3%)
1	E	0.44	0/1912	0.74	7/2595 (0.3%)
1	F	0.42	0/1912	0.72	4/2595 (0.2%)
1	G	0.41	0/1869	0.73	7/2534 (0.3%)
1	H	0.43	0/1831	0.72	4/2484 (0.2%)
1	I	0.41	0/1912	0.74	5/2595 (0.2%)
1	J	0.44	0/1912	0.76	5/2595 (0.2%)
1	K	0.43	0/1853	0.74	4/2515 (0.2%)
1	L	0.40	0/1912	0.74	6/2595 (0.2%)
All	All	0.42	0/22697	0.74	68/30799 (0.2%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	27	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	106	ASP	CB-CG-OD2	7.04	124.64	118.30
1	D	170	ASP	CB-CG-OD2	7.01	124.61	118.30
1	B	117	ASP	CB-CG-OD2	6.80	124.42	118.30
1	D	27	ASP	CB-CG-OD2	6.72	124.35	118.30
1	J	39	ASP	CB-CG-OD2	6.70	124.33	118.30
1	C	27	ASP	CB-CG-OD2	6.70	124.33	118.30
1	I	27	ASP	CB-CG-OD2	6.63	124.27	118.30
1	J	27	ASP	CB-CG-OD2	6.55	124.19	118.30
1	H	170	ASP	CB-CG-OD2	6.54	124.18	118.30
1	K	39	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	27	ASP	CB-CG-OD2	6.49	124.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	27	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	160	ASP	CB-CG-OD2	6.26	123.93	118.30
1	F	27	ASP	CB-CG-OD2	6.25	123.93	118.30
1	E	170	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	29	ASP	CB-CG-OD2	6.16	123.84	118.30
1	F	170	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	160	ASP	CB-CG-OD2	6.08	123.77	118.30
1	L	39	ASP	CB-CG-OD2	6.02	123.72	118.30
1	L	170	ASP	CB-CG-OD2	6.01	123.71	118.30
1	I	133	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	58	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	133	ASP	CB-CG-OD2	5.99	123.69	118.30
1	G	160	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	27	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	160	ASP	CB-CG-OD2	5.94	123.64	118.30
1	K	27	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	170	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	39	ASP	CB-CG-OD2	5.84	123.56	118.30
1	G	117	ASP	CB-CG-OD2	5.84	123.56	118.30
1	L	58	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	39	ASP	CB-CG-OD2	5.82	123.54	118.30
1	K	117	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	15	ASP	CB-CG-OD2	5.75	123.48	118.30
1	D	117	ASP	CB-CG-OD2	5.71	123.44	118.30
1	F	39	ASP	CB-CG-OD2	5.67	123.41	118.30
1	J	29	ASP	CB-CG-OD2	5.67	123.40	118.30
1	J	170	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	39	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	106	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	27	ASP	CB-CG-OD2	5.56	123.30	118.30
1	I	39	ASP	CB-CG-OD2	5.54	123.29	118.30
1	E	39	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	133	ASP	CB-CG-OD2	5.51	123.26	118.30
1	G	106	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	29	ASP	CB-CG-OD2	5.45	123.20	118.30
1	H	106	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	39	ASP	CB-CG-OD2	5.40	123.16	118.30
1	I	117	ASP	CB-CG-OD2	5.39	123.15	118.30
1	J	30	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	G	29	ASP	CB-CG-OD2	5.34	123.10	118.30
1	F	133	ASP	CB-CG-OD2	5.33	123.09	118.30
1	D	106	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	133	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	170	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	58	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	30	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	I	170	ASP	CB-CG-OD2	5.18	122.96	118.30
1	L	117	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	29	ASP	CB-CG-OD2	5.11	122.90	118.30
1	E	5	ASP	CB-CG-OD2	5.10	122.89	118.30
1	G	133	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	29	ASP	CB-CG-OD2	5.07	122.86	118.30
1	G	170	ASP	CB-CG-OD2	5.04	122.84	118.30
1	L	29	ASP	CB-CG-OD2	5.02	122.82	118.30
1	K	29	ASP	CB-CG-OD2	5.01	122.81	118.30
1	G	27	ASP	CB-CG-OD2	5.00	122.81	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	1847	0	1845	8	0
1	B	1880	0	1884	8	0
1	C	1851	0	1859	10	0
1	D	1880	0	1884	11	0
1	E	1880	0	1884	6	0
1	F	1880	0	1884	9	0
1	G	1839	0	1846	9	0
1	H	1801	0	1806	12	0
1	I	1880	0	1884	11	0
1	J	1880	0	1884	11	0
1	K	1822	0	1827	13	0
1	L	1880	0	1884	9	0
2	B	14	0	8	0	0
2	C	14	0	8	0	0
2	D	14	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	14	0	8	0	0
2	F	14	0	8	0	0
2	I	14	0	8	0	0
2	K	14	0	8	0	0
2	L	14	0	8	0	0
3	J	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	B	9	0	3	0	0
5	C	9	0	3	0	0
5	D	9	0	3	0	0
5	E	9	0	3	0	0
5	F	9	0	3	0	0
5	I	9	0	3	0	0
5	K	9	0	3	0	0
5	L	9	0	3	0	0
6	J	18	0	10	0	0
7	A	90	0	0	0	0
7	B	101	0	0	1	0
7	C	85	0	0	0	0
7	D	88	0	0	0	0
7	E	98	0	0	0	0
7	F	96	0	0	1	0
7	G	89	0	0	2	0
7	H	113	0	0	2	0
7	I	95	0	0	2	0
7	J	120	0	0	3	0
7	K	90	0	0	1	0
7	L	84	0	0	0	0
All	All	23681	0	22469	111	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 2.

All (111) 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:G:185:GLU:HA	1:G:188:GLN:HE21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ASP:OD2	1:C:250:ARG:HD3	1.87	0.73
7:G:310:HOH:O	1:I:186:GLU:HG3	1.92	0.68
1:G:152:HIS:HD2	7:G:335:HOH:O	1.80	0.65
1:K:170:ASP:HB2	7:K:1147:HOH:O	1.99	0.63
1:K:185:GLU:HA	1:K:188:GLN:HE21	1.64	0.62
1:A:185:GLU:HA	1:A:188:GLN:HE21	1.63	0.62
1:C:222:ASN:HD22	1:C:224:THR:H	1.47	0.62
1:J:186:GLU:OE1	7:J:2154:HOH:O	2.16	0.60
1:H:152:HIS:HD2	7:H:354:HOH:O	1.86	0.57
1:D:226:GLN:HE22	1:D:230:ASN:HD22	1.53	0.57
1:H:185:GLU:HA	1:H:188:GLN:HE21	1.70	0.56
1:E:158:SER:HB3	1:E:200:ALA:HB2	1.88	0.56
1:C:105:GLY:HA2	1:C:237:THR:OG1	2.08	0.54
1:D:102:ILE:O	1:D:222:ASN:ND2	2.40	0.54
1:F:185:GLU:HA	1:F:188:GLN:HE21	1.73	0.54
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.88	0.54
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.89	0.54
1:D:181:LYS:O	1:F:178:ARG:NH2	2.42	0.53
1:D:185:GLU:HA	1:D:188:GLN:HE21	1.73	0.52
1:J:108:LEU:HD22	1:J:152:HIS:HB2	1.91	0.52
1:I:158:SER:HB3	1:I:200:ALA:HB2	1.91	0.52
1:E:16:LEU:HD22	1:E:84:LEU:HB3	1.91	0.52
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.92	0.52
1:K:158:SER:HB3	1:K:200:ALA:HB2	1.90	0.52
1:C:91:ARG:HB3	1:C:215:MET:HG2	1.91	0.52
1:A:158:SER:HB3	1:A:200:ALA:HB2	1.91	0.51
1:G:91:ARG:HG2	1:G:215:MET:SD	2.50	0.51
1:J:158:SER:HB3	1:J:200:ALA:HB2	1.93	0.50
1:G:92:ILE:HD11	1:G:241:ALA:HB1	1.92	0.50
1:A:31:VAL:HG13	1:A:64:VAL:HG12	1.94	0.50
1:C:222:ASN:ND2	1:C:224:THR:H	2.11	0.49
1:L:30:ARG:HD3	1:L:238:GLU:OE2	2.12	0.49
1:H:152:HIS:CD2	7:H:354:HOH:O	2.64	0.49
1:C:58:ASP:OD2	1:C:250:ARG:CD	2.58	0.49
1:F:184:MET:O	1:F:188:GLN:HG3	2.13	0.48
1:K:44:LEU:HD11	1:K:54:ARG:HB2	1.95	0.48
1:E:49:GLU:HB3	1:F:49:GLU:HB3	1.96	0.48
1:I:251:ARG:HD3	7:I:2193:HOH:O	2.13	0.47
1:L:238:GLU:O	1:L:242:VAL:HG23	2.13	0.47
1:G:163:TYR:HB2	1:G:164:PRO:CD	2.45	0.47
1:B:163:TYR:HB2	1:B:164:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:GLU:O	1:J:242:VAL:HG23	2.15	0.47
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.97	0.46
1:I:238:GLU:O	1:I:242:VAL:HG23	2.15	0.46
1:K:230:ASN:O	1:K:231:ALA:CB	2.63	0.46
1:J:4:SER:N	7:J:2066:HOH:O	2.47	0.46
1:B:30:ARG:HD3	1:B:238:GLU:OE1	2.16	0.46
1:A:119:ALA:HB3	1:A:201:THR:OG1	2.16	0.46
1:H:158:SER:HB3	1:H:200:ALA:HB2	1.97	0.46
1:G:238:GLU:O	1:G:242:VAL:HG23	2.16	0.46
1:G:166:GLN:NE2	1:G:168:ARG:HH12	2.12	0.46
1:I:38:MET:HG2	1:I:57:LEU:HD13	1.98	0.46
1:A:71:GLY:N	1:A:72:PRO:CD	2.78	0.46
1:G:158:SER:HB3	1:G:200:ALA:HB2	1.98	0.45
1:F:15:ASP:HB3	1:F:44:LEU:HD13	1.98	0.45
1:A:113:SER:HA	1:A:156:THR:O	2.17	0.45
1:J:71:GLY:N	1:J:72:PRO:CD	2.79	0.45
1:B:71:GLY:N	1:B:72:PRO:CD	2.80	0.45
1:I:147:ILE:HD11	1:I:244:ILE:HD11	1.98	0.45
1:H:44:LEU:HD11	1:H:54:ARG:HB2	1.98	0.45
1:J:30:ARG:HD3	1:J:238:GLU:OE2	2.16	0.44
1:J:16:LEU:HD22	1:J:84:LEU:HB3	2.00	0.44
1:H:163:TYR:HB2	1:H:164:PRO:CD	2.47	0.44
1:H:238:GLU:O	1:H:242:VAL:HG23	2.18	0.44
1:B:22:ALA:HA	1:B:63:ILE:O	2.18	0.44
1:K:199:SER:O	1:K:203:LEU:HG	2.17	0.44
1:J:158:SER:HA	1:J:196:GLU:O	2.18	0.44
1:I:147:ILE:HD11	1:I:149:ALA:HB2	1.99	0.44
1:H:102:ILE:O	1:H:222:ASN:ND2	2.48	0.43
1:K:57:LEU:HB3	1:K:253:LEU:HD11	2.00	0.43
1:A:49:GLU:HB3	1:B:49:GLU:HB3	1.99	0.43
1:D:163:TYR:HB2	1:D:164:PRO:CD	2.48	0.43
1:E:132:ALA:HA	1:E:203:LEU:HD22	1.99	0.43
1:H:113:SER:HA	1:H:156:THR:O	2.17	0.43
1:K:71:GLY:N	1:K:72:PRO:CD	2.81	0.43
1:K:16:LEU:HG	1:K:63:ILE:HD11	2.01	0.43
1:C:163:TYR:HB2	1:C:164:PRO:CD	2.48	0.43
1:K:34:ILE:HG12	1:K:242:VAL:HG13	2.01	0.43
1:C:163:TYR:CB	1:C:164:PRO:CD	2.97	0.43
1:H:167:GLU:HG3	1:H:180:PHE:O	2.18	0.43
1:H:137:THR:O	1:H:141:VAL:HG23	2.19	0.43
1:B:14:ASN:HB2	7:B:2097:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD11	1:A:54:ARG:HB2	2.00	0.42
1:B:40:LYS:N	1:B:41:PRO:CD	2.82	0.42
1:I:108:LEU:HD22	1:I:152:HIS:HB2	2.01	0.42
1:E:40:LYS:N	1:E:41:PRO:CD	2.82	0.42
1:F:237:THR:HG22	7:F:2097:HOH:O	2.20	0.42
1:J:163:TYR:HB2	1:J:164:PRO:CD	2.49	0.42
1:K:79:GLU:HG2	1:L:163:TYR:CD2	2.55	0.42
1:D:91:ARG:HB3	1:D:215:MET:HG2	2.01	0.42
1:L:163:TYR:HB2	1:L:164:PRO:CD	2.50	0.42
1:D:71:GLY:N	1:D:72:PRO:CD	2.82	0.42
1:K:102:ILE:O	1:K:222:ASN:ND2	2.53	0.41
1:K:49:GLU:HB3	1:L:49:GLU:HB3	2.02	0.41
1:D:107:VAL:HG11	1:D:244:ILE:HD13	2.02	0.41
1:L:71:GLY:N	1:L:72:PRO:CD	2.83	0.41
1:C:22:ALA:HA	1:C:63:ILE:O	2.20	0.41
1:D:57:LEU:HB3	1:D:253:LEU:HD11	2.02	0.41
1:F:169:TYR:O	1:F:174:GLY:HA2	2.20	0.41
1:D:132:ALA:HA	1:D:203:LEU:HD22	2.03	0.41
1:I:71:GLY:N	1:I:72:PRO:CD	2.82	0.41
1:L:22:ALA:HA	1:L:63:ILE:O	2.21	0.41
1:F:31:VAL:HG13	1:F:64:VAL:HG12	2.01	0.41
7:J:2154:HOH:O	1:L:175:ARG:HD2	2.21	0.41
1:E:163:TYR:HB2	1:E:164:PRO:CD	2.51	0.41
1:I:4:SER:N	7:I:2167:HOH:O	2.54	0.41
1:H:25:PRO:O	1:H:66:SER:HA	2.21	0.40
1:L:158:SER:HB3	1:L:200:ALA:HB2	2.03	0.40
1:G:113:SER:HA	1:G:156:THR:O	2.22	0.40
1:I:49:GLU:HB3	1:J:49:GLU:HB3	2.03	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	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	39	46
1	B	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	39	46
1	C	242/253 (96%)	232 (96%)	9 (4%)	1 (0%)	39	46
1	D	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	39	46
1	E	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	39	46
1	F	248/253 (98%)	244 (98%)	3 (1%)	1 (0%)	39	46
1	G	241/253 (95%)	235 (98%)	5 (2%)	1 (0%)	39	46
1	H	236/253 (93%)	234 (99%)	1 (0%)	1 (0%)	39	46
1	I	248/253 (98%)	245 (99%)	2 (1%)	1 (0%)	39	46
1	J	248/253 (98%)	245 (99%)	2 (1%)	1 (0%)	39	46
1	K	239/253 (94%)	233 (98%)	5 (2%)	1 (0%)	39	46
1	L	248/253 (98%)	245 (99%)	2 (1%)	1 (0%)	39	46
All	All	2936/3036 (97%)	2877 (98%)	47 (2%)	12 (0%)	39	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	163	TYR
1	C	163	TYR
1	F	163	TYR
1	G	163	TYR
1	I	163	TYR
1	J	163	TYR
1	K	163	TYR
1	L	163	TYR
1	A	163	TYR
1	D	163	TYR
1	H	163	TYR
1	B	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	197/204 (97%)	188 (95%)	9 (5%)	33	42
1	B	201/204 (98%)	186 (92%)	15 (8%)	17	18
1	C	198/204 (97%)	180 (91%)	18 (9%)	12	11
1	D	201/204 (98%)	188 (94%)	13 (6%)	21	24
1	E	201/204 (98%)	190 (94%)	11 (6%)	27	32
1	F	201/204 (98%)	186 (92%)	15 (8%)	17	18
1	G	196/204 (96%)	182 (93%)	14 (7%)	18	20
1	H	192/204 (94%)	179 (93%)	13 (7%)	20	22
1	I	201/204 (98%)	192 (96%)	9 (4%)	34	43
1	J	201/204 (98%)	186 (92%)	15 (8%)	17	18
1	K	194/204 (95%)	186 (96%)	8 (4%)	37	48
1	L	201/204 (98%)	185 (92%)	16 (8%)	15	16
All	All	2384/2448 (97%)	2228 (94%)	156 (6%)	21	24

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	37	LEU
1	A	60	LYS
1	A	150	THR
1	A	196	GLU
1	A	227	GLU
1	A	239	SER
1	A	243	LYS
1	A	250	ARG
1	B	33	LYS
1	B	84	LEU
1	B	92	ILE
1	B	142	GLU
1	B	147	ILE
1	B	150	THR
1	B	175	ARG
1	B	181	LYS
1	B	186	GLU
1	B	196	GLU
1	B	226	GLN
1	B	232	GLU
1	B	235	LYS

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Mol	Chain	Res	Type
1	B	243	LYS
1	B	250	ARG
1	C	14	ASN
1	C	30	ARG
1	C	33	LYS
1	C	37	LEU
1	C	60	LYS
1	C	145	LYS
1	C	146	SER
1	C	147	ILE
1	C	175	ARG
1	C	186	GLU
1	C	196	GLU
1	C	215	MET
1	C	222	ASN
1	C	234	MET
1	C	235	LYS
1	C	236	GLN
1	C	239	SER
1	C	243	LYS
1	D	13	LYS
1	D	17	GLN
1	D	60	LYS
1	D	150	THR
1	D	175	ARG
1	D	196	GLU
1	D	215	MET
1	D	225	GLN
1	D	230	ASN
1	D	233	THR
1	D	236	GLN
1	D	239	SER
1	D	240	HIS
1	E	33	LYS
1	E	84	LEU
1	E	92	ILE
1	E	147	ILE
1	E	150	THR
1	E	175	ARG
1	E	196	GLU
1	E	234	MET
1	E	236	GLN

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Mol	Chain	Res	Type
1	E	243	LYS
1	E	250	ARG
1	F	13	LYS
1	F	33	LYS
1	F	62	VAL
1	F	84	LEU
1	F	92	ILE
1	F	145	LYS
1	F	150	THR
1	F	178	ARG
1	F	186	GLU
1	F	196	GLU
1	F	232	GLU
1	F	235	LYS
1	F	236	GLN
1	F	240	HIS
1	F	250	ARG
1	G	13	LYS
1	G	14	ASN
1	G	27	ASP
1	G	33	LYS
1	G	37	LEU
1	G	40	LYS
1	G	42	VAL
1	G	48	ARG
1	G	145	LYS
1	G	147	ILE
1	G	175	ARG
1	G	196	GLU
1	G	240	HIS
1	G	243	LYS
1	H	30	ARG
1	H	37	LEU
1	H	60	LYS
1	H	62	VAL
1	H	91	ARG
1	H	145	LYS
1	H	150	THR
1	H	167	GLU
1	H	175	ARG
1	H	196	GLU
1	H	236	GLN

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Mol	Chain	Res	Type
1	H	240	HIS
1	H	243	LYS
1	I	13	LYS
1	I	33	LYS
1	I	84	LEU
1	I	92	ILE
1	I	145	LYS
1	I	150	THR
1	I	186	GLU
1	I	196	GLU
1	I	250	ARG
1	J	4	SER
1	J	13	LYS
1	J	33	LYS
1	J	57	LEU
1	J	84	LEU
1	J	92	ILE
1	J	147	ILE
1	J	150	THR
1	J	175	ARG
1	J	178	ARG
1	J	181	LYS
1	J	186	GLU
1	J	196	GLU
1	J	240	HIS
1	J	250	ARG
1	K	13	LYS
1	K	33	LYS
1	K	84	LEU
1	K	92	ILE
1	K	150	THR
1	K	196	GLU
1	K	225	GLN
1	K	240	HIS
1	L	30	ARG
1	L	84	LEU
1	L	91	ARG
1	L	92	ILE
1	L	145	LYS
1	L	147	ILE
1	L	150	THR
1	L	175	ARG

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Mol	Chain	Res	Type
1	L	181	LYS
1	L	188	GLN
1	L	196	GLU
1	L	230	ASN
1	L	239	SER
1	L	243	LYS
1	L	245	VAL
1	L	250	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	152	HIS
1	A	166	GLN
1	A	188	GLN
1	A	225	GLN
1	A	226	GLN
1	C	188	GLN
1	C	222	ASN
1	D	188	GLN
1	D	230	ASN
1	E	188	GLN
1	F	188	GLN
1	F	225	GLN
1	F	236	GLN
1	G	103	ASN
1	G	166	GLN
1	G	188	GLN
1	G	225	GLN
1	H	14	ASN
1	H	17	GLN
1	H	103	ASN
1	H	152	HIS
1	H	166	GLN
1	H	188	GLN
1	H	225	GLN
1	I	14	ASN
1	I	188	GLN
1	I	226	GLN
1	J	236	GLN
1	K	188	GLN

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Mol	Chain	Res	Type
1	K	225	GLN
1	L	226	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 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$
5	URF	B	2011	-	5,9,9	3.54	1 (20%)	5,12,12	6.24	4 (80%)
2	R1P	B	2012	-	13,14,14	0.61	0	18,21,21	4.75	8 (44%)
5	URF	C	2081	-	5,9,9	3.80	1 (20%)	5,12,12	6.41	4 (80%)
2	R1P	C	2082	-	13,14,14	0.66	0	18,21,21	4.95	9 (50%)
5	URF	D	2021	-	5,9,9	3.75	1 (20%)	5,12,12	6.08	4 (80%)
2	R1P	D	2022	-	13,14,14	0.66	0	18,21,21	4.60	9 (50%)
5	URF	E	2031	-	5,9,9	3.39	1 (20%)	5,12,12	6.92	4 (80%)
2	R1P	E	2032	-	13,14,14	0.55	0	18,21,21	4.92	10 (55%)
5	URF	F	2001	-	5,9,9	3.23	1 (20%)	5,12,12	6.52	4 (80%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	R1P	F	2002	-	13,14,14	0.68	0	18,21,21	4.91	8 (44%)
5	URF	I	2041	-	5,9,9	3.83	1 (20%)	5,12,12	6.55	5 (100%)
2	R1P	I	2042	-	13,14,14	0.78	0	18,21,21	4.78	8 (44%)
6	5UD	J	2051	-	14,19,19	2.40	2 (14%)	13,28,28	4.17	11 (84%)
3	PO4	J	2052	-	4,4,4	0.45	0	6,6,6	0.28	0
5	URF	K	2061	-	5,9,9	3.16	1 (20%)	5,12,12	6.77	4 (80%)
2	R1P	K	2062	-	13,14,14	0.65	0	18,21,21	4.71	9 (50%)
5	URF	L	2071	-	5,9,9	3.41	1 (20%)	5,12,12	6.30	4 (80%)
2	R1P	L	2072	-	13,14,14	0.65	0	18,21,21	4.53	9 (50%)

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
5	URF	B	2011	-	-	0/0/0/0	0/1/1/1
2	R1P	B	2012	-	-	0/6/23/23	0/1/1/1
5	URF	C	2081	-	-	0/0/0/0	0/1/1/1
2	R1P	C	2082	-	-	0/6/23/23	0/1/1/1
5	URF	D	2021	-	-	0/0/0/0	0/1/1/1
2	R1P	D	2022	-	-	0/6/23/23	0/1/1/1
5	URF	E	2031	-	-	0/0/0/0	0/1/1/1
2	R1P	E	2032	-	-	0/6/23/23	0/1/1/1
5	URF	F	2001	-	-	0/0/0/0	0/1/1/1
2	R1P	F	2002	-	-	0/6/23/23	0/1/1/1
5	URF	I	2041	-	-	0/0/0/0	0/1/1/1
2	R1P	I	2042	-	-	0/6/23/23	0/1/1/1
6	5UD	J	2051	-	-	0/2/22/22	0/2/2/2
3	PO4	J	2052	-	-	0/0/0/0	0/0/0/0
5	URF	K	2061	-	-	0/0/0/0	0/1/1/1
2	R1P	K	2062	-	-	0/6/23/23	0/1/1/1
5	URF	L	2071	-	-	0/0/0/0	0/1/1/1
2	R1P	L	2072	-	-	0/6/23/23	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	2051	5UD	C6-C5	2.39	1.42	1.38
5	K	2061	URF	C4-C5	6.99	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2001	URF	C4-C5	7.07	1.47	1.38
5	L	2071	URF	C4-C5	7.57	1.47	1.38
5	E	2031	URF	C4-C5	7.58	1.47	1.38
5	B	2011	URF	C4-C5	7.62	1.47	1.38
6	J	2051	5UD	C4-C5	8.32	1.48	1.38
5	D	2021	URF	C4-C5	8.33	1.48	1.38
5	C	2081	URF	C4-C5	8.41	1.48	1.38
5	I	2041	URF	C4-C5	8.49	1.49	1.38

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2032	R1P	O4'-C1'-C2'	-12.75	86.87	104.78
2	F	2002	R1P	O4'-C1'-C2'	-12.65	87.01	104.78
2	C	2082	R1P	O4'-C1'-C2'	-12.26	87.55	104.78
5	E	2031	URF	N1-C2-N3	-12.15	120.58	128.33
5	K	2061	URF	N1-C2-N3	-12.05	120.65	128.33
5	F	2001	URF	N1-C2-N3	-11.72	120.86	128.33
2	K	2062	R1P	O4'-C1'-C2'	-11.69	88.36	104.78
2	B	2012	R1P	O4'-C1'-C2'	-11.65	88.42	104.78
5	I	2041	URF	N1-C2-N3	-11.49	121.00	128.33
5	L	2071	URF	N1-C2-N3	-11.40	121.06	128.33
2	I	2042	R1P	O4'-C1'-C2'	-11.35	88.84	104.78
5	C	2081	URF	N1-C2-N3	-11.19	121.19	128.33
2	D	2022	R1P	O4'-C1'-C2'	-10.99	89.35	104.78
2	L	2072	R1P	O4'-C1'-C2'	-10.81	89.60	104.78
5	D	2021	URF	N1-C2-N3	-10.72	121.49	128.33
5	B	2011	URF	N1-C2-N3	-10.60	121.57	128.33
6	J	2051	5UD	C5-C4-N3	-5.95	115.71	122.34
5	B	2011	URF	C5-C4-N3	-4.50	117.33	122.34
6	J	2051	5UD	O3'-C3'-C4'	-3.68	100.03	111.05
5	I	2041	URF	C5-C4-N3	-3.60	118.33	122.34
5	C	2081	URF	C5-C4-N3	-3.58	118.35	122.34
5	F	2001	URF	C5-C4-N3	-3.55	118.39	122.34
5	K	2061	URF	C5-C4-N3	-3.49	118.45	122.34
5	E	2031	URF	C5-C4-N3	-3.38	118.57	122.34
5	D	2021	URF	C5-C4-N3	-3.03	118.97	122.34
5	L	2071	URF	C5-C4-N3	-2.94	119.07	122.34
2	E	2032	R1P	O3'-C3'-C4'	-2.77	102.74	111.05
2	L	2072	R1P	O3'-C3'-C4'	-2.77	102.75	111.05
6	J	2051	5UD	F5-C5-C4	-2.71	113.53	118.56
6	J	2051	5UD	O4'-C4'-C3'	-2.65	99.80	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2082	R1P	O3'-C3'-C4'	-2.64	103.13	111.05
2	F	2002	R1P	O3'-C3'-C4'	-2.64	103.13	111.05
2	I	2042	R1P	O1'-P-O1P	-2.62	100.57	107.11
2	K	2062	R1P	O3'-C3'-C4'	-2.61	103.22	111.05
2	D	2022	R1P	O3'-C3'-C4'	-2.51	103.53	111.05
2	I	2042	R1P	O3'-C3'-C4'	-2.44	103.73	111.05
2	F	2002	R1P	O4'-C4'-C3'	-2.37	100.38	105.15
2	E	2032	R1P	O4'-C4'-C3'	-2.36	100.39	105.15
2	C	2082	R1P	O4'-C4'-C3'	-2.33	100.44	105.15
2	E	2032	R1P	O4'-C4'-C5'	-2.14	104.54	109.17
2	B	2012	R1P	O4'-C4'-C5'	-2.13	104.56	109.17
2	L	2072	R1P	O4'-C4'-C3'	-2.11	100.90	105.15
2	K	2062	R1P	O4'-C4'-C3'	-2.11	100.90	105.15
2	K	2062	R1P	O1'-P-O1P	-2.06	101.95	107.11
2	F	2002	R1P	O2'-C2'-C3'	2.09	118.61	111.83
2	B	2012	R1P	O3P-P-O2P	2.09	115.35	107.38
2	L	2072	R1P	O2'-C2'-C3'	2.10	118.66	111.83
2	C	2082	R1P	O5'-C5'-C4'	2.11	118.30	111.33
2	B	2012	R1P	O2'-C2'-C3'	2.11	118.68	111.83
2	I	2042	R1P	C5'-C4'-C3'	2.16	120.20	115.08
2	E	2032	R1P	O3P-P-O2P	2.17	115.65	107.38
2	L	2072	R1P	C5'-C4'-C3'	2.22	120.32	115.08
2	K	2062	R1P	O2'-C2'-C3'	2.23	119.07	111.83
6	J	2051	5UD	C2'-C3'-C4'	2.24	107.22	102.61
2	D	2022	R1P	O3P-P-O2P	2.24	115.93	107.38
2	F	2002	R1P	C1'-O4'-C4'	2.34	114.69	105.88
2	L	2072	R1P	O3P-P-O2P	2.37	116.41	107.38
2	K	2062	R1P	C5'-C4'-C3'	2.38	120.72	115.08
2	K	2062	R1P	C1'-O4'-C4'	2.41	114.95	105.88
2	D	2022	R1P	C1'-C2'-C3'	2.44	105.73	102.45
2	E	2032	R1P	C1'-O4'-C4'	2.44	115.06	105.88
5	I	2041	URF	F5-C5-C4	2.45	123.11	118.56
2	F	2002	R1P	C5'-C4'-C3'	2.46	120.90	115.08
6	J	2051	5UD	O2'-C2'-C3'	2.52	120.01	111.83
2	B	2012	R1P	C1'-O4'-C4'	2.53	115.37	105.88
2	D	2022	R1P	C1'-O4'-C4'	2.57	115.54	105.88
2	E	2032	R1P	O2'-C2'-C3'	2.57	120.20	111.83
2	C	2082	R1P	C5'-C4'-C3'	2.58	121.18	115.08
2	D	2022	R1P	O2'-C2'-C3'	2.58	120.21	111.83
6	J	2051	5UD	O5'-C5'-C4'	2.70	120.25	111.33
2	L	2072	R1P	C1'-O4'-C4'	2.75	116.24	105.88
2	D	2022	R1P	C5'-C4'-C3'	2.77	121.64	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2082	R1P	C1'-O4'-C4'	2.81	116.43	105.88
2	I	2042	R1P	C1'-C2'-C3'	2.87	106.31	102.45
2	B	2012	R1P	C5'-C4'-C3'	2.87	121.87	115.08
2	I	2042	R1P	C1'-O4'-C4'	3.05	117.36	105.88
2	E	2032	R1P	C5'-C4'-C3'	3.26	122.79	115.08
2	C	2082	R1P	C1'-C2'-C3'	3.44	107.08	102.45
6	J	2051	5UD	O3'-C3'-C2'	3.91	124.53	111.83
6	J	2051	5UD	C4'-O4'-C1'	4.06	114.18	109.72
5	E	2031	URF	C6-N1-C2	4.16	122.16	115.47
5	D	2021	URF	C6-N1-C2	4.27	122.33	115.47
5	C	2081	URF	C6-N1-C2	4.31	122.40	115.47
5	K	2061	URF	C6-N1-C2	4.32	122.42	115.47
5	B	2011	URF	C6-N1-C2	4.40	122.54	115.47
5	F	2001	URF	C6-N1-C2	4.41	122.57	115.47
5	L	2071	URF	C6-N1-C2	4.62	122.89	115.47
5	I	2041	URF	C6-N1-C2	4.77	123.14	115.47
6	J	2051	5UD	O4'-C1'-N1	5.76	120.23	108.08
5	L	2071	URF	C4-N3-C2	6.03	120.46	115.25
5	I	2041	URF	C4-N3-C2	6.38	120.76	115.25
5	D	2021	URF	C4-N3-C2	6.45	120.82	115.25
5	B	2011	URF	C4-N3-C2	6.51	120.88	115.25
5	F	2001	URF	C4-N3-C2	6.55	120.91	115.25
5	C	2081	URF	C4-N3-C2	6.94	121.25	115.25
5	K	2061	URF	C4-N3-C2	7.25	121.51	115.25
5	E	2031	URF	C4-N3-C2	7.85	122.03	115.25
6	J	2051	5UD	C4-N3-C2	8.81	122.86	115.25
2	B	2012	R1P	O4'-C1'-O1'	9.51	128.55	108.90
2	I	2042	R1P	O4'-C1'-O1'	9.76	129.06	108.90
2	L	2072	R1P	O1'-C1'-C2'	9.79	124.13	106.67
2	D	2022	R1P	O1'-C1'-C2'	9.94	124.40	106.67
2	E	2032	R1P	O4'-C1'-O1'	10.00	129.56	108.90
2	K	2062	R1P	O1'-C1'-C2'	10.03	124.55	106.67
2	C	2082	R1P	O1'-C1'-C2'	10.29	125.02	106.67
2	D	2022	R1P	O4'-C1'-O1'	10.41	130.40	108.90
2	L	2072	R1P	O4'-C1'-O1'	10.42	130.43	108.90
2	F	2002	R1P	O4'-C1'-O1'	10.53	130.65	108.90
2	K	2062	R1P	O4'-C1'-O1'	10.58	130.76	108.90
2	F	2002	R1P	O1'-C1'-C2'	10.60	125.58	106.67
2	E	2032	R1P	O1'-C1'-C2'	10.77	125.88	106.67
2	C	2082	R1P	O4'-C1'-O1'	11.26	132.17	108.90
2	B	2012	R1P	O1'-C1'-C2'	11.30	126.83	106.67
2	I	2042	R1P	O1'-C1'-C2'	11.31	126.83	106.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	246/253 (97%)	-0.01	9 (3%)	45	59	11, 19, 36, 63	0
1	B	250/253 (98%)	-0.25	3 (1%)	81	89	10, 18, 29, 35	0
1	C	246/253 (97%)	-0.06	10 (4%)	41	55	11, 19, 38, 66	0
1	D	250/253 (98%)	-0.11	9 (3%)	46	60	11, 20, 44, 63	0
1	E	250/253 (98%)	-0.21	7 (2%)	56	69	11, 17, 32, 50	0
1	F	250/253 (98%)	-0.23	11 (4%)	38	52	10, 15, 31, 58	0
1	G	245/253 (96%)	-0.03	9 (3%)	45	59	15, 23, 35, 62	0
1	H	240/253 (94%)	-0.22	5 (2%)	67	79	12, 19, 29, 42	0
1	I	250/253 (98%)	-0.25	5 (2%)	68	79	10, 17, 31, 51	0
1	J	250/253 (98%)	-0.37	3 (1%)	81	89	9, 15, 25, 41	0
1	K	243/253 (96%)	-0.24	5 (2%)	67	79	9, 16, 28, 39	0
1	L	250/253 (98%)	-0.07	11 (4%)	38	52	15, 21, 35, 55	0
All	All	2970/3036 (97%)	-0.17	87 (2%)	55	67	9, 19, 33, 66	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	ILE	7.1
1	G	232	GLU	6.0
1	F	232	GLU	5.9
1	A	230	ASN	5.6
1	L	233	THR	5.3
1	A	229	PRO	5.3
1	F	239	SER	5.2
1	L	231	ALA	5.1
1	K	239	SER	5.1
1	C	226	GLN	5.0
1	A	227	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	235	LYS	4.9
1	C	234	MET	4.8
1	C	236	GLN	4.7
1	D	235	LYS	4.6
1	F	233	THR	4.6
1	K	4	SER	4.1
1	D	232	GLU	4.1
1	F	235	LYS	4.0
1	D	231	ALA	4.0
1	I	232	GLU	4.0
1	F	236	GLN	4.0
1	C	229	PRO	4.0
1	A	226	GLN	3.8
1	E	237	THR	3.8
1	D	233	THR	3.7
1	G	235	LYS	3.7
1	K	231	ALA	3.5
1	J	232	GLU	3.5
1	F	231	ALA	3.5
1	C	235	LYS	3.4
1	B	14	ASN	3.4
1	L	148	GLY	3.3
1	D	14	ASN	3.3
1	I	231	ALA	3.3
1	C	228	ILE	3.2
1	L	236	GLN	3.1
1	F	237	THR	3.0
1	A	236	GLN	3.0
1	L	235	LYS	3.0
1	I	236	GLN	2.9
1	D	234	MET	2.9
1	D	230	ASN	2.8
1	G	234	MET	2.8
1	H	236	GLN	2.7
1	H	7	PHE	2.7
1	J	236	GLN	2.7
1	F	238	GLU	2.7
1	K	170	ASP	2.7
1	I	235	LYS	2.7
1	L	232	GLU	2.7
1	E	234	MET	2.6
1	B	232	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	239	SER	2.6
1	G	148	GLY	2.5
1	C	237	THR	2.5
1	I	233	THR	2.4
1	L	5	ASP	2.4
1	G	29	ASP	2.4
1	F	63	ILE	2.4
1	C	4	SER	2.3
1	L	239	SER	2.3
1	A	237	THR	2.3
1	G	233	THR	2.3
1	L	140	LEU	2.3
1	C	170	ASP	2.3
1	H	239	SER	2.2
1	L	234	MET	2.2
1	H	30	ARG	2.2
1	E	148	GLY	2.2
1	B	231	ALA	2.2
1	F	240	HIS	2.2
1	L	145	LYS	2.2
1	E	240	HIS	2.2
1	A	150	THR	2.1
1	A	14	ASN	2.1
1	G	40	LYS	2.1
1	C	224	THR	2.1
1	H	238	GLU	2.0
1	J	233	THR	2.0
1	G	252	LEU	2.0
1	F	234	MET	2.0
1	D	47	HIS	2.0
1	K	240	HIS	2.0
1	D	236	GLN	2.0
1	E	238	GLU	2.0
1	G	231	ALA	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	R1P	L	2072	14/14	0.93	0.19	4.64	38,38,41,42	2
2	R1P	D	2022	14/14	0.88	0.20	3.63	38,39,43,43	3
2	R1P	K	2062	14/14	0.85	0.21	3.41	31,32,39,40	2
2	R1P	C	2082	14/14	0.80	0.24	3.11	42,44,50,50	2
2	R1P	I	2042	14/14	0.95	0.15	2.82	27,29,33,33	2
2	R1P	E	2032	14/14	0.91	0.17	2.73	31,34,39,39	2
2	R1P	F	2002	14/14	0.94	0.15	2.66	30,32,38,39	2
2	R1P	B	2012	14/14	0.94	0.15	2.58	26,29,30,30	2
6	5UD	J	2051	18/18	0.91	0.16	1.76	29,31,33,35	2
3	PO4	J	2052	5/5	0.98	0.10	0.48	18,18,19,19	0
5	URF	K	2061	9/9	0.95	0.10	0.20	19,21,22,27	0
5	URF	C	2081	9/9	0.92	0.16	0.17	41,44,44,45	1
5	URF	B	2011	9/9	0.96	0.10	-0.38	11,13,15,17	0
5	URF	D	2021	9/9	0.95	0.10	-0.47	30,32,33,33	0
5	URF	F	2001	9/9	0.96	0.10	-0.63	18,22,23,25	0
5	URF	E	2031	9/9	0.97	0.09	-0.72	25,27,28,29	0
5	URF	L	2071	9/9	0.97	0.10	-0.76	27,28,29,32	0
5	URF	I	2041	9/9	0.97	0.07	-1.27	19,20,21,22	0
4	K	C	2102	1/1	0.99	0.05	-2.41	21,21,21,21	0
4	K	E	2103	1/1	0.99	0.03	-2.65	16,16,16,16	0
4	K	I	2104	1/1	1.00	0.03	-3.06	16,16,16,16	0
4	K	K	2105	1/1	0.99	0.03	-3.14	17,17,17,17	0
4	K	A	2101	1/1	0.99	0.03	-3.21	20,20,20,20	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.