



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2020 – 09:16 AM BST

PDB ID : 3QPB  
Title : Crystal Structure of Streptococcus Pyogenes Uridine Phosphorylase Reveals a Subclass of the NP-I Superfamily  
Authors : Tran, T.H.; Christoffersen, S.; Parker, W.B.; Piskur, J.; Serra, I.; Terreni, M.; Ealick, S.E.  
Deposited on : 2011-02-11  
Resolution : 1.82 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

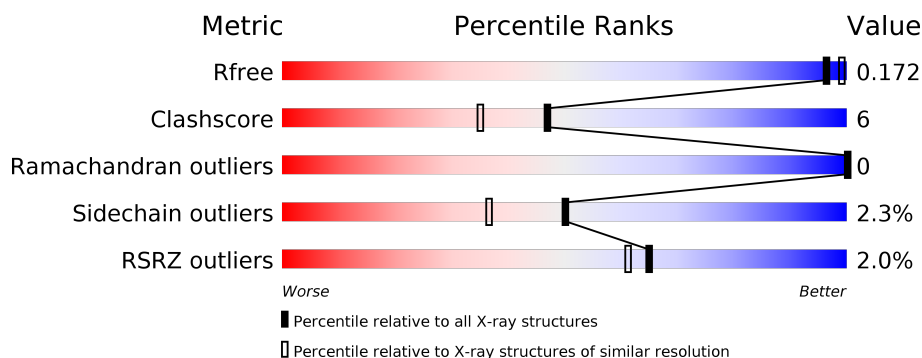
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	282	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>11%</div> </div> </div>
1	C	282	<div> <div></div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	D	282	<div> <div></div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>
1	E	282	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>12%</div> </div> </div>
1	F	282	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	282	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>•</div> <div>12%</div> </div> </div>
1	H	282	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div></div> <div>11%</div> </div> </div>
1	I	282	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div></div> <div>11%</div> </div> </div>
1	J	282	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>•</div> <div>12%</div> </div> </div>
1	K	282	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div></div> <div>12%</div> </div> </div>
1	L	282	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>•</div> <div>12%</div> </div> </div>
1	M	282	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>12%</div> </div> </div>
1	N	282	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div></div> <div>12%</div> </div> </div>
1	O	282	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>
1	P	282	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>
1	Q	282	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>
1	R	282	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div></div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37086 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
			1879	1177	325	365	12			
1	B	250	Total	C	N	O	S	0	0	0
			1879	1177	325	365	12			
1	C	254	Total	C	N	O	S	0	0	0
			1910	1196	329	373	12			
1	D	249	Total	C	N	O	S	0	0	0
			1870	1171	323	364	12			
1	E	249	Total	C	N	O	S	0	0	0
			1870	1171	323	364	12			
1	F	251	Total	C	N	O	S	0	0	0
			1888	1182	326	368	12			
1	G	249	Total	C	N	O	S	0	0	0
			1872	1172	324	364	12			
1	H	250	Total	C	N	O	S	0	0	0
			1879	1177	325	365	12			
1	I	250	Total	C	N	O	S	0	0	0
			1879	1177	325	365	12			
1	J	248	Total	C	N	O	S	0	0	0
			1863	1166	322	363	12			
1	K	249	Total	C	N	O	S	0	0	0
			1870	1171	323	364	12			
1	L	249	Total	C	N	O	S	0	0	0
			1872	1172	324	364	12			
1	M	249	Total	C	N	O	S	0	0	0
			1870	1171	323	364	12			
1	N	249	Total	C	N	O	S	0	0	0
			1872	1172	324	364	12			
1	O	249	Total	C	N	O	S	0	0	0
			1872	1172	324	364	12			
1	P	248	Total	C	N	O	S	0	0	0
			1863	1166	322	363	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	248	Total	C	N	O	S	0	0	0
			1854	1160	319	363	12			
1	R	246	Total	C	N	O	S	0	0	0
			1849	1160	319	358	12			

There are 414 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q5XA29
A	-21	GLY	-	expression tag	UNP Q5XA29
A	-20	SER	-	expression tag	UNP Q5XA29
A	-19	ASP	-	expression tag	UNP Q5XA29
A	-18	LYS	-	expression tag	UNP Q5XA29
A	-17	ILE	-	expression tag	UNP Q5XA29
A	-16	HIS	-	expression tag	UNP Q5XA29
A	-15	HIS	-	expression tag	UNP Q5XA29
A	-14	HIS	-	expression tag	UNP Q5XA29
A	-13	HIS	-	expression tag	UNP Q5XA29
A	-12	HIS	-	expression tag	UNP Q5XA29
A	-11	HIS	-	expression tag	UNP Q5XA29
A	-10	SER	-	expression tag	UNP Q5XA29
A	-9	SER	-	expression tag	UNP Q5XA29
A	-8	GLY	-	expression tag	UNP Q5XA29
A	-7	GLU	-	expression tag	UNP Q5XA29
A	-6	ASN	-	expression tag	UNP Q5XA29
A	-5	LEU	-	expression tag	UNP Q5XA29
A	-4	TYR	-	expression tag	UNP Q5XA29
A	-3	PHE	-	expression tag	UNP Q5XA29
A	-2	GLN	-	expression tag	UNP Q5XA29
A	-1	GLY	-	expression tag	UNP Q5XA29
A	0	HIS	-	expression tag	UNP Q5XA29
B	-22	MET	-	expression tag	UNP Q5XA29
B	-21	GLY	-	expression tag	UNP Q5XA29
B	-20	SER	-	expression tag	UNP Q5XA29
B	-19	ASP	-	expression tag	UNP Q5XA29
B	-18	LYS	-	expression tag	UNP Q5XA29
B	-17	ILE	-	expression tag	UNP Q5XA29
B	-16	HIS	-	expression tag	UNP Q5XA29
B	-15	HIS	-	expression tag	UNP Q5XA29
B	-14	HIS	-	expression tag	UNP Q5XA29
B	-13	HIS	-	expression tag	UNP Q5XA29
B	-12	HIS	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP Q5XA29
B	-10	SER	-	expression tag	UNP Q5XA29
B	-9	SER	-	expression tag	UNP Q5XA29
B	-8	GLY	-	expression tag	UNP Q5XA29
B	-7	GLU	-	expression tag	UNP Q5XA29
B	-6	ASN	-	expression tag	UNP Q5XA29
B	-5	LEU	-	expression tag	UNP Q5XA29
B	-4	TYR	-	expression tag	UNP Q5XA29
B	-3	PHE	-	expression tag	UNP Q5XA29
B	-2	GLN	-	expression tag	UNP Q5XA29
B	-1	GLY	-	expression tag	UNP Q5XA29
B	0	HIS	-	expression tag	UNP Q5XA29
C	-22	MET	-	expression tag	UNP Q5XA29
C	-21	GLY	-	expression tag	UNP Q5XA29
C	-20	SER	-	expression tag	UNP Q5XA29
C	-19	ASP	-	expression tag	UNP Q5XA29
C	-18	LYS	-	expression tag	UNP Q5XA29
C	-17	ILE	-	expression tag	UNP Q5XA29
C	-16	HIS	-	expression tag	UNP Q5XA29
C	-15	HIS	-	expression tag	UNP Q5XA29
C	-14	HIS	-	expression tag	UNP Q5XA29
C	-13	HIS	-	expression tag	UNP Q5XA29
C	-12	HIS	-	expression tag	UNP Q5XA29
C	-11	HIS	-	expression tag	UNP Q5XA29
C	-10	SER	-	expression tag	UNP Q5XA29
C	-9	SER	-	expression tag	UNP Q5XA29
C	-8	GLY	-	expression tag	UNP Q5XA29
C	-7	GLU	-	expression tag	UNP Q5XA29
C	-6	ASN	-	expression tag	UNP Q5XA29
C	-5	LEU	-	expression tag	UNP Q5XA29
C	-4	TYR	-	expression tag	UNP Q5XA29
C	-3	PHE	-	expression tag	UNP Q5XA29
C	-2	GLN	-	expression tag	UNP Q5XA29
C	-1	GLY	-	expression tag	UNP Q5XA29
C	0	HIS	-	expression tag	UNP Q5XA29
D	-22	MET	-	expression tag	UNP Q5XA29
D	-21	GLY	-	expression tag	UNP Q5XA29
D	-20	SER	-	expression tag	UNP Q5XA29
D	-19	ASP	-	expression tag	UNP Q5XA29
D	-18	LYS	-	expression tag	UNP Q5XA29
D	-17	ILE	-	expression tag	UNP Q5XA29
D	-16	HIS	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP Q5XA29
D	-14	HIS	-	expression tag	UNP Q5XA29
D	-13	HIS	-	expression tag	UNP Q5XA29
D	-12	HIS	-	expression tag	UNP Q5XA29
D	-11	HIS	-	expression tag	UNP Q5XA29
D	-10	SER	-	expression tag	UNP Q5XA29
D	-9	SER	-	expression tag	UNP Q5XA29
D	-8	GLY	-	expression tag	UNP Q5XA29
D	-7	GLU	-	expression tag	UNP Q5XA29
D	-6	ASN	-	expression tag	UNP Q5XA29
D	-5	LEU	-	expression tag	UNP Q5XA29
D	-4	TYR	-	expression tag	UNP Q5XA29
D	-3	PHE	-	expression tag	UNP Q5XA29
D	-2	GLN	-	expression tag	UNP Q5XA29
D	-1	GLY	-	expression tag	UNP Q5XA29
D	0	HIS	-	expression tag	UNP Q5XA29
E	-22	MET	-	expression tag	UNP Q5XA29
E	-21	GLY	-	expression tag	UNP Q5XA29
E	-20	SER	-	expression tag	UNP Q5XA29
E	-19	ASP	-	expression tag	UNP Q5XA29
E	-18	LYS	-	expression tag	UNP Q5XA29
E	-17	ILE	-	expression tag	UNP Q5XA29
E	-16	HIS	-	expression tag	UNP Q5XA29
E	-15	HIS	-	expression tag	UNP Q5XA29
E	-14	HIS	-	expression tag	UNP Q5XA29
E	-13	HIS	-	expression tag	UNP Q5XA29
E	-12	HIS	-	expression tag	UNP Q5XA29
E	-11	HIS	-	expression tag	UNP Q5XA29
E	-10	SER	-	expression tag	UNP Q5XA29
E	-9	SER	-	expression tag	UNP Q5XA29
E	-8	GLY	-	expression tag	UNP Q5XA29
E	-7	GLU	-	expression tag	UNP Q5XA29
E	-6	ASN	-	expression tag	UNP Q5XA29
E	-5	LEU	-	expression tag	UNP Q5XA29
E	-4	TYR	-	expression tag	UNP Q5XA29
E	-3	PHE	-	expression tag	UNP Q5XA29
E	-2	GLN	-	expression tag	UNP Q5XA29
E	-1	GLY	-	expression tag	UNP Q5XA29
E	0	HIS	-	expression tag	UNP Q5XA29
F	-22	MET	-	expression tag	UNP Q5XA29
F	-21	GLY	-	expression tag	UNP Q5XA29
F	-20	SER	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	ASP	-	expression tag	UNP Q5XA29
F	-18	LYS	-	expression tag	UNP Q5XA29
F	-17	ILE	-	expression tag	UNP Q5XA29
F	-16	HIS	-	expression tag	UNP Q5XA29
F	-15	HIS	-	expression tag	UNP Q5XA29
F	-14	HIS	-	expression tag	UNP Q5XA29
F	-13	HIS	-	expression tag	UNP Q5XA29
F	-12	HIS	-	expression tag	UNP Q5XA29
F	-11	HIS	-	expression tag	UNP Q5XA29
F	-10	SER	-	expression tag	UNP Q5XA29
F	-9	SER	-	expression tag	UNP Q5XA29
F	-8	GLY	-	expression tag	UNP Q5XA29
F	-7	GLU	-	expression tag	UNP Q5XA29
F	-6	ASN	-	expression tag	UNP Q5XA29
F	-5	LEU	-	expression tag	UNP Q5XA29
F	-4	TYR	-	expression tag	UNP Q5XA29
F	-3	PHE	-	expression tag	UNP Q5XA29
F	-2	GLN	-	expression tag	UNP Q5XA29
F	-1	GLY	-	expression tag	UNP Q5XA29
F	0	HIS	-	expression tag	UNP Q5XA29
G	-22	MET	-	expression tag	UNP Q5XA29
G	-21	GLY	-	expression tag	UNP Q5XA29
G	-20	SER	-	expression tag	UNP Q5XA29
G	-19	ASP	-	expression tag	UNP Q5XA29
G	-18	LYS	-	expression tag	UNP Q5XA29
G	-17	ILE	-	expression tag	UNP Q5XA29
G	-16	HIS	-	expression tag	UNP Q5XA29
G	-15	HIS	-	expression tag	UNP Q5XA29
G	-14	HIS	-	expression tag	UNP Q5XA29
G	-13	HIS	-	expression tag	UNP Q5XA29
G	-12	HIS	-	expression tag	UNP Q5XA29
G	-11	HIS	-	expression tag	UNP Q5XA29
G	-10	SER	-	expression tag	UNP Q5XA29
G	-9	SER	-	expression tag	UNP Q5XA29
G	-8	GLY	-	expression tag	UNP Q5XA29
G	-7	GLU	-	expression tag	UNP Q5XA29
G	-6	ASN	-	expression tag	UNP Q5XA29
G	-5	LEU	-	expression tag	UNP Q5XA29
G	-4	TYR	-	expression tag	UNP Q5XA29
G	-3	PHE	-	expression tag	UNP Q5XA29
G	-2	GLN	-	expression tag	UNP Q5XA29
G	-1	GLY	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q5XA29
H	-22	MET	-	expression tag	UNP Q5XA29
H	-21	GLY	-	expression tag	UNP Q5XA29
H	-20	SER	-	expression tag	UNP Q5XA29
H	-19	ASP	-	expression tag	UNP Q5XA29
H	-18	LYS	-	expression tag	UNP Q5XA29
H	-17	ILE	-	expression tag	UNP Q5XA29
H	-16	HIS	-	expression tag	UNP Q5XA29
H	-15	HIS	-	expression tag	UNP Q5XA29
H	-14	HIS	-	expression tag	UNP Q5XA29
H	-13	HIS	-	expression tag	UNP Q5XA29
H	-12	HIS	-	expression tag	UNP Q5XA29
H	-11	HIS	-	expression tag	UNP Q5XA29
H	-10	SER	-	expression tag	UNP Q5XA29
H	-9	SER	-	expression tag	UNP Q5XA29
H	-8	GLY	-	expression tag	UNP Q5XA29
H	-7	GLU	-	expression tag	UNP Q5XA29
H	-6	ASN	-	expression tag	UNP Q5XA29
H	-5	LEU	-	expression tag	UNP Q5XA29
H	-4	TYR	-	expression tag	UNP Q5XA29
H	-3	PHE	-	expression tag	UNP Q5XA29
H	-2	GLN	-	expression tag	UNP Q5XA29
H	-1	GLY	-	expression tag	UNP Q5XA29
H	0	HIS	-	expression tag	UNP Q5XA29
I	-22	MET	-	expression tag	UNP Q5XA29
I	-21	GLY	-	expression tag	UNP Q5XA29
I	-20	SER	-	expression tag	UNP Q5XA29
I	-19	ASP	-	expression tag	UNP Q5XA29
I	-18	LYS	-	expression tag	UNP Q5XA29
I	-17	ILE	-	expression tag	UNP Q5XA29
I	-16	HIS	-	expression tag	UNP Q5XA29
I	-15	HIS	-	expression tag	UNP Q5XA29
I	-14	HIS	-	expression tag	UNP Q5XA29
I	-13	HIS	-	expression tag	UNP Q5XA29
I	-12	HIS	-	expression tag	UNP Q5XA29
I	-11	HIS	-	expression tag	UNP Q5XA29
I	-10	SER	-	expression tag	UNP Q5XA29
I	-9	SER	-	expression tag	UNP Q5XA29
I	-8	GLY	-	expression tag	UNP Q5XA29
I	-7	GLU	-	expression tag	UNP Q5XA29
I	-6	ASN	-	expression tag	UNP Q5XA29
I	-5	LEU	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	TYR	-	expression tag	UNP Q5XA29
I	-3	PHE	-	expression tag	UNP Q5XA29
I	-2	GLN	-	expression tag	UNP Q5XA29
I	-1	GLY	-	expression tag	UNP Q5XA29
I	0	HIS	-	expression tag	UNP Q5XA29
J	-22	MET	-	expression tag	UNP Q5XA29
J	-21	GLY	-	expression tag	UNP Q5XA29
J	-20	SER	-	expression tag	UNP Q5XA29
J	-19	ASP	-	expression tag	UNP Q5XA29
J	-18	LYS	-	expression tag	UNP Q5XA29
J	-17	ILE	-	expression tag	UNP Q5XA29
J	-16	HIS	-	expression tag	UNP Q5XA29
J	-15	HIS	-	expression tag	UNP Q5XA29
J	-14	HIS	-	expression tag	UNP Q5XA29
J	-13	HIS	-	expression tag	UNP Q5XA29
J	-12	HIS	-	expression tag	UNP Q5XA29
J	-11	HIS	-	expression tag	UNP Q5XA29
J	-10	SER	-	expression tag	UNP Q5XA29
J	-9	SER	-	expression tag	UNP Q5XA29
J	-8	GLY	-	expression tag	UNP Q5XA29
J	-7	GLU	-	expression tag	UNP Q5XA29
J	-6	ASN	-	expression tag	UNP Q5XA29
J	-5	LEU	-	expression tag	UNP Q5XA29
J	-4	TYR	-	expression tag	UNP Q5XA29
J	-3	PHE	-	expression tag	UNP Q5XA29
J	-2	GLN	-	expression tag	UNP Q5XA29
J	-1	GLY	-	expression tag	UNP Q5XA29
J	0	HIS	-	expression tag	UNP Q5XA29
K	-22	MET	-	expression tag	UNP Q5XA29
K	-21	GLY	-	expression tag	UNP Q5XA29
K	-20	SER	-	expression tag	UNP Q5XA29
K	-19	ASP	-	expression tag	UNP Q5XA29
K	-18	LYS	-	expression tag	UNP Q5XA29
K	-17	ILE	-	expression tag	UNP Q5XA29
K	-16	HIS	-	expression tag	UNP Q5XA29
K	-15	HIS	-	expression tag	UNP Q5XA29
K	-14	HIS	-	expression tag	UNP Q5XA29
K	-13	HIS	-	expression tag	UNP Q5XA29
K	-12	HIS	-	expression tag	UNP Q5XA29
K	-11	HIS	-	expression tag	UNP Q5XA29
K	-10	SER	-	expression tag	UNP Q5XA29
K	-9	SER	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-8	GLY	-	expression tag	UNP Q5XA29
K	-7	GLU	-	expression tag	UNP Q5XA29
K	-6	ASN	-	expression tag	UNP Q5XA29
K	-5	LEU	-	expression tag	UNP Q5XA29
K	-4	TYR	-	expression tag	UNP Q5XA29
K	-3	PHE	-	expression tag	UNP Q5XA29
K	-2	GLN	-	expression tag	UNP Q5XA29
K	-1	GLY	-	expression tag	UNP Q5XA29
K	0	HIS	-	expression tag	UNP Q5XA29
L	-22	MET	-	expression tag	UNP Q5XA29
L	-21	GLY	-	expression tag	UNP Q5XA29
L	-20	SER	-	expression tag	UNP Q5XA29
L	-19	ASP	-	expression tag	UNP Q5XA29
L	-18	LYS	-	expression tag	UNP Q5XA29
L	-17	ILE	-	expression tag	UNP Q5XA29
L	-16	HIS	-	expression tag	UNP Q5XA29
L	-15	HIS	-	expression tag	UNP Q5XA29
L	-14	HIS	-	expression tag	UNP Q5XA29
L	-13	HIS	-	expression tag	UNP Q5XA29
L	-12	HIS	-	expression tag	UNP Q5XA29
L	-11	HIS	-	expression tag	UNP Q5XA29
L	-10	SER	-	expression tag	UNP Q5XA29
L	-9	SER	-	expression tag	UNP Q5XA29
L	-8	GLY	-	expression tag	UNP Q5XA29
L	-7	GLU	-	expression tag	UNP Q5XA29
L	-6	ASN	-	expression tag	UNP Q5XA29
L	-5	LEU	-	expression tag	UNP Q5XA29
L	-4	TYR	-	expression tag	UNP Q5XA29
L	-3	PHE	-	expression tag	UNP Q5XA29
L	-2	GLN	-	expression tag	UNP Q5XA29
L	-1	GLY	-	expression tag	UNP Q5XA29
L	0	HIS	-	expression tag	UNP Q5XA29
M	-22	MET	-	expression tag	UNP Q5XA29
M	-21	GLY	-	expression tag	UNP Q5XA29
M	-20	SER	-	expression tag	UNP Q5XA29
M	-19	ASP	-	expression tag	UNP Q5XA29
M	-18	LYS	-	expression tag	UNP Q5XA29
M	-17	ILE	-	expression tag	UNP Q5XA29
M	-16	HIS	-	expression tag	UNP Q5XA29
M	-15	HIS	-	expression tag	UNP Q5XA29
M	-14	HIS	-	expression tag	UNP Q5XA29
M	-13	HIS	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	HIS	-	expression tag	UNP Q5XA29
M	-11	HIS	-	expression tag	UNP Q5XA29
M	-10	SER	-	expression tag	UNP Q5XA29
M	-9	SER	-	expression tag	UNP Q5XA29
M	-8	GLY	-	expression tag	UNP Q5XA29
M	-7	GLU	-	expression tag	UNP Q5XA29
M	-6	ASN	-	expression tag	UNP Q5XA29
M	-5	LEU	-	expression tag	UNP Q5XA29
M	-4	TYR	-	expression tag	UNP Q5XA29
M	-3	PHE	-	expression tag	UNP Q5XA29
M	-2	GLN	-	expression tag	UNP Q5XA29
M	-1	GLY	-	expression tag	UNP Q5XA29
M	0	HIS	-	expression tag	UNP Q5XA29
N	-22	MET	-	expression tag	UNP Q5XA29
N	-21	GLY	-	expression tag	UNP Q5XA29
N	-20	SER	-	expression tag	UNP Q5XA29
N	-19	ASP	-	expression tag	UNP Q5XA29
N	-18	LYS	-	expression tag	UNP Q5XA29
N	-17	ILE	-	expression tag	UNP Q5XA29
N	-16	HIS	-	expression tag	UNP Q5XA29
N	-15	HIS	-	expression tag	UNP Q5XA29
N	-14	HIS	-	expression tag	UNP Q5XA29
N	-13	HIS	-	expression tag	UNP Q5XA29
N	-12	HIS	-	expression tag	UNP Q5XA29
N	-11	HIS	-	expression tag	UNP Q5XA29
N	-10	SER	-	expression tag	UNP Q5XA29
N	-9	SER	-	expression tag	UNP Q5XA29
N	-8	GLY	-	expression tag	UNP Q5XA29
N	-7	GLU	-	expression tag	UNP Q5XA29
N	-6	ASN	-	expression tag	UNP Q5XA29
N	-5	LEU	-	expression tag	UNP Q5XA29
N	-4	TYR	-	expression tag	UNP Q5XA29
N	-3	PHE	-	expression tag	UNP Q5XA29
N	-2	GLN	-	expression tag	UNP Q5XA29
N	-1	GLY	-	expression tag	UNP Q5XA29
N	0	HIS	-	expression tag	UNP Q5XA29
O	-22	MET	-	expression tag	UNP Q5XA29
O	-21	GLY	-	expression tag	UNP Q5XA29
O	-20	SER	-	expression tag	UNP Q5XA29
O	-19	ASP	-	expression tag	UNP Q5XA29
O	-18	LYS	-	expression tag	UNP Q5XA29
O	-17	ILE	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-16	HIS	-	expression tag	UNP Q5XA29
O	-15	HIS	-	expression tag	UNP Q5XA29
O	-14	HIS	-	expression tag	UNP Q5XA29
O	-13	HIS	-	expression tag	UNP Q5XA29
O	-12	HIS	-	expression tag	UNP Q5XA29
O	-11	HIS	-	expression tag	UNP Q5XA29
O	-10	SER	-	expression tag	UNP Q5XA29
O	-9	SER	-	expression tag	UNP Q5XA29
O	-8	GLY	-	expression tag	UNP Q5XA29
O	-7	GLU	-	expression tag	UNP Q5XA29
O	-6	ASN	-	expression tag	UNP Q5XA29
O	-5	LEU	-	expression tag	UNP Q5XA29
O	-4	TYR	-	expression tag	UNP Q5XA29
O	-3	PHE	-	expression tag	UNP Q5XA29
O	-2	GLN	-	expression tag	UNP Q5XA29
O	-1	GLY	-	expression tag	UNP Q5XA29
O	0	HIS	-	expression tag	UNP Q5XA29
P	-22	MET	-	expression tag	UNP Q5XA29
P	-21	GLY	-	expression tag	UNP Q5XA29
P	-20	SER	-	expression tag	UNP Q5XA29
P	-19	ASP	-	expression tag	UNP Q5XA29
P	-18	LYS	-	expression tag	UNP Q5XA29
P	-17	ILE	-	expression tag	UNP Q5XA29
P	-16	HIS	-	expression tag	UNP Q5XA29
P	-15	HIS	-	expression tag	UNP Q5XA29
P	-14	HIS	-	expression tag	UNP Q5XA29
P	-13	HIS	-	expression tag	UNP Q5XA29
P	-12	HIS	-	expression tag	UNP Q5XA29
P	-11	HIS	-	expression tag	UNP Q5XA29
P	-10	SER	-	expression tag	UNP Q5XA29
P	-9	SER	-	expression tag	UNP Q5XA29
P	-8	GLY	-	expression tag	UNP Q5XA29
P	-7	GLU	-	expression tag	UNP Q5XA29
P	-6	ASN	-	expression tag	UNP Q5XA29
P	-5	LEU	-	expression tag	UNP Q5XA29
P	-4	TYR	-	expression tag	UNP Q5XA29
P	-3	PHE	-	expression tag	UNP Q5XA29
P	-2	GLN	-	expression tag	UNP Q5XA29
P	-1	GLY	-	expression tag	UNP Q5XA29
P	0	HIS	-	expression tag	UNP Q5XA29
Q	-22	MET	-	expression tag	UNP Q5XA29
Q	-21	GLY	-	expression tag	UNP Q5XA29

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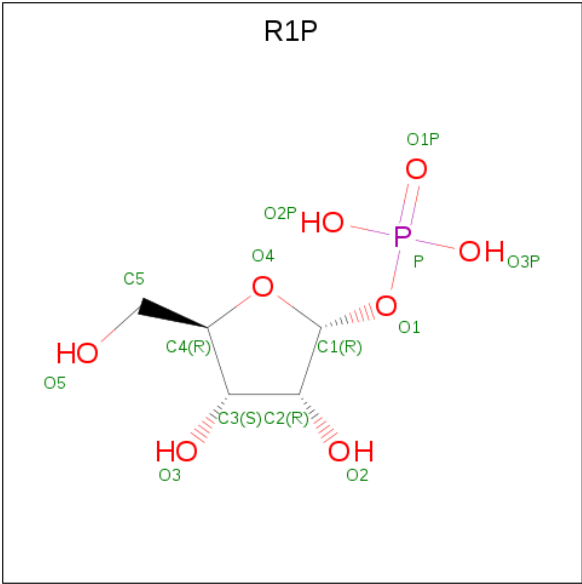
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-20	SER	-	expression tag	UNP Q5XA29
Q	-19	ASP	-	expression tag	UNP Q5XA29
Q	-18	LYS	-	expression tag	UNP Q5XA29
Q	-17	ILE	-	expression tag	UNP Q5XA29
Q	-16	HIS	-	expression tag	UNP Q5XA29
Q	-15	HIS	-	expression tag	UNP Q5XA29
Q	-14	HIS	-	expression tag	UNP Q5XA29
Q	-13	HIS	-	expression tag	UNP Q5XA29
Q	-12	HIS	-	expression tag	UNP Q5XA29
Q	-11	HIS	-	expression tag	UNP Q5XA29
Q	-10	SER	-	expression tag	UNP Q5XA29
Q	-9	SER	-	expression tag	UNP Q5XA29
Q	-8	GLY	-	expression tag	UNP Q5XA29
Q	-7	GLU	-	expression tag	UNP Q5XA29
Q	-6	ASN	-	expression tag	UNP Q5XA29
Q	-5	LEU	-	expression tag	UNP Q5XA29
Q	-4	TYR	-	expression tag	UNP Q5XA29
Q	-3	PHE	-	expression tag	UNP Q5XA29
Q	-2	GLN	-	expression tag	UNP Q5XA29
Q	-1	GLY	-	expression tag	UNP Q5XA29
Q	0	HIS	-	expression tag	UNP Q5XA29
R	-22	MET	-	expression tag	UNP Q5XA29
R	-21	GLY	-	expression tag	UNP Q5XA29
R	-20	SER	-	expression tag	UNP Q5XA29
R	-19	ASP	-	expression tag	UNP Q5XA29
R	-18	LYS	-	expression tag	UNP Q5XA29
R	-17	ILE	-	expression tag	UNP Q5XA29
R	-16	HIS	-	expression tag	UNP Q5XA29
R	-15	HIS	-	expression tag	UNP Q5XA29
R	-14	HIS	-	expression tag	UNP Q5XA29
R	-13	HIS	-	expression tag	UNP Q5XA29
R	-12	HIS	-	expression tag	UNP Q5XA29
R	-11	HIS	-	expression tag	UNP Q5XA29
R	-10	SER	-	expression tag	UNP Q5XA29
R	-9	SER	-	expression tag	UNP Q5XA29
R	-8	GLY	-	expression tag	UNP Q5XA29
R	-7	GLU	-	expression tag	UNP Q5XA29
R	-6	ASN	-	expression tag	UNP Q5XA29
R	-5	LEU	-	expression tag	UNP Q5XA29
R	-4	TYR	-	expression tag	UNP Q5XA29
R	-3	PHE	-	expression tag	UNP Q5XA29
R	-2	GLN	-	expression tag	UNP Q5XA29

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	GLY	-	expression tag	UNP Q5XA29
R	0	HIS	-	expression tag	UNP Q5XA29

- Molecule 2 is 1-O-phosphono-alpha-D-ribofuranose (three-letter code: R1P) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>8</sub>P).



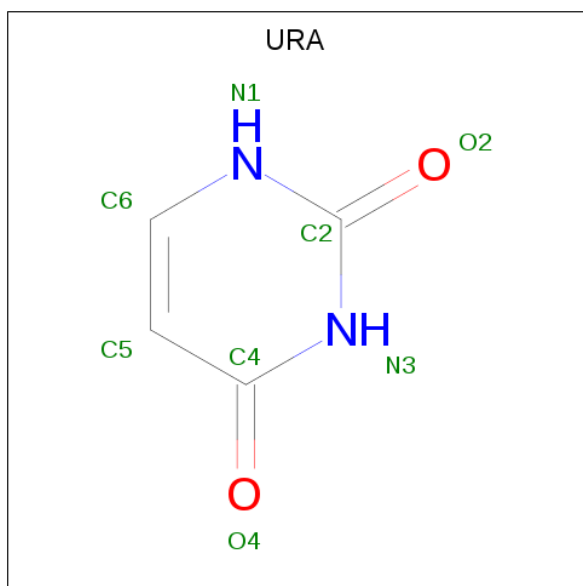
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			14	5	8	1		
2	B	1	Total	C	O	P	0	0
			14	5	8	1		
2	C	1	Total	C	O	P	0	0
			14	5	8	1		
2	D	1	Total	C	O	P	0	0
			14	5	8	1		
2	E	1	Total	C	O	P	0	0
			14	5	8	1		
2	F	1	Total	C	O	P	0	0
			14	5	8	1		
2	G	1	Total	C	O	P	0	0
			14	5	8	1		
2	H	1	Total	C	O	P	0	0
			14	5	8	1		
2	I	1	Total	C	O	P	0	0
			14	5	8	1		
2	J	1	Total	C	O	P	0	0
			14	5	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	M	1	Total	C	O	P	0	0
			14	5	8	1		
2	N	1	Total	C	O	P	0	0
			14	5	8	1		
2	O	1	Total	C	O	P	0	0
			14	5	8	1		
2	P	1	Total	C	O	P	0	0
			14	5	8	1		
2	Q	1	Total	C	O	P	0	0
			14	5	8	1		
2	R	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 3 is URACIL (three-letter code: URA) (formula:  $C_4H_4N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	2	2		
3	B	1	Total	C	N	O	0	0
			8	4	2	2		
3	C	1	Total	C	N	O	0	0
			8	4	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 8	C 4	N 2	O 2	0	0
3	E	1	Total 8	C 4	N 2	O 2	0	0
3	F	1	Total 8	C 4	N 2	O 2	0	0
3	G	1	Total 8	C 4	N 2	O 2	0	0
3	H	1	Total 8	C 4	N 2	O 2	0	0
3	I	1	Total 8	C 4	N 2	O 2	0	0
3	J	1	Total 8	C 4	N 2	O 2	0	0
3	K	1	Total 8	C 4	N 2	O 2	0	0
3	L	1	Total 8	C 4	N 2	O 2	0	0
3	M	1	Total 8	C 4	N 2	O 2	0	0
3	N	1	Total 8	C 4	N 2	O 2	0	0
3	O	1	Total 8	C 4	N 2	O 2	0	0
3	P	1	Total 8	C 4	N 2	O 2	0	0
3	Q	1	Total 8	C 4	N 2	O 2	0	0
3	R	1	Total 8	C 4	N 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	172	Total 172	O 172	0	0
4	B	176	Total 176	O 176	0	0
4	C	213	Total 213	O 213	0	0
4	D	170	Total 170	O 170	0	0

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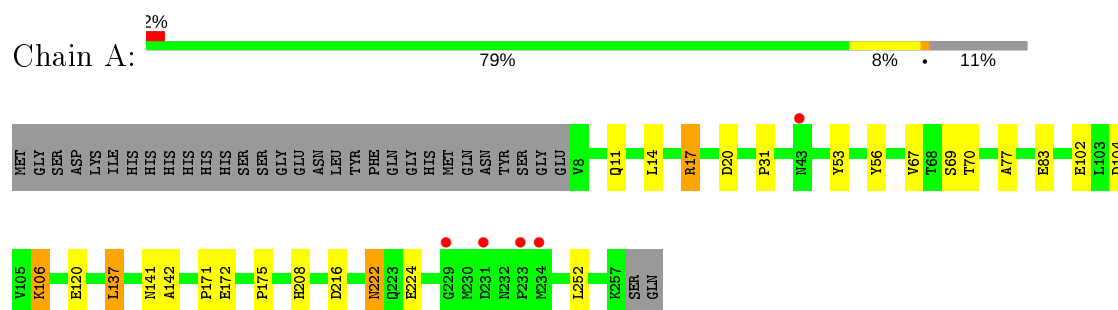
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	198	Total 198	O 198	0	0
4	F	207	Total 207	O 207	0	0
4	G	181	Total 181	O 181	0	0
4	H	151	Total 151	O 151	0	0
4	I	191	Total 191	O 191	0	0
4	J	199	Total 199	O 199	0	0
4	K	189	Total 189	O 189	0	0
4	L	188	Total 188	O 188	0	0
4	M	114	Total 114	O 114	0	0
4	N	120	Total 120	O 120	0	0
4	O	129	Total 129	O 129	0	0
4	P	103	Total 103	O 103	0	0
4	Q	139	Total 139	O 139	0	0
4	R	139	Total 139	O 139	0	0

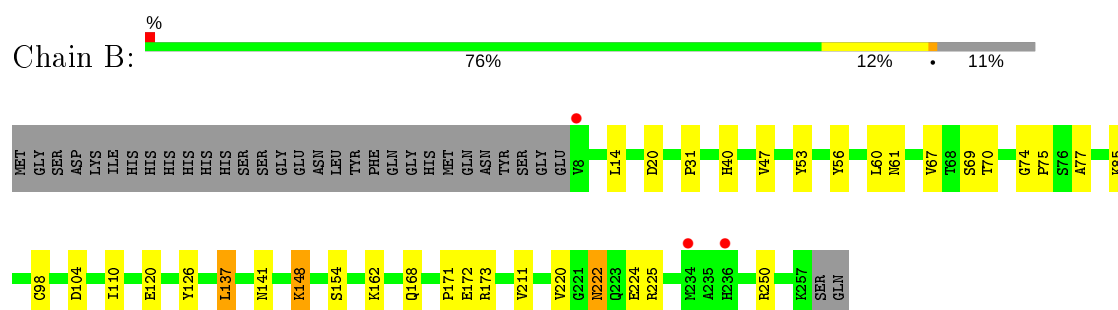
### 3 Residue-property plots [i](#)

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.

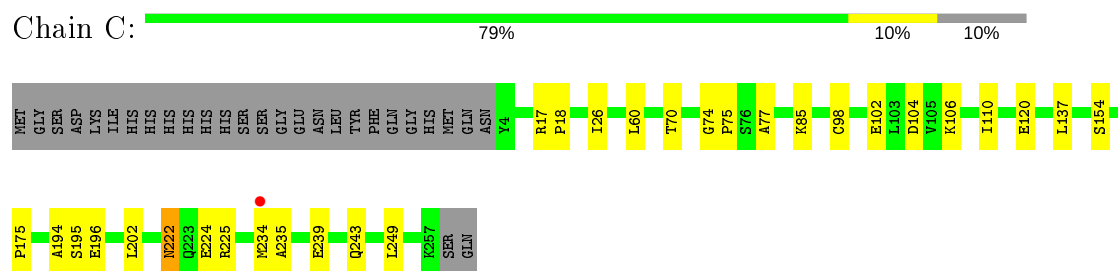
#### • Molecule 1: Uridine phosphorylase



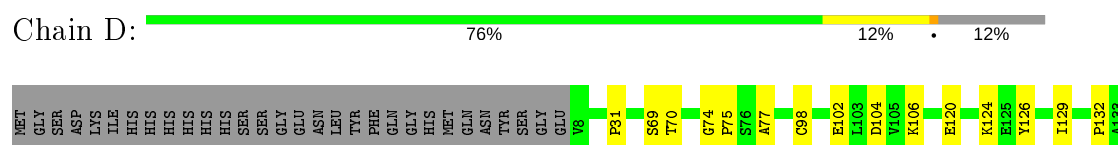
#### • Molecule 1: Uridine phosphorylase

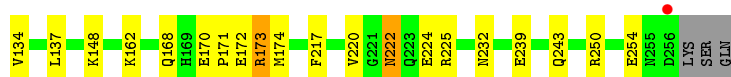


#### • Molecule 1: Uridine phosphorylase

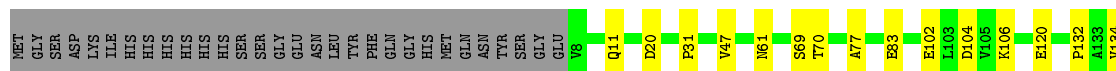
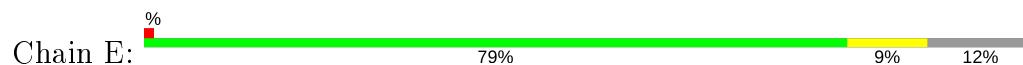


#### • Molecule 1: Uridine phosphorylase

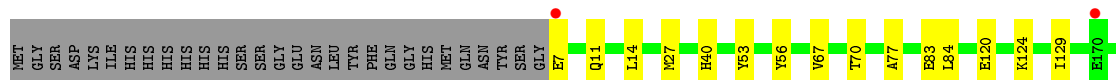
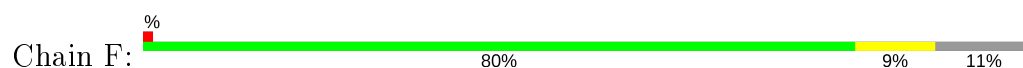




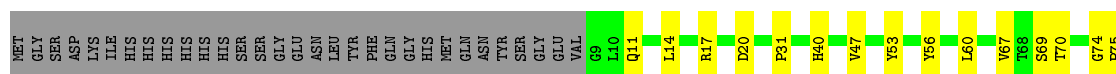
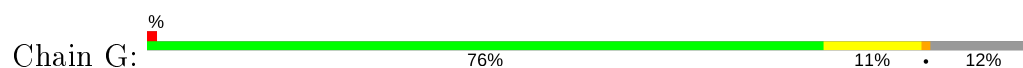
- Molecule 1: Uridine phosphorylase



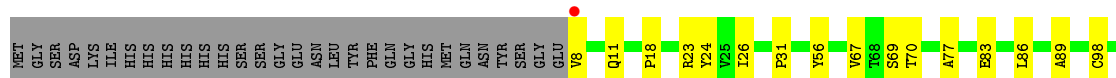
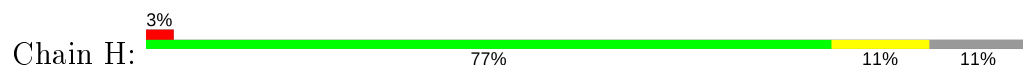
- Molecule 1: Uridine phosphorylase



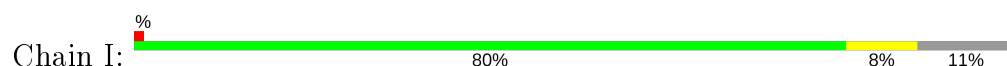
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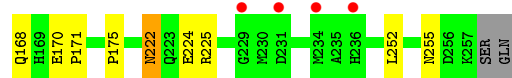
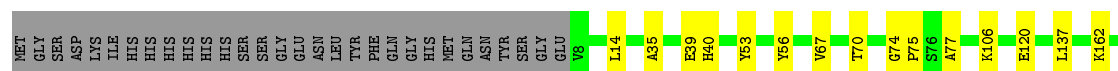


- Molecule 1: Uridine phosphorylase

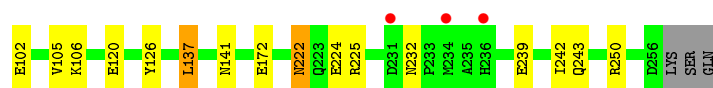
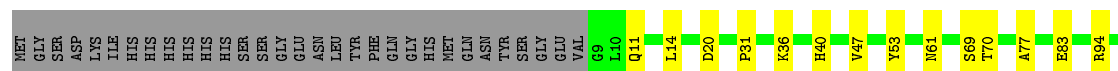
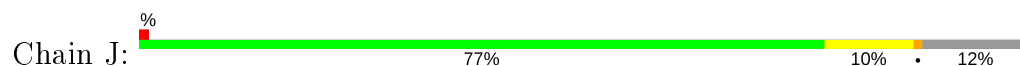


- Molecule 1: Uridine phosphorylase

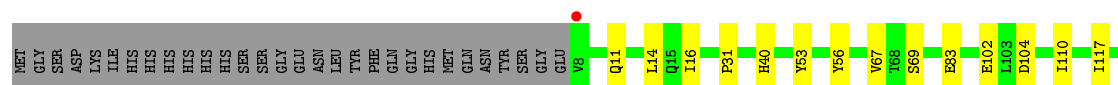
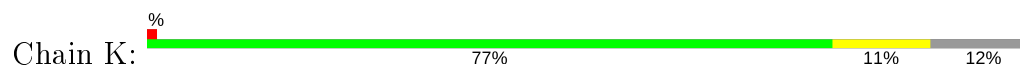




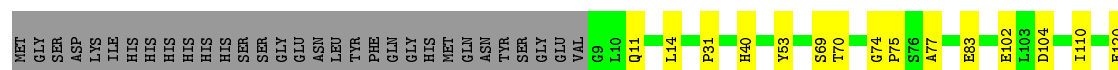
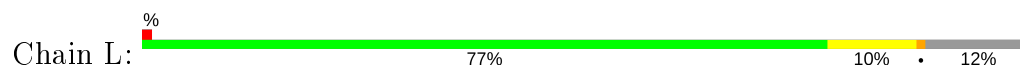
• Molecule 1: Uridine phosphorylase



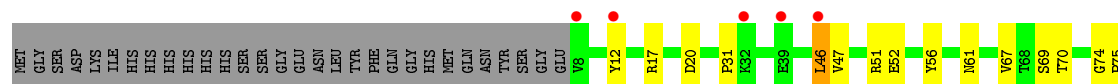
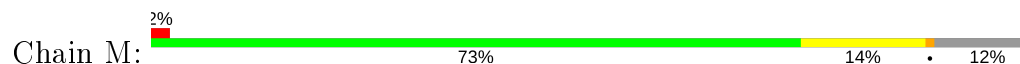
• Molecule 1: Uridine phosphorylase



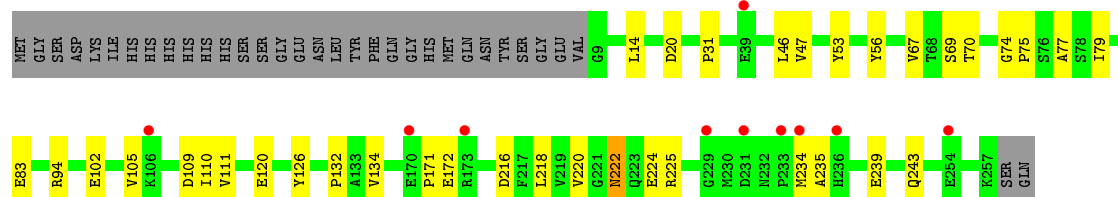
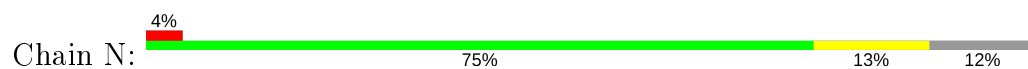
• Molecule 1: Uridine phosphorylase



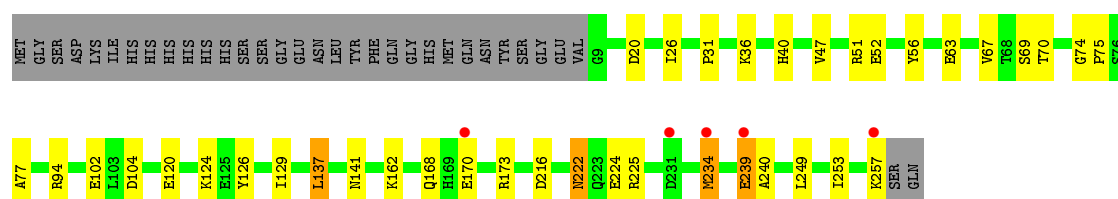
• Molecule 1: Uridine phosphorylase



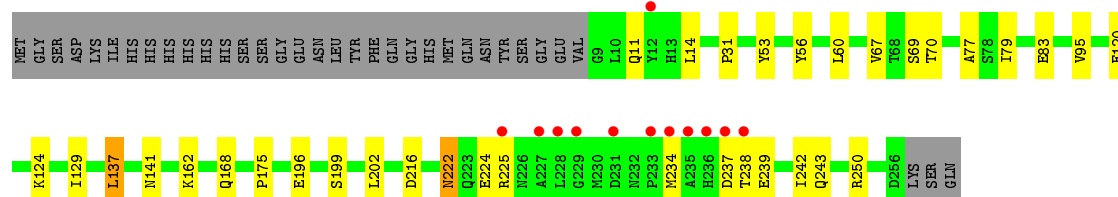
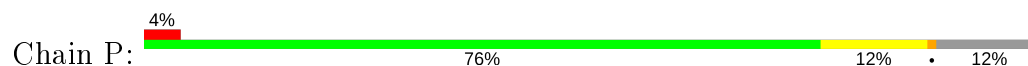
- Molecule 1: Uridine phosphorylase



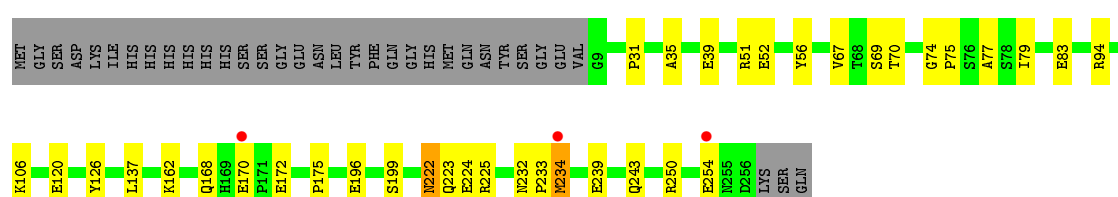
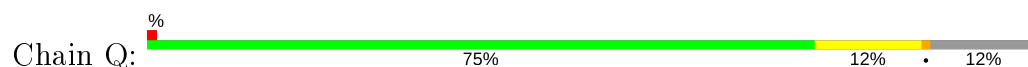
- Molecule 1: Uridine phosphorylase



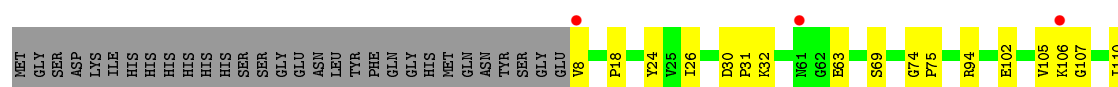
- Molecule 1: Uridine phosphorylase

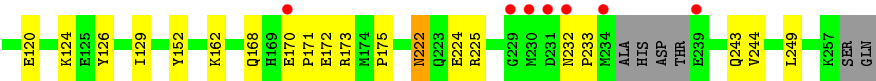


- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.02Å 91.58Å 170.18Å 78.46° 82.33° 60.12°	Depositor
Resolution (Å)	50.00 – 1.82 43.28 – 1.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.82) 95.2 (43.28-1.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 1.82Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.177 , 0.203 0.173 , 0.172	Depositor DCC
$R_{free}$ test set	20029 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.6	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for h-k,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	37086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: URA, 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	0.30	0/1911	0.60	0/2588
1	B	0.29	0/1911	0.60	0/2588
1	C	0.30	0/1943	0.61	0/2631
1	D	0.30	0/1902	0.61	0/2577
1	E	0.30	0/1902	0.60	0/2577
1	F	0.30	0/1920	0.61	0/2600
1	G	0.29	0/1904	0.60	0/2578
1	H	0.29	0/1911	0.60	0/2588
1	I	0.29	0/1911	0.60	0/2588
1	J	0.30	0/1895	0.61	0/2567
1	K	0.30	0/1902	0.61	0/2577
1	L	0.30	0/1904	0.60	0/2578
1	M	0.28	0/1902	0.56	0/2577
1	N	0.27	0/1904	0.56	0/2578
1	O	0.28	0/1904	0.56	0/2578
1	P	0.27	0/1895	0.56	0/2567
1	Q	0.28	0/1886	0.58	0/2556
1	R	0.27	0/1879	0.57	0/2542
All	All	0.29	0/34286	0.59	0/46435

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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	1879	0	1861	23	0
1	B	1879	0	1861	27	0
1	C	1910	0	1884	21	0
1	D	1870	0	1848	26	0
1	E	1870	0	1848	19	0
1	F	1888	0	1867	15	0
1	G	1872	0	1852	27	0
1	H	1879	0	1861	26	0
1	I	1879	0	1861	17	0
1	J	1863	0	1839	19	0
1	K	1870	0	1848	19	0
1	L	1872	0	1852	22	0
1	M	1870	0	1848	30	0
1	N	1872	0	1852	27	0
1	O	1872	0	1852	31	0
1	P	1863	0	1839	27	0
1	Q	1854	0	1819	25	0
1	R	1849	0	1837	34	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	0	0
2	E	14	0	0	0	0
2	F	14	0	0	0	0
2	G	14	0	0	0	0
2	H	14	0	0	0	0
2	I	14	0	0	0	0
2	J	14	0	0	0	0
2	K	14	0	0	0	0
2	L	14	0	0	0	0
2	M	14	0	0	0	0
2	N	14	0	0	0	0
2	O	14	0	0	0	0
2	P	14	0	0	0	0
2	Q	14	0	0	0	0
2	R	14	0	0	0	0
3	A	8	0	3	0	0
3	B	8	0	3	0	0
3	C	8	0	3	0	0
3	D	8	0	3	0	0
3	E	8	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	8	0	3	0	0
3	G	8	0	3	0	0
3	H	8	0	3	0	0
3	I	8	0	3	0	0
3	J	8	0	3	0	0
3	K	8	0	3	0	0
3	L	8	0	3	0	0
3	M	8	0	3	0	0
3	N	8	0	3	0	0
3	O	8	0	3	0	0
3	P	8	0	3	0	0
3	Q	8	0	3	0	0
3	R	8	0	3	0	0
4	A	172	0	0	3	0
4	B	176	0	0	1	0
4	C	213	0	0	3	0
4	D	170	0	0	0	0
4	E	198	0	0	0	0
4	F	207	0	0	2	0
4	G	181	0	0	1	0
4	H	151	0	0	2	0
4	I	191	0	0	2	0
4	J	199	0	0	1	0
4	K	189	0	0	2	0
4	L	188	0	0	1	0
4	M	114	0	0	0	0
4	N	120	0	0	0	0
4	O	129	0	0	1	0
4	P	103	0	0	0	0
4	Q	139	0	0	2	0
4	R	139	0	0	0	0
All	All	37086	0	33383	421	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 (421) 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:Q:168:GLN:HE21	1:Q:223:GLN:HE22	1.08	0.92
1:A:252:LEU:HG	4:A:2806:HOH:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:106:LYS:NZ	1:R:107:GLY:H	1.67	0.90
1:P:95:VAL:HG11	1:P:242:ILE:HD13	1.57	0.87
1:F:239:GLU:HG3	1:F:243:GLN:HE21	1.43	0.82
1:F:231:ASP:OD1	1:F:233:PRO:HD3	1.82	0.78
1:D:222:ASN:H	1:D:232:ASN:HD21	1.31	0.78
1:Q:168:GLN:HE21	1:Q:223:GLN:NE2	1.81	0.78
1:A:208:HIS:NE2	1:B:173:ARG:HD3	2.01	0.75
1:E:11:GLN:HE21	1:E:83:GLU:HG2	1.51	0.73
1:I:252:LEU:HA	4:I:278:HOH:O	1.88	0.73
1:A:11:GLN:HE21	1:A:83:GLU:HG2	1.54	0.72
1:J:222:ASN:H	1:J:232:ASN:HD21	1.38	0.71
1:B:148:LYS:HE3	1:B:148:LYS:HA	1.71	0.70
1:G:208:HIS:NE2	1:H:173:ARG:HD3	2.08	0.68
1:Q:35:ALA:O	1:Q:39:GLU:HG3	1.94	0.68
1:R:106:LYS:HE2	1:R:232:ASN:HA	1.76	0.68
1:L:257:LYS:HE2	1:L:257:LYS:HA	1.76	0.67
1:P:222:ASN:HD22	1:P:222:ASN:C	1.98	0.67
1:P:237:ASP:OD1	1:P:239:GLU:HG2	1.95	0.67
1:R:106:LYS:HZ2	1:R:107:GLY:H	1.43	0.66
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.60	0.66
1:F:11:GLN:HE21	1:F:83:GLU:HG2	1.61	0.66
1:N:14:LEU:HD23	1:N:53:TYR:HB3	1.78	0.65
1:H:11:GLN:HE21	1:H:83:GLU:HG2	1.61	0.65
1:R:8:VAL:HG23	1:R:18:PRO:HG2	1.79	0.65
1:O:222:ASN:HD21	1:O:224:GLU:HB2	1.60	0.64
1:R:106:LYS:HZ1	1:R:107:GLY:H	1.43	0.64
1:G:11:GLN:HE21	1:G:83:GLU:HG2	1.63	0.64
1:L:239:GLU:HG3	1:L:243:GLN:HE21	1.63	0.63
1:M:17:ARG:HG2	1:M:20:ASP:OD2	1.99	0.63
1:D:222:ASN:HD21	1:D:224:GLU:HB2	1.63	0.63
1:J:239:GLU:HG3	1:J:243:GLN:HE21	1.64	0.63
1:O:239:GLU:HG2	1:O:240:ALA:N	2.14	0.62
1:E:61:ASN:ND2	1:E:250:ARG:HH21	1.98	0.62
1:K:11:GLN:HE21	1:K:83:GLU:HG2	1.64	0.62
1:P:238:THR:O	1:P:242:ILE:HG12	2.00	0.62
1:A:222:ASN:HD22	1:A:222:ASN:C	2.03	0.62
1:L:11:GLN:HE21	1:L:83:GLU:HG2	1.65	0.61
1:P:222:ASN:HD21	1:P:224:GLU:HB2	1.64	0.61
1:P:137:LEU:HD22	1:P:141:ASN:HD21	1.65	0.61
1:M:79:ILE:O	1:M:83:GLU:HG3	2.01	0.61
1:H:222:ASN:C	1:H:222:ASN:HD22	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:11:GLN:HE21	1:J:83:GLU:HG2	1.66	0.60
1:N:220:VAL:HG13	1:N:235:ALA:O	2.00	0.60
1:H:170:GLU:HG3	1:H:173:ARG:HB3	1.84	0.60
1:D:239:GLU:HG3	1:D:243:GLN:HE21	1.67	0.60
1:C:98:CYS:SG	1:C:194:ALA:HB1	2.42	0.59
1:O:222:ASN:C	1:O:222:ASN:HD22	2.05	0.59
1:P:137:LEU:HD22	1:P:141:ASN:ND2	2.17	0.59
1:O:124:LYS:HE3	1:O:129:ILE:HD13	1.83	0.59
1:M:61:ASN:HD21	1:M:250:ARG:HG2	1.67	0.59
1:H:8:VAL:HG23	1:H:18:PRO:HG2	1.84	0.59
1:N:222:ASN:HD21	1:N:224:GLU:HB2	1.67	0.59
1:R:222:ASN:C	1:R:222:ASN:HD22	2.06	0.58
1:C:18:PRO:HD2	4:C:2597:HOH:O	2.02	0.58
1:Q:222:ASN:HD22	1:Q:222:ASN:C	2.07	0.58
1:J:36:LYS:HE3	1:J:242:ILE:HD12	1.84	0.58
1:D:173:ARG:C	1:D:173:ARG:HD3	2.24	0.58
1:O:234:MET:CE	1:O:234:MET:H	2.16	0.58
1:C:106:LYS:HE3	1:C:225:ARG:CZ	2.34	0.57
1:B:20:ASP:HB3	1:B:47:VAL:HG11	1.87	0.57
1:R:106:LYS:HE3	1:R:233:PRO:HD2	1.86	0.57
1:L:172:GLU:CD	1:L:172:GLU:H	2.08	0.57
1:I:222:ASN:HD21	1:I:224:GLU:HB2	1.70	0.57
1:G:222:ASN:C	1:G:222:ASN:HD22	2.09	0.56
1:R:162:LYS:HE3	1:R:168:GLN:HB2	1.87	0.56
1:C:106:LYS:HE3	1:C:225:ARG:NH2	2.20	0.56
1:M:46:LEU:O	1:M:46:LEU:HD22	2.06	0.56
1:I:222:ASN:HD22	1:I:222:ASN:C	2.08	0.56
1:P:124:LYS:HE3	1:P:129:ILE:HD13	1.88	0.56
1:D:171:PRO:HG2	1:D:172:GLU:OE2	2.06	0.56
1:N:14:LEU:HD23	1:N:53:TYR:CB	2.35	0.56
1:H:222:ASN:HD21	1:H:224:GLU:HB2	1.71	0.55
1:R:110:ILE:HD13	1:R:244:VAL:HG21	1.87	0.55
1:M:222:ASN:C	1:M:222:ASN:HD22	2.10	0.55
1:M:222:ASN:HD21	1:M:224:GLU:HB2	1.72	0.55
1:P:239:GLU:O	1:P:243:GLN:HG2	2.07	0.55
1:O:257:LYS:NZ	1:O:257:LYS:HB3	2.22	0.55
1:D:134:VAL:HG22	1:E:134:VAL:HG22	1.88	0.55
1:R:222:ASN:HD21	1:R:224:GLU:HB2	1.72	0.55
1:J:106:LYS:NZ	1:J:106:LYS:HB2	2.22	0.55
1:P:222:ASN:HB3	1:P:225:ARG:CD	2.37	0.55
1:J:137:LEU:HD22	1:J:141:ASN:ND2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASN:HD21	1:A:224:GLU:HB2	1.72	0.54
1:K:222:ASN:C	1:K:222:ASN:HD22	2.10	0.54
1:M:137:LEU:HD22	1:M:141:ASN:ND2	2.22	0.54
1:C:98:CYS:HG	1:C:195:SER:C	2.11	0.54
1:M:166:TYR:O	1:M:170:GLU:HG2	2.07	0.54
1:R:124:LYS:HE3	1:R:129:ILE:HD13	1.89	0.54
1:D:222:ASN:HD22	1:D:222:ASN:C	2.11	0.54
1:L:222:ASN:C	1:L:222:ASN:HD22	2.11	0.54
1:B:148:LYS:HE3	1:B:148:LYS:CA	2.37	0.54
1:M:56:TYR:HB2	1:M:67:VAL:CG1	2.37	0.54
1:A:106:LYS:HB3	1:A:106:LYS:NZ	2.23	0.54
1:O:162:LYS:HE3	1:O:168:GLN:OE1	2.08	0.54
1:C:102:GLU:HG3	1:C:104:ASP:H	1.74	0.53
1:L:222:ASN:HD21	1:L:224:GLU:HB2	1.72	0.53
1:C:98:CYS:SG	1:C:194:ALA:CB	2.97	0.53
1:E:106:LYS:HB2	1:E:106:LYS:NZ	2.24	0.53
1:K:239:GLU:HG3	1:K:243:GLN:HE21	1.73	0.53
1:P:70:THR:HB	1:P:77:ALA:HA	1.91	0.53
1:E:170:GLU:HG3	1:E:173:ARG:HB3	1.91	0.53
1:C:234:MET:HG2	1:C:235:ALA:N	2.24	0.52
1:D:172:GLU:H	1:D:172:GLU:CD	2.13	0.52
1:B:148:LYS:CE	1:B:148:LYS:HA	2.40	0.52
1:F:222:ASN:C	1:F:222:ASN:HD22	2.12	0.52
1:K:222:ASN:ND2	1:K:225:ARG:H	2.08	0.52
1:Q:79:ILE:O	1:Q:83:GLU:HG3	2.10	0.52
1:N:14:LEU:CD2	1:N:53:TYR:HB3	2.39	0.52
1:L:171:PRO:HG2	1:L:172:GLU:OE2	2.10	0.52
1:C:222:ASN:C	1:C:222:ASN:HD22	2.13	0.52
1:E:222:ASN:HD21	1:E:224:GLU:HB2	1.75	0.52
1:A:142:ALA:HB1	4:A:2806:HOH:O	2.09	0.52
1:E:225:ARG:NH2	1:E:231:ASP:OD2	2.43	0.52
1:B:222:ASN:HD22	1:B:222:ASN:C	2.13	0.51
1:E:61:ASN:ND2	1:E:250:ARG:NH2	2.57	0.51
1:H:106:LYS:HD3	1:H:225:ARG:CZ	2.41	0.51
1:J:222:ASN:HD21	1:J:224:GLU:HB2	1.76	0.51
1:F:27:MET:HE3	1:F:84:LEU:HD12	1.93	0.51
1:O:170:GLU:O	1:O:173:ARG:HG3	2.11	0.51
1:E:222:ASN:C	1:E:222:ASN:HD22	2.14	0.51
1:Q:222:ASN:ND2	1:Q:225:ARG:H	2.09	0.51
1:H:23:ARG:HG3	1:H:24:TYR:CD2	2.46	0.51
1:H:23:ARG:HA	1:H:89:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:222:ASN:C	1:N:222:ASN:HD22	2.14	0.51
1:L:222:ASN:ND2	1:L:225:ARG:H	2.09	0.50
1:M:237:ASP:OD1	1:M:239:GLU:HB2	2.11	0.50
1:P:222:ASN:ND2	1:P:224:GLU:H	2.09	0.50
1:O:222:ASN:ND2	1:O:224:GLU:H	2.09	0.50
1:A:172:GLU:CD	1:A:172:GLU:H	2.14	0.50
1:B:98:CYS:O	1:B:220:VAL:HG22	2.11	0.50
1:G:40:HIS:HD2	4:G:1228:HOH:O	1.94	0.50
1:G:17:ARG:HG2	1:G:20:ASP:OD2	2.12	0.50
1:R:106:LYS:NZ	1:R:107:GLY:N	2.48	0.50
1:M:61:ASN:ND2	1:M:250:ARG:HG2	2.26	0.50
1:N:46:LEU:HD23	1:N:47:VAL:N	2.26	0.50
1:A:137:LEU:HD22	1:A:141:ASN:ND2	2.26	0.50
1:E:61:ASN:HD21	1:E:250:ARG:HH21	1.60	0.50
1:G:20:ASP:HB3	1:G:47:VAL:HG11	1.93	0.49
1:R:94:ARG:HH11	1:R:94:ARG:HG3	1.76	0.49
1:G:208:HIS:NE2	1:H:173:ARG:CD	2.75	0.49
1:Q:233:PRO:HD2	4:Q:2290:HOH:O	2.12	0.49
1:K:223:GLN:HG2	4:K:264:HOH:O	2.12	0.49
1:R:170:GLU:OE1	1:R:173:ARG:HD3	2.12	0.49
1:G:170:GLU:HG2	1:G:170:GLU:O	2.12	0.49
1:N:239:GLU:HG2	1:N:243:GLN:HE21	1.77	0.49
1:E:239:GLU:HG3	1:E:243:GLN:HE21	1.77	0.49
1:J:222:ASN:C	1:J:222:ASN:HD22	2.16	0.49
1:L:137:LEU:HD22	1:L:141:ASN:ND2	2.27	0.49
1:R:106:LYS:HZ2	1:R:107:GLY:N	2.09	0.49
1:R:106:LYS:HE2	1:R:232:ASN:OD1	2.13	0.49
1:C:98:CYS:SG	1:C:195:SER:O	2.67	0.49
1:G:222:ASN:HD21	1:G:224:GLU:HB2	1.78	0.49
1:O:20:ASP:HB3	1:O:47:VAL:HG11	1.94	0.49
1:D:173:ARG:HD3	1:D:174:MET:N	2.27	0.48
1:Q:239:GLU:HG3	1:Q:243:GLN:HE21	1.78	0.48
1:A:171:PRO:HG2	1:A:172:GLU:OE2	2.13	0.48
1:C:239:GLU:HG3	1:C:243:GLN:HE21	1.78	0.48
1:G:170:GLU:OE2	1:G:173:ARG:NH1	2.46	0.48
1:G:172:GLU:CD	1:G:172:GLU:H	2.16	0.48
1:G:70:THR:HB	1:G:77:ALA:HA	1.93	0.48
1:Q:250:ARG:O	1:Q:254:GLU:HG3	2.14	0.48
1:N:46:LEU:HD23	1:N:46:LEU:C	2.33	0.48
1:I:222:ASN:ND2	1:I:224:GLU:H	2.11	0.48
1:J:70:THR:HB	1:J:77:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:GLU:HG3	1:L:104:ASP:H	1.78	0.48
1:M:70:THR:HB	1:M:77:ALA:HA	1.95	0.48
1:N:218:LEU:C	1:N:218:LEU:HD13	2.33	0.48
1:P:60:LEU:HD11	1:P:250:ARG:NH2	2.28	0.48
1:Q:222:ASN:HD21	1:Q:224:GLU:HB2	1.79	0.48
1:F:14:LEU:HD22	1:F:53:TYR:CG	2.49	0.48
1:G:257:LYS:C	1:G:257:LYS:HD3	2.34	0.48
1:N:14:LEU:HD12	1:N:83:GLU:HB2	1.95	0.48
1:O:56:TYR:HB2	1:O:67:VAL:CG1	2.44	0.48
1:E:172:GLU:H	1:E:172:GLU:CD	2.16	0.48
1:G:31:PRO:HA	1:G:69:SER:HB3	1.96	0.48
1:J:40:HIS:HD2	4:J:1926:HOH:O	1.95	0.48
1:L:31:PRO:HA	1:L:69:SER:HB3	1.96	0.48
1:D:170:GLU:O	1:D:173:ARG:HG3	2.14	0.48
1:K:250:ARG:O	1:K:254:GLU:HG3	2.14	0.48
1:B:172:GLU:H	1:B:172:GLU:CD	2.17	0.47
1:E:102:GLU:HG3	1:E:104:ASP:H	1.79	0.47
1:N:79:ILE:O	1:N:83:GLU:HG3	2.14	0.47
1:H:23:ARG:HG3	1:H:24:TYR:CE2	2.50	0.47
1:B:137:LEU:HD22	1:B:141:ASN:ND2	2.28	0.47
1:M:249:LEU:O	1:M:253:ILE:HG13	2.14	0.47
1:I:222:ASN:HD22	1:I:224:GLU:H	1.63	0.47
1:O:63:GLU:HG3	1:O:253:ILE:HG23	1.96	0.47
1:P:56:TYR:HB2	1:P:67:VAL:CG1	2.45	0.47
1:D:102:GLU:HG3	1:D:104:ASP:H	1.80	0.47
1:R:172:GLU:CD	1:R:172:GLU:H	2.18	0.47
1:F:222:ASN:ND2	1:F:225:ARG:H	2.12	0.46
1:L:14:LEU:HD22	1:L:53:TYR:CG	2.50	0.46
1:K:222:ASN:HD21	1:K:224:GLU:HB2	1.80	0.46
1:C:222:ASN:HD21	1:C:224:GLU:HB2	1.81	0.46
1:D:132:PRO:HB2	1:D:134:VAL:HG23	1.97	0.46
1:D:250:ARG:O	1:D:254:GLU:HG3	2.16	0.46
1:P:14:LEU:HD22	1:P:53:TYR:CG	2.51	0.46
1:K:102:GLU:HG3	1:K:104:ASP:H	1.79	0.46
1:M:218:LEU:C	1:M:218:LEU:HD13	2.35	0.46
1:N:94:ARG:HH11	1:N:94:ARG:HG3	1.79	0.46
1:A:17:ARG:HD2	1:A:20:ASP:OD2	2.16	0.46
1:C:70:THR:HB	1:C:77:ALA:HA	1.97	0.46
1:D:98:CYS:O	1:D:220:VAL:HG22	2.15	0.46
1:E:70:THR:HB	1:E:77:ALA:HA	1.97	0.46
1:G:170:GLU:OE2	1:G:173:ARG:CZ	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:222:ASN:ND2	1:J:225:ARG:H	2.13	0.46
1:K:175:PRO:HD2	1:L:126:TYR:O	2.16	0.46
1:M:106:LYS:HG2	1:M:109:ASP:OD2	2.16	0.46
1:O:234:MET:SD	1:O:234:MET:N	2.84	0.46
1:O:36:LYS:NZ	1:O:36:LYS:HB3	2.30	0.46
1:R:106:LYS:HG3	1:R:107:GLY:N	2.30	0.46
1:R:24:TYR:CE2	1:R:63:GLU:HG2	2.51	0.46
1:B:56:TYR:HB2	1:B:67:VAL:CG1	2.45	0.46
1:H:222:ASN:ND2	1:H:224:GLU:H	2.14	0.46
1:J:172:GLU:CD	1:J:172:GLU:H	2.19	0.46
1:A:14:LEU:HD22	1:A:53:TYR:CG	2.51	0.45
1:E:222:ASN:ND2	1:E:225:ARG:H	2.14	0.45
1:I:106:LYS:HE3	1:I:225:ARG:NH2	2.31	0.45
1:Q:175:PRO:HD2	1:R:126:TYR:O	2.15	0.45
1:M:31:PRO:HA	1:M:69:SER:HB3	1.99	0.45
1:O:222:ASN:HD22	1:O:224:GLU:N	2.14	0.45
1:H:98:CYS:O	1:H:220:VAL:HG22	2.16	0.45
1:Q:126:TYR:O	1:R:175:PRO:HD2	2.16	0.45
1:H:222:ASN:HD22	1:H:224:GLU:H	1.64	0.45
1:O:249:LEU:O	1:O:253:ILE:HG13	2.16	0.45
1:R:106:LYS:CE	1:R:233:PRO:HD2	2.45	0.45
1:M:162:LYS:HE3	1:M:168:GLN:OE1	2.17	0.45
1:M:46:LEU:C	1:M:46:LEU:HD22	2.36	0.45
1:R:171:PRO:HG2	1:R:172:GLU:OE2	2.16	0.45
1:K:56:TYR:HB2	1:K:67:VAL:CG1	2.47	0.45
1:N:102:GLU:HB3	1:N:105:VAL:HG23	1.98	0.45
1:R:222:ASN:HD22	1:R:224:GLU:H	1.65	0.45
1:D:162:LYS:HE3	1:D:168:GLN:OE1	2.16	0.45
1:I:14:LEU:HD22	1:I:53:TYR:CG	2.52	0.45
1:O:70:THR:HB	1:O:77:ALA:HA	1.98	0.45
1:P:162:LYS:HE3	1:P:168:GLN:OE1	2.16	0.45
1:A:70:THR:HB	1:A:77:ALA:HA	1.99	0.45
1:H:102:GLU:HG2	4:H:2256:HOH:O	2.17	0.44
1:I:35:ALA:O	1:I:39:GLU:HG2	2.16	0.44
1:O:257:LYS:HZ3	1:O:257:LYS:HB3	1.82	0.44
1:R:152:TYR:OH	1:R:243:GLN:NE2	2.50	0.44
1:J:61:ASN:OD1	1:J:250:ARG:NH2	2.49	0.44
1:N:109:ASP:C	1:N:110:ILE:HD12	2.37	0.44
1:Q:162:LYS:HE3	1:Q:168:GLN:OE1	2.17	0.44
1:A:222:ASN:ND2	1:A:224:GLU:H	2.15	0.44
1:J:14:LEU:HD22	1:J:53:TYR:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:222:ASN:HD22	1:O:224:GLU:H	1.64	0.44
1:E:132:PRO:HB2	1:E:134:VAL:HG23	1.98	0.44
1:H:31:PRO:HA	1:H:69:SER:HB3	1.99	0.44
1:B:110:ILE:O	1:B:154:SER:HA	2.18	0.44
1:E:11:GLN:NE2	1:E:83:GLU:HG2	2.28	0.44
1:L:40:HIS:HD2	4:L:1160:HOH:O	2.00	0.44
1:M:74:GLY:N	1:M:75:PRO:CD	2.81	0.44
1:N:111:VAL:O	1:N:216:ASP:HA	2.17	0.44
1:P:79:ILE:O	1:P:83:GLU:HG3	2.18	0.44
1:G:253:ILE:O	1:G:257:LYS:HG3	2.18	0.44
1:J:31:PRO:HA	1:J:69:SER:HB3	2.00	0.44
1:L:110:ILE:O	1:L:154:SER:HA	2.18	0.44
1:N:172:GLU:CD	1:N:172:GLU:H	2.21	0.44
1:P:222:ASN:HD22	1:P:224:GLU:H	1.65	0.44
1:R:106:LYS:HE3	1:R:233:PRO:CD	2.47	0.44
1:D:222:ASN:ND2	1:D:224:GLU:H	2.15	0.43
1:F:253:ILE:O	1:F:257:LYS:HG2	2.18	0.43
1:I:222:ASN:ND2	1:I:225:ARG:H	2.15	0.43
1:I:40:HIS:HD2	4:I:1145:HOH:O	2.01	0.43
1:G:56:TYR:HB2	1:G:67:VAL:CG1	2.48	0.43
1:H:162:LYS:HE3	1:H:168:GLN:OE1	2.18	0.43
1:P:196:GLU:OE2	1:P:199:SER:HB2	2.18	0.43
1:N:31:PRO:HA	1:N:69:SER:HB3	1.99	0.43
1:P:222:ASN:O	1:P:225:ARG:HG2	2.18	0.43
1:B:171:PRO:HG2	1:B:172:GLU:OE2	2.18	0.43
1:N:70:THR:HB	1:N:77:ALA:HA	2.00	0.43
1:Q:74:GLY:N	1:Q:75:PRO:CD	2.81	0.43
1:B:40:HIS:HD2	4:B:794:HOH:O	2.01	0.43
1:D:124:LYS:HE3	1:D:129:ILE:HD13	2.01	0.43
1:D:222:ASN:ND2	1:D:225:ARG:H	2.17	0.43
1:F:222:ASN:HD21	1:F:224:GLU:HB2	1.83	0.43
1:Q:232:ASN:N	1:Q:233:PRO:HD3	2.33	0.43
1:R:31:PRO:HA	1:R:69:SER:HB3	2.01	0.43
1:G:126:TYR:O	1:H:175:PRO:HD2	2.18	0.43
1:I:56:TYR:HB2	1:I:67:VAL:CG1	2.49	0.43
1:O:51:ARG:HB3	1:O:52:GLU:OE2	2.17	0.43
1:D:222:ASN:HD22	1:D:224:GLU:H	1.67	0.43
1:H:23:ARG:HG2	4:H:268:HOH:O	2.18	0.43
1:L:70:THR:HB	1:L:77:ALA:HA	2.00	0.43
1:N:132:PRO:HB2	1:N:134:VAL:HG13	2.00	0.43
1:Q:234:MET:CE	1:Q:234:MET:H	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:THR:HB	1:F:77:ALA:HA	2.00	0.43
1:L:222:ASN:ND2	1:L:224:GLU:H	2.16	0.43
1:A:31:PRO:HA	1:A:69:SER:HB3	2.00	0.43
1:B:70:THR:HB	1:B:77:ALA:HA	2.01	0.43
1:G:124:LYS:HE3	1:G:129:ILE:HD13	1.99	0.43
1:P:222:ASN:HB3	1:P:225:ARG:HG2	2.01	0.43
1:H:110:ILE:O	1:H:154:SER:HA	2.19	0.43
1:K:110:ILE:O	1:K:154:SER:HA	2.19	0.43
1:O:222:ASN:ND2	1:O:225:ARG:H	2.15	0.43
1:P:222:ASN:HD22	1:P:224:GLU:N	2.17	0.43
1:C:222:ASN:ND2	1:C:225:ARG:H	2.17	0.42
1:F:239:GLU:CG	1:F:243:GLN:HE21	2.21	0.42
1:F:56:TYR:HB2	1:F:67:VAL:CG1	2.49	0.42
1:G:171:PRO:HG2	1:G:172:GLU:OE2	2.19	0.42
1:Q:51:ARG:HB3	1:Q:52:GLU:OE2	2.19	0.42
1:R:24:TYR:HE2	1:R:63:GLU:HG2	1.83	0.42
1:H:162:LYS:HE3	1:H:168:GLN:HB2	2.01	0.42
1:O:137:LEU:HD22	1:O:141:ASN:ND2	2.34	0.42
1:A:102:GLU:HG3	1:A:104:ASP:H	1.84	0.42
1:B:222:ASN:HD21	1:B:224:GLU:HB2	1.83	0.42
1:C:175:PRO:HD2	1:D:126:TYR:O	2.19	0.42
1:I:70:THR:HB	1:I:77:ALA:HA	2.00	0.42
1:J:20:ASP:HB3	1:J:47:VAL:HG11	2.01	0.42
1:K:40:HIS:HD2	4:K:1938:HOH:O	2.02	0.42
1:A:106:LYS:HZ3	1:A:106:LYS:HB3	1.84	0.42
1:C:85:LYS:HD2	4:C:2052:HOH:O	2.20	0.42
1:P:95:VAL:HG22	1:P:216:ASP:OD1	2.19	0.42
1:A:56:TYR:HB2	1:A:67:VAL:CG1	2.50	0.42
1:G:222:ASN:ND2	1:G:225:ARG:H	2.17	0.42
1:Q:172:GLU:CD	1:Q:172:GLU:H	2.22	0.42
1:R:102:GLU:HB3	1:R:105:VAL:HG23	2.00	0.42
1:B:74:GLY:N	1:B:75:PRO:CD	2.83	0.42
1:G:74:GLY:N	1:G:75:PRO:CD	2.82	0.42
1:I:222:ASN:HD22	1:I:224:GLU:N	2.17	0.42
1:M:170:GLU:HG3	1:M:170:GLU:O	2.20	0.42
1:N:222:ASN:ND2	1:N:225:ARG:H	2.18	0.42
1:N:56:TYR:HB2	1:N:67:VAL:CG1	2.50	0.42
1:I:175:PRO:HD2	1:J:126:TYR:O	2.19	0.42
1:L:196:GLU:OE2	1:L:199:SER:HB2	2.19	0.42
1:M:110:ILE:O	1:M:154:SER:HA	2.19	0.42
1:M:51:ARG:HB3	1:M:52:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:175:PRO:HD2	1:N:126:TYR:O	2.20	0.42
1:A:17:ARG:CG	1:A:17:ARG:HH11	2.29	0.42
1:O:126:TYR:O	1:P:175:PRO:HD2	2.20	0.42
1:R:74:GLY:N	1:R:75:PRO:CD	2.83	0.42
1:A:142:ALA:CB	4:A:2806:HOH:O	2.67	0.42
1:D:148:LYS:HB3	1:D:148:LYS:NZ	2.35	0.42
1:G:60:LEU:HD21	1:G:246:VAL:HG13	2.01	0.42
1:M:172:GLU:CD	1:M:172:GLU:H	2.22	0.42
1:M:92:PHE:CD1	1:M:92:PHE:N	2.87	0.42
1:O:36:LYS:NZ	1:O:36:LYS:CB	2.83	0.42
1:B:61:ASN:OD1	1:B:250:ARG:NH2	2.53	0.42
1:P:31:PRO:HA	1:P:69:SER:HB3	2.01	0.42
1:R:106:LYS:HD2	1:R:225:ARG:HD3	2.02	0.42
1:A:222:ASN:HD22	1:A:224:GLU:H	1.68	0.41
1:M:222:ASN:ND2	1:M:225:ARG:H	2.18	0.41
1:N:74:GLY:N	1:N:75:PRO:CD	2.82	0.41
1:B:14:LEU:HD22	1:B:53:TYR:CG	2.54	0.41
1:B:85:LYS:HD3	1:B:211:VAL:HG11	2.00	0.41
1:C:60:LEU:HD12	1:C:60:LEU:HA	1.95	0.41
1:K:14:LEU:HB2	1:K:16:ILE:HG12	2.01	0.41
1:L:14:LEU:HD23	1:L:14:LEU:N	2.34	0.41
1:Q:94:ARG:HH11	1:Q:94:ARG:HG3	1.85	0.41
1:I:170:GLU:N	1:I:171:PRO:CD	2.82	0.41
1:L:74:GLY:N	1:L:75:PRO:CD	2.84	0.41
1:O:94:ARG:HH11	1:O:94:ARG:HG3	1.85	0.41
1:C:110:ILE:O	1:C:154:SER:HA	2.19	0.41
1:D:222:ASN:HD22	1:D:224:GLU:N	2.18	0.41
1:D:70:THR:HB	1:D:77:ALA:HA	2.02	0.41
1:H:56:TYR:HB2	1:H:67:VAL:CG1	2.49	0.41
1:H:70:THR:HB	1:H:77:ALA:HA	2.02	0.41
1:K:196:GLU:OE2	1:K:199:SER:HB2	2.20	0.41
1:N:20:ASP:HB3	1:N:47:VAL:HG11	2.00	0.41
1:Q:196:GLU:OE2	1:Q:199:SER:HB2	2.20	0.41
1:Q:56:TYR:HB2	1:Q:67:VAL:CG1	2.49	0.41
1:D:31:PRO:HA	1:D:69:SER:HB3	2.03	0.41
1:G:60:LEU:HA	1:G:60:LEU:HD12	1.92	0.41
1:M:46:LEU:HD13	1:M:46:LEU:O	2.21	0.41
1:O:74:GLY:N	1:O:75:PRO:CD	2.84	0.41
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.95	0.41
1:D:106:LYS:HE2	1:D:225:ARG:CZ	2.49	0.41
1:E:31:PRO:HA	1:E:69:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:GLU:CG	1:G:170:GLU:O	2.68	0.41
1:K:14:LEU:HD22	1:K:53:TYR:CG	2.55	0.41
1:M:222:ASN:ND2	1:M:224:GLU:H	2.19	0.41
1:N:67:VAL:O	1:N:67:VAL:HG13	2.21	0.41
1:Q:51:ARG:HA	1:R:30:ASP:OD1	2.21	0.41
1:C:17:ARG:HD3	4:C:1236:HOH:O	2.21	0.41
1:C:74:GLY:N	1:C:75:PRO:CD	2.84	0.41
1:H:222:ASN:HD22	1:H:224:GLU:N	2.19	0.41
1:O:102:GLU:HG3	1:O:104:ASP:H	1.85	0.41
1:O:26:ILE:HG13	1:O:249:LEU:HD11	2.02	0.41
1:G:170:GLU:OE2	1:G:173:ARG:HD3	2.21	0.41
1:H:26:ILE:HG13	1:H:249:LEU:HD11	2.02	0.41
1:J:94:ARG:HG3	1:J:94:ARG:HH11	1.86	0.41
1:Q:70:THR:HB	1:Q:77:ALA:HA	2.02	0.41
1:B:31:PRO:HA	1:B:69:SER:HB3	2.03	0.41
1:H:11:GLN:NE2	1:H:86:LEU:HD12	2.36	0.41
1:J:102:GLU:CG	1:J:105:VAL:HG23	2.50	0.41
1:Q:31:PRO:HA	1:Q:69:SER:HB3	2.02	0.41
1:B:148:LYS:HE3	1:B:148:LYS:O	2.20	0.41
1:F:124:LYS:HE3	1:F:129:ILE:HD13	2.02	0.41
1:G:14:LEU:HD22	1:G:53:TYR:CG	2.56	0.41
1:I:162:LYS:HE3	1:I:168:GLN:OE1	2.21	0.41
1:O:31:PRO:HA	1:O:69:SER:HB3	2.01	0.41
1:B:162:LYS:HE3	1:B:168:GLN:OE1	2.20	0.41
1:C:26:ILE:HG13	1:C:249:LEU:HD11	2.02	0.41
1:E:20:ASP:HB3	1:E:47:VAL:HG11	2.03	0.41
1:I:74:GLY:N	1:I:75:PRO:CD	2.84	0.41
1:K:31:PRO:HA	1:K:69:SER:HB3	2.02	0.41
1:P:11:GLN:HG3	1:P:83:GLU:HB3	2.03	0.41
1:A:175:PRO:HD2	1:B:126:TYR:O	2.21	0.40
1:R:106:LYS:CD	1:R:233:PRO:HD2	2.51	0.40
1:B:104:ASP:N	1:B:104:ASP:OD2	2.54	0.40
1:F:254:GLU:HG2	4:F:2582:HOH:O	2.21	0.40
1:F:40:HIS:HD2	4:F:279:HOH:O	2.03	0.40
1:L:162:LYS:HE3	1:L:168:GLN:OE1	2.21	0.40
1:M:20:ASP:HB3	1:M:47:VAL:HG11	2.04	0.40
1:N:171:PRO:HG2	1:N:172:GLU:OE2	2.21	0.40
1:P:225:ARG:HB3	1:P:225:ARG:HH11	1.85	0.40
1:R:26:ILE:HG13	1:R:249:LEU:HD11	2.03	0.40
1:B:14:LEU:N	1:B:14:LEU:HD23	2.36	0.40
1:D:74:GLY:N	1:D:75:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:GLU:H	1:K:172:GLU:CD	2.24	0.40
1:K:222:ASN:ND2	1:K:224:GLU:H	2.19	0.40
1:M:170:GLU:OE1	1:M:173:ARG:HD3	2.21	0.40
1:O:222:ASN:ND2	1:O:224:GLU:N	2.69	0.40
1:O:40:HIS:HD2	4:O:1940:HOH:O	2.04	0.40
1:Q:106:LYS:HB3	4:Q:2290:HOH:O	2.22	0.40
1:B:222:ASN:ND2	1:B:225:ARG:H	2.20	0.40
1:K:117:ILE:HB	1:K:160:GLN:HA	2.04	0.40
1:L:222:ASN:HD22	1:L:224:GLU:H	1.70	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	248/282 (88%)	240 (97%)	8 (3%)	0	100	100
1	B	248/282 (88%)	240 (97%)	8 (3%)	0	100	100
1	C	252/282 (89%)	246 (98%)	6 (2%)	0	100	100
1	D	247/282 (88%)	240 (97%)	7 (3%)	0	100	100
1	E	247/282 (88%)	241 (98%)	6 (2%)	0	100	100
1	F	249/282 (88%)	243 (98%)	6 (2%)	0	100	100
1	G	247/282 (88%)	240 (97%)	7 (3%)	0	100	100
1	H	248/282 (88%)	240 (97%)	8 (3%)	0	100	100
1	I	248/282 (88%)	241 (97%)	7 (3%)	0	100	100
1	J	246/282 (87%)	237 (96%)	9 (4%)	0	100	100
1	K	247/282 (88%)	238 (96%)	9 (4%)	0	100	100
1	L	247/282 (88%)	239 (97%)	8 (3%)	0	100	100
1	M	247/282 (88%)	239 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	247/282 (88%)	240 (97%)	7 (3%)	0	100	100
1	O	247/282 (88%)	240 (97%)	7 (3%)	0	100	100
1	P	246/282 (87%)	241 (98%)	5 (2%)	0	100	100
1	Q	246/282 (87%)	241 (98%)	5 (2%)	0	100	100
1	R	242/282 (86%)	236 (98%)	6 (2%)	0	100	100
All	All	4449/5076 (88%)	4322 (97%)	127 (3%)	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	196/224 (88%)	190 (97%)	6 (3%)	40	25
1	B	196/224 (88%)	192 (98%)	4 (2%)	55	43
1	C	199/224 (89%)	194 (98%)	5 (2%)	47	33
1	D	195/224 (87%)	190 (97%)	5 (3%)	46	32
1	E	195/224 (87%)	192 (98%)	3 (2%)	65	55
1	F	197/224 (88%)	194 (98%)	3 (2%)	65	55
1	G	195/224 (87%)	188 (96%)	7 (4%)	35	19
1	H	196/224 (88%)	193 (98%)	3 (2%)	65	55
1	I	196/224 (88%)	192 (98%)	4 (2%)	55	43
1	J	194/224 (87%)	191 (98%)	3 (2%)	65	55
1	K	195/224 (87%)	190 (97%)	5 (3%)	46	32
1	L	195/224 (87%)	191 (98%)	4 (2%)	53	41
1	M	195/224 (87%)	188 (96%)	7 (4%)	35	19
1	N	195/224 (87%)	192 (98%)	3 (2%)	65	55
1	O	195/224 (87%)	189 (97%)	6 (3%)	40	25
1	P	194/224 (87%)	189 (97%)	5 (3%)	46	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	192/224 (86%)	187 (97%)	5 (3%)	46	32
1	R	193/224 (86%)	190 (98%)	3 (2%)	62	53
All	All	3513/4032 (87%)	3432 (98%)	81 (2%)	50	37

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	106	LYS
1	A	120	GLU
1	A	137	LEU
1	A	216	ASP
1	A	222	ASN
1	B	120	GLU
1	B	137	LEU
1	B	148	LYS
1	B	222	ASN
1	C	120	GLU
1	C	137	LEU
1	C	196	GLU
1	C	202	LEU
1	C	222	ASN
1	D	120	GLU
1	D	137	LEU
1	D	173	ARG
1	D	217	PHE
1	D	222	ASN
1	E	120	GLU
1	E	222	ASN
1	E	234	MET
1	F	7	GLU
1	F	120	GLU
1	F	222	ASN
1	G	104	ASP
1	G	120	GLU
1	G	170	GLU
1	G	209	LEU
1	G	222	ASN
1	G	231	ASP
1	G	257	LYS
1	H	120	GLU

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Mol	Chain	Res	Type
1	H	218	LEU
1	H	222	ASN
1	I	120	GLU
1	I	137	LEU
1	I	222	ASN
1	I	255	ASN
1	J	120	GLU
1	J	137	LEU
1	J	222	ASN
1	K	120	GLU
1	K	137	LEU
1	K	202	LEU
1	K	222	ASN
1	K	234	MET
1	L	120	GLU
1	L	137	LEU
1	L	222	ASN
1	L	257	LYS
1	M	12	TYR
1	M	46	LEU
1	M	120	GLU
1	M	137	LEU
1	M	222	ASN
1	M	234	MET
1	M	239	GLU
1	N	120	GLU
1	N	222	ASN
1	N	234	MET
1	O	120	GLU
1	O	137	LEU
1	O	216	ASP
1	O	222	ASN
1	O	234	MET
1	O	239	GLU
1	P	120	GLU
1	P	137	LEU
1	P	202	LEU
1	P	222	ASN
1	P	234	MET
1	Q	120	GLU
1	Q	137	LEU
1	Q	170	GLU

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Mol	Chain	Res	Type
1	Q	222	ASN
1	Q	234	MET
1	R	32	LYS
1	R	120	GLU
1	R	222	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	40	HIS
1	A	61	ASN
1	A	222	ASN
1	A	255	ASN
1	B	11	GLN
1	B	222	ASN
1	C	11	GLN
1	C	222	ASN
1	C	255	ASN
1	D	11	GLN
1	D	222	ASN
1	D	232	ASN
1	D	236	HIS
1	D	243	GLN
1	D	255	ASN
1	E	11	GLN
1	E	40	HIS
1	E	61	ASN
1	E	145	ASN
1	E	222	ASN
1	E	255	ASN
1	F	11	GLN
1	F	40	HIS
1	F	61	ASN
1	F	145	ASN
1	F	222	ASN
1	F	243	GLN
1	F	255	ASN
1	G	11	GLN
1	G	40	HIS
1	G	222	ASN
1	H	11	GLN

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Mol	Chain	Res	Type
1	H	40	HIS
1	H	43	ASN
1	H	61	ASN
1	H	222	ASN
1	I	11	GLN
1	I	40	HIS
1	I	222	ASN
1	I	255	ASN
1	J	11	GLN
1	J	40	HIS
1	J	145	ASN
1	J	222	ASN
1	J	232	ASN
1	J	243	GLN
1	J	255	ASN
1	K	11	GLN
1	K	40	HIS
1	K	145	ASN
1	K	222	ASN
1	K	255	ASN
1	L	11	GLN
1	L	40	HIS
1	L	145	ASN
1	L	222	ASN
1	L	243	GLN
1	M	11	GLN
1	M	61	ASN
1	M	222	ASN
1	M	243	GLN
1	M	255	ASN
1	N	11	GLN
1	N	222	ASN
1	N	243	GLN
1	N	255	ASN
1	O	11	GLN
1	O	40	HIS
1	O	222	ASN
1	P	11	GLN
1	P	141	ASN
1	P	145	ASN
1	P	222	ASN
1	Q	11	GLN

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Mol	Chain	Res	Type
1	Q	141	ASN
1	Q	145	ASN
1	Q	222	ASN
1	Q	223	GLN
1	Q	255	ASN
1	R	11	GLN
1	R	15	GLN
1	R	40	HIS
1	R	145	ASN
1	R	222	ASN
1	R	243	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

36 ligands 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
3	URA	H	1255	-	6,8,8	2.21	2 (33%)	4,10,10	7.90	3 (75%)
3	URA	F	1255	-	6,8,8	2.19	2 (33%)	4,10,10	8.01	3 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	R1P	Q	1254	-	13,14,14	0.91	0	20,21,21	0.78	1 (5%)
3	URA	K	1255	-	6,8,8	2.20	2 (33%)	4,10,10	7.91	3 (75%)
3	URA	M	1255	-	6,8,8	2.18	2 (33%)	4,10,10	7.98	3 (75%)
2	R1P	L	1254	-	13,14,14	0.91	0	20,21,21	0.82	1 (5%)
3	URA	E	1255	-	6,8,8	2.21	2 (33%)	4,10,10	8.00	3 (75%)
3	URA	N	1255	-	6,8,8	2.20	2 (33%)	4,10,10	7.95	3 (75%)
2	R1P	O	1254	-	13,14,14	0.90	0	20,21,21	0.82	1 (5%)
3	URA	R	1255	-	6,8,8	2.21	2 (33%)	4,10,10	7.99	3 (75%)
2	R1P	P	1254	-	13,14,14	0.91	0	20,21,21	0.84	1 (5%)
3	URA	D	1255	-	6,8,8	2.19	2 (33%)	4,10,10	8.02	3 (75%)
2	R1P	N	1254	-	13,14,14	0.90	0	20,21,21	0.85	1 (5%)
3	URA	O	1255	-	6,8,8	2.21	2 (33%)	4,10,10	7.90	3 (75%)
2	R1P	B	1254	-	13,14,14	0.91	0	20,21,21	0.88	1 (5%)
2	R1P	M	1254	-	13,14,14	0.90	0	20,21,21	0.85	1 (5%)
3	URA	L	1255	-	6,8,8	2.20	2 (33%)	4,10,10	8.02	3 (75%)
3	URA	Q	1255	-	6,8,8	2.18	2 (33%)	4,10,10	7.89	3 (75%)
2	R1P	R	1254	-	13,14,14	0.90	0	20,21,21	0.89	1 (5%)
2	R1P	G	1254	-	13,14,14	0.91	0	20,21,21	0.81	1 (5%)
2	R1P	E	1254	-	13,14,14	0.90	0	20,21,21	0.83	1 (5%)
3	URA	I	1255	-	6,8,8	2.20	2 (33%)	4,10,10	7.96	3 (75%)
2	R1P	J	1254	-	13,14,14	0.92	0	20,21,21	0.83	1 (5%)
2	R1P	H	1254	-	13,14,14	0.90	0	20,21,21	0.80	1 (5%)
3	URA	B	1255	-	6,8,8	2.19	2 (33%)	4,10,10	7.90	3 (75%)
3	URA	P	1255	-	6,8,8	2.20	2 (33%)	4,10,10	7.97	3 (75%)
3	URA	G	1255	-	6,8,8	2.20	2 (33%)	4,10,10	8.01	3 (75%)
2	R1P	A	1254	-	13,14,14	0.92	0	20,21,21	0.81	1 (5%)
3	URA	J	1255	-	6,8,8	2.20	2 (33%)	4,10,10	7.96	3 (75%)
2	R1P	K	1254	-	13,14,14	0.91	0	20,21,21	0.82	1 (5%)
2	R1P	C	1254	-	13,14,14	0.91	0	20,21,21	0.83	1 (5%)
3	URA	A	1255	-	6,8,8	2.21	2 (33%)	4,10,10	7.94	3 (75%)
3	URA	C	1255	-	6,8,8	2.20	2 (33%)	4,10,10	7.96	3 (75%)
2	R1P	F	1254	-	13,14,14	0.91	0	20,21,21	0.81	1 (5%)
2	R1P	D	1254	-	13,14,14	0.91	0	20,21,21	0.81	1 (5%)
2	R1P	I	1254	-	13,14,14	0.91	0	20,21,21	0.83	1 (5%)

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	URA	H	1255	-	-	-	0/1/1/1
3	URA	F	1255	-	-	-	0/1/1/1
3	URA	K	1255	-	-	-	0/1/1/1
3	URA	M	1255	-	-	-	0/1/1/1
2	R1P	L	1254	-	-	0/6/23/23	0/1/1/1
3	URA	E	1255	-	-	-	0/1/1/1
3	URA	N	1255	-	-	-	0/1/1/1
2	R1P	O	1254	-	-	0/6/23/23	0/1/1/1
3	URA	R	1255	-	-	-	0/1/1/1
2	R1P	P	1254	-	-	2/6/23/23	0/1/1/1
3	URA	D	1255	-	-	-	0/1/1/1
2	R1P	N	1254	-	-	2/6/23/23	0/1/1/1
3	URA	O	1255	-	-	-	0/1/1/1
2	R1P	B	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	M	1254	-	-	1/6/23/23	0/1/1/1
3	URA	L	1255	-	-	-	0/1/1/1
3	URA	Q	1255	-	-	-	0/1/1/1
2	R1P	R	1254	-	-	3/6/23/23	0/1/1/1
2	R1P	G	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	E	1254	-	-	0/6/23/23	0/1/1/1
3	URA	I	1255	-	-	-	0/1/1/1
2	R1P	J	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	H	1254	-	-	1/6/23/23	0/1/1/1
3	URA	B	1255	-	-	-	0/1/1/1
3	URA	P	1255	-	-	-	0/1/1/1
3	URA	G	1255	-	-	-	0/1/1/1
2	R1P	A	1254	-	-	0/6/23/23	0/1/1/1
3	URA	J	1255	-	-	-	0/1/1/1
2	R1P	K	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	C	1254	-	-	0/6/23/23	0/1/1/1
3	URA	A	1255	-	-	-	0/1/1/1
2	R1P	Q	1254	-	-	0/6/23/23	0/1/1/1
3	URA	C	1255	-	-	-	0/1/1/1
2	R1P	F	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	D	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	I	1254	-	-	0/6/23/23	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1255	URA	C4-N3	4.30	1.40	1.33
3	H	1255	URA	C4-N3	4.30	1.40	1.33
3	R	1255	URA	C4-N3	4.30	1.40	1.33
3	O	1255	URA	C4-N3	4.29	1.40	1.33
3	N	1255	URA	C4-N3	4.28	1.40	1.33
3	P	1255	URA	C4-N3	4.28	1.40	1.33
3	G	1255	URA	C4-N3	4.27	1.40	1.33
3	E	1255	URA	C4-N3	4.27	1.40	1.33
3	J	1255	URA	C4-N3	4.26	1.40	1.33
3	I	1255	URA	C4-N3	4.26	1.40	1.33
3	D	1255	URA	C4-N3	4.26	1.40	1.33
3	K	1255	URA	C4-N3	4.25	1.40	1.33
3	L	1255	URA	C4-N3	4.25	1.40	1.33
3	B	1255	URA	C4-N3	4.25	1.40	1.33
3	F	1255	URA	C4-N3	4.23	1.40	1.33
3	M	1255	URA	C4-N3	4.23	1.40	1.33
3	C	1255	URA	C4-N3	4.22	1.40	1.33
3	Q	1255	URA	C4-N3	4.22	1.40	1.33
3	E	1255	URA	C6-N1	2.83	1.40	1.34
3	O	1255	URA	C6-N1	2.82	1.40	1.34
3	C	1255	URA	C6-N1	2.82	1.40	1.34
3	K	1255	URA	C6-N1	2.80	1.40	1.34
3	L	1255	URA	C6-N1	2.80	1.40	1.34
3	J	1255	URA	C6-N1	2.80	1.40	1.34
3	R	1255	URA	C6-N1	2.80	1.40	1.34
3	H	1255	URA	C6-N1	2.80	1.40	1.34
3	M	1255	URA	C6-N1	2.80	1.40	1.34
3	Q	1255	URA	C6-N1	2.79	1.40	1.34
3	I	1255	URA	C6-N1	2.79	1.40	1.34
3	N	1255	URA	C6-N1	2.79	1.40	1.34
3	G	1255	URA	C6-N1	2.78	1.40	1.34
3	F	1255	URA	C6-N1	2.78	1.40	1.34
3	A	1255	URA	C6-N1	2.78	1.40	1.34
3	B	1255	URA	C6-N1	2.78	1.40	1.34
3	D	1255	URA	C6-N1	2.76	1.40	1.34
3	P	1255	URA	C6-N1	2.76	1.40	1.34

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1255	URA	N1-C2-N3	-11.17	119.55	128.43
3	D	1255	URA	C6-N1-C2	11.14	119.91	114.42
3	L	1255	URA	C6-N1-C2	11.14	119.91	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1255	URA	N1-C2-N3	-11.12	119.59	128.43
3	F	1255	URA	N1-C2-N3	-11.09	119.61	128.43
3	J	1255	URA	N1-C2-N3	-11.09	119.62	128.43
3	E	1255	URA	C6-N1-C2	11.08	119.88	114.42
3	A	1255	URA	N1-C2-N3	-11.08	119.62	128.43
3	R	1255	URA	C6-N1-C2	11.07	119.88	114.42
3	E	1255	URA	N1-C2-N3	-11.06	119.63	128.43
3	F	1255	URA	C6-N1-C2	11.06	119.88	114.42
3	D	1255	URA	N1-C2-N3	-11.05	119.65	128.43
3	L	1255	URA	N1-C2-N3	-11.04	119.65	128.43
3	P	1255	URA	N1-C2-N3	-11.04	119.65	128.43
3	M	1255	URA	N1-C2-N3	-11.04	119.65	128.43
3	M	1255	URA	C6-N1-C2	11.04	119.86	114.42
3	I	1255	URA	C6-N1-C2	11.03	119.86	114.42
3	P	1255	URA	C6-N1-C2	11.03	119.86	114.42
3	R	1255	URA	N1-C2-N3	-11.03	119.66	128.43
3	B	1255	URA	N1-C2-N3	-11.02	119.67	128.43
3	Q	1255	URA	N1-C2-N3	-11.01	119.68	128.43
3	G	1255	URA	C6-N1-C2	11.01	119.85	114.42
3	O	1255	URA	N1-C2-N3	-11.00	119.69	128.43
3	I	1255	URA	N1-C2-N3	-11.00	119.69	128.43
3	N	1255	URA	C6-N1-C2	11.00	119.84	114.42
3	N	1255	URA	N1-C2-N3	-10.98	119.70	128.43
3	K	1255	URA	N1-C2-N3	-10.96	119.72	128.43
3	J	1255	URA	C6-N1-C2	10.96	119.82	114.42
3	H	1255	URA	N1-C2-N3	-10.95	119.72	128.43
3	C	1255	URA	C6-N1-C2	10.93	119.81	114.42
3	K	1255	URA	C6-N1-C2	10.92	119.81	114.42
3	A	1255	URA	C6-N1-C2	10.92	119.81	114.42
3	H	1255	URA	C6-N1-C2	10.91	119.80	114.42
3	B	1255	URA	C6-N1-C2	10.86	119.78	114.42
3	O	1255	URA	C6-N1-C2	10.85	119.77	114.42
3	Q	1255	URA	C6-N1-C2	10.82	119.75	114.42
3	L	1255	URA	C5-C6-N1	-3.03	120.19	123.96
3	D	1255	URA	C5-C6-N1	-3.00	120.23	123.96
3	I	1255	URA	C5-C6-N1	-3.00	120.24	123.96
3	K	1255	URA	C5-C6-N1	-2.99	120.24	123.96
3	F	1255	URA	C5-C6-N1	-2.99	120.25	123.96
3	R	1255	URA	C5-C6-N1	-2.99	120.25	123.96
3	H	1255	URA	C5-C6-N1	-2.99	120.25	123.96
3	E	1255	URA	C5-C6-N1	-2.98	120.25	123.96
3	N	1255	URA	C5-C6-N1	-2.98	120.26	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1255	URA	C5-C6-N1	-2.95	120.29	123.96
3	P	1255	URA	C5-C6-N1	-2.94	120.31	123.96
3	G	1255	URA	C5-C6-N1	-2.91	120.34	123.96
3	Q	1255	URA	C5-C6-N1	-2.91	120.34	123.96
3	O	1255	URA	C5-C6-N1	-2.90	120.35	123.96
3	J	1255	URA	C5-C6-N1	-2.90	120.36	123.96
3	C	1255	URA	C5-C6-N1	-2.89	120.36	123.96
3	B	1255	URA	C5-C6-N1	-2.89	120.37	123.96
3	A	1255	URA	C5-C6-N1	-2.89	120.37	123.96
2	R	1254	R1P	C2-C3-C4	-2.67	97.46	102.64
2	M	1254	R1P	C2-C3-C4	-2.64	97.52	102.64
2	P	1254	R1P	C2-C3-C4	-2.58	97.62	102.64
2	B	1254	R1P	C2-C3-C4	-2.57	97.64	102.64
2	O	1254	R1P	C2-C3-C4	-2.53	97.73	102.64
2	C	1254	R1P	C2-C3-C4	-2.52	97.74	102.64
2	G	1254	R1P	C2-C3-C4	-2.50	97.78	102.64
2	J	1254	R1P	C2-C3-C4	-2.48	97.82	102.64
2	L	1254	R1P	C2-C3-C4	-2.46	97.86	102.64
2	A	1254	R1P	C2-C3-C4	-2.45	97.88	102.64
2	E	1254	R1P	C2-C3-C4	-2.44	97.89	102.64
2	I	1254	R1P	C2-C3-C4	-2.43	97.93	102.64
2	N	1254	R1P	C2-C3-C4	-2.42	97.94	102.64
2	D	1254	R1P	C2-C3-C4	-2.35	98.08	102.64
2	K	1254	R1P	C2-C3-C4	-2.35	98.08	102.64
2	H	1254	R1P	C2-C3-C4	-2.33	98.11	102.64
2	Q	1254	R1P	C2-C3-C4	-2.29	98.20	102.64
2	F	1254	R1P	C2-C3-C4	-2.27	98.23	102.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	1254	R1P	C1-O1-P-O1P
2	N	1254	R1P	C1-O1-P-O1P
2	N	1254	R1P	C1-O1-P-O2P
2	R	1254	R1P	C1-O1-P-O1P
2	P	1254	R1P	C1-O1-P-O2P
2	M	1254	R1P	C1-O1-P-O2P
2	R	1254	R1P	C1-O1-P-O2P
2	R	1254	R1P	C1-O1-P-O3P
2	H	1254	R1P	C1-O1-P-O2P

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	250/282 (88%)	-0.21	5 (2%) 65 61	4, 10, 24, 35	0
1	B	250/282 (88%)	-0.40	3 (1%) 79 76	4, 10, 22, 31	0
1	C	254/282 (90%)	-0.42	1 (0%) 92 91	3, 8, 19, 30	0
1	D	249/282 (88%)	-0.39	1 (0%) 92 91	3, 9, 23, 34	0
1	E	249/282 (88%)	-0.41	2 (0%) 86 84	4, 9, 20, 28	0
1	F	251/282 (89%)	-0.39	4 (1%) 72 68	4, 9, 21, 37	0
1	G	249/282 (88%)	-0.33	4 (1%) 72 68	4, 10, 21, 32	0
1	H	250/282 (88%)	-0.19	8 (3%) 47 42	4, 11, 25, 36	0
1	I	250/282 (88%)	-0.26	4 (1%) 72 68	4, 10, 24, 34	0
1	J	248/282 (87%)	-0.44	3 (1%) 79 76	3, 9, 19, 28	0
1	K	249/282 (88%)	-0.42	2 (0%) 86 84	3, 9, 21, 30	0
1	L	249/282 (88%)	-0.36	4 (1%) 72 68	3, 9, 20, 32	0
1	M	249/282 (88%)	-0.03	7 (2%) 53 48	9, 16, 29, 35	0
1	N	249/282 (88%)	0.07	10 (4%) 38 32	8, 16, 32, 43	0
1	O	249/282 (88%)	-0.03	5 (2%) 65 61	8, 16, 31, 38	0
1	P	248/282 (87%)	0.09	12 (4%) 30 25	8, 17, 34, 45	0
1	Q	248/282 (87%)	-0.30	3 (1%) 79 76	7, 13, 25, 37	0
1	R	246/282 (87%)	-0.11	10 (4%) 37 31	7, 14, 31, 46	0
All	All	4487/5076 (88%)	-0.25	88 (1%) 65 61	3, 11, 26, 46	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	234	MET	7.8
1	R	234	MET	6.3
1	P	12	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	O	234	MET	5.2
1	P	236	HIS	5.0
1	N	234	MET	5.0
1	I	234	MET	4.8
1	P	235	ALA	4.7
1	P	231	ASP	4.5
1	N	231	ASP	4.2
1	K	234	MET	4.2
1	M	234	MET	4.1
1	A	231	ASP	3.9
1	H	231	ASP	3.8
1	L	234	MET	3.7
1	R	61	ASN	3.7
1	N	236	HIS	3.6
1	M	12	TYR	3.5
1	R	231	ASP	3.5
1	B	236	HIS	3.4
1	N	170	GLU	3.4
1	C	234	MET	3.3
1	F	234	MET	3.3
1	M	46	LEU	3.1
1	O	231	ASP	3.1
1	P	229	GLY	3.1
1	I	236	HIS	3.1
1	G	234	MET	3.0
1	B	234	MET	3.0
1	D	256	ASP	3.0
1	N	233	PRO	3.0
1	P	237	ASP	2.9
1	P	238	THR	2.9
1	R	8	VAL	2.9
1	A	234	MET	2.9
1	H	234	MET	2.9
1	I	231	ASP	2.9
1	E	231	ASP	2.8
1	H	229	GLY	2.8
1	N	173	ARG	2.8
1	F	257	LYS	2.8
1	F	7	GLU	2.8
1	M	8	VAL	2.8
1	H	233	PRO	2.8
1	I	229	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	104	ASP	2.7
1	L	257	LYS	2.7
1	J	234	MET	2.7
1	R	232	ASN	2.7
1	G	170	GLU	2.7
1	P	227	ALA	2.7
1	H	236	HIS	2.7
1	J	231	ASP	2.6
1	F	170	GLU	2.6
1	B	8	VAL	2.6
1	H	8	VAL	2.6
1	R	239	GLU	2.5
1	M	170	GLU	2.5
1	Q	170	GLU	2.5
1	H	170	GLU	2.5
1	A	229	GLY	2.5
1	P	228	LEU	2.4
1	M	32	LYS	2.4
1	R	170	GLU	2.4
1	O	257	LYS	2.4
1	G	236	HIS	2.4
1	K	8	VAL	2.4
1	Q	254	GLU	2.4
1	L	231	ASP	2.4
1	N	106	LYS	2.3
1	O	170	GLU	2.3
1	P	225	ARG	2.3
1	A	43	ASN	2.3
1	Q	234	MET	2.2
1	M	39	GLU	2.2
1	N	229	GLY	2.2
1	N	254	GLU	2.2
1	R	229	GLY	2.2
1	L	236	HIS	2.2
1	O	239	GLU	2.1
1	J	236	HIS	2.1
1	R	106	LYS	2.1
1	N	39	GLU	2.1
1	H	228	LEU	2.1
1	P	233	PRO	2.1
1	R	230	MET	2.1
1	A	233	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	170	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	R1P	R	1254	14/14	0.77	0.20	36,38,40,40	0
2	R1P	P	1254	14/14	0.87	0.16	26,30,31,32	0
2	R1P	N	1254	14/14	0.88	0.14	24,25,26,27	0
2	R1P	M	1254	14/14	0.93	0.12	18,21,23,23	0
2	R1P	G	1254	14/14	0.93	0.12	14,18,19,20	0
2	R1P	L	1254	14/14	0.94	0.11	12,15,17,17	0
2	R1P	O	1254	14/14	0.94	0.11	16,20,21,22	0
3	URA	O	1255	8/8	0.94	0.09	16,18,18,19	0
2	R1P	E	1254	14/14	0.94	0.11	10,15,18,19	0
2	R1P	H	1254	14/14	0.94	0.12	16,18,19,20	0
2	R1P	I	1254	14/14	0.94	0.10	10,14,15,16	0
2	R1P	B	1254	14/14	0.95	0.12	13,16,17,18	0
3	URA	P	1255	8/8	0.95	0.10	17,19,19,20	0
2	R1P	A	1254	14/14	0.95	0.11	13,18,19,19	0
2	R1P	K	1254	14/14	0.95	0.10	10,13,14,16	0
3	URA	C	1255	8/8	0.95	0.09	8,11,12,14	0
2	R1P	J	1254	14/14	0.95	0.10	11,14,17,17	0
3	URA	R	1255	8/8	0.96	0.08	19,22,22,23	0
3	URA	F	1255	8/8	0.96	0.08	8,10,12,14	0
2	R1P	C	1254	14/14	0.96	0.10	11,15,18,21	0
3	URA	M	1255	8/8	0.96	0.08	15,17,18,18	0
2	R1P	F	1254	14/14	0.96	0.09	9,11,13,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	R1P	D	1254	14/14	0.96	0.10	9,12,14,15	0
3	URA	G	1255	8/8	0.96	0.09	10,14,15,17	0
3	URA	J	1255	8/8	0.97	0.08	9,11,13,14	0
3	URA	N	1255	8/8	0.97	0.06	19,21,22,22	0
3	URA	H	1255	8/8	0.97	0.08	9,12,15,15	0
3	URA	A	1255	8/8	0.97	0.07	10,11,13,13	0
2	R1P	Q	1254	14/14	0.97	0.08	10,13,14,14	0
3	URA	Q	1255	8/8	0.97	0.08	11,12,13,14	0
3	URA	K	1255	8/8	0.97	0.07	8,12,13,16	0
3	URA	E	1255	8/8	0.97	0.07	10,12,13,16	0
3	URA	B	1255	8/8	0.98	0.07	11,15,15,16	0
3	URA	I	1255	8/8	0.98	0.07	12,14,15,16	0
3	URA	L	1255	8/8	0.98	0.06	10,11,12,12	0
3	URA	D	1255	8/8	0.98	0.07	9,11,13,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.