



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:28 PM UTC

PDB ID : 3QPB / pdb_00003qpb
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

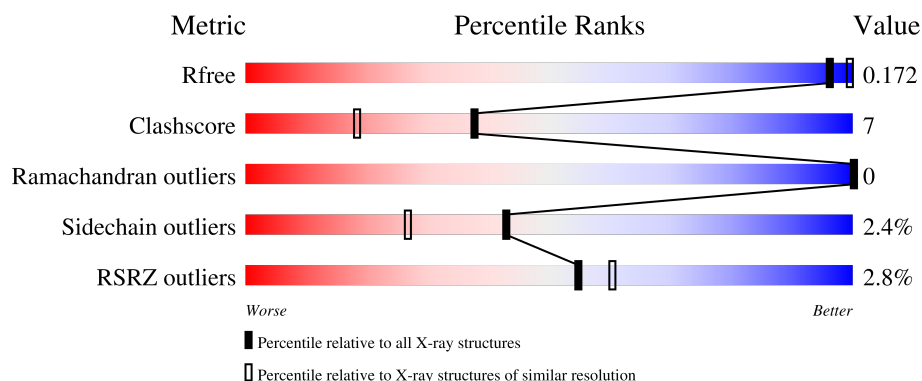
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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

Mol	Chain	Length	Quality of chain
1	A	282	2% 78% 9% 11%
1	B	282	2% 74% 13% 11%
1	C	282	% 77% 12% 10%
1	D	282	% 74% 13% 12%
1	E	282	% 77% 11% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	282	
1	G	282	
1	H	282	
1	I	282	
1	J	282	
1	K	282	
1	L	282	
1	M	282	
1	N	282	
1	O	282	
1	P	282	
1	Q	282	
1	R	282	

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
3	URA	A	1255	-	X	-	-
3	URA	B	1255	-	X	-	-
3	URA	C	1255	-	X	-	-
3	URA	D	1255	-	X	-	-
3	URA	E	1255	-	X	-	-
3	URA	F	1255	-	X	-	-
3	URA	G	1255	-	X	-	-
3	URA	H	1255	-	X	-	-
3	URA	I	1255	-	X	-	-
3	URA	J	1255	-	X	-	-
3	URA	K	1255	-	X	-	-
3	URA	L	1255	-	X	-	-
3	URA	M	1255	-	X	-	-
3	URA	N	1255	-	X	-	-
3	URA	O	1255	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	URA	P	1255	-	X	-	-
3	URA	Q	1255	-	X	-	-
3	URA	R	1255	-	X	-	-

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

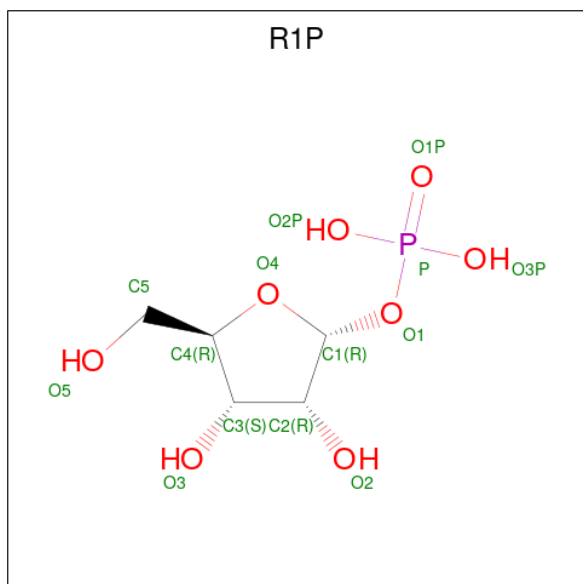
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-20	SER	-	expression tag	UNP Q5XA29
Q	-19	ASP	-	expression tag	UNP Q5XA29
Q	-18	LYS	-	expression tag	UNP Q5XA29
Q	-17	ILE	-	expression tag	UNP Q5XA29
Q	-16	HIS	-	expression tag	UNP Q5XA29
Q	-15	HIS	-	expression tag	UNP Q5XA29
Q	-14	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

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 (CCD ID: R1P) (formula: $C_5H_{11}O_8P$).



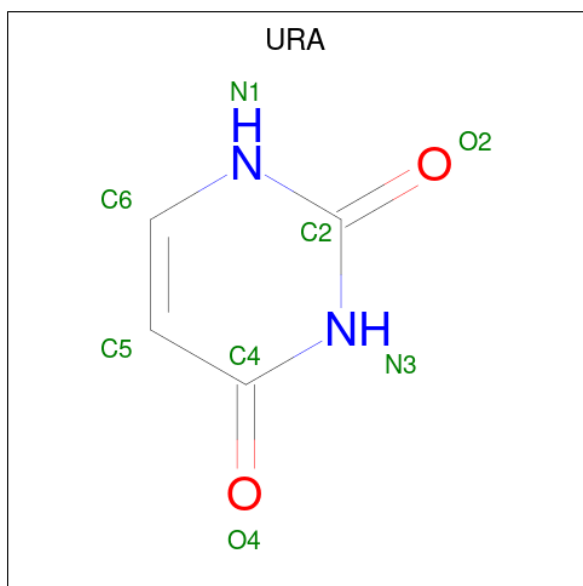
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			14	5	8	1		
2	B	1	Total	C	O	P	0	0
			14	5	8	1		
2	C	1	Total	C	O	P	0	0
			14	5	8	1		
2	D	1	Total	C	O	P	0	0
			14	5	8	1		
2	E	1	Total	C	O	P	0	0
			14	5	8	1		
2	F	1	Total	C	O	P	0	0
			14	5	8	1		
2	G	1	Total	C	O	P	0	0
			14	5	8	1		
2	H	1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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

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

Continued on next page...

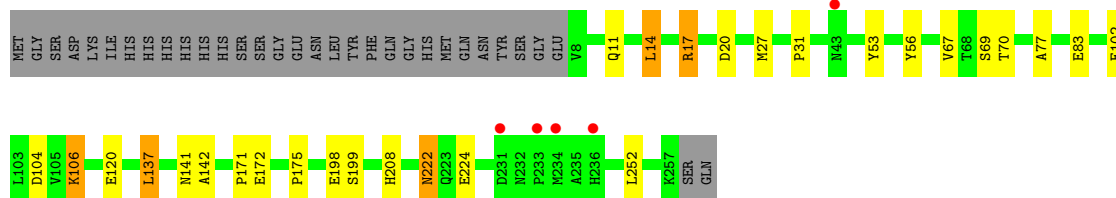
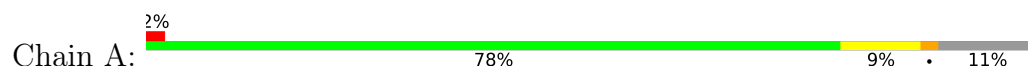
Continued from previous page...

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

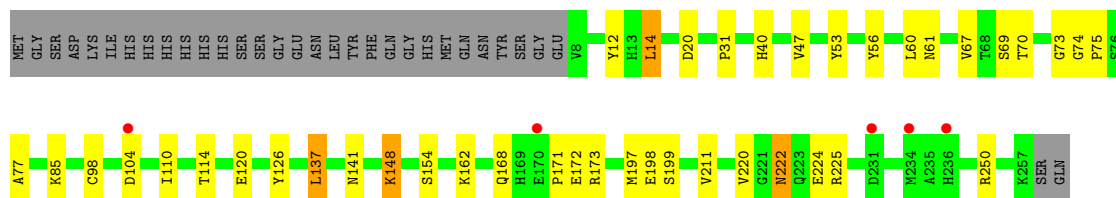
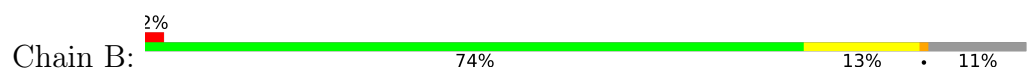
3 Residue-property plots [i](#)

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.

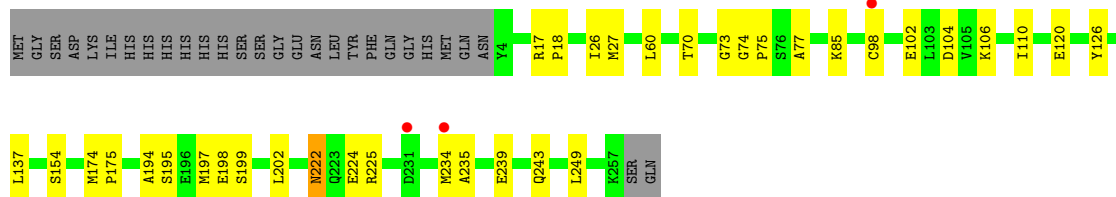
• Molecule 1: Uridine phosphorylase



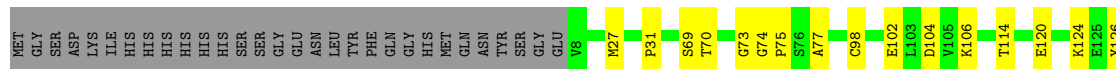
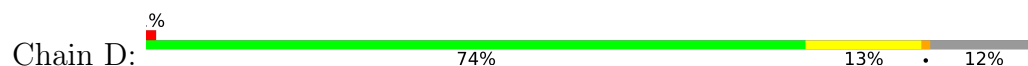
• Molecule 1: Uridine phosphorylase

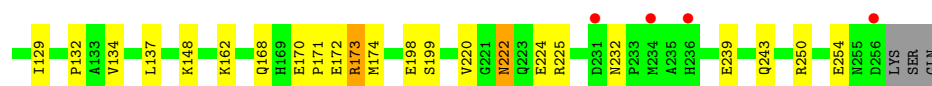


• Molecule 1: Uridine phosphorylase

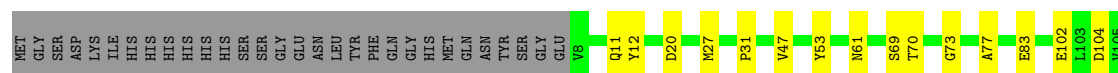
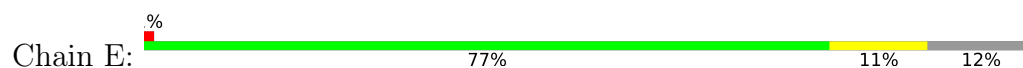


• Molecule 1: Uridine phosphorylase

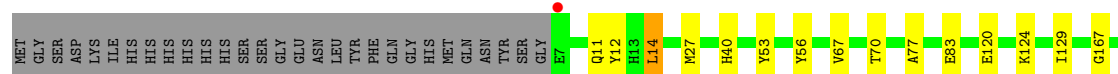
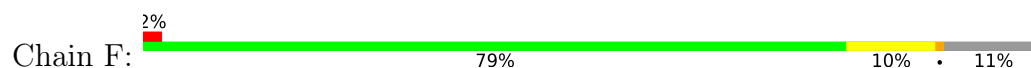




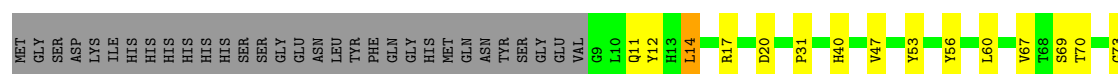
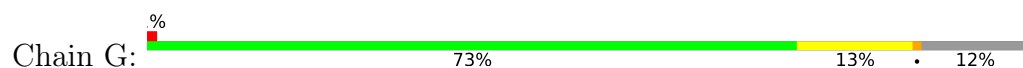
- Molecule 1: Uridine phosphorylase



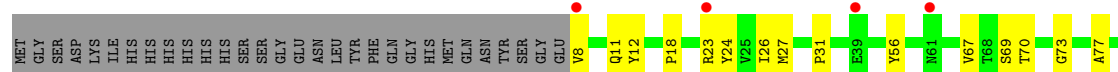
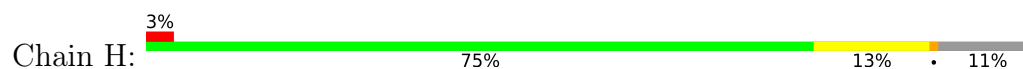
- Molecule 1: Uridine phosphorylase



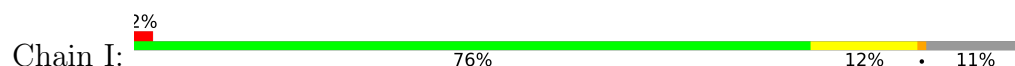
- Molecule 1: Uridine phosphorylase

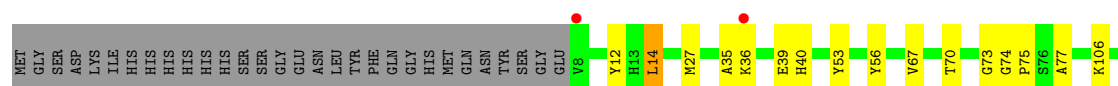


- Molecule 1: Uridine phosphorylase

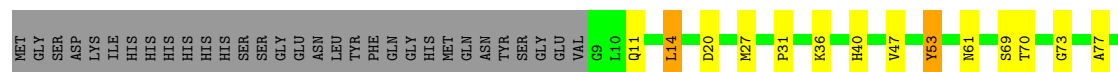
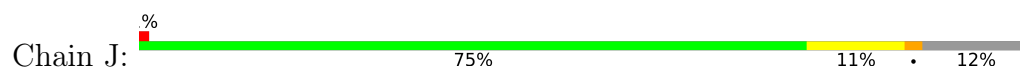


- Molecule 1: Uridine phosphorylase

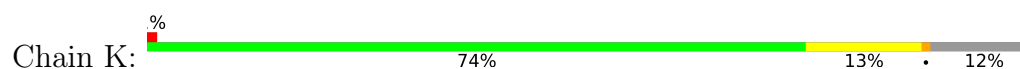




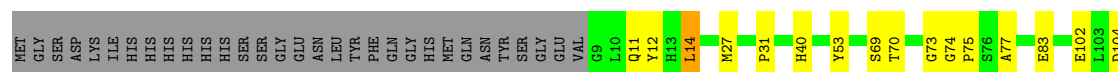
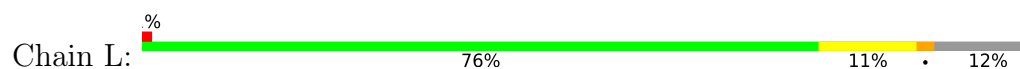
• Molecule 1: Uridine phosphorylase



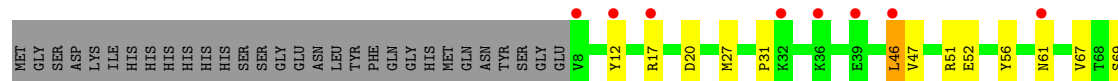
• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase

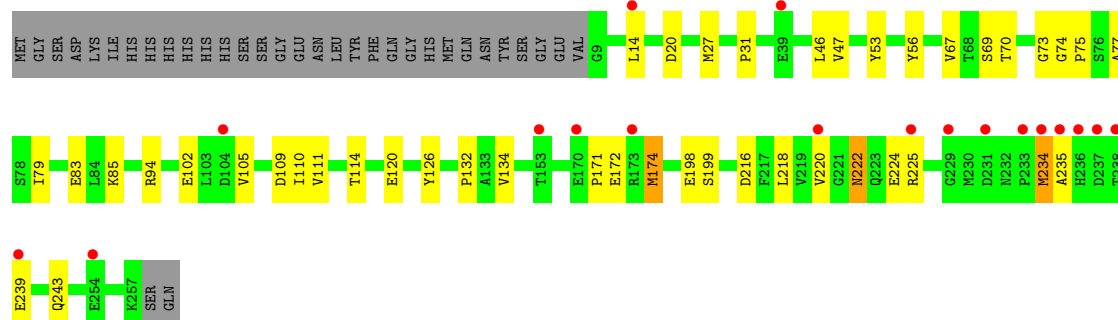


• Molecule 1: Uridine phosphorylase

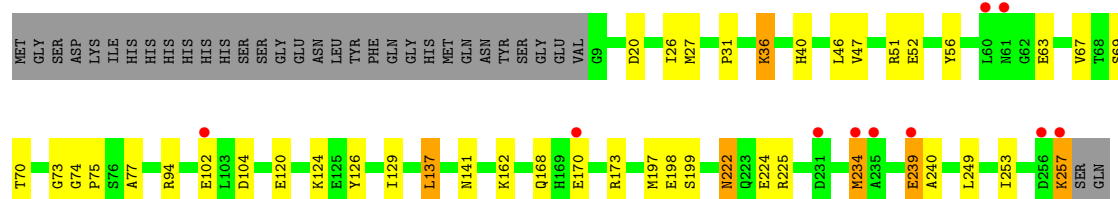
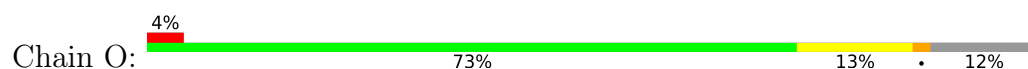




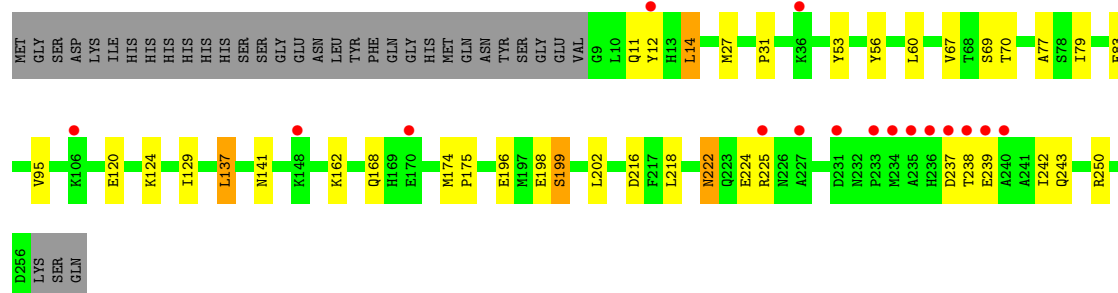
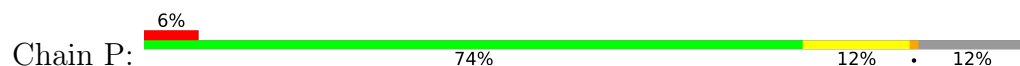
- Molecule 1: Uridine phosphorylase



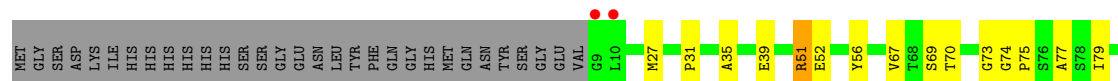
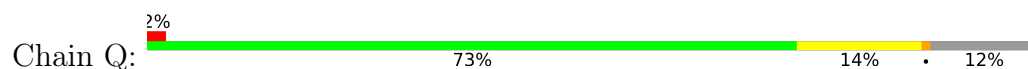
- Molecule 1: Uridine phosphorylase

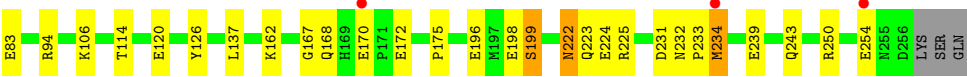


- Molecule 1: Uridine phosphorylase

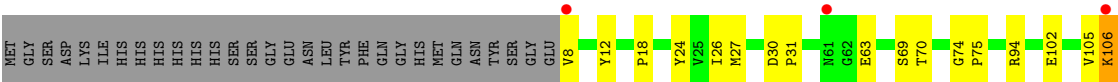


- Molecule 1: Uridine phosphorylase





● Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.02Å 91.58Å 170.18Å 78.46° 82.33° 60.12°	Depositor
Resolution (Å)	50.00 – 1.82 50.00 – 1.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.82) 95.5 (50.00-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	11.6	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R1P, URA

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	0.35	0/1911	0.86	2/2588 (0.1%)
1	B	0.34	0/1911	0.87	6/2588 (0.2%)
1	C	0.36	0/1943	0.86	4/2631 (0.2%)
1	D	0.35	0/1902	0.88	4/2577 (0.2%)
1	E	0.35	0/1902	0.86	7/2577 (0.3%)
1	F	0.35	0/1920	0.88	6/2600 (0.2%)
1	G	0.35	0/1904	0.87	8/2578 (0.3%)
1	H	0.35	0/1911	0.86	5/2588 (0.2%)
1	I	0.34	0/1911	0.88	6/2588 (0.2%)
1	J	0.35	0/1895	0.86	6/2567 (0.2%)
1	K	0.35	0/1902	0.88	7/2577 (0.3%)
1	L	0.36	0/1904	0.86	4/2578 (0.2%)
1	M	0.32	0/1902	0.85	4/2577 (0.2%)
1	N	0.32	0/1904	0.83	5/2578 (0.2%)
1	O	0.33	0/1904	0.83	4/2578 (0.2%)
1	P	0.32	0/1895	0.85	3/2567 (0.1%)
1	Q	0.33	0/1886	0.86	6/2556 (0.2%)
1	R	0.33	0/1879	0.84	5/2542 (0.2%)
All	All	0.34	0/34286	0.86	92/46435 (0.2%)

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	199	SER	N-CA-C	6.40	118.25	111.28
1	D	73	GLY	N-CA-C	6.35	120.04	111.72
1	F	167	GLY	N-CA-C	-6.34	106.80	114.66
1	Q	199	SER	N-CA-C	6.34	118.19	111.28
1	I	199	SER	N-CA-C	6.24	118.08	111.28
1	E	199	SER	N-CA-C	6.19	118.03	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	199	SER	N-CA-C	6.19	118.02	111.28
1	B	73	GLY	N-CA-C	6.04	119.63	111.72
1	G	199	SER	N-CA-C	6.01	117.83	111.28
1	C	198	GLU	N-CA-C	6.00	121.66	113.97
1	R	199	SER	N-CA-C	5.95	117.77	111.28
1	F	197	MET	N-CA-C	5.92	122.20	114.75
1	D	199	SER	N-CA-C	5.91	117.73	111.28
1	A	199	SER	N-CA-C	5.90	117.71	111.28
1	M	199	SER	N-CA-C	5.90	117.71	111.28
1	I	167	GLY	N-CA-C	-5.90	107.35	114.66
1	G	114	THR	N-CA-C	-5.85	105.98	113.23
1	M	198	GLU	N-CA-C	5.84	121.45	113.97
1	B	114	THR	N-CA-C	-5.81	106.02	113.23
1	M	167	GLY	N-CA-C	-5.78	107.49	114.66
1	B	197	MET	N-CA-C	5.76	122.01	114.75
1	R	12	TYR	N-CA-C	5.74	117.99	111.11
1	R	174	MET	N-CA-C	5.70	117.94	110.08
1	A	198	GLU	N-CA-C	5.68	121.24	113.97
1	K	197	MET	N-CA-C	5.68	121.90	114.75
1	Q	114	THR	N-CA-C	-5.66	106.21	113.23
1	L	199	SER	N-CA-C	5.63	117.42	111.28
1	I	12	TYR	N-CA-C	5.61	117.85	111.11
1	H	12	TYR	N-CA-C	5.60	117.83	111.11
1	K	199	SER	N-CA-C	5.59	117.38	111.28
1	R	198	GLU	N-CA-C	5.59	121.13	113.97
1	G	12	TYR	N-CA-C	5.58	117.81	111.11
1	C	199	SER	N-CA-C	5.58	117.36	111.28
1	J	73	GLY	N-CA-C	5.58	119.02	111.72
1	Q	51	ARG	CB-CA-C	-5.58	110.13	116.54
1	B	198	GLU	N-CA-C	5.56	121.09	113.97
1	E	198	GLU	N-CA-C	5.54	121.07	113.97
1	F	198	GLU	N-CA-C	5.54	121.06	113.97
1	F	174	MET	N-CA-C	5.54	117.54	109.84
1	C	197	MET	N-CA-C	5.53	121.72	114.75
1	N	114	THR	N-CA-C	-5.52	106.39	113.23
1	G	198	GLU	N-CA-C	5.51	121.02	113.97
1	B	12	TYR	N-CA-C	5.45	117.66	111.11
1	L	12	TYR	N-CA-C	5.45	117.64	111.11
1	J	198	GLU	N-CA-C	5.44	120.93	113.97
1	I	73	GLY	N-CA-C	5.43	119.45	112.18
1	J	199	SER	N-CA-C	5.43	117.95	111.71
1	K	167	GLY	N-CA-C	-5.42	107.93	114.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	73	GLY	N-CA-C	5.42	118.82	111.72
1	K	198	GLU	N-CA-C	5.40	120.88	113.97
1	G	167	GLY	N-CA-C	-5.38	107.98	114.66
1	G	174	MET	N-CA-C	5.37	117.30	109.84
1	K	12	TYR	N-CA-C	5.36	117.55	111.11
1	I	198	GLU	N-CA-C	5.36	120.82	113.97
1	I	174	MET	N-CA-C	5.35	117.28	109.84
1	P	199	SER	N-CA-C	5.35	117.11	111.28
1	C	73	GLY	N-CA-C	5.34	119.33	112.18
1	F	12	TYR	N-CA-C	5.33	117.51	111.11
1	F	199	SER	N-CA-C	5.30	117.06	111.28
1	G	197	MET	N-CA-C	5.29	121.42	114.75
1	O	73	GLY	N-CA-C	5.28	118.64	111.72
1	H	199	SER	N-CA-C	5.28	117.04	111.28
1	D	114	THR	N-CA-C	-5.27	106.69	113.23
1	P	198	GLU	N-CA-C	5.26	120.71	113.97
1	Q	198	GLU	N-CA-C	5.24	120.68	113.97
1	J	174	MET	N-CA-C	5.24	117.12	109.84
1	D	198	GLU	N-CA-C	5.24	120.67	113.97
1	E	174	MET	N-CA-C	5.24	117.12	109.84
1	L	114	THR	N-CA-C	-5.23	106.75	113.23
1	E	12	TYR	N-CA-C	5.20	117.35	111.11
1	M	114	THR	N-CA-C	-5.18	106.81	113.23
1	N	174	MET	N-CA-C	5.17	117.03	109.84
1	P	12	TYR	N-CA-C	5.16	117.31	111.11
1	J	114	THR	N-CA-C	-5.15	106.84	113.23
1	N	73	GLY	N-CA-C	5.15	119.08	112.18
1	N	198	GLU	N-CA-C	5.14	120.56	113.97
1	J	53	TYR	N-CA-C	5.14	117.31	107.75
1	L	73	GLY	N-CA-C	5.14	119.07	112.18
1	B	199	SER	N-CA-C	5.13	116.87	111.28
1	Q	73	GLY	N-CA-C	5.11	118.41	111.72
1	O	197	MET	N-CA-C	5.10	122.40	114.64
1	G	73	GLY	N-CA-C	5.10	118.40	111.72
1	E	73	GLY	N-CA-C	5.09	119.00	112.18
1	E	128	PRO	N-CA-C	-5.07	103.23	111.14
1	R	114	THR	N-CA-C	-5.07	106.94	113.23
1	H	198	GLU	N-CA-C	5.06	120.45	113.97
1	O	198	GLU	N-CA-C	5.05	120.44	113.97
1	H	225	ARG	N-CA-C	-5.03	105.88	111.36
1	E	53	TYR	N-CA-C	5.02	117.08	107.75
1	K	114	THR	N-CA-C	-5.02	107.01	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	167	GLY	N-CA-C	-5.02	107.84	115.66
1	H	73	GLY	N-CA-C	5.01	118.89	112.18

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	1879	0	1861	24	0
1	B	1879	0	1861	27	0
1	C	1910	0	1884	27	0
1	D	1870	0	1848	30	0
1	E	1870	0	1848	20	0
1	F	1888	0	1867	16	0
1	G	1872	0	1852	28	0
1	H	1879	0	1861	30	0
1	I	1879	0	1861	21	0
1	J	1863	0	1839	22	0
1	K	1870	0	1848	22	0
1	L	1872	0	1852	25	0
1	M	1870	0	1848	35	0
1	N	1872	0	1852	33	0
1	O	1872	0	1852	39	0
1	P	1863	0	1839	33	0
1	Q	1854	0	1819	27	0
1	R	1849	0	1837	35	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	469	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 7.

All (469) 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
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:R:106:LYS:HZ2	1:R:107:GLY:H	1.30	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:P:222:ASN:C	1:P:222:ASN:HD22	1.98	0.71
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:HA	1:L:257:LYS:HE2	1.76	0.67
1:P:237:ASP:OD1	1:P:239:GLU:HG2	1.95	0.67
1:A:222:ASN:C	1:A:222:ASN:HD22	2.03	0.66
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.60	0.66
1:A:27:MET:HE2	1:A:70:THR:HG22	1.78	0.66
1:F:11:GLN:HE21	1:F:83:GLU:HG2	1.61	0.66
1:H:222:ASN:C	1:H:222:ASN:HD22	2.04	0.65
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:C	1:O:222:ASN:HD22	2.05	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:222:ASN:HD21	1:O:224:GLU:HB2	1.60	0.64
1:C:98:CYS:HG	1:C:195:SER:C	2.06	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:R:222:ASN:C	1:R:222:ASN:HD22	2.06	0.63
1:H:27:MET:HE2	1:H:70:THR:HG22	1.80	0.63
1:M:17:ARG:HG2	1:M:20:ASP:OD2	1.99	0.63
1:Q:222:ASN:C	1:Q:222:ASN:HD22	2.07	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:D:173:ARG:HD3	1:D:173:ARG:C	2.24	0.62
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:L:172:GLU:CD	1:L:172:GLU:H	2.08	0.61
1:R:106:LYS:HZ2	1:R:107:GLY:N	1.97	0.61
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:G:222:ASN:C	1:G:222:ASN:HD22	2.09	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:N:234:MET:HE2	1:N:234:MET:O	2.01	0.60
1:I:222:ASN:C	1:I:222:ASN:HD22	2.08	0.60
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:A:27:MET:HE2	1:A:70:THR:CG2	2.32	0.60
1:I:27:MET:HE2	1:I:70:THR:HG22	1.84	0.60
1:D:239:GLU:HG3	1:D:243:GLN:HE21	1.67	0.60
1:M:222:ASN:C	1:M:222:ASN:HD22	2.10	0.60
1:C:98:CYS:SG	1:C:194:ALA:HB1	2.42	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:K:222:ASN:HD22	1:K:222:ASN:C	2.10	0.59
1:H:8:VAL:HG23	1:H:18:PRO:HG2	1.84	0.59
1:L:222:ASN:C	1:L:222:ASN:HD22	2.11	0.59
1:D:222:ASN:C	1:D:222:ASN:HD22	2.11	0.59
1:N:222:ASN:HD21	1:N:224:GLU:HB2	1.67	0.59
1:C:18:PRO:HD2	4:C:2597:HOH:O	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:36:LYS:HE3	1:J:242:ILE:HD12	1.84	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:D:172:GLU:CD	1:D:172:GLU:H	2.13	0.57
1:F:222:ASN:C	1:F:222:ASN:HD22	2.12	0.57
1:R:106:LYS:HE3	1:R:233:PRO:HD2	1.86	0.57
1:I:222:ASN:HD21	1:I:224:GLU:HB2	1.70	0.57
1:B:222:ASN:C	1:B:222:ASN:HD22	2.13	0.56
1:K:234:MET:HE3	1:K:234:MET:O	2.05	0.56
1:H:27:MET:HE2	1:H:70:THR:CG2	2.34	0.56
1:L:27:MET:HE2	1:L:70:THR:CG2	2.35	0.56
1:O:234:MET:H	1:O:234:MET:HE2	1.70	0.56
1:R:162:LYS:HE3	1:R:168:GLN:HB2	1.87	0.56
1:C:222:ASN:C	1:C:222:ASN:HD22	2.13	0.56
1:C:106:LYS:HE3	1:C:225:ARG:NH2	2.20	0.56
1:A:172:GLU:H	1:A:172:GLU:CD	2.14	0.56
1:F:27:MET:HE2	1:F:70:THR:HG22	1.88	0.56
1:M:46:LEU:O	1:M:46:LEU:HD22	2.06	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:E:222:ASN:C	1:E:222:ASN:HD22	2.14	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:N:222:ASN:C	1:N:222:ASN:HD22	2.14	0.55
1:R:110:ILE:HD13	1:R:244:VAL:HG21	1.87	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:HB2	1:J:106:LYS:NZ	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
1:A:222:ASN:HD21	1:A:224:GLU:HB2	1.72	0.54
1:M:137:LEU:HD22	1:M:141:ASN:ND2	2.22	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:B:148:LYS:HE3	1:B:148:LYS:CA	2.37	0.54
1:G:172:GLU:CD	1:G:172:GLU:H	2.16	0.54
1:M:56:TYR:HB2	1:M:67:VAL:CG1	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LYS:NZ	1:A:106:LYS:HB3	2.23	0.54
1:J:222:ASN:C	1:J:222:ASN:HD22	2.16	0.54
1:O:162:LYS:HE3	1:O:168:GLN:OE1	2.08	0.54
1:R:27:MET:HE2	1:R:70:THR:CG2	2.38	0.54
1:E:172:GLU:CD	1:E:172:GLU:H	2.16	0.53
1:C:102:GLU:HG3	1:C:104:ASP:H	1.74	0.53
1:I:27:MET:HE2	1:I:70:THR:CG2	2.38	0.53
1:N:46:LEU:HD23	1:N:46:LEU:C	2.33	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:N:218:LEU:HD13	1:N:218:LEU:C	2.33	0.53
1:G:257:LYS:HD3	1:G:257:LYS:C	2.34	0.53
1:K:239:GLU:HG3	1:K:243:GLN:HE21	1.73	0.53
1:L:27:MET:HE2	1:L:70:THR:HG22	1.89	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:B:148:LYS:HA	1:B:148:LYS:CE	2.40	0.52
1:B:172:GLU:CD	1:B:172:GLU:H	2.17	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: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:R:172:GLU:H	1:R:172:GLU:CD	2.18	0.51
1:M:218:LEU:C	1:M:218:LEU:HD13	2.35	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:J:27:MET:HE2	1:J:70:THR:HG22	1.93	0.51
1:R:106:LYS:HZ1	1:R:107:GLY:H	1.56	0.51
1:O:170:GLU:O	1:O:173:ARG:HG3	2.11	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:222:ASN:ND2	1:O:224:GLU:H	2.09	0.50
1:J:172:GLU:CD	1:J:172:GLU:H	2.19	0.50
1:K:27:MET:HE2	1:K:70:THR:HG22	1.93	0.50
1:B:98:CYS:O	1:B:220:VAL:HG22	2.11	0.50
1:O:27:MET:HE2	1:O:70:THR:HG22	1.94	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:M:61:ASN:ND2	1:M:250:ARG:HG2	2.26	0.50
1:M:234:MET:HE3	1:M:234:MET:O	2.12	0.50
1:N:46:LEU:HD23	1:N:47:VAL:N	2.26	0.50
1:R:106:LYS:NZ	1:R:107:GLY:N	2.48	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:M:46:LEU:HD22	1:M:46:LEU:C	2.36	0.50
1:G:20:ASP:HB3	1:G:47:VAL:HG11	1.93	0.49
1:R:94:ARG:HG3	1:R:94:ARG:HH11	1.76	0.49
1:C:27:MET:HE2	1:C:70:THR:HG22	1.93	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:N:27:MET:HE2	1:N:70:THR:HG22	1.94	0.49
1:R:170:GLU:OE1	1:R:173:ARG:HD3	2.12	0.49
1:G:170:GLU:O	1:G:170:GLU:HG2	2.12	0.49
1:M:27:MET:HE2	1:M:70:THR:HG22	1.94	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:27:MET:HE2	1:J:70:THR:CG2	2.42	0.49
1:N:109:ASP:C	1:N:110:ILE:HD12	2.37	0.49
1:L:137:LEU:HD22	1:L:141:ASN:ND2	2.27	0.49
1:R:106:LYS:HE2	1:R:232:ASN:OD1	2.13	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: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:70:THR:HB	1:G:77:ALA:HA	1.93	0.48
1:G:170:GLU:OE2	1:G:173:ARG:NH1	2.46	0.48
1:I:234:MET:HE3	1:I:236:HIS:CE1	2.48	0.48
1:Q:250:ARG:O	1:Q:254:GLU:HG3	2.14	0.48
1:C:27:MET:HE2	1:C:70:THR:CG2	2.42	0.48
1:N:172:GLU:CD	1:N:172:GLU:H	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:D:173:ARG:HD3	1:D:174:MET:N	2.27	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: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:P:27:MET:HE2	1:P:70:THR:HG22	1.96	0.47
1:D:102:GLU:HG3	1:D:104:ASP:H	1.80	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:Q:172:GLU:CD	1:Q:172:GLU:H	2.22	0.47
1:C:98:CYS:SG	1:C:195:SER:O	2.67	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:M:172:GLU:H	1:M:172:GLU:CD	2.22	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:C:126:TYR:CZ	1:D:174:MET:HE1	2.51	0.46
1:K:102:GLU:HG3	1:K:104:ASP:H	1.79	0.46
1:E:27:MET:HE2	1:E:70:THR:HG22	1.96	0.46
1:N:94:ARG:HG3	1:N:94:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O:126:TYR:CZ	1:P:174:MET:HE1	2.51	0.46
1:R:24:TYR:CE2	1:R:63:GLU:HG2	2.51	0.46
1:R:106:LYS:HG3	1:R:107:GLY:N	2.30	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:O:234:MET:HE2	1:O:234:MET:N	2.31	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:N:27:MET:HE2	1:N:70:THR:CG2	2.46	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:27:MET:HE2	1:O:70:THR:CG2	2.47	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: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:K:172:GLU:H	1:K:172:GLU:CD	2.24	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:K:174:MET:HE1	1:L:126:TYR:CZ	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:Q:27:MET:HE2	1:Q:70:THR:HG22	1.99	0.45
1:H:102:GLU:HG2	4:H:2256:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:35:ALA:O	1:I:39:GLU:HG2	2.16	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: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
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:O:46:LEU:C	1:O:46:LEU:HD23	2.42	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: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:40:HIS:HD2	4:I:1145:HOH:O	2.01	0.43
1:I:222:ASN:ND2	1:I:225:ARG:H	2.15	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:218:LEU:C	1:P:218:LEU:HD13	2.44	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:H:222:ASN:C	1:H:222:ASN:ND2	2.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:Q:234:MET:CE	2.30	0.43
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:M:174:MET:HE1	1:N:126:TYR:CE1	2.53	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:174:MET:HE1	1:D:126:TYR:CZ	2.54	0.42
1:C:222:ASN:ND2	1:C:225:ARG:H	2.17	0.42
1:F:56:TYR:HB2	1:F:67:VAL:CG1	2.49	0.42
1:F:239:GLU:CG	1:F:243:GLN:HE21	2.21	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:M:174:MET:HE1	1:N:126:TYR:CZ	2.54	0.42
1:N:85:LYS:HD3	1:N:85:LYS:C	2.44	0.42
1:C:85:LYS:HD2	4:C:2052:HOH:O	2.20	0.42
1:D:27:MET:HE2	1:D:70:THR:HG22	2.01	0.42
1:O:222:ASN:C	1:O:222:ASN:ND2	2.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:ASN:ND2	1:G:225:ARG:H	2.17	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:56:TYR:HB2	1:N:67:VAL:CG1	2.50	0.42
1:N:222:ASN:ND2	1:N:225:ARG:H	2.18	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:51:ARG:HB3	1:M:52:GLU:OE2	2.20	0.42
1:M:110:ILE:O	1:M:154:SER:HA	2.19	0.42
1:M:175:PRO:HD2	1:N:126:TYR:O	2.20	0.42
1:A:17:ARG:HH11	1:A:17:ARG:CG	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:NZ	1:D:148:LYS:HB3	2.35	0.42
1:G:60:LEU:HD21	1:G:246:VAL:HG13	2.01	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:O:126:TYR:CE1	1:P:174:MET:HE1	2.54	0.42
1:O:257:LYS:HB3	1:O:257:LYS:HZ3	1.85	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:HG3	1:Q:94:ARG:HH11	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:HG3	1:O:94:ARG:HH11	1.85	0.41
1:C:110:ILE:O	1:C:154:SER:HA	2.19	0.41
1:C:126:TYR:CE1	1:D:174:MET:HE1	2.55	0.41
1:D:70:THR:HB	1:D:77:ALA:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ASN:HD22	1:D:224:GLU:N	2.18	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:56:TYR:HB2	1:Q:67:VAL:CG1	2.49	0.41
1:Q:196:GLU:OE2	1:Q:199:SER:HB2	2.20	0.41
1:D:31:PRO:HA	1:D:69:SER:HB3	2.03	0.41
1:G:60:LEU:HD12	1:G:60:LEU:HA	1.92	0.41
1:M:46:LEU:O	1:M:46:LEU:HD13	2.21	0.41
1:O:74:GLY:N	1:O:75:PRO:CD	2.84	0.41
1:P:222:ASN:C	1:P:222:ASN:ND2	2.70	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
1:G:170:GLU:O	1:G:170:GLU:CG	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: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:26:ILE:HG13	1:O:249:LEU:HD11	2.02	0.41
1:O:102:GLU:HG3	1:O:104:ASP:H	1.85	0.41
1:G:126:TYR:CZ	1:H:174:MET:HE1	2.55	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:P:27:MET:HE2	1:P:70:THR:CG2	2.51	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: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:H:11:GLN:NE2	1:H:86:LEU:HD12	2.36	0.41
1:I:126:TYR:CZ	1:J:174:MET:HE1	2.56	0.41
1:I:162:LYS:HE3	1:I:168:GLN:OE1	2.21	0.41
1:J:102:GLU:CG	1:J:105:VAL:HG23	2.50	0.41
1:O:31:PRO:HA	1:O:69:SER:HB3	2.01	0.41
1:Q:31:PRO:HA	1:Q:69:SER:HB3	2.02	0.41
1:B:162:LYS:HE3	1:B:168:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:27:MET:HE2	1:F:70:THR:CG2	2.50	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:M:126:TYR:CE1	1:N:174:MET:HE1	2.56	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:40:HIS:HD2	4:F:279:HOH:O	2.03	0.40
1:F:254:GLU:HG2	4:F:2582:HOH:O	2.21	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:HH11	1:P:225:ARG:HB3	1.85	0.40
1:R:26:ILE:HG13	1:R:249:LEU:HD11	2.03	0.40
1:B:14:LEU:HD23	1:B:14:LEU:N	2.36	0.40
1:D:74:GLY:N	1:D:75:PRO:CD	2.84	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:40:HIS:HD2	4:O:1940:HOH:O	2.04	0.40
1:O:222:ASN:ND2	1:O:224:GLU:N	2.69	0.40
1:C:98:CYS:SG	1:C:195:SER:C	3.02	0.40
1:Q:106:LYS:HB3	4:Q:2290:HOH:O	2.22	0.40
1:Q:231:ASP:C	1:Q:233:PRO:HD3	2.46	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
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%)	35	17
1	B	196/224 (88%)	191 (97%)	5 (3%)	40	23
1	C	199/224 (89%)	195 (98%)	4 (2%)	48	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	195/224 (87%)	191 (98%)	4 (2%)	47	32
1	E	195/224 (87%)	193 (99%)	2 (1%)	68	60
1	F	197/224 (88%)	194 (98%)	3 (2%)	57	46
1	G	195/224 (87%)	188 (96%)	7 (4%)	31	13
1	H	196/224 (88%)	193 (98%)	3 (2%)	57	46
1	I	196/224 (88%)	190 (97%)	6 (3%)	35	17
1	J	194/224 (87%)	189 (97%)	5 (3%)	40	23
1	K	195/224 (87%)	190 (97%)	5 (3%)	40	23
1	L	195/224 (87%)	190 (97%)	5 (3%)	40	23
1	M	195/224 (87%)	188 (96%)	7 (4%)	31	13
1	N	195/224 (87%)	192 (98%)	3 (2%)	57	46
1	O	195/224 (87%)	188 (96%)	7 (4%)	31	13
1	P	194/224 (87%)	189 (97%)	5 (3%)	40	23
1	Q	192/224 (86%)	187 (97%)	5 (3%)	40	23
1	R	193/224 (86%)	190 (98%)	3 (2%)	55	44
All	All	3513/4032 (87%)	3428 (98%)	85 (2%)	43	27

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	17	ARG
1	A	106	LYS
1	A	120	GLU
1	A	137	LEU
1	A	222	ASN
1	B	14	LEU
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	202	LEU
1	C	222	ASN
1	D	120	GLU
1	D	137	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	173	ARG
1	D	222	ASN
1	E	120	GLU
1	E	222	ASN
1	F	14	LEU
1	F	120	GLU
1	F	222	ASN
1	G	14	LEU
1	G	104	ASP
1	G	120	GLU
1	G	170	GLU
1	G	209	LEU
1	G	222	ASN
1	G	257	LYS
1	H	120	GLU
1	H	218	LEU
1	H	222	ASN
1	I	14	LEU
1	I	36	LYS
1	I	120	GLU
1	I	137	LEU
1	I	222	ASN
1	I	255	ASN
1	J	14	LEU
1	J	106	LYS
1	J	120	GLU
1	J	137	LEU
1	J	222	ASN
1	K	14	LEU
1	K	120	GLU
1	K	137	LEU
1	K	202	LEU
1	K	222	ASN
1	L	14	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	218	LEU
1	M	222	ASN
1	M	239	GLU
1	N	120	GLU
1	N	222	ASN
1	N	234	MET
1	O	36	LYS
1	O	120	GLU
1	O	137	LEU
1	O	222	ASN
1	O	234	MET
1	O	239	GLU
1	O	257	LYS
1	P	14	LEU
1	P	120	GLU
1	P	137	LEU
1	P	202	LEU
1	P	222	ASN
1	Q	120	GLU
1	Q	137	LEU
1	Q	170	GLU
1	Q	222	ASN
1	Q	234	MET
1	R	106	LYS
1	R	120	GLU
1	R	222	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	40	HIS
1	A	43	ASN
1	A	61	ASN
1	A	141	ASN
1	A	222	ASN
1	A	255	ASN
1	B	222	ASN
1	C	15	GLN
1	C	141	ASN
1	C	222	ASN
1	C	226	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	243	GLN
1	C	255	ASN
1	D	145	ASN
1	D	222	ASN
1	D	232	ASN
1	D	243	GLN
1	D	255	ASN
1	E	11	GLN
1	E	15	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	226	ASN
1	F	243	GLN
1	F	255	ASN
1	G	11	GLN
1	G	40	HIS
1	G	222	ASN
1	G	243	GLN
1	H	11	GLN
1	H	40	HIS
1	H	43	ASN
1	H	61	ASN
1	H	169	HIS
1	H	222	ASN
1	H	243	GLN
1	I	11	GLN
1	I	222	ASN
1	I	236	HIS
1	I	255	ASN
1	J	11	GLN
1	J	40	HIS
1	J	145	ASN
1	J	222	ASN
1	J	226	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	232	ASN
1	J	243	GLN
1	J	255	ASN
1	K	11	GLN
1	K	40	HIS
1	K	61	ASN
1	K	145	ASN
1	K	222	ASN
1	K	226	ASN
1	K	255	ASN
1	L	11	GLN
1	L	40	HIS
1	L	145	ASN
1	L	222	ASN
1	L	226	ASN
1	L	243	GLN
1	M	61	ASN
1	M	169	HIS
1	M	208	HIS
1	M	222	ASN
1	N	15	GLN
1	N	222	ASN
1	N	243	GLN
1	N	255	ASN
1	O	40	HIS
1	O	169	HIS
1	O	222	ASN
1	O	226	ASN
1	P	141	ASN
1	P	145	ASN
1	P	222	ASN
1	Q	11	GLN
1	Q	141	ASN
1	Q	145	ASN
1	Q	222	ASN
1	Q	223	GLN
1	Q	243	GLN
1	Q	255	ASN
1	R	15	GLN
1	R	40	HIS
1	R	145	ASN
1	R	208	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	222	ASN
1	R	243	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	R1P	O	1254	-	13,14,14	0.93	0	21,21,21	0.85	1 (4%)
3	URA	C	1255	-	8,8,8	1.95	3 (37%)	10,10,10	3.15	6 (60%)
3	URA	K	1255	-	8,8,8	1.94	2 (25%)	10,10,10	3.19	6 (60%)
2	R1P	B	1254	-	13,14,14	0.93	0	21,21,21	0.92	2 (9%)
3	URA	D	1255	-	8,8,8	1.92	3 (37%)	10,10,10	3.17	6 (60%)
3	URA	L	1255	-	8,8,8	1.93	3 (37%)	10,10,10	3.17	6 (60%)
3	URA	R	1255	-	8,8,8	1.93	2 (25%)	10,10,10	3.17	6 (60%)
2	R1P	Q	1254	-	13,14,14	0.93	0	21,21,21	0.79	1 (4%)
2	R1P	E	1254	-	13,14,14	0.93	0	21,21,21	0.86	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	URA	J	1255	-	8,8,8	1.93	3 (37%)	10,10,10	3.14	6 (60%)
2	R1P	J	1254	-	13,14,14	0.94	0	21,21,21	0.86	1 (4%)
3	URA	G	1255	-	8,8,8	1.93	2 (25%)	10,10,10	3.11	6 (60%)
2	R1P	M	1254	-	13,14,14	0.92	0	21,21,21	0.89	1 (4%)
3	URA	M	1255	-	8,8,8	1.91	2 (25%)	10,10,10	3.17	6 (60%)
3	URA	N	1255	-	8,8,8	1.93	2 (25%)	10,10,10	3.18	6 (60%)
2	R1P	H	1254	-	13,14,14	0.92	0	21,21,21	0.83	1 (4%)
3	URA	H	1255	-	8,8,8	1.94	3 (37%)	10,10,10	3.18	6 (60%)
3	URA	O	1255	-	8,8,8	1.94	3 (37%)	10,10,10	3.17	6 (60%)
3	URA	Q	1255	-	8,8,8	1.92	2 (25%)	10,10,10	3.16	6 (60%)
3	URA	B	1255	-	8,8,8	1.93	3 (37%)	10,10,10	3.16	6 (60%)
3	URA	F	1255	-	8,8,8	1.94	3 (37%)	10,10,10	3.14	6 (60%)
2	R1P	L	1254	-	13,14,14	0.93	0	21,21,21	0.86	1 (4%)
2	R1P	R	1254	-	13,14,14	0.92	0	21,21,21	0.93	1 (4%)
2	R1P	C	1254	-	13,14,14	0.93	0	21,21,21	0.86	1 (4%)
2	R1P	D	1254	-	13,14,14	0.93	0	21,21,21	0.84	1 (4%)
3	URA	I	1255	-	8,8,8	1.93	2 (25%)	10,10,10	3.18	6 (60%)
2	R1P	F	1254	-	13,14,14	0.93	0	21,21,21	0.84	1 (4%)
3	URA	A	1255	-	8,8,8	1.94	2 (25%)	10,10,10	3.16	6 (60%)
2	R1P	G	1254	-	13,14,14	0.93	0	21,21,21	0.84	1 (4%)
2	R1P	K	1254	-	13,14,14	0.93	0	21,21,21	0.84	1 (4%)
3	URA	P	1255	-	8,8,8	1.92	3 (37%)	10,10,10	3.17	6 (60%)
2	R1P	P	1254	-	13,14,14	0.93	0	21,21,21	0.88	1 (4%)
2	R1P	N	1254	-	13,14,14	0.92	0	21,21,21	0.88	1 (4%)
2	R1P	A	1254	-	13,14,14	0.94	0	21,21,21	0.84	1 (4%)
2	R1P	I	1254	-	13,14,14	0.93	0	21,21,21	0.85	1 (4%)
3	URA	E	1255	-	8,8,8	1.94	2 (25%)	10,10,10	3.15	6 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	R1P	O	1254	-	-	0/6/23/23	0/1/1/1
3	URA	C	1255	-	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	URA	K	1255	-	-	-	0/1/1/1
2	R1P	B	1254	-	-	0/6/23/23	0/1/1/1
3	URA	D	1255	-	-	-	0/1/1/1
3	URA	L	1255	-	-	-	0/1/1/1
3	URA	R	1255	-	-	-	0/1/1/1
2	R1P	Q	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	E	1254	-	-	0/6/23/23	0/1/1/1
3	URA	J	1255	-	-	-	0/1/1/1
2	R1P	J	1254	-	-	0/6/23/23	0/1/1/1
3	URA	G	1255	-	-	-	0/1/1/1
2	R1P	M	1254	-	-	2/6/23/23	0/1/1/1
3	URA	M	1255	-	-	-	0/1/1/1
3	URA	N	1255	-	-	-	0/1/1/1
2	R1P	H	1254	-	-	1/6/23/23	0/1/1/1
3	URA	H	1255	-	-	-	0/1/1/1
3	URA	O	1255	-	-	-	0/1/1/1
3	URA	Q	1255	-	-	-	0/1/1/1
3	URA	B	1255	-	-	-	0/1/1/1
3	URA	F	1255	-	-	-	0/1/1/1
2	R1P	L	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	R	1254	-	-	2/6/23/23	0/1/1/1
2	R1P	C	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	D	1254	-	-	0/6/23/23	0/1/1/1
3	URA	I	1255	-	-	-	0/1/1/1
2	R1P	F	1254	-	-	0/6/23/23	0/1/1/1
3	URA	A	1255	-	-	-	0/1/1/1
2	R1P	G	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	K	1254	-	-	0/6/23/23	0/1/1/1
3	URA	P	1255	-	-	-	0/1/1/1
2	R1P	P	1254	-	-	1/6/23/23	0/1/1/1
2	R1P	N	1254	-	-	2/6/23/23	0/1/1/1
2	R1P	A	1254	-	-	0/6/23/23	0/1/1/1
2	R1P	I	1254	-	-	0/6/23/23	0/1/1/1
3	URA	E	1255	-	-	-	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1255	URA	C6-N1	3.04	1.40	1.36
3	O	1255	URA	C6-N1	3.03	1.40	1.36
3	C	1255	URA	C6-N1	3.02	1.40	1.36
3	K	1255	URA	C6-N1	3.00	1.40	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1255	URA	C6-N1	3.00	1.40	1.36
3	J	1255	URA	C6-N1	3.00	1.40	1.36
3	R	1255	URA	C6-N1	3.00	1.40	1.36
3	H	1255	URA	C6-N1	2.99	1.40	1.36
3	M	1255	URA	C6-N1	2.99	1.40	1.36
3	Q	1255	URA	C6-N1	2.99	1.40	1.36
3	I	1255	URA	C6-N1	2.99	1.40	1.36
3	N	1255	URA	C6-N1	2.98	1.40	1.36
3	G	1255	URA	C6-N1	2.97	1.40	1.36
3	A	1255	URA	C2-N1	2.97	1.40	1.36
3	F	1255	URA	C6-N1	2.97	1.40	1.36
3	A	1255	URA	C6-N1	2.97	1.40	1.36
3	C	1255	URA	C2-N1	2.96	1.40	1.36
3	B	1255	URA	C6-N1	2.96	1.40	1.36
3	H	1255	URA	C2-N1	2.96	1.40	1.36
3	F	1255	URA	C2-N1	2.95	1.40	1.36
3	D	1255	URA	C6-N1	2.94	1.40	1.36
3	P	1255	URA	C6-N1	2.94	1.40	1.36
3	D	1255	URA	C2-N1	2.92	1.40	1.36
3	B	1255	URA	C2-N1	2.91	1.40	1.36
3	G	1255	URA	C2-N1	2.91	1.40	1.36
3	Q	1255	URA	C2-N1	2.91	1.40	1.36
3	J	1255	URA	C2-N1	2.91	1.40	1.36
3	E	1255	URA	C2-N1	2.90	1.40	1.36
3	I	1255	URA	C2-N1	2.90	1.40	1.36
3	R	1255	URA	C2-N1	2.90	1.40	1.36
3	N	1255	URA	C2-N1	2.89	1.40	1.36
3	O	1255	URA	C2-N1	2.89	1.40	1.36
3	L	1255	URA	C2-N1	2.89	1.40	1.36
3	P	1255	URA	C2-N1	2.89	1.40	1.36
3	K	1255	URA	C2-N1	2.88	1.40	1.36
3	M	1255	URA	C2-N1	2.84	1.40	1.36
3	L	1255	URA	C6-C5	2.05	1.39	1.35
3	F	1255	URA	C6-C5	2.02	1.39	1.35
3	O	1255	URA	C6-C5	2.02	1.39	1.35
3	D	1255	URA	C6-C5	2.01	1.39	1.35
3	H	1255	URA	C6-C5	2.01	1.39	1.35
3	B	1255	URA	C6-C5	2.01	1.39	1.35
3	J	1255	URA	C6-C5	2.01	1.39	1.35
3	P	1255	URA	C6-C5	2.01	1.39	1.35
3	C	1255	URA	C6-C5	2.00	1.39	1.35

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1255	URA	C4-N3-C2	-5.77	119.96	125.55
3	D	1255	URA	C4-N3-C2	-5.76	119.97	125.55
3	I	1255	URA	C4-N3-C2	-5.76	119.97	125.55
3	R	1255	URA	C4-N3-C2	-5.75	119.97	125.55
3	N	1255	URA	C4-N3-C2	-5.72	120.00	125.55
3	P	1255	URA	C4-N3-C2	-5.72	120.00	125.55
3	M	1255	URA	C4-N3-C2	-5.72	120.00	125.55
3	L	1255	URA	C4-N3-C2	-5.72	120.00	125.55
3	H	1255	URA	C4-N3-C2	-5.72	120.01	125.55
3	E	1255	URA	C4-N3-C2	-5.70	120.02	125.55
3	F	1255	URA	C4-N3-C2	-5.68	120.04	125.55
3	B	1255	URA	C4-N3-C2	-5.67	120.05	125.55
3	O	1255	URA	C4-N3-C2	-5.66	120.06	125.55
3	A	1255	URA	C4-N3-C2	-5.66	120.07	125.55
3	C	1255	URA	C4-N3-C2	-5.65	120.07	125.55
3	J	1255	URA	C4-N3-C2	-5.65	120.08	125.55
3	Q	1255	URA	C4-N3-C2	-5.63	120.09	125.55
3	G	1255	URA	C4-N3-C2	-5.56	120.16	125.55
3	H	1255	URA	N1-C2-N3	4.32	119.72	115.17
3	K	1255	URA	N1-C2-N3	4.31	119.72	115.17
3	Q	1255	URA	C6-N1-C2	-4.31	119.75	122.40
3	N	1255	URA	N1-C2-N3	4.30	119.70	115.17
3	I	1255	URA	N1-C2-N3	4.29	119.69	115.17
3	O	1255	URA	N1-C2-N3	4.28	119.69	115.17
3	O	1255	URA	C6-N1-C2	-4.28	119.77	122.40
3	Q	1255	URA	N1-C2-N3	4.28	119.68	115.17
3	B	1255	URA	C6-N1-C2	-4.27	119.78	122.40
3	B	1255	URA	N1-C2-N3	4.27	119.67	115.17
3	R	1255	URA	N1-C2-N3	4.26	119.66	115.17
3	M	1255	URA	N1-C2-N3	4.25	119.65	115.17
3	P	1255	URA	N1-C2-N3	4.25	119.65	115.17
3	L	1255	URA	N1-C2-N3	4.25	119.65	115.17
3	D	1255	URA	N1-C2-N3	4.25	119.65	115.17
3	H	1255	URA	C6-N1-C2	-4.24	119.80	122.40
3	E	1255	URA	N1-C2-N3	4.23	119.63	115.17
3	A	1255	URA	C6-N1-C2	-4.23	119.81	122.40
3	K	1255	URA	C6-N1-C2	-4.23	119.81	122.40
3	A	1255	URA	N1-C2-N3	4.22	119.62	115.17
3	C	1255	URA	C6-N1-C2	-4.22	119.81	122.40
3	J	1255	URA	N1-C2-N3	4.22	119.62	115.17
3	F	1255	URA	N1-C2-N3	4.21	119.61	115.17
3	J	1255	URA	C6-N1-C2	-4.20	119.82	122.40
3	C	1255	URA	N1-C2-N3	4.19	119.59	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1255	URA	C6-N1-C2	-4.17	119.84	122.40
3	G	1255	URA	N1-C2-N3	4.16	119.55	115.17
3	G	1255	URA	C6-N1-C2	-4.16	119.85	122.40
3	P	1255	URA	C6-N1-C2	-4.14	119.86	122.40
3	I	1255	URA	C6-N1-C2	-4.14	119.86	122.40
3	M	1255	URA	C6-N1-C2	-4.13	119.86	122.40
3	F	1255	URA	C6-N1-C2	-4.11	119.88	122.40
3	R	1255	URA	C6-N1-C2	-4.11	119.88	122.40
3	E	1255	URA	C6-N1-C2	-4.10	119.88	122.40
3	L	1255	URA	C6-N1-C2	-4.05	119.91	122.40
3	D	1255	URA	C6-N1-C2	-4.05	119.91	122.40
3	D	1255	URA	C5-C4-N3	3.86	120.20	114.80
3	C	1255	URA	C5-C4-N3	3.85	120.19	114.80
3	M	1255	URA	C5-C4-N3	3.83	120.17	114.80
3	L	1255	URA	C5-C4-N3	3.83	120.17	114.80
3	E	1255	URA	C5-C4-N3	3.82	120.15	114.80
3	J	1255	URA	C5-C4-N3	3.82	120.15	114.80
3	F	1255	URA	C5-C4-N3	3.81	120.14	114.80
3	I	1255	URA	C5-C4-N3	3.81	120.14	114.80
3	P	1255	URA	C5-C4-N3	3.81	120.13	114.80
3	R	1255	URA	C5-C4-N3	3.80	120.13	114.80
3	A	1255	URA	C5-C4-N3	3.80	120.12	114.80
3	B	1255	URA	C5-C4-N3	3.80	120.12	114.80
3	K	1255	URA	C5-C4-N3	3.79	120.11	114.80
3	N	1255	URA	C5-C4-N3	3.77	120.08	114.80
3	O	1255	URA	C5-C4-N3	3.77	120.08	114.80
3	H	1255	URA	C5-C4-N3	3.77	120.08	114.80
3	G	1255	URA	C5-C4-N3	3.74	120.04	114.80
3	Q	1255	URA	C5-C4-N3	3.74	120.04	114.80
3	L	1255	URA	O4-C4-C5	-3.04	119.92	125.16
3	D	1255	URA	O4-C4-C5	-3.03	119.93	125.16
3	C	1255	URA	O4-C4-C5	-3.03	119.94	125.16
3	A	1255	URA	O4-C4-C5	-3.02	119.95	125.16
3	P	1255	URA	O4-C4-C5	-3.02	119.95	125.16
3	I	1255	URA	O4-C4-C5	-3.01	119.96	125.16
3	R	1255	URA	O4-C4-C5	-3.01	119.97	125.16
3	N	1255	URA	O4-C4-C5	-3.01	119.97	125.16
3	M	1255	URA	O4-C4-C5	-3.01	119.97	125.16
3	E	1255	URA	O4-C4-C5	-3.00	120.00	125.16
3	F	1255	URA	O4-C4-C5	-2.98	120.02	125.16
3	O	1255	URA	O4-C4-C5	-2.98	120.02	125.16
3	G	1255	URA	O4-C4-C5	-2.98	120.03	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1255	URA	O4-C4-C5	-2.97	120.04	125.16
3	B	1255	URA	O4-C4-C5	-2.95	120.08	125.16
3	Q	1255	URA	O4-C4-C5	-2.94	120.09	125.16
3	H	1255	URA	O4-C4-C5	-2.94	120.09	125.16
3	K	1255	URA	O4-C4-C5	-2.93	120.11	125.16
2	R	1254	R1P	C2-C3-C4	-2.67	97.46	102.61
2	M	1254	R1P	C2-C3-C4	-2.64	97.52	102.61
3	N	1255	URA	O2-C2-N1	-2.60	120.11	122.79
2	P	1254	R1P	C2-C3-C4	-2.58	97.62	102.61
3	L	1255	URA	O2-C2-N1	-2.58	120.13	122.79
3	A	1255	URA	O2-C2-N1	-2.57	120.13	122.79
2	B	1254	R1P	C2-C3-C4	-2.57	97.64	102.61
3	I	1255	URA	O2-C2-N1	-2.53	120.18	122.79
2	O	1254	R1P	C2-C3-C4	-2.52	97.73	102.61
2	C	1254	R1P	C2-C3-C4	-2.52	97.74	102.61
3	H	1255	URA	O2-C2-N1	-2.52	120.19	122.79
3	R	1255	URA	O2-C2-N1	-2.51	120.20	122.79
2	G	1254	R1P	C2-C3-C4	-2.50	97.78	102.61
2	J	1254	R1P	C2-C3-C4	-2.48	97.82	102.61
3	E	1255	URA	O2-C2-N1	-2.48	120.23	122.79
3	M	1255	URA	O2-C2-N1	-2.47	120.24	122.79
3	K	1255	URA	O2-C2-N1	-2.47	120.24	122.79
3	P	1255	URA	O2-C2-N1	-2.47	120.24	122.79
3	D	1255	URA	O2-C2-N1	-2.47	120.24	122.79
2	L	1254	R1P	C2-C3-C4	-2.46	97.86	102.61
2	A	1254	R1P	C2-C3-C4	-2.45	97.88	102.61
3	O	1255	URA	O2-C2-N1	-2.45	120.26	122.79
3	Q	1255	URA	O2-C2-N1	-2.45	120.27	122.79
2	E	1254	R1P	C2-C3-C4	-2.44	97.89	102.61
3	G	1255	URA	O2-C2-N1	-2.43	120.28	122.79
3	J	1255	URA	O2-C2-N1	-2.42	120.29	122.79
2	I	1254	R1P	C2-C3-C4	-2.42	97.93	102.61
2	N	1254	R1P	C2-C3-C4	-2.42	97.94	102.61
3	C	1255	URA	O2-C2-N1	-2.41	120.31	122.79
3	B	1255	URA	O2-C2-N1	-2.38	120.33	122.79
3	F	1255	URA	O2-C2-N1	-2.35	120.36	122.79
2	D	1254	R1P	C2-C3-C4	-2.34	98.08	102.61
2	K	1254	R1P	C2-C3-C4	-2.34	98.08	102.61
2	H	1254	R1P	C2-C3-C4	-2.33	98.11	102.61
2	Q	1254	R1P	C2-C3-C4	-2.28	98.20	102.61
2	F	1254	R1P	C2-C3-C4	-2.26	98.23	102.61
2	B	1254	R1P	O1-C1-C2	2.02	109.93	106.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/282 (88%)	-0.21	5 (2%) 65 71	4, 10, 24, 35	0
1	B	250/282 (88%)	-0.29	5 (2%) 65 71	4, 10, 22, 31	0
1	C	254/282 (90%)	-0.38	3 (1%) 76 82	3, 8, 19, 30	0
1	D	249/282 (88%)	-0.26	4 (1%) 70 77	3, 9, 23, 34	0
1	E	249/282 (88%)	-0.36	3 (1%) 76 82	4, 9, 20, 28	0
1	F	251/282 (89%)	-0.33	7 (2%) 55 60	4, 9, 21, 37	0
1	G	249/282 (88%)	-0.23	4 (1%) 70 77	4, 10, 21, 32	0
1	H	250/282 (88%)	-0.11	9 (3%) 46 53	4, 11, 25, 36	0
1	I	250/282 (88%)	-0.28	5 (2%) 65 71	4, 10, 24, 34	0
1	J	248/282 (87%)	-0.38	4 (1%) 70 77	3, 9, 19, 28	0
1	K	249/282 (88%)	-0.30	3 (1%) 76 82	3, 9, 21, 30	0
1	L	249/282 (88%)	-0.34	3 (1%) 76 82	3, 9, 20, 32	0
1	M	249/282 (88%)	0.21	11 (4%) 39 45	9, 16, 29, 35	0
1	N	249/282 (88%)	0.28	18 (7%) 21 24	8, 16, 32, 43	0
1	O	249/282 (88%)	0.21	10 (4%) 42 48	8, 16, 31, 38	0
1	P	248/282 (87%)	0.36	16 (6%) 25 28	8, 17, 34, 45	0
1	Q	248/282 (87%)	-0.10	5 (2%) 65 71	7, 13, 25, 37	0
1	R	246/282 (87%)	0.12	11 (4%) 38 44	7, 14, 31, 46	0
All	All	4487/5076 (88%)	-0.13	126 (2%) 55 60	3, 11, 26, 46	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	12	TYR	6.6
1	R	234	MET	6.2
1	P	234	MET	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	236	HIS	5.8
1	K	234	MET	5.6
1	L	234	MET	5.2
1	I	234	MET	5.1
1	H	170	GLU	5.1
1	O	234	MET	5.1
1	P	235	ALA	5.0
1	N	234	MET	4.9
1	M	46	LEU	4.8
1	D	256	ASP	4.7
1	C	98	CYS	4.4
1	N	231	ASP	4.3
1	A	231	ASP	4.2
1	R	61	ASN	4.1
1	F	170	GLU	4.0
1	G	104	ASP	4.0
1	P	237	ASP	4.0
1	G	170	GLU	4.0
1	R	231	ASP	3.9
1	P	231	ASP	3.9
1	M	234	MET	3.9
1	N	39	GLU	3.9
1	M	170	GLU	3.9
1	G	234	MET	3.9
1	M	12	TYR	3.8
1	F	7	GLU	3.7
1	H	236	HIS	3.7
1	C	234	MET	3.7
1	N	170	GLU	3.6
1	H	8	VAL	3.6
1	O	239	GLU	3.4
1	N	254	GLU	3.4
1	Q	170	GLU	3.4
1	L	257	LYS	3.4
1	N	239	GLU	3.4
1	F	234	MET	3.4
1	Q	9	GLY	3.3
1	E	231	ASP	3.3
1	H	231	ASP	3.3
1	M	32	LYS	3.2
1	I	236	HIS	3.2
1	H	234	MET	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	233	PRO	3.1
1	I	231	ASP	3.1
1	F	257	LYS	3.1
1	A	43	ASN	3.1
1	N	236	HIS	3.1
1	R	170	GLU	3.1
1	R	106	LYS	3.1
1	J	231	ASP	3.0
1	K	170	GLU	3.0
1	F	236	HIS	3.0
1	E	170	GLU	2.9
1	O	170	GLU	2.9
1	N	235	ALA	2.9
1	N	104	ASP	2.9
1	R	239	GLU	2.9
1	R	232	ASN	2.8
1	M	17	ARG	2.8
1	A	234	MET	2.8
1	P	148	LYS	2.8
1	O	231	ASP	2.8
1	R	228	LEU	2.8
1	M	39	GLU	2.8
1	L	231	ASP	2.8
1	N	237	ASP	2.8
1	R	8	VAL	2.8
1	H	61	ASN	2.7
1	M	36	LYS	2.7
1	P	227	ALA	2.7
1	N	229	GLY	2.7
1	J	234	MET	2.7
1	P	225	ARG	2.7
1	A	233	PRO	2.7
1	P	170	GLU	2.7
1	O	257	LYS	2.6
1	Q	10	LEU	2.6
1	D	234	MET	2.6
1	Q	254	GLU	2.6
1	G	257	LYS	2.6
1	Q	234	MET	2.5
1	F	231	ASP	2.5
1	H	233	PRO	2.5
1	O	61	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	231	ASP	2.5
1	P	239	GLU	2.4
1	P	238	THR	2.4
1	N	220	VAL	2.4
1	B	236	HIS	2.4
1	M	8	VAL	2.4
1	R	229	GLY	2.4
1	B	234	MET	2.4
1	B	104	ASP	2.3
1	K	256	ASP	2.3
1	J	170	GLU	2.3
1	O	235	ALA	2.3
1	M	256	ASP	2.3
1	C	231	ASP	2.3
1	B	170	GLU	2.3
1	P	36	LYS	2.3
1	P	106	LYS	2.3
1	N	153	THR	2.3
1	I	8	VAL	2.2
1	D	236	HIS	2.2
1	P	240	ALA	2.2
1	N	173	ARG	2.2
1	H	23	ARG	2.2
1	N	233	PRO	2.1
1	M	61	ASN	2.1
1	N	238	THR	2.1
1	H	39	GLU	2.1
1	O	102	GLU	2.1
1	N	14	LEU	2.1
1	I	36	LYS	2.1
1	E	234	MET	2.1
1	A	236	HIS	2.1
1	B	231	ASP	2.1
1	F	237	ASP	2.1
1	J	102	GLU	2.0
1	O	60	LEU	2.0
1	O	256	ASP	2.0
1	P	233	PRO	2.0
1	N	225	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	R1P	R	1254	14/14	0.80	0.17	36,38,40,40	0
2	R1P	P	1254	14/14	0.85	0.14	26,30,31,32	0
2	R1P	N	1254	14/14	0.89	0.13	24,25,26,27	0
2	R1P	O	1254	14/14	0.93	0.09	16,20,21,22	0
2	R1P	M	1254	14/14	0.93	0.10	18,21,23,23	0
2	R1P	H	1254	14/14	0.93	0.09	16,18,19,20	0
2	R1P	E	1254	14/14	0.94	0.09	10,15,18,19	0
2	R1P	G	1254	14/14	0.94	0.10	14,18,19,20	0
2	R1P	A	1254	14/14	0.94	0.09	13,18,19,19	0
2	R1P	I	1254	14/14	0.94	0.09	10,14,15,16	0
2	R1P	L	1254	14/14	0.94	0.09	12,15,17,17	0
2	R1P	B	1254	14/14	0.95	0.08	13,16,17,18	0
2	R1P	J	1254	14/14	0.95	0.07	11,14,17,17	0
2	R1P	K	1254	14/14	0.95	0.08	10,13,14,16	0
3	URA	C	1255	8/8	0.95	0.07	8,11,12,14	0
3	URA	M	1255	8/8	0.95	0.06	15,17,18,18	0
3	URA	O	1255	8/8	0.95	0.07	16,18,18,19	0
3	URA	P	1255	8/8	0.95	0.08	17,19,19,20	0
3	URA	R	1255	8/8	0.95	0.07	19,22,22,23	0
3	URA	E	1255	8/8	0.96	0.06	10,12,13,16	0
3	URA	F	1255	8/8	0.96	0.06	8,10,12,14	0
3	URA	H	1255	8/8	0.96	0.06	9,12,15,15	0
3	URA	J	1255	8/8	0.96	0.06	9,11,13,14	0
2	R1P	D	1254	14/14	0.96	0.07	9,12,14,15	0
3	URA	N	1255	8/8	0.96	0.06	19,21,22,22	0
2	R1P	Q	1254	14/14	0.96	0.07	10,13,14,14	0
2	R1P	C	1254	14/14	0.96	0.07	11,15,18,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	URA	Q	1255	8/8	0.96	0.06	11,12,13,14	0
2	R1P	F	1254	14/14	0.96	0.07	9,11,13,15	0
3	URA	G	1255	8/8	0.97	0.06	10,14,15,17	0
3	URA	D	1255	8/8	0.97	0.05	9,11,13,14	0
3	URA	I	1255	8/8	0.97	0.05	12,14,15,16	0
3	URA	B	1255	8/8	0.97	0.06	11,15,15,16	0
3	URA	A	1255	8/8	0.97	0.05	10,11,13,13	0
3	URA	K	1255	8/8	0.98	0.05	8,12,13,16	0
3	URA	L	1255	8/8	0.98	0.04	10,11,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.