



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:33 AM GMT

PDB ID : 2HWU  
Title : Crystal structure of the uridine phosphorylase from Salmonella typhimurium  
in complex with uridine and phosphate ion at 2.91Å resolution  
Authors : Timofeev, V.I.; Gabdulkhakov, A.G.; Dontsova, M.V.; Mikhailov, A.M.  
Deposited on : 2006-08-02  
Resolution : 2.91 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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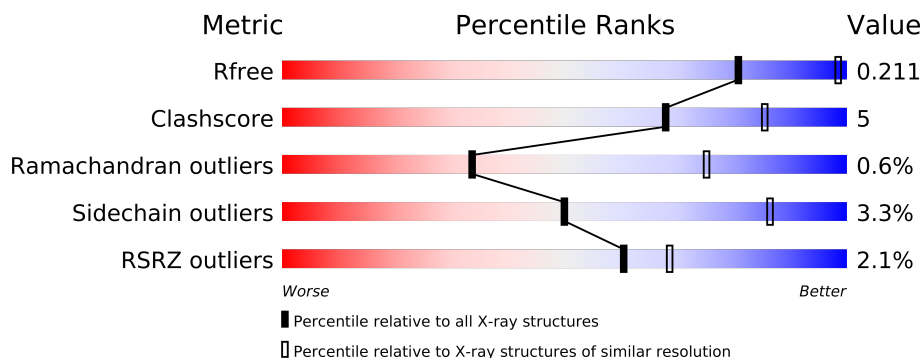
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.91 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))
$R_{free}$	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	253	
1	B	253	
1	C	253	
1	D	253	
1	E	253	
1	F	253	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	A	1	-	X

## 2 Entry composition

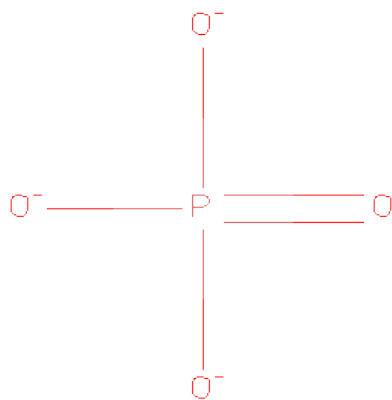
There are 4 unique types of molecules in this entry. The entry contains 11194 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

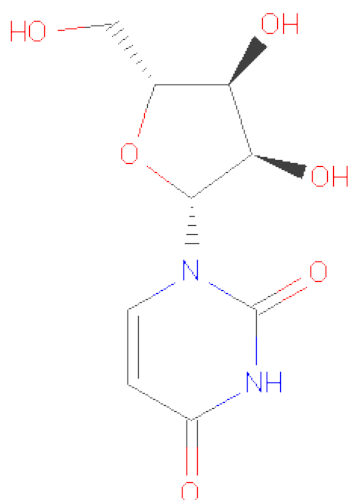
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1900	1188	334	365	13			
1	B	242	Total	C	N	O	S	0	1	0
			1816	1138	320	347	11			
1	C	243	Total	C	N	O	S	0	1	0
			1825	1143	322	348	12			
1	D	244	Total	C	N	O	S	0	0	0
			1833	1147	323	351	12			
1	E	242	Total	C	N	O	S	0	0	0
			1815	1136	321	347	11			
1	F	242	Total	C	N	O	S	0	1	0
			1816	1139	320	346	11			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is URIDINE (three-letter code: URI) (formula:  $C_9H_{12}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	2	6		
3	B	1	Total	C	N	O	0	0
			17	9	2	6		
3	C	1	Total	C	N	O	0	0
			17	9	2	6		
3	D	1	Total	C	N	O	0	0
			17	9	2	6		
3	E	1	Total	C	N	O	0	0
			17	9	2	6		
3	F	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	18	Total	O	0	0
			18	18		
4	C	13	Total	O	0	0
			13	13		

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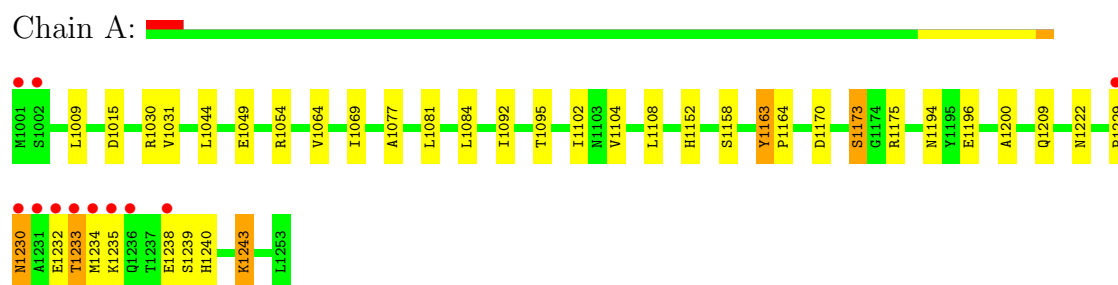
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	11	Total 11	O 11	0	0
4	E	14	Total 14	O 14	0	0
4	F	12	Total 12	O 12	0	0

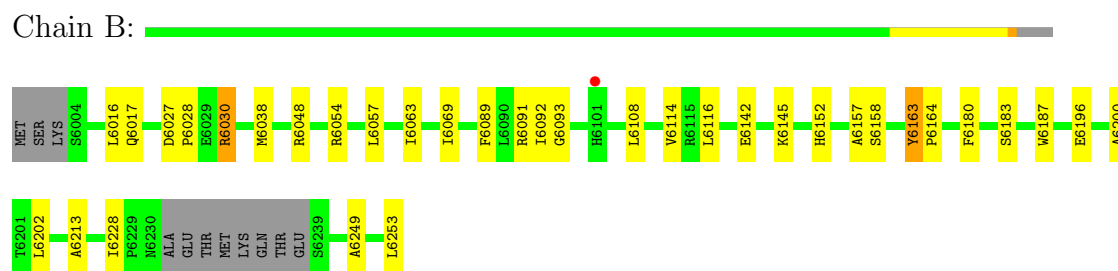
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

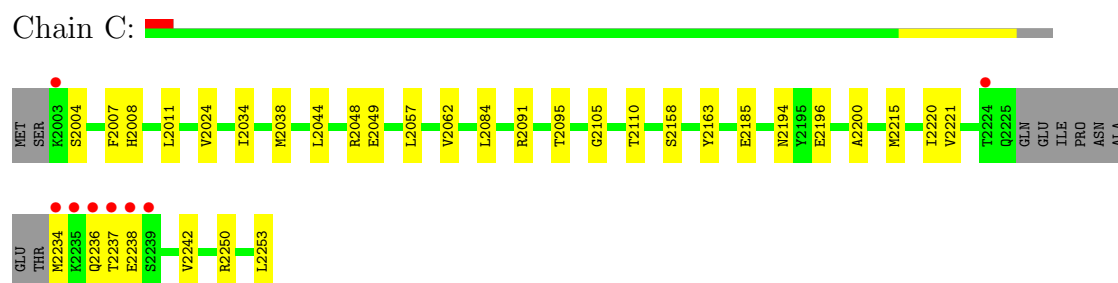
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

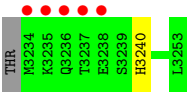


- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase





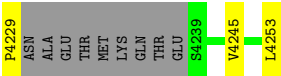
● Molecule 1: Uridine phosphorylase

Chain E:



● Molecule 1: Uridine phosphorylase

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.88Å 123.99Å 134.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.91 – 2.91 19.97 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.7 (90.91-2.91) 98.1 (19.97-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.208 , 0.256 0.203 , 0.211	Depositor DCC
$R_{free}$ test set	1625 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 32493 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.31	0/1930	0.50	0/2613
1	B	0.30	0/1849	0.48	0/2505
1	C	0.31	0/1858	0.49	0/2513
1	D	0.31	0/1861	0.50	0/2518
1	E	0.31	0/1842	0.50	0/2492
1	F	0.31	0/1850	0.49	0/2505
All	All	0.31	0/11190	0.49	0/15146

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1900	0	1914	21	0
1	B	1816	0	1826	18	0
1	C	1825	0	1844	16	0
1	D	1833	0	1844	17	0
1	E	1815	0	1828	14	0
1	F	1816	0	1833	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
3	A	17	0	12	1	0
3	B	17	0	12	1	0
3	C	17	0	12	1	0
3	D	17	0	12	1	0
3	E	17	0	12	1	0
3	F	17	0	12	2	0
4	A	14	0	0	0	0
4	B	18	0	0	0	0
4	C	13	0	0	0	0
4	D	11	0	0	0	0
4	E	14	0	0	0	0
4	F	12	0	0	0	0
All	All	11194	0	11161	108	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (108) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:4228:ILE:HB	1:F:4229:PRO:HD3	1.35	1.07
1:A:1232:GLU:HB2	1:A:1235:LYS:HB2	1.59	0.84
1:F:4228:ILE:HB	1:F:4229:PRO:CD	2.18	0.73
3:A:201:URI:O2	3:A:201:URI:H2'	1.88	0.72
3:F:206:URI:H2'	3:F:206:URI:O2	1.90	0.69
1:A:1173:SER:OG	1:A:1175:ARG:HG2	1.93	0.69
3:B:202:URI:O2	3:B:202:URI:H2'	1.91	0.68
1:F:4228:ILE:CB	1:F:4229:PRO:HD3	2.20	0.66
1:A:1234:MET:HG2	1:A:1238:GLU:HB2	1.80	0.64
1:B:6069:ILE:HD11	1:D:3048:ARG:HD3	1.78	0.64
1:A:1230:ASN:O	1:A:1233:THR:HG22	1.99	0.62
1:D:3038:MET:HG2	1:D:3057:LEU:HD13	1.82	0.62
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.82	0.61
1:A:1104:VAL:HG11	1:A:1229:PRO:HG3	1.82	0.61
1:F:4038:MET:HG2	1:F:4057:LEU:HD13	1.82	0.60
1:E:5105:GLY:HA2	1:E:5237:THR:HG23	1.83	0.60
1:C:2234:MET:N	1:C:2237:THR:HG1	1.98	0.60
1:B:6038:MET:HG2	1:B:6057:LEU:HD13	1.84	0.60
1:C:2091:ARG:HG2	1:C:2215:MET:SD	2.43	0.59
3:E:205:URI:O2	3:E:205:URI:H2'	2.02	0.58
1:F:4226:GLN:HE22	1:F:4229:PRO:HD2	1.68	0.58
1:B:6158:SER:HB3	1:B:6200:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.87	0.57
1:D:3158:SER:HB3	1:D:3200:ALA:HB2	1.89	0.55
1:B:6030:ARG:HH22	1:B:6093:GLY:HA2	1.71	0.55
1:F:4062:VAL:HG22	1:F:4253:LEU:HD21	1.90	0.54
1:E:5044:LEU:HD11	1:E:5054:ARG:HB2	1.88	0.54
1:A:1163:TYR:HB2	1:A:1164:PRO:HD3	1.90	0.54
1:A:1239:SER:O	1:A:1243:LYS:HB2	2.09	0.53
1:C:2048:ARG:HB3	1:C:2049:GLU:OE1	2.09	0.53
1:F:4226:GLN:NE2	1:F:4229:PRO:HD2	2.24	0.52
1:E:5199:SER:HB3	1:E:5215:MET:SD	2.50	0.52
1:A:1049:GLU:HB3	1:F:4049:GLU:HB3	1.91	0.52
1:B:6017:GLN:HG3	1:B:6054:ARG:CD	2.40	0.52
1:D:3186:GLU:OE2	1:E:5178:ARG:HB2	2.11	0.51
1:A:1015:ASP:O	1:A:1054:ARG:HD3	2.11	0.51
1:F:4158:SER:HB3	1:F:4200:ALA:HB2	1.93	0.51
1:C:2057:LEU:HG	1:C:2250:ARG:HG3	1.93	0.51
1:E:5030:ARG:HE	1:E:5238:GLU:HG2	1.75	0.50
1:B:6249:ALA:O	1:B:6253:LEU:HG	2.11	0.50
1:C:2158:SER:HB3	1:C:2200:ALA:HB2	1.93	0.49
1:B:6048:ARG:HD3	1:D:3069:ILE:HD11	1.92	0.49
1:F:4163:TYR:HB2	1:F:4164:PRO:HD3	1.95	0.49
1:B:6017:GLN:HG3	1:B:6054:ARG:HD3	1.95	0.49
1:E:5089:PHE:O	1:E:5213:ALA:HA	2.13	0.48
1:B:6016:LEU:HA	1:B:6063:ILE:HD11	1.96	0.48
1:C:2011:LEU:HD21	1:C:2044:LEU:HB3	1.95	0.48
1:C:2038:MET:HG2	1:C:2057:LEU:HD13	1.96	0.47
1:C:2220:ILE:HG13	1:C:2221:VAL:H	1.79	0.47
1:C:2105:GLY:HA2	1:C:2237:THR:HG23	1.95	0.47
1:D:3114:VAL:HB	1:D:3157:ALA:HA	1.95	0.47
1:B:6108:LEU:HD22	1:B:6152:HIS:HB2	1.96	0.47
1:E:5015:ASP:HB3	1:E:5044:LEU:HD22	1.97	0.47
1:B:6163:TYR:HB2	1:B:6164:PRO:HD3	1.95	0.47
1:E:5144:ALA:HA	1:E:5244:ILE:HG12	1.97	0.47
1:E:5095:THR:OG1	1:E:5194:ASN:HB2	2.15	0.47
1:C:2034:ILE:HG12	1:C:2242:VAL:HG13	1.97	0.46
1:C:2038:MET:SD	1:C:2062:VAL:HG21	2.55	0.46
1:F:4163:TYR:HB2	1:F:4164:PRO:CD	2.45	0.46
1:F:4007:PHE:HD2	1:F:4008:HIS:CE1	2.34	0.46
1:A:1102:ILE:O	1:A:1222:ASN:ND2	2.49	0.46
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.46	0.46
1:A:1108:LEU:HD22	1:A:1152:HIS:HB2	1.98	0.45
1:B:6163:TYR:HB2	1:B:6164:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:3009:LEU:HD21	1:D:3077:ALA:HA	1.97	0.45
3:C:203:URI:O5'	1:E:5008:HIS:NE2	2.39	0.45
1:F:4094:THR:O	3:F:206:URI:H1'	2.17	0.45
1:A:1230:ASN:C	1:A:1230:ASN:HD22	2.21	0.45
1:A:1031:VAL:HG13	1:A:1064:VAL:HG12	1.99	0.45
1:F:4044:LEU:HD11	1:F:4054:ARG:HB2	1.98	0.44
1:D:3184:MET:HG3	1:D:3195:TYR:HE2	1.81	0.44
1:B:6114:VAL:HB	1:B:6157:ALA:HA	1.98	0.44
1:F:4016:LEU:HG	1:F:4063:ILE:HG13	2.00	0.44
1:A:1044:LEU:HD11	1:A:1054:ARG:HB2	2.00	0.43
1:F:4028:PRO:HA	1:F:4066:SER:HB3	1.99	0.43
1:D:3091:ARG:CZ	1:D:3198:GLU:HB2	2.48	0.43
1:A:1095:THR:OG1	1:A:1194:ASN:HB2	2.18	0.43
1:C:2110:THR:HB	1:C:2215:MET:HB3	2.01	0.43
1:E:5224:THR:O	1:E:5225:GLN:HB2	2.17	0.43
1:B:6089:PHE:O	1:B:6213:ALA:HA	2.19	0.43
3:D:204:URI:O2	3:D:204:URI:H2'	2.18	0.43
1:D:3187:TRP:HD1	1:D:3195:TYR:HH	1.64	0.42
1:B:6180:PHE:HA	1:B:6183:SER:HB3	2.01	0.42
1:C:2220:ILE:HG13	1:C:2221:VAL:N	2.34	0.42
1:F:4099:GLN:HB2	1:F:4102:ILE:HD12	2.01	0.42
1:E:5108:LEU:HD22	1:E:5152:HIS:HB2	2.01	0.42
1:C:2007:PHE:HD2	1:C:2008:HIS:CE1	2.38	0.42
1:F:4223:ARG:HA	1:F:4226:GLN:O	2.20	0.42
1:E:5205:MET:O	1:E:5209:GLN:HB2	2.19	0.42
1:D:3170:ASP:OD1	1:D:3227:GLU:OE2	2.38	0.42
1:B:6027:ASP:HA	1:B:6028:PRO:HD2	1.86	0.42
1:D:3038:MET:HB2	1:D:3055:ALA:HB1	2.01	0.41
1:D:3098:ILE:HD12	1:D:3188:GLN:HG3	2.03	0.41
1:B:6091:ARG:HB2	1:B:6202:LEU:HD22	2.03	0.41
1:D:3163:TYR:HB2	1:D:3164:PRO:CD	2.51	0.41
1:D:3099:GLN:HA	1:D:3100:PRO:HD3	1.92	0.41
1:A:1009:LEU:HD21	1:A:1077:ALA:HA	2.02	0.41
1:D:3163:TYR:HB2	1:D:3164:PRO:HD3	2.03	0.41
1:B:6116:LEU:HD21	1:B:6187:TRP:CZ2	2.55	0.41
1:A:1209:GLN:HG2	1:F:4175:ARG:HH21	1.86	0.40
1:A:1081:LEU:HA	1:A:1084:LEU:HD12	2.02	0.40
1:C:2095:THR:OG1	1:C:2194:ASN:HB2	2.21	0.40
1:A:1069:ILE:HD11	1:F:4048:ARG:HD3	2.02	0.40
1:C:2062:VAL:HG12	1:C:2253:LEU:HD21	2.04	0.40
1:F:4017:GLN:HB2	1:F:4054:ARG:HD2	2.04	0.40
1:F:4065:CYS:HB3	1:F:4081:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:4114:VAL:HB	1:F:4157:ALA:HA	2.04	0.40
1:D:3016:LEU:HG	1:D:3063:ILE:HG13	2.04	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	251/253 (99%)	242 (96%)	8 (3%)	1 (0%)	43	82
1	B	239/253 (94%)	232 (97%)	6 (2%)	1 (0%)	43	82
1	C	240/253 (95%)	233 (97%)	5 (2%)	2 (1%)	27	67
1	D	240/253 (95%)	230 (96%)	9 (4%)	1 (0%)	43	82
1	E	238/253 (94%)	229 (96%)	7 (3%)	2 (1%)	27	67
1	F	239/253 (94%)	227 (95%)	10 (4%)	2 (1%)	27	67
All	All	1447/1518 (95%)	1393 (96%)	45 (3%)	9 (1%)	33	75

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	5225	GLN
1	F	4228	ILE
1	A	1163	TYR
1	B	6163	TYR
1	E	5163	TYR
1	F	4163	TYR
1	C	2004	SER
1	C	2163	TYR
1	D	3163	TYR

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/202 (100%)	193 (96%)	9 (4%)	38	76
1	B	193/202 (96%)	187 (97%)	6 (3%)	52	87
1	C	194/202 (96%)	188 (97%)	6 (3%)	52	87
1	D	194/202 (96%)	190 (98%)	4 (2%)	66	92
1	E	192/202 (95%)	184 (96%)	8 (4%)	40	79
1	F	193/202 (96%)	188 (97%)	5 (3%)	59	90
All	All	1168/1212 (96%)	1130 (97%)	38 (3%)	50	86

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1030	ARG
1	A	1092	ILE
1	A	1170	ASP
1	A	1173	SER
1	A	1196	GLU
1	A	1230	ASN
1	A	1233	THR
1	A	1240	HIS
1	A	1243	LYS
1	B	6030	ARG
1	B	6092	ILE
1	B	6142	GLU
1	B	6145	LYS
1	B	6196	GLU
1	B	6228	ILE
1	C	2024	VAL
1	C	2084	LEU
1	C	2185	GLU
1	C	2196	GLU
1	C	2236	GLN
1	C	2238	GLU
1	D	3092	ILE
1	D	3170	ASP

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Mol	Chain	Res	Type
1	D	3196	GLU
1	D	3240	HIS
1	E	5029	GLU
1	E	5030	ARG
1	E	5103	ASN
1	E	5170	ASP
1	E	5196	GLU
1	E	5215	MET
1	E	5226	GLN
1	E	5240	HIS
1	F	4003	LYS
1	F	4092	ILE
1	F	4146	SER
1	F	4196	GLU
1	F	4245	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1230	ASN
1	B	6226	GLN
1	B	6240	HIS
1	D	3226	GLN
1	D	3240	HIS
1	E	5047	HIS
1	E	5188	GLN
1	E	5226	GLN
1	F	4047	HIS
1	F	4226	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	PO4	A	1	-	4,4,4	0.27	0	6,6,6	0.31	0
3	URI	A	201	-	18,18,18	1.27	2 (11%)	22,26,26	2.80	4 (18%)
3	URI	B	202	-	18,18,18	1.32	2 (11%)	22,26,26	2.86	3 (13%)
3	URI	C	203	-	18,18,18	1.28	2 (11%)	22,26,26	2.59	3 (13%)
3	URI	D	204	-	18,18,18	1.28	2 (11%)	22,26,26	2.82	3 (13%)
3	URI	E	205	-	18,18,18	1.32	2 (11%)	22,26,26	2.74	3 (13%)
3	URI	F	206	-	18,18,18	1.27	2 (11%)	22,26,26	2.86	3 (13%)

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	PO4	A	1	-	-	0/0/0/0	0/0/0/0
3	URI	A	201	-	-	1/4/22/22	0/2/2/2
3	URI	B	202	-	-	1/4/22/22	0/2/2/2
3	URI	C	203	-	-	0/4/22/22	0/2/2/2
3	URI	D	204	-	-	0/4/22/22	0/2/2/2
3	URI	E	205	-	-	0/4/22/22	0/2/2/2
3	URI	F	206	-	-	1/4/22/22	0/2/2/2

All (12) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	205	URI	C2-N1	4.41	1.43	1.38
3	B	202	URI	C2-N1	4.39	1.43	1.38
3	C	203	URI	C2-N1	4.25	1.43	1.38
3	D	204	URI	C2-N1	4.25	1.43	1.38
3	F	206	URI	C2-N1	4.20	1.43	1.38
3	A	201	URI	C2-N1	4.18	1.43	1.38
3	E	205	URI	C6-C5	2.29	1.39	1.36
3	A	201	URI	C6-C5	2.24	1.39	1.36
3	B	202	URI	C6-C5	2.24	1.39	1.36
3	F	206	URI	C6-C5	2.22	1.39	1.36
3	C	203	URI	C6-C5	2.20	1.39	1.36
3	D	204	URI	C6-C5	2.19	1.39	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	URI	C2-N1-C1'	11.46	125.39	118.21
3	F	206	URI	C2-N1-C1'	11.32	125.31	118.21
3	D	204	URI	C2-N1-C1'	11.18	125.22	118.21
3	A	201	URI	C2-N1-C1'	10.94	125.06	118.21
3	E	205	URI	C2-N1-C1'	10.78	124.97	118.21
3	C	203	URI	C2-N1-C1'	10.00	124.48	118.21
3	E	205	URI	N3-C2-N1	4.93	120.08	115.97
3	D	204	URI	N3-C2-N1	4.76	119.94	115.97
3	B	202	URI	N3-C2-N1	4.76	119.94	115.97
3	A	201	URI	N3-C2-N1	4.73	119.92	115.97
3	C	203	URI	N3-C2-N1	4.67	119.87	115.97
3	F	206	URI	N3-C2-N1	4.57	119.79	115.97
3	A	201	URI	C3'-C2'-C1'	3.37	106.19	100.91
3	F	206	URI	C3'-C2'-C1'	3.23	105.95	100.91
3	C	203	URI	C3'-C2'-C1'	3.13	105.81	100.91
3	E	205	URI	C3'-C2'-C1'	3.13	105.81	100.91
3	D	204	URI	C3'-C2'-C1'	3.01	105.61	100.91
3	B	202	URI	C3'-C2'-C1'	2.71	105.15	100.91
3	A	201	URI	C4'-O4'-C1'	2.04	111.97	109.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	URI	C2'-C1'-N1-C6
3	F	206	URI	C2'-C1'-N1-C6
3	A	201	URI	C2'-C1'-N1-C6

There are no ring outliers.

## 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	253/253 (100%)	-0.27	11 (4%) 34 40	2, 3, 32, 49	0
1	B	242/253 (95%)	-0.41	1 (0%) 90 94	2, 3, 11, 15	0
1	C	243/253 (96%)	-0.21	8 (3%) 44 52	2, 5, 15, 54	0
1	D	244/253 (96%)	-0.23	7 (2%) 49 58	2, 4, 19, 58	0
1	E	242/253 (95%)	-0.35	4 (1%) 67 76	2, 3, 12, 39	0
1	F	242/253 (95%)	-0.49	0 100 100	2, 3, 9, 12	0
All	All	1466/1518 (96%)	-0.33	31 (2%) 60 68	2, 3, 14, 58	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3234	MET	6.1
1	E	5236	GLN	5.7
1	A	1234	MET	5.1
1	A	1231	ALA	5.1
1	D	3238	GLU	4.5
1	C	2236	GLN	4.3
1	E	5237	THR	4.0
1	A	1235	LYS	3.9
1	A	1236	GLN	3.9
1	C	2235	LYS	3.8
1	A	1230	ASN	3.8
1	E	5239	SER	3.7
1	C	2237	THR	3.7
1	D	3237	THR	3.6
1	A	1229	PRO	3.5
1	A	1232	GLU	3.5
1	D	3236	GLN	3.4
1	D	3235	LYS	2.9
1	C	2238	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	5238	GLU	2.7
1	A	1238	GLU	2.7
1	A	1002	SER	2.6
1	A	1233	THR	2.6
1	B	6101	HIS	2.6
1	A	1001	MET	2.6
1	D	3004	SER	2.5
1	C	2239	SER	2.5
1	C	2234	MET	2.4
1	D	3005	ASP	2.2
1	C	2224	THR	2.1
1	C	2003	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	A	1	5/5	0.24	2.36	50,51,51,51	0
3	URI	E	205	17/17	0.15	-0.04	12,12,12,12	0
3	URI	B	202	17/17	0.13	-0.38	7,8,8,8	0
3	URI	F	206	17/17	0.13	-0.39	7,7,7,8	0
3	URI	D	204	17/17	0.13	-0.62	12,12,12,12	0
3	URI	C	203	17/17	0.13	-0.82	10,10,10,10	0
3	URI	A	201	17/17	0.11	-1.42	8,9,9,9	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.