Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:39 AM GMT

PDB ID	:	2RJ3
Title	:	Crystal Structure of the Uridine Phosphorylase from Salmonella Typhimurium in Complex with Uracil and Phosphate Ion at 2.49A Resolution
Authors	:	Timofeev, V.I.; Pavlyuk, B.P.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Mikhailov, A.M.
Deposited on	:	2007-10-14
Resolution	:	2.51 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

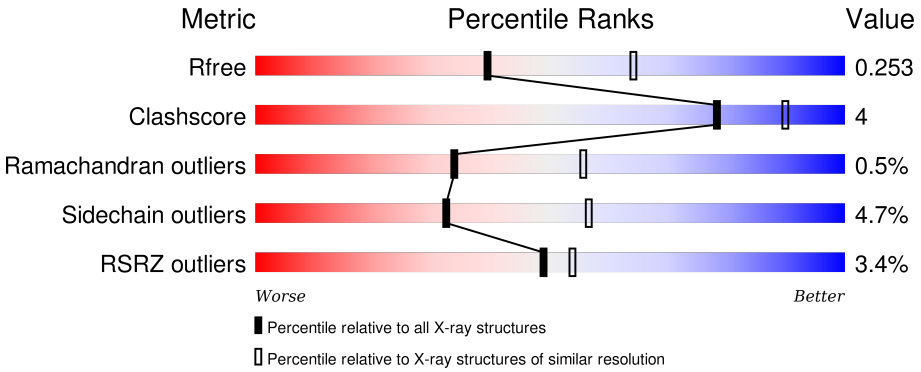
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	252	3% 89% 8%
1	B	252	3% 87% 11%
1	C	252	5% 90% 8%
1	D	252	3% 90% 8%
1	E	252	4% 86% 11%

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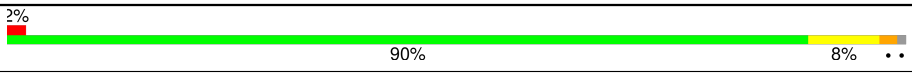
Mol	Chain	Length	Quality of chain
1	F	252	

2 Entry composition (i)

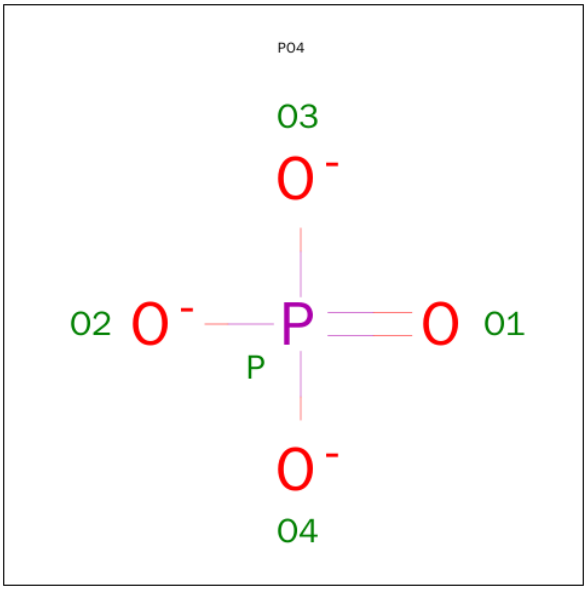
There are 4 unique types of molecules in this entry. The entry contains 11513 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

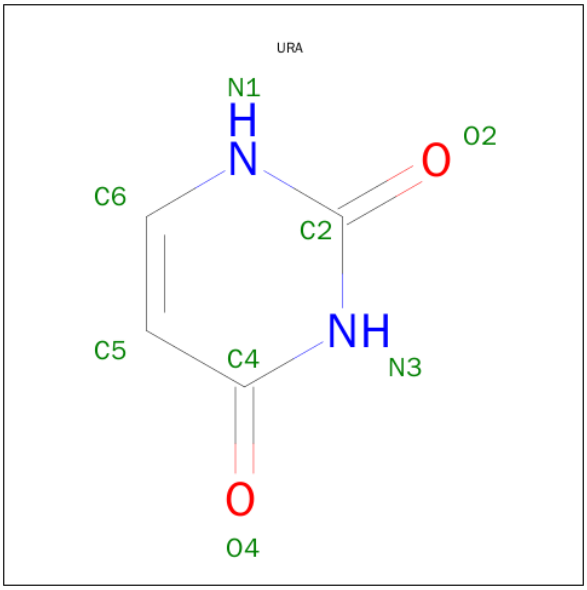
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	C	249	Total	C	N	O	S	0	0	0
			1867	1168	328	359	12			
1	D	248	Total	C	N	O	S	0	0	0
			1864	1167	328	357	12			
1	F	249	Total	C	N	O	S	0	0	0
			1871	1171	329	359	12			
1	E	249	Total	C	N	O	S	0	0	0
			1871	1171	329	359	12			
1	B	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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



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

- Molecule 4 is water.

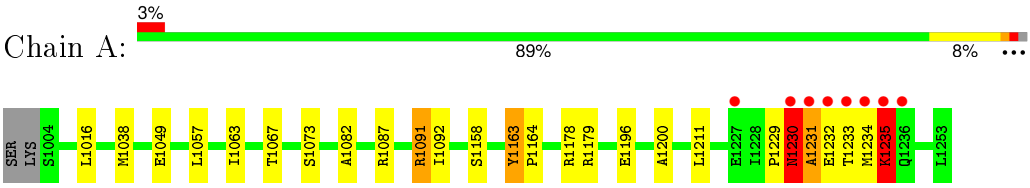
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	39	Total O 39 39	0	0
4	B	37	Total O 37 37	0	0
4	C	31	Total O 31 31	0	0
4	D	45	Total O 45 45	0	0
4	E	28	Total O 28 28	0	0
4	F	38	Total O 38 38	0	0

3 Residue-property plots (i)

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

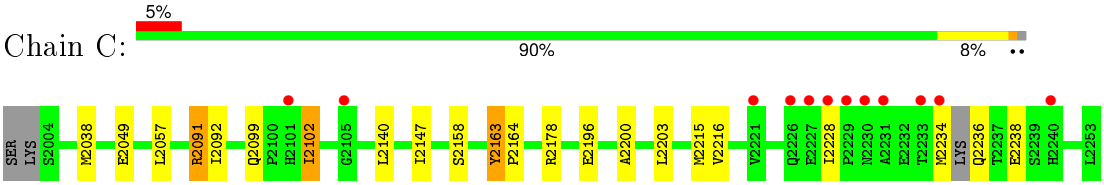
- Molecule 1: Uridine phosphorylase

Chain A:



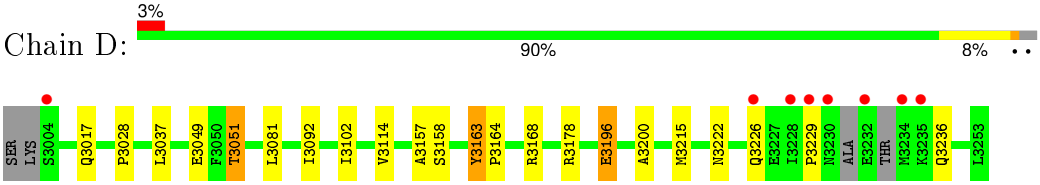
- Molecule 1: Uridine phosphorylase

Chain C:



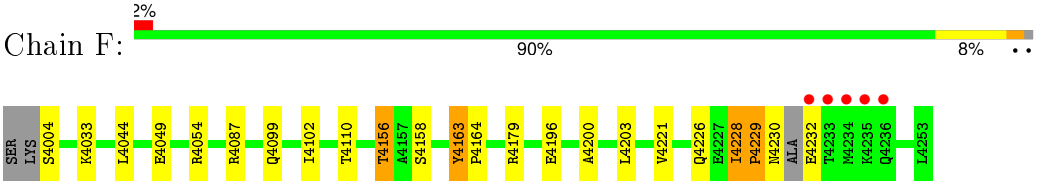
- Molecule 1: Uridine phosphorylase

Chain D:



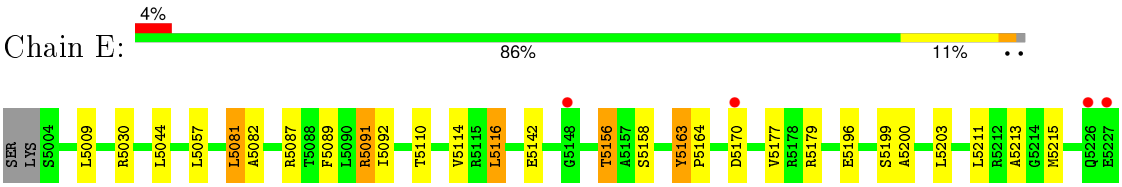
- Molecule 1: Uridine phosphorylase

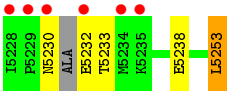
Chain F:



- Molecule 1: Uridine phosphorylase

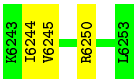
Chain E:





• Molecule 1: Uridine phosphorylase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.00Å 124.26Å 133.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.98 – 2.51 15.98 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.98-2.51) 97.2 (15.98-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	11.16 (at 2.52Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.257 0.218 , 0.253	Depositor DCC
R_{free} test set	2491 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 49812 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11513	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, 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	0.37	0/1906	0.72	6/2584 (0.2%)
1	B	0.38	0/1906	0.60	3/2584 (0.1%)
1	C	0.33	0/1896	0.49	0/2570
1	D	0.36	0/1892	0.51	0/2561
1	E	0.35	0/1900	0.54	0/2574
1	F	0.40	1/1900 (0.1%)	0.54	0/2574
All	All	0.37	1/11400 (0.0%)	0.57	9/15447 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	F	0	1
All	All	1	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	4232	GLU	CG-CD	5.41	1.60	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1235	LYS	N-CA-C	13.53	147.53	111.00
1	A	1230	ASN	N-CA-C	13.08	146.32	111.00
1	A	1235	LYS	CB-CA-C	-10.69	89.02	110.40
1	B	6235	LYS	N-CA-C	-9.71	84.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	6236	GLN	N-CA-C	8.06	132.76	111.00
1	B	6236	GLN	N-CA-CB	-7.36	97.35	110.60
1	A	1230	ASN	C-N-CA	6.09	136.93	121.70
1	A	1235	LYS	C-N-CA	5.88	136.40	121.70
1	A	1231	ALA	N-CA-CB	-5.46	102.45	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1230	ASN	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1229	PRO	Peptide
1	A	1230	ASN	Peptide
1	A	1235	LYS	Peptide
1	F	4229	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1876	0	1887	21	0
1	B	1876	0	1887	18	0
1	C	1867	0	1873	13	0
1	D	1864	0	1873	8	0
1	E	1871	0	1881	14	0
1	F	1871	0	1881	11	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	8	0	3	0	0
3	B	8	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	8	0	3	0	0
3	E	8	0	3	0	0
3	F	8	0	3	0	0
4	A	39	0	0	1	0
4	B	37	0	0	1	0
4	C	31	0	0	0	0
4	D	45	0	0	0	0
4	E	28	0	0	0	0
4	F	38	0	0	0	0
All	All	11513	0	11297	82	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 4.

All (82) 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:A:1230:ASN:HB3	1:A:1232:GLU:HG2	1.34	1.05
1:E:5091:ARG:HG2	1:E:5215:MET:HG3	1.51	0.91
1:B:6071:GLY:CA	1:B:6201:THR:HG21	2.07	0.84
1:B:6071:GLY:HA3	1:B:6201:THR:HG21	1.60	0.84
1:C:2091:ARG:HB3	1:C:2215:MET:HG3	1.59	0.84
1:E:5163:TYR:HB2	1:E:5164:PRO:HD3	1.64	0.79
1:A:1232:GLU:HA	1:A:1235:LYS:CB	2.15	0.77
1:B:6216:VAL:HG21	1:B:6244:ILE:HD11	1.73	0.69
1:E:5082:ALA:O	1:E:5087:ARG:NH2	2.30	0.64
1:F:4158:SER:HB3	1:F:4200:ALA:HB2	1.80	0.63
1:B:6071:GLY:HA2	1:B:6201:THR:HG21	1.79	0.63
1:B:6158:SER:HB3	1:B:6200:ALA:HB2	1.81	0.62
1:A:1232:GLU:HA	1:A:1235:LYS:HB2	1.81	0.62
1:C:2158:SER:HB3	1:C:2200:ALA:HB2	1.82	0.61
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.81	0.61
1:A:1091:ARG:HD3	4:A:9003:HOH:O	2.00	0.60
1:B:6077:ALA:O	1:B:6081:LEU:HB2	2.02	0.60
1:E:5230:ASN:O	1:E:5232:GLU:N	2.35	0.59
1:B:6201:THR:HG22	4:B:9210:HOH:O	2.04	0.58
1:A:1230:ASN:C	1:A:1230:ASN:OD1	2.42	0.57
1:F:4226:GLN:HE22	1:F:4230:ASN:HB2	1.70	0.56
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.36	0.56
1:F:4110:THR:HG23	1:F:4156:THR:HG23	1.87	0.54
1:F:4221:VAL:HB	1:F:4229:PRO:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5057:LEU:HB3	1:E:5253:LEU:HD21	1.88	0.54
1:A:1163:TYR:HB2	1:A:1164:PRO:HD3	1.90	0.54
1:E:5091:ARG:HG2	1:E:5215:MET:CG	2.31	0.54
1:B:6038:MET:HG2	1:B:6057:LEU:HD13	1.90	0.53
1:A:1067:THR:O	1:A:1073:SER:HB3	2.09	0.53
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.91	0.53
1:A:1232:GLU:HA	1:A:1235:LYS:HB3	1.91	0.52
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.92	0.51
1:B:6016:LEU:HD11	1:B:6084:LEU:HB3	1.94	0.50
1:E:5163:TYR:CB	1:E:5164:PRO:HD3	2.39	0.50
1:D:3102:ILE:O	1:D:3222:ASN:ND2	2.42	0.50
1:D:3049:GLU:HB3	1:B:6049:GLU:HB3	1.93	0.50
1:D:3114:VAL:HB	1:D:3157:ALA:HA	1.93	0.49
1:A:1231:ALA:O	1:A:1235:LYS:HB2	2.12	0.49
1:E:5199:SER:HB3	1:E:5215:MET:SD	2.53	0.49
1:B:6057:LEU:HG	1:B:6250:ARG:HG2	1.96	0.48
1:F:4163:TYR:HB2	1:F:4164:PRO:CD	2.45	0.47
1:C:2140:LEU:HD22	1:C:2216:VAL:HB	1.95	0.47
1:B:6016:LEU:HD13	1:B:6086:ILE:CD1	2.44	0.47
1:F:4163:TYR:HB2	1:F:4164:PRO:HD3	1.95	0.47
1:A:1232:GLU:CA	1:A:1235:LYS:HB2	2.44	0.47
1:D:3158:SER:HB3	1:D:3200:ALA:HB2	1.98	0.46
1:C:2147:ILE:HG22	1:C:2147:ILE:O	2.15	0.46
1:C:2163:TYR:HB2	1:C:2164:PRO:CD	2.45	0.46
1:E:5089:PHE:O	1:E:5213:ALA:HA	2.16	0.45
1:B:6049:GLU:HG3	1:B:6068:GLY:HA3	1.98	0.45
1:E:5009:LEU:CD1	1:E:5081:LEU:HD13	2.46	0.45
1:C:2234:MET:O	1:C:2236:GLN:N	2.50	0.45
1:C:2099:GLN:HB2	1:C:2102:ILE:HG13	1.98	0.45
1:C:2163:TYR:HB2	1:C:2164:PRO:HD3	1.99	0.45
1:D:3028:PRO:HB3	1:D:3051:THR:HG23	1.99	0.44
1:A:1082:ALA:O	1:A:1087:ARG:NH2	2.51	0.44
1:E:5110:THR:HG23	1:E:5156:THR:HG23	2.00	0.44
1:A:1235:LYS:O	1:A:1235:LYS:HD2	2.17	0.44
1:A:1163:TYR:CB	1:A:1164:PRO:CD	2.96	0.43
1:B:6016:LEU:HA	1:B:6063:ILE:HD11	2.00	0.43
1:D:3196:GLU:HG2	1:D:3215:MET:HE2	2.00	0.43
1:A:1049:GLU:HB3	1:F:4049:GLU:HB3	2.01	0.43
1:C:2038:MET:HG2	1:C:2057:LEU:HD13	2.01	0.43
1:A:1230:ASN:CB	1:A:1232:GLU:HG2	2.25	0.43
1:F:4228:ILE:HD13	1:F:4229:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5114:VAL:HG12	1:E:5116:LEU:HD13	2.01	0.43
1:A:1178:ARG:O	1:C:2178:ARG:NH2	2.51	0.43
1:C:2091:ARG:CB	1:C:2215:MET:HG3	2.40	0.42
1:B:6163:TYR:HB2	1:B:6164:PRO:HD3	2.00	0.42
1:D:3163:TYR:HB2	1:D:3164:PRO:HD3	2.00	0.42
1:F:4228:ILE:HA	1:F:4229:PRO:HD3	1.83	0.42
1:D:3163:TYR:HA	1:D:3168:ARG:HD2	2.02	0.42
1:F:4099:GLN:HB2	1:F:4102:ILE:HD12	2.02	0.42
1:C:2234:MET:HB3	1:C:2238:GLU:HB2	2.01	0.42
1:C:2228:ILE:H	1:C:2228:ILE:HG13	1.64	0.42
1:B:6242:VAL:O	1:B:6245:VAL:HG12	2.20	0.41
1:F:4044:LEU:HD11	1:F:4054:ARG:HB2	2.03	0.41
1:E:5030:ARG:HD3	1:E:5238:GLU:OE1	2.21	0.41
1:A:1235:LYS:C	1:A:1235:LYS:HD2	2.37	0.41
1:A:1016:LEU:HG	1:A:1063:ILE:HG13	2.03	0.41
1:B:6233:THR:HG23	1:B:6234:MET:HG3	2.03	0.41
1:B:6016:LEU:HD13	1:B:6086:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/252 (98%)	241 (97%)	5 (2%)	2 (1%)	24	41
1	B	248/252 (98%)	239 (96%)	8 (3%)	1 (0%)	39	61
1	C	245/252 (97%)	235 (96%)	9 (4%)	1 (0%)	39	61
1	D	243/252 (96%)	234 (96%)	7 (3%)	2 (1%)	24	41
1	E	245/252 (97%)	235 (96%)	9 (4%)	1 (0%)	39	61
1	F	245/252 (97%)	239 (98%)	5 (2%)	1 (0%)	39	61
All	All	1474/1512 (98%)	1423 (96%)	43 (3%)	8 (0%)	34	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1163	TYR
1	C	2163	TYR
1	D	3163	TYR
1	F	4163	TYR
1	E	5163	TYR
1	B	6163	TYR
1	A	1233	THR
1	D	3229	PRO

5.3.2 Protein sidechains (i)

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	199/201 (99%)	192 (96%)	7 (4%)	43 70
1	B	199/201 (99%)	188 (94%)	11 (6%)	27 48
1	C	198/201 (98%)	192 (97%)	6 (3%)	48 76
1	D	198/201 (98%)	189 (96%)	9 (4%)	34 59
1	E	199/201 (99%)	184 (92%)	15 (8%)	17 31
1	F	199/201 (99%)	191 (96%)	8 (4%)	38 64
All	All	1192/1206 (99%)	1136 (95%)	56 (5%)	32 56

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1091	ARG
1	A	1092	ILE
1	A	1179	ARG
1	A	1196	GLU
1	A	1211	LEU
1	A	1234	MET
1	A	1235	LYS
1	C	2049	GLU
1	C	2091	ARG

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Mol	Chain	Res	Type
1	C	2092	ILE
1	C	2102	ILE
1	C	2196	GLU
1	C	2203	LEU
1	D	3017	GLN
1	D	3037	LEU
1	D	3051	THR
1	D	3081	LEU
1	D	3092	ILE
1	D	3178	ARG
1	D	3196	GLU
1	D	3226	GLN
1	D	3236	GLN
1	F	4004	SER
1	F	4033	LYS
1	F	4087	ARG
1	F	4156	THR
1	F	4179	ARG
1	F	4196	GLU
1	F	4203	LEU
1	F	4228	ILE
1	E	5044	LEU
1	E	5081	LEU
1	E	5091	ARG
1	E	5092	ILE
1	E	5116	LEU
1	E	5142	GLU
1	E	5156	THR
1	E	5170	ASP
1	E	5177	VAL
1	E	5179	ARG
1	E	5196	GLU
1	E	5203	LEU
1	E	5211	LEU
1	E	5233	THR
1	E	5253	LEU
1	B	6011	LEU
1	B	6092	ILE
1	B	6145	LYS
1	B	6153	VAL
1	B	6184	MET
1	B	6196	GLU

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Mol	Chain	Res	Type
1	B	6201	THR
1	B	6203	LEU
1	B	6234	MET
1	B	6235	LYS
1	B	6236	GLN

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	1047	HIS
1	C	2230	ASN
1	F	4226	GLN
1	F	4230	ASN
1	F	4240	HIS
1	E	5017	GLN
1	E	5188	GLN
1	E	5236	GLN
1	B	6103	ASN
1	B	6225	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 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	7001	-	4,4,4	0.50	0	6,6,6	0.27	0
3	URA	A	8001	-	4,8,8	0.49	0	6,10,10	7.85	4 (66%)
2	PO4	B	7006	-	4,4,4	0.55	0	6,6,6	0.27	0
3	URA	B	8006	-	4,8,8	0.45	0	6,10,10	7.68	4 (66%)
2	PO4	C	7002	-	4,4,4	0.43	0	6,6,6	0.27	0
2	PO4	D	7003	-	4,4,4	0.54	0	6,6,6	0.27	0
3	URA	D	8003	-	4,8,8	0.56	0	6,10,10	7.83	4 (66%)
2	PO4	E	7005	-	4,4,4	0.49	0	6,6,6	0.28	0
3	URA	E	8005	-	4,8,8	0.54	0	6,10,10	7.99	4 (66%)
2	PO4	F	7004	-	4,4,4	0.45	0	6,6,6	0.28	0
3	URA	F	8004	-	4,8,8	0.54	0	6,10,10	7.88	4 (66%)

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	7001	-	-	0/0/0/0	0/0/0/0
3	URA	A	8001	-	-	0/0/0/0	0/1/1/1
2	PO4	B	7006	-	-	0/0/0/0	0/0/0/0
3	URA	B	8006	-	-	0/0/0/0	0/1/1/1
2	PO4	C	7002	-	-	0/0/0/0	0/0/0/0
2	PO4	D	7003	-	-	0/0/0/0	0/0/0/0
3	URA	D	8003	-	-	0/0/0/0	0/1/1/1
2	PO4	E	7005	-	-	0/0/0/0	0/0/0/0
3	URA	E	8005	-	-	0/0/0/0	0/1/1/1
2	PO4	F	7004	-	-	0/0/0/0	0/0/0/0
3	URA	F	8004	-	-	0/0/0/0	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	8005	URA	N1-C2-N3	-11.87	120.76	128.33
3	D	8003	URA	N1-C2-N3	-11.76	120.83	128.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	8001	URA	N1-C2-N3	-11.72	120.86	128.33
3	F	8004	URA	N1-C2-N3	-11.68	120.88	128.33
3	B	8006	URA	N1-C2-N3	-11.49	121.00	128.33
3	E	8005	URA	C5-C6-N1	-4.06	119.26	123.90
3	F	8004	URA	C5-C6-N1	-3.97	119.37	123.90
3	B	8006	URA	C5-C6-N1	-3.93	119.41	123.90
3	A	8001	URA	C5-C6-N1	-3.90	119.45	123.90
3	D	8003	URA	C5-C6-N1	-3.73	119.64	123.90
3	F	8004	URA	C4-N3-C2	6.20	120.28	114.14
3	D	8003	URA	C4-N3-C2	6.39	120.47	114.14
3	B	8006	URA	C4-N3-C2	6.43	120.51	114.14
3	A	8001	URA	C4-N3-C2	6.47	120.55	114.14
3	E	8005	URA	C4-N3-C2	6.57	120.65	114.14
3	B	8006	URA	C6-N1-C2	12.75	120.67	114.40
3	D	8003	URA	C6-N1-C2	13.14	120.86	114.40
3	A	8001	URA	C6-N1-C2	13.17	120.88	114.40
3	E	8005	URA	C6-N1-C2	13.41	121.00	114.40
3	F	8004	URA	C6-N1-C2	13.43	121.01	114.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	250/252 (99%)	-0.31	8 (3%) 51 56	3, 11, 33, 46	0
1	B	250/252 (99%)	-0.18	8 (3%) 51 56	6, 13, 28, 45	0
1	C	249/252 (98%)	0.09	12 (4%) 34 39	8, 20, 45, 57	0
1	D	248/252 (98%)	-0.13	8 (3%) 51 56	6, 15, 39, 52	0
1	E	249/252 (98%)	-0.14	10 (4%) 42 47	6, 14, 38, 52	0
1	F	249/252 (98%)	-0.24	5 (2%) 68 72	5, 12, 28, 45	0
All	All	1495/1512 (98%)	-0.15	51 (3%) 49 54	3, 14, 37, 57	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1234	MET	10.4
1	C	2231	ALA	10.4
1	B	6233	THR	8.1
1	D	3230	ASN	7.4
1	B	6234	MET	5.9
1	F	4233	THR	5.8
1	C	2230	ASN	5.7
1	D	3226	GLN	5.2
1	B	6237	THR	5.1
1	D	3228	ILE	4.9
1	E	5226	GLN	4.8
1	B	6231	ALA	4.6
1	F	4232	GLU	4.4
1	B	6236	GLN	4.2
1	D	3232	GLU	4.2
1	B	6232	GLU	4.0
1	C	2234	MET	4.0
1	C	2226	GLN	3.9
1	F	4235	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	3229	PRO	3.8
1	C	2227	GLU	3.6
1	C	2233	THR	3.6
1	C	2228	ILE	3.5
1	E	5227	GLU	3.4
1	E	5229	PRO	3.4
1	A	1236	GLN	3.4
1	A	1235	LYS	3.3
1	E	5228	ILE	3.3
1	C	2229	PRO	3.3
1	C	2221	VAL	3.2
1	A	1233	THR	3.2
1	A	1231	ALA	3.2
1	D	3235	LYS	3.1
1	D	3004	SER	3.1
1	E	5230	ASN	3.1
1	E	5170	ASP	3.0
1	A	1230	ASN	3.0
1	E	5234	MET	2.8
1	A	1232	GLU	2.6
1	F	4234	MET	2.6
1	C	2101	HIS	2.6
1	E	5232	GLU	2.6
1	B	6235	LYS	2.5
1	A	1227	GLU	2.4
1	D	3234	MET	2.3
1	F	4236	GLN	2.3
1	B	6238	GLU	2.3
1	E	5148	GLY	2.3
1	C	2105	GLY	2.1
1	E	5235	LYS	2.1
1	C	2240	HIS	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	C	7002	5/5	0.92	0.18	1.09	51,51,51,52	0
3	URA	B	8006	8/8	0.95	0.13	0.79	11,11,12,12	0
3	URA	E	8005	8/8	0.93	0.18	0.69	30,31,31,31	0
3	URA	F	8004	8/8	0.96	0.12	0.16	4,5,6,6	0
3	URA	D	8003	8/8	0.97	0.11	-0.73	11,11,11,11	0
2	PO4	F	7004	5/5	0.99	0.07	-2.11	8,8,10,10	0
2	PO4	E	7005	5/5	0.99	0.07	-2.31	23,23,23,23	0
2	PO4	B	7006	5/5	0.99	0.06	-2.63	14,14,15,15	0
2	PO4	A	7001	5/5	0.99	0.07	-2.89	6,6,7,7	0
2	PO4	D	7003	5/5	0.99	0.07	-3.48	10,10,11,11	0
3	URA	A	8001	8/8	0.98	0.06	-3.61	8,8,8,8	0

6.5 Other polymers

There are no such residues in this entry.