



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:46 PM GMT

PDB ID : 1Y1R
Title : Crystal Structure of the Uridine Phosphorylase from Salmonella Typhimurium
in Complex with Inhibitor and Phosphate Ion at 2.11Å Resolution
Authors : Dontsova, M.V.; Gabdoulkhakov, A.G.; Kachalova, G.S.; Betzel, C.; Ealick,
S.E.; Mikhailov, A.M.
Deposited on : 2004-11-19
Resolution : 2.11 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

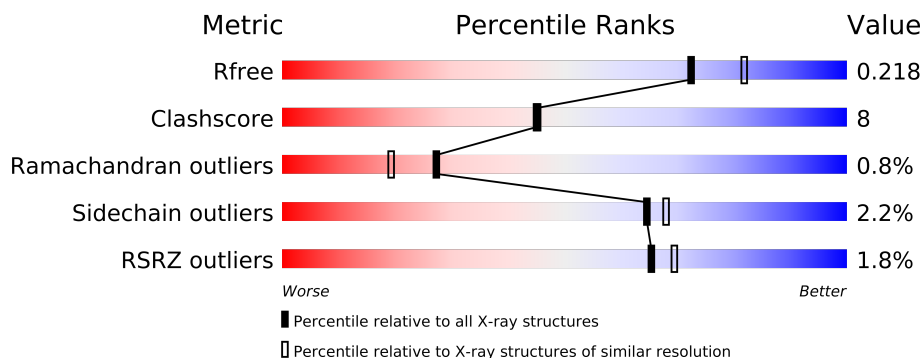
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.11 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	3409 (2.14-2.10)
Clashscore	79885	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (2.14-2.10)

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. 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	D	703	-	X
2	PO4	F	704	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
3	ANU	B	707	-	X
3	ANU	D	706	-	X

2 Entry composition

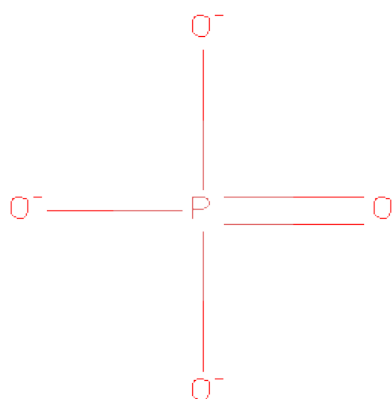
There are 4 unique types of molecules in this entry. The entry contains 11625 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

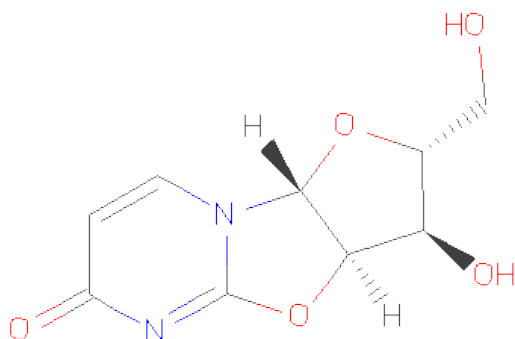
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1886	1180	332	362	12			
1	C	243	Total	C	N	O	S	0	0	0
			1824	1143	322	347	12			
1	D	241	Total	C	N	O	S	0	0	0
			1806	1132	318	344	12			
1	F	240	Total	C	N	O	S	0	0	0
			1800	1128	318	343	11			
1	E	241	Total	C	N	O	S	0	0	0
			1807	1132	319	345	11			
1	B	242	Total	C	N	O	S	0	0	0
			1814	1137	320	346	11			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is 2,2'-ANHYDROURIDINE (three-letter code: ANU) (formula: C₉H₁₀N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			16	9	2	5		
3	B	1	Total	C	N	O	0	0
			16	9	2	5		

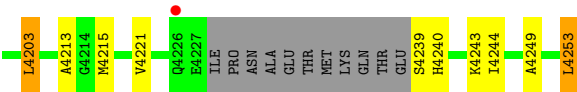
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	116	Total	O	0	0
			116	116		
4	C	109	Total	O	0	0
			109	109		
4	D	82	Total	O	0	0
			82	82		
4	E	117	Total	O	0	0
			117	117		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	95	Total	O	0	0
			95	95		



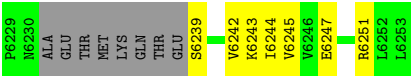
• Molecule 1: Uridine phosphorylase

Chain E:



• Molecule 1: Uridine phosphorylase

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.88Å 124.07Å 134.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.75 – 2.11 28.75 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.5 (28.75-2.11) 98.3 (28.75-2.09)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.219 0.180 , 0.218	Depositor DCC
R_{free} test set	4192 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 86957 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11625	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: ANU, PO4

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	0.39	0/1916	0.69	0/2595
1	B	0.40	0/1843	0.65	0/2497
1	C	0.38	0/1852	0.64	0/2505
1	D	0.37	0/1834	0.63	0/2482
1	E	0.39	0/1835	0.67	1/2484 (0.0%)
1	F	0.39	0/1828	0.65	0/2474
All	All	0.39	0/11108	0.66	1/15037 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5021	LEU	CA-CB-CG	5.32	127.53	115.30

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	1886	0	1900	40	0
1	B	1814	0	1825	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1824	0	1843	26	0
1	D	1806	0	1822	46	0
1	E	1807	0	1821	24	0
1	F	1800	0	1814	32	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
3	B	16	0	10	3	0
3	D	16	0	10	2	0
4	A	122	0	0	2	0
4	B	116	0	0	2	0
4	C	109	0	0	1	0
4	D	82	0	0	0	0
4	E	117	0	0	1	0
4	F	95	0	0	1	0
All	All	11625	0	11045	185	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 8.

All (185) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1229:PRO:HB2	1:A:1233:THR:HG22	1.21	1.13
1:D:3049:GLU:HG2	1:B:6049:GLU:HG2	1.27	1.08
1:D:3100:PRO:HG3	1:D:3224:THR:HG21	1.52	0.92
1:F:4091:ARG:HB3	1:F:4215:MET:HG3	1.53	0.89
1:A:1229:PRO:HB2	1:A:1233:THR:CG2	2.03	0.87
1:A:1049:GLU:HB2	1:F:4049:GLU:CD	1.97	0.85
1:A:1229:PRO:CB	1:A:1233:THR:HG22	2.04	0.85
1:D:3049:GLU:CG	1:B:6049:GLU:HG2	2.06	0.83
1:D:3234:MET:HG3	1:D:3235:LYS:H	1.43	0.83
1:D:3049:GLU:HG2	1:B:6049:GLU:CG	2.09	0.81
1:A:1178:ARG:HA	1:A:1181:LYS:HE2	1.68	0.75
1:C:2094:THR:HG21	1:C:2238:GLU:HG2	1.69	0.75
1:D:3196:GLU:HA	3:D:706:ANU:O2	1.87	0.74
1:D:3238:GLU:O	1:D:3242:VAL:HG23	1.91	0.70
1:C:2158:SER:HB3	1:C:2200:ALA:HB2	1.74	0.69
1:F:4158:SER:HB3	1:F:4200:ALA:HB2	1.74	0.69
1:B:6108:LEU:HD22	1:B:6152:HIS:HB2	1.74	0.69
1:E:5060:LYS:HD3	1:E:5253:LEU:HB3	1.75	0.69
1:A:1027:ASP:HB3	1:A:1030:ARG:HG2	1.74	0.68
1:F:4249:ALA:O	1:F:4253:LEU:HD22	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:6170:ASP:HB2	1:B:6227:GLU:OE1	1.94	0.68
1:E:5060:LYS:HB2	1:E:5253:LEU:HD13	1.74	0.68
1:C:2094:THR:CG2	1:C:2238:GLU:HG2	2.26	0.66
1:D:3158:SER:HB3	1:D:3200:ALA:HB2	1.77	0.66
1:D:3234:MET:HG3	1:D:3235:LYS:N	2.12	0.65
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.78	0.64
1:C:2249:ALA:O	1:C:2253:LEU:HD13	1.98	0.64
1:D:3069:ILE:HD11	1:B:6048:ARG:HD3	1.80	0.63
1:A:1049:GLU:HB2	1:F:4049:GLU:OE2	1.98	0.63
1:E:5048:ARG:HB3	1:E:5049:GLU:OE1	1.97	0.63
1:B:6239:SER:O	1:B:6243:LYS:HG3	2.00	0.62
1:A:1049:GLU:CD	1:F:4049:GLU:HB2	2.20	0.62
1:C:2048:ARG:HD2	4:C:411:HOH:O	2.00	0.61
1:A:1037:LEU:HD22	1:A:1242:VAL:HG12	1.83	0.61
1:F:4179:ARG:HD2	4:F:379:HOH:O	1.99	0.61
1:D:3092:ILE:HD13	1:D:3093:GLY:N	2.15	0.61
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.83	0.60
1:A:1179:ARG:HD3	4:A:273:HOH:O	2.02	0.59
1:D:3060:LYS:HD2	1:D:3253:LEU:HB3	1.85	0.59
1:E:5092:ILE:HD11	1:E:5241:ALA:HB1	1.84	0.58
1:D:3105:GLY:HA2	1:D:3237:THR:OG1	2.03	0.58
1:E:5184:MET:O	1:E:5188:GLN:HG3	2.04	0.58
1:B:6158:SER:HB3	1:B:6200:ALA:HB2	1.85	0.58
1:D:3048:ARG:HB3	1:D:3049:GLU:OE1	2.03	0.57
1:A:1142:GLU:HB3	1:A:1251:ARG:NH1	2.19	0.57
1:A:1238:GLU:O	1:A:1242:VAL:HG23	2.04	0.57
1:A:1069:ILE:HD11	1:F:4048:ARG:HD3	1.86	0.56
1:E:5181:LYS:NZ	1:E:5181:LYS:HB2	2.21	0.55
1:A:1049:GLU:CD	1:A:1068:GLY:HA2	2.28	0.55
1:D:3013:LYS:HB3	1:D:3013:LYS:NZ	2.22	0.54
1:C:2138:THR:O	1:C:2142:GLU:HG2	2.07	0.54
1:E:5049:GLU:HG3	1:E:5068:GLY:HA3	1.89	0.53
1:E:5060:LYS:HE2	1:E:5253:LEU:OXT	2.08	0.53
1:A:1027:ASP:HB3	1:A:1030:ARG:CG	2.37	0.53
1:B:6030:ARG:HH12	1:B:6093:GLY:HA2	1.73	0.53
1:F:4007:PHE:N	1:F:4007:PHE:CD2	2.77	0.53
3:B:707:ANU:H2'	3:B:707:ANU:O5'	2.08	0.52
1:C:2234:MET:HG3	1:C:2238:GLU:OE2	2.09	0.52
1:D:3092:ILE:C	1:D:3092:ILE:HD13	2.30	0.52
1:B:6167:GLU:HG2	1:B:6169:TYR:CE1	2.45	0.51
1:D:3163:TYR:HB2	1:D:3164:PRO:CD	2.40	0.51
1:D:3142:GLU:HB3	1:D:3251:ARG:NH1	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:6069:ILE:CD1	3:B:707:ANU:H5'1	2.41	0.51
1:F:4038:MET:HG2	1:F:4057:LEU:HD13	1.92	0.51
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.93	0.51
1:D:3089:PHE:O	1:D:3213:ALA:HA	2.10	0.50
1:F:4028:PRO:HA	1:F:4066:SER:HB3	1.93	0.50
1:A:1031:VAL:HG13	1:A:1064:VAL:HG12	1.94	0.50
1:F:4044:LEU:HD11	1:F:4054:ARG:HB2	1.93	0.49
1:F:4003:LYS:HD2	1:F:4004:SER:N	2.27	0.49
1:A:1220:ILE:O	1:A:1229:PRO:HG2	2.13	0.49
1:C:2238:GLU:O	1:C:2242:VAL:HG23	2.11	0.49
1:B:6242:VAL:O	1:B:6245:VAL:HG12	2.13	0.49
1:E:5163:TYR:HB2	1:E:5164:PRO:CD	2.42	0.49
1:F:4060:LYS:HD2	1:F:4253:LEU:HB3	1.93	0.49
1:B:6108:LEU:CD2	1:B:6152:HIS:HB2	2.42	0.49
1:F:4179:ARG:O	1:F:4179:ARG:HG3	2.11	0.49
1:B:6099:GLN:HB3	1:B:6101:HIS:CE1	2.48	0.48
1:C:2057:LEU:HB3	1:C:2253:LEU:HD21	1.94	0.48
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.43	0.48
1:C:2093:GLY:O	1:C:2217:ALA:HA	2.13	0.48
1:D:3049:GLU:CB	1:B:6049:GLU:HG2	2.43	0.48
1:D:3221:VAL:HG22	1:D:3222:ASN:N	2.28	0.48
1:D:3100:PRO:CG	1:D:3224:THR:HG21	2.34	0.48
1:A:1048:ARG:HB3	1:F:4049:GLU:OE1	2.14	0.48
1:F:4012:THR:O	1:F:4015:ASP:HB2	2.13	0.48
1:F:4199:SER:O	1:F:4203:LEU:HB2	2.14	0.48
1:F:4163:TYR:HB2	1:F:4164:PRO:CD	2.44	0.47
1:C:2057:LEU:HB3	1:C:2253:LEU:CD2	2.45	0.47
1:C:2022:ALA:HA	1:C:2063:ILE:O	2.14	0.47
1:E:5021:LEU:HD13	1:E:5022:ALA:N	2.29	0.47
1:B:6048:ARG:HB3	1:B:6049:GLU:OE2	2.15	0.47
1:D:3048:ARG:HD3	1:B:6069:ILE:HD11	1.97	0.47
1:A:1143:ALA:O	1:A:1147:ILE:HD13	2.15	0.47
1:D:3239:SER:O	1:D:3243:LYS:HG3	2.15	0.46
1:D:3114:VAL:HB	1:D:3157:ALA:HA	1.97	0.46
1:F:4007:PHE:HD2	1:F:4007:PHE:N	2.14	0.46
1:A:1006:VAL:HG21	1:A:1009:LEU:HB2	1.96	0.46
1:C:2163:TYR:HB2	1:C:2164:PRO:CD	2.45	0.46
1:B:6176:VAL:O	1:B:6181:LYS:HE2	2.16	0.46
1:D:3049:GLU:HB3	1:B:6049:GLU:HG2	1.98	0.46
1:C:2178:ARG:HA	1:C:2181:LYS:HE2	1.98	0.46
1:F:4030:ARG:O	1:F:4034:ILE:HG13	2.16	0.45
1:D:3049:GLU:HG2	1:B:6049:GLU:CB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2116:LEU:HB2	1:C:2158:SER:O	2.16	0.45
1:B:6030:ARG:O	1:B:6034:ILE:HG13	2.16	0.45
1:F:4178:ARG:HB2	1:E:5186:GLU:OE2	2.17	0.45
1:A:1183:SER:HA	1:A:1186:GLU:OE1	2.16	0.45
1:D:3043:LYS:HB2	1:D:3053:TRP:CZ2	2.51	0.45
1:B:6163:TYR:HB2	1:B:6164:PRO:CD	2.47	0.45
1:E:5140:LEU:HD23	1:E:5248:ALA:CB	2.47	0.45
1:A:1242:VAL:O	1:A:1245:VAL:HG12	2.16	0.45
1:F:4031:VAL:HG21	1:F:4051:THR:O	2.17	0.45
1:C:2147:ILE:O	1:C:2147:ILE:CG2	2.65	0.44
1:D:3184:MET:O	1:D:3188:GLN:HG3	2.18	0.44
1:F:4108:LEU:CD2	1:F:4152:HIS:HB2	2.47	0.44
1:E:5223:ARG:C	1:E:5225:GLN:H	2.21	0.44
1:E:5141:VAL:HG12	1:E:5145:LYS:HE3	1.99	0.44
1:A:1092:ILE:CD1	1:A:1242:VAL:HG22	2.48	0.44
1:E:5093:GLY:O	1:E:5217:ALA:HA	2.17	0.44
1:F:4092:ILE:HD13	1:F:4093:GLY:N	2.33	0.44
1:A:1012:THR:O	1:A:1015:ASP:HB2	2.17	0.44
1:D:3013:LYS:HD2	1:D:3084:LEU:HA	2.00	0.44
1:C:2143:ALA:O	1:C:2147:ILE:HD13	2.18	0.44
1:A:1096:GLY:HA2	1:A:1221:VAL:O	2.18	0.44
1:D:3197:MET:HB2	3:D:706:ANU:H3'	1.99	0.43
1:C:2221:VAL:HG22	1:C:2222:ASN:N	2.33	0.43
1:E:5168:ARG:HD2	4:E:536:HOH:O	2.18	0.43
1:C:2242:VAL:O	1:C:2245:VAL:HG12	2.18	0.43
1:B:6028:PRO:HA	1:B:6066:SER:HB3	2.00	0.43
1:B:6031:VAL:HG13	1:B:6064:VAL:HG12	2.01	0.43
1:A:1091:ARG:NH1	1:A:1091:ARG:HG3	2.33	0.43
1:A:1229:PRO:HB2	1:A:1233:THR:CB	2.47	0.43
1:A:1049:GLU:HB2	1:F:4049:GLU:CG	2.48	0.43
1:D:3239:SER:OG	1:D:3243:LYS:HE3	2.18	0.43
1:E:5016:LEU:HG	1:E:5063:ILE:HG13	2.00	0.43
1:E:5236:GLN:HA	1:E:5236:GLN:OE1	2.18	0.43
1:A:1049:GLU:OE2	1:F:4049:GLU:HB2	2.19	0.43
1:B:6251:ARG:HG3	1:B:6251:ARG:HH11	1.84	0.43
1:A:1229:PRO:O	1:A:1230:ASN:C	2.57	0.42
1:A:1091:ARG:HH11	1:A:1091:ARG:HG3	1.83	0.42
1:E:5024:VAL:O	1:E:5024:VAL:HG23	2.19	0.42
1:E:5167:GLU:HG2	1:E:5167:GLU:O	2.19	0.42
1:B:6170:ASP:HB3	4:B:410:HOH:O	2.20	0.42
1:F:4092:ILE:HD13	1:F:4092:ILE:C	2.39	0.42
1:D:3038:MET:SD	1:D:3062:VAL:HG21	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:6227:GLU:O	1:B:6228:ILE:HD13	2.20	0.42
1:C:2222:ASN:CG	1:C:2225:GLN:HG3	2.40	0.42
1:F:4089:PHE:O	1:F:4213:ALA:HA	2.20	0.42
1:D:3142:GLU:HB3	1:D:3251:ARG:HH12	1.84	0.42
1:D:3220:ILE:HG13	1:D:3221:VAL:HG12	2.02	0.42
1:B:6069:ILE:HD13	3:B:707:ANU:H5'1	2.02	0.41
1:C:2060:LYS:HD2	1:C:2253:LEU:HB3	2.01	0.41
1:A:1007:PHE:HD2	1:A:1008:HIS:CE1	2.37	0.41
1:B:6021:LEU:HD23	1:B:6021:LEU:C	2.41	0.41
1:D:3004:SER:OG	1:D:3010:GLY:HA2	2.20	0.41
1:D:3234:MET:O	1:D:3235:LYS:C	2.59	0.41
1:C:2092:ILE:HD12	1:C:2216:VAL:HG13	2.02	0.41
1:A:1089:PHE:O	1:A:1213:ALA:HA	2.21	0.41
1:F:4114:VAL:HB	1:F:4157:ALA:HA	2.02	0.41
1:B:6137:THR:O	1:B:6141:VAL:HG23	2.20	0.41
1:A:1236:GLN:HB3	4:A:354:HOH:O	2.20	0.41
1:D:3242:VAL:O	1:D:3246:VAL:HG23	2.21	0.41
1:C:2140:LEU:HD22	1:C:2216:VAL:HB	2.02	0.41
1:E:5163:TYR:HB2	1:E:5164:PRO:HD3	2.02	0.41
1:A:1149:ALA:HB2	1:A:1240:HIS:NE2	2.36	0.41
1:F:4239:SER:O	1:F:4243:LYS:HG3	2.21	0.41
1:D:3049:GLU:HG2	1:B:6049:GLU:HB3	2.03	0.41
1:A:1091:ARG:HD3	1:A:1215:MET:SD	2.61	0.41
1:D:3071:GLY:N	1:D:3072:PRO:CD	2.84	0.41
1:D:3074:THR:O	1:D:3078:VAL:HG23	2.21	0.41
1:D:3013:LYS:CD	1:D:3084:LEU:HA	2.51	0.41
1:D:3181:LYS:HB2	1:D:3181:LYS:HE3	1.87	0.41
1:B:6177:VAL:HG22	4:B:114:HOH:O	2.20	0.41
1:B:6107:VAL:HG21	1:B:6244:ILE:HD12	2.02	0.41
1:D:3099:GLN:HB3	1:D:3101:HIS:CE1	2.56	0.41
1:C:2057:LEU:HD22	1:C:2250:ARG:HG3	2.03	0.40
1:D:3057:LEU:HB3	1:D:3253:LEU:HD11	2.02	0.40
1:E:5060:LYS:HD3	1:E:5253:LEU:CB	2.48	0.40
1:E:5022:ALA:HA	1:E:5063:ILE:O	2.21	0.40
1:F:4240:HIS:O	1:F:4244:ILE:HG13	2.20	0.40
1:A:1060:LYS:HB2	1:A:1253:LEU:HD13	2.03	0.40
1:C:2096:GLY:HA2	1:C:2221:VAL:O	2.22	0.40
1:D:3167:GLU:HG2	1:D:3169:TYR:CE1	2.56	0.40
1:C:2092:ILE:HD11	1:C:2241:ALA:HB1	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	249/253 (98%)	237 (95%)	9 (4%)	3 (1%)	19	11
1	B	238/253 (94%)	232 (98%)	5 (2%)	1 (0%)	43	39
1	C	239/253 (94%)	234 (98%)	4 (2%)	1 (0%)	43	39
1	D	237/253 (94%)	231 (98%)	4 (2%)	2 (1%)	27	19
1	E	237/253 (94%)	231 (98%)	4 (2%)	2 (1%)	27	19
1	F	236/253 (93%)	226 (96%)	8 (3%)	2 (1%)	27	19
All	All	1436/1518 (95%)	1391 (97%)	34 (2%)	11 (1%)	27	19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1230	ASN
1	A	1235	LYS
1	A	1163	TYR
1	D	3163	TYR
1	D	3235	LYS
1	E	5163	TYR
1	F	4163	TYR
1	B	6163	TYR
1	C	2163	TYR
1	F	4221	VAL
1	E	5224	THR

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	200/202 (99%)	194 (97%)	6 (3%)	53	55
1	B	192/202 (95%)	187 (97%)	5 (3%)	59	61
1	C	193/202 (96%)	189 (98%)	4 (2%)	66	69
1	D	191/202 (95%)	187 (98%)	4 (2%)	66	69
1	E	191/202 (95%)	189 (99%)	2 (1%)	85	90
1	F	190/202 (94%)	186 (98%)	4 (2%)	66	69
All	All	1157/1212 (96%)	1132 (98%)	25 (2%)	64	68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1092	ILE
1	A	1179	ARG
1	A	1181	LYS
1	A	1196	GLU
1	A	1215	MET
1	A	1230	ASN
1	C	2057	LEU
1	C	2196	GLU
1	C	2250	ARG
1	C	2253	LEU
1	D	3013	LYS
1	D	3030	ARG
1	D	3092	ILE
1	D	3215	MET
1	F	4092	ILE
1	F	4196	GLU
1	F	4203	LEU
1	F	4253	LEU
1	E	5021	LEU
1	E	5044	LEU
1	B	6049	GLU
1	B	6142	GLU
1	B	6170	ASP
1	B	6196	GLU
1	B	6247	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1225	GLN
1	A	1230	ASN
1	F	4188	GLN
1	F	4225	GLN
1	F	4226	GLN
1	E	5014	ASN
1	E	5020	GLN
1	E	5103	ASN
1	B	6188	GLN
1	B	6225	GLN
1	B	6226	GLN
1	B	6230	ASN

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 ⓘ

5 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	B	705	-	4,4,4	0.76	0	6,6,6	0.31	0
3	ANU	B	707	-	18,18,18	1.55	3 (16%)	25,27,27	5.01	15 (60%)
2	PO4	D	703	-	4,4,4	0.66	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANU	D	706	-	18,18,18	1.58	4 (22%)	25,27,27	4.94	15 (60%)
2	PO4	F	704	-	4,4,4	0.67	0	6,6,6	0.31	0

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	B	705	-	-	0/0/0/0	0/0/0/0
3	ANU	B	707	-	-	0/2/26/26	0/0/3/3
2	PO4	D	703	-	-	0/0/0/0	0/0/0/0
3	ANU	D	706	-	-	0/2/26/26	0/0/3/3
2	PO4	F	704	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	707	ANU	C2-N3	4.12	1.41	1.32
3	D	706	ANU	C2-N3	3.79	1.40	1.32
3	D	706	ANU	C6-C5	2.92	1.40	1.36
3	B	707	ANU	C6-N1	2.76	1.40	1.35
3	D	706	ANU	C6-N1	2.58	1.40	1.35
3	B	707	ANU	C6-C5	2.54	1.40	1.36
3	D	706	ANU	C2-N1	2.01	1.41	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	706	ANU	O2-C2'-C3'	12.69	129.40	110.48
3	B	707	ANU	O2-C2'-C3'	11.65	127.84	110.48
3	B	707	ANU	C2-O2-C2'	-9.85	96.41	106.84
3	D	706	ANU	O4'-C1'-C2'	-9.03	98.51	106.95
3	D	706	ANU	C2-O2-C2'	-8.52	97.81	106.84
3	B	707	ANU	C2'-C1'-N1	-8.09	93.94	100.98
3	B	707	ANU	O4'-C1'-C2'	-8.07	99.40	106.95
3	B	707	ANU	N3-C2-N1	-7.62	118.54	126.59
3	D	706	ANU	N3-C2-N1	-7.15	119.05	126.59
3	D	706	ANU	O4'-C1'-N1	6.75	118.53	111.87
3	D	706	ANU	C2'-C1'-N1	-6.63	95.21	100.98
3	B	707	ANU	O2-C2'-C1'	-6.55	97.89	105.23
3	B	707	ANU	O4'-C1'-N1	6.48	118.26	111.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	706	ANU	C4-N3-C2	6.11	119.81	114.17
3	B	707	ANU	C4-N3-C2	5.80	119.52	114.17
3	B	707	ANU	C2-N1-C1'	-5.24	104.56	112.26
3	D	706	ANU	O2-C2'-C1'	-5.12	99.50	105.23
3	D	706	ANU	C2-N1-C1'	-4.57	105.54	112.26
3	D	706	ANU	O2-C2-N3	3.57	132.70	120.95
3	D	706	ANU	C6-N1-C1'	3.56	133.38	125.06
3	B	707	ANU	O2-C2-N3	3.55	132.64	120.95
3	B	707	ANU	C6-N1-C1'	3.54	133.34	125.06
3	D	706	ANU	C5'-C4'-C3'	-3.44	106.62	115.06
3	D	706	ANU	C4'-O4'-C1'	-3.14	106.34	109.75
3	B	707	ANU	C4'-O4'-C1'	-3.14	106.34	109.75
3	D	706	ANU	C2'-C3'-C4'	-3.13	94.52	101.94
3	D	706	ANU	C3'-C2'-C1'	-2.66	97.56	102.73
3	B	707	ANU	C2'-C3'-C4'	-2.29	96.51	101.94
3	B	707	ANU	C5'-C4'-C3'	-2.22	109.61	115.06
3	B	707	ANU	C3'-C2'-C1'	-2.20	98.45	102.73

There are no chirality outliers.

There are no torsion outliers.

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, 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	251/253 (99%)	-0.02	6 (2%) 56 61	7, 15, 58, 99	0
1	B	242/253 (95%)	-0.17	0 100 100	9, 15, 36, 55	0
1	C	243/253 (96%)	0.07	6 (2%) 54 59	8, 18, 42, 85	0
1	D	241/253 (95%)	0.06	9 (3%) 39 43	9, 17, 48, 89	0
1	E	241/253 (95%)	-0.12	2 (0%) 83 87	7, 15, 41, 61	0
1	F	240/253 (94%)	-0.04	3 (1%) 74 78	8, 18, 41, 70	0
All	All	1458/1518 (96%)	-0.04	26 (1%) 65 69	7, 16, 43, 99	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1231	ALA	8.4
1	D	3234	MET	7.6
1	A	1234	MET	7.3
1	A	1233	THR	5.9
1	D	3235	LYS	5.1
1	C	2234	MET	4.8
1	A	1230	ASN	3.8
1	F	4003	LYS	3.4
1	A	1235	LYS	3.4
1	C	2236	GLN	3.2
1	D	3236	GLN	3.2
1	C	2235	LYS	3.1
1	E	5236	GLN	3.1
1	A	1236	GLN	2.9
1	D	3220	ILE	2.7
1	D	3224	THR	2.4
1	D	3221	VAL	2.3
1	F	4007	PHE	2.3
1	C	2101	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	4226	GLN	2.2
1	E	5225	GLN	2.2
1	D	3237	THR	2.2
1	D	3004	SER	2.2
1	C	2225	GLN	2.1
1	C	2059	GLY	2.1
1	D	3094	THR	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ANU	D	706	16/16	0.49	6.73	20,20,20,20	0
3	ANU	B	707	16/16	0.18	4.15	20,20,20,20	0
2	PO4	D	703	5/5	0.29	3.24	20,20,20,20	0
2	PO4	F	704	5/5	0.24	2.29	20,20,20,20	0
2	PO4	B	705	5/5	0.11	0.38	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.