



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 01:10 AM EDT

PDB ID : 2PGA
Title : X-ray Structure of the Uridine Phosphorylase From SALMONELLA TY-PHIMURIUM in Complex with Inhibitor and Phosphate and Potassium Ion at 1.74 Å Resolution
Authors : Timofeev, V.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.
Deposited on : unknown
Resolution : 1.74 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

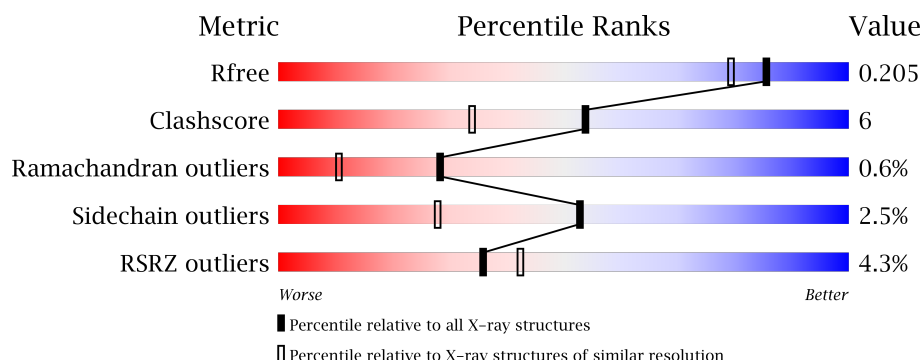
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	100719	2694 (1.76-1.72)
Clashscore	112137	2854 (1.76-1.72)
Ramachandran outliers	110173	2824 (1.76-1.72)
Sidechain outliers	110143	2824 (1.76-1.72)
RSRZ outliers	101464	2705 (1.76-1.72)

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 $\leq 5\%$. 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	253	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	253	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	C	253	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>•</div> </div> </div>
1	D	253	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	E	253	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	253	

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
2	K	A	8002	-	-	-	X
2	K	B	8001	-	-	-	X
2	K	E	8221	-	-	-	X
4	ANU	B	7016	-	-	-	X
4	ANU	D	7013	-	-	-	X
4	ANU	F	7014	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11631 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
			1877	1174	330	361	12			
1	B	241	Total	C	N	O	S	0	1	0
			1810	1135	319	345	11			
1	C	243	Total	C	N	O	S	0	1	0
			1825	1143	322	348	12			
1	D	241	Total	C	N	O	S	0	0	0
			1806	1132	318	344	12			
1	E	241	Total	C	N	O	S	0	0	0
			1807	1132	319	345	11			
1	F	240	Total	C	N	O	S	0	1	0
			1801	1128	318	344	11			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

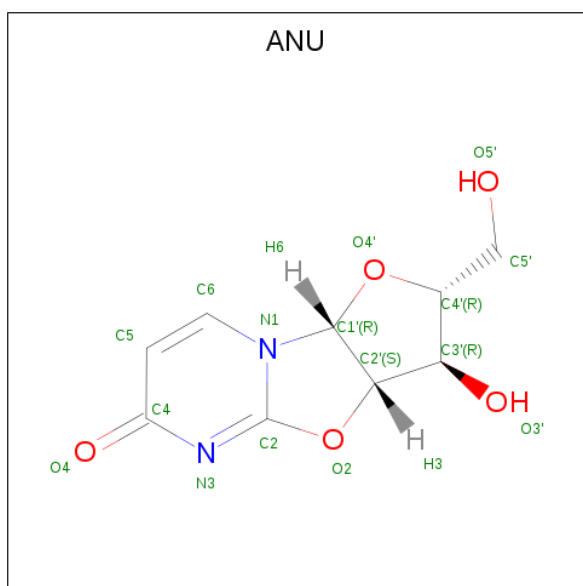
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is 2,2'-Anhydro-(1-beta-D-arabinofuranosyl)uracil (three-letter code: ANU) (formula: C₉H₁₀N₂O₅).



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

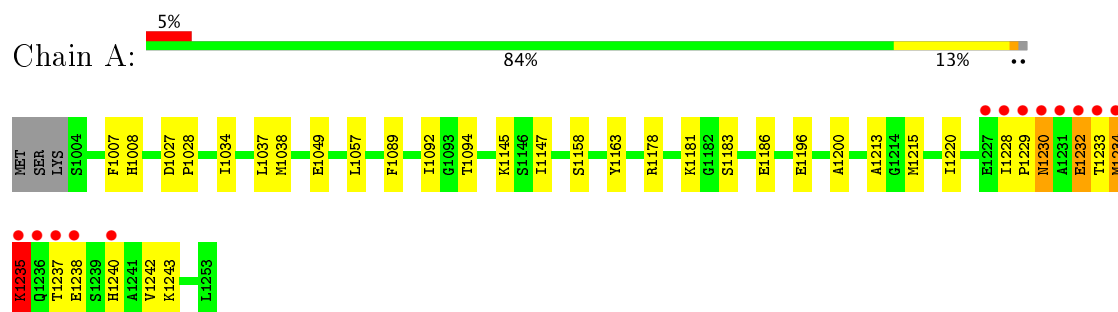
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	129	Total	O	0	0
			129	129		
5	B	115	Total	O	0	0
			115	115		
5	C	89	Total	O	0	0
			89	89		
5	D	94	Total	O	0	0
			94	94		
5	E	116	Total	O	0	0
			116	116		
5	F	96	Total	O	0	0
			96	96		

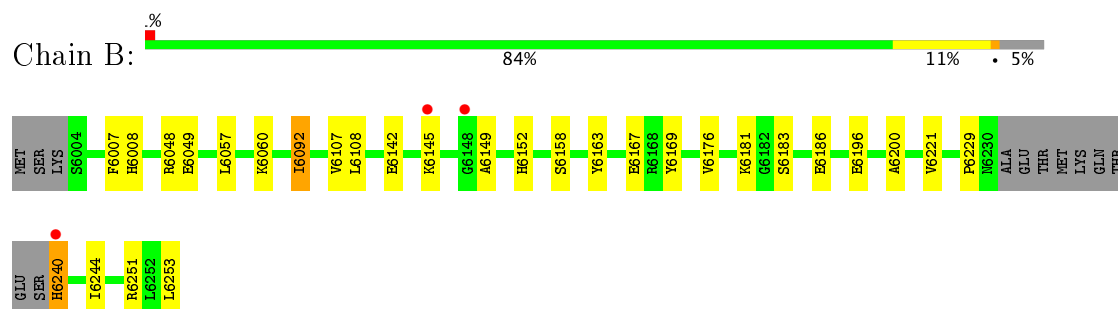
3 Residue-property plots [i](#)

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

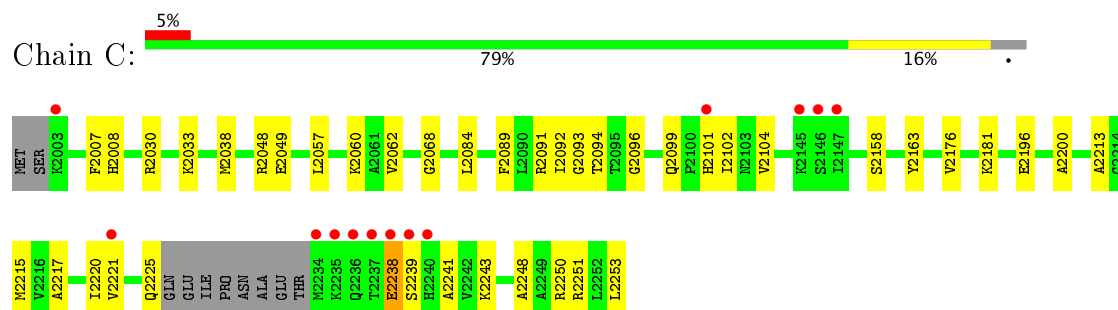
- Molecule 1: Uridine phosphorylase



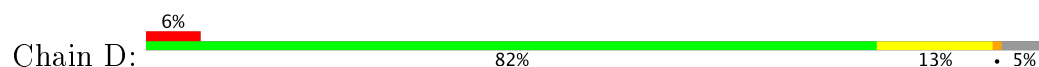
- Molecule 1: Uridine phosphorylase

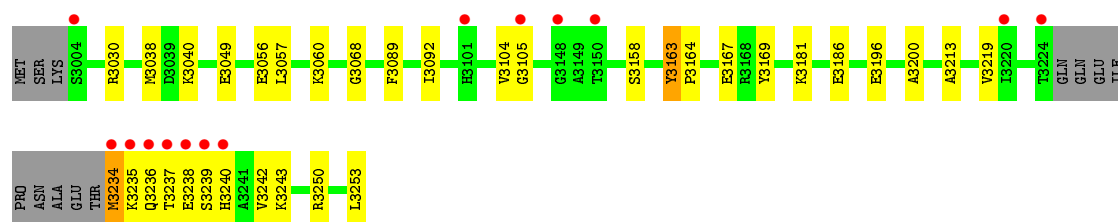


- Molecule 1: Uridine phosphorylase

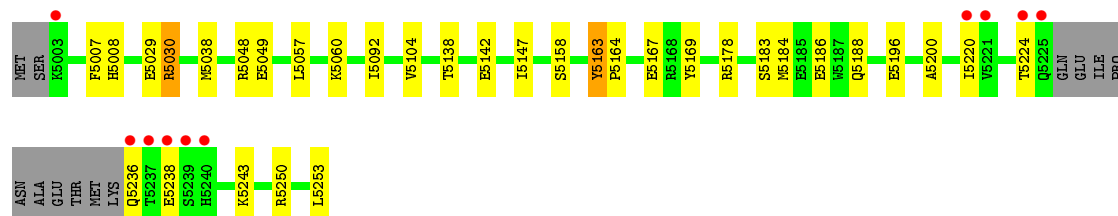
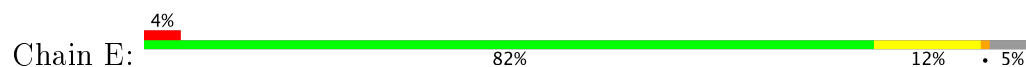


- Molecule 1: Uridine phosphorylase

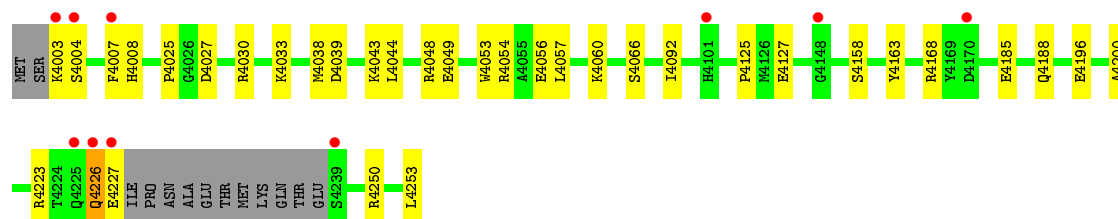
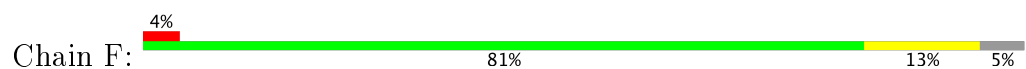




• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.79Å 124.07Å 134.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.74 6.00 – 1.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.74) 95.5 (6.00-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.74Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.210 0.176 , 0.205	Depositor DCC
R_{free} test set	7049 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.77 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11631	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 5.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ANU, K, 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	0.32	0/1907	0.53	0/2584
1	B	0.33	0/1843	0.53	0/2497
1	C	0.31	0/1858	0.51	0/2513
1	D	0.32	0/1834	0.52	0/2482
1	E	0.34	0/1835	0.55	0/2484
1	F	0.32	0/1834	0.52	0/2482
All	All	0.32	0/11111	0.53	0/15042

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1877	0	1887	29	0
1	B	1810	0	1821	15	0
1	C	1825	0	1844	27	0
1	D	1806	0	1822	26	0
1	E	1807	0	1821	21	0
1	F	1801	0	1815	20	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	E	1	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
4	B	16	0	10	0	0
4	D	16	0	10	0	0
4	F	16	0	10	0	0
5	A	129	0	0	1	0
5	B	115	0	0	0	0
5	C	89	0	0	0	0
5	D	94	0	0	0	0
5	E	116	0	0	0	0
5	F	96	0	0	0	0
All	All	11631	0	11040	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (135) 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:1220:ILE:HG21	1:A:1234:MET:HG3	1.47	0.96
1:A:1094:THR:HG21	1:A:1234:MET:HG2	1.51	0.90
1:A:1178:ARG:HA	1:A:1181:LYS:HE2	1.58	0.86
1:D:3234:MET:CE	1:D:3234:MET:HA	2.08	0.83
1:D:3234:MET:N	1:D:3237:THR:HG1	1.77	0.82
1:C:2038:MET:HG2	1:C:2057:LEU:HD13	1.64	0.78
1:A:1037:LEU:HD22	1:A:1242:VAL:HG12	1.70	0.74
1:B:6176:VAL:O	1:B:6181:LYS:HE2	1.89	0.72
1:F:4007:PHE:HD2	1:F:4008:HIS:CE1	2.12	0.68
1:F:4030:ARG:HH11	1:F:4033:LYS:HE3	1.58	0.68
1:C:2099:GLN:HB3	1:C:2101:HIS:NE2	2.10	0.67
1:E:5048:ARG:HB3	1:E:5049:GLU:OE1	1.95	0.66
1:C:2038:MET:SD	1:C:2062:VAL:HG21	2.38	0.63
1:D:3234:MET:HA	1:D:3234:MET:HE2	1.79	0.63
1:D:3105:GLY:HA2	1:D:3237:THR:HG23	1.81	0.62
1:F:4223:ARG:HA	1:F:4226:GLN:O	2.00	0.62
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.82	0.62
1:C:2239:SER:O	1:C:2243:LYS:HG3	1.99	0.62
1:C:2101:HIS:CD2	1:C:2101:HIS:H	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5184:MET:O	1:E:5188:GLN:HG3	2.01	0.60
1:F:4060:LYS:HD3	1:F:4253:LEU:HB3	1.84	0.60
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.83	0.60
1:C:2048:ARG:HB3	1:C:2049:GLU:OE1	2.02	0.60
1:C:2007:PHE:HD2	1:C:2008:HIS:CE1	2.20	0.59
1:C:2104:VAL:HG13	1:C:2220:ILE:HA	1.82	0.59
1:F:4030:ARG:NH1	1:F:4033:LYS:HE3	2.18	0.59
1:D:3057:LEU:HG	1:D:3250:ARG:HG2	1.83	0.58
1:D:3239:SER:O	1:D:3243:LYS:HG3	2.02	0.58
1:D:3057:LEU:HB3	1:D:3253:LEU:HD11	1.85	0.58
1:F:4044:LEU:HD11	1:F:4054:ARG:HB2	1.86	0.58
1:E:5030:ARG:HE	1:E:5238:GLU:CG	2.16	0.58
1:C:2158:SER:HB3	1:C:2200:ALA:HB2	1.88	0.56
1:F:4057:LEU:HG	1:F:4250:ARG:HG2	1.88	0.56
1:E:5057:LEU:HD22	1:E:5250:ARG:NH1	2.21	0.55
1:D:3104:VAL:HA	1:D:3219:VAL:HG12	1.87	0.55
1:B:6158:SER:HB3	1:B:6200:ALA:HB2	1.89	0.55
1:E:5038:MET:HG2	1:E:5057:LEU:HD21	1.90	0.54
1:D:3060:LYS:HD2	1:D:3253:LEU:HB3	1.90	0.53
1:E:5104:VAL:HG13	1:E:5220:ILE:HA	1.90	0.53
1:A:1094:THR:HG21	1:A:1234:MET:CG	2.33	0.53
1:E:5147:ILE:HG21	1:E:5243:LYS:HD2	1.89	0.53
1:A:1007:PHE:HD2	1:A:1008:HIS:CE1	2.26	0.53
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.90	0.53
1:D:3038:MET:HG2	1:D:3057:LEU:HD13	1.90	0.53
1:F:4038:MET:HG2	1:F:4057:LEU:HD13	1.92	0.52
1:D:3158:SER:HB3	1:D:3200:ALA:HB2	1.92	0.51
1:D:3105:GLY:HA2	1:D:3237:THR:CG2	2.41	0.51
1:B:6167:GLU:HG2	1:B:6169:TYR:CE1	2.45	0.51
1:E:5147:ILE:HD13	1:E:5243:LYS:HD2	1.93	0.51
1:C:2030:ARG:HD2	1:C:2033:LYS:HZ1	1.76	0.50
1:D:3235:LYS:HD3	1:D:3236:GLN:N	2.26	0.50
1:A:1094:THR:HB	1:A:1220:ILE:HD13	1.94	0.50
1:A:1235:LYS:H	1:A:1235:LYS:CD	2.26	0.49
1:D:3163:TYR:HB2	1:D:3164:PRO:CD	2.43	0.49
1:E:5060:LYS:HB2	1:E:5253:LEU:HD13	1.94	0.49
1:E:5236:GLN:O	1:E:5236:GLN:HG3	2.13	0.49
1:B:6049:GLU:HB3	1:D:3049:GLU:HB3	1.96	0.48
1:C:2094:THR:HG21	1:C:2238:GLU:HG2	1.96	0.48
1:F:4185:GLU:HA	1:F:4188:GLN:OE1	2.13	0.48
1:B:6048:ARG:HB3	1:B:6049:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4158:SER:HB3	1:F:4200:ALA:HB2	1.96	0.48
1:C:2094:THR:CG2	1:C:2238:GLU:HG2	2.43	0.47
1:A:1232:GLU:CB	1:A:1235:LYS:HG2	2.44	0.47
1:F:4168:ARG:HG2	1:F:4227:GLU:HG2	1.96	0.47
1:E:5030:ARG:HE	1:E:5238:GLU:HG3	1.79	0.47
1:F:4003:LYS:HD2	1:F:4004:SER:HB3	1.96	0.47
1:A:1034:ILE:HG12	1:A:1242:VAL:HG13	1.96	0.47
1:A:1229:PRO:HB2	1:A:1233:THR:HA	1.95	0.47
1:E:5030:ARG:NE	1:E:5238:GLU:HG3	2.29	0.47
1:C:2220:ILE:HG13	1:C:2221:VAL:HG22	1.96	0.46
1:E:5163:TYR:HB2	1:E:5164:PRO:CD	2.45	0.46
1:A:1049:GLU:HB3	1:F:4049:GLU:HB3	1.96	0.46
1:C:2176:VAL:O	1:C:2181:LYS:HG3	2.16	0.46
1:A:1220:ILE:HD13	1:A:1234:MET:HG3	1.97	0.46
1:F:4048:ARG:HB3	1:F:4049:GLU:OE1	2.16	0.46
1:C:2096:GLY:HA2	1:C:2221:VAL:HG23	1.97	0.46
1:A:1230:ASN:OD1	1:A:1232:GLU:HG3	2.16	0.46
1:A:1220:ILE:CG2	1:A:1234:MET:HA	2.46	0.46
1:B:6108:LEU:HD22	1:B:6152:HIS:HB2	1.98	0.46
1:C:2057:LEU:HB3	1:C:2253:LEU:HD11	1.98	0.46
1:A:1234:MET:O	1:A:1237:THR:N	2.49	0.45
1:D:3049:GLU:HG3	1:D:3068:GLY:HA3	1.98	0.45
1:B:6176:VAL:H	1:B:6181:LYS:NZ	2.14	0.45
1:C:2099:GLN:HB2	1:C:2102:ILE:HD12	1.98	0.45
1:C:2049:GLU:HG3	1:C:2068:GLY:HA3	1.99	0.45
1:E:5007:PHE:HD2	1:E:5008:HIS:CE1	2.35	0.45
1:A:1232:GLU:HB2	1:A:1235:LYS:HG2	1.98	0.45
1:D:3238:GLU:O	1:D:3242:VAL:HG23	2.17	0.44
1:C:2099:GLN:HB3	1:C:2101:HIS:CD2	2.52	0.44
1:F:4025:PRO:O	1:F:4066:SER:HA	2.18	0.44
1:F:4007:PHE:CD2	1:F:4008:HIS:CE1	3.01	0.44
1:C:2093:GLY:O	1:C:2217:ALA:HA	2.17	0.44
1:E:5183:SER:HA	1:E:5186:GLU:OE1	2.17	0.44
1:B:6007:PHE:HD1	1:B:6008:HIS:CE1	2.36	0.44
1:B:6057:LEU:HB3	1:B:6253:LEU:HD11	2.00	0.43
1:A:1027:ASP:HA	1:A:1028:PRO:HD2	1.93	0.43
1:B:6221:VAL:HB	1:B:6229:PRO:HG3	2.01	0.43
1:D:3235:LYS:C	1:D:3235:LYS:HD3	2.38	0.43
1:C:2049:GLU:OE1	1:C:2049:GLU:N	2.51	0.43
1:C:2057:LEU:HG	1:C:2250:ARG:HG3	1.99	0.43
1:F:4027:ASP:HB3	1:F:4030:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3181:LYS:HE3	1:D:3181:LYS:HB2	1.67	0.43
1:F:4039:ASP:HB2	1:F:4056:GLU:HB3	2.00	0.43
1:C:2248:ALA:HA	1:C:2251:ARG:HD2	2.01	0.43
1:E:5253:LEU:HD23	1:E:5253:LEU:HA	1.87	0.43
1:A:1147:ILE:HG13	1:A:1243:LYS:HG2	2.01	0.43
1:C:2060:LYS:HD2	1:C:2253:LEU:HB3	2.01	0.43
1:C:2091:ARG:HG2	1:C:2215:MET:SD	2.59	0.42
1:A:1228:ILE:HA	1:A:1229:PRO:HD2	1.87	0.42
1:A:1235:LYS:N	1:A:1235:LYS:CD	2.81	0.42
1:D:3163:TYR:CB	1:D:3164:PRO:CD	2.97	0.42
1:D:3089:PHE:O	1:D:3213:ALA:HA	2.19	0.42
1:D:3234:MET:HE3	1:D:3234:MET:HA	1.98	0.42
1:F:4125:PRO:HB2	1:F:4127:GLU:OE1	2.19	0.42
1:F:4043:LYS:HB2	1:F:4053:TRP:CE2	2.54	0.42
1:E:5138:THR:O	1:E:5142:GLU:HG3	2.19	0.42
1:A:1089:PHE:O	1:A:1213:ALA:HA	2.20	0.42
1:C:2089:PHE:O	1:C:2213:ALA:HA	2.20	0.41
1:B:6092:ILE:HD13	1:B:6092:ILE:C	2.41	0.41
1:E:5167:GLU:HG2	1:E:5169:TYR:CE1	2.55	0.41
1:B:6149:ALA:HB2	1:B:6240:HIS:HD2	1.86	0.41
1:D:3186:GLU:OE2	1:E:5178:ARG:HB2	2.21	0.41
1:A:1145:LYS:HD3	5:A:8071:HOH:O	2.21	0.41
1:C:2092:ILE:HD11	1:C:2241:ALA:HB1	2.03	0.41
1:E:5163:TYR:CB	1:E:5164:PRO:CD	2.99	0.41
1:A:1238:GLU:O	1:A:1242:VAL:HG23	2.21	0.41
1:B:6060:LYS:HD2	1:B:6253:LEU:HB3	2.03	0.40
1:B:6107:VAL:HG21	1:B:6244:ILE:HD12	2.03	0.40
1:D:3040:LYS:HE3	1:D:3056:GLU:CD	2.41	0.40
1:A:1183:SER:HA	1:A:1186:GLU:OE1	2.22	0.40
1:A:1235:LYS:N	1:A:1235:LYS:HD2	2.33	0.40
1:D:3030:ARG:HG2	1:D:3030:ARG:O	2.22	0.40
1:A:1229:PRO:HG2	1:A:1233:THR:HG22	2.02	0.40
1:B:6183:SER:HA	1:B:6186:GLU:OE1	2.22	0.40
1:D:3167:GLU:HG2	1:D:3169:TYR:CE1	2.57	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	248/253 (98%)	239 (96%)	6 (2%)	3 (1%)	15	3
1	B	238/253 (94%)	234 (98%)	3 (1%)	1 (0%)	38	19
1	C	240/253 (95%)	237 (99%)	2 (1%)	1 (0%)	38	19
1	D	237/253 (94%)	233 (98%)	3 (1%)	1 (0%)	38	19
1	E	237/253 (94%)	231 (98%)	5 (2%)	1 (0%)	38	19
1	F	237/253 (94%)	230 (97%)	6 (2%)	1 (0%)	38	19
All	All	1437/1518 (95%)	1404 (98%)	25 (2%)	8 (1%)	28	10

All (8) Ramachandran outliers are listed below:

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

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	199/202 (98%)	192 (96%)	7 (4%)	41 15
1	B	192/202 (95%)	186 (97%)	6 (3%)	45 19
1	C	194/202 (96%)	190 (98%)	4 (2%)	59 35
1	D	191/202 (95%)	187 (98%)	4 (2%)	59 35
1	E	191/202 (95%)	186 (97%)	5 (3%)	51 26
1	F	191/202 (95%)	188 (98%)	3 (2%)	68 49
All	All	1158/1212 (96%)	1129 (98%)	29 (2%)	53 28

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1092	ILE
1	A	1196	GLU
1	A	1215	MET
1	A	1232	GLU
1	A	1234	MET
1	A	1235	LYS
1	A	1240	HIS
1	B	6092	ILE
1	B	6142	GLU
1	B	6145	LYS
1	B	6196	GLU
1	B	6240	HIS
1	B	6251	ARG
1	C	2084	LEU
1	C	2196	GLU
1	C	2225	GLN
1	C	2238	GLU
1	D	3092	ILE
1	D	3196	GLU
1	D	3234	MET
1	D	3240	HIS
1	E	5029	GLU
1	E	5030	ARG
1	E	5092	ILE
1	E	5196	GLU
1	E	5224	THR
1	F	4092	ILE

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Mol	Chain	Res	Type
1	F	4196	GLU
1	F	4226	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	6101	HIS
1	B	6240	HIS
1	C	2240	HIS
1	D	3240	HIS
1	E	5225	GLN
1	F	4240	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	B	7006	-	4,4,4	0.72	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ANU	B	7016	-	13,18,18	2.07	2 (15%)	15,27,27	2.37	4 (26%)
3	PO4	D	7003	-	4,4,4	0.80	0	6,6,6	0.51	0
4	ANU	D	7013	-	13,18,18	2.23	1 (7%)	15,27,27	2.27	4 (26%)
3	PO4	F	7004	-	4,4,4	0.69	0	6,6,6	0.37	0
4	ANU	F	7014	-	13,18,18	2.20	1 (7%)	15,27,27	1.92	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	B	7006	-	-	0/0/0/0	0/0/0/0
4	ANU	B	7016	-	-	0/2/26/26	0/2/3/3
3	PO4	D	7003	-	-	0/0/0/0	0/0/0/0
4	ANU	D	7013	-	-	0/2/26/26	0/2/3/3
3	PO4	F	7004	-	-	0/0/0/0	0/0/0/0
4	ANU	F	7014	-	-	0/2/26/26	0/2/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	7016	ANU	O2-C2'	-2.01	1.43	1.46
4	B	7016	ANU	C2-N3	6.73	1.45	1.32
4	F	7014	ANU	C2-N3	7.23	1.46	1.32
4	D	7013	ANU	C2-N3	7.37	1.46	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	7016	ANU	O2-C2'-C3'	-4.78	103.60	110.51
4	D	7013	ANU	O2-C2'-C3'	-3.49	105.46	110.51
4	F	7014	ANU	O2-C2'-C3'	-3.07	106.07	110.51
4	D	7013	ANU	C5'-C4'-C3'	-2.78	108.34	115.05
4	B	7016	ANU	C5'-C4'-C3'	-2.59	108.79	115.05
4	F	7014	ANU	C5'-C4'-C3'	-2.31	109.47	115.05
4	D	7013	ANU	O2-C2'-C1'	3.03	108.59	105.24
4	F	7014	ANU	O2-C2'-C1'	3.26	108.84	105.24
4	B	7016	ANU	O2-C2'-C1'	3.60	109.23	105.24
4	F	7014	ANU	C4-N3-C2	4.92	118.36	114.13
4	B	7016	ANU	C4-N3-C2	5.74	119.06	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	7013	ANU	C4-N3-C2	6.06	119.34	114.13

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 [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	250/253 (98%)	-0.17	13 (5%) 28 34	10, 16, 41, 64	0
1	B	241/253 (95%)	-0.38	3 (1%) 79 85	10, 17, 31, 40	0
1	C	243/253 (96%)	0.08	13 (5%) 27 33	12, 22, 41, 62	0
1	D	241/253 (95%)	-0.02	14 (5%) 24 29	11, 20, 38, 64	0
1	E	241/253 (95%)	-0.21	10 (4%) 38 44	10, 17, 34, 59	0
1	F	240/253 (94%)	-0.16	10 (4%) 37 43	10, 19, 36, 48	0
All	All	1456/1518 (95%)	-0.15	63 (4%) 36 42	10, 18, 38, 64	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3234	MET	13.9
1	A	1231	ALA	9.0
1	C	2236	GLN	8.2
1	A	1233	THR	7.6
1	A	1234	MET	7.4
1	C	2234	MET	7.1
1	D	3236	GLN	7.0
1	A	1230	ASN	6.4
1	D	3237	THR	6.4
1	D	3235	LYS	6.1
1	A	1232	GLU	6.0
1	D	3238	GLU	5.7
1	E	5236	GLN	5.3
1	F	4003	LYS	5.0
1	F	4239	SER	5.0
1	C	2003	LYS	4.9
1	E	5238	GLU	4.4
1	A	1228	ILE	4.2
1	E	5237	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	3239	SER	4.2
1	C	2235	LYS	4.1
1	A	1229	PRO	4.1
1	A	1236	GLN	3.9
1	C	2101	HIS	3.9
1	E	5240	HIS	3.9
1	C	2240	HIS	3.6
1	E	5224	THR	3.6
1	C	2221	VAL	3.5
1	C	2238	GLU	3.4
1	F	4148	GLY	3.3
1	E	5225	GLN	3.3
1	A	1238	GLU	3.3
1	F	4007	PHE	3.2
1	D	3240	HIS	3.2
1	A	1235	LYS	3.2
1	D	3148	GLY	3.2
1	F	4226	GLN	3.1
1	D	3105	GLY	3.0
1	F	4004	SER	2.9
1	E	5221	VAL	2.8
1	D	3224	THR	2.8
1	E	5003	LYS	2.8
1	B	6240	HIS	2.8
1	B	6145	LYS	2.8
1	C	2145	LYS	2.8
1	D	3150	THR	2.7
1	C	2237	THR	2.6
1	C	2147	ILE	2.6
1	E	5239	SER	2.6
1	D	3101	HIS	2.4
1	C	2146	SER	2.4
1	F	4227	GLU	2.4
1	A	1240	HIS	2.4
1	C	2239	SER	2.4
1	E	5220	ILE	2.3
1	A	1227	GLU	2.3
1	A	1237	THR	2.2
1	F	4170	ASP	2.2
1	F	4225	GLN	2.1
1	D	3220	ILE	2.1
1	F	4101	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	6148	GLY	2.0
1	D	3004	SER	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	K	E	8221	1/1	0.96	0.23	4.81	34,34,34,34	0
4	ANU	F	7014	16/16	0.89	0.17	3.58	20,24,27,27	0
2	K	A	8002	1/1	0.99	0.14	3.03	21,21,21,21	0
4	ANU	B	7016	16/16	0.96	0.09	2.68	13,16,18,19	0
4	ANU	D	7013	16/16	0.84	0.18	2.39	21,25,29,29	0
2	K	B	8001	1/1	0.99	0.13	2.30	18,18,18,18	0
3	PO4	F	7004	5/5	0.97	0.11	1.73	24,25,26,27	0
3	PO4	D	7003	5/5	0.95	0.11	0.85	22,26,27,28	0
3	PO4	B	7006	5/5	0.98	0.08	0.18	17,17,18,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.