W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:47 AM GMT

PDB ID	:	3C74
Title	:	X-ray structure of the uridine phosphorylase from salmonella typhimurium in complex with 2,2'-anhydrouridine at 2.38a resolution
Authors	:	Lashkov, A.A.; Mikhailov, A.M.
Deposited on	:	2008-02-06
Resolution	:	2.38 Å(reported)

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

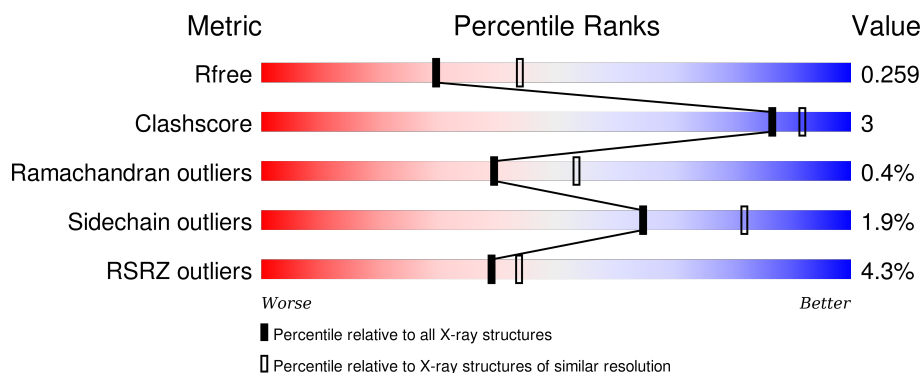|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.38 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.
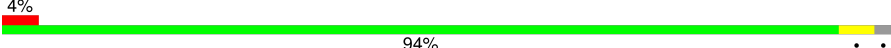
Metric	Percentile Ranks	Value
Rfree		0.259
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		1.9%
RSRZ outliers		4.3%

Worse   *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	253	6% / 91% · ·
1	B	253	5% / 85% 10% · ·
1	C	253	2% / 86% 9% · ·
1	D	253	3% / 90% 8% ··
1	E	253	5% / 89% 6% · 5%

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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	ANU	A	1516	X	-	-	-
2	ANU	B	1516	X	-	-	-
2	ANU	C	1516	X	-	-	-
2	ANU	D	1516	X	-	-	-
2	ANU	E	1516	X	-	-	-
2	ANU	F	1516	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11475 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.
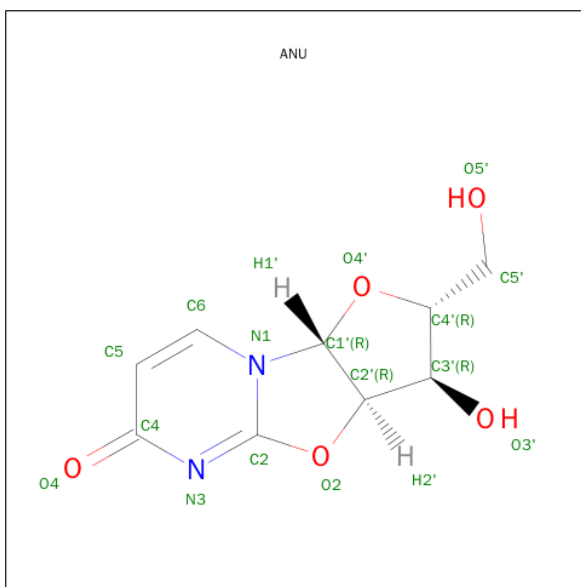
- Molecule 1 is a protein called Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1814	1138	319	346	11			
1	B	244	Total	C	N	O	S	0	0	0
			1827	1145	322	349	11			
1	C	243	Total	C	N	O	S	0	0	0
			1818	1140	321	346	11			
1	D	251	Total	C	N	O	S	0	0	0
			1885	1180	332	361	12			
1	E	241	Total	C	N	O	S	0	0	0
			1805	1133	318	343	11			
1	F	248	Total	C	N	O	S	0	0	0
			1856	1163	327	354	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	LYS	-	expression tag	UNP P0A1F6
B	2001	LYS	-	expression tag	UNP P0A1F6
C	3001	LYS	-	expression tag	UNP P0A1F6
D	4001	LYS	-	expression tag	UNP P0A1F6
E	5001	LYS	-	expression tag	UNP P0A1F6
F	6001	LYS	-	expression tag	UNP P0A1F6

- Molecule 2 is 2,2'-ANHYDROURIDINE (three-letter code: ANU) (formula: $C_9H_{10}N_2O_5$).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	48	Total 48	O 48	0	0
3	C	59	Total 59	O 59	0	0
3	D	82	Total 82	O 82	0	0
3	E	61	Total 61	O 61	0	0
3	F	67	Total 67	O 67	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.
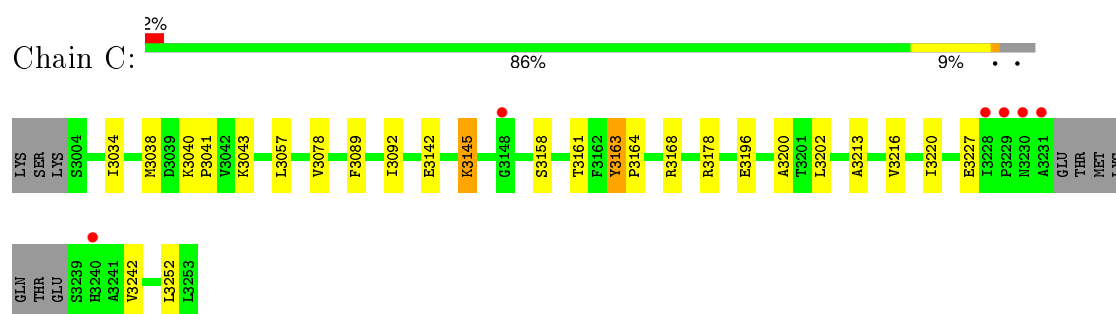
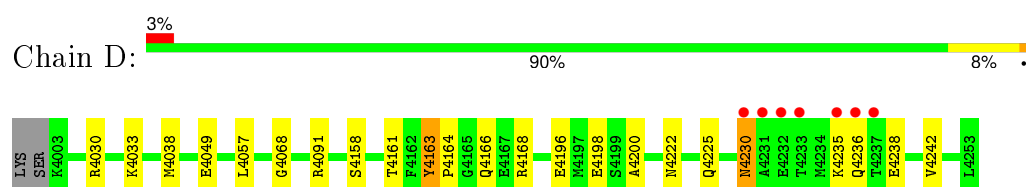- Molecule 1: Uridine phosphorylase
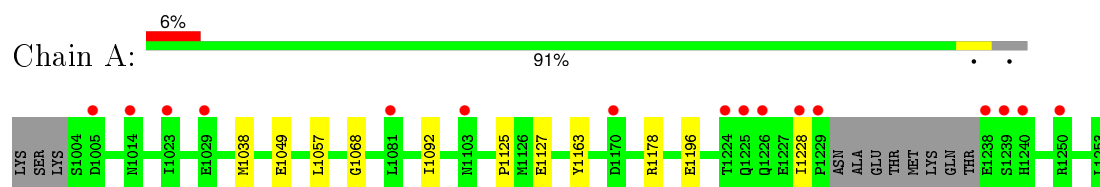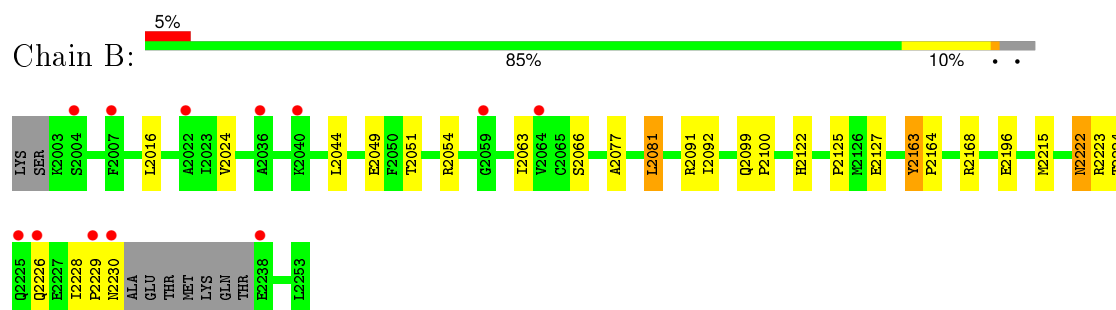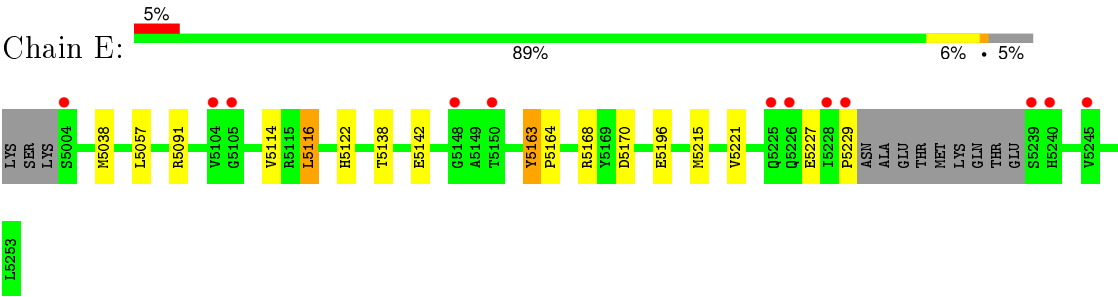

- Molecule 1: Uridine phosphorylase

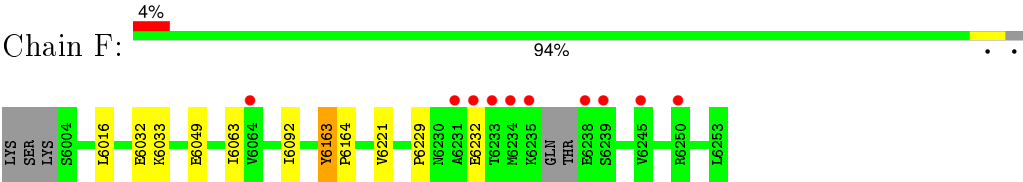- Molecule 1: Uridine phosphorylase

- Molecule 1: Uridine phosphorylase

- Molecule 1: Uridine phosphorylase

Chain E:

• Molecule 1: Uridine phosphorylase

Chain F:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.37Å 125.31Å 135.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.38 19.94 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.94-2.38) 98.4 (19.94-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.22 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.258 0.210 , 0.259	Depositor DCC
R_{free} test set	1849 reflections (3.12%)	DCC
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	1 of 61088 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11475	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0/1843	0.51	0/2498
1	B	0.37	0/1856	0.53	0/2516
1	C	0.37	0/1847	0.54	0/2504
1	D	0.37	0/1915	0.51	0/2595
1	E	0.37	0/1834	0.52	0/2486
1	F	0.37	0/1885	0.51	0/2554
All	All	0.37	0/11180	0.52	0/15153

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	1814	0	1825	6	0
1	B	1827	0	1833	17	0
1	C	1818	0	1830	13	0
1	D	1885	0	1900	14	0
1	E	1805	0	1819	9	0
1	F	1856	0	1867	7	0
2	A	16	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	10	0	0
2	C	16	0	10	0	0
2	D	16	0	10	0	0
2	E	16	0	10	0	0
2	F	16	0	10	0	0
3	A	57	0	0	0	0
3	B	48	0	0	0	0
3	C	59	0	0	0	0
3	D	82	0	0	0	0
3	E	61	0	0	0	0
3	F	67	0	0	0	0
All	All	11475	0	11134	60	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 3.

All (60) 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:B:2163:TYR:HB2	1:B:2164:PRO:HD3	1.65	0.79
1:E:5163:TYR:HB2	1:E:5164:PRO:HD3	1.65	0.78
1:F:6163:TYR:HB2	1:F:6164:PRO:HD3	1.69	0.74
1:F:6221:VAL:HB	1:F:6229:PRO:HG3	1.73	0.71
1:C:3163:TYR:HB2	1:C:3164:PRO:HD3	1.71	0.70
1:B:2091:ARG:HG2	1:B:2215:MET:SD	2.34	0.67
1:F:6032:GLU:HG3	1:F:6033:LYS:HE3	1.78	0.64
1:D:4030:ARG:NH1	1:D:4033:LYS:HD3	2.16	0.61
1:E:5221:VAL:HB	1:E:5229:PRO:HG3	1.84	0.60
1:A:1049:GLU:HG3	1:F:6049:GLU:HG3	1.83	0.59
1:D:4230:ASN:H	1:D:4230:ASN:HD22	1.54	0.55
1:A:1125:PRO:HB2	1:A:1127:GLU:OE2	2.05	0.55
1:C:3040:LYS:N	1:C:3041:PRO:HD3	2.21	0.55
1:C:3034:ILE:HG12	1:C:3242:VAL:HG13	1.88	0.55
1:E:5163:TYR:CB	1:E:5164:PRO:HD3	2.36	0.55
1:B:2077:ALA:O	1:B:2081:LEU:HB2	2.08	0.54
1:E:5091:ARG:HG2	1:E:5215:MET:SD	2.48	0.54
1:E:5114:VAL:HG12	1:E:5116:LEU:HD13	1.90	0.54
1:B:2051:THR:H	1:B:2066:SER:HB3	1.75	0.51
1:A:1178:ARG:O	1:C:3178:ARG:NH2	2.43	0.51
1:C:3158:SER:HB3	1:C:3200:ALA:HB2	1.93	0.50
1:C:3078:VAL:HG21	1:C:3202:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5138:THR:O	1:E:5142:GLU:HG2	2.12	0.50
1:B:2125:PRO:HB2	1:B:2127:GLU:OE2	2.12	0.50
1:D:4038:MET:HG2	1:D:4057:LEU:HD13	1.93	0.49
1:E:5168:ARG:NH1	1:E:5227:GLU:O	2.46	0.49
1:D:4030:ARG:HH21	1:D:4242:VAL:HG21	1.77	0.48
1:F:6163:TYR:CB	1:F:6164:PRO:HD3	2.43	0.48
1:A:1049:GLU:HG3	1:F:6049:GLU:CG	2.44	0.48
1:B:2223:ARG:HA	1:B:2226:GLN:O	2.13	0.48
1:C:3038:MET:HG2	1:C:3057:LEU:HD13	1.96	0.48
1:D:4163:TYR:HB2	1:D:4164:PRO:HD3	1.96	0.48
1:B:2163:TYR:CB	1:B:2164:PRO:HD3	2.41	0.47
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.98	0.45
1:C:3142:GLU:O	1:C:3145:LYS:HD3	2.15	0.45
1:A:1049:GLU:HG2	1:A:1068:GLY:HA3	1.99	0.45
1:F:6016:LEU:HA	1:F:6063:ILE:HD11	1.99	0.44
1:B:2163:TYR:HA	1:B:2168:ARG:HD2	2.00	0.44
1:B:2049:GLU:HB3	1:D:4049:GLU:HB3	1.99	0.44
1:C:3161:THR:OG1	1:E:5122:HIS:HD2	2.00	0.44
1:D:4091:ARG:CZ	1:D:4198:GLU:HG3	2.48	0.44
1:B:2016:LEU:HG	1:B:2063:ILE:HD11	2.01	0.43
1:C:3089:PHE:O	1:C:3213:ALA:HA	2.19	0.43
1:B:2122:HIS:HD2	1:D:4161:THR:OG1	2.02	0.42
1:C:3163:TYR:CB	1:C:3164:PRO:HD3	2.45	0.42
1:C:3168:ARG:NH1	1:C:3227:GLU:O	2.52	0.42
1:B:2222:ASN:HD22	1:B:2224:THR:H	1.67	0.42
1:D:4238:GLU:O	1:D:4242:VAL:HG23	2.20	0.42
1:B:2044:LEU:HD11	1:B:2054:ARG:HB2	2.02	0.42
1:E:5038:MET:HG2	1:E:5057:LEU:HD13	2.01	0.41
1:C:3092:ILE:HA	1:C:3216:VAL:O	2.20	0.41
1:B:2226:GLN:NE2	1:B:2228:ILE:O	2.52	0.41
1:D:4158:SER:HB3	1:D:4200:ALA:HB2	2.02	0.41
1:D:4222:ASN:HB3	1:D:4225:GLN:HG2	2.02	0.41
1:D:4163:TYR:HB2	1:D:4164:PRO:CD	2.51	0.41
1:B:2228:ILE:HA	1:B:2229:PRO:HD3	1.89	0.41
1:B:2099:GLN:HA	1:B:2100:PRO:HD3	1.91	0.41
1:D:4166:GLN:OE1	1:D:4168:ARG:NH1	2.55	0.40
1:B:2024:VAL:O	1:B:2091:ARG:HD2	2.22	0.40
1:D:4049:GLU:HG3	1:D:4068:GLY:HA3	2.03	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	238/253 (94%)	234 (98%)	3 (1%)	1 (0%)	39	53
1	B	240/253 (95%)	235 (98%)	4 (2%)	1 (0%)	39	53
1	C	239/253 (94%)	234 (98%)	4 (2%)	1 (0%)	39	53
1	D	249/253 (98%)	246 (99%)	2 (1%)	1 (0%)	39	53
1	E	237/253 (94%)	231 (98%)	5 (2%)	1 (0%)	39	53
1	F	244/253 (96%)	238 (98%)	5 (2%)	1 (0%)	39	53
All	All	1447/1518 (95%)	1418 (98%)	23 (2%)	6 (0%)	39	53

All (6) Ramachandran outliers are listed below:

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

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	192/202 (95%)	189 (98%)	3 (2%)	70	85
1	B	193/202 (96%)	188 (97%)	5 (3%)	54	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	192/202 (95%)	187 (97%)	5 (3%)	54	73
1	D	200/202 (99%)	196 (98%)	4 (2%)	63	80
1	E	191/202 (95%)	188 (98%)	3 (2%)	70	85
1	F	196/202 (97%)	194 (99%)	2 (1%)	82	92
All	All	1164/1212 (96%)	1142 (98%)	22 (2%)	65	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1092	ILE
1	A	1196	GLU
1	A	1228	ILE
1	B	2081	LEU
1	B	2092	ILE
1	B	2196	GLU
1	B	2222	ASN
1	B	2230	ASN
1	C	3043	LYS
1	C	3145	LYS
1	C	3196	GLU
1	C	3220	ILE
1	C	3252	LEU
1	D	4196	GLU
1	D	4230	ASN
1	D	4235	LYS
1	D	4236	GLN
1	E	5116	LEU
1	E	5170	ASP
1	E	5196	GLU
1	F	6092	ILE
1	F	6232	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1083	GLN
1	A	1209	GLN
1	A	1226	GLN
1	B	2122	HIS
1	B	2209	GLN

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Mol	Chain	Res	Type
1	B	2222	ASN
1	B	2230	ASN
1	C	3047	HIS
1	C	3122	HIS
1	C	3209	GLN
1	C	3226	GLN
1	D	4047	HIS
1	D	4083	GLN
1	D	4122	HIS
1	D	4209	GLN
1	D	4230	ASN
1	D	4236	GLN
1	E	5122	HIS
1	E	5166	GLN
1	E	5209	GLN
1	F	6083	GLN
1	F	6209	GLN
1	F	6226	GLN

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)

6 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	ANU	A	1516	-	13,18,18	2.59	2 (15%)	16,27,27	2.17	4 (25%)
2	ANU	B	1516	-	13,18,18	2.50	2 (15%)	16,27,27	2.06	3 (18%)
2	ANU	C	1516	-	13,18,18	2.65	3 (23%)	16,27,27	2.08	3 (18%)
2	ANU	D	1516	-	13,18,18	2.61	2 (15%)	16,27,27	2.05	3 (18%)
2	ANU	E	1516	-	13,18,18	2.58	2 (15%)	16,27,27	2.15	4 (25%)
2	ANU	F	1516	-	13,18,18	2.67	3 (23%)	16,27,27	2.08	3 (18%)

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	ANU	A	1516	-	1/1/4/4	0/2/26/26	0/2/3/3
2	ANU	B	1516	-	1/1/4/4	0/2/26/26	0/2/3/3
2	ANU	C	1516	-	1/1/4/4	0/2/26/26	0/2/3/3
2	ANU	D	1516	-	1/1/4/4	0/2/26/26	0/2/3/3
2	ANU	E	1516	-	1/1/4/4	0/2/26/26	0/2/3/3
2	ANU	F	1516	-	1/1/4/4	0/2/26/26	0/2/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1516	ANU	O4'-C1'	2.39	1.44	1.41
2	F	1516	ANU	O4'-C1'	2.46	1.44	1.41
2	B	1516	ANU	O2-C2	4.51	1.42	1.35
2	D	1516	ANU	O2-C2	4.84	1.42	1.35
2	F	1516	ANU	O2-C2	4.89	1.42	1.35
2	A	1516	ANU	O2-C2	4.92	1.42	1.35
2	E	1516	ANU	O2-C2	4.96	1.42	1.35
2	C	1516	ANU	O2-C2	5.03	1.43	1.35
2	B	1516	ANU	C2-N3	7.37	1.47	1.32
2	A	1516	ANU	C2-N3	7.46	1.47	1.32
2	E	1516	ANU	C2-N3	7.51	1.47	1.32
2	C	1516	ANU	C2-N3	7.52	1.47	1.32
2	D	1516	ANU	C2-N3	7.60	1.47	1.32
2	F	1516	ANU	C2-N3	7.62	1.47	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1516	ANU	C5'-C4'-C3'	-2.36	109.50	115.08
2	D	1516	ANU	C5'-C4'-C3'	-2.21	109.85	115.08
2	B	1516	ANU	C5'-C4'-C3'	-2.18	109.93	115.08
2	E	1516	ANU	C5'-C4'-C3'	-2.08	110.16	115.08
2	A	1516	ANU	C3'-C2'-C1'	2.17	106.92	102.73
2	E	1516	ANU	C4'-O4'-C1'	2.40	112.36	109.72
2	A	1516	ANU	C4'-O4'-C1'	2.41	112.36	109.72
2	D	1516	ANU	O2-C2'-C1'	2.47	108.06	105.28
2	F	1516	ANU	C4'-O4'-C1'	2.49	112.46	109.72
2	B	1516	ANU	O2-C2'-C1'	2.71	108.33	105.28
2	A	1516	ANU	O2-C2'-C1'	2.75	108.38	105.28
2	F	1516	ANU	O2-C2'-C1'	2.85	108.49	105.28
2	E	1516	ANU	O2-C2'-C1'	2.91	108.56	105.28
2	C	1516	ANU	O2-C2'-C1'	3.00	108.66	105.28
2	B	1516	ANU	C4-N3-C2	6.22	120.31	114.14
2	F	1516	ANU	C4-N3-C2	6.25	120.33	114.14
2	C	1516	ANU	C4-N3-C2	6.27	120.35	114.14
2	D	1516	ANU	C4-N3-C2	6.40	120.48	114.14
2	E	1516	ANU	C4-N3-C2	6.55	120.63	114.14
2	A	1516	ANU	C4-N3-C2	6.69	120.77	114.14

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1516	ANU	C2'
2	E	1516	ANU	C2'
2	B	1516	ANU	C2'
2	A	1516	ANU	C2'
2	C	1516	ANU	C2'
2	D	1516	ANU	C2'

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	242/253 (95%)	0.30	16 (6%)	22	25	27, 36, 49, 60	0
1	B	244/253 (96%)	0.16	12 (4%)	33	38	24, 34, 48, 58	0
1	C	243/253 (96%)	0.10	6 (2%)	61	64	24, 31, 42, 56	0
1	D	251/253 (99%)	0.13	7 (2%)	56	59	24, 31, 53, 64	0
1	E	241/253 (95%)	0.25	12 (4%)	32	37	25, 34, 45, 55	0
1	F	248/253 (98%)	0.23	10 (4%)	42	47	24, 32, 47, 63	0
All	All	1469/1518 (96%)	0.20	63 (4%)	39	44	24, 33, 48, 64	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6233	THR	8.8
1	A	1238	GLU	7.5
1	C	3231	ALA	7.5
1	F	6234	MET	6.8
1	F	6235	LYS	6.3
1	A	1239	SER	6.1
1	F	6231	ALA	5.7
1	D	4231	ALA	5.1
1	F	6232	GLU	5.1
1	D	4235	LYS	4.9
1	C	3230	ASN	4.9
1	D	4232	GLU	4.7
1	D	4230	ASN	4.3
1	A	1228	ILE	4.3
1	D	4236	GLN	4.1
1	E	5225	GLN	4.1
1	D	4233	THR	4.0
1	A	1229	PRO	3.8
1	F	6239	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	3148	GLY	3.7
1	B	2004	SER	3.7
1	E	5104	VAL	3.6
1	E	5226	GLN	3.6
1	B	2238	GLU	3.4
1	F	6064	VAL	3.3
1	F	6238	GLU	3.3
1	A	1225	GLN	3.2
1	E	5239	SER	3.2
1	B	2230	ASN	3.1
1	E	5245	VAL	3.1
1	E	5150	THR	3.0
1	E	5004	SER	3.0
1	A	1005	ASP	3.0
1	D	4237	THR	2.9
1	E	5105	GLY	2.9
1	C	3240	HIS	2.7
1	A	1224	THR	2.7
1	F	6245	VAL	2.6
1	C	3229	PRO	2.5
1	B	2064	VAL	2.5
1	E	5240	HIS	2.4
1	B	2007	PHE	2.4
1	A	1250	ARG	2.4
1	B	2059	GLY	2.3
1	B	2226	GLN	2.3
1	A	1240	HIS	2.3
1	A	1014	ASN	2.3
1	E	5229	PRO	2.3
1	A	1226	GLN	2.3
1	B	2036	ALA	2.2
1	B	2229	PRO	2.2
1	A	1103	ASN	2.2
1	A	1081	LEU	2.2
1	A	1170	ASP	2.2
1	A	1023	ILE	2.2
1	E	5228	ILE	2.2
1	E	5148	GLY	2.2
1	B	2225	GLN	2.1
1	B	2022	ALA	2.1
1	B	2040	LYS	2.1
1	F	6250	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	3228	ILE	2.1
1	A	1029	GLU	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	ANU	C	1516	16/16	0.89	0.18	1.31	37,37,38,38	0
2	ANU	F	1516	16/16	0.92	0.16	1.12	32,33,34,34	0
2	ANU	E	1516	16/16	0.83	0.17	0.94	41,42,42,43	0
2	ANU	D	1516	16/16	0.87	0.14	0.45	41,42,42,42	0
2	ANU	A	1516	16/16	0.91	0.14	0.42	32,33,33,33	0
2	ANU	B	1516	16/16	0.94	0.12	-0.50	36,36,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.