



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:03 am GMT

PDB ID : 2HRD  
Title : Crystal structure of the uridine phosphorylase from *Salmonella typhimurium* in complex with thymine and phosphate ion at 1.70Å resolution  
Authors : Timofeev, V.I.; Gabdulkhakov, A.G.; Mikhailov, A.M.  
Deposited on : 2006-07-20  
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

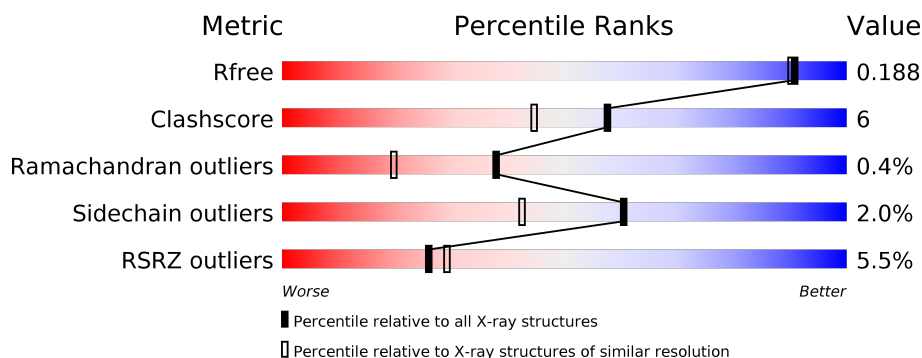
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>7%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	B	253	<div> <div>3%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	C	253	<div> <div>7%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	D	253	<div> <div>5%</div> <div>87%</div> <div>8%</div> <div>..</div> </div>
1	E	253	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	F	253	<div> <div>4%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>

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
3	TDR	A	901[A]	-	-	-	X
3	TDR	A	901[B]	-	-	-	X
3	TDR	B	902	-	-	X	X
3	TDR	C	903[A]	-	-	-	X
3	TDR	C	903[B]	-	-	-	X
3	TDR	D	904[A]	-	-	-	X
3	TDR	D	904[B]	-	-	-	X
3	TDR	E	905[A]	-	-	-	X
3	TDR	E	905[B]	-	-	-	X
3	TDR	F	906[A]	-	-	-	X
3	TDR	F	906[B]	-	-	X	X
4	1PE	B	1001	-	-	X	X
5	GOL	A	1254	-	-	-	X
5	GOL	C	1013	-	-	-	X
5	GOL	E	1015	-	-	-	X
5	GOL	F	1011	-	-	-	X

## 2 Entry composition [i](#)

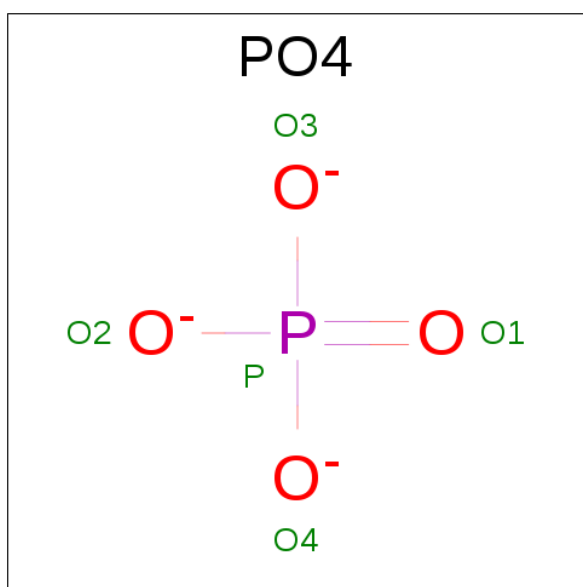
There are 6 unique types of molecules in this entry. The entry contains 12584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

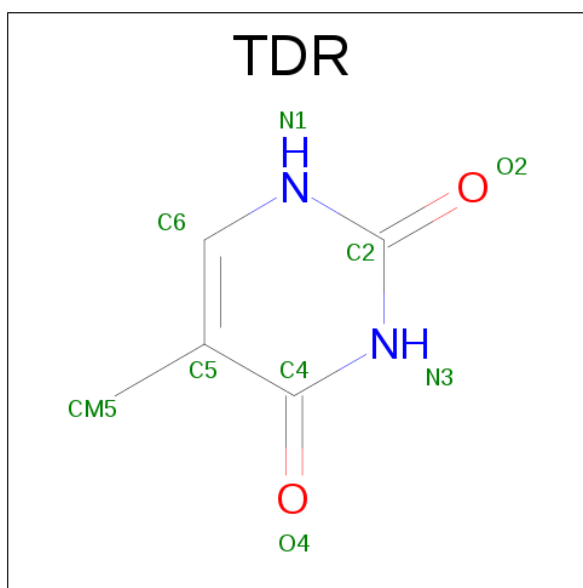
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	16	0
			1973	1244	342	375	12			
1	B	246	Total	C	N	O	S	0	18	0
			1939	1223	337	368	11			
1	C	245	Total	C	N	O	S	0	17	0
			1947	1233	342	361	11			
1	D	244	Total	C	N	O	S	0	18	0
			1937	1219	335	372	11			
1	E	252	Total	C	N	O	S	0	18	0
			1991	1256	343	380	12			
1	F	245	Total	C	N	O	S	0	11	0
			1893	1195	328	359	11			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	1
			10	8	2		
2	A	1	Total	O	P	0	1
			10	8	2		

- Molecule 3 is THYMINE (three-letter code: TDR) (formula:  $C_5H_6N_2O_2$ ).



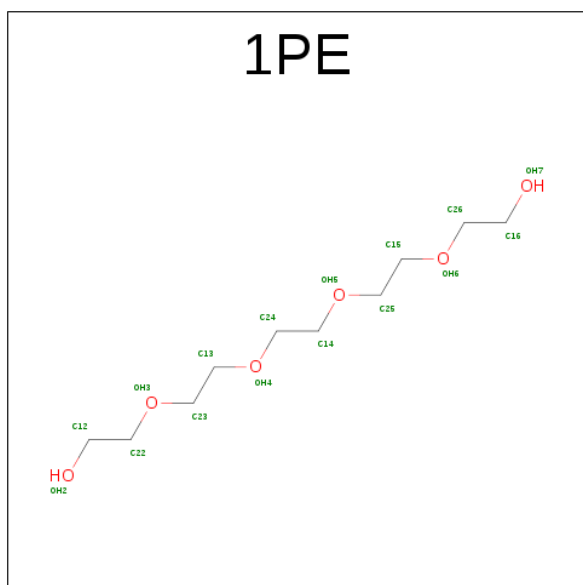
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			18	10	4	4		
3	B	1	Total	C	N	O	0	0
			9	5	2	2		
3	C	1	Total	C	N	O	0	1
			18	10	4	4		
3	D	1	Total	C	N	O	0	1
			18	10	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	1
			18	10	4	4		
3	F	1	Total	C	N	O	0	1
			18	10	4	4		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

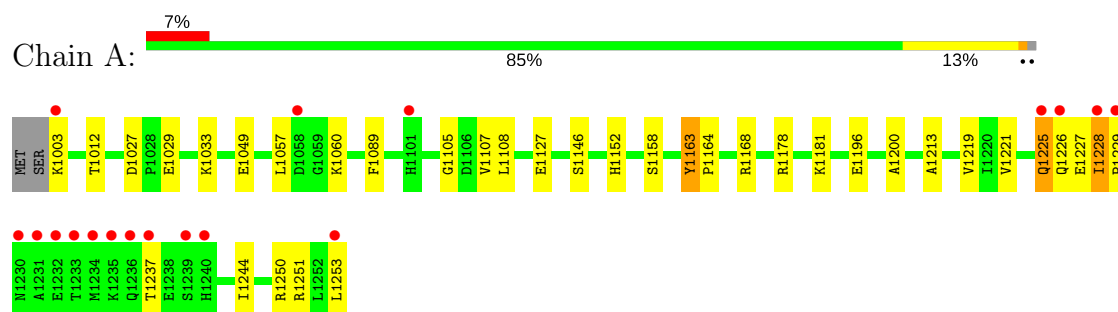
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	126	Total	O	0	1
			127	127		
6	B	136	Total	O	0	0
			136	136		
6	C	91	Total	O	0	0
			91	91		
6	D	111	Total	O	0	1
			112	112		
6	E	123	Total	O	0	2
			125	125		
6	F	118	Total	O	0	0
			118	118		

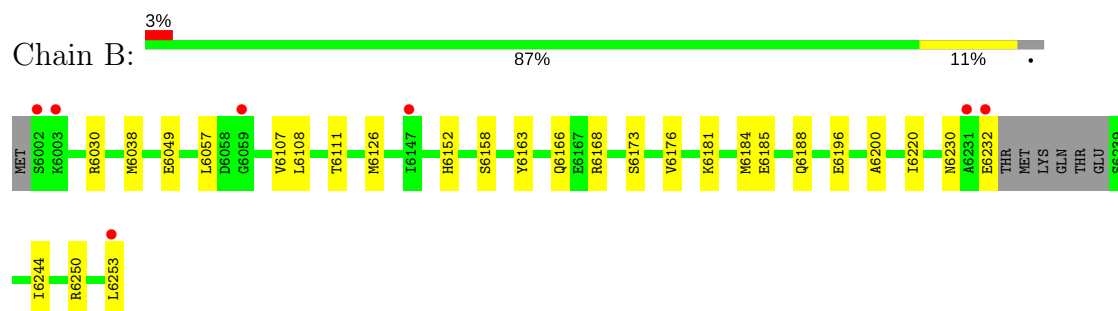
### 3 Residue-property plots [i](#)

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.

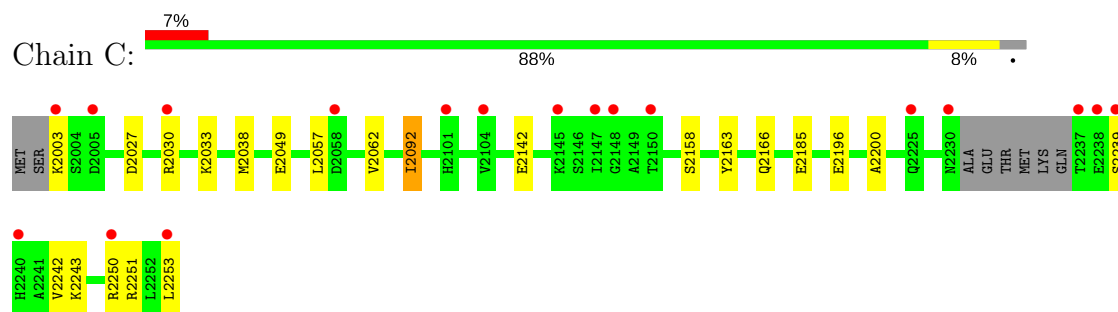
#### • Molecule 1: Uridine phosphorylase



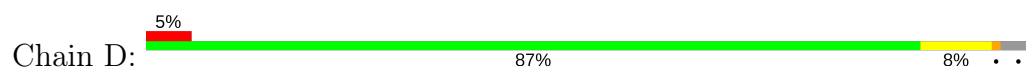
#### • Molecule 1: Uridine phosphorylase



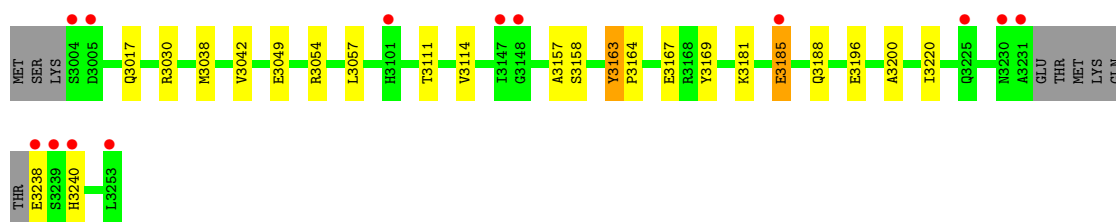
#### • Molecule 1: Uridine phosphorylase



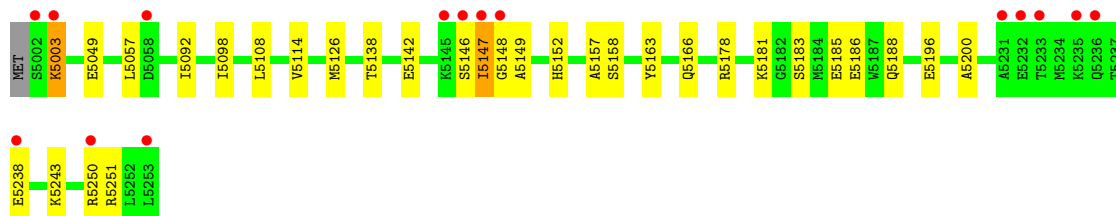
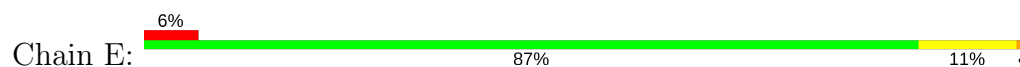
#### • Molecule 1: Uridine phosphorylase



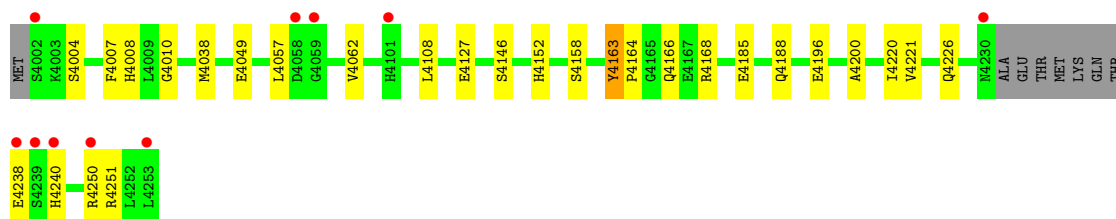
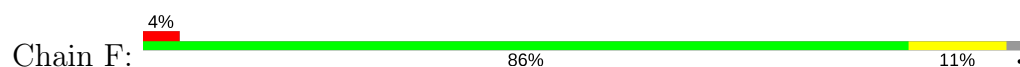




• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.20Å 123.40Å 133.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 19.83 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.70) 100.0 (19.83-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.17 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.166 , 0.189 0.165 , 0.188	Depositor DCC
$R_{free}$ test set	7980 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	7.7	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, 1PE, TDR

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	0.33	0/2051	0.53	0/2772
1	B	0.33	0/2019	0.52	0/2728
1	C	0.32	0/2023	0.51	0/2736
1	D	0.33	0/2018	0.52	0/2731
1	E	0.33	0/2066	0.53	0/2793
1	F	0.33	0/1953	0.54	0/2644
All	All	0.33	0/12130	0.52	0/16404

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

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	1973	0	2035	37	0
1	B	1939	0	1999	26	0
1	C	1947	0	2014	15	0
1	D	1937	0	1971	11	0
1	E	1991	0	2054	27	0
1	F	1893	0	1926	20	0
2	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	15	0	0	0	0
3	A	18	0	12	0	0
3	B	9	0	6	5	0
3	C	18	0	12	1	0
3	D	18	0	12	2	0
3	E	18	0	12	3	0
3	F	18	0	12	6	0
4	B	16	0	22	7	0
5	A	6	0	8	0	0
5	B	6	0	8	1	0
5	C	6	0	8	1	0
5	E	6	0	8	0	0
5	F	6	0	8	1	0
6	A	127	0	0	0	0
6	B	136	0	0	0	0
6	C	91	0	0	1	0
6	D	112	0	0	1	0
6	E	125	0	0	2	0
6	F	118	0	0	3	0
All	All	12584	0	12127	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.

The worst 5 of 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:B:6185[B]:GLU:HG2	4:B:1001:1PE:C16	1.56	1.32
1:B:6185[B]:GLU:CG	4:B:1001:1PE:H161	1.64	1.28
1:E:5147[A]:ILE:CD1	1:E:5243[A]:LYS:HD2	1.83	1.08
1:E:5147[A]:ILE:HD12	1:E:5243[A]:LYS:HD2	1.36	1.06
1:E:5098[B]:ILE:HG22	1:E:5188[B]:GLN:HG2	1.32	1.06

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	265/253 (105%)	262 (99%)	2 (1%)	1 (0%)	38	20
1	B	259/253 (102%)	256 (99%)	2 (1%)	1 (0%)	38	20
1	C	259/253 (102%)	255 (98%)	3 (1%)	1 (0%)	38	20
1	D	258/253 (102%)	253 (98%)	4 (2%)	1 (0%)	38	20
1	E	268/253 (106%)	263 (98%)	4 (2%)	1 (0%)	38	20
1	F	251/253 (99%)	246 (98%)	4 (2%)	1 (0%)	38	20
All	All	1560/1518 (103%)	1535 (98%)	19 (1%)	6 (0%)	38	20

5 of 6 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/202 (106%)	212 (99%)	3 (1%)	71	58
1	B	212/202 (105%)	208 (98%)	4 (2%)	62	45
1	C	211/202 (104%)	207 (98%)	4 (2%)	62	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	211/202 (104%)	203 (96%)	8 (4%)	38	16
1	E	217/202 (107%)	211 (97%)	6 (3%)	49	28
1	F	204/202 (101%)	201 (98%)	3 (2%)	70	55
All	All	1270/1212 (105%)	1242 (98%)	28 (2%)	60	38

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3017[B]	GLN
1	D	3185[B]	GLU
1	F	4196	GLU
1	D	3181	LYS
1	D	3185[A]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1225	GLN
1	C	2226	GLN
1	E	5225	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](#)

27 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	$\# Z  > 2$
5	GOL	A	1254	-	5,5,5	0.38	0	5,5,5	0.28	0
2	PO4	A	801	-	4,4,4	0.82	0	6,6,6	0.23	0
2	PO4	A	808[A]	-	4,4,4	0.78	0	6,6,6	0.41	0
2	PO4	A	808[B]	-	4,4,4	0.81	0	6,6,6	0.38	0
3	TDR	A	901[A]	-	7,9,9	0.91	0	7,12,12	5.59	5 (71%)
3	TDR	A	901[B]	-	7,9,9	0.95	0	7,12,12	5.54	5 (71%)
4	1PE	B	1001	-	15,15,15	0.46	0	14,14,14	0.27	0
5	GOL	B	1014	-	5,5,5	0.38	0	5,5,5	0.23	0
2	PO4	B	802	-	4,4,4	0.80	0	6,6,6	0.51	0
3	TDR	B	902	-	7,9,9	1.06	0	7,12,12	5.44	5 (71%)
5	GOL	C	1013	-	5,5,5	0.37	0	5,5,5	0.26	0
2	PO4	C	803	-	4,4,4	0.79	0	6,6,6	0.47	0
3	TDR	C	903[A]	-	7,9,9	0.90	0	7,12,12	5.63	5 (71%)
3	TDR	C	903[B]	-	7,9,9	0.98	0	7,12,12	5.58	5 (71%)
2	PO4	D	804	-	4,4,4	0.85	0	6,6,6	0.45	0
3	TDR	D	904[A]	-	7,9,9	0.93	0	7,12,12	5.51	5 (71%)
3	TDR	D	904[B]	-	7,9,9	0.96	0	7,12,12	5.57	5 (71%)
5	GOL	E	1015	-	5,5,5	0.33	0	5,5,5	0.25	0
2	PO4	E	805	-	4,4,4	0.80	0	6,6,6	0.39	0
3	TDR	E	905[A]	-	7,9,9	0.91	0	7,12,12	5.43	5 (71%)
3	TDR	E	905[B]	-	7,9,9	0.98	0	7,12,12	5.57	5 (71%)
5	GOL	F	1011	-	5,5,5	0.35	0	5,5,5	0.20	0
2	PO4	F	806	-	4,4,4	0.79	0	6,6,6	0.38	0
2	PO4	F	807[A]	-	4,4,4	0.81	0	6,6,6	0.32	0
2	PO4	F	807[B]	-	4,4,4	0.77	0	6,6,6	0.38	0
3	TDR	F	906[A]	-	7,9,9	0.92	0	7,12,12	5.51	5 (71%)
3	TDR	F	906[B]	-	7,9,9	0.98	0	7,12,12	5.55	5 (71%)

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
5	GOL	A	1254	-	-	0/4/4/4	0/0/0/0
2	PO4	A	801	-	-	0/0/0/0	0/0/0/0
2	PO4	A	808[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	A	808[B]	-	-	0/0/0/0	0/0/0/0
3	TDR	A	901[A]	-	-	0/0/0/0	0/1/1/1
3	TDR	A	901[B]	-	-	0/0/0/0	0/1/1/1
4	1PE	B	1001	-	-	0/13/13/13	0/0/0/0
5	GOL	B	1014	-	-	0/4/4/4	0/0/0/0
2	PO4	B	802	-	-	0/0/0/0	0/0/0/0
3	TDR	B	902	-	-	0/0/0/0	0/1/1/1
5	GOL	C	1013	-	-	0/4/4/4	0/0/0/0
2	PO4	C	803	-	-	0/0/0/0	0/0/0/0
3	TDR	C	903[A]	-	-	0/0/0/0	0/1/1/1
3	TDR	C	903[B]	-	-	0/0/0/0	0/1/1/1
2	PO4	D	804	-	-	0/0/0/0	0/0/0/0
3	TDR	D	904[A]	-	-	0/0/0/0	0/1/1/1
3	TDR	D	904[B]	-	-	0/0/0/0	0/1/1/1
5	GOL	E	1015	-	-	0/4/4/4	0/0/0/0
2	PO4	E	805	-	-	0/0/0/0	0/0/0/0
3	TDR	E	905[A]	-	-	0/0/0/0	0/1/1/1
3	TDR	E	905[B]	-	-	0/0/0/0	0/1/1/1
5	GOL	F	1011	-	-	0/4/4/4	0/0/0/0
2	PO4	F	806	-	-	0/0/0/0	0/0/0/0
2	PO4	F	807[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	F	807[B]	-	-	0/0/0/0	0/0/0/0
3	TDR	F	906[A]	-	-	0/0/0/0	0/1/1/1
3	TDR	F	906[B]	-	-	0/0/0/0	0/1/1/1

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	TDR	N1-C2-N3	-9.04	121.90	128.40
3	A	901[A]	TDR	N1-C2-N3	-8.85	122.03	128.40
3	C	903[A]	TDR	N1-C2-N3	-8.83	122.05	128.40
3	F	906[A]	TDR	N1-C2-N3	-8.75	122.11	128.40
3	F	906[B]	TDR	N1-C2-N3	-8.73	122.12	128.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 29 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	1PE	7	0
5	B	1014	GOL	1	0
2	B	802	PO4	1	0
3	B	902	TDR	5	0
5	C	1013	GOL	1	0
3	C	903[A]	TDR	1	0
2	D	804	PO4	1	0
3	D	904[A]	TDR	1	0
3	D	904[B]	TDR	1	0
3	E	905[A]	TDR	1	0
3	E	905[B]	TDR	2	0
5	F	1011	GOL	1	0
3	F	906[A]	TDR	2	0
3	F	906[B]	TDR	4	0

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	251/253 (99%)	0.12	18 (7%) 16 19	2, 5, 21, 39	4 (1%)
1	B	246/253 (97%)	-0.01	7 (2%) 53 59	2, 5, 17, 31	0
1	C	245/253 (96%)	0.29	18 (7%) 16 19	2, 8, 23, 39	1 (0%)
1	D	244/253 (96%)	0.13	13 (5%) 27 31	2, 7, 19, 33	0
1	E	252/253 (99%)	0.02	15 (5%) 23 25	2, 5, 20, 27	0
1	F	245/253 (96%)	-0.06	10 (4%) 38 43	2, 5, 16, 31	0
All	All	1483/1518 (97%)	0.08	81 (5%) 26 29	2, 6, 20, 39	5 (0%)

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2237	THR	14.1
1	A	1228	ILE	11.4
1	D	3004	SER	9.7
1	E	5002	SER	8.8
1	A	1233	THR	7.4

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	F	1011	6/6	0.67	0.27	25.19	33,33,33,34	0
3	TDR	E	905[A]	9/9	0.74	0.26	18.98	10,10,10,10	9
3	TDR	E	905[B]	9/9	0.74	0.26	16.65	17,17,17,17	9
3	TDR	F	906[A]	9/9	0.81	0.26	16.29	11,11,11,12	9
5	GOL	A	1254	6/6	0.73	0.25	16.28	35,35,35,35	0
3	TDR	F	906[B]	9/9	0.81	0.26	14.54	8,9,9,10	9
3	TDR	B	902	9/9	0.74	0.26	13.82	12,12,13,15	0
5	GOL	C	1013	6/6	0.87	0.18	13.46	33,33,33,34	0
4	1PE	B	1001	16/16	0.51	0.49	10.21	9,27,33,33	16
3	TDR	D	904[B]	9/9	0.80	0.26	9.51	17,17,17,17	9
3	TDR	D	904[A]	9/9	0.80	0.26	9.29	8,8,9,9	9
3	TDR	C	903[B]	9/9	0.69	0.32	7.72	21,21,21,21	9
3	TDR	C	903[A]	9/9	0.69	0.32	7.56	19,20,20,20	9
5	GOL	E	1015	6/6	0.72	0.16	6.78	41,42,42,42	0
3	TDR	A	901[B]	9/9	0.80	0.27	4.18	17,17,17,17	9
3	TDR	A	901[A]	9/9	0.80	0.27	4.09	14,15,15,15	9
2	PO4	D	804	5/5	0.99	0.07	-0.54	7,7,7,7	0
2	PO4	B	802	5/5	0.99	0.05	-0.77	7,7,8,8	0
2	PO4	E	805	5/5	0.99	0.05	-1.17	5,5,6,7	0
2	PO4	F	806	5/5	0.99	0.05	-1.73	5,6,7,7	0
2	PO4	A	801	5/5	0.99	0.06	-1.99	4,4,4,5	0
2	PO4	C	803	5/5	0.99	0.05	-2.31	8,8,9,9	0
2	PO4	F	807[B]	5/5	0.90	0.19	-	17,17,18,18	5
2	PO4	F	807[A]	5/5	0.90	0.19	-	15,15,16,16	5
2	PO4	A	808[A]	5/5	0.92	0.18	-	15,15,15,15	5
5	GOL	B	1014	6/6	0.74	0.26	-	41,42,42,42	0
2	PO4	A	808[B]	5/5	0.92	0.18	-	23,23,23,23	5

## 6.5 Other polymers

There are no such residues in this entry.