



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:11 PM GMT

PDB ID : 4RDI  
Title : Crystal structure of E. coli tRNA N6-threonylcarbamoyladenosine dehydratase, TcdA  
Authors : Park, S.Y.; Kim, S.; Lee, H.  
Deposited on : 2014-09-19  
Resolution : 1.95 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](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

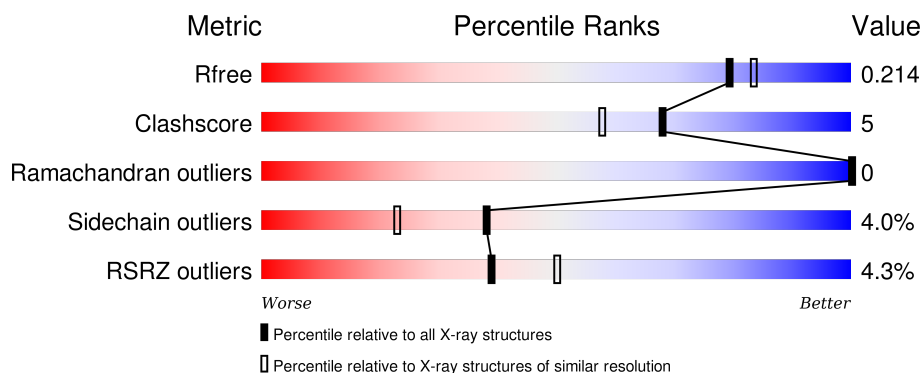
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	288	<div> <div>2%</div> <div>75%</div> <div>10%</div> <div>15%</div> </div>
1	B	288	<div> <div>5%</div> <div>75%</div> <div>9%</div> <div>16%</div> </div>
1	C	288	<div> <div>5%</div> <div>74%</div> <div>9%</div> <div>16%</div> </div>
1	D	288	<div> <div>3%</div> <div>75%</div> <div>7%</div> <div>17%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8053 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 tRNA threonylcarbamoyladenine dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	Se	0	1	0
			1849	1163	330	344	6	6			
1	B	243	Total	C	N	O	S	Se	0	1	0
			1828	1152	326	338	6	6			
1	C	243	Total	C	N	O	S	Se	0	0	0
			1825	1150	326	338	5	6			
1	D	239	Total	C	N	O	S	Se	0	1	0
			1793	1127	322	332	6	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP Q46927
A	-18	GLY	-	EXPRESSION TAG	UNP Q46927
A	-17	SER	-	EXPRESSION TAG	UNP Q46927
A	-16	SER	-	EXPRESSION TAG	UNP Q46927
A	-15	HIS	-	EXPRESSION TAG	UNP Q46927
A	-14	HIS	-	EXPRESSION TAG	UNP Q46927
A	-13	HIS	-	EXPRESSION TAG	UNP Q46927
A	-12	HIS	-	EXPRESSION TAG	UNP Q46927
A	-11	HIS	-	EXPRESSION TAG	UNP Q46927
A	-10	HIS	-	EXPRESSION TAG	UNP Q46927
A	-9	SER	-	EXPRESSION TAG	UNP Q46927
A	-8	SER	-	EXPRESSION TAG	UNP Q46927
A	-7	GLY	-	EXPRESSION TAG	UNP Q46927
A	-6	LEU	-	EXPRESSION TAG	UNP Q46927
A	-5	VAL	-	EXPRESSION TAG	UNP Q46927
A	-4	PRO	-	EXPRESSION TAG	UNP Q46927
A	-3	ARG	-	EXPRESSION TAG	UNP Q46927
A	-2	GLY	-	EXPRESSION TAG	UNP Q46927
A	-1	SER	-	EXPRESSION TAG	UNP Q46927
A	0	HIS	-	EXPRESSION TAG	UNP Q46927
B	-19	MSE	-	EXPRESSION TAG	UNP Q46927

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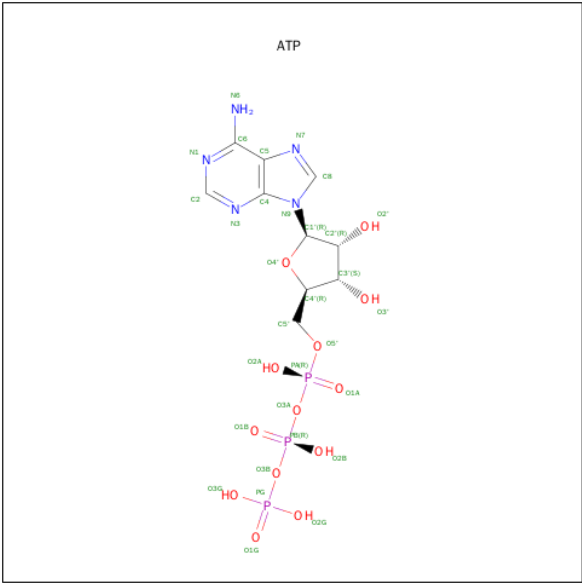
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q46927
B	-17	SER	-	EXPRESSION TAG	UNP Q46927
B	-16	SER	-	EXPRESSION TAG	UNP Q46927
B	-15	HIS	-	EXPRESSION TAG	UNP Q46927
B	-14	HIS	-	EXPRESSION TAG	UNP Q46927
B	-13	HIS	-	EXPRESSION TAG	UNP Q46927
B	-12	HIS	-	EXPRESSION TAG	UNP Q46927
B	-11	HIS	-	EXPRESSION TAG	UNP Q46927
B	-10	HIS	-	EXPRESSION TAG	UNP Q46927
B	-9	SER	-	EXPRESSION TAG	UNP Q46927
B	-8	SER	-	EXPRESSION TAG	UNP Q46927
B	-7	GLY	-	EXPRESSION TAG	UNP Q46927
B	-6	LEU	-	EXPRESSION TAG	UNP Q46927
B	-5	VAL	-	EXPRESSION TAG	UNP Q46927
B	-4	PRO	-	EXPRESSION TAG	UNP Q46927
B	-3	ARG	-	EXPRESSION TAG	UNP Q46927
B	-2	GLY	-	EXPRESSION TAG	UNP Q46927
B	-1	SER	-	EXPRESSION TAG	UNP Q46927
B	0	HIS	-	EXPRESSION TAG	UNP Q46927
C	-19	MSE	-	EXPRESSION TAG	UNP Q46927
C	-18	GLY	-	EXPRESSION TAG	UNP Q46927
C	-17	SER	-	EXPRESSION TAG	UNP Q46927
C	-16	SER	-	EXPRESSION TAG	UNP Q46927
C	-15	HIS	-	EXPRESSION TAG	UNP Q46927
C	-14	HIS	-	EXPRESSION TAG	UNP Q46927
C	-13	HIS	-	EXPRESSION TAG	UNP Q46927
C	-12	HIS	-	EXPRESSION TAG	UNP Q46927
C	-11	HIS	-	EXPRESSION TAG	UNP Q46927
C	-10	HIS	-	EXPRESSION TAG	UNP Q46927
C	-9	SER	-	EXPRESSION TAG	UNP Q46927
C	-8	SER	-	EXPRESSION TAG	UNP Q46927
C	-7	GLY	-	EXPRESSION TAG	UNP Q46927
C	-6	LEU	-	EXPRESSION TAG	UNP Q46927
C	-5	VAL	-	EXPRESSION TAG	UNP Q46927
C	-4	PRO	-	EXPRESSION TAG	UNP Q46927
C	-3	ARG	-	EXPRESSION TAG	UNP Q46927
C	-2	GLY	-	EXPRESSION TAG	UNP Q46927
C	-1	SER	-	EXPRESSION TAG	UNP Q46927
C	0	HIS	-	EXPRESSION TAG	UNP Q46927
D	-19	MSE	-	EXPRESSION TAG	UNP Q46927
D	-18	GLY	-	EXPRESSION TAG	UNP Q46927
D	-17	SER	-	EXPRESSION TAG	UNP Q46927

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP Q46927
D	-15	HIS	-	EXPRESSION TAG	UNP Q46927
D	-14	HIS	-	EXPRESSION TAG	UNP Q46927
D	-13	HIS	-	EXPRESSION TAG	UNP Q46927
D	-12	HIS	-	EXPRESSION TAG	UNP Q46927
D	-11	HIS	-	EXPRESSION TAG	UNP Q46927
D	-10	HIS	-	EXPRESSION TAG	UNP Q46927
D	-9	SER	-	EXPRESSION TAG	UNP Q46927
D	-8	SER	-	EXPRESSION TAG	UNP Q46927
D	-7	GLY	-	EXPRESSION TAG	UNP Q46927
D	-6	LEU	-	EXPRESSION TAG	UNP Q46927
D	-5	VAL	-	EXPRESSION TAG	UNP Q46927
D	-4	PRO	-	EXPRESSION TAG	UNP Q46927
D	-3	ARG	-	EXPRESSION TAG	UNP Q46927
D	-2	GLY	-	EXPRESSION TAG	UNP Q46927
D	-1	SER	-	EXPRESSION TAG	UNP Q46927
D	0	HIS	-	EXPRESSION TAG	UNP Q46927

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	158	Total	O	0	0
			158	158		
4	B	162	Total	O	0	0
			162	162		
4	C	151	Total	O	0	0
			151	151		

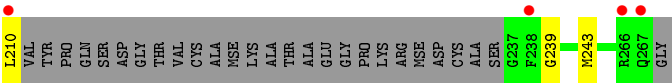
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	139	Total	O	0	0
			139	139		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.71Å 97.04Å 84.22Å 90.00° 111.83° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 28.49 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-1.95) 98.5 (28.49-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.52 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.156 , 0.209 0.164 , 0.214	Depositor DCC
$R_{free}$ test set	3548 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.9	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 70426 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8053	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	1.03	0/1872	0.98	4/2524 (0.2%)
1	B	0.92	0/1851	0.99	1/2496 (0.0%)
1	C	0.88	0/1845	0.94	4/2488 (0.2%)
1	D	0.95	0/1814	0.94	3/2444 (0.1%)
All	All	0.95	0/7382	0.96	12/9952 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	12	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	143	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	D	160	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	175	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	64	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	D	94	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	12	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	72	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	182	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	12	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	175	ASP	C-N-CD	5.01	138.91	128.40

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	1849	0	1888	19	0
1	B	1828	0	1870	21	0
1	C	1825	0	1865	21	0
1	D	1793	0	1831	12	0
2	A	31	0	12	2	0
2	B	31	0	12	1	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	158	0	0	4	0
4	B	162	0	0	0	0
4	C	151	0	0	3	0
4	D	139	0	0	4	0
All	All	8053	0	7534	70	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 5.

All (70) 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:C:62:MSE:HE3	1:C:108:PHE:CD2	1.85	1.12
1:C:62:MSE:CE	1:C:108:PHE:CD2	2.55	0.90
1:D:62:MSE:HE3	1:D:107:ASP:HA	1.53	0.87
1:B:120:VAL:HG11	1:B:122:TYR:CZ	2.22	0.74
1:C:62:MSE:HE3	1:C:108:PHE:CE2	2.23	0.72
1:C:62:MSE:HE2	1:C:108:PHE:N	2.04	0.72
1:A:62:MSE:HE2	1:A:108:PHE:CD2	2.31	0.66
1:B:120:VAL:CG1	1:B:122:TYR:CE2	2.80	0.64
1:C:158:GLN:OE1	1:C:206:SER:HB3	1.99	0.62
1:B:120:VAL:CG1	1:B:122:TYR:CZ	2.82	0.61
1:A:101:ARG:NH1	4:A:435:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HH11	1:B:184:ARG:HG3	1.64	0.61
1:D:12:ARG:NH2	4:D:538:HOH:O	2.33	0.61
1:C:62:MSE:CE	1:C:108:PHE:CG	2.84	0.59
1:A:78:ARG:HD3	1:B:98:PRO:HG3	1.84	0.58
1:A:62:MSE:HE2	1:A:108:PHE:CE2	2.37	0.58
1:C:19:LEU:HB2	1:D:239:GLY:HA3	1.85	0.58
1:A:133:ARG:HG3	4:A:494:HOH:O	2.02	0.58
1:A:194:ASN:C	1:A:194:ASN:HD22	2.08	0.57
1:B:184:ARG:CG	1:B:184:ARG:HH11	2.21	0.53
1:A:119:SER:HA	4:A:543:HOH:O	2.08	0.52
1:C:62:MSE:HE2	1:C:108:PHE:H	1.76	0.51
1:C:36:VAL:CG1	1:C:129:ILE:HD11	2.40	0.51
1:A:133:ARG:HG2	1:A:184:ARG:NH2	2.26	0.50
1:B:185:LEU:HB3	1:B:191:VAL:HB	1.93	0.50
1:D:3:VAL:N	4:D:411:HOH:O	2.45	0.50
1:C:173:ILE:HD12	1:C:174:GLN:HG2	1.94	0.49
1:D:127:ASP:OD2	1:D:151:THR:OG1	2.20	0.49
1:A:133:ARG:HG2	1:A:184:ARG:CZ	2.43	0.49
1:B:186:LYS:CD	1:B:192:VAL:HG12	2.43	0.48
2:A:301:ATP:O1G	4:A:492:HOH:O	2.20	0.48
1:B:184:ARG:CG	1:B:184:ARG:NH1	2.77	0.47
1:A:263:LYS:O	1:A:267:GLN:HG3	2.14	0.47
1:A:62:MSE:CE	1:A:108:PHE:CE2	2.98	0.47
1:C:101:ARG:NH1	4:C:446:HOH:O	2.44	0.47
1:A:85:LYS:NZ	2:A:301:ATP:O2B	2.49	0.46
1:C:48:ALA:HB1	1:D:243:MSE:SE	2.66	0.46
1:B:170:ALA:HB2	1:B:199:LEU:HG	1.98	0.46
1:A:133:ARG:N	1:A:134:PRO:HD2	2.31	0.46
1:B:186:LYS:HD2	1:B:192:VAL:HG12	1.97	0.46
1:B:85:LYS:NZ	2:B:301:ATP:O2B	2.47	0.45
1:D:12:ARG:NH1	4:D:451:HOH:O	2.37	0.45
1:B:129:ILE:HG21	1:B:129:ILE:HD13	1.63	0.45
1:A:167:THR:HG23	1:A:168:ASP:O	2.17	0.44
1:C:17:ALA:HB2	1:C:25:LEU:HD22	2.00	0.44
1:C:266:ARG:O	1:C:267:GLN:CB	2.66	0.43
1:B:194:ASN:HD22	1:B:194:ASN:HA	1.63	0.43
1:C:36:VAL:HG12	1:C:129:ILE:HD11	2.00	0.43
1:C:170:ALA:HA	1:C:182:ARG:HD3	1.99	0.43
1:C:194:ASN:HD22	1:C:194:ASN:C	2.22	0.43
1:A:116:GLN:NE2	1:A:116:GLN:H	2.17	0.43
1:C:182:ARG:O	4:C:434:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG21	1:B:138:LEU:HA	2.01	0.42
1:D:191:VAL:HG12	1:D:199:LEU:HD22	2.01	0.42
1:C:19:LEU:HD21	1:D:159:ILE:HG22	2.02	0.42
1:B:120:VAL:HG11	1:B:122:TYR:OH	2.19	0.42
1:D:209:ALA:O	1:D:210:LEU:CB	2.68	0.41
1:A:176:PRO:HD2	1:A:210:LEU:HD21	2.01	0.41
1:B:167:THR:HG23	1:B:168:ASP:O	2.20	0.41
1:B:120:VAL:HG13	1:B:122:TYR:CE2	2.55	0.41
1:A:153:GLY:HA3	1:A:175:ASP:OD2	2.20	0.41
1:D:158:GLN:OE1	1:D:206:SER:HB3	2.21	0.41
1:A:139:ILE:CD1	1:A:181:LEU:HD21	2.50	0.41
1:C:36:VAL:HG11	1:C:129:ILE:HD11	2.02	0.41
1:C:147:ILE:HG23	4:C:453:HOH:O	2.21	0.41
1:D:11:GLN:HG3	4:D:491:HOH:O	2.21	0.41
1:B:194:ASN:HB2	1:B:198:LYS:H	1.86	0.41
1:B:184:ARG:NE	1:B:188:ASP:OD2	2.48	0.40
1:B:210:LEU:HD23	1:B:238:PHE:CZ	2.56	0.40
1:A:36:VAL:HG12	1:A:129:ILE:CG2	2.52	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	243/288 (84%)	238 (98%)	5 (2%)	0	100	100
1	B	240/288 (83%)	233 (97%)	7 (3%)	0	100	100
1	C	239/288 (83%)	235 (98%)	4 (2%)	0	100	100
1	D	236/288 (82%)	233 (99%)	3 (1%)	0	100	100
All	All	958/1152 (83%)	939 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	194/215 (90%)	187 (96%)	7 (4%)	42	28
1	B	191/215 (89%)	183 (96%)	8 (4%)	36	21
1	C	190/215 (88%)	180 (95%)	10 (5%)	28	13
1	D	186/215 (86%)	181 (97%)	5 (3%)	52	41
All	All	761/860 (88%)	731 (96%)	30 (4%)	38	24

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	124	TYR
1	A	146	LYS
1	A	152	THR
1	A	194	ASN
1	A	196	LYS
1	A	210	LEU
1	B	23	LYS
1	B	116	GLN
1	B	124	TYR
1	B	131	SER
1	B	133	ARG
1	B	180	LYS
1	B	184	ARG
1	B	194	ASN
1	C	2	SER
1	C	62	MSE
1	C	75	HIS
1	C	124	TYR
1	C	131	SER
1	C	133	ARG
1	C	149	LEU
1	C	194	ASN
1	C	210	LEU

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Mol	Chain	Res	Type
1	C	266	ARG
1	D	10	ARG
1	D	72	ARG
1	D	124	TYR
1	D	159	ILE
1	D	188	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	194	ASN
1	B	194	ASN
1	C	26	GLN
1	C	194	ASN

### 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](#)

8 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	ATP	A	301	-	26,33,33	0.97	1 (3%)	26,52,52	2.52	9 (34%)
3	GOL	A	302	-	5,5,5	0.82	0	5,5,5	0.51	0
2	ATP	B	301	-	26,33,33	1.13	2 (7%)	26,52,52	2.49	7 (26%)
3	GOL	B	302	-	5,5,5	1.09	0	5,5,5	0.84	0
2	ATP	C	301	-	26,33,33	1.37	4 (15%)	26,52,52	2.33	6 (23%)
3	GOL	C	302	-	5,5,5	0.83	0	5,5,5	0.95	0
2	ATP	D	301	-	26,33,33	1.26	3 (11%)	26,52,52	2.43	7 (26%)
3	GOL	D	302	-	5,5,5	0.87	0	5,5,5	1.09	1 (20%)

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	ATP	A	301	-	-	0/18/38/38	0/3/3/3
3	GOL	A	302	-	-	0/4/4/4	0/0/0/0
2	ATP	B	301	-	-	0/18/38/38	0/3/3/3
3	GOL	B	302	-	-	0/4/4/4	0/0/0/0
2	ATP	C	301	-	-	0/18/38/38	0/3/3/3
3	GOL	C	302	-	-	0/4/4/4	0/0/0/0
2	ATP	D	301	-	-	0/18/38/38	0/3/3/3
3	GOL	D	302	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ATP	PA-O1A	-2.32	1.42	1.51
2	C	301	ATP	C2'-C1'	-2.28	1.50	1.53
2	C	301	ATP	O4'-C4'	-2.15	1.40	1.45
2	D	301	ATP	O3'-C3'	2.46	1.48	1.43
2	D	301	ATP	O4'-C1'	2.50	1.44	1.41
2	A	301	ATP	C5-C4	2.55	1.46	1.40
2	B	301	ATP	C2-N3	2.69	1.36	1.32
2	C	301	ATP	C5-C4	2.98	1.47	1.40
2	D	301	ATP	C5-C4	3.10	1.47	1.40
2	C	301	ATP	O4'-C1'	3.10	1.45	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ATP	N3-C2-N1	-9.51	121.40	128.87
2	C	301	ATP	N3-C2-N1	-9.24	121.61	128.87
2	D	301	ATP	N3-C2-N1	-8.59	122.13	128.87
2	A	301	ATP	N3-C2-N1	-8.24	122.39	128.87
2	B	301	ATP	C1'-N9-C4	-5.03	121.20	126.81
2	A	301	ATP	C1'-N9-C4	-5.00	121.23	126.81
2	D	301	ATP	C4'-O4'-C1'	-3.25	106.20	109.64
2	A	301	ATP	C4'-O4'-C1'	-2.79	106.68	109.64
2	D	301	ATP	C1'-N9-C4	-2.66	123.84	126.81
2	C	301	ATP	C1'-N9-C4	-2.02	124.55	126.81
2	A	301	ATP	O2A-PA-O1A	2.03	123.12	112.56
3	D	302	GOL	C3-C2-C1	2.06	119.74	111.06
2	A	301	ATP	C2-N1-C6	2.10	122.52	118.77
2	B	301	ATP	C2-N1-C6	2.13	122.56	118.77
2	A	301	ATP	O2'-C2'-C3'	2.18	118.91	111.86
2	B	301	ATP	O3G-PG-O2G	2.25	115.72	107.44
2	A	301	ATP	N6-C6-N1	2.35	122.45	118.52
2	D	301	ATP	O2A-PA-O1A	2.35	124.81	112.56
2	B	301	ATP	N6-C6-N1	2.38	122.51	118.52
2	D	301	ATP	N6-C6-N1	2.41	122.55	118.52
2	B	301	ATP	O2B-PB-O1B	2.41	125.10	112.56
2	C	301	ATP	O2B-PB-O3A	2.54	116.15	105.27
2	B	301	ATP	O2B-PB-O3A	2.61	116.46	105.27
2	A	301	ATP	O3G-PG-O2G	2.80	117.71	107.44
2	C	301	ATP	C2-N1-C6	2.82	123.80	118.77
2	C	301	ATP	O2A-PA-O1A	2.83	127.30	112.56
2	C	301	ATP	O3G-PG-O1G	2.91	120.11	110.63
2	D	301	ATP	O2B-PB-O3A	3.52	120.33	105.27
2	A	301	ATP	O2B-PB-O3A	4.61	125.01	105.27
2	D	301	ATP	O3G-PG-O2G	4.70	124.68	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ATP	2	0
2	B	301	ATP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	240/288 (83%)	-0.11	6 (2%) 61 71	10, 18, 41, 62	0
1	B	237/288 (82%)	0.04	13 (5%) 29 40	11, 21, 53, 76	0
1	C	237/288 (82%)	0.21	14 (5%) 26 36	14, 25, 52, 72	0
1	D	233/288 (80%)	0.04	8 (3%) 49 60	14, 24, 43, 79	0
All	All	947/1152 (82%)	0.04	41 (4%) 39 50	10, 22, 47, 79	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	267	GLN	5.6
1	A	236	SER	5.3
1	D	267	GLN	5.3
1	B	212	TYR	5.2
1	C	237	GLY	5.1
1	C	212	TYR	4.8
1	B	266	ARG	4.5
1	A	195	SER	4.4
1	D	266	ARG	4.4
1	C	238	PHE	4.4
1	B	267	GLN	4.3
1	D	238	PHE	4.1
1	B	195	SER	4.1
1	D	195	SER	4.0
1	A	267	GLN	3.8
1	C	2	SER	3.7
1	C	195	SER	3.6
1	A	192	VAL	3.3
1	B	213	PRO	3.1
1	B	196	LYS	3.1
1	B	187	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	266	ARG	3.0
1	B	237	GLY	2.9
1	B	265	ALA	2.9
1	D	197	GLY	2.9
1	C	265	ALA	2.8
1	C	211	VAL	2.8
1	B	2	SER	2.7
1	D	196	LYS	2.7
1	C	213	PRO	2.4
1	B	186	LYS	2.4
1	C	126	ILE	2.3
1	A	190	GLY	2.2
1	C	179	ALA	2.2
1	D	210	LEU	2.2
1	A	215	SER	2.1
1	C	190	GLY	2.1
1	B	4	VAL	2.1
1	B	191	VAL	2.1
1	C	175	ASP	2.0
1	D	190	GLY	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, 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
2	ATP	D	301	31/31	0.92	0.10	0.18	22,27,50,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ATP	B	301	31/31	0.95	0.10	-0.09	16,21,52,54	0
3	GOL	C	302	6/6	0.93	0.10	-0.10	27,30,33,33	0
3	GOL	B	302	6/6	0.93	0.09	-0.43	21,25,28,29	0
3	GOL	A	302	6/6	0.95	0.08	-0.47	16,19,22,23	0
3	GOL	D	302	6/6	0.91	0.10	-0.47	27,31,33,34	0
2	ATP	A	301	31/31	0.94	0.08	-0.50	17,18,35,40	0
2	ATP	C	301	31/31	0.96	0.08	-0.93	16,21,47,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.