



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2017 – 02:48 PM EST

PDB ID : 4D79
Title : Crystal structure of E. coli tRNA N6-threonylcarbamoyladenosine dehydratase, TcdA, in complex with ATP at 1.768 Angstroem resolution
Authors : Lopez-Esteva, M.; Arda, A.; Savko, M.; Round, A.; Shepard, W.; Bruix, M.; Coll, M.; Fernandez, F.J.; Jimenez-Barbero, J.; Vega, M.C.
Deposited on : 2014-11-21
Resolution : 1.77 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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-20028442

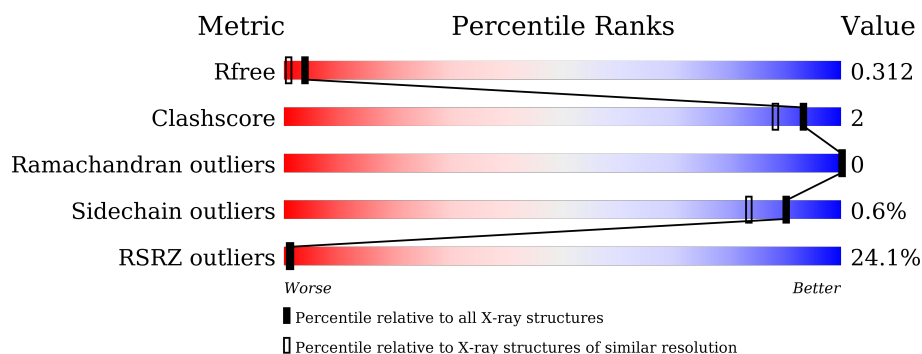
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	276	<div> <div>7%</div> <div>86%</div> <div>12%</div> </div>
1	B	276	<div> <div>11%</div> <div>82%</div> <div>7%</div> <div>11%</div> </div>
1	C	276	<div> <div>30%</div> <div>88%</div> <div>9%</div> </div>
1	D	276	<div> <div>38%</div> <div>86%</div> <div>12%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	B	401	-	-	-	X
3	ATP	C	401	-	-	-	X
4	GOL	A	501	-	-	-	X
4	GOL	A	502	-	-	-	X
4	GOL	B	502	-	-	-	X
4	GOL	C	502	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8167 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 THREONYLCARBAMOYLADENOSINE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	3	0
			1846	1161	332	341	12			
1	B	247	Total	C	N	O	S	0	3	0
			1872	1176	334	350	12			
1	C	252	Total	C	N	O	S	0	4	1
			1923	1210	348	353	12			
1	D	244	Total	C	N	O	S	0	1	0
			1843	1160	329	343	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	LEU	-	EXPRESSION TAG	UNP Q46927
A	270	GLU	-	EXPRESSION TAG	UNP Q46927
A	271	HIS	-	EXPRESSION TAG	UNP Q46927
A	272	HIS	-	EXPRESSION TAG	UNP Q46927
A	273	HIS	-	EXPRESSION TAG	UNP Q46927
A	274	HIS	-	EXPRESSION TAG	UNP Q46927
A	275	HIS	-	EXPRESSION TAG	UNP Q46927
A	276	HIS	-	EXPRESSION TAG	UNP Q46927
B	269	LEU	-	EXPRESSION TAG	UNP Q46927
B	270	GLU	-	EXPRESSION TAG	UNP Q46927
B	271	HIS	-	EXPRESSION TAG	UNP Q46927
B	272	HIS	-	EXPRESSION TAG	UNP Q46927
B	273	HIS	-	EXPRESSION TAG	UNP Q46927
B	274	HIS	-	EXPRESSION TAG	UNP Q46927
B	275	HIS	-	EXPRESSION TAG	UNP Q46927
B	276	HIS	-	EXPRESSION TAG	UNP Q46927
C	269	LEU	-	EXPRESSION TAG	UNP Q46927
C	270	GLU	-	EXPRESSION TAG	UNP Q46927
C	271	HIS	-	EXPRESSION TAG	UNP Q46927
C	272	HIS	-	EXPRESSION TAG	UNP Q46927

Continued on next page...

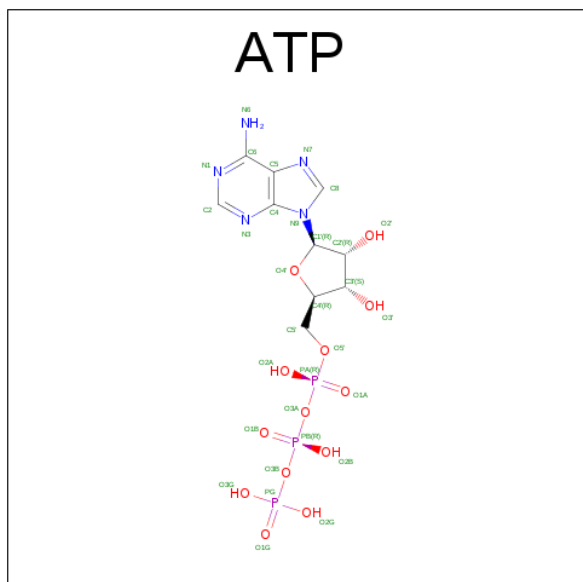
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	273	HIS	-	EXPRESSION TAG	UNP Q46927
C	274	HIS	-	EXPRESSION TAG	UNP Q46927
C	275	HIS	-	EXPRESSION TAG	UNP Q46927
C	276	HIS	-	EXPRESSION TAG	UNP Q46927
D	269	LEU	-	EXPRESSION TAG	UNP Q46927
D	270	GLU	-	EXPRESSION TAG	UNP Q46927
D	271	HIS	-	EXPRESSION TAG	UNP Q46927
D	272	HIS	-	EXPRESSION TAG	UNP Q46927
D	273	HIS	-	EXPRESSION TAG	UNP Q46927
D	274	HIS	-	EXPRESSION TAG	UNP Q46927
D	275	HIS	-	EXPRESSION TAG	UNP Q46927
D	276	HIS	-	EXPRESSION TAG	UNP Q46927

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

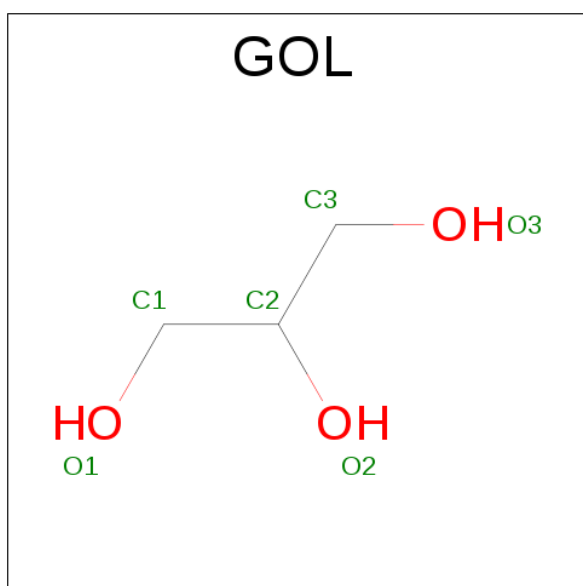
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Na 1	0	0
5	D	1	Total 1	Na 1	0	0


- Molecule 6 is water.

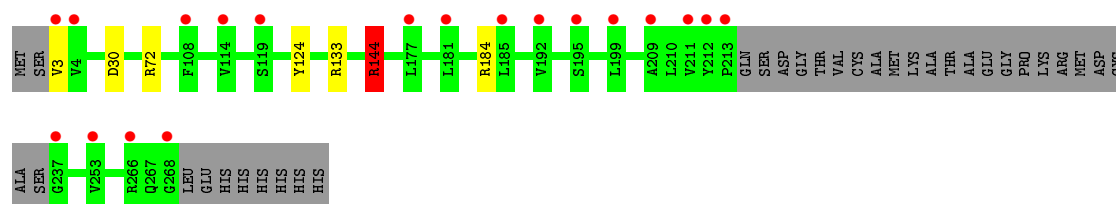
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total 123	O 123	0	0
6	B	140	Total 140	O 140	0	0
6	C	144	Total 144	O 144	0	0
6	D	104	Total 104	O 104	0	0

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 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.

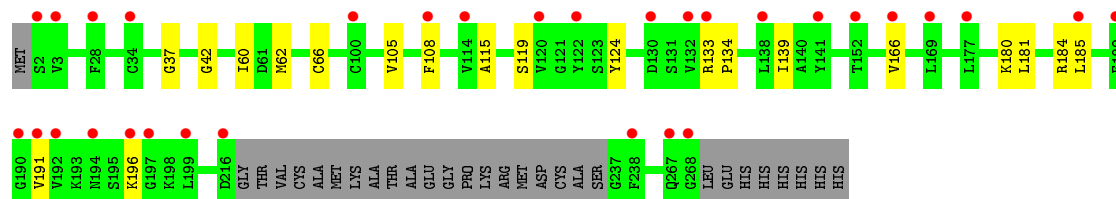
- Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

Chain A: 




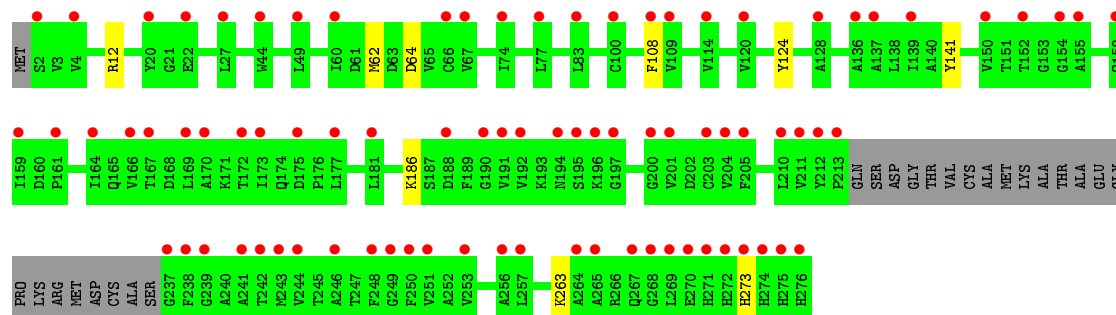
- Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

Chain B: 




- Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

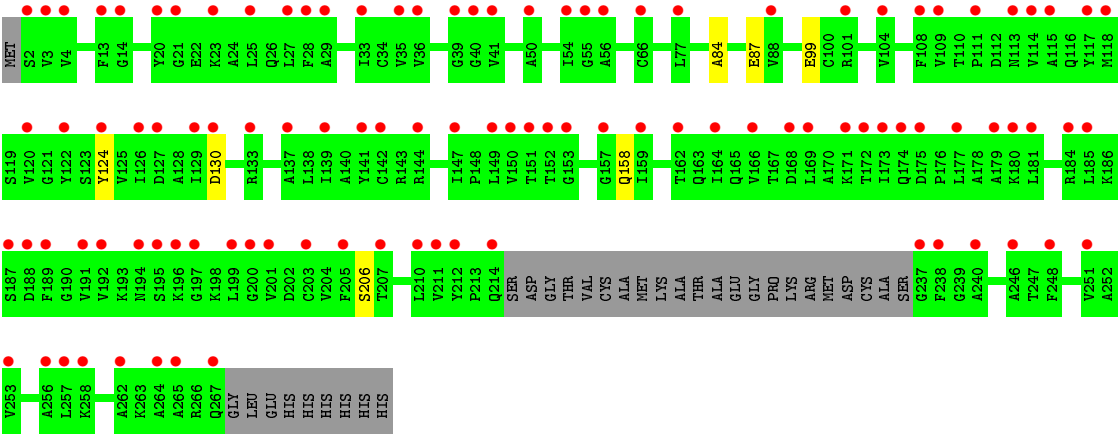
Chain C: 



- Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.69 Å 97.16 Å 83.19 Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	41.13 – 1.77 77.34 – 1.77	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.13-1.77) 95.0 (77.34-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 1.77 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.142 , 0.183 0.297 , 0.312	Depositor DCC
R_{free} test set	4502 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8167	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 4.41% 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: GOL, K, ATP, NA

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	0.52	0/1872	0.73	4/2533 (0.2%)
1	B	0.49	0/1898	0.65	0/2570
1	C	0.48	0/1957	0.63	0/2651
1	D	0.46	0/1869	0.64	0/2530
All	All	0.49	0/7596	0.66	4/10284 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144[A]	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	144[B]	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	144[A]	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	144[B]	ARG	NE-CZ-NH1	6.81	123.70	120.30

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	1846	0	1883	6	0
1	B	1872	0	1903	14	0
1	C	1923	0	1947	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1843	0	1878	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	1	0
3	B	31	0	12	0	0
3	C	31	0	12	2	0
3	D	31	0	12	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	6	0	8	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	123	0	0	0	0
6	B	140	0	0	3	0
6	C	144	0	0	3	1
6	D	104	0	0	1	2
All	All	8167	0	7715	29	3

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 2.

All (29) 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:66[A]:CYS:SG	6:B:2046:HOH:O	2.31	0.87
1:A:133:ARG:CG	1:A:184:ARG:HH12	2.18	0.57
1:C:108:PHE:HB2	3:C:401:ATP:C6	2.42	0.55
1:A:133:ARG:HG3	1:A:184:ARG:HH12	1.72	0.54
1:B:180:LYS:HG3	6:B:2106:HOH:O	2.11	0.51
1:B:133:ARG:HG2	1:B:184:ARG:HH12	1.77	0.50
1:C:186:LYS:NZ	6:C:2120:HOH:O	2.44	0.50
1:B:133:ARG:HB2	1:B:134:PRO:CD	2.42	0.50
1:C:108:PHE:HB2	3:C:401:ATP:N6	2.27	0.49
1:B:133:ARG:HB2	1:B:134:PRO:HD3	1.95	0.48
1:C:12:ARG:NH2	6:C:2019:HOH:O	2.46	0.48
1:B:196:LYS:NZ	1:D:130:ASP:OD2	2.46	0.48
1:B:139:ILE:CD1	1:B:181:LEU:HD21	2.45	0.47
1:A:72:ARG:NH2	3:A:401:ATP:O3B	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HG2	1:A:184:ARG:NH1	2.31	0.46
1:A:144[A]:ARG:CG	1:A:144[A]:ARG:HH11	2.29	0.46
1:B:37:GLY:O	1:B:42:GLY:HA3	2.17	0.45
1:D:99:GLU:OE2	6:D:2048:HOH:O	2.21	0.45
1:C:62:MET:SD	1:C:108:PHE:HD1	2.40	0.45
1:B:166[B]:VAL:HG21	6:B:2126:HOH:O	2.18	0.44
1:A:3:VAL:N	1:A:30:ASP:OD1	2.52	0.43
1:B:62:MET:HG2	1:B:108:PHE:CZ	2.54	0.42
1:B:115:ALA:O	1:B:119:SER:OG	2.27	0.42
1:C:263:LYS:NZ	6:C:2138:HOH:O	2.53	0.41
1:B:185:LEU:HB3	1:B:191:VAL:HB	2.03	0.41
1:B:62:MET:CG	1:B:108:PHE:CE2	3.04	0.41
1:D:158:GLN:OE1	1:D:206:SER:HB3	2.22	0.40
1:B:60:ILE:HG12	1:B:105:VAL:HB	2.03	0.40
1:D:84:ALA:HB3	1:D:87[B]:GLU:HG3	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2100:HOH:O	6:D:2003:HOH:O[2_657]	1.82	0.38
1:C:64:ASP:OD1	1:C:273:HIS:ND1[2_647]	2.00	0.20
1:C:141:TYR:OH	6:D:2048:HOH:O[2_657]	2.19	0.01

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	242/276 (88%)	237 (98%)	5 (2%)	0	100	100
1	B	246/276 (89%)	241 (98%)	5 (2%)	0	100	100
1	C	252/276 (91%)	248 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	241/276 (87%)	237 (98%)	4 (2%)	0	100	100
All	All	981/1104 (89%)	963 (98%)	18 (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	192/216 (89%)	189 (98%)	3 (2%)	70	52
1	B	196/216 (91%)	195 (100%)	1 (0%)	92	87
1	C	201/216 (93%)	200 (100%)	1 (0%)	92	87
1	D	192/216 (89%)	191 (100%)	1 (0%)	92	87
All	All	781/864 (90%)	775 (99%)	6 (1%)	90	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	TYR
1	A	144[A]	ARG
1	A	144[B]	ARG
1	B	124	TYR
1	C	124	TYR
1	D	124	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	ATP	A	401	-	26,33,33	1.14	3 (11%)	26,52,52	2.07	4 (15%)
4	GOL	A	501	-	5,5,5	0.37	0	5,5,5	0.45	0
4	GOL	A	502	-	5,5,5	0.51	0	5,5,5	0.34	0
3	ATP	B	401	-	26,33,33	1.20	2 (7%)	26,52,52	2.15	4 (15%)
4	GOL	B	501	-	5,5,5	0.48	0	5,5,5	0.42	0
4	GOL	B	502	-	5,5,5	0.33	0	5,5,5	0.56	0
3	ATP	C	401	-	26,33,33	1.06	2 (7%)	26,52,52	2.00	4 (15%)
4	GOL	C	501	-	5,5,5	0.68	0	5,5,5	0.62	0
4	GOL	C	502	-	5,5,5	0.33	0	5,5,5	0.39	0
3	ATP	D	401	-	26,33,33	1.09	2 (7%)	26,52,52	2.51	7 (26%)
4	GOL	D	501	-	5,5,5	0.47	0	5,5,5	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	401	-	-	0/18/38/38	0/3/3/3
4	GOL	A	501	-	-	0/4/4/4	0/0/0/0
4	GOL	A	502	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	401	-	-	0/18/38/38	0/3/3/3
4	GOL	B	501	-	-	0/4/4/4	0/0/0/0
4	GOL	B	502	-	-	0/4/4/4	0/0/0/0
3	ATP	C	401	-	-	0/18/38/38	0/3/3/3
4	GOL	C	501	-	-	0/4/4/4	0/0/0/0
4	GOL	C	502	-	-	0/4/4/4	0/0/0/0
3	ATP	D	401	-	-	0/18/38/38	0/3/3/3
4	GOL	D	501	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ATP	C2-N1	2.02	1.37	1.33
3	A	401	ATP	C2-N3	2.22	1.36	1.32
3	A	401	ATP	O4'-C1'	2.24	1.44	1.41
3	C	401	ATP	O4'-C1'	2.56	1.44	1.41
3	C	401	ATP	C5-C4	2.82	1.46	1.40
3	D	401	ATP	C5-C4	2.96	1.47	1.40
3	B	401	ATP	O4'-C1'	3.13	1.45	1.41
3	B	401	ATP	C5-C4	3.17	1.47	1.40
3	A	401	ATP	C5-C4	3.20	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ATP	N3-C2-N1	-9.22	121.63	128.87
3	A	401	ATP	N3-C2-N1	-8.30	122.35	128.87
3	B	401	ATP	N3-C2-N1	-7.71	122.81	128.87
3	C	401	ATP	N3-C2-N1	-7.47	123.00	128.87
3	D	401	ATP	C1'-N9-C4	-5.69	120.46	126.81
3	D	401	ATP	C4'-O4'-C1'	-2.65	106.83	109.64
3	A	401	ATP	C1'-N9-C4	-2.54	123.97	126.81
3	C	401	ATP	C4'-O4'-C1'	-2.51	106.98	109.64
3	D	401	ATP	O2A-PA-O3A	2.04	114.00	105.27
3	A	401	ATP	O3G-PG-O2G	2.11	115.20	107.44
3	B	401	ATP	O3G-PG-O2G	2.20	115.53	107.44
3	D	401	ATP	O2B-PB-O3A	2.30	115.14	105.27
3	D	401	ATP	C2-N1-C6	2.49	123.21	118.77
3	B	401	ATP	C1'-N9-C4	2.54	129.64	126.81
3	D	401	ATP	N6-C6-N1	3.07	123.67	118.52
3	C	401	ATP	N6-C6-N1	3.17	123.84	118.52
3	A	401	ATP	N6-C6-N1	3.37	124.17	118.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	401	ATP	O4'-C1'-N9	3.56	114.84	108.11
3	B	401	ATP	O4'-C1'-N9	5.34	118.19	108.11

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
3	A	401	ATP	1	0
3	C	401	ATP	2	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

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	243/276 (88%)	0.94	19 (7%)	16 20	17, 28, 67, 116	0
1	B	247/276 (89%)	1.05	31 (12%)	5 7	16, 25, 59, 112	0
1	C	252/276 (91%)	1.79	83 (32%)	0 1	17, 27, 75, 102	0
1	D	244/276 (88%)	2.01	105 (43%)	0 0	17, 29, 60, 112	0
All	All	986/1104 (89%)	1.45	238 (24%)	1 1	16, 27, 67, 116	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	VAL	6.3
1	D	189	PHE	6.2
1	C	201	VAL	5.7
1	C	197	GLY	5.7
1	D	199	LEU	5.5
1	A	268	GLY	5.4
1	C	108	PHE	5.3
1	D	264	ALA	5.1
1	D	169	LEU	5.0
1	A	3	VAL	4.9
1	C	275	HIS	4.9
1	C	2	SER	4.9
1	C	276	HIS	4.9
1	C	211	VAL	4.8
1	D	196	LYS	4.5
1	D	152	THR	4.5
1	A	195	SER	4.5
1	D	137	ALA	4.5
1	D	2	SER	4.4
1	D	265	ALA	4.4
1	D	185	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	270	GLU	4.2
1	D	184	ARG	4.2
1	C	212	TYR	4.1
1	D	109	VAL	4.0
1	C	271	HIS	3.9
1	C	213	PRO	3.9
1	D	120	VAL	3.9
1	C	170	ALA	3.9
1	C	273	HIS	3.9
1	D	149	LEU	3.9
1	D	267	GLN	3.9
1	C	196	LYS	3.8
1	A	266	ARG	3.8
1	C	67[A]	VAL	3.8
1	D	205	PHE	3.8
1	D	195	SER	3.8
1	A	237	GLY	3.8
1	C	4	VAL	3.7
1	D	212	TYR	3.7
1	D	139	ILE	3.7
1	A	181	LEU	3.6
1	C	210	LEU	3.6
1	C	246	ALA	3.6
1	C	152	THR	3.6
1	C	177	LEU	3.6
1	C	269	LEU	3.6
1	D	192	VAL	3.6
1	A	119	SER	3.6
1	A	199	LEU	3.6
1	C	204	VAL	3.6
1	D	122	TYR	3.5
1	C	257	LEU	3.5
1	A	211	VAL	3.5
1	C	120	VAL	3.5
1	C	248	PHE	3.5
1	C	155	ALA	3.5
1	B	216	ASP	3.5
1	D	25	LEU	3.4
1	C	203	CYS	3.4
1	C	173	ILE	3.4
1	B	2	SER	3.4
1	D	211	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	28	PHE	3.4
1	C	164	ILE	3.3
1	C	128	ALA	3.3
1	C	274	HIS	3.3
1	B	192	VAL	3.3
1	A	4	VAL	3.3
1	B	190	GLY	3.3
1	D	157	GLY	3.3
1	D	238	PHE	3.2
1	D	4	VAL	3.2
1	C	195	SER	3.2
1	C	205	PHE	3.2
1	D	151	THR	3.2
1	B	133	ARG	3.1
1	C	194	ASN	3.1
1	C	191	VAL	3.1
1	D	187	SER	3.1
1	D	35	VAL	3.1
1	D	172	THR	3.1
1	D	114	VAL	3.1
1	D	194	ASN	3.1
1	D	246	ALA	3.1
1	C	267	GLN	3.0
1	C	137	ALA	3.0
1	D	41	VAL	3.0
1	D	150	VAL	3.0
1	D	144	ARG	3.0
1	C	250	PHE	3.0
1	D	214	GLN	3.0
1	C	167	THR	3.0
1	A	192	VAL	3.0
1	C	77	LEU	3.0
1	D	181	LEU	3.0
1	D	180	LYS	3.0
1	B	268	GLY	2.9
1	D	124	TYR	2.9
1	D	66	CYS	2.9
1	C	253	VAL	2.8
1	D	257	LEU	2.8
1	D	173	ILE	2.8
1	C	49	LEU	2.8
1	D	36	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	54	ILE	2.8
1	D	141	TYR	2.8
1	D	177	LEU	2.8
1	C	66[A]	CYS	2.8
1	C	264	ALA	2.8
1	C	159	ILE	2.8
1	D	129	ILE	2.8
1	B	185	LEU	2.8
1	D	23	LYS	2.8
1	C	238	PHE	2.8
1	D	256	ALA	2.8
1	C	100	CYS	2.8
1	D	142	CYS	2.8
1	C	154	GLY	2.7
1	D	171	LYS	2.7
1	B	100	CYS	2.7
1	D	33	ILE	2.7
1	D	147	ILE	2.7
1	D	159	ILE	2.7
1	C	20	TYR	2.7
1	D	210	LEU	2.7
1	C	237	GLY	2.7
1	C	268	GLY	2.7
1	D	40	GLY	2.7
1	C	22	GLU	2.7
1	D	203	CYS	2.7
1	B	122	TYR	2.7
1	C	27	LEU	2.7
1	D	113	ASN	2.7
1	D	175	ASP	2.7
1	D	248	PHE	2.7
1	B	169	LEU	2.6
1	D	56	ALA	2.6
1	B	120	VAL	2.6
1	B	194	ASN	2.6
1	B	191	VAL	2.6
1	C	166	VAL	2.6
1	C	244	VAL	2.6
1	C	136	ALA	2.6
1	C	172	THR	2.6
1	B	267	GLN	2.6
1	D	133	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	189	PHE	2.5
1	C	272	HIS	2.5
1	C	242	THR	2.5
1	B	238	PHE	2.5
1	C	192	VAL	2.5
1	B	197	GLY	2.5
1	D	108	PHE	2.5
1	D	164	ILE	2.5
1	D	166	VAL	2.5
1	D	237	GLY	2.5
1	A	209	ALA	2.5
1	D	162	THR	2.5
1	C	181	LEU	2.5
1	C	161	PRO	2.4
1	B	130	ASP	2.4
1	D	174	GLN	2.4
1	C	190	GLY	2.4
1	D	111	PRO	2.4
1	C	74	ILE	2.4
1	D	126	ILE	2.4
1	C	200	GLY	2.4
1	A	213	PRO	2.4
1	A	177	LEU	2.4
1	D	13	PHE	2.4
1	B	138	LEU	2.4
1	C	169	LEU	2.4
1	D	117	TYR	2.4
1	C	241	ALA	2.4
1	D	77	LEU	2.3
1	D	168	ASP	2.3
1	A	212	TYR	2.3
1	D	115	ALA	2.3
1	D	207	THR	2.3
1	D	201	VAL	2.3
1	A	108	PHE	2.3
1	D	130	ASP	2.3
1	D	14	GLY	2.3
1	D	188	ASP	2.3
1	D	127	ASP	2.3
1	C	83	LEU	2.2
1	D	262	ALA	2.2
1	D	21	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	153	GLY	2.2
1	B	108	PHE	2.2
1	A	114	VAL	2.2
1	D	27	LEU	2.2
1	C	60	ILE	2.2
1	C	139	ILE	2.2
1	C	249	GLY	2.2
1	D	200	GLY	2.2
1	B	166[A]	VAL	2.2
1	C	175	ASP	2.2
1	D	20	TYR	2.2
1	C	188	ASP	2.2
1	D	118	MET	2.2
1	C	114	VAL	2.2
1	D	251	VAL	2.2
1	D	253	VAL	2.2
1	B	196	LYS	2.2
1	B	28	PHE	2.1
1	B	199	LEU	2.1
1	C	256	ALA	2.1
1	B	34	CYS	2.1
1	C	150	VAL	2.1
1	D	3	VAL	2.1
1	D	104	VAL	2.1
1	B	152	THR	2.1
1	B	177	LEU	2.1
1	D	258	LYS	2.1
1	C	265	ALA	2.1
1	C	158	GLN	2.1
1	B	132	VAL	2.1
1	D	50	ALA	2.1
1	D	240	ALA	2.1
1	D	101	ARG	2.1
1	B	141	TYR	2.1
1	C	44	TRP	2.1
1	D	88	VAL	2.1
1	C	239	GLY	2.0
1	C	243	MET	2.0
1	D	29	ALA	2.0
1	D	55	GLY	2.0
1	A	253	VAL	2.0
1	B	3	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	109	VAL	2.0
1	A	185	LEU	2.0
1	D	39	GLY	2.0
1	D	197	GLY	2.0
1	D	179	ALA	2.0
1	B	114	VAL	2.0
1	C	251	VAL	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
4	GOL	B	502	6/6	0.41	0.36	12.27	37,70,103,109	0
4	GOL	C	502	6/6	0.58	0.31	7.92	38,59,65,68	0
4	GOL	A	501	6/6	0.86	0.24	4.83	34,44,58,85	0
4	GOL	A	502	6/6	0.83	0.18	2.81	29,55,72,73	0
3	ATP	C	401	31/31	0.79	0.26	2.69	27,66,179,229	0
3	ATP	B	401	31/31	0.88	0.21	2.63	25,60,177,208	0
5	NA	D	302	1/1	0.35	0.23	1.82	24,24,24,24	0
2	K	B	301	1/1	0.65	0.16	1.04	18,18,18,18	1
3	ATP	A	401	31/31	0.84	0.16	0.83	24,37,130,182	0
5	NA	B	302	1/1	0.75	0.14	0.68	23,23,23,23	0
4	GOL	C	501	6/6	0.64	0.20	0.45	29,39,54,63	0
4	GOL	B	501	6/6	0.77	0.15	0.38	24,27,34,44	0
4	GOL	D	501	6/6	0.61	0.20	-0.21	31,41,46,81	0
2	K	A	301	1/1	0.81	0.12	-0.69	18,18,18,18	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ATP	D	401	31/31	0.81	0.16	-0.75	21,28,76,99	0
2	K	C	301	1/1	0.61	0.17	-1.07	20,20,20,20	1
2	K	D	301	1/1	0.68	0.16	-1.21	24,24,24,24	1

6.5 Other polymers [i](#)

There are no such residues in this entry.