Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 12:45 PM EST

PDB ID	:	1QF6
Title	:	STRUCTURE OF E. COLI THREONYL-TRNA SYNTHETASE COMPLEXED WITH ITS COGNATE TRNA
Authors	:	Sankaranarayanan, R.; Dock-Bregeon, A.C.; Rees, B.; Moras, D.
Deposited on	:	1999-04-06
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

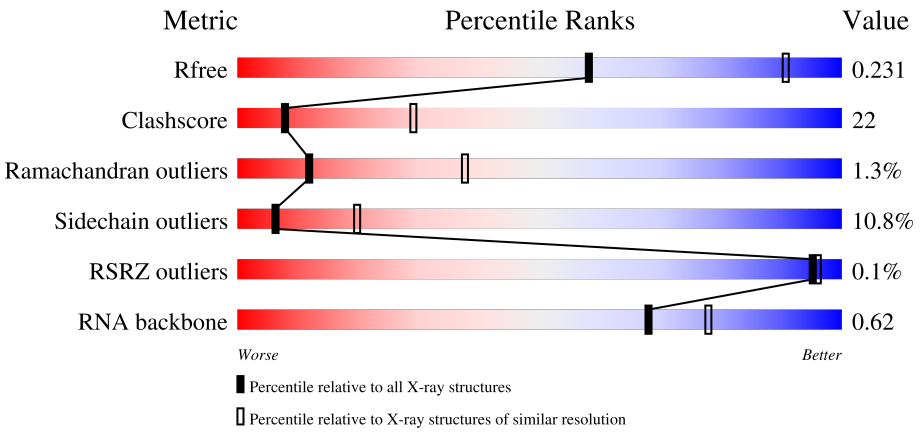
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	B	76	51% 36% 9% •
2	A	642	53% 40% 7%

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
1	H2U	B	16	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7093 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 RNA chain called THREONINE TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	76	1633	731	288	538	76	0	0	0

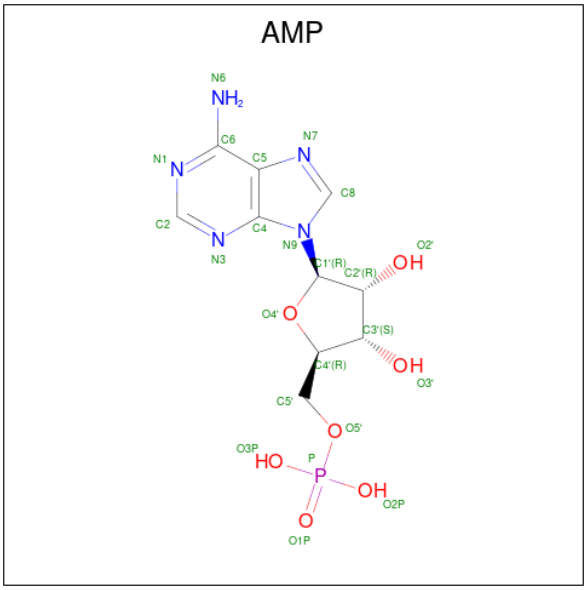
- Molecule 2 is a protein called THREONYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	641	5192	3274	915	968	35	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	23	10	5	7	1	0	0

- Molecule 5 is water.

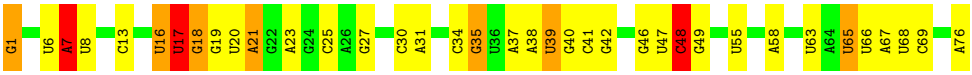
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	80	80	80	0	0
5	A	164	Total	O	0	0
			164	164		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

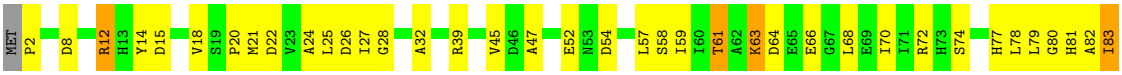
- Molecule 1: THREONINE TRNA

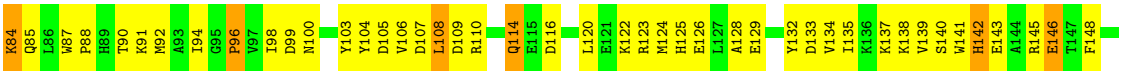
Chain B:

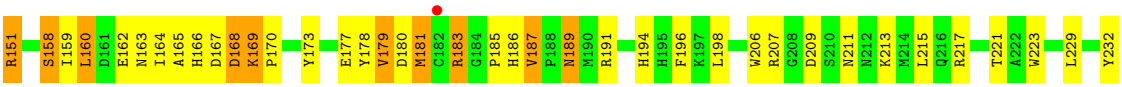


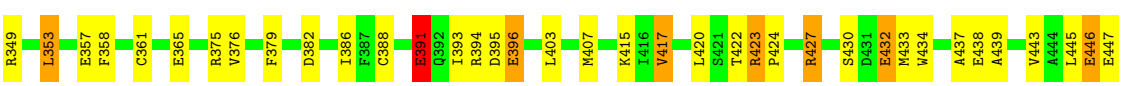
- Molecule 2: THREONYL-TRNA SYNTHETASE

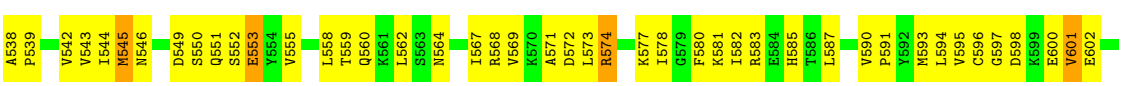
Chain A:











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.67Å 162.67Å 128.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 29.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.90) 91.8 (29.90-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.72Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.195 , 0.239 0.189 , 0.231	Depositor DCC
R_{free} test set	3592 reflections (6.76%)	wwPDB-VP
Wilson B-factor (Å^2)	56.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7093	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: AMP, G7M, ZN, PSU, AET, 5MU, H2U

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	B	0.72	1/1649 (0.1%)	0.81	3/2567 (0.1%)
2	A	0.68	9/5308 (0.2%)	0.80	4/7158 (0.1%)
All	All	0.69	10/6957 (0.1%)	0.81	7/9725 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	2	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	146	GLU	CG-CD	8.38	1.64	1.51
2	A	146	GLU	CD-OE2	8.08	1.34	1.25
2	A	391	GLU	CD-OE1	7.33	1.33	1.25
1	B	1	G	OP3-P	-6.81	1.52	1.61
2	A	146	GLU	CD-OE1	6.53	1.32	1.25
2	A	391	GLU	CG-CD	6.44	1.61	1.51
2	A	391	GLU	CD-OE2	6.03	1.32	1.25
2	A	641	GLU	CD-OE2	5.93	1.32	1.25
2	A	432	GLU	CD-OE2	5.85	1.32	1.25
2	A	432	GLU	CG-CD	5.03	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	7	A	C2'-C3'-O3'	10.06	131.62	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	48	C	C2'-C3'-O3'	9.36	130.10	109.50
2	A	358	PHE	N-CA-C	-5.95	94.93	111.00
2	A	613	GLY	N-CA-C	-5.47	99.42	113.10
1	B	21	A	N9-C1'-C2'	5.40	121.02	114.00
2	A	329	ILE	N-CA-C	-5.14	97.12	111.00
2	A	322	SER	N-CA-C	-5.04	97.38	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	7	A	C3'
1	B	48	C	C3'

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	G	Sidechain
1	B	19	G	Sidechain
1	B	21	A	Sidechain
1	B	25	C	Sidechain
1	B	27	G	Sidechain
1	B	58	A	Sidechain
1	B	63	U	Sidechain
1	B	65	U	Sidechain

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	B	1633	0	835	16	0
2	A	5192	0	5073	258	0
3	A	1	0	0	0	0
4	A	23	0	12	2	0
5	A	164	0	0	4	0
5	B	80	0	0	0	0
All	All	7093	0	5920	273	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 22.

All (273) 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)
2:A:143:GLU:HB3	5:A:1144:HOH:O	1.64	0.98
2:A:125:HIS:O	2:A:129:GLU:HG2	1.69	0.92
2:A:158:SER:O	2:A:162:GLU:HG2	1.72	0.88
2:A:21:MET:O	2:A:25:LEU:HD12	1.74	0.88
2:A:145:ARG:HG2	2:A:145:ARG:HH11	1.39	0.88
2:A:544:ILE:HD12	2:A:559:THR:HG22	1.57	0.86
2:A:61:THR:HG22	2:A:63:LYS:H	1.41	0.85
2:A:543:VAL:HG21	2:A:585:HIS:HD2	1.42	0.84
2:A:543:VAL:HG21	2:A:585:HIS:CD2	2.14	0.83
2:A:538:ALA:O	2:A:568:ARG:NH1	2.12	0.82
2:A:83:ILE:HG12	2:A:120:LEU:HD11	1.62	0.80
2:A:148:PHE:CE2	2:A:181:MET:HG2	2.17	0.80
2:A:229:LEU:C	2:A:229:LEU:HD23	2.03	0.79
2:A:79:LEU:HG	2:A:124:MET:HE1	1.65	0.78
2:A:66:GLU:O	2:A:70:ILE:HG12	1.84	0.78
1:B:17:H2U:H5”	1:B:18:G:OP2	1.84	0.78
2:A:555:VAL:O	2:A:559:THR:HG23	1.84	0.78
2:A:550:SER:HB2	2:A:551:GLN:NE2	2.01	0.76
2:A:301:ARG:HG3	2:A:328:CYS:SG	2.26	0.75
2:A:430:SER:OG	2:A:433:MET:HG3	1.86	0.74
2:A:25:LEU:HD12	2:A:25:LEU:H	1.53	0.74
1:B:47:U:H4’	1:B:48:C:H5’	1.69	0.74
2:A:559:THR:HG21	2:A:571:ALA:HB2	1.68	0.74
2:A:79:LEU:HA	2:A:124:MET:HE2	1.71	0.72
2:A:610:THR:CG2	2:A:614:LYS:HB3	2.19	0.72
2:A:139:VAL:HB	5:A:1144:HOH:O	1.88	0.72
2:A:233:LEU:H	2:A:233:LEU:CD2	2.02	0.72
2:A:574:ARG:HH11	2:A:574:ARG:HG3	1.53	0.72
2:A:255:HIS:ND1	2:A:267:HIS:HE1	1.88	0.72
2:A:417:VAL:HG22	2:A:469:THR:HG23	1.71	0.72
2:A:572:ASP:OD1	2:A:574:ARG:HG3	1.90	0.71
2:A:229:LEU:O	2:A:233:LEU:HD23	1.90	0.71
2:A:616:LEU:HD22	2:A:641:GLU:HG3	1.72	0.71
2:A:423:ARG:HD2	2:A:438:GLU:OE2	1.90	0.71
2:A:233:LEU:HD22	2:A:233:LEU:N	2.04	0.70
1:B:35:G:C6	2:A:597:GLY:HA3	2.25	0.70
2:A:122:LYS:O	2:A:126:GLU:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:94:ILE:HG22	2:A:96:PRO:HD3	1.73	0.70
2:A:79:LEU:HA	2:A:124:MET:CE	2.21	0.70
2:A:20:PRO:HG2	2:A:47:ALA:HA	1.73	0.70
2:A:148:PHE:CZ	2:A:181:MET:HG2	2.25	0.70
1:B:6:U:O2'	1:B:7:A:H5'	1.93	0.68
2:A:610:THR:HG23	2:A:613:GLY:H	1.60	0.67
2:A:621:VAL:O	2:A:624:VAL:HG22	1.95	0.67
2:A:610:THR:HG22	2:A:614:LYS:HB3	1.74	0.67
2:A:139:VAL:O	2:A:169:LYS:HA	1.95	0.66
2:A:90:THR:HG23	2:A:106:VAL:HG13	1.78	0.66
2:A:514:ILE:HG22	2:A:515:LEU:HD23	1.78	0.65
2:A:85:GLN:HE21	2:A:123:ARG:HH11	1.42	0.65
2:A:70:ILE:CD1	2:A:185:PRO:HG2	2.27	0.65
2:A:639:GLN:HB2	2:A:642:GLU:OE2	1.97	0.65
2:A:110:ARG:HG2	2:A:110:ARG:HH11	1.61	0.64
2:A:613:GLY:O	2:A:614:LYS:HB2	1.96	0.64
2:A:591:PRO:HG3	2:A:611:ARG:HH12	1.63	0.64
2:A:61:THR:CG2	2:A:63:LYS:H	2.10	0.64
2:A:12:ARG:HB3	2:A:14:TYR:HE1	1.63	0.63
1:B:65:U:H2'	1:B:66:U:C6	2.33	0.63
2:A:532:PHE:HD2	2:A:611:ARG:HE	1.47	0.63
2:A:59:ILE:N	2:A:59:ILE:HD12	2.13	0.62
2:A:422:THR:O	2:A:458:GLU:O	2.17	0.62
2:A:465:LYS:HG2	2:A:484:GLN:HG2	1.82	0.62
2:A:145:ARG:HG2	2:A:145:ARG:NH1	2.12	0.62
2:A:84:LYS:HE2	2:A:90:THR:O	2.00	0.61
2:A:233:LEU:CD2	2:A:233:LEU:N	2.62	0.61
2:A:459:GLY:HA2	2:A:465:LYS:HD3	1.83	0.61
2:A:114:GLN:O	2:A:114:GLN:HG2	2.00	0.60
2:A:221:THR:CG2	2:A:223:TRP:HE1	2.14	0.60
1:B:66:U:H2'	1:B:67:A:C8	2.37	0.60
2:A:583:ARG:HG3	2:A:583:ARG:HH11	1.67	0.60
1:B:41:C:O2'	1:B:42:G:H5'	2.01	0.59
2:A:233:LEU:H	2:A:233:LEU:HD22	1.62	0.59
2:A:434:TRP:O	2:A:438:GLU:HG3	2.02	0.59
2:A:221:THR:HG21	2:A:223:TRP:HE1	1.68	0.59
2:A:572:ASP:OD2	2:A:574:ARG:NH1	2.35	0.59
2:A:407:MET:CE	2:A:514:ILE:HG21	2.32	0.59
2:A:85:GLN:NE2	2:A:123:ARG:HD2	2.18	0.58
2:A:229:LEU:HD23	2:A:229:LEU:O	2.03	0.58
2:A:590:VAL:O	2:A:611:ARG:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:83:ILE:HG12	2:A:120:LEU:CD1	2.34	0.58
2:A:229:LEU:C	2:A:229:LEU:CD2	2.72	0.57
2:A:334:CYS:HB2	2:A:335:PRO:CD	2.34	0.57
2:A:63:LYS:HG2	2:A:64:ASP:N	2.18	0.57
2:A:78:LEU:HG	2:A:124:MET:HG3	1.86	0.57
2:A:545:MET:HE1	2:A:582:ILE:HD13	1.86	0.57
2:A:546:ASN:HB3	2:A:555:VAL:HG21	1.86	0.56
2:A:542:VAL:O	2:A:569:VAL:HG23	2.05	0.56
2:A:544:ILE:HG12	2:A:594:LEU:HB2	1.88	0.56
2:A:544:ILE:HG22	2:A:555:VAL:HG13	1.88	0.56
2:A:90:THR:HG23	2:A:106:VAL:CG1	2.36	0.56
2:A:134:VAL:HG21	2:A:187:VAL:HG12	1.87	0.56
2:A:242:ARG:NH1	2:A:527:GLU:O	2.39	0.56
2:A:543:VAL:HG23	2:A:590:VAL:HG11	1.87	0.56
2:A:552:SER:HB2	2:A:573:LEU:HD13	1.87	0.55
2:A:12:ARG:HG2	2:A:14:TYR:OH	2.07	0.55
2:A:608:VAL:CG1	2:A:616:LEU:HD12	2.36	0.55
2:A:128:ALA:O	2:A:194:HIS:HE1	1.89	0.55
2:A:301:ARG:HD2	2:A:310:TRP:CH2	2.42	0.55
2:A:132:TYR:O	2:A:189:ASN:HB2	2.08	0.54
2:A:320:THR:HG22	2:A:321:SER:N	2.22	0.54
2:A:598:ASP:HA	2:A:601:VAL:HG23	1.89	0.54
2:A:608:VAL:HG12	2:A:616:LEU:HD12	1.89	0.54
2:A:633:ARG:HD3	2:A:633:ARG:C	2.28	0.54
2:A:610:THR:HG21	2:A:614:LYS:HB3	1.90	0.54
2:A:639:GLN:O	2:A:642:GLU:HG2	2.08	0.54
2:A:105:ASP:OD1	2:A:217:ARG:HB2	2.08	0.53
2:A:258:GLU:O	2:A:261:PRO:HD3	2.08	0.53
2:A:520:ARG:NH1	4:A:1002:AMP:H2'	2.24	0.53
2:A:551:GLN:HG2	2:A:596:CYS:O	2.08	0.53
2:A:591:PRO:HG3	2:A:611:ARG:NH1	2.23	0.53
2:A:349:ARG:HG3	2:A:349:ARG:HH11	1.74	0.53
2:A:382:ASP:O	2:A:382:ASP:CG	2.47	0.53
2:A:632:ILE:HG22	2:A:633:ARG:N	2.22	0.53
2:A:100:ASN:O	2:A:221:THR:HG23	2.08	0.53
2:A:601:VAL:HG12	2:A:602:GLU:N	2.24	0.53
1:B:39:U:H2'	1:B:40:G:H8	1.74	0.53
2:A:551:GLN:H	2:A:551:GLN:CD	2.12	0.53
2:A:600:GLU:O	2:A:601:VAL:O	2.25	0.53
2:A:320:THR:HG22	2:A:321:SER:H	1.73	0.52
2:A:39:ARG:HB3	2:A:58:SER:OG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:U:H2'	1:B:40:G:C8	2.45	0.52
2:A:14:TYR:CD2	2:A:18:VAL:HG11	2.44	0.52
2:A:335:PRO:O	2:A:339:GLN:HG2	2.10	0.52
2:A:229:LEU:HD23	2:A:233:LEU:HD23	1.90	0.52
2:A:574:ARG:HG3	2:A:574:ARG:NH1	2.25	0.52
2:A:417:VAL:HG13	2:A:471:TYR:HE1	1.74	0.51
2:A:560:GLN:O	2:A:564:ASN:ND2	2.44	0.51
2:A:631:GLU:OE2	2:A:639:GLN:HA	2.09	0.51
2:A:77:HIS:CE1	2:A:180:ASP:HB3	2.45	0.51
2:A:59:ILE:N	2:A:59:ILE:CD1	2.73	0.51
2:A:151:ARG:HH22	2:A:178:TYR:HA	1.76	0.51
2:A:229:LEU:HD23	2:A:233:LEU:CD2	2.40	0.51
2:A:301:ARG:HD2	2:A:310:TRP:CZ2	2.46	0.51
2:A:407:MET:SD	2:A:514:ILE:HG21	2.51	0.50
2:A:349:ARG:HG3	2:A:349:ARG:NH1	2.26	0.50
2:A:85:GLN:HE22	2:A:123:ARG:HD2	1.76	0.50
2:A:277:LEU:HB2	2:A:518:MET:HE1	1.94	0.50
2:A:243:ASP:OD2	2:A:245:ARG:HB2	2.12	0.50
2:A:135:ILE:HG21	2:A:137:LYS:HE2	1.94	0.49
2:A:234:GLN:OE1	2:A:234:GLN:HA	2.11	0.49
2:A:145:ARG:NH1	2:A:145:ARG:CG	2.72	0.49
2:A:120:LEU:HD23	2:A:198:LEU:HD11	1.93	0.49
2:A:160:LEU:HD13	2:A:164:ILE:HD12	1.94	0.49
2:A:80:GLY:HA2	2:A:92:MET:HE1	1.93	0.49
2:A:138:LYS:NZ	2:A:169:LYS:HD3	2.28	0.49
2:A:79:LEU:C	2:A:79:LEU:HD23	2.32	0.49
2:A:91:LYS:HB2	2:A:107:ASP:HB3	1.93	0.49
2:A:460:ALA:HB1	2:A:462:TYR:CE1	2.48	0.49
2:A:621:VAL:HG12	2:A:622:ASN:N	2.26	0.49
2:A:28:GLY:HA3	5:A:1129:HOH:O	2.12	0.49
2:A:110:ARG:HG2	2:A:110:ARG:NH1	2.25	0.48
2:A:120:LEU:HD23	2:A:198:LEU:CD1	2.43	0.48
2:A:70:ILE:HG23	2:A:185:PRO:O	2.13	0.48
2:A:45:VAL:HG12	5:A:1040:HOH:O	2.13	0.48
2:A:594:LEU:HB3	2:A:606:VAL:HG11	1.95	0.48
2:A:598:ASP:HA	2:A:601:VAL:CG2	2.42	0.48
2:A:544:ILE:CD1	2:A:559:THR:HG22	2.36	0.48
2:A:57:LEU:HG	2:A:58:SER:N	2.28	0.48
2:A:57:LEU:HD12	2:A:58:SER:H	1.79	0.48
2:A:587:LEU:HD12	2:A:587:LEU:HA	1.68	0.48
1:B:65:U:H2'	1:B:66:U:H6	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:135:ILE:HD12	2:A:135:ILE:N	2.29	0.48
2:A:560:GLN:HG3	2:A:564:ASN:HD21	1.79	0.47
2:A:22:ASP:HA	2:A:25:LEU:HD13	1.96	0.47
2:A:246:LYS:O	2:A:250:GLN:HG3	2.14	0.47
2:A:489:LEU:N	2:A:490:PRO:HD2	2.29	0.47
2:A:141:TRP:CH2	2:A:145:ARG:HD2	2.49	0.47
2:A:465:LYS:CG	2:A:484:GLN:HG2	2.44	0.47
2:A:159:ILE:O	2:A:163:ASN:HB2	2.14	0.47
2:A:446:GLU:HG3	2:A:447:GLU:N	2.30	0.47
2:A:85:GLN:HE21	2:A:123:ARG:NH1	2.12	0.47
2:A:424:PRO:HG2	2:A:427:ARG:HB3	1.95	0.47
2:A:594:LEU:HD13	2:A:606:VAL:HG11	1.96	0.47
2:A:610:THR:HG23	2:A:613:GLY:N	2.27	0.47
2:A:233:LEU:H	2:A:233:LEU:HD23	1.80	0.47
2:A:423:ARG:NH2	2:A:434:TRP:HB2	2.30	0.47
2:A:501:ASP:OD1	2:A:503:GLU:HB2	2.14	0.47
2:A:534:PRO:O	2:A:535:THR:C	2.53	0.47
2:A:594:LEU:CD2	2:A:608:VAL:HG22	2.45	0.47
2:A:262:GLY:C	2:A:263:MET:HG2	2.35	0.46
2:A:465:LYS:NZ	2:A:467:GLU:OE2	2.48	0.46
2:A:221:THR:HG22	2:A:223:TRP:NE1	2.30	0.46
2:A:254:TYR:HB2	2:A:265:PHE:O	2.15	0.46
1:B:30:C:H2'	1:B:31:A:H8	1.81	0.46
2:A:446:GLU:CG	2:A:447:GLU:N	2.77	0.46
2:A:165:ALA:O	2:A:167:ASP:N	2.49	0.45
2:A:221:THR:HG21	2:A:232:TYR:CD2	2.51	0.45
2:A:189:ASN:ND2	2:A:191:ARG:H	2.14	0.45
2:A:486:ASP:OD2	2:A:489:LEU:HB2	2.17	0.45
2:A:497:TYR:CZ	2:A:505:LYS:HB2	2.51	0.45
2:A:553:GLU:O	2:A:553:GLU:HG2	2.15	0.45
2:A:74:SER:OG	2:A:187:VAL:HB	2.15	0.45
2:A:78:LEU:O	2:A:81:HIS:HB3	2.17	0.45
2:A:25:LEU:O	2:A:28:GLY:N	2.49	0.45
2:A:288:TYR:CD1	2:A:288:TYR:N	2.83	0.45
2:A:386:ILE:HG21	2:A:396:GLU:HG3	1.99	0.45
2:A:539:PRO:O	2:A:568:ARG:HD2	2.16	0.45
2:A:82:ALA:HB1	2:A:123:ARG:HG3	1.98	0.45
2:A:330:LYS:HA	2:A:331:PRO:HD3	1.56	0.45
2:A:624:VAL:O	2:A:628:LEU:HG	2.17	0.44
2:A:545:MET:HE2	2:A:581:LYS:HB2	1.99	0.44
2:A:600:GLU:O	2:A:601:VAL:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:12:ARG:HB3	2:A:14:TYR:CE1	2.48	0.44
2:A:391:GLU:CD	2:A:391:GLU:H	2.20	0.44
2:A:432:GLU:CD	2:A:432:GLU:N	2.71	0.44
2:A:551:GLN:HG3	2:A:601:VAL:CG2	2.48	0.44
2:A:124:MET:HG2	2:A:196:PHE:CZ	2.53	0.44
2:A:255:HIS:ND1	2:A:267:HIS:CE1	2.77	0.44
2:A:595:VAL:HB	2:A:607:ALA:HB3	2.00	0.44
1:B:66:U:H2'	1:B:67:A:H8	1.82	0.43
2:A:57:LEU:CG	2:A:58:SER:N	2.81	0.43
2:A:594:LEU:HB3	2:A:606:VAL:CG1	2.48	0.43
1:B:68:U:H2'	1:B:69:C:H6	1.81	0.43
2:A:21:MET:O	2:A:24:ALA:HB3	2.18	0.43
2:A:133:ASP:HA	2:A:189:ASN:HB2	2.00	0.43
2:A:213:LYS:HG2	2:A:215:LEU:HD23	2.00	0.43
2:A:638:LYS:HD3	2:A:638:LYS:H	1.84	0.43
2:A:168:ASP:O	2:A:170:PRO:HD2	2.17	0.43
2:A:321:SER:OG	2:A:326:GLU:HG2	2.18	0.43
2:A:242:ARG:CZ	2:A:530:ALA:HB2	2.48	0.43
2:A:582:ILE:HD13	2:A:593:MET:HE2	1.99	0.43
2:A:585:HIS:HB2	2:A:593:MET:CE	2.49	0.43
2:A:25:LEU:O	2:A:27:ILE:N	2.52	0.43
2:A:353:LEU:HD12	2:A:353:LEU:C	2.39	0.43
2:A:103:TYR:CD1	2:A:103:TYR:C	2.91	0.43
2:A:415:LYS:HE2	2:A:471:TYR:CE1	2.53	0.43
2:A:158:SER:HB3	2:A:162:GLU:OE2	2.18	0.43
2:A:173:TYR:CE2	2:A:186:HIS:HB2	2.53	0.42
2:A:87:TRP:CH2	2:A:116:ASP:HB3	2.54	0.42
2:A:591:PRO:HA	2:A:611:ARG:HH11	1.84	0.42
2:A:386:ILE:HG21	2:A:396:GLU:CG	2.50	0.42
2:A:82:ALA:O	2:A:83:ILE:C	2.57	0.42
2:A:497:TYR:CE1	2:A:505:LYS:HB2	2.54	0.42
2:A:298:MET:HA	2:A:328:CYS:O	2.20	0.42
2:A:332:MET:HA	2:A:361:CYS:SG	2.59	0.42
2:A:567:ILE:HD12	2:A:567:ILE:N	2.34	0.42
2:A:209:ASP:OD1	2:A:211:ASN:HB2	2.19	0.42
2:A:21:MET:O	2:A:25:LEU:CD1	2.56	0.42
2:A:84:LYS:CE	2:A:90:THR:O	2.66	0.42
2:A:143:GLU:HA	2:A:146:GLU:HB2	2.00	0.42
2:A:439:ALA:O	2:A:443:VAL:HG23	2.20	0.42
2:A:534:PRO:O	2:A:536:TRP:N	2.52	0.42
2:A:337:HIS:HE2	2:A:357:GLU:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:84:LYS:O	2:A:88:PRO:HG3	2.19	0.42
2:A:151:ARG:NH2	2:A:179:VAL:H	2.17	0.42
2:A:537:LEU:HD23	2:A:537:LEU:HA	1.89	0.42
2:A:379:PHE:HB2	2:A:517:SER:HB2	2.02	0.41
2:A:393:ILE:O	2:A:394:ARG:C	2.58	0.41
2:A:562:LEU:HB3	2:A:569:VAL:HG11	2.00	0.41
2:A:90:THR:CG2	2:A:106:VAL:HG13	2.46	0.41
2:A:58:SER:C	2:A:59:ILE:HD12	2.41	0.41
2:A:108:LEU:HD23	2:A:109:ASP:H	1.85	0.41
2:A:479:GLN:HG2	4:A:1002:AMP:O3'	2.19	0.41
2:A:558:LEU:HD21	2:A:606:VAL:HG21	2.01	0.41
2:A:544:ILE:HB	2:A:559:THR:HG22	2.02	0.41
1:B:68:U:H2'	1:B:69:C:C6	2.56	0.41
2:A:348:TYR:CE2	2:A:500:GLU:HG3	2.56	0.41
2:A:83:ILE:CG2	2:A:84:LYS:N	2.82	0.41
2:A:255:HIS:O	2:A:265:PHE:HB2	2.20	0.41
2:A:365:GLU:OE1	2:A:375:ARG:NH2	2.50	0.41
2:A:623:GLU:O	2:A:627:LYS:HG3	2.20	0.41
1:B:67:A:H2'	1:B:68:U:C6	2.55	0.41
2:A:2:PRO:N	2:A:14:TYR:O	2.53	0.41
2:A:140:SER:C	2:A:142:HIS:H	2.24	0.41
2:A:437:ALA:HB2	2:A:487:PHE:CE2	2.56	0.41
2:A:479:GLN:NE2	2:A:482:THR:HG21	2.35	0.41
1:B:17:H2U:C5'	1:B:18:G:OP2	2.63	0.41
2:A:388:CYS:O	2:A:508:VAL:HB	2.20	0.40
2:A:403:LEU:HG	2:A:407:MET:HE3	2.03	0.40
2:A:577:LYS:O	2:A:580:PHE:N	2.54	0.40
2:A:206:TRP:CE2	2:A:207:ARG:HG2	2.56	0.40
2:A:242:ARG:NH1	2:A:530:ALA:HB2	2.36	0.40
2:A:25:LEU:HA	2:A:32:ALA:HB2	2.04	0.40
2:A:284:LYS:HD3	2:A:284:LYS:HA	1.98	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
2	A	639/642 (100%)	561 (88%)	70 (11%)	8 (1%)	12 37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	183	ARG
2	A	601	VAL
2	A	614	LYS
2	A	605	LYS
2	A	26	ASP
2	A	166	HIS
2	A	535	THR
2	A	54	ASP

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
2	A	557/558 (100%)	497 (89%)	60 (11%)	6 20

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	8	ASP
2	A	12	ARG
2	A	15	ASP
2	A	52	GLU
2	A	61	THR
2	A	63	LYS
2	A	68	LEU
2	A	72	ARG
2	A	83	ILE
2	A	84	LYS
2	A	96	PRO

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Mol	Chain	Res	Type
2	A	98	ILE
2	A	99	ASP
2	A	104	TYR
2	A	108	LEU
2	A	114	GLN
2	A	142	HIS
2	A	151	ARG
2	A	158	SER
2	A	160	LEU
2	A	168	ASP
2	A	169	LYS
2	A	177	GLU
2	A	179	VAL
2	A	181	MET
2	A	183	ARG
2	A	187	VAL
2	A	189	ASN
2	A	233	LEU
2	A	263	MET
2	A	267	HIS
2	A	279	VAL
2	A	326	GLU
2	A	332	MET
2	A	343	GLN
2	A	353	LEU
2	A	376	VAL
2	A	391	GLU
2	A	395	ASP
2	A	396	GLU
2	A	417	VAL
2	A	420	LEU
2	A	423	ARG
2	A	427	ARG
2	A	445	LEU
2	A	446	GLU
2	A	458	GLU
2	A	469	THR
2	A	485	LEU
2	A	494	SER
2	A	500	GLU
2	A	512	ARG
2	A	519	GLU

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Mol	Chain	Res	Type
2	A	545	MET
2	A	549	ASP
2	A	553	GLU
2	A	574	ARG
2	A	578	ILE
2	A	609	ARG
2	A	638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	56	GLN
2	A	77	HIS
2	A	85	GLN
2	A	114	GLN
2	A	125	HIS
2	A	194	HIS
2	A	250	GLN
2	A	257	GLN
2	A	267	HIS
2	A	291	GLN
2	A	342	ASN
2	A	371	HIS
2	A	381	GLN
2	A	398	ASN
2	A	556	ASN
2	A	560	GLN
2	A	564	ASN
2	A	585	HIS
2	A	639	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	75/76 (98%)	13 (17%)	3 (4%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	8	U

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Mol	Chain	Res	Type
1	B	13	C
1	B	16	H2U
1	B	17	H2U
1	B	18	G
1	B	20	H2U
1	B	23	A
1	B	34	C
1	B	35	G
1	B	38	A
1	B	39	U
1	B	49	G
1	B	76	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	7	A
1	B	38	A
1	B	48	C

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

7 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	H2U	B	17	1	18,21,22	0.75	1 (5%)	21,30,33	1.26	2 (9%)
1	H2U	B	20	1	18,21,22	0.60	0	21,30,33	0.85	0
1	G7M	B	46	1	20,26,27	1.08	2 (10%)	17,39,42	0.43	0
1	AET	B	37	1	28,35,36	1.57	7 (25%)	31,51,54	2.24	8 (25%)
1	H2U	B	16	1	18,21,22	1.00	1 (5%)	21,30,33	0.79	1 (4%)
1	PSU	B	55	1	18,21,22	1.92	1 (5%)	22,30,33	0.85	1 (4%)
1	5MU	B	54	1	19,22,23	0.51	0	28,32,35	0.56	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
1	H2U	B	17	1	-	4/7/38/39	0/2/2/2
1	H2U	B	20	1	-	3/7/38/39	0/2/2/2
1	G7M	B	46	1	-	0/3/25/26	0/3/3/3
1	AET	B	37	1	-	5/23/45/46	0/3/3/3
1	H2U	B	16	1	-	2/7/38/39	0/2/2/2
1	PSU	B	55	1	-	0/7/25/26	0/2/2/2
1	5MU	B	54	1	-	0/7/25/26	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	PSU	C6-N1	-7.71	1.23	1.36
1	B	37	AET	CM6-N6	-3.47	1.40	1.46
1	B	16	H2U	C2-N1	3.44	1.40	1.35
1	B	37	AET	O2'-C2'	3.39	1.51	1.43
1	B	37	AET	C6-N1	3.06	1.37	1.33
1	B	46	G7M	C8-N9	2.63	1.38	1.33
1	B	17	H2U	C2-N1	2.38	1.39	1.35
1	B	46	G7M	C8-N7	2.22	1.37	1.33
1	B	37	AET	C10-N6	2.18	1.40	1.37
1	B	37	AET	O10-C10	2.18	1.27	1.23
1	B	37	AET	C2-N3	2.12	1.35	1.32
1	B	37	AET	C8-N7	-2.04	1.31	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	AET	O3'-C3'-C4'	5.58	127.18	111.05
1	B	37	AET	O3'-C3'-C2'	-5.19	95.02	111.82
1	B	37	AET	C3'-C2'-C1'	4.37	107.56	100.98
1	B	37	AET	C15-C14-C12	4.31	120.98	112.29
1	B	17	H2U	N3-C2-N1	-4.06	112.36	116.65
1	B	37	AET	O14-C14-C12	3.76	116.67	109.13
1	B	37	AET	N1-C6-N6	3.46	120.11	116.36
1	B	37	AET	N11-C10-N6	2.75	118.04	114.04
1	B	55	PSU	C5-C6-N1	2.64	126.06	122.11
1	B	17	H2U	O3'-C3'-C2'	-2.50	103.73	111.82
1	B	16	H2U	N3-C2-N1	-2.41	114.11	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	AET	O14-C14-C15	-2.18	103.29	109.74

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	17	H2U	O4'-C1'-N1-C2
1	B	17	H2U	O4'-C1'-N1-C6
1	B	17	H2U	C2'-C1'-N1-C2
1	B	37	AET	C5-C6-N6-C10
1	B	37	AET	N1-C6-N6-C10
1	B	20	H2U	O4'-C4'-C5'-O5'
1	B	20	H2U	C3'-C4'-C5'-O5'
1	B	17	H2U	C2'-C1'-N1-C6
1	B	37	AET	C14-C12-C13-ODA
1	B	37	AET	N1-C6-N6-CM6
1	B	16	H2U	C3'-C4'-C5'-O5'
1	B	37	AET	C14-C12-C13-ODB
1	B	16	H2U	O4'-C4'-C5'-O5'
1	B	20	H2U	C2'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	17	H2U	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	AMP	A	1002	-	22,25,25	0.78	0	25,38,38	1.05	2 (8%)

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
4	AMP	A	1002	-	-	0/6/26/26	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1002	AMP	C5-C6-N6	2.79	124.60	120.35
4	A	1002	AMP	O2P-P-O1P	2.35	119.88	110.68

There are no chirality outliers.

There are no torsion outliers.

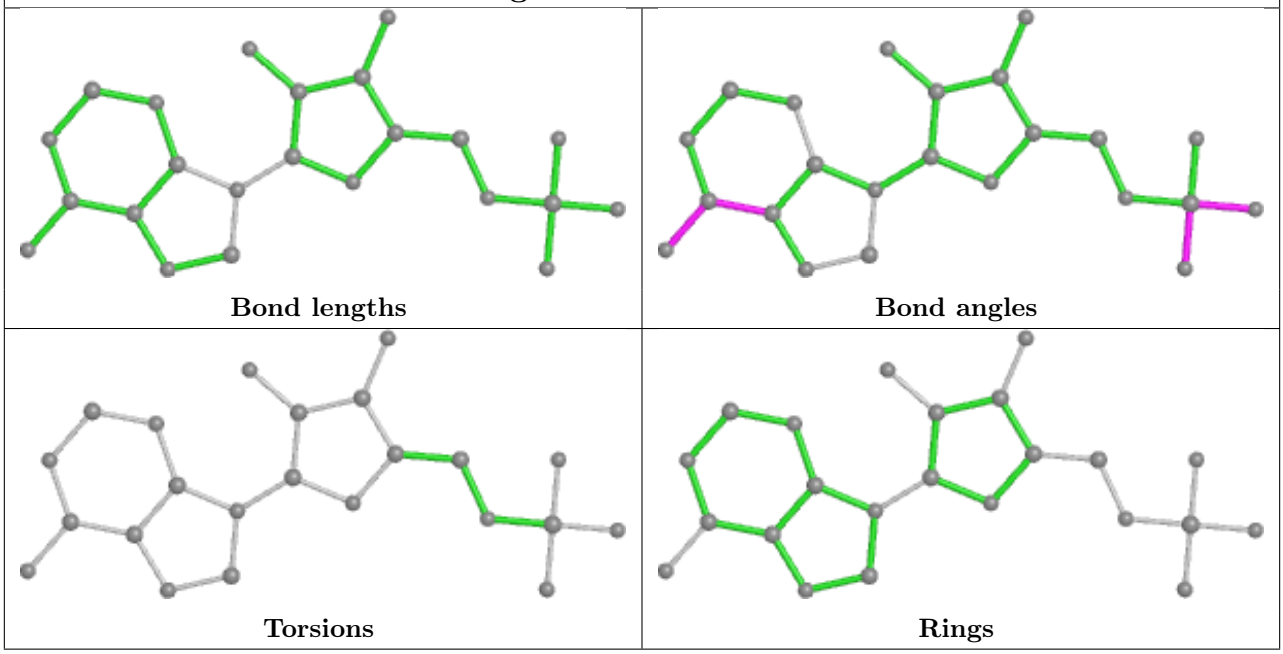
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	AMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AMP A 1002



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	B	69/76 (90%)	-0.51	0 100 100	29, 46, 86, 94	0
2	A	641/642 (99%)	-0.42	1 (0%) 95 95	23, 49, 81, 97	0
All	All	710/718 (98%)	-0.43	1 (0%) 95 96	23, 49, 83, 97	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	182	CYS	2.4

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
1	H2U	B	16	20/21	0.79	0.51	83,100,100,100	0
1	H2U	B	17	20/21	0.83	0.25	84,98,100,100	0
1	AET	B	37	33/34	0.90	0.17	84,90,100,100	0
1	H2U	B	20	20/21	0.96	0.13	50,55,58,61	0
1	G7M	B	46	24/25	0.97	0.12	43,48,62,64	0
1	5MU	B	54	21/22	0.98	0.12	17,36,47,49	0
1	PSU	B	55	20/21	0.98	0.10	31,45,52,53	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

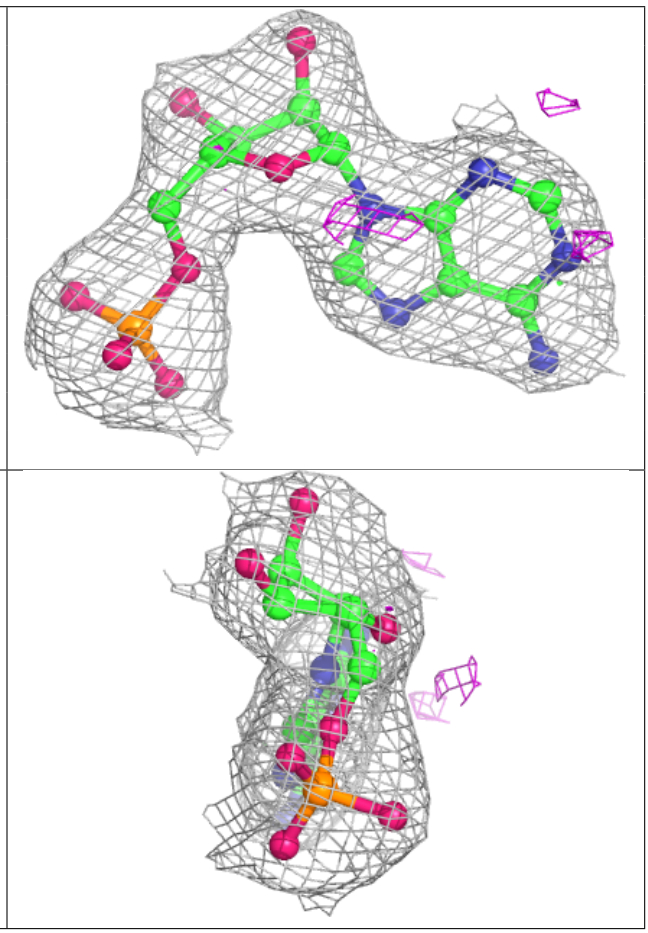
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AMP	A	1002	23/23	0.98	0.26	35,39,42,43	0
3	ZN	A	1001	1/1	0.99	0.22	38,38,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AMP A 1002:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.