



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:41 am BST

PDB ID : 1H4Q
Title : Prolyl-tRNA synthetase from *Thermus thermophilus* complexed with tRNA^{Pro}(CGG), ATP and prolinol
Authors : Yaremchuk, A.; Tukalo, M.; Cusack, S.
Deposited on : 2001-05-13
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

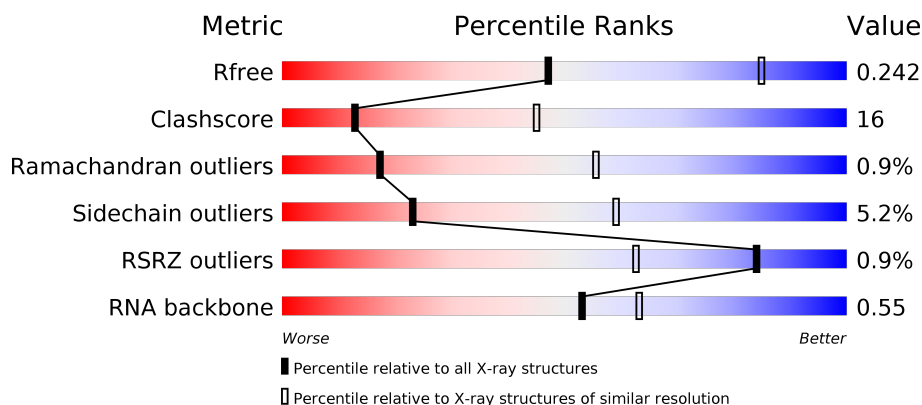
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 ≥ 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 $\leq 5\%$. 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	477	<div> <div>65%</div> <div>29%</div> <div>• •</div> </div>
1	B	477	<div> <div>59%</div> <div>35%</div> <div>• •</div> </div>
2	T	77	<div> <div>8%</div> <div>38%</div> <div>31%</div> <div>12%</div> <div>6%</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9027 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.

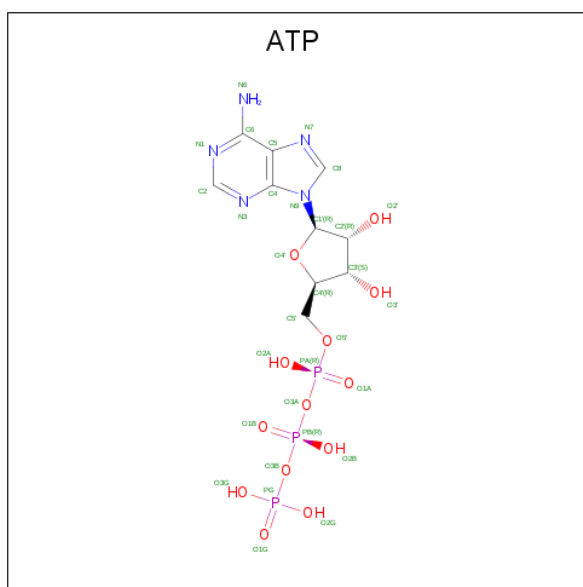
- Molecule 1 is a protein called PROLYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	78	0	0
			3743	2397	654	681	11			
1	B	464	Total	C	N	O	S	72	0	0
			3736	2393	653	679	11			

- Molecule 2 is a RNA chain called TRNAPRO(CGG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	67	Total	C	N	O	P	0	0	0
			1436	640	262	468	66			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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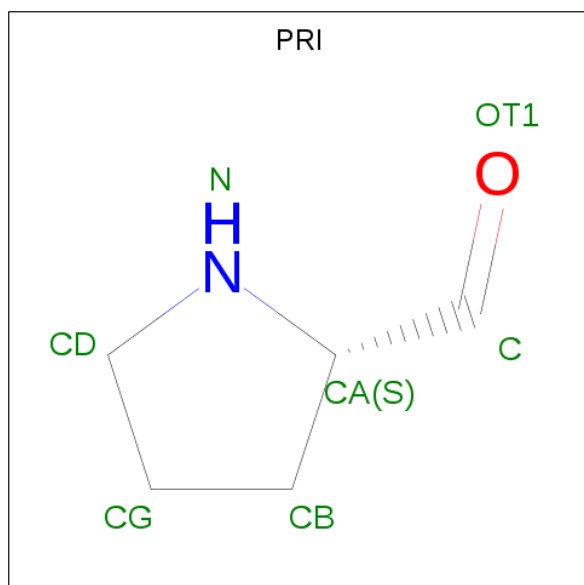
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PYRROLIDINE-2-CARBALDEHYDE (three-letter code: PRI) (formula: C₅H₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	5	1	1		
5	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

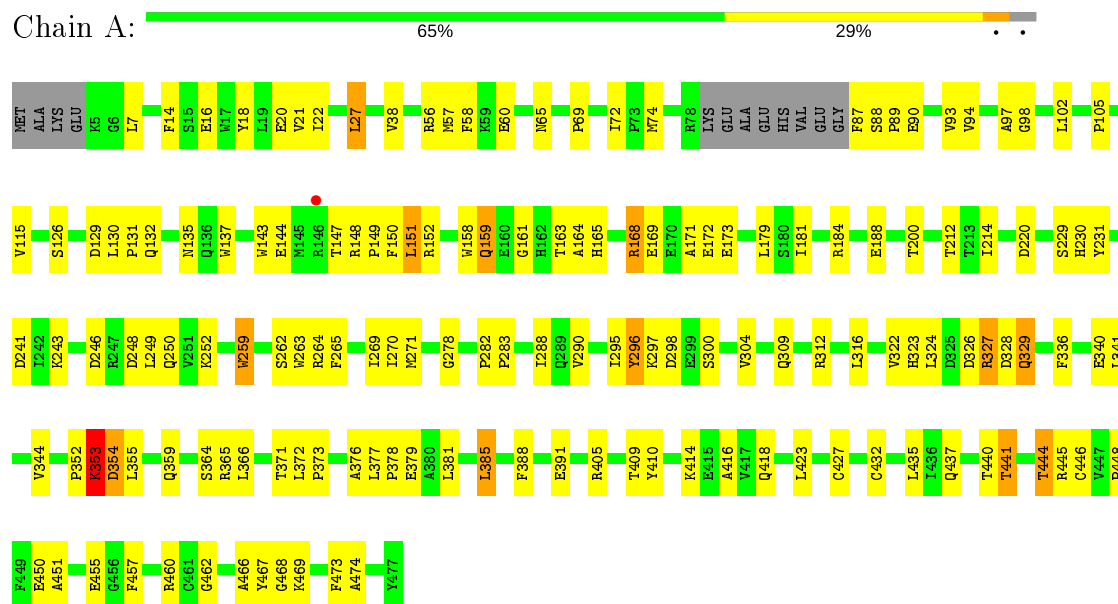
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total	O	0	0
			13	13		
7	B	8	Total	O	0	0
			8	8		
7	T	3	Total	O	0	0
			3	3		

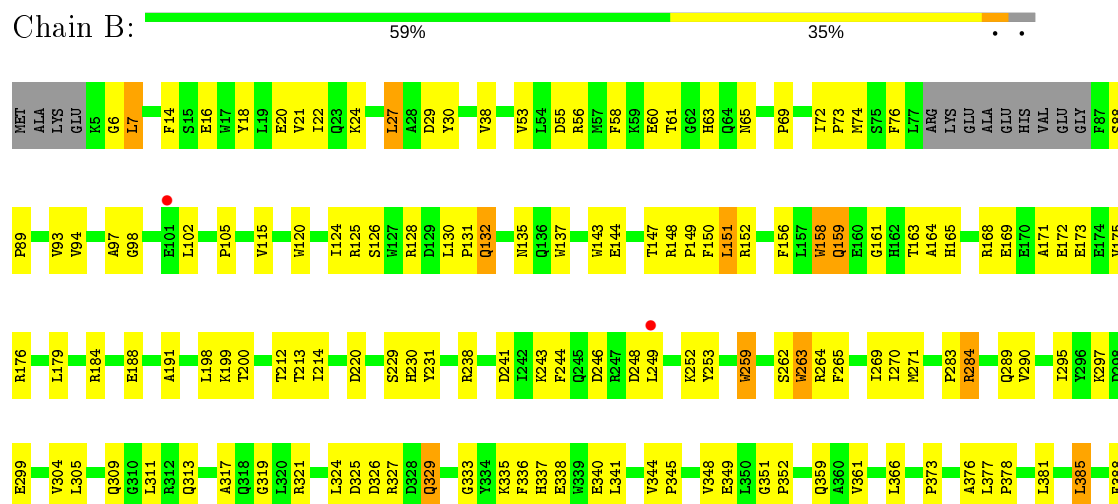
3 Residue-property plots

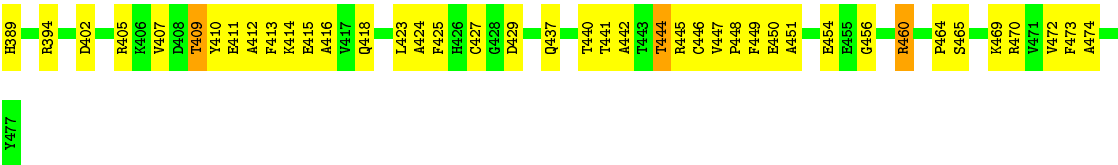
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PROLYL-TRNA SYNTHETASE

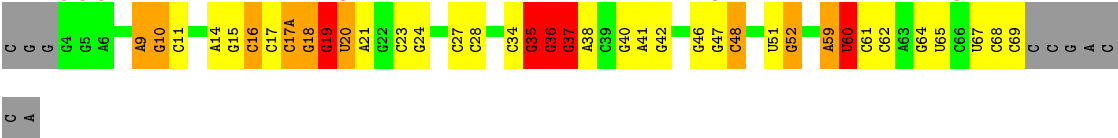


• Molecule 1: PROLYL-TRNA SYNTHETASE





● Molecule 2: TRNAPRO(CGCG)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.29 Å 141.29 Å 237.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.00) 99.8 (19.98-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.98 Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.221 , 0.254 0.211 , 0.242	Depositor DCC
R_{free} test set	2452 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9027	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: 5MU, ZN, PRI, SO4, ATP, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/3840	0.66	0/5204
1	B	0.37	0/3833	0.64	0/5194
2	T	0.41	0/1560	0.91	6/2434 (0.2%)
All	All	0.38	0/9233	0.71	6/12832 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	37	G	N9-C1'-C2'	7.32	123.52	114.00
2	T	35	G	N9-C1'-C2'	7.26	123.44	114.00
2	T	36	G	N9-C1'-C2'	6.10	121.93	114.00
2	T	19	G	N9-C1'-C2'	5.98	121.77	114.00
2	T	48	C	N1-C1'-C2'	5.39	121.01	114.00
2	T	60	U	C5'-C4'-C3'	-5.23	107.63	116.00

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	3743	0	3664	115	0
1	B	3736	0	3661	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	1436	0	730	34	0
3	A	31	0	12	3	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	7	0	9	2	0
5	B	7	0	9	2	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	13	0	0	0	0
7	B	8	0	0	0	0
7	T	3	0	0	0	0
All	All	9027	0	8097	274	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 16.

All (274) 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:A:168:ARG:HB3	1:A:168:ARG:HH11	1.20	1.02
1:B:120:TRP:NE1	1:B:132:GLN:HG2	1.81	0.94
1:A:353:LYS:HG3	1:A:354:ASP:H	1.33	0.92
1:A:97:ALA:HB3	1:A:102:LEU:HD21	1.59	0.84
1:B:97:ALA:HB3	1:B:102:LEU:HD21	1.59	0.82
1:A:262:SER:OG	3:A:1478:ATP:H1'	1.78	0.82
2:T:18:G:O2'	2:T:19:G:H5'	1.82	0.80
1:B:425:PHE:HZ	1:B:454:GLU:HB3	1.46	0.79
1:A:290:VAL:HG21	1:A:381:LEU:HD13	1.64	0.78
1:B:407:VAL:HG11	1:B:413:PHE:HA	1.64	0.78
1:A:57:MET:CE	1:A:181:ILE:HG23	2.15	0.76
1:B:425:PHE:CZ	1:B:454:GLU:HB3	2.20	0.76
1:B:120:TRP:CE2	1:B:132:GLN:HG2	2.21	0.75
2:T:51:U:H2'	2:T:52:G:O4'	1.87	0.75
1:A:290:VAL:HG21	1:A:381:LEU:CD1	2.18	0.72
1:A:329:GLN:HG2	1:B:128:ARG:CZ	2.20	0.72
1:A:56:ARG:O	1:A:60:GLU:HG3	1.90	0.71
1:B:152:ARG:HH21	1:B:264:ARG:HH22	1.40	0.70
1:B:168:ARG:O	1:B:172:GLU:HG3	1.91	0.70
1:A:168:ARG:HB3	1:A:168:ARG:NH1	2.02	0.68
1:A:377:LEU:HB3	1:A:378:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:HH21	1:A:264:ARG:HH22	1.41	0.68
1:A:58:PHE:HE2	1:A:159:GLN:HG3	1.59	0.67
1:B:290:VAL:HG21	1:B:381:LEU:HD13	1.76	0.67
1:A:57:MET:HE1	1:A:181:ILE:HG23	1.75	0.67
1:B:58:PHE:HE2	1:B:159:GLN:HG3	1.60	0.67
1:B:238:ARG:HG2	1:B:253:TYR:CE1	2.29	0.67
1:B:179:LEU:HD22	1:B:212:THR:HB	1.75	0.66
1:A:354:ASP:HB3	1:A:359:GLN:O	1.95	0.66
1:A:437:GLN:O	1:A:441:THR:HA	1.95	0.66
1:B:410:TYR:CE2	1:B:414:LYS:HE3	2.31	0.66
1:B:241:ASP:OD1	1:B:243:LYS:HE3	1.96	0.65
1:A:457:PHE:HB3	1:A:462:GLY:O	1.96	0.65
1:B:137:TRP:CZ3	1:B:159:GLN:HB2	2.32	0.65
1:A:241:ASP:OD1	1:A:243:LYS:HE3	1.97	0.65
1:A:168:ARG:CB	1:A:168:ARG:HH11	2.05	0.65
1:B:198:LEU:HB2	1:B:449:PHE:HE2	1.62	0.64
1:B:305:LEU:O	1:B:309:GLN:HG3	1.96	0.64
1:B:137:TRP:CE3	1:B:159:GLN:HB2	2.32	0.64
1:A:336:PHE:O	1:A:340:GLU:HG3	1.98	0.64
1:A:137:TRP:CE3	1:A:159:GLN:HB2	2.33	0.63
1:A:179:LEU:HD22	1:A:212:THR:HB	1.79	0.63
2:T:46:G:H3'	2:T:47:G:H21	1.62	0.63
1:B:262:SER:OG	3:B:1478:ATP:H1'	1.99	0.63
1:B:56:ARG:O	1:B:60:GLU:HG3	1.99	0.62
1:A:137:TRP:CZ3	1:A:159:GLN:HB2	2.33	0.62
1:A:448:PRO:HG2	1:A:451:ALA:HB2	1.80	0.62
1:B:324:LEU:HG	1:B:326:ASP:OD1	2.00	0.62
1:B:437:GLN:O	1:B:441:THR:HA	1.99	0.61
1:A:451:ALA:HB3	1:A:469:LYS:HD3	1.82	0.60
2:T:64:G:H2'	2:T:65:U:C6	2.36	0.60
1:B:150:PHE:O	1:B:264:ARG:HA	2.02	0.59
1:B:451:ALA:HB3	1:B:469:LYS:HD3	1.84	0.59
1:B:72:ILE:HG12	1:B:115:VAL:CG2	2.33	0.59
1:A:150:PHE:O	1:A:264:ARG:HA	2.03	0.58
1:B:168:ARG:HG3	1:B:231:TYR:OH	2.04	0.58
2:T:17(A):C:H5''	2:T:18:G:OP2	2.03	0.58
1:A:353:LYS:HG3	1:A:354:ASP:N	2.12	0.58
1:B:120:TRP:NE1	1:B:132:GLN:CG	2.62	0.58
2:T:9:A:H4'	2:T:10:G:OP1	2.03	0.58
1:B:184:ARG:HG3	1:B:188:GLU:OE2	2.04	0.58
1:A:126:SER:O	1:A:129:ASP:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:CYS:SG	1:B:429:ASP:HB3	2.43	0.57
2:T:20:U:H4'	2:T:21:A:H5'	1.86	0.57
1:B:329:GLN:H	1:B:329:GLN:NE2	2.02	0.57
1:A:405:ARG:HD3	1:A:416:ALA:HB2	1.86	0.57
1:A:329:GLN:HG2	1:B:128:ARG:NH2	2.20	0.56
1:A:353:LYS:NZ	1:A:353:LYS:HB3	2.20	0.56
1:B:124:ILE:O	1:B:125:ARG:NH1	2.38	0.56
1:A:296:TYR:O	1:A:297:LYS:HG3	2.05	0.56
3:A:1478:ATP:PA	5:A:1480:PRI:HO'T	2.46	0.56
1:B:143:TRP:O	1:B:144:GLU:HG3	2.05	0.56
1:B:311:LEU:HD21	1:B:348:VAL:HG11	1.88	0.56
1:A:72:ILE:HG12	1:A:115:VAL:CG2	2.36	0.56
1:A:18:TYR:O	1:A:21:VAL:HG12	2.06	0.55
1:B:18:TYR:O	1:B:21:VAL:HG12	2.06	0.55
1:B:295:ILE:O	1:B:352:PRO:HD3	2.06	0.55
1:B:407:VAL:HG23	1:B:424:ALA:HB2	1.89	0.55
1:A:466:ALA:O	1:A:468:GLY:N	2.39	0.55
1:A:248:ASP:O	1:A:249:LEU:HB2	2.07	0.55
1:A:283:PRO:HB3	1:A:385:LEU:HD12	1.89	0.55
1:B:132:GLN:O	1:B:163:THR:HA	2.07	0.55
1:A:143:TRP:O	1:A:144:GLU:HG3	2.07	0.55
1:B:176:ARG:NH2	1:B:449:PHE:CD1	2.75	0.55
1:A:184:ARG:HG3	1:A:188:GLU:OE2	2.07	0.54
1:B:212:THR:OG1	1:B:229:SER:HB3	2.07	0.54
1:B:72:ILE:HG12	1:B:115:VAL:HG21	1.89	0.54
2:T:10:G:H2'	2:T:11:C:H6	1.71	0.54
1:A:132:GLN:O	1:A:163:THR:HA	2.08	0.54
1:B:24:LYS:HB3	1:B:341:LEU:HD21	1.89	0.54
1:B:448:PRO:HG2	1:B:451:ALA:HB2	1.88	0.54
1:A:212:THR:OG1	1:A:229:SER:HB3	2.08	0.54
2:T:17:C:H2'	2:T:17(A):C:H5	1.72	0.54
2:T:16:C:O2'	2:T:60:U:O3'	2.26	0.53
1:A:168:ARG:HG3	1:A:231:TYR:OH	2.09	0.53
1:B:289:GLN:HG3	1:B:321:ARG:HB2	1.90	0.53
1:B:313:GLN:NE2	1:B:313:GLN:HA	2.22	0.53
1:A:353:LYS:O	1:A:355:LEU:N	2.42	0.53
1:A:98:GLY:HA2	1:B:89:PRO:O	2.09	0.53
2:T:27:C:H2'	2:T:28:C:H6	1.73	0.53
1:B:244:PHE:CE2	1:B:252:LYS:HG3	2.44	0.53
1:A:169:GLU:O	1:A:173:GLU:HG3	2.09	0.53
1:A:56:ARG:NH1	1:A:57:MET:HG2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:O	1:A:327:ARG:C	2.48	0.53
1:B:238:ARG:NH1	1:B:253:TYR:HE1	2.07	0.53
2:T:23:C:H2'	2:T:24:G:C8	2.44	0.52
1:A:278:GLY:HA3	1:A:341:LEU:HD12	1.91	0.52
1:B:169:GLU:O	1:B:173:GLU:HG3	2.09	0.52
1:A:312:ARG:NH1	1:A:316:LEU:HD11	2.24	0.52
1:A:38:VAL:HG22	1:B:69:PRO:HD3	1.91	0.52
1:A:246:ASP:HB2	1:A:252:LYS:HE2	1.92	0.52
1:A:373:PRO:HG2	1:A:376:ALA:CB	2.40	0.52
1:A:414:LYS:O	1:A:418:GLN:HG2	2.10	0.52
1:A:18:TYR:CZ	1:A:22:ILE:HD11	2.46	0.51
1:A:57:MET:HE3	1:A:181:ILE:HG23	1.89	0.51
2:T:64:G:H2'	2:T:65:U:H6	1.73	0.51
1:B:14:PHE:CD2	1:B:220:ASP:HB3	2.45	0.51
1:B:243:LYS:HG2	1:B:253:TYR:CE2	2.45	0.51
1:B:161:GLY:HA3	1:B:259:TRP:CZ3	2.45	0.51
1:A:161:GLY:HA3	1:A:259:TRP:CZ3	2.46	0.51
1:B:132:GLN:HB2	1:B:164:ALA:HB3	1.93	0.51
1:B:284:ARG:NH1	1:B:389:HIS:CD2	2.79	0.51
2:T:17:C:H2'	2:T:17(A):C:C5	2.46	0.51
1:B:65:ASN:HA	1:B:135:ASN:O	2.10	0.51
1:B:243:LYS:HE2	1:B:253:TYR:CE2	2.46	0.50
1:B:73:PRO:HB2	1:B:76:PHE:CD1	2.45	0.50
1:B:325:ASP:OD1	1:B:335:LYS:HE2	2.11	0.50
1:B:373:PRO:HG2	1:B:376:ALA:HB3	1.93	0.50
1:A:371:THR:O	1:A:372:LEU:HD23	2.11	0.50
1:B:265:PHE:O	1:B:269:ILE:HG13	2.12	0.50
1:A:14:PHE:CD2	1:A:220:ASP:HB3	2.46	0.50
1:B:147:THR:HG22	1:B:148:ARG:N	2.27	0.50
1:B:414:LYS:O	1:B:418:GLN:HG2	2.12	0.50
1:A:262:SER:CB	3:A:1478:ATP:H1'	2.41	0.50
1:B:191:ALA:HB2	1:B:389:HIS:CE1	2.47	0.49
1:A:365:ARG:HH11	1:A:365:ARG:HG3	1.77	0.49
1:A:377:LEU:CB	1:A:378:PRO:HD3	2.43	0.49
1:A:56:ARG:HH22	1:A:184:ARG:HH22	1.60	0.49
2:T:52:G:O6	2:T:62:C:N3	2.46	0.49
1:A:147:THR:HG22	1:A:148:ARG:N	2.26	0.49
1:A:353:LYS:CG	1:A:354:ASP:H	2.15	0.49
1:A:72:ILE:HG12	1:A:115:VAL:HG21	1.94	0.49
1:A:377:LEU:HB3	1:A:378:PRO:CD	2.42	0.49
1:A:445:ARG:HA	1:A:445:ARG:NE	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:THR:HG23	1:B:412:ALA:HB2	1.95	0.49
1:A:58:PHE:CE2	1:A:159:GLN:HG3	2.46	0.49
1:B:447:VAL:HG12	1:B:469:LYS:HD2	1.95	0.49
2:T:10:G:H2'	2:T:11:C:C6	2.48	0.49
2:T:59:A:H2'	2:T:60:U:O5'	2.13	0.49
1:B:53:VAL:HA	1:B:56:ARG:HH12	1.78	0.48
1:A:329:GLN:CD	1:A:329:GLN:H	2.17	0.48
1:B:405:ARG:HD3	1:B:416:ALA:HB2	1.95	0.48
1:B:283:PRO:HB3	1:B:385:LEU:HD12	1.96	0.48
1:A:365:ARG:HG3	1:A:365:ARG:O	2.14	0.48
1:B:125:ARG:O	1:B:244:PHE:HA	2.13	0.48
2:T:41:A:H2'	2:T:42:G:O4'	2.14	0.48
1:A:14:PHE:CG	1:A:220:ASP:HB3	2.49	0.48
1:B:120:TRP:HE1	1:B:132:GLN:CG	2.24	0.48
2:T:17:C:N3	2:T:17(A):C:N4	2.62	0.47
1:B:385:LEU:O	1:B:388:PHE:HB3	2.14	0.47
1:B:18:TYR:CZ	1:B:22:ILE:HD11	2.49	0.47
1:A:65:ASN:HA	1:A:135:ASN:O	2.14	0.47
1:A:282:PRO:HA	1:A:283:PRO:HD3	1.75	0.47
2:T:27:C:H2'	2:T:28:C:C6	2.48	0.47
1:B:445:ARG:HA	1:B:445:ARG:NE	2.28	0.47
1:A:22:ILE:HD13	1:A:149:PRO:HB2	1.96	0.47
1:B:349:GLU:HB2	1:B:361:VAL:HB	1.97	0.47
1:B:200:THR:HG23	1:B:444:THR:HG21	1.96	0.47
1:B:473:PHE:O	1:B:474:ALA:HB2	2.14	0.47
1:A:427:CYS:O	1:A:466:ALA:HB2	2.15	0.47
1:B:246:ASP:HB3	1:B:248:ASP:OD2	2.14	0.47
1:B:377:LEU:HB3	1:B:378:PRO:HD3	1.97	0.47
1:A:295:ILE:O	1:A:352:PRO:HD3	2.15	0.47
1:B:88:SER:OG	1:B:89:PRO:HD2	2.15	0.47
1:A:69:PRO:HD3	1:B:38:VAL:HG22	1.96	0.46
1:B:6:GLY:O	1:B:7:LEU:HB2	2.15	0.46
1:A:296:TYR:HA	1:A:352:PRO:HG3	1.96	0.46
1:A:366:LEU:HD13	1:A:388:PHE:CZ	2.50	0.46
2:T:23:C:H2'	2:T:24:G:H8	1.80	0.46
2:T:67:U:H2'	2:T:68:C:C6	2.51	0.46
1:B:14:PHE:CG	1:B:220:ASP:HB3	2.51	0.46
1:B:151:LEU:HD12	1:B:151:LEU:HA	1.75	0.46
2:T:48:C:C5	2:T:59:A:H5"	2.50	0.46
1:B:22:ILE:HD13	1:B:149:PRO:HB2	1.98	0.46
1:B:249:LEU:N	1:B:249:LEU:HD22	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ALA:C	1:B:319:GLY:H	2.18	0.46
2:T:46:G:H3'	2:T:47:G:N2	2.29	0.46
1:A:248:ASP:OD2	1:A:250:GLN:HB2	2.16	0.46
1:A:448:PRO:CG	1:A:451:ALA:HB2	2.46	0.45
1:A:93:VAL:O	1:B:94:VAL:HA	2.16	0.45
1:B:448:PRO:CG	1:B:451:ALA:HB2	2.45	0.45
1:A:366:LEU:HD23	1:A:391:GLU:HG2	1.98	0.45
1:A:200:THR:HG23	1:A:444:THR:HG21	1.97	0.45
1:A:151:LEU:HD12	1:A:151:LEU:HA	1.75	0.45
1:A:297:LYS:O	1:A:300:SER:N	2.47	0.45
1:A:168:ARG:O	1:A:172:GLU:HG3	2.17	0.45
1:A:94:VAL:HA	1:B:93:VAL:O	2.17	0.45
1:B:407:VAL:CG2	1:B:424:ALA:HB2	2.47	0.45
1:B:456:GLY:H	1:B:465:SER:CB	2.30	0.45
1:A:265:PHE:O	1:A:269:ILE:HG13	2.16	0.45
1:B:132:GLN:CA	1:B:132:GLN:HE21	2.29	0.45
1:A:296:TYR:HB3	1:A:304:VAL:HG21	1.98	0.44
1:B:338:GLU:O	1:B:341:LEU:HB3	2.17	0.44
2:T:36:G:H4'	2:T:37:G:O5'	2.17	0.44
1:A:309:GLN:HE21	1:A:324:LEU:HD23	1.82	0.44
2:T:16:C:O3'	2:T:60:U:O2'	2.31	0.44
1:A:473:PHE:O	1:A:474:ALA:HB2	2.17	0.44
1:B:445:ARG:O	1:B:446:CYS:HB3	2.17	0.44
1:A:445:ARG:O	1:A:446:CYS:HB3	2.17	0.44
1:A:16:GLU:O	1:A:20:GLU:HG3	2.17	0.44
1:A:130:LEU:HB3	1:A:131:PRO:HA	2.00	0.44
1:A:373:PRO:HG2	1:A:376:ALA:HB3	2.00	0.44
1:A:440:THR:C	1:A:441:THR:HG23	2.38	0.44
1:A:89:PRO:O	1:B:98:GLY:HA2	2.18	0.44
1:A:87:PHE:O	1:A:88:SER:C	2.56	0.43
1:B:61:THR:HG1	1:B:63:HIS:CE1	2.36	0.43
2:T:40:G:H2'	2:T:41:A:C8	2.53	0.43
1:A:161:GLY:HA3	1:A:259:TRP:CH2	2.53	0.43
1:B:27:LEU:HD23	1:B:270:ILE:HD11	2.00	0.43
1:A:151:LEU:HD21	1:A:271:MET:CE	2.48	0.43
1:B:158:TRP:CZ3	5:B:1480:PRI:HCG2	2.53	0.43
1:A:432:CYS:O	1:A:435:LEU:HB3	2.18	0.43
1:B:243:LYS:HE2	1:B:253:TYR:HE2	1.84	0.43
1:A:373:PRO:HG2	1:A:376:ALA:HB2	2.01	0.43
1:B:373:PRO:HG2	1:B:376:ALA:CB	2.47	0.43
1:B:448:PRO:HD3	1:B:472:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:HIS:CD2	5:A:1480:PRI:HCB2	2.53	0.43
1:B:214:ILE:O	1:B:214:ILE:HG13	2.18	0.43
1:B:297:LYS:HA	2:T:34:C:C5	2.53	0.43
1:B:336:PHE:O	1:B:340:GLU:HG3	2.18	0.43
1:B:333:GLY:O	1:B:337:HIS:HD2	2.01	0.43
1:A:364:SER:C	1:A:366:LEU:H	2.20	0.43
1:B:161:GLY:HA3	1:B:259:TRP:CH2	2.53	0.43
1:B:16:GLU:O	1:B:20:GLU:HG3	2.18	0.43
1:B:351:GLY:HA3	2:T:35:G:C6	2.53	0.43
1:B:448:PRO:HG2	1:B:451:ALA:CB	2.48	0.42
1:B:423:LEU:O	1:B:470:ARG:HD3	2.20	0.42
1:A:27:LEU:HD23	1:A:270:ILE:HD11	2.02	0.42
1:B:171:ALA:O	1:B:175:VAL:HG23	2.18	0.42
1:B:58:PHE:HE2	1:B:159:GLN:CG	2.31	0.42
1:B:130:LEU:HB3	1:B:131:PRO:HA	2.02	0.42
1:B:411:GLU:O	1:B:415:GLU:HG3	2.20	0.42
1:A:165:HIS:CD2	1:A:171:ALA:HA	2.55	0.42
1:A:410:TYR:O	1:A:414:LYS:HG3	2.20	0.42
1:B:165:HIS:CD2	1:B:171:ALA:HA	2.54	0.42
1:B:29:ASP:OD1	1:B:30:TYR:N	2.51	0.42
1:B:385:LEU:HD13	1:B:385:LEU:HA	1.75	0.42
2:T:18:G:HO2'	2:T:19:G:H5'	1.84	0.42
1:B:149:PRO:O	1:B:150:PHE:HB2	2.20	0.42
1:B:74:MET:HB2	1:B:105:PRO:O	2.20	0.42
2:T:14:A:C2'	2:T:15:G:H5'	2.50	0.42
2:T:17(A):C:H4'	2:T:18:G:OP1	2.19	0.42
1:B:230:HIS:CD2	5:B:1480:PRI:HCB2	2.55	0.41
1:A:74:MET:HB2	1:A:105:PRO:O	2.20	0.41
1:B:440:THR:C	1:B:442:ALA:H	2.24	0.41
1:B:156:PHE:HA	1:B:263:TRP:CZ2	2.56	0.41
1:B:409:THR:O	1:B:412:ALA:N	2.51	0.41
1:B:151:LEU:HD21	1:B:271:MET:CE	2.50	0.41
1:B:394:ARG:HH11	1:B:394:ARG:HG3	1.86	0.41
2:T:59:A:C2'	2:T:60:U:O5'	2.69	0.41
1:B:326:ASP:O	1:B:327:ARG:C	2.59	0.41
2:T:17:C:C4	2:T:17(A):C:C4	3.08	0.41
1:A:288:ILE:HB	1:A:344:VAL:HG22	2.02	0.41
1:B:344:VAL:HA	1:B:345:PRO:HD3	1.90	0.41
1:A:132:GLN:HB2	1:A:164:ALA:HB3	2.03	0.40
1:A:381:LEU:HA	1:A:381:LEU:HD23	1.84	0.40
1:A:214:ILE:HG13	1:A:214:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LEU:HD23	1:A:460:ARG:HD3	2.03	0.40
1:B:199:LYS:HE2	1:B:213:THR:HG21	2.03	0.40
1:B:410:TYR:CE1	1:B:460:ARG:HG3	2.56	0.40
1:B:132:GLN:CB	1:B:164:ALA:HB3	2.51	0.40
1:B:448:PRO:HB2	1:B:451:ALA:HB2	2.02	0.40
1:A:322:VAL:HG22	1:A:323:HIS:N	2.36	0.40
1:B:304:VAL:HG21	1:B:352:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/477 (97%)	419 (91%)	36 (8%)	6 (1%)	12	45
1	B	460/477 (96%)	415 (90%)	43 (9%)	2 (0%)	34	72
All	All	921/954 (96%)	834 (91%)	79 (9%)	8 (1%)	17	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASP
1	A	298	ASP
1	A	327	ARG
1	A	467	TYR
1	B	7	LEU
1	A	90	GLU
1	A	353	LYS
1	B	464	PRO

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	383/395 (97%)	363 (95%)	20 (5%)	23	59
1	B	383/395 (97%)	363 (95%)	20 (5%)	23	59
All	All	766/790 (97%)	726 (95%)	40 (5%)	23	59

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	27	LEU
1	A	151	LEU
1	A	158	TRP
1	A	159	GLN
1	A	168	ARG
1	A	259	TRP
1	A	263	TRP
1	A	296	TYR
1	A	328	ASP
1	A	329	GLN
1	A	353	LYS
1	A	379	GLU
1	A	385	LEU
1	A	409	THR
1	A	423	LEU
1	A	441	THR
1	A	444	THR
1	A	450	GLU
1	A	455	GLU
1	B	27	LEU
1	B	55	ASP
1	B	126	SER
1	B	132	GLN
1	B	151	LEU
1	B	158	TRP
1	B	159	GLN

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Mol	Chain	Res	Type
1	B	259	TRP
1	B	263	TRP
1	B	284	ARG
1	B	299	GLU
1	B	329	GLN
1	B	359	GLN
1	B	366	LEU
1	B	385	LEU
1	B	402	ASP
1	B	409	THR
1	B	444	THR
1	B	450	GLU
1	B	460	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	159	GLN
1	A	235	ASN
1	A	255	HIS
1	A	309	GLN
1	A	329	GLN
1	A	337	HIS
1	B	12	GLN
1	B	132	GLN
1	B	159	GLN
1	B	235	ASN
1	B	255	HIS
1	B	313	GLN
1	B	329	GLN
1	B	337	HIS
1	B	359	GLN
1	B	389	HIS
1	B	403	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	T	66/77 (85%)	13 (19%)	6 (9%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	T	9	A
2	T	10	G
2	T	17(A)	C
2	T	18	G
2	T	20	U
2	T	35	G
2	T	36	G
2	T	37	G
2	T	38	A
2	T	52	G
2	T	59	A
2	T	61	C
2	T	69	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	T	9	A
2	T	16	C
2	T	17(A)	C
2	T	19	G
2	T	20	U
2	T	60	U

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

2 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
2	5MU	T	54	2	15,22,23	1.19	2 (13%)	16,32,35	3.67	2 (12%)
2	PSU	T	55	2	17,21,22	1.77	3 (17%)	20,30,33	5.42	5 (25%)

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	5MU	T	54	2	-	0/5/25/26	0/2/2/2
2	PSU	T	55	2	-	0/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	55	PSU	C5-C1'	-5.70	1.47	1.52
2	T	54	5MU	C4-N3	3.27	1.38	1.33
2	T	55	PSU	C2-N1	2.73	1.43	1.38
2	T	55	PSU	C4-N3	2.56	1.37	1.33
2	T	54	5MU	C6-C5	-2.15	1.34	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	55	PSU	N1-C2-N3	-17.26	114.71	128.43
2	T	54	5MU	C4-N3-C2	14.32	127.23	115.14
2	T	55	PSU	C4-N3-C2	14.12	127.06	115.14
2	T	55	PSU	C5-C4-N3	-8.16	114.85	125.36
2	T	55	PSU	C6-N1-C2	2.66	119.75	115.36
2	T	54	5MU	C5M-C5-C6	2.05	123.01	118.68
2	T	55	PSU	C5-C1'-C2'	-2.02	111.72	115.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	1478	-	26,33,33	0.58	0	31,52,52	1.03	2 (6%)
3	ATP	B	1478	-	26,33,33	0.58	0	31,52,52	1.02	2 (6%)
6	SO4	B	1481	-	4,4,4	0.27	0	6,6,6	0.10	0
6	SO4	A	1481	-	4,4,4	0.29	0	6,6,6	0.07	0
5	PRI	A	1480	-	5,7,7	0.78	0	7,8,8	1.54	1 (14%)
5	PRI	B	1480	-	5,7,7	0.72	0	7,8,8	1.27	1 (14%)

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	1478	-	-	3/18/38/38	0/3/3/3
3	ATP	B	1478	-	-	4/18/38/38	0/3/3/3
5	PRI	B	1480	-	-	0/0/9/9	0/1/1/1
5	PRI	A	1480	-	-	0/0/9/9	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	1480	PRI	OT1-C-CA	-3.23	116.31	124.78
5	B	1480	PRI	OT1-C-CA	-2.58	118.01	124.78
3	A	1478	ATP	C5-C6-N6	2.54	124.21	120.35
3	B	1478	ATP	C5-C6-N6	2.48	124.11	120.35
3	B	1478	ATP	O3G-PG-O2G	2.35	116.62	107.64
3	A	1478	ATP	O3G-PG-O2G	2.24	116.19	107.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

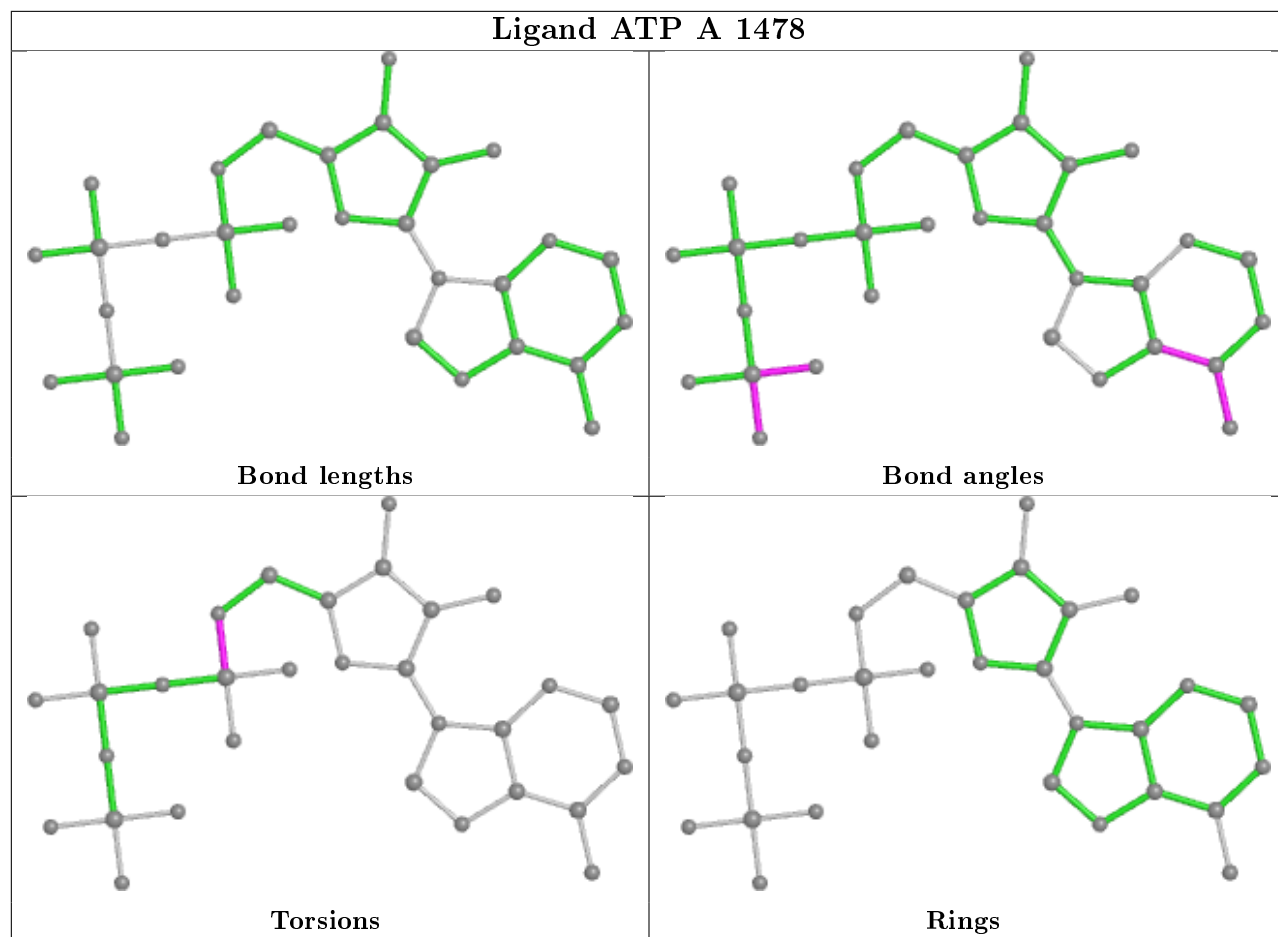
Mol	Chain	Res	Type	Atoms
3	A	1478	ATP	C5'-O5'-PA-O1A
3	A	1478	ATP	C5'-O5'-PA-O2A
3	B	1478	ATP	C5'-O5'-PA-O2A
3	A	1478	ATP	C5'-O5'-PA-O3A
3	B	1478	ATP	C5'-O5'-PA-O3A
3	B	1478	ATP	C5'-O5'-PA-O1A
3	B	1478	ATP	C4'-C5'-O5'-PA

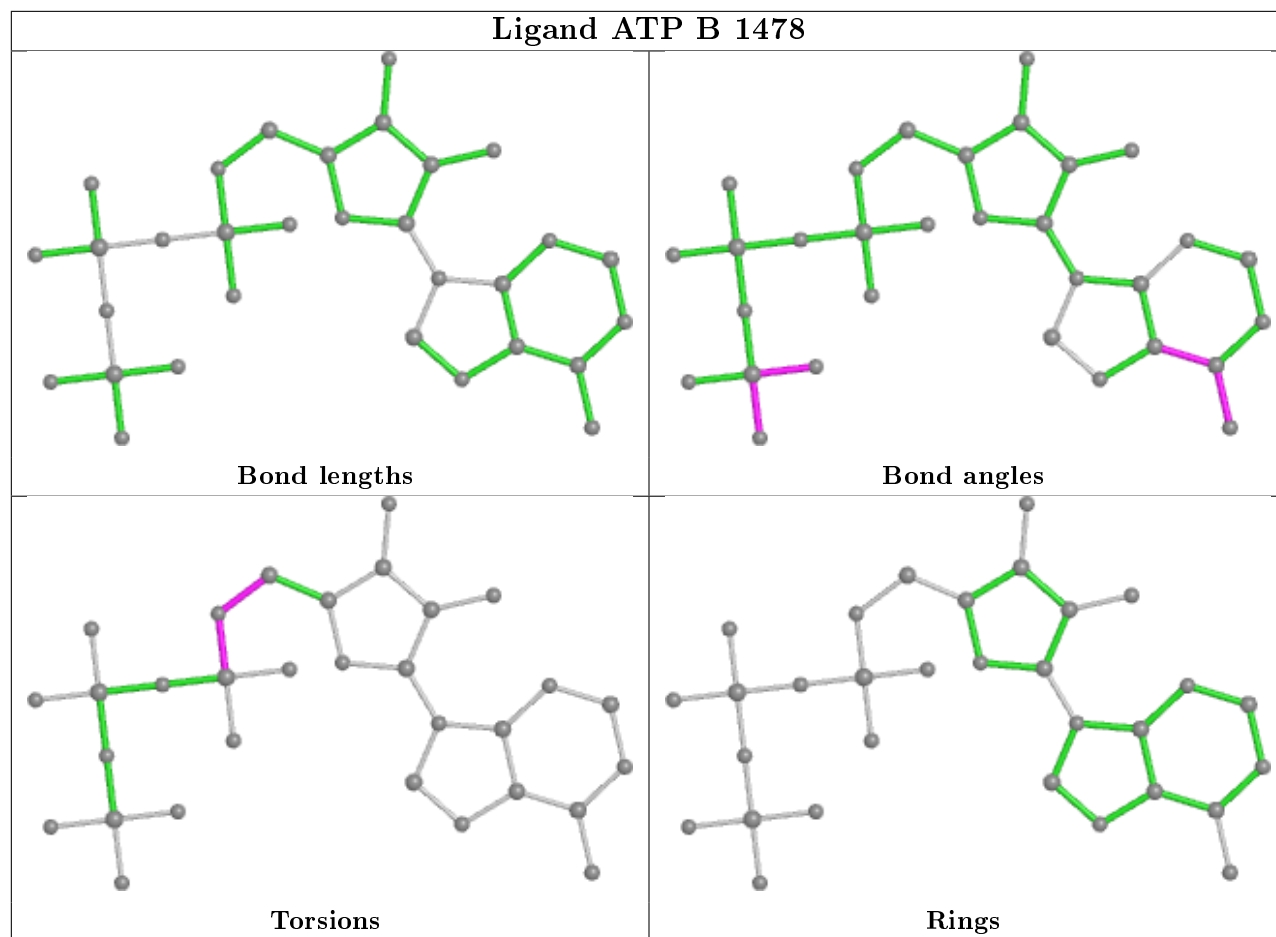
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1478	ATP	3	0
3	B	1478	ATP	1	0
5	A	1480	PRI	2	0
5	B	1480	PRI	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 than 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.





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	464/477 (97%)	-0.43	1 (0%) 95 87	21, 46, 81, 107	17 (3%)
1	B	463/477 (97%)	-0.34	2 (0%) 92 79	25, 50, 85, 104	14 (3%)
2	T	65/77 (84%)	0.24	6 (9%) 9 3	27, 62, 93, 108	7 (10%)
All	All	992/1031 (96%)	-0.34	9 (0%) 84 63	21, 49, 85, 108	38 (3%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	4	G	4.5
2	T	5	G	3.9
2	T	20	U	2.5
1	B	101	GLU	2.3
2	T	6	A	2.3
1	A	146	ARG	2.3
2	T	47	G	2.3
1	B	249	LEU	2.2
2	T	66	C	2.1

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

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
2	5MU	T	54	21/22	0.96	0.16	27,46,66,68	0
2	PSU	T	55	20/21	0.98	0.15	39,48,55,58	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

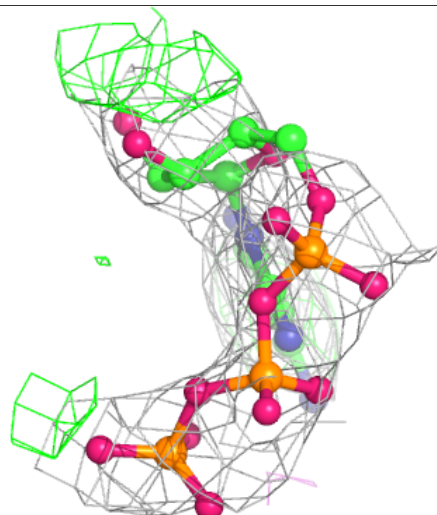
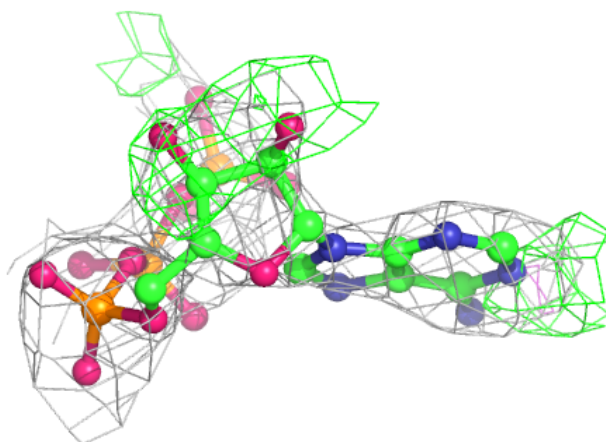
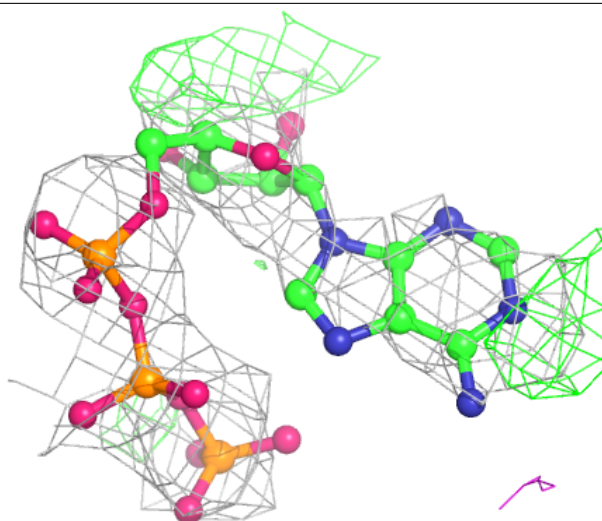
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ATP	B	1478	31/31	0.72	0.36	69,86,105,106	31
4	ZN	B	1479	1/1	0.75	0.07	88,88,88,88	0
3	ATP	A	1478	31/31	0.79	0.33	54,62,95,97	31
5	PRI	B	1480	7/7	0.90	0.27	58,59,60,60	7
5	PRI	A	1480	7/7	0.92	0.20	26,31,40,44	7
6	SO4	A	1481	5/5	0.94	0.14	75,75,78,78	5
4	ZN	A	1479	1/1	0.94	0.08	59,59,59,59	0
6	SO4	B	1481	5/5	0.95	0.14	56,59,61,61	5

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.

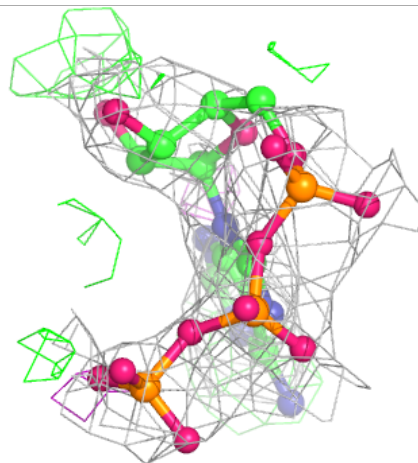
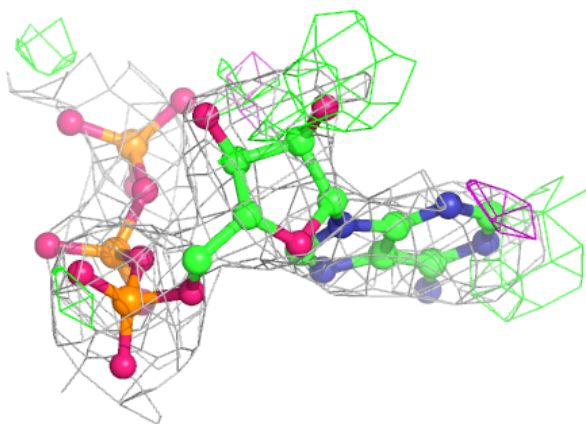
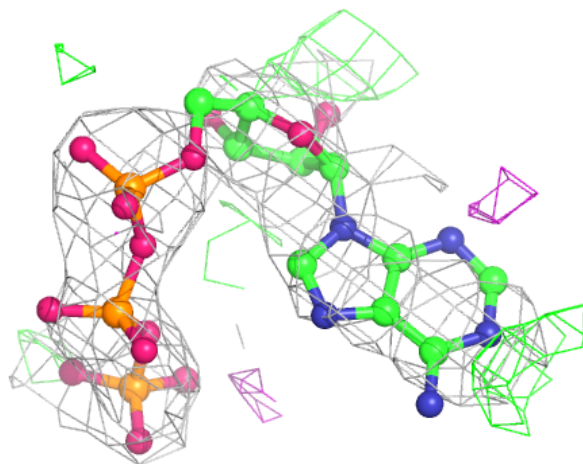
Electron density around ATP B 1478:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP A 1478:

$2mF_o-DF_c$ (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.