



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:23 AM GMT

PDB ID : 1H4Q  
Title : PROLYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS  
COMPLEXED WITH TRNAPRO(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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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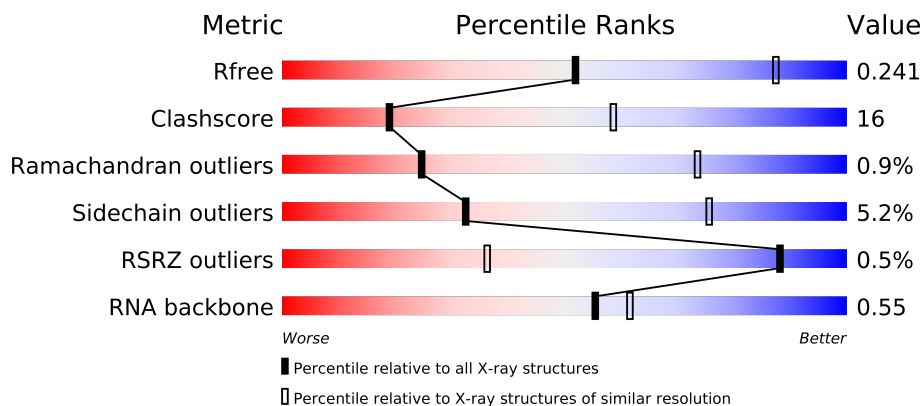
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance




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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	477	
1	B	477	
2	T	77	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ATP	A	1478	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 9027 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

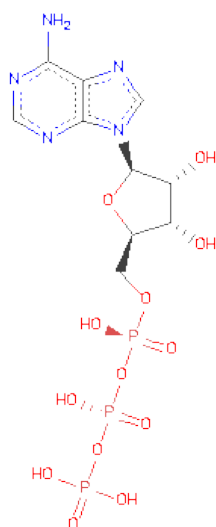
- Molecule 1 is a protein called PROLYL-TRNA SYNTHETASE.

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<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

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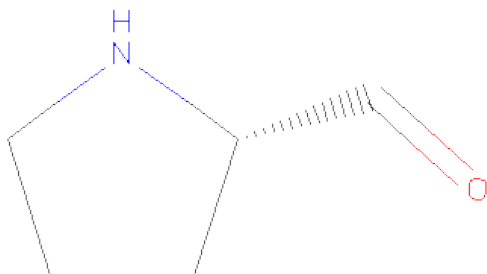
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

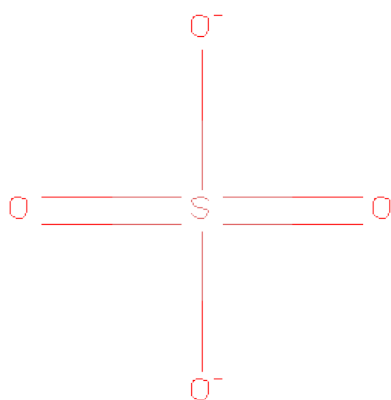
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PYRROLIDINE-2-CARBALDEHYDE (three-letter code: PRI) (formula: C<sub>5</sub>H<sub>9</sub>NO).



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: O<sub>4</sub>S).



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.

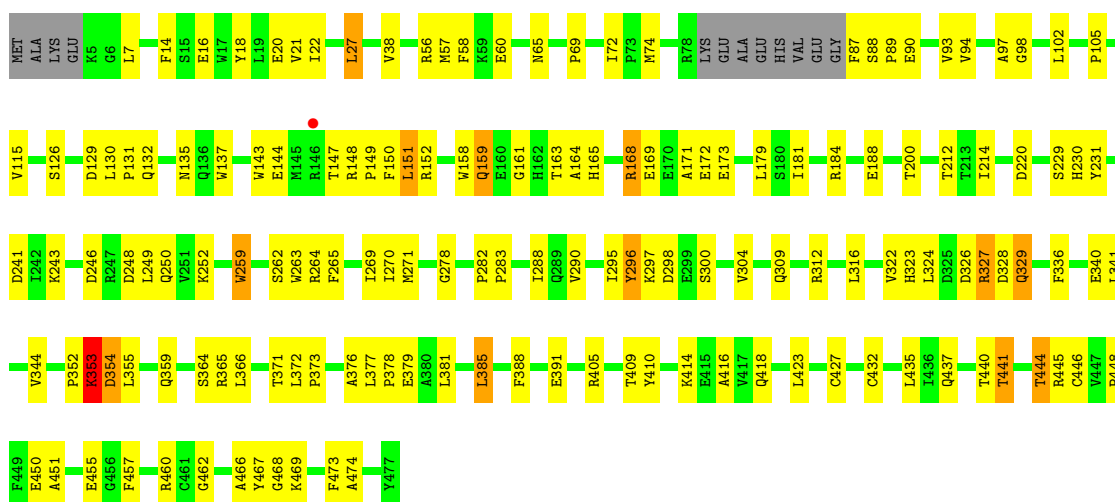
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total	O	0	0
			13	13		
7	B	8	Total	O	0	0
			8	8		
7	T	3	Total	O	0	0
			3	3		

### 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 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.

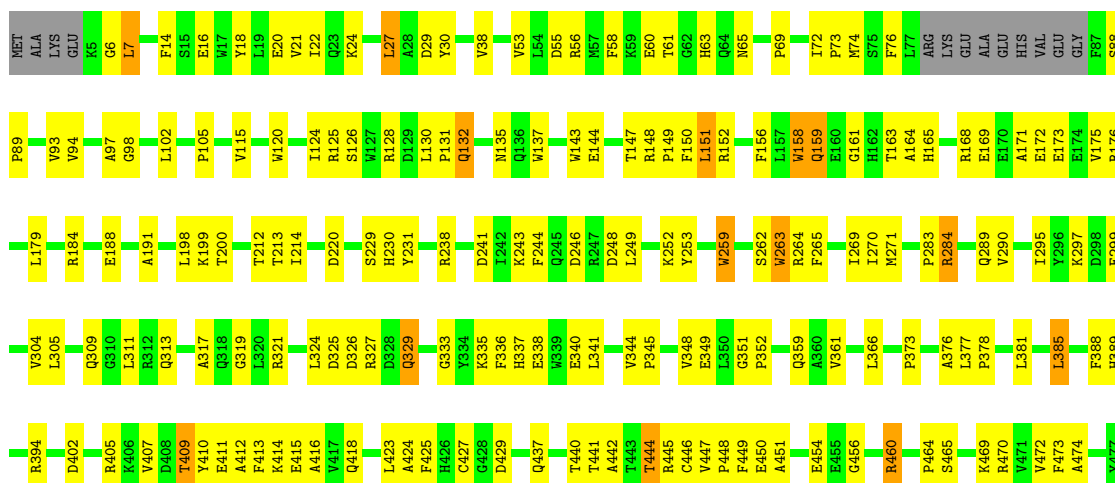
#### • Molecule 1: PROLYL-TRNA SYNTHETASE

Chain A:



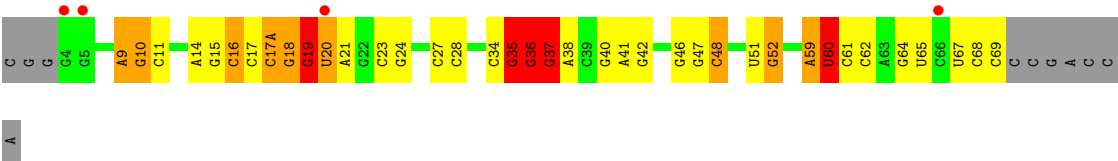
#### • Molecule 1: PROLYL-TRNA SYNTHETASE

Chain B:



#### • Molecule 2: TRNAPRO(CGCG)

Chain T:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.29Å 141.29Å 237.56Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.71 (at 2.98Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.221 , 0.254 0.213 , 0.241	Depositor DCC
$R_{free}$ test set	2452 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48592 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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



## 5 Model quality

### 5.1 Standard geometry

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( $^{\circ}$ )	Ideal( $^{\circ}$ )
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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (274) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:152:ARG:HH21	1:A:264:ARG:HH22	1.41	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:T:46:G:H3'	2:T:47:G:H21	1.62	0.63
1:A:179:LEU:HD22	1:A:212:THR:HB	1.79	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:B:120:TRP:NE1	1:B:132:GLN:CG	2.62	0.58
1:A:353:LYS:HG3	1:A:354:ASP:N	2.12	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:18:TYR:O	1:B:21:VAL:HG12	2.06	0.55
1:A:18:TYR:O	1:A: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:B:132:GLN:O	1:B:163:THR:HA	2.07	0.55
1:A:283:PRO:HB3	1:A:385:LEU:HD12	1.89	0.55
1:A:248:ASP:O	1:A:249:LEU:HB2	2.07	0.55
1:B:176:ARG:NH2	1:B:449:PHE:CD1	2.75	0.55
1:A:143:TRP:O	1:A:144:GLU:HG3	2.07	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
2:T:17:C:H2'	2:T:17(A):C:H5	1.72	0.54
1:A:212:THR:OG1	1:A:229:SER:HB3	2.08	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:313:GLN:NE2	1:B:313:GLN:HA	2.22	0.53
1:B:289:GLN:HG3	1:B:321:ARG:HB2	1.90	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:56:ARG:NH1	1:A:57:MET:HG2	2.24	0.53
1:A:169:GLU:O	1:A:173:GLU:HG3	2.09	0.53
1:B:238:ARG:NH1	1:B:253:TYR:HE1	2.07	0.53
1:A:326:ASP:O	1:A:327:ARG:C	2.48	0.53
2:T:23:C:H2'	2:T:24:G:C8	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:38:VAL:HG22	1:B:69:PRO:HD3	1.91	0.52
1:A:312:ARG:NH1	1:A:316:LEU:HD11	2.24	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:243:LYS:HG2	1:B:253:TYR:CE2	2.45	0.51
1:B:14:PHE:CD2	1:B:220:ASP:HB3	2.45	0.51
1:B:161:GLY:HA3	1:B:259:TRP:CZ3	2.45	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
1:A:161:GLY:HA3	1:A:259:TRP:CZ3	2.46	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:B:414:LYS:O	1:B:418:GLN:HG2	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: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:56:ARG:HH22	1:A:184:ARG:HH22	1.60	0.49
1:A:377:LEU:CB	1:A:378:PRO:HD3	2.43	0.49
1:A:365:ARG:HH11	1:A:365:ARG:HG3	1.77	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:B:409:THR:HG23	1:B:412:ALA:HB2	1.95	0.49
1:A:445:ARG:HA	1:A:445:ARG:NE	2.28	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:65:ASN:HA	1:A:135:ASN:O	2.14	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:A:427:CYS:O	1:A:466:ALA:HB2	2.15	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: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
2:T:23:C:H2'	2:T:24:G:H8	1.80	0.46
1:A:366:LEU:HD13	1:A:388:PHE:CZ	2.50	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
2:T:48:C:C5	2:T:59:A:H5''	2.50	0.46
1:B:151:LEU:HA	1:B:151:LEU:HD12	1.75	0.46
1:B:22:ILE:HD13	1:B:149:PRO:HB2	1.98	0.46
2:T:46:G:H3'	2:T:47:G:N2	2.29	0.46
1:B:249:LEU:N	1:B:249:LEU:HD22	2.30	0.46
1:B:317:ALA:C	1:B:319:GLY:H	2.18	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:B:448:PRO:CG	1:B:451:ALA:HB2	2.45	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:VAL:O	1:B:94:VAL:HA	2.16	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:297:LYS:O	1:A:300:SER:N	2.47	0.45
1:A:151:LEU:HD12	1:A:151:LEU:HA	1.75	0.45
1:A:168:ARG:O	1:A:172:GLU:HG3	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:94:VAL:HA	1:B:93:VAL:O	2.17	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:440:THR:C	1:A:441:THR:HG23	2.38	0.44
1:A:373:PRO:HG2	1:A:376:ALA:HB3	2.00	0.44
1:A:130:LEU:HB3	1:A:131:PRO:HA	2.00	0.44
1:A:89:PRO:O	1:B:98:GLY:HA2	2.18	0.44
2:T:40:G:H2'	2:T:41:A:C8	2.53	0.43
1:B:61:THR:HG1	1:B:63:HIS:CE1	2.36	0.43
1:A:87:PHE:O	1:A:88:SER:C	2.56	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:B:243:LYS:HE2	1:B:253:TYR:HE2	1.84	0.43
1:A:432:CYS:O	1:A:435:LEU:HB3	2.18	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
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:B:161:GLY:HA3	1:B:259:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:364:SER:C	1:A:366:LEU:H	2.20	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:B:58:PHE:HE2	1:B:159:GLN:CG	2.31	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: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
2:T:18:G:HO2'	2:T:19:G:H5'	1.84	0.42
1:A:410:TYR:O	1:A:414:LYS:HG3	2.20	0.42
1:B:385:LEU:HD13	1:B:385:LEU:HA	1.75	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:A:165:HIS:CD2	1:A:171:ALA:HA	2.55	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:17(A):C:H4'	2:T:18:G:OP1	2.19	0.42
2:T:14:A:C2'	2:T:15:G:H5'	2.50	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
2:T:59:A:C2'	2:T:60:U:O5'	2.69	0.41
1:B:394:ARG:HH11	1:B:394:ARG:HG3	1.86	0.41
2:T:17:C:C4	2:T:17(A):C:C4	3.08	0.41
1:B:326:ASP:O	1:B:327:ARG:C	2.59	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:381:LEU:HD23	1:A:381:LEU:HA	1.84	0.40
1:A:132:GLN:HB2	1:A:164:ALA:HB3	2.03	0.40
1:B:410:TYR:CE1	1:B:460:ARG:HG3	2.56	0.40
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:A:214:ILE:HG13	1:A:214:ILE:O	2.22	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:B:304:VAL:HG21	1:B:352:PRO:HG3	2.02	0.40
1:A:322:VAL:HG22	1:A:323:HIS:N	2.36	0.40



There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/477 (97%)	419 (91%)	36 (8%)	6 (1%)	18	62
1	B	460/477 (96%)	415 (90%)	43 (9%)	2 (0%)	43	87
All	All	921/954 (96%)	834 (91%)	79 (9%)	8 (1%)	25	73

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%)	32	75
1	B	383/395 (97%)	363 (95%)	20 (5%)	32	75
All	All	766/790 (97%)	726 (95%)	40 (5%)	32	75

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
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	20,22,23	0.87	1 (5%)	25,32,35	1.10	4 (16%)
2	PSU	T	55	2	19,21,22	1.17	2 (10%)	23,30,33	1.10	3 (13%)

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	-	0/6/25/26	0/2/2/2
2	PSU	T	55	2	-	0/8/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	55	PSU	C2-N1	3.21	1.43	1.37
2	T	54	5MU	C6-C5	-2.19	1.34	1.40
2	T	55	PSU	P-OP1	2.09	1.49	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	54	5MU	C6-N1-C2	-2.45	121.71	122.41
2	T	55	PSU	C5-C1'-C2'	-2.21	111.72	115.61
2	T	55	PSU	C5-C4-N3	-2.20	114.85	118.86
2	T	54	5MU	N3-C2-N1	-2.13	114.19	115.97
2	T	54	5MU	C5M-C5-C6	2.08	123.01	118.59
2	T	54	5MU	C5-C6-N1	2.03	123.56	121.59
2	T	55	PSU	C6-C5-C4	2.02	121.05	116.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	33,33,33	0.65	0	52,52,52	0.92	1 (1%)
5	PRI	A	1480	-	7,7,7	1.22	1 (14%)	8,8,8	1.63	1 (12%)
6	SO4	A	1481	-	4,4,4	0.30	0	6,6,6	0.07	0
3	ATP	B	1478	-	33,33,33	0.61	0	52,52,52	0.87	1 (1%)
5	PRI	B	1480	-	7,7,7	1.38	1 (14%)	8,8,8	1.39	1 (12%)
6	SO4	B	1481	-	4,4,4	0.30	0	6,6,6	0.10	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	1478	-	-	0/22/38/38	0/1/3/3
5	PRI	A	1480	-	-	0/1/9/9	0/1/1/1
6	SO4	A	1481	-	-	0/0/0/0	0/0/0/0
3	ATP	B	1478	-	-	0/22/38/38	0/1/3/3
5	PRI	B	1480	-	-	0/1/9/9	0/1/1/1
6	SO4	B	1481	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1480	PRI	CA-C	3.31	1.53	1.50
5	A	1480	PRI	CA-C	2.76	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1480	PRI	OT1-C-CA	-3.50	116.31	125.47
5	B	1480	PRI	OT1-C-CA	-2.85	118.01	125.47
3	B	1478	ATP	O3G-PG-O2G	2.31	116.62	107.61
3	A	1478	ATP	O3G-PG-O2G	2.20	116.19	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	464/477 (97%)	-0.32	1 (0%) 93 54	21, 46, 81, 107	17 (3%)
1	B	463/477 (97%)	-0.26	0 100 100	25, 50, 85, 104	14 (3%)
2	T	67/77 (87%)	0.03	4 (5%) 21 5	27, 61, 93, 108	7 (10%)
All	All	994/1031 (96%)	-0.27	5 (0%) 88 36	21, 49, 85, 108	38 (3%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	4	G	4.2
2	T	5	G	3.0
2	T	20	U	2.1
2	T	66	C	2.1
1	A	146	ARG	2.0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	5MU	T	54	21/22	0.18	0.94	27,46,66,68	0
2	PSU	T	55	20/21	0.16	0.09	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	A	1478	31/31	0.34	2.35	54,62,95,97	31
3	ATP	B	1478	31/31	0.34	1.57	69,86,105,106	31
5	PRI	B	1480	7/7	0.27	0.96	58,59,60,60	7
5	PRI	A	1480	7/7	0.23	0.21	26,31,40,44	7
6	SO4	B	1481	5/5	0.11	-1.43	56,59,61,61	5
4	ZN	B	1479	1/1	0.07	-1.96	88,88,88,88	0
4	ZN	A	1479	1/1	0.09	-2.05	59,59,59,59	0
6	SO4	A	1481	5/5	0.12	-5.03	75,75,78,78	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.