



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:50 AM GMT

PDB ID : 1B23
Title : E. coli cysteinyl-tRNA and T. aquaticus elongation factor EF-TU:GTP ternary complex
Authors : Nissen, P.; Kjeldgaard, M.; Thirup, S.; Nyborg, J.
Deposited on : 1998-12-04
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

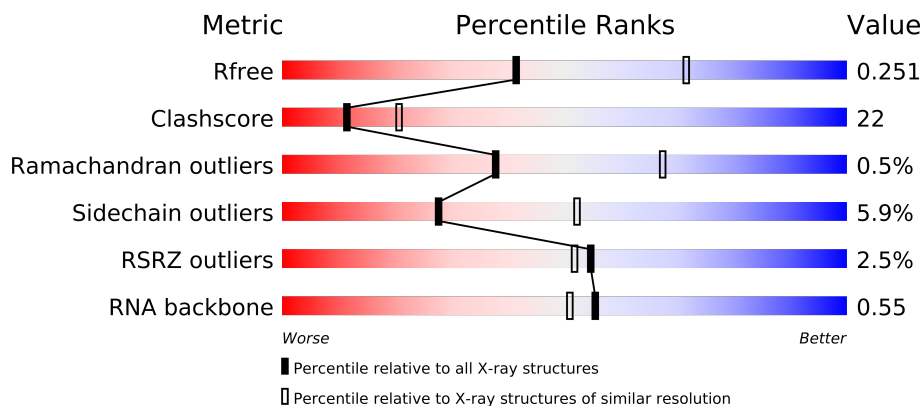
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)
RNA backbone	1838	1002 (3.12-2.08)

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. 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	R	74	
2	P	405	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	P	409	-	X
5	CYS	R	976	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5040 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 RNA chain called CYSTEINYL TRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	R	74	Total	C	N	O	P	S	5	0	0
			1584	710	280	518	74	2			

- Molecule 2 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	405	Total	C	N	O	S	0	0	0
			3144	1986	548	598	12			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

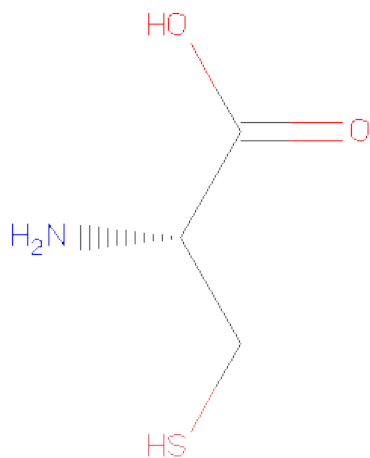
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Mg	0	0
			1	1		
3	R	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		

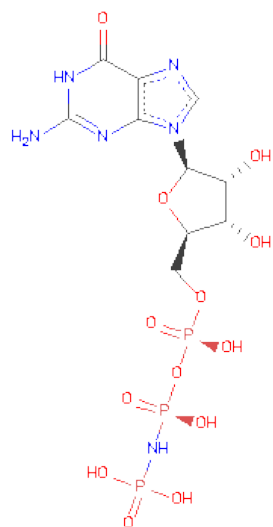
- Molecule 5 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	R	1	Total	C	N	O	S	0	0
			6	3	1	1	1		

- Molecule 6 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter

code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	P	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

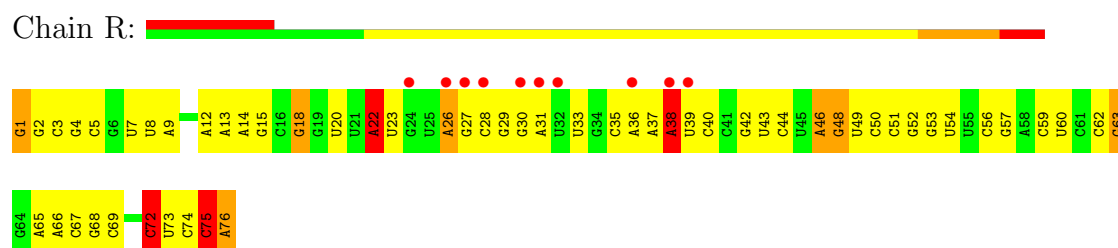
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	174	Total	O	0	0
			174	174		
7	R	87	Total	O	0	0
			87	87		

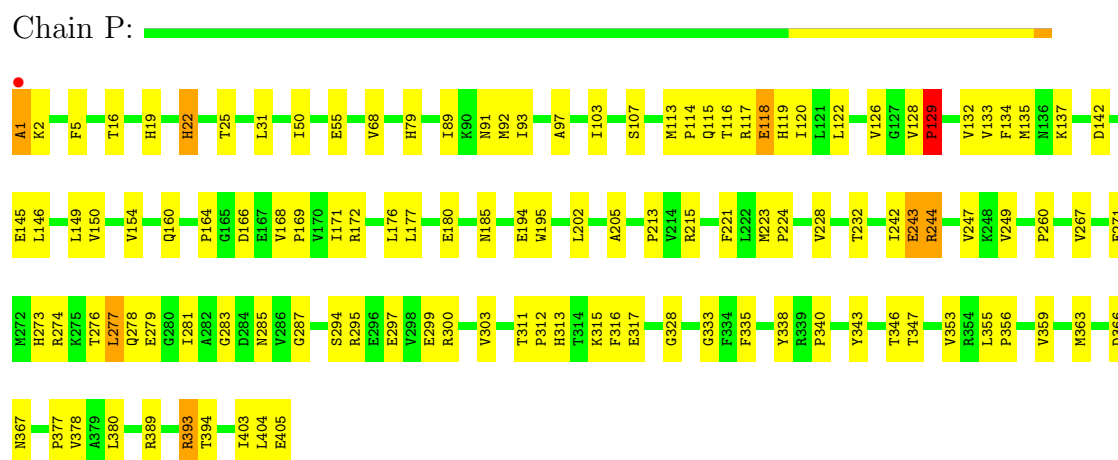
3 Residue-property plots

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: CYSTEINYL TRNA



• Molecule 2: ELONGATION FACTOR TU



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.75Å 132.98Å 154.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 38.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.0 (10.00-2.60) 89.2 (38.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.61Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.263 0.202 , 0.251	Depositor DCC
R_{free} test set	1424 reflections (8.54%)	DCC
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.976	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.5	EDS
Estimated twinning fraction	0.031 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18103 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5040	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, GNP, MIA, MG, H2U, SO4, 4SU, 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	R	1.03	6/1580 (0.4%)	1.36	14/2458 (0.6%)
2	P	0.35	1/3204 (0.0%)	0.65	1/4345 (0.0%)
All	All	0.66	7/4784 (0.1%)	0.97	15/6803 (0.2%)

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	R	0	1
2	P	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	75	C	C1'-N1	23.98	1.84	1.48
1	R	7	U	C1'-N1	-17.00	1.23	1.46
1	R	75	C	O5'-C5'	16.03	1.70	1.44
1	R	72	C	C1'-N1	13.31	1.68	1.48
1	R	22	A	N9-C4	-10.79	1.31	1.37
2	P	1	ALA	C-N	-7.50	1.16	1.34
1	R	1	G	OP3-P	-7.10	1.52	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	75	C	O4'-C1'-N1	24.97	128.18	108.20
1	R	75	C	O5'-C5'-C4'	-24.31	65.50	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	75	C	P-O5'-C5'	-19.72	89.35	120.90
1	R	75	C	C4'-C3'-O3'	19.06	151.13	113.00
1	R	7	U	C2-N1-C1'	18.61	140.03	117.70
1	R	7	U	N1-C1'-C2'	18.02	137.42	114.00
1	R	7	U	C6-N1-C1'	-16.32	98.35	121.20
2	P	1	ALA	C-N-CA	15.56	160.61	121.70
1	R	75	C	C2'-C3'-O3'	-10.27	86.90	109.50
1	R	75	C	P-O3'-C3'	9.77	131.42	119.70
1	R	22	A	C8-N9-C4	6.83	108.53	105.80
1	R	72	C	N1-C1'-C2'	-6.61	104.72	112.00
1	R	75	C	C2-N1-C1'	6.44	125.88	118.80
1	R	75	C	C6-N1-C1'	-5.96	113.65	120.80
1	R	38	A	N9-C1'-C2'	-5.37	106.10	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	1	ALA	Peptide
1	R	72	C	Sidechain

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	R	1584	0	814	118	0
2	P	3144	0	3159	83	0
3	P	1	0	0	0	0
3	R	2	0	0	0	0
4	P	10	0	0	0	0
5	R	6	0	4	3	0
6	P	32	0	13	3	0
7	P	174	0	0	6	0
7	R	87	0	0	6	0
All	All	5040	0	3990	193	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 22.

All (193) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:72:C:N4	1:R:73:U:C4	1.77	1.52
1:R:72:C:N1	1:R:72:C:C1'	1.68	1.50
1:R:72:C:C4	1:R:73:U:C5	2.06	1.44
1:R:75:C:O5'	1:R:75:C:C5'	1.70	1.38
1:R:75:C:C1'	1:R:75:C:N1	1.84	1.35
1:R:75:C:O5'	1:R:75:C:C4'	1.74	1.33
1:R:72:C:N4	1:R:73:U:O4	1.57	1.32
1:R:62:C:C2'	1:R:63:G:H5''	1.60	1.30
1:R:75:C:N4	2:P:232:THR:OG1	1.70	1.24
1:R:75:C:H4'	1:R:75:C:OP1	1.36	1.23
1:R:75:C:P	1:R:75:C:C5'	2.31	1.18
1:R:75:C:P	1:R:75:C:H4'	1.83	1.18
1:R:72:C:C4	1:R:73:U:C4	2.27	1.16
1:R:75:C:P	1:R:75:C:C4'	2.40	1.07
1:R:72:C:C5	1:R:73:U:C5	2.45	1.04
1:R:62:C:H2'	1:R:63:G:C5'	1.86	1.04
1:R:62:C:H2'	1:R:63:G:H5''	1.05	1.03
1:R:38:A:H5''	7:R:1012:HOH:O	1.61	0.98
1:R:75:C:C4'	1:R:75:C:OP1	2.12	0.97
1:R:50:C:H2'	1:R:51:C:H6	1.31	0.94
1:R:75:C:H42	2:P:232:THR:CB	1.85	0.90
1:R:72:C:C5	1:R:73:U:H5	1.90	0.88
1:R:31:A:H5''	7:R:980:HOH:O	1.75	0.87
1:R:75:C:N4	2:P:232:THR:HG1	1.73	0.86
1:R:75:C:O5'	1:R:75:C:O4'	1.94	0.85
2:P:113:MET:HB3	2:P:114:PRO:HD2	1.58	0.84
1:R:14:A:H2'	1:R:15:G:C8	2.12	0.82
1:R:72:C:C1'	1:R:72:C:C6	2.62	0.82
1:R:37:MIA:H5'	7:R:987:HOH:O	1.79	0.81
1:R:73:U:O2'	1:R:74:C:H5'	1.80	0.80
2:P:312:PRO:HB2	2:P:377:PRO:HB2	1.65	0.79
1:R:73:U:C2'	1:R:74:C:H5'	2.13	0.79
1:R:50:C:H2'	1:R:51:C:C6	2.17	0.77
1:R:75:C:C1'	1:R:75:C:C6	2.70	0.75
1:R:68:G:O2'	1:R:69:C:H5'	1.87	0.74
1:R:42:G:O2'	1:R:43:U:H5'	1.88	0.73
1:R:72:C:C2	1:R:72:C:C1'	2.69	0.73
2:P:171:ILE:HD11	2:P:205:ALA:HB2	1.72	0.72
1:R:63:G:H8	1:R:63:G:H5'	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:72:C:N1	1:R:72:C:C2'	2.55	0.70
2:P:122:LEU:O	2:P:126:VAL:HG23	1.92	0.70
2:P:260:PRO:HD2	7:P:515:HOH:O	1.92	0.70
1:R:72:C:N3	1:R:73:U:C5	2.58	0.69
1:R:8:4SU:H5''	1:R:49:U:OP2	1.93	0.69
1:R:75:C:H5'	1:R:75:C:P	2.31	0.69
1:R:22:A:H8	1:R:22:A:H5'	1.57	0.69
1:R:2:G:H2'	1:R:3:C:C6	2.28	0.69
1:R:22:A:H2'	1:R:23:U:H5'	1.74	0.68
1:R:1:G:H4'	2:P:91:ASN:HD21	1.59	0.68
1:R:43:U:H2'	1:R:44:C:C6	2.29	0.67
1:R:75:C:H42	2:P:232:THR:HG1	1.28	0.67
5:R:976:CYS:SG	5:R:976:CYS:O	2.52	0.67
1:R:62:C:O2'	1:R:63:G:H5''	1.94	0.67
1:R:20:H2U:N3	7:R:1049:HOH:O	2.29	0.65
2:P:145:GLU:O	2:P:149:LEU:HD13	1.98	0.64
1:R:1:G:H4'	2:P:91:ASN:ND2	2.12	0.63
1:R:62:C:C3'	1:R:63:G:H5''	2.29	0.63
2:P:89:ILE:O	2:P:93:ILE:HG12	1.99	0.63
1:R:26:A:H2'	1:R:27:G:C8	2.34	0.62
2:P:313:HIS:CD2	2:P:403:ILE:HG21	2.35	0.62
1:R:26:A:H2'	1:R:27:G:H8	1.65	0.61
2:P:19:HIS:HD2	2:P:115:GLN:H	1.48	0.61
1:R:22:A:C2'	1:R:23:U:H5'	2.31	0.61
1:R:54:5MU:OP2	1:R:54:5MU:H71	2.01	0.61
2:P:228:VAL:HG21	2:P:299:GLU:HA	1.83	0.61
1:R:8:4SU:O2'	1:R:46:A:H1'	2.01	0.60
2:P:405:GLU:HB2	7:P:569:HOH:O	2.01	0.60
1:R:29:G:O2'	1:R:30:G:H5'	2.01	0.60
2:P:5:PHE:HB3	2:P:277:LEU:HD23	1.85	0.59
2:P:25:THR:HG23	2:P:50:ILE:HG21	1.83	0.59
2:P:117:ARG:HH12	2:P:160:GLN:NE2	2.00	0.59
5:R:976:CYS:N	2:P:273:HIS:H	2.01	0.59
1:R:48:G:OP2	1:R:48:G:H8	1.85	0.59
1:R:33:U:O2	1:R:36:A:H8	1.86	0.58
1:R:75:C:OP1	1:R:75:C:C5'	2.48	0.58
1:R:59:C:H6	1:R:59:C:O5'	1.87	0.57
2:P:378:VAL:HG13	2:P:380:LEU:HD13	1.86	0.57
2:P:137:LYS:HE2	6:P:406:GNP:C4	2.33	0.57
1:R:2:G:H2'	1:R:3:C:H6	1.68	0.57
2:P:68:VAL:HG23	2:P:79:HIS:HB3	1.87	0.57
2:P:224:PRO:HA	2:P:303:VAL:HG22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:63:G:C8	1:R:63:G:H5'	2.39	0.56
1:R:65:A:H1'	7:R:1038:HOH:O	2.05	0.56
1:R:73:U:C5	1:R:74:C:C5	2.94	0.56
1:R:14:A:N6	1:R:46:A:C2	2.74	0.56
1:R:33:U:O2	1:R:36:A:C8	2.58	0.56
2:P:221:PHE:CZ	2:P:223:MET:HB2	2.40	0.56
2:P:356:PRO:HD2	2:P:359:VAL:CG2	2.36	0.56
1:R:73:U:H2'	1:R:74:C:H5'	1.89	0.55
1:R:73:U:H2'	1:R:74:C:O4'	2.06	0.55
1:R:22:A:H2'	1:R:23:U:C5'	2.36	0.55
2:P:137:LYS:HG2	6:P:406:GNP:C6	2.36	0.54
1:R:39:PSU:H2'	1:R:40:C:C6	2.42	0.54
2:P:171:ILE:CD1	2:P:202:LEU:HA	2.37	0.54
1:R:65:A:O2'	1:R:66:A:H5'	2.08	0.54
1:R:73:U:C4	1:R:74:C:C5	2.97	0.53
2:P:97:ALA:HA	2:P:126:VAL:HG12	1.90	0.53
2:P:389:ARG:HG2	2:P:394:THR:HA	1.90	0.53
1:R:59:C:C2'	1:R:60:U:H5'	2.38	0.53
2:P:378:VAL:HG23	7:P:504:HOH:O	2.09	0.53
2:P:279:GLU:HG3	2:P:279:GLU:O	2.08	0.53
1:R:72:C:C4	1:R:73:U:C6	2.87	0.52
2:P:343:TYR:HE1	2:P:389:ARG:HB2	1.73	0.52
1:R:59:C:H2'	1:R:60:U:H5'	1.90	0.52
1:R:72:C:N3	1:R:73:U:C6	2.78	0.51
2:P:113:MET:HB3	2:P:114:PRO:CD	2.35	0.51
2:P:31:LEU:HD21	2:P:202:LEU:HD23	1.92	0.51
1:R:18:G:H1'	1:R:57:G:N2	2.26	0.51
1:R:28:C:O2'	1:R:29:G:H5'	2.10	0.51
2:P:378:VAL:HG13	2:P:380:LEU:CD1	2.41	0.51
2:P:22:HIS:CD2	2:P:107:SER:H	2.28	0.51
2:P:356:PRO:HD2	2:P:359:VAL:HG22	1.93	0.51
2:P:243:GLU:HB3	2:P:244:ARG:HD3	1.92	0.50
1:R:43:U:C4	1:R:44:C:N4	2.79	0.50
1:R:73:U:C2	1:R:74:C:C6	3.00	0.50
1:R:50:C:C2	1:R:51:C:C5	2.99	0.50
2:P:294:SER:OG	2:P:297:GLU:HG3	2.11	0.50
1:R:72:C:C2'	1:R:73:U:H5'	2.41	0.50
2:P:277:LEU:HG	7:P:472:HOH:O	2.11	0.50
1:R:36:A:C2	1:R:37:MIA:H1'	2.47	0.50
1:R:56:C:C4	1:R:57:G:N7	2.80	0.49
1:R:51:C:O2	1:R:52:G:C8	2.65	0.49
1:R:39:PSU:H2'	1:R:40:C:H6	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:62:C:C2'	1:R:63:G:C5'	2.55	0.49
2:P:117:ARG:HH12	2:P:160:GLN:HE22	1.60	0.49
1:R:4:G:O2'	1:R:5:C:H5'	2.14	0.48
2:P:277:LEU:HD13	2:P:278:GLN:N	2.28	0.48
2:P:353:VAL:HG12	2:P:355:LEU:HD12	1.95	0.48
1:R:73:U:H2'	1:R:74:C:C5'	2.43	0.48
1:R:33:U:H2'	1:R:35:C:H5	1.79	0.48
5:R:976:CYS:HB3	2:P:285:ASN:OD1	2.14	0.48
1:R:22:A:C8	1:R:22:A:H5'	2.45	0.47
1:R:66:A:H2'	1:R:67:C:C6	2.48	0.47
1:R:54:5MU:O5'	1:R:54:5MU:H6	1.98	0.47
2:P:164:PRO:O	2:P:168:VAL:HG23	2.14	0.47
2:P:5:PHE:HB3	2:P:277:LEU:CD2	2.45	0.47
2:P:103:ILE:HA	2:P:132:VAL:O	2.15	0.47
2:P:278:GLN:HB3	7:P:490:HOH:O	2.15	0.47
2:P:300:ARG:HD3	2:P:346:THR:O	2.16	0.46
2:P:176:LEU:HB2	6:P:406:GNP:C5	2.45	0.46
1:R:67:C:O2'	1:R:68:G:H5'	2.15	0.46
2:P:135:MET:HB2	2:P:172:ARG:HA	1.96	0.46
2:P:128:VAL:HA	2:P:129:PRO:HD3	1.71	0.46
2:P:166:ASP:HB2	7:P:421:HOH:O	2.15	0.46
1:R:67:C:H2'	1:R:68:G:H8	1.80	0.46
1:R:4:G:H2'	1:R:5:C:C6	2.50	0.46
2:P:213:PRO:HD2	2:P:215:ARG:NH2	2.31	0.46
1:R:1:G:C4'	2:P:91:ASN:HD21	2.27	0.45
2:P:249:VAL:HA	2:P:267:VAL:HG23	1.98	0.45
1:R:12:A:O2'	1:R:13:A:H5'	2.16	0.45
2:P:116:THR:O	2:P:120:ILE:HG13	2.17	0.45
1:R:1:G:H5''	2:P:300:ARG:NH2	2.32	0.45
1:R:72:C:C2	1:R:73:U:C6	3.05	0.44
1:R:46:A:H8	1:R:46:A:H5'	1.82	0.44
2:P:176:LEU:O	2:P:180:GLU:HG3	2.18	0.44
1:R:4:G:H1'	7:R:1034:HOH:O	2.18	0.44
1:R:8:4SU:H6	1:R:8:4SU:H3'	1.98	0.44
1:R:27:G:C6	1:R:28:C:C4	3.06	0.43
2:P:328:GLY:O	2:P:393:ARG:HB2	2.17	0.43
1:R:51:C:C2	1:R:52:G:C8	3.05	0.43
2:P:150:VAL:O	2:P:154:VAL:HG23	2.17	0.43
1:R:35:C:C4	1:R:36:A:C8	3.07	0.43
1:R:22:A:H2'	1:R:23:U:O4'	2.17	0.43
2:P:271:GLU:HG2	2:P:276:THR:HA	2.01	0.43
2:P:404:LEU:O	2:P:405:GLU:HB3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:215:ARG:NH1	2:P:283:GLY:HA3	2.34	0.43
1:R:72:C:N3	1:R:73:U:C4	2.83	0.43
1:R:53:G:O2'	1:R:54:5MU:H5''	2.18	0.43
2:P:315:LYS:O	2:P:316:PHE:HB3	2.19	0.43
1:R:73:U:C2'	1:R:74:C:C5'	2.90	0.43
1:R:9:A:N6	1:R:46:A:C2	2.86	0.43
1:R:49:U:H2'	1:R:50:C:C6	2.53	0.43
2:P:117:ARG:HG3	2:P:118:GLU:N	2.34	0.42
2:P:177:LEU:HD23	2:P:195:TRP:CE2	2.54	0.42
2:P:168:VAL:HA	2:P:169:PRO:HD3	1.85	0.42
2:P:247:VAL:HG13	2:P:247:VAL:O	2.18	0.42
1:R:39:PSU:C4	1:R:40:C:C5	3.08	0.42
1:R:73:U:H2'	1:R:74:C:H6	1.85	0.42
1:R:76:A:C2	2:P:287:GLY:O	2.73	0.42
2:P:115:GLN:HA	2:P:118:GLU:HB2	2.02	0.42
2:P:133:VAL:HG12	2:P:134:PHE:N	2.34	0.42
1:R:14:A:N6	1:R:46:A:H2	2.19	0.41
2:P:343:TYR:HA	2:P:347:THR:O	2.20	0.41
2:P:171:ILE:HD13	2:P:202:LEU:HA	2.02	0.41
1:R:75:C:C1'	1:R:75:C:C2	2.89	0.41
1:R:75:C:O2'	1:R:76:A:P	2.78	0.41
2:P:194:GLU:HG3	2:P:195:TRP:N	2.35	0.41
2:P:333:GLY:HA3	2:P:363:MET:SD	2.61	0.41
2:P:311:THR:HA	2:P:312:PRO:HD2	1.90	0.41
2:P:93:ILE:CD1	2:P:122:LEU:HD13	2.51	0.40
2:P:363:MET:O	2:P:366:ASP:HB2	2.22	0.40
2:P:338:TYR:CE2	2:P:340:PRO:HG3	2.56	0.40
2:P:242:ILE:HD12	2:P:281:ILE:O	2.21	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
2	P	403/405 (100%)	370 (92%)	31 (8%)	2 (0%)	38 67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	2	LYS
2	P	129	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	
2	P	338/338 (100%)	319 (94%)	19 (6%)	30	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	16	THR
2	P	22	HIS
2	P	55	GLU
2	P	92	MET
2	P	118	GLU
2	P	119	HIS
2	P	129	PRO
2	P	142	ASP
2	P	146	LEU
2	P	185	ASN
2	P	243	GLU
2	P	244	ARG
2	P	274	ARG
2	P	277	LEU
2	P	295	ARG
2	P	317	GLU
2	P	335	PHE
2	P	367	ASN
2	P	393	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	19	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	22	HIS
2	P	41	ASN
2	P	91	ASN
2	P	98	GLN
2	P	115	GLN
2	P	160	GLN
2	P	185	ASN
2	P	341	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	72/74 (97%)	9 (12%)	1 (1%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	18	G
1	R	22	A
1	R	26	A
1	R	38	A
1	R	46	A
1	R	48	G
1	R	63	G
1	R	75	C
1	R	76	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	75	C

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

8 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	R	20	1	19,21,22	0.56	0	27,30,33	0.71	1 (3%)
1	H2U	R	21	1	19,21,22	0.69	0	27,30,33	0.65	0
1	PSU	R	32	1	19,21,22	1.64	3 (15%)	23,30,33	1.13	2 (8%)
1	MIA	R	37	1	29,31,32	1.40	4 (13%)	41,44,47	2.08	9 (21%)
1	PSU	R	39	1	19,21,22	1.60	2 (10%)	23,30,33	1.06	2 (8%)
1	5MU	R	54	1	20,22,23	0.94	2 (10%)	25,32,35	1.22	2 (8%)
1	PSU	R	55	1	19,21,22	1.69	2 (10%)	23,30,33	1.00	2 (8%)
1	4SU	R	8	1	19,21,22	1.04	1 (5%)	23,30,33	26.82	1 (4%)

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	R	20	1	-	0/8/38/39	0/2/2/2
1	H2U	R	21	1	-	0/8/38/39	0/2/2/2
1	PSU	R	32	1	-	0/8/25/26	0/2/2/2
1	MIA	R	37	1	-	0/16/33/34	0/1/3/3
1	PSU	R	39	1	-	0/8/25/26	0/2/2/2
1	5MU	R	54	1	-	0/6/25/26	0/2/2/2
1	PSU	R	55	1	-	0/8/25/26	0/2/2/2
1	4SU	R	8	1	-	0/6/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	55	PSU	C6-N1	6.45	1.38	1.32
1	R	32	PSU	C6-N1	6.07	1.37	1.32
1	R	39	PSU	C6-N1	6.03	1.37	1.32
1	R	37	MIA	C12-N6	4.27	1.56	1.46
1	R	37	MIA	C6-N1	3.58	1.38	1.33
1	R	8	4SU	C5-C4	3.25	1.43	1.38
1	R	37	MIA	C6-C5	-2.44	1.39	1.44
1	R	54	5MU	P-OP1	2.39	1.49	1.46
1	R	32	PSU	C6-C5	-2.37	1.34	1.38
1	R	37	MIA	P-OP1	2.29	1.49	1.46
1	R	54	5MU	C6-C5	-2.28	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	39	PSU	C6-C5	-2.27	1.34	1.38
1	R	55	PSU	C6-C5	-2.19	1.34	1.38
1	R	32	PSU	P-OP1	2.15	1.49	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	8	4SU	C4-N3-C2	128.58	127.10	121.60
1	R	37	MIA	C12-N6-C6	-9.92	110.28	123.25
1	R	54	5MU	C6-N1-C2	-3.96	121.28	122.41
1	R	37	MIA	C5-C6-N6	3.12	125.95	120.34
1	R	37	MIA	C2-N3-C4	-3.10	110.75	115.24
1	R	37	MIA	C5-C6-N1	-3.04	117.12	120.45
1	R	39	PSU	C5-C1'-C2'	-2.88	110.53	115.61
1	R	37	MIA	C13-C12-N6	2.60	120.94	111.65
1	R	32	PSU	O4'-C1'-C5	2.51	112.67	109.55
1	R	37	MIA	C2'-C1'-N9	-2.43	107.02	113.27
1	R	32	PSU	C5-C4-N3	-2.41	114.48	118.86
1	R	39	PSU	C5-C4-N3	-2.34	114.59	118.86
1	R	55	PSU	C5-C4-N3	-2.31	114.65	118.86
1	R	54	5MU	C5-C6-N1	2.30	123.83	121.59
1	R	55	PSU	C5-C1'-C2'	-2.26	111.61	115.61
1	R	37	MIA	C11-S10-C2	2.23	103.87	102.26
1	R	37	MIA	C15-C14-C13	2.23	128.13	111.39
1	R	37	MIA	C2-N1-C6	2.22	119.16	115.55
1	R	20	H2U	N3-C2-N1	-2.17	114.58	116.71

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
6	GNP	P	406	3	34,34,34	21.32	5 (14%)	50,54,54	5.15	9 (18%)
4	SO4	P	408	-	4,4,4	1.30	0	6,6,6	0.10	0
4	SO4	P	409	-	4,4,4	1.37	0	6,6,6	0.10	0
5	CYS	R	976	1	5,5,6	7.43	2 (40%)	3,5,7	3.28	1 (33%)

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
6	GNP	P	406	3	-	0/18/38/38	0/1/3/3
4	SO4	P	408	-	-	0/0/0/0	0/0/0/0
4	SO4	P	409	-	-	0/0/0/0	0/0/0/0
5	CYS	R	976	1	-	0/2/4/6	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	406	GNP	PB-O3A	123.93	3.34	1.59
5	R	976	CYS	O-C	16.41	1.22	1.11
6	P	406	GNP	PA-O3A	-5.86	1.49	1.59
6	P	406	GNP	PG-O1G	5.20	1.52	1.46
6	P	406	GNP	PB-O1B	2.43	1.49	1.46
5	R	976	CYS	CA-C	2.31	1.52	1.48
6	P	406	GNP	PB-O2B	-2.20	1.48	1.55

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	406	GNP	C6-C5-N7	-25.34	130.73	134.14
6	P	406	GNP	PA-O3A-PB	-22.36	55.42	131.81
6	P	406	GNP	O3A-PB-N3B	7.87	128.41	106.59
6	P	406	GNP	O2B-PB-O3A	-6.83	72.74	105.14
5	R	976	CYS	C-CA-N	-5.68	108.16	113.83
6	P	406	GNP	O2B-PB-O1B	4.03	119.19	109.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	406	GNP	O1G-PG-N3B	-3.53	106.49	111.83
6	P	406	GNP	C6-N1-C2	3.28	125.25	119.51
6	P	406	GNP	O1B-PB-N3B	-2.48	108.09	111.83
6	P	406	GNP	C2-N3-C4	-2.17	112.05	115.09

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, 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	R	73/74 (98%)	0.53	10 (13%) 4 2	44, 72, 99, 100	0
2	P	405/405 (100%)	-0.17	1 (0%) 93 94	26, 45, 74, 97	0
All	All	478/479 (99%)	-0.07	11 (2%) 54 54	26, 48, 85, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	1	ALA	13.8
1	R	36	A	3.8
1	R	26	A	3.3
1	R	31	A	3.0
1	R	38	A	2.8
1	R	32	PSU	2.7
1	R	39	PSU	2.4
1	R	24	G	2.4
1	R	28	C	2.4
1	R	30	G	2.2
1	R	27	G	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	H2U	R	20	20/21	0.25	10.62	61,73,74,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	5MU	R	54	21/22	0.16	1.41	45,49,50,52	0
1	PSU	R	39	20/21	0.30	0.85	98,100,100,100	0
1	H2U	R	21	20/21	0.21	0.73	80,85,87,88	0
1	MIA	R	37	29/30	0.30	0.69	96,98,100,100	5
1	PSU	R	32	20/21	0.31	0.47	95,98,100,100	0
1	PSU	R	55	20/21	0.13	-0.23	56,63,67,67	0
1	4SU	R	8	20/21	0.15	-0.48	67,72,83,85	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	P	409	5/5	0.30	6.53	23,23,23,28	5
5	CYS	R	976	6/7	0.28	2.30	64,65,67,68	0
4	SO4	P	408	5/5	0.17	0.20	31,31,32,33	5
3	MG	R	77	1/1	0.20	0.08	55,55,55,55	0
3	MG	R	179	1/1	0.17	-0.28	54,54,54,54	1
6	GNP	P	406	32/32	0.11	-1.06	30,38,44,45	0
3	MG	P	407	1/1	0.08	-2.16	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.