



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:59 PM UTC

PDB ID : 4KR7 / pdb_00004kr7
Title : Crystal structure of a 4-thiouridine synthetase - RNA complex with bound ATP
Authors : Neumann, P.; Ficner, R.; Lakomek, K.
Deposited on : 2013-05-16
Resolution : 3.42 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

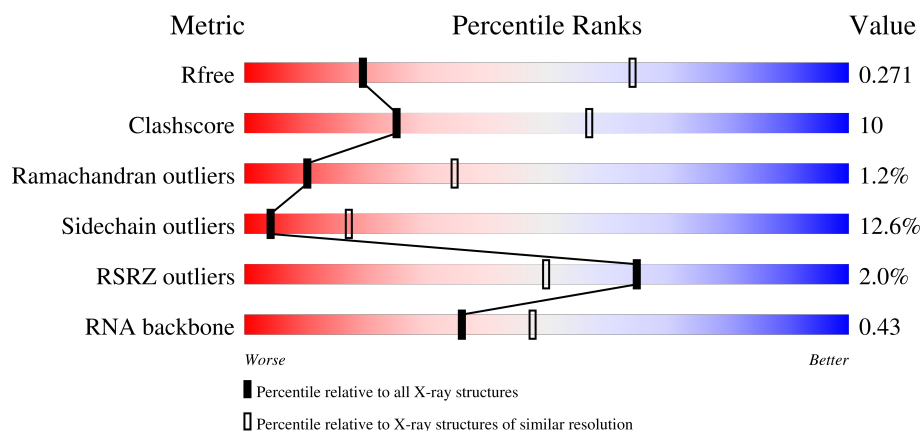
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	388	68% 28% • •
1	B	388	67% 28% • •
2	M	39	10% 38% 33% 26% •
2	X	39	8% 44% 33% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7924 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 Probable tRNA sulfurtransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3099	1996	530	568	5			
1	B	386	Total	C	N	O	S	0	0	0
			3099	1996	530	568	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	LYS	engineered mutation	UNP Q9X220
B	2	GLU	LYS	engineered mutation	UNP Q9X220

- Molecule 2 is a RNA chain called RNA (39-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	39	Total	C	N	O	P	0	0	0
			831	372	153	268	38			
2	X	39	Total	C	N	O	P	0	0	0
			831	372	153	268	38			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

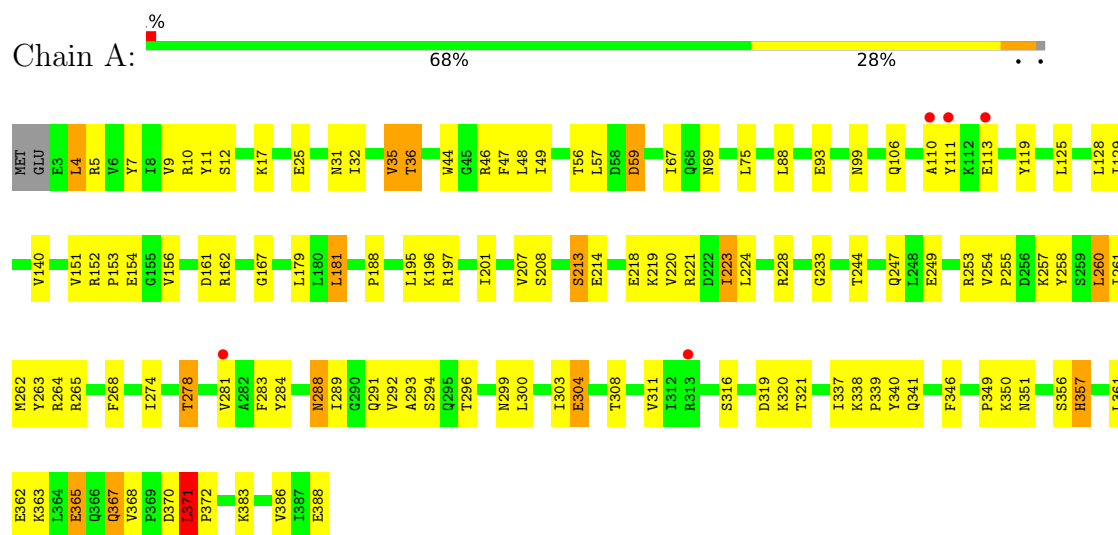
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

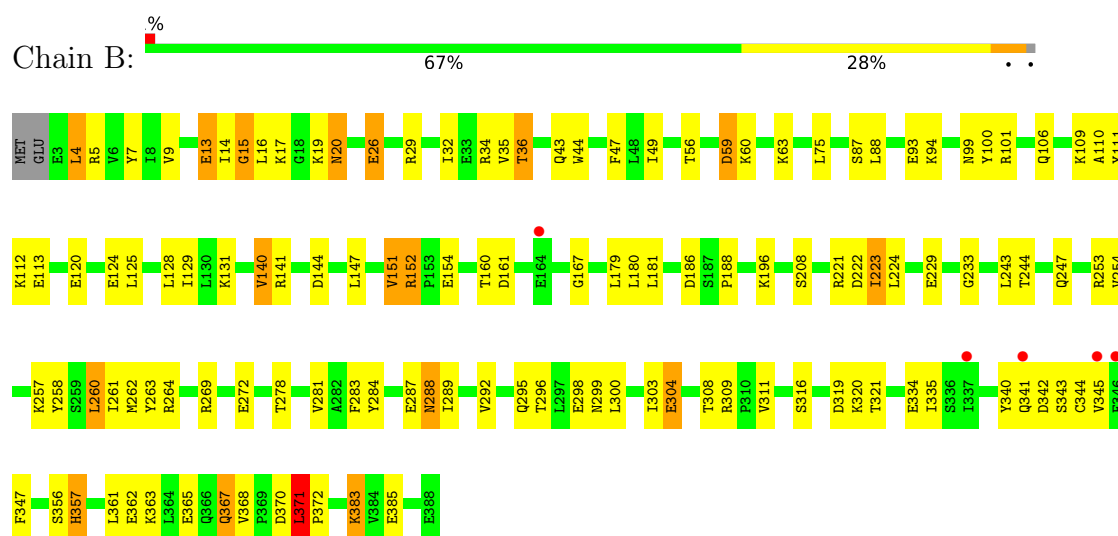
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Probable tRNA sulfurtransferase

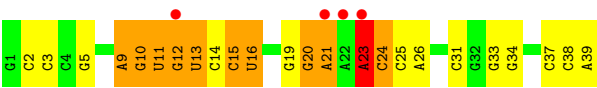


• Molecule 1: Probable tRNA sulfurtransferase

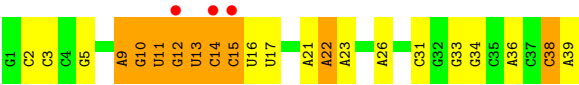


• Molecule 2: RNA (39-MER)





● Molecule 2: RNA (39-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.17Å 113.22Å 133.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.39 – 3.42 29.39 – 3.42	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.39-3.42) 97.8 (29.39-3.42)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.230 , 0.274 0.231 , 0.271	Depositor DCC
R_{free} test set	1065 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 113.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7924	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0.42	0/3158	0.81	5/4254 (0.1%)
1	B	0.42	0/3158	0.82	5/4254 (0.1%)
2	M	0.21	0/929	0.52	1/1447 (0.1%)
2	X	0.20	0/929	0.53	0/1447
All	All	0.39	0/8174	0.75	11/11402 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	23	A	O4'-C1'-N9	8.58	121.37	108.50
1	B	347	PHE	N-CA-C	-6.47	105.39	113.28
1	B	295	GLN	N-CA-C	6.30	117.84	110.41
1	A	340	TYR	N-CA-C	-6.13	104.17	112.26
1	A	371	LEU	CA-C-N	-5.97	112.86	119.19
1	A	371	LEU	C-N-CA	-5.97	112.86	119.19
1	A	289	ILE	N-CA-C	5.86	114.79	106.53
1	B	371	LEU	CA-C-N	-5.62	112.72	118.85
1	B	371	LEU	C-N-CA	-5.62	112.72	118.85
1	B	140	VAL	N-CA-C	-5.22	108.42	113.53
1	A	11	TYR	N-CA-C	5.16	117.44	110.06

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3099	0	3202	62	1
1	B	3099	0	3202	60	0
2	M	831	0	425	16	0
2	X	831	0	425	17	1
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	7924	0	7278	147	1

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 10.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:10:G:H3'	2:X:11:U:H5''	1.62	0.82
1:A:181:LEU:HD11	1:A:220:VAL:HG13	1.63	0.78
1:A:371:LEU:HD23	1:A:372:PRO:HD3	1.68	0.76
1:A:283:PHE:HB2	1:A:311:VAL:HG12	1.65	0.75
1:B:188:PRO:HG3	1:B:223:ILE:HD12	1.67	0.75
2:M:13:U:O2'	2:M:15:C:N3	2.20	0.74
1:B:371:LEU:HD23	1:B:372:PRO:HD3	1.68	0.74
2:X:12:G:H3'	2:X:13:U:C5'	2.17	0.73
1:B:283:PHE:HB2	1:B:311:VAL:HG12	1.72	0.72
1:B:243:LEU:HB3	1:B:247:GLN:HE21	1.54	0.72
1:A:288:ASN:ND2	1:A:291:GLN:OE1	2.22	0.72
1:A:188:PRO:HG3	1:A:223:ILE:HD12	1.72	0.71
1:A:10:ARG:HD2	1:A:69:ASN:HD21	1.53	0.71
1:A:350:LYS:HD3	2:X:12:G:H8	1.57	0.70
1:A:196:LYS:NZ	1:B:319:ASP:OD1	2.24	0.70
1:A:181:LEU:HD13	1:A:223:ILE:HD11	1.75	0.69
2:X:10:G:H3'	2:X:11:U:C5'	2.22	0.69
1:A:319:ASP:OD1	1:B:196:LYS:NZ	2.26	0.68
2:M:3:C:H42	2:M:33:G:H1	1.37	0.68
2:X:9:A:O4'	2:X:10:G:N2	2.26	0.68
2:X:12:G:H1	2:X:15:C:H41	1.40	0.67
2:X:3:C:H42	2:X:33:G:H1	1.43	0.67
2:M:23:A:O2'	2:M:24:C:O5'	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:SER:H	1:B:345:VAL:HG23	1.62	0.65
1:B:288:ASN:HD21	1:B:320:LYS:NZ	1.95	0.64
1:B:180:LEU:O	3:B:401:ATP:O2'	2.08	0.64
1:A:32:ILE:O	1:A:36:THR:OG1	2.16	0.63
1:B:88:LEU:HD21	1:B:128:LEU:HG	1.79	0.63
1:B:288:ASN:HD21	1:B:320:LYS:HZ3	1.47	0.63
1:A:288:ASN:N	1:A:288:ASN:OD1	2.32	0.63
1:A:195:LEU:HD21	1:A:201:ILE:HG12	1.81	0.62
1:B:288:ASN:N	1:B:288:ASN:OD1	2.33	0.61
1:A:257:LYS:HG3	1:A:258:TYR:HD1	1.66	0.61
1:B:9:VAL:HB	1:B:47:PHE:HB2	1.83	0.61
1:A:356:SER:OG	1:A:357:HIS:N	2.33	0.60
1:B:32:ILE:O	1:B:36:THR:OG1	2.18	0.60
1:B:94:LYS:NZ	1:B:161:ASP:OD1	2.27	0.60
1:B:186:ASP:OD1	1:B:320:LYS:NZ	2.35	0.59
1:A:265:ARG:NH2	1:A:365:GLU:OE2	2.36	0.59
2:M:12:G:HO2'	2:M:13:U:P	2.27	0.58
1:A:338:LYS:N	1:A:339:PRO:HD2	2.19	0.57
1:A:350:LYS:HD3	2:X:12:G:C8	2.37	0.57
1:A:88:LEU:HD21	1:A:128:LEU:HG	1.86	0.57
1:B:59:ASP:OD2	1:B:59:ASP:N	2.36	0.56
1:A:257:LYS:HE2	1:A:258:TYR:HE1	1.70	0.56
2:X:13:U:H2'	2:X:13:U:O2	2.05	0.56
1:A:257:LYS:HG3	1:A:258:TYR:CD1	2.42	0.55
1:B:14:ILE:HG23	1:B:15:GLY:H	1.72	0.54
1:A:218:GLU:OE2	1:A:221:ARG:NH1	2.41	0.54
1:B:264:ARG:NH2	1:B:287:GLU:OE1	2.40	0.54
1:B:63:LYS:HD2	1:B:229:GLU:HB3	1.89	0.54
1:B:88:LEU:HD23	1:B:129:ILE:HD13	1.90	0.53
1:A:264:ARG:NH2	3:A:401:ATP:O2A	2.38	0.53
2:X:14:C:H4'	2:X:15:C:C2	2.44	0.52
2:X:10:G:C8	2:X:11:U:H5''	2.44	0.52
1:A:293:ALA:HB2	1:B:19:LYS:HD2	1.92	0.52
1:A:59:ASP:OD2	1:A:59:ASP:N	2.42	0.51
1:A:197:ARG:HB3	1:B:289:ILE:O	2.11	0.51
1:B:370:ASP:OD1	1:B:370:ASP:N	2.34	0.51
1:B:26:GLU:OE1	1:B:29:ARG:NH2	2.43	0.51
2:M:9:A:H4'	2:M:10:G:O4'	2.10	0.51
1:A:9:VAL:HB	1:A:47:PHE:HB2	1.93	0.50
1:B:257:LYS:HG3	1:B:258:TYR:HD1	1.77	0.50
1:B:111:TYR:CE2	1:B:113:GLU:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:SER:OG	1:B:357:HIS:N	2.33	0.50
1:B:208:SER:OG	1:B:247:GLN:NE2	2.45	0.49
1:A:370:ASP:OD1	1:A:370:ASP:N	2.36	0.49
1:B:257:LYS:HE2	1:B:258:TYR:HE1	1.77	0.49
2:M:15:C:H3'	2:M:16:U:C5'	2.41	0.49
2:X:5:G:H1	2:X:31:C:H42	1.60	0.49
2:X:12:G:H3'	2:X:13:U:H5'	1.95	0.49
1:A:213:SER:HB2	1:A:341:GLN:HB3	1.94	0.49
2:M:25:C:H2'	2:M:26:A:C8	2.48	0.49
1:B:299:ASN:O	1:B:303:ILE:HG13	2.12	0.49
1:A:111:TYR:HD1	1:A:153:PRO:HD3	1.78	0.49
1:A:228:ARG:NH1	1:A:233:GLY:O	2.45	0.49
1:A:299:ASN:O	1:A:303:ILE:HG13	2.13	0.49
1:A:274:ILE:O	1:A:278:THR:OG1	2.25	0.48
1:A:5:ARG:HH22	1:A:93:GLU:CD	2.21	0.48
1:B:257:LYS:HG3	1:B:258:TYR:CD1	2.48	0.48
1:A:386:VAL:HG12	1:A:388:GLU:HG2	1.96	0.48
1:A:7:TYR:HB2	1:A:49:ILE:HB	1.95	0.48
2:M:5:G:H1	2:M:31:C:H42	1.61	0.47
2:X:14:C:H4'	2:X:15:C:N3	2.29	0.47
1:A:110:ALA:HB3	1:A:152:ARG:HA	1.96	0.47
1:B:5:ARG:HH22	1:B:93:GLU:CD	2.23	0.47
1:A:44:TRP:CZ3	1:A:48:LEU:HD11	2.49	0.47
1:A:253:ARG:HB3	1:A:367:GLN:HB3	1.97	0.47
1:B:7:TYR:HB2	1:B:49:ILE:HB	1.97	0.47
1:A:125:LEU:O	1:A:129:ILE:HG12	2.15	0.47
1:B:179:LEU:HD12	1:B:284:TYR:O	2.15	0.47
1:B:13:GLU:H	1:B:13:GLU:HG2	1.35	0.46
1:B:125:LEU:O	1:B:129:ILE:HG12	2.16	0.46
1:A:4:LEU:HD12	1:A:75:LEU:HB3	1.98	0.46
1:B:60:LYS:HD2	1:B:60:LYS:H	1.81	0.45
2:X:12:G:H1	2:X:15:C:N4	2.12	0.45
1:B:222:ASP:HB3	1:B:335:ILE:HD13	1.97	0.45
1:B:253:ARG:HB3	1:B:367:GLN:HB3	1.98	0.45
1:B:341:GLN:HG3	1:B:342:ASP:N	2.31	0.45
1:B:221:ARG:HE	1:B:385:GLU:CD	2.24	0.45
1:B:262:MET:HE1	1:B:365:GLU:HG2	1.99	0.45
1:B:272:GLU:HG3	1:B:309:ARG:HD2	1.97	0.45
1:B:87:SER:HB3	1:B:147:LEU:HD21	1.99	0.45
1:B:264:ARG:HH22	1:B:287:GLU:CD	2.24	0.45
1:B:304:GLU:O	1:B:304:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HB2	1:A:349:PRO:HG3	1.98	0.44
2:M:10:G:H2'	2:M:11:U:H5'	2.00	0.44
2:M:19:G:H1	2:M:24:C:H42	1.65	0.44
2:M:12:G:O2'	2:M:13:U:P	2.74	0.44
1:B:109:LYS:HA	1:B:151:VAL:HG13	2.00	0.44
1:B:110:ALA:HB3	1:B:152:ARG:HG3	1.99	0.43
1:B:224:LEU:HD12	1:B:224:LEU:HA	1.82	0.43
1:B:261:ILE:HB	1:B:361:LEU:HD21	1.99	0.43
1:A:88:LEU:HD23	1:A:129:ILE:HD13	2.01	0.43
1:A:179:LEU:HD12	1:A:284:TYR:O	2.18	0.43
1:A:208:SER:OG	1:A:247:GLN:OE1	2.37	0.43
1:A:304:GLU:O	1:A:304:GLU:HG3	2.17	0.43
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.81	0.43
1:B:383:LYS:HE3	1:B:383:LYS:HB2	1.81	0.43
1:B:100:TYR:HB3	1:B:144:ASP:HB3	2.01	0.42
1:B:4:LEU:HD12	1:B:75:LEU:HB3	2.01	0.42
2:X:2:C:H42	2:X:34:G:H1	1.65	0.42
1:A:268:PHE:CD2	1:A:303:ILE:HG22	2.54	0.42
1:A:260:LEU:HA	1:A:263:TYR:CD2	2.55	0.42
1:A:281:VAL:HG11	1:B:298:GLU:HG2	2.01	0.42
2:M:20:G:H1	2:M:21:A:HO2'	1.61	0.42
1:A:151:VAL:HG13	1:A:156:VAL:HG22	2.02	0.42
1:A:161:ASP:OD2	1:A:161:ASP:N	2.52	0.42
1:B:260:LEU:HA	1:B:263:TYR:CD2	2.55	0.42
2:M:20:G:C2	2:M:21:A:H4'	2.54	0.42
2:M:2:C:H42	2:M:34:G:H1	1.68	0.41
1:A:36:THR:HG21	1:A:57:LEU:HD13	2.03	0.41
2:M:19:G:H1	2:M:24:C:N4	2.18	0.41
1:B:34:ARG:HD2	1:B:233:GLY:HA3	2.02	0.41
1:A:262:MET:SD	1:A:361:LEU:HD23	2.60	0.41
1:B:43:GLN:HG2	1:B:44:TRP:CD2	2.56	0.41
1:A:31:ASN:O	1:A:35:VAL:HG13	2.21	0.41
2:X:22:A:N3	2:X:22:A:H2'	2.36	0.41
1:B:120:GLU:O	1:B:124:GLU:HG3	2.21	0.41
1:B:269:ARG:NH2	1:B:365:GLU:OE1	2.49	0.41
1:A:219:LYS:HD2	1:A:339:PRO:HB3	2.02	0.41
1:A:261:ILE:HB	1:A:361:LEU:HD21	2.03	0.41
1:A:5:ARG:NH2	1:A:93:GLU:OE2	2.54	0.40
1:A:249:GLU:O	1:A:253:ARG:HD3	2.21	0.40
1:A:337:ILE:C	1:A:339:PRO:HD2	2.47	0.40
1:A:9:VAL:HG13	1:A:67:ILE:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TYR:CE2	2:M:37:C:H4'	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LYS:NZ	2:X:38:C:O2'[3_544]	2.08	0.12

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	384/388 (99%)	362 (94%)	17 (4%)	5 (1%)	9	33
1	B	384/388 (99%)	362 (94%)	18 (5%)	4 (1%)	12	39
All	All	768/776 (99%)	724 (94%)	35 (5%)	9 (1%)	10	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	GLU
1	A	346	PHE
1	A	12	SER
1	B	17	LYS
1	A	167	GLY
1	B	15	GLY
1	B	20	ASN
1	B	167	GLY
1	A	255	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	340/342 (99%)	299 (88%)	41 (12%)	5	18
1	B	340/342 (99%)	295 (87%)	45 (13%)	4	15
All	All	680/684 (99%)	594 (87%)	86 (13%)	4	17

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	17	LYS
1	A	25	GLU
1	A	35	VAL
1	A	36	THR
1	A	46	ARG
1	A	56	THR
1	A	59	ASP
1	A	99	ASN
1	A	106	GLN
1	A	113	GLU
1	A	140	VAL
1	A	154	GLU
1	A	162	ARG
1	A	181	LEU
1	A	207	VAL
1	A	213	SER
1	A	223	ILE
1	A	244	THR
1	A	254	VAL
1	A	260	LEU
1	A	278	THR
1	A	288	ASN
1	A	292	VAL
1	A	294	SER
1	A	296	THR
1	A	300	LEU

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Mol	Chain	Res	Type
1	A	304	GLU
1	A	308	THR
1	A	316	SER
1	A	320	LYS
1	A	321	THR
1	A	351	ASN
1	A	357	HIS
1	A	362	GLU
1	A	363	LYS
1	A	365	GLU
1	A	367	GLN
1	A	368	VAL
1	A	371	LEU
1	A	383	LYS
1	B	4	LEU
1	B	13	GLU
1	B	16	LEU
1	B	20	ASN
1	B	26	GLU
1	B	35	VAL
1	B	36	THR
1	B	56	THR
1	B	59	ASP
1	B	99	ASN
1	B	101	ARG
1	B	106	GLN
1	B	112	LYS
1	B	131	LYS
1	B	140	VAL
1	B	141	ARG
1	B	151	VAL
1	B	152	ARG
1	B	154	GLU
1	B	160	THR
1	B	181	LEU
1	B	223	ILE
1	B	244	THR
1	B	254	VAL
1	B	260	LEU
1	B	278	THR
1	B	281	VAL
1	B	288	ASN

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Mol	Chain	Res	Type
1	B	292	VAL
1	B	296	THR
1	B	300	LEU
1	B	304	GLU
1	B	308	THR
1	B	316	SER
1	B	321	THR
1	B	334	GLU
1	B	340	TYR
1	B	344	CYS
1	B	357	HIS
1	B	362	GLU
1	B	363	LYS
1	B	367	GLN
1	B	368	VAL
1	B	371	LEU
1	B	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	B	247	GLN
1	B	288	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	M	38/39 (97%)	13 (34%)	3 (7%)
2	X	38/39 (97%)	15 (39%)	4 (10%)
All	All	76/78 (97%)	28 (36%)	7 (9%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	M	9	A
2	M	10	G
2	M	11	U
2	M	12	G
2	M	13	U

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Mol	Chain	Res	Type
2	M	14	C
2	M	15	C
2	M	16	U
2	M	20	G
2	M	21	A
2	M	23	A
2	M	24	C
2	M	39	A
2	X	9	A
2	X	10	G
2	X	11	U
2	X	12	G
2	X	13	U
2	X	14	C
2	X	15	C
2	X	16	U
2	X	17	U
2	X	21	A
2	X	22	A
2	X	23	A
2	X	26	A
2	X	36	A
2	X	39	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	M	9	A
2	M	12	G
2	M	38	C
2	X	9	A
2	X	13	U
2	X	21	A
2	X	38	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	401	4	32,33,33	1.80	7 (21%)	48,52,52	1.80	10 (20%)
3	ATP	A	401	4	32,33,33	1.55	8 (25%)	48,52,52	1.80	11 (22%)

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	B	401	4	-	7/22/38/38	0/3/3/3
3	ATP	A	401	4	-	5/22/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ATP	PB-O3B	5.80	1.65	1.59
3	B	401	ATP	C5-C4	4.62	1.47	1.39
3	A	401	ATP	C5-C4	4.55	1.47	1.39
3	A	401	ATP	PB-O3B	3.46	1.63	1.59
3	B	401	ATP	PB-O3A	3.01	1.62	1.59
3	B	401	ATP	PA-O3A	2.90	1.62	1.59
3	B	401	ATP	C5-C6	2.62	1.48	1.41
3	A	401	ATP	C5-C6	2.55	1.48	1.41
3	A	401	ATP	PA-O3A	2.52	1.62	1.59
3	A	401	ATP	PB-O3A	2.42	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ATP	C8-N7	2.36	1.36	1.31
3	A	401	ATP	C5-N7	-2.36	1.34	1.39
3	A	401	ATP	C8-N7	2.35	1.36	1.31
3	B	401	ATP	C5-N7	-2.17	1.35	1.39
3	A	401	ATP	C4-N9	-2.00	1.33	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ATP	C5-C4-N3	-6.02	118.43	126.72
3	A	401	ATP	C5-C4-N3	-5.49	119.15	126.72
3	B	401	ATP	N3-C4-N9	4.69	135.15	127.17
3	A	401	ATP	N3-C4-N9	4.25	134.40	127.17
3	A	401	ATP	C2'-C1'-N9	-3.99	103.40	113.30
3	B	401	ATP	C2-N3-C4	3.68	120.81	111.83
3	A	401	ATP	C2-N3-C4	3.60	120.61	111.83
3	A	401	ATP	C4-C5-N7	-3.46	106.63	110.58
3	A	401	ATP	N3-C2-N1	-3.44	123.37	128.58
3	B	401	ATP	C4-C5-N7	-3.34	106.76	110.58
3	B	401	ATP	N3-C2-N1	-2.96	124.10	128.58
3	B	401	ATP	C2'-C1'-N9	-2.87	106.18	113.30
3	B	401	ATP	C3'-C2'-C1'	2.70	106.56	101.46
3	A	401	ATP	C4-N9-C8	2.57	108.44	105.74
3	B	401	ATP	C4-N9-C8	2.53	108.40	105.74
3	A	401	ATP	C5-N7-C8	2.45	107.30	103.45
3	B	401	ATP	C5-N7-C8	2.30	107.06	103.45
3	A	401	ATP	C2-N1-C6	2.20	122.34	118.73
3	A	401	ATP	C6-C5-N7	2.18	136.29	132.09
3	B	401	ATP	O3A-PB-O1B	-2.17	104.18	110.70
3	A	401	ATP	C3'-C2'-C1'	2.06	105.36	101.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ATP	C5'-O5'-PA-O1A
3	A	401	ATP	C5'-O5'-PA-O2A
3	A	401	ATP	C5'-O5'-PA-O3A
3	B	401	ATP	O4'-C4'-C5'-O5'
3	A	401	ATP	PB-O3A-PA-O5'
3	B	401	ATP	C5'-O5'-PA-O1A
3	B	401	ATP	C5'-O5'-PA-O2A

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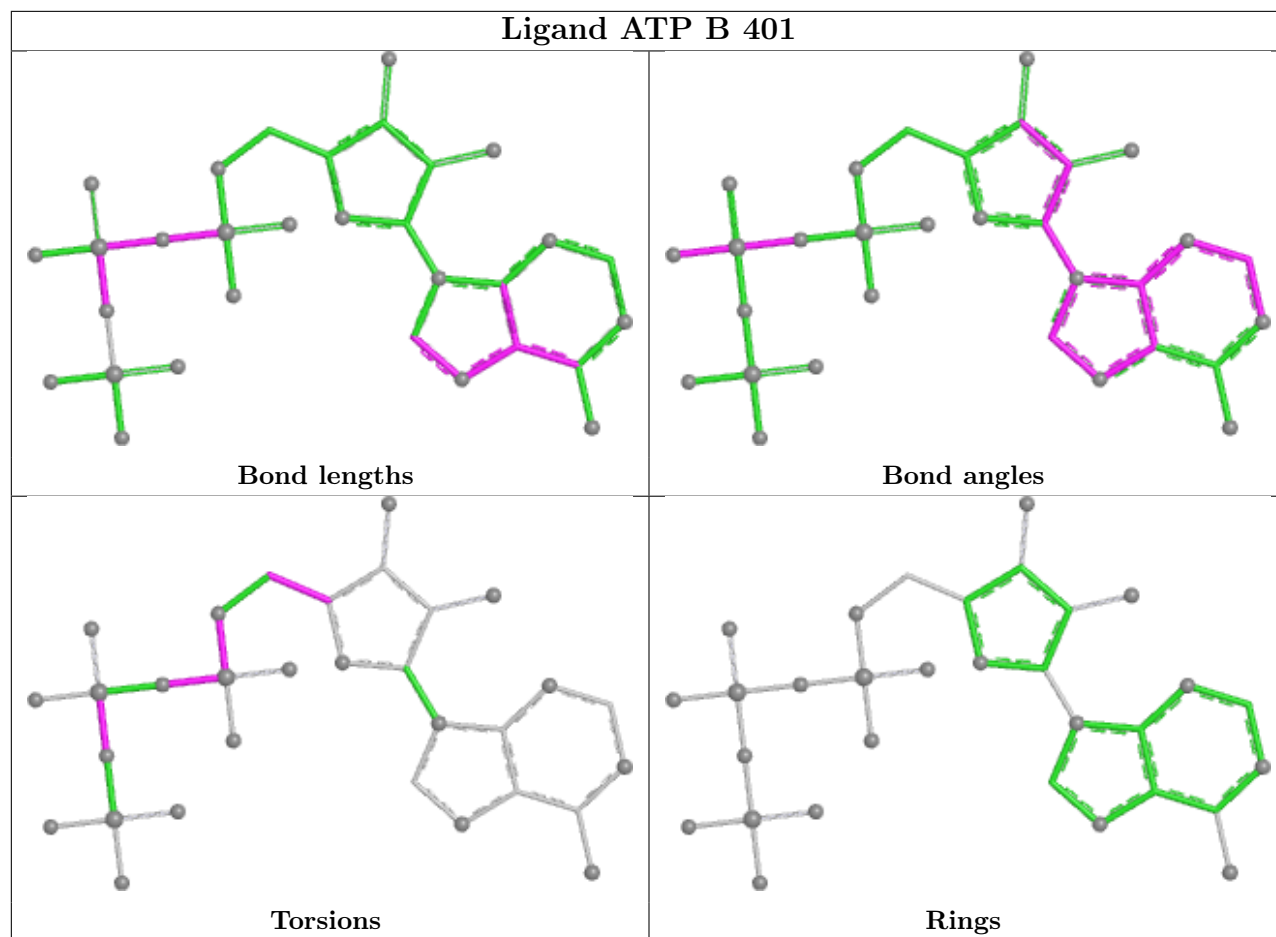
Mol	Chain	Res	Type	Atoms
3	B	401	ATP	C5'-O5'-PA-O3A
3	B	401	ATP	PG-O3B-PB-O2B
3	B	401	ATP	PB-O3A-PA-O2A
3	B	401	ATP	C3'-C4'-C5'-O5'
3	A	401	ATP	PB-O3A-PA-O2A

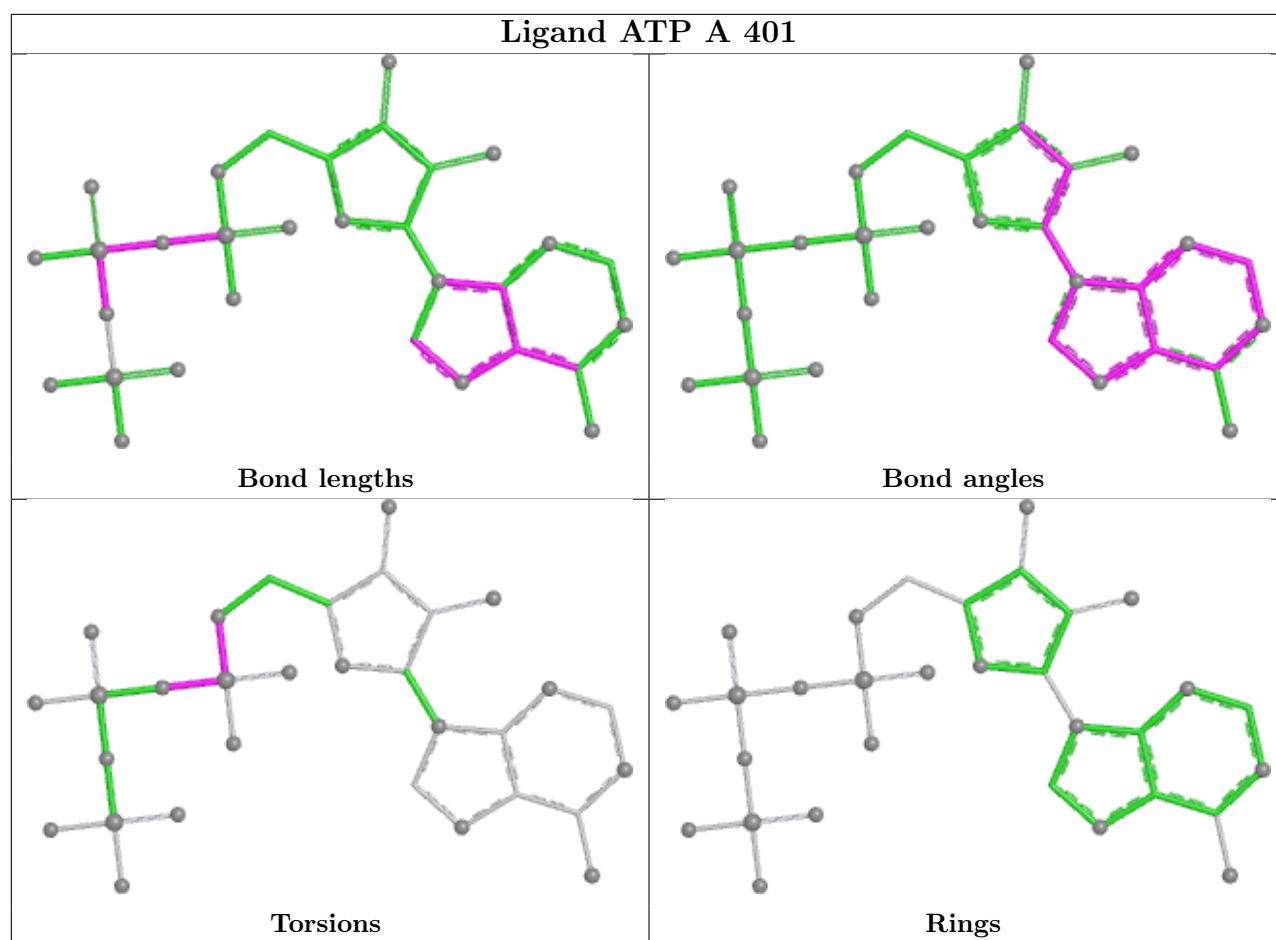
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ATP	1	0
3	A	401	ATP	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/388 (99%)	-0.05	5 (1%) 75 61	42, 83, 141, 195	0
1	B	386/388 (99%)	-0.05	5 (1%) 75 61	43, 87, 143, 198	0
2	M	39/39 (100%)	0.74	4 (10%) 12 12	79, 120, 216, 257	0
2	X	39/39 (100%)	0.64	3 (7%) 19 16	106, 152, 223, 229	0
All	All	850/854 (99%)	0.02	17 (2%) 65 50	42, 88, 157, 257	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	22	A	4.3
1	B	337	ILE	3.5
2	X	14	C	3.3
2	M	12	G	3.0
1	B	346	PHE	2.9
2	M	21	A	2.9
1	A	113	GLU	2.7
2	X	15	C	2.7
2	X	12	G	2.7
1	A	111	TYR	2.6
1	A	110	ALA	2.4
1	B	345	VAL	2.4
1	B	341	GLN	2.3
1	A	313	ARG	2.2
1	B	164	GLU	2.1
2	M	23	A	2.1
1	A	281	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

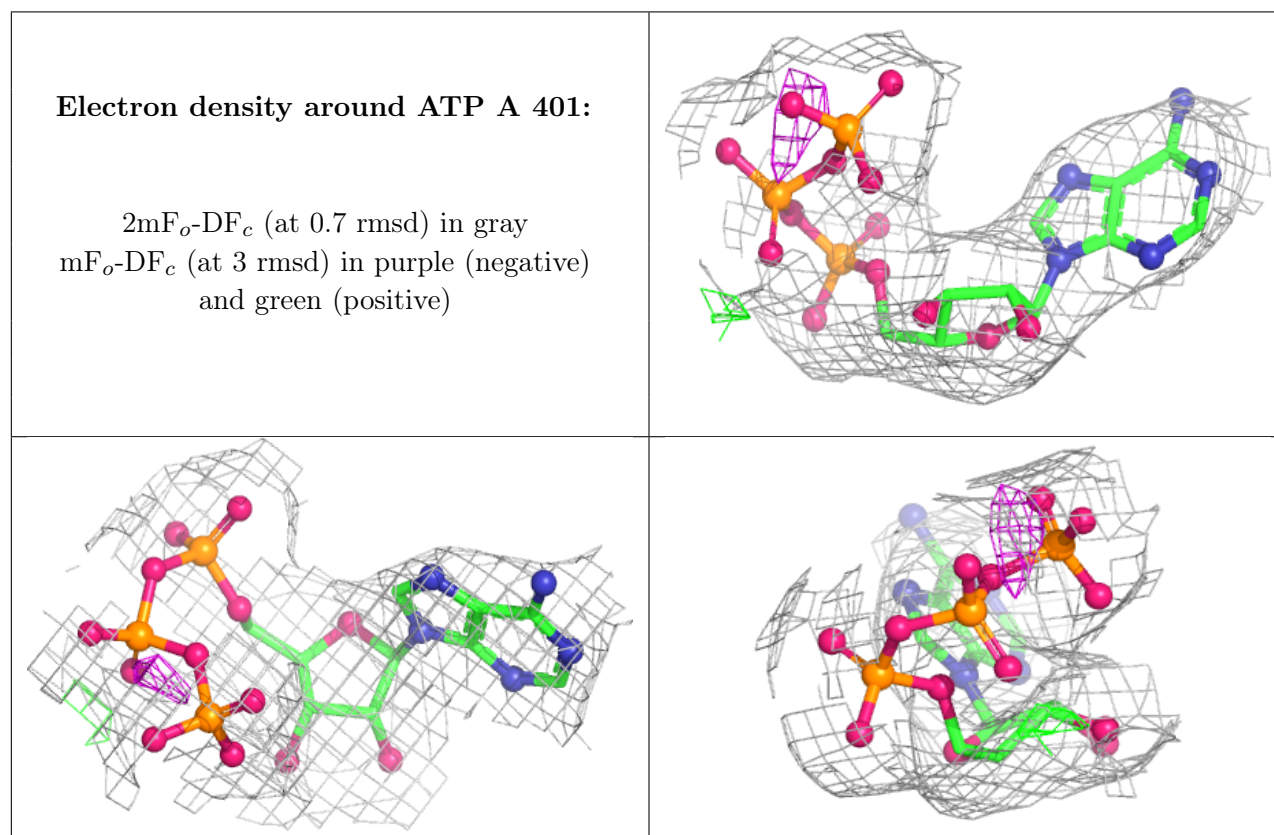
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

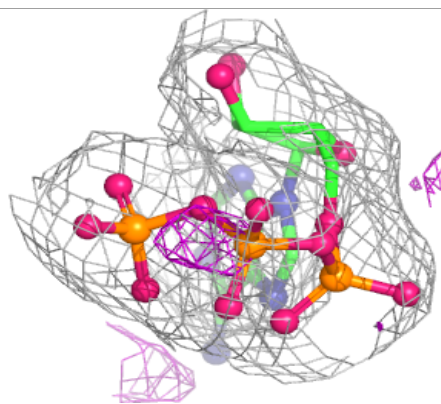
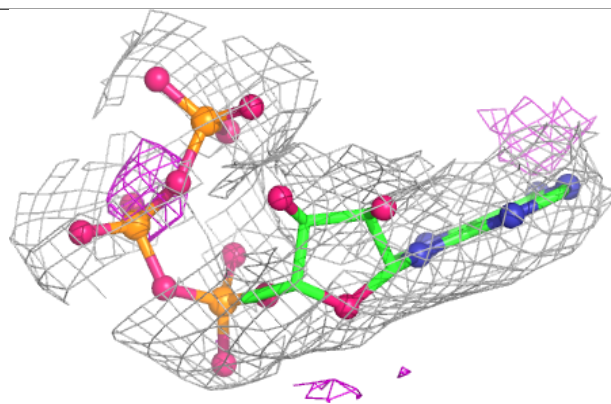
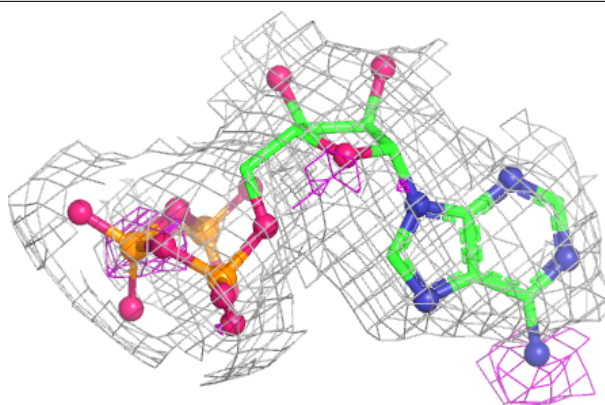
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	402	1/1	0.76	0.08	71,71,71,71	0
3	ATP	A	401	31/31	0.89	0.09	99,102,106,107	0
4	MG	B	402	1/1	0.90	0.08	65,65,65,65	0
3	ATP	B	401	31/31	0.91	0.09	85,88,90,92	0

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



Electron density around ATP B 401:

$2mF_o - DF_c$ (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.