



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:54 AM UTC

PDB ID : 4D79 / pdb_00004d79
Title : Crystal structure of E. coli tRNA N6-threonylcarbamoyladenosine dehydratase, TcdA, in complex with ATP at 1.768 Angstroem resolution
Authors : Lopez-Esteva, M.; Arda, A.; Savko, M.; Round, A.; Shepard, W.; Bruix, M.; Coll, M.; Fernandez, F.J.; Jimenez-Barbero, J.; Vega, M.C.
Deposited on : 2014-11-21
Resolution : 1.77 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

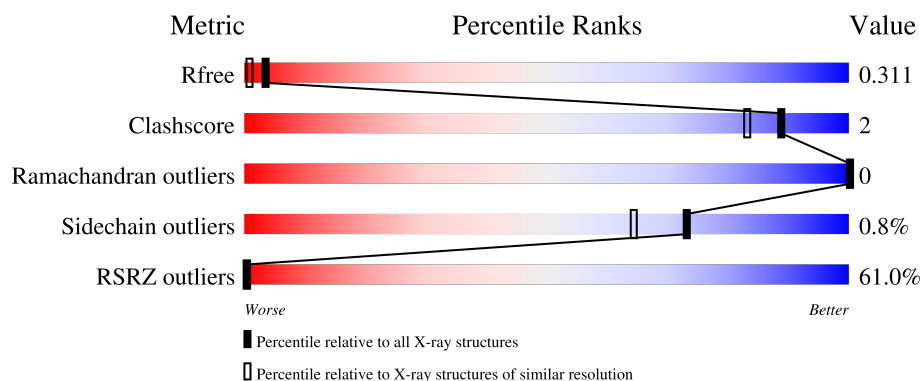
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	276	31% 85% 12%
1	B	276	41% 82% 11%
1	C	276	71% 88% 9%
1	D	276	75% 85% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8167 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 TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	3	0
			1846	1161	332	341	12			
1	B	247	Total	C	N	O	S	0	3	0
			1872	1176	334	350	12			
1	C	252	Total	C	N	O	S	0	4	1
			1923	1210	348	353	12			
1	D	244	Total	C	N	O	S	0	1	0
			1843	1160	329	343	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	LEU	-	expression tag	UNP Q46927
A	270	GLU	-	expression tag	UNP Q46927
A	271	HIS	-	expression tag	UNP Q46927
A	272	HIS	-	expression tag	UNP Q46927
A	273	HIS	-	expression tag	UNP Q46927
A	274	HIS	-	expression tag	UNP Q46927
A	275	HIS	-	expression tag	UNP Q46927
A	276	HIS	-	expression tag	UNP Q46927
B	269	LEU	-	expression tag	UNP Q46927
B	270	GLU	-	expression tag	UNP Q46927
B	271	HIS	-	expression tag	UNP Q46927
B	272	HIS	-	expression tag	UNP Q46927
B	273	HIS	-	expression tag	UNP Q46927
B	274	HIS	-	expression tag	UNP Q46927
B	275	HIS	-	expression tag	UNP Q46927
B	276	HIS	-	expression tag	UNP Q46927
C	269	LEU	-	expression tag	UNP Q46927
C	270	GLU	-	expression tag	UNP Q46927
C	271	HIS	-	expression tag	UNP Q46927
C	272	HIS	-	expression tag	UNP Q46927

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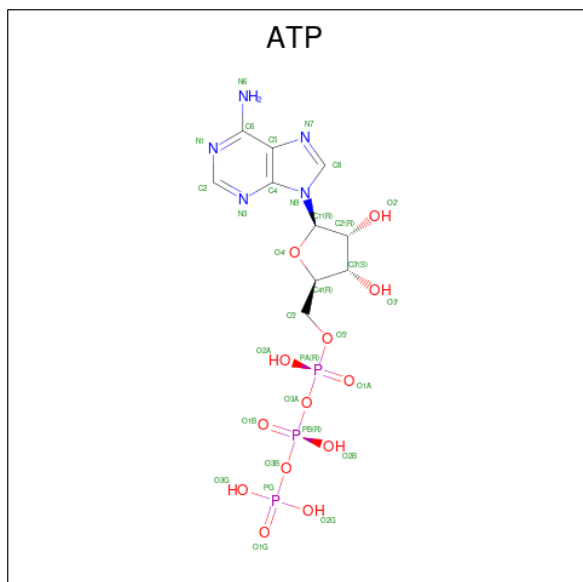
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Chain	Residue	Modelled	Actual	Comment	Reference
C	273	HIS	-	expression tag	UNP Q46927
C	274	HIS	-	expression tag	UNP Q46927
C	275	HIS	-	expression tag	UNP Q46927
C	276	HIS	-	expression tag	UNP Q46927
D	269	LEU	-	expression tag	UNP Q46927
D	270	GLU	-	expression tag	UNP Q46927
D	271	HIS	-	expression tag	UNP Q46927
D	272	HIS	-	expression tag	UNP Q46927
D	273	HIS	-	expression tag	UNP Q46927
D	274	HIS	-	expression tag	UNP Q46927
D	275	HIS	-	expression tag	UNP Q46927
D	276	HIS	-	expression tag	UNP Q46927

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

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



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Na 1	0	0
5	D	1	Total 1	Na 1	0	0

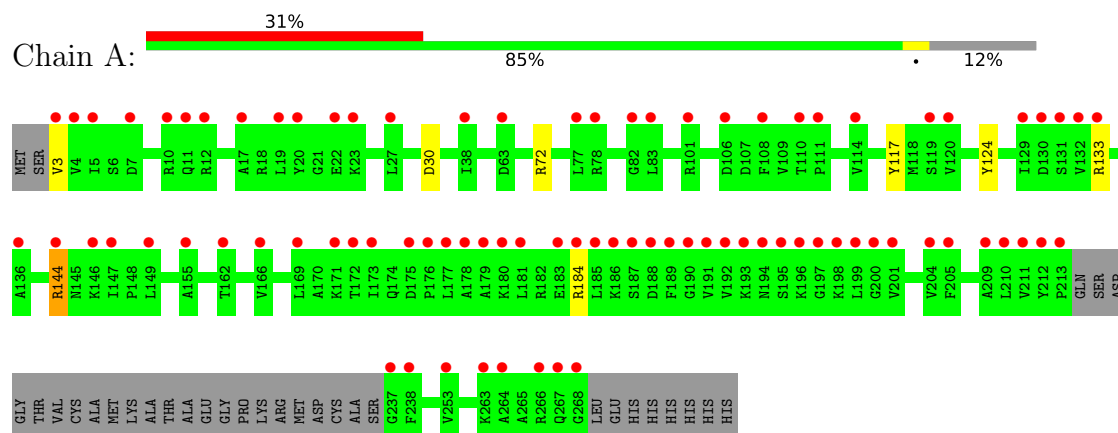
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total 123	O 123	0	0
6	B	140	Total 140	O 140	0	0
6	C	144	Total 144	O 144	0	0
6	D	104	Total 104	O 104	0	0

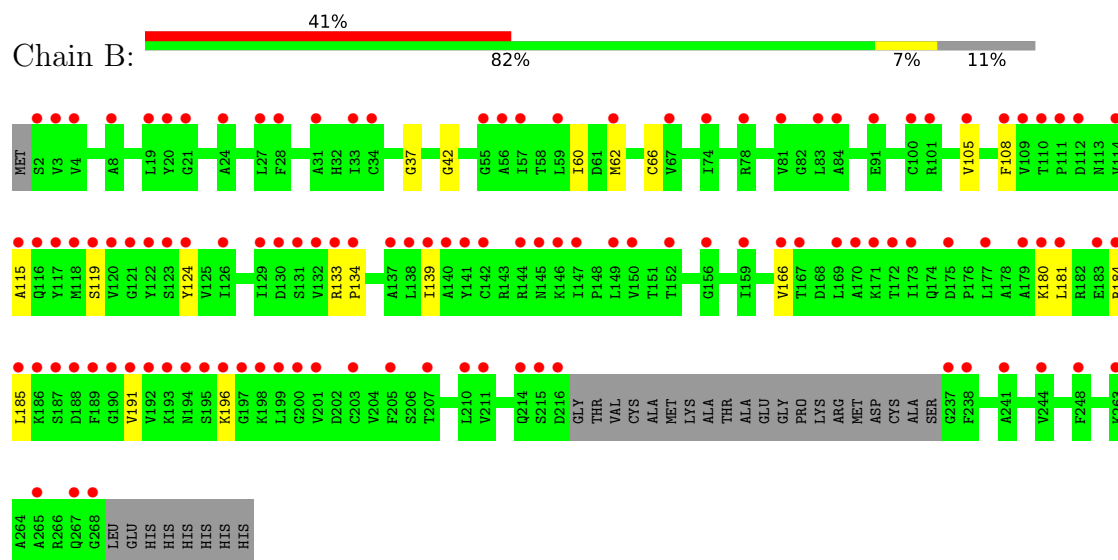
3 Residue-property plots

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.

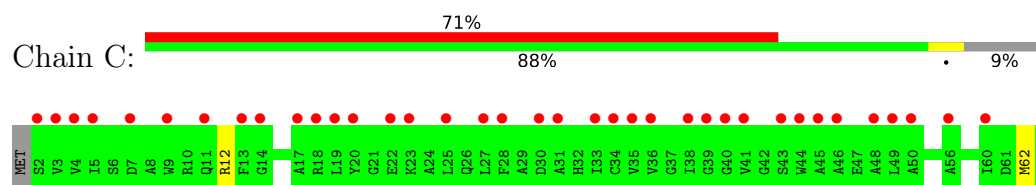
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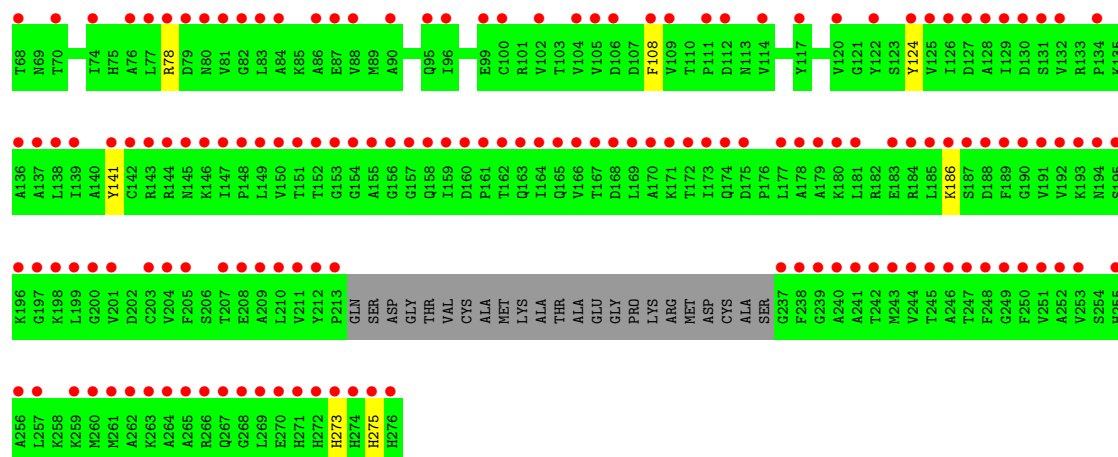


• Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE

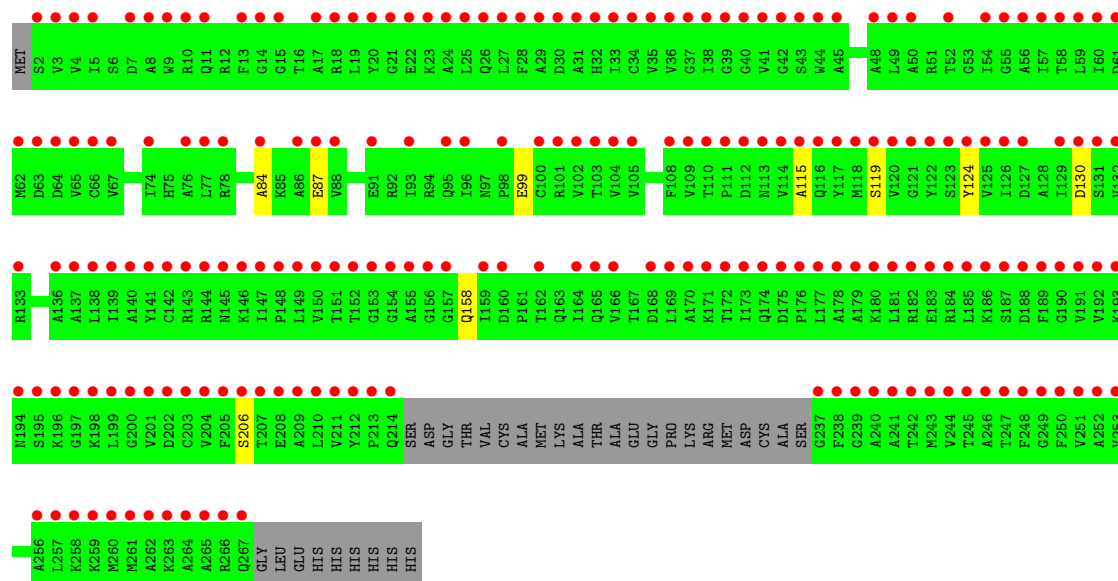
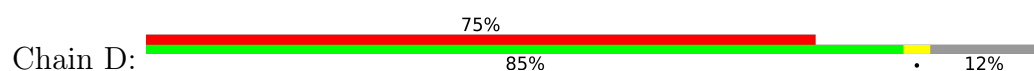


• Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE





• Molecule 1: TRNA THREONYLCARBAMOYLADENOSINE DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.69Å 97.16Å 83.19Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	41.13 – 1.77 41.13 – 1.77	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.13-1.77) 95.0 (41.13-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 1.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.142 , 0.183 0.297 , 0.311	Depositor DCC
R_{free} test set	4502 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8167	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: GOL, K, NA, 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	0.53	1/1872 (0.1%)	0.61	0/2533
1	B	0.48	0/1898	0.61	0/2570
1	C	0.47	1/1957 (0.1%)	0.59	0/2651
1	D	0.44	0/1869	0.59	0/2530
All	All	0.48	2/7596 (0.0%)	0.60	0/10284

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	275	HIS	C-N	-6.87	1.23	1.33
1	A	117	TYR	C-O	-5.80	1.17	1.24

There are no bond angle outliers.

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	1846	0	1883	6	0
1	B	1872	0	1903	14	0
1	C	1923	0	1947	5	2
1	D	1843	0	1878	5	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	1	0
3	B	31	0	12	0	0
3	C	31	0	12	2	0
3	D	31	0	12	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	6	0	8	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	123	0	0	0	0
6	B	140	0	0	3	0
6	C	144	0	0	2	1
6	D	104	0	0	1	2
All	All	8167	0	7715	29	3

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 2.

All (29) 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:B:66[A]:CYS:SG	6:B:2046:HOH:O	2.31	0.87
1:A:133:ARG:CG	1:A:184:ARG:HH12	2.18	0.57
1:C:108:PHE:HB2	3:C:401:ATP:C6	2.42	0.55
1:A:133:ARG:HG3	1:A:184:ARG:HH12	1.72	0.54
1:B:180:LYS:HG3	6:B:2106:HOH:O	2.11	0.51
1:B:133:ARG:HG2	1:B:184:ARG:HH12	1.77	0.50
1:C:186:LYS:NZ	6:C:2120:HOH:O	2.44	0.50
1:B:133:ARG:HB2	1:B:134:PRO:CD	2.42	0.50
1:C:108:PHE:HB2	3:C:401:ATP:N6	2.27	0.49
1:B:133:ARG:HB2	1:B:134:PRO:HD3	1.95	0.48
1:B:196:LYS:NZ	1:D:130:ASP:OD2	2.46	0.48
1:C:12:ARG:NH2	6:C:2019:HOH:O	2.46	0.48
1:B:139:ILE:CD1	1:B:181:LEU:HD21	2.45	0.47
1:A:72:ARG:NH2	3:A:401:ATP:O3B	2.48	0.46
1:A:133:ARG:HG2	1:A:184:ARG:NH1	2.31	0.46
1:A:144[A]:ARG:CG	1:A:144[A]:ARG:HH11	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLY:O	1:B:42:GLY:HA3	2.17	0.45
1:D:99:GLU:OE2	6:D:2048:HOH:O	2.21	0.45
1:C:62:MET:SD	1:C:108:PHE:HD1	2.40	0.45
1:B:166[B]:VAL:HG21	6:B:2126:HOH:O	2.18	0.44
1:A:3:VAL:N	1:A:30:ASP:OD1	2.52	0.43
1:B:115:ALA:O	1:B:119:SER:OG	2.27	0.43
1:B:62:MET:HG2	1:B:108:PHE:CZ	2.54	0.42
1:D:115:ALA:O	1:D:119:SER:OG	2.30	0.41
1:B:185:LEU:HB3	1:B:191:VAL:HB	2.03	0.41
1:B:62:MET:CG	1:B:108:PHE:CE2	3.04	0.41
1:D:158:GLN:OE1	1:D:206:SER:HB3	2.22	0.40
1:B:60:ILE:HG12	1:B:105:VAL:HB	2.03	0.40
1:D:84:ALA:HB3	1:D:87[B]:GLU:HG3	2.03	0.40

All (3) 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)
6:C:2100:HOH:O	6:D:2003:HOH:O[2_657]	1.82	0.38
1:C:64:ASP:OD1	1:C:273:HIS:ND1[2_647]	2.00	0.20
1:C:141:TYR:OH	6:D:2048:HOH:O[2_657]	2.19	0.01

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	242/276 (88%)	237 (98%)	5 (2%)	0	100	100
1	B	246/276 (89%)	241 (98%)	5 (2%)	0	100	100
1	C	252/276 (91%)	248 (98%)	4 (2%)	0	100	100
1	D	241/276 (87%)	237 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	981/1104 (89%)	963 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	192/216 (89%)	189 (98%)	3 (2%)	55	38
1	B	196/216 (91%)	195 (100%)	1 (0%)	81	75
1	C	201/216 (93%)	199 (99%)	2 (1%)	68	56
1	D	192/216 (89%)	191 (100%)	1 (0%)	81	75
All	All	781/864 (90%)	774 (99%)	7 (1%)	73	60

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	TYR
1	A	144[A]	ARG
1	A	144[B]	ARG
1	B	124	TYR
1	C	78	ARG
1	C	124	TYR
1	D	124	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	GLN
1	C	145	ASN
1	C	273	HIS
1	D	165	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	D	501	-	5,5,5	0.49	0	5,5,5	0.32	0
3	ATP	B	401	-	32,33,33	1.42	4 (12%)	48,52,52	2.13	8 (16%)
3	ATP	D	401	-	32,33,33	1.39	4 (12%)	48,52,52	2.08	16 (33%)
4	GOL	C	502	-	5,5,5	0.34	0	5,5,5	0.46	0
4	GOL	A	501	-	5,5,5	0.42	0	5,5,5	0.44	0
4	GOL	C	501	-	5,5,5	0.69	0	5,5,5	0.70	0
3	ATP	A	401	-	32,33,33	1.44	5 (15%)	48,52,52	1.82	8 (16%)
3	ATP	C	401	-	32,33,33	1.51	7 (21%)	48,52,52	2.03	9 (18%)
4	GOL	B	502	-	5,5,5	0.34	0	5,5,5	0.67	0
4	GOL	B	501	-	5,5,5	0.50	0	5,5,5	0.46	0
4	GOL	A	502	-	5,5,5	0.50	0	5,5,5	0.43	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
4	GOL	D	501	-	-	0/4/4/4	-
3	ATP	B	401	-	-	4/22/38/38	0/3/3/3
3	ATP	D	401	-	-	3/22/38/38	0/3/3/3
4	GOL	C	502	-	-	2/4/4/4	-
4	GOL	A	501	-	-	0/4/4/4	-
4	GOL	C	501	-	-	0/4/4/4	-
3	ATP	A	401	-	-	6/22/38/38	0/3/3/3
3	ATP	C	401	-	-	6/22/38/38	0/3/3/3
4	GOL	B	502	-	-	2/4/4/4	-
4	GOL	B	501	-	-	0/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ATP	C5-C4	4.84	1.47	1.39
3	B	401	ATP	C5-C4	4.80	1.47	1.39
3	D	401	ATP	C5-C4	4.54	1.47	1.39
3	C	401	ATP	C5-C4	4.35	1.46	1.39
3	C	401	ATP	C5-N7	-3.16	1.33	1.39
3	B	401	ATP	C5-N7	-2.79	1.34	1.39
3	D	401	ATP	C5-N7	-2.74	1.34	1.39
3	C	401	ATP	C8-N7	2.59	1.36	1.31
3	C	401	ATP	PA-O3A	2.55	1.62	1.59
3	C	401	ATP	PB-O3A	2.54	1.62	1.59
3	B	401	ATP	C8-N7	2.43	1.36	1.31
3	C	401	ATP	PB-O3B	2.38	1.62	1.59
3	B	401	ATP	C5-C6	2.24	1.47	1.41
3	A	401	ATP	C5-C6	2.19	1.47	1.41
3	D	401	ATP	C8-N7	2.18	1.35	1.31
3	D	401	ATP	C2-N1	2.17	1.37	1.33
3	A	401	ATP	PB-O3B	2.14	1.61	1.59
3	C	401	ATP	C5-C6	2.14	1.46	1.41
3	A	401	ATP	C5-N7	-2.09	1.35	1.39
3	A	401	ATP	C8-N7	2.06	1.35	1.31

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ATP	C5-C4-N3	-7.53	116.36	126.72
3	B	401	ATP	C5-C4-N3	-7.43	116.48	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ATP	N3-C4-N9	6.44	138.12	127.17
3	C	401	ATP	N3-C4-N9	6.04	137.45	127.17
3	D	401	ATP	C4-N9-C8	5.54	111.55	105.74
3	B	401	ATP	O4'-C1'-N9	5.26	118.19	108.09
3	A	401	ATP	N3-C4-N9	5.13	135.89	127.17
3	D	401	ATP	N3-C4-N9	4.90	135.51	127.17
3	A	401	ATP	C5-C4-N3	-4.87	120.00	126.72
3	D	401	ATP	N3-C2-N1	-4.60	121.63	128.58
3	C	401	ATP	C2-N3-C4	4.40	122.57	111.83
3	B	401	ATP	C2-N3-C4	4.28	122.29	111.83
3	A	401	ATP	C4-N9-C8	4.27	110.22	105.74
3	D	401	ATP	C5-C4-N3	-4.23	120.89	126.72
3	A	401	ATP	N3-C2-N1	-4.12	122.35	128.58
3	D	401	ATP	N9-C8-N7	-3.87	108.44	113.94
3	B	401	ATP	N3-C2-N1	-3.81	122.81	128.58
3	C	401	ATP	N3-C2-N1	-3.69	123.00	128.58
3	C	401	ATP	O4'-C1'-N9	3.51	114.84	108.09
3	A	401	ATP	C2-N3-C4	3.48	120.33	111.83
3	D	401	ATP	C2-N3-C4	3.31	119.93	111.83
3	D	401	ATP	C5-N7-C8	3.14	108.39	103.45
3	D	401	ATP	O2B-PB-O3A	2.91	115.14	107.27
3	D	401	ATP	C2-N1-C6	2.73	123.21	118.73
3	D	401	ATP	C4-N9-C1'	-2.64	120.46	126.63
3	A	401	ATP	C5-C6-N6	-2.60	116.84	123.29
3	A	401	ATP	N6-C6-N1	2.60	124.17	118.38
3	D	401	ATP	O3A-PA-O1A	-2.54	103.06	110.70
3	D	401	ATP	O2A-PA-O3A	2.49	114.00	107.27
3	C	401	ATP	N6-C6-N1	2.45	123.84	118.38
3	C	401	ATP	C5-C6-N6	-2.41	117.33	123.29
3	C	401	ATP	C4-C5-N7	-2.39	107.85	110.58
3	D	401	ATP	N6-C6-N1	2.38	123.67	118.38
3	B	401	ATP	O4'-C1'-C2'	-2.38	101.53	106.62
3	A	401	ATP	N9-C8-N7	-2.24	110.75	113.94
3	D	401	ATP	C4-C5-N7	-2.24	108.02	110.58
3	C	401	ATP	C5-N7-C8	2.15	106.83	103.45
3	B	401	ATP	O3G-PG-O2G	2.06	115.53	107.80
3	D	401	ATP	C5-C4-N9	-2.03	103.60	105.81
3	D	401	ATP	C5-C6-N6	-2.03	118.27	123.29
3	B	401	ATP	O2B-PB-O1B	2.02	121.84	112.44

There are no chirality outliers.

All (25) 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-O3A
3	B	401	ATP	C5'-O5'-PA-O1A
3	B	401	ATP	C5'-O5'-PA-O3A
3	C	401	ATP	C5'-O5'-PA-O1A
4	A	502	GOL	C1-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3
4	B	502	GOL	O2-C2-C3-O3
4	C	502	GOL	O2-C2-C3-O3
4	B	502	GOL	C1-C2-C3-O3
4	C	502	GOL	C1-C2-C3-O3
3	A	401	ATP	PB-O3A-PA-O5'
3	B	401	ATP	PB-O3A-PA-O5'
3	C	401	ATP	PB-O3A-PA-O5'
3	D	401	ATP	PB-O3A-PA-O5'
3	A	401	ATP	C5'-O5'-PA-O2A
3	B	401	ATP	C5'-O5'-PA-O2A
3	C	401	ATP	C5'-O5'-PA-O2A
3	C	401	ATP	C5'-O5'-PA-O3A
3	D	401	ATP	PA-O3A-PB-O2B
3	A	401	ATP	PB-O3A-PA-O2A
3	C	401	ATP	PB-O3A-PA-O2A
3	D	401	ATP	PA-O3A-PB-O1B
3	C	401	ATP	O4'-C4'-C5'-O5'
3	A	401	ATP	O4'-C4'-C5'-O5'

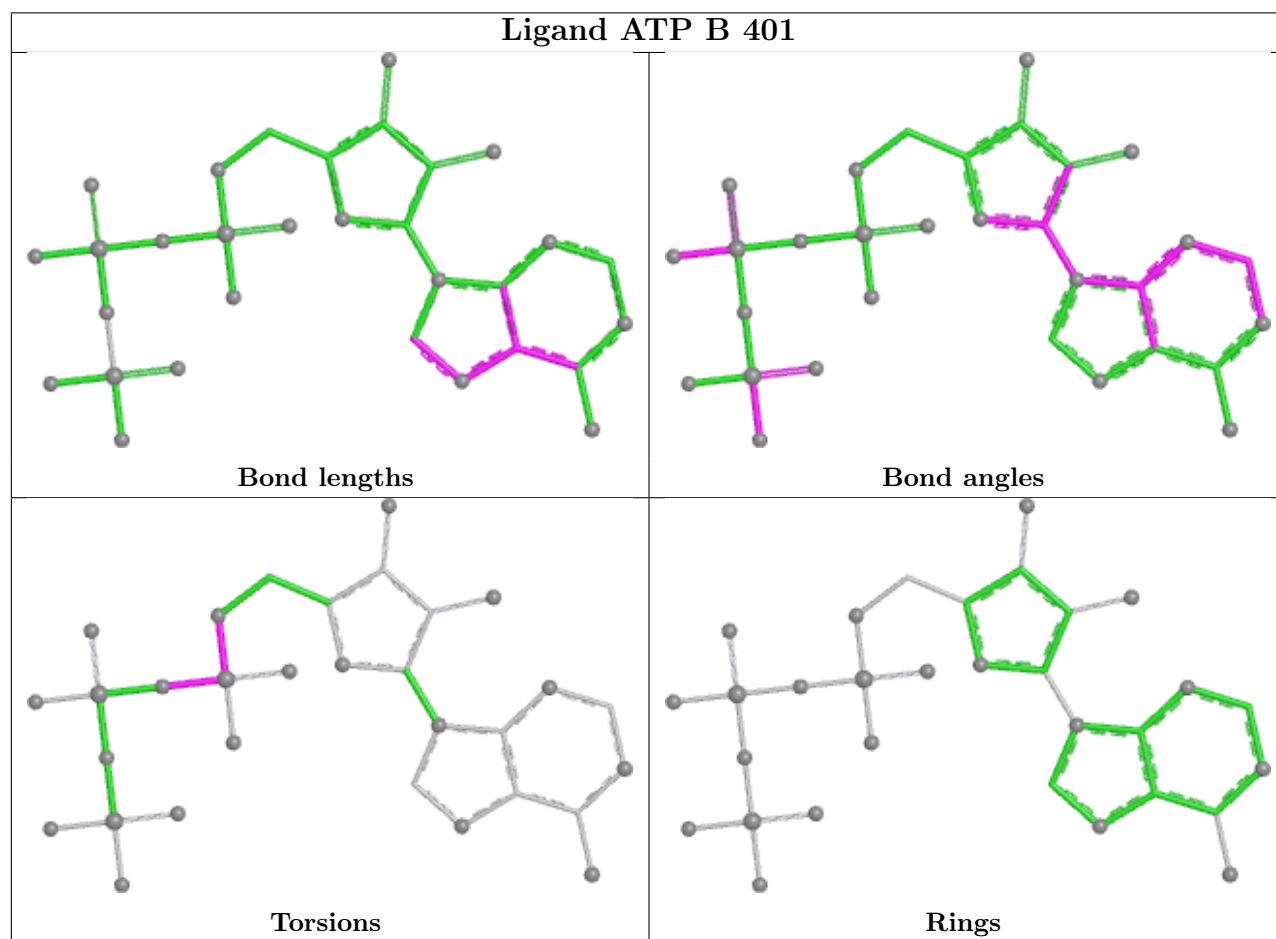
There are no ring outliers.

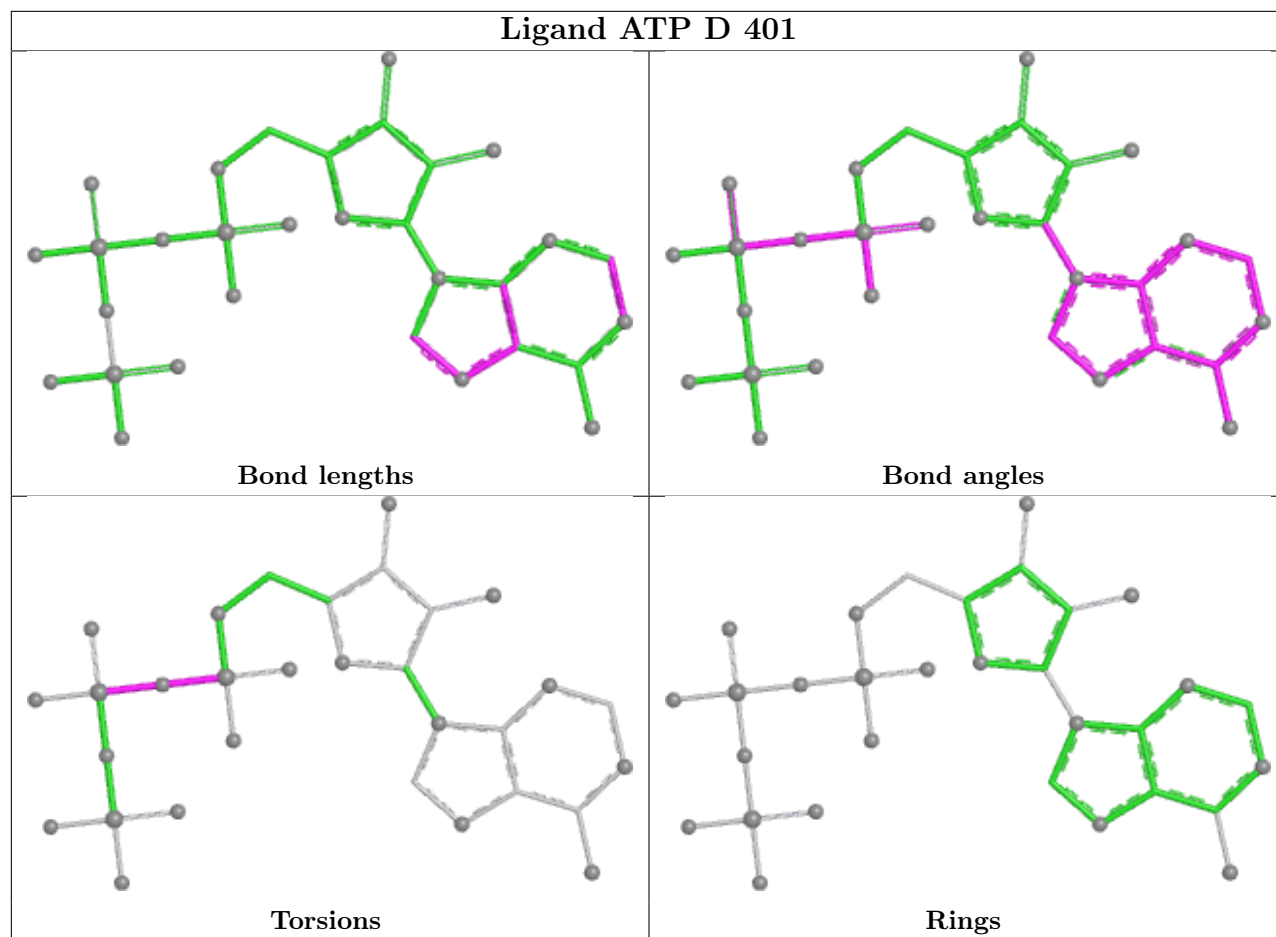
2 monomers are involved in 3 short contacts:

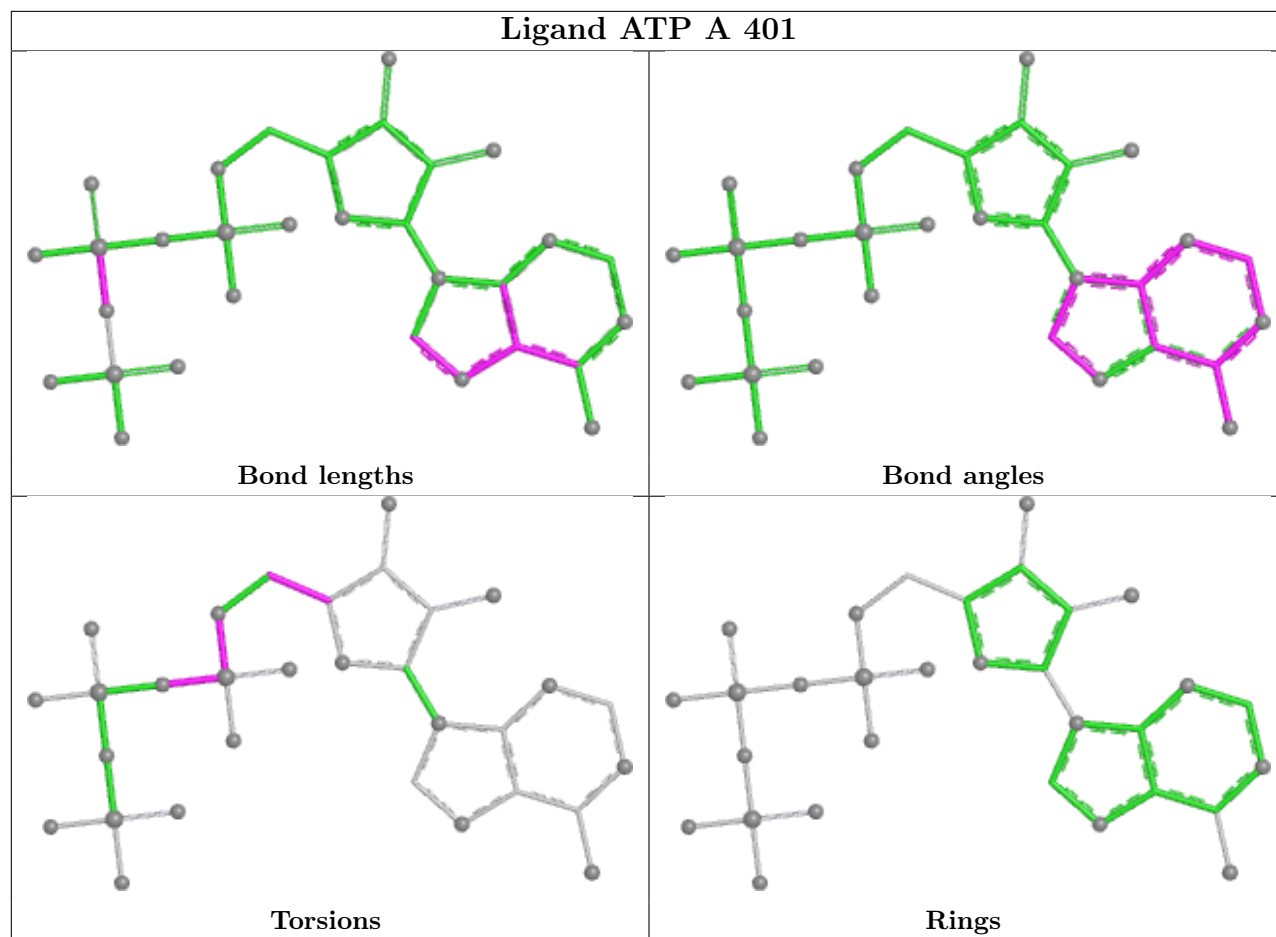
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ATP	1	0
3	C	401	ATP	2	0

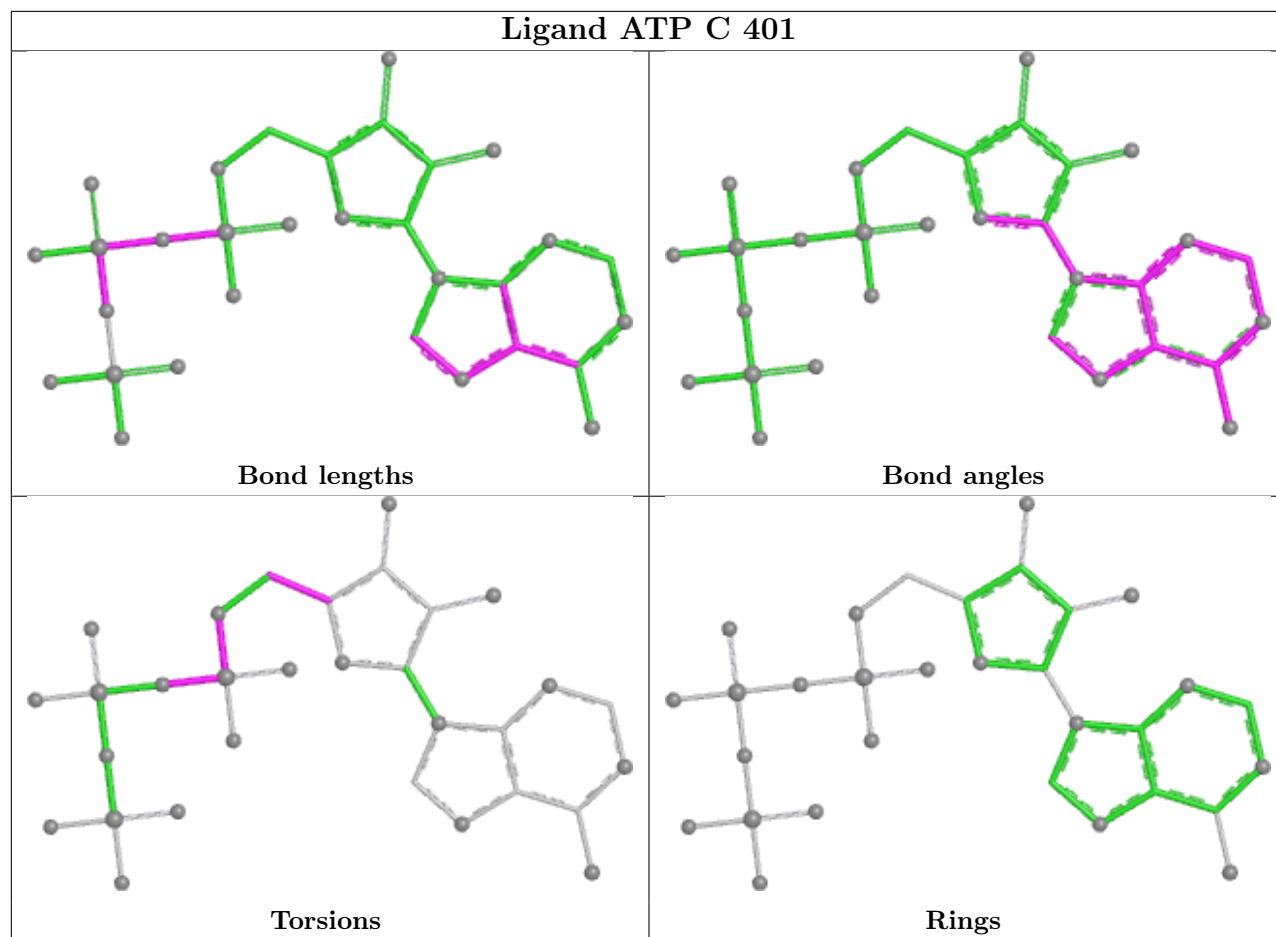
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	243/276 (88%)	1.87	85 (34%) 1 1	10, 28, 67, 116	3 (1%)
1	B	247/276 (89%)	2.08	114 (46%) 0 0	12, 25, 59, 112	3 (1%)
1	C	252/276 (91%)	2.86	195 (77%) 0 0	13, 27, 75, 102	4 (1%)
1	D	244/276 (88%)	3.15	207 (84%) 0 0	17, 29, 60, 112	1 (0%)
All	All	986/1104 (89%)	2.49	601 (60%) 0 0	10, 27, 67, 116	11 (1%)

All (601) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	211	VAL	8.1
1	D	189	PHE	7.8
1	C	213	PRO	7.1
1	B	120	VAL	6.8
1	D	192	VAL	6.8
1	C	120	VAL	6.6
1	D	137	ALA	6.5
1	A	268	GLY	6.4
1	C	108	PHE	6.3
1	D	173	ILE	6.2
1	D	149	LEU	6.2
1	D	129	ILE	6.1
1	D	210	LEU	5.9
1	B	192	VAL	5.9
1	C	201	VAL	5.9
1	D	169	LEU	5.8
1	C	173	ILE	5.7
1	A	3	VAL	5.7
1	A	192	VAL	5.6
1	C	269	LEU	5.6
1	C	238	PHE	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	199	LEU	5.5
1	D	212	TYR	5.5
1	D	214	GLN	5.5
1	D	152	THR	5.5
1	D	109	VAL	5.4
1	B	190	GLY	5.4
1	A	213	PRO	5.4
1	D	191	VAL	5.3
1	D	2	SER	5.3
1	A	120	VAL	5.2
1	A	4	VAL	5.2
1	C	275	HIS	5.2
1	D	120	VAL	5.1
1	A	237	GLY	5.1
1	C	212	TYR	5.1
1	C	161	PRO	5.0
1	D	180	LYS	5.0
1	B	268	GLY	4.9
1	A	211	VAL	4.9
1	A	210	LEU	4.9
1	C	210	LEU	4.8
1	B	166[A]	VAL	4.8
1	C	271	HIS	4.8
1	C	274	HIS	4.8
1	B	194	ASN	4.8
1	D	36	VAL	4.8
1	C	197	GLY	4.7
1	D	150	VAL	4.7
1	C	248	PHE	4.7
1	D	114	VAL	4.7
1	C	132	VAL	4.6
1	C	204	VAL	4.6
1	D	184	ARG	4.6
1	D	185	LEU	4.6
1	D	205	PHE	4.6
1	D	168	ASP	4.6
1	D	264	ALA	4.6
1	C	159	ILE	4.6
1	B	62	MET	4.6
1	C	152	THR	4.5
1	B	216	ASP	4.5
1	A	131	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	267	GLN	4.5
1	D	181	LEU	4.5
1	D	267	GLN	4.5
1	D	121	GLY	4.5
1	D	122	TYR	4.5
1	D	33	ILE	4.5
1	D	159	ILE	4.5
1	C	67[A]	VAL	4.4
1	C	164	ILE	4.4
1	D	196	LYS	4.4
1	B	132	VAL	4.4
1	D	115	ALA	4.4
1	A	119	SER	4.4
1	A	195	SER	4.4
1	A	209	ALA	4.4
1	D	171	LYS	4.4
1	D	174	GLN	4.3
1	C	177	LEU	4.3
1	D	4	VAL	4.3
1	D	193	LYS	4.3
1	A	212	TYR	4.3
1	D	28	PHE	4.3
1	C	4	VAL	4.3
1	C	192	VAL	4.3
1	A	199	LEU	4.3
1	D	265	ALA	4.2
1	A	181	LEU	4.2
1	C	246	ALA	4.2
1	B	196	LYS	4.2
1	D	117	TYR	4.2
1	B	108	PHE	4.2
1	B	189	PHE	4.2
1	D	41	VAL	4.2
1	D	23	LYS	4.2
1	B	130	ASP	4.2
1	C	167	THR	4.2
1	D	238	PHE	4.1
1	C	237	GLY	4.1
1	D	67	VAL	4.1
1	D	142	CYS	4.1
1	B	169	LEU	4.1
1	C	273	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	2	SER	4.1
1	A	173	ILE	4.1
1	C	77	LEU	4.1
1	D	177	LEU	4.1
1	C	131	SER	4.1
1	C	205	PHE	4.1
1	B	191	VAL	4.1
1	D	211	VAL	4.1
1	C	241	ALA	4.0
1	D	151	THR	4.0
1	A	191	VAL	4.0
1	C	109	VAL	4.0
1	C	203	CYS	4.0
1	D	153	GLY	4.0
1	D	197	GLY	4.0
1	C	208	GLU	4.0
1	B	195	SER	4.0
1	C	170	ALA	4.0
1	D	56	ALA	4.0
1	C	199	LEU	3.9
1	D	194	ASN	3.9
1	D	201	VAL	3.9
1	D	25	LEU	3.9
1	B	2	SER	3.9
1	D	124	TYR	3.9
1	A	133	ARG	3.9
1	C	257	LEU	3.9
1	C	209	ALA	3.8
1	D	165	GLN	3.8
1	D	14	GLY	3.8
1	D	146	LYS	3.8
1	D	126	ILE	3.8
1	D	139	ILE	3.8
1	B	171	LYS	3.8
1	D	157	GLY	3.8
1	D	237	GLY	3.8
1	C	137	ALA	3.8
1	D	246	ALA	3.8
1	D	147	ILE	3.7
1	C	253	VAL	3.7
1	D	35	VAL	3.7
1	C	155	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	122	TYR	3.7
1	B	144	ARG	3.7
1	D	21	GLY	3.7
1	D	200	GLY	3.7
1	C	114	VAL	3.7
1	C	191	VAL	3.7
1	D	131	SER	3.7
1	D	195	SER	3.7
1	B	170	ALA	3.7
1	C	276	HIS	3.7
1	D	203	CYS	3.7
1	C	188	ASP	3.7
1	D	3	VAL	3.7
1	D	104	VAL	3.7
1	B	111	PRO	3.7
1	C	158	GLN	3.7
1	B	117	TYR	3.7
1	D	113	ASN	3.7
1	B	133	ARG	3.6
1	B	185	LEU	3.6
1	D	257	LEU	3.6
1	D	119	SER	3.6
1	B	186	LYS	3.6
1	C	100	CYS	3.6
1	C	272	HIS	3.6
1	D	54	ILE	3.6
1	A	108	PHE	3.6
1	C	22	GLU	3.6
1	D	241	ALA	3.6
1	C	190	GLY	3.6
1	C	266	ARG	3.6
1	B	193	LYS	3.6
1	C	189	PHE	3.6
1	D	101	ARG	3.6
1	D	179	ALA	3.6
1	D	87[A]	GLU	3.6
1	C	20	TYR	3.6
1	D	5	ILE	3.5
1	C	250	PHE	3.5
1	C	3	VAL	3.5
1	B	184	ARG	3.5
1	D	187	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	270	GLU	3.5
1	C	139	ILE	3.5
1	D	170	ALA	3.5
1	D	256	ALA	3.5
1	C	63[A]	ASP	3.5
1	D	175	ASP	3.5
1	A	132	VAL	3.5
1	B	3	VAL	3.5
1	C	81	VAL	3.5
1	D	138	LEU	3.5
1	C	183	GLU	3.5
1	D	141	TYR	3.5
1	C	265	ALA	3.5
1	D	240	ALA	3.5
1	C	74	ILE	3.5
1	C	196	LYS	3.5
1	C	138	LEU	3.5
1	D	172	THR	3.5
1	B	188	ASP	3.4
1	C	175	ASP	3.4
1	D	258	LYS	3.4
1	D	209	ALA	3.4
1	C	181	LEU	3.4
1	D	166	VAL	3.4
1	D	251	VAL	3.4
1	C	242	THR	3.4
1	D	207	THR	3.4
1	C	194	ASN	3.4
1	C	264	ALA	3.4
1	D	133	ARG	3.4
1	D	13	PHE	3.4
1	D	108	PHE	3.4
1	C	83	LEU	3.4
1	A	193	LYS	3.4
1	C	82	GLY	3.4
1	C	172	THR	3.4
1	C	239	GLY	3.4
1	C	249	GLY	3.4
1	C	66[A]	CYS	3.4
1	B	265	ALA	3.4
1	B	116	GLN	3.4
1	C	27	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	197	GLY	3.4
1	B	67	VAL	3.4
1	B	109	VAL	3.4
1	A	179	ALA	3.3
1	A	264	ALA	3.3
1	C	136	ALA	3.3
1	C	141	TYR	3.3
1	A	106	ASP	3.3
1	D	22	GLU	3.3
1	D	188	ASP	3.3
1	B	238	PHE	3.3
1	A	266	ARG	3.3
1	C	134	PRO	3.3
1	D	262	ALA	3.3
1	D	144	ARG	3.3
1	B	199	LEU	3.3
1	A	189	PHE	3.3
1	C	23	LYS	3.3
1	C	187	SER	3.3
1	C	169	LEU	3.3
1	C	174	GLN	3.3
1	D	148	PRO	3.3
1	D	34	CYS	3.3
1	C	102	VAL	3.3
1	C	195	SER	3.2
1	A	185	LEU	3.2
1	B	180	LYS	3.2
1	D	213	PRO	3.2
1	D	27	LEU	3.2
1	D	183	GLU	3.2
1	D	248	PHE	3.2
1	C	154	GLY	3.2
1	D	29	ALA	3.2
1	A	187	SER	3.2
1	A	188	ASP	3.2
1	B	91	GLU	3.2
1	C	60	ILE	3.2
1	C	95	GLN	3.2
1	C	267	GLN	3.2
1	D	263	LYS	3.2
1	B	119	SER	3.2
1	D	140	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	23	LYS	3.1
1	A	180	LYS	3.1
1	D	111	PRO	3.1
1	D	198	LYS	3.1
1	C	156	GLY	3.1
1	D	130	ASP	3.1
1	C	86	ALA	3.1
1	D	86	ALA	3.1
1	B	152	THR	3.1
1	C	80	ASN	3.1
1	C	166	VAL	3.1
1	D	20	TYR	3.1
1	A	155	ALA	3.1
1	D	178	ALA	3.1
1	A	186	LYS	3.1
1	C	193	LYS	3.1
1	D	186	LYS	3.1
1	B	114	VAL	3.1
1	C	165	GLN	3.1
1	A	198	LYS	3.1
1	D	24	ALA	3.1
1	D	252	ALA	3.1
1	A	183	GLU	3.1
1	C	125	VAL	3.0
1	A	184	ARG	3.0
1	B	78	ARG	3.0
1	A	129	ILE	3.0
1	C	49	LEU	3.0
1	D	31	ALA	3.0
1	C	207	THR	3.0
1	D	110	THR	3.0
1	D	63	ASP	3.0
1	D	127	ASP	3.0
1	A	267	GLN	3.0
1	C	251	VAL	3.0
1	C	268	GLY	3.0
1	B	183	GLU	3.0
1	A	110	THR	3.0
1	B	210	LEU	3.0
1	C	128	ALA	3.0
1	C	256	ALA	3.0
1	D	112	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	3.0
1	D	9	TRP	3.0
1	C	247	THR	3.0
1	B	138	LEU	3.0
1	D	77	LEU	3.0
1	D	96	ILE	3.0
1	A	171	LYS	3.0
1	D	66	CYS	3.0
1	D	40	GLY	3.0
1	D	7	ASP	2.9
1	D	88	VAL	2.9
1	D	125	VAL	2.9
1	C	151	THR	2.9
1	C	179	ALA	2.9
1	B	177	LEU	2.9
1	A	194	ASN	2.9
1	C	184	ARG	2.9
1	D	61	ASP	2.9
1	B	215	SER	2.9
1	C	245	THR	2.9
1	D	253	VAL	2.9
1	D	8	ALA	2.9
1	A	5	ILE	2.9
1	C	200	GLY	2.9
1	D	143	ARG	2.9
1	D	266	ARG	2.9
1	C	255	HIS	2.9
1	B	150	VAL	2.9
1	A	144[A]	ARG	2.9
1	D	190	GLY	2.9
1	A	177	LEU	2.9
1	A	130	ASP	2.9
1	C	44	TRP	2.9
1	B	28	PHE	2.8
1	C	144	ARG	2.8
1	D	48	ALA	2.8
1	C	263	LYS	2.8
1	D	202	ASP	2.8
1	B	141	TYR	2.8
1	B	27	LEU	2.8
1	B	134	PRO	2.8
1	C	111	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	164	ILE	2.8
1	D	78	ARG	2.8
1	B	214	GLN	2.8
1	D	247	THR	2.8
1	A	196	LYS	2.8
1	C	7	ASP	2.8
1	B	56	ALA	2.8
1	B	200	GLY	2.8
1	C	31	ALA	2.8
1	C	48	ALA	2.8
1	B	4	VAL	2.8
1	C	150	VAL	2.8
1	B	34	CYS	2.8
1	B	100	CYS	2.8
1	A	147	ILE	2.8
1	D	103	THR	2.8
1	D	260	MET	2.8
1	B	175	ASP	2.8
1	A	82	GLY	2.8
1	B	105	VAL	2.8
1	C	244	VAL	2.8
1	D	65	VAL	2.8
1	C	261	MET	2.8
1	C	112	ASP	2.8
1	D	58	THR	2.8
1	B	131	SER	2.8
1	D	136	ALA	2.7
1	C	104	VAL	2.7
1	D	259	LYS	2.7
1	A	83	LEU	2.7
1	B	20	TYR	2.7
1	C	168	ASP	2.7
1	C	38	ILE	2.7
1	A	190	GLY	2.7
1	D	154	GLY	2.7
1	D	50	ALA	2.7
1	D	84	ALA	2.7
1	D	118	MET	2.7
1	D	176	PRO	2.7
1	D	44	TRP	2.7
1	D	105	VAL	2.7
1	D	132	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	203	CYS	2.7
1	C	19	LEU	2.7
1	D	100	CYS	2.7
1	A	10	ARG	2.7
1	B	33	ILE	2.7
1	B	126	ILE	2.7
1	D	55	GLY	2.7
1	A	7	ASP	2.7
1	A	169	LEU	2.7
1	B	142	CYS	2.7
1	B	149	LEU	2.7
1	C	41	VAL	2.7
1	C	162	THR	2.7
1	D	39	GLY	2.7
1	B	57	ILE	2.7
1	C	5	ILE	2.7
1	D	57	ILE	2.7
1	D	64	ASP	2.7
1	B	179	ALA	2.7
1	C	262	ALA	2.7
1	D	182	ARG	2.6
1	B	205	PHE	2.6
1	A	197	GLY	2.6
1	B	198	LYS	2.6
1	C	185	LEU	2.6
1	D	60	ILE	2.6
1	A	175	ASP	2.6
1	A	176	PRO	2.6
1	D	206	SER	2.6
1	C	186	LYS	2.6
1	C	157	GLY	2.6
1	C	96	ILE	2.6
1	D	155	ALA	2.6
1	C	148	PRO	2.6
1	C	180	LYS	2.6
1	D	98	PRO	2.6
1	B	118	MET	2.6
1	A	63	ASP	2.6
1	C	160	ASP	2.6
1	A	114	VAL	2.6
1	B	124	TYR	2.6
1	C	124	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	204	VAL	2.6
1	C	129	ILE	2.6
1	D	156	GLY	2.5
1	B	110	THR	2.5
1	D	162	THR	2.5
1	B	123	SER	2.5
1	C	149[A]	LEU	2.5
1	C	198	LYS	2.5
1	B	241	ALA	2.5
1	C	252	ALA	2.5
1	D	145	ASN	2.5
1	C	11	GLN	2.5
1	C	64	ASP	2.5
1	B	147	ILE	2.5
1	D	38	ILE	2.5
1	C	153	GLY	2.5
1	D	249	GLY	2.5
1	C	243	MET	2.5
1	C	25	LEU	2.5
1	C	28	PHE	2.5
1	C	46	ALA	2.5
1	C	50	ALA	2.5
1	B	139	ILE	2.5
1	B	263	LYS	2.5
1	C	147	ILE	2.5
1	C	87	GLU	2.5
1	A	172	THR	2.5
1	B	207	THR	2.5
1	D	245	THR	2.5
1	A	22	GLU	2.4
1	A	205	PHE	2.4
1	C	171	LYS	2.4
1	A	200	GLY	2.4
1	B	121	GLY	2.4
1	C	18	ARG	2.4
1	D	37	GLY	2.4
1	C	68	THR	2.4
1	D	93	ILE	2.4
1	C	127	ASP	2.4
1	C	34	CYS	2.4
1	C	142	CYS	2.4
1	C	9	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	19	LEU	2.4
1	D	42	GLY	2.4
1	A	238	PHE	2.4
1	B	137	ALA	2.4
1	C	145	ASN	2.4
1	C	163	GLN	2.4
1	C	117	TYR	2.4
1	D	244	VAL	2.4
1	D	30	ASP	2.4
1	A	111	PRO	2.4
1	D	123	SER	2.4
1	D	49	LEU	2.4
1	C	78	ARG	2.4
1	C	143	ARG	2.4
1	C	259	LYS	2.4
1	C	33	ILE	2.4
1	D	116	GLN	2.3
1	C	39	GLY	2.3
1	D	91	GLU	2.3
1	B	84	ALA	2.3
1	C	17	ALA	2.3
1	C	130	ASP	2.3
1	C	240	ALA	2.3
1	C	260	MET	2.3
1	D	62	MET	2.3
1	A	253	VAL	2.3
1	C	35	VAL	2.3
1	C	36	VAL	2.3
1	D	95	GLN	2.3
1	B	21	GLY	2.3
1	C	99	GLU	2.3
1	D	18	ARG	2.3
1	D	160	ASP	2.3
1	B	172	THR	2.3
1	D	242	THR	2.3
1	A	178	ALA	2.3
1	B	24	ALA	2.3
1	B	115	ALA	2.3
1	C	84	ALA	2.3
1	A	149	LEU	2.3
1	B	59	LEU	2.3
1	B	83	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	159	ILE	2.3
1	B	237	GLY	2.3
1	C	79	ASP	2.3
1	B	31	ALA	2.3
1	B	181	LEU	2.3
1	A	101	ARG	2.3
1	B	187	SER	2.3
1	B	55	GLY	2.3
1	D	15	GLY	2.3
1	D	26	GLN	2.2
1	D	32	HIS	2.2
1	B	140	ALA	2.2
1	C	43	SER	2.2
1	C	146	LYS	2.2
1	B	156	GLY	2.2
1	C	40	GLY	2.2
1	A	20	TYR	2.2
1	C	122	TYR	2.2
1	A	166	VAL	2.2
1	C	70	THR	2.2
1	B	145	ASN	2.2
1	C	76	ALA	2.2
1	C	178	ALA	2.2
1	D	76	ALA	2.2
1	D	52	THR	2.2
1	A	146	LYS	2.2
1	B	81	VAL	2.2
1	B	146	LYS	2.2
1	B	244	VAL	2.2
1	C	56	ALA	2.2
1	A	78	ARG	2.2
1	B	173	ILE	2.2
1	C	65	VAL	2.1
1	D	17	ALA	2.1
1	B	112	ASP	2.1
1	C	13	PHE	2.1
1	C	106	ASP	2.1
1	D	243	MET	2.1
1	A	11	GLN	2.1
1	A	12	ARG	2.1
1	A	204	VAL	2.1
1	D	45	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	14	GLY	2.1
1	D	239	GLY	2.1
1	C	30	ASP	2.1
1	D	43	SER	2.1
1	B	101	ARG	2.1
1	D	10	ARG	2.1
1	A	38	ILE	2.1
1	B	74	ILE	2.1
1	A	17	ALA	2.1
1	A	136	ALA	2.1
1	C	45	ALA	2.1
1	D	208	GLU	2.1
1	D	261	MET	2.1
1	A	19	LEU	2.1
1	A	27	LEU	2.1
1	B	167	THR	2.1
1	B	248	PHE	2.1
1	B	129	ILE	2.1
1	D	74	ILE	2.1
1	A	201	VAL	2.0
1	B	201	VAL	2.0
1	B	211	VAL	2.0
1	C	105	VAL	2.0
1	A	77	LEU	2.0
1	B	19	LEU	2.0
1	D	59	LEU	2.0
1	A	162	THR	2.0
1	D	11	GLN	2.0
1	C	126	ILE	2.0
1	D	250	PHE	2.0
1	B	8	ALA	2.0
1	C	90	ALA	2.0
1	D	102	VAL	2.0
1	A	263	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

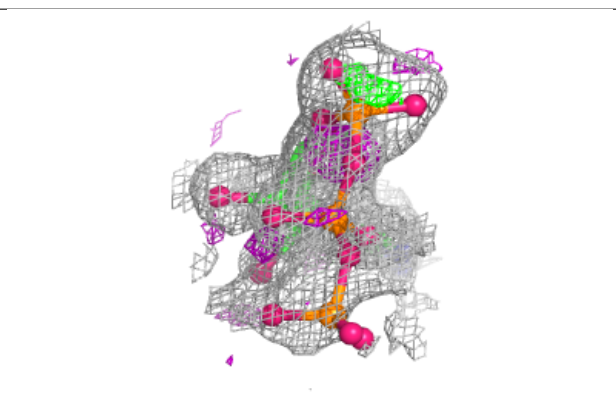
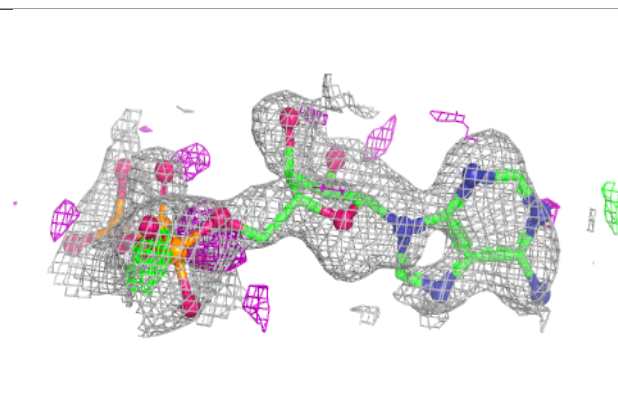
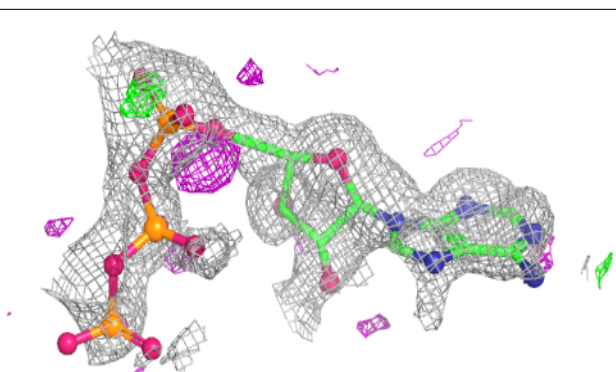
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	D	302	1/1	0.61	0.24	24,24,24,24	0
4	GOL	B	502	6/6	0.62	0.33	37,70,103,109	0
2	K	B	301	1/1	0.63	0.14	18,18,18,18	1
2	K	C	301	1/1	0.66	0.16	20,20,20,20	1
4	GOL	C	502	6/6	0.67	0.29	38,59,65,68	0
4	GOL	C	501	6/6	0.67	0.21	29,39,54,63	0
2	K	D	301	1/1	0.69	0.15	24,24,24,24	1
4	GOL	D	501	6/6	0.70	0.21	31,41,46,81	0
3	ATP	C	401	31/31	0.76	0.20	27,66,179,229	0
4	GOL	A	501	6/6	0.79	0.20	34,44,58,85	0
3	ATP	D	401	31/31	0.81	0.15	21,28,76,99	0
2	K	A	301	1/1	0.82	0.10	18,18,18,18	1
5	NA	B	302	1/1	0.82	0.12	23,23,23,23	0
3	ATP	B	401	31/31	0.82	0.16	25,60,177,208	0
4	GOL	A	502	6/6	0.83	0.18	29,55,72,73	0
4	GOL	B	501	6/6	0.83	0.15	24,27,34,44	0
3	ATP	A	401	31/31	0.84	0.15	24,37,130,182	0

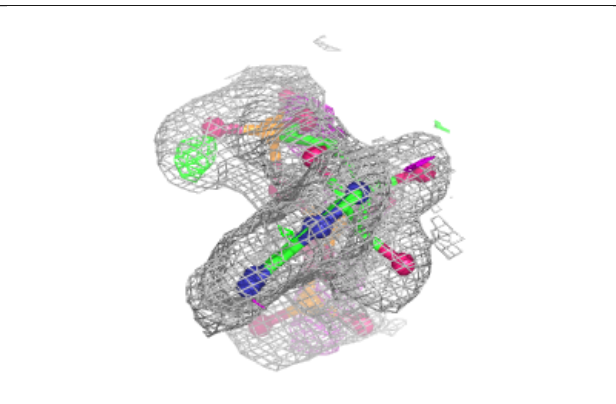
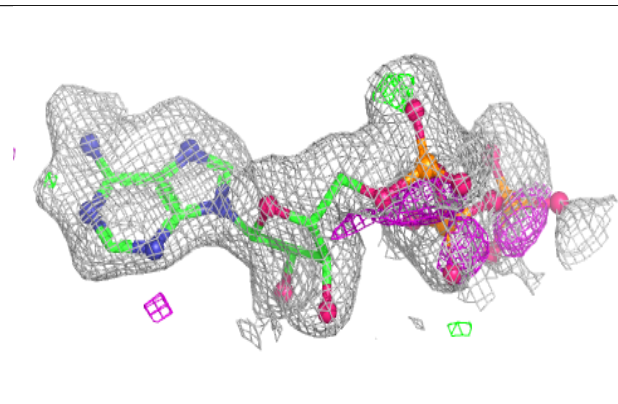
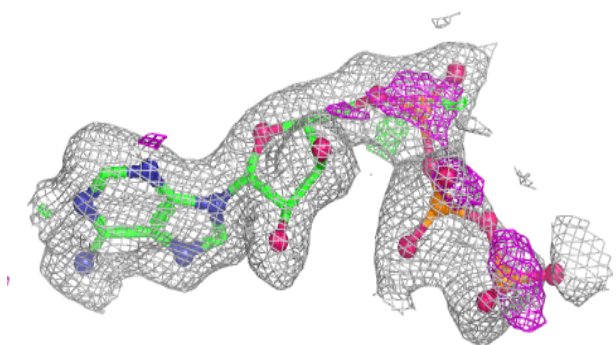
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 401:

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

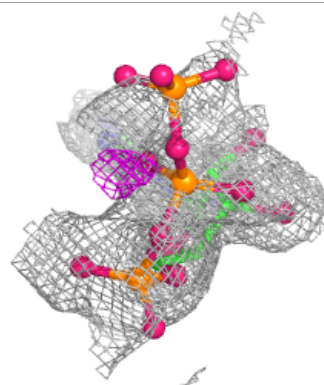
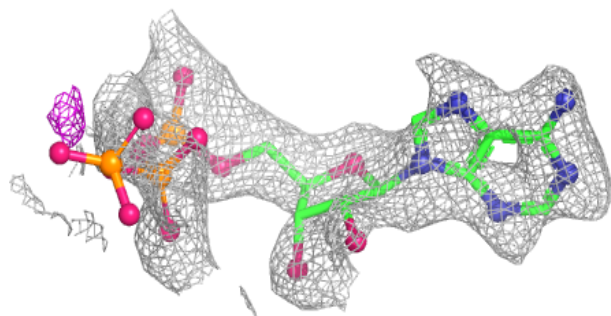
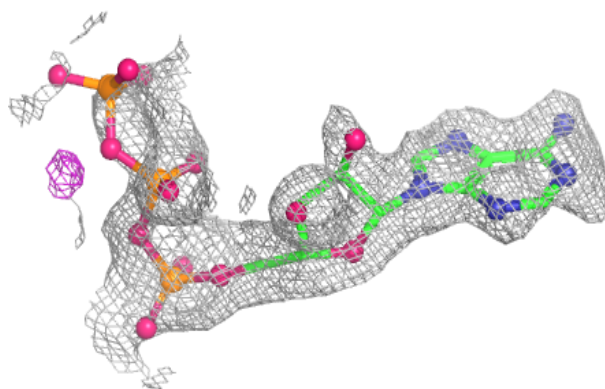
**Electron density around ATP D 401:**

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

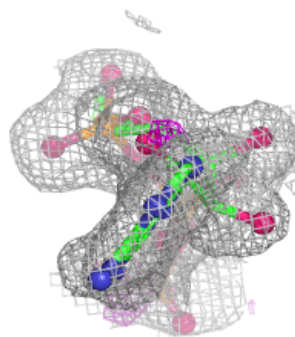
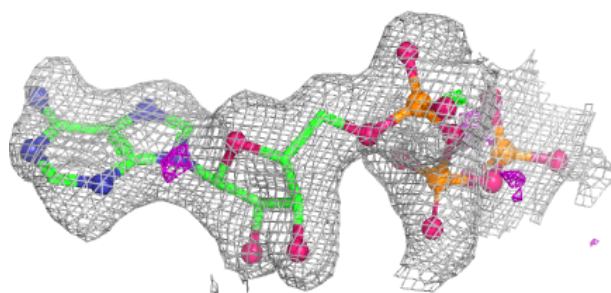
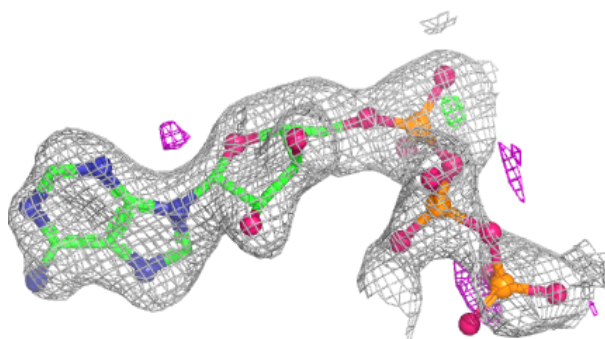


Electron density around ATP B 401:

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

**Electron density around ATP A 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.