W O R L D W I D E

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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 10:25 am GMT

PDB ID	:	2J3M
Title	:	PROLYL-TRNA SYNTHETASE FROM ENTEROCOCCUS FAECALIS COMPLEXED WITH ATP, manganese and prolinol
Authors	:	Crepin, T.; Yaremchuk, A.; Tukalo, M.; Cusack, S.
Deposited on	:	2006-08-22
Resolution	:	2.30 Å(reported)

PERCENTILES INFOmissingINFO

1 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9247 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	1	0
			4396	2772	742	862	20			
1	B	558	Total	C	N	O	S	0	0	0
			4406	2775	745	865	21			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
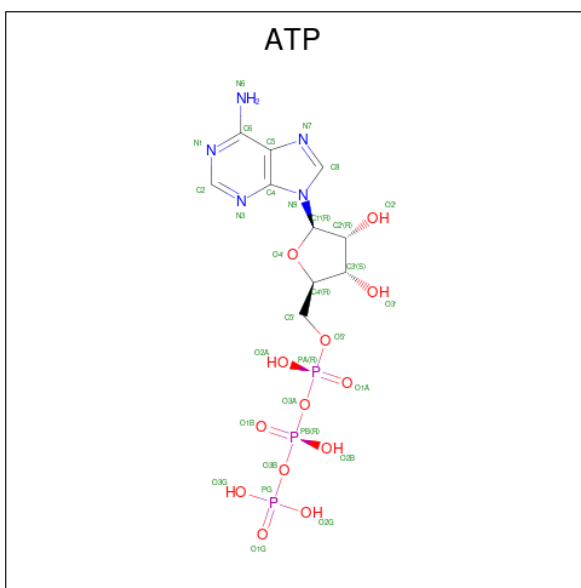
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is PYRROLIDINE-2-CARBALDEHYDE (three-letter code: PRI) (formula: C_5H_9NO).

PRI

OT1

N

H

N

CD

C

CA(S)

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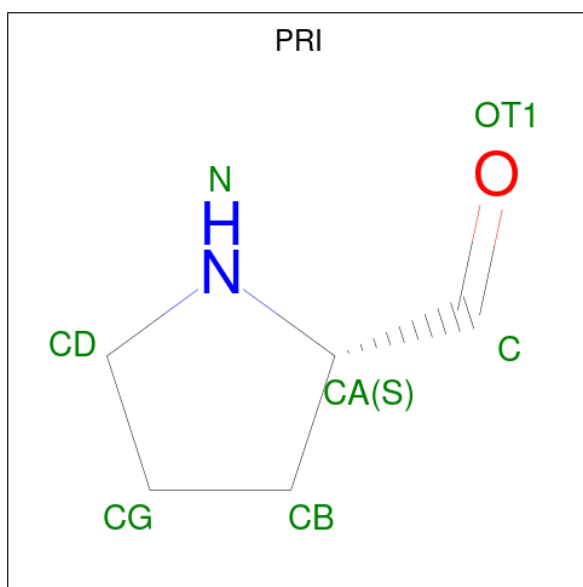
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 7	C 5	N 1	O 1	0	0
3	B	1	Total 7	C 5	N 1	O 1	0	0

• Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mn 2	0	0
4	B	4	Total 4	Mn 4	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	201	Total 201	O 201	0	0
5	B	162	Total 162	O 162	0	0

2 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: PROLYL-TRNA SYNTHETASE
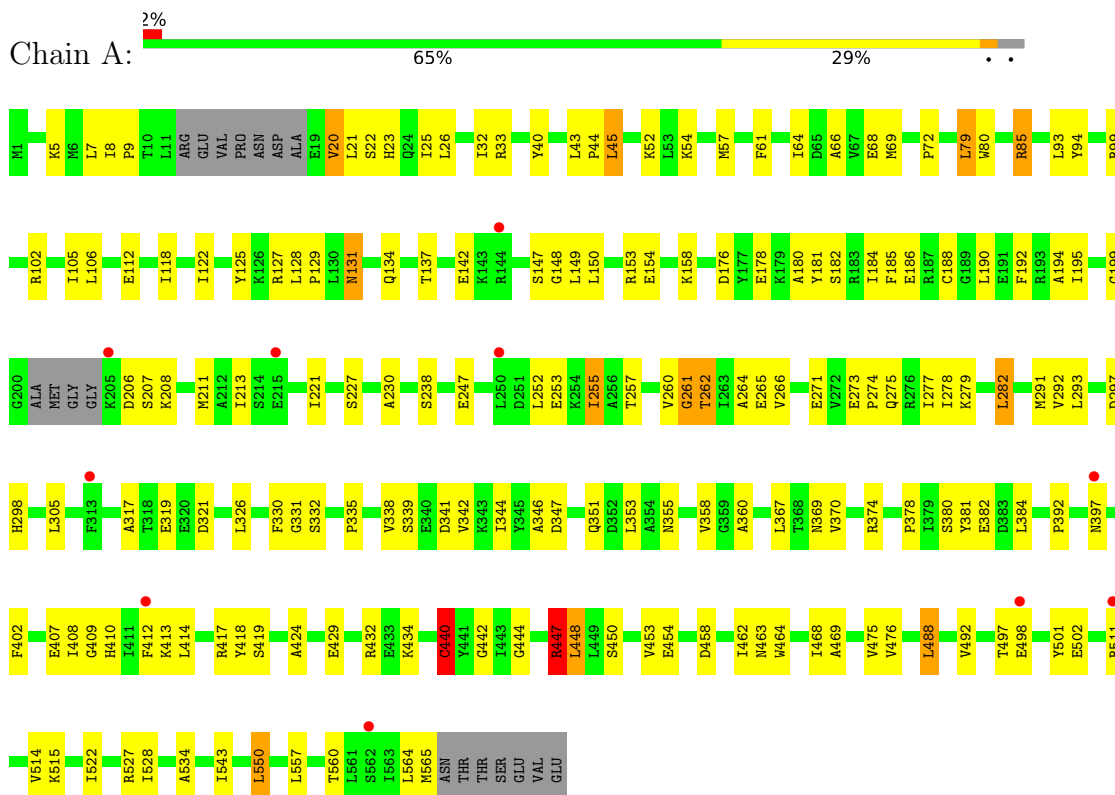
- Molecule 1: PROLYL-TRNA SYNTHETASE
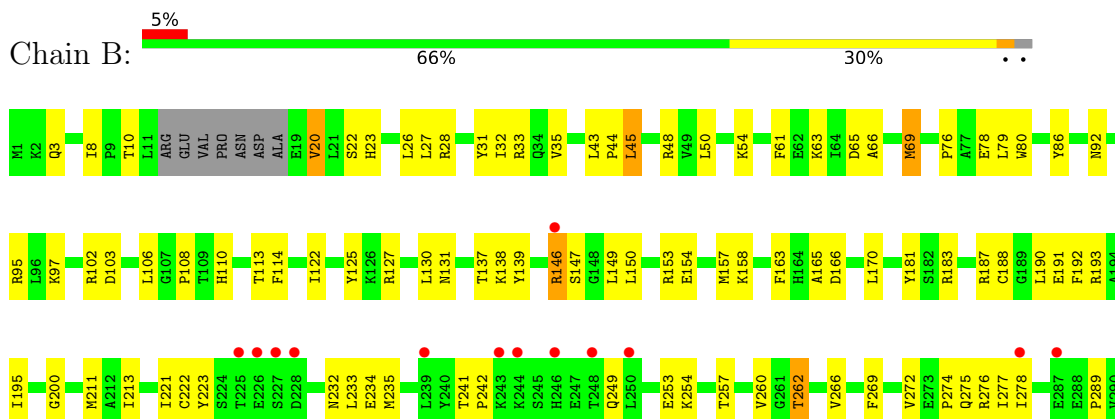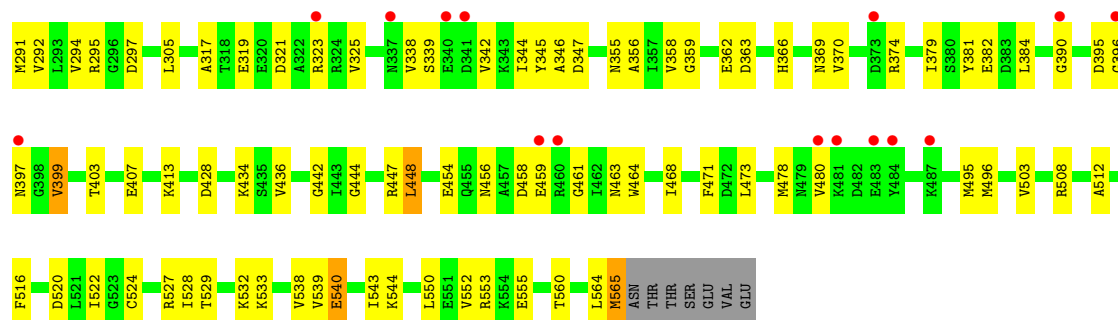
3   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.58Å 92.68Å 101.22Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	29.49 – 2.30 29.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.49-2.30) 100.0 (29.44-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.36 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.260 0.190 , 0.251	Depositor DCC
R_{free} test set	1894 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 34.9	EDS
L-test for twinning[2]	$<\lvert L \rvert> = 0.47$, $<L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9247	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<\lvert L \rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

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	0.81	2/4468 (0.0%)	0.84	3/6027 (0.0%)
1	B	0.77	2/4478 (0.0%)	0.81	1/6041 (0.0%)
All	All	0.79	4/8946 (0.0%)	0.83	4/12068 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	CYS	CB-SG	-5.64	1.72	1.81
1	B	407	GLU	CG-CD	-5.39	1.43	1.51
1	B	540	GLU	CG-CD	5.13	1.59	1.51
1	A	271	GLU	CG-CD	5.05	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	447	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	85	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	130	LEU	CB-CG-CD1	-5.07	102.38	111.00

There are no chirality outliers.

There are no planarity outliers.

4.2 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	4396	0	4350	136	2
1	B	4406	0	4363	135	1
2	A	31	0	12	2	0
2	B	31	0	12	5	0
3	A	7	0	9	2	0
3	B	7	0	9	7	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
5	A	201	0	0	7	0
5	B	162	0	0	4	0
All	All	9247	0	8755	267	2

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 15.

The worst 5 of 267 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:146:ARG:H	1:B:146:ARG:HD2	1.05	1.12
1:A:543:ILE:HD12	1:A:565:MET:HE1	1.44	0.95
1:A:25:ILE:HD13	1:A:462:ILE:HG12	1.50	0.93
1:B:146:ARG:HD2	1:B:146:ARG:N	1.84	0.92
1:A:255:ILE:HB	5:A:2101:HOH:O	1.74	0.85

All (2) 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:432:ARG:NH2	1:B:200:GLY:O[1_655]	1.91	0.29
1:A:102:ARG:NH1	1:A:273:GLU:OE2[2_655]	2.16	0.04

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	549/572 (96%)	530 (96%)	18 (3%)	1 (0%)	47	58
1	B	554/572 (97%)	524 (95%)	26 (5%)	4 (1%)	22	26
All	All	1103/1144 (96%)	1054 (96%)	44 (4%)	5 (0%)	29	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	GLY
1	B	242	PRO
1	B	20	VAL
1	B	262	THR
1	A	261	GLY

4.3.2 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	474/487 (97%)	458 (97%)	16 (3%)	37	51
1	B	474/487 (97%)	457 (96%)	17 (4%)	35	49
All	All	948/974 (97%)	915 (96%)	33 (4%)	36	50

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	458	ASP
1	B	532	LYS
1	B	565	MET
1	A	447	ARG
1	A	440	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN

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Mol	Chain	Res	Type
1	B	92	ASN
1	B	456	ASN
1	B	131	ASN
1	A	337	ASN

4.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6   Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
3	PRI	B	1566	-	5,7,7	0.52	0	7,8,8	1.34	0
2	ATP	B	701	4	26,33,33	0.93	0	31,52,52	1.44	5 (16%)
2	ATP	A	701	4	26,33,33	0.86	1 (3%)	31,52,52	1.60	5 (16%)
3	PRI	A	1566	-	5,7,7	0.88	0	7,8,8	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PRI	B	1566	-	-	0/0/9/9	0/1/1/1
2	ATP	B	701	4	-	5/18/38/38	0/3/3/3
2	ATP	A	701	4	-	3/18/38/38	0/3/3/3
3	PRI	A	1566	-	-	0/0/9/9	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ATP	C5-C4	2.28	1.46	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	ATP	N3-C2-N1	-4.69	121.35	128.68
2	B	701	ATP	N3-C2-N1	-3.67	122.95	128.68
2	A	701	ATP	C2-N1-C6	3.45	124.65	118.75
2	B	701	ATP	C4-C5-N7	-2.84	106.44	109.40
2	A	701	ATP	PB-O3B-PG	-2.51	124.22	132.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ATP	C5'-O5'-PA-O1A
2	B	701	ATP	C5'-O5'-PA-O1A
2	B	701	ATP	C5'-O5'-PA-O3A
2	A	701	ATP	C5'-O5'-PA-O2A
2	B	701	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1566	PRI	7	0
2	B	701	ATP	5	0
2	A	701	ATP	2	0
3	A	1566	PRI	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ATP B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 701

Bond lengths

Bond angles

Torsions

Rings
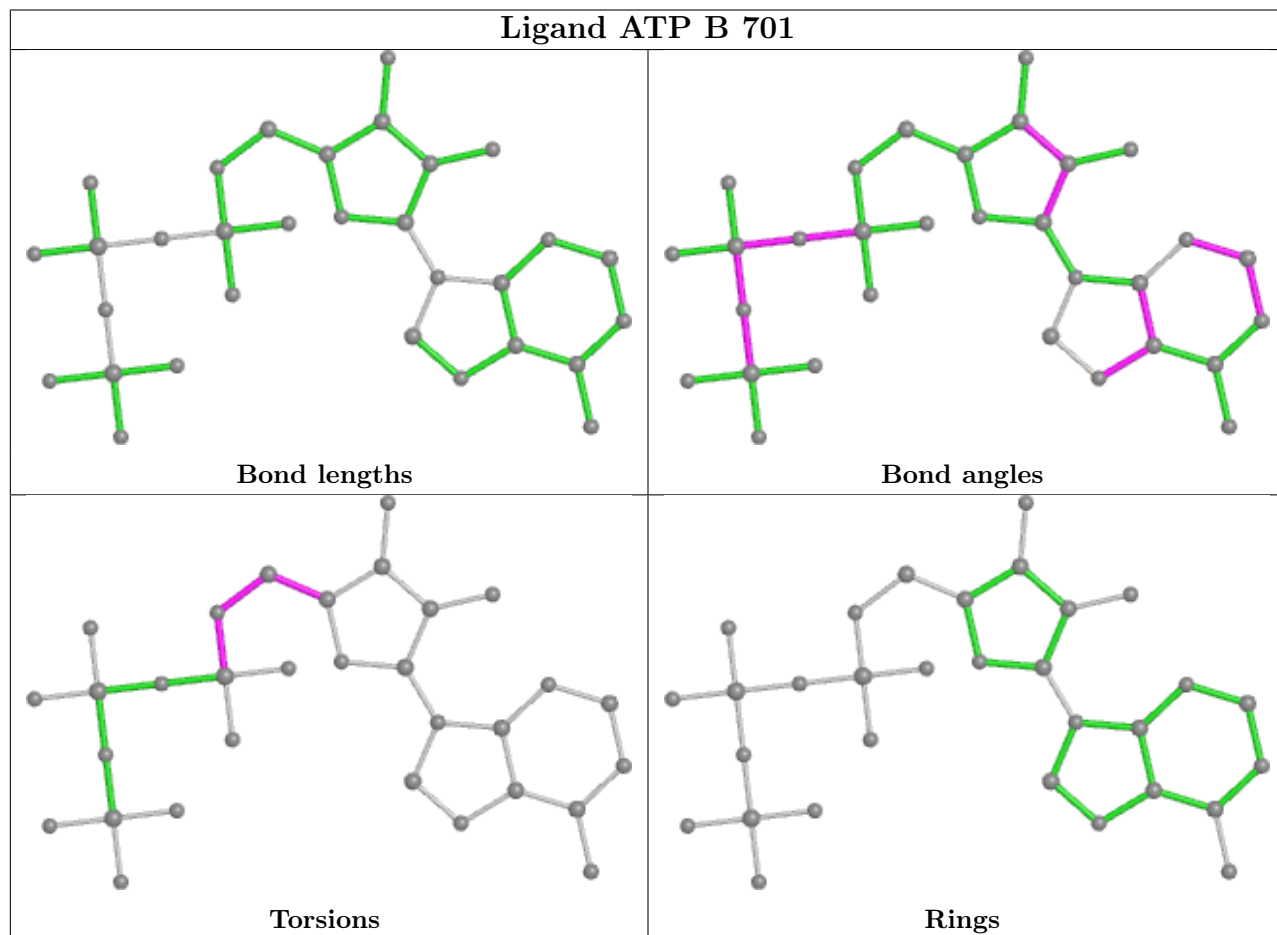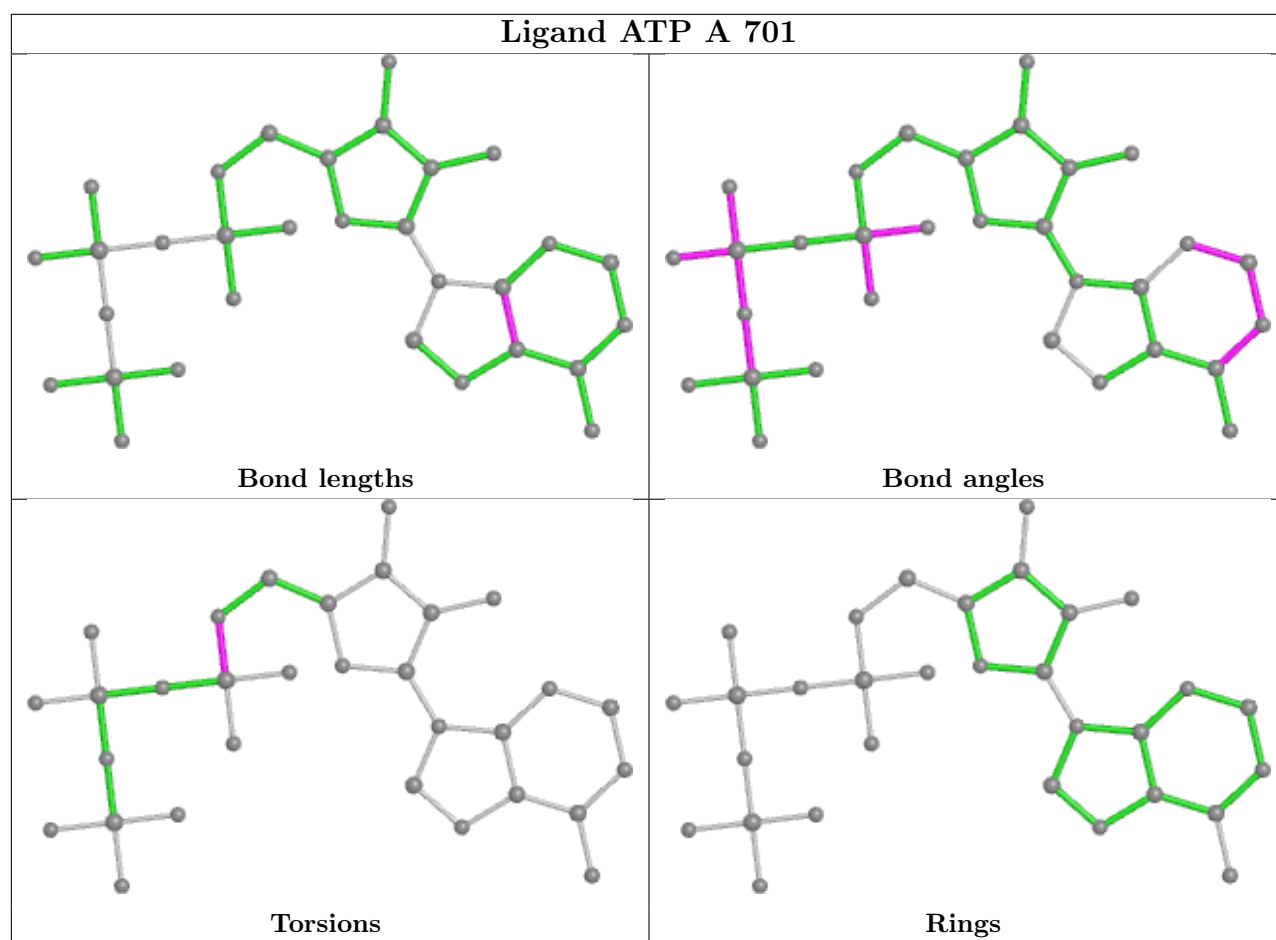
4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	554/572 (96%)	0.11	10 (1%)	68	74	7, 19, 30, 40	0
1	B	558/572 (97%)	0.33	28 (5%)	28	35	8, 22, 42, 63	0
All	All	1112/1144 (97%)	0.22	38 (3%)	45	52	7, 21, 37, 63	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	HIS	6.3
1	B	248	THR	4.3
1	B	484	TYR	3.8
1	A	412[A]	PHE	3.5
1	B	244	LYS	3.5

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

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

5.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.4 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(Å^2)	Q<0.9
3	PRI	A	1566	7/7	0.86	0.45	58,58,59,59	0
3	PRI	B	1566	7/7	0.90	0.28	38,38,38,39	0
2	ATP	A	701	31/31	0.98	0.12	7,11,18,20	0
2	ATP	B	701	31/31	0.98	0.10	5,14,19,23	0
4	MN	A	1567	1/1	0.98	0.10	17,17,17,17	0
4	MN	A	1568	1/1	0.98	0.09	22,22,22,22	0
4	MN	B	1568	1/1	0.98	0.07	28,28,28,28	0
4	MN	B	1569	1/1	0.98	0.07	29,29,29,29	0
4	MN	B	1570	1/1	0.98	0.08	24,24,24,24	0
4	MN	B	1567	1/1	0.99	0.06	23,23,23,23	0

5.5　Other polymers ⓘ

There are no such residues in this entry.