



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:15 AM UTC

PDB ID : 2QUI / pdb_00002qui
Title : Crystal structures of human tryptophanyl-tRNA synthetase in complex with
Tryptophanamide and ATP
Authors : Shen, N.; Ding, J.P.
Deposited on : 2007-08-05
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

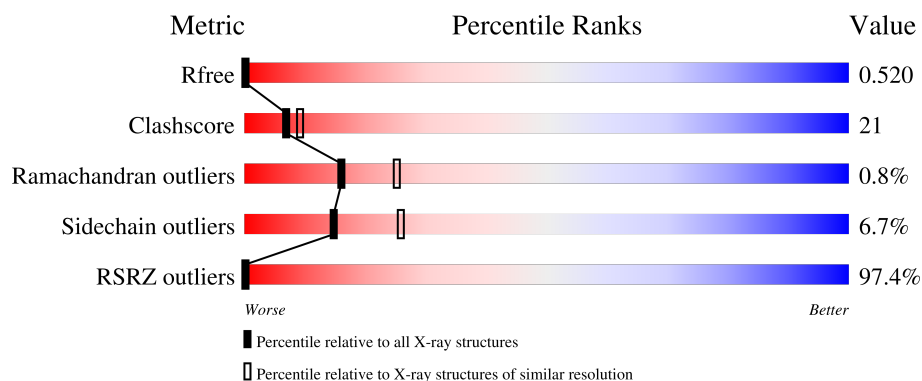
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	477	79% 19% 56% 7% 18%
1	B	477	78% 27% 46% 6% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LTN	A	501	-	X	X	-
3	LTN	B	478	-	X	-	-
4	ATP	A	502	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6469 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3127	2005	525	582	15			
1	B	379	Total	C	N	O	S	0	0	0
			3054	1960	519	560	15			

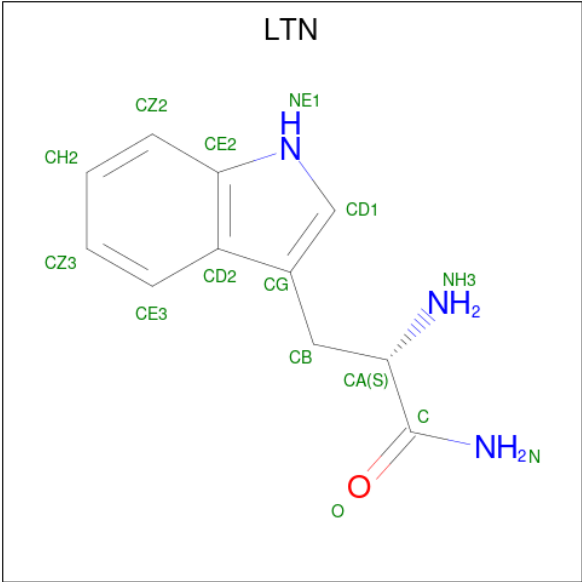
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	472	HIS	-	expression tag	UNP P23381
A	473	HIS	-	expression tag	UNP P23381
A	474	HIS	-	expression tag	UNP P23381
A	475	HIS	-	expression tag	UNP P23381
A	476	HIS	-	expression tag	UNP P23381
A	477	HIS	-	expression tag	UNP P23381
B	472	HIS	-	expression tag	UNP P23381
B	473	HIS	-	expression tag	UNP P23381
B	474	HIS	-	expression tag	UNP P23381
B	475	HIS	-	expression tag	UNP P23381
B	476	HIS	-	expression tag	UNP P23381
B	477	HIS	-	expression tag	UNP P23381

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

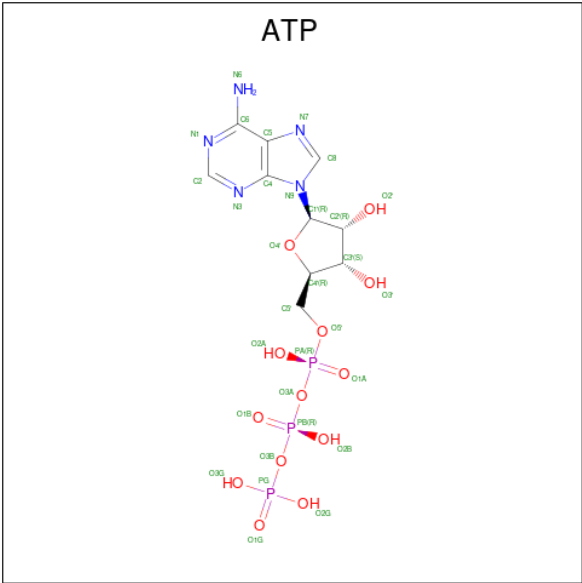
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is L-TRYPTOPHANAMIDE (CCD ID: LTN) (formula: C₁₁H₁₃N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	3	1		
3	B	1	Total	C	N	O	0	0
			15	11	3	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

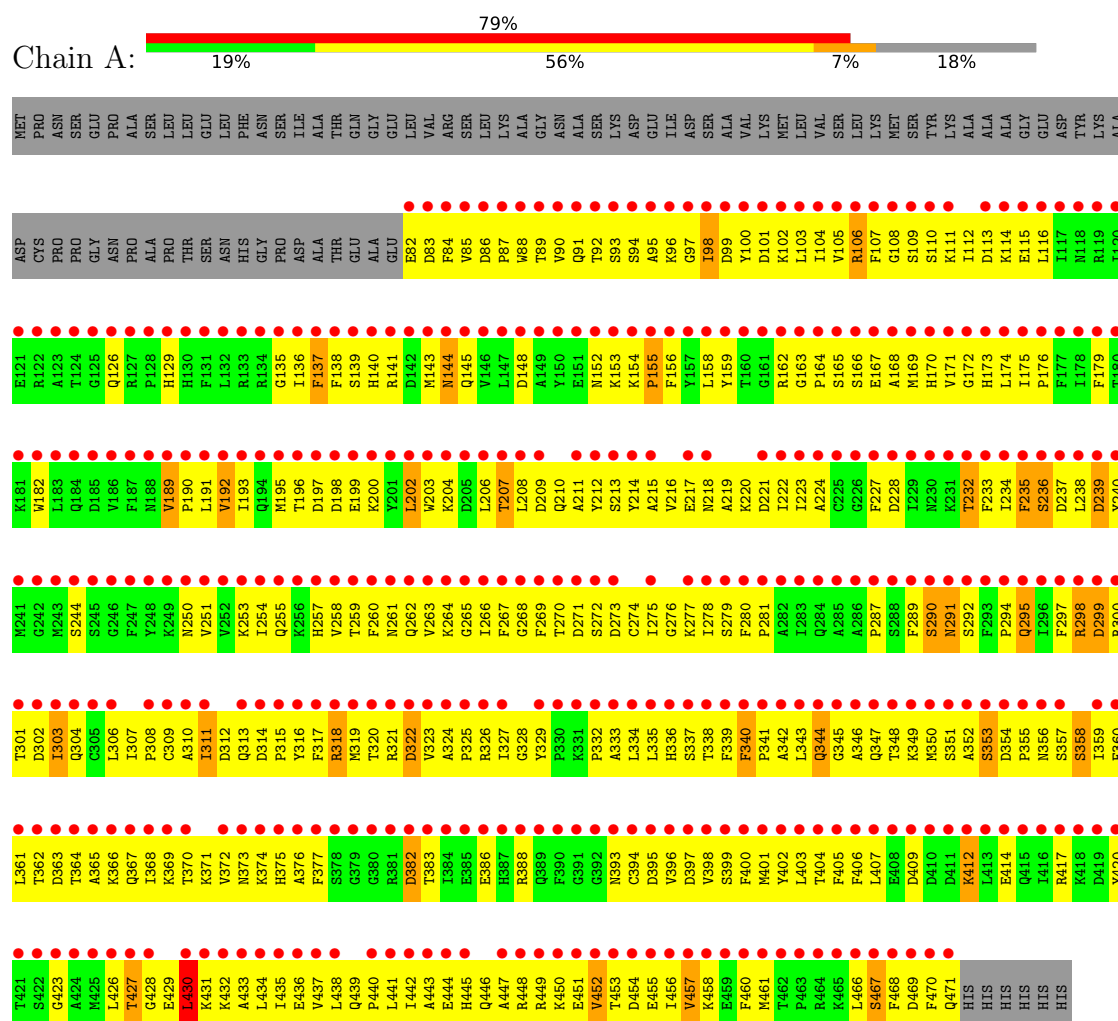


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total 120	O 120	0	0
5	B	106	Total 106	O 106	0	0

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: Tryptophanyl-tRNA synthetase



T421	L361	T301	W241	K181	E121	ASP
S422	T362	D302	G242	W182	R122	CYS
G423	D363	D303	M243	L183	A123	PRO
A424	T364	Q304	S244	Q184	T124	PRO
N425	A365	C305	G245	D185	G125	GLY
L426	K366	L306	G246	V186	Q126	ASN
T427	Q367	I307	F247	F187	F127	PRO
G428	I368	F308	Y248	N188	P128	ALA
E429	K369	C309	K249	V189	H129	ALA
L430	T370	A310	N250	P190	H130	PRO
K431	K371	I311	V251	L191	F131	THR
K432	V372	D312	V252	V192	L132	ASN
N433	N373	Q313	K253	I193	R133	HIS
L434	K374	D314	I254	Q194	R134	GLY
L435	H375	F315	Q255	M195	G135	PRO
E436	A376	Y316	K256	T196	I136	ASP
V437	F377	R317	H257	D197	F137	ALA
L438	S378	R318	V258	D198	F138	THR
Q439	G379	M319	T259	E199	S139	GLU
P440	G380	T320	F260	K200	H140	ALA
L441	R381	R321	N261	Y201	R141	GLU
L442	D382	D322	Q262	L202	D142	GLU
A443	T383	V323	V263	M203	M143	ASP
E444	I384	A324	K264	K204	N144	PHE
H445	F385	P325	G265	D205	Q145	VAL
Q446	E386	R326	I266	L206	V146	ASP
A447	H387	I327	F267	T207	L147	PRO
R448	R388	G328	G268	L208	D148	TRP
R449	Q389	Y329	F269	D209	A149	THR
K450	F390	P330	T270	Q210	Y150	VAL
E451	G391	K331	D271	A211	E151	GLN
V452	G392	P332	S272	Y212	N152	THR
T453	N393	A333	D273	S213	K153	SER
D454	C394	L334	C274	Y214	K154	SER
E455	D395	L335	I275	A215	P155	ALA
L456	V396	H336	G276	V216	F156	ALA
V457	D397	S337	K277	E217	Y157	LYS
K458	V398	T338	I278	N218	L158	I98
E459	S399	F339	I279	A219	Y159	D99
F460	F400	P340	F280	K220	T160	Y100
M461	M401	A341	P281	D221	G161	D101
T462	Y402	A342	A282	I222	R162	K102
P463	L403	L343	I283	I223	G163	L103
R464	T404	Q344	Q284	A224	P164	L104
K465	F405	G345	A285	C225	S165	V105
L466	F406	A346	A286	G226	S166	V106
S467	L407	Q347	P287	F227	E167	F107
F468	E408	T348	S288	D228	A168	G108
D469	D409	K349	F289	I229	M169	S109
F470	D410	M350	S290	N230	H170	S110
Q471	D411	S351	N291	K231	V171	K111
H472	K412	A352	S292	T232	G172	I112
H473	L413	S353	F293	F233	H173	D113
H474	E414	D354	P294	I234	L174	K114
H475	Q415	P355	Q295	F235	I175	E115
HIS	T416	N356	I296	S236	P176	E116
HIS	R417	S357	F297	D237	F177	I117
HIS	K418	S358	R298	L238	I178	M118
HIS	D419	I359	D299	D239	F179	M119
HIS	Y420	F360	R300	Y240	T180	I120

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.70Å 79.70Å 383.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.40) 95.2 (50.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.238 0.508 , 0.520	Depositor DCC
R_{free} test set	2417 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.54 , 497.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.48	EDS
Total number of atoms	6469	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: LTN, ATP, MG

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	0/3204	0.95	11/4331 (0.3%)
1	B	0.44	0/3132	0.94	12/4230 (0.3%)
All	All	0.43	0/6336	0.95	23/8561 (0.3%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	ARG	N-CA-C	-10.11	100.34	111.36
1	A	318	ARG	N-CA-C	-10.07	100.38	111.36
1	B	292	SER	N-CA-C	-8.50	102.91	113.28
1	B	375	HIS	N-CA-C	6.06	121.72	113.97
1	B	438	LEU	N-CA-C	5.98	117.59	111.14

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	3127	0	3049	131	2188
1	B	3054	0	2978	135	1612
2	A	1	0	0	0	0
3	A	15	0	11	1	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	11	1	0
4	A	31	0	12	10	77
5	A	120	0	0	8	109
5	B	106	0	0	4	88
All	All	6469	0	6061	261	3584

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 21.

The worst 5 of 261 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:250:ASN:HD21	1:B:291:ASN:ND2	1.59	0.98
1:A:207:THR:HG22	1:A:210:GLN:H	1.35	0.90
1:A:165:SER:HB2	4:A:502:ATP:O3G	1.73	0.88
1:B:457:VAL:HG12	1:B:461:MET:HE2	1.56	0.88
1:A:250:ASN:HD21	1:A:291:ASN:ND2	1.73	0.87

The worst 5 of 3584 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:318:ARG:N	1:A:442:ILE:CG2[3_365]	0.14	2.06
1:A:322:ASP:N	1:A:443:ALA:O[3_365]	0.19	2.01
1:A:138:PHE:CA	1:A:431:LYS:CG[3_365]	0.20	2.00
1:A:140:HIS:O	1:A:435:ILE:C[3_365]	0.20	2.00
1:A:164:PRO:O	1:A:273:ASP:CG[4_435]	0.20	2.00

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/477 (81%)	366 (94%)	18 (5%)	4 (1%)	12	20
1	B	377/477 (79%)	359 (95%)	16 (4%)	2 (0%)	24	37
All	All	765/954 (80%)	725 (95%)	34 (4%)	6 (1%)	16	25

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	SER
1	B	351	SER
1	A	298	ARG
1	A	353	SER
1	B	350	MET

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	340/416 (82%)	320 (94%)	20 (6%)	18	31
1	B	331/416 (80%)	306 (92%)	25 (8%)	12	21
All	All	671/832 (81%)	626 (93%)	45 (7%)	15	26

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239	ASP
1	B	348	THR
1	B	291	ASN
1	B	301	THR
1	B	393	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	GLN

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Mol	Chain	Res	Type
1	B	375	HIS
1	B	255	GLN
1	B	445	HIS
1	B	344	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	LTN	A	501	-	16,16,16	3.43	11 (68%)	22,22,22	2.35	9 (40%)
3	LTN	B	478	-	16,16,16	3.52	11 (68%)	22,22,22	2.38	9 (40%)
4	ATP	A	502	-	32,33,33	1.20	2 (6%)	48,52,52	1.73	10 (20%)

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	LTN	A	501	-	-	2/8/8/8	0/2/2/2
3	LTN	B	478	-	-	3/8/8/8	0/2/2/2
4	ATP	A	502	-	-	0/22/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	478	LTN	O-C	8.37	1.38	1.23
3	A	501	LTN	O-C	8.18	1.38	1.23
3	B	478	LTN	C-N	-4.58	1.22	1.32
3	A	501	LTN	C-N	-4.54	1.22	1.32
3	B	478	LTN	CD2-CG	-4.50	1.36	1.44

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	478	LTN	CD2-CG-CD1	5.78	112.08	106.16
3	A	501	LTN	CD2-CG-CD1	5.63	111.91	106.16
3	B	478	LTN	CE2-CD2-CG	-5.47	101.64	107.17
3	A	501	LTN	CE2-CD2-CG	-5.34	101.78	107.17
4	A	502	ATP	C5-C4-N3	-5.25	119.49	126.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	LTN	O-C-CA-NH3
3	B	478	LTN	O-C-CA-NH3
3	A	501	LTN	O-C-CA-CB
3	B	478	LTN	O-C-CA-CB
3	B	478	LTN	N-C-CA-CB

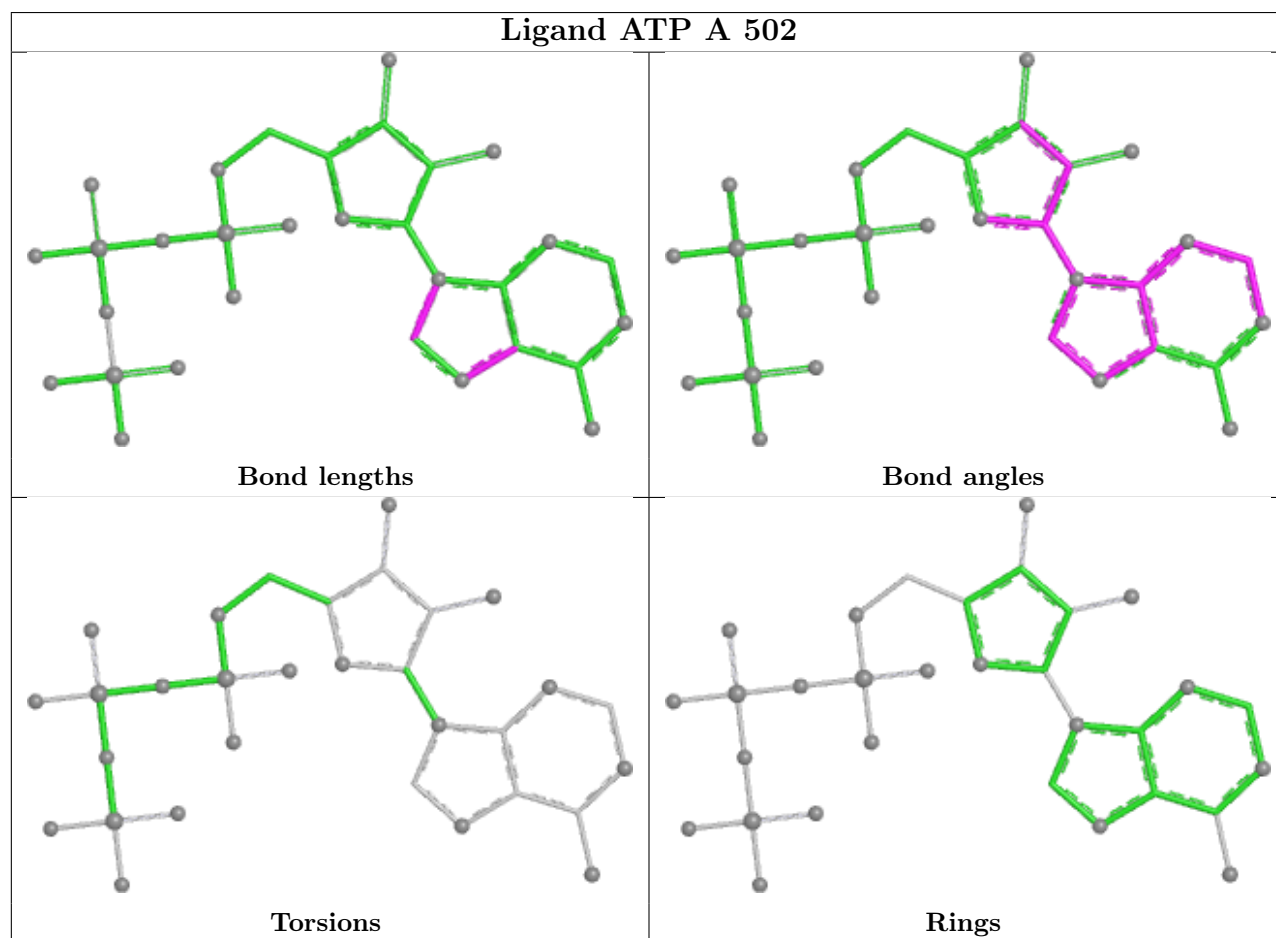
There are no ring outliers.

3 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	LTN	1	7
3	B	478	LTN	1	0
4	A	502	ATP	10	77

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	390/477 (81%)	5.06	375 (96%) 0 0	33, 46, 93, 179	0
1	B	379/477 (79%)	5.55	374 (98%) 0 0	33, 48, 69, 92	0
All	All	769/954 (80%)	5.30	749 (97%) 0 0	33, 47, 80, 179	0

The worst 5 of 749 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	PHE	13.5
1	A	88	TRP	12.6
1	A	452	VAL	12.5
1	A	353	SER	12.2
1	B	426	LEU	11.4

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](#)

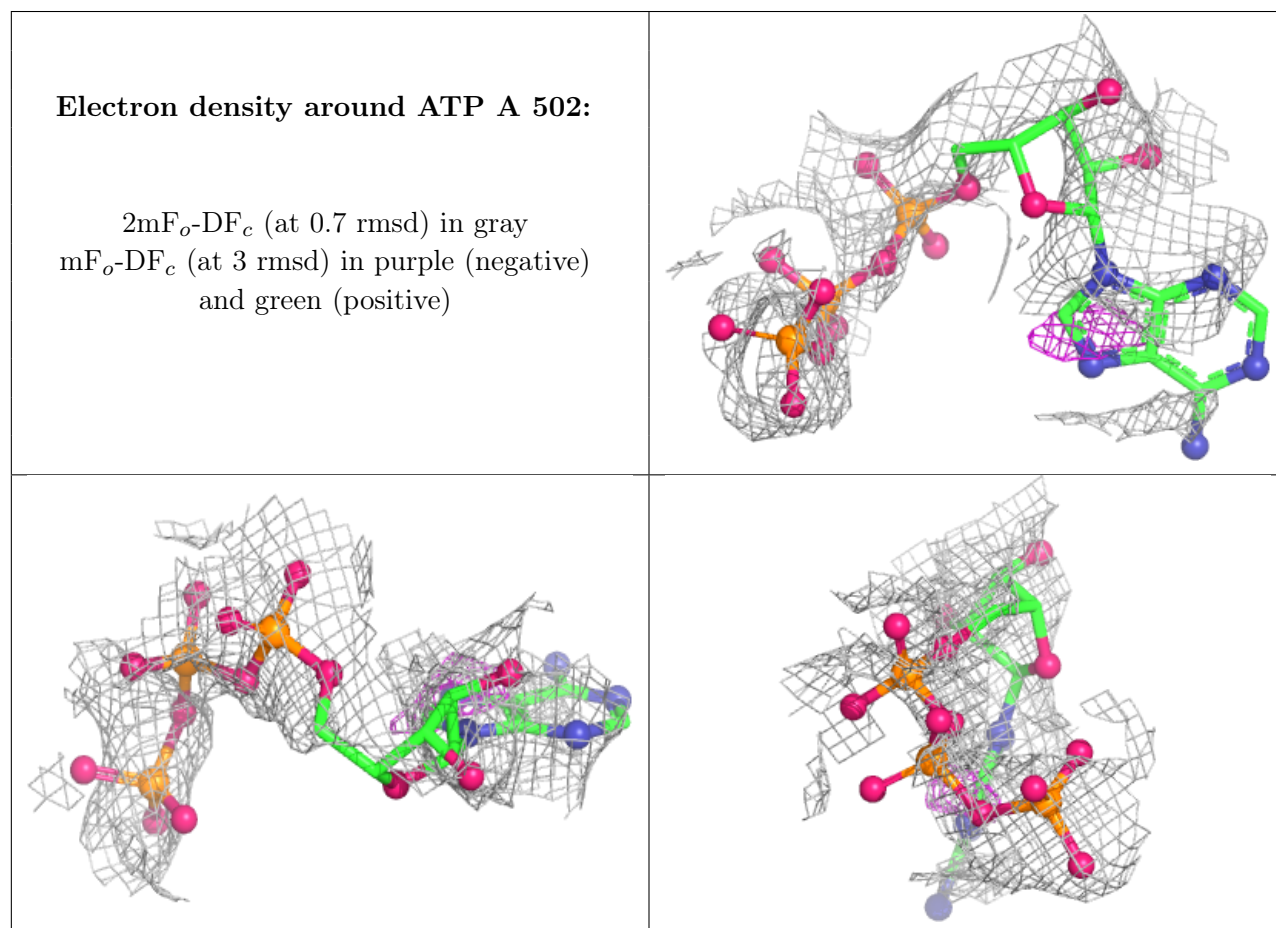
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
4	ATP	A	502	31/31	0.55	0.46	118,121,140,141	0
3	LTN	B	478	15/15	0.63	0.29	41,44,45,49	0
3	LTN	A	501	15/15	0.69	0.36	37,40,42,42	0
2	MG	A	500	1/1	0.84	0.46	74,74,74,74	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.