



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 02:01 PM EST

PDB ID : 2QUI
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

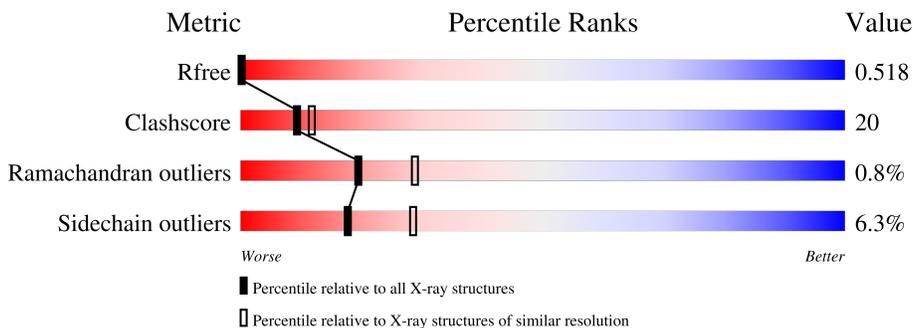
1 Overall quality at a glance

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	477	20% (green), 58% (yellow), 18% (grey)
1	B	477	28% (green), 48% (yellow), 21% (grey)

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	-
4	ATP	A	502	-	-	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
			Total	C	N	O	S			
1	A	390	3127	2005	525	582	15	0	0	0
1	B	379	3054	1960	519	560	15	0	0	0

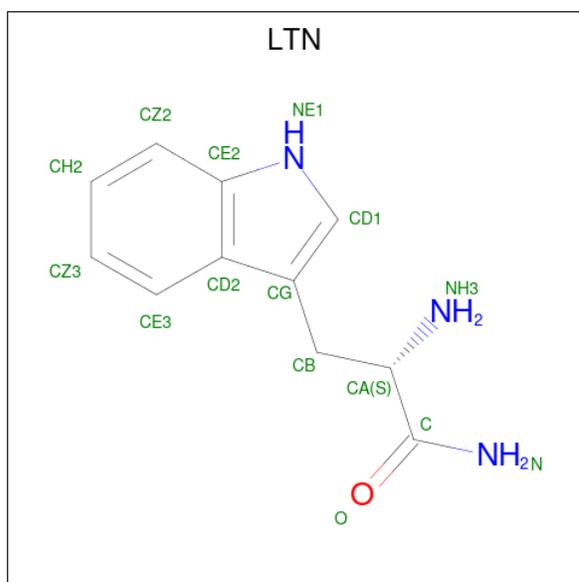
There are 12 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

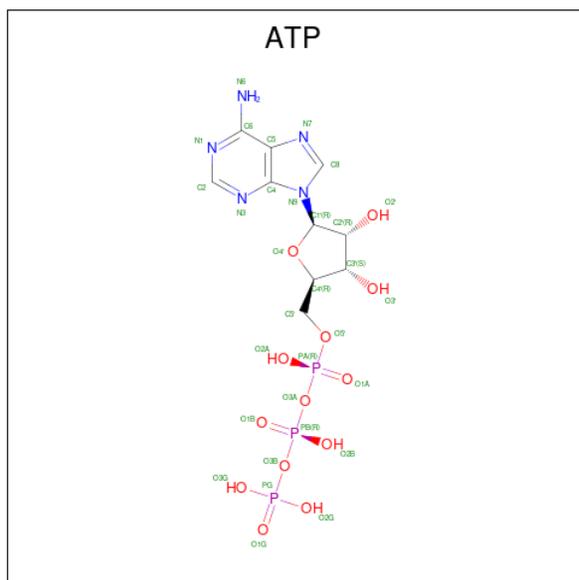
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is L-TRYPTOPHANAMIDE (three-letter code: LTN) (formula: C₁₁H₁₃N₃O).



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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

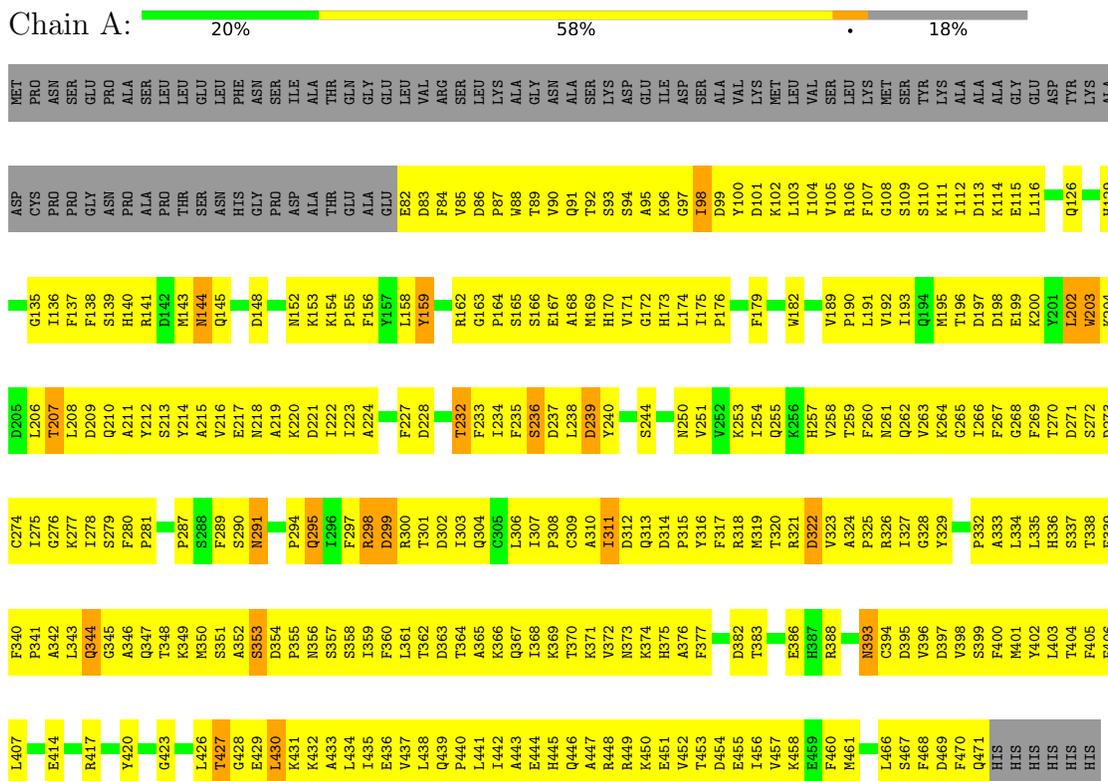
- Molecule 5 is water.

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

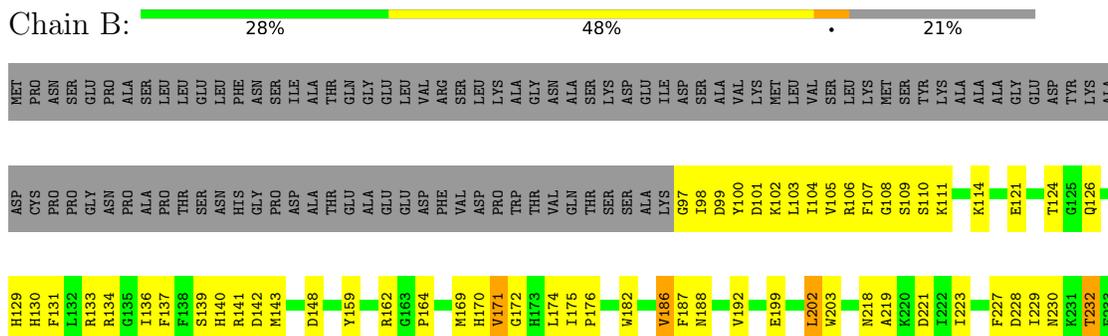
3 Residue-property plots [i](#)

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. 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. 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



- Molecule 1: Tryptophanyl-tRNA synthetase



I234	I235	I236	I237	I238	I239	I240	I241	I242	I243	I244	I245	I246	I247	I248	I249	I250	I251	I252	I253	I254	I255	I256	I257	I258	I259	I260	I261	I262	I263	I264	I265	I266	I267	I268	I269	I270	I271	I272	I273	I274	I275	I276	I277	I278	I279	I280	I281	I282	I283	I284	I285	I286	I287	I288	I289	I290	I291	I292	I293	I294	I295	I296	I297	I298	I299	I300	I301	I302	I303	I304	I305	I306	I307	I308	I309	I310	I311	I312	I313	I314	I315	I316	I317	I318	I319	I320	I321	I322	I323	I324	I325	I326	I327	I328	I329	I330	I331	I332	I333	I334	I335	I336	I337	I338	I339	I340	I341	I342	I343	I344	I345	I346	I347	I348	I349	I350	I351	I352	I353	I354	I355	I356	I357	I358	I359	I360	I361	I362	I363	I364	I365	I366	I367	I368	I369	I370	I371	I372	I373	I374	I375	I376	I377	I378	I379	I380	I381	I382	I383	I384	I385	I386	I387	I388	I389	I390	I391	I392	I393	I394	I395	I396	I397	I398	I399	I400	I401	I402	I403	I404	I405	I406	I407	I408	I409	I410	I411	I412	I413	I414	I415	I416	I417	I418	I419	I420	I421	I422	I423	I424	I425	I426	I427	I428	I429	I430	I431	I432	I433	I434	I435	I436	I437	I438	I439	I440	I441	I442	I443	I444	I445	I446	I447	I448	I449	I450	I451	I452	I453	I454	I455	I456	I457	I458	I459	I460	I461	I462	I463	I464	I465	I466	I467	I468	I469	I470	I471	I472	I473	I474	I475	I476	I477	I478	I479	I480	I481	I482	I483	I484	I485	I486	I487	I488	I489	I490	I491	I492	I493	I494	I495	I496	I497	I498	I499	I500	I501	I502	I503	I504	I505	I506	I507	I508	I509	I510	I511	I512	I513	I514	I515	I516	I517	I518	I519	I520	I521	I522	I523	I524	I525	I526	I527	I528	I529	I530	I531	I532	I533	I534	I535	I536	I537	I538	I539	I540	I541	I542	I543	I544	I545	I546	I547	I548	I549	I550	I551	I552	I553	I554	I555	I556	I557	I558	I559	I560	I561	I562	I563	I564	I565	I566	I567	I568	I569	I570	I571	I572	I573	I574	I575	I576	I577	I578	I579	I580	I581	I582	I583	I584	I585	I586	I587	I588	I589	I590	I591	I592	I593	I594	I595	I596	I597	I598	I599	I600	I601	I602	I603	I604	I605	I606	I607	I608	I609	I610	I611	I612	I613	I614	I615	I616	I617	I618	I619	I620	I621	I622	I623	I624	I625	I626	I627	I628	I629	I630	I631	I632	I633	I634	I635	I636	I637	I638	I639	I640	I641	I642	I643	I644	I645	I646	I647	I648	I649	I650	I651	I652	I653	I654	I655	I656	I657	I658	I659	I660	I661	I662	I663	I664	I665	I666	I667	I668	I669	I670	I671	I672	I673	I674	I675	I676	I677	I678	I679	I680	I681	I682	I683	I684	I685	I686	I687	I688	I689	I690	I691	I692	I693	I694	I695	I696	I697	I698	I699	I700	I701	I702	I703	I704	I705	I706	I707	I708	I709	I710	I711	I712	I713	I714	I715	I716	I717	I718	I719	I720	I721	I722	I723	I724	I725	I726	I727	I728	I729	I730	I731	I732	I733	I734	I735	I736	I737	I738	I739	I740	I741	I742	I743	I744	I745	I746	I747	I748	I749	I750	I751	I752	I753	I754	I755	I756	I757	I758	I759	I760	I761	I762	I763	I764	I765	I766	I767	I768	I769	I770	I771	I772	I773	I774	I775	I776	I777	I778	I779	I780	I781	I782	I783	I784	I785	I786	I787	I788	I789	I790	I791	I792	I793	I794	I795	I796	I797	I798	I799	I800	I801	I802	I803	I804	I805	I806	I807	I808	I809	I810	I811	I812	I813	I814	I815	I816	I817	I818	I819	I820	I821	I822	I823	I824	I825	I826	I827	I828	I829	I830	I831	I832	I833	I834	I835	I836	I837	I838	I839	I840	I841	I842	I843	I844	I845	I846	I847	I848	I849	I850	I851	I852	I853	I854	I855	I856	I857	I858	I859	I860	I861	I862	I863	I864	I865	I866	I867	I868	I869	I870	I871	I872	I873	I874	I875	I876	I877	I878	I879	I880	I881	I882	I883	I884	I885	I886	I887	I888	I889	I890	I891	I892	I893	I894	I895	I896	I897	I898	I899	I900	I901	I902	I903	I904	I905	I906	I907	I908	I909	I910	I911	I912	I913	I914	I915	I916	I917	I918	I919	I920	I921	I922	I923	I924	I925	I926	I927	I928	I929	I930	I931	I932	I933	I934	I935	I936	I937	I938	I939	I940	I941	I942	I943	I944	I945	I946	I947	I948	I949	I950	I951	I952	I953	I954	I955	I956	I957	I958	I959	I960	I961	I962	I963	I964	I965	I966	I967	I968	I969	I970	I971	I972	I973	I974	I975	I976	I977	I978	I979	I980	I981	I982	I983	I984	I985	I986	I987	I988	I989	I990	I991	I992	I993	I994	I995	I996	I997	I998	I999	I1000
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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 48.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.40) 95.1 (48.57-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.238 0.507 , 0.518	Depositor DCC
R_{free} test set	2417 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtrriage
Anisotropy	0.490	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.55	EDS
Total number of atoms	6469	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage'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

5.1 Standard geometry

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

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	0.38	0/3204	0.61	0/4331
1	B	0.39	0/3132	0.61	0/4230
All	All	0.38	0/6336	0.61	0/8561

There are no bond length outliers.

There are no bond angle outliers.

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	3127	0	3049	123	2188
1	B	3054	0	2978	126	1612
2	A	1	0	0	0	0
3	A	15	0	11	1	7
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	244	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 20.

The worst 5 of 244 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:A:250:ASN:HD21	1:A:291:ASN:ND2	1.73	0.87
1:A:344:GLN:HE22	1:A:357:SER:HA	1.40	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 [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	388/477 (81%)	366 (94%)	18 (5%)	4 (1%)	15	23
1	B	377/477 (79%)	359 (95%)	16 (4%)	2 (0%)	29	41
All	All	765/954 (80%)	725 (95%)	34 (4%)	6 (1%)	19	29

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	SER
1	B	351	SER

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

5.3.2 Protein sidechains [i](#)

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%)	323 (95%)	17 (5%)	24	40
1	B	331/416 (80%)	306 (92%)	25 (8%)	13	20
All	All	671/832 (81%)	629 (94%)	42 (6%)	18	28

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	291	ASN
1	B	354	ASP
1	B	295	GLN
1	B	311	ILE
1	B	407	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
1	B	445	HIS
1	B	261	ASN
1	B	474	HIS
1	B	356	ASN

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 monosaccharides 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	-	15,16,16	2.88	8 (53%)	17,22,22	1.54	4 (23%)
4	ATP	A	502	-	26,33,33	0.96	1 (3%)	31,52,52	1.59	5 (16%)
3	LTN	B	478	-	15,16,16	2.95	8 (53%)	17,22,22	1.58	4 (23%)

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	-	-	2/7/8/8	0/2/2/2
4	ATP	A	502	-	-	0/18/38/38	0/3/3/3
3	LTN	B	478	-	-	2/7/8/8	0/2/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	478	LTN	O-C	7.98	1.38	1.23
3	A	501	LTN	O-C	7.81	1.38	1.23
3	B	478	LTN	C-N	-4.30	1.22	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	LTN	C-N	-4.26	1.22	1.32
3	B	478	LTN	CH2-CZ2	3.88	1.45	1.36

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	ATP	N3-C2-N1	-4.45	121.72	128.68
4	A	502	ATP	PA-O3A-PB	-3.80	119.79	132.83
4	A	502	ATP	PB-O3B-PG	-3.52	120.74	132.83
3	B	478	LTN	CB-CG-CD1	-3.35	123.82	127.97
3	B	478	LTN	O-C-N	-3.15	117.53	123.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

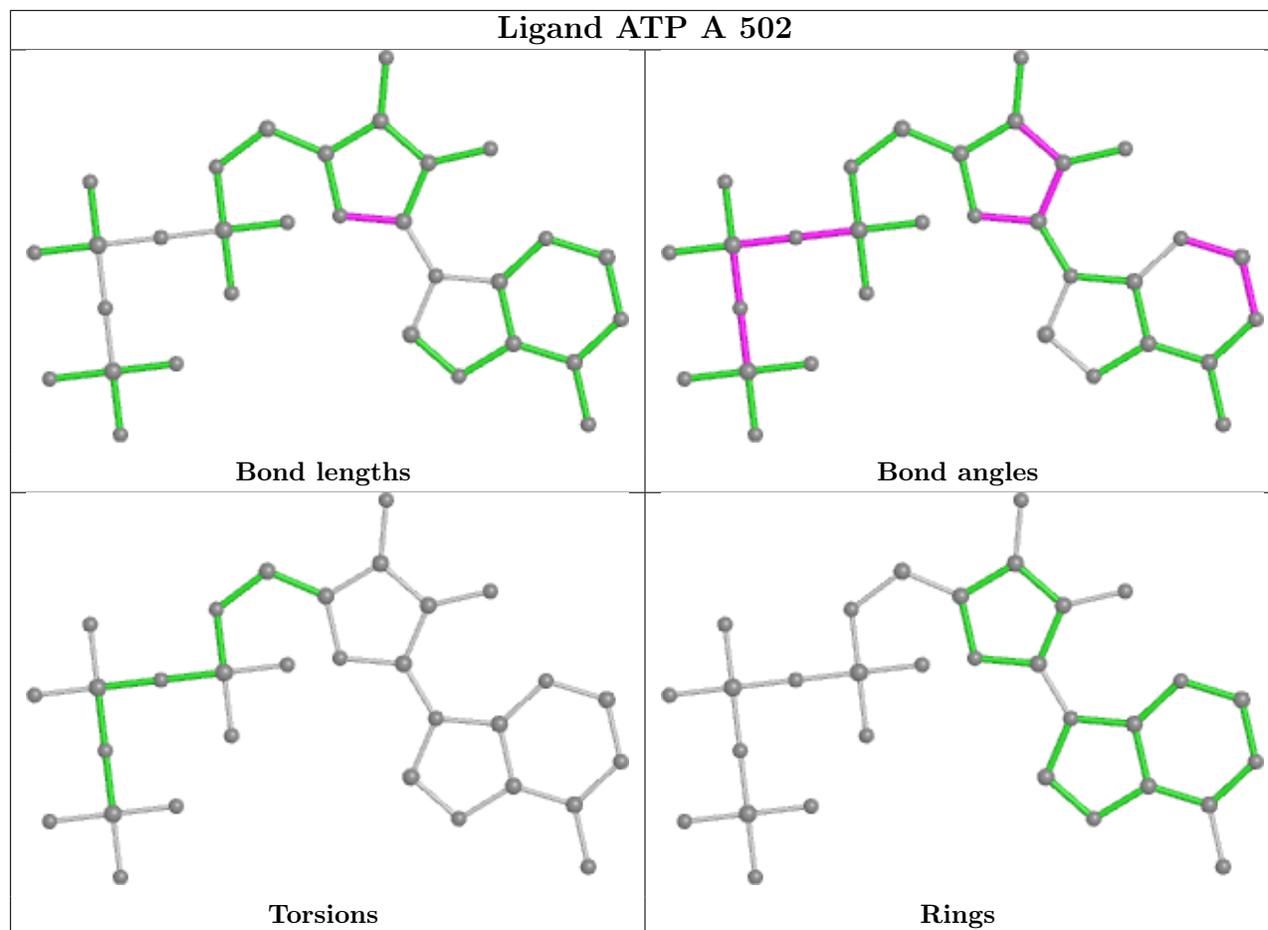
Mol	Chain	Res	Type	Atoms
3	A	501	LTN	O-C-CA-NH3
3	B	478	LTN	O-C-CA-NH3
3	A	501	LTN	O-C-CA-CB
3	B	478	LTN	O-C-CA-CB

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
4	A	502	ATP	10	77
3	B	478	LTN	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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

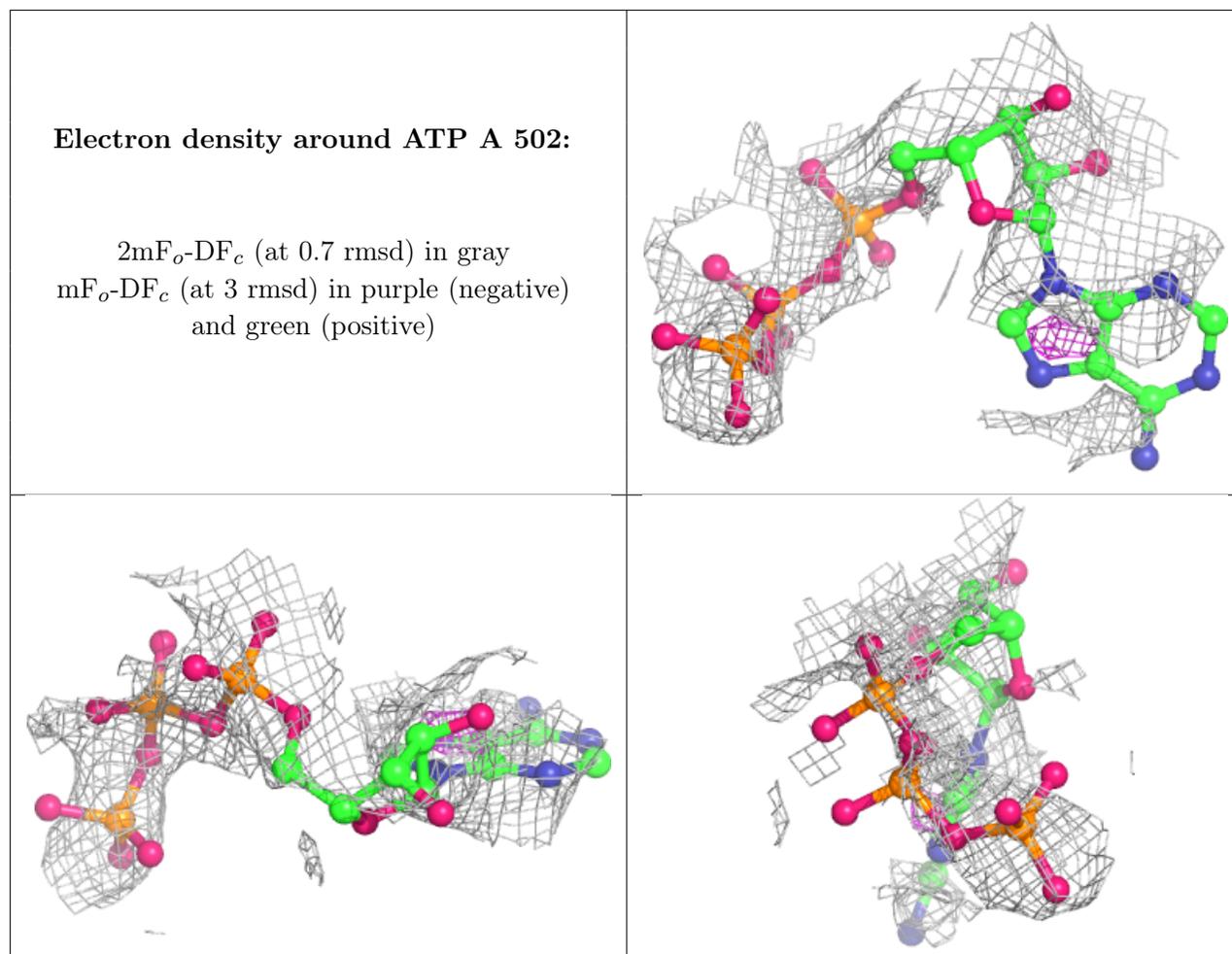
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.