



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:35 am BST

PDB ID : 3ZGZ  
Title : Ternary complex of E. coli leucyl-tRNA synthetase, tRNA(leu) and toxic moiety from agrocin 84 (TM84) in aminoacylation-like conformation  
Authors : Chopra, S.; Palencia, A.; Virus, C.; Tripathy, A.; Temple, B.R.; Velazquez-Campoy, A.; Cusack, S.; Reader, J.S.  
Deposited on : 2012-12-19  
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](mailto: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 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)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

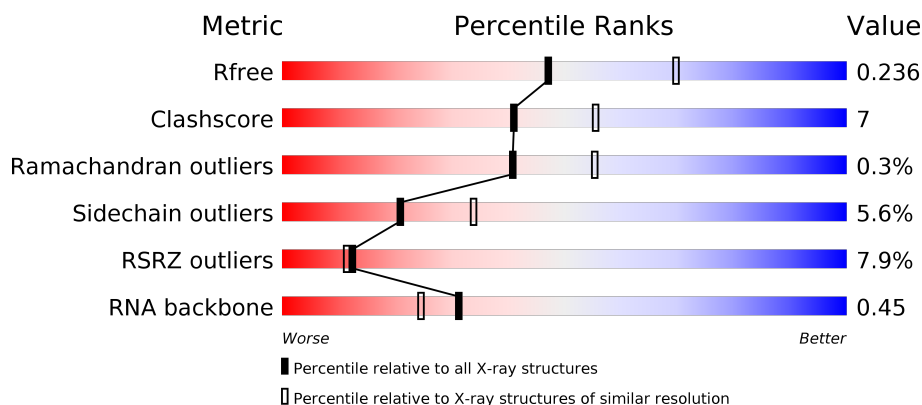
# 1 Overall quality at a glance

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)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	880	<div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	D	880	<div> <div>14%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	B	88	<div> <div>3%</div> <div>57%</div> <div>30%</div> <div>7%</div> <div>7%</div> </div>
2	E	88	<div> <div>8%</div> <div>70%</div> <div>19%</div> <div>•</div> <div>9%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17522 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 LEUCINE-TRNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	0	0
			6834	4339	1159	1291	45			
1	D	867	Total	C	N	O	S	0	0	0
			6881	4369	1168	1299	45			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07813
A	-18	GLY	-	expression tag	UNP P07813
A	-17	SER	-	expression tag	UNP P07813
A	-16	SER	-	expression tag	UNP P07813
A	-15	HIS	-	expression tag	UNP P07813
A	-14	HIS	-	expression tag	UNP P07813
A	-13	HIS	-	expression tag	UNP P07813
A	-12	HIS	-	expression tag	UNP P07813
A	-11	HIS	-	expression tag	UNP P07813
A	-10	HIS	-	expression tag	UNP P07813
A	-9	SER	-	expression tag	UNP P07813
A	-8	SER	-	expression tag	UNP P07813
A	-7	GLY	-	expression tag	UNP P07813
A	-6	LEU	-	expression tag	UNP P07813
A	-5	VAL	-	expression tag	UNP P07813
A	-4	PRO	-	expression tag	UNP P07813
A	-3	ARG	-	expression tag	UNP P07813
A	-2	GLY	-	expression tag	UNP P07813
A	-1	SER	-	expression tag	UNP P07813
A	0	HIS	-	expression tag	UNP P07813
D	-19	MET	-	expression tag	UNP P07813
D	-18	GLY	-	expression tag	UNP P07813
D	-17	SER	-	expression tag	UNP P07813
D	-16	SER	-	expression tag	UNP P07813
D	-15	HIS	-	expression tag	UNP P07813

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	HIS	-	expression tag	UNP P07813
D	-13	HIS	-	expression tag	UNP P07813
D	-12	HIS	-	expression tag	UNP P07813
D	-11	HIS	-	expression tag	UNP P07813
D	-10	HIS	-	expression tag	UNP P07813
D	-9	SER	-	expression tag	UNP P07813
D	-8	SER	-	expression tag	UNP P07813
D	-7	GLY	-	expression tag	UNP P07813
D	-6	LEU	-	expression tag	UNP P07813
D	-5	VAL	-	expression tag	UNP P07813
D	-4	PRO	-	expression tag	UNP P07813
D	-3	ARG	-	expression tag	UNP P07813
D	-2	GLY	-	expression tag	UNP P07813
D	-1	SER	-	expression tag	UNP P07813
D	0	HIS	-	expression tag	UNP P07813

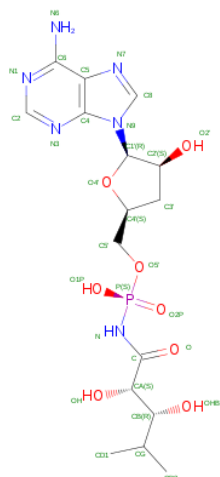
- Molecule 2 is a RNA chain called TRNA-LEU UAA ISOACCEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	P	0	0	1
			1692	749	304	558	81			
2	E	80	Total	C	N	O	P	0	0	1
			1675	743	304	549	79			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is [(2S,4S,5R)-5-(6-aminopurin-9-yl)-4-oxidanyl-oxolan-2-yl]methoxy-N-[(2S,3R)-4-methyl-2,3-bis(oxidanyl)pentanoyl]phosphonamidic acid (three-letter code: 84T) (formula: C<sub>16</sub>H<sub>25</sub>N<sub>6</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 16	N 6	O 8	P 1	0	0
4	D	1	Total 31	C 16	N 6	O 8	P 1	0	0

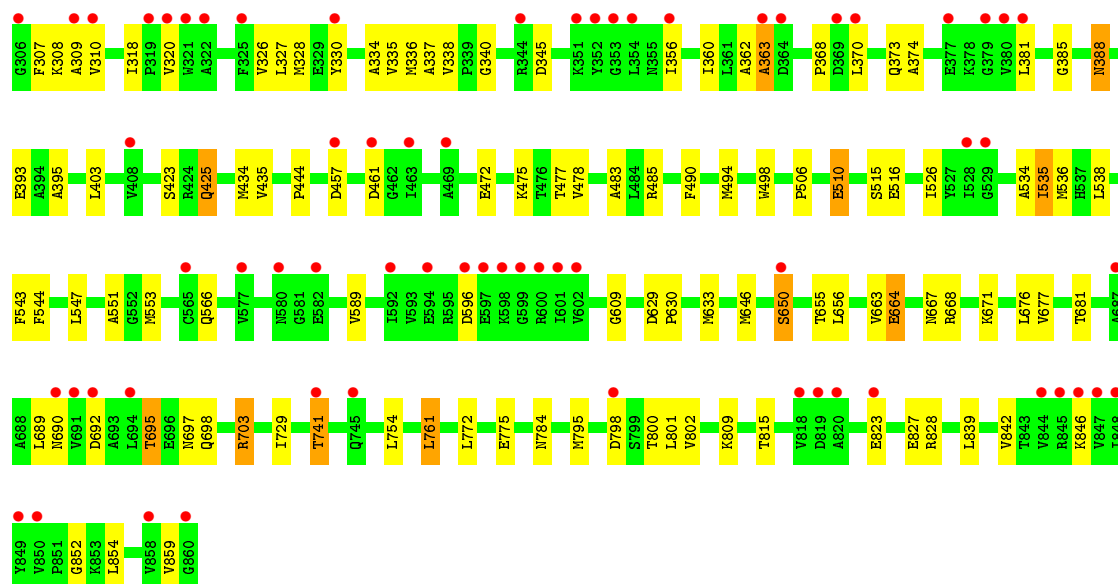
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	5	Total Mg 5 5	0	0
5	E	2	Total Mg 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	247	Total O 247 247	0	0
6	B	75	Total O 75 75	0	0
6	D	42	Total O 42 42	0	0
6	E	5	Total O 5 5	0	0

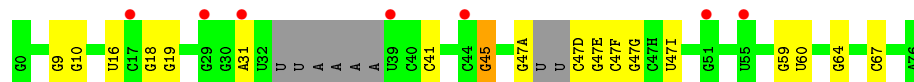




• Molecule 2: TRNA-LEU UAA ISOACCEPTOR



• Molecule 2: TRNA-LEU UAA ISOACCEPTOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.58Å 68.19Å 226.22Å 90.00° 105.53° 90.00°	Depositor
Resolution (Å)	43.59 – 2.40 43.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (43.59-2.40) 93.3 (43.59-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, $R_{free}$	0.187 , 0.238 0.187 , 0.236	Depositor DCC
$R_{free}$ test set	4280 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, 84T, 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	0.74	1/6995 (0.0%)	0.85	12/9497 (0.1%)
1	D	0.56	1/7043 (0.0%)	0.65	0/9562
2	B	0.54	1/1887 (0.1%)	0.99	9/2939 (0.3%)
2	E	0.31	0/1869	0.76	0/2911
All	All	0.62	3/17794 (0.0%)	0.78	21/24909 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	C	O3'-P	-5.64	1.54	1.61
1	A	585	TRP	CD2-CE2	5.47	1.48	1.41
1	D	498	TRP	CD2-CE2	5.02	1.47	1.41

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASP	N-CA-CB	-12.27	88.52	110.60
1	A	179	CYS	N-CA-C	-10.79	81.86	111.00
1	A	180	ASP	N-CA-C	7.79	132.02	111.00
1	A	668	ARG	NE-CZ-NH1	7.65	124.13	120.30
2	B	0	G	O3'-P-O5'	-7.56	89.64	104.00

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	6834	0	6687	107	0
1	D	6881	0	6733	114	0
2	B	1692	0	853	11	0
2	E	1675	0	848	3	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	24	2	0
4	D	31	0	24	0	0
5	B	5	0	0	0	0
5	E	2	0	0	0	0
6	A	247	0	0	8	0
6	B	75	0	0	0	0
6	D	42	0	0	2	0
6	E	5	0	0	1	0
All	All	17522	0	15169	228	0

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 7.

The worst 5 of 228 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:D:262:ALA:HB3	1:D:328:MET:HE2	1.27	1.11
1:A:434:MET:HE2	1:A:444:PRO:HA	1.41	1.02
1:D:262:ALA:HB3	1:D:328:MET:CE	1.93	0.98
1:A:729:ILE:HD13	1:A:761:LEU:HD13	1.43	0.97
1:A:161:ASN:ND2	1:A:181:THR:HG21	1.81	0.95

There are no symmetry-related clashes.

## 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	858/880 (98%)	834 (97%)	23 (3%)	1 (0%)	51	68
1	D	863/880 (98%)	816 (95%)	42 (5%)	5 (1%)	25	36
All	All	1721/1760 (98%)	1650 (96%)	65 (4%)	6 (0%)	41	55

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	363	ALA
1	A	439	ASP
1	D	284	GLU
1	D	393	GLU
1	D	535	ILE

### 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	724/741 (98%)	688 (95%)	36 (5%)	24	40
1	D	729/741 (98%)	683 (94%)	46 (6%)	18	28
All	All	1453/1482 (98%)	1371 (94%)	82 (6%)	21	34

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	36	TYR
1	D	181	THR
1	D	798	ASP
1	D	84	LEU
1	D	153	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	659	GLN
1	D	690	ASN
1	A	697	ASN
1	A	555	ASN
1	D	392	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	76/88 (86%)	12 (15%)	1 (1%)
2	E	75/88 (85%)	15 (20%)	1 (1%)
All	All	151/176 (85%)	27 (17%)	2 (1%)

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	10	G
2	B	16	U
2	B	19	G
2	B	41	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	47(G)	G
2	E	60	U

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	84T	A	1862	-	29,33,33	1.33	3 (10%)	31,49,49	2.14	11 (35%)
4	84T	D	1862	-	29,33,33	1.34	3 (10%)	31,49,49	1.74	4 (12%)

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	84T	A	1862	-	-	1/21/39/39	0/3/3/3
4	84T	D	1862	-	-	1/21/39/39	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1862	84T	C2'-C1'	-3.93	1.50	1.54
4	D	1862	84T	P-O2P	3.43	1.51	1.46
4	A	1862	84T	C2'-C1'	-3.24	1.51	1.54
4	A	1862	84T	P-O2P	2.68	1.50	1.46
4	A	1862	84T	P-O1P	-2.62	1.49	1.56

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1862	84T	O1P-P-O2P	6.13	122.77	109.92
4	D	1862	84T	N3-C2-N1	-4.77	121.23	128.68
4	A	1862	84T	N3-C2-N1	-4.64	121.42	128.68
4	A	1862	84T	O1P-P-O2P	3.77	117.83	109.92
4	A	1862	84T	C4-C5-N7	-3.68	105.56	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

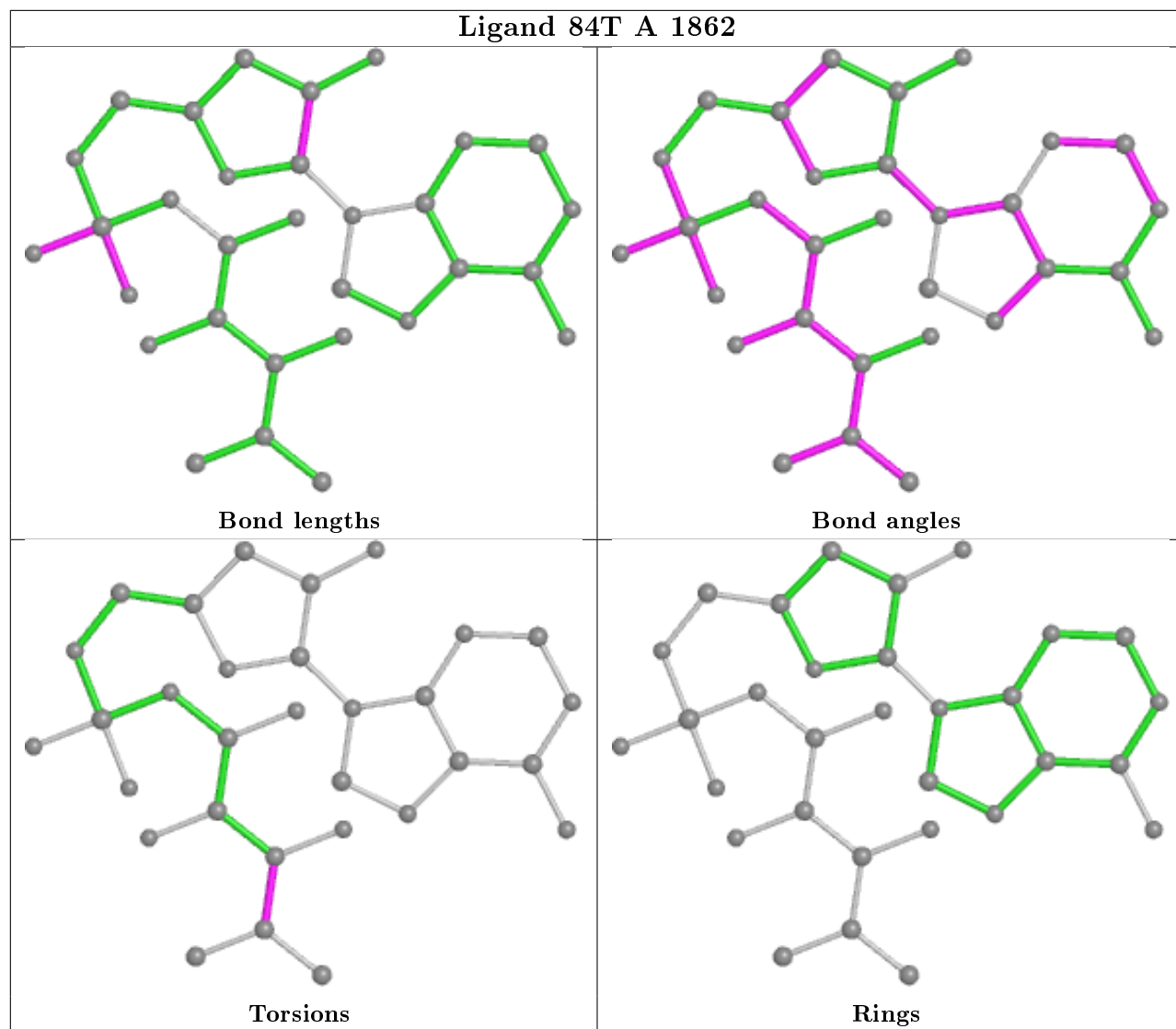
Mol	Chain	Res	Type	Atoms
4	A	1862	84T	OHB-CB-CG-CD1
4	D	1862	84T	C-N-P-O2P

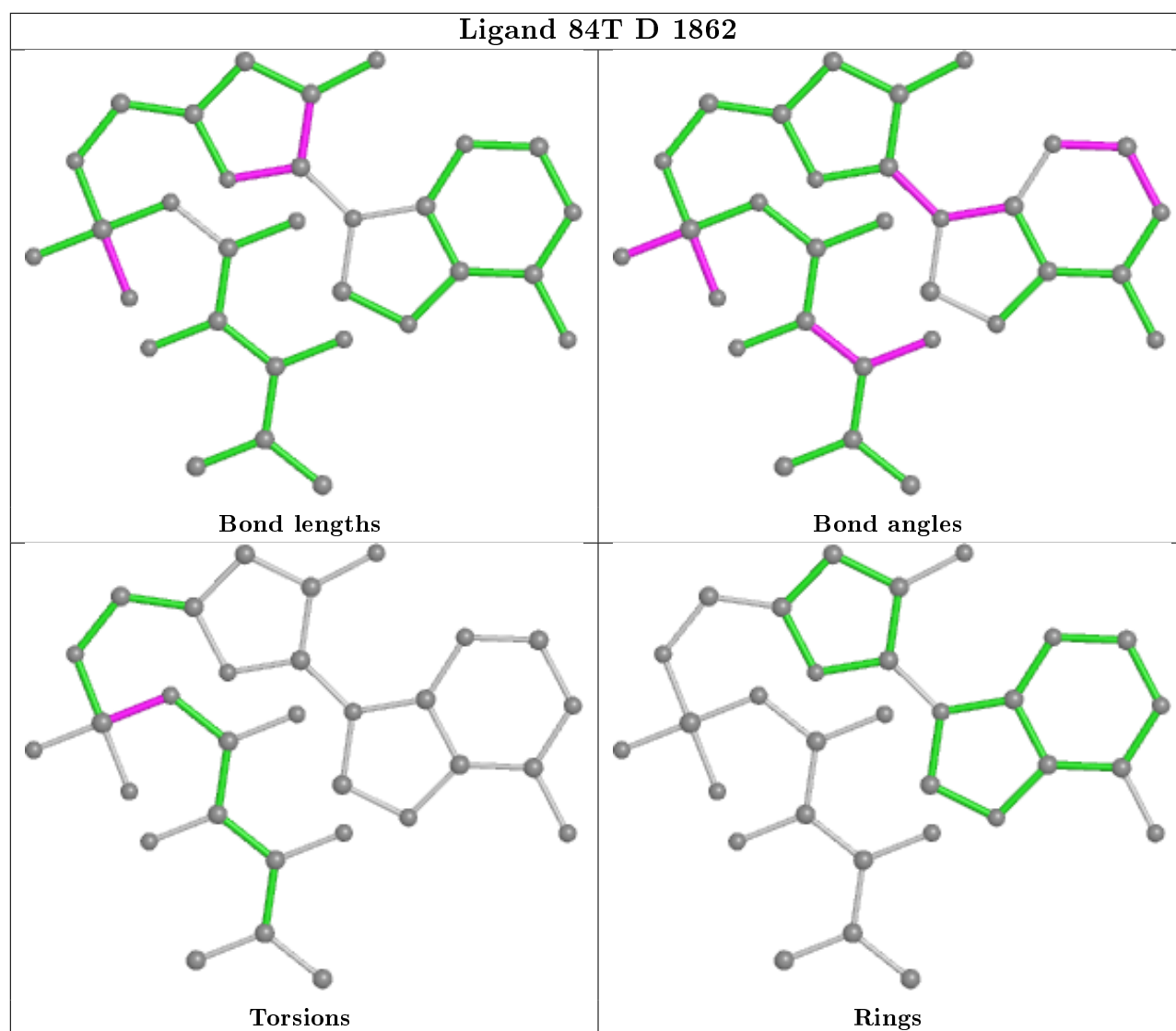
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1862	84T	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	860/880 (97%)	0.04	13 (1%) 73 72	19, 35, 67, 122	0
1	D	867/880 (98%)	0.78	126 (14%) 2 2	39, 66, 116, 153	0
2	B	82/88 (93%)	-0.30	3 (3%) 41 41	24, 39, 92, 120	0
2	E	80/88 (90%)	0.45	7 (8%) 10 9	48, 78, 105, 118	0
All	All	1889/1936 (97%)	0.38	149 (7%) 12 11	19, 51, 108, 153	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	303	VAL	8.4
1	D	596	ASP	7.2
1	D	860	GLY	6.2
1	D	177	TRP	5.7
1	D	463	ILE	5.7

### 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](#)

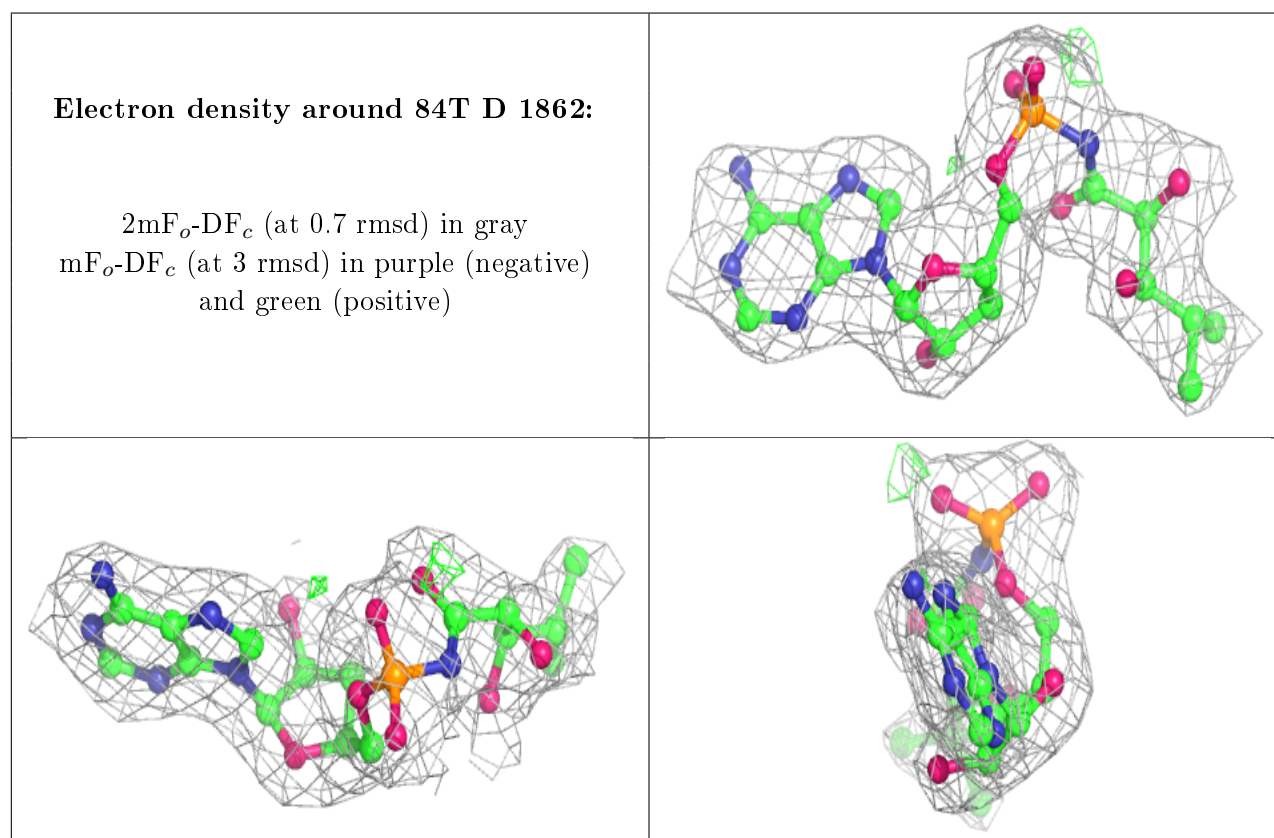
There are no carbohydrates in this entry.

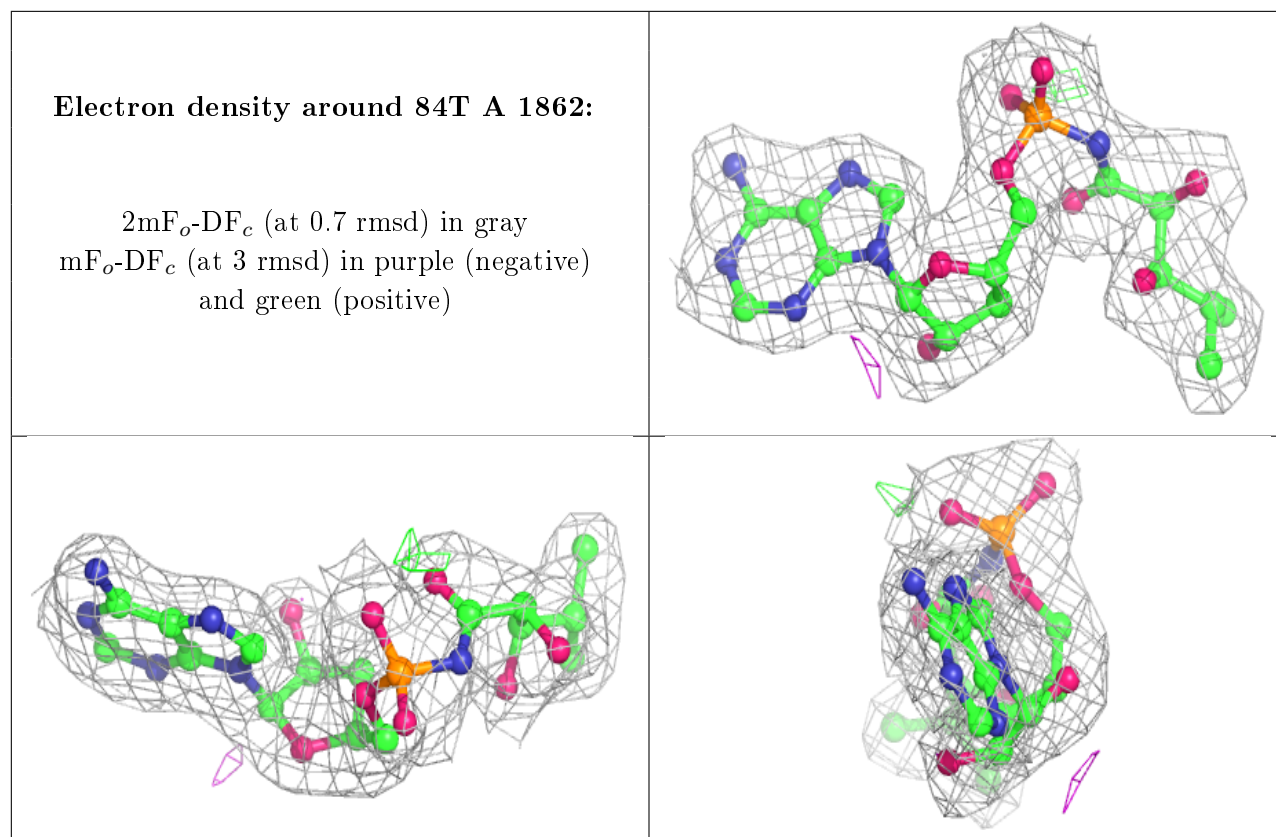
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	MG	E	1078	1/1	0.70	0.32	59,59,59,59	0
5	MG	B	1078	1/1	0.76	0.12	62,62,62,62	0
3	ZN	D	1861	1/1	0.83	0.14	125,125,125,125	0
3	ZN	A	1861	1/1	0.85	0.09	118,118,118,118	0
5	MG	B	1081	1/1	0.88	0.09	55,55,55,55	0
5	MG	B	1079	1/1	0.89	0.07	43,43,43,43	0
5	MG	E	1077	1/1	0.90	0.15	60,60,60,60	0
5	MG	B	1077	1/1	0.95	0.09	32,32,32,32	0
5	MG	B	1080	1/1	0.98	0.05	41,41,41,41	0
4	84T	D	1862	31/31	0.98	0.20	38,39,41,43	0
4	84T	A	1862	31/31	0.98	0.20	18,19,22,23	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.