



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:11 PM UTC

PDB ID : 4CQN / pdb_00004cqn
Title : Crystal structure of the E.coli LeuRS-tRNA complex with the non- cognate
isoleucyl adenylate analogue
Authors : Palencia, A.; Cusack, S.; Cvetic, N.; Haslaz, I.; Gruic-Sovulj, I.
Deposited on : 2014-02-20
Resolution : 2.50 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

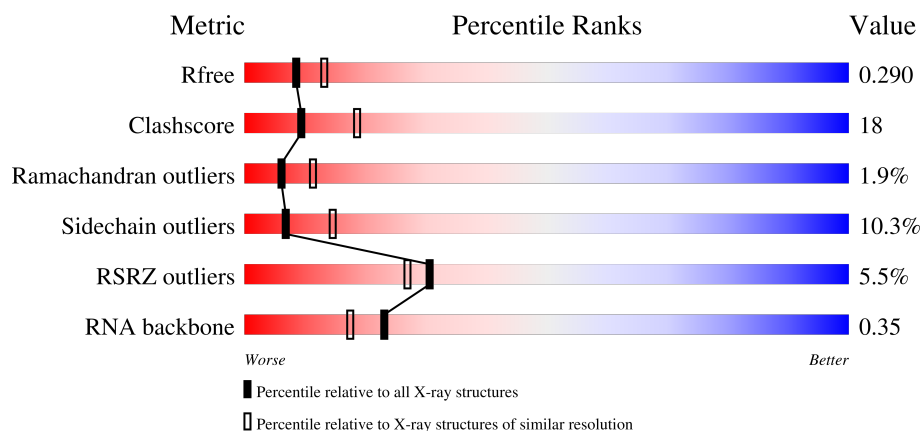
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	880	 53% 39% 5% .
1	D	880	 11% 58% 35% 5% .
2	B	82	 4% 38% 41% 18% .
2	E	82	 32% 52% 12% .

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
4	ILA	A	1863	X	-	X	-
4	ILA	D	1863	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17558 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	2	0
			6844	4345	1161	1293	45			
1	D	860	Total	C	N	O	S	0	0	0
			6834	4339	1158	1292	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

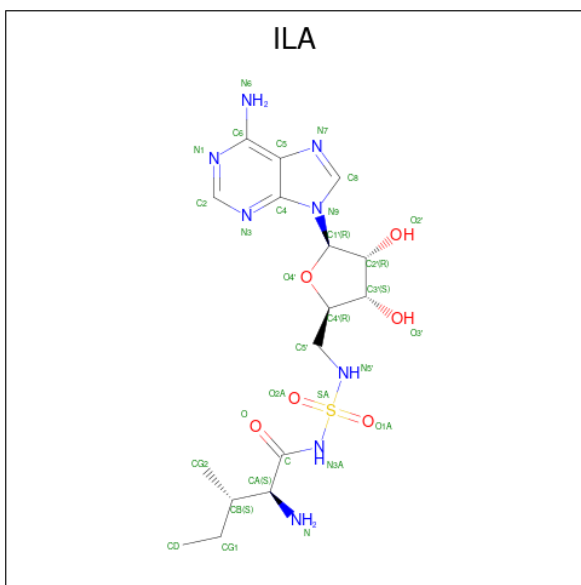
- Molecule 2 is a RNA chain called ESCHERICHIA COLI TRNA-LEU UAA ISOACCEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	P	0	0	0
			1755	781	317	575	82			
2	E	79	Total	C	N	O	P	0	0	0
			1691	752	305	555	79			

- Molecule 3 is ZINC ION (CCD ID: 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 N-[ISOLEUCINYL]-N'-[ADENOSYL]-DIAMINOSUFONE (CCD ID: ILA) (formula: C₁₆H₂₆N₈O₆S).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

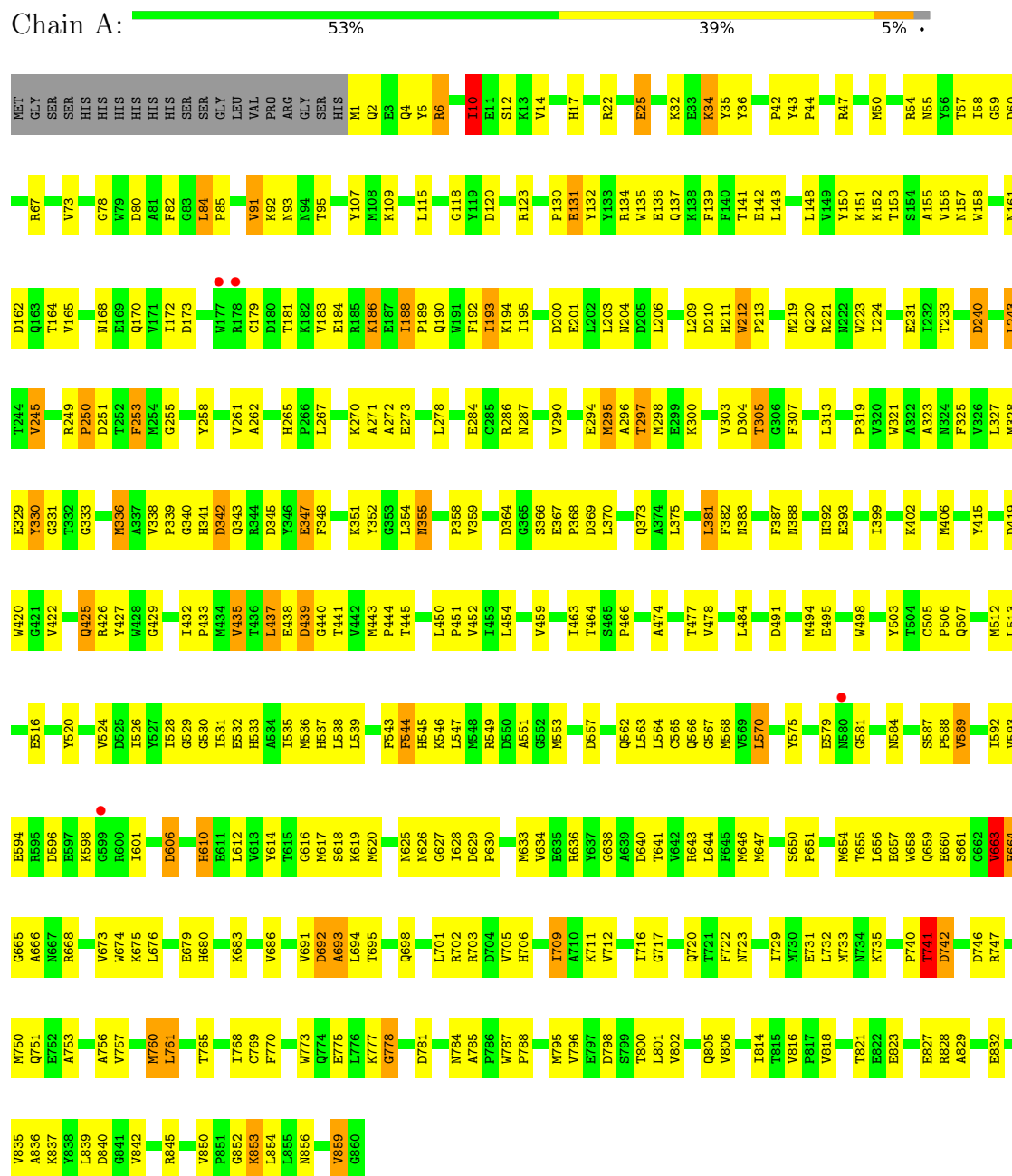
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	233	Total	O	0	0
			233	233		
6	B	57	Total	O	0	0
			57	57		
6	D	16	Total	O	0	0
			16	16		

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: LEUCINE-TRNA LIGASE



Chain D: 11% 58% 35% 5%

The visualization displays a hierarchical tree structure of 1000 items, each represented by a colored bar with a label. The items are grouped into 100 clusters, each containing 10 items. The colors of the bars represent different categories or values, with a legend at the top showing a gradient from green to red. The labels on the bars are alphanumeric codes, such as 'T815', 'W858', 'P368', etc. The visualization is designed to show the distribution and relationships between these items across different categories.

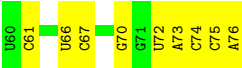
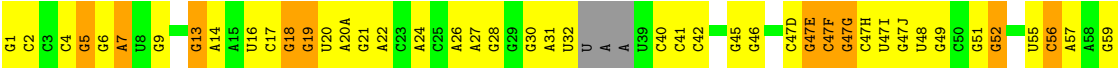
Chain B:

Color	Percentage
Green	4%
Yellow	38%
Orange	41%
Red	18%

.



● Molecule 2: ESCHERICHIA COLI TRNA-LEU UAA ISOACCEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.62Å 67.58Å 224.59Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	46.49 – 2.50 46.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.49-2.50) 97.1 (46.49-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.214 , 0.290 0.214 , 0.290	Depositor DCC
R_{free} test set	3828 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17558	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: ILA, MG, ZN

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	0.93	1/7014 (0.0%)	1.19	37/9520 (0.4%)
1	D	0.50	0/6995	0.92	8/9495 (0.1%)
2	B	0.55	1/1959 (0.1%)	1.06	18/3047 (0.6%)
2	E	0.41	0/1887	0.75	0/2935
All	All	0.70	2/17855 (0.0%)	1.03	63/24997 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	PHE	N-CA	-6.80	1.38	1.46
2	B	12	G	O3'-P	-5.18	1.53	1.61

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20(A)	A	C4'-C3'-O3'	-7.86	101.20	113.00
2	B	75	C	C2'-C3'-O3'	-7.40	102.60	113.70
1	A	717	GLY	N-CA-C	7.30	123.72	114.66
2	B	5	G	C3'-C2'-O2'	6.83	120.94	110.70
2	B	5	G	C1'-C2'-O2'	6.59	118.28	108.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	592	ILE	Peptide
1	A	80	ASP	Peptide

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	6844	0	6696	279	0
1	D	6834	0	6683	238	0
2	B	1755	0	890	38	0
2	E	1691	0	858	38	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	52	12	0
4	D	62	0	52	7	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	A	233	0	0	15	0
6	B	57	0	0	1	0
6	D	16	0	0	2	0
All	All	17558	0	15231	581	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 18.

The worst 5 of 581 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:A:422:VAL:HG11	1:A:494:MET:HE1	1.36	1.06
1:A:267:LEU:HD21	1:A:305:THR:HG21	1.40	1.00
1:A:553:MET:HE2	6:A:2052:HOH:O	1.59	0.98
1:A:801:LEU:C	1:A:801:LEU:HD23	1.90	0.97
1:A:342:ASP:HB2	4:A:1863:ILA:CG2	1.96	0.95

There are no symmetry-related clashes.

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	860/880 (98%)	797 (93%)	54 (6%)	9 (1%)	12	24
1	D	858/880 (98%)	716 (83%)	119 (14%)	23 (3%)	4	6
All	All	1718/1760 (98%)	1513 (88%)	173 (10%)	32 (2%)	6	11

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ASP
1	A	693	ALA
1	D	237	ASN
1	D	463	ILE
1	A	161	ASN

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	726/741 (98%)	648 (89%)	78 (11%)	6	13
1	D	723/741 (98%)	652 (90%)	71 (10%)	7	16
All	All	1449/1482 (98%)	1300 (90%)	149 (10%)	7	14

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	372	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	793	LYS
1	D	413	VAL
1	D	646	MET
1	A	570	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	372	GLN
1	D	533	HIS
1	D	507	GLN
1	D	562	GLN
1	A	831	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	81/82 (98%)	15 (18%)	6 (7%)
2	E	76/82 (92%)	21 (27%)	3 (3%)
All	All	157/164 (95%)	36 (22%)	9 (5%)

5 of 36 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	11	U
2	B	15	A
2	B	16	U
2	B	17	C

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	47(E)	G
2	E	48	U
2	B	37	A
2	B	47(D)	C
2	B	47(E)	G

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 8 ligands modelled in this entry, 4 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	$\# Z > 2$
4	ILA	D	1863	-	33,33,33	2.08	8 (24%)	44,49,49	2.12	11 (25%)
4	ILA	D	1862	-	33,33,33	2.03	6 (18%)	44,49,49	2.18	11 (25%)
4	ILA	A	1863	-	33,33,33	2.18	6 (18%)	44,49,49	2.92	21 (47%)
4	ILA	A	1862	-	33,33,33	2.45	8 (24%)	44,49,49	3.00	19 (43%)

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	ILA	D	1863	-	1/1/8/10	7/25/41/41	0/3/3/3
4	ILA	D	1862	-	-	10/25/41/41	0/3/3/3
4	ILA	A	1863	-	1/1/8/10	1/25/41/41	0/3/3/3
4	ILA	A	1862	-	-	6/25/41/41	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1862	ILA	SA-N5'	-8.58	1.51	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1862	ILA	SA-N5'	-7.13	1.52	1.61
4	D	1863	ILA	SA-N5'	-6.77	1.53	1.61
4	A	1863	ILA	SA-N5'	-6.72	1.53	1.61
4	A	1862	ILA	SA-N3A	-6.15	1.52	1.63

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1862	ILA	O2A-SA-O1A	-11.18	103.88	120.34
4	D	1862	ILA	O2A-SA-O1A	-7.31	109.57	120.34
4	D	1863	ILA	O2A-SA-O1A	-7.06	109.95	120.34
4	A	1863	ILA	N1-C2-N3	-6.96	118.05	128.58
4	A	1863	ILA	O2A-SA-O1A	-6.83	110.28	120.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1863	ILA	CB
4	D	1863	ILA	CB

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1862	ILA	O-C-CA-CB
4	A	1862	ILA	N3A-C-CA-CB
4	A	1863	ILA	C5'-N5'-SA-N3A
4	D	1862	ILA	CG2-CB-CG1-CD
4	D	1862	ILA	C-N3A-SA-O2A

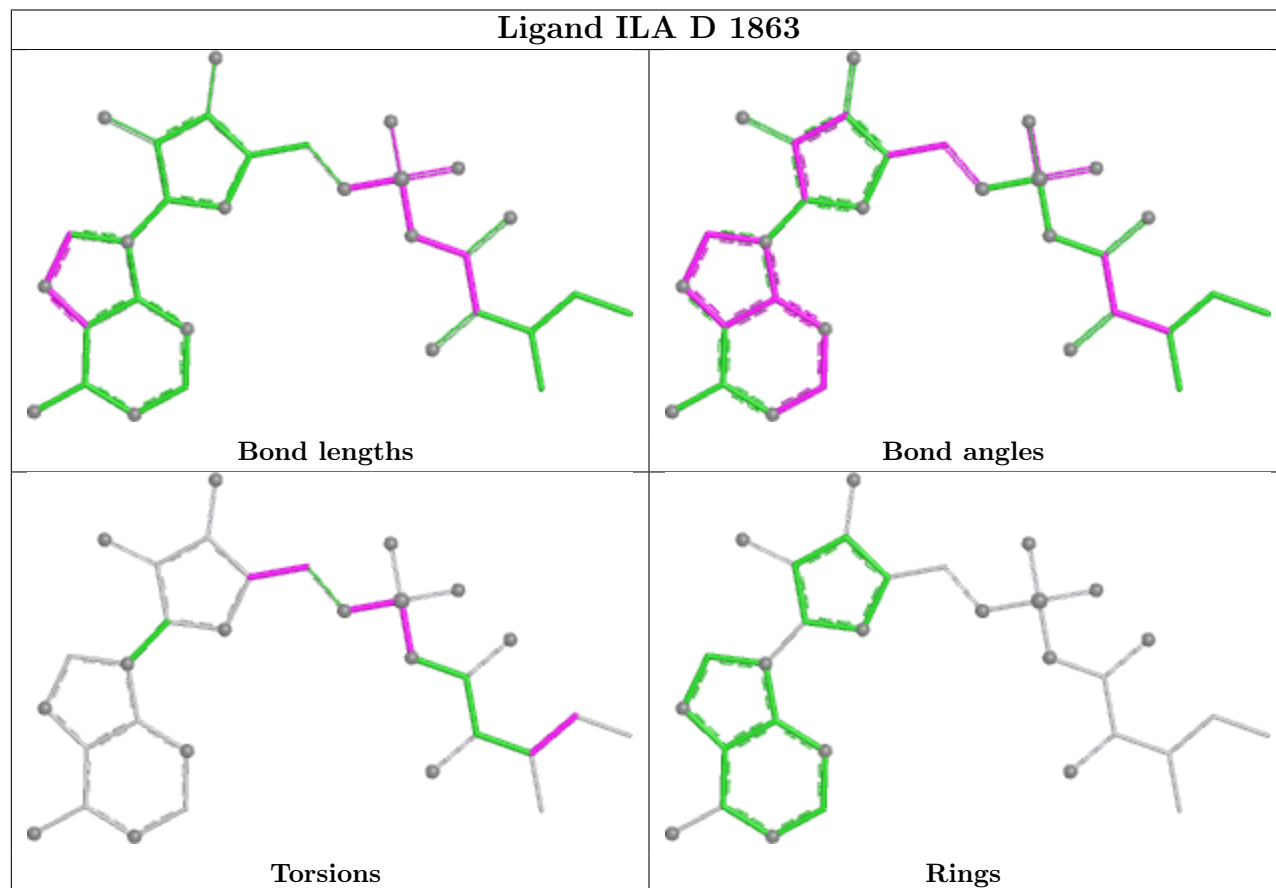
There are no ring outliers.

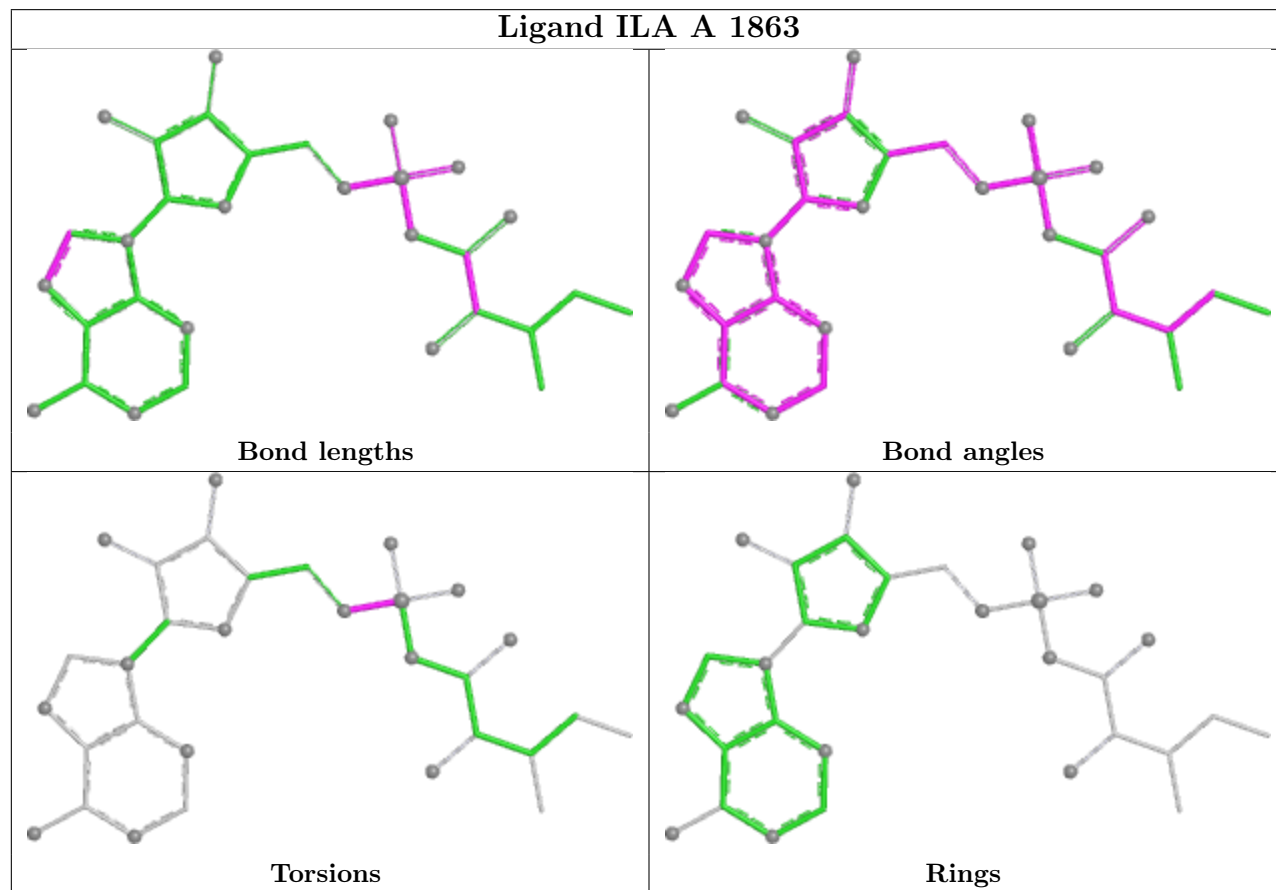
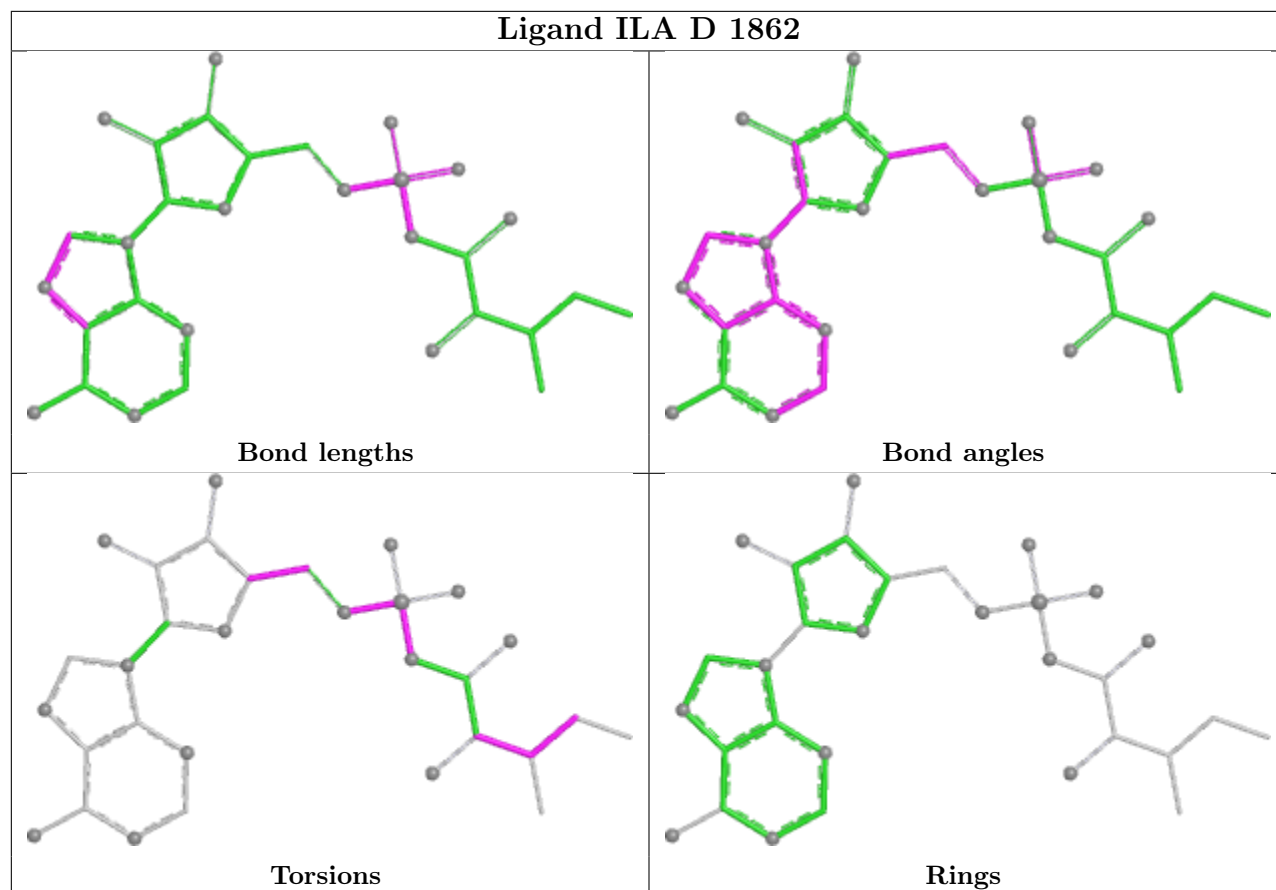
4 monomers are involved in 19 short contacts:

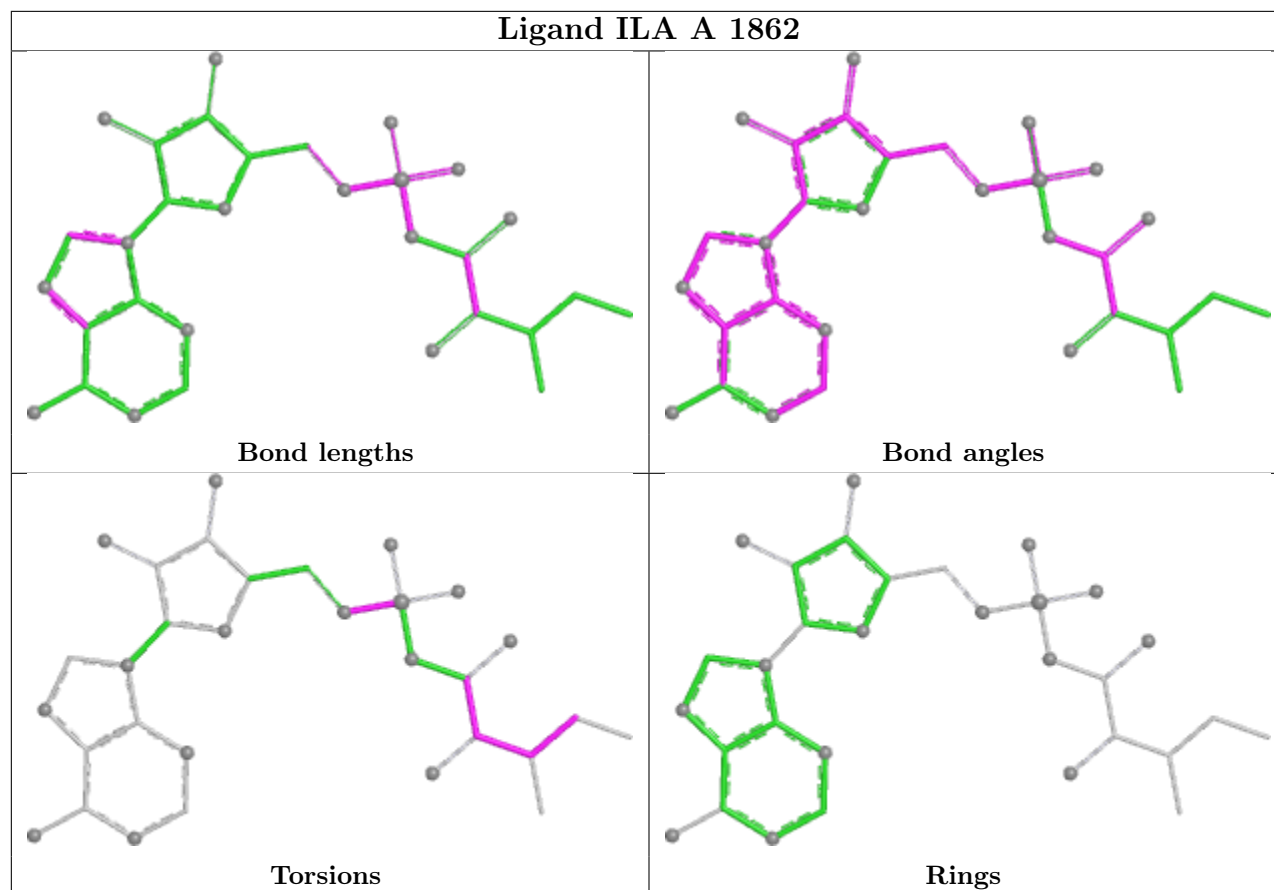
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1863	ILA	4	0
4	D	1862	ILA	3	0
4	A	1863	ILA	11	0
4	A	1862	ILA	1	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	33:U	O3'	37:A	P	11.93
1	B	47(A):G	O3'	47(D):C	P	10.54
1	E	47(A):G	O3'	47(D):C	P	9.54

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	860/880 (97%)	-0.39	4 (0%) 87 85	6, 19, 48, 99	2 (0%)
1	D	860/880 (97%)	0.96	97 (11%) 10 8	36, 71, 111, 142	0
2	B	82/82 (100%)	-0.60	3 (3%) 45 40	9, 21, 72, 116	0
2	E	79/82 (96%)	0.56	0 100 100	56, 79, 125, 142	0
All	All	1881/1924 (97%)	0.26	104 (5%) 30 27	6, 47, 105, 142	2 (0%)

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	322	ALA	4.7
1	D	290	VAL	4.2
1	D	810	VAL	4.0
1	D	291	ALA	3.8
1	D	858	VAL	3.7

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](#)

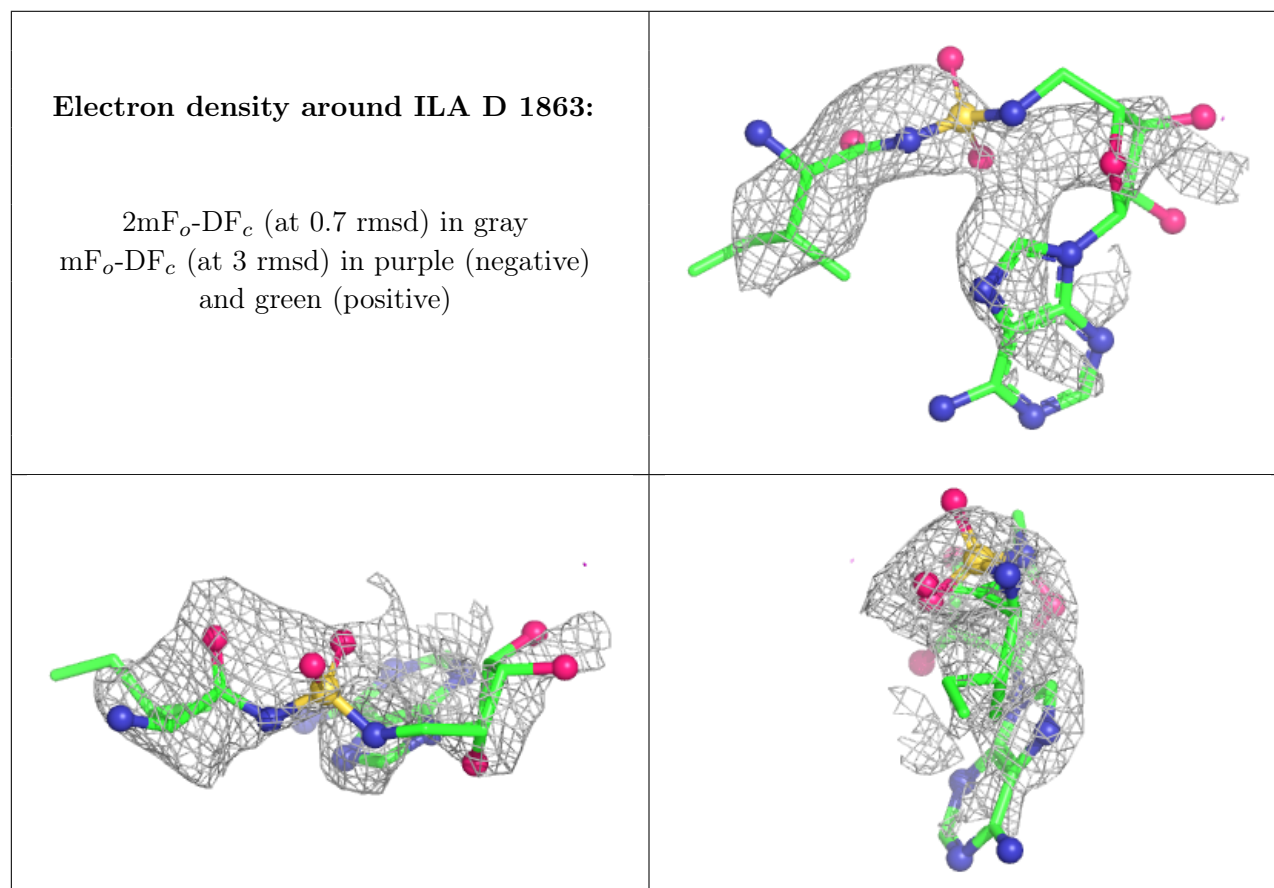
There are no oligosaccharides in this entry.

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.

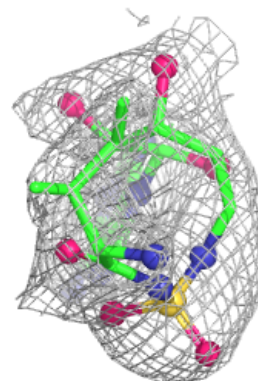
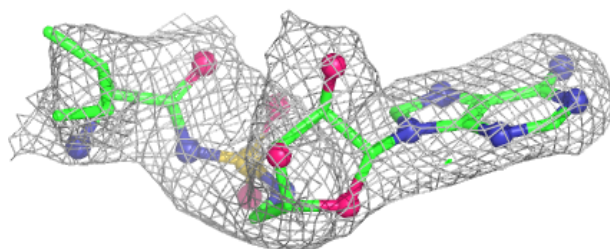
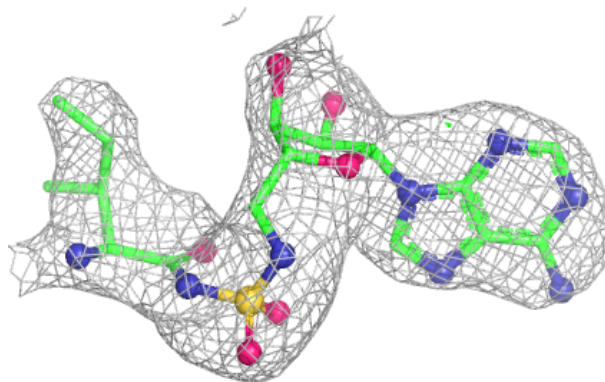
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ILA	D	1863	31/31	0.72	0.17	104,151,160,160	0
5	MG	E	1077	1/1	0.89	0.07	52,52,52,52	0
4	ILA	D	1862	31/31	0.91	0.09	38,48,56,61	0
3	ZN	D	1861	1/1	0.93	0.05	100,100,100,100	0
4	ILA	A	1863	31/31	0.94	0.08	21,28,32,36	0
5	MG	B	1077	1/1	0.96	0.05	25,25,25,25	0
4	ILA	A	1862	31/31	0.97	0.06	7,10,11,11	0
3	ZN	A	1861	1/1	0.98	0.04	65,65,65,65	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.



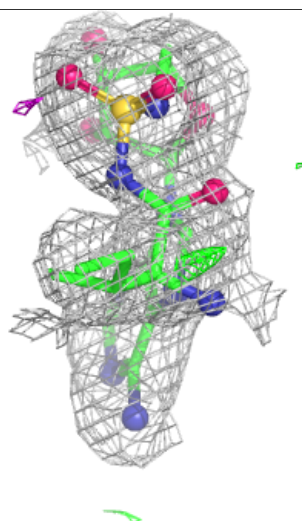
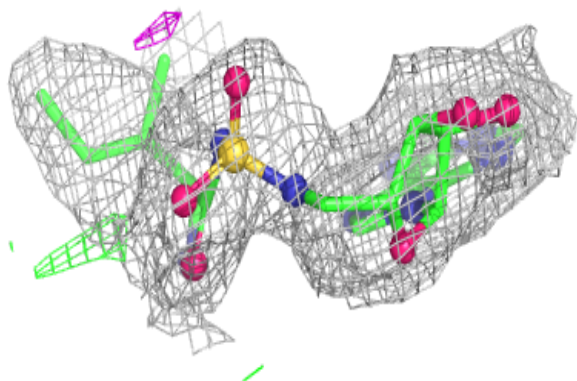
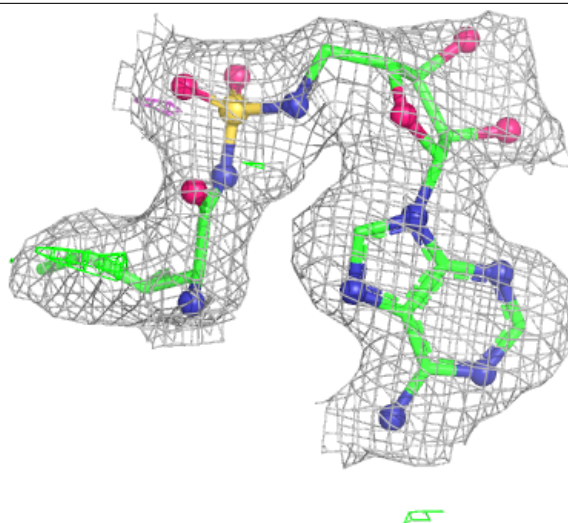
Electron density around ILA D 1862:

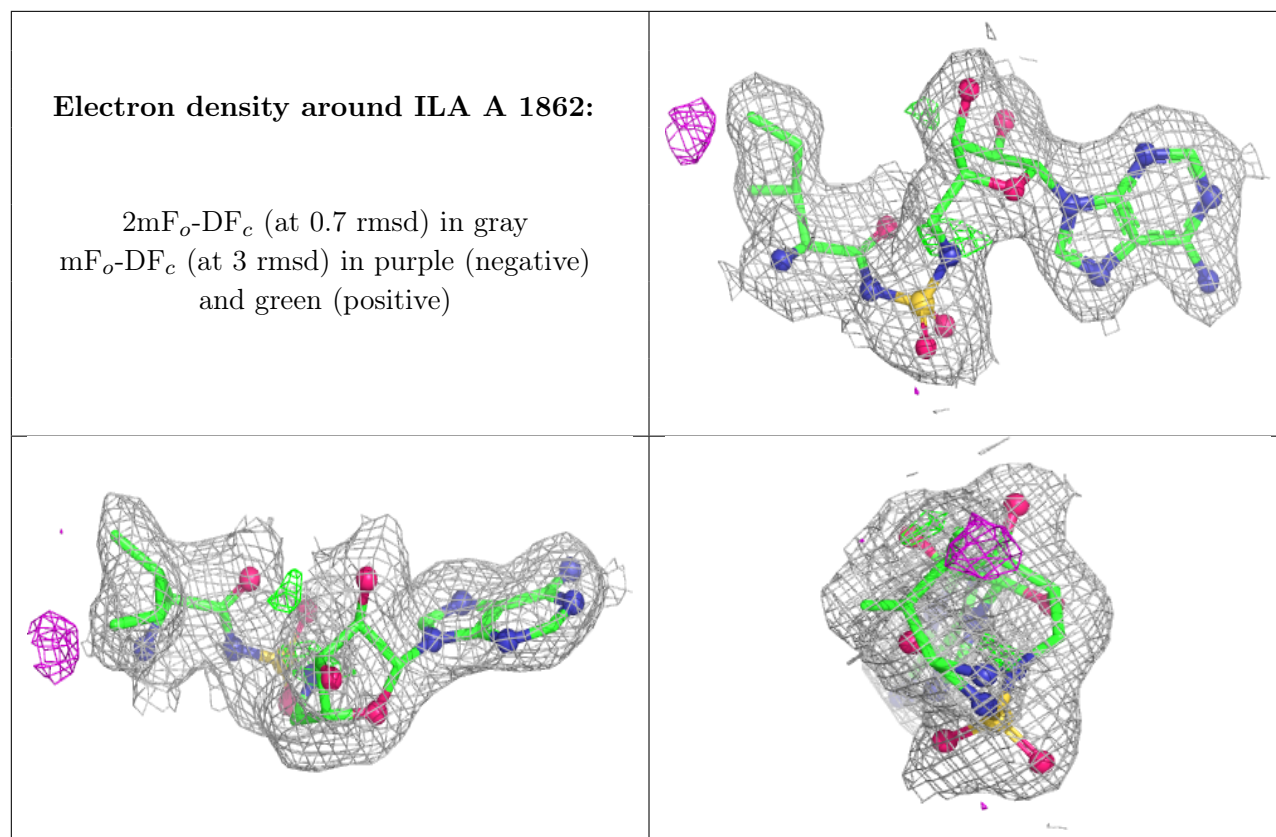
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ILA A 1863:

$2mF_o-DF_c$ (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.