Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:34 am BST

PDB ID	:	5OMW
Title	:	Mutant T252A of E. coli leucyl-tRNA synthetase, tRNA(leu) and leucyl-adenylate analogue in the aminoacylation conformation
Authors	:	Palencia, A.; Cusack, S.
Deposited on	:	2017-08-02
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references ⓘ) were used in the production of this report:

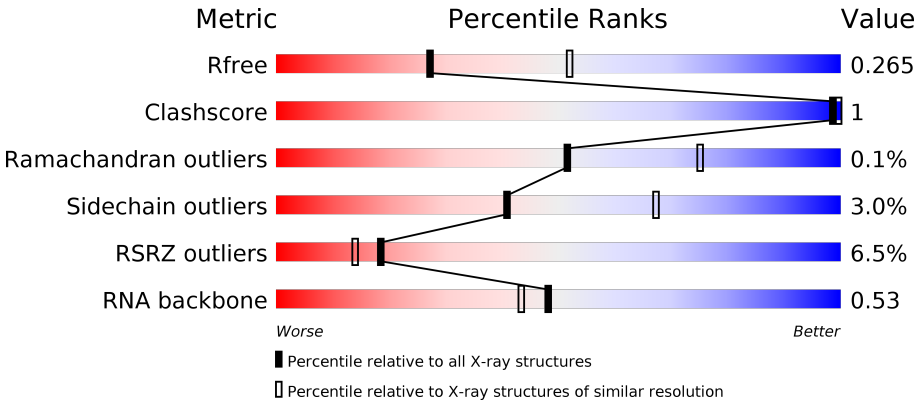
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 >=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 <=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	3%, 93%, 5%
1	D	880	11%, 94%
2	B	87	3%, 84%, 11%, 5%
2	E	87	6%, 78%, 10%, 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17141 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
			6833	4338	1159	1291	45			
1	D	860	Total	C	N	O	S	0	0	0
			6833	4338	1159	1291	45			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	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
A	252	ALA	THR	engineered mutation	UNP P07813
D	-19	MET	-	initiating methionine	UNP P07813
D	-18	GLY	-	expression tag	UNP P07813
D	-17	SER	-	expression tag	UNP P07813
D	-16	SER	-	expression tag	UNP P07813

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP P07813
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
D	252	ALA	THR	engineered mutation	UNP P07813

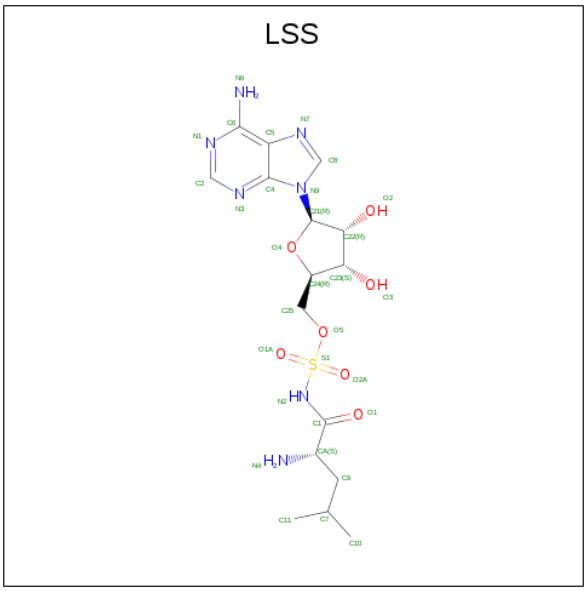
- Molecule 2 is a RNA chain called L-leucyl-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	P	0	0	0
			1777	791	322	581	83			
2	E	77	Total	C	N	O	P	0	0	0
			1632	724	295	536	77			

- 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 5'-O-(L-leucylsulfamoyl)adenosine (three-letter code: LSS) (formula: $C_{16}H_{25}N_7O_7S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 31 16 7 7 1	0	0
4	D	1	Total C N O S 31 16 7 7 1	0	0

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

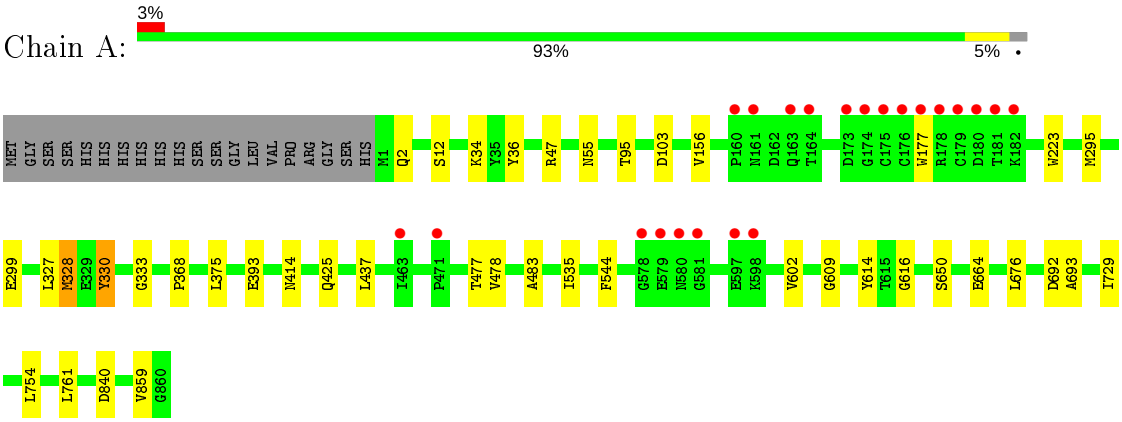
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

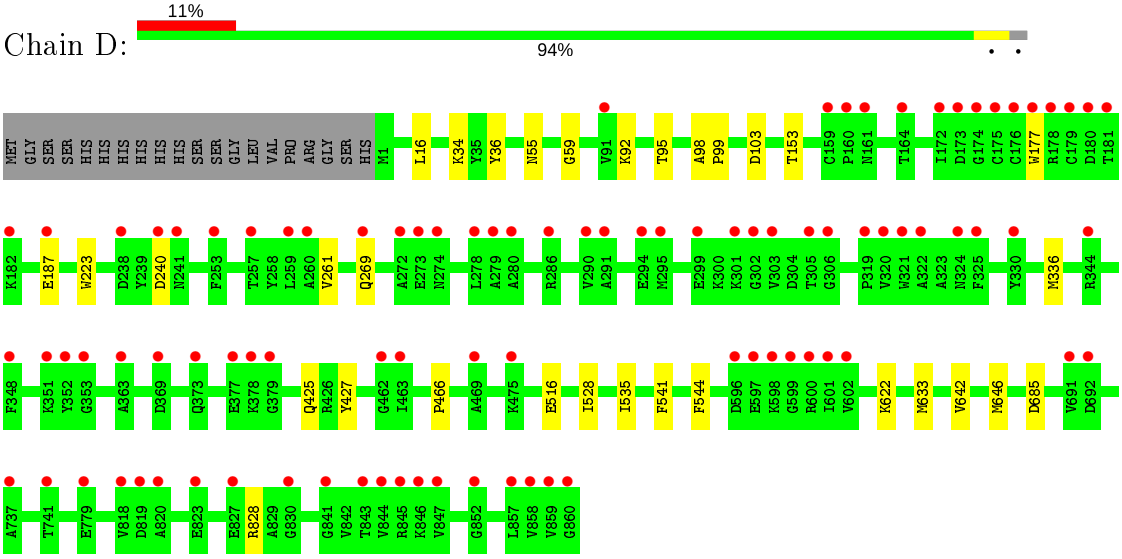
- Molecule 1: Leucine–tRNA ligase

Chain A:



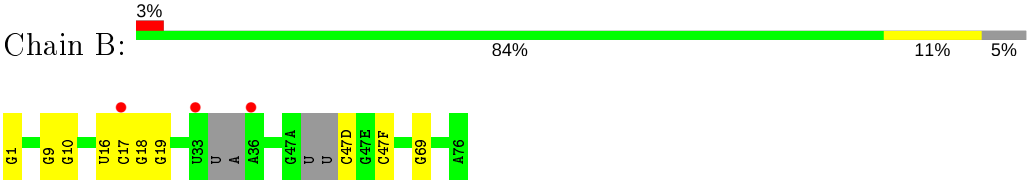
- Molecule 1: Leucine–tRNA ligase

Chain D:



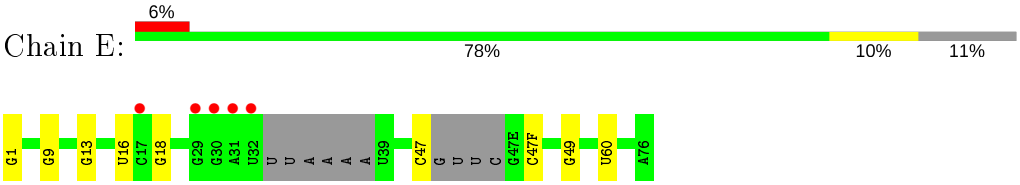
- Molecule 2: L-leucyl-tRNA

Chain B:



• Molecule 2: L-leucyl-tRNA

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.25Å 68.91Å 228.33Å 90.00° 104.93° 90.00°	Depositor
Resolution (Å)	220.62 – 2.60 47.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (220.62-2.60) 99.8 (47.27-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.219 , 0.264 0.224 , 0.265	Depositor DCC
R_{free} test set	3665 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17141	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, MG, LSS

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	0/6994	0.64	0/9494
1	D	0.39	0/6994	0.58	0/9494
2	B	0.39	1/1984 (0.1%)	0.70	0/3086
2	E	0.33	1/1821 (0.1%)	0.66	0/2833
All	All	0.40	2/17793 (0.0%)	0.63	0/24907

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	G	OP3-P	-10.08	1.49	1.61
2	B	1	G	OP3-P	-9.80	1.49	1.61

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	6833	0	6686	10	0
1	D	6833	0	6686	6	0
2	B	1777	0	901	1	0
2	E	1632	0	825	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	31	0	25	0	0
4	D	31	0	25	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
All	All	17141	0	15148	17	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 1.

All (17) 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:368:PRO:HB3	1:A:375:LEU:HD22	1.75	0.68
1:A:676:LEU:HD23	1:A:754:LEU:HD21	1.77	0.67
1:A:437:LEU:HD23	1:A:483:ALA:HB2	1.75	0.66
1:A:295:MET:SD	1:A:327:LEU:HD11	2.48	0.53
2:B:47(D):C:O4'	2:B:47(D):C:O2	2.28	0.52
1:A:437:LEU:HD21	1:A:478:VAL:HB	1.94	0.50
1:A:223:TRP:CD2	1:A:535:ILE:HG21	2.50	0.47
1:D:98:ALA:HB3	1:D:99:PRO:HD3	1.97	0.45
1:A:729:ILE:HG21	1:A:761:LEU:HD13	1.99	0.45
1:A:328:MET:HE2	1:A:333:GLY:HA3	2.01	0.43
1:A:327:LEU:HD12	1:A:330:TYR:CE2	2.54	0.42
1:D:223:TRP:CD2	1:D:535:ILE:HG21	2.54	0.42
1:D:153:THR:CG2	1:D:187:GLU:HB3	2.49	0.41
1:D:427:TYR:HB2	1:D:466:PRO:HD2	2.02	0.41
1:D:59:GLY:HA2	1:D:528:ILE:HD13	2.03	0.41
1:A:614:TYR:CZ	1:A:616:GLY:HA2	2.55	0.41
1:D:633:MET:HE2	1:D:642:VAL:HG13	2.04	0.41

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%)	830 (97%)	26 (3%)	2 (0%)	47 71
1	D	858/880 (98%)	829 (97%)	29 (3%)	0	100 100
All	All	1716/1760 (98%)	1659 (97%)	55 (3%)	2 (0%)	51 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	693	ALA
1	A	609	GLY

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	723/740 (98%)	699 (97%)	24 (3%)	38 64
1	D	723/740 (98%)	703 (97%)	20 (3%)	43 69
All	All	1446/1480 (98%)	1402 (97%)	44 (3%)	41 67

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	12	SER
1	A	34	LYS
1	A	36	TYR
1	A	47	ARG
1	A	55	ASN
1	A	95	THR
1	A	103	ASP
1	A	156	VAL
1	A	177	TRP
1	A	299	GLU

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Mol	Chain	Res	Type
1	A	328	MET
1	A	330	TYR
1	A	393	GLU
1	A	414	ASN
1	A	425	GLN
1	A	477	THR
1	A	544	PHE
1	A	602	VAL
1	A	650	SER
1	A	664	GLU
1	A	692	ASP
1	A	840	ASP
1	A	859	VAL
1	D	16	LEU
1	D	34	LYS
1	D	36	TYR
1	D	55	ASN
1	D	92	LYS
1	D	95	THR
1	D	103	ASP
1	D	177	TRP
1	D	240	ASP
1	D	261	VAL
1	D	269	GLN
1	D	336	MET
1	D	425	GLN
1	D	516	GLU
1	D	541	PHE
1	D	544	PHE
1	D	622	LYS
1	D	646	MET
1	D	685	ASP
1	D	828	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	555	ASN
1	A	625	ASN
1	D	75	GLN
1	D	110	ASN

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Mol	Chain	Res	Type
1	D	383	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	80/87 (91%)	8 (10%)	1 (1%)
2	E	73/87 (83%)	7 (9%)	1 (1%)
All	All	153/174 (87%)	15 (9%)	2 (1%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	10	G
2	B	16	U
2	B	17	C
2	B	18	G
2	B	19	G
2	B	47(F)	C
2	B	69	G
2	E	9	G
2	E	13	G
2	E	16	U
2	E	18	G
2	E	47	C
2	E	47(F)	C
2	E	49	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	17	C
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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	LSS	A	901	-	30,33,33	1.08	3 (10%)	33,49,49	1.84	3 (9%)
4	LSS	D	901	-	30,33,33	1.28	3 (10%)	33,49,49	1.81	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	LSS	A	901	-	-	2/18/39/39	0/3/3/3
4	LSS	D	901	-	-	1/18/39/39	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	LSS	S1-N2	-3.65	1.53	1.59
4	A	901	LSS	S1-N2	-2.80	1.54	1.59
4	D	901	LSS	O5-S1	-2.69	1.54	1.59
4	A	901	LSS	O5-S1	-2.54	1.54	1.59
4	D	901	LSS	O1A-S1	2.31	1.44	1.42
4	A	901	LSS	O4-C21	2.15	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	LSS	O2A-S1-O1A	-7.85	108.53	120.76
4	D	901	LSS	O2A-S1-O1A	-7.51	109.06	120.76
4	D	901	LSS	N3-C2-N1	-4.58	121.52	128.68
4	A	901	LSS	N3-C2-N1	-3.88	122.61	128.68
4	A	901	LSS	C25-O5-S1	3.11	123.79	117.37
4	D	901	LSS	C25-O5-S1	2.75	123.06	117.37
4	D	901	LSS	C21-N9-C4	-2.26	122.66	126.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

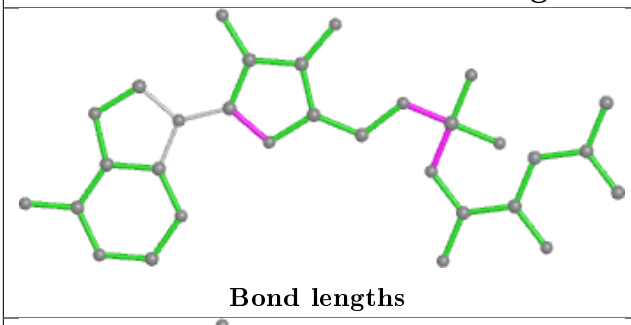
Mol	Chain	Res	Type	Atoms
4	D	901	LSS	C25-O5-S1-N2
4	A	901	LSS	C25-O5-S1-N2
4	A	901	LSS	N2-C1-CA-N4

There are no ring outliers.

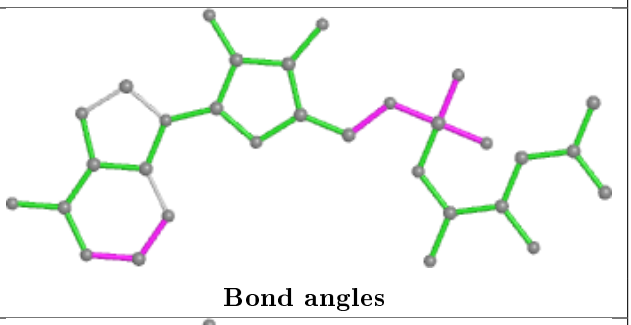
No monomer is involved in short contacts.

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.

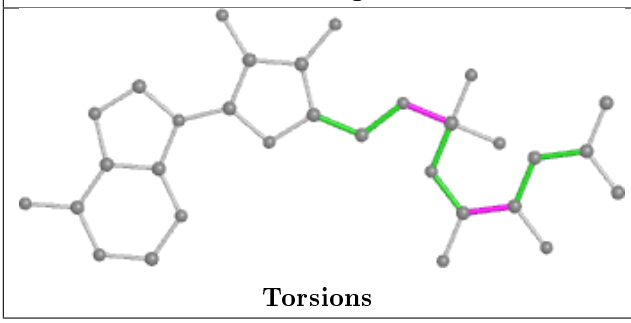
Ligand LSS A 901



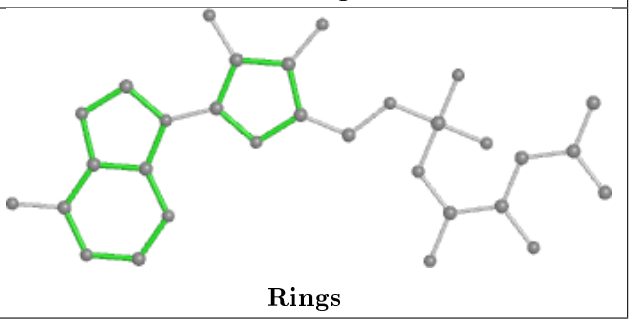
Bond lengths



Bond angles

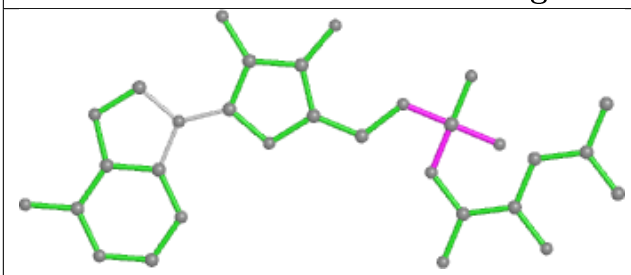


Torsions

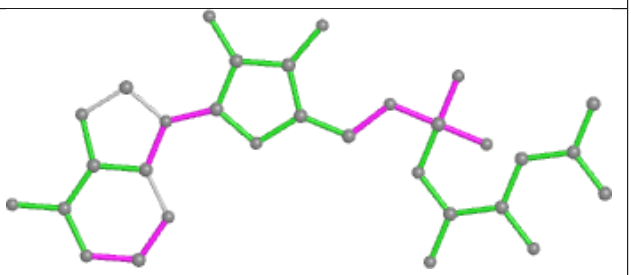


Rings

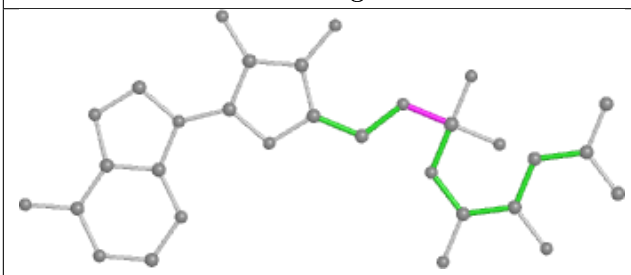
Ligand LSS D 901



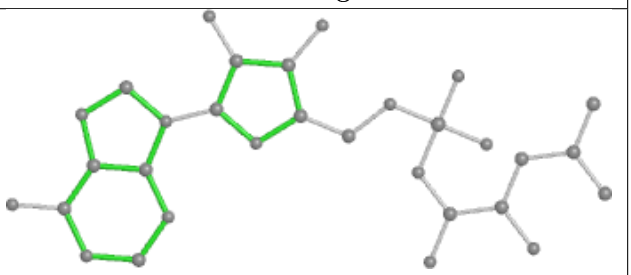
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 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, 95^{th} 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%)	-0.03	22 (2%) 56 50	21, 38, 76, 174	0
1	D	860/880 (97%)	0.56	93 (10%) 5 3	43, 74, 119, 179	0
2	B	83/87 (95%)	-0.40	3 (3%) 42 35	24, 37, 103, 157	0
2	E	77/87 (88%)	0.06	5 (6%) 18 14	52, 79, 114, 159	0
All	All	1880/1934 (97%)	0.23	123 (6%) 18 14	21, 58, 114, 179	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	860	GLY	23.4
1	A	175	CYS	11.3
1	D	173	ASP	10.1
1	A	173	ASP	9.9
1	D	174	GLY	9.7
1	A	176	CYS	9.6
1	D	177	TRP	7.9
1	A	177	TRP	7.8
1	A	174	GLY	7.5
1	D	175	CYS	7.3
1	D	291	ALA	6.8
1	D	178	ARG	6.8
1	D	463	ILE	6.2
1	D	600	ARG	6.2
1	D	172	ILE	6.0
1	D	597	GLU	5.7
1	D	599	GLY	5.3
1	D	598	LYS	4.9
1	D	279	ALA	4.8
2	B	17	C	4.4
2	B	36	A	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	692	ASP	4.4
1	A	580	ASN	4.3
1	D	303	VAL	4.3
1	D	847	VAL	4.3
1	D	324	ASN	4.2
1	D	859	VAL	4.1
1	D	845	ARG	4.1
1	D	819	ASP	3.9
1	D	259	LEU	3.8
1	D	377	GLU	3.7
1	D	325	PHE	3.7
1	D	841	GLY	3.6
1	A	180	ASP	3.6
1	D	353	GLY	3.5
1	D	179	CYS	3.5
1	A	578	GLY	3.4
1	A	579	GLU	3.4
1	A	181	THR	3.4
1	D	176	CYS	3.3
1	D	238	ASP	3.3
1	D	369	ASP	3.3
1	A	598	LYS	3.3
1	A	178	ARG	3.3
1	D	352	TYR	3.2
1	A	163	GLN	3.2
1	D	294	GLU	3.2
2	E	32	U	3.2
1	D	691	VAL	3.2
1	D	820	ALA	3.1
1	A	161	ASN	3.1
1	A	463	ILE	3.0
1	A	597	GLU	3.0
1	D	280	ALA	3.0
1	A	179	CYS	3.0
1	D	823	GLU	3.0
1	D	272	ALA	3.0
1	D	278	LEU	3.0
1	D	741	THR	2.9
1	D	257	THR	2.9
1	D	818	VAL	2.9
1	D	596	ASP	2.9
1	D	290	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	180	ASP	2.9
1	D	269	GLN	2.8
1	D	601	ILE	2.8
1	D	241	ASN	2.8
1	D	321	TRP	2.8
1	D	181	THR	2.8
1	D	301	LYS	2.8
1	D	161	ASN	2.7
2	E	30	G	2.7
1	D	363	ALA	2.7
1	D	320	VAL	2.7
1	D	852	GLY	2.7
1	A	160	PRO	2.7
1	D	344	ARG	2.7
1	D	843	THR	2.7
1	D	830	GLY	2.6
1	D	260	ALA	2.6
1	D	379	GLY	2.6
1	D	299	GLU	2.6
1	D	322	ALA	2.6
1	D	305	THR	2.6
1	A	471	PRO	2.6
2	E	17	C	2.6
1	A	164	THR	2.5
1	D	844	VAL	2.5
1	D	302	GLY	2.5
1	D	469	ALA	2.5
1	D	857	LEU	2.4
1	D	602	VAL	2.4
1	D	159	CYS	2.4
1	A	581	GLY	2.4
1	D	160	PRO	2.4
1	D	187	GLU	2.4
1	D	462	GLY	2.3
1	D	240	ASP	2.3
1	D	182	LYS	2.3
1	D	779	GLU	2.3
2	E	29	G	2.3
1	D	737	ALA	2.3
1	D	164	THR	2.3
1	D	286	ARG	2.3
1	D	306	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	182	LYS	2.3
1	D	348	PHE	2.3
1	D	295	MET	2.2
1	D	330	TYR	2.2
1	D	858	VAL	2.2
1	D	274	ASN	2.2
1	D	846	LYS	2.1
1	D	475	LYS	2.1
1	D	351	LYS	2.1
1	D	378	LYS	2.1
1	D	91	VAL	2.1
2	B	33	U	2.1
1	D	827	GLU	2.1
1	D	253	PHE	2.0
1	D	373	GLN	2.0
2	E	31	A	2.0
1	D	273	GLU	2.0
1	D	319	PRO	2.0

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^{th} 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	ZN	D	900	1/1	0.21	0.39	205,205,205,205	0
3	ZN	A	900	1/1	0.60	0.35	164,164,164,164	0
5	MG	E	101	1/1	0.75	0.15	59,59,59,59	0
5	MG	B	101	1/1	0.81	0.12	47,47,47,47	0
4	LSS	D	901	31/31	0.96	0.18	48,50,54,55	0

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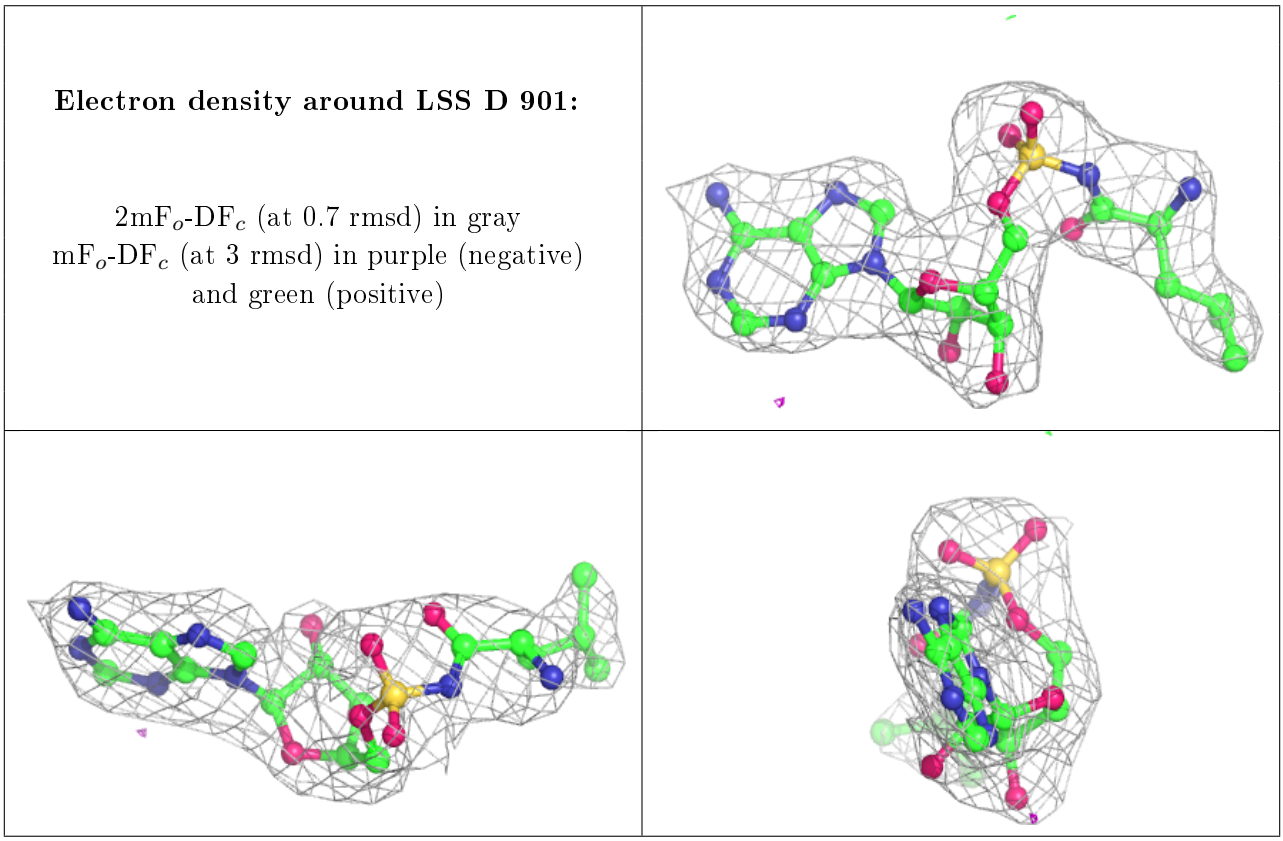
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LSS	A	901	31/31	0.98	0.18	22,25,28,28	0

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.

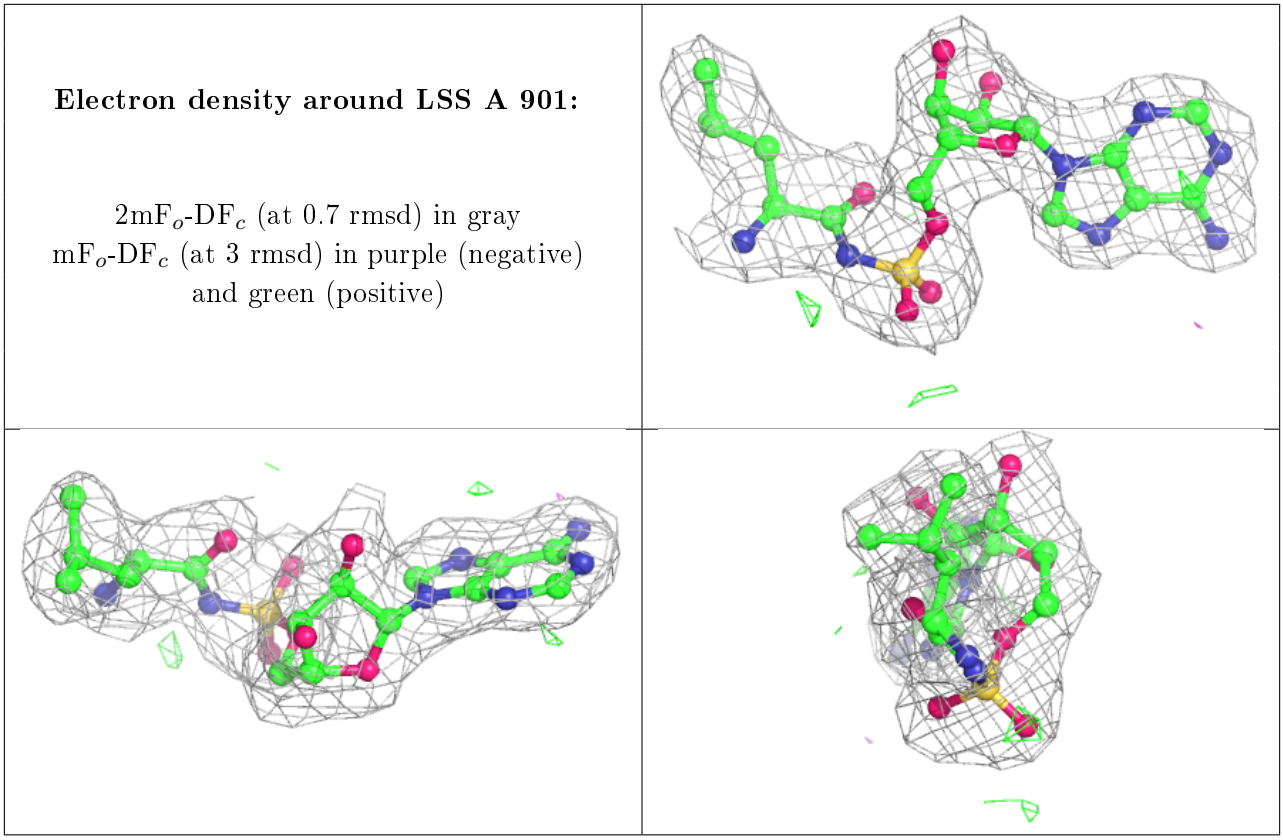
Electron density around LSS D 901:

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



Electron density around LSS A 901:

$2mF_o$-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.