wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 04:08 AM JST

PDB ID	:	6KQY
Title	:	Crystal structure of human leucyl-tRNA synthetase, Leucine-bound form
Authors	:	Kim, S.; Son, J.; Kim, S.; Hwang, K.Y.
Deposited on	:	2019-08-20
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

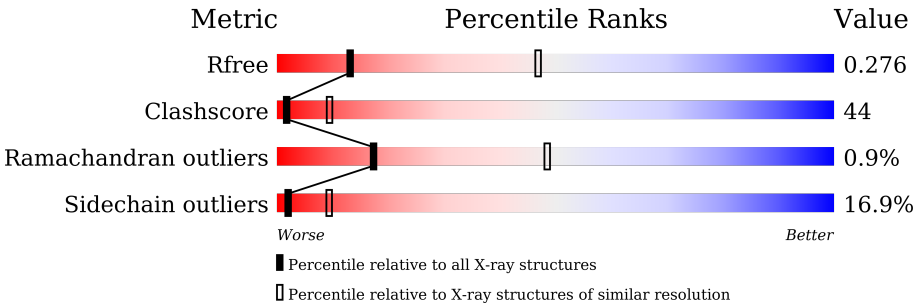
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1188	30% 45% 10% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8558 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.

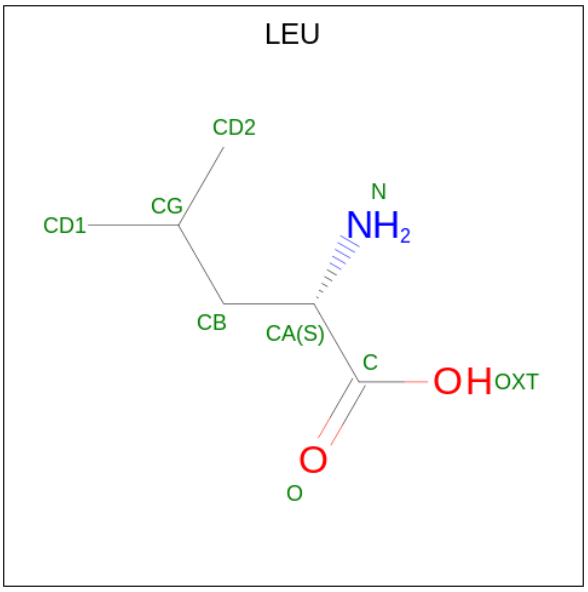
- Molecule 1 is a protein called Leucine–tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1002	Total	C	N	O	S	0	0	0
			8088	5204	1343	1488	53			

There are 12 discrepancies between the modelled and reference sequences:

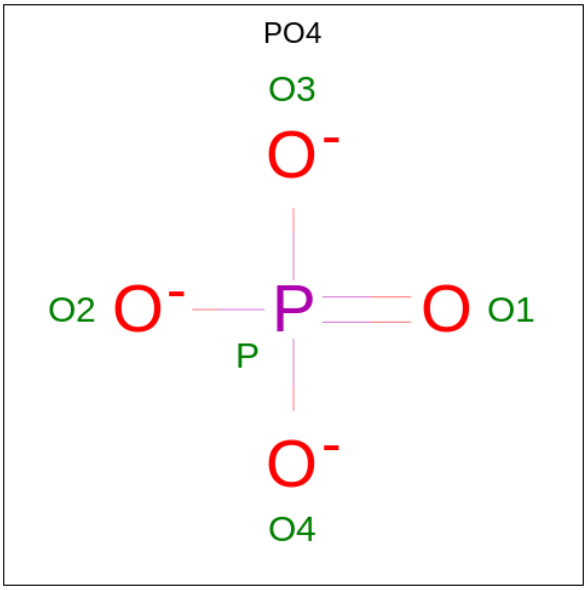
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9P2J5
A	-10	ARG	-	expression tag	UNP Q9P2J5
A	-9	GLY	-	expression tag	UNP Q9P2J5
A	-8	SER	-	expression tag	UNP Q9P2J5
A	-7	HIS	-	expression tag	UNP Q9P2J5
A	-6	HIS	-	expression tag	UNP Q9P2J5
A	-5	HIS	-	expression tag	UNP Q9P2J5
A	-4	HIS	-	expression tag	UNP Q9P2J5
A	-3	HIS	-	expression tag	UNP Q9P2J5
A	-2	HIS	-	expression tag	UNP Q9P2J5
A	-1	GLY	-	expression tag	UNP Q9P2J5
A	0	SER	-	expression tag	UNP Q9P2J5

- Molecule 2 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 6 1 2	0	0
2	A	1	Total C N O 9 6 1 2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

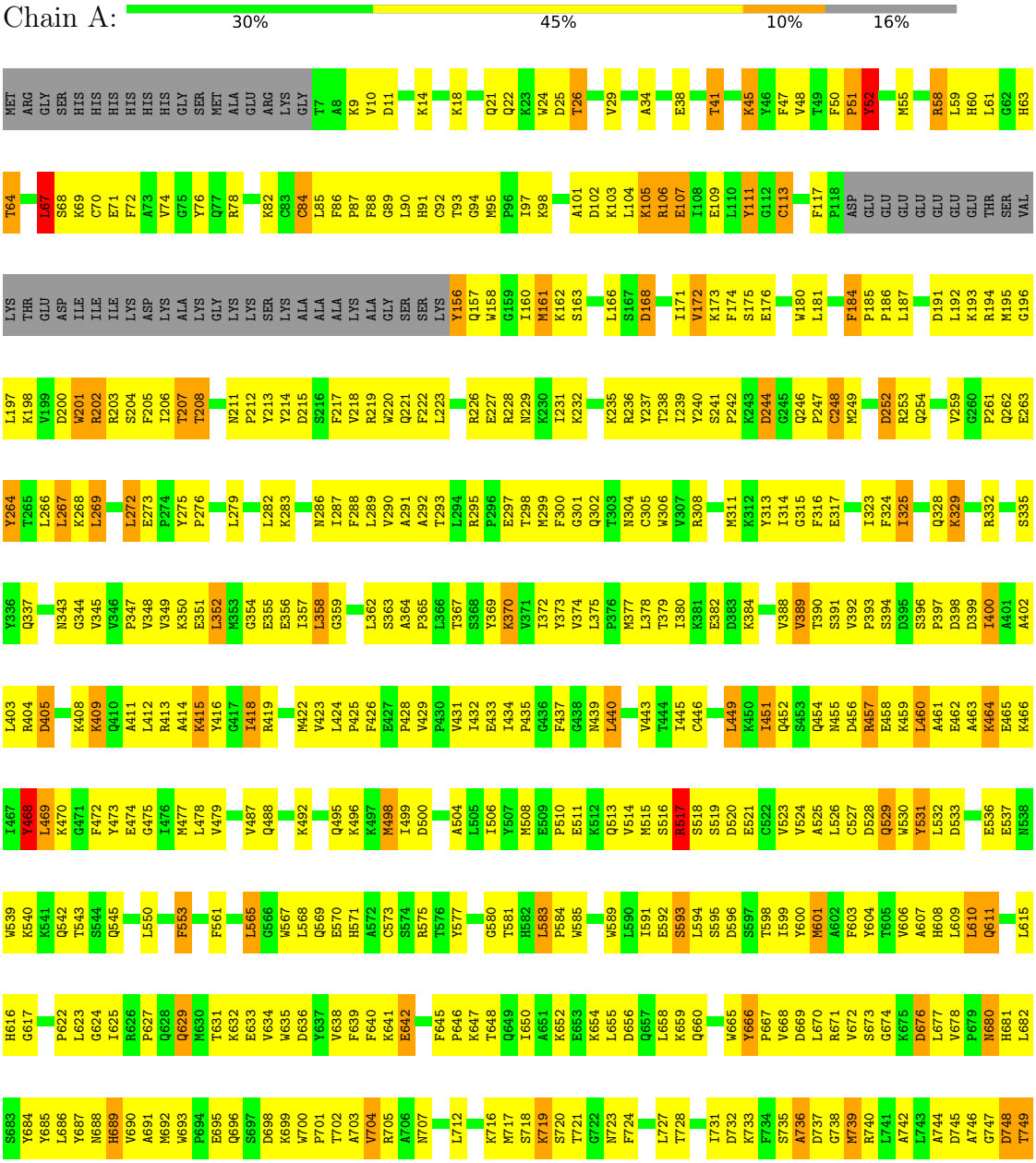
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	447	Total O 447 447	0	0

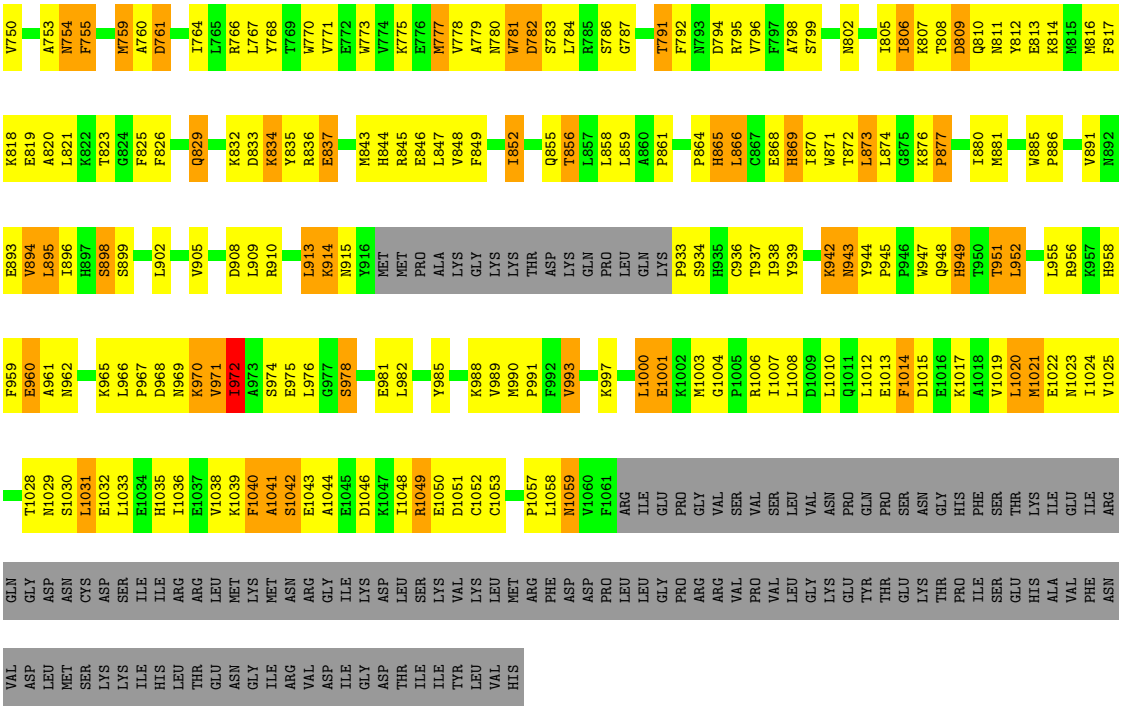
3 Residue-property plots (i)

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: Leucine–tRNA ligase, cytoplasmic

Chain A:




V750 A753 N754 F755 M759 A760 D761 I764 L765 R766 L767 Y768 T769 W770 V771 E772 W773 V774 K775 E776 M777 V778 A779 N780 W781 D782 S783 L784 R785 S786 G787 T791 F792 N793 D794 R795 V796 F797 A798 S799 N802 I805 I806 K807 T808 D809 Q810 N811 Y812 E813 K814 M815 M816 F817
K818 E819 A820 L821 K822 T823 G824 F825 F826 Q829 K832 D833 K834 Y835 R836 E837 M843 H844 R845 E846 L847 V848 F849 I852 Q855 T856 L857 L858 L859 A860 P861 P864 H865 L866 C867 E868 H869 I870 W871 T872 L873 L874 G875 K876 P877 I880 M881 W885 P886 V891 N892
E893 V894 L895 I896 H897 S898 S899 L902 V905 D908 L909 R910 L913 K914 N915 Y916 MET MET PRO ALA LYS GLY LYS LYS THR ASP LYS GLN PRO LEU GLN LYS P933 S934 H935 C936 T937 I938 Y939 K942 N943 Y944 P945 P946 W947 Q948 H949 T950 T951 L952 L955 R956 K957 H958
F959 E960 A961 N962 K965 L966 P967 D968 N969 K970 V971 I972 A973 S974 E975 L976 G977 S978 E981 L982 Y985 K988 V989 M990 P991 F992 V993 K997 L1000 E1001 K1002 M1003 G1004 P1005 R1006 I1007 L1008 D1009 L1010 Q1011 L1012 E1013 P1014 D1015 E1016 K1017 A1018 V1019 L1020 M1021 E1022 N1023 I1024 V1025
T1028 N1029 S1030 L1031 E1032 L1033 E1034 H1035 I1036 E1037 V1038 K1039 F1040 A1041 S1042 E1043 A1044 E1045 D1046 K1047 I1048 R1049 E1050 D1051 C1052 C1053 P1057 L1058 N1059 V1060 F1061 ARG ILE GLU PRO GLY VAL SER VAL SER LEU VAL ASN PRO GLN PRO SER ASN GLY HIS PHE SER THR LYS ILE GLU ILE ARG
GLN GLY ASP ASN CYS ASP SER ILE ILE ARG LEU THR GLU ASN GLY ILE ARG VAL ASP ILE GLY ASP THR ILE ILE TYR LEU VAL HIS
VAL ASP LEU MET SER LYS LYS ILE ILE HIS LEU THR GLU ASN GLY ILE ARG VAL ASP ILE LYS ASP LEU SER LYS VAL LYS LEU MET ARG PHE ASP ASP PRO LEU LEU GLY PRO ARG ARG VAL PRO VAL LEU GLY LYS GLU TYR THR GLU LYS THR PRO ILE SER GLU HIS ALA VAL PHE ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.74Å 123.74Å 536.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.76 – 3.30 49.76 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.76-3.30) 94.7 (49.76-2.83)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.251 , 0.276 0.249 , 0.276	Depositor DCC
R_{free} test set	1937 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.08 , 10.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.27$, $< L^2 > = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.53	EDS
Total number of atoms	8558	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: PO4

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	0.60	0/8288	0.79	9/11203 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1041	ALA	N-CA-CB	6.66	119.42	110.10
1	A	52	TYR	CA-CB-CG	6.27	125.32	113.40
1	A	565	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	67	LEU	CA-CB-CG	6.19	129.55	115.30
1	A	1041	ALA	CB-CA-C	5.81	118.81	110.10

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	8088	0	8046	708	6
2	A	18	0	20	4	0
3	A	5	0	0	0	0
4	A	447	0	0	77	0
All	All	8558	0	8066	708	6

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 44.

The worst 5 of 708 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:446:CYS:CB	1:A:451:ILE:HD12	1.49	1.42
1:A:958:HIS:HE1	1:A:962:ASN:ND2	1.06	1.42
1:A:958:HIS:CE1	1:A:962:ASN:ND2	1.87	1.39
1:A:446:CYS:CB	1:A:451:ILE:CD1	2.08	1.22
1:A:958:HIS:CE1	1:A:962:ASN:HD22	1.55	1.19

The worst 5 of 6 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:455:ASN:CG	1:A:877:PRO:CG[8_545]	1.09	1.11
1:A:455:ASN:OD1	1:A:877:PRO:CG[8_545]	1.34	0.86
1:A:455:ASN:ND2	1:A:877:PRO:CB[8_545]	1.52	0.68
1:A:455:ASN:ND2	1:A:877:PRO:CG[8_545]	1.65	0.55
1:A:455:ASN:CG	1:A:877:PRO:CB[8_545]	1.89	0.31

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	996/1188 (84%)	817 (82%)	170 (17%)	9 (1%)	17 48

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	TYR
1	A	517	ARG
1	A	1013	GLU

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Mol	Chain	Res	Type
1	A	736	ALA
1	A	877	PRO

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	883/1047 (84%)	733 (83%)	150 (17%)	2 9

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	869	HIS
1	A	1040	PHE
1	A	898	SER
1	A	970	LYS
1	A	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	689	HIS
1	A	696	GLN
1	A	962	ASN
1	A	958	HIS
1	A	569	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	LEU	A	1202	-	7,8,8	0.88	1 (14%)	9,10,10	1.36	2 (22%)
3	PO4	A	1203	-	4,4,4	0.82	0	6,6,6	0.44	0
2	LEU	A	1201	-	7,8,8	0.88	0	9,10,10	1.30	2 (22%)

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
2	LEU	A	1202	-	-	4/8/8/8	-
2	LEU	A	1201	-	-	1/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1202	LEU	OXT-C	-2.03	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1202	LEU	OXT-C-O	-3.42	116.33	124.09
2	A	1201	LEU	OXT-C-O	-3.09	117.07	124.09
2	A	1201	LEU	OXT-C-CA	2.23	120.98	113.38
2	A	1202	LEU	OXT-C-CA	2.06	120.41	113.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	LEU	N-CA-CB-CG
2	A	1202	LEU	O-C-CA-N
2	A	1202	LEU	OXT-C-CA-N
2	A	1202	LEU	OXT-C-CA-CB
2	A	1202	LEU	O-C-CA-CB

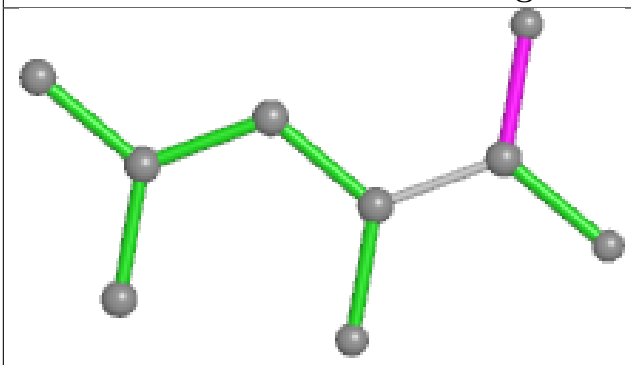
There are no ring outliers.

1 monomer is involved in 4 short contacts:

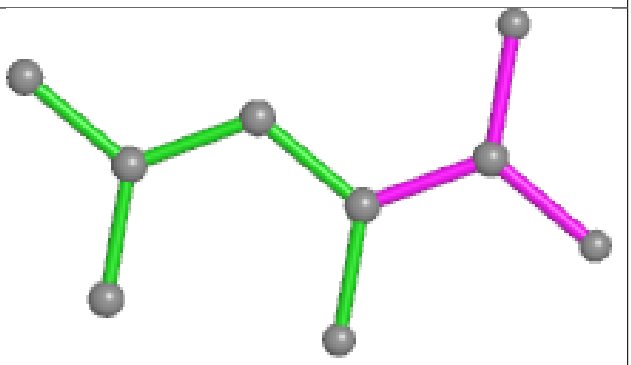
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1202	LEU	4	0

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 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.

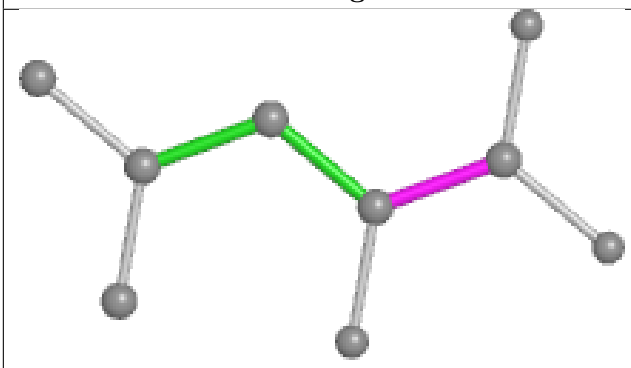
Ligand LEU A 1202



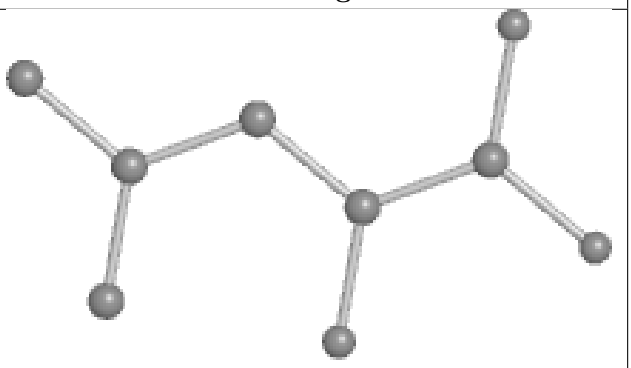
Bond lengths



Bond angles

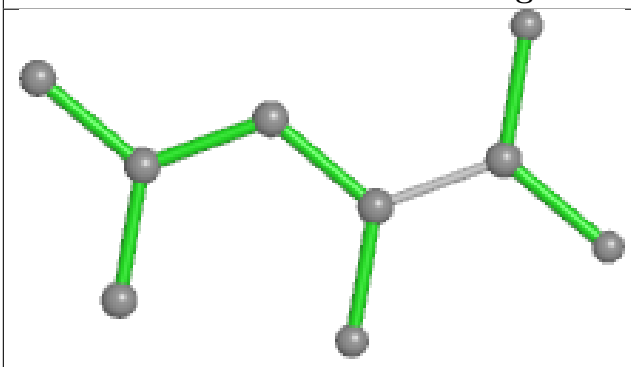


Torsions

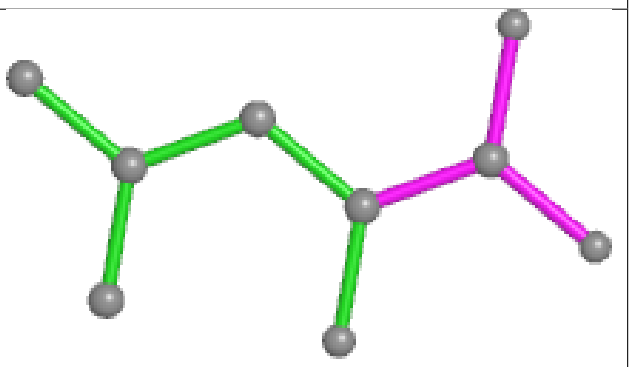


Rings

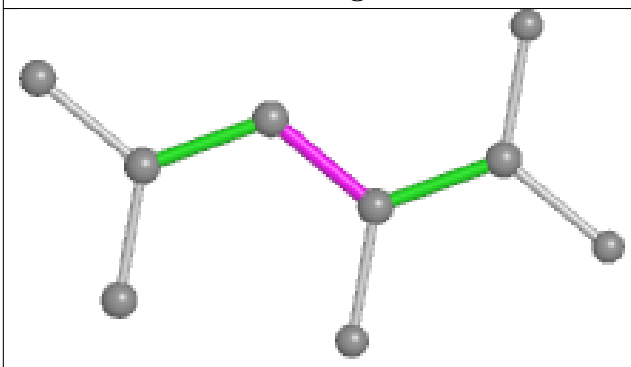
Ligand LEU A 1201



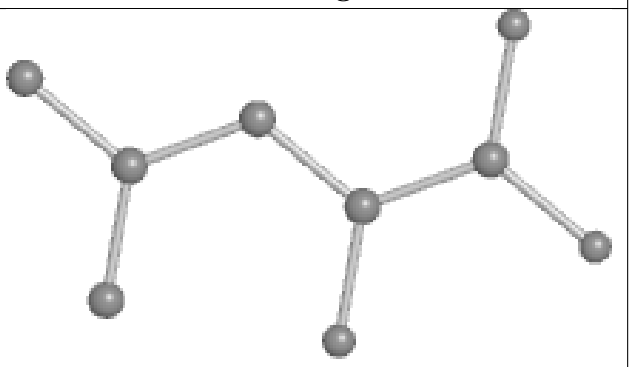
Bond lengths



Bond angles



Torsions



Rings

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.

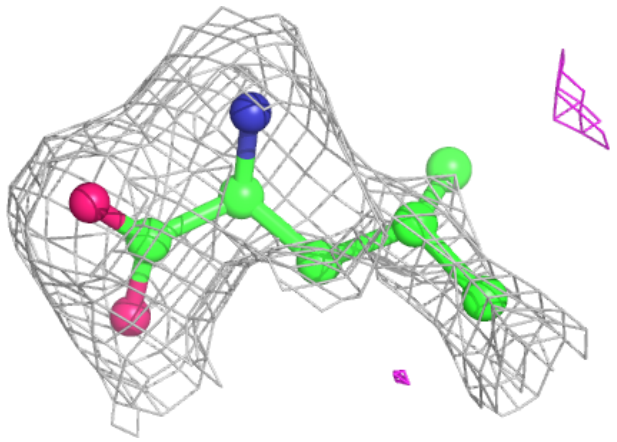
6.4 Ligands

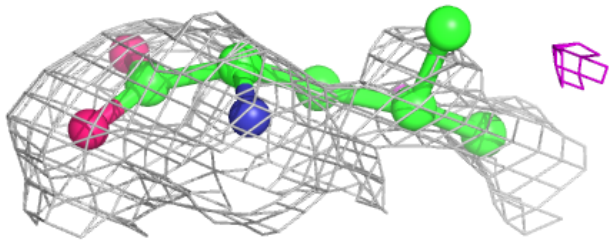
Unable to reproduce the depositors R factor - this section is therefore empty.

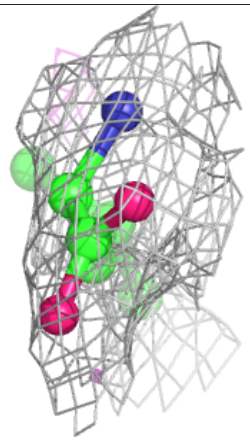
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LEU A 1201:

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

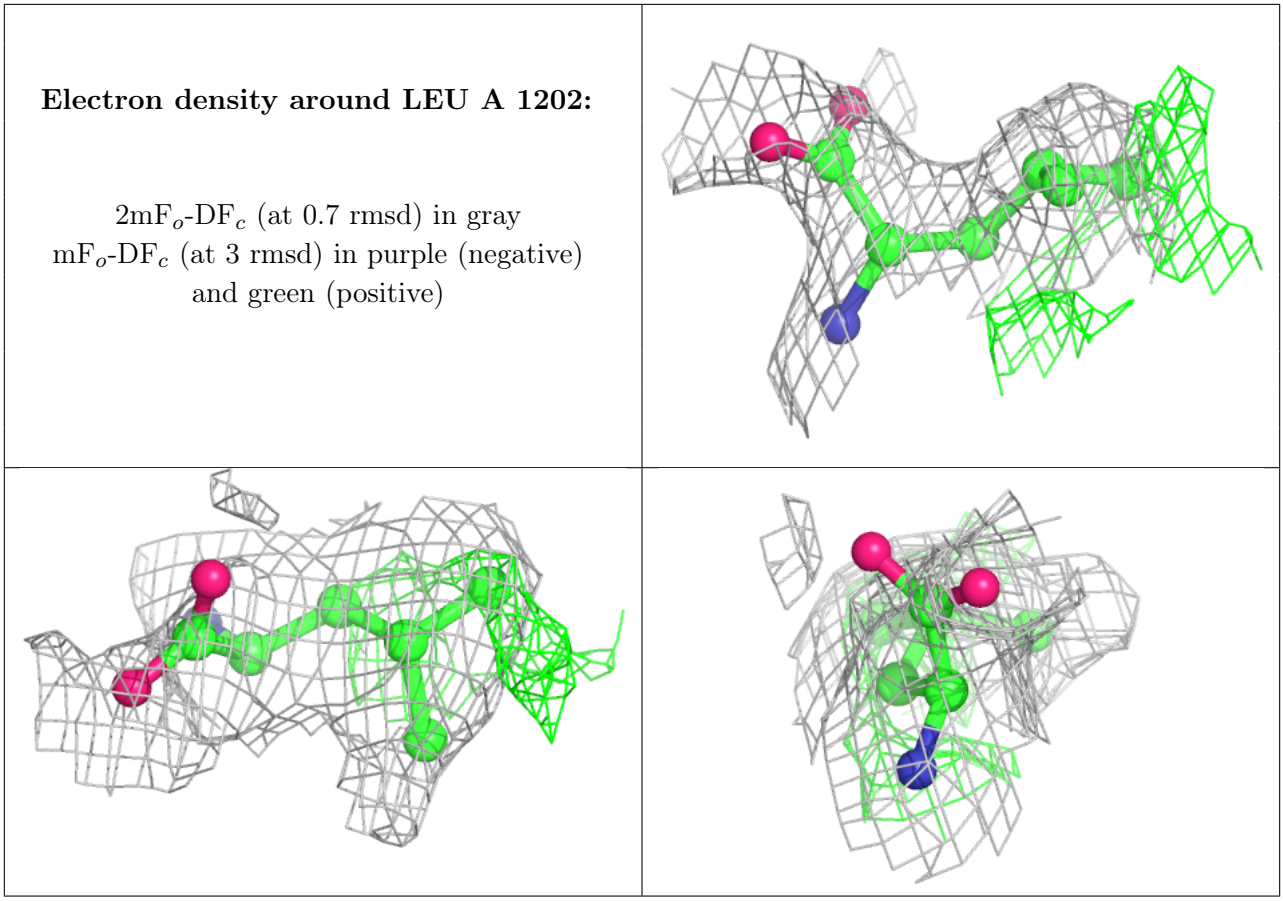






Electron density around LEU A 1202:

$2mF_o$-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)

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