Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:52 PM GMT

PDB ID	:	4ARC
Title	:	Ternary complex of E. coli leucyl-tRNA synthetase, tRNA(leu) and leucine in the editing conformation
Authors	:	Palencia, A.; Crepin, T.; Vu, M.T.; Lincecum Jr, T.L.; Martinis, S.A.; Cusack, S.
Deposited on	:	2012-04-23
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

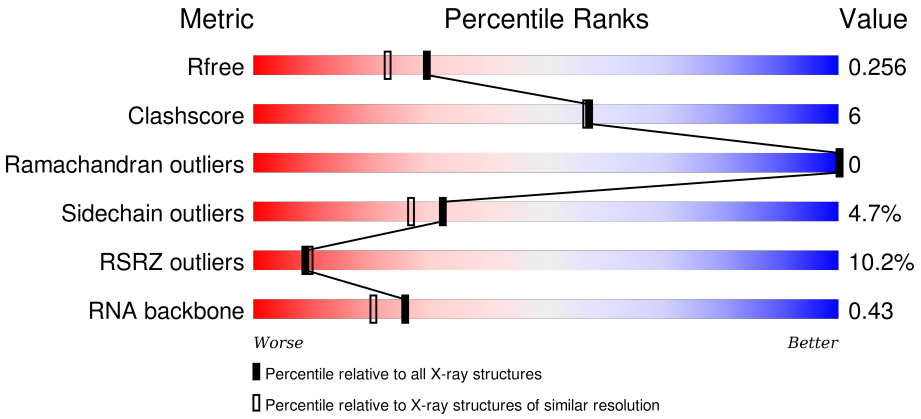
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)
RNA backbone	2183	1002 (2.72-1.30)

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. 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	8% 80% 11% • 8%
2	B	87	22% 39% 31% 10% • 18%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8406 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	813	Total	C	N	O	S	0	0	0
			6465	4118	1091	1218	38			

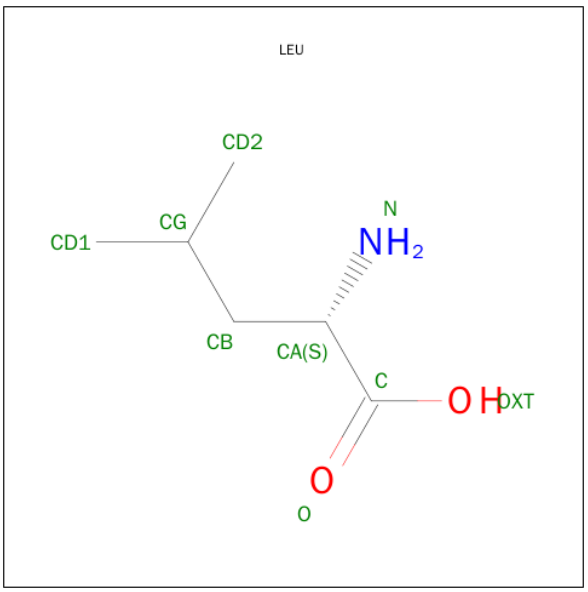
There are 20 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called TRNA-LEU5 (UAA ISOACCEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	P	0	0	0
			1516	675	271	499	71			

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is water.

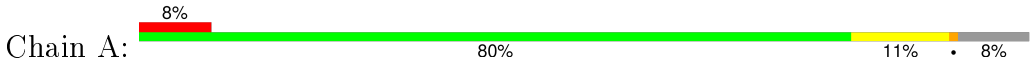
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	385	Total O 385 385	0	0
5	B	30	Total O 30 30	0	0

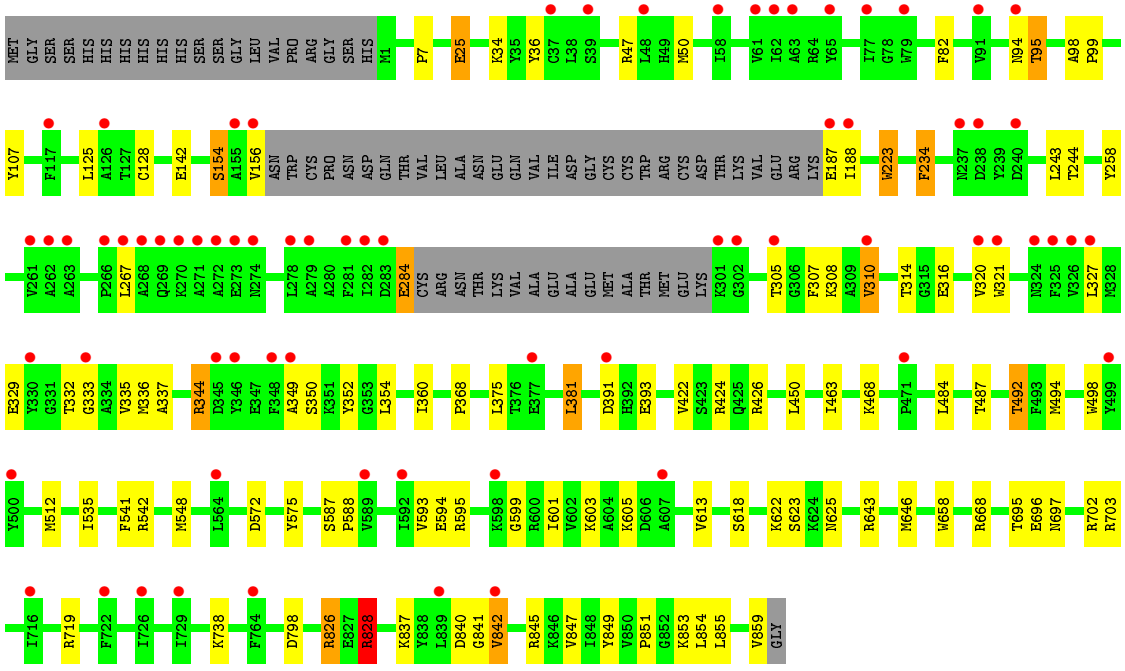
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

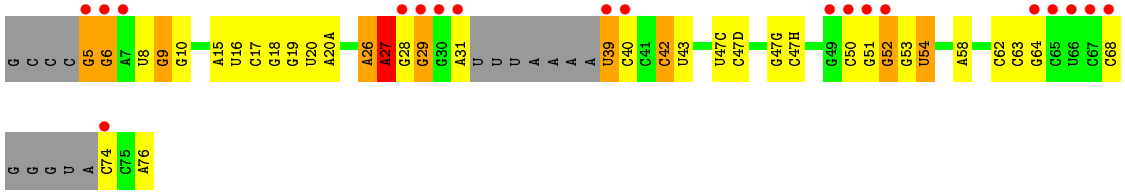
Chain A:





- Molecule 2: TRNA-LEU5 (UAA ISOACCEPTOR)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.08Å 119.37Å 141.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.57 – 2.00 45.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.57-2.00) 99.3 (45.57-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.210 , 0.257 0.208 , 0.256	Depositor DCC
R_{free} test set	4411 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 87918 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8406	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.84	3/6619 (0.0%)	0.85	12/8986 (0.1%)
2	B	0.48	0/1691	1.03	10/2630 (0.4%)
All	All	0.78	3/8310 (0.0%)	0.90	22/11616 (0.2%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	TRP	CD2-CE2	5.40	1.47	1.41
1	A	25	GLU	CD-OE1	5.24	1.31	1.25
1	A	223	TRP	CD2-CE2	5.24	1.47	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	58	A	O5'-P-OP2	-9.43	97.21	105.70
1	A	542	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	424	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	542	ARG	NE-CZ-NH1	7.05	123.82	120.30
2	B	27	A	P-O3'-C3'	6.63	127.66	119.70
1	A	826	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	B	58	A	O3'-P-O5'	-6.43	91.78	104.00
2	B	39	U	P-O3'-C3'	6.26	127.21	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	20	U	O5'-P-OP1	6.14	118.07	110.70
2	B	54	U	OP2-P-O3'	6.11	118.65	105.20
1	A	828	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	B	26	A	OP1-P-O3'	5.99	118.39	105.20
1	A	643	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	B	5	G	P-O3'-C3'	5.94	126.82	119.70
1	A	643	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	719	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	703	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	344	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	719	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	702	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	B	74	C	P-O3'-C3'	5.18	125.92	119.70
2	B	15	A	P-O3'-C3'	-5.04	113.65	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ASN	Peptide

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	6465	0	6331	75	0
2	B	1516	0	770	18	0
3	A	9	0	10	0	0
4	B	1	0	0	0	0
5	A	385	0	0	19	0
5	B	30	0	0	1	0
All	All	8406	0	7111	90	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 6.

All (90) 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:512:MET:HE2	1:A:548:MET:SD	1.98	1.03
2:B:26:A:H2'	2:B:27:A:H5'	1.41	0.98
1:A:468:LYS:HZ3	1:A:487:THR:HG23	1.33	0.93
1:A:234:PHE:HB2	5:A:2157:HOH:O	1.71	0.90
2:B:26:A:C2'	2:B:27:A:H5'	2.03	0.88
1:A:575:TYR:CZ	1:A:613:VAL:HG11	2.08	0.88
1:A:468:LYS:NZ	1:A:487:THR:HG23	1.95	0.81
1:A:223:TRP:CE3	1:A:535:ILE:HD12	2.16	0.81
1:A:512:MET:CE	1:A:548:MET:SD	2.69	0.80
1:A:695:THR:HG22	5:A:2317:HOH:O	1.82	0.80
1:A:95:THR:HG21	5:A:2088:HOH:O	1.82	0.79
1:A:243:LEU:HB3	5:A:2157:HOH:O	1.92	0.70
1:A:575:TYR:CE1	1:A:613:VAL:HG11	2.25	0.70
1:A:492:THR:HG23	5:A:2082:HOH:O	1.92	0.70
1:A:840:ASP:HB3	5:A:2383:HOH:O	1.94	0.68
2:B:52:G:N2	2:B:63:C:C2	2.62	0.68
1:A:695:THR:CG2	5:A:2317:HOH:O	2.40	0.65
1:A:593:VAL:HG12	1:A:594:GLU:N	2.10	0.65
1:A:244:THR:HG22	1:A:332:THR:HG21	1.76	0.65
1:A:422:VAL:HG11	1:A:494:MET:HE1	1.80	0.64
1:A:593:VAL:HG11	1:A:601:ILE:HG12	1.81	0.62
1:A:593:VAL:HG13	1:A:601:ILE:HG23	1.80	0.62
1:A:841:GLY:O	1:A:842:VAL:HG13	1.99	0.61
1:A:142:GLU:HG2	5:A:2111:HOH:O	1.99	0.61
1:A:267:LEU:HD21	1:A:305:THR:HG21	1.84	0.60
1:A:98:ALA:HB3	1:A:99:PRO:CD	2.34	0.58
1:A:593:VAL:CG1	1:A:594:GLU:N	2.67	0.58
1:A:349:ALA:HA	5:A:2189:HOH:O	2.03	0.58
1:A:492:THR:CG2	5:A:2082:HOH:O	2.50	0.57
1:A:156:VAL:HG21	5:A:2123:HOH:O	2.06	0.55
1:A:142:GLU:CG	5:A:2111:HOH:O	2.55	0.54
1:A:393:GLU:CD	1:A:393:GLU:H	2.11	0.54
1:A:352:TYR:HB2	5:A:2189:HOH:O	2.07	0.54
1:A:25:GLU:OE1	5:A:2029:HOH:O	2.18	0.54
1:A:391:ASP:HB3	5:A:2205:HOH:O	2.09	0.53
2:B:43:U:O2'	5:B:2022:HOH:O	2.19	0.52
1:A:463:ILE:N	1:A:463:ILE:HD12	2.25	0.52
1:A:595:ARG:HD2	1:A:599:GLY:O	2.10	0.51
2:B:28:G:H2'	2:B:29:G:O4'	2.11	0.51
1:A:695:THR:HG22	1:A:697:ASN:H	1.76	0.50
1:A:393:GLU:CD	1:A:393:GLU:N	2.66	0.50
1:A:828:ARG:HH11	1:A:828:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47(G):G:H2'	2:B:47(H):C:C6	2.48	0.49
1:A:847:VAL:HB	5:A:2373:HOH:O	2.12	0.49
1:A:98:ALA:HB3	1:A:99:PRO:HD3	1.95	0.49
1:A:223:TRP:CD2	1:A:535:ILE:HD12	2.48	0.49
1:A:50:MET:HE1	1:A:646:MET:SD	2.53	0.48
1:A:50:MET:HE1	1:A:658:TRP:CZ3	2.48	0.48
1:A:695:THR:HG22	1:A:696:GLU:N	2.29	0.48
2:B:8:U:O2'	2:B:20(A):A:N1	2.37	0.48
1:A:828:ARG:CG	1:A:828:ARG:HH11	2.27	0.48
2:B:5:G:H3'	2:B:6:G:H5"	1.95	0.47
1:A:828:ARG:HG3	1:A:828:ARG:NH1	2.30	0.47
1:A:572:ASP:O	1:A:588:PRO:HG3	2.15	0.47
1:A:360:ILE:HD13	1:A:381:LEU:HD22	1.96	0.46
1:A:587:SER:HA	1:A:625:ASN:O	2.16	0.46
1:A:50:MET:CE	1:A:646:MET:SD	3.04	0.46
1:A:575:TYR:CE1	1:A:613:VAL:CG1	2.98	0.45
2:B:53:G:C2	2:B:62:C:C2	3.04	0.45
1:A:267:LEU:HD23	1:A:267:LEU:C	2.36	0.45
1:A:344:ARG:NH2	2:B:76:A:N3	2.64	0.45
1:A:284:GLU:HA	5:A:2177:HOH:O	2.17	0.45
2:B:52:G:N2	2:B:63:C:O2	2.49	0.45
1:A:354:LEU:HD12	5:A:2189:HOH:O	2.16	0.45
1:A:668:ARG:HD3	5:A:2300:HOH:O	2.17	0.45
1:A:575:TYR:CZ	1:A:613:VAL:CG1	2.93	0.45
1:A:314:THR:OG1	1:A:316:GLU:OE1	2.34	0.45
1:A:82:PHE:CE2	1:A:128:CYS:HA	2.52	0.45
1:A:498:TRP:CE3	1:A:512:MET:HE3	2.53	0.44
2:B:51:G:C4	2:B:64:G:N2	2.86	0.44
1:A:849:TYR:CZ	1:A:851:PRO:HA	2.53	0.44
2:B:39:U:H2'	2:B:40:C:C6	2.54	0.43
2:B:10:G:C6	2:B:26:A:C2	3.07	0.42
1:A:368:PRO:HB3	1:A:375:LEU:HD22	2.00	0.42
1:A:426:ARG:HA	1:A:426:ARG:HD2	1.83	0.42
1:A:47:ARG:NH2	1:A:107:TYR:OH	2.52	0.42
1:A:327:LEU:O	1:A:333:GLY:HA2	2.20	0.42
1:A:258:TYR:CZ	1:A:337:ALA:HB1	2.55	0.42
2:B:53:G:O2'	2:B:54:U:H5'	2.20	0.42
1:A:154:SER:O	1:A:187:GLU:HA	2.19	0.42
1:A:738:LYS:HE2	2:B:42:C:OP2	2.21	0.41
1:A:310:VAL:HG12	1:A:310:VAL:O	2.20	0.41
1:A:575:TYR:O	1:A:613:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:LYS:HE2	2:B:19:G:O2'	2.21	0.41
2:B:9:G:N3	2:B:9:G:H2'	2.36	0.41
1:A:847:VAL:HG11	1:A:855:LEU:HD11	2.03	0.40
1:A:125:LEU:HA	1:A:125:LEU:HD23	1.93	0.40
1:A:305:THR:HG22	1:A:307:PHE:H	1.86	0.40
1:A:305:THR:HB	1:A:320:VAL:O	2.21	0.40
1:A:360:ILE:CD1	1:A:381:LEU:HD22	2.52	0.40

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	807/880 (92%)	783 (97%)	24 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	683/741 (92%)	651 (95%)	32 (5%)	32 27

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	34	LYS
1	A	36	TYR
1	A	95	THR
1	A	154	SER
1	A	188	ILE
1	A	234	PHE
1	A	284	GLU
1	A	308	LYS
1	A	310	VAL
1	A	329	GLU
1	A	335	VAL
1	A	336	MET
1	A	350	SER
1	A	381	LEU
1	A	450	LEU
1	A	484	LEU
1	A	492	THR
1	A	541	PHE
1	A	603	LYS
1	A	605	LYS
1	A	618	SER
1	A	622	LYS
1	A	623	SER
1	A	798	ASP
1	A	826	ARG
1	A	828	ARG
1	A	837	LYS
1	A	842	VAL
1	A	845	ARG
1	A	854	LEU
1	A	859	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	68/87 (78%)	13 (19%)	3 (4%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	G
2	B	9	G
2	B	16	U
2	B	17	C
2	B	18	G
2	B	27	A
2	B	29	G
2	B	31	A
2	B	42	C
2	B	47(D)	C
2	B	50	C
2	B	52	G
2	B	68	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	16	U
2	B	29	G
2	B	47(C)	U

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LEU	A	1001	-	5,8,8	0.34	0	5,10,10	1.67	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LEU	A	1001	-	-	0/4/8/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	LEU	CG-CB-CA	3.17	121.56	114.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	813/880 (92%)	0.74	71 (8%) 13 13	20, 38, 72, 100	0
2	B	71/87 (81%)	1.17	19 (26%) 1 1	31, 65, 104, 144	0
All	All	884/967 (91%)	0.78	90 (10%) 9 9	20, 41, 79, 144	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	ALA	9.0
1	A	279	ALA	8.8
1	A	278	LEU	6.5
1	A	267	LEU	6.4
1	A	283	ASP	6.3
1	A	240	ASP	6.2
1	A	281	PHE	5.9
1	A	269	GLN	5.7
1	A	282	ILE	5.7
1	A	156	VAL	5.5
1	A	262	ALA	5.4
2	B	6	G	5.2
2	B	5	G	5.2
1	A	325	PHE	5.2
1	A	327	LEU	5.0
1	A	94	ASN	4.7
1	A	305	THR	4.5
1	A	188	ILE	4.4
1	A	349	ALA	4.2
1	A	346	TYR	4.1
2	B	64	G	4.1
2	B	31	A	4.1
2	B	74	C	4.0
2	B	65	C	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	270	LYS	4.0
2	B	30	G	3.9
1	A	274	ASN	3.7
2	B	68	C	3.7
1	A	261	VAL	3.7
1	A	348	PHE	3.6
1	A	326	VAL	3.5
2	B	29	G	3.3
1	A	499	TYR	3.3
2	B	51	G	3.3
1	A	592	ILE	3.3
1	A	272	ALA	3.2
1	A	330	TYR	3.2
1	A	598	LYS	3.2
1	A	155	ALA	3.1
1	A	589	VAL	3.1
2	B	39	U	3.0
1	A	273	GLU	2.9
1	A	607	ALA	2.8
1	A	391	ASP	2.7
1	A	263	ALA	2.7
1	A	377	GLU	2.7
1	A	62	ILE	2.7
1	A	839	LEU	2.6
1	A	238	ASP	2.6
2	B	67	C	2.6
1	A	764	PHE	2.6
1	A	310	VAL	2.6
1	A	77	ILE	2.5
1	A	91	VAL	2.5
2	B	40	C	2.5
1	A	320	VAL	2.5
1	A	268	ALA	2.4
1	A	302	GLY	2.4
1	A	500	TYR	2.4
1	A	58	ILE	2.4
1	A	117	PHE	2.4
1	A	237	ASN	2.4
1	A	471	PRO	2.4
1	A	716	ILE	2.4
1	A	79	TRP	2.4
2	B	66	U	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	266	PRO	2.3
1	A	324	ASN	2.3
1	A	37	CYS	2.3
2	B	28	G	2.3
1	A	726	ILE	2.3
1	A	729	ILE	2.3
1	A	345	ASP	2.2
1	A	48	LEU	2.2
2	B	52	G	2.2
1	A	61	VAL	2.2
2	B	7	A	2.2
1	A	564	LEU	2.2
1	A	187	GLU	2.2
1	A	39	SER	2.1
2	B	50	C	2.1
1	A	321	TRP	2.1
1	A	126	ALA	2.1
1	A	722	PHE	2.1
1	A	63	ALA	2.1
2	B	49	G	2.1
1	A	842	VAL	2.1
1	A	65	TYR	2.0
1	A	301	LYS	2.0
1	A	333	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	LEU	A	1001	9/9	0.90	0.18	0.40	27,33,41,42	0
4	MG	B	1077	1/1	0.85	0.06	-	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.