



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:39 am GMT

PDB ID : 3ZJU  
Title : Ternary complex of E .coli leucyl-tRNA synthetase, tRNA(Leu) and the benzoxaborole AN3016 in the editing conformation  
Authors : Cusack, S.; Palencia, A.; Crepin, T.; Hernandez, V.; Akama, T.; Baker, S.J.; Bu, W.; Feng, L.; Freund, Y.R.; Liu, L.; Meewan, M.; Mohan, M.; Mao, W.; Rock, F.L.; Sexton, H.; Sheoran, A.; Zhang, Y.; Zhang, Y.; Zhou, Y.; Nieman, J.A.; Anugula, M.R.; Keramane, E.M.; Savariraj, K.; Reddy, D.S.; Sharma, R.; Subedi, R.; Singh, R.; OLeary, A.; Simon, N.L.; DeMarsh, P.L.; Mushtaq, S.; Warner, M.; Livermore, D.M.; Alley, M.R.K.; Plattner, J.J.  
Deposited on : 2013-01-18  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

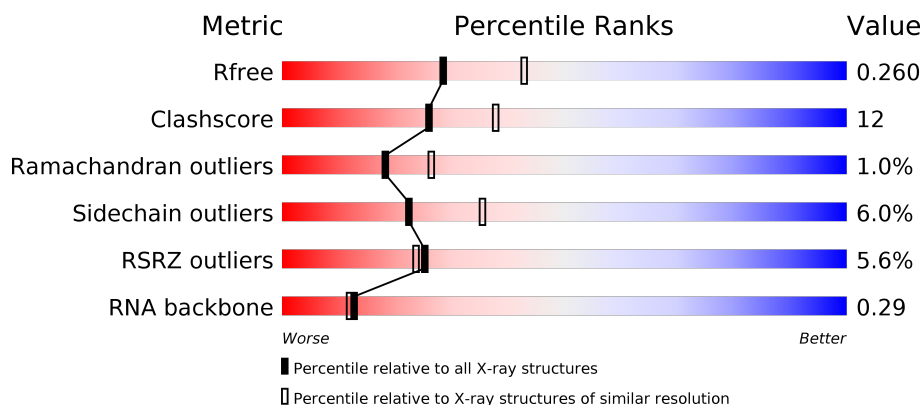
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


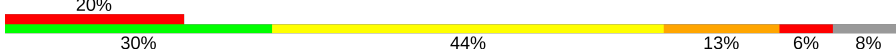
The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)
RNA backbone	2435	1034 (2.86-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
2	B	87	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8359 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 LEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C	N	O	S	0	0	0
			6517	4147	1103	1228	39			

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 TRNALEU5 UAA ISOACCEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	80	Total	B	C	N	O	P	0	0
			1724	1	771	307	565	80		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total 108	O 108	0	0
4	B	8	Total 8	O 8	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.72Å 120.03Å 142.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.40) 98.8 (29.87-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0085	Depositor
R, $R_{free}$	0.207 , 0.261 0.207 , 0.260	Depositor DCC
$R_{free}$ test set	2645 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8359	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DJF

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	0.72	0/6671	0.60	1/9054 (0.0%)
2	B	1.08	1/1884 (0.1%)	1.41	15/2934 (0.5%)
All	All	0.81	1/8555 (0.0%)	0.87	16/11988 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	A	O5'-C5'	-5.21	1.34	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47(A)	G	O4'-C1'-N9	8.14	114.72	108.20
2	B	28	G	C1'-O4'-C4'	-6.79	104.47	109.90
2	B	28	G	O4'-C1'-N9	6.76	113.61	108.20
2	B	12	G	C3'-C2'-C1'	-6.15	96.58	101.50
2	B	14	A	C5'-C4'-O4'	-6.14	101.73	109.10
2	B	55	U	O4'-C1'-N1	5.66	112.73	108.20
2	B	28	G	C4'-C3'-C2'	-5.58	97.02	102.60
2	B	4	C	C4'-C3'-C2'	-5.51	97.09	102.60
2	B	70	G	C4'-C3'-C2'	-5.45	97.15	102.60
2	B	4	C	O4'-C1'-N1	5.44	112.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	22	A	O4'-C1'-N9	5.35	112.48	108.20
2	B	27	A	C3'-C2'-C1'	5.32	105.76	101.50
2	B	47(C)	U	O4'-C1'-N1	5.27	112.41	108.20
2	B	12	G	O4'-C4'-C3'	-5.26	98.74	104.00
2	B	41	C	O4'-C1'-N1	5.24	112.39	108.20
1	A	381	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	ASP	Peptide
1	A	94	ASN	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	6517	0	6379	142	1
2	B	1724	0	877	43	0
3	A	2	0	0	0	0
4	A	108	0	0	4	1
4	B	8	0	0	2	0
All	All	8359	0	7256	182	2

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 12.

All (182) 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:595:ARG:HH11	1:A:595:ARG:HG3	1.00	1.15
2:B:65:C:C6	2:B:65:C:H5''	1.92	1.04
1:A:509:LYS:O	1:A:510:GLU:HB2	1.61	0.99
1:A:695:THR:HG22	1:A:697:ASN:H	1.30	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ARG:HH11	1:A:426:ARG:HG2	1.29	0.97
1:A:188:ILE:HG13	1:A:189:PRO:HD2	1.48	0.96
1:A:595:ARG:HH11	1:A:595:ARG:CG	1.79	0.94
1:A:314:THR:HG21	1:A:316:GLU:OE1	1.69	0.92
2:B:65:C:H6	2:B:65:C:H5''	1.34	0.91
1:A:468:LYS:HG2	1:A:487:THR:HG21	1.56	0.88
1:A:468:LYS:HZ3	1:A:487:THR:HG22	1.40	0.87
1:A:468:LYS:NZ	1:A:487:THR:HG22	1.89	0.87
1:A:595:ARG:NH1	1:A:595:ARG:HG3	1.79	0.86
1:A:599:GLY:O	1:A:600:ARG:HB2	1.74	0.85
1:A:426:ARG:HH11	1:A:426:ARG:CG	1.88	0.85
1:A:188:ILE:HG13	1:A:189:PRO:CD	2.08	0.83
2:B:18:G:H21	2:B:58:A:H5'	1.44	0.83
1:A:843:THR:O	1:A:860:GLY:HA2	1.80	0.81
1:A:480:GLY:O	1:A:481:MET:HB3	1.81	0.79
1:A:534:ALA:HA	1:A:538:LEU:HD12	1.65	0.78
1:A:314:THR:CG2	1:A:316:GLU:OE1	2.31	0.78
1:A:468:LYS:HG2	1:A:487:THR:CG2	2.14	0.76
1:A:48:LEU:H	1:A:111:GLN:HE22	1.32	0.76
1:A:49:HIS:H	1:A:52:HIS:HD2	1.30	0.76
1:A:50:MET:HE1	1:A:658:TRP:CE3	2.23	0.74
1:A:529:GLY:O	1:A:565:CYS:HA	1.89	0.73
4:A:2079:HOH:O	2:B:13:G:H4'	1.88	0.72
2:B:40:C:H2'	2:B:41:C:C6	2.23	0.72
1:A:50:MET:CE	1:A:658:TRP:CE3	2.75	0.70
2:B:18:G:N2	2:B:58:A:H5'	2.06	0.70
1:A:468:LYS:CG	1:A:487:THR:CG2	2.69	0.69
1:A:468:LYS:HG3	1:A:487:THR:HG23	1.75	0.69
2:B:39:U:C5	4:B:2008:HOH:O	2.45	0.69
1:A:509:LYS:HG2	1:A:510:GLU:H	1.58	0.68
1:A:519:ASN:HD21	1:A:555:ASN:H	1.41	0.68
1:A:706:HIS:CD2	1:A:791:ASP:H	2.13	0.67
1:A:215:THR:HG22	1:A:219:MET:CE	2.24	0.67
1:A:555:ASN:ND2	4:A:2063:HOH:O	2.28	0.66
1:A:299:GLU:HA	1:A:299:GLU:OE1	1.94	0.66
1:A:423:SER:O	1:A:424:ARG:HD3	1.96	0.66
1:A:314:THR:CB	1:A:316:GLU:OE1	2.44	0.66
1:A:426:ARG:NH1	1:A:426:ARG:HG2	2.06	0.66
2:B:65:C:C6	2:B:65:C:C5'	2.77	0.65
1:A:599:GLY:O	1:A:600:ARG:CB	2.45	0.64
1:A:509:LYS:O	1:A:510:GLU:CB	2.41	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:ARG:HH11	1:A:845:ARG:CG	2.11	0.64
1:A:509:LYS:HG2	1:A:510:GLU:N	2.14	0.62
2:B:11:U:O2'	2:B:12:G:H5'	1.99	0.62
2:B:2:C:H2'	2:B:3:C:H6	1.64	0.61
1:A:690:ASN:H	1:A:745:GLN:HE22	1.47	0.61
1:A:711:LYS:HD3	4:A:2090:HOH:O	2.00	0.60
1:A:215:THR:HG22	1:A:219:MET:HE1	1.83	0.60
1:A:695:THR:HG22	1:A:697:ASN:N	2.12	0.59
1:A:633:MET:HE1	1:A:637:TYR:HE2	1.68	0.58
1:A:600:ARG:HH11	1:A:602:VAL:HG12	1.67	0.58
1:A:570:LEU:HB2	1:A:617:MET:HE2	1.87	0.57
2:B:28:G:H2'	2:B:29:G:O4'	2.04	0.57
1:A:859:VAL:HG13	1:A:860:GLY:HA3	1.87	0.57
1:A:706:HIS:HD2	1:A:791:ASP:H	1.53	0.56
1:A:193:ILE:HD12	1:A:422:VAL:HG11	1.87	0.56
2:B:40:C:H2'	2:B:41:C:H6	1.67	0.56
1:A:468:LYS:NZ	1:A:487:THR:CG2	2.66	0.56
2:B:2:C:H2'	2:B:3:C:C6	2.40	0.56
1:A:1:MET:HG3	1:A:775:GLU:HG3	1.87	0.56
1:A:314:THR:HB	1:A:316:GLU:OE1	2.05	0.56
1:A:633:MET:CE	1:A:658:TRP:HZ2	2.18	0.56
1:A:49:HIS:H	1:A:52:HIS:CD2	2.18	0.55
2:B:13:G:H2'	2:B:14:A:H5''	1.89	0.55
1:A:596:ASP:CG	1:A:597:GLU:N	2.60	0.55
1:A:816:VAL:HG22	1:A:817:PRO:HD2	1.89	0.54
2:B:27:A:H61	2:B:43:U:H3	1.54	0.54
1:A:223:TRP:CE3	1:A:535:ILE:HD12	2.43	0.54
2:B:47:C:O5'	2:B:47:C:H6	1.89	0.54
1:A:336:MET:HG3	1:A:336:MET:O	2.06	0.54
2:B:26:A:H3'	2:B:27:A:H5''	1.90	0.54
1:A:480:GLY:O	1:A:481:MET:CB	2.56	0.53
1:A:136:GLU:OE2	1:A:495:GLU:OE2	2.27	0.53
1:A:44:PRO:HA	1:A:108:MET:SD	2.49	0.53
1:A:50:MET:CE	1:A:658:TRP:CZ3	2.91	0.53
2:B:42:C:H2'	2:B:43:U:C6	2.43	0.53
1:A:34:LYS:C	1:A:34:LYS:HD2	2.30	0.52
1:A:155:ALA:HA	1:A:187:GLU:HA	1.90	0.52
2:B:47(F):C:C2	2:B:47(G):G:C8	2.97	0.52
1:A:426:ARG:NH1	1:A:426:ARG:CG	2.59	0.52
1:A:695:THR:HG22	1:A:696:GLU:N	2.24	0.52
1:A:378:LYS:HD2	1:A:392:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:THR:O	1:A:860:GLY:CA	2.56	0.51
1:A:1:MET:HE2	1:A:775:GLU:HB3	1.94	0.50
1:A:633:MET:HE3	1:A:658:TRP:HZ2	1.76	0.50
1:A:215:THR:HG22	1:A:219:MET:HE2	1.93	0.50
1:A:314:THR:HG22	1:A:316:GLU:HB3	1.93	0.50
1:A:259:LEU:CD2	1:A:336:MET:HA	2.42	0.50
1:A:465:SER:HB3	1:A:468:LYS:HD2	1.94	0.50
1:A:468:LYS:CG	1:A:487:THR:HG23	2.32	0.49
1:A:805:GLN:HE22	2:B:19:G:H21	1.60	0.49
1:A:299:GLU:N	1:A:300:LYS:HE3	2.28	0.49
1:A:570:LEU:O	1:A:617:MET:HE1	2.13	0.49
1:A:811:ARG:NH1	1:A:838:TYR:CE1	2.81	0.49
1:A:50:MET:HE1	1:A:658:TRP:CZ3	2.47	0.48
2:B:27:A:H2'	2:B:28:G:O4'	2.13	0.48
1:A:426:ARG:HA	1:A:426:ARG:HD3	1.67	0.48
1:A:387:PHE:HA	1:A:390:LEU:HD12	1.96	0.48
1:A:336:MET:O	1:A:336:MET:CG	2.61	0.48
1:A:828:ARG:NH1	4:A:2105:HOH:O	2.47	0.48
1:A:43:TYR:CD1	1:A:44:PRO:HD2	2.49	0.48
1:A:50:MET:HE3	1:A:658:TRP:CE3	2.46	0.48
1:A:108:MET:HA	1:A:111:GLN:HE21	1.79	0.47
2:B:27:A:N6	2:B:43:U:H3	2.13	0.47
1:A:470:ASP:OD1	1:A:471:PRO:HD2	2.15	0.47
1:A:299:GLU:CA	1:A:299:GLU:OE1	2.60	0.47
1:A:842:VAL:HG22	1:A:860:GLY:HA3	1.96	0.47
1:A:259:LEU:HD23	1:A:336:MET:HA	1.97	0.47
1:A:260:ALA:HB3	1:A:335:VAL:HG22	1.96	0.46
2:B:47(G):G:H2'	2:B:47(H):C:C6	2.51	0.46
1:A:695:THR:CG2	1:A:696:GLU:N	2.77	0.46
1:A:845:ARG:HH11	1:A:845:ARG:HG3	1.81	0.46
1:A:98:ALA:HB3	1:A:99:PRO:CD	2.46	0.46
1:A:94:ASN:N	1:A:94:ASN:OD1	2.45	0.46
2:B:52:G:N2	2:B:63:C:C2	2.83	0.46
1:A:144:TYR:HA	1:A:149:VAL:HB	1.97	0.46
2:B:52:G:H1	2:B:62:C:H42	1.62	0.46
1:A:845:ARG:CG	1:A:845:ARG:NH1	2.74	0.46
2:B:11:U:C2'	2:B:12:G:H5'	2.45	0.46
2:B:39:U:H2'	2:B:39:U:O2	2.16	0.46
1:A:595:ARG:NH1	1:A:595:ARG:CG	2.51	0.45
1:A:667:ASN:OD1	1:A:671:LYS:HE3	2.15	0.45
2:B:76:DJF:H18	2:B:76:DJF:H15	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47(F):C:H2'	2:B:47(G):G:H8	1.80	0.45
1:A:338:VAL:HG12	1:A:338:VAL:O	2.16	0.45
1:A:519:ASN:ND2	1:A:555:ASN:H	2.10	0.45
1:A:357:LYS:HA	1:A:358:PRO:HD3	1.88	0.45
1:A:351:LYS:HG2	1:A:351:LYS:O	2.17	0.45
1:A:842:VAL:HG22	1:A:860:GLY:O	2.17	0.45
1:A:50:MET:HE3	1:A:658:TRP:CZ3	2.52	0.44
1:A:282:ILE:HG22	1:A:282:ILE:O	2.17	0.44
1:A:543:PHE:CZ	1:A:547:LEU:HD11	2.53	0.44
2:B:76:DJF:O21	2:B:76:DJF:H5'A	2.16	0.44
1:A:191:TRP:H	1:A:423:SER:HG	1.61	0.44
2:B:8:U:H2'	2:B:21:G:N2	2.32	0.44
1:A:443:MET:HB2	1:A:444:PRO:HD2	2.00	0.44
2:B:30:G:H2'	2:B:31:A:H5'	1.98	0.44
1:A:729:ILE:HD13	1:A:761:LEU:HD13	2.00	0.43
1:A:48:LEU:H	1:A:111:GLN:NE2	2.08	0.43
1:A:845:ARG:HG2	1:A:845:ARG:NH1	2.33	0.43
2:B:52:G:H1	2:B:62:C:N4	2.16	0.43
1:A:677:VAL:HG11	1:A:772:LEU:HD22	2.00	0.43
2:B:72:U:O2'	2:B:73:A:H5'	2.19	0.43
1:A:82:PHE:CG	1:A:429:GLY:HA2	2.54	0.43
1:A:686:VAL:HG12	1:A:747:ARG:NH1	2.33	0.43
1:A:252:THR:HG22	1:A:360:ILE:HD11	2.01	0.43
1:A:41:LEU:HD13	1:A:499:TYR:CD2	2.53	0.43
1:A:461:ASP:O	1:A:463:ILE:N	2.51	0.43
1:A:267:LEU:C	1:A:267:LEU:HD23	2.39	0.42
1:A:847:VAL:HG11	1:A:855:LEU:HD11	2.02	0.42
1:A:239:TYR:HE2	1:A:241:ASN:HB3	1.85	0.42
2:B:4:C:H2'	2:B:5:G:O4'	2.20	0.42
1:A:261:VAL:HG22	1:A:265:HIS:CG	2.55	0.42
1:A:393:GLU:CD	1:A:393:GLU:H	2.22	0.42
1:A:658:TRP:CZ2	1:A:663:VAL:HG21	2.54	0.42
1:A:845:ARG:HH11	1:A:845:ARG:HG2	1.84	0.42
1:A:247:THR:HG1	2:B:76:DJF:C10	2.32	0.42
1:A:428:TRP:CE3	1:A:428:TRP:HA	2.55	0.41
1:A:474:ALA:HB1	1:A:484:LEU:HD23	2.02	0.41
2:B:10:G:C6	2:B:26:A:C2	3.08	0.41
1:A:84:LEU:N	1:A:85:PRO:CD	2.84	0.41
2:B:39:U:H5	4:B:2008:HOH:O	1.96	0.41
1:A:236:VAL:HB	1:A:239:TYR:HB3	2.03	0.41
1:A:755:LEU:HD22	1:A:773:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:MET:HE1	1:A:660:GLU:OE2	2.21	0.41
2:B:58:A:H1'	2:B:60:U:OP2	2.20	0.41
1:A:239:TYR:CE2	1:A:241:ASN:HB3	2.56	0.41
1:A:834:LEU:H	1:A:834:LEU:HG	1.65	0.41
1:A:344:ARG:HH22	2:B:76:DJF:H1'	1.85	0.41
1:A:690:ASN:C	1:A:690:ASN:OD1	2.59	0.41
2:B:76:DJF:O17	2:B:76:DJF:H4'	2.21	0.41
1:A:54:ARG:HB2	1:A:646:MET:CE	2.51	0.41
1:A:454:LEU:HA	1:A:455:PRO:HD3	1.89	0.41
1:A:570:LEU:HB2	1:A:617:MET:CE	2.50	0.40
1:A:811:ARG:NH1	1:A:838:TYR:CZ	2.89	0.40
2:B:12:G:H2'	2:B:13:G:O4'	2.21	0.40
2:B:41:C:H6	2:B:41:C:OP2	2.05	0.40
1:A:351:LYS:CG	1:A:351:LYS:O	2.70	0.40

All (2) 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)
4:A:2028:HOH:O	4:A:2071:HOH:O[4_455]	1.59	0.61
1:A:506:PRO:O	1:A:579:GLU:OE1[4_455]	2.16	0.04

## 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	814/880 (92%)	766 (94%)	40 (5%)	8 (1%)	18 26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	GLY

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Mol	Chain	Res	Type
1	A	600	ARG
1	A	463	ILE
1	A	595	ARG
1	A	597	GLU
1	A	480	GLY
1	A	481	MET
1	A	601	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	688/741 (93%)	647 (94%)	41 (6%)	22	35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	12	SER
1	A	34	LYS
1	A	36	TYR
1	A	92	LYS
1	A	94	ASN
1	A	95	THR
1	A	240	ASP
1	A	261	VAL
1	A	284	GLU
1	A	286	ARG
1	A	299	GLU
1	A	344	ARG
1	A	376	THR
1	A	383	ASN
1	A	423	SER
1	A	426	ARG
1	A	443	MET
1	A	450	LEU

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Mol	Chain	Res	Type
1	A	477	THR
1	A	484	LEU
1	A	487	THR
1	A	510	GLU
1	A	541	PHE
1	A	544	PHE
1	A	589	VAL
1	A	595	ARG
1	A	596	ASP
1	A	613	VAL
1	A	618	SER
1	A	646	MET
1	A	711	LYS
1	A	761	LEU
1	A	779	GLU
1	A	793	LYS
1	A	811	ARG
1	A	828	ARG
1	A	837	LYS
1	A	845	ARG
1	A	854	LEU
1	A	859	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	52	HIS
1	A	72	ASN
1	A	104	ASN
1	A	111	GLN
1	A	274	ASN
1	A	519	ASN
1	A	555	ASN
1	A	706	HIS
1	A	745	GLN
1	A	762	ASN
1	A	805	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	77/87 (88%)	27 (35%)	0

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	3	C
2	B	4	C
2	B	5	G
2	B	6	G
2	B	9	G
2	B	13	G
2	B	14	A
2	B	15	A
2	B	20	U
2	B	27	A
2	B	28	G
2	B	40	C
2	B	41	C
2	B	44	C
2	B	47(D)	C
2	B	47(E)	G
2	B	50	C
2	B	51	G
2	B	52	G
2	B	58	A
2	B	65	C
2	B	68	C
2	B	70	G
2	B	71	G
2	B	73	A
2	B	74	C

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	DJF	B	76	2	28,41,42	0.87	0	27,61,64	2.78	4 (14%)

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	DJF	B	76	2	-	0/8/52/53	0/6/6/6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	76	DJF	N3-C2-N1	-8.58	121.39	128.86
2	B	76	DJF	O17-C16-C15	-3.19	117.14	124.00
2	B	76	DJF	C4-C5-N7	-2.99	106.52	109.41
2	B	76	DJF	O17-C16-C12	9.85	124.06	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	76	DJF	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	820/880 (93%)	0.05	33 (4%) 39 38	16, 35, 70, 128	0
2	B	79/87 (90%)	0.72	17 (21%) 1 1	28, 64, 119, 132	0
All	All	899/967 (92%)	0.11	50 (5%) 25 24	16, 36, 78, 132	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	ARG	5.6
2	B	31	A	5.0
1	A	287	ASN	5.0
2	B	65	C	4.7
2	B	30	G	4.4
1	A	841	GLY	4.1
1	A	761	LEU	3.8
1	A	594	GLU	3.8
1	A	597	GLU	3.7
2	B	41	C	3.7
1	A	288	THR	3.7
1	A	285	CYS	3.6
2	B	2	C	3.6
2	B	1	G	3.5
1	A	279	ALA	3.5
2	B	73	A	3.4
1	A	283	ASP	3.4
1	A	94	ASN	3.2
1	A	860	GLY	3.1
1	A	240	ASP	3.1
2	B	29	G	3.0
2	B	40	C	3.0
2	B	42	C	2.9
1	A	765	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	644	LEU	2.7
2	B	64	G	2.7
1	A	764	PHE	2.7
1	A	187	GLU	2.6
2	B	47(E)	G	2.5
1	A	362	ALA	2.5
1	A	280	ALA	2.5
1	A	479	ASN	2.5
1	A	91	VAL	2.4
2	B	53	G	2.4
1	A	476	THR	2.4
1	A	482	PRO	2.4
1	A	61	VAL	2.3
1	A	833	HIS	2.3
2	B	39	U	2.3
1	A	440	GLY	2.3
1	A	441	THR	2.3
1	A	57	THR	2.3
1	A	238	ASP	2.2
1	A	481	MET	2.2
1	A	836	ALA	2.2
2	B	71	G	2.2
1	A	600	ARG	2.1
2	B	72	U	2.1
2	B	52	G	2.1
1	A	670	LEU	2.1

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

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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	DJF	B	76	36/37	0.97	0.14	-	29,34,45,54	0

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	1861	1/1	0.87	0.15	1.49	47,47,47,47	0
3	MG	A	1862	1/1	0.80	0.12	-0.77	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.