Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 PM GMT

PDB ID	:	3ZJV
Title	:	Ternary complex of E .coli leucyl-tRNA synthetase, tRNA(Leu) and the benzoxaborole AN3213 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	:	2.31 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 ⓘ symbol.

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

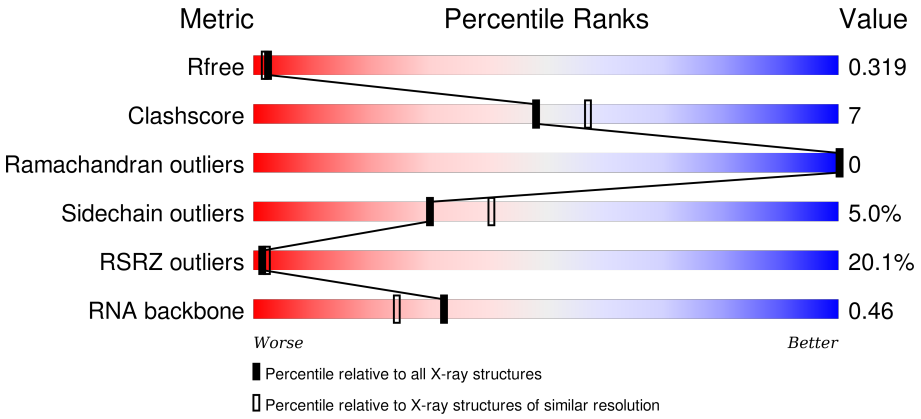
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)
RNA backbone	2183	1031 (2.86-1.78)

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	15% 79% 13% • 8%
2	B	87	54% 52% 32% 10% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8707 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	1	0
			6469	4118	1094	1218	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	85	Total	B	C	N	O	P	0	0	0
			1833	1	820	327	600	85			

- Molecule 3 is water.

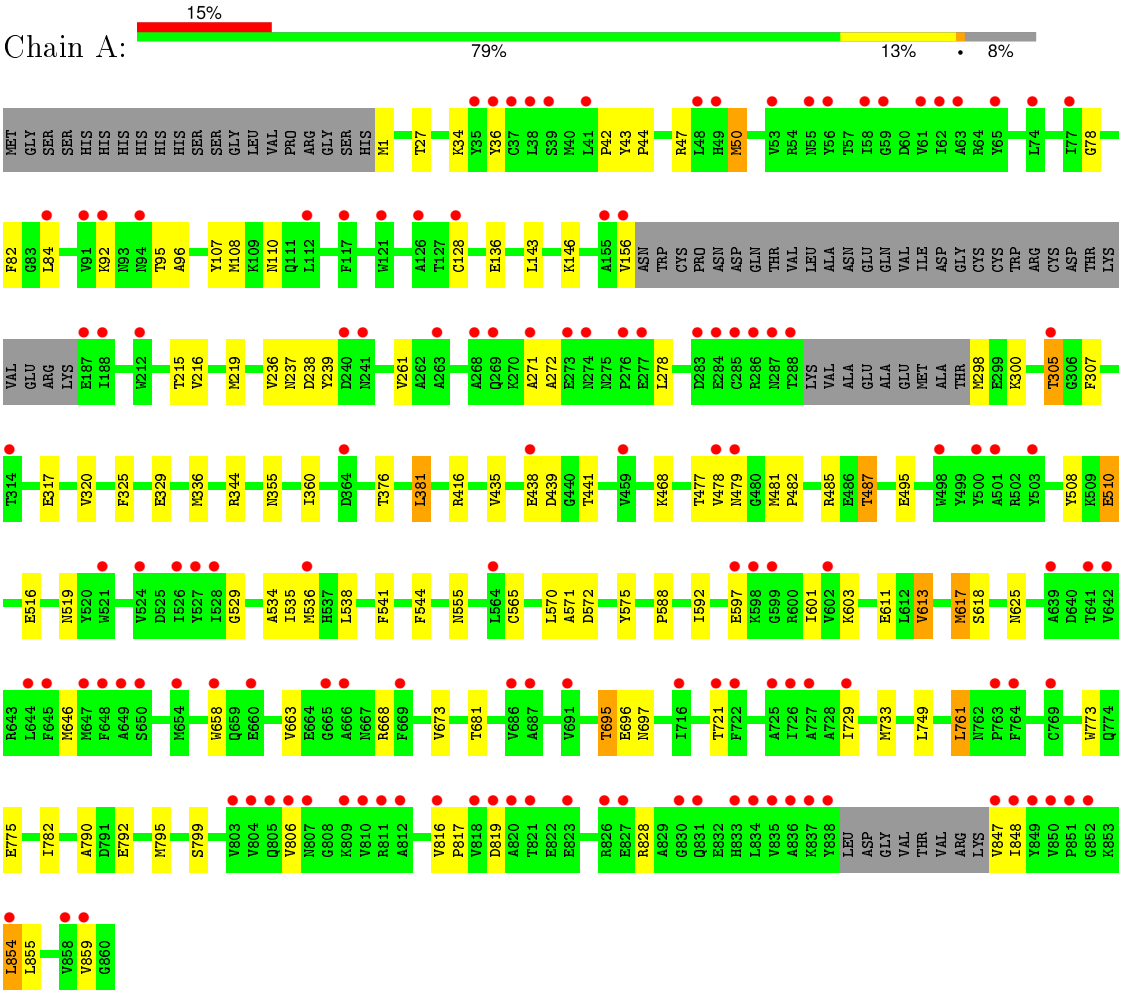
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	374	Total O 374 374	0	0
3	B	31	Total O 31 31	0	0

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.

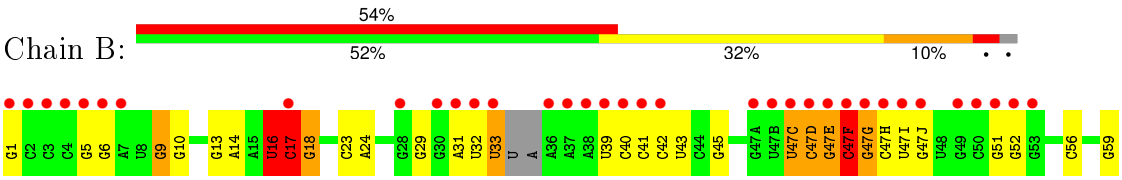
- Molecule 1: LEUCINE–TRNA LIGASE

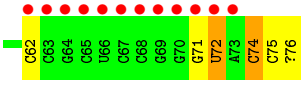
Chain A:



- Molecule 2: TRNALEU5 UAA ISOACCEPTOR

Chain B:




C62
C63
G64
C65
U66
C67
C68
G69
G70
G71
U72
A73
C74
C75
?76

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.37Å 76.94Å 90.71Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	88.74 – 2.31 45.51 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (88.74-2.31) 99.9 (45.51-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.6.0111	Depositor
R, R_{free}	0.200 , 0.247 0.282 , 0.319	Depositor DCC
R_{free} test set	2693 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.2	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 52865 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8707	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: 365

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	0/6626	0.68	1/8992 (0.0%)
2	B	0.91	4/2004 (0.2%)	1.47	23/3119 (0.7%)
All	All	0.68	4/8630 (0.0%)	0.95	24/12111 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	31	A	C6-N6	-11.93	1.24	1.33
2	B	1	G	OP3-P	-10.46	1.48	1.61
2	B	14	A	O5'-C5'	-6.85	1.31	1.42
2	B	31	A	C6-N1	6.68	1.40	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	31	A	C5-C6-N1	-11.19	112.11	117.70
2	B	31	A	N1-C2-N3	-10.69	123.96	129.30
2	B	31	A	C6-N1-C2	9.71	124.43	118.60
2	B	14	A	C5'-C4'-C3'	-8.70	102.08	116.00
2	B	47(H)	C	O4'-C1'-N1	7.67	114.34	108.20
2	B	9	G	O4'-C1'-N9	7.04	113.83	108.20
2	B	40	C	O4'-C1'-N1	6.78	113.63	108.20
2	B	47(G)	G	O4'-C1'-N9	6.41	113.33	108.20
2	B	72	U	O4'-C1'-N1	6.41	113.33	108.20
2	B	10	G	C4'-C3'-C2'	-6.29	96.31	102.60
2	B	16	U	P-O3'-C3'	6.20	127.14	119.70
2	B	17	C	N1-C1'-C2'	6.06	121.88	114.00
2	B	24	A	O5'-P-OP1	-5.79	100.49	105.70
2	B	47(J)	G	O4'-C1'-N9	5.77	112.82	108.20
2	B	14	A	P-O5'-C5'	-5.68	111.81	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	23	C	C6-N1-C2	-5.58	118.07	120.30
2	B	23	C	O5'-P-OP2	-5.58	100.68	105.70
2	B	31	A	C5-C6-N6	5.41	128.03	123.70
2	B	47(I)	U	O4'-C1'-N1	5.22	112.38	108.20
2	B	13	G	O3'-P-O5'	-5.18	94.15	104.00
1	A	416	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	B	59	G	O4'-C1'-N9	5.11	112.29	108.20
2	B	13	G	O4'-C1'-N9	5.04	112.23	108.20
2	B	47(F)	C	O4'-C1'-N1	5.02	112.22	108.20

There are no chirality outliers.

There are no planarity outliers.

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	6469	0	6320	105	0
2	B	1833	0	931	10	0
3	A	374	0	0	15	0
3	B	31	0	0	1	0
All	All	8707	0	7251	113	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 7.

All (113) 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:854:LEU:HD23	1:A:854:LEU:C	1.51	1.22
1:A:854:LEU:HD23	1:A:854:LEU:O	1.61	0.98
1:A:571:ALA:N	1:A:617:MET:HE1	1.78	0.98
1:A:468:LYS:HZ3	1:A:487:THR:HG23	1.28	0.98
1:A:854:LEU:CD2	1:A:854:LEU:C	2.30	0.96
1:A:570:LEU:C	1:A:617:MET:HE1	1.88	0.94
1:A:468:LYS:NZ	1:A:487:THR:HG23	1.83	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:VAL:HG12	1:A:817:PRO:HD2	1.55	0.88
2:B:33:U:O3'	3:B:2020:HOH:O	1.90	0.88
1:A:468:LYS:NZ	1:A:487:THR:CG2	2.39	0.85
1:A:468:LYS:HZ3	1:A:487:THR:CG2	1.90	0.84
1:A:854:LEU:HD23	1:A:855:LEU:N	1.94	0.81
1:A:439:ASP:H	1:A:481:MET:HE1	1.46	0.80
1:A:305:THR:HG23	1:A:307:PHE:H	1.49	0.77
1:A:355:ASN:HB2	3:A:2187:HOH:O	1.84	0.76
1:A:439:ASP:H	1:A:481:MET:CE	2.00	0.74
1:A:305:THR:HG22	1:A:320:VAL:O	1.88	0.73
1:A:236:VAL:HB	1:A:239:TYR:HB3	1.71	0.73
1:A:1:MET:HE1	1:A:775:GLU:HB3	1.73	0.70
1:A:571:ALA:N	1:A:617:MET:CE	2.52	0.70
1:A:50:MET:HE3	1:A:50:MET:HA	1.74	0.69
1:A:571:ALA:CA	1:A:617:MET:HE1	2.22	0.69
1:A:215:THR:O	1:A:219:MET:HE3	1.92	0.69
1:A:571:ALA:C	1:A:617:MET:HE3	2.13	0.69
1:A:1:MET:CE	1:A:775:GLU:HB3	2.23	0.67
1:A:479:ASN:ND2	3:A:2235:HOH:O	2.28	0.66
1:A:816:VAL:HG12	1:A:817:PRO:CD	2.25	0.66
1:A:360:ILE:HD13	1:A:381:LEU:HD22	1.79	0.65
1:A:438:GLU:CG	1:A:481:MET:HE2	2.28	0.63
1:A:360:ILE:CD1	1:A:381:LEU:HD22	2.30	0.61
2:B:16:U:H2'	2:B:17:C:C5	2.35	0.61
1:A:438:GLU:HG3	1:A:481:MET:HE2	1.81	0.61
1:A:1:MET:HE1	1:A:775:GLU:CB	2.30	0.60
1:A:617:MET:HE3	1:A:617:MET:HA	1.83	0.60
1:A:508:TYR:CZ	1:A:510:GLU:HB2	2.36	0.60
1:A:438:GLU:HG3	1:A:481:MET:CE	2.32	0.59
1:A:82:PHE:CE2	1:A:128:CYS:HA	2.38	0.58
1:A:468:LYS:HG2	1:A:487:THR:CG2	2.33	0.58
1:A:571:ALA:CA	1:A:617:MET:CE	2.82	0.57
1:A:695:THR:HG22	1:A:697:ASN:H	1.71	0.56
1:A:344:ARG:HB3	3:A:2183:HOH:O	2.06	0.56
1:A:695:THR:HG22	1:A:697:ASN:N	2.20	0.55
1:A:110:ASN:ND2	3:A:2088:HOH:O	2.22	0.55
1:A:534:ALA:HA	1:A:538:LEU:HD12	1.87	0.55
1:A:575:TYR:CE2	1:A:613:VAL:HG22	2.41	0.55
1:A:854:LEU:O	1:A:854:LEU:CD2	2.44	0.55
1:A:695:THR:HG21	3:A:2332:HOH:O	2.07	0.54
1:A:806:VAL:CG1	1:A:859:VAL:HG22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LYS:HZ2	1:A:487:THR:CG2	2.16	0.54
1:A:27:THR:HG22	3:A:2031:HOH:O	2.07	0.54
1:A:570:LEU:CB	1:A:617:MET:HE2	2.39	0.53
2:B:47(C):U:H4'	2:B:47(D):C:OP1	2.08	0.52
1:A:729:ILE:HD13	1:A:761:LEU:HD13	1.90	0.52
2:B:17:C:H5"	2:B:18:G:OP1	2.09	0.52
1:A:271:ALA:HB2	1:A:307:PHE:CE2	2.45	0.51
1:A:47:ARG:NH2	1:A:107:TYR:OH	2.44	0.51
1:A:216:VAL:HA	1:A:219:MET:HE3	1.92	0.51
1:A:854:LEU:HD23	1:A:855:LEU:CA	2.41	0.51
1:A:570:LEU:HB3	1:A:617:MET:HE2	1.93	0.51
1:A:300:LYS:HE2	2:B:74:C:N3	2.26	0.51
2:B:47(E):G:H2'	2:B:47(F):C:O4'	2.11	0.51
1:A:658:TRP:CZ2	1:A:663:VAL:HG21	2.46	0.51
1:A:439:ASP:HB3	1:A:441:THR:HG23	1.92	0.50
1:A:806:VAL:HG12	1:A:859:VAL:CG2	2.40	0.50
1:A:792:GLU:OE2	1:A:795:MET:HE3	2.11	0.50
1:A:42:PRO:HD2	1:A:78:GLY:O	2.13	0.49
1:A:136:GLU:OE2	1:A:495:GLU:OE2	2.31	0.48
1:A:298:MET:N	3:A:2170:HOH:O	2.46	0.48
1:A:695:THR:HG21	3:A:2333:HOH:O	2.14	0.48
1:A:272:ALA:N	1:A:278:LEU:HD23	2.29	0.48
1:A:854:LEU:CD2	1:A:855:LEU:N	2.69	0.47
1:A:468:LYS:HG2	1:A:487:THR:HG23	1.96	0.47
1:A:792:GLU:CD	1:A:795:MET:HE3	2.34	0.47
1:A:611:GLU:HG2	3:A:2295:HOH:O	2.13	0.47
1:A:799:SER:HA	1:A:817:PRO:HA	1.97	0.47
1:A:438:GLU:HG2	1:A:481:MET:HE2	1.96	0.47
1:A:571:ALA:C	1:A:617:MET:CE	2.82	0.46
1:A:529:GLY:O	1:A:565:CYS:HA	2.15	0.46
1:A:617:MET:HB3	1:A:617:MET:HE2	1.64	0.46
1:A:485:ARG:HB2	3:A:2215:HOH:O	2.15	0.46
2:B:16:U:H2'	2:B:17:C:H5	1.81	0.46
1:A:95:THR:HG23	1:A:96:ALA:N	2.30	0.46
1:A:43:TYR:CD1	1:A:44:PRO:HD2	2.51	0.46
1:A:773:TRP:HB2	1:A:782:ILE:HD12	1.98	0.46
1:A:695:THR:CG2	1:A:696:GLU:N	2.79	0.45
1:A:816:VAL:CG1	1:A:817:PRO:CD	2.95	0.44
1:A:790:ALA:HB1	1:A:795:MET:HE2	1.99	0.44
1:A:519:ASN:OD1	1:A:555:ASN:HB2	2.16	0.44
1:A:592:ILE:N	1:A:592:ILE:HD12	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE3	1:A:681:THR:OG1	2.18	0.43
1:A:601:ILE:HD12	3:A:2297:HOH:O	2.17	0.43
1:A:481:MET:CG	1:A:482:PRO:HD2	2.48	0.43
1:A:721:THR:HA	3:A:2343:HOH:O	2.19	0.43
1:A:215:THR:C	1:A:219:MET:HE3	2.38	0.43
1:A:468:LYS:CE	1:A:487:THR:HG23	2.48	0.42
1:A:617:MET:CE	1:A:617:MET:HA	2.49	0.42
1:A:305:THR:CG2	1:A:320:VAL:O	2.63	0.42
2:B:75:C:OP2	2:B:76:365:H22A	2.20	0.42
1:A:146:LYS:NZ	3:A:2109:HOH:O	2.42	0.42
1:A:749:LEU:C	1:A:749:LEU:HD23	2.39	0.42
1:A:238:ASP:N	3:A:2153:HOH:O	1.93	0.42
1:A:1:MET:HE2	1:A:775:GLU:HB3	2.00	0.42
1:A:325:PHE:CE2	3:A:2183:HOH:O	2.70	0.42
1:A:668:ARG:HD3	2:B:39:U:OP2	2.19	0.42
1:A:572:ASP:O	1:A:588:PRO:HG3	2.21	0.41
1:A:237:ASN:ND2	1:A:317:GLU:OE2	2.53	0.41
1:A:617:MET:CA	1:A:617:MET:CE	2.97	0.41
1:A:478:VAL:N	1:A:481:MET:O	2.44	0.41
1:A:673:VAL:HG22	1:A:733:MET:HE2	2.01	0.41
1:A:468:LYS:NZ	1:A:487:THR:HG22	2.31	0.41
2:B:71:G:C6	2:B:72:U:C5	3.09	0.41
1:A:847:VAL:C	1:A:848:ILE:HD13	2.41	0.41
1:A:44:PRO:HA	1:A:108:MET:SD	2.61	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	806/880 (92%)	790 (98%)	16 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	682/741 (92%)	648 (95%)	34 (5%)	30 41

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	36	TYR
1	A	50	MET
1	A	84	LEU
1	A	92	LYS
1	A	143	LEU
1	A	156	VAL
1	A	261	VAL
1	A	305	THR
1	A	329	GLU
1	A	336	MET
1	A	376	THR
1	A	381	LEU
1	A	435	VAL
1	A	477	THR
1	A	487	THR
1	A	510	GLU
1	A	516	GLU
1	A	535	ILE
1	A	536	MET
1	A	541	PHE
1	A	544	PHE
1	A	597	GLU
1	A	603	LYS
1	A	613	VAL
1	A	617	MET
1	A	618	SER

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Mol	Chain	Res	Type
1	A	625	ASN
1	A	646	MET
1	A	695	THR
1	A	761	LEU
1	A	819	ASP
1	A	828	ARG
1	A	854	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	479	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	82/87 (94%)	22 (26%)	3 (3%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	5	G
2	B	6	G
2	B	9	G
2	B	16	U
2	B	17	C
2	B	18	G
2	B	29	G
2	B	32	U
2	B	33	U
2	B	41	C
2	B	42	C
2	B	43	U
2	B	45	G
2	B	47(D)	C
2	B	47(E)	G
2	B	47(F)	C
2	B	47(G)	G
2	B	51	G
2	B	52	G

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Mol	Chain	Res	Type
2	B	56	C
2	B	62	C
2	B	74	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	5	G
2	B	16	U
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)

There are no ligands in this entry.

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

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%)	1.15	133 (16%) 2 4	33, 38, 54, 91	0
2	B	84/87 (96%)	2.61	47 (55%) 0 0	35, 42, 51, 56	0
All	All	897/967 (92%)	1.29	180 (20%) 1 2	33, 38, 54, 91	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	835	VAL	7.5
1	A	94	ASN	7.0
2	B	36	A	6.7
1	A	811	ARG	6.4
1	A	858	VAL	6.3
2	B	2	C	6.0
1	A	818	VAL	6.0
1	A	859	VAL	6.0
2	B	1	G	5.9
1	A	836	ALA	5.9
2	B	65	C	5.8
1	A	837	LYS	5.8
1	A	812	ALA	5.8
2	B	73	A	5.7
2	B	31	A	5.6
2	B	71	G	5.6
2	B	3	C	5.3
1	A	156	VAL	5.0
1	A	819	ASP	4.9
2	B	63	C	4.9
2	B	32	U	4.8
2	B	47(E)	G	4.7
2	B	51	G	4.7
2	B	70	G	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	850	VAL	4.6
2	B	50	C	4.6
1	A	274	ASN	4.5
1	A	849	TYR	4.5
2	B	72	U	4.5
1	A	806	VAL	4.5
2	B	64	G	4.4
2	B	47(F)	C	4.4
2	B	37	A	4.3
2	B	33	U	4.3
1	A	536	MET	4.2
2	B	41	C	4.2
2	B	6	G	4.2
2	B	52	G	4.2
2	B	38	A	4.2
1	A	268	ALA	4.1
2	B	49	G	4.1
1	A	91	VAL	4.1
1	A	479	ASN	4.0
2	B	17	C	4.0
1	A	155	ALA	4.0
1	A	838	TYR	3.9
2	B	53	G	3.9
2	B	30	G	3.9
2	B	5	G	3.8
2	B	47(D)	C	3.8
1	A	807	ASN	3.8
2	B	69	G	3.8
1	A	852	GLY	3.8
1	A	810	VAL	3.7
2	B	4	C	3.7
1	A	269	GLN	3.7
1	A	288	THR	3.7
1	A	809	LYS	3.7
2	B	47(G)	G	3.6
2	B	67	C	3.6
2	B	40	C	3.6
2	B	66	U	3.5
1	A	848	ILE	3.5
2	B	62	C	3.4
2	B	42	C	3.4
1	A	644	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	47(H)	C	3.3
1	A	62	ILE	3.3
2	B	7	A	3.3
1	A	645	PHE	3.2
1	A	41	LEU	3.2
1	A	823	GLU	3.1
1	A	827	GLU	3.1
1	A	816	VAL	3.1
1	A	37	CYS	3.1
1	A	49[A]	HIS	3.1
1	A	56	TYR	3.0
1	A	687	ALA	3.0
1	A	833	HIS	3.0
1	A	277	GLU	3.0
1	A	854	LEU	3.0
1	A	53	VAL	2.9
1	A	285	CYS	2.9
1	A	821	THR	2.9
1	A	686	VAL	2.9
1	A	820	ALA	2.8
1	A	804	VAL	2.8
1	A	805	GLN	2.8
1	A	597	GLU	2.8
1	A	273	GLU	2.8
1	A	284	GLU	2.7
1	A	276	PRO	2.7
1	A	459	VAL	2.6
1	A	501	ALA	2.6
1	A	598	LYS	2.6
1	A	38	LEU	2.6
1	A	92	LYS	2.6
1	A	188	ILE	2.6
1	A	35	TYR	2.5
2	B	47(A)	G	2.5
1	A	128	CYS	2.5
1	A	642	VAL	2.5
1	A	847	VAL	2.5
1	A	648	PHE	2.5
2	B	39	U	2.5
1	A	725	ALA	2.5
1	A	500	TYR	2.5
1	A	763	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	691	VAL	2.5
1	A	117	PHE	2.5
1	A	36	TYR	2.4
1	A	478	VAL	2.4
1	A	528	ILE	2.4
1	A	764	PHE	2.4
1	A	826	ARG	2.4
1	A	498	TRP	2.4
1	A	669	PHE	2.4
1	A	503	TYR	2.4
1	A	526	ILE	2.4
2	B	68	C	2.4
1	A	721	THR	2.4
1	A	74	LEU	2.3
1	A	524	VAL	2.3
1	A	283	ASP	2.3
1	A	314	THR	2.3
1	A	564	LEU	2.3
1	A	438	GLU	2.3
1	A	287	ASN	2.3
1	A	305	THR	2.3
1	A	654	MET	2.3
2	B	47(B)	U	2.3
1	A	660	GLU	2.3
1	A	58	ILE	2.3
1	A	649	ALA	2.3
1	A	641	THR	2.2
1	A	61	VAL	2.2
1	A	240	ASP	2.2
1	A	851	PRO	2.2
1	A	521	TRP	2.2
1	A	63	ALA	2.2
1	A	666	ALA	2.2
1	A	729	ILE	2.2
1	A	769	CYS	2.2
1	A	830	GLY	2.2
1	A	126	ALA	2.2
1	A	602	VAL	2.2
1	A	665	GLY	2.2
1	A	271	ALA	2.2
1	A	658	TRP	2.2
2	B	47(J)	G	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	59	GLY	2.2
1	A	727	ALA	2.2
1	A	716	ILE	2.2
1	A	121	TRP	2.2
1	A	286	ARG	2.2
1	A	48	LEU	2.2
1	A	647	MET	2.2
1	A	650	SER	2.2
1	A	639	ALA	2.2
1	A	77	ILE	2.1
1	A	803	VAL	2.1
2	B	47(C)	U	2.1
2	B	47(I)	U	2.1
1	A	65	TYR	2.1
1	A	187	GLU	2.1
1	A	599	GLY	2.1
1	A	364	ASP	2.1
1	A	831	GLN	2.1
1	A	722	PHE	2.1
1	A	84	LEU	2.1
1	A	527	TYR	2.1
1	A	263	ALA	2.1
1	A	55	ASN	2.1
1	A	112	LEU	2.1
2	B	28	G	2.1
1	A	39	SER	2.1
1	A	726	ILE	2.1
1	A	241	ASN	2.0
1	A	212	TRP	2.0
1	A	834	LEU	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.