



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:31 PM UTC

PDB ID : 3ZJV / pdb_00003zjv
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12

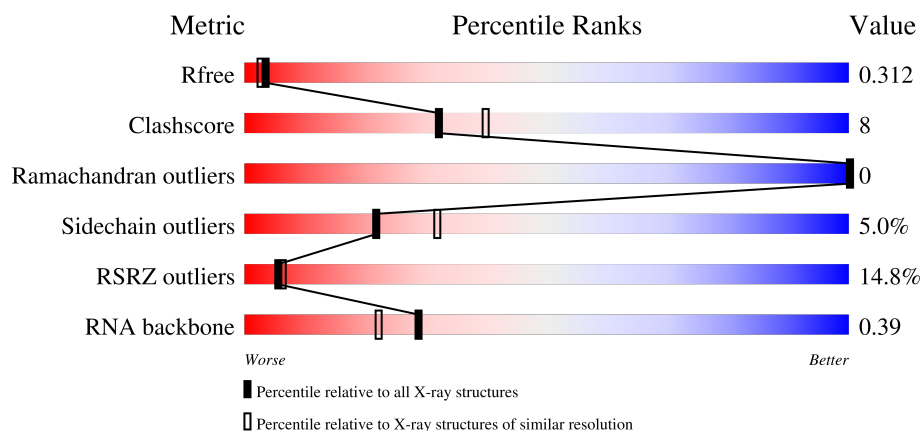
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)
RNA backbone	3983	1116 (2.64-2.00)

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 $\leq 5\%$. 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	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	B	87	33% 61% 26% 9% ..

2 Entry composition

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
			Total	C	N	O	S			
1	A	813	6469	4118	1094	1218	39	0	1	0

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
			Total	B	C	N	O	P		
2	B	85	1833	1	820	327	600	85	0	0

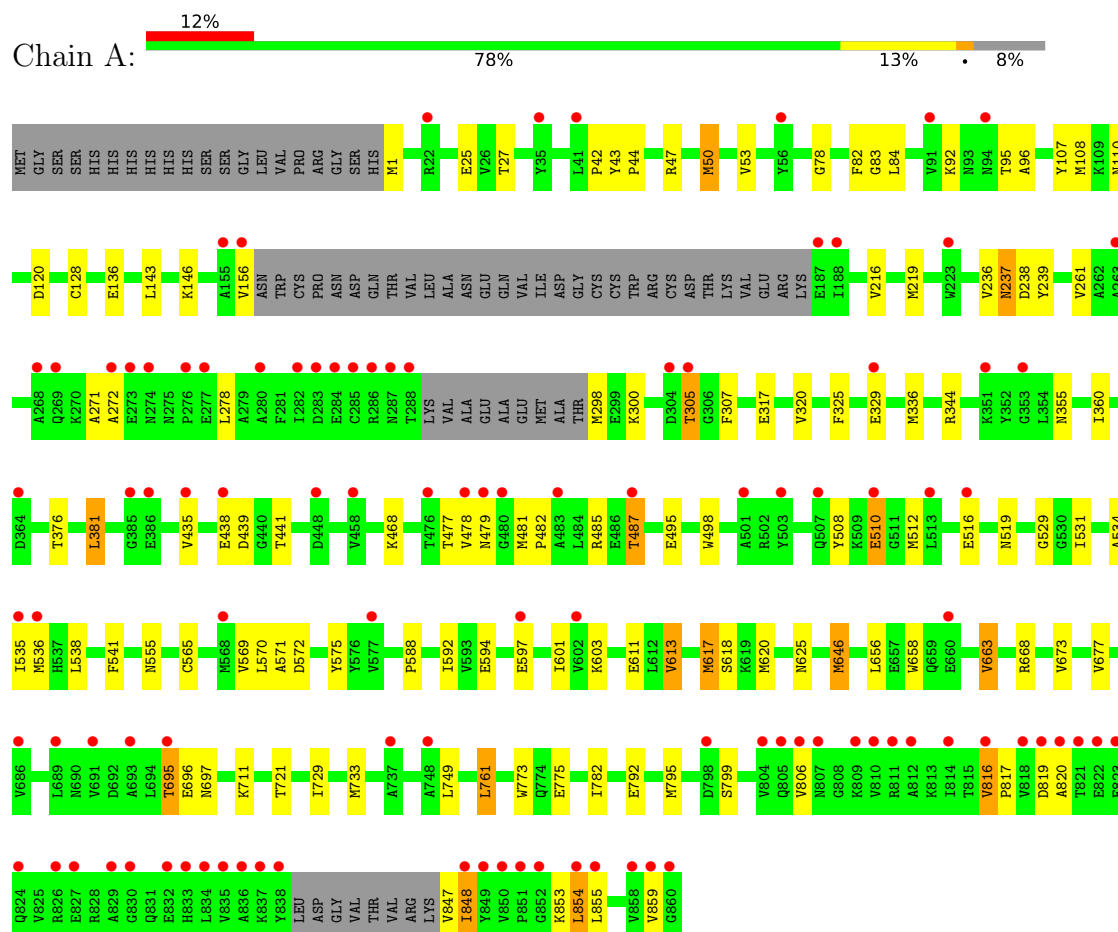
- Molecule 3 is water.

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

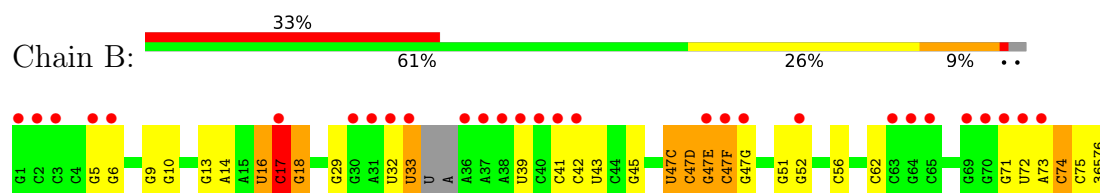
3 Residue-property plots

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 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



• Molecule 2: TRNALEU5 UAA ISOACCEPTOR



4 Data and refinement statistics

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 88.60 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (88.74-2.31) 99.9 (88.60-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.6.0111	Depositor
R, R_{free}	0.200 , 0.247 0.280 , 0.312	Depositor DCC
R_{free} test set	2693 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.74	0/6626	0.85	4/8992 (0.0%)
2	B	0.65	1/2004 (0.0%)	1.14	6/3119 (0.2%)
All	All	0.72	1/8630 (0.0%)	0.93	10/12111 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	A	O5'-C5'	-7.04	1.31	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	14	A	C5'-C4'-C3'	-9.28	102.08	116.00
1	A	237	ASN	N-CA-C	8.26	119.91	111.07
2	B	17	C	N1-C1'-C2'	6.59	121.88	112.00
2	B	13	G	O3'-P-O5'	-6.56	94.15	104.00
1	A	820	ALA	N-CA-C	6.46	119.60	110.23
2	B	10	G	C4'-C3'-C2'	-6.29	96.31	102.60
2	B	14	A	P-O5'-C5'	-6.06	111.81	120.90
1	A	83	GLY	N-CA-C	5.90	118.04	112.08
1	A	663	VAL	CB-CA-C	-5.46	104.77	112.14
2	B	73	A	C2'-C3'-O3'	5.30	117.46	109.50

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	6469	0	6320	116	0
2	B	1833	0	931	10	0
3	A	374	0	0	16	0
3	B	31	0	0	1	0
All	All	8707	0	7251	124	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 8.

All (124) 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:C	1:A:854:LEU:HD23	1.51	1.27
1:A:571:ALA:N	1:A:617:MET:HE1	1.73	1.01
1:A:1:MET:HE2	1:A:775:GLU:HB3	1.42	1.01
1:A:854:LEU:C	1:A:854:LEU:CD2	2.30	1.00
1:A:854:LEU:HD23	1:A:854:LEU:O	1.61	0.98
1:A:570:LEU:C	1:A:617:MET:HE1	1.94	0.91
1:A:468:LYS:NZ	1:A:487:THR:HG23	1.83	0.90
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:1:MET:HE2	1:A:775:GLU:CB	2.06	0.85
1:A:571:ALA:CA	1:A:617:MET:HE1	2.08	0.83
1:A:854:LEU:HD23	1:A:855:LEU:N	1.94	0.81
1:A:468:LYS:HZ3	1:A:487:THR:HG23	1.47	0.80
1:A:1:MET:HE1	1:A:677:VAL:HG12	1.64	0.79
1:A:305:THR:HG23	1:A:307:PHE:H	1.49	0.77
1:A:468:LYS:HZ2	1:A:487:THR:CG2	1.97	0.77
1:A:355:ASN:HB2	3:A:2187:HOH:O	1.84	0.76
1:A:438:GLU:HG3	1:A:481:MET:HE3	1.68	0.75
1:A:439:ASP:H	1:A:481:MET:CE	2.00	0.75
1:A:236:VAL:HB	1:A:239:TYR:HB3	1.71	0.73
1:A:305:THR:HG22	1:A:320:VAL:O	1.88	0.73
1:A:216:VAL:HA	1:A:219:MET:HE3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:MET:HE3	1:A:617:MET:HA	1.71	0.71
1:A:673:VAL:HG22	1:A:733:MET:HE2	1.71	0.70
1:A:571:ALA:N	1:A:617:MET:CE	2.52	0.70
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:50:MET:HE3	1:A:50:MET:HA	1.78	0.66
1:A:439:ASP:CG	1:A:481:MET:HE1	2.21	0.65
1:A:360:ILE:HD13	1:A:381:LEU:HD22	1.79	0.65
1:A:1:MET:HE2	1:A:775:GLU:CG	2.28	0.64
1:A:570:LEU:CB	1:A:617:MET:HE2	2.28	0.63
1:A:439:ASP:H	1:A:481:MET:HE1	1.64	0.62
1:A:792:GLU:OE2	1:A:795:MET:HE3	2.00	0.61
1:A:360:ILE:CD1	1:A:381:LEU:HD22	2.30	0.61
1:A:1:MET:CE	1:A:775:GLU:HB3	2.23	0.61
2:B:16:U:H2'	2:B:17:C:C5	2.35	0.61
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:571:ALA:C	1:A:617:MET:HE3	2.28	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:792:GLU:CD	1:A:795:MET:HE3	2.29	0.57
1:A:570:LEU:HB3	1:A:617:MET:HE2	1.87	0.56
1:A:468:LYS:HZ3	1:A:487:THR:CG2	2.09	0.56
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:110:ASN:ND2	3:A:2088:HOH:O	2.22	0.55
1:A:695:THR:HG22	1:A:697:ASN:N	2.20	0.55
1:A:534:ALA:HA	1:A:538:LEU:HD12	1.87	0.55
1:A:571:ALA:CA	1:A:617:MET:CE	2.82	0.55
1:A:575:TYR:CE2	1:A:613:VAL:HG22	2.41	0.55
1:A:854:LEU:CD2	1:A:854:LEU:O	2.44	0.55
1:A:695:THR:HG21	3:A:2332:HOH:O	2.07	0.54
1:A:617:MET:HE3	1:A:617:MET:CA	2.37	0.54
1:A:806:VAL:CG1	1:A:859:VAL:HG22	2.37	0.54
1:A:27:THR:HG22	3:A:2031:HOH:O	2.07	0.54
1:A:570:LEU:HB2	1:A:617:MET:HE2	1.91	0.53
1:A:729:ILE:HD13	1:A:761:LEU:HD13	1.90	0.52
2:B:47(C):U:H4'	2:B:47(D):C:OP2	2.08	0.52
1:A:571:ALA:C	1:A:617:MET:CE	2.82	0.52
2:B:17:C:H5''	2:B:18:G:OP2	2.09	0.52
1:A:146:LYS:NZ	3:A:2109:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:711:LYS:NZ	3:A:2336:HOH:O	2.31	0.51
1:A:854:LEU:HD23	1:A:855:LEU:CA	2.41	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:1:MET:HE2	1:A:775:GLU:HG3	1.94	0.49
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:570:LEU:C	1:A:617:MET:CE	2.78	0.48
1:A:298:MET:N	3:A:2170:HOH:O	2.46	0.48
1:A:272:ALA:N	1:A:278:LEU:HD23	2.29	0.48
1:A:695:THR:HG21	3:A:2333:HOH:O	2.14	0.48
1:A:854:LEU:CD2	1:A:855:LEU:N	2.69	0.47
1:A:219:MET:HE1	1:A:531:ILE:HD11	1.95	0.47
1:A:468:LYS:HG2	1:A:487:THR:HG23	1.96	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:749:LEU:C	1:A:749:LEU:HD23	2.39	0.46
1:A:498:TRP:CE3	1:A:512:MET:HE3	2.51	0.46
1:A:529:GLY:O	1:A:565:CYS:HA	2.15	0.46
1:A:439:ASP:H	1:A:481:MET:HE2	1.80	0.46
1:A:485:ARG:HB2	3:A:2215:HOH:O	2.15	0.46
1:A:95:THR:HG23	1:A:96:ALA:N	2.30	0.46
2:B:16:U:H2'	2:B:17:C:H5	1.81	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:847:VAL:C	1:A:848:ILE:HD13	2.41	0.45
1:A:569:VAL:HG12	1:A:620:MET:HE3	1.97	0.45
1:A:617:MET:HE2	1:A:617:MET:HB3	1.76	0.45
1:A:816:VAL:CG1	1:A:817:PRO:CD	2.95	0.44
1:A:519:ASN:OD1	1:A:555:ASN:HB2	2.16	0.44
1:A:592:ILE:HD12	1:A:592:ILE:N	2.31	0.44
1:A:519:ASN:CG	1:A:555:ASN:HB2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LYS:CE	1:A:487:THR:HG23	2.48	0.42
1:A:25:GLU:HA	1:A:120:ASP:CG	2.44	0.42
1:A:305:THR:CG2	1:A:320:VAL:O	2.63	0.42
2:B:75:C:OP1	2:B:76:365:H22A	2.20	0.42
1:A:238:ASP:N	3:A:2153:HOH:O	1.93	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:OP1	2.19	0.42
1:A:656:LEU:C	1:A:656:LEU:HD23	2.44	0.42
1:A:237:ASN:ND2	1:A:317:GLU:OE2	2.53	0.41
1:A:572:ASP:O	1:A:588:PRO:HG3	2.21	0.41
1:A:478:VAL:N	1:A:481:MET:O	2.44	0.41
1:A:617:MET:CE	1:A:617:MET:CA	2.97	0.41
1:A:646:MET:HE2	1:A:656:LEU:HD13	2.01	0.41
1:A:50:MET:HE3	1:A:53:VAL:HB	2.03	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:438:GLU:CG	1:A:481:MET:HE3	2.45	0.41
1:A:44:PRO:HA	1:A:108:MET:SD	2.61	0.40
1:A:571:ALA:HA	1:A:617:MET:HE1	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	22	32

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

Mol	Chain	Res	Type
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	594	GLU
1	A	597	GLU
1	A	603	LYS
1	A	613	VAL
1	A	617	MET
1	A	618	SER
1	A	625	ASN
1	A	646	MET
1	A	695	THR
1	A	761	LEU
1	A	816	VAL

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Mol	Chain	Res	Type
1	A	819	ASP
1	A	848	ILE
1	A	853	LYS
1	A	854	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	190	GLN
1	A	479	ASN
1	A	824	GLN

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 oligosaccharides 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, 95th 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%)	1.20	104 (12%) 7 8	21, 38, 54, 91	1 (0%)
2	B	84/87 (96%)	1.49	29 (34%) 1 1	35, 42, 51, 56	0
All	All	897/967 (92%)	1.22	133 (14%) 5 6	21, 38, 54, 91	1 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	ASN	6.7
1	A	155	ALA	5.2
1	A	811	ARG	5.1
1	A	859	VAL	5.1
1	A	837	LYS	4.9
1	A	849	TYR	4.9
1	A	156	VAL	4.8
1	A	268	ALA	4.6
1	A	818	VAL	4.5
1	A	835	VAL	4.3
1	A	274	ASN	4.2
1	A	269	GLN	4.2
1	A	850	VAL	4.1
1	A	812	ALA	4.1
1	A	838	TYR	4.0
1	A	479	ASN	4.0
1	A	836	ALA	3.9
1	A	806	VAL	3.9
1	A	852	GLY	3.7
1	A	536	MET	3.6
1	A	438	GLU	3.6
1	A	819	ASP	3.5
1	A	277	GLU	3.4
1	A	848	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	830	GLY	3.3
1	A	858	VAL	3.3
1	A	288	THR	3.3
2	B	31	A	3.3
1	A	287	ASN	3.2
2	B	1	G	3.2
1	A	810	VAL	3.1
1	A	827	GLU	3.1
2	B	72	U	3.1
2	B	2	C	3.0
2	B	40	C	3.0
2	B	33	U	3.0
2	B	70	G	3.0
2	B	71	G	3.0
1	A	478	VAL	3.0
1	A	364	ASP	3.0
1	A	823	GLU	2.9
1	A	860	GLY	2.9
2	B	42	C	2.9
2	B	36	A	2.9
1	A	816	VAL	2.9
1	A	188	ILE	2.8
2	B	32	U	2.8
1	A	480	GLY	2.8
1	A	805	GLN	2.8
1	A	276	PRO	2.8
1	A	284	GLU	2.8
1	A	834	LEU	2.7
2	B	17	C	2.7
1	A	448	ASP	2.7
2	B	37	A	2.7
1	A	820	ALA	2.7
2	B	41	C	2.7
1	A	283	ASP	2.7
1	A	821	THR	2.7
1	A	501	ALA	2.6
1	A	854	LEU	2.6
2	B	39	U	2.6
1	A	273	GLU	2.6
1	A	597	GLU	2.6
1	A	829	ALA	2.6
1	A	833	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	38	A	2.6
1	A	798	ASP	2.6
1	A	91	VAL	2.6
1	A	851	PRO	2.6
1	A	809	LYS	2.5
1	A	263	ALA	2.5
1	A	386	GLU	2.4
1	A	535	ILE	2.4
1	A	41	LEU	2.4
2	B	3	C	2.4
2	B	63	C	2.4
1	A	602	VAL	2.4
1	A	507	GLN	2.4
1	A	510	GLU	2.4
2	B	69	G	2.3
2	B	73	A	2.3
1	A	286	ARG	2.3
1	A	826	ARG	2.3
1	A	187	GLU	2.3
1	A	285	CYS	2.3
1	A	824	GLN	2.3
1	A	458	VAL	2.3
1	A	689	LEU	2.3
2	B	52	G	2.3
1	A	272	ALA	2.3
2	B	30	G	2.2
1	A	353	GLY	2.2
1	A	483	ALA	2.2
1	A	822	GLU	2.2
1	A	304	ASP	2.2
2	B	47(E)	G	2.2
2	B	47(F)	C	2.2
1	A	305	THR	2.2
1	A	35	TYR	2.2
1	A	855	LEU	2.2
1	A	435	VAL	2.2
1	A	22	ARG	2.2
1	A	807	ASN	2.2
1	A	385	GLY	2.2
2	B	64	G	2.2
1	A	814	ILE	2.2
1	A	804	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	568	MET	2.2
2	B	6	G	2.2
1	A	56	TYR	2.1
1	A	832	GLU	2.1
1	A	693	ALA	2.1
1	A	695	THR	2.1
1	A	503	TYR	2.1
1	A	516	GLU	2.1
1	A	660	GLU	2.1
1	A	223	TRP	2.1
1	A	691	VAL	2.1
2	B	65	C	2.1
2	B	5	G	2.1
1	A	513	LEU	2.1
1	A	476	THR	2.1
1	A	487	THR	2.1
1	A	280	ALA	2.1
2	B	47(G)	G	2.1
1	A	329	GLU	2.1
1	A	577	VAL	2.1
1	A	748	ALA	2.0
1	A	282	ILE	2.0
1	A	686	VAL	2.0
1	A	737	ALA	2.0
1	A	351	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.