Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 05:56 AM EDT

PDB ID	:	1JNP
Title	:	Crystal Structure of Murine Tcl1 at 2.5 Resolution
Authors	:	Petock, J.M.; Torshin, I.Y.; Wang, Y.F.; DuBois, G.C.; Croce, C.M.; Harrison, R.W.; Weber, I.T.
Deposited on	:	2001-07-24
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	Percentile Ranks	Value
Clashscore		72
Ramachandran outliers		5.1%
Sidechain outliers		38.5%
RSRZ outliers		4.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution
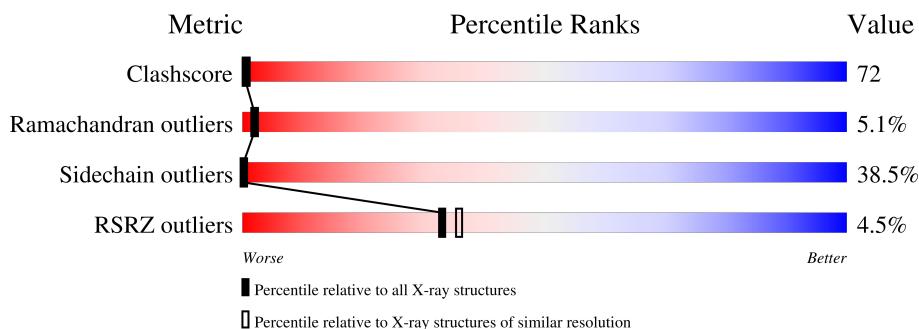
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	116	4% / 18% 45% 21% · 13%
1	B	116	3% / 9% 42% 34% · 13%
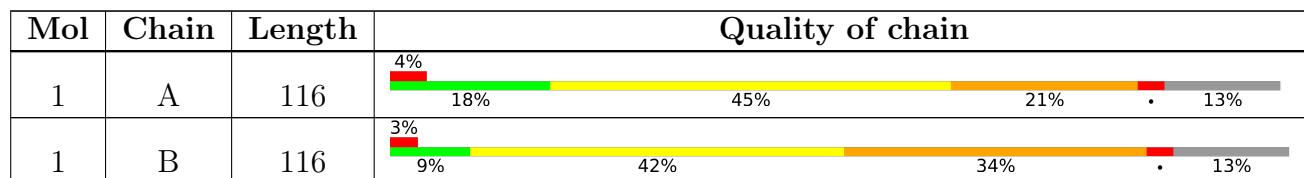
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 1801 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 T-CELL LEUKEMIA/LYMPHOMA PROTEIN 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			876	572	148	152	4			
1	B	101	Total	C	N	O	S	3	0	0
			876	572	148	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	CYS	engineered mutation	UNP P56280
B	285	ALA	CYS	engineered mutation	UNP P56280

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	28	Total	O	0	0
			28	28		
2	B	21	Total	O	0	0
			21	21		

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: T-CELL LEUKEMIA/LYMPHOMA PROTEIN 1A

Chain A:

• Molecule 1: T-CELL LEUKEMIA/LYMPHOMA PROTEIN 1A

Chain B:
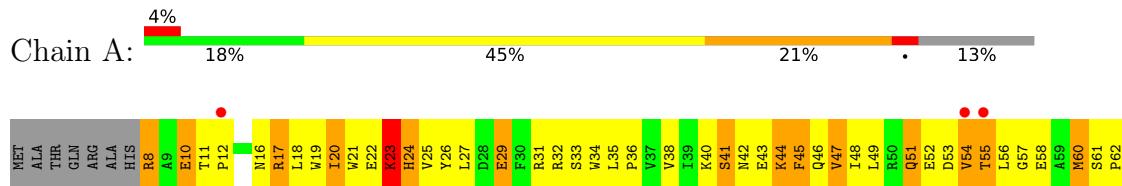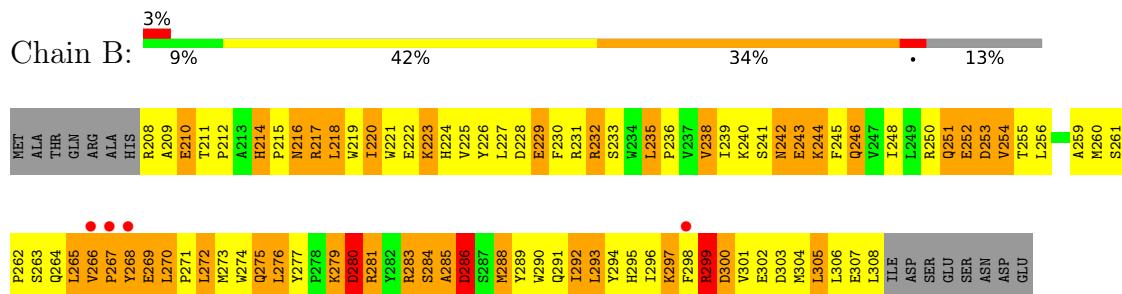
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.32Å　　115.91Å　　37.95Å 90.00°　　115.15°　　90.00°	Depositor
Resolution (Å)	10.00　–　2.50 9.49　–　2.50	Depositor EDS
% Data completeness (in resolution range)	92.1 (10.00-2.50) 88.8 (9.49-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	4.58 (at 2.49Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.226　,　　0.236 0.217　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å²)	27.5	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.13 , 118.8	EDS
L-test for twinning [2]	$<|L|> = 0.55$, $<L^2> = 0.39$	Xtriage
Estimated twinning fraction	0.089 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	1801	wwPDB-VP
Average B, all atoms (Å²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.35	0/904	1.05	4/1229 (0.3%)
1	B	0.32	0/904	0.95	1/1229 (0.1%)
All	All	0.34	0/1808	1.00	5/2458 (0.2%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	LYS	C-N-CA	11.10	149.46	121.70
1	A	65	LEU	C-N-CA	7.67	140.88	121.70
1	B	299	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	68	TYR	CA-CB-CG	5.24	123.35	113.40
1	A	68	TYR	CB-CG-CD1	5.08	124.05	121.00

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	876	0	861	103	0
1	B	876	0	863	149	0
2	A	28	0	0	3	0
2	B	21	0	0	2	0
All	All	1801	0	1724	249	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 72.

All (249) 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:B:279:LYS:HD3	1:B:281:ARG:HB2	1.41	1.02
1:A:10:GLU:HA	1:A:96:ILE:HA	1.42	1.00
1:A:61:SER:HB2	1:A:64:GLN:HG3	1.54	0.88
1:A:66:VAL:HG13	1:A:67:PRO:HD3	1.56	0.88
1:B:238:VAL:H	1:B:248:ILE:HG22	1.39	0.87
1:A:38:VAL:HB	1:A:48:ILE:HD12	1.61	0.83
1:B:222:GLU:HA	1:B:260:MET:HG3	1.60	0.82
1:B:255:THR:O	1:B:256:LEU:HD23	1.84	0.78
1:B:299:ARG:O	1:B:301:VAL:HG23	1.83	0.78
1:B:243:GLU:O	1:B:244:LYS:HE3	1.83	0.77
1:B:293:LEU:HG	1:B:305:LEU:HB3	1.67	0.76
1:B:236:PRO:HA	1:B:248:ILE:O	1.86	0.75
1:B:272:LEU:HD22	1:B:272:LEU:H	1.51	0.75
1:B:297:LYS:HA	1:B:301:VAL:O	1.87	0.74
1:A:22:GLU:HA	1:A:60:MET:HE3	1.70	0.74
1:B:221:TRP:HB3	1:B:225:VAL:HG12	1.71	0.73
1:B:226:TYR:OH	1:B:270:LEU:HB3	1.88	0.73
1:A:54:VAL:HG13	1:A:56:LEU:N	2.04	0.72
1:B:261:SER:H	1:B:264:GLN:NE2	1.89	0.71
1:B:275:GLN:NE2	1:B:283:ARG:HD3	2.06	0.71
1:B:262:PRO:HA	1:B:265:LEU:HD11	1.72	0.70
1:B:228:ASP:OD2	1:B:230:PHE:HB2	1.92	0.70
1:B:230:PHE:HB3	1:B:232:ARG:HD2	1.73	0.69
1:B:254:VAL:O	1:B:256:LEU:HG	1.93	0.69
1:A:48:ILE:HG13	1:A:105:LEU:HD12	1.74	0.68
1:B:217:ARG:HH11	1:B:217:ARG:HB2	1.59	0.68
1:B:217:ARG:O	1:B:228:ASP:HA	1.95	0.67
1:A:80:ASP:OD2	1:A:92:ILE:HG21	1.94	0.67
1:B:261:SER:H	1:B:264:GLN:HE21	1.42	0.66
1:B:232:ARG:HH11	1:B:232:ARG:HA	1.60	0.66
1:B:220:ILE:HD12	1:B:225:VAL:O	1.95	0.65
1:A:65:LEU:HB3	1:A:66:VAL:HA	1.78	0.65
1:B:268:TYR:HB3	1:B:270:LEU:O	1.97	0.64
1:B:288:MET:HB3	1:B:308:LEU:HD21	1.80	0.64
1:A:90:TRP:NE1	1:A:108:LEU:HD12	2.13	0.64
1:A:90:TRP:CE2	1:A:108:LEU:HB2	2.33	0.64
1:B:250:ARG:HB2	1:B:303:ASP:OD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TRP:CZ3	1:A:104:MET:HB2	2.33	0.64
1:A:29:GLU:HA	1:B:289:TYR:OH	1.98	0.63
1:B:228:ASP:HB2	1:B:229:GLU:OE2	1.98	0.63
1:B:292:ILE:HA	1:B:306:LEU:HD12	1.80	0.63
1:B:279:LYS:HG3	1:B:280:ASP:N	2.14	0.62
1:B:294:TYR:O	1:B:304:MET:HA	1.98	0.62
1:B:233:SER:O	1:B:251:GLN:HA	1.99	0.62
1:A:24:HIS:O	1:A:36:PRO:HD2	1.99	0.62
1:B:292:ILE:HG13	1:B:304:MET:SD	2.39	0.62
1:A:88:MET:SD	1:A:108:LEU:HD11	2.40	0.62
1:A:53:ASP:O	1:A:54:VAL:HG23	2.00	0.61
1:B:209:ALA:HB3	1:B:297:LYS:O	2.00	0.61
1:B:223:LYS:HD2	1:B:268:TYR:CD1	2.36	0.60
1:B:279:LYS:HG3	1:B:280:ASP:H	1.66	0.60
1:A:73:MET:HB3	1:A:85:ALA:HB2	1.84	0.60
1:B:240:LYS:HB2	1:B:246:GLN:HB3	1.83	0.60
1:A:93:LEU:HB2	1:A:105:LEU:O	2.02	0.60
1:A:54:VAL:HG22	1:A:56:LEU:HG	1.83	0.59
1:A:22:GLU:OE1	1:A:56:LEU:HD13	2.02	0.59
1:B:218:LEU:O	1:B:273:MET:HG2	2.02	0.59
1:A:73:MET:HG3	1:A:74:TRP:N	2.18	0.59
1:B:220:ILE:HD13	1:B:226:TYR:CZ	2.38	0.59
1:A:27:LEU:HD12	1:A:33:SER:HA	1.84	0.59
1:B:233:SER:HB2	1:B:253:ASP:HA	1.85	0.58
1:B:279:LYS:CE	1:B:281:ARG:HD2	2.34	0.58
1:A:93:LEU:CB	1:A:105:LEU:HD23	2.34	0.58
1:A:25:VAL:HG13	1:A:35:LEU:CD2	2.34	0.58
1:B:245:PHE:CD2	1:B:308:LEU:HD12	2.39	0.58
1:B:268:TYR:CZ	1:B:270:LEU:HB2	2.39	0.57
1:B:297:LYS:HZ2	1:B:300:ASP:HA	1.69	0.57
1:B:227:LEU:HD23	1:B:231:ARG:HG3	1.87	0.57
1:B:242:ASN:O	1:B:243:GLU:HG3	2.03	0.57
1:A:20:ILE:CG2	1:A:72:LEU:HG	2.34	0.57
1:A:35:LEU:O	1:A:49:LEU:HA	2.05	0.57
1:B:246:GLN:HG3	1:B:305:LEU:CD1	2.35	0.57
1:B:240:LYS:HZ3	1:B:246:GLN:HB3	1.70	0.56
1:A:79:LYS:HD3	1:A:81:ARG:HB2	1.87	0.56
1:B:286:ASP:OD1	1:B:288:MET:HB2	2.05	0.56
1:A:31:ARG:HG3	1:B:275:GLN:HE22	1.70	0.56
1:B:240:LYS:HE2	1:B:246:GLN:HG2	1.87	0.56
1:B:293:LEU:CG	1:B:305:LEU:HB3	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HE2	1:A:23:LYS:H	1.70	0.55
1:A:31:ARG:HB2	1:B:283:ARG:CZ	2.36	0.55
1:B:265:LEU:HD11	1:B:272:LEU:HD12	1.87	0.55
1:B:217:ARG:HB2	1:B:217:ARG:NH1	2.21	0.55
1:B:227:LEU:HA	1:B:232:ARG:O	2.06	0.55
1:A:38:VAL:HB	1:A:48:ILE:CD1	2.36	0.55
1:A:24:HIS:HB3	1:A:25:VAL:HG23	1.89	0.54
1:B:294:TYR:CZ	1:B:305:LEU:HD23	2.42	0.54
1:A:94:TYR:HB2	1:A:96:ILE:HG23	1.89	0.54
1:A:23:LYS:HG2	1:A:24:HIS:HB2	1.90	0.54
1:A:43:GLU:OE2	1:A:43:GLU:HA	2.08	0.54
1:B:221:TRP:CD1	1:B:256:LEU:HD13	2.42	0.54
1:A:76:LEU:HD11	1:A:80:ASP:HA	1.90	0.53
1:A:98:PHE:O	1:A:101:VAL:HB	2.07	0.53
1:B:238:VAL:HG22	1:B:248:ILE:HB	1.90	0.53
1:B:221:TRP:CZ3	1:B:259:ALA:HB2	2.44	0.53
1:B:261:SER:O	1:B:265:LEU:HG	2.07	0.53
1:B:290:TRP:HA	1:B:307:GLU:O	2.08	0.53
1:A:83:ARG:NE	1:A:87:SER:HA	2.24	0.53
1:A:8:ARG:HA	1:A:97:LYS:O	2.09	0.53
1:B:296:ILE:O	1:B:302:GLU:HA	2.09	0.53
1:B:286:ASP:OD2	1:B:288:MET:HG2	2.09	0.53
1:A:47:VAL:HG12	1:A:90:TRP:HZ3	1.75	0.52
1:B:215:PRO:HD2	1:B:304:MET:HE1	1.91	0.52
1:B:293:LEU:HD12	1:B:294:TYR:HD2	1.74	0.52
1:B:246:GLN:HG3	1:B:305:LEU:HD11	1.91	0.52
1:A:68:TYR:HB2	2:A:1002:HOH:O	2.09	0.52
1:B:219:TRP:HZ3	1:B:229:GLU:N	2.08	0.52
1:B:226:TYR:O	1:B:227:LEU:HD12	2.09	0.52
1:B:289:TYR:O	1:B:308:LEU:HD23	2.09	0.52
1:B:239:ILE:HA	1:B:246:GLN:O	2.09	0.52
1:A:62:PRO:O	1:A:66:VAL:HB	2.10	0.52
1:B:230:PHE:CB	1:B:232:ARG:HD2	2.40	0.52
1:A:97:LYS:O	1:A:98:PHE:HD2	1.92	0.52
1:B:297:LYS:NZ	1:B:300:ASP:HA	2.24	0.51
1:B:220:ILE:HD13	1:B:226:TYR:CE1	2.45	0.51
1:B:233:SER:CB	1:B:253:ASP:HA	2.40	0.51
1:A:20:ILE:HD12	1:A:22:GLU:O	2.09	0.51
1:A:88:MET:CE	1:A:108:LEU:HD11	2.40	0.51
1:A:25:VAL:HG13	1:A:35:LEU:HD22	1.93	0.51
1:B:219:TRP:HA	1:B:273:MET:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HB	1:A:72:LEU:O	2.11	0.51
1:A:20:ILE:HG22	1:A:72:LEU:HG	1.93	0.51
1:A:23:LYS:H	1:A:23:LYS:CD	2.24	0.51
1:A:91:GLN:HG2	1:A:92:ILE:N	2.26	0.50
1:B:279:LYS:NZ	1:B:281:ARG:HD2	2.26	0.50
1:A:10:GLU:OE1	1:A:10:GLU:O	2.30	0.50
1:A:40:LYS:O	1:A:45:PHE:HA	2.11	0.50
1:A:45:PHE:CE1	1:A:108:LEU:HD22	2.47	0.50
1:B:217:ARG:HD2	1:B:273:MET:CE	2.40	0.50
1:B:235:LEU:HD23	1:B:252:GLU:HG3	1.93	0.50
1:A:23:LYS:H	1:A:23:LYS:CE	2.25	0.50
1:B:232:ARG:HH11	1:B:232:ARG:CA	2.24	0.50
1:B:297:LYS:CG	1:B:302:GLU:HG2	2.42	0.50
1:A:23:LYS:NZ	1:A:23:LYS:HB3	2.21	0.50
1:A:22:GLU:HA	1:A:60:MET:CE	2.40	0.49
1:B:240:LYS:HB2	1:B:246:GLN:CB	2.41	0.49
1:A:88:MET:CE	1:A:108:LEU:HD21	2.42	0.49
1:A:101:VAL:HG12	1:A:101:VAL:O	2.11	0.49
1:A:54:VAL:CG1	1:A:56:LEU:HB2	2.43	0.49
1:B:216:ASN:HB2	1:B:276:LEU:HD22	1.95	0.49
1:B:262:PRO:HA	1:B:265:LEU:CD1	2.40	0.49
1:A:97:LYS:HG3	1:A:102:GLU:HG3	1.94	0.48
1:B:279:LYS:O	1:B:280:ASP:OD2	2.30	0.48
1:B:279:LYS:HE2	1:B:280:ASP:HB2	1.96	0.48
1:A:90:TRP:CD2	1:A:108:LEU:HB2	2.48	0.48
1:B:298:PHE:O	1:B:299:ARG:HB2	2.14	0.48
1:B:261:SER:HB3	1:B:264:GLN:HE21	1.79	0.47
1:A:23:LYS:HE2	1:A:23:LYS:N	2.29	0.47
1:A:97:LYS:HZ3	1:A:100:ASP:HA	1.79	0.47
1:B:235:LEU:HD12	2:B:1029:HOH:O	2.14	0.47
1:B:284:SER:OG	1:B:290:TRP:NE1	2.46	0.47
1:A:20:ILE:HD12	1:A:25:VAL:O	2.14	0.47
1:A:88:MET:HE2	1:A:108:LEU:HD21	1.97	0.47
1:A:92:ILE:HG23	1:A:92:ILE:O	2.15	0.47
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.75	0.47
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.70	0.47
1:A:32:ARG:HE	1:A:51:GLN:CD	2.19	0.46
1:B:221:TRP:CH2	1:B:259:ALA:HB2	2.50	0.46
1:A:20:ILE:HD13	1:A:26:TYR:CG	2.50	0.46
1:B:220:ILE:HG12	1:B:268:TYR:HE2	1.80	0.46
1:B:240:LYS:CE	1:B:246:GLN:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:HG3	1:B:273:MET:SD	2.56	0.46
1:B:233:SER:OG	1:B:254:VAL:HG22	2.16	0.46
1:A:79:LYS:HE2	1:A:81:ARG:NE	2.30	0.46
1:A:17:ARG:HD3	1:A:29:GLU:HG3	1.98	0.46
1:A:16:ASN:N	1:A:29:GLU:OE2	2.49	0.46
1:B:285:ALA:O	1:B:286:ASP:HB3	2.16	0.46
1:B:261:SER:HB3	1:B:264:GLN:HB2	1.99	0.45
1:A:32:ARG:NH2	1:A:51:GLN:OE1	2.49	0.45
1:B:210:GLU:HA	1:B:296:ILE:HG22	1.99	0.45
1:A:23:LYS:HG2	1:A:24:HIS:N	2.32	0.45
1:A:44:LYS:O	1:A:44:LYS:HD3	2.17	0.45
1:A:93:LEU:HD23	1:A:107:GLU:HB2	1.97	0.45
1:A:11:THR:N	1:A:95:HIS:O	2.50	0.45
1:B:293:LEU:HD12	1:B:294:TYR:CD2	2.50	0.45
1:A:10:GLU:OE1	1:A:10:GLU:N	2.50	0.45
1:A:97:LYS:HG2	1:A:102:GLU:HA	1.98	0.45
1:B:216:ASN:OD1	1:B:217:ARG:NH1	2.50	0.45
1:B:224:HIS:N	1:B:268:TYR:OH	2.50	0.44
1:A:18:LEU:HD12	1:A:26:TYR:HB3	1.97	0.44
1:B:220:ILE:HG12	1:B:268:TYR:CE2	2.51	0.44
1:B:228:ASP:O	1:B:231:ARG:N	2.50	0.44
1:B:275:GLN:HE22	1:B:283:ARG:HD3	1.77	0.44
1:B:284:SER:O	1:B:286:ASP:N	2.50	0.44
1:A:8:ARG:O	1:A:98:PHE:HE2	2.00	0.44
1:A:21:TRP:CE3	1:A:27:LEU:HB2	2.53	0.44
1:A:40:LYS:NZ	1:A:41:SER:O	2.50	0.44
1:B:218:LEU:HB2	1:B:274:TRP:HB2	1.98	0.44
1:A:54:VAL:HA	1:A:55:THR:OG1	2.17	0.44
1:B:267:PRO:HD3	2:B:1013:HOH:O	2.16	0.44
1:B:221:TRP:CB	1:B:225:VAL:HG12	2.44	0.44
1:B:231:ARG:HH11	1:B:231:ARG:HD3	1.65	0.44
1:A:35:LEU:HB3	2:A:1001:HOH:O	2.17	0.44
1:A:20:ILE:N	1:A:72:LEU:O	2.49	0.43
1:B:208:ARG:O	1:B:208:ARG:HG3	2.11	0.43
1:A:19:TRP:O	1:A:26:TYR:HD2	2.01	0.43
1:A:20:ILE:HD13	1:A:26:TYR:CD2	2.54	0.43
1:B:268:TYR:CE1	1:B:270:LEU:HB2	2.53	0.43
1:B:291:GLN:N	1:B:307:GLU:O	2.49	0.43
1:B:292:ILE:HG13	1:B:304:MET:CG	2.49	0.43
1:A:66:VAL:HG22	1:A:67:PRO:N	2.33	0.43
1:B:208:ARG:NE	1:B:299:ARG:HH21	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HG21	1:B:272:LEU:HA	1.99	0.43
1:B:272:LEU:N	1:B:272:LEU:HD13	2.34	0.43
1:B:276:LEU:HD23	1:B:276:LEU:O	2.18	0.43
1:B:216:ASN:HA	1:B:276:LEU:HB3	2.00	0.43
1:B:279:LYS:HB2	1:B:279:LYS:HE3	1.53	0.43
1:B:214:HIS:HA	1:B:295:HIS:CE1	2.54	0.43
1:B:292:ILE:HB	1:B:306:LEU:CD1	2.49	0.43
1:B:251:GLN:HB2	1:B:302:GLU:HB2	2.00	0.42
1:B:292:ILE:HB	1:B:306:LEU:HD11	2.00	0.42
1:A:34:TRP:C	1:A:35:LEU:HD23	2.39	0.42
1:B:268:TYR:HD1	1:B:269:GLU:H	1.67	0.42
1:B:220:ILE:CG2	1:B:272:LEU:HA	2.49	0.42
1:A:57:GLY:O	1:A:58:GLU:HB3	2.19	0.42
1:A:68:TYR:HD2	2:A:1002:HOH:O	2.02	0.42
1:B:304:MET:HB3	1:B:304:MET:HE3	1.90	0.42
1:A:40:LYS:HG3	1:A:41:SER:N	2.35	0.42
1:B:242:ASN:H	1:B:242:ASN:ND2	2.16	0.42
1:B:279:LYS:HE2	1:B:281:ARG:HD2	2.01	0.42
1:B:275:GLN:HE21	1:B:277:TYR:HE1	1.68	0.41
1:B:220:ILE:HG23	1:B:220:ILE:O	2.20	0.41
1:B:224:HIS:O	1:B:225:VAL:HG23	2.20	0.41
1:B:292:ILE:O	1:B:292:ILE:HG12	2.20	0.41
1:B:296:ILE:HD12	1:B:303:ASP:HB2	2.02	0.41
1:B:219:TRP:O	1:B:226:TYR:HA	2.20	0.41
1:B:294:TYR:OH	1:B:305:LEU:HD23	2.19	0.41
1:A:20:ILE:HD13	1:A:20:ILE:HA	1.85	0.41
1:A:60:MET:HE3	1:A:60:MET:HB3	1.83	0.41
1:A:23:LYS:HA	1:A:65:LEU:HD21	2.02	0.41
1:A:20:ILE:HD11	1:A:68:TYR:OH	2.21	0.41
1:A:48:ILE:HG13	1:A:105:LEU:CD1	2.44	0.41
1:A:44:LYS:NZ	1:A:46:GLN:NE2	2.68	0.41
1:B:220:ILE:HD13	1:B:226:TYR:CE2	2.56	0.41
1:A:17:ARG:HD3	1:A:29:GLU:CG	2.51	0.41
1:B:231:ARG:O	1:B:231:ARG:HG2	2.21	0.41
1:B:235:LEU:N	1:B:250:ARG:O	2.49	0.41
1:B:244:LYS:HD3	1:B:244:LYS:HA	1.67	0.41
1:B:296:ILE:CD1	1:B:303:ASP:HB2	2.51	0.41
1:B:208:ARG:HD2	1:B:299:ARG:HH21	1.86	0.41
1:B:209:ALA:O	1:B:296:ILE:HA	2.21	0.40
1:B:245:PHE:HD2	1:B:308:LEU:HD12	1.85	0.40
1:A:47:VAL:HG12	1:A:90:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PRO:HG3	1:A:72:LEU:HD13	2.03	0.40
1:B:226:TYR:OH	1:B:271:PRO:O	2.29	0.40
1:B:279:LYS:HG3	1:B:281:ARG:H	1.86	0.40
1:A:83:ARG:CZ	1:A:87:SER:HA	2.51	0.40
1:A:94:TYR:CD1	1:A:96:ILE:HG12	2.56	0.40
1:B:238:VAL:H	1:B:248:ILE:CG2	2.22	0.40
1:B:292:ILE:HA	1:B:305:LEU:O	2.22	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	99/116 (85%)	82 (83%)	15 (15%)	2 (2%)	7	12
1	B	99/116 (85%)	82 (83%)	9 (9%)	8 (8%)	1	1
All	All	198/232 (85%)	164 (83%)	24 (12%)	10 (5%)	2	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	ASP
1	B	286	ASP
1	A	12	PRO
1	B	243	GLU
1	B	285	ALA
1	A	66	VAL
1	B	212	PRO
1	B	252	GLU
1	B	267	PRO
1	B	266	VAL

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	96/109 (88%)	63 (66%)	33 (34%)	0	0
1	B	96/109 (88%)	55 (57%)	41 (43%)	0	0
All	All	192/218 (88%)	118 (62%)	74 (38%)	0	0

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	10	GLU
1	A	17	ARG
1	A	20	ILE
1	A	23	LYS
1	A	24	HIS
1	A	29	GLU
1	A	41	SER
1	A	42	ASN
1	A	44	LYS
1	A	45	PHE
1	A	47	VAL
1	A	51	GLN
1	A	52	GLU
1	A	54	VAL
1	A	55	THR
1	A	60	MET
1	A	63	SER
1	A	64	GLN
1	A	65	LEU
1	A	66	VAL
1	A	68	TYR
1	A	72	LEU
1	A	73	MET
1	A	74	TRP
1	A	79	LYS
1	A	86	ASP

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Mol	Chain	Res	Type
1	A	88	MET
1	A	93	LEU
1	A	97	LYS
1	A	99	ARG
1	A	104	MET
1	A	105	LEU
1	B	210	GLU
1	B	211	THR
1	B	214	HIS
1	B	216	ASN
1	B	217	ARG
1	B	218	LEU
1	B	220	ILE
1	B	223	LYS
1	B	229	GLU
1	B	232	ARG
1	B	235	LEU
1	B	238	VAL
1	B	241	SER
1	B	242	ASN
1	B	244	LYS
1	B	246	GLN
1	B	251	GLN
1	B	253	ASP
1	B	254	VAL
1	B	263	SER
1	B	265	LEU
1	B	266	VAL
1	B	268	TYR
1	B	269	GLU
1	B	270	LEU
1	B	272	LEU
1	B	275	GLN
1	B	276	LEU
1	B	279	LYS
1	B	280	ASP
1	B	281	ARG
1	B	283	ARG
1	B	284	SER
1	B	286	ASP
1	B	288	MET
1	B	292	ILE

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Mol	Chain	Res	Type
1	B	293	LEU
1	B	297	LYS
1	B	299	ARG
1	B	300	ASP
1	B	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	75	GLN
1	B	242	ASN
1	B	246	GLN
1	B	264	GLN
1	B	275	GLN
1	B	291	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	101/116 (87%)	0.34	5 (4%)	28	30	20, 35, 61, 74	0
1	B	101/116 (87%)	0.26	4 (3%)	38	41	17, 35, 60, 89	1 (0%)
All	All	202/232 (87%)	0.30	9 (4%)	33	36	17, 35, 61, 89	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	VAL	5.5
1	A	54	VAL	4.6
1	B	268	TYR	4.2
1	A	55	THR	3.6
1	B	266	VAL	3.1
1	B	267	PRO	3.0
1	A	12	PRO	2.8
1	A	99	ARG	2.0
1	B	298	PHE	2.0

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

There are no ligands in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.5 Other polymers ⓘ

There are no such residues in this entry.