



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:29 AM UTC

PDB ID : 1QAJ / pdb_00001qaj
Title : CRYSTAL STRUCTURES OF THE N-TERMINAL FRAGMENT FROM
MOLONEY MURINE LEUKEMIA VIRUS REVERSE TRANSCRIPTASE
COMPLEXED WITH NUCLEIC ACID: FUNCTIONAL IMPLICATIONS
FOR TEMPLATE-PRIMER BINDING TO THE FINGERS DOMAIN
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giadis, M.M.
Deposited on : 1999-03-18
Resolution : 2.30 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
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
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

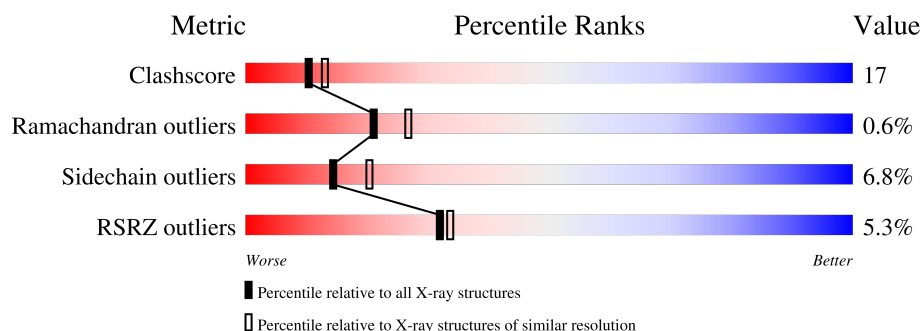
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	C	8	25% 75%
1	D	8	100%
2	A	259	3% 69% 26% 5%
2	B	259	8% 61% 32% 5% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4856 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 DNA chain called DNA (5'-D(*CP*AP*TP*GP*CP*AP*TP*G)-3').

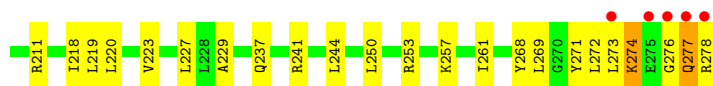
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			
1	D	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			

- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	259	Total	C	N	O	S	0	0	0
			2069	1327	362	372	8			
2	B	257	Total	C	N	O	S	0	0	0
			2059	1322	360	369	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	12	Total	O	0	0
			12	12		
3	D	10	Total	O	0	0
			10	10		
3	A	238	Total	O	0	0
			238	238		
3	B	146	Total	O	0	0
			146	146		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.87Å 63.59Å 73.40Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.30) 98.5 (20.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.259 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4856	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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 [i](#)

5.1 Standard geometry [i](#)

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	C	0.26	0/180	0.67	0/276
1	D	0.26	0/180	0.71	0/276
2	A	0.56	2/2126 (0.1%)	1.16	25/2896 (0.9%)
2	B	0.66	5/2116 (0.2%)	1.18	29/2883 (1.0%)
All	All	0.59	7/4602 (0.2%)	1.14	54/6331 (0.9%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	96	THR	CA-C	6.85	1.61	1.52
2	A	22	HIS	CB-CG	6.58	1.59	1.50
2	B	129	VAL	CA-C	6.35	1.58	1.52
2	B	130	PRO	CA-C	-6.13	1.44	1.52
2	A	277	GLN	N-CA	6.06	1.53	1.46
2	B	100	PRO	CA-C	-5.90	1.46	1.53
2	B	97	PRO	CA-C	-5.05	1.45	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	260	GLN	OE1-CD-NE2	-10.65	111.95	122.60
2	A	263	GLN	OE1-CD-NE2	-10.39	112.21	122.60
2	B	113	GLN	OE1-CD-NE2	-10.32	112.28	122.60
2	A	221	GLN	OE1-CD-NE2	-10.19	112.41	122.60
2	A	277	GLN	OE1-CD-NE2	-10.08	112.52	122.60
2	A	238	GLN	OE1-CD-NE2	-10.05	112.55	122.60
2	B	165	GLN	OE1-CD-NE2	-10.05	112.55	122.60
2	B	182	GLN	OE1-CD-NE2	-9.74	112.86	122.60
2	B	144	GLN	OE1-CD-NE2	-9.74	112.86	122.60
2	A	237	GLN	OE1-CD-NE2	-9.59	113.01	122.60
2	A	265	GLN	OE1-CD-NE2	-9.51	113.09	122.60
2	A	245	GLN	OE1-CD-NE2	-9.20	113.41	122.60
2	B	100	PRO	CA-N-CD	-8.62	99.94	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	111	PRO	CA-N-CD	-8.43	100.20	112.00
2	A	22	HIS	N-CA-C	-8.10	103.92	113.88
2	B	113	GLN	CG-CD-NE2	7.27	127.31	116.40
2	B	261	ILE	N-CA-C	7.08	118.33	107.99
2	B	97	PRO	CA-N-CD	-7.08	102.09	112.00
2	A	190	GLN	N-CA-C	-6.99	100.13	110.48
2	A	263	GLN	CG-CD-NE2	6.89	126.74	116.40
2	A	221	GLN	CG-CD-NE2	6.86	126.69	116.40
2	B	144	GLN	CG-CD-NE2	6.79	126.58	116.40
2	B	165	GLN	CG-CD-NE2	6.75	126.53	116.40
2	A	274	LYS	N-CA-C	-6.71	98.39	109.80
2	A	260	GLN	CG-CD-NE2	6.62	126.33	116.40
2	B	182	GLN	CG-CD-NE2	6.57	126.26	116.40
2	A	237	GLN	CG-CD-NE2	6.52	126.18	116.40
2	A	277	GLN	CG-CD-NE2	6.50	126.14	116.40
2	A	193	LYS	N-CA-C	6.41	119.08	111.71
2	A	238	GLN	CG-CD-NE2	6.38	125.97	116.40
2	A	261	ILE	N-CA-C	6.31	117.38	108.36
2	A	265	GLN	CG-CD-NE2	6.27	125.81	116.40
2	B	171	GLU	N-CA-C	6.18	119.59	109.76
2	A	245	GLN	CG-CD-NE2	6.14	125.60	116.40
2	B	175	PRO	CA-N-CD	-6.13	103.42	112.00
2	B	100	PRO	CB-CA-C	-6.08	102.79	112.27
2	B	48	LEU	N-CA-C	6.04	119.36	109.76
2	B	127	PRO	CA-C-N	-5.87	113.39	122.49
2	B	127	PRO	C-N-CA	-5.87	113.39	122.49
2	B	127	PRO	CA-N-CD	-5.79	103.89	112.00
2	B	131	ASN	N-CA-C	-5.78	102.77	109.93
2	A	146	TYR	N-CA-C	5.64	118.76	109.85
2	B	130	PRO	CA-N-CD	-5.63	104.12	112.00
2	B	111	PRO	CA-C-N	-5.56	115.09	122.98
2	B	111	PRO	C-N-CA	-5.56	115.09	122.98
2	A	96	THR	CA-C-N	5.54	125.47	119.76
2	A	96	THR	C-N-CA	5.54	125.47	119.76
2	B	29	PHE	CA-C-N	5.53	124.72	118.97
2	B	29	PHE	C-N-CA	5.53	124.72	118.97
2	B	189	PRO	N-CA-C	5.32	119.06	111.13
2	B	100	PRO	N-CA-CB	5.27	106.23	102.65
2	B	56	SER	N-CA-C	5.25	117.06	110.24
2	B	140	PRO	CB-CA-C	5.24	117.32	110.92
2	A	167	LEU	N-CA-C	5.11	117.59	111.71

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	C	161	0	92	5	0
1	D	161	0	92	0	0
2	A	2069	0	2080	63	0
2	B	2059	0	2072	82	0
3	A	238	0	0	7	0
3	B	146	0	0	6	0
3	C	12	0	0	0	0
3	D	10	0	0	0	0
All	All	4856	0	4336	149	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 17.

All (149) 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)
2:A:173:ARG:HH11	2:A:173:ARG:HB3	1.39	0.87
2:B:272:LEU:HD23	2:B:278:ARG:HD2	1.59	0.85
2:A:272:LEU:HD21	2:A:274:LYS:HE2	1.57	0.83
2:B:161:HIS:HD2	2:B:163:THR:H	1.25	0.80
2:A:71:ARG:NH2	2:A:173:ARG:H	1.79	0.79
2:A:173:ARG:HH11	2:A:173:ARG:CB	1.97	0.79
2:B:274:LYS:HD2	2:B:274:LYS:H	1.48	0.78
2:B:78:ILE:O	2:B:82:LEU:HD23	1.84	0.78
1:C:3:DT:H1'	1:C:4:DG:N7	2.00	0.77
2:A:173:ARG:HH11	2:A:173:ARG:CG	1.99	0.74
2:B:43:VAL:HG23	2:B:44:ARG:HE	1.50	0.74
2:B:75:LYS:NZ	2:B:176:GLU:HG3	2.02	0.73
2:B:62:LYS:HD2	2:B:62:LYS:H	1.55	0.72
2:A:173:ARG:HB3	2:A:173:ARG:NH1	2.05	0.72
2:B:61:ILE:HD11	2:B:117:GLU:HG3	1.70	0.72
2:B:101:VAL:HG12	2:B:102:LYS:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:MET:HE3	2:B:86:ILE:HD11	1.73	0.71
2:A:135:LEU:HG	2:A:220:LEU:HG	1.73	0.70
2:B:174:ASP:OD1	2:B:176:GLU:HG2	1.91	0.70
2:B:62:LYS:HD2	2:B:62:LYS:N	2.06	0.70
2:A:64:TYR:CE2	2:A:99:LEU:HD11	2.30	0.66
2:A:71:ARG:HH22	2:A:173:ARG:H	1.43	0.66
2:B:102:LYS:O	2:B:103:LYS:HG2	1.96	0.66
2:A:172:TRP:O	2:A:173:ARG:HD2	1.97	0.65
2:B:272:LEU:HG	2:B:274:LYS:HE3	1.77	0.65
2:A:273:LEU:N	2:A:273:LEU:HD23	2.12	0.64
2:A:145:TRP:NE1	2:A:264:LYS:HE3	2.13	0.63
2:B:274:LYS:HD2	2:B:274:LYS:N	2.14	0.62
2:A:23:MET:HE3	2:A:23:MET:H	1.63	0.62
2:A:174:ASP:OD1	2:A:176:GLU:HB3	2.01	0.60
2:A:245:GLN:HE21	2:A:249:ASN:HD21	1.48	0.60
2:A:173:ARG:HG2	3:A:449:HOH:O	2.01	0.60
2:B:101:VAL:CG1	2:B:102:LYS:H	2.15	0.60
2:A:272:LEU:O	2:A:278:ARG:N	2.32	0.60
2:A:173:ARG:HH11	2:A:173:ARG:HG3	1.67	0.60
2:A:83:ASP:OD1	2:B:161:HIS:HE1	1.85	0.59
2:A:132:PRO:O	2:A:136:LEU:HD13	2.01	0.59
2:B:161:HIS:CD2	2:B:163:THR:H	2.15	0.59
2:B:101:VAL:HG12	2:B:102:LYS:H	1.67	0.59
2:B:101:VAL:CG1	2:B:102:LYS:N	2.64	0.59
2:B:57:THR:HG22	3:B:289:HOH:O	2.04	0.58
2:B:237:GLN:O	2:B:241:ARG:HG3	2.03	0.58
2:B:82:LEU:HD22	2:B:87:LEU:HB2	1.84	0.58
1:C:6:DA:H4'	1:C:7:DT:OP1	2.03	0.58
1:C:1:DC:H2''	1:C:2:DA:C8	2.40	0.57
2:B:74:ILE:HG23	2:B:111:PRO:HG3	1.87	0.57
2:B:272:LEU:CG	2:B:274:LYS:HE3	2.35	0.56
2:A:161:HIS:HD2	2:A:163:THR:H	1.53	0.56
2:A:274:LYS:C	2:A:276:GLY:H	2.15	0.55
2:B:75:LYS:N	2:B:76:PRO:HD2	2.22	0.55
2:A:207:LEU:HD13	2:A:219:LEU:HD21	1.88	0.55
2:A:179:ILE:HD12	2:A:183:LEU:HD21	1.87	0.54
2:B:176:GLU:HB2	3:B:396:HOH:O	2.06	0.54
2:A:64:TYR:HE2	2:A:99:LEU:HD11	1.71	0.54
2:B:82:LEU:HD21	2:B:183:LEU:HD13	1.88	0.54
2:B:131:ASN:HB3	2:B:134:ASN:HD22	1.72	0.54
2:B:187:ARG:NH1	3:B:372:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:VAL:HG21	2:B:112:VAL:HG21	1.90	0.53
2:B:62:LYS:H	2:B:62:LYS:CD	2.16	0.53
2:A:277:GLN:O	2:A:278:ARG:OXT	2.27	0.53
2:B:22:HIS:HB3	2:B:25:TRP:CD1	2.43	0.53
2:A:161:HIS:CD2	2:A:163:THR:HG23	2.44	0.53
2:B:74:ILE:HD11	2:B:100:PRO:HA	1.91	0.53
2:B:80:ARG:O	2:B:84:GLN:HG3	2.09	0.53
2:A:245:GLN:HE21	2:A:249:ASN:ND2	2.07	0.53
2:A:145:TRP:CE2	2:A:264:LYS:HE3	2.44	0.52
2:B:227:LEU:C	2:B:227:LEU:HD23	2.34	0.52
2:A:75:LYS:HB3	2:A:76:PRO:HD3	1.91	0.52
2:A:120:LYS:HG3	3:A:318:HOH:O	2.10	0.52
1:C:3:DT:H1'	1:C:4:DG:C8	2.44	0.52
2:B:174:ASP:CG	2:B:176:GLU:HG2	2.34	0.52
2:B:177:MET:O	2:B:177:MET:HE3	2.09	0.51
2:A:273:LEU:HD23	2:A:273:LEU:H	1.73	0.51
2:B:39:MET:HE3	2:B:86:ILE:CD1	2.40	0.51
2:A:35:GLU:OE2	2:A:257:LYS:HG3	2.10	0.51
2:B:273:LEU:HB2	3:B:418:HOH:O	2.10	0.50
2:B:195:SER:HB2	2:B:196:PRO:HD3	1.93	0.50
2:A:161:HIS:CD2	2:A:163:THR:H	2.29	0.49
2:A:274:LYS:O	2:A:276:GLY:N	2.45	0.49
2:A:103:LYS:HB3	2:A:106:THR:OG1	2.13	0.49
2:A:173:ARG:NH1	3:A:450:HOH:O	2.45	0.49
2:A:57:THR:HG23	2:A:58:PRO:HD2	1.94	0.48
2:B:273:LEU:HB3	2:B:277:GLN:OE1	2.12	0.48
2:A:94:TRP:CE2	2:A:167:LEU:HD23	2.49	0.48
2:A:227:LEU:C	2:A:227:LEU:HD23	2.38	0.48
2:B:268:TYR:CE1	2:B:269:LEU:HD13	2.49	0.48
2:B:43:VAL:CG2	2:B:44:ARG:HE	2.22	0.48
2:B:274:LYS:C	2:B:276:GLY:H	2.22	0.48
2:A:272:LEU:CD2	2:A:274:LYS:HE2	2.36	0.47
2:B:41:LEU:C	2:B:41:LEU:HD23	2.39	0.47
2:A:71:ARG:NH2	2:A:173:ARG:N	2.54	0.47
2:B:102:LYS:HG2	2:B:103:LYS:N	2.29	0.47
2:B:68:GLN:O	2:B:72:LEU:HG	2.15	0.47
2:B:51:PRO:HD2	3:B:324:HOH:O	2.14	0.46
2:B:99:LEU:HD22	2:B:99:LEU:N	2.29	0.46
2:B:131:ASN:HB3	2:B:134:ASN:ND2	2.29	0.46
2:A:173:ARG:HE	2:A:180:SER:C	2.22	0.46
2:A:22:HIS:H	2:A:23:MET:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:245:GLN:NE2	2:A:249:ASN:HD21	2.14	0.45
2:B:176:GLU:N	2:B:176:GLU:OE1	2.49	0.45
2:A:69:GLU:H	2:A:69:GLU:CD	2.24	0.45
2:A:98:LEU:HD12	2:A:98:LEU:HA	1.84	0.45
2:B:61:ILE:HD11	2:B:117:GLU:CG	2.42	0.45
2:B:101:VAL:O	2:B:109:TYR:HD1	1.99	0.45
2:B:106:THR:HG23	2:B:107:ASN:N	2.32	0.45
2:B:273:LEU:HD23	2:B:273:LEU:N	2.31	0.45
2:A:166:PRO:HG3	3:A:302:HOH:O	2.16	0.45
2:A:236:CYS:SG	2:A:262:CYS:HA	2.55	0.45
2:B:75:LYS:HZ1	2:B:176:GLU:HG3	1.80	0.45
2:B:32:ALA:HB2	2:B:244:LEU:O	2.17	0.45
2:B:62:LYS:N	2:B:62:LYS:CD	2.72	0.45
2:B:211:ARG:NH1	2:B:219:LEU:HB3	2.33	0.44
2:A:272:LEU:HD21	2:A:274:LYS:CE	2.37	0.44
2:B:80:ARG:CZ	2:B:80:ARG:HB2	2.47	0.44
2:B:158:LEU:HD11	2:B:199:PHE:HA	1.98	0.44
2:B:136:LEU:HD12	2:B:271:TYR:CD2	2.53	0.44
2:A:52:LEU:HD21	2:A:167:LEU:HD21	1.98	0.44
2:A:173:ARG:CG	2:A:173:ARG:NH1	2.69	0.44
2:A:274:LYS:C	2:A:276:GLY:N	2.76	0.44
2:B:74:ILE:HG12	2:B:111:PRO:HD3	2.00	0.44
2:B:139:LEU:O	2:B:141:PRO:HD3	2.18	0.44
2:B:187:ARG:CG	2:B:187:ARG:HH11	2.31	0.44
2:B:187:ARG:HH11	2:B:187:ARG:HG2	1.82	0.44
2:B:106:THR:HG23	2:B:107:ASN:H	1.83	0.43
2:A:165:GLN:N	2:A:166:PRO:CD	2.81	0.43
2:B:257:LYS:HD3	3:B:295:HOH:O	2.18	0.43
2:A:223:VAL:HG12	2:A:224:ASP:N	2.34	0.43
2:A:272:LEU:CD2	2:A:274:LYS:CE	2.97	0.43
2:B:77:HIS:O	2:B:81:LEU:HD22	2.19	0.42
2:B:102:LYS:HD2	2:B:102:LYS:C	2.44	0.42
2:B:206:ASP:HB3	2:B:250:LEU:HD13	2.01	0.42
2:A:173:ARG:NH1	2:A:173:ARG:HG3	2.32	0.42
2:B:75:LYS:HZ3	2:B:176:GLU:HG3	1.81	0.42
2:B:133:TYR:C	2:B:135:LEU:H	2.28	0.42
2:B:273:LEU:HD23	2:B:273:LEU:H	1.85	0.42
2:A:57:THR:HG22	3:A:281:HOH:O	2.19	0.42
2:B:133:TYR:C	2:B:135:LEU:N	2.78	0.42
2:A:29:PHE:O	2:A:33:TRP:CD1	2.73	0.42
2:A:103:LYS:HA	2:A:104:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:LEU:CD2	2:B:274:LYS:HE3	2.50	0.42
2:B:218:ILE:HB	2:B:229:ALA:HB3	2.01	0.41
2:B:175:PRO:HB2	2:B:176:GLU:OE1	2.19	0.41
2:B:38:GLY:O	2:B:253:ARG:HG3	2.20	0.41
2:B:70:ALA:C	2:B:72:LEU:H	2.28	0.41
2:A:20:GLY:N	3:A:438:HOH:O	2.54	0.40
2:A:195:SER:HB2	2:A:196:PRO:HD3	2.03	0.40
2:B:103:LYS:HB2	2:B:108:ASP:HB2	2.04	0.40
1:C:3:DT:H4'	1:C:4:DG:OP1	2.22	0.40
2:A:177:MET:HG3	3:A:344:HOH:O	2.21	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	
2	A	257/259 (99%)	248 (96%)	7 (3%)	2 (1%)	16	20
2	B	255/259 (98%)	237 (93%)	17 (7%)	1 (0%)	30	38
All	All	512/518 (99%)	485 (95%)	24 (5%)	3 (1%)	21	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	GLU
2	B	223	VAL
2	A	223	VAL

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	
2	A	227/227 (100%)	213 (94%)	14 (6%)	16	24
2	B	226/227 (100%)	209 (92%)	17 (8%)	12	17
All	All	453/454 (100%)	422 (93%)	31 (7%)	14	20

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	21	SER
2	A	23	MET
2	A	68	GLN
2	A	81	LEU
2	A	96	THR
2	A	102	LYS
2	A	103	LYS
2	A	116	ARG
2	A	124	ASP
2	A	147	THR
2	A	173	ARG
2	A	269	LEU
2	A	273	LEU
2	A	275	GLU
2	B	57	THR
2	B	62	LYS
2	B	81	LEU
2	B	96	THR
2	B	97	PRO
2	B	100	PRO
2	B	102	LYS
2	B	111	PRO
2	B	130	PRO
2	B	132	PRO
2	B	140	PRO
2	B	166	PRO
2	B	173	ARG

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Mol	Chain	Res	Type
2	B	176	GLU
2	B	220	LEU
2	B	274	LYS
2	B	277	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	31	GLN
2	A	68	GLN
2	A	84	GLN
2	A	91	GLN
2	A	126	HIS
2	A	134	ASN
2	A	161	HIS
2	A	213	GLN
2	A	249	ASN
2	A	277	GLN
2	B	22	HIS
2	B	68	GLN
2	B	107	ASN
2	B	126	HIS
2	B	134	ASN
2	B	144	GLN
2	B	161	HIS
2	B	190	GLN
2	B	204	HIS
2	B	245	GLN
2	B	249	ASN
2	B	265	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 [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	C	8/8 (100%)	0.90	0 100 100	39, 53, 64, 77	0
1	D	8/8 (100%)	-0.25	0 100 100	31, 45, 46, 52	0
2	A	259/259 (100%)	-0.09	7 (2%) 56 58	13, 24, 52, 72	0
2	B	257/259 (99%)	0.41	21 (8%) 17 19	15, 34, 74, 96	0
All	All	532/534 (99%)	0.16	28 (5%) 32 34	13, 30, 67, 96	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	20	GLY	5.1
2	B	133	TYR	4.7
2	B	109	TYR	4.5
2	B	276	GLY	4.3
2	A	21	SER	4.0
2	B	106	THR	4.0
2	A	276	GLY	3.8
2	B	104	PRO	3.6
2	B	273	LEU	3.2
2	B	102	LYS	3.1
2	A	277	GLN	2.9
2	B	277	GLN	2.9
2	B	175	PRO	2.7
2	B	105	GLY	2.6
2	B	99	LEU	2.6
2	A	275	GLU	2.6
2	B	177	MET	2.4
2	B	275	GLU	2.4
2	B	103	LYS	2.3
2	B	138	GLY	2.3
2	B	278	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	179	ILE	2.3
2	B	74	ILE	2.2
2	B	69	GLU	2.2
2	B	22	HIS	2.0
2	A	64	TYR	2.0
2	A	23	MET	2.0
2	B	130	PRO	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.