



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:04 PM UTC

PDB ID : 1MUH / pdb_00001muh
Title : CRYSTAL STRUCTURE OF TN5 TRANSPOSASE COMPLEXED WITH
TRANSPOSON END DNA
Authors : Thoden, J.B.; Holden, H.M.; Davies, D.R.; Goryshin, I.Y.; Reznikoff, W.S.;
Rayment, I.
Deposited on : 2002-09-23
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

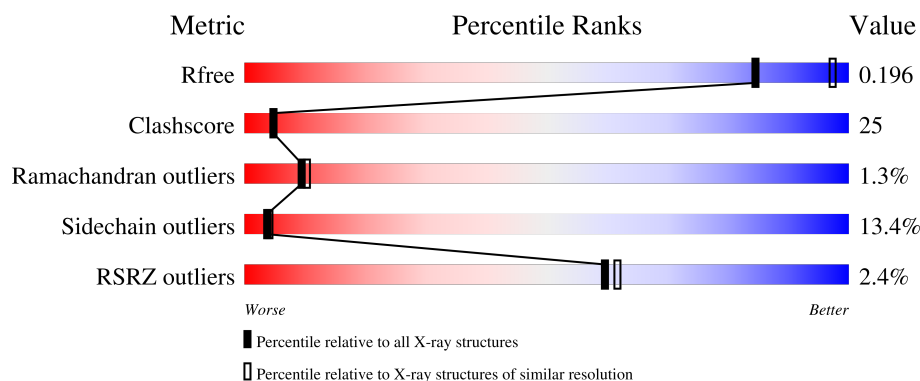
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

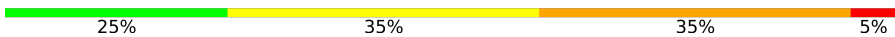
The reported resolution of this entry is 2.30 Å.

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))
R_{free}	180053	6319 (2.30-2.30)
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	B	20	
2	C	20	
3	A	481	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4691 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 TRANSFERRED STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	20	Total	C	N	O	P	0	0	0
			413	198	78	118	19			

- Molecule 2 is a DNA chain called DNA NON-TRANSFERRED STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			401	194	70	118	19			

- Molecule 3 is a protein called Tn5 transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	455	Total	C	N	O	S	0	1	0
			3569	2250	653	654	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	LYS	GLU	engineered mutation	UNP Q46731
A	56	ALA	MET	engineered mutation	UNP Q46731
A	372	PRO	LEU	engineered mutation	UNP Q46731
A	477	GLY	-	cloning artifact	UNP Q46731

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

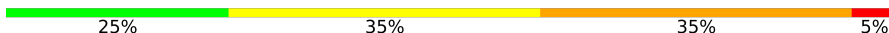
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	27	Total 27	O 27	0	0
6	C	22	Total 22	O 22	0	0
6	A	257	Total 257	O 257	0	0

3 Residue-property plots

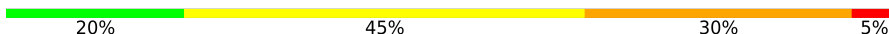
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA TRANSFERRED STRAND

Chain B: 



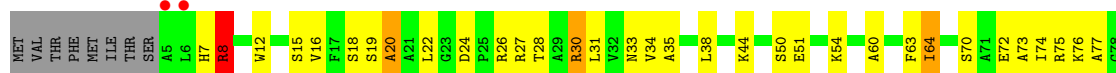
• Molecule 2: DNA NON-TRANSFERRED STRAND

Chain C: 



• Molecule 3: Tn5 transposase

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.70Å 113.70Å 228.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.30) 99.7 (30.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 2.31Å)	Xtriage
Refinement program	TNT, CNS	Depositor
R, R_{free}	0.204 , 0.267 0.199 , 0.196	Depositor DCC
R_{free} test set	4023 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 147.7	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	0.95	EDS
Total number of atoms	4691	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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](#)

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

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	B	0.75	0/464	2.18	24/716 (3.4%)
2	C	0.75	0/448	1.96	21/688 (3.1%)
3	A	1.27	2/3642 (0.1%)	1.92	77/4914 (1.6%)
All	All	1.19	2/4554 (0.0%)	1.96	122/6318 (1.9%)

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	B	0	1
2	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	250	ARG	NE-CZ	5.38	1.39	1.33
3	A	64	ILE	CA-CB	-5.05	1.48	1.54

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	DA	C4-N9-C1'	-19.41	97.94	127.05
1	B	19	DA	C8-N9-C1'	14.72	149.14	127.05
1	B	1	DG	C4-N9-C1'	-13.71	106.44	127.00
1	B	1	DG	C8-N9-C1'	12.61	145.92	127.00
2	C	4	DA	C8-N9-C1'	11.80	144.75	127.05
2	C	4	DA	C4-N9-C1'	-10.98	110.57	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	DA	C4-N9-C1'	-10.02	112.02	127.05
3	A	7	HIS	N-CA-C	9.73	123.34	110.88
2	C	18	DG	C4-N9-C1'	-9.49	112.76	127.00
3	A	288	ASN	O-C-N	9.49	125.89	121.53
3	A	64	ILE	CA-C-N	-9.28	108.12	122.60
3	A	64	ILE	C-N-CA	-9.28	108.12	122.60
2	C	2	DT	C6-N1-C1'	-9.05	105.77	119.35
3	A	276	ASN	N-CA-C	-8.95	98.89	111.24
1	B	2	DA	C8-N9-C1'	8.79	140.23	127.05
3	A	89	PHE	O-C-N	8.78	129.35	121.80
3	A	156	ASP	CA-CB-CG	-8.45	104.15	112.60
1	B	5	DT	C2-N1-C1'	-8.44	106.69	119.35
2	C	2	DT	C5'-C4'-C3'	8.37	127.45	114.90
1	B	4	DT	C5'-C4'-C3'	-8.30	102.45	114.90
2	C	15	DC	P-O5'-C5'	-8.30	107.55	120.00
2	C	18	DG	P-O5'-C5'	-8.22	107.67	120.00
3	A	321	HIS	CA-CB-CG	-8.05	105.75	113.80
2	C	18	DG	C8-N9-C1'	7.90	138.85	127.00
2	C	2	DT	C2-N1-C1'	7.72	130.94	119.35
3	A	288	ASN	CA-CB-CG	-7.72	104.88	112.60
1	B	5	DT	P-O3'-C3'	7.63	131.64	120.20
3	A	395	THR	O-C-N	7.54	130.24	122.09
1	B	4	DT	C2-N1-C1'	7.54	130.66	119.35
3	A	89	PHE	CA-C-N	7.53	129.25	119.84
3	A	89	PHE	C-N-CA	7.53	129.25	119.84
3	A	307	GLU	N-CA-C	7.47	120.14	111.02
1	B	4	DT	C6-N1-C1'	-7.11	108.68	119.35
1	B	14	DG	P-O5'-C5'	-7.06	109.40	120.00
3	A	289	PRO	O-C-N	6.99	124.44	121.15
3	A	256	ARG	CA-CB-CG	-6.95	100.21	114.10
3	A	396	VAL	N-CA-C	6.87	117.84	111.45
3	A	461	ASP	CA-CB-CG	6.82	119.42	112.60
3	A	83	VAL	CB-CA-C	-6.81	103.26	111.97
3	A	151	PRO	CB-CA-C	-6.67	102.70	111.23
1	B	13	DA	C4-N9-C1'	-6.66	117.06	127.05
1	B	19	DA	O5'-C5'-C4'	6.66	120.79	110.80
3	A	173	ARG	CB-CA-C	-6.64	100.19	110.81
1	B	19	DA	N9-C1'-C2'	-6.61	103.58	113.50
2	C	15	DC	C5'-C4'-O4'	-6.49	99.67	109.40
2	C	11	DT	N1-C1'-C2'	-6.47	103.80	113.50
3	A	391	GLN	CA-C-N	-6.43	111.03	122.74
3	A	391	GLN	C-N-CA	-6.43	111.03	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	DC	P-O5'-C5'	-6.42	110.36	120.00
3	A	125	TRP	N-CA-C	-6.40	99.28	109.59
3	A	95	ILE	N-CA-CB	6.38	120.08	110.13
3	A	400	ASP	CA-C-N	-6.36	112.17	120.44
3	A	400	ASP	C-N-CA	-6.36	112.17	120.44
1	B	9	DT	C6-N1-C1'	-6.30	109.91	119.35
3	A	256	ARG	N-CA-CB	6.24	120.16	110.12
1	B	5	DT	C6-N1-C1'	6.22	128.69	119.35
2	C	5	DC	P-O5'-C5'	-6.19	110.71	120.00
3	A	395	THR	N-CA-C	-6.07	104.59	111.14
1	B	13	DA	C8-N9-C1'	6.05	136.13	127.05
3	A	133	GLU	CB-CA-C	5.97	119.59	109.80
3	A	241	ILE	CA-C-O	5.96	122.67	119.15
3	A	93	LEU	CA-C-N	-5.94	114.35	123.14
3	A	93	LEU	C-N-CA	-5.94	114.35	123.14
2	C	1	DC	C2-N1-C1'	5.92	128.58	119.70
3	A	147	TRP	CB-CA-C	-5.91	99.50	109.50
1	B	17	DT	C4'-C3'-O3'	-5.90	101.15	110.00
3	A	153	ASP	O-C-N	5.88	127.82	121.12
3	A	280	ASN	CA-CB-CG	-5.85	106.75	112.60
1	B	11	DT	P-O3'-C3'	-5.83	111.45	120.20
2	C	1	DC	C6-N1-C1'	-5.83	110.96	119.70
3	A	128	SER	CB-CA-C	-5.82	97.86	109.33
2	C	11	DT	P-O3'-C3'	5.81	128.91	120.20
2	C	8	DT	O4'-C1'-N1	-5.79	99.72	108.40
2	C	18	DG	P-O3'-C3'	-5.77	111.55	120.20
3	A	422	LEU	N-CA-C	-5.76	105.00	111.28
3	A	398	THR	CA-C-N	5.75	125.87	119.32
3	A	398	THR	C-N-CA	5.75	125.87	119.32
2	C	10	DA	P-O5'-C5'	-5.72	111.41	120.00
3	A	85	LEU	CB-CA-C	-5.71	101.32	110.79
1	B	6	DG	O4'-C1'-N9	-5.69	99.87	108.40
3	A	441	THR	N-CA-C	-5.62	106.42	113.72
3	A	106	GLN	N-CA-C	5.61	117.84	111.11
3	A	367	ARG	CD-NE-CZ	-5.58	116.58	124.40
1	B	19	DA	C4'-C3'-O3'	5.56	118.33	110.00
3	A	63	PHE	CA-C-N	-5.55	112.36	121.19
3	A	63	PHE	C-N-CA	-5.55	112.36	121.19
3	A	230	ASN	CA-CB-CG	-5.55	107.05	112.60
3	A	252	LYS	N-CA-CB	5.47	118.78	109.87
3	A	250	ARG	CD-NE-CZ	5.45	132.03	124.40
3	A	169	ALA	CA-C-N	-5.45	112.98	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	169	ALA	C-N-CA	-5.45	112.98	120.28
2	C	10	DA	N9-C1'-C2'	-5.42	105.36	113.50
3	A	262	SER	CA-C-N	-5.41	114.83	122.94
3	A	262	SER	C-N-CA	-5.41	114.83	122.94
3	A	456	LEU	CA-C-N	-5.38	112.00	120.60
3	A	456	LEU	C-N-CA	-5.38	112.00	120.60
3	A	33	ASN	O-C-N	5.34	127.57	122.07
3	A	239	ILE	CA-C-N	-5.30	115.14	122.30
3	A	239	ILE	C-N-CA	-5.30	115.14	122.30
3	A	118	GLN	CB-CA-C	-5.30	101.77	110.72
3	A	351	ARG	CA-C-O	5.30	126.06	119.97
3	A	344	GLU	N-CA-C	5.28	119.35	113.02
3	A	245	GLY	N-CA-C	-5.27	103.11	112.54
3	A	427	MET	CA-CB-CG	-5.21	103.68	114.10
3	A	8	ARG	CD-NE-CZ	5.21	131.69	124.40
3	A	226	ASP	O-C-N	5.20	127.63	122.12
3	A	465	ALA	O-C-N	5.19	127.70	122.09
3	A	435	PHE	N-CA-C	5.19	117.87	110.24
3	A	406	GLY	CA-C-N	-5.15	112.98	120.29
3	A	406	GLY	C-N-CA	-5.15	112.98	120.29
3	A	224	LEU	CA-C-N	-5.14	113.60	120.54
3	A	224	LEU	C-N-CA	-5.14	113.60	120.54
3	A	182	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	13	DA	P-O3'-C3'	-5.05	112.62	120.20
3	A	151	PRO	N-CA-CB	5.04	107.74	103.35
3	A	20	ALA	CA-C-N	-5.03	114.61	122.16
3	A	20	ALA	C-N-CA	-5.03	114.61	122.16
1	B	3	DC	C2-N1-C1'	-5.03	112.16	119.70
3	A	270	ILE	CB-CA-C	-5.03	101.43	110.48
3	A	232	PRO	CB-CA-C	-5.02	104.40	110.98
2	C	2	DT	C2'-C3'-O3'	-5.01	103.98	111.50
3	A	463	PHE	N-CA-C	-5.01	105.51	110.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	19	DA	Sidechain
2	C	11	DT	Sidechain

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	B	413	0	227	12	0
2	C	401	0	228	22	0
3	A	3569	0	3601	185	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	257	0	0	7	0
6	B	27	0	0	0	0
6	C	22	0	0	3	0
All	All	4691	0	4056	213	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 25.

All (213) 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)
3:A:189:ARG:HB3	3:A:212:LYS:HB2	1.22	1.19
1:B:4:DT:H5''	1:B:4:DT:H6	1.31	0.94
3:A:194:HIS:CD2	3:A:274:GLN:HG3	2.02	0.94
3:A:194:HIS:CE1	3:A:274:GLN:HB2	2.08	0.88
3:A:472:GLN:HG3	3:A:474:ILE:HD11	1.55	0.88
3:A:189:ARG:CB	3:A:212:LYS:HB2	2.04	0.88
3:A:472:GLN:HG3	3:A:474:ILE:CD1	2.07	0.82
1:B:4:DT:H5''	1:B:4:DT:C6	2.16	0.80
2:C:14:DA:H1'	2:C:15:DC:H5''	1.61	0.80
3:A:189:ARG:HB3	3:A:212:LYS:CB	2.10	0.79
3:A:308:SER:OG	3:A:311:GLN:HG3	1.84	0.77
3:A:107:VAL:HG23	3:A:346:PRO:HD3	1.65	0.77
3:A:370:PHE:HE2	3:A:396:VAL:HG11	1.51	0.76
3:A:367:ARG:HB2	3:A:449:LEU:HD12	1.67	0.75
3:A:8:ARG:HH12	3:A:401:GLU:CD	1.97	0.72
2:C:14:DA:H1'	2:C:15:DC:C5'	2.20	0.71
3:A:22:LEU:HD12	3:A:28:THR:HA	1.73	0.70
2:C:5:DC:OP1	3:A:367:ARG:NH2	2.25	0.70
3:A:473:GLY:C	3:A:474:ILE:HG13	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:DA:H2'	6:C:195:HOH:O	1.91	0.70
3:A:106:GLN:O	3:A:109:GLU:HG3	1.90	0.70
3:A:370:PHE:CE2	3:A:396:VAL:HG11	2.26	0.69
3:A:426:TYR:HD2	3:A:427:MET:HG2	1.56	0.69
3:A:468:ASP:O	3:A:472:GLN:HG2	1.93	0.68
3:A:414:LYS:O	3:A:417:GLU:HG2	1.93	0.68
3:A:80:MET:HE1	3:A:175:ARG:HD3	1.77	0.67
3:A:106:GLN:HG3	6:A:678:HOH:O	1.94	0.67
3:A:260:LYS:NZ	3:A:260:LYS:HB3	2.10	0.66
3:A:75:ARG:NH2	3:A:350:GLU:OE2	2.28	0.66
3:A:398:THR:OG1	3:A:401:GLU:HG2	1.96	0.66
3:A:244:LYS:HE2	3:A:246:VAL:CG1	2.27	0.65
3:A:20:ALA:HB3	3:A:28:THR:HG23	1.78	0.65
3:A:464:LEU:N	3:A:464:LEU:HD23	2.12	0.63
3:A:188:ASP:HB2	6:A:579:HOH:O	2.00	0.62
3:A:466:ALA:O	3:A:467:LYS:C	2.41	0.62
3:A:22:LEU:HD12	3:A:28:THR:CA	2.30	0.61
3:A:231:GLN:HB3	3:A:232:PRO:HD2	1.83	0.60
3:A:20:ALA:HA	3:A:77:ALA:HB2	1.83	0.60
3:A:473:GLY:O	3:A:474:ILE:HG13	2.01	0.59
3:A:194:HIS:NE2	3:A:274:GLN:HG3	2.18	0.59
3:A:31:LEU:HD12	3:A:31:LEU:O	2.04	0.58
3:A:392:SER:O	3:A:395:THR:OG1	2.18	0.58
3:A:70:SER:O	3:A:74:ILE:HG13	2.04	0.58
3:A:476:ILE:HG12	3:A:477:GLY:H	1.69	0.58
3:A:84:LYS:O	3:A:87:GLN:HB2	2.04	0.58
3:A:398:THR:O	3:A:402:CYS:HB2	2.04	0.58
3:A:91:GLU:HB3	3:A:134:ALA:HB3	1.84	0.57
2:C:14:DA:C1'	2:C:15:DC:H5''	2.31	0.57
3:A:107:VAL:CG2	3:A:346:PRO:HD3	2.34	0.57
3:A:426:TYR:CE1	3:A:449:LEU:HD11	2.40	0.57
3:A:193:ILE:HG22	3:A:196:TYR:H	1.70	0.56
3:A:314:ARG:HA	6:A:675:HOH:O	2.03	0.56
3:A:201:LEU:O	3:A:202:ALA:C	2.46	0.56
3:A:194:HIS:NE2	3:A:274:GLN:HB2	2.21	0.55
3:A:8:ARG:NH2	3:A:401:GLU:OE2	2.35	0.55
3:A:425:ALA:O	3:A:429:ILE:HG13	2.07	0.54
3:A:173:ARG:HA	3:A:180:MET:CG	2.37	0.54
3:A:112:GLY:O	3:A:122:ARG:HB3	2.08	0.54
3:A:398:THR:HB	3:A:399:PRO:HD2	1.89	0.54
3:A:244:LYS:HE2	3:A:246:VAL:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:DT:H3'	2:C:3:DG:H5'	1.90	0.53
3:A:104:ARG:HG2	3:A:121:SER:OG	2.07	0.53
3:A:275:GLY:O	3:A:276:ASN:C	2.48	0.53
3:A:401:GLU:O	3:A:402:CYS:C	2.51	0.53
3:A:81:GLN:HA	3:A:81:GLN:HE21	1.73	0.53
2:C:18:DG:C2'	2:C:19:DT:H72	2.39	0.53
3:A:90:PRO:O	3:A:182:ASN:HB3	2.09	0.53
3:A:81:GLN:HA	3:A:81:GLN:NE2	2.24	0.52
3:A:246:VAL:HG23	3:A:254:LYS:HG2	1.90	0.52
3:A:83:VAL:O	3:A:86:ALA:HB3	2.09	0.52
3:A:472:GLN:HG3	3:A:474:ILE:HD12	1.89	0.52
2:C:17:DA:H8	6:C:195:HOH:O	1.93	0.52
3:A:460:LEU:O	3:A:463:PHE:HB3	2.11	0.51
3:A:270:ILE:CG1	3:A:279:LEU:HD23	2.40	0.51
3:A:466:ALA:C	3:A:470:MET:HE3	2.35	0.51
2:C:18:DG:H2'	2:C:19:DT:H72	1.93	0.51
3:A:133:GLU:O	3:A:137:PHE:HA	2.10	0.51
3:A:275:GLY:CA	3:A:277:ILE:HG23	2.40	0.51
3:A:437:ASP:OD2	3:A:440:ARG:HA	2.11	0.51
3:A:24:ASP:OD1	3:A:26:ARG:HB2	2.10	0.50
3:A:270:ILE:HD11	3:A:279:LEU:HD21	1.93	0.50
3:A:466:ALA:O	3:A:467:LYS:O	2.30	0.50
3:A:247:VAL:HG12	3:A:248:ASP:N	2.25	0.50
3:A:280:ASN:HB3	3:A:306:VAL:HG21	1.93	0.50
3:A:164:LYS:O	3:A:165:TRP:C	2.53	0.49
3:A:189:ARG:HG3	6:A:579:HOH:O	2.13	0.49
3:A:427:MET:O	3:A:431:ARG:HG3	2.11	0.49
3:A:116:SER:O	3:A:119:ASP:HB2	2.12	0.49
3:A:191:ALA:O	3:A:193:ILE:N	2.46	0.49
3:A:314:ARG:O	3:A:318:ILE:HG13	2.13	0.49
3:A:300:LEU:C	3:A:301:LEU:HD23	2.37	0.49
1:B:19:DA:H2'	1:B:20:DG:O4'	2.13	0.48
1:B:1:DG:H2''	1:B:2:DA:OP2	2.13	0.48
3:A:469:LEU:HA	3:A:474:ILE:HD12	1.95	0.48
3:A:163:GLY:HA2	3:A:166:LEU:HD12	1.95	0.48
3:A:50:SER:O	3:A:51:GLU:C	2.55	0.48
3:A:272:LEU:O	3:A:276:ASN:HA	2.14	0.48
3:A:31:LEU:HD12	3:A:31:LEU:C	2.38	0.48
3:A:280:ASN:HB3	3:A:306:VAL:CG2	2.44	0.48
3:A:437:ASP:CG	3:A:440:ARG:HA	2.39	0.48
3:A:19:SER:O	3:A:20:ALA:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:288:ASN:N	3:A:289:PRO:HD3	2.29	0.48
3:A:423:GLN:O	3:A:424:TRP:C	2.55	0.48
2:C:20:DC:O5'	2:C:20:DC:H2'	2.13	0.47
3:A:95:ILE:O	3:A:129:VAL:HA	2.14	0.47
1:B:6:DG:H2''	1:B:7:DT:O5'	2.14	0.47
3:A:111:LEU:HD13	3:A:123:GLY:HA2	1.96	0.47
3:A:153:ASP:O	3:A:156:ASP:HB2	2.15	0.47
3:A:246:VAL:HG23	3:A:254:LYS:CG	2.45	0.47
3:A:285:GLU:HG3	3:A:297:LYS:HB2	1.97	0.47
3:A:404:LEU:O	3:A:405:LEU:C	2.56	0.47
3:A:476:ILE:CG1	3:A:477:GLY:N	2.77	0.47
3:A:200:LYS:HA	3:A:200:LYS:HD2	1.75	0.47
3:A:200:LYS:NZ	3:A:205:GLU:HB3	2.30	0.47
1:B:20:DG:N3	3:A:323:TRP:HH2	2.13	0.47
3:A:144:HIS:ND1	6:A:497:HOH:O	2.35	0.47
3:A:241:ILE:CD1	3:A:261:ALA:HB2	2.45	0.47
3:A:405:LEU:HD21	3:A:428:ALA:HB3	1.97	0.47
3:A:467:LYS:O	3:A:468:ASP:C	2.56	0.47
3:A:30:ARG:HG2	6:A:488:HOH:O	2.15	0.46
3:A:430:ALA:HA	3:A:449:LEU:HD23	1.96	0.46
1:B:2:DA:H2''	1:B:3:DC:OP2	2.14	0.46
3:A:476:ILE:HG12	3:A:477:GLY:N	2.30	0.46
3:A:114:LEU:HD12	3:A:122:ARG:HA	1.98	0.46
3:A:181:SER:HA	6:A:626:HOH:O	2.14	0.46
3:A:197:LEU:O	3:A:198:GLN:C	2.58	0.46
3:A:324:ARG:O	3:A:324:ARG:HG3	2.13	0.46
3:A:194:HIS:O	3:A:195:ALA:C	2.54	0.46
3:A:474:ILE:HG22	3:A:475:LYS:N	2.31	0.46
3:A:467:LYS:O	3:A:470:MET:HG2	2.15	0.46
2:C:2:DT:H73	3:A:263:LEU:CD2	2.45	0.46
2:C:18:DG:C2'	2:C:19:DT:C7	2.95	0.45
3:A:114:LEU:HD11	3:A:122:ARG:C	2.41	0.45
2:C:14:DA:C2'	2:C:15:DC:H5''	2.45	0.45
3:A:260:LYS:NZ	3:A:260:LYS:CB	2.79	0.45
2:C:11:DT:H6	2:C:11:DT:H2'	1.43	0.45
3:A:418:LYS:O	3:A:420:GLY:N	2.50	0.45
3:A:12:TRP:O	3:A:15:SER:OG	2.29	0.45
3:A:92:LEU:HD23	3:A:133:GLU:HA	1.99	0.45
3:A:196:TYR:O	3:A:197:LEU:C	2.60	0.45
3:A:288:ASN:N	3:A:289:PRO:CD	2.79	0.45
3:A:241:ILE:HB	3:A:259:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:ILE:HG12	3:A:279:LEU:HD23	1.98	0.45
3:A:275:GLY:HA3	3:A:277:ILE:HG23	1.99	0.45
2:C:18:DG:H2''	2:C:19:DT:C7	2.47	0.45
3:A:70:SER:O	3:A:73:ALA:HB3	2.16	0.45
2:C:4:DA:H2''	2:C:5:DC:O5'	2.18	0.44
3:A:398:THR:H	3:A:401:GLU:HG3	1.82	0.44
3:A:16:VAL:HA	3:A:81:GLN:HG2	1.99	0.44
3:A:30:ARG:HA	3:A:30:ARG:HD3	1.78	0.44
3:A:304:GLU:HA	3:A:305:PRO:HD2	1.74	0.44
1:B:12:DA:OP2	3:A:440:ARG:NH1	2.44	0.44
3:A:60:ALA:O	3:A:64:ILE:HG23	2.17	0.44
3:A:164:LYS:CG	3:A:165:TRP:N	2.79	0.44
3:A:399:PRO:O	3:A:403:GLN:HB2	2.17	0.44
3:A:173:ARG:O	3:A:174:LEU:C	2.58	0.44
1:B:1:DG:H5'	1:B:1:DG:C8	2.53	0.44
3:A:153:ASP:OD1	3:A:154:PRO:HD2	2.18	0.44
2:C:10:DA:H2'	2:C:11:DT:H71	2.00	0.43
3:A:246:VAL:CG2	3:A:254:LYS:HG3	2.48	0.43
3:A:228:LEU:HD12	3:A:299:LEU:HD11	2.00	0.43
3:A:275:GLY:C	3:A:277:ILE:HG23	2.43	0.43
3:A:38:LEU:HD23	3:A:38:LEU:HA	1.79	0.43
3:A:264:SER:O	3:A:284:ALA:HA	2.18	0.43
3:A:398:THR:H	3:A:401:GLU:CG	2.31	0.43
3:A:418:LYS:O	3:A:419:ALA:C	2.57	0.43
2:C:15:DC:H5'	2:C:15:DC:C6	2.53	0.43
3:A:8:ARG:NH1	3:A:401:GLU:OE2	2.50	0.43
3:A:274:GLN:C	3:A:276:ASN:H	2.26	0.43
3:A:468:ASP:OD1	3:A:472:GLN:OE1	2.37	0.43
3:A:76:LYS:O	3:A:77:ALA:C	2.59	0.43
3:A:239:ILE:HD11	3:A:296:LEU:CD1	2.49	0.43
3:A:333:LYS:O	3:A:334:THR:C	2.59	0.43
3:A:467:LYS:O	3:A:469:LEU:N	2.52	0.43
3:A:28:THR:O	3:A:31:LEU:HB3	2.19	0.43
3:A:176:MET:HE3	3:A:179:MET:HB3	1.99	0.43
3:A:272:LEU:HB2	3:A:277:ILE:HG12	2.00	0.43
3:A:270:ILE:HD11	3:A:279:LEU:CD2	2.48	0.43
3:A:197:LEU:HD23	3:A:197:LEU:HA	1.80	0.42
3:A:114:LEU:HD12	3:A:122:ARG:CA	2.49	0.42
3:A:274:GLN:C	3:A:276:ASN:N	2.77	0.42
3:A:200:LYS:HZ1	3:A:205:GLU:HB3	1.84	0.42
3:A:273:LYS:CG	3:A:274:GLN:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:469:LEU:O	3:A:474:ILE:HD12	2.19	0.42
3:A:12:TRP:CE2	3:A:362:ARG:HD2	2.55	0.42
3:A:272:LEU:HD23	3:A:272:LEU:HA	1.71	0.42
3:A:188:ASP:HA	3:A:319:TYR:OH	2.18	0.42
3:A:79:ALA:O	3:A:82:THR:N	2.52	0.42
3:A:243:GLN:NE2	3:A:255:ASN:OD1	2.44	0.42
3:A:125:TRP:HB2	3:A:148:TRP:CE2	2.55	0.42
3:A:22:LEU:HD12	3:A:28:THR:N	2.35	0.41
3:A:194:HIS:O	3:A:198:GLN:HB2	2.19	0.41
3:A:246:VAL:HG22	3:A:254:LYS:O	2.21	0.41
1:B:12:DA:C2	2:C:10:DA:C2	3.08	0.41
2:C:14:DA:C2'	2:C:15:DC:C5'	2.98	0.41
3:A:27:ARG:O	3:A:28:THR:C	2.62	0.41
3:A:87:GLN:HA	3:A:179:MET:SD	2.60	0.41
3:A:173:ARG:HA	3:A:180:MET:HG3	2.03	0.41
3:A:397:LEU:HB3	3:A:401:GLU:HG3	2.01	0.41
3:A:267:SER:HB2	3:A:306:VAL:HB	2.03	0.41
1:B:13:DA:H2''	1:B:14:DG:C8	2.56	0.41
2:C:16:DA:H2''	6:C:195:HOH:O	2.21	0.41
3:A:169:ALA:O	3:A:170:ALA:C	2.59	0.41
3:A:224:LEU:O	3:A:225:TYR:C	2.58	0.41
3:A:247:VAL:CG1	3:A:248:ASP:N	2.83	0.41
3:A:291:LYS:HE2	3:A:291:LYS:HB2	1.72	0.41
1:B:2:DA:H1'	1:B:3:DC:H5'	2.03	0.41
3:A:111:LEU:HB3	3:A:123:GLY:HA2	2.03	0.40
3:A:469:LEU:N	3:A:469:LEU:HD23	2.29	0.40
2:C:5:DC:O3'	3:A:445:SER:HB3	2.21	0.40
3:A:27:ARG:HH11	3:A:27:ARG:HD2	1.73	0.40
3:A:34:VAL:O	3:A:35:ALA:C	2.65	0.40
3:A:263:LEU:N	3:A:263:LEU:HD12	2.36	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	
3	A	452/481 (94%)	423 (94%)	23 (5%)	6 (1%)	9	10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	274	GLN
3	A	192	ASP
3	A	468	ASP
3	A	467	LYS
3	A	473	GLY
3	A	292	GLY

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	
3	A	367/393 (93%)	318 (87%)	49 (13%)	4	4

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	8	ARG
3	A	18	SER
3	A	30	ARG
3	A	44	LYS
3	A	54	LYS
3	A	72	GLU
3	A	80	MET
3	A	84	LYS
3	A	88	GLU
3	A	95	ILE
3	A	118	GLN
3	A	119	ASP
3	A	131	LEU

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Mol	Chain	Res	Type
3	A	132	LEU
3	A	136	THR
3	A	159	GLU
3	A	166	LEU
3	A	178	SER
3	A	180	MET
3	A	187	CYS
3	A	200	LYS
3	A	206	ARG
3	A	240	SER
3	A	241	ILE
3	A	252	LYS
3	A	260	LYS
3	A	264	SER
3	A	269	ARG
3	A	270	ILE
3	A	273	LYS
3	A	274	GLN
3	A	277	ILE
3	A	279	LEU
3	A	291	LYS
3	A	293	GLU
3	A	297	LYS
3	A	301	LEU
3	A	343	MET
3	A	367	ARG
3	A	371	THR
3	A	392	SER
3	A	395	THR
3	A	410	LYS
3	A	413	ARG
3	A	414	LYS
3	A	427	MET
3	A	436	MET
3	A	475	LYS
3	A	476	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	81	GLN
3	A	231	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

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 [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 [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, 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	B	20/20 (100%)	-0.65	0 100 100	33, 46, 84, 97	0
2	C	20/20 (100%)	-0.41	0 100 100	34, 56, 78, 90	0
3	A	455/481 (94%)	-0.08	12 (2%) 57 59	26, 47, 90, 100	1 (0%)
All	All	495/521 (95%)	-0.12	12 (2%) 59 62	26, 47, 90, 100	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	476	ILE	3.7
3	A	474	ILE	3.6
3	A	372	PRO	2.9
3	A	477	GLY	2.8
3	A	5	ALA	2.6
3	A	294	THR	2.6
3	A	293	GLU	2.3
3	A	366	LEU	2.3
3	A	292	GLY	2.2
3	A	6	LEU	2.2
3	A	473	GLY	2.1
3	A	415	ARG	2.1

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](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
5	MG	A	479	1/1	0.98	0.04	50,50,50,50	0
4	MN	A	478	1/1	1.00	0.02	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.