Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:57 PM GMT

PDB ID	:	1MUS
Title	:	crystal structure of Tn5 transposase complexed with resolved outside end DNA
Authors	:	Holden, H.M.; Thoden, J.B.; Steiniger-White, M.; Reznikoff, W.S.; Lovell, S.; Rayment, I.
Deposited on	:	2002-09-24
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

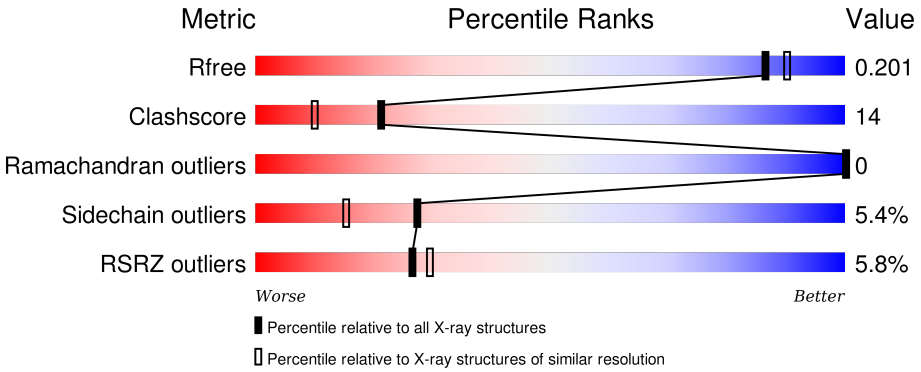
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	20	5%, 15%, 40%, 45%
2	C	20	10%, 50%, 40%
3	A	477	6%, 66%, 25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5060 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
			405	194	70	121	20			

- Molecule 3 is a protein called Tn5 transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	458	Total	C	N	O	S	0	4	0
			3611	2276	664	658	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	LYS	GLU	ENGINEERED	UNP Q46731
A	56	ALA	MET	ENGINEERED	UNP Q46731
A	119	LYS	ASP	ENGINEERED	UNP Q46731
A	120	ALA	LYS	ENGINEERED	UNP Q46731
A	345	LYS	GLU	ENGINEERED	UNP Q46731
A	372	PRO	LEU	ENGINEERED	UNP Q46731
A	477	GLY	-	CLONING ARTIFACT	UNP Q46731

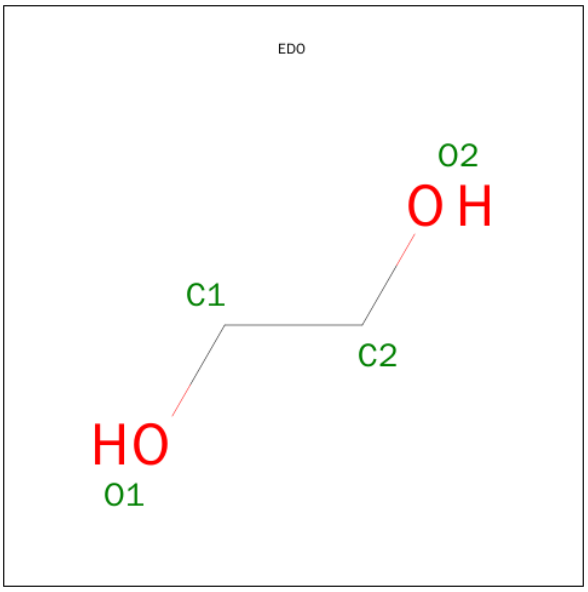
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

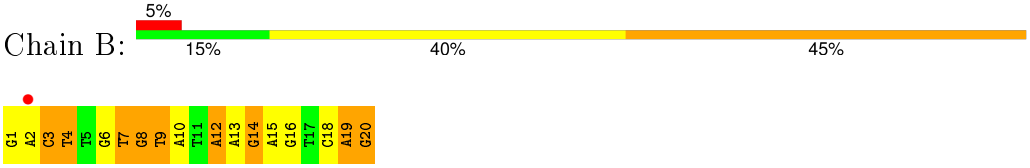
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	494	Total O 494 494	0	0
7	B	71	Total O 71 71	0	0
7	C	50	Total O 50 50	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

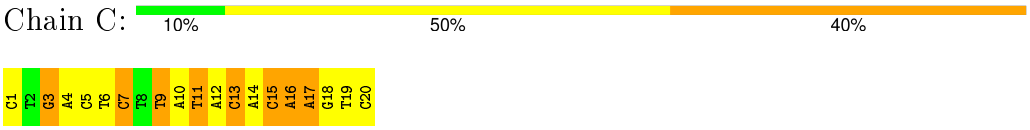
- Molecule 1: DNA transferred strand

Chain B:



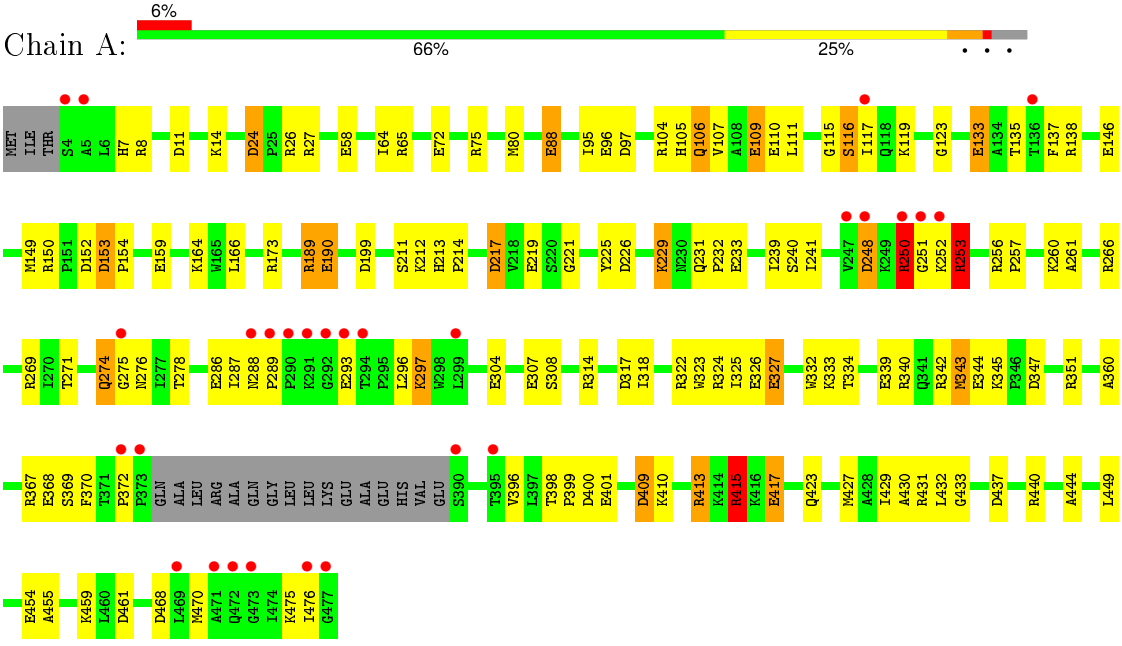
- Molecule 2: DNA non-transferred strand

Chain C:



- Molecule 3: Tn5 transposase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	112.70Å 112.70Å 235.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.90 25.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	85.5 (30.00-1.90) 85.7 (25.42-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 1.91Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.191 , 0.249 0.205 , 0.201	Depositor DCC
R_{free} test set	5942 reflections (10.94%)	DCC
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 89.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 60265 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5060	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.34	1/464 (0.2%)	2.06	22/716 (3.1%)
2	C	1.52	4/452 (0.9%)	2.49	31/692 (4.5%)
3	A	0.97	23/3698 (0.6%)	1.45	50/4985 (1.0%)
All	All	1.08	28/4614 (0.6%)	1.67	103/6393 (1.6%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DC	OP3-P	-7.92	1.51	1.61
3	A	344	GLU	CD-OE2	7.07	1.33	1.25
3	A	219	GLU	CD-OE2	6.54	1.32	1.25
3	A	454	GLU	CD-OE2	6.44	1.32	1.25
3	A	304	GLU	CD-OE2	6.43	1.32	1.25
3	A	190	GLU	CD-OE2	6.36	1.32	1.25
3	A	326	GLU	CD-OE2	6.29	1.32	1.25
3	A	110	GLU	CD-OE2	6.03	1.32	1.25
3	A	339	GLU	CD-OE2	5.94	1.32	1.25
3	A	233	GLU	CD-OE2	5.92	1.32	1.25
3	A	293	GLU	CD-OE2	5.90	1.32	1.25
3	A	307	GLU	CD-OE2	5.86	1.32	1.25
3	A	368	GLU	CD-OE2	5.79	1.32	1.25
3	A	88	GLU	CD-OE2	5.75	1.31	1.25
3	A	159	GLU	CD-OE2	5.63	1.31	1.25
2	C	4	DA	N3-C4	-5.59	1.31	1.34
3	A	327	GLU	CD-OE2	5.49	1.31	1.25
3	A	286	GLU	CD-OE2	5.45	1.31	1.25
2	C	16	DA	C5-C6	-5.37	1.36	1.41
3	A	96	GLU	CD-OE2	5.37	1.31	1.25
3	A	417	GLU	CD-OE2	5.32	1.31	1.25
3	A	401	GLU	CD-OE2	5.32	1.31	1.25
3	A	72	GLU	CD-OE2	5.26	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	58	GLU	CD-OE2	5.21	1.31	1.25
2	C	5	DC	C3'-O3'	-5.16	1.37	1.44
3	A	109[A]	GLU	CD-OE2	5.13	1.31	1.25
3	A	109[B]	GLU	CD-OE2	5.13	1.31	1.25
1	B	8	DG	C3'-O3'	-5.07	1.37	1.44

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	16	DA	O4'-C1'-N9	-15.99	96.81	108.00
2	C	15	DC	C2-N1-C1'	-13.11	104.38	118.80
2	C	20	DC	C2-N1-C1'	-12.97	104.53	118.80
3	A	324	ARG	NE-CZ-NH1	12.06	126.33	120.30
3	A	27	ARG	NE-CZ-NH2	-11.65	114.48	120.30
2	C	15	DC	C6-N1-C1'	10.85	133.82	120.80
3	A	413	ARG	NE-CZ-NH1	10.11	125.35	120.30
3	A	250	ARG	NE-CZ-NH1	9.95	125.28	120.30
2	C	13	DC	C6-N1-C1'	-9.46	109.44	120.80
1	B	14	DG	C8-N9-C1'	9.34	139.14	127.00
2	C	20	DC	C6-N1-C1'	9.29	131.94	120.80
3	A	253	ARG	NE-CZ-NH1	9.16	124.88	120.30
3	A	324	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	B	4	DT	C6-C5-C7	-9.12	117.43	122.90
2	C	1	DC	OP1-P-OP2	-9.12	105.92	119.60
1	B	14	DG	C4-N9-C1'	-8.69	115.20	126.50
2	C	13	DC	C2-N1-C1'	8.50	128.15	118.80
3	A	24	ASP	CB-CG-OD2	-8.49	110.66	118.30
3	A	351	ARG	NE-CZ-NH2	-8.40	116.10	120.30
3	A	27	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	9	DT	P-O5'-C5'	-8.21	107.77	120.90
3	A	217	ASP	CB-CG-OD2	-8.08	111.03	118.30
3	A	189	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	B	15	DA	O4'-C1'-N9	-7.87	102.49	108.00
2	C	7	DC	C2-N1-C1'	-7.87	110.15	118.80
2	C	20	DC	C6-N1-C2	7.83	123.43	120.30
3	A	400	ASP	CB-CG-OD2	-7.75	111.33	118.30
3	A	250	ARG	NE-CZ-NH2	-7.62	116.49	120.30
3	A	150	ARG	NE-CZ-NH2	-7.55	116.53	120.30
3	A	415[A]	ARG	NE-CZ-NH1	7.51	124.06	120.30
3	A	415[B]	ARG	NE-CZ-NH1	7.51	124.06	120.30
2	C	7	DC	C6-N1-C1'	7.46	129.75	120.80
3	A	437	ASP	CB-CG-OD2	-7.44	111.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	75	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	4	DT	C4-C5-C7	7.29	123.37	119.00
2	C	12	DA	C8-N9-C4	7.08	108.63	105.80
3	A	97	ASP	CB-CG-OD2	-7.02	111.98	118.30
3	A	65	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	A	468	ASP	CB-CG-OD2	-6.85	112.13	118.30
3	A	317	ASP	CB-CG-OD1	6.83	124.44	118.30
1	B	7	DT	O4'-C1'-N1	-6.75	103.27	108.00
3	A	152	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	B	7	DT	C6-N1-C1'	-6.65	110.43	120.40
3	A	253	ARG	NE-CZ-NH2	-6.63	116.98	120.30
3	A	347	ASP	CB-CG-OD2	-6.61	112.35	118.30
3	A	413	ARG	NE-CZ-NH2	-6.57	117.02	120.30
3	A	65	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	C	15	DC	P-O3'-C3'	-6.53	111.86	119.70
3	A	440	ARG	NE-CZ-NH1	6.51	123.56	120.30
3	A	153	ASP	CB-CG-OD2	-6.48	112.47	118.30
3	A	217	ASP	CB-CG-OD1	6.41	124.07	118.30
2	C	11	DT	C6-N1-C1'	-6.38	110.83	120.40
3	A	24	ASP	CB-CG-OD1	6.36	124.03	118.30
3	A	97	ASP	CB-CG-OD1	6.35	124.01	118.30
1	B	9	DT	C5'-C4'-O4'	-6.32	97.29	109.30
1	B	7	DT	C2-N1-C1'	6.27	128.23	118.20
3	A	152	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	12	DA	P-O3'-C3'	6.23	127.18	119.70
2	C	1	DC	O4'-C1'-N1	6.23	112.36	108.00
3	A	342	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	C	3	DG	O4'-C1'-N9	-6.11	103.72	108.00
2	C	9	DT	C6-N1-C1'	-6.11	111.24	120.40
2	C	11	DT	C4-C5-C7	6.11	122.66	119.00
2	C	9	DT	N3-C4-O4	-6.03	116.28	119.90
2	C	5	DC	C6-N1-C2	6.03	122.71	120.30
2	C	9	DT	C1'-O4'-C4'	-6.02	104.08	110.10
3	A	317	ASP	CB-CG-OD2	-6.02	112.88	118.30
2	C	11	DT	O5'-P-OP2	-5.97	100.33	105.70
2	C	9	DT	N3-C2-O2	-5.94	118.74	122.30
3	A	409	ASP	CB-CG-OD1	5.93	123.64	118.30
3	A	256	ARG	N-CA-CB	5.86	121.15	110.60
3	A	461	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	20	DG	O4'-C1'-C2'	5.81	110.55	105.90
1	B	16	DG	O4'-C1'-N9	-5.75	103.98	108.00
3	A	133	GLU	N-CA-CB	5.73	120.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	226	ASP	CB-CG-OD1	5.64	123.38	118.30
3	A	437	ASP	CB-CG-OD1	5.63	123.36	118.30
1	B	7	DT	P-O3'-C3'	5.62	126.44	119.70
2	C	12	DA	N7-C8-N9	-5.61	111.00	113.80
1	B	19	DA	C2-N3-C4	-5.60	107.80	110.60
1	B	10	DA	N1-C2-N3	-5.58	126.51	129.30
3	A	199	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	18	DC	C2-N1-C1'	-5.56	112.69	118.80
3	A	248	ASP	CB-CG-OD2	-5.55	113.31	118.30
2	C	11	DT	O4'-C1'-N1	5.53	111.87	108.00
1	B	8	DG	C5-C6-O6	5.51	131.91	128.60
3	A	153	ASP	CB-CG-OD1	5.47	123.23	118.30
3	A	468	ASP	CB-CG-OD1	5.44	123.19	118.30
3	A	226	ASP	CB-CG-OD2	-5.43	113.41	118.30
3	A	322	ARG	NE-CZ-NH1	5.40	123.00	120.30
3	A	248	ASP	CB-CG-OD1	5.40	123.16	118.30
3	A	461	ASP	CB-CG-OD2	-5.35	113.48	118.30
2	C	4	DA	O4'-C1'-C2'	-5.28	101.68	105.90
2	C	13	DC	C6-N1-C2	5.27	122.41	120.30
3	A	340	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	C	5	DC	C5-C6-N1	-5.23	118.39	121.00
1	B	4	DT	C4'-C3'-C2'	-5.16	98.46	103.10
1	B	8	DG	C8-N9-C1'	5.14	133.69	127.00
2	C	12	DA	O5'-P-OP2	-5.14	101.07	105.70
1	B	3	DC	P-O5'-C5'	-5.12	112.71	120.90
1	B	19	DA	N1-C6-N6	5.07	121.64	118.60
2	C	17	DA	O4'-C1'-N9	5.05	111.54	108.00
2	C	12	DA	O4'-C1'-N9	-5.03	104.48	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	413	0	227	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	405	0	227	14	0
3	A	3611	0	3661	88	1
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	12	0	18	3	0
7	A	494	0	0	18	0
7	B	71	0	0	2	0
7	C	50	0	0	1	0
All	All	5060	0	4133	122	1

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 14.

All (122) 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:C:9:DT:H2"	2:C:10:DA:H5"	1.40	1.01
1:B:4:DT:H6	1:B:4:DT:H5"	1.25	0.98
1:B:4:DT:C6	1:B:4:DT:H5"	2.07	0.89
3:A:115:GLY:HA3	3:A:119:LYS:HD2	1.56	0.88
3:A:274:GLN:NE2	3:A:274:GLN:H	1.77	0.81
3:A:116[B]:SER:OG	3:A:119:LYS:HG3	1.85	0.77
3:A:274:GLN:HE21	3:A:274:GLN:H	1.30	0.77
3:A:106:GLN:O	3:A:109[A]:GLU:HG2	1.85	0.76
3:A:149:MET:HE2	7:A:828:HOH:O	1.85	0.76
3:A:253:ARG:HG3	7:A:924:HOH:O	1.85	0.75
3:A:189:ARG:HB3	3:A:212:LYS:HB2	1.67	0.74
3:A:398:THR:HB	3:A:399:PRO:HD2	1.68	0.74
3:A:475:LYS:HG2	3:A:476:ILE:N	2.02	0.74
1:B:2:DA:C2'	1:B:3:DC:H5"	2.18	0.73
3:A:415[B]:ARG:HG2	3:A:415[B]:ARG:HH11	1.54	0.73
2:C:14:DA:H2"	2:C:15:DC:H5"	1.71	0.72
3:A:119:LYS:HB3	7:A:588:HOH:O	1.92	0.70
3:A:271:THR:OG1	3:A:278:THR:HG22	1.92	0.69
3:A:225:TYR:CZ	3:A:229:LYS:HD2	2.27	0.69
3:A:116[A]:SER:OG	3:A:119:LYS:HE2	1.92	0.69
1:B:2:DA:H2"	1:B:3:DC:H5"	1.74	0.68
3:A:117:ILE:HG13	7:A:742:HOH:O	1.93	0.68
1:B:8:DG:H2"	1:B:9:DT:H5'	1.76	0.67
3:A:239:ILE:HD11	3:A:296:LEU:HD13	1.76	0.67
1:B:3:DC:H2'	1:B:4:DT:H72	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:15:DC:H2"	2:C:16:DA:O5'	1.96	0.64
1:B:8:DG:H2"	1:B:9:DT:C5'	2.28	0.63
1:B:20:DG:OP2	3:A:333:LYS:NZ	2.30	0.63
3:A:470:MET:HB3	7:A:968:HOH:O	1.98	0.63
1:B:1:DG:H2"	1:B:2:DA:OP2	2.00	0.62
2:C:16:DA:H2"	2:C:17:DA:O5'	1.99	0.62
3:A:239:ILE:HD11	3:A:296:LEU:CD1	2.29	0.62
1:B:2:DA:H2"	1:B:3:DC:C5'	2.31	0.61
1:B:9:DT:H5'	7:B:59:HOH:O	2.01	0.61
3:A:455:ALA:O	3:A:459:LYS:HG3	2.02	0.60
3:A:115:GLY:HA3	3:A:119:LYS:CD	2.30	0.59
3:A:370:PHE:O	3:A:372:PRO:HD3	2.03	0.58
3:A:423:GLN:HG2	7:A:903:HOH:O	2.02	0.58
2:C:10:DA:H2'	2:C:11:DT:H72	1.85	0.57
3:A:217:ASP:O	3:A:221:GLY:N	2.36	0.57
3:A:104:ARG:HG3	7:A:589:HOH:O	2.04	0.57
3:A:213:HIS:HB3	3:A:214:PRO:HD2	1.86	0.57
3:A:250:ARG:HH11	3:A:250:ARG:HG2	1.70	0.57
1:B:12:DA:N3	7:B:34:HOH:O	2.33	0.56
1:B:6:DG:H2"	1:B:7:DT:O5'	2.05	0.55
3:A:415[B]:ARG:HH11	3:A:415[B]:ARG:CG	2.19	0.54
3:A:297:LYS:HE2	7:A:872:HOH:O	2.07	0.54
3:A:253:ARG:N	7:A:924:HOH:O	2.28	0.54
2:C:10:DA:H2'	2:C:11:DT:C7	2.38	0.54
1:B:13:DA:H2"	1:B:14:DG:C8	2.43	0.53
3:A:88:GLU:HB2	7:A:959:HOH:O	2.09	0.53
1:B:3:DC:H2"	1:B:4:DT:O5'	2.09	0.53
3:A:241:ILE:HD11	3:A:296:LEU:HD11	1.91	0.52
3:A:275:GLY:O	3:A:276:ASN:C	2.45	0.52
3:A:239:ILE:HG12	3:A:261:ALA:HB3	1.91	0.51
3:A:413:ARG:HG3	3:A:417:GLU:HG3	1.91	0.51
3:A:398:THR:HB	3:A:399:PRO:CD	2.39	0.51
3:A:138:ARG:HH12	3:A:369:SER:HA	1.76	0.51
1:B:2:DA:C2	1:B:3:DC:C2	2.99	0.50
3:A:345:LYS:HD2	7:A:824:HOH:O	2.11	0.50
3:A:250:ARG:NH2	7:A:840:HOH:O	2.41	0.50
3:A:7:HIS:CE1	3:A:396:VAL:HG13	2.47	0.50
3:A:24:ASP:OD1	3:A:26:ARG:HB2	2.10	0.50
1:B:3:DC:C2'	1:B:4:DT:H72	2.42	0.50
1:B:2:DA:H1'	1:B:3:DC:H5"	1.94	0.49
3:A:95:ILE:HG21	3:A:325:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:DG:C2'	1:B:9:DT:H5"	2.42	0.49
3:A:332:TRP:HA	3:A:360:ALA:HB2	1.94	0.49
2:C:3:DG:H4'	3:A:323:TRP:CD2	2.47	0.49
2:C:14:DA:C2'	2:C:15:DC:H5"	2.41	0.49
3:A:166:LEU:HD12	7:A:620:HOH:O	2.13	0.48
3:A:288:ASN:N	3:A:289:PRO:CD	2.77	0.48
3:A:345:LYS:HG2	7:A:875:HOH:O	2.15	0.47
3:A:288:ASN:N	3:A:289:PRO:HD3	2.29	0.47
3:A:367:ARG:NH1	3:A:444:ALA:O	2.46	0.47
3:A:8:ARG:NE	3:A:11:ASP:OD2	2.41	0.47
3:A:225:TYR:CZ	3:A:229:LYS:CD	2.97	0.47
3:A:225:TYR:CE2	3:A:229:LYS:HD3	2.49	0.47
3:A:146:GLU:OE2	6:A:484:EDO:H22	2.15	0.47
3:A:250:ARG:CG	3:A:250:ARG:HH11	2.28	0.46
3:A:105:HIS:CD2	3:A:107:VAL:HG12	2.51	0.46
2:C:9:DT:C2'	2:C:10:DA:H5"	2.29	0.46
3:A:95:ILE:CG2	3:A:325:ILE:HB	2.46	0.46
3:A:248:ASP:OD1	3:A:251:GLY:N	2.49	0.46
3:A:64:ILE:HD12	3:A:343:MET:HG2	1.98	0.45
3:A:314:ARG:O	3:A:318:ILE:HG13	2.17	0.45
3:A:296:LEU:HD21	6:A:482:EDO:O2	2.16	0.45
3:A:225:TYR:CE2	3:A:229:LYS:CD	3.00	0.45
1:B:2:DA:C1'	1:B:3:DC:H5"	2.46	0.45
3:A:345:LYS:HD3	7:A:875:HOH:O	2.16	0.45
3:A:231:GLN:O	3:A:266:ARG:NH1	2.50	0.44
3:A:274:GLN:N	3:A:274:GLN:HE21	2.07	0.44
2:C:9:DT:H2"	2:C:10:DA:C5'	2.29	0.44
1:B:8:DG:H1'	1:B:9:DT:H5"	1.99	0.44
3:A:133:GLU:O	3:A:137:PHE:HA	2.18	0.44
2:C:18:DG:H2"	2:C:19:DT:H5'	2.00	0.44
3:A:413:ARG:CG	3:A:417:GLU:HG3	2.48	0.43
3:A:115:GLY:CA	3:A:119:LYS:HD2	2.37	0.43
2:C:15:DC:H1'	7:C:41:HOH:O	2.18	0.43
2:C:6:DT:H2"	2:C:7:DC:C6	2.53	0.43
2:C:13:DC:H2'	2:C:13:DC:H6	1.60	0.43
3:A:308:SER:HA	7:A:666:HOH:O	2.18	0.43
3:A:257:PRO:HG3	7:A:745:HOH:O	2.18	0.43
3:A:427:MET:O	3:A:431:ARG:HG3	2.19	0.43
3:A:88:GLU:HG2	3:A:88:GLU:O	2.19	0.42
3:A:327:GLU:HA	7:A:560:HOH:O	2.18	0.42
3:A:287:ILE:C	3:A:289:PRO:HD3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:ASP:OD1	3:A:154:PRO:HD2	2.19	0.42
3:A:429:ILE:O	3:A:432:LEU:HB2	2.20	0.42
1:B:19:DA:OP1	3:A:334:THR:OG1	2.29	0.42
3:A:231:GLN:HB3	3:A:232:PRO:HD2	2.01	0.42
3:A:409:ASP:O	3:A:410:LYS:C	2.56	0.42
3:A:430:ALA:O	3:A:433:GLY:N	2.52	0.42
3:A:432:LEU:HD23	3:A:432:LEU:HA	1.91	0.41
3:A:153:ASP:HA	3:A:154:PRO:HD3	1.92	0.41
3:A:111:LEU:HB3	3:A:123:GLY:HA2	2.03	0.41
1:B:3:DC:C6	1:B:4:DT:H72	2.56	0.41
3:A:164:LYS:HB3	6:A:484:EDO:H21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:470:MET:SD	3:A:470:MET:SD[12_555]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	458/477 (96%)	444 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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
3	A	375/388 (97%)	353 (94%)	22 (6%)	24 12

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	14	LYS
3	A	80	MET
3	A	106	GLN
3	A	116[A]	SER
3	A	116[B]	SER
3	A	135	THR
3	A	173	ARG
3	A	190	GLU
3	A	211	SER
3	A	229	LYS
3	A	240	SER
3	A	250	ARG
3	A	252	LYS
3	A	253	ARG
3	A	260	LYS
3	A	269	ARG
3	A	274	GLN
3	A	297	LYS
3	A	343	MET
3	A	415[A]	ARG
3	A	415[B]	ARG
3	A	449	LEU

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

Mol	Chain	Res	Type
3	A	57	GLN
3	A	81	GLN
3	A	274	GLN
3	A	403	GLN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	A	482	-	3,3,3	0.39	0	2,2,2	0.35	0
6	EDO	A	483	-	3,3,3	0.66	0	2,2,2	0.58	0
6	EDO	A	484	-	3,3,3	0.56	0	2,2,2	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	482	-	-	0/1/1/1	0/0/0/0
6	EDO	A	483	-	-	0/1/1/1	0/0/0/0
6	EDO	A	484	-	-	0/1/1/1	0/0/0/0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	482	EDO	1	0
6	A	484	EDO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	20/20 (100%)	-0.23	1 (5%) 32 35	23, 30, 65, 71	0
2	C	20/20 (100%)	-0.34	0 100 100	20, 36, 55, 71	0
3	A	458/477 (96%)	0.17	28 (6%) 25 27	16, 28, 64, 99	0
All	All	498/517 (96%)	0.13	29 (5%) 26 29	16, 28, 64, 99	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	291	LYS	6.0
3	A	294	THR	5.2
3	A	251	GLY	4.8
3	A	473	GLY	3.8
3	A	250	ARG	3.7
3	A	292	GLY	3.7
3	A	390	SER	3.7
3	A	373	PRO	3.7
3	A	477	GLY	3.5
3	A	288	ASN	3.2
3	A	248	ASP	3.1
3	A	476	ILE	3.1
3	A	252	LYS	3.1
3	A	275	GLY	3.1
3	A	247	VAL	2.9
3	A	4	SER	2.8
3	A	289	PRO	2.7
3	A	5	ALA	2.5
3	A	136	THR	2.5
1	B	2	DA	2.5
3	A	290	PRO	2.4
3	A	299	LEU	2.4
3	A	395	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	469	LEU	2.3
3	A	117	ILE	2.1
3	A	472	GLN	2.1
3	A	471	ALA	2.1
3	A	293	GLU	2.1
3	A	372	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
6	EDO	A	483	4/4	0.96	0.10	1.84	19,25,31,31	0
6	EDO	A	482	4/4	0.94	0.12	-0.39	45,66,66,72	0
6	EDO	A	484	4/4	0.92	0.11	-0.44	24,34,47,55	0
4	MN	A	478	1/1	0.99	0.03	-3.40	21,21,21,21	0
4	MN	A	479	1/1	0.99	0.03	-3.55	22,22,22,22	0
5	MG	A	480	1/1	0.98	0.05	-	15,15,15,15	1
5	MG	A	481	1/1	0.98	0.07	-	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.