



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 07:54 pm GMT

PDB ID : 3GX4  
Title : Crystal Structure Analysis of S. Pombe ATL in complex with DNA  
Authors : Tubbs, J.L.; Arvai, A.S.; Tainer, J.A.  
Deposited on : 2009-04-01  
Resolution : 2.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

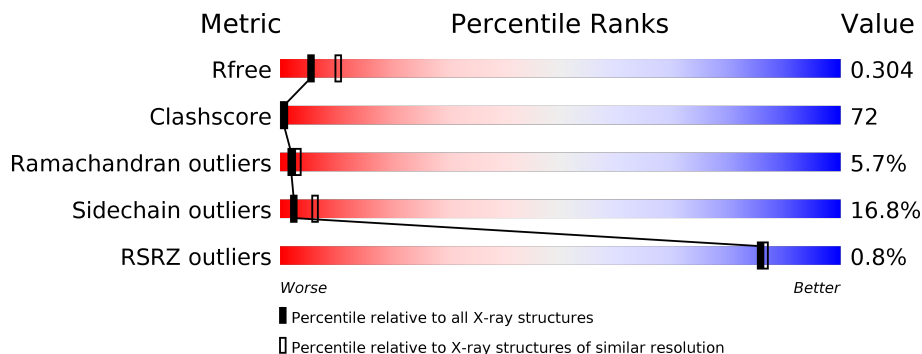
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	X	116	
2	Y	13	
3	Z	13	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NCO	Y	302	-	-	X	X
4	NCO	Z	303	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1455 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 Alkyltransferase-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	108	Total	C	N	O	S	0	0	0
			890	563	156	165	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	109	GLY	-	EXPRESSION TAG	UNP Q9UTN9
X	110	SER	-	EXPRESSION TAG	UNP Q9UTN9
X	111	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	112	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	113	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	114	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	115	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	116	HIS	-	EXPRESSION TAG	UNP Q9UTN9

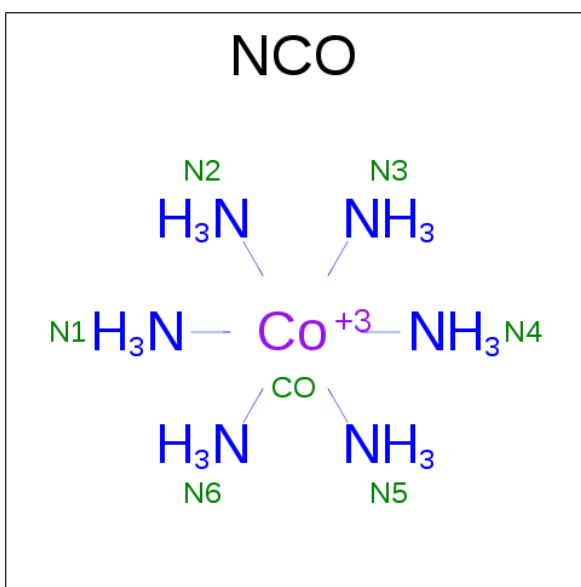
- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*CP\*CP\*AP\*TP\*GP\*(6OG)P\*CP\*TP\*AP\*GP\*TP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	13	Total	C	N	O	P	0	0	0
			266	128	50	76	12			

- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*TP\*AP\*CP\*TP\*AP\*GP\*CP\*CP\*AP\*TP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			

- Molecule 4 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: CoH<sub>18</sub>N<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	Y	1	Total	Co	N	0	0
			7	1	6		
4	Z	1	Total	Co	N	0	0
			7	1	6		

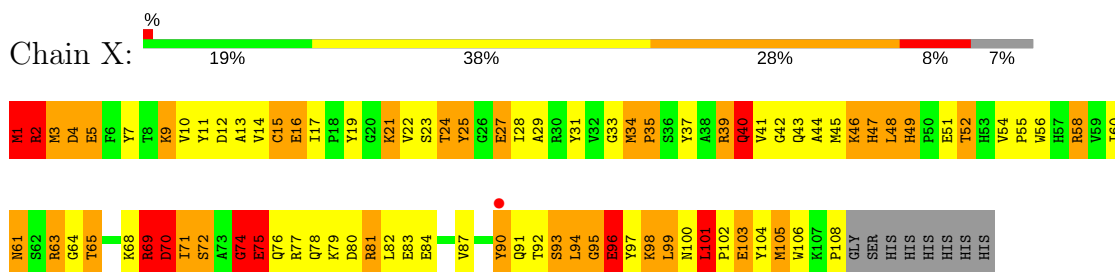
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	19	Total	O	0	0
			19	19		
5	Y	2	Total	O	0	0
			2	2		
5	Z	2	Total	O	0	0
			2	2		

### 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 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.

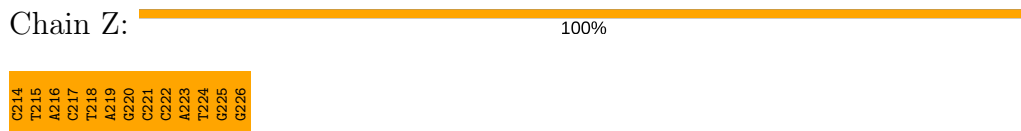
- Molecule 1: Alkyltransferase-like protein 1



- Molecule 2: DNA (5'-D(\*GP\*CP\*CP\*AP\*TP\*GP\*(6OG)P\*CP\*TP\*AP\*GP\*TP\*A)-3')



- Molecule 3: DNA (5'-D(\*CP\*TP\*AP\*CP\*TP\*AP\*GP\*CP\*CP\*AP\*TP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.73Å 59.73Å 238.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.04 – 2.70 39.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.04-2.70) 88.6 (39.04-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.227 , 0.296 0.232 , 0.304	Depositor DCC
$R_{free}$ test set	373 reflections (5.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6OG, NCO

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	X	2.28	41/913 (4.5%)	1.98	30/1232 (2.4%)
2	Y	3.80	52/271 (19.2%)	2.84	33/414 (8.0%)
3	Z	3.98	59/293 (20.1%)	2.85	35/450 (7.8%)
All	All	3.00	152/1477 (10.3%)	2.38	98/2096 (4.7%)

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	X	0	2

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	90	TYR	CE2-CZ	9.65	1.51	1.38
3	Z	220	DG	C3'-O3'	-9.10	1.32	1.44
1	X	90	TYR	CE1-CZ	9.02	1.50	1.38
2	Y	210	DA	P-O5'	-8.75	1.50	1.59
1	X	84	GLU	CD-OE1	8.54	1.35	1.25
3	Z	221	DC	O3'-P	-8.52	1.50	1.61
1	X	84	GLU	CG-CD	8.27	1.64	1.51
3	Z	215	DT	C4-C5	-8.22	1.37	1.45
1	X	98	LYS	CB-CG	-7.85	1.31	1.52
3	Z	216	DA	C3'-O3'	-7.76	1.33	1.44
3	Z	221	DC	C3'-O3'	-7.61	1.34	1.44
1	X	75	GLU	N-CA	7.57	1.61	1.46
3	Z	219	DA	N7-C5	-7.53	1.34	1.39
2	Y	209	DT	P-O5'	-7.52	1.52	1.59
1	X	40	GLN	C-O	7.46	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	217	DC	N3-C4	-7.42	1.28	1.33
3	Z	224	DT	C4-C5	-7.37	1.38	1.45
3	Z	223	DA	P-O5'	-7.22	1.52	1.59
1	X	56	TRP	CB-CG	-7.15	1.37	1.50
2	Y	208	DC	P-O5'	-7.12	1.52	1.59
1	X	22	VAL	CB-CG2	7.08	1.67	1.52
3	Z	222	DC	N1-C6	-7.03	1.32	1.37
3	Z	222	DC	N3-C4	-6.98	1.29	1.33
3	Z	219	DA	N3-C4	-6.97	1.30	1.34
2	Y	208	DC	N3-C4	-6.96	1.29	1.33
1	X	7	TYR	CE2-CZ	6.88	1.47	1.38
2	Y	201	DG	N9-C8	-6.84	1.33	1.37
1	X	27	GLU	CD-OE1	6.83	1.33	1.25
3	Z	219	DA	N9-C4	-6.82	1.33	1.37
3	Z	221	DC	N3-C4	-6.82	1.29	1.33
1	X	84	GLU	CD-OE2	6.81	1.33	1.25
2	Y	206	DG	C3'-O3'	-6.81	1.35	1.44
3	Z	222	DC	P-O5'	-6.79	1.52	1.59
2	Y	206	DG	N7-C5	-6.77	1.35	1.39
2	Y	208	DC	N1-C6	-6.77	1.33	1.37
3	Z	216	DA	C5-C4	-6.77	1.34	1.38
1	X	11	TYR	CD2-CE2	6.76	1.49	1.39
2	Y	208	DC	C2-N3	-6.75	1.30	1.35
3	Z	221	DC	N1-C6	-6.74	1.33	1.37
1	X	103	GLU	CG-CD	6.69	1.61	1.51
3	Z	224	DT	N1-C2	-6.69	1.32	1.38
3	Z	223	DA	N3-C4	-6.63	1.30	1.34
3	Z	220	DG	N7-C5	-6.61	1.35	1.39
2	Y	208	DC	C2-O2	-6.59	1.18	1.24
1	X	2	ARG	CG-CD	6.57	1.68	1.51
2	Y	209	DT	N1-C2	-6.49	1.32	1.38
1	X	90	TYR	CG-CD1	6.48	1.47	1.39
2	Y	204	DA	C6-N1	-6.45	1.31	1.35
1	X	39	ARG	CZ-NH1	6.44	1.41	1.33
3	Z	223	DA	C6-N1	-6.42	1.31	1.35
3	Z	216	DA	N3-C4	-6.39	1.31	1.34
3	Z	219	DA	C5-C6	-6.39	1.35	1.41
2	Y	210	DA	N3-C4	-6.39	1.31	1.34
3	Z	221	DC	C2-N3	-6.36	1.30	1.35
3	Z	223	DA	N9-C8	-6.36	1.32	1.37
3	Z	220	DG	N1-C2	-6.35	1.32	1.37
2	Y	212	DT	C4-C5	-6.35	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	217	DC	N1-C6	-6.34	1.33	1.37
3	Z	224	DT	P-O5'	-6.30	1.53	1.59
2	Y	205	DT	C3'-O3'	-6.25	1.35	1.44
2	Y	201	DG	N7-C5	-6.24	1.35	1.39
3	Z	218	DT	N1-C2	-6.21	1.33	1.38
2	Y	205	DT	C4-C5	-6.20	1.39	1.45
3	Z	216	DA	C6-N1	-6.20	1.31	1.35
1	X	75	GLU	CD-OE1	6.19	1.32	1.25
1	X	39	ARG	CB-CG	-6.17	1.35	1.52
3	Z	223	DA	C3'-O3'	-6.16	1.35	1.44
2	Y	204	DA	N3-C4	-6.15	1.31	1.34
2	Y	210	DA	C5-C4	-6.15	1.34	1.38
2	Y	211	DG	N9-C4	-6.11	1.33	1.38
3	Z	220	DG	C8-N7	-6.11	1.27	1.30
3	Z	218	DT	C2-N3	-6.08	1.32	1.37
1	X	75	GLU	CG-CD	6.08	1.61	1.51
2	Y	209	DT	N1-C6	-6.06	1.34	1.38
1	X	105	MET	CA-CB	-6.06	1.40	1.53
2	Y	209	DT	C2-O2	-6.04	1.17	1.22
3	Z	217	DC	C3'-O3'	-6.02	1.36	1.44
3	Z	219	DA	C6-N1	-6.02	1.31	1.35
3	Z	224	DT	N3-C4	-6.01	1.33	1.38
1	X	104	TYR	CG-CD2	5.98	1.47	1.39
3	Z	214	DC	C3'-O3'	-5.95	1.36	1.44
3	Z	221	DC	C2-O2	-5.95	1.19	1.24
2	Y	208	DC	C4-C5	-5.93	1.38	1.43
2	Y	206	DG	C8-N7	-5.92	1.27	1.30
2	Y	206	DG	N1-C2	-5.90	1.33	1.37
1	X	65	THR	C-O	5.89	1.34	1.23
3	Z	220	DG	C6-N1	-5.88	1.35	1.39
2	Y	213	DA	C3'-O3'	-5.87	1.36	1.44
1	X	16	GLU	CB-CG	5.87	1.63	1.52
3	Z	224	DT	C2-N3	-5.85	1.33	1.37
1	X	46	LYS	N-CA	-5.84	1.34	1.46
2	Y	208	DC	N1-C2	-5.84	1.34	1.40
2	Y	213	DA	N7-C5	-5.77	1.35	1.39
3	Z	216	DA	P-O5'	-5.75	1.53	1.59
2	Y	206	DG	C6-N1	-5.73	1.35	1.39
2	Y	206	DG	C5-C4	-5.71	1.34	1.38
2	Y	210	DA	C3'-O3'	-5.71	1.36	1.44
3	Z	220	DG	P-O5'	-5.68	1.54	1.59
3	Z	223	DA	O3'-P	-5.65	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	223	DA	C8-N7	-5.63	1.27	1.31
3	Z	222	DC	C2-N3	-5.60	1.31	1.35
1	X	90	TYR	CD2-CE2	5.59	1.47	1.39
1	X	103	GLU	CD-OE2	5.57	1.31	1.25
3	Z	225	DG	C5-C4	-5.56	1.34	1.38
3	Z	216	DA	N9-C8	-5.51	1.33	1.37
1	X	72	SER	CA-C	5.50	1.67	1.52
2	Y	211	DG	C5-C6	-5.50	1.36	1.42
2	Y	213	DA	C5-C4	-5.50	1.34	1.38
3	Z	218	DT	N1-C6	-5.48	1.34	1.38
2	Y	212	DT	N1-C2	-5.48	1.33	1.38
2	Y	211	DG	C3'-O3'	-5.47	1.36	1.44
2	Y	211	DG	C8-N7	-5.46	1.27	1.30
2	Y	213	DA	N9-C8	-5.46	1.33	1.37
1	X	21	LYS	C-O	5.46	1.33	1.23
3	Z	215	DT	C4-O4	-5.44	1.18	1.23
2	Y	206	DG	N9-C8	-5.43	1.34	1.37
2	Y	201	DG	C3'-O3'	-5.42	1.36	1.44
1	X	35	PRO	CG-CD	5.42	1.68	1.50
2	Y	211	DG	N7-C5	-5.41	1.36	1.39
2	Y	212	DT	C1'-N1	-5.40	1.39	1.47
2	Y	211	DG	C5-C4	-5.39	1.34	1.38
2	Y	208	DC	O3'-P	-5.38	1.54	1.61
3	Z	215	DT	N1-C2	-5.38	1.33	1.38
2	Y	202	DC	C3'-O3'	-5.35	1.36	1.44
3	Z	223	DA	C5-C4	-5.31	1.35	1.38
3	Z	220	DG	N9-C8	-5.31	1.34	1.37
2	Y	205	DT	N3-C4	-5.31	1.34	1.38
2	Y	211	DG	N9-C8	-5.27	1.34	1.37
3	Z	216	DA	N7-C5	-5.27	1.36	1.39
1	X	16	GLU	C-O	5.24	1.33	1.23
1	X	70	ASP	CB-CG	5.23	1.62	1.51
2	Y	204	DA	N9-C4	-5.22	1.34	1.37
1	X	19	TYR	CD1-CE1	5.21	1.47	1.39
1	X	96	GLU	CD-OE2	5.14	1.31	1.25
2	Y	204	DA	N7-C5	-5.14	1.36	1.39
1	X	93	SER	CB-OG	5.14	1.49	1.42
3	Z	224	DT	N1-C6	-5.13	1.34	1.38
2	Y	208	DC	P-OP1	-5.12	1.40	1.49
1	X	11	TYR	CG-CD2	5.12	1.45	1.39
3	Z	218	DT	N3-C4	-5.12	1.34	1.38
1	X	21	LYS	CE-NZ	5.10	1.61	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	83	GLU	CG-CD	5.08	1.59	1.51
3	Z	219	DA	P-O5'	-5.08	1.54	1.59
2	Y	212	DT	C5-C7	-5.06	1.47	1.50
1	X	31	TYR	CD1-CE1	5.05	1.47	1.39
1	X	96	GLU	CG-CD	-5.05	1.44	1.51
2	Y	213	DA	P-O5'	-5.05	1.54	1.59
3	Z	221	DC	P-O5'	-5.04	1.54	1.59
3	Z	218	DT	C2-O2	-5.03	1.18	1.22
3	Z	220	DG	O3'-P	-5.01	1.55	1.61
1	X	5	GLU	CB-CG	-5.00	1.42	1.52
2	Y	213	DA	N3-C4	-5.00	1.31	1.34

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2	ARG	NE-CZ-NH1	13.92	127.26	120.30
2	Y	211	DG	O4'-C4'-C3'	-12.99	98.20	106.00
2	Y	210	DA	O4'-C1'-N9	12.73	116.91	108.00
3	Z	215	DT	C5-C4-O4	-11.90	116.57	124.90
3	Z	222	DC	O4'-C1'-N1	11.58	116.10	108.00
3	Z	217	DC	O4'-C1'-N1	11.30	115.91	108.00
2	Y	206	DG	O4'-C4'-C3'	-11.17	99.30	106.00
2	Y	206	DG	O4'-C1'-N9	10.86	115.60	108.00
3	Z	219	DA	O4'-C1'-N9	10.64	115.45	108.00
2	Y	212	DT	O4'-C1'-N1	-10.32	100.78	108.00
1	X	4	ASP	CB-CG-OD2	-10.09	109.22	118.30
3	Z	215	DT	N3-C4-O4	10.04	125.93	119.90
1	X	58	ARG	NE-CZ-NH2	-9.64	115.48	120.30
3	Z	214	DC	O4'-C4'-C3'	-9.49	100.30	106.00
1	X	4	ASP	CB-CG-OD1	9.47	126.83	118.30
1	X	2	ARG	NE-CZ-NH2	-9.35	115.63	120.30
3	Z	226	DG	O4'-C1'-C2'	-9.04	98.67	105.90
3	Z	221	DC	O4'-C1'-N1	-8.95	101.73	108.00
3	Z	216	DA	O4'-C1'-N9	8.77	114.14	108.00
2	Y	206	DG	C4'-C3'-C2'	-8.60	95.36	103.10
1	X	15	CYS	CA-CB-SG	-8.48	98.74	114.00
2	Y	211	DG	O4'-C1'-N9	-8.40	102.12	108.00
3	Z	216	DA	O4'-C4'-C3'	-8.30	101.02	106.00
3	Z	222	DC	C4'-C3'-C2'	-8.26	95.67	103.10
2	Y	208	DC	O4'-C1'-C2'	-8.00	99.50	105.90
3	Z	221	DC	O4'-C4'-C3'	-7.97	101.22	106.00
3	Z	225	DG	O4'-C1'-N9	7.90	113.53	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	202	DC	O4'-C4'-C3'	-7.84	101.29	106.00
2	Y	205	DT	C5-C4-O4	-7.75	119.47	124.90
3	Z	219	DA	O4'-C4'-C3'	-7.67	101.39	106.00
3	Z	217	DC	P-O5'-C5'	-7.52	108.87	120.90
1	X	75	GLU	CB-CA-C	-7.43	95.55	110.40
3	Z	224	DT	N3-C4-O4	7.30	124.28	119.90
2	Y	209	DT	O4'-C1'-C2'	-7.25	100.10	105.90
3	Z	219	DA	C4'-C3'-C2'	-7.20	96.62	103.10
2	Y	205	DT	O4'-C4'-C3'	-7.13	101.65	104.50
2	Y	204	DA	O4'-C1'-C2'	-7.11	100.21	105.90
3	Z	219	DA	C3'-C2'-C1'	-7.01	94.08	102.50
2	Y	213	DA	O4'-C1'-N9	6.98	112.89	108.00
3	Z	219	DA	C2-N3-C4	-6.85	107.17	110.60
2	Y	211	DG	C4-C5-N7	6.79	113.52	110.80
2	Y	212	DT	O4'-C1'-C2'	-6.74	100.51	105.90
2	Y	205	DT	O4'-C1'-N1	6.70	112.69	108.00
1	X	69	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	X	74	GLY	N-CA-C	6.66	129.76	113.10
3	Z	215	DT	O4'-C1'-C2'	-6.66	100.57	105.90
3	Z	224	DT	C4-C5-C7	-6.61	115.03	119.00
3	Z	217	DC	P-O3'-C3'	-6.55	111.84	119.70
2	Y	203	DC	O4'-C1'-C2'	-6.49	100.71	105.90
2	Y	205	DT	N3-C4-O4	6.37	123.72	119.90
1	X	47	HIS	CB-CA-C	-6.36	97.69	110.40
2	Y	208	DC	OP1-P-OP2	-6.31	110.14	119.60
2	Y	205	DT	C4'-C3'-C2'	-6.30	97.43	103.10
3	Z	221	DC	P-O3'-C3'	-6.26	112.19	119.70
1	X	49	HIS	C-N-CD	6.24	141.51	128.40
1	X	105	MET	CA-CB-CG	-6.21	102.73	113.30
3	Z	218	DT	C4'-C3'-C2'	-6.19	97.53	103.10
1	X	39	ARG	NE-CZ-NH1	-6.15	117.23	120.30
1	X	63	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	Z	215	DT	C4-C5-C7	-6.07	115.36	119.00
1	X	70	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	X	25	TYR	CD1-CE1-CZ	-5.99	114.41	119.80
2	Y	211	DG	C4'-C3'-C2'	5.98	108.48	103.10
2	Y	208	DC	O5'-P-OP2	-5.97	100.33	105.70
1	X	39	ARG	CD-NE-CZ	5.95	131.93	123.60
2	Y	206	DG	C8-N9-C4	-5.93	104.03	106.40
3	Z	218	DT	P-O5'-C5'	-5.93	111.41	120.90
3	Z	224	DT	C5-C4-O4	-5.93	120.75	124.90
1	X	34	MET	CG-SD-CE	5.92	109.68	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	46	LYS	CD-CE-NZ	-5.87	98.19	111.70
2	Y	202	DC	N3-C4-C5	5.87	124.25	121.90
1	X	98	LYS	CD-CE-NZ	-5.85	98.25	111.70
2	Y	212	DT	N3-C4-O4	5.79	123.37	119.90
2	Y	202	DC	O4'-C1'-N1	-5.74	103.99	108.00
1	X	39	ARG	NE-CZ-NH2	5.68	123.14	120.30
3	Z	215	DT	C6-C5-C7	5.68	126.31	122.90
1	X	63	ARG	CG-CD-NE	-5.63	99.99	111.80
1	X	94	LEU	CA-CB-CG	5.59	128.16	115.30
1	X	1	MET	CG-SD-CE	5.49	108.99	100.20
3	Z	220	DG	P-O5'-C5'	-5.46	112.16	120.90
2	Y	204	DA	C4'-C3'-C2'	-5.43	98.21	103.10
1	X	12	ASP	CB-CG-OD1	-5.35	113.48	118.30
3	Z	217	DC	C5-C4-N4	5.35	123.94	120.20
1	X	9	LYS	CD-CE-NZ	-5.35	99.40	111.70
2	Y	211	DG	C5-N7-C8	-5.34	101.63	104.30
3	Z	226	DG	P-O5'-C5'	-5.31	112.41	120.90
3	Z	219	DA	C5-N7-C8	-5.30	101.25	103.90
2	Y	205	DT	N3-C2-O2	-5.29	119.12	122.30
1	X	101	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	X	10	VAL	CA-CB-CG2	-5.17	103.14	110.90
2	Y	201	DG	O4'-C4'-C3'	-5.14	102.45	104.50
2	Y	211	DG	N9-C4-C5	-5.11	103.36	105.40
1	X	80	ASP	CB-CG-OD1	-5.10	113.71	118.30
3	Z	219	DA	N1-C6-N6	5.08	121.65	118.60
1	X	47	HIS	C-N-CA	-5.04	109.09	121.70
3	Z	219	DA	C4-C5-N7	5.04	113.22	110.70
2	Y	204	DA	C3'-C2'-C1'	-5.04	96.46	102.50
3	Z	215	DT	N3-C2-O2	5.00	125.30	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	74	GLY	Peptide
1	X	75	GLU	Peptide

## 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	X	890	0	868	111	0
2	Y	266	0	150	47	0
3	Z	262	0	148	38	0
4	Y	7	0	0	14	0
4	Z	7	0	0	1	0
5	X	19	0	0	0	0
5	Y	2	0	0	0	0
5	Z	2	0	0	0	0
All	All	1455	0	1166	181	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 (181) 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:X:71:ILE:CD1	1:X:71:ILE:CG1	1.76	1.61
2:Y:206:DG:H2''	4:Y:302:NCO:N3	1.38	1.36
2:Y:211:DG:H2''	2:Y:212:DT:C5'	1.59	1.30
2:Y:205:DT:H2''	2:Y:206:DG:H5''	1.29	1.12
2:Y:211:DG:C2'	2:Y:212:DT:H5''	1.81	1.10
3:Z:217:DC:H2''	3:Z:218:DT:OP2	1.52	1.10
1:X:93:SER:O	1:X:94:LEU:HB2	1.49	1.10
2:Y:206:DG:H4'	2:Y:206:DG:OP1	1.42	1.08
2:Y:211:DG:C2'	2:Y:212:DT:C5'	2.30	1.08
1:X:70:ASP:O	1:X:71:ILE:C	1.91	1.07
3:Z:216:DA:H5'	3:Z:216:DA:C8	1.95	1.01
3:Z:216:DA:H5'	3:Z:216:DA:H8	1.23	1.01
2:Y:211:DG:H2''	2:Y:212:DT:H5''	1.04	1.00
1:X:69:ARG:HB2	1:X:69:ARG:HH11	1.29	0.97
2:Y:209:DT:H3	3:Z:219:DA:N6	1.62	0.96
2:Y:211:DG:C2'	2:Y:212:DT:H5'	1.97	0.94
3:Z:215:DT:H2''	3:Z:216:DA:H5''	1.50	0.92
1:X:24:THR:CG2	1:X:27:GLU:H	1.83	0.92
1:X:46:LYS:HE3	2:Y:207:6OG:OP1	1.70	0.92
3:Z:216:DA:H2''	3:Z:217:DC:H5'	1.53	0.90
1:X:24:THR:HG23	1:X:27:GLU:H	1.37	0.89
2:Y:211:DG:H2''	2:Y:212:DT:H5'	1.54	0.88
1:X:93:SER:O	1:X:94:LEU:CB	2.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:105:MET:HG3	1:X:106:TRP:N	1.88	0.86
2:Y:206:DG:C2'	4:Y:302:NCO:N3	2.34	0.85
1:X:106:TRP:CZ2	1:X:108:PRO:HB3	2.10	0.85
1:X:24:THR:HG22	1:X:27:GLU:HB2	1.57	0.84
1:X:34:MET:HA	1:X:34:MET:HE2	1.60	0.84
1:X:70:ASP:O	1:X:72:SER:N	2.11	0.83
1:X:99:LEU:HD12	1:X:99:LEU:C	2.00	0.82
2:Y:209:DT:H3	3:Z:219:DA:H62	0.83	0.81
1:X:49:HIS:O	1:X:52:THR:HG22	1.81	0.80
1:X:24:THR:HG22	1:X:27:GLU:CB	2.12	0.79
1:X:39:ARG:NH1	4:Y:302:NCO:N2	2.31	0.79
1:X:68:LYS:O	1:X:70:ASP:N	2.16	0.79
3:Z:217:DC:C2'	3:Z:218:DT:OP2	2.30	0.79
1:X:101:LEU:N	1:X:102:PRO:CD	2.46	0.78
1:X:49:HIS:HB3	1:X:51:GLU:OE2	1.84	0.78
1:X:1:MET:HG2	1:X:2:ARG:N	1.96	0.77
2:Y:205:DT:H2''	2:Y:206:DG:C5'	2.13	0.76
2:Y:209:DT:N3	3:Z:219:DA:N6	2.29	0.75
3:Z:215:DT:H2''	3:Z:216:DA:C5'	2.16	0.75
3:Z:218:DT:H5''	3:Z:218:DT:H6	1.52	0.75
2:Y:202:DC:H2''	2:Y:203:DC:H5'	1.70	0.73
3:Z:216:DA:H2''	3:Z:217:DC:C5'	2.17	0.73
1:X:101:LEU:HB3	1:X:102:PRO:HD3	1.68	0.73
2:Y:209:DT:C4	3:Z:219:DA:N6	2.56	0.73
3:Z:221:DC:C2'	3:Z:222:DC:H5'	2.17	0.73
1:X:25:TYR:HB2	2:Y:209:DT:OP1	1.88	0.72
1:X:33:GLY:O	1:X:35:PRO:HD3	1.89	0.72
3:Z:220:DG:H2''	3:Z:221:DC:O5'	1.90	0.71
3:Z:215:DT:C2'	3:Z:216:DA:H5''	2.21	0.71
1:X:99:LEU:CD1	1:X:99:LEU:C	2.59	0.70
2:Y:208:DC:O5'	4:Y:302:NCO:N6	2.24	0.69
2:Y:206:DG:H1'	4:Y:302:NCO:N5	2.07	0.69
1:X:98:LYS:HG3	1:X:99:LEU:N	2.08	0.68
3:Z:216:DA:C5'	3:Z:216:DA:C8	2.73	0.68
2:Y:203:DC:H2''	2:Y:204:DA:C8	2.29	0.68
1:X:24:THR:HG22	1:X:27:GLU:CG	2.23	0.67
2:Y:207:6OG:H3'	4:Y:302:NCO:N6	2.10	0.67
1:X:2:ARG:NH1	1:X:4:ASP:OD1	2.30	0.65
3:Z:218:DT:H2''	3:Z:219:DA:H5'	1.79	0.65
1:X:15:CYS:SG	1:X:54:VAL:HG13	2.37	0.65
2:Y:203:DC:H42	3:Z:225:DG:H1	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:106:TRP:CE2	1:X:108:PRO:HB3	2.32	0.64
1:X:39:ARG:HA	4:Y:302:NCO:N1	2.14	0.63
3:Z:221:DC:H2'	3:Z:222:DC:H5'	1.79	0.63
2:Y:206:DG:C4'	2:Y:206:DG:OP1	2.30	0.63
2:Y:203:DC:N4	3:Z:225:DG:H1	1.97	0.62
2:Y:211:DG:N2	3:Z:217:DC:O2	2.29	0.62
1:X:68:LYS:O	1:X:69:ARG:C	2.32	0.62
1:X:34:MET:HA	1:X:34:MET:CE	2.29	0.62
2:Y:210:DA:H2''	2:Y:211:DG:O5'	2.00	0.62
1:X:98:LYS:CG	1:X:99:LEU:N	2.62	0.61
1:X:95:GLY:O	1:X:96:GLU:C	2.38	0.61
2:Y:211:DG:H2'	2:Y:212:DT:H5'	1.82	0.60
1:X:69:ARG:CB	1:X:69:ARG:HH11	2.11	0.60
1:X:99:LEU:O	1:X:99:LEU:HD12	2.01	0.59
2:Y:210:DA:H5''	2:Y:210:DA:C8	2.38	0.58
2:Y:205:DT:C6	2:Y:205:DT:H5'	2.39	0.58
3:Z:218:DT:C6	3:Z:218:DT:H5''	2.39	0.57
3:Z:224:DT:H2''	3:Z:225:DG:C8	2.40	0.57
1:X:79:LYS:C	1:X:81:ARG:H	2.06	0.57
1:X:47:HIS:CD2	1:X:47:HIS:N	2.71	0.57
1:X:60:ILE:HB	1:X:65:THR:O	2.04	0.56
2:Y:211:DG:C3'	2:Y:212:DT:C5'	2.82	0.56
1:X:61:ASN:ND2	1:X:63:ARG:HD3	2.20	0.56
2:Y:208:DC:P	4:Y:302:NCO:N6	2.78	0.56
1:X:37:TYR:O	1:X:41:VAL:HG23	2.06	0.56
1:X:49:HIS:C	1:X:51:GLU:H	2.10	0.55
1:X:70:ASP:O	1:X:71:ILE:O	2.22	0.55
1:X:46:LYS:CE	2:Y:207:6OG:OP1	2.51	0.55
1:X:39:ARG:CA	4:Y:302:NCO:N1	2.69	0.55
1:X:101:LEU:H	1:X:102:PRO:CD	2.19	0.55
1:X:101:LEU:N	1:X:102:PRO:HD2	2.21	0.55
2:Y:206:DG:C8	2:Y:206:DG:H5''	2.42	0.55
1:X:92:THR:HB	1:X:94:LEU:O	2.07	0.55
1:X:39:ARG:HB2	1:X:40:GLN:NE2	2.22	0.54
2:Y:210:DA:H5''	2:Y:210:DA:H8	1.71	0.54
2:Y:206:DG:N3	4:Y:302:NCO:N5	2.56	0.54
1:X:1:MET:CG	1:X:2:ARG:N	2.71	0.54
1:X:90:TYR:CD1	1:X:90:TYR:N	2.76	0.53
3:Z:221:DC:C2'	3:Z:222:DC:C5'	2.86	0.53
1:X:25:TYR:HD1	1:X:61:ASN:HA	1.73	0.53
2:Y:205:DT:H6	2:Y:205:DT:H5'	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:39:ARG:HB3	4:Y:302:NCO:N1	2.23	0.53
1:X:79:LYS:HD3	1:X:97:TYR:CZ	2.42	0.53
1:X:14:VAL:HG12	1:X:55:PRO:HD2	1.91	0.53
1:X:68:LYS:C	1:X:70:ASP:H	2.12	0.53
1:X:75:GLU:CG	1:X:75:GLU:O	2.47	0.52
1:X:21:LYS:O	1:X:58:ARG:HD2	2.09	0.52
1:X:24:THR:HG22	1:X:27:GLU:H	1.70	0.52
1:X:45:MET:O	1:X:46:LYS:C	2.47	0.52
1:X:79:LYS:C	1:X:81:ARG:N	2.60	0.52
1:X:49:HIS:O	1:X:51:GLU:N	2.43	0.51
1:X:61:ASN:ND2	1:X:63:ARG:H	2.08	0.51
1:X:33:GLY:O	1:X:34:MET:HE3	2.11	0.51
1:X:101:LEU:HD12	1:X:105:MET:HB2	1.91	0.51
1:X:3:MET:HG3	3:Z:224:DT:OP1	2.11	0.51
1:X:23:SER:OG	1:X:24:THR:N	2.43	0.51
2:Y:204:DA:H2'	2:Y:204:DA:O5'	2.10	0.51
1:X:39:ARG:NE	4:Y:302:NCO:N2	2.59	0.51
1:X:1:MET:HG3	1:X:5:GLU:HB2	1.92	0.50
1:X:98:LYS:HG3	1:X:99:LEU:H	1.74	0.50
1:X:33:GLY:C	1:X:35:PRO:HD3	2.31	0.50
1:X:49:HIS:C	1:X:51:GLU:N	2.65	0.50
3:Z:214:DC:O4'	3:Z:214:DC:O2	2.29	0.50
2:Y:204:DA:H1'	2:Y:205:DT:H5''	1.94	0.50
1:X:25:TYR:CD1	1:X:61:ASN:HA	2.47	0.49
1:X:64:GLY:CA	1:X:101:LEU:HD22	2.42	0.49
1:X:101:LEU:N	1:X:102:PRO:HD3	2.27	0.49
1:X:13:ALA:O	1:X:16:GLU:HB2	2.13	0.49
3:Z:226:DG:O6	4:Z:303:NCO:N3	2.46	0.49
1:X:45:MET:O	1:X:48:LEU:HD12	2.13	0.49
1:X:43:GLN:O	1:X:44:ALA:C	2.50	0.49
1:X:24:THR:CG2	1:X:27:GLU:HG2	2.43	0.48
1:X:92:THR:OG1	1:X:96:GLU:HB2	2.12	0.48
1:X:28:ILE:O	1:X:29:ALA:C	2.50	0.48
1:X:24:THR:HG22	1:X:27:GLU:HG2	1.93	0.48
3:Z:223:DA:H2''	3:Z:224:DT:C5'	2.44	0.48
2:Y:206:DG:H5'	2:Y:206:DG:H2'	1.61	0.47
3:Z:216:DA:H2''	3:Z:217:DC:OP2	2.15	0.47
1:X:39:ARG:CB	4:Y:302:NCO:N1	2.77	0.47
3:Z:219:DA:H5'	3:Z:219:DA:H2'	1.56	0.47
3:Z:223:DA:H2''	3:Z:224:DT:H5'	1.96	0.47
1:X:24:THR:CG2	1:X:27:GLU:N	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:82:LEU:O	1:X:87:VAL:HB	2.15	0.46
1:X:92:THR:HG22	1:X:93:SER:O	2.15	0.46
1:X:39:ARG:HD2	3:Z:221:DC:O2	2.16	0.46
1:X:39:ARG:CZ	4:Y:302:NCO:N2	2.78	0.46
1:X:37:TYR:HD2	1:X:40:GLN:HG3	1.80	0.45
2:Y:207:6OG:H2'	2:Y:207:6OG:H5'	1.18	0.45
1:X:61:ASN:HD21	1:X:63:ARG:HD3	1.79	0.45
2:Y:205:DT:C2'	2:Y:206:DG:H5''	2.21	0.45
3:Z:216:DA:C2'	3:Z:217:DC:C5'	2.93	0.45
1:X:37:TYR:CD1	1:X:37:TYR:N	2.85	0.44
1:X:79:LYS:HD3	1:X:97:TYR:CE2	2.52	0.44
1:X:101:LEU:HB3	1:X:102:PRO:CD	2.43	0.44
1:X:14:VAL:CG1	1:X:54:VAL:HG12	2.47	0.44
1:X:101:LEU:H	1:X:102:PRO:HD3	1.81	0.44
1:X:69:ARG:NH2	1:X:78:GLN:OE1	2.49	0.43
3:Z:216:DA:C5'	3:Z:216:DA:H8	2.10	0.43
1:X:75:GLU:HG2	1:X:76:GLN:N	2.17	0.43
3:Z:221:DC:C3'	3:Z:222:DC:H5'	2.48	0.43
1:X:42:GLY:O	1:X:45:MET:HB2	2.19	0.43
1:X:14:VAL:O	1:X:17:ILE:HG13	2.19	0.43
1:X:100:ASN:OD1	1:X:103:GLU:N	2.40	0.42
1:X:74:GLY:O	1:X:77:ARG:HB2	2.20	0.42
1:X:37:TYR:CD2	1:X:40:GLN:HG3	2.54	0.42
1:X:43:GLN:O	1:X:47:HIS:CD2	2.73	0.41
1:X:97:TYR:HD1	1:X:97:TYR:HA	1.50	0.41
3:Z:214:DC:H2'	3:Z:215:DT:C6	2.55	0.41
1:X:70:ASP:OD2	2:Y:206:DG:H3'	2.21	0.41
1:X:45:MET:O	2:Y:207:6OG:H3	2.20	0.41
3:Z:216:DA:H1'	3:Z:217:DC:H5''	2.03	0.41
1:X:68:LYS:C	1:X:70:ASP:N	2.66	0.41
1:X:28:ILE:HD12	1:X:28:ILE:HG23	1.61	0.41
2:Y:202:DC:H2''	2:Y:203:DC:C5'	2.47	0.41
1:X:64:GLY:HA3	1:X:101:LEU:HD22	2.03	0.40
1:X:25:TYR:OH	2:Y:207:6OG:H1'	2.21	0.40
2:Y:207:6OG:C5'	2:Y:207:6OG:H8	2.51	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	X	106/116 (91%)	82 (77%)	18 (17%)	6 (6%)	<b>2</b> <b>3</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	70	ASP
1	X	71	ILE
1	X	75	GLU
1	X	95	GLY
1	X	74	GLY
1	X	96	GLU

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	X	95/102 (93%)	79 (83%)	16 (17%)	<b>2</b> <b>6</b>

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	1	MET
1	X	2	ARG
1	X	3	MET
1	X	9	LYS
1	X	24	THR

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Mol	Chain	Res	Type
1	X	40	GLN
1	X	48	LEU
1	X	52	THR
1	X	61	ASN
1	X	69	ARG
1	X	70	ASP
1	X	75	GLU
1	X	81	ARG
1	X	91	GLN
1	X	99	LEU
1	X	101	LEU

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

Mol	Chain	Res	Type
1	X	40	GLN
1	X	47	HIS
1	X	76	GLN
1	X	91	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z  > 2$
2	6OG	Y	207	2	17,25,26	1.40	4 (23%)	20,36,39	3.36	10 (50%)

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
2	6OG	Y	207	2	-	0/5/23/24	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	207	6OG	C5-C4	-2.09	1.35	1.40
2	Y	207	6OG	C2'-C3'	-2.04	1.47	1.52
2	Y	207	6OG	C6-N1	2.39	1.36	1.31
2	Y	207	6OG	C8-N7	2.81	1.39	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	207	6OG	C4-C5-N7	-5.48	104.11	109.41
2	Y	207	6OG	C2'-C3'-C4'	-4.39	93.38	102.73
2	Y	207	6OG	O4'-C1'-C2'	-3.17	100.17	106.25
2	Y	207	6OG	C2'-C1'-N9	-3.01	107.13	114.23
2	Y	207	6OG	O3'-C3'-C2'	-2.94	100.15	110.83
2	Y	207	6OG	O4'-C4'-C5'	-2.93	99.52	109.40
2	Y	207	6OG	O6-C6-N1	-2.78	115.21	119.03
2	Y	207	6OG	N3-C2-N1	-2.68	123.55	127.46
2	Y	207	6OG	N2-C2-N1	2.35	121.00	117.24
2	Y	207	6OG	C2-N3-C4	10.04	126.88	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	207	6OG	7	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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	$\# Z  > 2$
4	NCO	Y	302	-	6,6,6	0.95	0	0,15,15	0.00	-
4	NCO	Z	303	-	6,6,6	3.24	5 (83%)	0,15,15	0.00	-

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
4	NCO	Y	302	-	-	0/0/0/0	0/0/0/0
4	NCO	Z	303	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	303	NCO	CO-N4	2.21	2.05	1.97
4	Z	303	NCO	CO-N2	2.69	2.07	1.97
4	Z	303	NCO	CO-N3	3.43	2.10	1.97
4	Z	303	NCO	CO-N1	4.11	2.13	1.97
4	Z	303	NCO	CO-N6	4.34	2.14	1.97

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 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	302	NCO	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	303	NCO	1	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	108/116 (93%)	-0.22	1 (0%) 84 85	21, 38, 56, 62	0
2	Y	12/13 (92%)	-0.65	0 100 100	26, 38, 43, 50	0
3	Z	13/13 (100%)	-0.87	0 100 100	21, 37, 49, 53	0
All	All	133/142 (93%)	-0.32	1 (0%) 86 86	21, 38, 55, 62	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	90	TYR	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	6OG	Y	207	23/24	0.98	0.15	-	19,27,32,41	0

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NCO	Y	302	7/7	0.82	0.72	16.59	127,129,131,132	0
4	NCO	Z	303	7/7	0.81	0.45	7.36	103,105,107,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.