



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:18 am BST

PDB ID : 5A39  
Title : Structure of Rad14 in complex with cisplatin containing DNA  
Authors : Koch, S.C.; Kuper, J.; Gasteiger, K.L.; Wichlein, N.; Strasser, R.; Eisen, D.; Geiger, S.; Schneider, S.; Kisker, C.; Carell, T.  
Deposited on : 2015-05-28  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

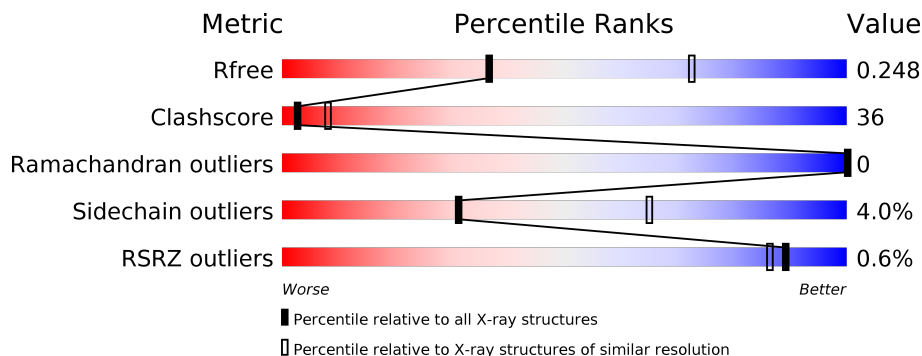
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.




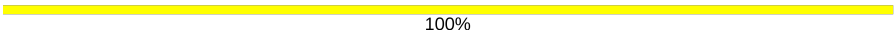
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	A	115	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 11%, yellow 88%, green 100%);"></div> <div style="margin-left: 10px;"> <p>7%</p> <p>88%</p> <p>11%</p> </div> </div>
1	B	115	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 90%, yellow 99%, green 100%);"></div> <div style="margin-left: 10px;"> <p>90%</p> <p>9%</p> </div> </div>
2	C	15	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 80%, orange 100%);"></div> <div style="margin-left: 10px;"> <p>80%</p> <p>20%</p> </div> </div>
2	D	15	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, orange 87%, yellow 97%, green 100%);"></div> <div style="margin-left: 10px;"> <p>7%</p> <p>80%</p> <p>20%</p> </div> </div>
3	E	13	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 23%, yellow 77%, green 100%);"></div> <div style="margin-left: 10px;"> <p>23%</p> <p>77%</p> </div> </div>
3	F	13	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 23%, yellow 77%, green 100%);"></div> <div style="margin-left: 10px;"> <p>23%</p> <p>77%</p> </div> </div>

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Mol	Chain	Length	Quality of chain
4	G	13	 8% 92%
4	H	13	 100%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4088 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 DNA REPAIR PROTEIN RAD14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	114	Total 940	C 594	N 161	O 177	S 8	0	0	0
1	B	115	Total 936	C 591	N 159	O 178	S 8	0	0	0

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	15	Total 557	C 270	N 93	O 168	P 26	0	15	0
2	D	15	Total 557	C 270	N 93	O 168	P 26	0	15	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	13	Total 270	C 128	N 52	O 77	P 13	0	13	0
3	F	13	Total 270	C 128	N 52	O 77	P 13	0	13	0

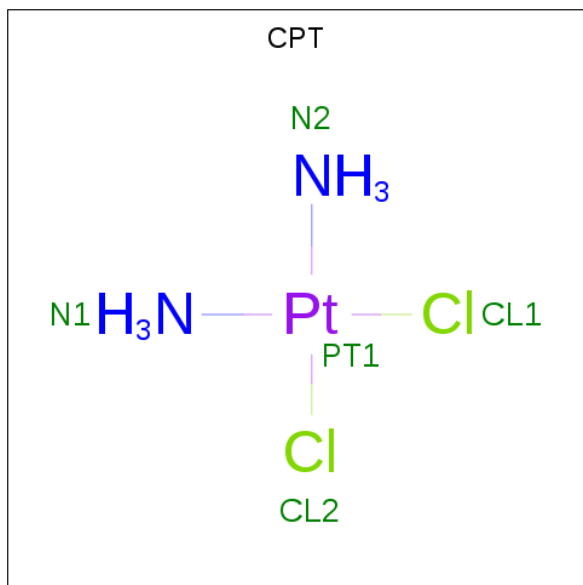
- Molecule 4 is a DNA chain called 5'-D(\*DGP\*AP\*TP\*GP\*AP\*CP\*CP\*GP\*TP\*AP\*GP\*AP\*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	G	13	Total 272	C 128	N 55	O 76	P 13	0	13	0
4	H	13	Total 272	C 128	N 55	O 76	P 13	0	13	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	A	1	Total Zn 1 1	0	0

- Molecule 6 is Cisplatin (three-letter code: CPT) (formula:  $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$ ).

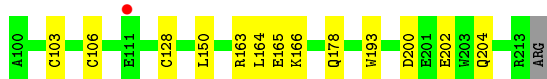
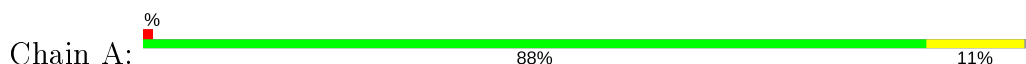


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total N Pt 3 2 1	0	0
6	C	1	Total N Pt 3 2 1	0	0
6	D	1	Total N Pt 3 2 1	0	0
6	D	1	Total N Pt 3 2 1	0	0

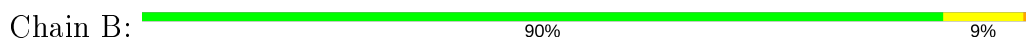
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

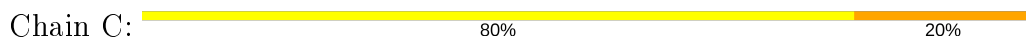
- Molecule 1: DNA REPAIR PROTEIN RAD14



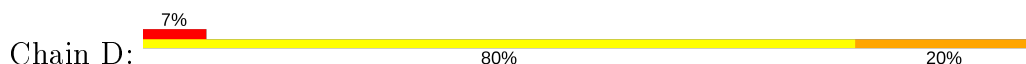
- Molecule 1: DNA REPAIR PROTEIN RAD14



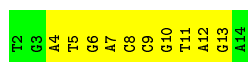
- Molecule 2: DNA



- Molecule 2: DNA

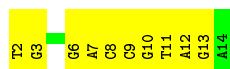


- Molecule 3: 5'-D(\*DTP\*GP\*AP\*TP\*GP\*AP\*CP\*CP\*GP\*TP\*AP\*GP\*AP)-3'



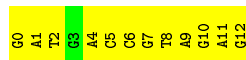
- Molecule 3: 5'-D(\*DTP\*GP\*AP\*TP\*GP\*AP\*CP\*CP\*GP\*TP\*AP\*GP\*AP)-3'





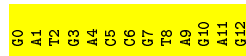
- Molecule 4: 5'-D(\*DGP\*AP\*TP\*GP\*AP\*CP\*CP\*GP\*TP\*AP\*GP\*AP\*GP)-3'

Chain G: 8% 92%



- Molecule 4: 5'-D(\*DGP\*AP\*TP\*GP\*AP\*CP\*CP\*GP\*TP\*AP\*GP\*AP\*GP)-3'

Chain H: 100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.42Å 54.42Å 130.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.42 – 2.80 36.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (54.42-2.80) 99.7 (36.92-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.213 , 0.256 0.209 , 0.248	Depositor DCC
$R_{free}$ test set	430 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtrriage
Anisotropy	0.180	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 25.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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 i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.81	0/964	0.83	0/1297
1	B	0.86	0/959	0.82	0/1292
2	C	1.79	22/622 (3.5%)	2.61	41/951 (4.3%)
2	D	1.76	24/622 (3.9%)	2.76	40/951 (4.2%)
3	E	0.24	0/303	0.69	0/466
3	F	0.33	0/303	0.73	0/466
4	G	0.27	0/306	0.75	0/471
4	H	0.35	0/306	0.73	0/471
All	All	1.11	46/4385 (1.0%)	1.61	81/6365 (1.3%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8[A]	DG	C5-C4	14.25	1.48	1.38
2	C	8[B]	DG	C5-C4	14.25	1.48	1.38
2	D	8[C]	DG	C5-C4	13.81	1.48	1.38
2	D	8[D]	DG	C5-C4	13.81	1.48	1.38
2	D	9[C]	DG	C5-C4	11.79	1.46	1.38
2	D	9[D]	DG	C5-C4	11.79	1.46	1.38
2	C	9[A]	DG	C5-C4	10.94	1.46	1.38
2	C	9[B]	DG	C5-C4	10.94	1.46	1.38
2	C	8[A]	DG	C8-N7	9.93	1.36	1.30
2	C	8[B]	DG	C8-N7	9.93	1.36	1.30
2	C	9[A]	DG	C8-N7	9.76	1.36	1.30
2	C	9[B]	DG	C8-N7	9.76	1.36	1.30
2	D	9[C]	DG	C8-N7	9.52	1.36	1.30
2	D	9[D]	DG	C8-N7	9.52	1.36	1.30
2	D	8[C]	DG	C8-N7	9.12	1.36	1.30
2	D	8[D]	DG	C8-N7	9.12	1.36	1.30
2	C	9[A]	DG	N7-C5	-8.69	1.34	1.39
2	C	9[B]	DG	N7-C5	-8.69	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9[A]	DG	N9-C4	-7.37	1.32	1.38
2	C	9[B]	DG	N9-C4	-7.37	1.32	1.38
2	C	9[A]	DG	C6-N1	-7.24	1.34	1.39
2	C	9[B]	DG	C6-N1	-7.24	1.34	1.39
2	D	9[C]	DG	C6-N1	-7.01	1.34	1.39
2	D	9[D]	DG	C6-N1	-7.01	1.34	1.39
2	D	9[C]	DG	N9-C4	-6.83	1.32	1.38
2	D	9[D]	DG	N9-C4	-6.83	1.32	1.38
2	C	8[A]	DG	C6-N1	-6.77	1.34	1.39
2	C	8[B]	DG	C6-N1	-6.77	1.34	1.39
2	D	9[C]	DG	N7-C5	-6.41	1.35	1.39
2	D	9[D]	DG	N7-C5	-6.41	1.35	1.39
2	D	8[C]	DG	C5-C6	6.41	1.48	1.42
2	D	8[D]	DG	C5-C6	6.41	1.48	1.42
2	D	8[C]	DG	C6-N1	-6.24	1.35	1.39
2	D	8[D]	DG	C6-N1	-6.24	1.35	1.39
2	C	8[A]	DG	C5-C6	6.23	1.48	1.42
2	C	8[B]	DG	C5-C6	6.23	1.48	1.42
2	D	8[C]	DG	N7-C5	-6.07	1.35	1.39
2	D	8[D]	DG	N7-C5	-6.07	1.35	1.39
2	C	8[A]	DG	N9-C4	-6.00	1.33	1.38
2	C	8[B]	DG	N9-C4	-6.00	1.33	1.38
2	D	9[C]	DG	C5-C6	5.86	1.48	1.42
2	D	9[D]	DG	C5-C6	5.86	1.48	1.42
2	D	8[C]	DG	N9-C4	-5.18	1.33	1.38
2	D	8[D]	DG	N9-C4	-5.18	1.33	1.38
2	C	9[A]	DG	C5-C6	5.12	1.47	1.42
2	C	9[B]	DG	C5-C6	5.12	1.47	1.42

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9[C]	DG	C2-N3-C4	18.09	120.94	111.90
2	D	9[D]	DG	C2-N3-C4	18.09	120.94	111.90
2	D	8[C]	DG	N3-C4-C5	-17.88	119.66	128.60
2	D	8[D]	DG	N3-C4-C5	-17.88	119.66	128.60
2	D	8[C]	DG	C2-N3-C4	17.68	120.74	111.90
2	D	8[D]	DG	C2-N3-C4	17.68	120.74	111.90
2	C	9[A]	DG	N3-C4-C5	-17.39	119.90	128.60
2	C	9[B]	DG	N3-C4-C5	-17.39	119.90	128.60
2	D	9[C]	DG	N3-C4-C5	-17.18	120.01	128.60
2	D	9[D]	DG	N3-C4-C5	-17.18	120.01	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9[A]	DG	C2-N3-C4	17.00	120.40	111.90
2	C	9[B]	DG	C2-N3-C4	17.00	120.40	111.90
2	C	8[A]	DG	C2-N3-C4	15.90	119.85	111.90
2	C	8[B]	DG	C2-N3-C4	15.90	119.85	111.90
2	C	8[A]	DG	N3-C4-C5	-15.73	120.73	128.60
2	C	8[B]	DG	N3-C4-C5	-15.73	120.73	128.60
2	D	9[C]	DG	C5-C6-N1	14.32	118.66	111.50
2	D	9[D]	DG	C5-C6-N1	14.32	118.66	111.50
2	C	9[A]	DG	C5-C6-O6	-13.91	120.25	128.60
2	C	9[B]	DG	C5-C6-O6	-13.91	120.25	128.60
2	C	8[A]	DG	C5-C6-N1	13.56	118.28	111.50
2	C	8[B]	DG	C5-C6-N1	13.56	118.28	111.50
2	D	9[C]	DG	C5-C6-O6	-13.56	120.47	128.60
2	D	9[D]	DG	C5-C6-O6	-13.56	120.47	128.60
2	D	8[C]	DG	N3-C4-N9	13.39	134.03	126.00
2	D	8[D]	DG	N3-C4-N9	13.39	134.03	126.00
2	D	8[C]	DG	C5-C6-N1	12.92	117.96	111.50
2	D	8[D]	DG	C5-C6-N1	12.92	117.96	111.50
2	D	9[C]	DG	C6-C5-N7	12.85	138.11	130.40
2	D	9[D]	DG	C6-C5-N7	12.85	138.11	130.40
2	C	8[A]	DG	C5-C6-O6	-12.84	120.90	128.60
2	C	8[B]	DG	C5-C6-O6	-12.84	120.90	128.60
2	C	9[A]	DG	C5-C6-N1	12.48	117.74	111.50
2	C	9[B]	DG	C5-C6-N1	12.48	117.74	111.50
2	D	8[C]	DG	C5-C6-O6	-12.13	121.32	128.60
2	D	8[D]	DG	C5-C6-O6	-12.13	121.32	128.60
2	D	9[C]	DG	C4-C5-N7	-11.79	106.08	110.80
2	D	9[D]	DG	C4-C5-N7	-11.79	106.08	110.80
2	C	8[A]	DG	C6-C5-N7	11.61	137.37	130.40
2	C	8[B]	DG	C6-C5-N7	11.61	137.37	130.40
2	C	8[A]	DG	N3-C4-N9	11.60	132.96	126.00
2	C	8[B]	DG	N3-C4-N9	11.60	132.96	126.00
2	C	9[A]	DG	N3-C4-N9	11.53	132.92	126.00
2	C	9[B]	DG	N3-C4-N9	11.53	132.92	126.00
2	D	8[C]	DG	O4'-C1'-N9	11.27	115.89	108.00
2	D	8[D]	DG	O4'-C1'-N9	11.27	115.89	108.00
2	D	9[C]	DG	N3-C4-N9	11.26	132.76	126.00
2	D	9[D]	DG	N3-C4-N9	11.26	132.76	126.00
2	D	8[C]	DG	C6-C5-N7	10.87	136.92	130.40
2	D	8[D]	DG	C6-C5-N7	10.87	136.92	130.40
2	C	9[A]	DG	C4-C5-N7	-10.70	106.52	110.80
2	C	9[B]	DG	C4-C5-N7	-10.70	106.52	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9[A]	DG	C6-C5-N7	10.31	136.58	130.40
2	C	9[B]	DG	C6-C5-N7	10.31	136.58	130.40
2	D	8[C]	DG	C4-C5-N7	-10.15	106.74	110.80
2	D	8[D]	DG	C4-C5-N7	-10.15	106.74	110.80
2	C	8[A]	DG	C4-C5-N7	-9.14	107.14	110.80
2	C	8[B]	DG	C4-C5-N7	-9.14	107.14	110.80
2	C	8[A]	DG	O4'-C1'-N9	9.02	114.31	108.00
2	C	8[B]	DG	O4'-C1'-N9	9.02	114.31	108.00
2	C	9[A]	DG	C5-N7-C8	6.18	107.39	104.30
2	C	9[B]	DG	C5-N7-C8	6.18	107.39	104.30
2	D	9[C]	DG	C5-N7-C8	5.71	107.16	104.30
2	D	9[D]	DG	C5-N7-C8	5.71	107.16	104.30
2	D	8[C]	DG	C5-N7-C8	5.71	107.15	104.30
2	D	8[D]	DG	C5-N7-C8	5.71	107.15	104.30
2	D	1[C]	DT	C5'-C4'-C3'	5.54	124.07	114.10
2	C	8[A]	DG	C4-C5-C6	-5.52	115.49	118.80
2	C	8[B]	DG	C4-C5-C6	-5.52	115.49	118.80
2	D	1[C]	DT	C5'-C4'-O4'	5.52	119.78	109.30
2	C	9[A]	DG	N7-C8-N9	-5.36	110.42	113.10
2	C	9[B]	DG	N7-C8-N9	-5.36	110.42	113.10
2	C	8[A]	DG	C8-N9-C4	5.34	108.54	106.40
2	C	8[B]	DG	C8-N9-C4	5.34	108.54	106.40
2	D	8[C]	DG	C8-N9-C4	5.28	108.51	106.40
2	D	8[D]	DG	C8-N9-C4	5.28	108.51	106.40
2	D	9[C]	DG	C8-N9-C4	5.25	108.50	106.40
2	D	9[D]	DG	C8-N9-C4	5.25	108.50	106.40
2	C	1[A]	DT	C5'-C4'-C3'	5.23	123.52	114.10
2	C	9[A]	DG	C8-N9-C4	5.22	108.49	106.40
2	C	9[B]	DG	C8-N9-C4	5.22	108.49	106.40

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	A	940	0	889	5	0
1	B	936	0	875	8	0
2	C	557	0	289	71	0
2	D	557	0	291	82	0
3	E	270	0	126	28	0
3	F	270	0	122	40	0
4	G	272	0	123	30	0
4	H	272	0	123	21	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	C	6	0	0	2	0
6	D	6	0	0	1	0
All	All	4088	0	2838	241	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 36.

All (241) 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:D:5[C]:DT:H2''	2:D:6[C]:DA:C8	1.37	1.57
2:D:8[D]:DG:N2	3:F:10[D]:DG:C2	1.88	1.37
3:F:8[D]:DC:H2''	3:F:9[D]:DC:C5'	1.65	1.26
2:C:5[A]:DT:H2''	2:C:6[A]:DA:C8	1.75	1.20
2:D:8[C]:DG:C2'	2:D:9[C]:DG:H5''	1.72	1.20
2:D:5[C]:DT:C2'	2:D:6[C]:DA:C8	2.27	1.16
2:D:5[C]:DT:H2''	2:D:6[C]:DA:N7	1.64	1.11
4:H:7[C]:DG:H2'	4:H:8[C]:DT:C7	1.84	1.07
4:H:7[C]:DG:H2'	4:H:8[C]:DT:H71	1.37	1.07
3:F:8[D]:DC:C2'	3:F:9[D]:DC:H5'	1.86	1.06
2:C:2[B]:DC:C3'	2:C:3[B]:DT:H5'	1.88	1.04
2:D:5[C]:DT:C2'	2:D:6[C]:DA:N7	2.19	1.04
2:C:8[B]:DG:N3	3:E:10[B]:DG:N2	1.84	1.03
4:G:0[A]:DG:N2	4:G:1[A]:DA:N3	2.06	1.02
2:D:8[C]:DG:H2''	2:D:9[C]:DG:H5''	1.03	1.01
2:C:1[A]:DT:H3'	2:C:2[A]:DC:H5'	1.44	0.99
2:D:2[D]:DC:H3'	2:D:2[D]:DC:O2	1.62	0.98
3:F:8[D]:DC:H2''	3:F:9[D]:DC:H5'	1.02	0.98
2:C:2[B]:DC:H3'	2:C:3[B]:DT:H5'	1.45	0.98
4:H:10[C]:DG:H1'	4:H:11[C]:DA:H5'	1.47	0.96
3:E:11[B]:DT:H2''	3:E:12[B]:DA:C8	2.03	0.94
2:D:9[D]:DG:C8	2:D:10[D]:DT:C7	2.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9[D]:DG:C8	2:D:10[D]:DT:H73	2.04	0.92
2:D:8[C]:DG:H2''	2:D:9[C]:DG:C5'	1.96	0.92
2:D:1[C]:DT:H3'	2:D:2[C]:DC:H5'	1.52	0.91
2:C:5[A]:DT:C2'	2:C:6[A]:DA:C8	2.54	0.91
2:C:5[A]:DT:H2''	2:C:6[A]:DA:H8	1.24	0.91
4:G:0[A]:DG:N2	4:G:1[A]:DA:C2	2.40	0.90
2:D:8[C]:DG:C2'	2:D:9[C]:DG:C5'	2.50	0.89
4:H:7[C]:DG:C2'	4:H:8[C]:DT:H71	2.03	0.89
2:D:2[D]:DC:O2	2:D:2[D]:DC:C3'	2.21	0.87
2:C:10[B]:DT:N3	3:E:7[B]:DA:N1	2.23	0.86
2:C:2[B]:DC:C2'	2:C:3[B]:DT:H5'	2.06	0.85
2:D:8[D]:DG:N2	3:F:10[D]:DG:N2	2.25	0.83
2:D:4[D]:DC:N3	3:F:13[D]:DG:N1	2.25	0.83
2:D:12[D]:DA:C8	2:D:13[D]:DT:H73	2.14	0.82
4:G:0[A]:DG:N2	4:G:1[A]:DA:C4	2.49	0.81
2:D:5[C]:DT:H2''	2:D:6[C]:DA:H8	1.04	0.81
4:G:5[A]:DC:H2''	4:G:6[A]:DC:H5'	1.61	0.80
2:C:9[B]:DG:N7	6:C:1015:CPT:N2	2.28	0.80
2:D:5[D]:DT:N3	3:F:12[D]:DA:N1	2.30	0.80
2:D:13[C]:DT:C5	2:D:14[C]:DC:N4	2.50	0.79
2:D:9[D]:DG:C8	2:D:10[D]:DT:H71	2.18	0.79
2:D:4[D]:DC:N4	3:F:13[D]:DG:O6	2.18	0.77
2:C:12[B]:DA:C2	3:E:6[B]:DG:N2	2.52	0.77
4:G:0[A]:DG:C2	4:G:1[A]:DA:C4	2.74	0.76
2:C:10[A]:DT:O4	4:G:4[A]:DA:N6	2.19	0.76
3:F:6[D]:DG:H2''	3:F:7[D]:DA:C8	2.22	0.75
2:D:12[D]:DA:C8	2:D:13[D]:DT:C7	2.69	0.75
2:D:9[D]:DG:C8	6:D:1015:CPT:N2	2.51	0.75
4:G:5[A]:DC:C2'	4:G:6[A]:DC:H5'	2.16	0.75
2:D:12[D]:DA:H2'	2:D:13[D]:DT:H71	1.67	0.75
2:C:1[A]:DT:H3'	2:C:2[A]:DC:C5'	2.16	0.75
2:C:7[B]:DC:N4	3:E:10[B]:DG:O6	2.20	0.74
2:D:8[D]:DG:N2	3:F:10[D]:DG:N3	2.36	0.74
3:E:8[B]:DC:H2''	3:E:9[B]:DC:H5'	1.68	0.74
2:D:8[D]:DG:N2	3:F:10[D]:DG:N1	2.33	0.74
2:D:12[D]:DA:C2'	2:D:13[D]:DT:H71	2.17	0.74
3:F:12[D]:DA:H2''	3:F:13[D]:DG:H5'	1.71	0.73
2:C:6[B]:DA:N1	3:E:11[B]:DT:N3	2.37	0.73
4:H:7[C]:DG:H2''	4:H:8[C]:DT:C6	2.22	0.73
2:C:1[A]:DT:C3'	2:C:2[A]:DC:C5'	2.66	0.73
2:C:6[A]:DA:C2'	2:C:7[A]:DC:H5'	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2[B]:DC:C3'	2:C:3[B]:DT:C5'	2.65	0.72
2:D:1[C]:DT:H3'	2:D:2[C]:DC:C5'	2.19	0.72
2:C:2[B]:DC:C2'	2:C:3[B]:DT:C5'	2.68	0.72
2:D:4[D]:DC:O2	3:F:13[D]:DG:N2	2.22	0.72
2:D:9[D]:DG:N9	2:D:10[D]:DT:H71	2.05	0.72
2:D:4[C]:DC:O2	2:D:5[C]:DT:C2	2.43	0.70
2:D:5[D]:DT:O4	3:F:12[D]:DA:N6	2.24	0.70
2:C:6[A]:DA:H2''	2:C:7[A]:DC:H5'	1.71	0.70
3:F:6[D]:DG:C2'	3:F:7[D]:DA:C8	2.74	0.70
2:C:1[A]:DT:C3'	2:C:2[A]:DC:H5'	2.20	0.69
2:C:10[B]:DT:O4	3:E:7[B]:DA:N6	2.26	0.68
2:C:9[B]:DG:C8	6:C:1015:CPT:N2	2.61	0.68
4:H:10[C]:DG:C1'	4:H:11[C]:DA:H5'	2.21	0.68
2:C:5[B]:DT:H2''	2:C:6[B]:DA:C8	2.28	0.68
2:C:4[A]:DC:O2	2:C:5[A]:DT:C2	2.46	0.68
2:C:10[B]:DT:C4	3:E:7[B]:DA:N1	2.63	0.67
2:C:11[B]:DC:N3	3:E:6[B]:DG:N1	2.43	0.66
2:C:1[A]:DT:C2'	2:C:2[A]:DC:H5''	2.26	0.66
4:H:7[C]:DG:C2'	4:H:8[C]:DT:C7	2.65	0.66
2:C:5[A]:DT:H2''	2:C:6[A]:DA:N7	2.08	0.65
3:F:9[D]:DC:C6	3:F:10[D]:DG:N7	2.64	0.65
2:D:4[C]:DC:C2	2:D:5[C]:DT:C2	2.84	0.65
2:D:9[D]:DG:N7	2:D:10[D]:DT:H73	2.12	0.65
2:D:4[C]:DC:C2'	2:D:5[C]:DT:C6	2.80	0.64
2:D:9[D]:DG:N9	2:D:10[D]:DT:C7	2.59	0.64
2:C:13[A]:DT:C5	2:C:14[A]:DC:N4	2.66	0.64
2:C:5[A]:DT:C1'	2:C:6[A]:DA:C8	2.81	0.64
2:C:10[B]:DT:N3	3:E:7[B]:DA:C2	2.66	0.64
4:H:4[C]:DA:H2''	4:H:5[C]:DC:O5'	1.96	0.64
3:F:8[D]:DC:H2''	3:F:9[D]:DC:H5''	1.71	0.64
2:C:5[B]:DT:O2	3:E:13[B]:DG:N2	2.31	0.63
2:C:13[A]:DT:H2''	2:C:14[A]:DC:C6	2.33	0.63
2:C:2[B]:DC:H2''	2:C:3[B]:DT:H5''	1.81	0.62
3:F:6[D]:DG:H2''	3:F:7[D]:DA:H8	1.64	0.62
2:C:10[B]:DT:O4	3:E:7[B]:DA:N1	2.31	0.62
3:E:6[B]:DG:H2''	3:E:7[B]:DA:C8	2.33	0.62
4:H:7[C]:DG:C2'	4:H:8[C]:DT:C5	2.83	0.62
4:G:0[A]:DG:C2	4:G:1[A]:DA:C5	2.87	0.62
2:C:13[B]:DT:C2	2:C:14[B]:DC:N3	2.68	0.61
1:A:106:CYS:HB3	1:A:128:CYS:SG	2.40	0.61
4:H:7[C]:DG:H2'	4:H:8[C]:DT:C5	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2[D]:DT:H2''	3:F:3[D]:DG:C5'	2.30	0.61
2:D:1[C]:DT:C3'	2:D:2[C]:DC:H5'	2.29	0.61
4:G:0[A]:DG:N1	4:G:1[A]:DA:C6	2.69	0.60
2:C:11[B]:DC:O2	3:E:6[B]:DG:N2	2.35	0.60
2:D:4[C]:DC:C2	2:D:5[C]:DT:N3	2.70	0.59
2:D:4[C]:DC:H2'	2:D:5[C]:DT:C6	2.37	0.59
2:C:7[B]:DC:N3	3:E:10[B]:DG:N1	2.50	0.59
3:F:2[D]:DT:H2''	3:F:3[D]:DG:H5''	1.84	0.59
2:C:5[A]:DT:H1'	2:C:6[A]:DA:C8	2.38	0.59
2:D:4[C]:DC:H2''	2:D:5[C]:DT:C6	2.38	0.58
4:G:10[A]:DG:H2''	4:G:11[A]:DA:OP2	2.01	0.58
2:C:13[B]:DT:H2''	2:C:14[B]:DC:C6	2.38	0.58
3:E:8[B]:DC:H2''	3:E:9[B]:DC:C5'	2.34	0.58
2:C:6[B]:DA:H2''	2:C:7[B]:DC:C6	2.37	0.58
2:D:5[C]:DT:C1'	2:D:6[C]:DA:C8	2.86	0.58
2:D:9[D]:DG:C2'	2:D:10[D]:DT:H71	2.34	0.58
2:D:4[C]:DC:H2''	2:D:5[C]:DT:O4'	2.04	0.58
4:H:8[C]:DT:H2''	4:H:9[C]:DA:C8	2.39	0.56
4:G:6[A]:DC:H2''	4:G:7[A]:DG:O5'	2.05	0.56
2:C:4[A]:DC:C2	2:C:5[A]:DT:N3	2.72	0.56
4:H:0[C]:DG:N2	4:H:1[C]:DA:C2	2.73	0.56
2:C:3[A]:DT:C2	4:G:12[A]:DG:N2	2.73	0.56
2:C:2[B]:DC:H2''	2:C:3[B]:DT:C5'	2.36	0.56
2:D:7[D]:DC:O2	3:F:10[D]:DG:N2	2.39	0.56
3:F:12[D]:DA:H2''	3:F:13[D]:DG:C5'	2.36	0.56
4:G:11[A]:DA:H2''	4:G:12[A]:DG:OP2	2.04	0.55
2:C:12[A]:DA:H2''	2:C:13[A]:DT:C6	2.40	0.55
4:G:4[A]:DA:N7	4:G:5[A]:DC:N4	2.54	0.55
2:C:11[B]:DC:N4	3:E:6[B]:DG:O6	2.40	0.55
2:D:8[C]:DG:H2'	2:D:9[C]:DG:C5'	2.35	0.55
3:F:9[D]:DC:H1'	3:F:10[D]:DG:C8	2.42	0.55
2:D:2[D]:DC:C4'	2:D:2[D]:DC:O2	2.55	0.55
4:G:6[A]:DC:C2'	4:G:7[A]:DG:O5'	2.54	0.55
2:C:6[A]:DA:C2	4:G:9[A]:DA:C2	2.95	0.55
2:D:11[D]:DC:C2	2:D:12[D]:DA:C6	2.96	0.54
2:D:8[C]:DG:H2'	2:D:9[C]:DG:H5''	1.81	0.54
2:D:12[D]:DA:N1	3:F:6[D]:DG:N1	2.53	0.54
2:C:5[B]:DT:C2	3:E:13[B]:DG:N2	2.76	0.54
2:D:8[C]:DG:C8	2:D:9[C]:DG:C8	2.96	0.53
4:H:8[C]:DT:H2''	4:H:9[C]:DA:H8	1.73	0.53
2:C:13[A]:DT:H2''	2:C:14[A]:DC:C5	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4[C]:DC:H2'	2:D:5[C]:DT:C5	2.44	0.53
2:C:9[A]:DG:C2	2:C:10[A]:DT:C2	2.98	0.52
2:D:11[D]:DC:O2	2:D:12[D]:DA:C2	2.63	0.52
2:C:5[A]:DT:C2'	2:C:6[A]:DA:N7	2.69	0.52
2:D:10[D]:DT:N3	3:F:7[D]:DA:N1	2.58	0.52
3:E:11[B]:DT:C2'	3:E:12[B]:DA:C8	2.88	0.52
2:C:8[A]:DG:N2	4:G:7[A]:DG:C2	2.78	0.52
2:D:3[C]:DT:C2	2:D:4[C]:DC:C5	2.98	0.51
4:G:4[A]:DA:C5	4:G:5[A]:DC:N4	2.78	0.51
4:G:0[A]:DG:C2	4:G:1[A]:DA:C2	2.98	0.51
2:D:10[D]:DT:H2''	2:D:11[D]:DC:H6	1.76	0.51
2:D:9[D]:DG:C1'	2:D:10[D]:DT:H71	2.41	0.51
4:H:2[C]:DT:H2''	4:H:3[C]:DG:C8	2.46	0.51
4:G:1[A]:DA:H2''	4:G:2[A]:DT:OP2	2.11	0.51
4:H:7[C]:DG:C2'	4:H:8[C]:DT:C6	2.92	0.50
4:H:11[C]:DA:C2	4:H:12[C]:DG:C4	2.99	0.50
3:E:11[B]:DT:H2''	3:E:12[B]:DA:H8	1.69	0.50
1:B:102:LYS:HG2	1:B:110:ILE:CD1	2.41	0.50
2:C:13[B]:DT:O2	2:C:14[B]:DC:C2	2.65	0.49
4:G:10[A]:DG:C2'	4:G:11[A]:DA:OP2	2.59	0.49
2:C:4[A]:DC:C2	2:C:5[A]:DT:C2	3.00	0.49
2:C:10[B]:DT:O4	3:E:7[B]:DA:C6	2.65	0.49
2:C:8[A]:DG:H8	2:C:8[A]:DG:H5''	1.78	0.48
2:D:11[D]:DC:N3	3:F:6[D]:DG:N1	2.62	0.48
3:F:9[D]:DC:C1'	3:F:10[D]:DG:C8	2.96	0.48
2:C:2[B]:DC:O2	2:C:2[B]:DC:O4'	2.27	0.48
2:D:5[C]:DT:C1'	2:D:6[C]:DA:N7	2.74	0.48
1:B:174:PHE:CZ	2:C:15[B]:DA:C5	3.02	0.48
1:A:165:GLU:HG2	1:A:178:GLN:HG2	1.95	0.48
2:C:8[A]:DG:C3'	2:C:9[A]:DG:H5'	2.44	0.48
4:H:6[C]:DC:H2''	4:H:7[C]:DG:H5''	1.95	0.48
2:C:12[B]:DA:C8	2:C:13[B]:DT:C7	2.96	0.48
2:D:13[C]:DT:C7	2:D:14[C]:DC:N4	2.77	0.48
3:F:6[D]:DG:C2'	3:F:7[D]:DA:H8	2.23	0.47
1:B:106:CYS:O	1:B:107:HIS:HB2	2.14	0.47
2:C:1[A]:DT:C2'	2:C:2[A]:DC:C5'	2.91	0.47
3:F:11[D]:DT:H2''	3:F:12[D]:DA:C8	2.50	0.47
2:D:10[D]:DT:H2''	2:D:11[D]:DC:C6	2.49	0.47
2:C:8[A]:DG:H5''	2:C:8[A]:DG:C8	2.50	0.47
2:D:1[C]:DT:C3'	2:D:2[C]:DC:C5'	2.88	0.47
2:D:5[C]:DT:H2'	2:D:6[C]:DA:N7	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:TRP:CE3	1:A:202:GLU:HG3	2.50	0.46
4:G:4[A]:DA:C8	4:G:5[A]:DC:N4	2.84	0.46
3:F:8[D]:DC:C2'	3:F:9[D]:DC:C5'	2.60	0.46
1:B:165:GLU:HG2	1:B:178:GLN:HG2	1.97	0.46
2:C:6[B]:DA:N6	3:E:11[B]:DT:O4	2.49	0.46
1:A:200:ASP:O	1:A:204:GLN:HG3	2.15	0.46
2:D:6[D]:DA:N1	3:F:11[D]:DT:N3	2.64	0.45
2:D:8[D]:DG:H21	3:F:10[D]:DG:N2	2.06	0.45
2:D:11[D]:DC:O2	3:F:6[D]:DG:N2	2.49	0.45
2:C:1[A]:DT:H2''	2:C:2[A]:DC:H5''	1.96	0.45
2:D:9[C]:DG:C2	2:D:10[C]:DT:C2	3.05	0.45
4:G:11[A]:DA:C2'	4:G:12[A]:DG:OP2	2.65	0.45
3:E:4[B]:DA:C8	3:E:5[B]:DT:H72	2.51	0.45
2:D:5[C]:DT:O2	4:H:10[C]:DG:N2	2.49	0.45
2:D:7[D]:DC:N3	3:F:10[D]:DG:N1	2.65	0.45
4:G:0[A]:DG:N1	4:G:1[A]:DA:N1	2.65	0.45
2:D:14[D]:DC:H2''	2:D:15[D]:DA:C8	2.52	0.44
4:G:10[A]:DG:C6	4:G:11[A]:DA:C6	3.05	0.44
4:G:4[A]:DA:H2''	4:G:5[A]:DC:C5	2.53	0.44
2:D:4[C]:DC:O2	2:D:5[C]:DT:O2	2.35	0.44
3:E:12[B]:DA:OP2	3:E:12[B]:DA:H8	2.01	0.43
2:D:5[C]:DT:C2'	2:D:6[C]:DA:H8	1.95	0.43
4:G:0[A]:DG:C2	4:G:1[A]:DA:C6	3.07	0.43
4:G:7[A]:DG:H2''	4:G:8[A]:DT:H6	1.83	0.43
4:G:4[A]:DA:H2''	4:G:5[A]:DC:C6	2.53	0.43
2:C:13[B]:DT:C2	2:C:14[B]:DC:C2	3.06	0.43
3:F:6[D]:DG:H2'	3:F:7[D]:DA:C8	2.52	0.43
1:A:193:TRP:CZ3	1:A:202:GLU:HG3	2.53	0.43
2:D:9[D]:DG:C5	2:D:10[D]:DT:H73	2.54	0.43
2:C:8[B]:DG:N1	3:E:9[B]:DC:N3	2.66	0.42
1:B:170:HIS:CD2	4:G:0[A]:DG:C8	3.07	0.42
1:B:158:GLU:HA	1:B:163:ARG:HH12	1.83	0.42
2:D:8[D]:DG:O6	2:D:9[D]:DG:O6	2.38	0.42
2:C:8[A]:DG:C2'	2:C:9[A]:DG:H5'	2.50	0.42
2:C:12[B]:DA:H2'	2:C:13[B]:DT:H71	2.02	0.42
1:B:102:LYS:HG2	1:B:110:ILE:HD12	2.02	0.42
2:C:2[A]:DC:C6	2:C:3[A]:DT:H72	2.54	0.42
2:D:6[D]:DA:H2''	2:D:7[D]:DC:C6	2.55	0.42
2:D:5[D]:DT:H2''	2:D:6[D]:DA:C8	2.56	0.41
2:D:4[D]:DC:C2	3:F:13[D]:DG:N2	2.86	0.41
4:H:8[C]:DT:C2'	4:H:9[C]:DA:C8	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13[D]:DT:C2	2:D:14[D]:DC:C2	3.08	0.41
2:C:8[A]:DG:H2'	2:C:9[A]:DG:H5'	2.03	0.41
2:D:2[D]:DC:C2	2:D:2[D]:DC:C3'	3.02	0.41
3:E:11[B]:DT:H2''	3:E:12[B]:DA:N7	2.31	0.41
1:B:206:ARG:HD3	4:H:7[C]:DG:OP1	2.21	0.41
3:F:11[D]:DT:H2''	3:F:12[D]:DA:H8	1.84	0.41
2:D:1[C]:DT:C5'	2:D:2[C]:DC:OP2	2.69	0.41
3:F:9[D]:DC:H2''	3:F:10[D]:DG:H8	1.84	0.41
3:F:9[D]:DC:N1	3:F:10[D]:DG:N7	2.68	0.41
3:E:6[B]:DG:C5	3:E:7[B]:DA:C6	3.09	0.40
2:D:10[C]:DT:C2	2:D:11[C]:DC:C5	3.09	0.40
3:F:12[D]:DA:C2'	3:F:13[D]:DG:H5'	2.45	0.40
2:D:14[C]:DC:H2'	2:D:14[C]:DC:H6	1.79	0.40
4:H:7[C]:DG:H5''	4:H:7[C]:DG:C8	2.56	0.40

There are no symmetry-related clashes.

## 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	
1	A	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
1	B	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
All	All	225/230 (98%)	218 (97%)	7 (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	
1	A	102/104 (98%)	97 (95%)	5 (5%)	25	57
1	B	100/104 (96%)	97 (97%)	3 (3%)	41	75
All	All	202/208 (97%)	194 (96%)	8 (4%)	31	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	CYS
1	A	150	LEU
1	A	163	ARG
1	A	164	LEU
1	A	166	LYS
1	B	110	ILE
1	B	163	ARG
1	B	164	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	CPT	C	1016	6	0,2,4	0.00	-	-		
6	CPT	D	1016	6	0,2,4	0.00	-	-		
6	CPT	D	1015	6	0,2,4	0.00	-	-		
6	CPT	C	1015	6	0,2,4	0.00	-	-		

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	D	1015	CPT	1	0
6	C	1015	CPT	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 [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	A	114/115 (99%)	-0.43	1 (0%) 84   80	34, 49, 90, 109	0
1	B	115/115 (100%)	-0.53	0 100   100	32, 48, 87, 93	1 (0%)
2	C	15/15 (100%)	-0.59	0 100   100	24, 50, 75, 75	15 (100%)
2	D	15/15 (100%)	-0.20	1 (6%) 17   10	15, 61, 80, 86	15 (100%)
3	E	13/13 (100%)	-0.70	0 100   100	58, 63, 70, 74	13 (100%)
3	F	13/13 (100%)	-0.83	0 100   100	46, 54, 60, 68	13 (100%)
4	G	13/13 (100%)	-0.61	0 100   100	46, 54, 72, 74	13 (100%)
4	H	13/13 (100%)	-0.79	0 100   100	41, 45, 48, 53	13 (100%)
All	All	311/312 (99%)	-0.51	2 (0%) 89   86	15, 50, 86, 109	83 (26%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1[C]	DT	5.2
1	A	111	GLU	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZN	B	300	1/1	0.95	0.29	84,84,84,84	0
6	CPT	C	1016	3/5	0.97	0.12	50,50,50,54	3
6	CPT	D	1016	3/5	0.98	0.11	44,44,44,46	3
6	CPT	D	1015	3/5	0.99	0.08	40,40,41,44	3
6	CPT	C	1015	3/5	0.99	0.15	42,42,43,44	3
5	ZN	A	300	1/1	0.99	0.15	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.