W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 12, 2017 – 07:17 pm GMT

PDB ID	:	4E1U
Title	:	[Ru(bpy)2 dppz]2+ bound to DNA
Authors	:	Song, H.; Kaiser, J.T.; Barton, J.K.
Deposited on	:	2012-03-07
Resolution	:	0.92 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 (i) symbol.

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

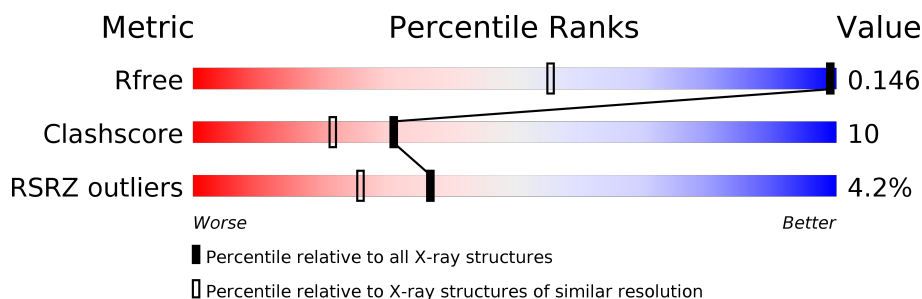|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 0.92 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	Percentile Ranks	Value
Rfree		0.146
Clashscore		10
RSRZ outliers		4.2%

Worse   *Better*

▍ Percentile relative to all X-ray structures

⃥ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1109 (1.08-0.76)
Clashscore	112137	1057 (1.06-0.78)
RSRZ outliers	101464	1117 (1.08-0.76)

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	A	12	42% 42% 17%
1	B	12	8% 42% 42% 17%

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:

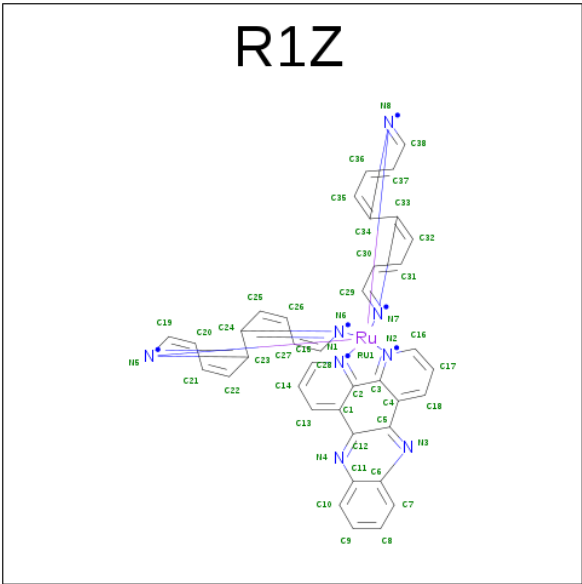| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BA	A	106	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1649 atoms, of which 515 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 5'-D(*CP*GP*GP*AP*AP*AP*TP*TP*AP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	12	Total 575	C 177	H 204	N 75	O 102	P 17	0	6	0
1	B	12	Total 510	C 157	H 181	N 65	O 92	P 15	0	4	0

- Molecule 2 is DELTA-[RU(BPY)2DPPZ]2+ (three-letter code: R1Z) (formula: $C_{38}H_{26}N_8Ru$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 73	C 38	H 26	N 8	Ru 1	0	0
2	A	1	Total 73	C 38	H 26	N 8	Ru 1	0	0
2	A	1	Total 73	C 38	H 26	N 8	Ru 1	0	0
2	A	1	Total 73	C 38	H 26	N 8	Ru 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 73	C 38	H 26	N 8	Ru 1	0	0

• Molecule 3 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ba 1	0	0
3	A	1	Total 1	Ba 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total 86	O 86	0	0
4	B	111	Total 111	O 111	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.
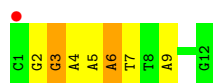
• Molecule 1: 5'-D(*CP*GP*GP*AP*AP*AP*TP*TP*AP*CP*CP*G)-3'

Chain A:
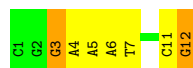
• Molecule 1: 5'-D(*CP*GP*GP*AP*AP*AP*TP*TP*AP*CP*CP*G)-3'

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	24.04Å　24.80Å　37.52Å 74.67°　84.42°　76.21°	Depositor
Resolution (Å)	23.33　–　0.92 36.16　–　0.92	Depositor EDS
% Data completeness (in resolution range)	81.7 (23.33-0.92) 72.5 (36.16-0.92)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 0.92Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.140　,　0.149 0.136　,　0.146	Depositor DCC
R_{free} test set	2384 reflections (5.53%)	DCC
Wilson B-factor (Å^2)	10.6	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 31.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	1649	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.68% 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, 0.333 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: R1Z, BA

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	1.16	1/417 (0.2%)	1.47	4/640 (0.6%)
1	B	0.79	0/370	1.64	7/570 (1.2%)
All	All	1.00	1/787 (0.1%)	1.55	11/1210 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	DC	O3'-P	14.06	1.78	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3[A]	DG	O4'-C1'-N9	12.10	116.47	108.00
1	B	3[B]	DG	O4'-C1'-N9	12.10	116.47	108.00
1	A	3[A]	DG	O4'-C1'-N9	6.98	112.89	108.00
1	A	3[B]	DG	O4'-C1'-N9	6.98	112.89	108.00
1	B	4	DA	O4'-C1'-N9	-6.37	103.54	108.00
1	B	3[A]	DG	C1'-O4'-C4'	-5.70	104.40	110.10
1	B	3[B]	DG	C1'-O4'-C4'	-5.70	104.40	110.10
1	A	12[A]	DG	C5-C6-O6	-5.35	125.39	128.60
1	A	12[B]	DG	C5-C6-O6	-5.35	125.39	128.60
1	B	6	DA	O4'-C1'-N9	5.30	111.71	108.00
1	B	9	DA	N9-C4-C5	-5.02	103.79	105.80

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	371	204	204	9	0
1	B	329	181	181	6	0
2	A	235	130	130	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	86	0	0	4	4
4	B	111	0	0	2	4
All	All	1134	515	515	15	4

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 10.

All (15) 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:A:12[B]:DG:OP2	4:A:271:HOH:O	1.94	0.82
1:A:5[A]:DA:H2"	1:A:6[A]:DA:OP2	1.88	0.74
1:A:7[B]:DT:P	4:A:242:HOH:O	2.47	0.72
1:A:7[B]:DT:OP1	4:A:242:HOH:O	2.16	0.61
1:A:3[B]:DG:C8	2:A:102:R1Z:C7	2.92	0.53
1:B:6:DA:H4'	1:B:7[A]:DT:OP1	2.07	0.53
1:A:12[A]:DG:OP2	4:A:271:HOH:O	2.19	0.52
1:B:3[A]:DG:H5'	4:B:1031:HOH:O	2.10	0.51
1:B:3[A]:DG:C5'	4:B:1031:HOH:O	2.59	0.49
2:A:105:R1Z:H291	1:B:2[A]:DG:N3	2.28	0.48
1:A:4[A]:DA:H2"	1:A:5[A]:DA:H5'	1.96	0.48
2:A:104:R1Z:H291	1:B:5[A]:DA:N3	2.32	0.45
1:A:4[A]:DA:C2'	1:A:5[A]:DA:H5'	2.50	0.41
2:A:104:R1Z:C10	1:B:3[B]:DG:C8	3.03	0.41
1:A:3[A]:DG:C8	2:A:102:R1Z:C7	3.04	0.41

All (4) 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)
4:A:270:HOH:O	4:B:1078:HOH:O[1_655]	1.07	1.13
4:A:254:HOH:O	4:B:1055:HOH:O[1_545]	1.30	0.90
4:A:268:HOH:O	4:B:1079:HOH:O[1_664]	1.79	0.41
4:A:249:HOH:O	4:B:1111:HOH:O[1_545]	1.94	0.26

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
2	R1Z	A	101	-	52,58,58	3.92	23 (44%)	58,97,97	2.87	22 (37%)
2	R1Z	A	102	-	52,58,58	3.88	20 (38%)	58,97,97	2.87	23 (39%)
2	R1Z	A	103	-	52,58,58	4.00	20 (38%)	58,97,97	2.68	20 (34%)
2	R1Z	A	104	-	52,58,58	3.99	21 (40%)	58,97,97	2.80	20 (34%)
2	R1Z	A	105	-	52,58,58	3.99	20 (38%)	58,97,97	2.70	20 (34%)

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	R1Z	A	101	-	-	0/0/112/112	0/12/12/12
2	R1Z	A	102	-	-	0/0/112/112	0/12/12/12
2	R1Z	A	103	-	-	0/0/112/112	0/12/12/12
2	R1Z	A	104	-	-	0/0/112/112	0/12/12/12
2	R1Z	A	105	-	-	0/0/112/112	0/12/12/12

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	103	R1Z	C19-N5	-11.01	1.32	1.48
2	A	105	R1Z	C19-N5	-10.98	1.32	1.48
2	A	101	R1Z	C19-N5	-10.90	1.32	1.48
2	A	104	R1Z	C19-N5	-10.88	1.32	1.48
2	A	104	R1Z	C38-N8	-10.81	1.32	1.48
2	A	101	R1Z	C38-N8	-10.80	1.32	1.48
2	A	103	R1Z	C38-N8	-10.78	1.32	1.48
2	A	105	R1Z	C38-N8	-10.71	1.33	1.48
2	A	102	R1Z	C38-N8	-10.69	1.33	1.48
2	A	102	R1Z	C19-N5	-10.23	1.33	1.48
2	A	105	R1Z	C29-N7	-10.21	1.33	1.48
2	A	101	R1Z	C29-N7	-9.93	1.34	1.48
2	A	104	R1Z	C29-N7	-9.73	1.34	1.48
2	A	105	R1Z	C28-N6	-9.69	1.34	1.48
2	A	103	R1Z	C28-N6	-9.67	1.34	1.48
2	A	102	R1Z	C28-N6	-9.63	1.34	1.48
2	A	104	R1Z	C28-N6	-9.63	1.34	1.48
2	A	103	R1Z	C29-N7	-9.46	1.34	1.48
2	A	102	R1Z	C29-N7	-9.16	1.35	1.48
2	A	101	R1Z	C28-N6	-8.69	1.36	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	104	R1Z	C35-C34	-8.04	1.35	1.53
2	A	105	R1Z	C35-C34	-7.74	1.36	1.53
2	A	103	R1Z	C35-C34	-7.73	1.36	1.53
2	A	102	R1Z	C35-C34	-7.69	1.36	1.53
2	A	101	R1Z	C22-C23	-7.69	1.36	1.53
2	A	102	R1Z	C22-C23	-7.67	1.36	1.53
2	A	101	R1Z	C35-C34	-7.61	1.36	1.53
2	A	104	R1Z	C22-C23	-7.55	1.36	1.53
2	A	103	R1Z	C22-C23	-7.52	1.36	1.53
2	A	105	R1Z	C22-C23	-7.44	1.37	1.53
2	A	103	R1Z	C25-C24	-7.05	1.37	1.53
2	A	104	R1Z	C25-C24	-6.59	1.38	1.53
2	A	104	R1Z	C32-C33	-6.58	1.38	1.53
2	A	103	R1Z	C32-C33	-6.53	1.38	1.53
2	A	105	R1Z	C32-C33	-6.53	1.38	1.53
2	A	102	R1Z	C25-C24	-6.49	1.39	1.53
2	A	101	R1Z	C32-C33	-6.28	1.39	1.53
2	A	105	R1Z	C25-C24	-6.12	1.39	1.53
2	A	102	R1Z	C32-C33	-5.97	1.40	1.53
2	A	101	R1Z	C25-C24	-5.79	1.40	1.53
2	A	103	R1Z	C26-C25	-5.52	1.38	1.53
2	A	105	R1Z	C26-C25	-5.45	1.38	1.53
2	A	101	R1Z	C31-C32	-5.39	1.38	1.53
2	A	104	R1Z	C31-C32	-5.38	1.39	1.53
2	A	102	R1Z	C26-C25	-5.26	1.39	1.53
2	A	105	R1Z	C31-C32	-5.22	1.39	1.53
2	A	103	R1Z	C31-C32	-5.21	1.39	1.53
2	A	101	R1Z	C26-C25	-5.21	1.39	1.53
2	A	102	R1Z	C31-C32	-5.20	1.39	1.53
2	A	104	R1Z	C26-C25	-5.02	1.39	1.53
2	A	103	R1Z	C36-C37	-4.55	1.33	1.51
2	A	102	R1Z	C20-C21	-4.55	1.33	1.51
2	A	103	R1Z	C20-C21	-4.51	1.33	1.51
2	A	104	R1Z	C20-C21	-4.50	1.33	1.51
2	A	102	R1Z	C36-C37	-4.48	1.33	1.51
2	A	105	R1Z	C36-C37	-4.46	1.33	1.51
2	A	101	R1Z	C36-C37	-4.44	1.33	1.51
2	A	104	R1Z	C36-C37	-4.44	1.33	1.51
2	A	101	R1Z	C20-C21	-4.25	1.34	1.51
2	A	105	R1Z	C20-C21	-4.18	1.34	1.51
2	A	105	R1Z	C29-C30	-3.65	1.37	1.51
2	A	105	R1Z	C28-C27	-3.58	1.38	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	102	R1Z	C29-C30	-3.52	1.38	1.51
2	A	104	R1Z	C28-C27	-3.46	1.38	1.51
2	A	104	R1Z	C31-C30	-3.45	1.37	1.51
2	A	102	R1Z	C28-C27	-3.45	1.38	1.51
2	A	103	R1Z	C28-C27	-3.45	1.38	1.51
2	A	101	R1Z	C31-C30	-3.41	1.37	1.51
2	A	104	R1Z	C27-C26	-3.36	1.38	1.51
2	A	105	R1Z	C31-C30	-3.35	1.38	1.51
2	A	101	R1Z	C29-C30	-3.33	1.39	1.51
2	A	103	R1Z	C29-C30	-3.32	1.39	1.51
2	A	101	R1Z	C27-C26	-3.32	1.38	1.51
2	A	104	R1Z	C29-C30	-3.30	1.39	1.51
2	A	102	R1Z	C27-C26	-3.22	1.38	1.51
2	A	103	R1Z	C27-C26	-3.20	1.38	1.51
2	A	101	R1Z	C28-C27	-3.17	1.39	1.51
2	A	102	R1Z	C31-C30	-3.16	1.38	1.51
2	A	103	R1Z	C31-C30	-3.15	1.38	1.51
2	A	105	R1Z	C27-C26	-3.14	1.38	1.51
2	A	105	R1Z	C21-C22	-2.98	1.45	1.53
2	A	105	R1Z	C36-C35	-2.93	1.45	1.53
2	A	104	R1Z	C21-C22	-2.86	1.45	1.53
2	A	103	R1Z	C36-C35	-2.83	1.45	1.53
2	A	104	R1Z	C36-C35	-2.73	1.46	1.53
2	A	103	R1Z	C21-C22	-2.67	1.46	1.53
2	A	101	R1Z	C3-C2	-2.64	1.37	1.43
2	A	102	R1Z	RU1-N8	-2.64	2.02	2.12
2	A	101	R1Z	C36-C35	-2.57	1.46	1.53
2	A	103	R1Z	RU1-N5	-2.54	2.02	2.12
2	A	103	R1Z	RU1-N8	-2.53	2.02	2.12
2	A	102	R1Z	C36-C35	-2.50	1.46	1.53
2	A	101	R1Z	RU1-N5	-2.42	2.03	2.12
2	A	102	R1Z	C21-C22	-2.30	1.47	1.53
2	A	104	R1Z	RU1-N7	-2.25	2.03	2.12
2	A	104	R1Z	RU1-N5	-2.20	2.04	2.12
2	A	101	R1Z	C4-C5	-2.19	1.40	1.45
2	A	102	R1Z	C3-C2	-2.17	1.38	1.43
2	A	101	R1Z	C21-C22	-2.15	1.47	1.53
2	A	101	R1Z	C3-N2	-2.13	1.34	1.37
2	A	104	R1Z	C24-C23	-2.09	1.46	1.52
2	A	105	R1Z	RU1-N8	-2.04	2.04	2.12
2	A	105	R1Z	RU1-N5	-2.02	2.04	2.12
2	A	101	R1Z	RU1-N6	-2.00	2.04	2.12

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	102	R1Z	C1-C12-C5	-2.42	117.83	120.04
2	A	101	R1Z	C16-C17-C18	-2.38	115.97	119.39
2	A	102	R1Z	C2-C1-C12	2.35	121.87	119.15
2	A	101	R1Z	C3-C2-N1	2.37	119.25	116.57
2	A	102	R1Z	C3-C4-C5	2.46	122.00	119.15
2	A	103	R1Z	C33-C34-N8	2.52	112.83	109.07
2	A	103	R1Z	C24-C23-N5	2.61	112.97	109.07
2	A	104	R1Z	C24-C23-N5	2.79	113.24	109.07
2	A	105	R1Z	C33-C34-N8	2.81	113.27	109.07
2	A	101	R1Z	C33-C34-N8	3.06	113.64	109.07
2	A	103	R1Z	C26-C25-C24	3.12	116.93	111.22
2	A	105	R1Z	C31-C32-C33	3.19	117.04	111.22
2	A	105	R1Z	C24-C23-N5	3.36	114.09	109.07
2	A	102	R1Z	C26-C25-C24	3.39	117.42	111.22
2	A	102	R1Z	C34-C33-N7	3.44	114.21	109.07
2	A	102	R1Z	C31-C32-C33	3.46	117.54	111.22
2	A	103	R1Z	C31-C32-C33	3.59	117.77	111.22
2	A	104	R1Z	C31-C32-C33	3.63	117.85	111.22
2	A	103	R1Z	C20-C21-C22	3.67	119.00	111.42
2	A	105	R1Z	C36-C35-C34	3.68	117.94	111.22
2	A	105	R1Z	C26-C25-C24	3.68	117.94	111.22
2	A	101	R1Z	C28-C27-C26	3.70	117.17	111.43
2	A	103	R1Z	C37-C36-C35	3.72	119.12	111.42
2	A	101	R1Z	C30-C31-C32	3.74	119.16	111.42
2	A	105	R1Z	C20-C21-C22	3.75	119.18	111.42
2	A	101	R1Z	C31-C32-C33	3.76	118.09	111.22
2	A	101	R1Z	C26-C25-C24	3.77	118.11	111.22
2	A	104	R1Z	C27-C26-C25	3.78	119.24	111.42
2	A	104	R1Z	C21-C22-C23	3.81	118.19	111.22
2	A	104	R1Z	C33-C34-N8	3.88	114.86	109.07
2	A	105	R1Z	C37-C38-N8	3.90	119.36	113.00
2	A	105	R1Z	C30-C31-C32	3.91	119.50	111.42
2	A	104	R1Z	C28-C27-C26	3.92	117.51	111.43
2	A	105	R1Z	C27-C26-C25	3.92	119.53	111.42
2	A	104	R1Z	C34-C33-N7	3.93	114.94	109.07
2	A	103	R1Z	C30-C31-C32	3.98	119.65	111.42
2	A	104	R1Z	C37-C36-C35	3.98	119.65	111.42
2	A	104	R1Z	C29-C30-C31	3.99	117.62	111.43
2	A	102	R1Z	C19-C20-C21	4.00	117.63	111.43
2	A	102	R1Z	C23-C24-N6	4.01	115.06	109.07
2	A	103	R1Z	C23-C24-N6	4.04	115.11	109.07
2	A	102	R1Z	C30-C31-C32	4.05	119.79	111.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	104	R1Z	C26-C25-C24	4.06	118.64	111.22
2	A	105	R1Z	C37-C36-C35	4.07	119.83	111.42
2	A	101	R1Z	C20-C19-N5	4.11	119.70	113.00
2	A	104	R1Z	C23-C24-N6	4.18	115.32	109.07
2	A	101	R1Z	C36-C35-C34	4.19	118.88	111.22
2	A	104	R1Z	C30-C31-C32	4.20	120.10	111.42
2	A	105	R1Z	C34-C33-N7	4.20	115.35	109.07
2	A	103	R1Z	C36-C35-C34	4.20	118.90	111.22
2	A	102	R1Z	C28-C27-C26	4.21	117.96	111.43
2	A	104	R1Z	C20-C21-C22	4.24	120.19	111.42
2	A	101	R1Z	C24-C23-N5	4.26	115.44	109.07
2	A	103	R1Z	C27-C26-C25	4.27	120.25	111.42
2	A	101	R1Z	C27-C26-C25	4.30	120.30	111.42
2	A	102	R1Z	C27-C26-C25	4.31	120.34	111.42
2	A	105	R1Z	C23-C24-N6	4.33	115.53	109.07
2	A	105	R1Z	C21-C22-C23	4.34	119.15	111.22
2	A	104	R1Z	C36-C35-C34	4.35	119.17	111.22
2	A	102	R1Z	C36-C35-C34	4.35	119.17	111.22
2	A	103	R1Z	C21-C22-C23	4.38	119.23	111.22
2	A	105	R1Z	C20-C19-N5	4.38	120.14	113.00
2	A	102	R1Z	C21-C22-C23	4.41	119.28	111.22
2	A	101	R1Z	C29-C30-C31	4.43	118.30	111.43
2	A	101	R1Z	C19-C20-C21	4.45	118.33	111.43
2	A	102	R1Z	C37-C38-N8	4.45	120.25	113.00
2	A	101	R1Z	C37-C36-C35	4.45	120.62	111.42
2	A	104	R1Z	C37-C38-N8	4.47	120.29	113.00
2	A	101	R1Z	C34-C33-N7	4.50	115.79	109.07
2	A	102	R1Z	C38-C37-C36	4.51	118.42	111.43
2	A	102	R1Z	C24-C23-N5	4.51	115.81	109.07
2	A	102	R1Z	C29-C30-C31	4.52	118.44	111.43
2	A	101	R1Z	C21-C22-C23	4.56	119.55	111.22
2	A	103	R1Z	C28-C27-C26	4.58	118.54	111.43
2	A	103	R1Z	C37-C38-N8	4.61	120.52	113.00
2	A	105	R1Z	C28-C27-C26	4.62	118.60	111.43
2	A	101	R1Z	C20-C21-C22	4.65	121.04	111.42
2	A	103	R1Z	C34-C33-N7	4.65	116.02	109.07
2	A	101	R1Z	C37-C38-N8	4.71	120.68	113.00
2	A	101	R1Z	C38-C37-C36	4.84	118.93	111.43
2	A	105	R1Z	C29-C30-C31	4.90	119.03	111.43
2	A	102	R1Z	C37-C36-C35	4.96	121.68	111.42
2	A	102	R1Z	C20-C21-C22	4.97	121.70	111.42
2	A	102	R1Z	C20-C19-N5	4.98	121.11	113.00

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	104	R1Z	C19-C20-C21	4.99	119.17	111.43
2	A	103	R1Z	C29-C30-C31	5.10	119.34	111.43
2	A	103	R1Z	C20-C19-N5	5.19	121.46	113.00
2	A	104	R1Z	C38-C37-C36	5.25	119.57	111.43
2	A	104	R1Z	C20-C19-N5	5.29	121.63	113.00
2	A	103	R1Z	C30-C29-N7	5.35	121.72	113.00
2	A	101	R1Z	C23-C24-N6	5.49	117.26	109.07
2	A	103	R1Z	C19-C20-C21	5.54	120.02	111.43
2	A	103	R1Z	C27-C28-N6	5.61	122.14	113.00
2	A	105	R1Z	C19-C20-C21	5.65	120.20	111.43
2	A	103	R1Z	C38-C37-C36	5.77	120.38	111.43
2	A	102	R1Z	C33-C34-N8	5.98	118.00	109.07
2	A	105	R1Z	C38-C37-C36	6.11	120.91	111.43
2	A	105	R1Z	C30-C29-N7	6.13	123.00	113.00
2	A	102	R1Z	C30-C29-N7	6.24	123.17	113.00
2	A	105	R1Z	C27-C28-N6	6.33	123.32	113.00
2	A	102	R1Z	C27-C28-N6	6.38	123.40	113.00
2	A	104	R1Z	C30-C29-N7	6.79	124.07	113.00
2	A	101	R1Z	C30-C29-N7	7.09	124.56	113.00
2	A	101	R1Z	C27-C28-N6	7.36	125.00	113.00
2	A	104	R1Z	C27-C28-N6	7.48	125.20	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	102	R1Z	2	0
2	A	104	R1Z	2	0
2	A	105	R1Z	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	12/12 (100%)	-0.33	0	100	100	11, 14, 16, 17	1 (8%)
1	B	12/12 (100%)	-0.09	1 (8%)	12	11	13, 15, 21, 26	0
All	All	24/24 (100%)	-0.21	1 (4%)	37	26	11, 15, 17, 26	1 (4%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	DC	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BA	A	106	1/1	0.99	0.11	4.16	14,14,14,14	1
2	R1Z	A	101	47/47	0.99	0.07	-0.12	12,18,23,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	R1Z	A	105	47/47	1.00	0.06	-0.41	9,12,18,19	0
2	R1Z	A	104	47/47	1.00	0.06	-0.45	9,12,17,19	0
2	R1Z	A	102	47/47	1.00	0.06	-1.03	12,15,19,21	0
2	R1Z	A	103	47/47	1.00	0.06	-1.04	9,12,17,19	0
3	BA	B	101	1/1	1.00	0.04	-1.92	19,19,19,19	1

6.5 Other polymers ⓘ

There are no such residues in this entry.