



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:32 PM GMT

PDB ID : 2R2S
Title : Co(III)bleomycinB2 bound to d(ATTAGTTATAACTAAT) complexed with MMLV RT catalytic fragment
Authors : Goodwin, K.D.; Lewis, M.A.; Long, E.C.; Georgiadis, M.M.
Deposited on : 2007-08-27
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

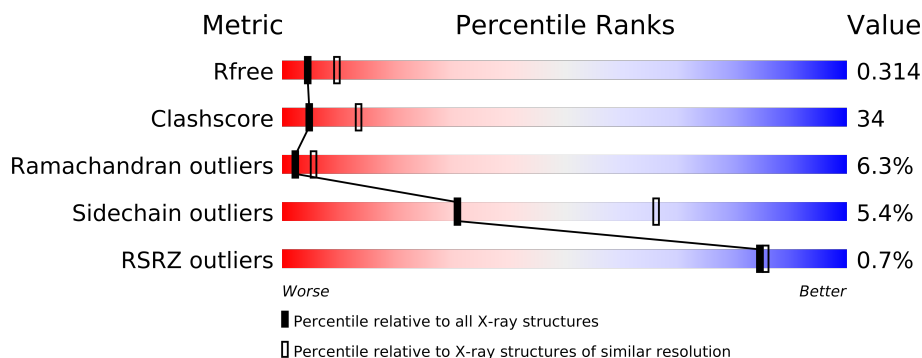
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	7	
2	G	8	
3	A	255	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2494 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*DAP*DTP*DTP*DAP*DGP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	7	Total	C	N	O	P	0	0	0
			141	70	23	42	6			

- Molecule 2 is a DNA chain called DNA (5'-D(P*DTP*DAP*DAP*DCP*DTP*DAP*DAP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	0
			163	79	29	47	8			

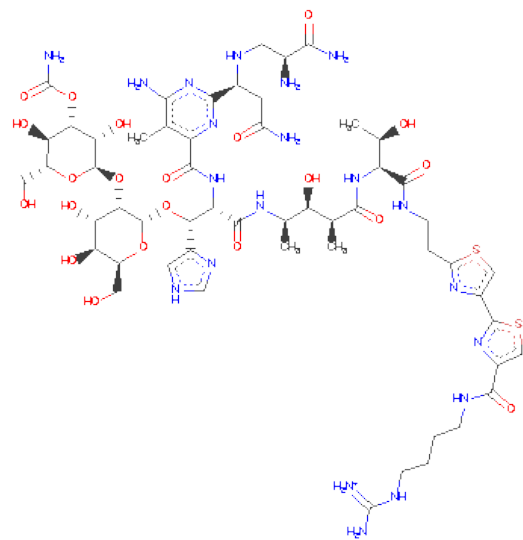
- Molecule 3 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	255	Total	C	N	O	S	0	0	0
			2041	1311	356	367	7			

- Molecule 4 is COBALT (III) ION (three-letter code: 3CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Co	0	0
			1	1		

- Molecule 5 is BLEOMYCIN B2 (three-letter code: BLB) (formula: C₅₅H₈₅N₂₀O₂₁S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	98	55	20	21	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	42	Total	O	
			42	42	0
6	B	5	Total	O	
			5	5	0
6	G	3	Total	O	
			3	3	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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 (5'-D(*DAP*DTP*DTP*DAP*DGP*DTP*DT)-3')

Chain B: 

A1
T2
T3
A4
G5
T6
T7

- Molecule 2: DNA (5'-D(P*DTP*DAP*DAP*DCP*DTP*DAP*DAP*DT)-3')

Chain G: 

T9
A10
A11
C12
T13
A14
A15
T16

- Molecule 3: Reverse transcriptase

Chain A: 

T24
W25
L26
S27
D28
F29
P30
Q31
A32
W33
A34
E35
L41
P51
L52
K53
T57
P58
V59
S60
I61
K62
Q63
Y64
P65
M66
A70
R71
L72
K75
P76
Q79
R80
L81
P89
P93
W94
N95
T96
P97
V101
K102
K103
P104
G105
T106
M107
D108
R116

R121
V122
P127
N131
P132
L135
L136
L139
S142
H143
Q144
Y145
Y146
L151
K152
F156
L160
H161
P162
S164
Q165
P166
L167
F168
W172
R173
D174
P175
E176
M177
G178
I179
S180
G181
Q182
L183
T184
W185
T186
R187
L188
F192
K193
N194
S195
P196
T197
E201

A202
L203
H204
R205
D206
R211
I212
Q213
L217
L220
Q221
Y222
D224
L227
A230
T231
S232
E233
Q237
L250
A254
S255
A256
K257
K258
C262
Q263
K264
Q265
V266
K267
G270
Y271
L272
L273
K274
E275
G276
Q277
R278

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	52.30Å 144.51Å 50.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 42.37 – 2.78	Depositor EDS
% Data completeness (in resolution range)	91.8 (50.00-2.80) 90.4 (42.37-2.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.308 0.227 , 0.314	Depositor DCC
R_{free} test set	477 reflections (5.47%)	DCC
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.2	EDS
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 9717 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2494	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3CO, BLB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.51	0/157	0.74	0/241
2	G	0.39	0/181	0.61	0/274
3	A	0.44	0/2097	0.67	0/2858
All	All	0.44	0/2435	0.67	0/3373

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	6	DT	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	141	0	83	17	0
2	G	163	0	93	13	0
3	A	2041	0	2056	129	0
4	B	1	0	0	0	0
5	B	98	0	76	12	0
6	A	42	0	0	3	0
6	B	5	0	0	0	0
6	G	3	0	0	2	0
All	All	2494	0	2308	161	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 161 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:9:BLB:C7	5:B:9:BLB:C6	1.76	1.55
2:G:11:DA:H2''	2:G:12:DC:H5'	1.42	1.01
3:A:62:LYS:HZ2	3:A:63:GLN:H	1.00	0.98
3:A:89:PRO:HA	3:A:183:LEU:HD23	1.63	0.80
3:A:174:ASP:HB2	3:A:179:ILE:HD12	1.67	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	253/255 (99%)	220 (87%)	17 (7%)	16 (6%)	2 5

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	177	MET
3	A	179	ILE
3	A	180	SER

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Mol	Chain	Res	Type
3	A	104	PRO
3	A	106	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	224/224 (100%)	212 (95%)	12 (5%)	31	66

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	102	LYS
3	A	131	ASN
3	A	177	MET
3	A	80	ARG
3	A	163	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	143	HIS
3	A	221	GLN
3	A	204	HIS
3	A	84	GLN
3	A	144	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
5	BLB	B	9	4	103,103,103	4.58	50 (48%)	139,145,145	5.64	72 (51%)

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
5	BLB	B	9	4	3/3/28/35	1/93/144/144	0/6/6/6

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	9	BLB	C7-C6	14.09	1.76	1.50
5	B	9	BLB	C10-NG	12.62	1.55	1.34
5	B	9	BLB	C46-NO	12.42	1.49	1.31
5	B	9	BLB	C7-NG	11.57	1.55	1.34
5	B	9	BLB	C13-C14	11.10	1.64	1.54

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	9	BLB	C14-C27-NJ	27.36	132.16	120.44
5	B	9	BLB	C3-NC-C6	20.58	137.03	113.67
5	B	9	BLB	C42-C43-S43	-18.96	104.52	121.29
5	B	9	BLB	C33-C34-C36	17.98	135.13	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	9	BLB	C41-NM-C40	13.89	151.10	122.57

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	9	BLB	C33
5	B	9	BLB	C37
5	B	9	BLB	C31

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	9	BLB	O49-C49-C48-NO

There are no ring outliers.

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	B	7/7 (100%)	-0.33	0 100 100	31, 35, 55, 74	0
2	G	8/8 (100%)	0.19	1 (12%) 5 4	32, 56, 82, 85	0
3	A	255/255 (100%)	-0.18	1 (0%) 90 91	19, 37, 69, 86	0
All	All	270/270 (100%)	-0.17	2 (0%) 84 85	19, 37, 69, 86	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	180	SER	4.2
2	G	10	DA	2.4

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	BLB	B	9	98/98	0.24	0.37	45,91,96,97	0
4	3CO	B	8	1/1	0.08	-	94,94,94,94	0

6.5 Other polymers ⓘ

There are no such residues in this entry.