



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:15 am BST

PDB ID : 1REK
Title : Crystal structure of cAMP-dependent protein kinase complexed with balanol analog 8
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Deposited on : 2003-11-06
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

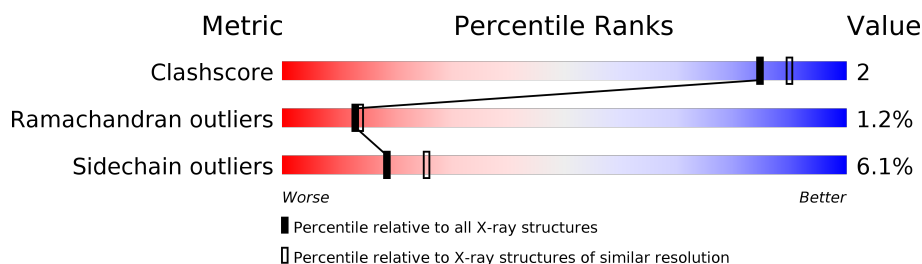
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	350	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2808 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.

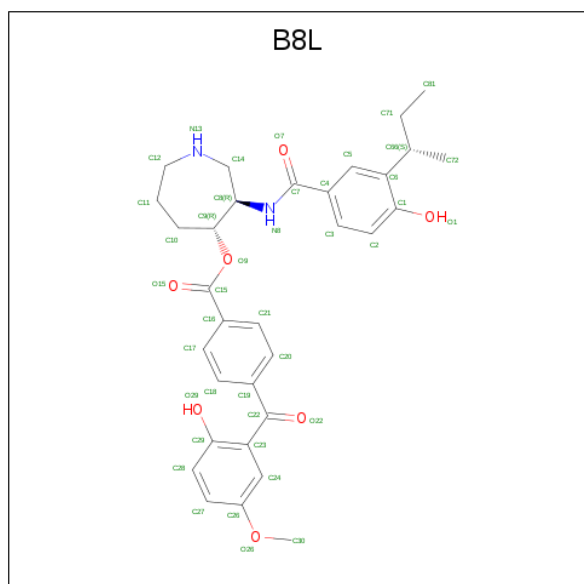
- Molecule 1 is a protein called cAMP-dependent protein kinase, alpha-catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	338	2663	1722	444	487	2	8	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

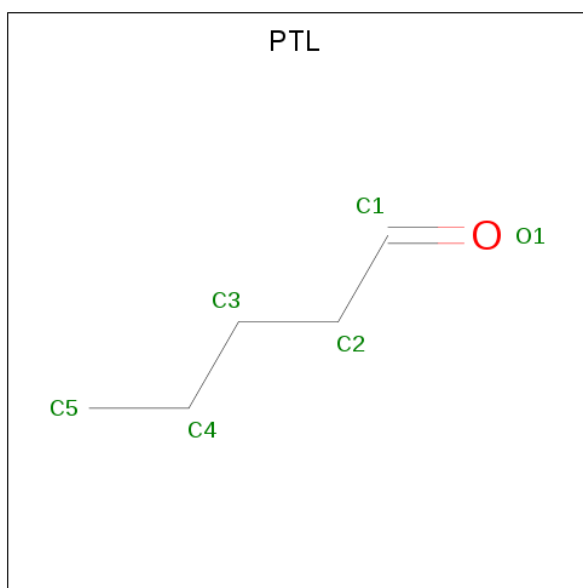
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	TPO	THR	MODIFIED RESIDUE	UNP P05132
A	338	SEP	SER	MODIFIED RESIDUE	UNP P05132

- Molecule 2 is 3-[(3-SEC-BUTYL-4-HYDROXYBENZOYL)AMINO]AZEPAN-4-YL 4-(2-HYDROXY-5-METHOXYBENZOYL)BENZOATE (three-letter code: B8L) (formula: $C_{32}H_{36}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	41	32	2	7	0	0

- Molecule 3 is PENTANAL (three-letter code: PTL) (formula: C₅H₁₀O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 5 5	0	0

- Molecule 4 is water.

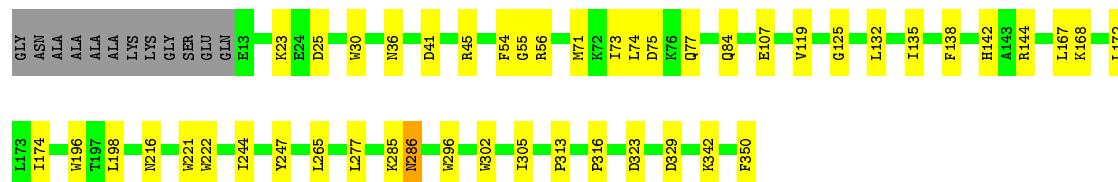
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	99	Total O 99 99	0	0

i

Note EDS was not executed.

- Molecule 1: cAMP-dependent protein kinase, alpha-catalytic subunit

83% 13% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.60 Å 71.90 Å 98.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2808	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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: TPO, PTL, B8L, SEP

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	0.73	0/2708	1.28	25/3670 (0.7%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	TRP	CD1-CG-CD2	10.30	114.54	106.30
1	A	302	TRP	CE2-CD2-CG	-9.54	99.67	107.30
1	A	30	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	A	30	TRP	CD1-CG-CD2	8.55	113.14	106.30
1	A	196	TRP	CD1-CG-CD2	8.51	113.10	106.30

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	2663	0	2517	12	0
2	A	41	0	36	0	0
3	A	5	0	9	0	0
4	A	99	0	0	1	0
All	All	2808	0	2562	12	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 2.

The worst 5 of 12 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:54:PHE:HZ	1:A:84:GLN:HG3	1.55	0.71
1:A:84:GLN:HA	4:A:517:HOH:O	1.99	0.62
1:A:135:ILE:HD11	1:A:138:PHE:HD1	1.71	0.55
1:A:142:HIS:CD2	1:A:313:PRO:HG2	2.42	0.55
1:A:77:GLN:OE1	1:A:342:LYS:HG2	2.11	0.50

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	334/350 (95%)	309 (92%)	21 (6%)	4 (1%)	13 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	LYS
1	A	323	ASP
1	A	286	ASN
1	A	125	GLY

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	263/303 (87%)	247 (94%)	16 (6%)	18	25

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	198	LEU
1	A	286	ASN
1	A	107	GLU
1	A	305	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	87	HIS
1	A	115	ASN
1	A	176	GLN
1	A	216	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	197	1	8,10,11	1.19	0	10,14,16	1.32	1 (10%)
1	SEP	A	338	1	8,9,10	1.05	0	8,12,14	3.13	3 (37%)

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
1	TPO	A	197	1	-	2/9/11/13	-
1	SEP	A	338	1	-	3/5/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	SEP	OG-CB-CA	7.66	115.60	108.14
1	A	338	SEP	O2P-P-OG	-2.64	99.71	106.73
1	A	338	SEP	O3P-P-O2P	2.20	116.05	107.64
1	A	197	TPO	O3P-P-O2P	2.15	115.87	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	197	TPO	O-C-CA-CB
1	A	338	SEP	CA-CB-OG-P
1	A	197	TPO	C-CA-CB-CG2
1	A	338	SEP	N-CA-CB-OG
1	A	338	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
2	B8L	A	351	-	41,44,44	2.16	8 (19%)	54,61,61	1.66	6 (11%)
3	PTL	A	352	-	4,4,5	0.39	0	3,3,4	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8L	A	351	-	-	7/32/44/44	0/4/4/4
3	PTL	A	352	-	-	0/2/2/3	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	351	B8L	O9-C15	5.86	1.46	1.34
2	A	351	B8L	C19-C22	-4.97	1.41	1.49
2	A	351	B8L	C23-C22	-4.65	1.40	1.50
2	A	351	B8L	C16-C15	-4.29	1.39	1.50
2	A	351	B8L	C4-C7	-4.24	1.41	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	351	B8L	C29-C23-C22	7.59	126.31	119.96
2	A	351	B8L	O9-C15-C16	5.34	120.55	111.92
2	A	351	B8L	C30-O26-C26	2.58	123.12	117.51
2	A	351	B8L	C5-C6-C1	2.31	118.96	116.92
2	A	351	B8L	C23-C22-C19	2.22	123.20	119.53

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	351	B8L	C16-C15-O9-C9
2	A	351	B8L	O15-C15-C16-C17

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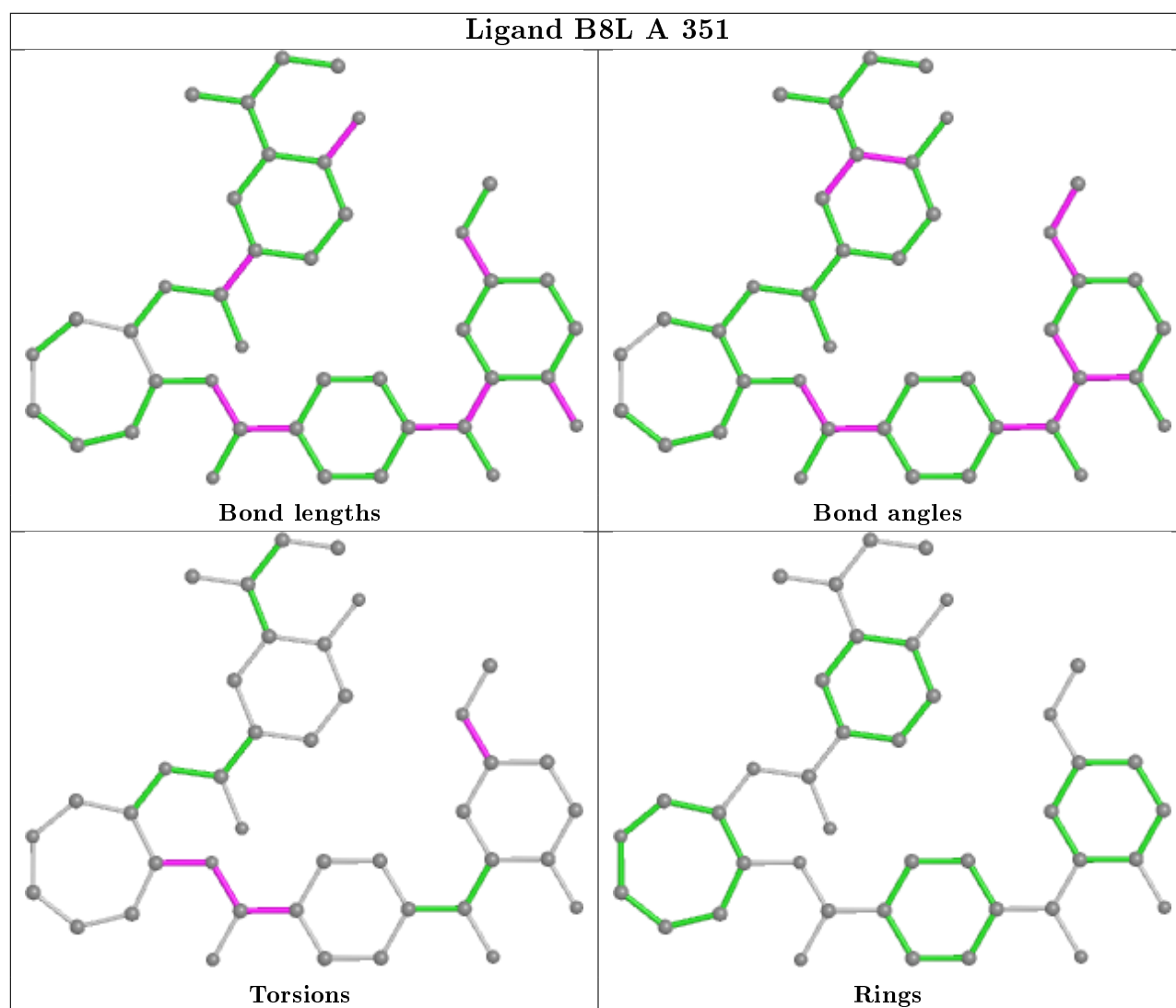
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Mol	Chain	Res	Type	Atoms
2	A	351	B8L	O15-C15-C16-C21
2	A	351	B8L	C24-C26-O26-C30
2	A	351	B8L	C27-C26-O26-C30

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.