



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 10:57 AM BST

PDB ID : 1RE8
Title : Crystal structure of cAMP-dependent protein kinase complexed with balanol analog 2
Authors : Akamine, P.; Madhusudan; Brunton, L.L.; Ou, H.D.; Canaves, J.M.; Xuong, N.H.; Taylor, S.S.
Deposited on : 2003-11-06
Resolution : 2.10 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

<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) : 2.13

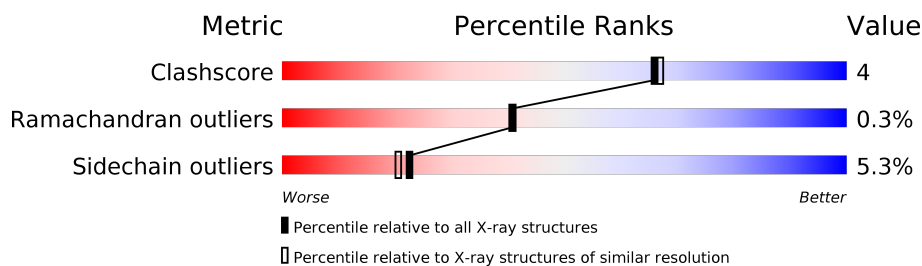
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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	

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
2	BD2	A	351	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3050 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.

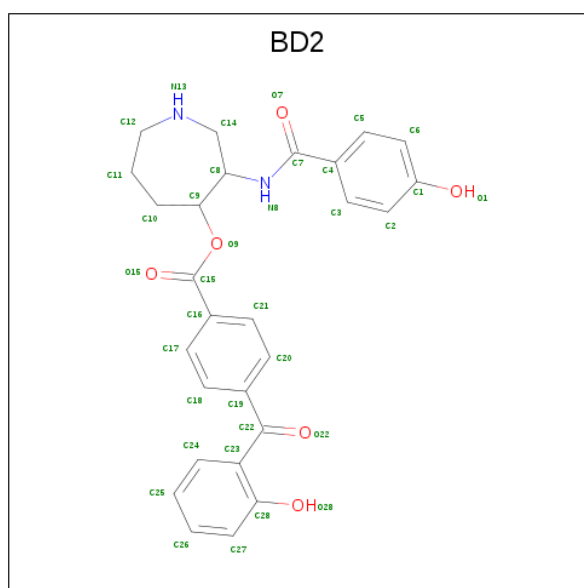
- Molecule 1 is a protein called cAMP-dependent protein kinase, alpha-catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	339	2733	1770	452	501	2	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

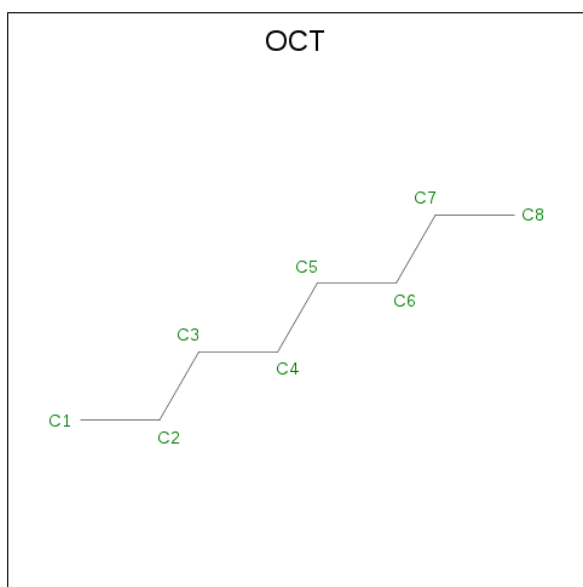
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	TPO	THR	MODIFIED RESIDUE	UNP P05132
A	338	SEP	SER	MODIFIED RESIDUE	UNP P05132

- Molecule 2 is 3-[(4-HYDROXYBENZOYL)AMINO]AZEPAN-4-YL 4-(2-HYDROXYBENZOYL)BENZOATE (three-letter code: BD2) (formula: C₂₇H₂₆N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	35	27	2	6	0	0

- Molecule 3 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0

- Molecule 4 is water.

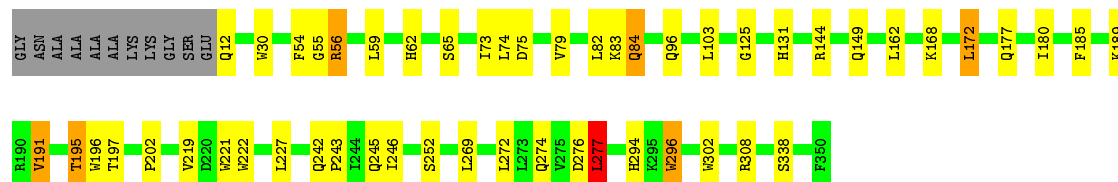
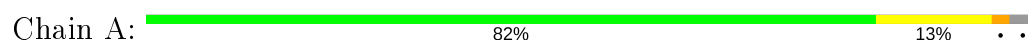
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	275	Total O 275 275	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

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



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	51.80 Å 71.60 Å 97.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3050	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP, OCT, BD2

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	0.67	0/2781	1.21	25/3761 (0.7%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	A	221	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	A	196	TRP	CE2-CD2-CG	-8.15	100.78	107.30
1	A	221	TRP	CE2-CD2-CG	-8.08	100.84	107.30
1	A	296	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	A	196	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	A	30	TRP	CD1-CG-CD2	7.93	112.65	106.30
1	A	277	LEU	CA-CB-CG	7.88	133.43	115.30
1	A	296	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	30	TRP	CE2-CD2-CG	-7.73	101.12	107.30
1	A	222	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	302	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	A	222	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	A	144	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	221	TRP	CG-CD2-CE3	6.16	139.45	133.90
1	A	144	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	196	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	A	222	TRP	CG-CD2-CE3	5.82	139.14	133.90
1	A	84	GLN	CA-CB-CG	5.72	125.99	113.40
1	A	196	TRP	CB-CG-CD1	-5.72	119.57	127.00
1	A	296	TRP	CG-CD2-CE3	5.69	139.02	133.90
1	A	221	TRP	CB-CG-CD1	-5.63	119.68	127.00
1	A	252	SER	CA-C-N	5.62	127.45	116.20
1	A	30	TRP	CG-CD2-CE3	5.42	138.78	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	TRP	CB-CG-CD1	-5.07	120.40	127.00

There are no chirality outliers.

There are no planarity outliers.

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	A	2733	0	2637	22	0
2	A	35	0	22	0	0
3	A	7	0	13	0	0
4	A	275	0	0	2	0
All	All	3050	0	2672	22	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 4.

All (22) 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:149:GLN:HE22	1:A:180:ILE:H	1.34	0.76
1:A:82:LEU:O	1:A:84:GLN:HG2	1.88	0.74
1:A:294:HIS:HD2	1:A:296:TRP:H	1.45	0.63
1:A:277:LEU:HD12	4:A:632:HOH:O	1.99	0.61
1:A:149:GLN:NE2	1:A:180:ILE:H	2.00	0.60
1:A:191:VAL:HG11	1:A:195:THR:HG23	1.84	0.60
1:A:189:LYS:HD3	1:A:195:THR:HG21	1.85	0.57
1:A:274:GLN:HE21	1:A:276:ASP:H	1.52	0.56
1:A:62:HIS:HD2	1:A:65:SER:H	1.58	0.52
1:A:242:GLN:H	1:A:245:GLN:HE21	1.57	0.52
1:A:294:HIS:CD2	1:A:296:TRP:H	2.29	0.48
1:A:103:LEU:HD22	1:A:185:PHE:HZ	1.80	0.46
1:A:125:GLY:O	1:A:131:HIS:HE1	1.99	0.45
1:A:56:ARG:HD2	4:A:399:HOH:O	2.16	0.44
1:A:54:PHE:CE2	1:A:84:GLN:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:H	1:A:245:GLN:NE2	2.16	0.42
1:A:243:PRO:HA	1:A:246:ILE:HD12	2.02	0.42
1:A:177:GLN:HE21	1:A:308:ARG:NH2	2.17	0.42
1:A:168:LYS:O	1:A:172:LEU:HD22	2.21	0.41
1:A:55:GLY:HA3	1:A:73:ILE:O	2.20	0.41
1:A:62:HIS:CD2	1:A:65:SER:H	2.36	0.40
1:A:75:ASP:O	1:A:79:VAL:HG23	2.22	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	335/350 (96%)	320 (96%)	14 (4%)	1 (0%)	41 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	LYS

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	282/303 (93%)	267 (95%)	15 (5%)	22 20

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	56	ARG
1	A	59	LEU
1	A	74	LEU
1	A	96	GLN
1	A	162	LEU
1	A	172	LEU
1	A	191	VAL
1	A	195	THR
1	A	202	PRO
1	A	219	VAL
1	A	227	LEU
1	A	269	LEU
1	A	272	LEU
1	A	277	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	36	ASN
1	A	42	GLN
1	A	62	HIS
1	A	87	HIS
1	A	96	GLN
1	A	131	HIS
1	A	149	GLN
1	A	171	ASN
1	A	177	GLN
1	A	181	GLN
1	A	245	GLN
1	A	274	GLN
1	A	283	ASN
1	A	294	HIS
1	A	326	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	SEP	A	338	1	8,9,10	0.99	0	8,12,14	2.58	2 (25%)
1	TPO	A	197	1	8,10,11	1.15	0	10,14,16	1.22	1 (10%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	SEP	OG-CB-CA	6.30	114.27	108.14
1	A	197	TPO	CG2-CB-CA	-2.10	109.03	113.16
1	A	338	SEP	O3P-P-O2P	2.07	115.57	107.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides 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	$\# Z > 2$
3	OCT	A	555	-	6,6,7	0.35	0	5,5,6	0.55	0
2	BD2	A	351	-	35,38,38	1.99	5 (14%)	47,52,52	1.98	8 (17%)

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
3	OCT	A	555	-	-	2/4/4/5	-
2	BD2	A	351	-	2/2/5/7	6/24/36/36	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	351	BD2	C19-C22	-5.62	1.39	1.49
2	A	351	BD2	C4-C7	-5.27	1.39	1.50
2	A	351	BD2	C23-C22	-4.74	1.40	1.50
2	A	351	BD2	C16-C15	-4.45	1.39	1.50
2	A	351	BD2	O9-C15	4.12	1.43	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	351	BD2	O9-C9-C10	6.43	120.68	108.03
2	A	351	BD2	O9-C9-C8	6.31	119.65	107.18
2	A	351	BD2	C14-C8-N8	5.62	120.19	109.61
2	A	351	BD2	O9-C15-C16	4.94	119.89	111.92
2	A	351	BD2	C10-C9-C8	3.02	119.64	114.87
2	A	351	BD2	C9-O9-C15	-2.78	112.55	117.38
2	A	351	BD2	C23-C22-C19	2.11	123.02	119.53
2	A	351	BD2	O9-C15-O15	-2.06	120.16	123.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	351	BD2	C8
2	A	351	BD2	C9

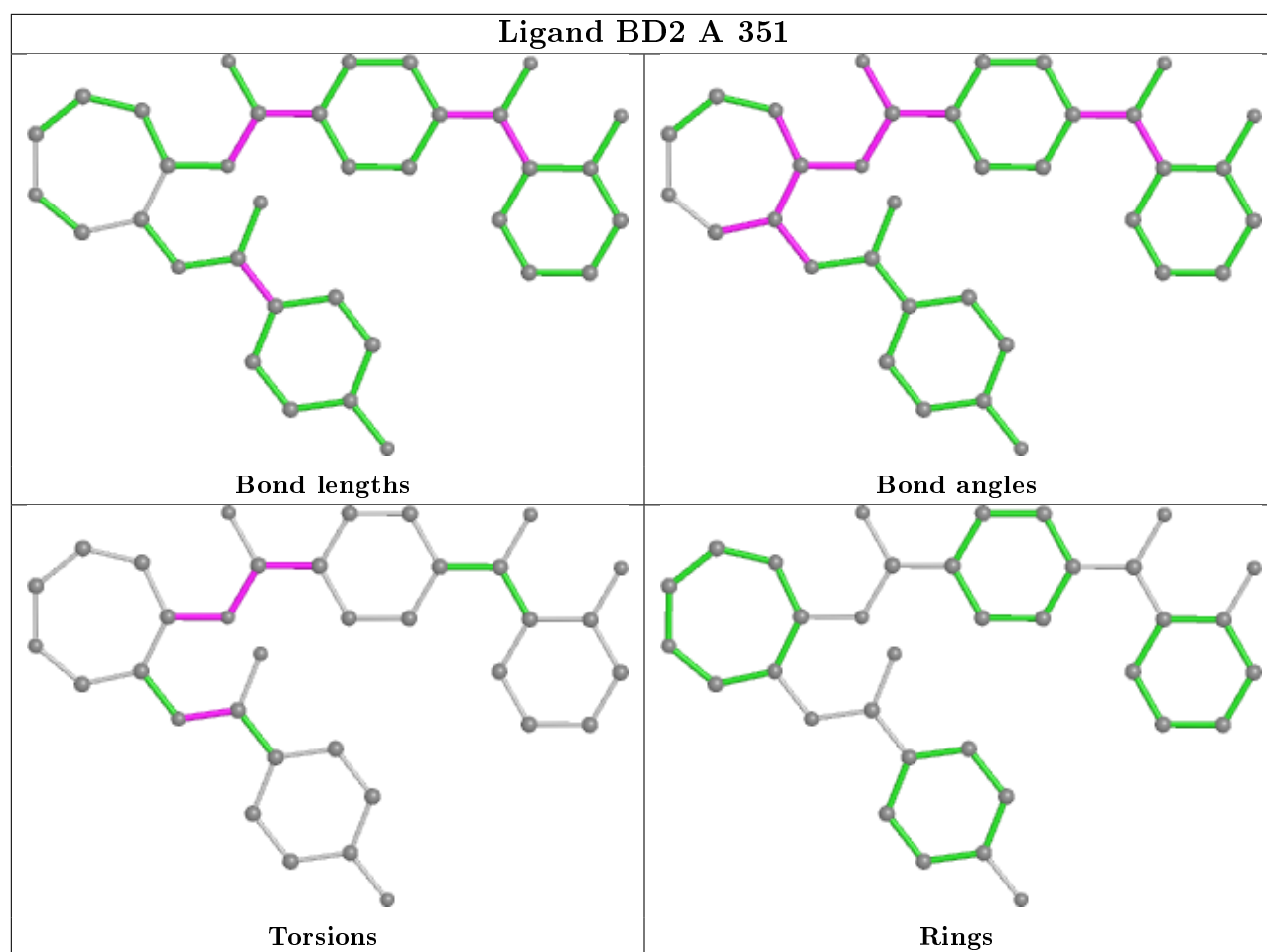
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	351	BD2	C10-C9-O9-C15
2	A	351	BD2	C16-C15-O9-C9
2	A	351	BD2	O15-C15-O9-C9
2	A	351	BD2	C4-C7-N8-C8
2	A	351	BD2	O7-C7-N8-C8
3	A	555	OCT	C2-C3-C4-C5
2	A	351	BD2	O9-C15-C16-C17
3	A	555	OCT	C4-C5-C6-C7

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.