



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 09:34 PM UTC

PDB ID : 2VHU / pdb_00002vhu
Title : P4 PROTEIN FROM BACTERIOPHAGE PHI12 K241C mutant in complex with ADP and MgCl
Authors : Kainov, D.E.; Mancini, E.J.; Telenius, J.; Lisal, J.; Grimes, J.M.; Bamford, D.H.; Stuart, D.I.; Tuma, R.
Deposited on : 2007-11-25
Resolution : 2.75 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

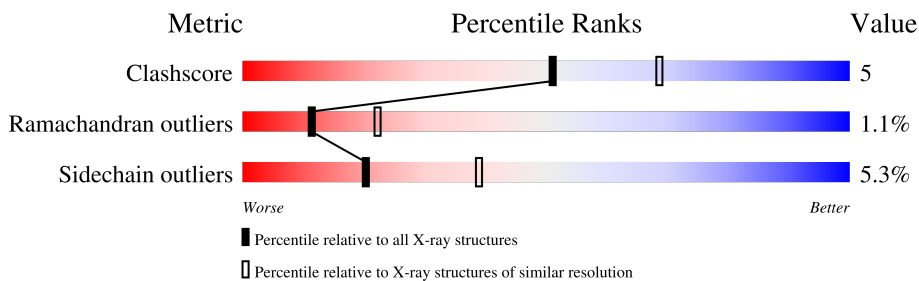
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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 of 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	331	 73% 13% • 13%
1	B	331	 76% 10% • 13%
1	C	331	 71% 15% • 13%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6772 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.

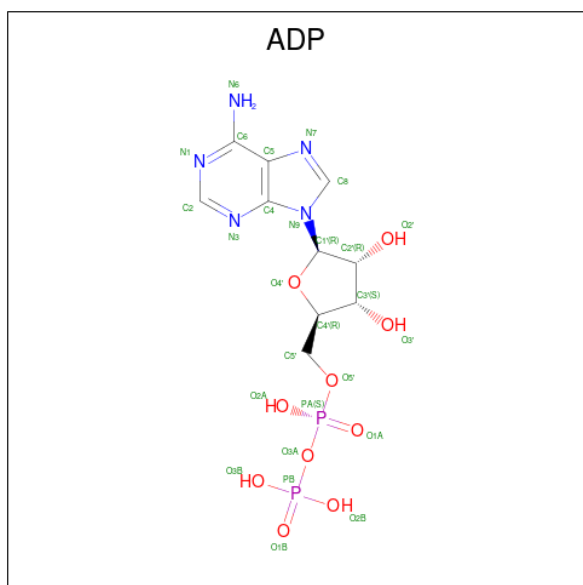
- Molecule 1 is a protein called NTPASE P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	1
			2168	1358	378	424	8			
1	B	289	Total	C	N	O	S	0	0	1
			2168	1358	378	424	8			
1	C	289	Total	C	N	O	S	0	0	1
			2168	1358	378	424	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	CYS	LYS	engineered mutation	UNP Q94M05
B	241	CYS	LYS	engineered mutation	UNP Q94M05
C	241	CYS	LYS	engineered mutation	UNP Q94M05

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	60	Total	O	0	0
			60	60		
4	C	58	Total	O	0	0
			58	58		

Lys	Thr	His
Asn	Thr	L37
Asp	Ser	E38
Leu	Gly	S39
Leu	Gly	V40
Ser	I207	P45
Val	S208	V58
Leu	D217	K61
Arg	A222	R65
Arg	A222	I66
Leu	C227	V67
Thr	C227	L106
Ser	L233	S123
Asn	N234	V126
	N238	K131
	D239	G132
	C241	M133
	I242	S134
	V243	L139
	E244	L143
	K247	G159
	S250	T167
	R251	F172
	S252	V173
	S256	I176
	W267	A179
	Q268	M180
	V269	I186
	Q278	V187
	T281	T188
	T298	D189
	S299	S190
	K300	L191
	Gln	A192
	Ser	N193
	Ser	V194
	Lys	T195
	Ala	Gly
	Ile	Ala
	Gln	Ala
	Thr	Gly
	Val	Gly
	Ile	Asn

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.30 Å 128.49 Å 158.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.75	Depositor
% Data completeness (in resolution range)	97.6 (100.00-2.75)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6772	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: MG, ADP

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	0.55	1/2205 (0.0%)	0.79	0/2988
1	B	0.56	1/2205 (0.0%)	0.84	0/2988
1	C	0.57	1/2205 (0.0%)	0.82	0/2988
All	All	0.56	3/6615 (0.0%)	0.82	0/8964

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	SER	C-N	-6.52	1.24	1.33
1	B	299	SER	C-N	-6.49	1.24	1.33
1	C	299	SER	C-N	-6.32	1.24	1.33

There are no bond angle outliers.

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	2168	0	2139	25	0
1	B	2168	0	2138	19	0
1	C	2168	0	2138	26	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	66	0	0	1	0
4	B	60	0	0	4	0
4	C	58	0	0	1	0
All	All	6772	0	6451	68	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 5.

The worst 5 of 68 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:C:65:ARG:HD2	4:C:2037:HOH:O	1.77	0.84
1:C:195:ILE:HD12	1:C:233:LEU:HD11	1.61	0.80
1:A:192:LYS:HE2	1:A:193:ASN:OD1	1.83	0.77
1:A:172:PHE:CZ	1:A:176:ILE:HD11	2.20	0.76
1:C:172:PHE:CE1	1:C:176:ILE:HD11	2.28	0.69

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	285/331 (86%)	266 (93%)	17 (6%)	2 (1%)	18	34
1	B	285/331 (86%)	268 (94%)	14 (5%)	3 (1%)	11	22
1	C	285/331 (86%)	271 (95%)	10 (4%)	4 (1%)	9	17
All	All	855/993 (86%)	805 (94%)	41 (5%)	9 (1%)	11	22

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	SER
1	A	133	ASN
1	C	133	ASN
1	C	240	ASP
1	C	251	ARG

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	
1	A	234/265 (88%)	223 (95%)	11 (5%)	23	45
1	B	234/265 (88%)	222 (95%)	12 (5%)	21	40
1	C	234/265 (88%)	220 (94%)	14 (6%)	17	32
All	All	702/795 (88%)	665 (95%)	37 (5%)	20	39

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	192	LYS
1	C	278	GLN
1	C	194	VAL
1	C	217	ASP
1	B	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	234	ASN
1	C	22	HIS
1	C	291	HIS
1	C	133	ASN
1	B	3	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	ADP	C	1301	3	28,29,29	1.52	5 (17%)	43,45,45	1.83	9 (20%)
2	ADP	A	1301	3	28,29,29	1.53	5 (17%)	43,45,45	1.91	9 (20%)
2	ADP	B	1300	3	28,29,29	1.56	5 (17%)	43,45,45	1.80	7 (16%)

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	ADP	C	1301	3	-	8/16/32/32	0/3/3/3
2	ADP	A	1301	3	-	8/16/32/32	0/3/3/3
2	ADP	B	1300	3	-	7/16/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1300	ADP	C5-C4	4.95	1.47	1.39
2	A	1301	ADP	C5-C4	4.85	1.47	1.39
2	C	1301	ADP	C5-C4	4.84	1.47	1.39
2	B	1300	ADP	PA-O3A	3.35	1.63	1.59
2	A	1301	ADP	PA-O3A	3.07	1.62	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	ADP	C5-C4-N3	-6.27	118.08	126.72
2	B	1300	ADP	C5-C4-N3	-6.07	118.36	126.72
2	C	1301	ADP	C5-C4-N3	-5.55	119.08	126.72
2	B	1300	ADP	N3-C4-N9	4.89	135.49	127.17
2	A	1301	ADP	N3-C4-N9	4.82	135.37	127.17

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ADP	PA-O3A-PB-O2B
2	A	1301	ADP	C5'-O5'-PA-O1A
2	A	1301	ADP	O4'-C4'-C5'-O5'
2	B	1300	ADP	PA-O3A-PB-O2B
2	B	1300	ADP	C5'-O5'-PA-O1A

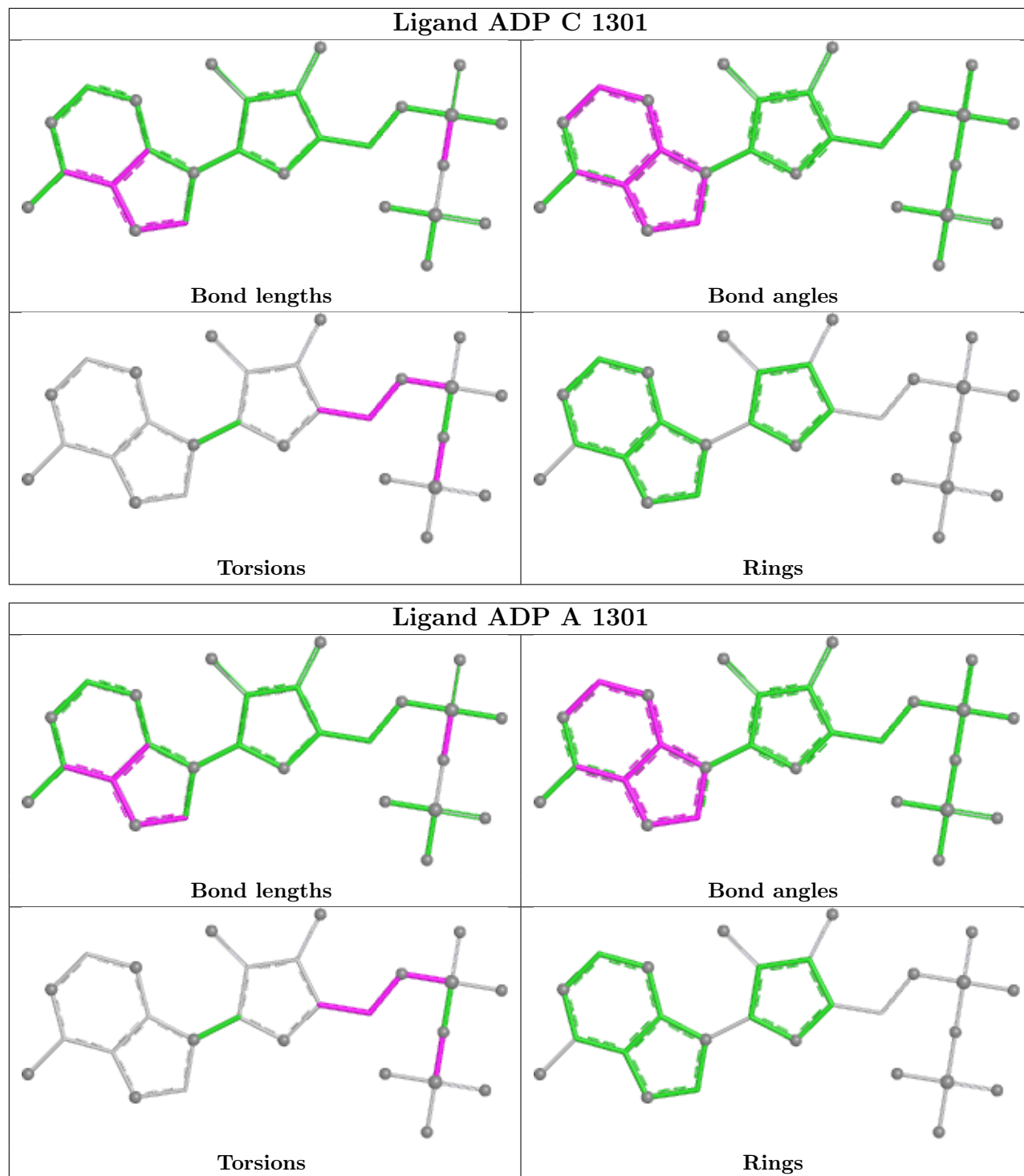
There are no ring outliers.

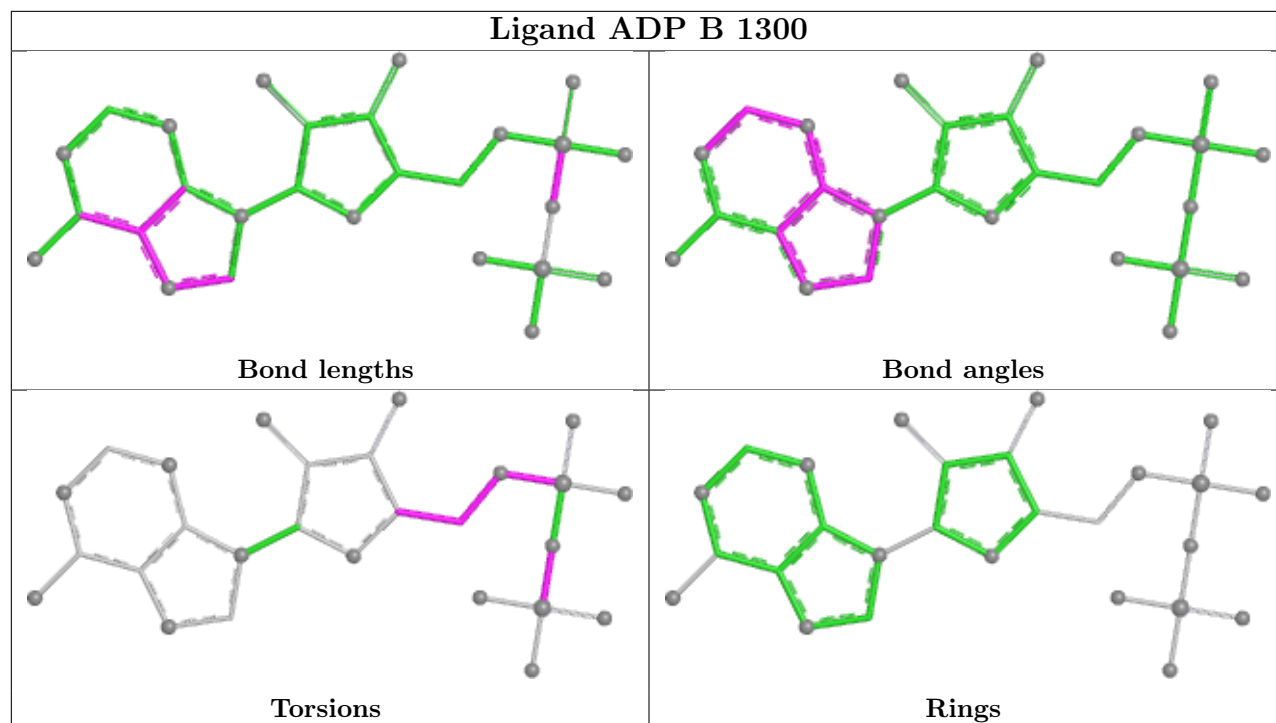
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	ADP	2	0
2	A	1301	ADP	1	0

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.