



# Full wwPDB EM Validation Report ⓘ

Dec 22, 2024 – 12:07 AM JST

PDB ID : 8ZF0  
EMDB ID : EMD-60049  
Title : pRib-ADP bound OsEDS1-PAD4-ADR1 complex  
Authors : Xu, W.Y.; Zhang, Y.  
Deposited on : 2024-05-07  
Resolution : 2.96 Å (reported)  
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

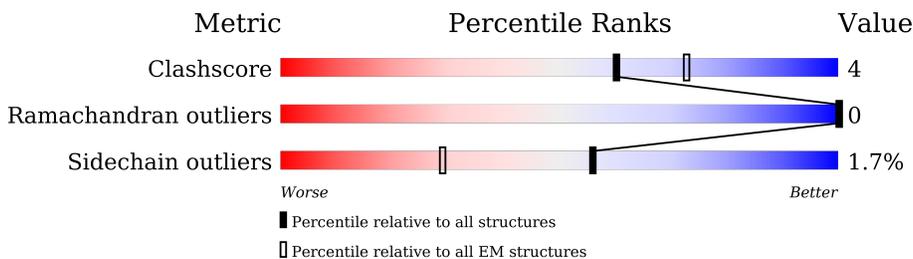
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.96 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	859	
2	B	621	
3	C	659	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12657 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RPW8 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	424	3277	2076	557	627	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	HIS	LEU	conflict	UNP A0A0E0JBT6

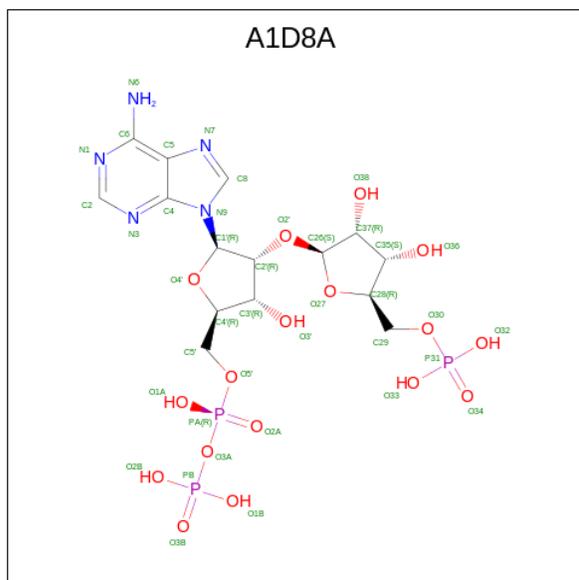
- Molecule 2 is a protein called EDS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	600	4636	2935	803	878	20	0	0

- Molecule 3 is a protein called Lipase-like PAD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	626	4704	2972	855	857	20	0	0

- Molecule 4 is [(2R,3R,4R,5R)-5-(6-aminopurin-9-yl)-4-[(2S,3R,4S,5R)-3,4-bis(oxidanyl)-5-(phosphonooxymethyl)oxolan-2-yl]oxy-3-oxidanyl-oxolan-2-yl]methyl phosphono hydrogen phosphate (three-letter code: A1D8A) (formula: C<sub>15</sub>H<sub>24</sub>N<sub>5</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	B	1	40	15	5	17	3	0

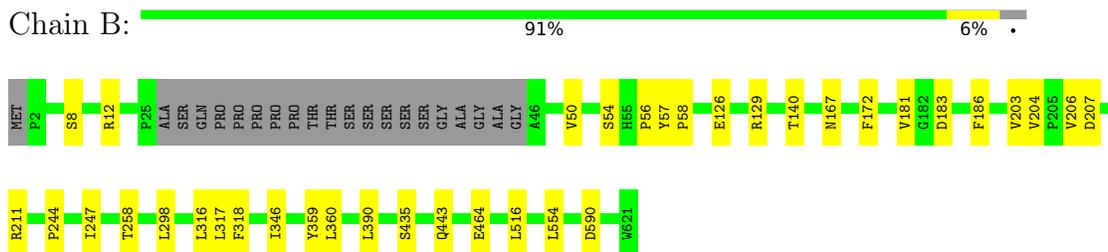
### 3 Residue-property plots [i](#)

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.

- Molecule 1: RPW8 domain-containing protein

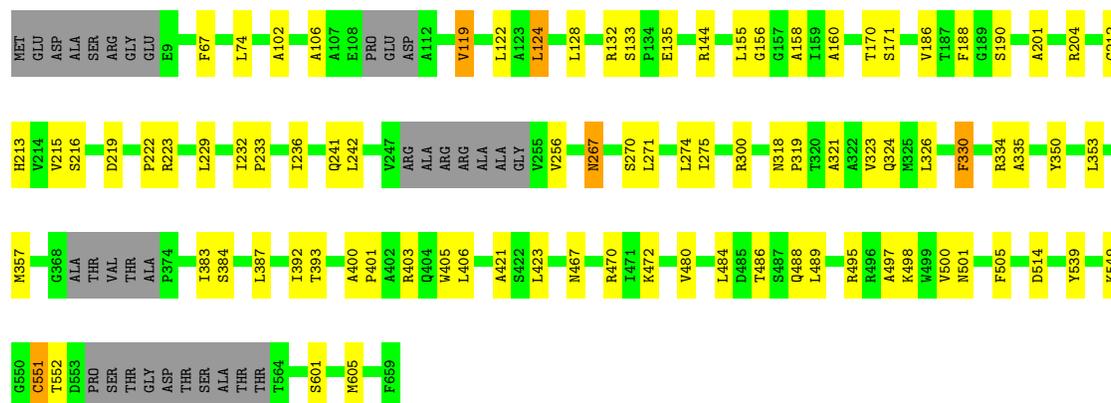


- Molecule 2: EDS1



- Molecule 3: Lipase-like PAD4

Chain C:  82% 13% 5%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1D8A

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	0.24	0/3338	0.46	0/4544
2	B	0.24	0/4750	0.44	0/6457
3	C	0.24	0/4812	0.47	0/6536
All	All	0.24	0/12900	0.46	0/17537

There are no bond length outliers.

There are no bond angle outliers.

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	3277	0	3226	41	0
2	B	4636	0	4465	18	0
3	C	4704	0	4576	51	0
4	B	40	0	0	0	0
All	All	12657	0	12267	108	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 (108) 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:612:LEU:HB2	1:A:639:ASN:HB3	1.75	0.68
3:C:201:ALA:HA	3:C:204:ARG:HE	1.59	0.66
3:C:216:SER:HB3	3:C:219:ASP:HB2	1.77	0.66
3:C:102:ALA:O	3:C:106:ALA:HB2	1.94	0.66
3:C:353:LEU:O	3:C:357:MET:HG3	1.95	0.65
1:A:474:LEU:HD12	1:A:525:PHE:HB2	1.77	0.65
2:B:464:GLU:HG3	3:C:421:ALA:HB1	1.79	0.64
1:A:606:ALA:HB2	1:A:630:TYR:HB3	1.79	0.63
1:A:466:PHE:O	1:A:534:ARG:NH1	2.32	0.63
3:C:74:LEU:HD21	3:C:242:LEU:HD23	1.80	0.63
1:A:664:LYS:NZ	1:A:690:LYS:O	2.31	0.63
1:A:576:GLN:HA	1:A:598:ALA:HA	1.82	0.61
3:C:216:SER:O	3:C:223:ARG:NH2	2.34	0.61
1:A:553:VAL:HA	1:A:579:SER:HB3	1.82	0.60
3:C:334:ARG:HG3	3:C:335:ALA:H	1.68	0.58
3:C:219:ASP:O	3:C:223:ARG:NH1	2.37	0.58
3:C:271:LEU:O	3:C:275:ILE:HG22	2.04	0.57
1:A:487:LEU:HB3	1:A:492:ALA:HB2	1.86	0.57
3:C:423:LEU:HD11	3:C:480:VAL:HG22	1.87	0.57
2:B:207:ASP:O	2:B:211:ARG:NH1	2.36	0.56
1:A:600:VAL:HG23	1:A:624:ALA:HB3	1.86	0.56
3:C:67:PHE:HB2	3:C:160:ALA:HB2	1.87	0.56
3:C:156:GLY:H	3:C:241:GLN:HE22	1.54	0.56
3:C:229:LEU:HA	3:C:232:ILE:HG12	1.88	0.56
3:C:144:ARG:NH2	3:C:170:THR:OG1	2.40	0.55
3:C:133:SER:OG	3:C:135:GLU:OE1	2.21	0.55
3:C:242:LEU:HD11	3:C:256:VAL:HG13	1.89	0.55
3:C:601:SER:O	3:C:605:MET:HG3	2.08	0.54
2:B:211:ARG:HH21	2:B:317:LEU:HA	1.72	0.54
3:C:212:CYS:SG	3:C:213:HIS:N	2.79	0.54
1:A:458:GLU:HB2	1:A:551:ARG:HH22	1.72	0.53
3:C:514:ASP:OD2	3:C:539:TYR:OH	2.22	0.53
1:A:724:LEU:HD13	1:A:727:ILE:HD11	1.92	0.52
2:B:54:SER:HA	2:B:58:PRO:HA	1.92	0.52
2:B:50:VAL:HG21	2:B:126:GLU:HG2	1.92	0.52
1:A:662:LEU:HD12	1:A:663:PRO:HD2	1.92	0.51
1:A:452:LEU:HD12	1:A:456:VAL:HG21	1.90	0.51
3:C:497:ALA:O	3:C:501:ASN:ND2	2.43	0.51
1:A:752:ARG:HA	1:A:776:ASP:HB3	1.92	0.51
2:B:316:LEU:HD21	2:B:390:LEU:HD11	1.93	0.51
3:C:158:ALA:HB2	3:C:190:SER:HB2	1.92	0.51
1:A:820:LEU:HB3	1:A:843:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:387:LEU:HB3	3:C:392:ILE:HD11	1.92	0.50
1:A:650:ARG:HA	1:A:672:LEU:HA	1.94	0.50
3:C:275:ILE:HD13	3:C:330:PHE:HE2	1.77	0.49
3:C:119:VAL:HG11	3:C:124:LEU:HD23	1.94	0.49
2:B:258:THR:HG22	2:B:318:PHE:HB2	1.95	0.49
2:B:244:PRO:HG2	2:B:247:ILE:HG13	1.95	0.49
1:A:458:GLU:HG3	1:A:485:HIS:CE1	2.48	0.48
3:C:233:PRO:HB2	3:C:236:ILE:HG22	1.95	0.48
1:A:598:ALA:HB3	1:A:619:MET:HG3	1.95	0.48
3:C:270:SER:O	3:C:274:LEU:HG	2.14	0.48
2:B:183:ASP:H	2:B:186:PHE:HB3	1.78	0.47
1:A:619:MET:SD	1:A:619:MET:N	2.88	0.47
3:C:223:ARG:HB2	3:C:275:ILE:HD11	1.97	0.47
3:C:484:LEU:HG	3:C:489:LEU:HD12	1.96	0.46
3:C:318:ASN:HB3	3:C:321:ALA:HB3	1.97	0.46
3:C:383:ILE:HG23	3:C:406:LEU:HD12	1.97	0.46
1:A:618:THR:OG1	1:A:619:MET:SD	2.74	0.46
3:C:384:SER:HB3	3:C:403:ARG:HH22	1.81	0.46
3:C:188:PHE:HE2	3:C:350:TYR:HB3	1.81	0.46
1:A:850:GLU:OE2	3:C:472:LYS:NZ	2.49	0.45
1:A:455:LYS:O	1:A:458:GLU:HG2	2.16	0.45
1:A:858:VAL:O	1:A:859:ASP:C	2.54	0.45
1:A:477:LEU:O	1:A:480:ILE:HG13	2.16	0.45
1:A:508:VAL:HB	1:A:526:SER:OG	2.16	0.45
1:A:644:THR:HG22	1:A:667:ILE:HD12	1.99	0.45
3:C:495:ARG:HH22	3:C:552:THR:HG21	1.82	0.45
3:C:467:ASN:OD1	3:C:470:ARG:NH2	2.45	0.45
1:A:619:MET:H	1:A:619:MET:CE	2.30	0.44
3:C:334:ARG:HH21	3:C:393:THR:HG22	1.81	0.44
1:A:439:THR:HA	1:A:443:GLU:HB2	2.00	0.44
3:C:267:ASN:HB3	3:C:270:SER:HB2	2.00	0.44
3:C:186:VAL:C	3:C:188:PHE:H	2.20	0.44
2:B:8:SER:O	2:B:12:ARG:HG3	2.18	0.43
1:A:619:MET:H	1:A:619:MET:HE1	1.84	0.43
2:B:435:SER:OG	2:B:590:ASP:OD2	2.37	0.43
2:B:554:LEU:HD12	2:B:554:LEU:HA	1.90	0.43
3:C:324:GLN:HB3	3:C:405:TRP:CE3	2.54	0.43
3:C:486:THR:HG22	3:C:488:GLN:HG3	2.01	0.43
2:B:56:PRO:HG2	2:B:57:TYR:CD1	2.55	0.42
1:A:746:HIS:O	1:A:746:HIS:ND1	2.52	0.42
1:A:820:LEU:HD23	1:A:820:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:VAL:HG12	2:B:206:VAL:H	1.84	0.42
2:B:129:ARG:NE	2:B:129:ARG:HA	2.34	0.42
3:C:400:ALA:HB3	3:C:401:PRO:HD3	2.02	0.42
3:C:498:LYS:HA	3:C:501:ASN:HD21	1.83	0.42
1:A:842:ASP:OD1	1:A:842:ASP:N	2.53	0.42
1:A:709:ILE:HD13	1:A:709:ILE:HA	1.86	0.42
1:A:470:LYS:HD3	1:A:470:LYS:HA	1.78	0.41
3:C:319:PRO:O	3:C:323:VAL:HG23	2.20	0.41
1:A:682:LEU:HD22	1:A:686:LEU:HD22	2.03	0.41
2:B:360:LEU:HD23	2:B:360:LEU:HA	1.79	0.41
3:C:128:LEU:O	3:C:132:ARG:HG3	2.20	0.41
3:C:551:CYS:SG	3:C:552:THR:N	2.94	0.41
1:A:462:ASP:OD1	1:A:551:ARG:NH2	2.49	0.41
2:B:298:LEU:HD11	2:B:346:ILE:HD11	2.02	0.41
3:C:122:LEU:HG	3:C:155:LEU:HD21	2.02	0.41
3:C:500:VAL:HG21	3:C:549:LYS:HD2	2.03	0.41
1:A:473:PRO:HB2	1:A:476:VAL:HG22	2.03	0.41
3:C:215:VAL:HG11	3:C:326:LEU:HD11	2.02	0.41
1:A:456:VAL:HG22	1:A:495:ILE:HD12	2.03	0.40
3:C:215:VAL:HG13	3:C:222:PRO:HG2	2.03	0.40
1:A:625:LEU:HB3	1:A:652:LEU:HD12	2.04	0.40
2:B:516:LEU:HD23	2:B:516:LEU:HA	1.87	0.40
1:A:615:PHE:O	1:A:618:THR:OG1	2.23	0.40
1:A:763:PRO:HA	1:A:764:PRO:HD3	2.00	0.40
3:C:300:ARG:HD3	3:C:300:ARG:HA	1.82	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 PDB entries followed by that with respect to all EM entries.

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	422/859 (49%)	413 (98%)	9 (2%)	0	100   100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	596/621 (96%)	591 (99%)	5 (1%)	0	100	100
3	C	616/659 (94%)	599 (97%)	17 (3%)	0	100	100
All	All	1634/2139 (76%)	1603 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	364/741 (49%)	356 (98%)	8 (2%)	47	69
2	B	489/520 (94%)	482 (99%)	7 (1%)	62	79
3	C	466/517 (90%)	459 (98%)	7 (2%)	60	78
All	All	1319/1778 (74%)	1297 (98%)	22 (2%)	56	76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	466	PHE
1	A	478	ILE
1	A	519	TYR
1	A	589	ASP
1	A	610	TYR
1	A	619	MET
1	A	826	ASP
1	A	853	ASN
2	B	140	THR
2	B	167	ASN
2	B	172	PHE
2	B	181	VAL
2	B	203	VAL
2	B	359	TYR
2	B	443	GLN
3	C	119	VAL

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Mol	Chain	Res	Type
3	C	124	LEU
3	C	171	SER
3	C	267	ASN
3	C	330	PHE
3	C	505	PHE
3	C	551	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	GLN

### 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](#)

1 ligand is 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$
4	A1D8A	B	701	-	37,43,43	3.20	12 (32%)	50,67,67	1.29	5 (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
4	A1D8A	B	701	-	-	8/22/58/58	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	A1D8A	O4'-C1'	-8.99	1.28	1.41
4	B	701	A1D8A	C35-C28	-8.52	1.31	1.53
4	B	701	A1D8A	O27-C26	8.24	1.56	1.41
4	B	701	A1D8A	O27-C28	5.53	1.57	1.45
4	B	701	A1D8A	O3'-C3'	4.64	1.53	1.43
4	B	701	A1D8A	C37-C35	4.27	1.65	1.53
4	B	701	A1D8A	C6-N6	4.07	1.48	1.34
4	B	701	A1D8A	O4'-C4'	3.51	1.52	1.45
4	B	701	A1D8A	C5'-C4'	-2.96	1.42	1.51
4	B	701	A1D8A	P31-O30	2.51	1.68	1.60
4	B	701	A1D8A	C26-C37	-2.41	1.49	1.52
4	B	701	A1D8A	PB-O2B	-2.02	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	A1D8A	N3-C2-N1	-4.50	121.64	128.68
4	B	701	A1D8A	O27-C26-C37	-3.37	100.64	104.98
4	B	701	A1D8A	C26-O2'-C2'	-2.74	111.18	117.96
4	B	701	A1D8A	C4-C5-N7	-2.53	106.77	109.40
4	B	701	A1D8A	PA-O3A-PB	-2.13	125.52	132.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	A1D8A	C3'-C4'-C5'-O5'
4	B	701	A1D8A	O4'-C4'-C5'-O5'
4	B	701	A1D8A	PA-O3A-PB-O1B
4	B	701	A1D8A	PA-O3A-PB-O2B
4	B	701	A1D8A	C4'-C5'-O5'-PA
4	B	701	A1D8A	O27-C28-C29-O30

*Continued on next page...*

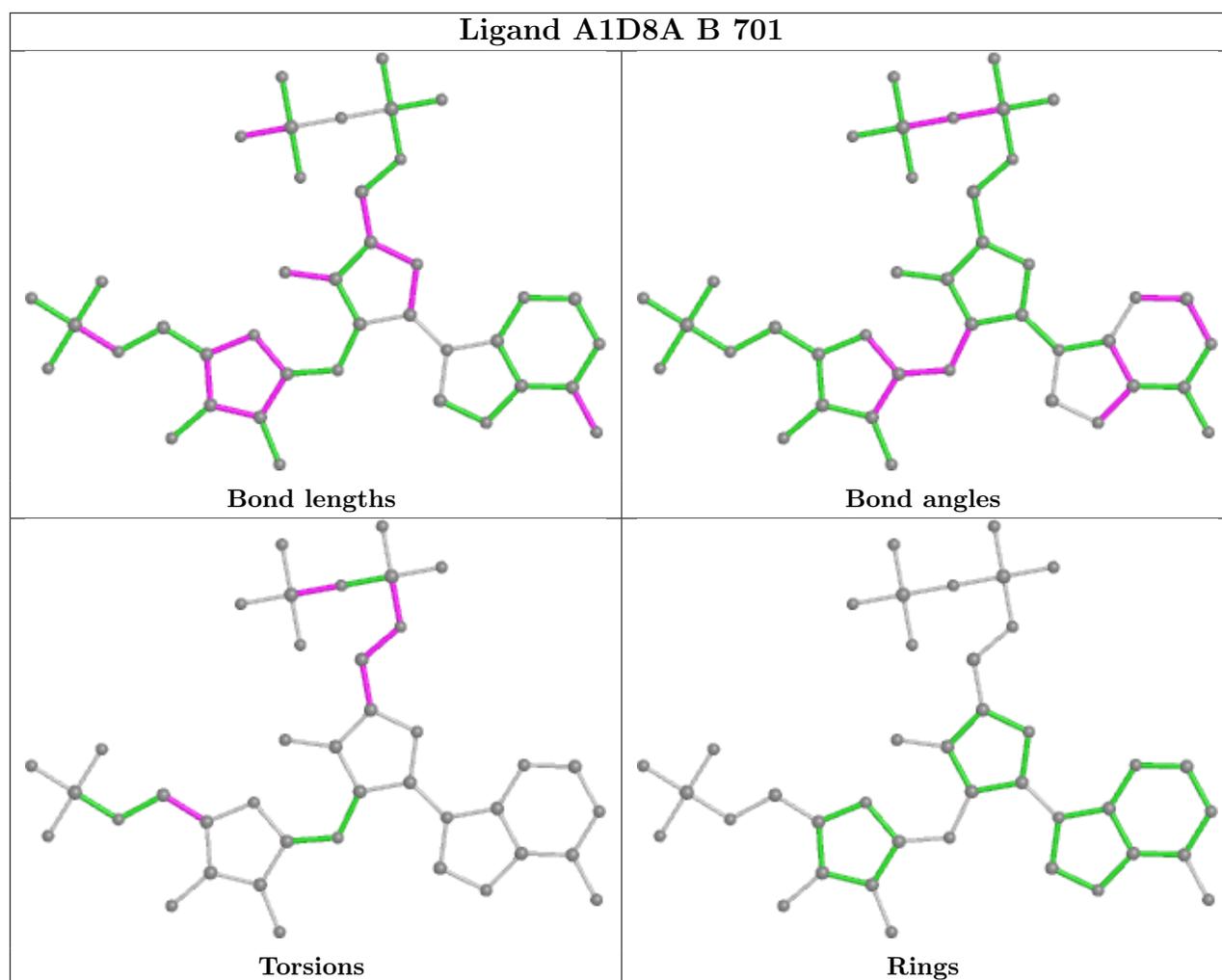
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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
4	B	701	A1D8A	C5'-O5'-PA-O2A
4	B	701	A1D8A	PA-O3A-PB-O3B

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.