



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 06:52 PM EST

PDB ID : 3U06  
Title : Crystal structure of the kinesin-14 NcdG347D  
Authors : Liu, H.-L.; Pemble IV, C.W.; Endow, S.A.  
Deposited on : 2011-09-28  
Resolution : 2.35 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](mailto: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>.

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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) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

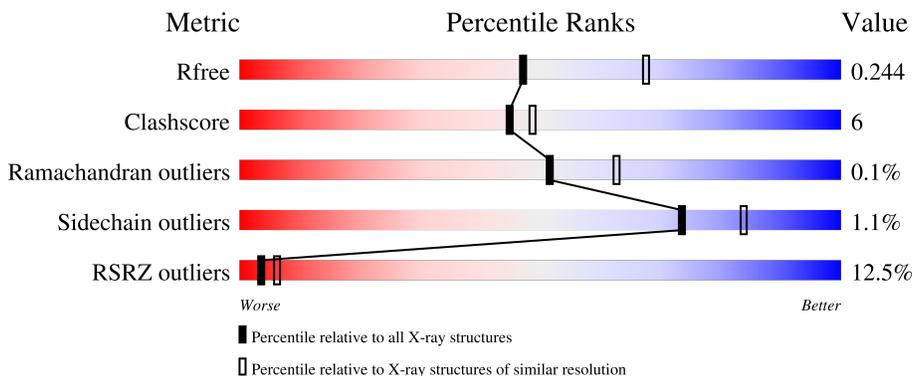
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	412	
1	B	412	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11469 atoms, of which 5633 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.

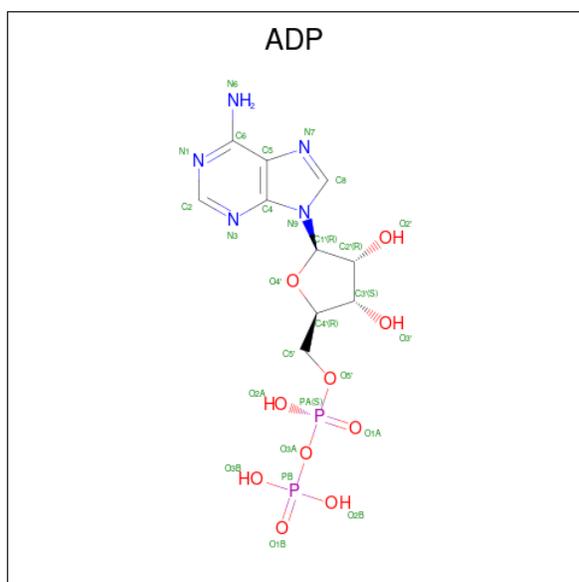
- Molecule 1 is a protein called Protein claret segregational.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	359	5715	1789	2840	506	559	21	0	0	0
1	B	344	5483	1721	2729	480	532	21	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	MET	-	expression tag	UNP P20480
A	290	GLY	-	expression tag	UNP P20480
A	291	SER	-	expression tag	UNP P20480
A	292	MET	-	expression tag	UNP P20480
A	347	ASP	GLY	engineered mutation	UNP P20480
B	289	MET	-	expression tag	UNP P20480
B	290	GLY	-	expression tag	UNP P20480
B	291	SER	-	expression tag	UNP P20480
B	292	MET	-	expression tag	UNP P20480
B	347	ASP	GLY	engineered mutation	UNP P20480

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

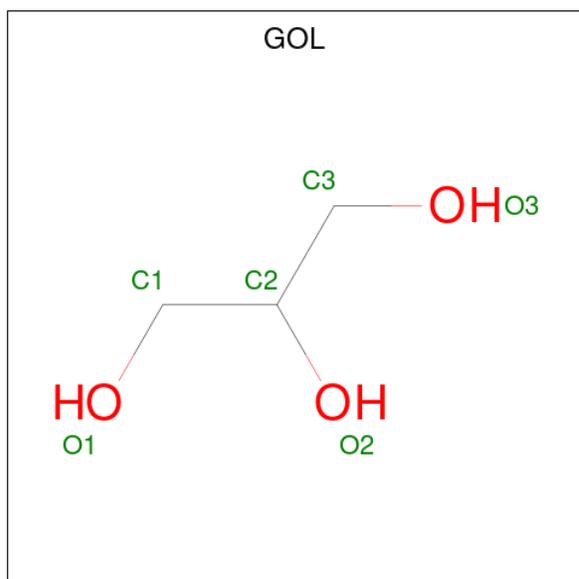


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	39	10	12	5	10	2	0	0
2	B	1	39	10	12	5	10	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total	O	0	0
			88	88		
5	B	34	Total	O	0	0
			34	34		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.54Å 67.09Å 94.37Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	46.62 – 2.35 46.62 – 2.34	Depositor EDS
% Data completeness (in resolution range)	86.1 (46.62-2.35) 86.1 (46.62-2.34)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.7.2_868	Depositor
R, $R_{free}$	0.216 , 0.250 0.216 , 0.244	Depositor DCC
$R_{free}$ test set	1818 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, GOL

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	0.23	0/2920	0.42	0/3936
1	B	0.23	0/2802	0.43	0/3778
All	All	0.23	0/5722	0.42	0/7714

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	2875	2840	2828	30	0
1	B	2754	2729	2718	44	0
2	A	27	12	12	0	0
2	B	27	12	12	1	0
3	A	1	0	0	0	0
4	A	24	32	32	0	0
4	B	6	8	8	0	0
5	A	88	0	0	1	0
5	B	34	0	0	1	0
All	All	5836	5633	5610	73	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 6.

All (73) 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:B:567:GLU:OE1	1:B:567:GLU:N	2.29	0.66
1:B:359:LEU:HD21	2:B:1:ADP:H1'	1.81	0.62
1:B:645:ILE:HD11	1:B:660:SER:HB3	1.82	0.62
1:B:458:VAL:HG22	1:B:528:LEU:HD23	1.82	0.62
1:B:301:VAL:O	1:B:305:GLN:HG3	2.02	0.60
1:B:525:PRO:O	1:B:529:ARG:HG3	2.02	0.59
1:A:552:ARG:HD3	1:A:599:ILE:CG2	2.33	0.58
1:A:346:ARG:O	1:A:347:ASP:HB2	2.04	0.58
1:A:403:HIS:HB2	1:A:404:PRO:CD	2.34	0.57
1:B:631:LEU:O	1:B:635:LEU:N	2.37	0.57
1:B:353:CYS:HA	1:B:645:ILE:HG23	1.87	0.57
1:B:454:ILE:HB	1:B:455:PRO:HD3	1.87	0.56
1:A:454:ILE:HB	1:A:455:PRO:HD3	1.87	0.56
1:B:632:MET:HB3	1:B:633:PRO:HD3	1.88	0.55
1:A:403:HIS:HB2	1:A:404:PRO:HD2	1.89	0.55
1:B:599:ILE:N	1:B:599:ILE:HD12	2.22	0.54
1:B:403:HIS:CG	1:B:404:PRO:HD2	2.43	0.54
1:B:601:ARG:O	1:B:604:SER:N	2.41	0.54
1:A:512:ILE:HD12	1:A:512:ILE:C	2.29	0.53
1:B:416:SER:OG	1:B:417:PRO:HD3	2.09	0.53
1:B:489:LEU:HD11	1:B:626:LYS:HD3	1.92	0.51
1:B:519:GLU:O	1:B:520:GLU:HG2	2.10	0.51
1:A:552:ARG:HD3	1:A:599:ILE:HG22	1.91	0.50
1:B:356:ARG:O	1:B:649:PRO:HG3	2.12	0.50
1:B:569:GLN:HG3	1:B:569:GLN:O	2.12	0.50
1:B:366:MET:SD	1:B:383:ILE:HD13	2.52	0.50
1:A:671:LYS:O	1:A:672:MET:CB	2.60	0.49
1:A:346:ARG:O	1:A:347:ASP:CB	2.61	0.49
1:B:520:GLU:HG3	1:B:531:LEU:HD21	1.94	0.49
1:A:552:ARG:HG2	1:A:599:ILE:HG23	1.95	0.49
1:A:374:ASP:OD1	1:A:377:THR:N	2.46	0.49
1:A:621:PRO:HB2	1:A:624:ASN:ND2	2.28	0.49
1:B:454:ILE:HG12	1:B:578:LEU:HD13	1.96	0.47
1:A:671:LYS:O	1:A:672:MET:HB2	2.12	0.47
1:B:605:GLU:O	1:B:609:VAL:HG23	2.14	0.47
1:B:520:GLU:HG3	1:B:531:LEU:CD2	2.45	0.47
1:B:347:ASP:HA	1:B:639:SER:HB3	1.97	0.47
1:B:631:LEU:O	1:B:635:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ALA:O	1:B:579:VAL:HA	2.14	0.47
1:A:300:VAL:HG23	1:B:300:VAL:CG1	2.46	0.46
1:B:567:GLU:HG2	1:B:567:GLU:O	2.16	0.46
1:B:350:ARG:HD2	1:B:639:SER:O	2.16	0.45
1:A:370:TRP:CH2	1:A:647:VAL:HG11	2.51	0.45
1:A:484:ILE:HG12	1:A:489:LEU:HD23	1.99	0.45
1:A:498:LYS:HD2	1:A:516:ASN:O	2.16	0.45
1:A:654:PHE:O	1:A:658:VAL:HG23	2.17	0.45
1:A:321:LEU:HG	1:A:325:LYS:HE3	1.98	0.44
1:B:552:ARG:HA	1:B:582:ALA:HB1	1.99	0.44
1:B:491:ASP:HB3	1:B:517:ILE:HD12	1.99	0.44
1:B:376:SER:HB2	1:B:398:PHE:O	2.18	0.44
1:B:601:ARG:O	1:B:602:SER:C	2.56	0.44
1:A:355:ILE:HD12	1:A:647:VAL:CG1	2.48	0.44
1:B:447:VAL:HG23	1:B:449:GLU:HG2	2.00	0.44
1:B:611:LEU:O	1:B:615:GLN:HG2	2.18	0.44
1:A:524:ASP:HB2	1:A:525:PRO:HD2	2.00	0.43
1:B:416:SER:N	1:B:417:PRO:CD	2.81	0.43
1:A:429:CYS:HB3	1:A:431:PHE:CE2	2.53	0.43
1:B:539:ARG:CZ	1:B:555:ALA:HB2	2.48	0.43
1:A:623:ARG:NH1	5:A:65:HOH:O	2.51	0.43
1:A:444:MET:HA	1:A:444:MET:HE2	2.01	0.42
1:B:478:LYS:HB2	1:B:560:GLU:HB3	2.01	0.42
1:B:391:MET:O	5:B:57:HOH:O	2.22	0.42
1:A:369:THR:HB	1:A:381:GLN:HB2	2.01	0.42
1:A:416:SER:N	1:A:417:PRO:CD	2.82	0.42
1:B:632:MET:HB3	1:B:633:PRO:CD	2.48	0.42
1:B:403:HIS:CD2	1:B:404:PRO:HD2	2.55	0.42
1:A:621:PRO:HB2	1:A:624:ASN:CG	2.41	0.41
1:B:416:SER:HB2	1:B:460:LEU:HD22	2.02	0.41
1:B:348:ASN:O	1:B:639:SER:HA	2.21	0.41
1:A:376:SER:HB3	1:A:398:PHE:O	2.21	0.40
1:B:658:VAL:O	1:B:662:ARG:HG3	2.22	0.40
1:A:416:SER:OG	1:A:417:PRO:HD3	2.21	0.40
1:A:447:VAL:HB	1:A:448:PRO:HD2	2.04	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	351/412 (85%)	343 (98%)	7 (2%)	1 (0%)	41	47
1	B	335/412 (81%)	319 (95%)	16 (5%)	0	100	100
All	All	686/824 (83%)	662 (96%)	23 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	ASP

### 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	328/373 (88%)	327 (100%)	1 (0%)	92	96
1	B	316/373 (85%)	310 (98%)	6 (2%)	57	68
All	All	644/746 (86%)	637 (99%)	7 (1%)	73	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	552	ARG
1	B	340	ASN
1	B	414	MET
1	B	419	ILE
1	B	427	ASN

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Mol	Chain	Res	Type
1	B	482	LEU
1	B	600	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	314	ASN
1	B	330	GLN
1	B	598	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	A	1	3	24,29,29	0.97	1 (4%)	29,45,45	1.47	5 (17%)
4	GOL	A	2	-	5,5,5	0.41	0	5,5,5	0.31	0
4	GOL	A	3	-	5,5,5	0.36	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	4	-	5,5,5	0.37	0	5,5,5	0.25	0
4	GOL	A	702	-	5,5,5	0.37	0	5,5,5	0.25	0
2	ADP	B	1	-	24,29,29	0.96	1 (4%)	29,45,45	1.54	4 (13%)
4	GOL	B	5	-	5,5,5	0.38	0	5,5,5	0.22	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	ADP	A	1	3	-	0/12/32/32	0/3/3/3
4	GOL	A	2	-	-	0/4/4/4	-
4	GOL	A	3	-	-	0/4/4/4	-
4	GOL	A	4	-	-	3/4/4/4	-
4	GOL	A	702	-	-	2/4/4/4	-
2	ADP	B	1	-	-	3/12/32/32	0/3/3/3
4	GOL	B	5	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ADP	C5-C4	2.47	1.47	1.40
2	B	1	ADP	C5-C4	2.42	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ADP	N3-C2-N1	-3.74	122.83	128.68
2	B	1	ADP	PA-O3A-PB	-3.72	120.08	132.83
2	B	1	ADP	N3-C2-N1	-3.62	123.01	128.68
2	B	1	ADP	C3'-C2'-C1'	3.21	105.81	100.98
2	A	1	ADP	PA-O3A-PB	-3.18	121.91	132.83
2	A	1	ADP	C3'-C2'-C1'	2.84	105.25	100.98
2	A	1	ADP	C4-C5-N7	-2.71	106.57	109.40
2	B	1	ADP	C4-C5-N7	-2.58	106.71	109.40
2	A	1	ADP	C2-N1-C6	2.12	122.38	118.75

There are no chirality outliers.

All (12) torsion outliers are listed below:

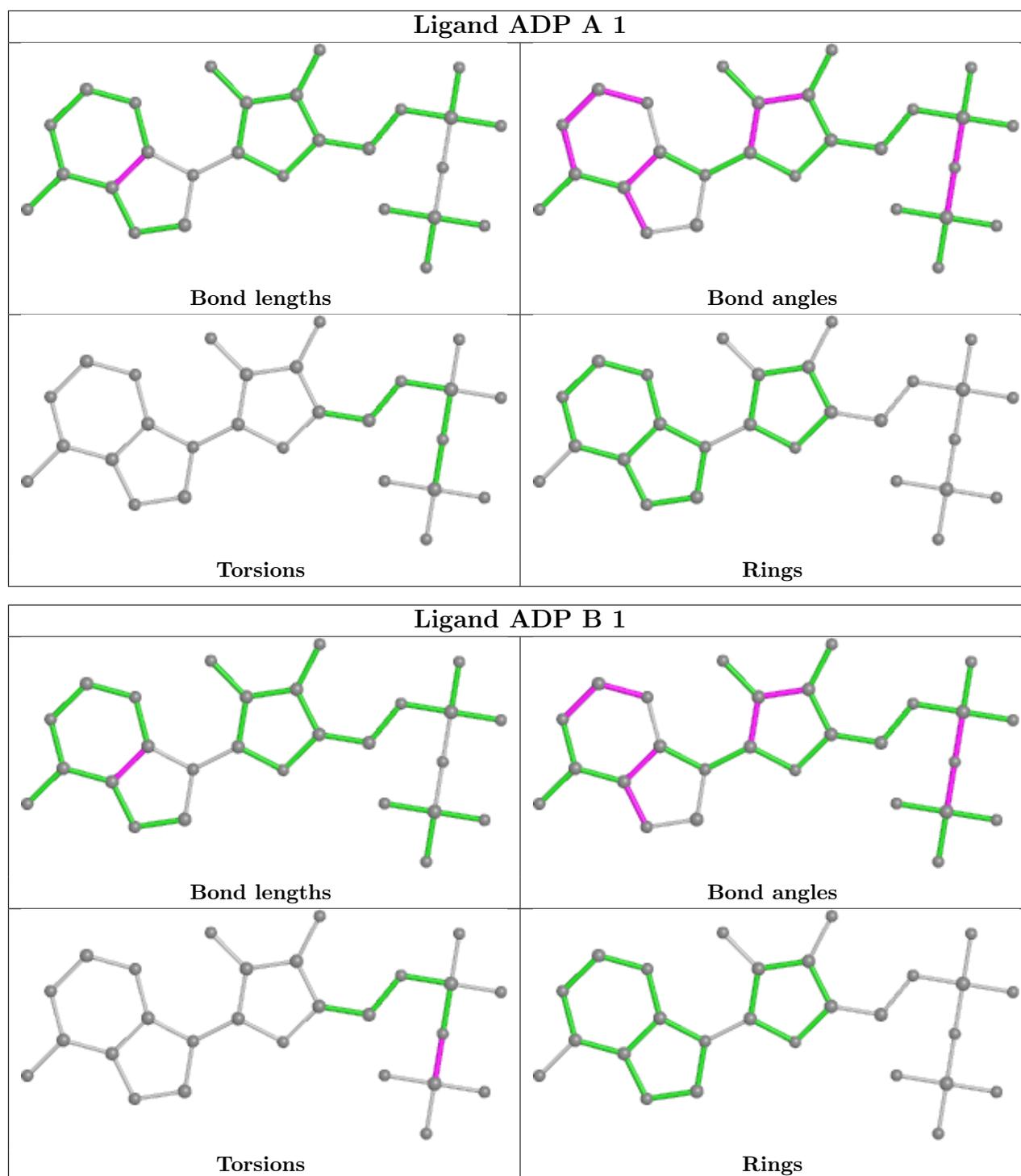
Mol	Chain	Res	Type	Atoms
2	B	1	ADP	PA-O3A-PB-O3B
4	A	702	GOL	C1-C2-C3-O3
4	B	5	GOL	O1-C1-C2-C3
4	A	4	GOL	C1-C2-C3-O3
4	B	5	GOL	C1-C2-C3-O3
4	A	702	GOL	O2-C2-C3-O3
4	B	5	GOL	O1-C1-C2-O2
4	A	4	GOL	O2-C2-C3-O3
4	A	4	GOL	O1-C1-C2-O2
4	B	5	GOL	O2-C2-C3-O3
2	B	1	ADP	PA-O3A-PB-O1B
2	B	1	ADP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/412 (87%)	0.74	16 (4%) 33 46	33, 51, 92, 122	0
1	B	344/412 (83%)	1.21	72 (20%) 1 1	34, 70, 120, 140	0
All	All	703/824 (85%)	0.97	88 (12%) 3 6	33, 57, 114, 140	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	514	VAL	5.9
1	B	471	LEU	5.0
1	B	549	ARG	5.0
1	B	513	TYR	4.9
1	B	561	LEU	4.8
1	B	311	LEU	4.6
1	B	566	ALA	4.6
1	B	515	SER	4.3
1	B	475	TYR	4.2
1	B	571	ILE	4.2
1	B	630	LEU	4.0
1	B	474	GLU	4.0
1	B	631	LEU	3.9
1	A	618	ASP	3.8
1	B	469	ARG	3.7
1	B	574	GLY	3.7
1	B	481	PHE	3.6
1	A	619	HIS	3.5
1	B	477	ILE	3.4
1	B	450	SER	3.3
1	A	306	ARG	3.3
1	B	493	LEU	3.3
1	B	603	LEU	3.2
1	B	634	SER	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	479	ALA	3.1
1	B	562	ILE	3.1
1	B	619	HIS	3.1
1	B	488	VAL	3.1
1	B	516	ASN	3.0
1	B	563	GLY	3.0
1	B	489	LEU	2.9
1	B	321	LEU	2.9
1	B	531	LEU	2.9
1	B	569	GLN	2.9
1	B	468	TYR	2.9
1	A	507	ASN	2.9
1	B	312	ARG	2.9
1	B	568	LYS	2.7
1	B	645	ILE	2.7
1	A	316	GLN	2.7
1	B	673	THR	2.7
1	B	362	GLU	2.6
1	B	425	GLY	2.6
1	B	423	LEU	2.6
1	B	523	LEU	2.6
1	B	600	ASN	2.6
1	B	389	SER	2.5
1	B	573	VAL	2.5
1	B	419	ILE	2.5
1	A	549	ARG	2.5
1	B	470	ASN	2.5
1	B	473	TRP	2.5
1	A	672	MET	2.4
1	B	556	VAL	2.4
1	B	572	SER	2.4
1	A	392	GLY	2.4
1	A	546	GLY	2.4
1	B	618	ASP	2.4
1	B	319	ALA	2.4
1	B	490	TYR	2.4
1	B	519	GLU	2.4
1	B	517	ILE	2.3
1	B	560	GLU	2.3
1	B	310	LEU	2.3
1	B	338	LEU	2.3
1	A	309	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	667	VAL	2.2
1	B	553	SER	2.2
1	A	305	GLN	2.2
1	B	449	GLU	2.2
1	B	390	LYS	2.2
1	B	564	ARG	2.2
1	B	458	VAL	2.2
1	A	419	ILE	2.2
1	B	478	LYS	2.2
1	B	316	GLN	2.2
1	B	518	THR	2.2
1	B	635	LEU	2.1
1	B	522	VAL	2.1
1	A	359	LEU	2.1
1	A	548	GLU	2.1
1	B	318	ALA	2.1
1	B	526	ASN	2.1
1	A	537	MET	2.1
1	A	497	GLN	2.0
1	B	383	ILE	2.0
1	B	492	LEU	2.0
1	B	525	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

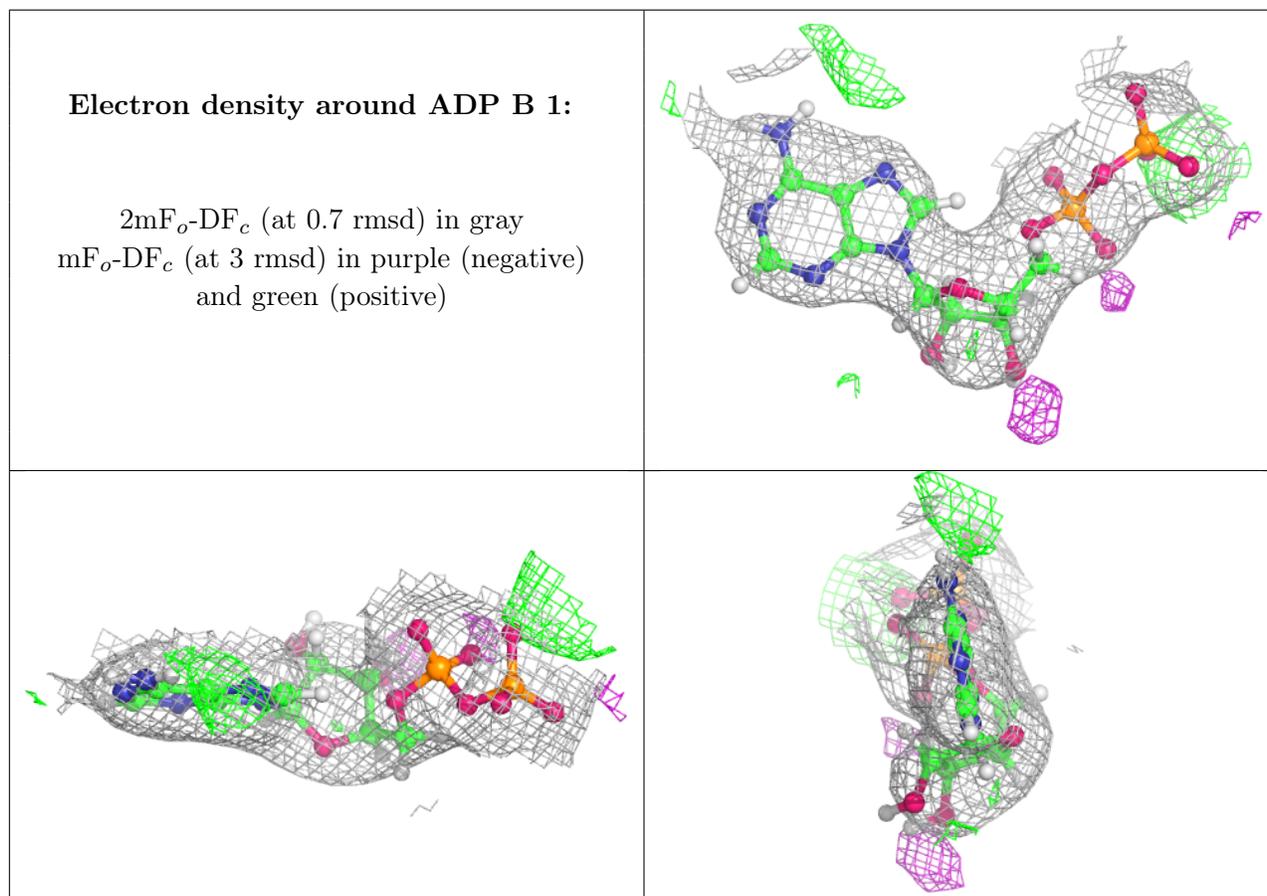
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	4	6/6	0.69	0.24	79,95,96,96	0

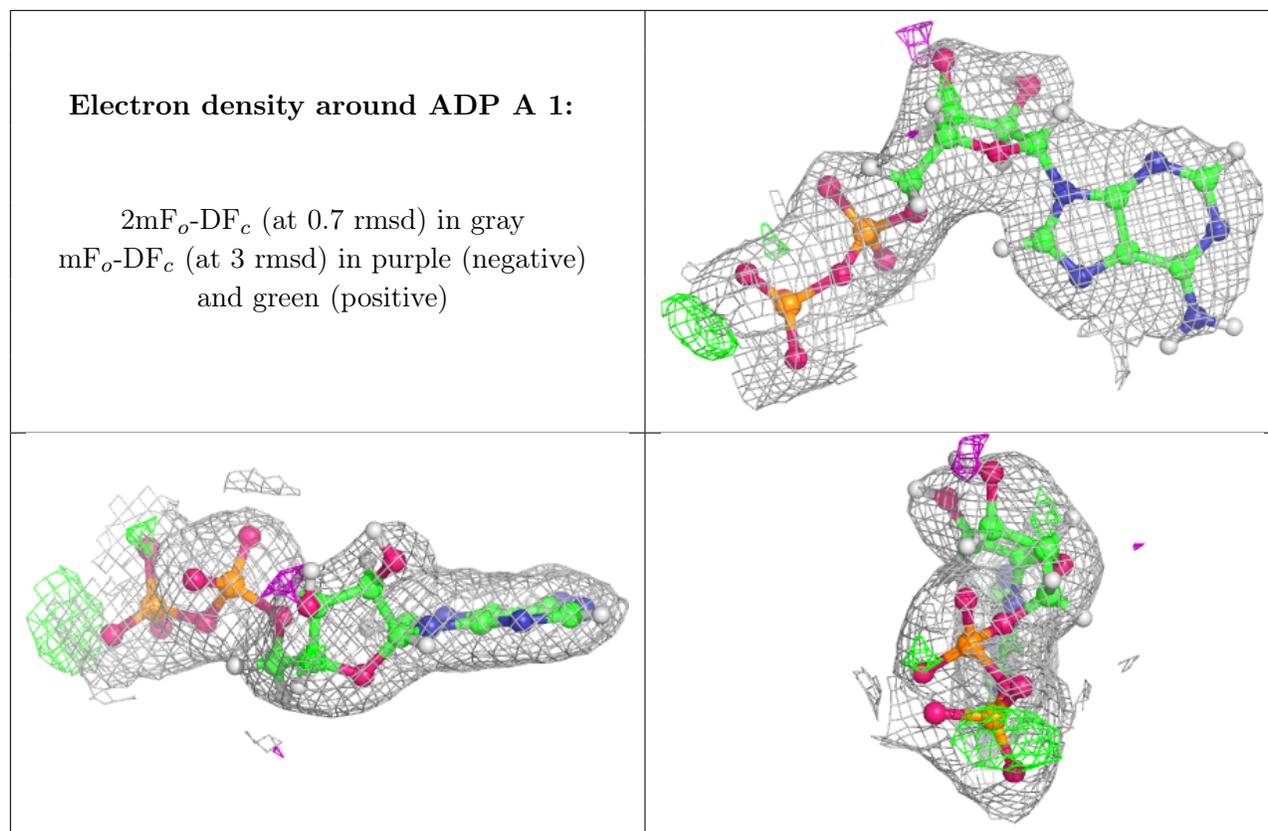
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	2	6/6	0.78	0.27	80,96,98,99	0
4	GOL	B	5	6/6	0.84	0.26	70,84,87,88	0
3	MG	A	701	1/1	0.90	0.16	50,50,50,50	0
4	GOL	A	3	6/6	0.90	0.15	44,53,55,56	0
4	GOL	A	702	6/6	0.93	0.23	66,79,80,82	0
2	ADP	B	1	27/27	0.95	0.21	60,69,84,87	0
2	ADP	A	1	27/27	0.97	0.18	35,47,62,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.