



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:34 AM UTC

PDB ID : 3U06 / pdb_00003u06
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

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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

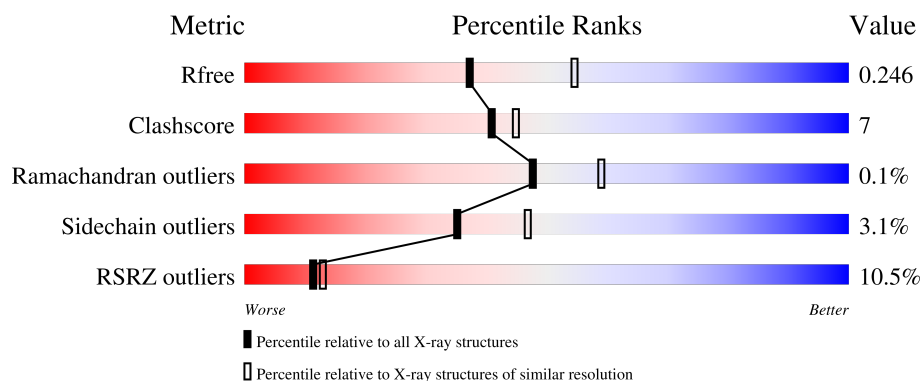
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 ≥ 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	4% 76% 10% • 13%
1	B	412	14% 66% 17% • 17%

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
1	A	359	Total	C	H	N	O	S	0	0	0
			5715	1789	2840	506	559	21			
1	B	344	Total	C	H	N	O	S	0	1	0
			5483	1721	2729	480	532	21			

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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

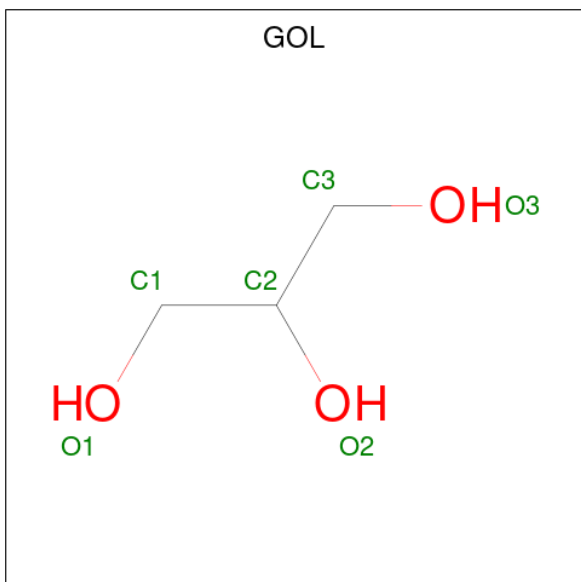


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
2	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0

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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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		

- Molecule 1: Protein claret segregational



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.54Å 67.09Å 94.37Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	46.62 – 2.35 46.62 – 2.35	Depositor EDS
% Data completeness (in resolution range)	86.1 (46.62-2.35) 87.1 (46.62-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.7.2 _868	Depositor
R, R_{free}	0.216 , 0.250 0.217 , 0.246	Depositor DCC
R_{free} test set	1818 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11469	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, 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	0.29	0/2920	0.64	0/3936
1	B	0.29	0/2802	0.68	0/3778
All	All	0.29	0/5722	0.66	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	45	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	74	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 7.

All (74) 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:512:ILE:HD12	1:A:512:ILE:C	2.29	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:A:444:MET:HA	1:A:444:MET:HE2	1.88	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: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:601:ARG:O	1:B:602:SER:C	2.56	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:621:PRO:HB2	1:A:624:ASN:CG	2.41	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: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: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:B:643:MET:HE1	1:B:667:VAL:HG21	2.02	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%)	36	43
1	B	335/412 (81%)	319 (95%)	16 (5%)	0	100	100
All	All	686/824 (83%)	662 (96%)	23 (3%)	1 (0%)	48	59

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%)	321 (98%)	7 (2%)	47	61
1	B	316/373 (85%)	303 (96%)	13 (4%)	27	36
All	All	644/746 (86%)	624 (97%)	20 (3%)	35	47

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	VAL
1	A	307	THR
1	A	310	LEU
1	A	312	ARG
1	A	552	ARG

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Mol	Chain	Res	Type
1	A	647	VAL
1	A	668	ASN
1	B	326	GLU
1	B	340	ASN
1	B	350	ARG
1	B	390	LYS
1	B	414	MET
1	B	419	ILE
1	B	427	ASN
1	B	482	LEU
1	B	531	LEU
1	B	537	MET
1	B	599	ILE
1	B	600	ASN
1	B	647	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	420	GLN
1	A	629	HIS
1	A	646	ASN
1	B	327	GLN
1	B	330	GLN
1	B	554	HIS
1	B	577	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 oligosaccharides in this entry.

5.6 Ligand geometry

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
4	GOL	A	3	-	5,5,5	0.37	0	5,5,5	0.23	0
4	GOL	A	2	-	5,5,5	0.42	0	5,5,5	0.34	0
2	ADP	B	1	-	28,29,29	1.40	4 (14%)	43,45,45	1.90	11 (25%)
4	GOL	A	4	-	5,5,5	0.37	0	5,5,5	0.28	0
2	ADP	A	1	3	28,29,29	1.42	5 (17%)	43,45,45	1.86	11 (25%)
4	GOL	B	5	-	5,5,5	0.38	0	5,5,5	0.24	0
4	GOL	A	702	-	5,5,5	0.38	0	5,5,5	0.28	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
4	GOL	A	3	-	-	0/4/4/4	-
4	GOL	A	2	-	-	0/4/4/4	-
2	ADP	B	1	-	-	3/16/32/32	0/3/3/3
4	GOL	A	4	-	-	3/4/4/4	-
2	ADP	A	1	3	-	0/16/32/32	0/3/3/3
4	GOL	B	5	-	-	4/4/4/4	-
4	GOL	A	702	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ADP	C5-C4	4.70	1.47	1.39
2	B	1	ADP	C5-C4	4.62	1.47	1.39
2	A	1	ADP	C5-C6	2.77	1.48	1.41
2	B	1	ADP	C5-C6	2.67	1.48	1.41
2	A	1	ADP	C8-N7	2.44	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	ADP	C5-N7	-2.38	1.34	1.39
2	B	1	ADP	C8-N7	2.32	1.36	1.31
2	A	1	ADP	C5-N7	-2.13	1.35	1.39
2	A	1	ADP	PA-O3A	2.03	1.61	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ADP	C5-C4-N3	-5.89	118.60	126.72
2	A	1	ADP	C5-C4-N3	-5.73	118.82	126.72
2	B	1	ADP	N3-C4-N9	4.75	135.25	127.17
2	A	1	ADP	N3-C4-N9	4.55	134.91	127.17
2	B	1	ADP	C2-N3-C4	3.88	121.31	111.83
2	A	1	ADP	C2-N3-C4	3.88	121.30	111.83
2	A	1	ADP	N3-C2-N1	-3.80	122.83	128.58
2	B	1	ADP	N3-C2-N1	-3.68	123.01	128.58
2	A	1	ADP	C4-C5-N7	-3.51	106.57	110.58
2	B	1	ADP	C4-C5-N7	-3.38	106.71	110.58
2	A	1	ADP	C4-N9-C8	2.84	108.72	105.74
2	B	1	ADP	C4-N9-C8	2.76	108.63	105.74
2	B	1	ADP	C5-N7-C8	2.70	107.69	103.45
2	A	1	ADP	C5-N7-C8	2.66	107.63	103.45
2	B	1	ADP	C3'-C2'-C1'	2.30	105.81	101.46
2	A	1	ADP	C2-N1-C6	2.22	122.38	118.73
2	A	1	ADP	C6-C5-N7	2.21	136.35	132.09
2	B	1	ADP	N9-C8-N7	-2.20	110.81	113.94
2	A	1	ADP	N9-C8-N7	-2.20	110.82	113.94
2	B	1	ADP	C2-N1-C6	2.06	122.11	118.73
2	B	1	ADP	C6-C5-N7	2.05	136.03	132.09
2	A	1	ADP	C3'-C2'-C1'	2.00	105.25	101.46

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

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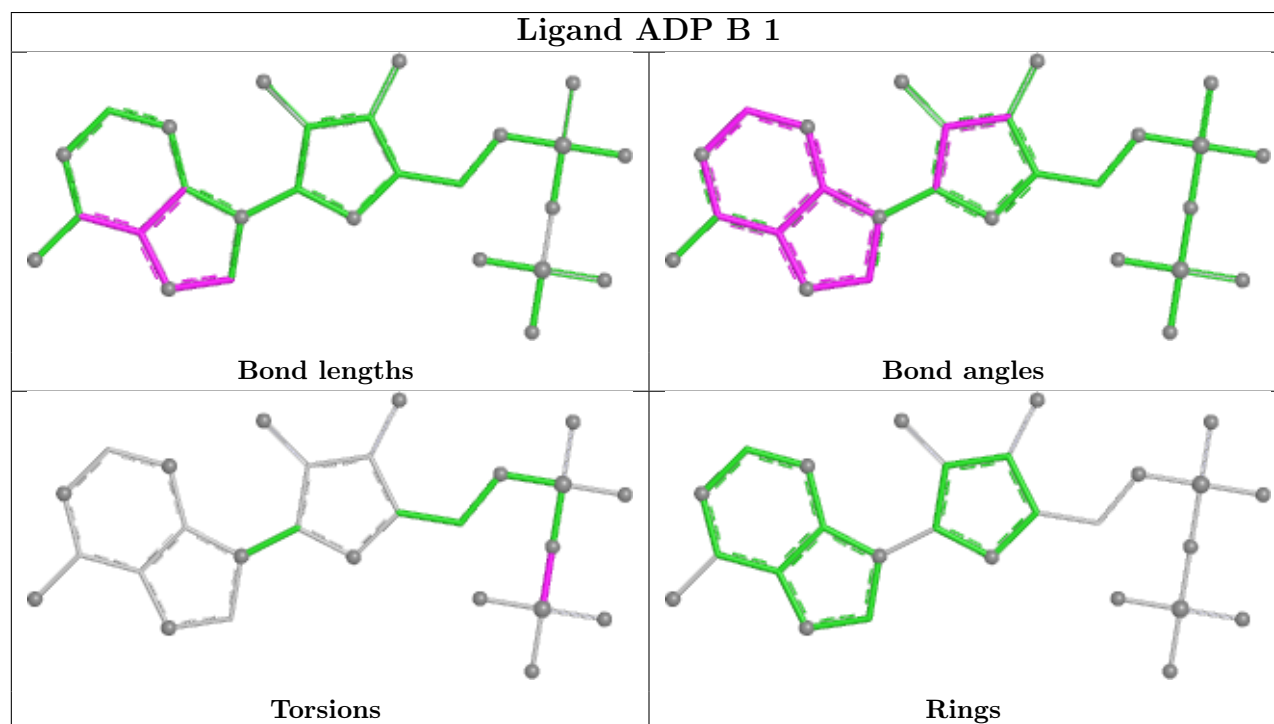
Mol	Chain	Res	Type	Atoms
4	A	4	GOL	O2-C2-C3-O3
4	A	4	GOL	O1-C1-C2-O2
4	B	5	GOL	O2-C2-C3-O3
2	B	1	ADP	PA-O3A-PB-O1B
2	B	1	ADP	PA-O3A-PB-O2B

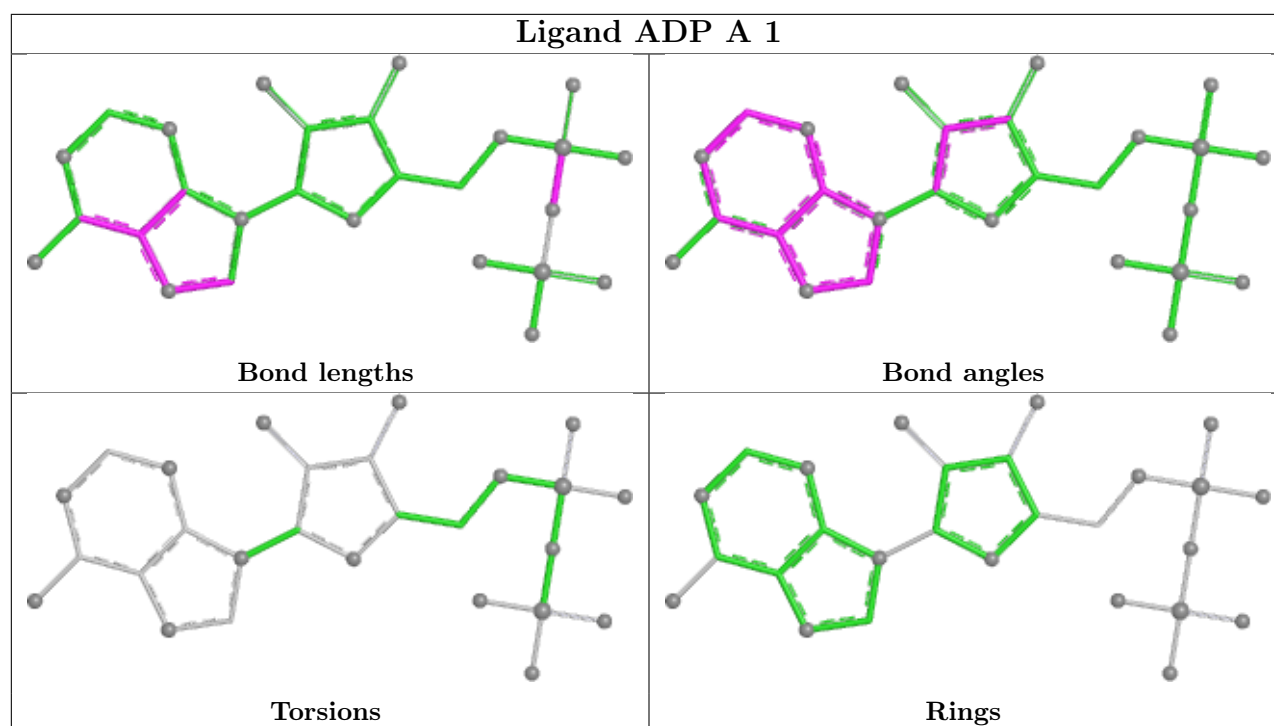
There are no ring outliers.

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 [i](#)

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, 95th 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 ²)	Q<0.9
1	A	359/412 (87%)	0.40	16 (4%) 38 44	36, 56, 99, 139	0
1	B	344/412 (83%)	1.07	58 (16%) 4 4	32, 76, 133, 151	1 (0%)
All	All	703/824 (85%)	0.73	74 (10%) 11 13	32, 62, 124, 151	1 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	599	ILE	5.5
1	B	631	LEU	5.0
1	B	673	THR	4.9
1	A	546	GLY	4.8
1	B	539	ARG	4.7
1	A	384	ASP	4.4
1	B	603	LEU	4.4
1	B	587	PRO	4.2
1	A	392	GLY	3.9
1	B	619	HIS	3.9
1	B	471	LEU	3.8
1	B	561	LEU	3.6
1	B	634	SER	3.6
1	A	672	MET	3.5
1	A	586	SER	3.5
1	A	507	ASN	3.5
1	B	517	ILE	3.4
1	B	518	THR	3.4
1	B	514	VAL	3.4
1	B	630	LEU	3.3
1	B	600	ASN	3.3
1	A	383	ILE	3.3
1	B	481	PHE	3.3
1	B	388	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	670	CYS	3.2
1	B	450	SER	3.2
1	B	635	LEU	3.2
1	B	550	SER	3.2
1	B	568	LYS	3.2
1	B	667	VAL	3.2
1	B	493	LEU	3.1
1	B	361	SER	3.1
1	A	597	LYS	3.1
1	B	475	TYR	3.1
1	B	623	ARG	3.0
1	B	549	ARG	3.0
1	B	333[A]	MET	2.9
1	B	384	ASP	2.8
1	B	489	LEU	2.7
1	A	508	ASN	2.6
1	B	448	PRO	2.6
1	B	530	HIS	2.6
1	B	566	ALA	2.5
1	B	462	PHE	2.5
1	B	513	TYR	2.5
1	B	531	LEU	2.5
1	B	479	ALA	2.5
1	A	359	LEU	2.4
1	B	523	LEU	2.4
1	A	619	HIS	2.4
1	B	419	ILE	2.4
1	B	313	CYS	2.3
1	B	571	ILE	2.3
1	B	389	SER	2.3
1	A	636	GLY	2.3
1	B	449	GLU	2.3
1	A	549	ARG	2.2
1	B	617	GLN	2.2
1	B	548	GLU	2.2
1	A	540	ALA	2.2
1	A	364	ASN	2.2
1	B	474	GLU	2.1
1	B	524	ASP	2.1
1	B	473	TRP	2.1
1	B	569	GLN	2.1
1	B	519	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	316	GLN	2.1
1	B	645	ILE	2.1
1	B	629	HIS	2.0
1	B	525	PRO	2.0
1	B	488	VAL	2.0
1	B	515	SER	2.0
1	B	338	LEU	2.0
1	B	466	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

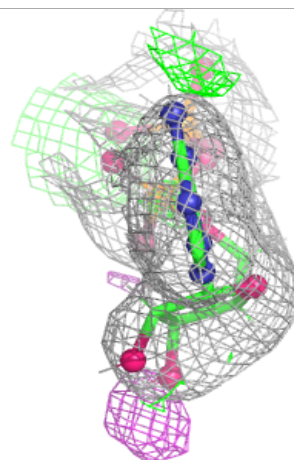
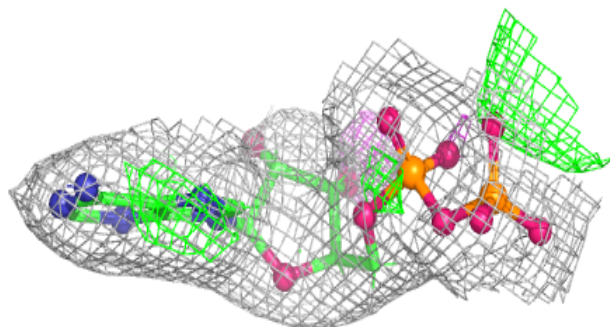
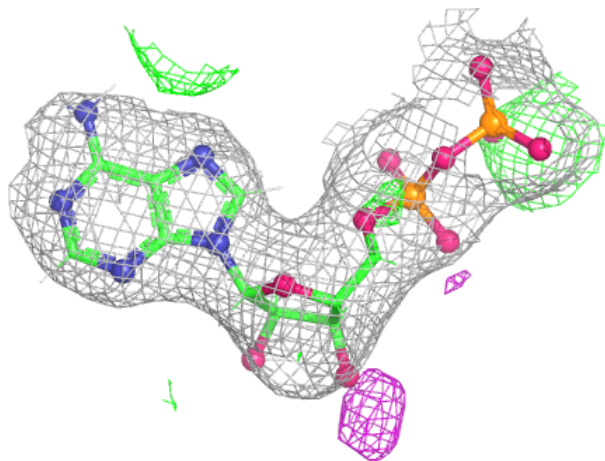
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

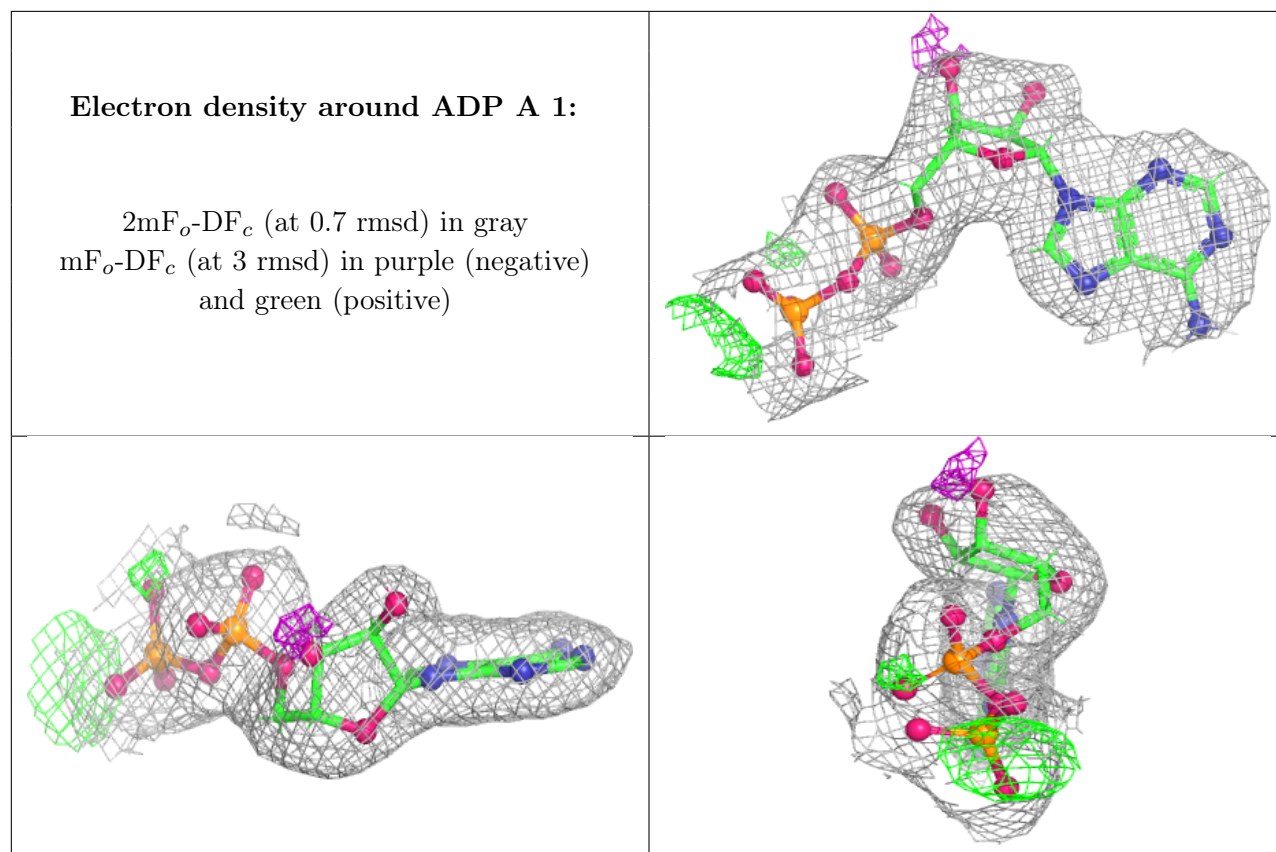
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	4	6/6	0.79	0.24	79,95,96,96	0
4	GOL	A	2	6/6	0.82	0.16	80,96,98,99	0
4	GOL	B	5	6/6	0.86	0.18	70,84,87,88	0
2	ADP	B	1	27/27	0.88	0.12	60,69,84,87	0
4	GOL	A	3	6/6	0.89	0.12	44,53,55,56	0
4	GOL	A	702	6/6	0.93	0.13	66,79,80,82	0
2	ADP	A	1	27/27	0.95	0.09	35,47,62,63	0
3	MG	A	701	1/1	0.99	0.06	50,50,50,50	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.

Electron density around ADP B 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.