



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:44 AM UTC

PDB ID : 5W3D / pdb_00005w3d
Title : The structure of kinesin-14 wild-type Ncd-ADP dimer
Authors : Park, H.W.; Ma, Z.; Chacko, J.; Jiang, S.M.; Robinson, R.C.; Endow, S.A.
Deposited on : 2017-06-07
Resolution : 2.79 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

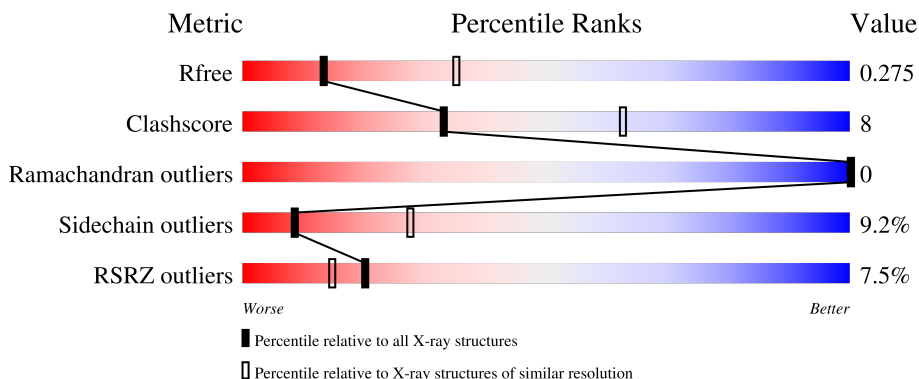
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	3% 65% 18% • 14%
1	B	412	9% 60% 14% • 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5346 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 Protein claret segregational.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2830	1764	497	549	20			
1	B	313	Total	C	N	O	S	0	0	0
			2460	1541	425	477	17			

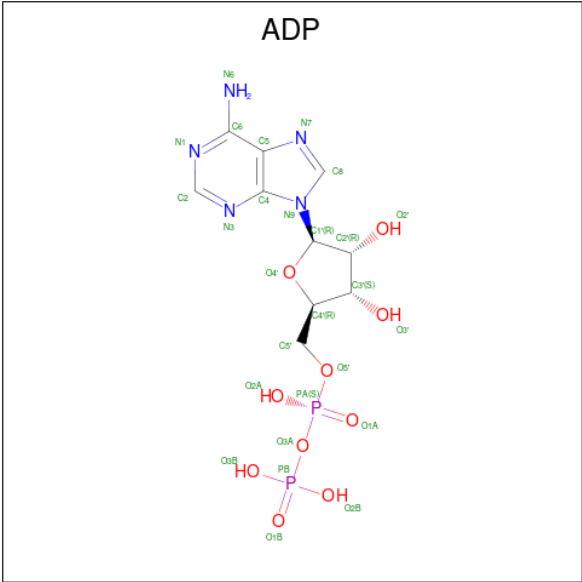
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	MET	-	initiating methionine	UNP P20480
A	290	GLY	-	expression tag	UNP P20480
A	291	SER	-	expression tag	UNP P20480
A	292	MET	-	expression tag	UNP P20480
A	697	ASN	SER	conflict	UNP P20480
B	289	MET	-	initiating methionine	UNP P20480
B	290	GLY	-	expression tag	UNP P20480
B	291	SER	-	expression tag	UNP P20480
B	292	MET	-	expression tag	UNP P20480
B	697	ASN	SER	conflict	UNP P20480

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.27Å 67.25Å 94.42Å 90.00° 97.92° 90.00°	Depositor
Resolution (Å)	46.80 – 2.79 46.80 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.80-2.79) 99.1 (46.80-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.235 , 0.280 0.236 , 0.275	Depositor DCC
R_{free} test set	1288 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5346	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: 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	0.61	0/2876	0.84	6/3879 (0.2%)
1	B	0.54	0/2498	0.86	5/3371 (0.1%)
All	All	0.58	0/5374	0.85	11/7250 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	487	GLU	N-CA-C	8.79	123.67	113.38
1	A	485	TYR	CB-CA-C	-8.26	98.56	110.62
1	B	423	LEU	N-CA-C	-6.57	104.05	111.14
1	B	653	CYS	CB-CA-C	-6.18	100.12	110.56
1	B	486	ASN	N-CA-C	6.07	117.85	109.54
1	B	665	ALA	N-CA-C	5.50	116.96	111.07
1	A	486	ASN	N-CA-C	-5.42	103.92	111.52
1	A	505	ALA	CB-CA-C	5.36	121.88	110.19
1	A	485	TYR	N-CA-C	5.36	117.07	107.80
1	A	486	ASN	N-CA-CB	5.32	120.00	111.91
1	B	415	VAL	CB-CA-C	-5.05	103.48	110.95

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	2830	0	2779	48	2
1	B	2460	0	2378	35	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	1	0
All	All	5346	0	5181	82	2

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 8.

All (82) 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:611:LEU:O	1:B:615:GLN:HG3	1.02	1.17
1:B:611:LEU:O	1:B:615:GLN:CG	1.99	1.09
1:A:488:VAL:HG23	1:A:490:TYR:CE1	2.04	0.93
1:B:420:GLN:HA	1:B:423:LEU:HD12	1.56	0.88
1:A:488:VAL:CG2	1:A:490:TYR:CE1	2.70	0.75
1:B:622:TYR:CB	1:B:623:ARG:HA	2.17	0.74
1:B:352:PHE:CD2	1:B:642:LEU:HD11	2.26	0.69
1:B:376:SER:HB2	1:B:398:PHE:O	1.93	0.69
1:A:488:VAL:CG2	1:A:490:TYR:CZ	2.77	0.67
1:A:427:ASN:C	1:A:428:ILE:HD12	2.20	0.67
1:A:359:LEU:HD23	1:A:362:GLU:H	1.63	0.64
1:A:488:VAL:HG21	1:A:490:TYR:OH	2.00	0.62
1:A:488:VAL:HG23	1:A:490:TYR:CZ	2.34	0.62
1:B:621:PRO:C	1:B:622:TYR:HD2	2.08	0.61
1:A:365:ARG:HB2	1:A:650:PHE:CD1	2.36	0.61
1:B:486:ASN:OD1	1:B:486:ASN:O	2.18	0.61
1:A:366:MET:HE3	1:A:366:MET:HA	1.82	0.60
1:A:622:TYR:CG	1:A:632:MET:HG3	2.36	0.60
1:B:625:SER:HB3	1:B:628:THR:OG1	2.02	0.59
1:B:622:TYR:CD2	1:B:622:TYR:N	2.71	0.58
1:B:352:PHE:CE2	1:B:642:LEU:HD11	2.39	0.57
1:A:526:ASN:OD1	1:A:529:ARG:NH1	2.37	0.57
1:A:360:GLU:H	1:A:360:GLU:CD	2.14	0.56
1:A:349:ILE:C	1:A:349:ILE:HD13	2.32	0.55
1:A:488:VAL:CG2	1:A:490:TYR:OH	2.55	0.54
1:A:437:GLY:N	3:A:802:ADP:O1B	2.40	0.54
1:B:621:PRO:C	1:B:622:TYR:CD2	2.85	0.54
1:A:621:PRO:HB2	1:A:624:ASN:CG	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLU:OE1	1:A:360:GLU:N	2.36	0.53
1:B:603:LEU:O	1:B:607:THR:HG23	2.08	0.53
1:A:439:GLY:CA	3:A:802:ADP:O1A	2.58	0.51
1:A:299:GLU:OE2	1:B:304:ARG:NH2	2.43	0.51
1:A:485:TYR:CZ	1:A:549:ARG:HG3	2.46	0.51
1:A:524:ASP:HB2	1:A:525:PRO:HD2	1.93	0.51
1:A:454:ILE:HB	1:A:455:PRO:HD3	1.93	0.50
1:B:473:TRP:HE1	1:B:563:GLY:C	2.19	0.50
1:A:554:HIS:CD2	1:A:582:ALA:H	2.30	0.49
1:A:622:TYR:CD1	1:A:632:MET:HG3	2.47	0.49
1:A:374:ASP:OD1	1:A:377:THR:N	2.45	0.49
1:A:342:VAL:O	1:A:346:ARG:HG3	2.12	0.49
1:B:425:GLY:HA2	1:B:573:VAL:O	2.14	0.48
1:A:403:HIS:HB2	1:A:404:PRO:CD	2.44	0.48
1:B:622:TYR:CB	1:B:623:ARG:CA	2.92	0.47
1:A:436:THR:OG1	1:A:585:GLU:OE2	2.23	0.47
1:A:525:PRO:HB2	1:A:529:ARG:NH2	2.29	0.46
1:B:444:MET:HE2	1:B:444:MET:HA	1.97	0.46
1:A:380:LEU:HD12	1:A:380:LEU:H	1.80	0.46
1:A:482:LEU:C	1:A:482:LEU:HD12	2.40	0.46
1:A:487:GLU:HG3	1:A:626:LYS:HD3	1.96	0.46
1:A:538:ASN:N	1:A:538:ASN:OD1	2.49	0.46
1:B:435:GLN:O	1:B:438:SER:OG	2.33	0.46
1:A:491:ASP:OD1	1:A:491:ASP:C	2.58	0.46
1:B:379:GLU:CG	1:B:381:GLN:HE21	2.29	0.46
1:A:356:ARG:NE	1:A:437:GLY:O	2.45	0.46
1:B:492:LEU:O	1:B:493:LEU:HD23	2.16	0.45
1:B:352:PHE:CZ	1:B:414:MET:HG2	2.52	0.45
1:B:486:ASN:H	1:B:488:VAL:HG12	1.81	0.45
1:B:625:SER:OG	1:B:626:LYS:N	2.50	0.45
1:B:439:GLY:N	3:B:802:ADP:O2A	2.50	0.45
1:A:481:PHE:CD1	1:A:481:PHE:N	2.84	0.45
1:B:427:ASN:C	1:B:428:ILE:HD12	2.41	0.45
1:B:610:ILE:HG22	1:B:614:LEU:HD12	1.99	0.45
1:B:482:LEU:N	1:B:482:LEU:HD23	2.30	0.44
1:B:442:TYR:O	1:B:446:GLY:HA2	2.17	0.44
1:A:668:ASN:HD22	1:A:668:ASN:N	2.14	0.44
1:A:439:GLY:HA2	3:A:802:ADP:O1A	2.17	0.44
1:A:613:LEU:HD13	1:A:620:ILE:CD1	2.48	0.44
1:A:365:ARG:NH2	1:A:652:ASP:OD1	2.50	0.44
1:A:668:ASN:HD22	1:A:668:ASN:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:VAL:HG13	1:B:527:HIS:CD2	2.52	0.43
1:A:471:LEU:HD12	1:A:471:LEU:N	2.32	0.43
1:A:403:HIS:HB2	1:A:404:PRO:HD2	2.00	0.43
1:A:408:GLN:HA	1:A:408:GLN:OE1	2.18	0.43
1:A:654:PHE:O	1:A:658:VAL:HG23	2.19	0.42
1:B:429:CYS:HB2	1:B:641:THR:HB	2.02	0.41
1:A:621:PRO:HB2	1:A:624:ASN:ND2	2.36	0.41
1:B:349:ILE:O	1:B:349:ILE:HG23	2.21	0.41
1:B:486:ASN:OD1	1:B:486:ASN:C	2.64	0.41
1:B:631:LEU:O	1:B:633:PRO:HD3	2.20	0.41
1:A:485:TYR:O	1:A:488:VAL:HG22	2.21	0.40
1:B:622:TYR:HB2	1:B:623:ARG:HA	2.00	0.40
1:A:411:ILE:HG23	1:A:644:PHE:CZ	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASN:CB	1:B:624:ASN:OD1[2_565]	1.69	0.51
1:A:364:ASN:CG	1:B:624:ASN:OD1[2_565]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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	346/412 (84%)	336 (97%)	10 (3%)	0	100	100
1	B	295/412 (72%)	263 (89%)	32 (11%)	0	100	100
All	All	641/824 (78%)	599 (93%)	42 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	322/372 (87%)	286 (89%)	36 (11%)	6	19
1	B	275/372 (74%)	256 (93%)	19 (7%)	14	41
All	All	597/744 (80%)	542 (91%)	55 (9%)	8	27

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	THR
1	A	307	THR
1	A	310	LEU
1	A	311	LEU
1	A	325	LYS
1	A	338	LEU
1	A	349	ILE
1	A	355	ILE
1	A	359	LEU
1	A	366	MET
1	A	368	CYS
1	A	371	THR
1	A	380	LEU
1	A	384	ASP
1	A	405	LEU
1	A	447	VAL
1	A	459	ASP
1	A	461	LEU
1	A	487	GLU
1	A	489	LEU
1	A	495	ASN
1	A	501	GLU
1	A	512	ILE
1	A	528	LEU
1	A	532	MET
1	A	537	MET
1	A	538	ASN

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Mol	Chain	Res	Type
1	A	550	SER
1	A	571	ILE
1	A	573	VAL
1	A	613	LEU
1	A	625	SER
1	A	642	LEU
1	A	648	SER
1	A	666	SER
1	A	668	ASN
1	B	296	LEU
1	B	300	VAL
1	B	310	LEU
1	B	315	GLU
1	B	326	GLU
1	B	368	CYS
1	B	393	GLN
1	B	395	ILE
1	B	474	GLU
1	B	488	VAL
1	B	521	THR
1	B	539	ARG
1	B	559	LEU
1	B	562	ILE
1	B	585	GLU
1	B	614	LEU
1	B	622	TYR
1	B	641	THR
1	B	659	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	HIS
1	A	393	GLN
1	A	470	ASN
1	A	495	ASN
1	A	497	GLN
1	A	510	ASN
1	A	516	ASN
1	A	554	HIS
1	A	577	ASN
1	A	608	ASN

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Mol	Chain	Res	Type
1	A	629	HIS
1	A	668	ASN
1	B	305	GLN
1	B	327	GLN
1	B	364	ASN
1	B	381	GLN
1	B	394	GLN
1	B	538	ASN
1	B	577	ASN
1	B	615	GLN
1	B	655	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	ADP	B	802	2	28,29,29	1.41	6 (21%)	43,45,45	1.91	10 (23%)
3	ADP	A	802	2	28,29,29	1.54	6 (21%)	43,45,45	2.08	14 (32%)

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	ADP	B	802	2	-	5/16/32/32	0/3/3/3
3	ADP	A	802	2	-	6/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	ADP	C5-C4	4.58	1.47	1.39
3	B	802	ADP	C5-C4	4.42	1.47	1.39
3	A	802	ADP	C5-C6	2.83	1.48	1.41
3	B	802	ADP	C5-C6	2.75	1.48	1.41
3	A	802	ADP	C5-N7	-2.68	1.34	1.39
3	A	802	ADP	PA-O3A	2.32	1.62	1.59
3	B	802	ADP	C8-N7	2.32	1.36	1.31
3	A	802	ADP	C8-N7	2.29	1.36	1.31
3	A	802	ADP	C4-N9	-2.18	1.33	1.37
3	B	802	ADP	C4-N9	-2.10	1.33	1.37
3	B	802	ADP	C5-N7	-2.04	1.35	1.39
3	B	802	ADP	PA-O3A	2.04	1.61	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	ADP	C5-C4-N3	-6.25	118.12	126.72
3	B	802	ADP	C5-C4-N3	-5.42	119.25	126.72
3	A	802	ADP	N3-C4-N9	5.24	136.08	127.17
3	B	802	ADP	N3-C4-N9	4.47	134.76	127.17
3	A	802	ADP	C2-N3-C4	4.08	121.78	111.83
3	B	802	ADP	C2-N3-C4	3.85	121.24	111.83
3	B	802	ADP	N3-C2-N1	-3.85	122.76	128.58
3	A	802	ADP	N3-C2-N1	-3.73	122.93	128.58
3	B	802	ADP	C4-N9-C8	3.68	109.60	105.74
3	B	802	ADP	C4-C5-N7	-3.59	106.48	110.58
3	A	802	ADP	C4-N9-C8	3.13	109.03	105.74
3	A	802	ADP	C4-C5-N7	-3.12	107.02	110.58
3	B	802	ADP	C5-N7-C8	2.84	107.91	103.45
3	B	802	ADP	N9-C8-N7	-2.76	110.02	113.94
3	B	802	ADP	C6-C5-N7	2.58	137.06	132.09
3	A	802	ADP	C2'-C3'-C4'	2.47	107.39	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	ADP	O3A-PA-O1A	-2.46	103.31	110.70
3	A	802	ADP	O2A-PA-O3A	2.44	113.87	107.27
3	A	802	ADP	C5-N7-C8	2.37	107.18	103.45
3	A	802	ADP	N9-C8-N7	-2.09	110.97	113.94
3	A	802	ADP	O3B-PB-O3A	2.05	111.50	104.64
3	A	802	ADP	O3A-PB-O1B	-2.02	100.40	111.04
3	A	802	ADP	C3'-C2'-C1'	2.00	105.25	101.46
3	B	802	ADP	O4'-C1'-N9	2.00	111.93	108.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	ADP	C5'-O5'-PA-O2A
3	A	802	ADP	C5'-O5'-PA-O3A
3	B	802	ADP	C5'-O5'-PA-O3A
3	A	802	ADP	O4'-C4'-C5'-O5'
3	B	802	ADP	O4'-C4'-C5'-O5'
3	B	802	ADP	C3'-C4'-C5'-O5'
3	A	802	ADP	C3'-C4'-C5'-O5'
3	A	802	ADP	C5'-O5'-PA-O1A
3	B	802	ADP	C5'-O5'-PA-O1A
3	A	802	ADP	C4'-C5'-O5'-PA
3	B	802	ADP	C4'-C5'-O5'-PA

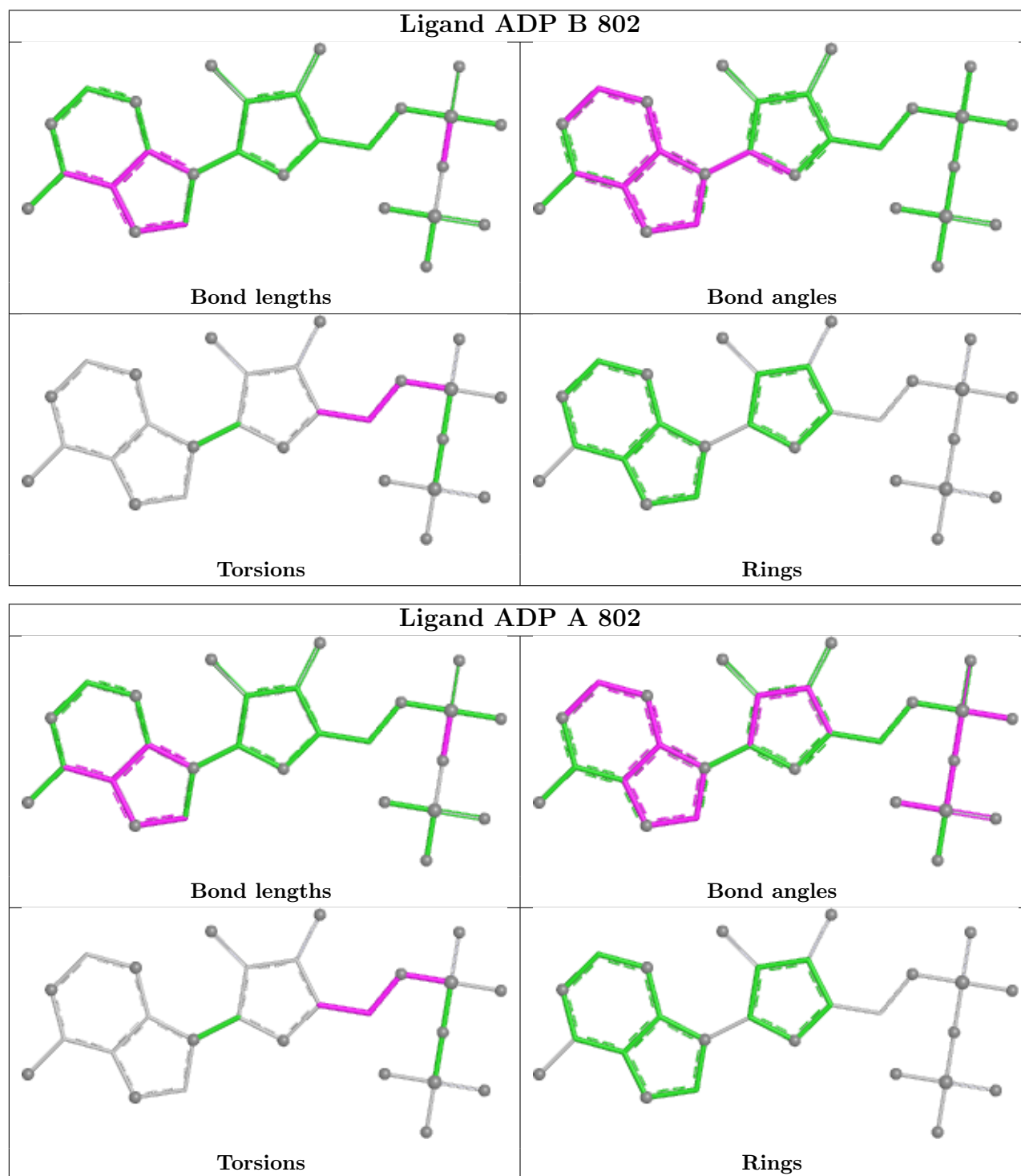
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	ADP	1	0
3	A	802	ADP	3	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 ⓘ

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, 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	354/412 (85%)	0.24	11 (3%) 51 41	45, 69, 103, 115	0
1	B	313/412 (75%)	0.87	39 (12%) 8 6	51, 91, 129, 140	0
All	All	667/824 (80%)	0.54	50 (7%) 20 15	45, 78, 123, 140	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	621	PRO	5.9
1	B	472	GLY	4.1
1	A	600	ASN	4.1
1	B	600	ASN	4.0
1	B	540	ALA	4.0
1	B	385	ALA	3.8
1	A	362	GLU	3.7
1	B	613	LEU	3.6
1	B	622	TYR	3.6
1	B	485	TYR	3.6
1	A	361	SER	3.6
1	B	587	PRO	3.4
1	B	633	PRO	3.3
1	B	611	LEU	3.2
1	B	579	VAL	3.2
1	A	359	LEU	3.1
1	B	468	TYR	3.1
1	A	367	CYS	3.0
1	B	431	PHE	3.0
1	B	550	SER	2.9
1	B	391	MET	2.9
1	B	602	SER	2.7
1	B	493	LEU	2.7
1	B	523	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	529	ARG	2.7
1	A	599	ILE	2.7
1	B	614	LEU	2.6
1	A	360	GLU	2.5
1	A	587	PRO	2.5
1	B	462	PHE	2.5
1	B	414	MET	2.5
1	B	669	SER	2.5
1	B	451	VAL	2.5
1	A	292	MET	2.5
1	A	383	ILE	2.4
1	B	481	PHE	2.4
1	B	641	THR	2.4
1	B	565	HIS	2.3
1	B	531	LEU	2.3
1	B	556	VAL	2.3
1	B	578	LEU	2.2
1	B	551	SER	2.2
1	B	353	CYS	2.2
1	B	651	GLN	2.2
1	B	366	MET	2.1
1	B	532	MET	2.1
1	B	612	ALA	2.1
1	A	580	ASP	2.1
1	B	573	VAL	2.1
1	B	572	SER	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](#)

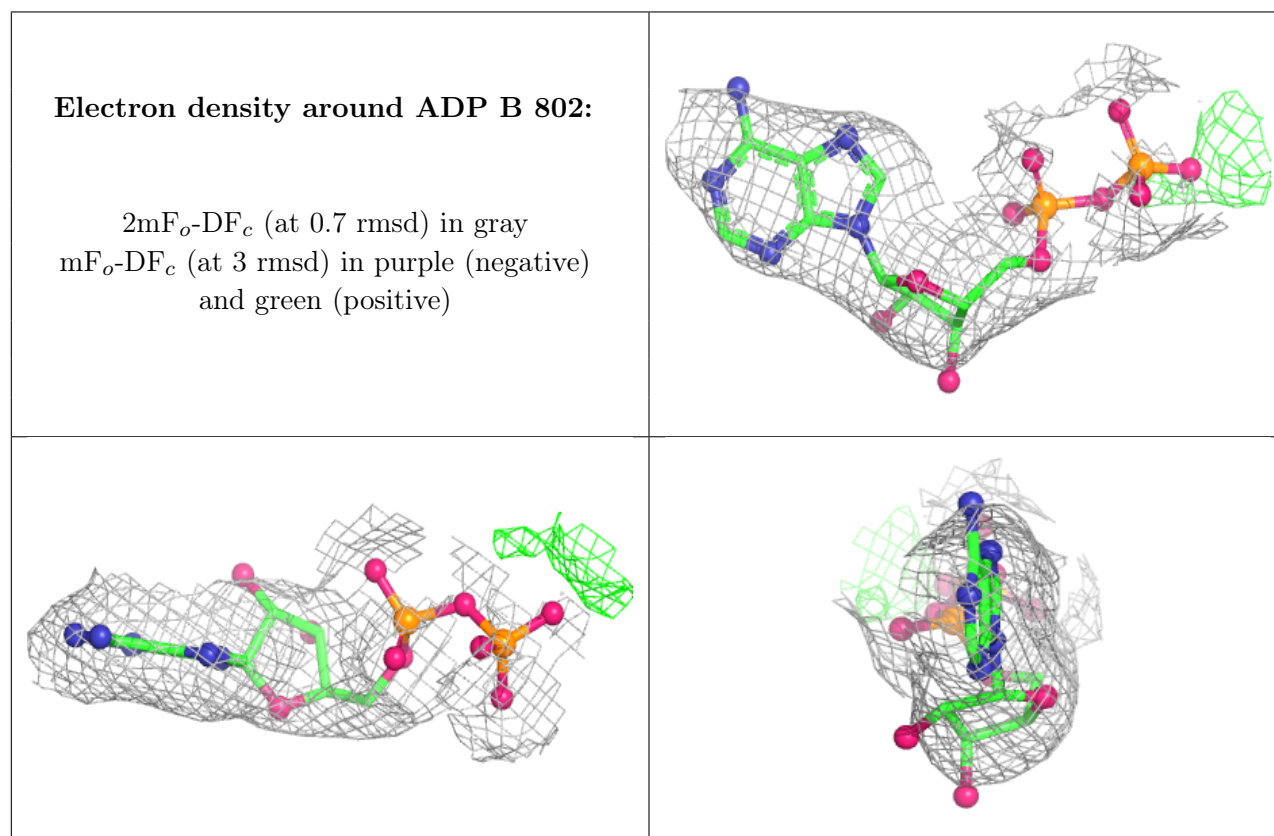
There are no oligosaccharides in this entry.

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.

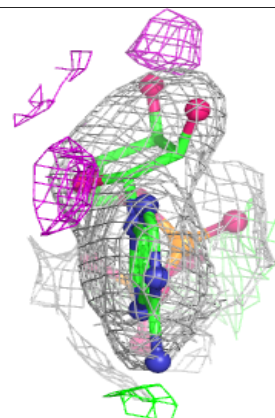
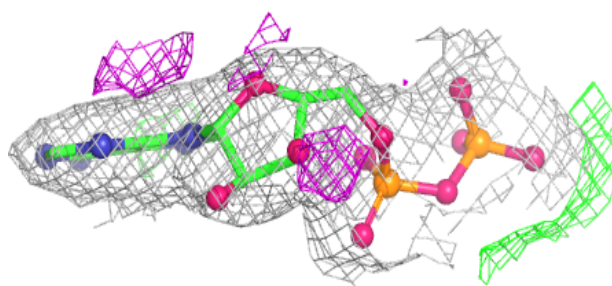
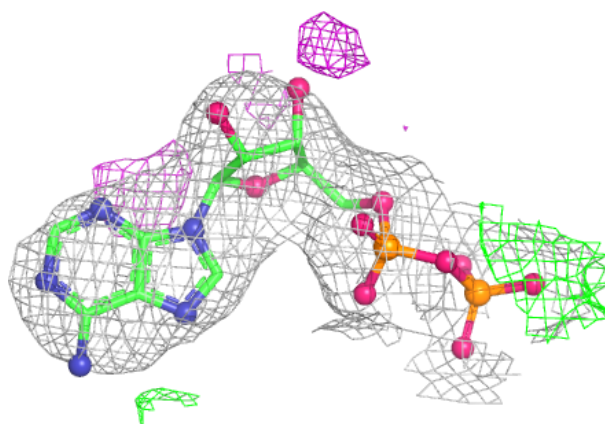
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	801	1/1	0.78	0.26	82,82,82,82	0
2	MG	A	801	1/1	0.82	0.26	63,63,63,63	0
3	ADP	B	802	27/27	0.90	0.11	83,100,105,107	0
3	ADP	A	802	27/27	0.92	0.11	65,73,81,86	0

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 A 802:

$2mF_o - DF_c$ (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.