Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 03:44 pm BST

PDB ID	:	2KIN
Title	:	KINESIN (MONOMERIC) FROM RATTUS NORVEGICUS
Authors	:	Sack, S.; Muller, J.; Kozielski, F.; Marx, A.; Thormahlen, M.; Biou, V.; Mandelkow, E.-M.; Brady, S.T.; Mandelkow, E.
Deposited on	:	1997-04-28
Resolution	:	2.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

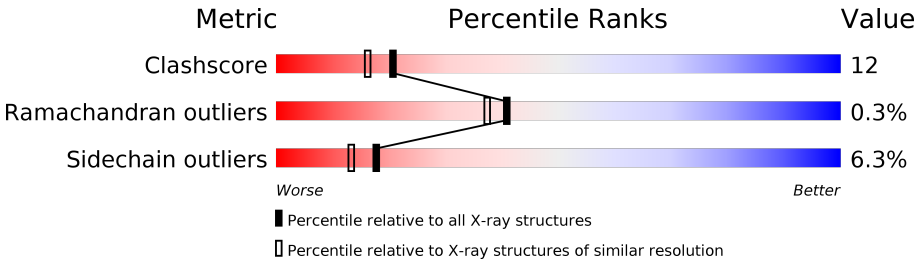
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	79% 17% .
2	B	100	69% 21% 8% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2933 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.

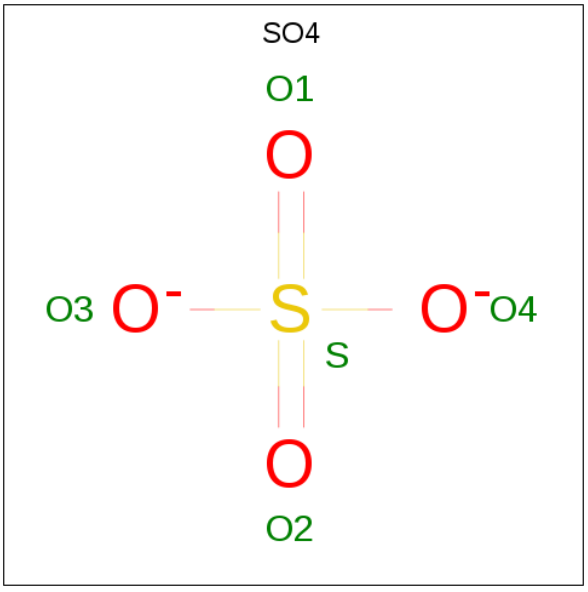
- Molecule 1 is a protein called KINESIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	2	0
			1908	1206	328	364	10			

- Molecule 2 is a protein called KINESIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			778	483	136	154	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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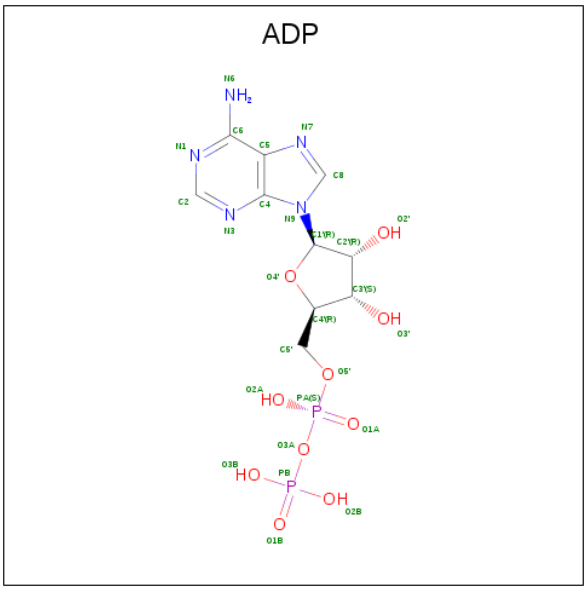
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	147	Total O 147 147	0	0
5	B	58	Total O 58 58	0	0

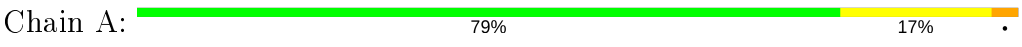
3 Residue-property plots (i)

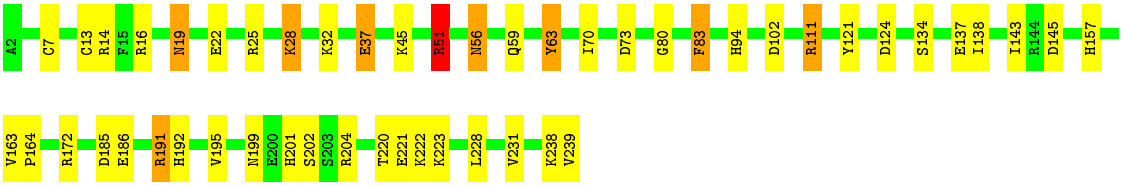
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: KINESIN

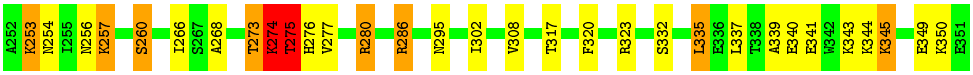
Chain A:





- Molecule 2: KINESIN

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.56Å 73.67Å 74.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2933	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.85	0/1953	1.57	27/2634 (1.0%)
2	B	0.80	0/786	1.38	7/1056 (0.7%)
All	All	0.84	0/2739	1.52	34/3690 (0.9%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	ASP	CB-CG-OD1	12.34	129.41	118.30
1	A	111	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	A	16	ARG	NE-CZ-NH2	10.73	125.67	120.30
1	A	51	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	102	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	172	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	191[A]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	191[B]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	B	286	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	A	51	ARG	CA-CB-CG	6.86	128.48	113.40
1	A	73	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	134	SER	N-CA-CB	6.56	120.33	110.50
1	A	37	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	111	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	239	VAL	CA-C-O	-6.38	106.69	120.10
1	A	111	ARG	CD-NE-CZ	-6.38	114.67	123.60
1	A	51	ARG	CD-NE-CZ	6.31	132.44	123.60
1	A	185	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	102	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	25	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	63	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	A	25	ARG	NE-CZ-NH1	5.95	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	323	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	195	VAL	CA-CB-CG2	-5.68	102.38	110.90
1	A	124	ASP	CB-CG-OD1	5.52	123.27	118.30
2	B	260	SER	N-CA-CB	5.46	118.69	110.50
1	A	73	ASP	CB-CG-OD1	5.39	123.15	118.30
2	B	275	THR	N-CA-CB	5.30	120.37	110.30
1	A	83	PHE	N-CA-CB	5.26	120.06	110.60
2	B	317	THR	CA-CB-CG2	-5.16	105.18	112.40
1	A	121	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	A	51	ARG	CG-CD-NE	-5.15	100.98	111.80
2	B	335	LEU	CA-CB-CG	5.09	127.01	115.30
2	B	286	ARG	CD-NE-CZ	-5.03	116.55	123.60

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	1908	0	1898	45	0
2	B	778	0	801	36	0
3	A	15	0	0	1	0
4	A	27	0	12	0	0
5	A	147	0	0	10	0
5	B	58	0	0	7	0
All	All	2933	0	2711	67	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 12.

All (67) 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:238:LYS:HE3	5:A:615:HOH:O	1.37	1.21
1:A:28:LYS:HE2	2:B:308:VAL:HG11	1.18	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:LYS:HD3	5:B:186:HOH:O	0.95	1.12
1:A:28:LYS:CE	2:B:308:VAL:HG11	1.83	1.07
1:A:28:LYS:HE2	2:B:308:VAL:CG1	1.96	0.95
1:A:222:LYS:HG2	2:B:337:LEU:CD2	1.99	0.93
1:A:37:GLU:HG3	5:A:588:HOH:O	1.71	0.90
1:A:56:ASN:HD22	1:A:56:ASN:H	1.21	0.88
2:B:273:THR:OG1	5:B:176:HOH:O	1.93	0.86
2:B:295:ASN:HD21	2:B:332:SER:H	1.27	0.82
1:A:28:LYS:CD	2:B:308:VAL:CG1	2.62	0.78
1:A:28:LYS:CD	2:B:308:VAL:HG11	2.13	0.77
1:A:222:LYS:HG2	2:B:337:LEU:HD23	1.67	0.76
1:A:186:GLU:OE2	5:A:603:HOH:O	2.04	0.76
1:A:204:ARG:HE	2:B:256:ASN:ND2	1.87	0.73
1:A:56:ASN:ND2	1:A:56:ASN:H	1.92	0.68
2:B:345:LYS:CD	5:B:186:HOH:O	1.78	0.68
2:B:275:THR:O	5:B:176:HOH:O	2.12	0.67
2:B:295:ASN:ND2	2:B:332:SER:H	1.93	0.66
1:A:204:ARG:HE	2:B:256:ASN:HD21	1.41	0.66
1:A:14:ARG:HH12	1:A:59:GLN:HE22	1.45	0.65
1:A:94:HIS:HD2	5:A:646:HOH:O	1.82	0.63
1:A:28:LYS:HD3	2:B:308:VAL:HB	1.81	0.62
1:A:19:ASN:ND2	1:A:22:GLU:H	1.98	0.62
2:B:340:GLU:HG3	2:B:344:LYS:NZ	2.16	0.61
1:A:28:LYS:H	1:A:28:LYS:HD2	1.66	0.59
1:A:220:THR:O	1:A:221:GLU:HB2	2.02	0.59
1:A:191[B]:ARG:NH2	1:A:202:SER:HA	2.17	0.58
2:B:274:LYS:HA	2:B:277:VAL:HG23	1.85	0.58
1:A:28:LYS:CE	2:B:308:VAL:CG1	2.64	0.57
2:B:345:LYS:CE	5:B:186:HOH:O	2.34	0.56
1:A:192:HIS:HE1	3:A:504:SO4:O3	1.88	0.56
1:A:28:LYS:HD3	2:B:308:VAL:CG1	2.36	0.56
2:B:268:ALA:O	2:B:273:THR:HG23	2.06	0.55
1:A:138:ILE:HG12	1:A:143:ILE:HG12	1.89	0.54
1:A:28:LYS:HD3	2:B:308:VAL:CB	2.38	0.54
2:B:345:LYS:HE2	5:B:186:HOH:O	2.04	0.54
2:B:341:GLU:HG3	5:B:56:HOH:O	2.08	0.53
2:B:340:GLU:O	2:B:344:LYS:HG3	2.08	0.53
1:A:28:LYS:CD	1:A:28:LYS:H	2.22	0.52
1:A:238:LYS:CE	5:A:615:HOH:O	2.20	0.52
1:A:192:HIS:HD2	5:A:530:HOH:O	1.93	0.51
1:A:14:ARG:HH12	1:A:59:GLN:NE2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:HG12	5:A:590:HOH:O	2.12	0.50
1:A:19:ASN:HD22	1:A:19:ASN:C	2.16	0.50
2:B:339:ALA:O	2:B:343:LYS:HG3	2.13	0.49
1:A:13:CYS:HA	2:B:302:ILE:HG13	1.94	0.48
2:B:253:LYS:HZ1	2:B:257:LYS:HA	1.80	0.47
1:A:51:ARG:HD3	5:A:641:HOH:O	2.13	0.47
2:B:274:LYS:HA	2:B:277:VAL:CG2	2.45	0.47
1:A:80:GLY:O	1:A:228:LEU:HA	2.16	0.46
1:A:19:ASN:HD22	1:A:22:GLU:H	1.62	0.45
1:A:63:TYR:HB2	1:A:111:ARG:HD2	1.99	0.45
1:A:94:HIS:HE1	5:A:596:HOH:O	2.00	0.45
1:A:157:HIS:O	1:A:164:PRO:HA	2.18	0.43
1:A:32:LYS:HE2	5:A:614:HOH:O	2.18	0.43
2:B:253:LYS:HG3	2:B:254:ASN:N	2.33	0.43
2:B:345:LYS:O	2:B:349:GLU:HG2	2.19	0.43
2:B:280:ARG:HA	2:B:286:ARG:HD2	2.01	0.42
1:A:137:GLU:OE1	1:A:201:HIS:HE1	2.02	0.42
1:A:137:GLU:OE1	1:A:191[B]:ARG:HD2	2.19	0.42
2:B:280:ARG:HG2	2:B:286:ARG:HD2	2.02	0.41
2:B:273:THR:O	2:B:274:LYS:C	2.58	0.41
2:B:266:ILE:HG12	2:B:320:PHE:CE1	2.55	0.41
1:A:56:ASN:HD22	1:A:56:ASN:N	2.00	0.41
1:A:163:VAL:HA	1:A:164:PRO:HD3	1.90	0.40
1:A:83:PHE:HB3	1:A:231:VAL:HB	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	238/238 (100%)	231 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	98/100 (98%)	96 (98%)	1 (1%)	1 (1%)	15 9
All	All	336/338 (99%)	327 (97%)	8 (2%)	1 (0%)	41 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	274	LYS

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	215/213 (101%)	207 (96%)	8 (4%)	34 32
2	B	89/89 (100%)	78 (88%)	11 (12%)	4 2
All	All	304/302 (101%)	285 (94%)	19 (6%)	18 13

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	CYS
1	A	19	ASN
1	A	28	LYS
1	A	45	LYS
1	A	51	ARG
1	A	56	ASN
1	A	199	ASN
1	A	223	LYS
2	B	253	LYS
2	B	257	LYS
2	B	260	SER
2	B	273	THR
2	B	274	LYS
2	B	275	THR
2	B	276	HIS

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Mol	Chain	Res	Type
2	B	280	ARG
2	B	335	LEU
2	B	345	LYS
2	B	350	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	56	ASN
1	A	59	GLN
1	A	94	HIS
1	A	101	HIS
1	A	126	ASN
1	A	192	HIS
1	A	201	HIS
2	B	254	ASN
2	B	256	ASN
2	B	289	GLN
2	B	295	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are 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	$\#\|Z\| > 2$
3	SO4	A	502	-	4,4,4	0.49	0	6,6,6	0.44	0
4	ADP	A	400	-	24,29,29	1.57	4 (16%)	29,45,45	2.11	11 (37%)
3	SO4	A	505	-	4,4,4	0.69	0	6,6,6	0.46	0
3	SO4	A	504	-	4,4,4	0.64	0	6,6,6	0.85	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	ADP	A	400	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	ADP	C2'-C3'	4.03	1.64	1.53
4	A	400	ADP	PA-O2A	-3.07	1.40	1.55
4	A	400	ADP	C8-N7	-2.35	1.30	1.34
4	A	400	ADP	O4'-C1'	2.08	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	400	ADP	C4-C5-N7	4.61	114.20	109.40
4	A	400	ADP	N6-C6-N1	3.90	126.68	118.57
4	A	400	ADP	C2-N1-C6	3.55	124.83	118.75
4	A	400	ADP	O3'-C3'-C2'	-3.53	100.41	111.82
4	A	400	ADP	N3-C2-N1	-3.51	123.20	128.68
4	A	400	ADP	C2'-C3'-C4'	-2.79	97.22	102.64
4	A	400	ADP	O5'-PA-O1A	-2.47	99.42	109.07
4	A	400	ADP	C5-C6-N1	-2.36	115.00	120.35
4	A	400	ADP	PA-O3A-PB	-2.35	124.77	132.83
4	A	400	ADP	O5'-C5'-C4'	-2.24	101.30	108.99
4	A	400	ADP	C5'-C4'-C3'	-2.16	107.09	115.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	400	ADP	PA-O3A-PB-O2B
4	A	400	ADP	PA-O3A-PB-O3B
4	A	400	ADP	C5'-O5'-PA-O2A
4	A	400	ADP	PA-O3A-PB-O1B

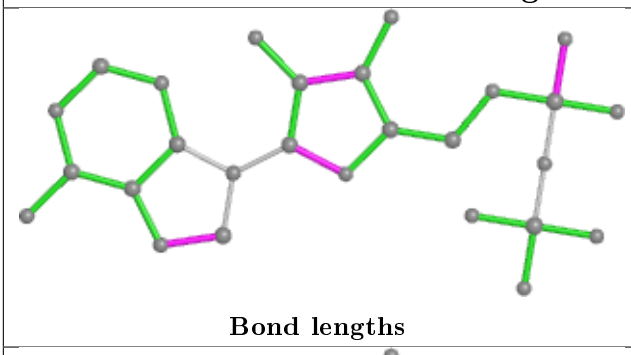
There are no ring outliers.

1 monomer is involved in 1 short contact:

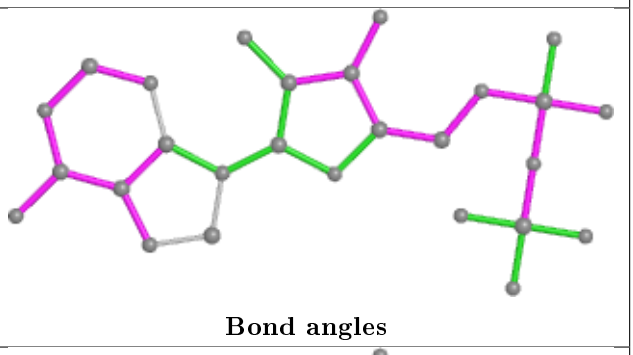
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	SO4	1	0

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 then 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.

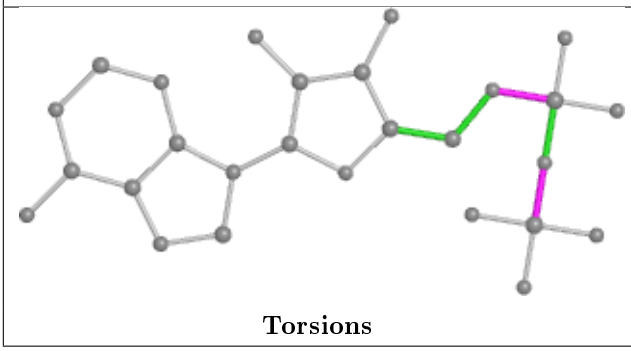
Ligand ADP A 400



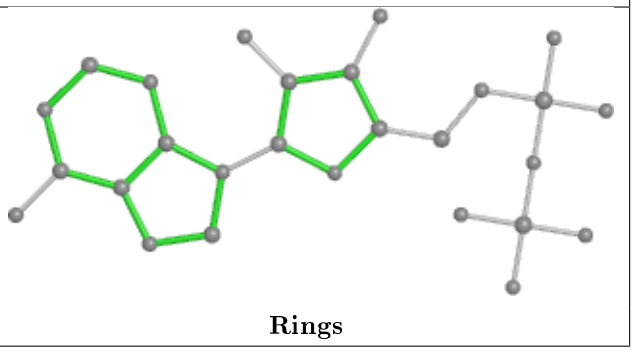
Bond lengths



Bond angles



Torsions



Rings

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

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.