



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:30 PM UTC

PDB ID : 1Q0B / pdb_00001q0b
Title : Crystal structure of the motor protein KSP in complex with ADP and monastrol
Authors : Yan, Y.; Sardana, V.; Xu, B.; Halczenko, W.; Homnick, C.; Buser, C.A.; Hartman, G.D.; Huber, H.E.; Kuo, L.C.
Deposited on : 2003-07-15
Resolution : 1.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

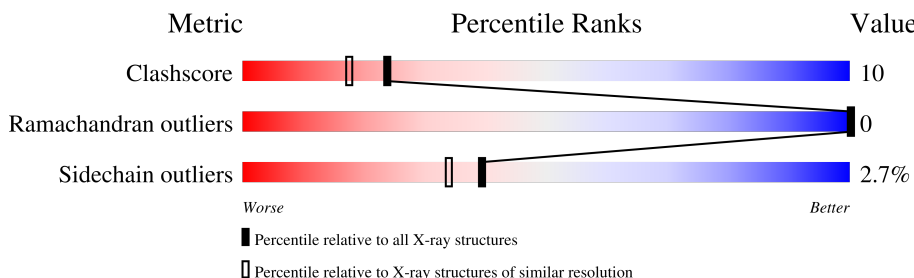
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	367	 69% 20% • 10%
1	B	367	 69% 20% • 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5825 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.

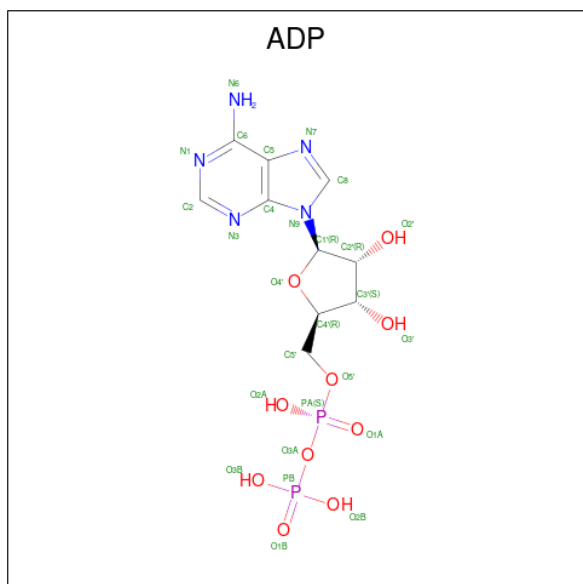
- Molecule 1 is a protein called Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2599	1628	453	508	10			
1	B	335	Total	C	N	O	S	0	0	0
			2630	1647	458	515	10			

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

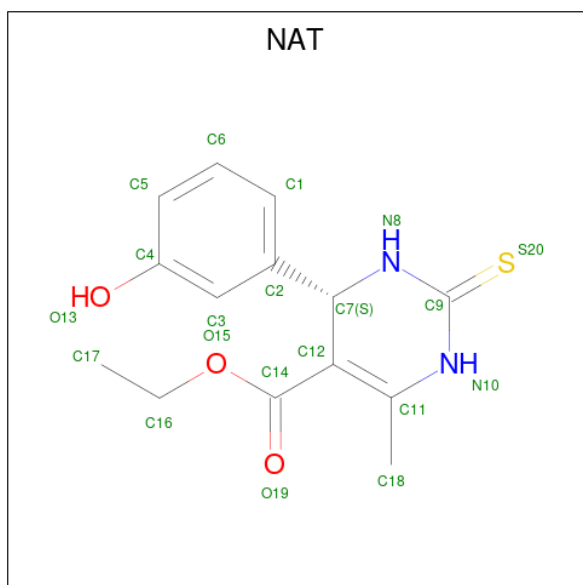
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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		

- Molecule 4 is ETHYL 4-(3-HYDROXYPHENYL)-6-METHYL-2-THIOXO-1,2,3,4-TETRAHYDOPYRIMIDINE-5-CARBOXYLATE (CCD ID: NAT) (formula: $C_{14}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	14	2	3	1		
4	B	1	Total	C	N	O	S	0	0
			20	14	2	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total	O	0	0
			250	250		
5	B	250	Total	O	0	0
			250	250		

4 Data and refinement statistics

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	69.30 Å 79.50 Å 159.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	99.0 (20.00-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5825	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: MG, ADP, NAT

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	0.35	0/2637	0.88	7/3564 (0.2%)
1	B	0.36	0/2669	0.90	8/3609 (0.2%)
All	All	0.35	0/5306	0.89	15/7173 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	VAL	N-CA-C	7.08	117.69	110.82
1	B	210	VAL	N-CA-C	6.97	117.07	110.30
1	B	126	THR	N-CA-C	-6.92	101.21	110.55
1	A	126	THR	N-CA-C	-6.84	101.31	110.55
1	B	135	ILE	N-CA-C	6.56	116.71	110.42
1	A	135	ILE	N-CA-C	6.52	116.68	110.42
1	A	86	VAL	N-CA-C	6.15	116.31	110.53
1	B	85	VAL	N-CA-C	6.13	117.49	111.67
1	A	264	VAL	N-CA-C	5.86	116.30	107.80
1	A	191	LYS	N-CA-C	5.74	120.28	113.28
1	A	210	VAL	N-CA-C	5.46	115.60	110.30
1	A	122	ASN	N-CA-C	5.23	118.93	112.24
1	B	264	VAL	N-CA-C	5.15	115.38	108.17
1	B	44	ASP	CA-C-N	5.06	124.23	118.97
1	B	44	ASP	C-N-CA	5.06	124.23	118.97

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	2599	0	2627	53	0
1	B	2630	0	2655	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	20	0	15	2	0
4	B	20	0	15	2	0
5	A	250	0	0	3	0
5	B	250	0	0	1	0
All	All	5825	0	5336	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 10.

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:B:162:GLU:HG3	1:B:171:LEU:HD13	1.42	0.97
1:B:152:THR:HG21	1:B:245:MET:HE2	1.53	0.90
1:B:49:GLU:HG2	1:B:67:THR:HG22	1.52	0.89
1:B:94:ILE:HG23	1:B:245:MET:HE1	1.58	0.84
1:A:81:VAL:O	1:A:85:VAL:HG12	1.77	0.84
1:A:45:PRO:HA	1:A:71:VAL:HG13	1.61	0.82
1:A:92:GLU:HA	1:A:95:MET:HE3	1.64	0.80
1:B:92:GLU:HG3	1:B:329:ARG:NH1	1.99	0.78
1:B:327:ARG:HD3	1:B:364:GLU:OE2	1.83	0.77
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.67	0.76
1:B:162:GLU:HG3	1:B:171:LEU:CD1	2.18	0.73
1:A:48:LYS:HA	1:A:71:VAL:HG12	1.72	0.71
1:A:114:THR:HG22	1:A:115:MET:HE2	1.73	0.71
1:B:70:MET:HE1	1:B:84:SER:HB3	1.74	0.69
1:B:246:LYS:HG2	1:B:256:VAL:HG12	1.76	0.67
1:B:184:MET:HE2	1:B:318:ARG:CZ	2.25	0.67
4:A:604:NAT:H181	4:A:604:NAT:O15	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLY:H	1:A:361:ASN:HD21	1.44	0.65
1:A:115:MET:HE1	1:A:333:ILE:HD12	1.79	0.64
1:B:92:GLU:HA	1:B:95:MET:HE3	1.79	0.64
1:A:207:LYS:HB3	1:A:207:LYS:NZ	2.12	0.64
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.80	0.64
1:A:173:ASN:ND2	1:A:175:SER:H	1.95	0.63
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.78	0.63
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.80	0.63
1:A:45:PRO:HA	1:A:71:VAL:CG1	2.28	0.63
1:A:87:CYS:HB3	1:A:88:PRO:HD3	1.81	0.63
1:A:209:GLU:HA	1:A:212:GLN:HE21	1.64	0.63
1:B:40:ILE:HD13	1:B:340:SER:HA	1.80	0.63
1:A:22:VAL:HG12	1:A:70:MET:HB2	1.82	0.61
1:A:162:GLU:HG3	1:A:171:LEU:HD23	1.83	0.61
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.67	0.60
1:A:178:VAL:HG23	1:A:227:LEU:HD12	1.84	0.59
1:B:29:ASN:ND2	1:B:32:GLU:H	2.01	0.58
1:B:29:ASN:C	1:B:29:ASN:HD22	2.11	0.58
1:A:207:LYS:HB3	1:A:207:LYS:HZ3	1.67	0.58
1:B:57:LEU:O	1:B:61:SER:HB3	2.04	0.58
1:B:172:LEU:O	1:B:174:PRO:HD3	2.05	0.57
1:B:92:GLU:HG3	1:B:329:ARG:HH11	1.68	0.57
1:B:97:TYR:CZ	1:B:365:VAL:HG23	2.41	0.56
1:A:186:ASP:CG	1:A:312:ARG:HH22	2.15	0.55
1:B:257:LYS:HG2	5:B:777:HOH:O	2.06	0.55
1:B:19:ILE:HD11	1:B:332:ILE:HG13	1.89	0.54
1:B:97:TYR:CE1	1:B:365:VAL:HG23	2.42	0.54
1:B:191:LYS:HG2	1:B:192:ARG:NH1	2.22	0.54
1:B:260:LYS:HE2	1:B:262:ASN:HD21	1.73	0.54
1:A:34:LYS:HB2	1:A:34:LYS:NZ	2.23	0.54
1:A:44:ASP:OD2	1:A:47:ARG:HD3	2.09	0.53
1:B:147:LEU:HD11	1:B:245:MET:HE3	1.91	0.53
1:B:305:ARG:HH22	1:B:360:LEU:HD22	1.74	0.53
1:B:55:GLY:O	1:B:61:SER:HB2	2.09	0.53
1:A:70:MET:HE1	1:A:84:SER:HB3	1.91	0.52
1:B:184:MET:HE3	1:B:194:VAL:HG11	1.91	0.52
1:A:190:ASN:OD1	1:A:190:ASN:N	2.42	0.52
1:A:173:ASN:C	1:A:173:ASN:HD22	2.18	0.52
1:A:325:GLY:H	1:A:361:ASN:ND2	2.07	0.52
1:A:40:ILE:HD13	1:A:340:SER:HA	1.92	0.51
1:B:29:ASN:HD22	1:B:32:GLU:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASN:HD21	1:B:32:GLU:HG3	1.75	0.51
1:A:172:LEU:HB3	1:A:202:ILE:CD1	2.43	0.49
1:B:147:LEU:CD1	1:B:245:MET:HE3	2.42	0.48
1:A:29:ASN:OD1	1:A:32:GLU:HG3	2.13	0.48
1:A:184:MET:HE3	1:A:318:ARG:CZ	2.43	0.48
4:B:605:NAT:O15	4:B:605:NAT:H181	2.13	0.48
1:A:321:GLN:NE2	5:A:790:HOH:O	2.45	0.48
1:A:249:THR:HB	1:A:253:GLU:OE1	2.13	0.48
1:B:305:ARG:HH22	1:B:360:LEU:CD2	2.27	0.47
1:A:361:ASN:C	1:A:362:LYS:HG3	2.40	0.47
1:B:305:ARG:NH2	1:B:360:LEU:HD22	2.29	0.47
1:A:249:THR:HG22	1:A:250:ILE:N	2.29	0.47
1:B:119:ARG:HG2	4:B:605:NAT:H161	1.97	0.47
1:A:251:ASP:HB2	1:A:253:GLU:OE1	2.14	0.46
1:A:258:ILE:HD12	1:A:258:ILE:N	2.29	0.46
1:B:343:LEU:CD2	1:B:347:LEU:HD22	2.46	0.46
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.98	0.44
1:A:153:GLU:HB3	1:A:246:LYS:HB3	2.00	0.44
1:B:130:ASP:HA	1:B:131:PRO:HD3	1.87	0.44
1:B:148:THR:HG23	1:B:149:ASP:N	2.32	0.44
1:A:85:VAL:HG13	1:A:86:VAL:N	2.33	0.44
1:B:106:GLN:HG3	1:B:109:THR:HG23	1.99	0.44
1:B:162:GLU:CD	1:B:171:LEU:HD22	2.42	0.44
1:A:247:GLU:O	1:A:254:GLU:HA	2.17	0.44
1:B:244:HIS:ND1	1:B:258:ILE:HG12	2.33	0.44
1:A:115:MET:CE	1:A:135:ILE:HD12	2.48	0.43
1:B:237:SER:HB3	1:B:265:ASP:HB3	2.00	0.43
1:A:184:MET:HE1	1:A:318:ARG:HD3	2.00	0.43
1:A:186:ASP:O	1:A:188:PRO:HD3	2.19	0.43
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.82	0.43
1:B:327:ARG:O	1:B:363:PRO:HA	2.18	0.43
1:B:44:ASP:OD2	1:B:46:VAL:HG22	2.18	0.43
1:B:365:VAL:CG1	1:B:366:ASN:N	2.80	0.43
1:B:163:ILE:HG12	1:B:168:LEU:CD2	2.49	0.42
1:A:172:LEU:HB3	1:A:202:ILE:HD11	2.00	0.42
1:A:209:GLU:O	1:A:213:ILE:HG13	2.19	0.42
1:A:221:ARG:HD3	5:A:830:HOH:O	2.18	0.42
1:A:48:LYS:HA	1:A:71:VAL:CG1	2.45	0.42
1:A:22:VAL:CG2	1:A:333:ILE:HG12	2.48	0.42
1:A:180:GLU:HG2	5:A:812:HOH:O	2.19	0.42
1:A:245:MET:HE3	1:A:257:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ALA:HB2	4:A:604:NAT:H182	2.02	0.41
1:B:46:VAL:HG23	1:B:47:ARG:N	2.34	0.41
1:B:70:MET:CE	1:B:84:SER:HB3	2.47	0.41
1:B:19:ILE:HG13	1:B:330:THR:O	2.21	0.41
1:B:57:LEU:CD2	1:B:58:ALA:H	2.34	0.41
1:B:192:ARG:HE	1:B:321:GLN:HE22	1.69	0.41
1:A:139:THR:O	1:A:143:ILE:HG13	2.21	0.40
1:A:257:LYS:C	1:A:258:ILE:HD12	2.47	0.40
1:B:323:SER:HA	1:B:328:THR: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	327/367 (89%)	320 (98%)	7 (2%)	0	100	100
1	B	331/367 (90%)	325 (98%)	6 (2%)	0	100	100
All	All	658/734 (90%)	645 (98%)	13 (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 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	293/321 (91%)	287 (98%)	6 (2%)	48	46
1	B	297/321 (92%)	287 (97%)	10 (3%)	32	25
All	All	590/642 (92%)	574 (97%)	16 (3%)	39	34

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	57	LEU
1	A	140	LEU
1	A	190	ASN
1	A	207	LYS
1	A	289	ASN
1	B	29	ASN
1	B	57	LEU
1	B	162	GLU
1	B	288	ILE
1	B	289	ASN
1	B	343	LEU
1	B	347	LEU
1	B	350	LEU
1	B	362	LYS
1	B	365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	98	ASN
1	A	122	ASN
1	A	173	ASN
1	A	183	GLN
1	A	212	GLN
1	A	229	ASN
1	A	244	HIS
1	A	262	ASN
1	A	289	ASN
1	A	308	HIS
1	A	321	GLN
1	A	361	ASN
1	B	20	GLN

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Mol	Chain	Res	Type
1	B	29	ASN
1	B	98	ASN
1	B	141	HIS
1	B	262	ASN
1	B	271	ASN
1	B	289	ASN
1	B	290	GLN
1	B	342	ASN
1	B	358	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 [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	NAT	B	605	-	21,21,21	2.76	10 (47%)	29,29,29	2.32	9 (31%)
3	ADP	A	601	2	28,29,29	1.63	7 (25%)	43,45,45	2.02	9 (20%)
4	NAT	A	604	-	21,21,21	2.75	9 (42%)	29,29,29	2.24	11 (37%)
3	ADP	B	600	2	28,29,29	1.64	5 (17%)	43,45,45	2.00	9 (20%)

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	NAT	B	605	-	-	0/11/27/27	0/2/2/2
3	ADP	A	601	2	-	6/16/32/32	0/3/3/3
4	NAT	A	604	-	-	0/11/27/27	0/2/2/2
3	ADP	B	600	2	-	6/16/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	NAT	C11-N10	6.22	1.46	1.38
4	B	605	NAT	C11-N10	6.20	1.46	1.38
4	B	605	NAT	C3-C4	5.15	1.46	1.39
4	A	604	NAT	C1-C2	4.66	1.46	1.39
4	A	604	NAT	C3-C4	4.63	1.46	1.39
4	B	605	NAT	C1-C2	4.45	1.46	1.39
3	B	600	ADP	C5-N7	-4.45	1.31	1.39
3	A	601	ADP	C5-N7	-4.39	1.31	1.39
4	B	605	NAT	C6-C1	4.32	1.46	1.38
4	A	604	NAT	C6-C1	3.91	1.45	1.38
4	A	604	NAT	C6-C5	3.91	1.45	1.38
4	A	604	NAT	C3-C2	3.57	1.44	1.39
4	B	605	NAT	C3-C2	3.50	1.44	1.39
4	B	605	NAT	C6-C5	3.44	1.44	1.38
4	A	604	NAT	C5-C4	3.20	1.45	1.39
3	B	600	ADP	C4-N9	-3.15	1.31	1.37
3	A	601	ADP	C4-N9	-3.06	1.31	1.37
4	B	605	NAT	C5-C4	2.83	1.44	1.39
4	A	604	NAT	C9-N8	2.60	1.35	1.33
4	B	605	NAT	C2-C7	-2.50	1.48	1.52
4	A	604	NAT	C2-C7	-2.47	1.49	1.52
4	B	605	NAT	C9-N8	2.36	1.35	1.33
3	A	601	ADP	C5'-C4'	2.28	1.58	1.51
3	B	600	ADP	C5'-C4'	2.25	1.58	1.51
3	B	600	ADP	PA-O3A	-2.21	1.57	1.59
3	A	601	ADP	PA-O2A	-2.16	1.45	1.55
3	A	601	ADP	C5-C4	2.12	1.42	1.39
3	A	601	ADP	C4-N3	2.07	1.38	1.34
3	A	601	ADP	PB-O3B	-2.06	1.47	1.54
3	B	600	ADP	PB-O3B	-2.02	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	NAT	C14-C12	2.01	1.51	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ADP	N3-C2-N1	-6.96	118.05	128.58
3	B	600	ADP	N3-C2-N1	-6.92	118.11	128.58
4	A	604	NAT	C16-O15-C14	6.30	127.39	116.49
4	B	605	NAT	C16-O15-C14	5.80	126.52	116.49
4	B	605	NAT	C12-C7-N8	5.23	113.62	109.07
3	A	601	ADP	C5-C4-N3	-4.98	119.86	126.72
3	B	600	ADP	C5-C4-N3	-4.96	119.88	126.72
4	A	604	NAT	C12-C7-N8	4.87	113.31	109.07
4	B	605	NAT	O15-C14-C12	4.40	120.19	112.28
3	A	601	ADP	C2-N3-C4	4.34	122.43	111.83
3	B	600	ADP	C2-N3-C4	4.33	122.40	111.83
3	B	600	ADP	N3-C4-N9	3.93	133.85	127.17
3	A	601	ADP	N3-C4-N9	3.93	133.85	127.17
4	A	604	NAT	N10-C9-N8	3.82	119.01	116.22
4	B	605	NAT	N10-C9-N8	3.79	118.99	116.22
4	B	605	NAT	C4-C3-C2	-3.35	117.20	120.09
4	A	604	NAT	C9-N10-C11	-3.22	121.93	123.83
3	B	600	ADP	C5-N7-C8	3.17	108.43	103.45
3	A	601	ADP	C5-N7-C8	3.17	108.43	103.45
4	B	605	NAT	O19-C14-C12	-3.16	118.53	125.20
3	A	601	ADP	N9-C8-N7	-2.98	109.72	113.94
4	A	604	NAT	C4-C3-C2	-2.97	117.52	120.09
3	B	600	ADP	N9-C8-N7	-2.97	109.73	113.94
4	A	604	NAT	O15-C14-C12	2.90	117.50	112.28
4	A	604	NAT	C5-C6-C1	-2.86	116.57	120.24
4	B	605	NAT	C5-C6-C1	-2.72	116.75	120.24
3	B	600	ADP	C4-C5-N7	-2.53	107.69	110.58
4	A	604	NAT	O19-C14-C12	-2.53	119.87	125.20
3	A	601	ADP	C4-C5-N7	-2.52	107.70	110.58
4	A	604	NAT	S20-C9-N10	-2.27	119.20	122.11
4	A	604	NAT	C1-C2-C3	2.16	121.23	118.74
4	B	605	NAT	C9-N10-C11	-2.13	122.58	123.83
4	B	605	NAT	C1-C2-C3	2.13	121.20	118.74
3	B	600	ADP	C2-N1-C6	2.11	122.20	118.73
4	A	604	NAT	C6-C5-C4	2.07	122.08	119.29
3	A	601	ADP	C2-N1-C6	2.06	122.11	118.73
3	B	600	ADP	C4-N9-C8	2.06	107.90	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ADP	C4-N9-C8	2.02	107.86	105.74

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	C5'-O5'-PA-O1A
3	A	601	ADP	C5'-O5'-PA-O2A
3	A	601	ADP	C5'-O5'-PA-O3A
3	B	600	ADP	C5'-O5'-PA-O1A
3	B	600	ADP	C5'-O5'-PA-O2A
3	B	600	ADP	C5'-O5'-PA-O3A
3	A	601	ADP	O4'-C4'-C5'-O5'
3	A	601	ADP	C3'-C4'-C5'-O5'
3	B	600	ADP	O4'-C4'-C5'-O5'
3	B	600	ADP	C3'-C4'-C5'-O5'
3	A	601	ADP	PA-O3A-PB-O2B
3	B	600	ADP	PA-O3A-PB-O2B

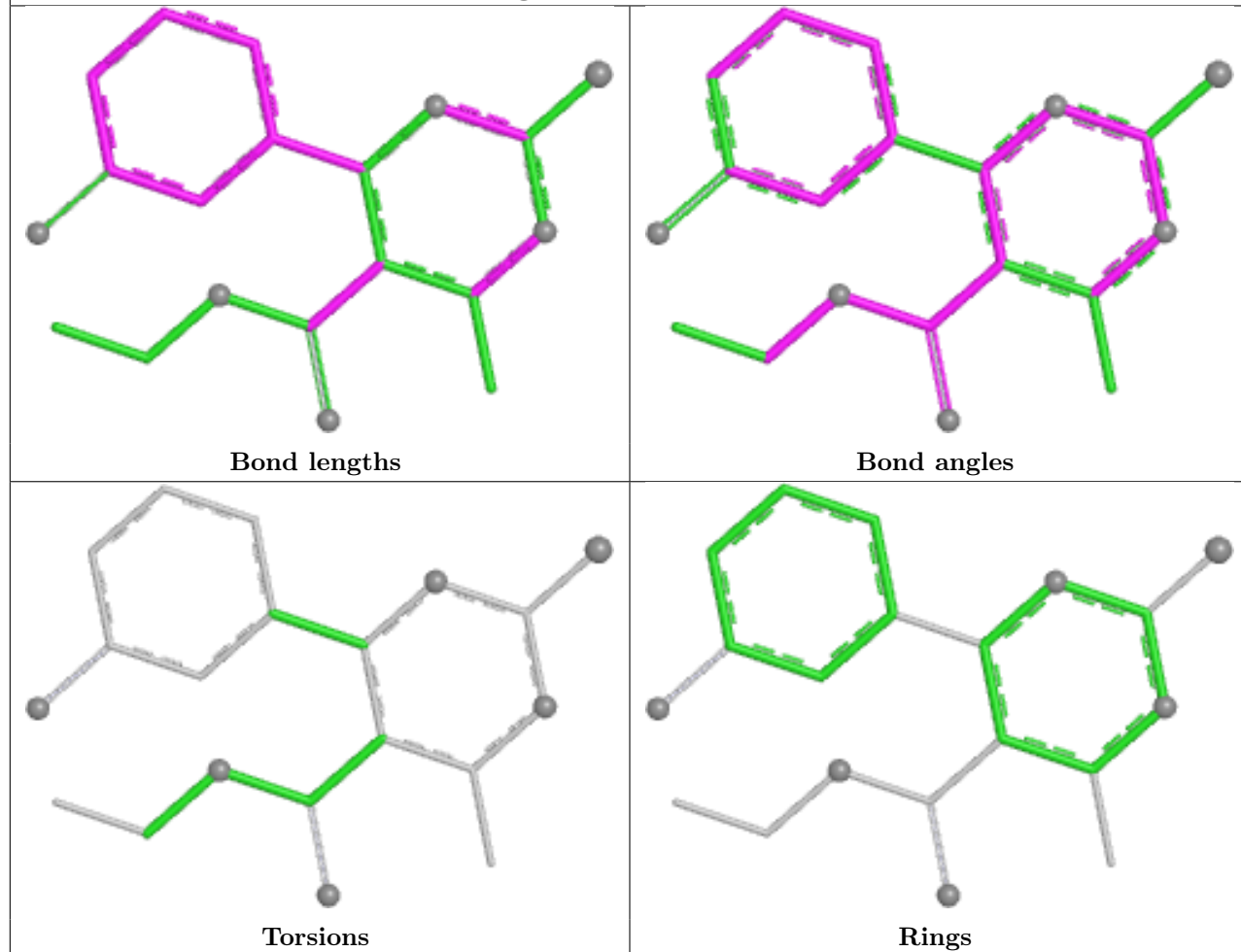
There are no ring outliers.

2 monomers are involved in 4 short contacts:

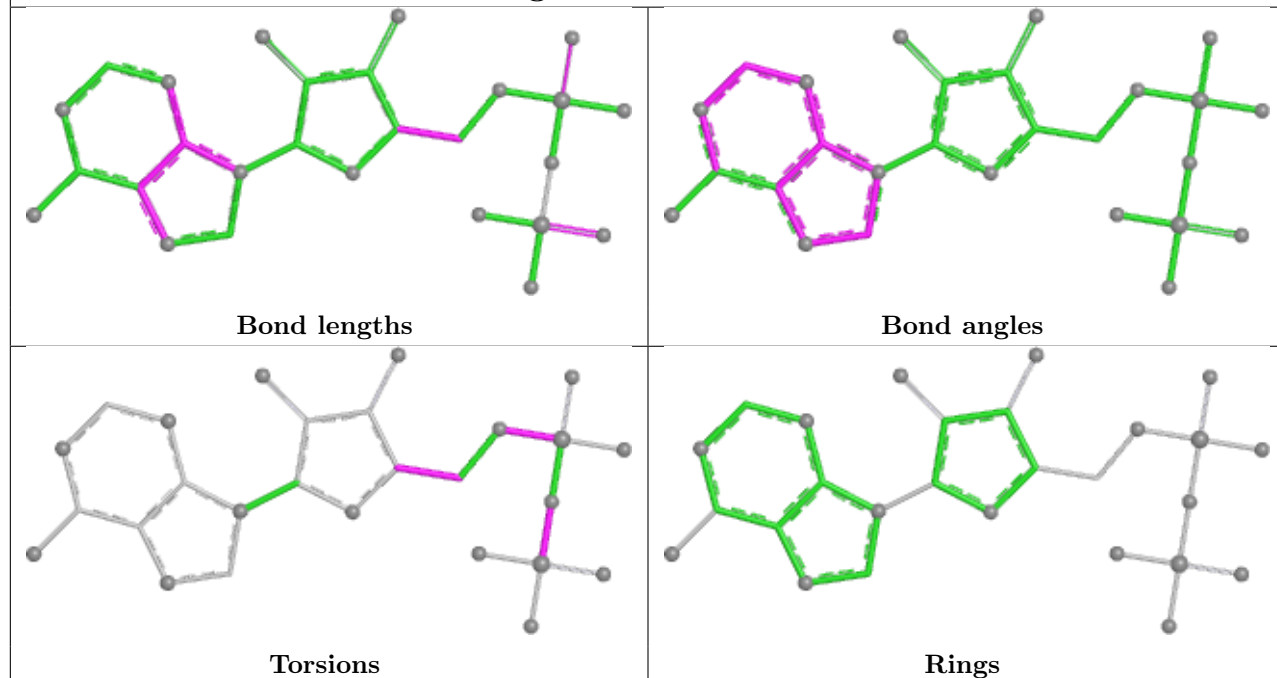
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	NAT	2	0
4	A	604	NAT	2	0

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.

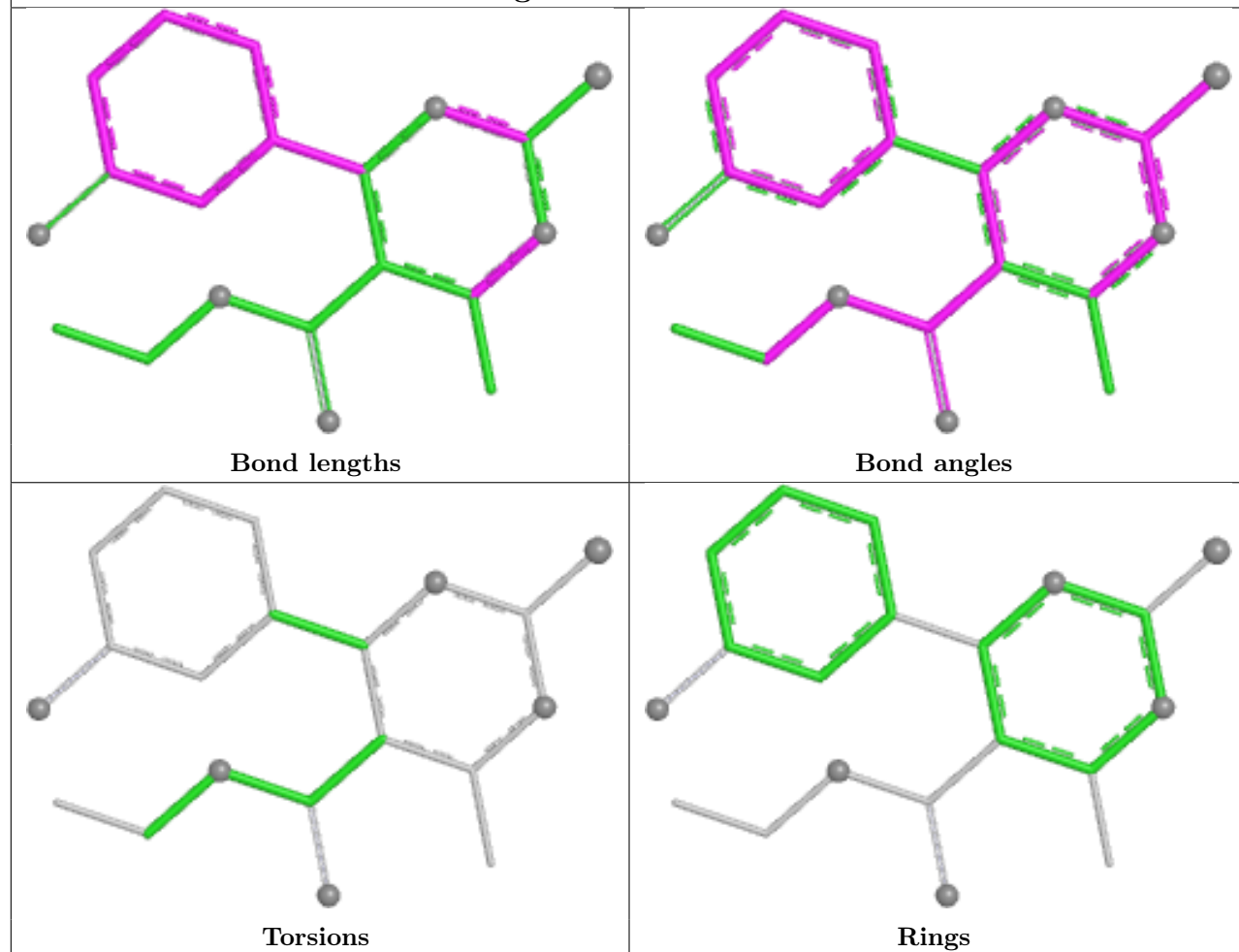
Ligand NAT B 605



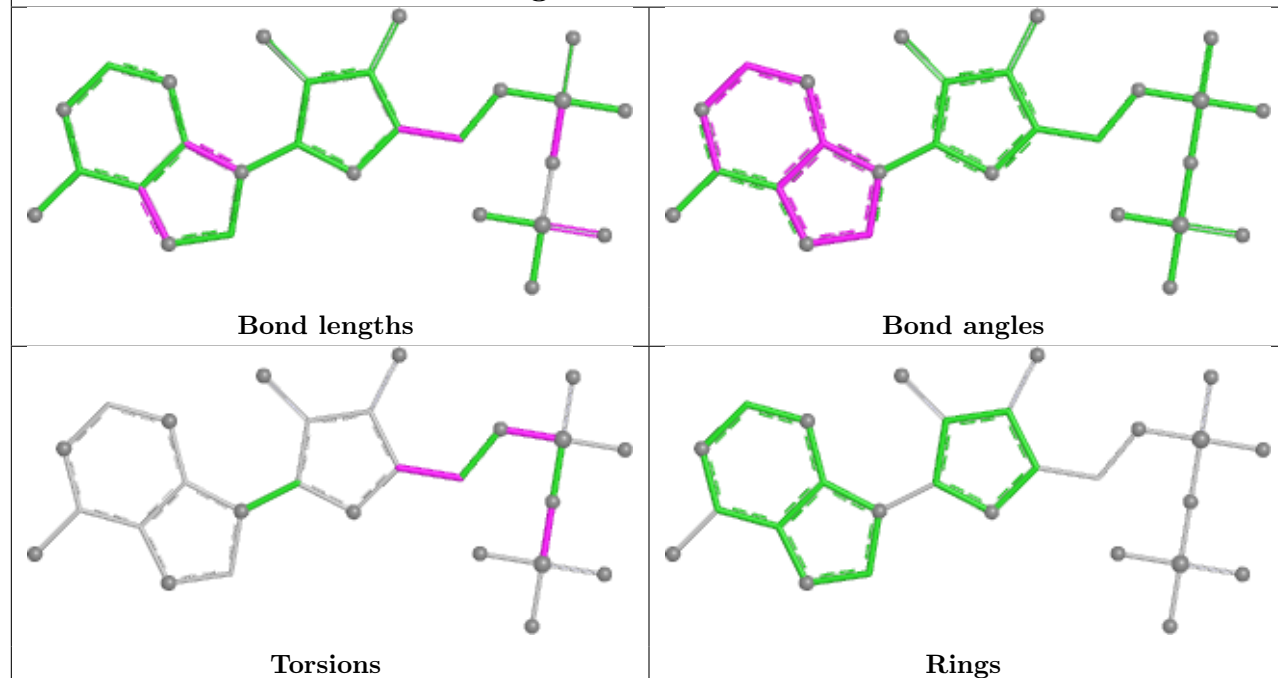
Ligand ADP A 601



Ligand NAT A 604



Ligand ADP B 600



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

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.