Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 07:23 am GMT

PDB ID	:	2J9E
Title	:	Structure of GlnK1 with bound effectors indicates regulatory mechanism for ammonia uptake
Authors	:	Yildiz, O.; Kalthoff, C.; Raunser, S.; Kuehlbrandt, W.
Deposited on	:	2006-11-07
Resolution	:	1.62 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:

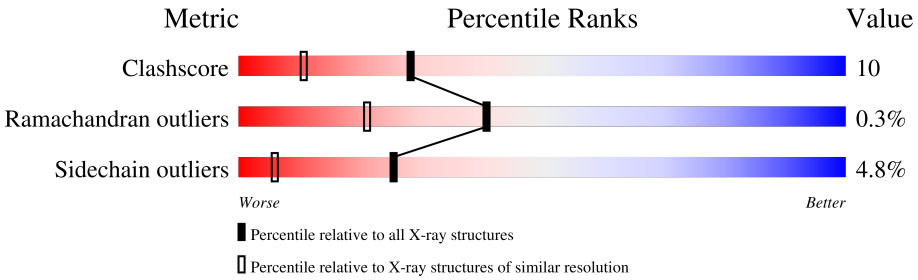
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.62 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	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	84% 8% • 6%
1	B	119	85% 12% • •
1	C	119	82% 15% • •

2 Entry composition (i)

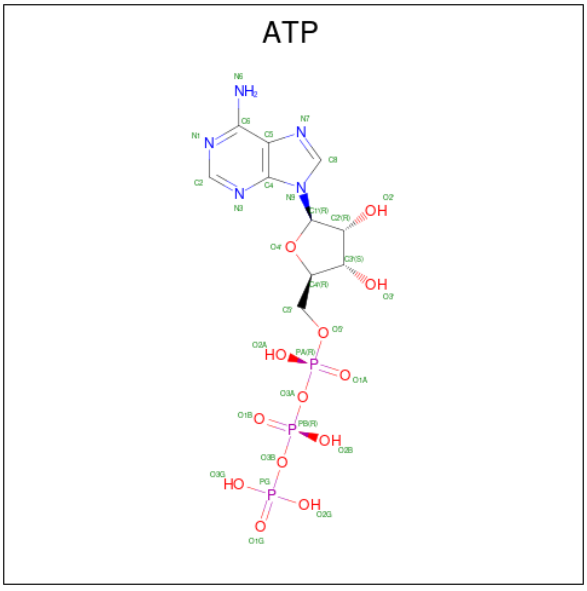
There are 8 unique types of molecules in this entry. The entry contains 3320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	9	0
			903	579	149	171	4			
1	B	119	Total	C	N	O	S	0	8	0
			973	618	168	183	4			
1	C	116	Total	C	N	O	S	0	7	0
			939	600	160	175	4			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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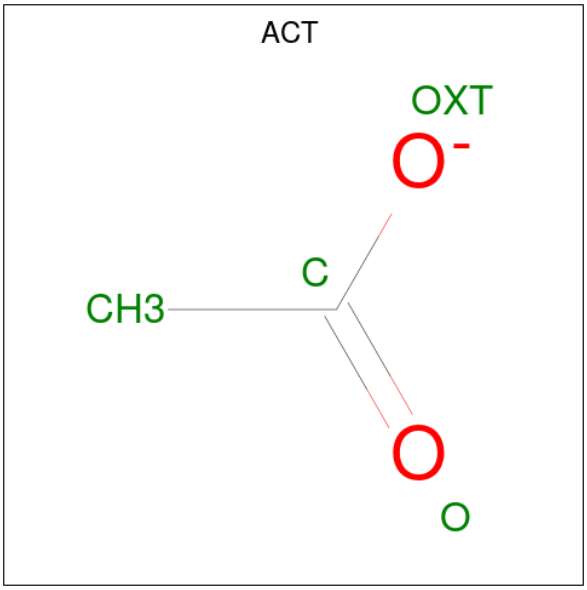
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	C	2	Total	Cl	0	0
			2	2		

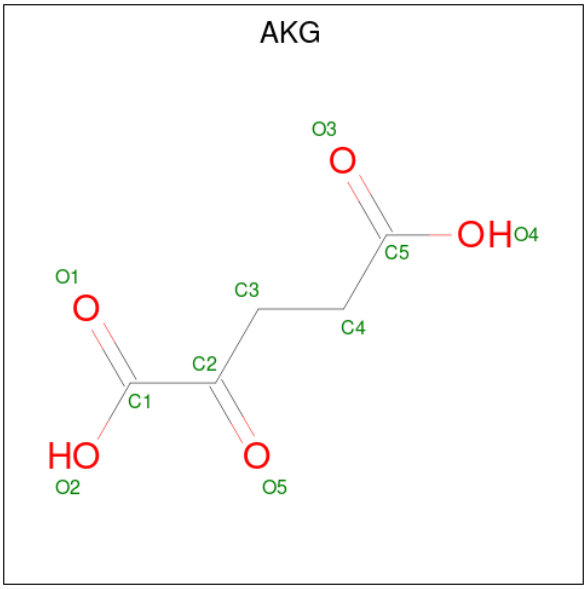
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Mg 1 1	0	0

- Molecule 7 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 10 5 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	112	Total O 112 112	0	0
8	B	137	Total O 137 137	0	0
8	C	143	Total O 143 143	0	0

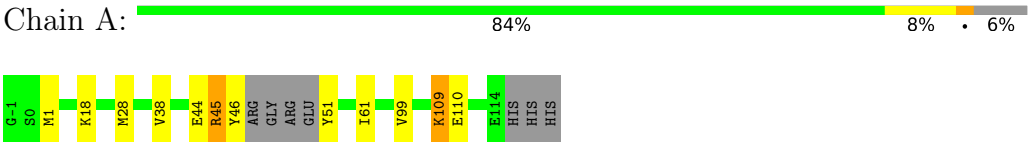
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

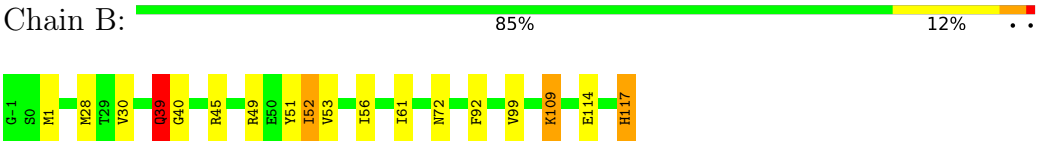
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain A:



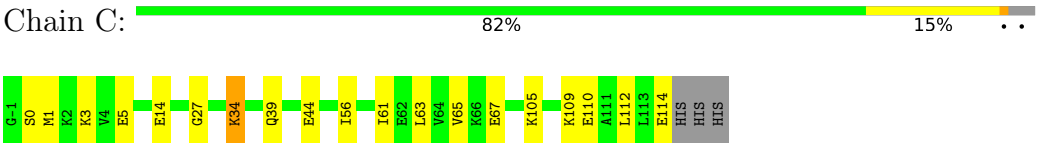
• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain B:



• Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain C:



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	60.40Å 77.80Å 82.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 1.62	Depositor
% Data completeness (in resolution range)	100.0 (19.89-1.62)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.142 , 0.190	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3320	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: ATP, ACT, AKG, CL, NA, MG

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	0/936	0.70	0/1257
1	B	0.60	0/1007	0.71	0/1351
1	C	0.63	0/967	0.75	0/1296
All	All	0.61	0/2910	0.72	0/3904

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	39	GLN	Peptide

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	903	0	972	18	0
1	B	973	0	1038	22	0
1	C	939	0	1024	18	0
2	A	31	0	12	2	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
3	A	4	0	3	0	0
4	A	2	0	0	0	0
4	C	2	0	0	1	0
5	B	1	0	0	0	0
6	C	1	0	0	0	0
7	C	10	0	4	1	0
8	A	112	0	0	6	0
8	B	137	0	0	8	0
8	C	143	0	0	6	0
All	All	3320	0	3077	59	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 (59) 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:28:MET:HE2	1:B:61[A]:ILE:HG23	1.55	0.86
1:C:5:GLU:OE1	8:C:2010:HOH:O	1.96	0.82
1:B:72:ASN:HB3	8:B:2087:HOH:O	1.83	0.76
2:A:1115:ATP:PA	8:A:2107:HOH:O	2.46	0.73
7:C:1119:AKG:O5	8:C:2143:HOH:O	2.04	0.73
1:C:14:GLU:OE2	8:C:2024:HOH:O	2.09	0.71
1:B:72:ASN:CB	8:B:2087:HOH:O	2.40	0.69
1:B:28:MET:HE2	1:B:61[A]:ILE:CG2	2.22	0.69
2:A:1115:ATP:O2G	8:A:2105:HOH:O	2.13	0.65
1:B:30:VAL:O	1:C:34[A]:LYS:HD3	1.98	0.64
1:A:109:LYS:N	1:A:109:LYS:HD3	2.13	0.62
1:C:3:LYS:HE2	8:C:2010:HOH:O	2.00	0.60
1:C:27:GLY:O	1:C:63[A]:LEU:CD1	2.52	0.58
1:B:28:MET:CE	1:B:61[A]:ILE:CG2	2.82	0.58
1:A:28:MET:CE	1:A:61:ILE:HG23	2.34	0.58
1:B:109:LYS:HG2	8:B:2129:HOH:O	2.06	0.55
1:C:1:MET:HE1	1:C:112:LEU:HG	1.88	0.55
1:B:117:HIS:N	1:B:117:HIS:HD1	2.05	0.54
1:B:1[B]:MET:HE2	8:B:2110:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:O	1:A:51:TYR:N	2.40	0.54
1:A:109:LYS:N	1:A:109:LYS:CD	2.71	0.53
1:A:28:MET:HE3	1:A:61:ILE:HG23	1.89	0.53
1:A:44:GLU:HA	1:A:45:ARG:CB	2.38	0.53
1:C:63[A]:LEU:HD11	8:C:2036:HOH:O	2.09	0.52
1:B:1[B]:MET:CE	1:B:99:VAL:HG23	2.40	0.52
1:B:1[B]:MET:HE3	1:B:99:VAL:HG23	1.92	0.52
1:B:52:ILE:HD12	1:B:53:VAL:N	2.25	0.51
1:A:1[A]:MET:SD	1:A:99[A]:VAL:HG21	2.50	0.51
1:A:1[A]:MET:SD	1:A:99[A]:VAL:CG2	3.00	0.50
1:A:38:VAL:HB	8:A:2107:HOH:O	2.12	0.49
1:A:99[B]:VAL:HG12	1:B:92:PHE:HD1	1.78	0.48
1:A:1[A]:MET:CE	1:A:99[A]:VAL:HG23	2.43	0.48
1:B:39:GLN:HG2	1:B:40:GLY:CA	2.43	0.48
1:A:18:LYS:NZ	8:A:2020:HOH:O	2.44	0.48
1:C:34[A]:LYS:CD	1:C:34[A]:LYS:H	2.28	0.47
1:B:49:ARG:HD3	1:B:51:TYR:CZ	2.50	0.47
1:A:109:LYS:CD	1:A:109:LYS:H	2.25	0.47
1:C:44:GLU:CD	1:C:56:ILE:HD13	2.35	0.47
1:A:110[A]:GLU:OE1	8:A:2099:HOH:O	2.20	0.46
4:C:1117:CL:CL	8:C:2010:HOH:O	2.58	0.46
1:B:117:HIS:N	1:B:117:HIS:ND1	2.63	0.46
1:C:1:MET:HE2	1:C:112:LEU:HD21	1.97	0.46
1:A:28:MET:HE1	1:A:61:ILE:CG2	2.45	0.45
1:A:109:LYS:H	1:A:109:LYS:HZ2	1.64	0.45
1:B:1[B]:MET:CE	8:B:2110:HOH:O	2.65	0.45
1:B:30:VAL:HG22	1:B:61[B]:ILE:HG22	2.00	0.44
1:B:114:GLU:HG3	1:C:39:GLN:HG3	2.00	0.43
1:C:61[B]:ILE:HG22	1:C:63[B]:LEU:HD22	2.01	0.43
1:B:56:ILE:HD11	8:B:2075:HOH:O	2.18	0.43
1:A:28:MET:HE1	1:A:61:ILE:HG23	2.01	0.42
8:B:2051:HOH:O	1:C:34[A]:LYS:CE	2.67	0.42
1:B:114:GLU:CG	1:B:117:HIS:HE1	2.32	0.42
1:C:63[A]:LEU:HG	1:C:65:VAL:HG13	2.00	0.42
1:A:18:LYS:CE	8:A:2020:HOH:O	2.67	0.42
1:B:28:MET:CE	1:B:61[A]:ILE:HG21	2.50	0.41
1:C:27:GLY:O	1:C:63[A]:LEU:HD12	2.19	0.41
8:B:2051:HOH:O	1:C:34[A]:LYS:HE3	2.22	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	117/119 (98%)	115 (98%)	1 (1%)	1 (1%)	17 4
1	B	125/119 (105%)	124 (99%)	1 (1%)	0	100 100
1	C	121/119 (102%)	120 (99%)	1 (1%)	0	100 100
All	All	363/357 (102%)	359 (99%)	3 (1%)	1 (0%)	41 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ARG

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	102/102 (100%)	100 (98%)	2 (2%)	55 29
1	B	110/102 (108%)	105 (96%)	5 (4%)	27 7
1	C	106/102 (104%)	98 (92%)	8 (8%)	13 2
All	All	318/306 (104%)	303 (95%)	15 (5%)	25 6

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TYR
1	A	109	LYS

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Mol	Chain	Res	Type
1	B	39	GLN
1	B	45	ARG
1	B	52	ILE
1	B	109	LYS
1	B	117	HIS
1	C	0	SER
1	C	34[A]	LYS
1	C	34[B]	LYS
1	C	67	GLU
1	C	105	LYS
1	C	109	LYS
1	C	110	GLU
1	C	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	39	GLN
1	C	80	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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	ATP	A	1115	-	26,33,33	1.00	2 (7%)	31,52,52	1.60	5 (16%)
2	ATP	B	1118	-	26,33,33	0.90	1 (3%)	31,52,52	1.81	8 (25%)
2	ATP	C	1115	6	26,33,33	1.02	1 (3%)	31,52,52	1.27	2 (6%)
7	AKG	C	1119	-	9,9,9	1.97	1 (11%)	11,11,11	1.29	0
3	ACT	A	1116	-	3,3,3	0.90	0	3,3,3	0.60	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	ATP	C	1115	6	-	2/18/38/38	0/3/3/3
2	ATP	A	1115	-	-	0/18/38/38	0/3/3/3
2	ATP	B	1118	-	-	2/18/38/38	0/3/3/3
7	AKG	C	1119	-	-	5/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1119	AKG	C2-C1	-5.06	1.46	1.53
2	C	1115	ATP	O4'-C1'	3.26	1.45	1.41
2	A	1115	ATP	C5-C4	2.24	1.46	1.40
2	A	1115	ATP	C2'-C1'	-2.17	1.50	1.53
2	B	1118	ATP	C5-C4	2.16	1.46	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1118	ATP	PB-O3B-PG	-5.27	114.74	132.83
2	A	1115	ATP	N3-C2-N1	-4.41	121.79	128.68
2	A	1115	ATP	PB-O3B-PG	-4.18	118.47	132.83
2	B	1118	ATP	N3-C2-N1	-3.77	122.78	128.68
2	C	1115	ATP	N3-C2-N1	-3.67	122.95	128.68
2	B	1118	ATP	PA-O3A-PB	-2.95	122.70	132.83
2	B	1118	ATP	O2B-PB-O1B	2.95	126.81	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1115	ATP	PA-O3A-PB	-2.86	123.02	132.83
2	B	1118	ATP	C2-N1-C6	2.77	123.49	118.75
2	C	1115	ATP	C1'-N9-C4	-2.45	122.33	126.64
2	B	1118	ATP	O2A-PA-O1A	2.36	123.92	112.24
2	B	1118	ATP	O3B-PG-O1G	-2.28	98.52	111.19
2	B	1118	ATP	C1'-N9-C4	-2.25	122.68	126.64
2	A	1115	ATP	C2-N1-C6	2.24	122.59	118.75
2	A	1115	ATP	O2B-PB-O1B	2.04	122.33	112.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1115	ATP	C5'-O5'-PA-O3A
7	C	1119	AKG	O1-C1-C2-O5
7	C	1119	AKG	O1-C1-C2-C3
7	C	1119	AKG	O2-C1-C2-O5
7	C	1119	AKG	O2-C1-C2-C3
2	B	1118	ATP	PB-O3A-PA-O1A
2	C	1115	ATP	C5'-O5'-PA-O1A
2	B	1118	ATP	PG-O3B-PB-O2B
7	C	1119	AKG	C2-C3-C4-C5

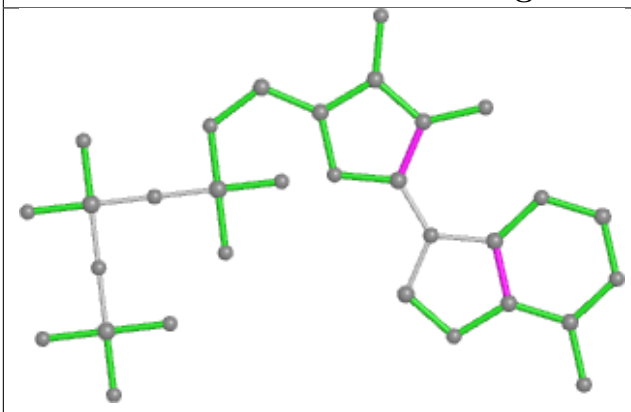
There are no ring outliers.

2 monomers are involved in 3 short contacts:

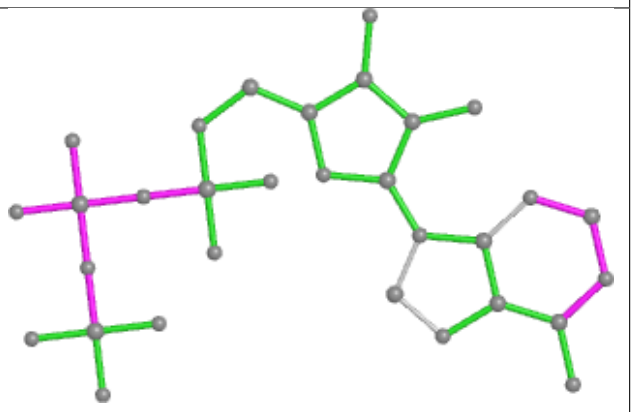
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1115	ATP	2	0
7	C	1119	AKG	1	0

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.

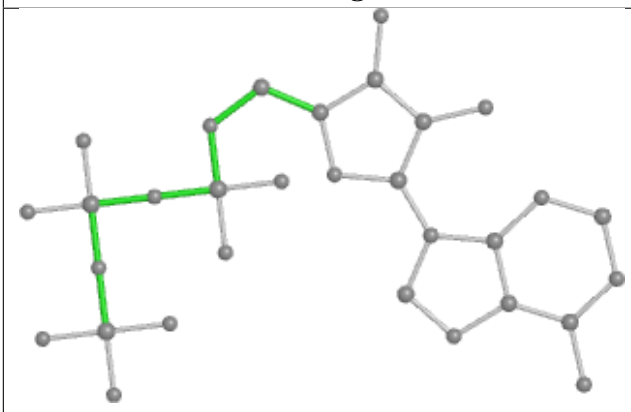
Ligand ATP A 1115



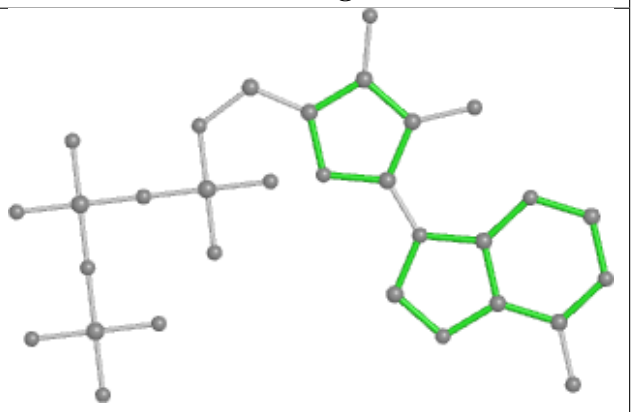
Bond lengths



Bond angles

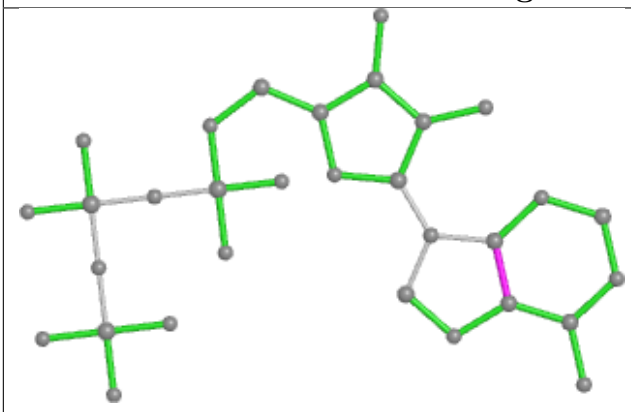


Torsions

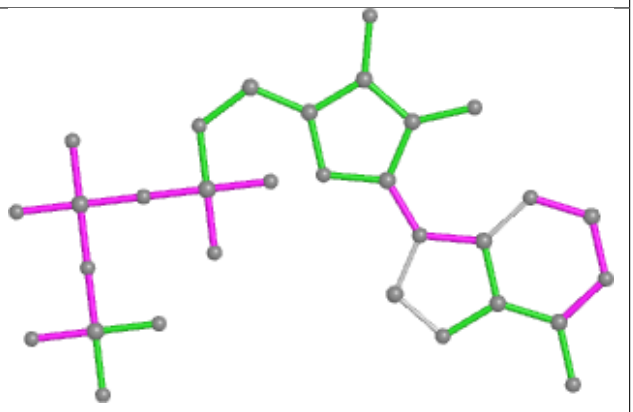


Rings

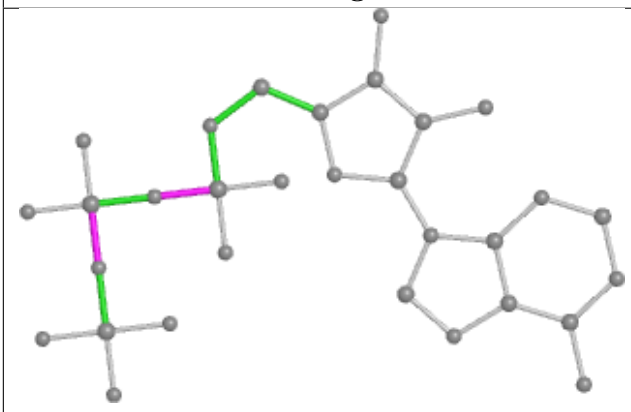
Ligand ATP B 1118



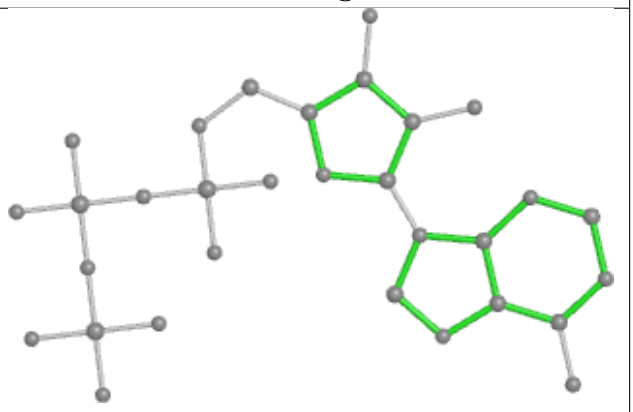
Bond lengths



Bond angles

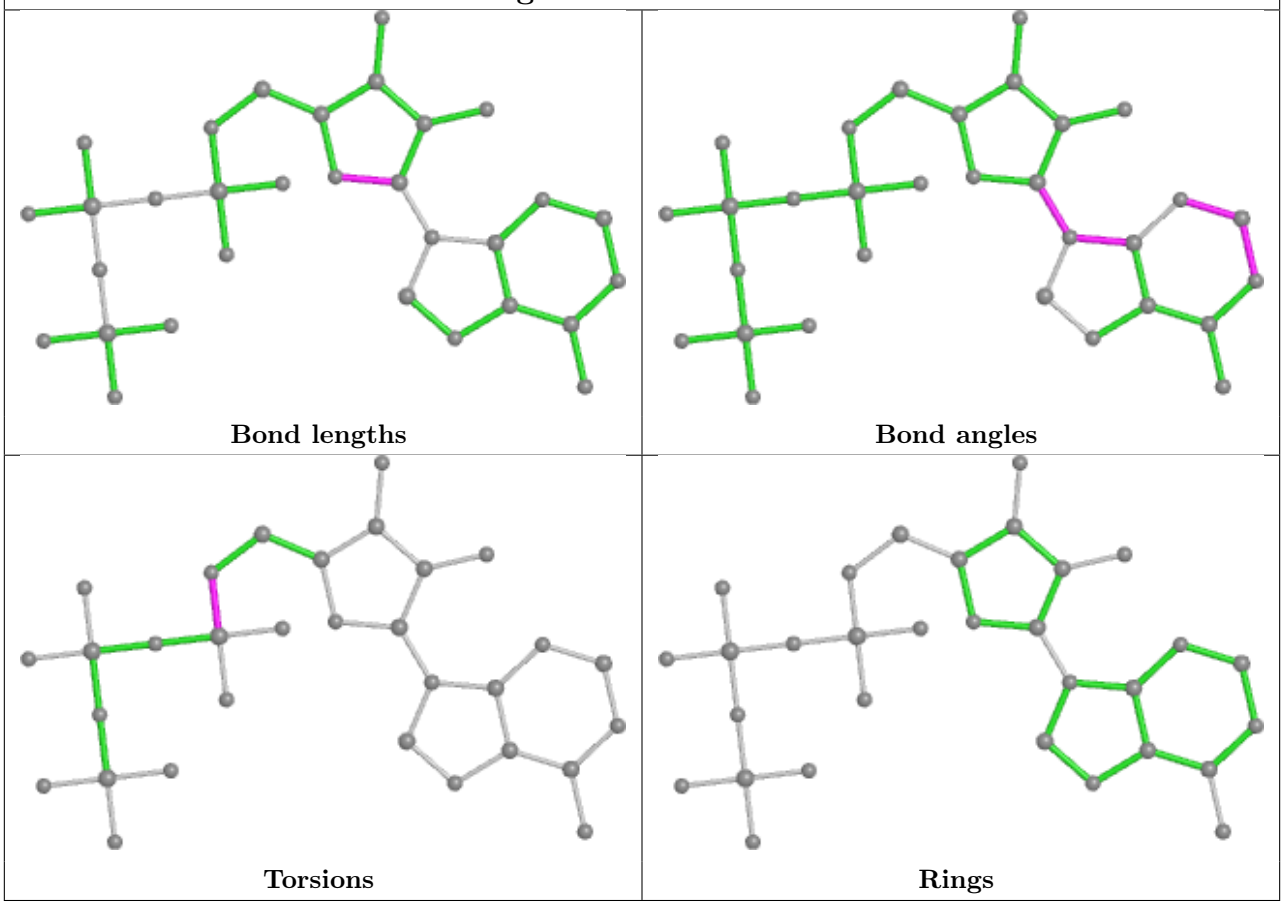


Torsions



Rings

Ligand ATP C 1115



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.