wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 10:57 pm GMT

PDB ID	:	2BUF
Title	:	Arginine Feed-Back Inhibitable Acetylglutamate Kinase
Authors	:	Ramon-Maiques, S.; Fernandez-Murga, M.L.; Vagin, A.; Fita, I.; Rubio, V.
Deposited on	:	2005-06-12
Resolution	:	2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

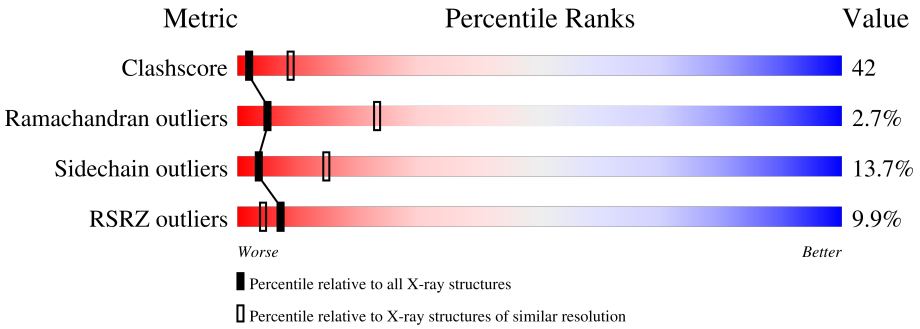
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.95 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	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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% 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	300	3% 45% 44% 8%
1	B	300	3% 46% 46% 7%
1	C	300	56% 37% 6%
1	D	300	60% 31% 7%
1	E	300	5% 48% 40% 8%
1	F	300	7% 47% 41% 9%
1	G	300	8% 48% 41% 8%

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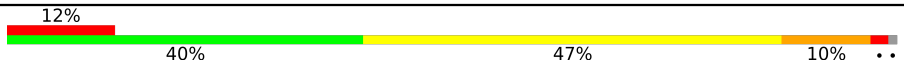
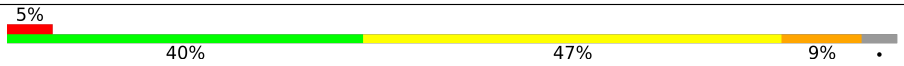
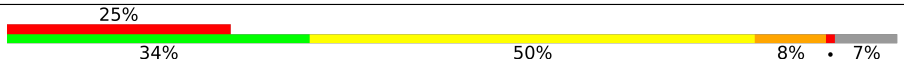
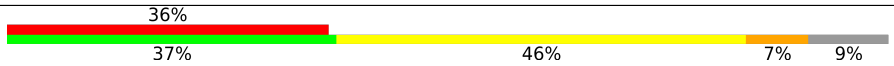
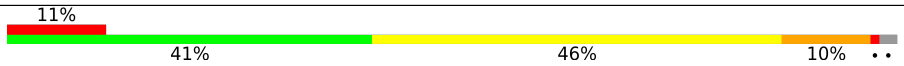
Mol	Chain	Length	Quality of chain
1	H	300	
1	I	300	
1	J	300	
1	K	300	
1	L	300	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NLG	F	1300	-	-	-	X
2	NLG	G	1301	-	X	-	-
2	NLG	H	1299	-	X	X	X
2	NLG	K	1298	-	-	-	X
2	NLG	L	1302	-	X	-	-
3	ADP	H	1297	-	-	-	X
3	ADP	J	1298	-	-	X	-

2 Entry composition (i)

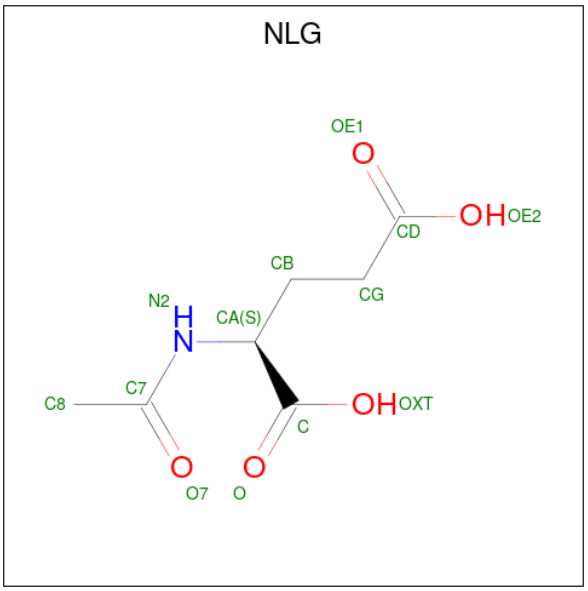
There are 5 unique types of molecules in this entry. The entry contains 25923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLGLUTAMATE KINASE.

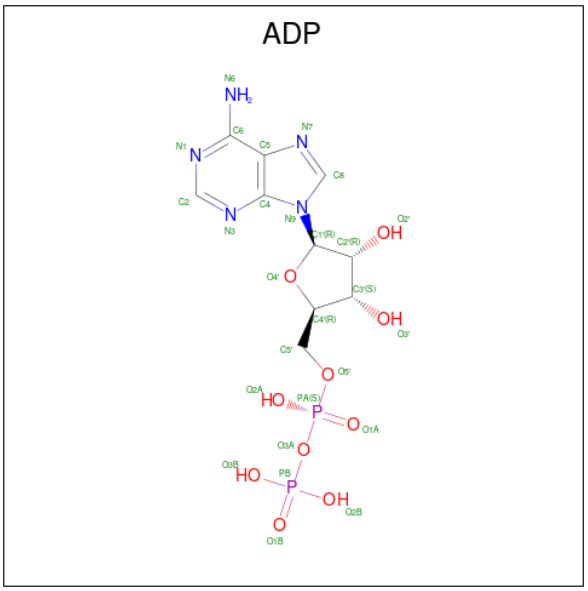
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2159	1359	382	408	10			
1	B	297	Total	C	N	O	S	0	0	1
			2177	1371	379	416	11			
1	C	299	Total	C	N	O	S	0	0	1
			2201	1386	385	419	11			
1	D	295	Total	C	N	O	S	0	0	1
			2170	1367	381	412	10			
1	E	288	Total	C	N	O	S	0	0	1
			2106	1327	368	401	10			
1	F	292	Total	C	N	O	S	0	0	1
			2131	1343	373	405	10			
1	G	298	Total	C	N	O	S	0	0	1
			2186	1377	380	418	11			
1	H	296	Total	C	N	O	S	0	0	1
			2173	1370	377	415	11			
1	I	289	Total	C	N	O	S	0	0	1
			2110	1331	366	403	10			
1	J	280	Total	C	N	O	S	0	0	1
			2015	1266	354	385	10			
1	K	274	Total	C	N	O	S	0	0	1
			1918	1206	339	365	8			
1	L	294	Total	C	N	O	S	0	0	1
			2163	1363	380	410	10			

- Molecule 2 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula: $C_7H_{11}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 13 7 1 5	0	0
2	B	1	Total C N O 13 7 1 5	0	0
2	D	1	Total C N O 13 7 1 5	0	0
2	E	1	Total C N O 13 7 1 5	0	0
2	F	1	Total C N O 13 7 1 5	0	0
2	G	1	Total C N O 13 7 1 5	0	0
2	H	1	Total C N O 13 7 1 5	0	0
2	I	1	Total C N O 13 7 1 5	0	0
2	K	1	Total C N O 13 7 1 5	0	0
2	L	1	Total C N O 13 7 1 5	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

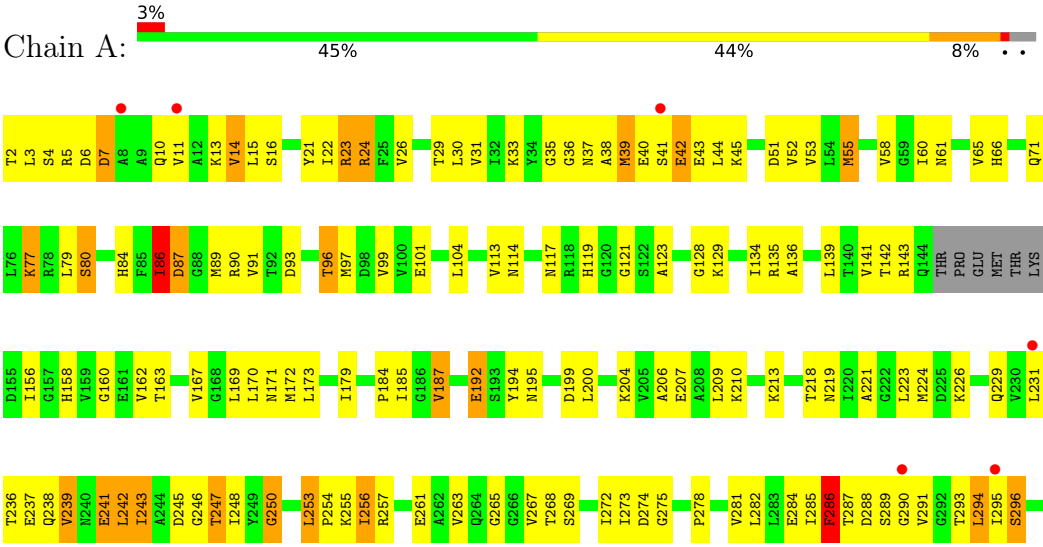
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0
5	L	1	Total Cl 1 1	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

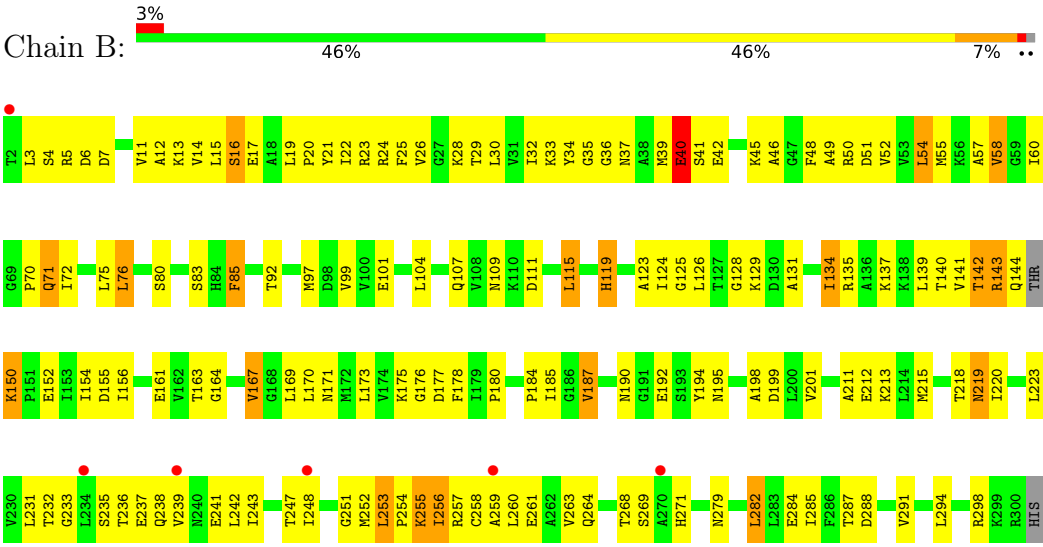
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain A:



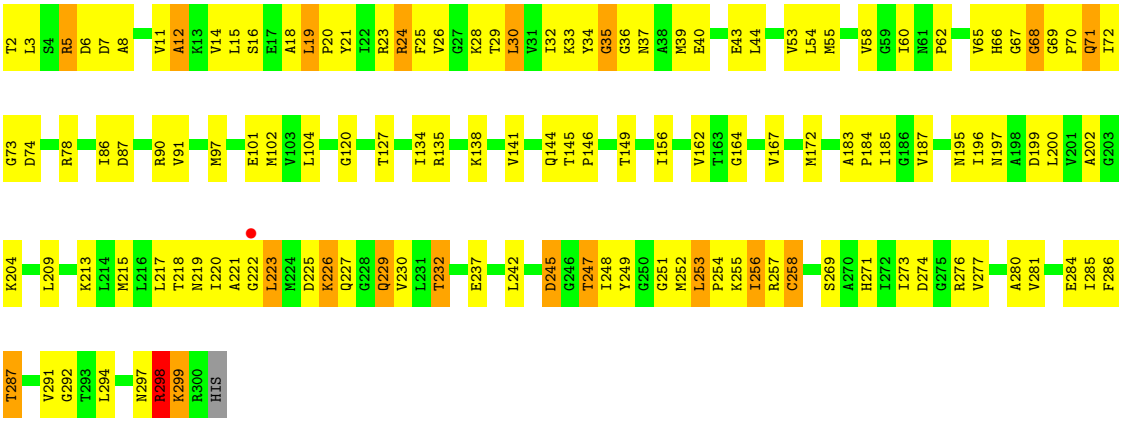
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain B:



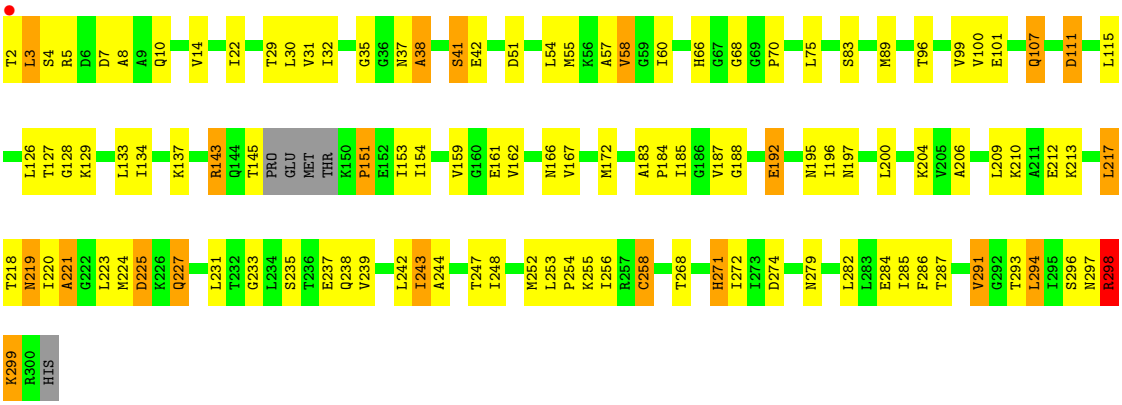
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain C:



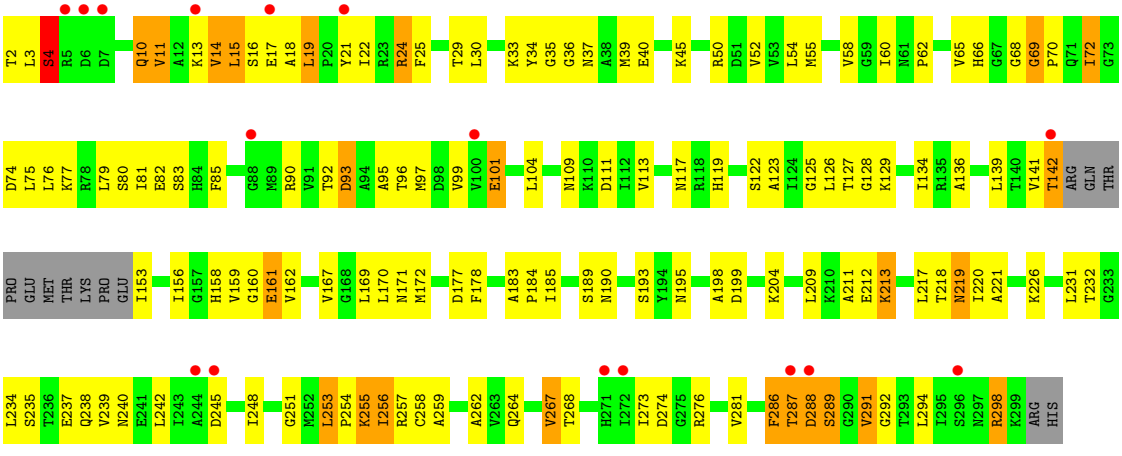
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain D:



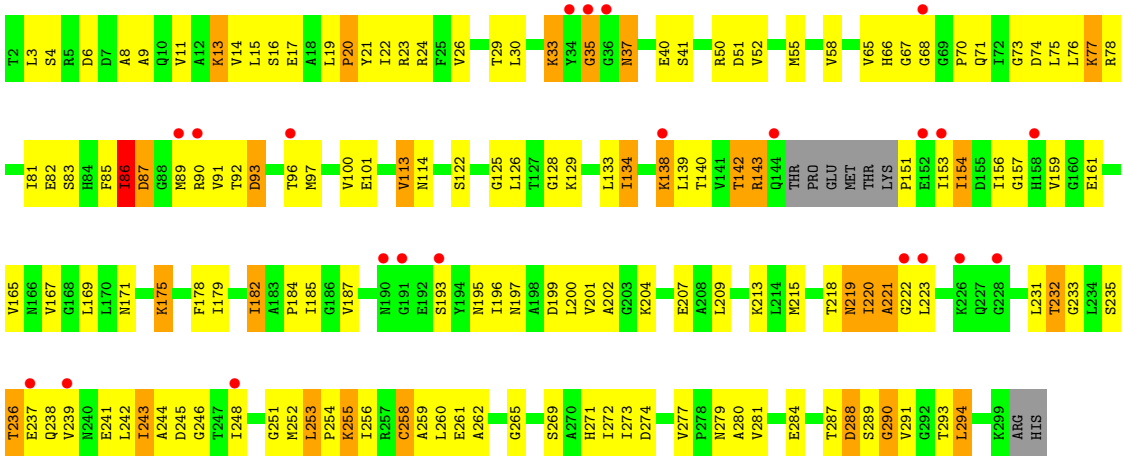
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain E:



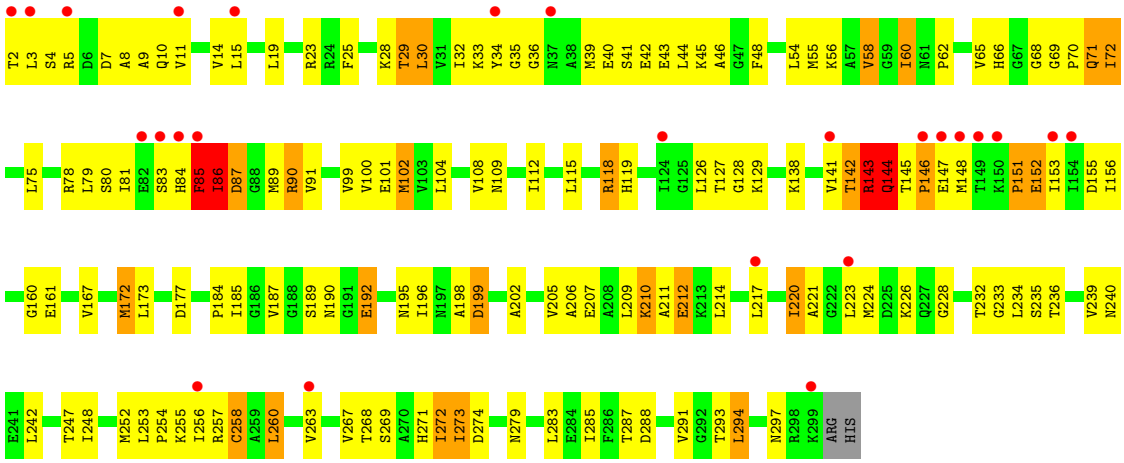
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain F:



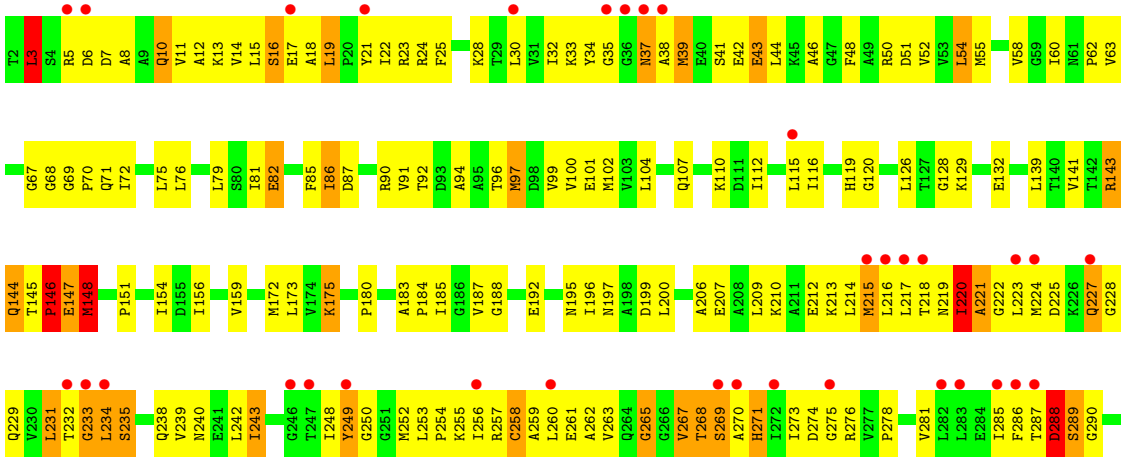
• Molecule 1: ACETYLGLUTAMATE KINASE

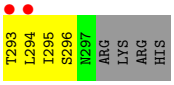
Chain G:



• Molecule 1: ACETYLGLUTAMATE KINASE

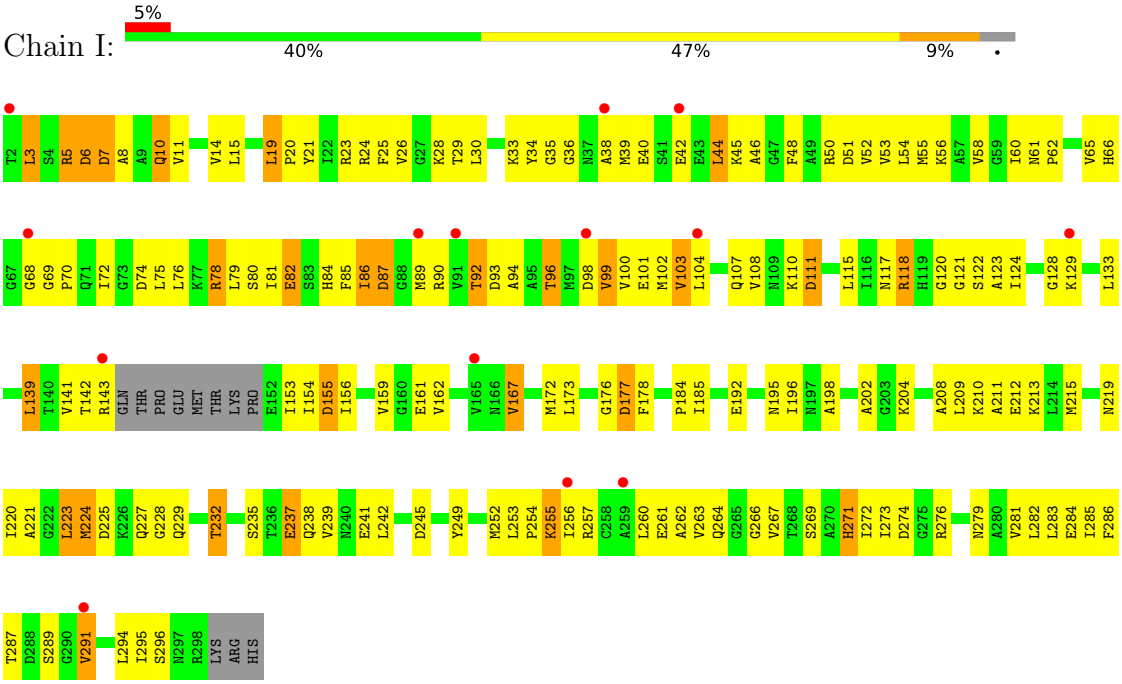
Chain H:





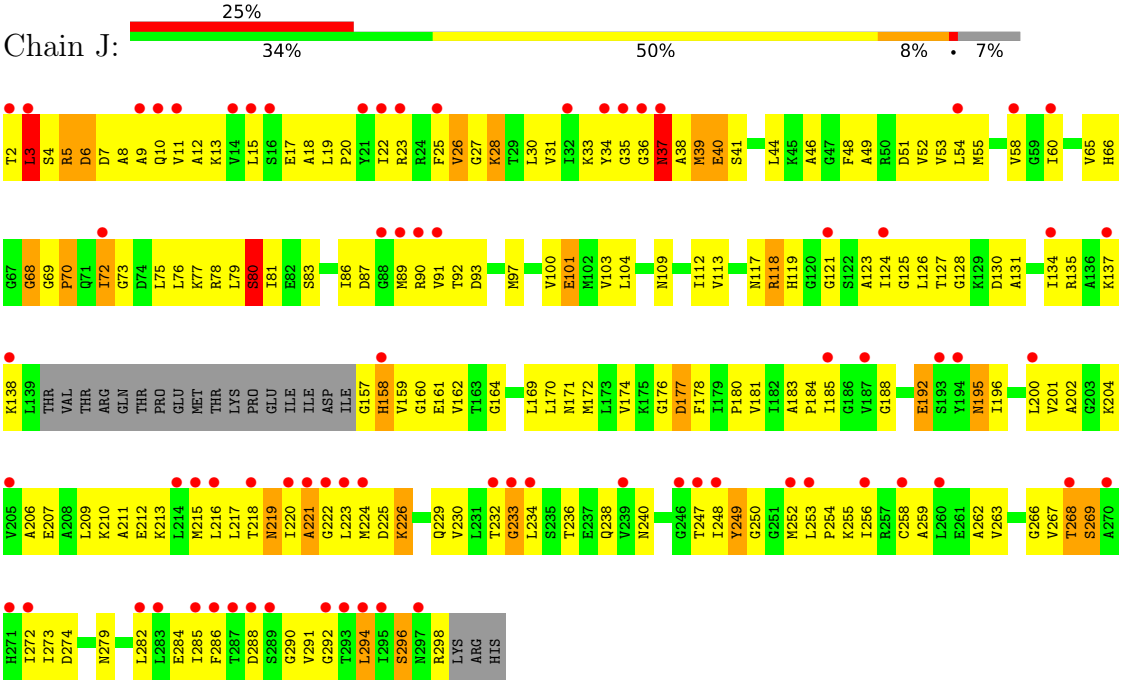
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain I:



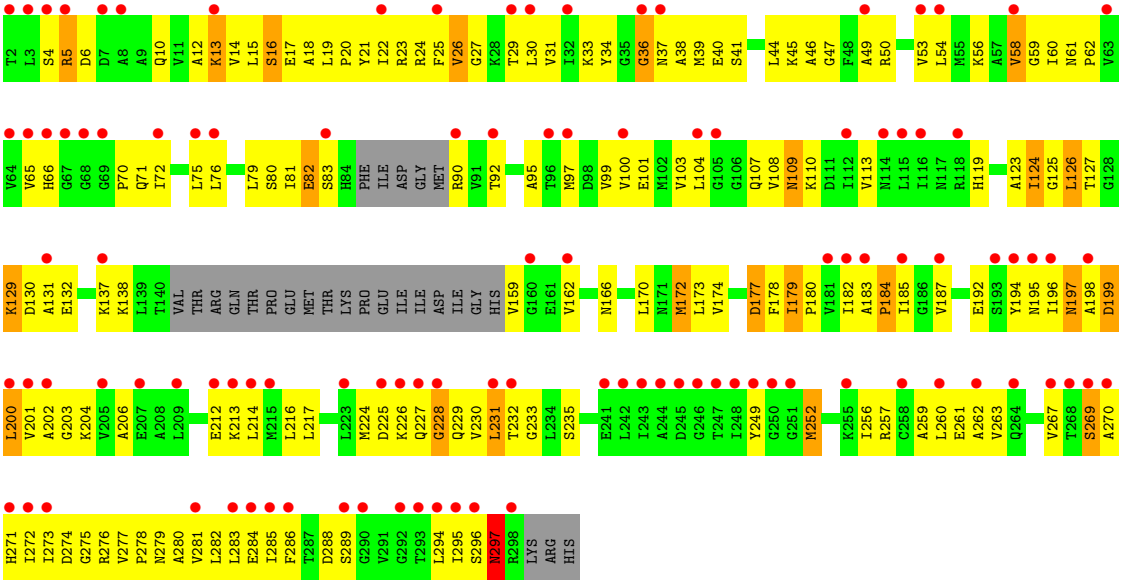
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain J:



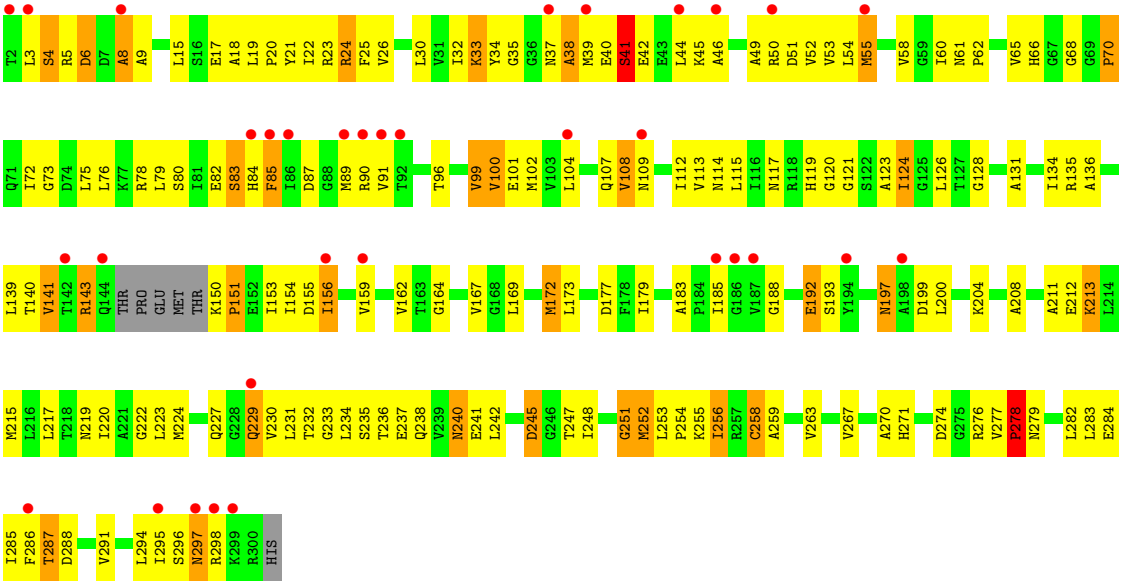
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain K:



- Molecule 1: ACETYLGLUTAMATE KINASE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.86Å 98.78Å 162.90Å 91.49° 92.03° 107.56°	Depositor
Resolution (Å)	18.00 – 2.95 80.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (18.00-2.95) 96.1 (80.13-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.82Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.249 , 0.267 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	78.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 79.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	25923	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, NLG, ADP, 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	0.54	0/2179	0.90	2/2940 (0.1%)
1	B	0.55	0/2197	0.94	5/2969 (0.2%)
1	C	0.57	0/2223	0.85	3/3005 (0.1%)
1	D	0.56	0/2190	0.89	3/2958 (0.1%)
1	E	0.55	1/2125 (0.0%)	0.95	5/2872 (0.2%)
1	F	0.46	0/2151	0.86	3/2907 (0.1%)
1	G	0.50	0/2208	0.91	6/2987 (0.2%)
1	H	0.54	0/2195	0.96	5/2969 (0.2%)
1	I	0.53	0/2129	0.91	4/2878 (0.1%)
1	J	0.50	0/2033	0.89	2/2747 (0.1%)
1	K	0.57	2/1934 (0.1%)	0.87	3/2620 (0.1%)
1	L	0.52	0/2183	0.88	2/2948 (0.1%)
All	All	0.53	3/25747 (0.0%)	0.90	43/34800 (0.1%)

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	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	138	LYS	N-CA	10.40	1.67	1.46
1	E	4	SER	C-O	-5.61	1.12	1.23
1	K	137	LYS	CA-C	5.45	1.67	1.52

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	THR	N-CA-C	10.29	138.78	111.00
1	E	298	ARG	N-CA-C	9.62	136.97	111.00
1	D	298	ARG	N-CA-C	-9.19	86.20	111.00
1	E	3	LEU	N-CA-C	-7.76	90.04	111.00
1	K	4	SER	N-CA-C	7.48	131.19	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	85	PHE	Sidechain

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	2159	0	2259	162	0
1	B	2177	0	2265	184	0
1	C	2201	0	2302	142	0
1	D	2170	0	2272	116	0
1	E	2106	0	2196	150	0
1	F	2131	0	2213	190	0
1	G	2186	0	2278	197	0
1	H	2173	0	2270	238	0
1	I	2110	0	2195	220	0
1	J	2015	0	2071	279	0
1	K	1918	0	1917	266	0
1	L	2163	0	2265	220	0
2	A	13	0	9	0	0
2	B	13	0	9	0	0
2	D	13	0	9	1	0
2	E	13	0	9	0	0
2	F	13	0	9	3	0
2	G	13	0	9	4	0
2	H	13	0	9	6	0
2	I	13	0	9	1	0
2	K	13	0	9	4	0
2	L	13	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	2	0
3	C	27	0	12	2	0
3	D	27	0	12	0	0
3	E	27	0	12	3	0
3	F	27	0	12	2	0
3	G	27	0	12	1	0
3	H	27	0	12	5	0
3	I	27	0	12	0	0
3	J	27	0	12	13	0
3	L	27	0	12	3	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	L	1	0	0	0	0
All	All	25923	0	26713	2195	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 42.

The worst 5 of 2195 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:J:282:LEU:CD2	1:K:12:ALA:HA	1.69	1.22
1:K:34:TYR:CE1	1:K:37:ASN:HB2	1.80	1.15
1:J:223:LEU:HD11	1:J:248:ILE:HG12	1.17	1.14
1:D:14:VAL:HG11	1:F:11:VAL:HG21	1.30	1.13
1:L:54:LEU:HD21	1:L:286:PHE:CZ	1.82	1.13

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	288/300 (96%)	249 (86%)	34 (12%)	5 (2%)	9 34
1	B	293/300 (98%)	268 (92%)	23 (8%)	2 (1%)	22 56
1	C	297/300 (99%)	272 (92%)	20 (7%)	5 (2%)	9 34
1	D	291/300 (97%)	272 (94%)	14 (5%)	5 (2%)	9 34
1	E	284/300 (95%)	250 (88%)	28 (10%)	6 (2%)	7 29
1	F	288/300 (96%)	242 (84%)	38 (13%)	8 (3%)	5 22
1	G	296/300 (99%)	254 (86%)	33 (11%)	9 (3%)	4 20
1	H	294/300 (98%)	243 (83%)	36 (12%)	15 (5%)	2 9
1	I	285/300 (95%)	254 (89%)	28 (10%)	3 (1%)	14 46
1	J	276/300 (92%)	221 (80%)	40 (14%)	15 (5%)	2 9
1	K	268/300 (89%)	221 (82%)	36 (13%)	11 (4%)	3 13
1	L	290/300 (97%)	243 (84%)	37 (13%)	10 (3%)	3 17
All	All	3450/3600 (96%)	2989 (87%)	367 (11%)	94 (3%)	5 23

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	D	38	ALA
1	D	221	ALA
1	E	4	SER
1	E	289	SER

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	231/239 (97%)	193 (84%)	38 (16%)	2 9
1	B	233/239 (98%)	200 (86%)	33 (14%)	3 13
1	C	237/239 (99%)	215 (91%)	22 (9%)	9 30
1	D	233/239 (98%)	205 (88%)	28 (12%)	5 19
1	E	225/239 (94%)	188 (84%)	37 (16%)	2 9
1	F	226/239 (95%)	197 (87%)	29 (13%)	4 17
1	G	235/239 (98%)	197 (84%)	38 (16%)	2 10
1	H	234/239 (98%)	201 (86%)	33 (14%)	3 14
1	I	225/239 (94%)	194 (86%)	31 (14%)	3 14
1	J	210/239 (88%)	191 (91%)	19 (9%)	9 32
1	K	188/239 (79%)	164 (87%)	24 (13%)	4 17
1	L	232/239 (97%)	194 (84%)	38 (16%)	2 9
All	All	2709/2868 (94%)	2339 (86%)	370 (14%)	3 15

5 of 370 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	37	ASN
1	I	237	GLU
1	H	132	GLU
1	I	7	ASP
1	J	192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	117	ASN
1	L	197	ASN
1	E	238	GLN
1	E	171	ASN
1	L	227	GLN

5.3.3 RNA

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 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 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	D	1300	4	24,29,29	1.82	3 (12%)	29,45,45	2.00	6 (20%)
3	ADP	G	1299	4	24,29,29	1.86	5 (20%)	29,45,45	2.04	7 (24%)
3	ADP	F	1299	-	24,29,29	1.93	4 (16%)	29,45,45	2.04	5 (17%)
3	ADP	J	1298	-	24,29,29	2.66	8 (33%)	29,45,45	2.24	9 (31%)
3	ADP	C	1300	4	24,29,29	2.00	5 (20%)	29,45,45	2.20	6 (20%)
2	NLG	A	1302	-	12,12,12	4.05	7 (58%)	15,15,15	4.26	8 (53%)
2	NLG	L	1302	-	12,12,12	4.14	7 (58%)	15,15,15	4.21	8 (53%)
2	NLG	B	1302	-	12,12,12	4.19	6 (50%)	15,15,15	4.22	7 (46%)
3	ADP	B	1300	4	24,29,29	1.97	5 (20%)	29,45,45	2.08	5 (17%)
3	ADP	E	1299	4	24,29,29	2.05	6 (25%)	29,45,45	2.08	6 (20%)
3	ADP	L	1300	4	24,29,29	1.98	5 (20%)	29,45,45	2.07	6 (20%)
2	NLG	E	1301	-	12,12,12	4.18	6 (50%)	15,15,15	4.22	7 (46%)
2	NLG	K	1298	-	12,12,12	4.00	5 (41%)	15,15,15	4.42	9 (60%)
3	ADP	I	1298	4	24,29,29	1.79	4 (16%)	29,45,45	1.95	6 (20%)
3	ADP	H	1297	4	24,29,29	1.91	6 (25%)	29,45,45	2.11	8 (27%)
2	NLG	I	1300	-	12,12,12	4.07	5 (41%)	15,15,15	4.27	9 (60%)
2	NLG	F	1300	-	12,12,12	4.09	5 (41%)	15,15,15	4.27	9 (60%)
2	NLG	G	1301	-	12,12,12	4.11	6 (50%)	15,15,15	4.32	10 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NLG	H	1299	-	12,12,12	4.27	7 (58%)	15,15,15	4.27	9 (60%)
2	NLG	D	1302	-	12,12,12	4.10	5 (41%)	15,15,15	4.23	8 (53%)

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	D	1300	4	-	4/12/32/32	0/3/3/3
3	ADP	G	1299	4	-	1/12/32/32	0/3/3/3
3	ADP	F	1299	-	-	1/12/32/32	0/3/3/3
3	ADP	J	1298	-	-	2/12/32/32	0/3/3/3
3	ADP	C	1300	4	-	2/12/32/32	0/3/3/3
2	NLG	A	1302	-	-	0/13/13/13	-
2	NLG	L	1302	-	-	1/13/13/13	-
2	NLG	B	1302	-	-	0/13/13/13	-
3	ADP	B	1300	4	-	2/12/32/32	0/3/3/3
3	ADP	E	1299	4	-	1/12/32/32	0/3/3/3
3	ADP	L	1300	4	-	3/12/32/32	0/3/3/3
2	NLG	E	1301	-	-	0/13/13/13	-
2	NLG	K	1298	-	-	1/13/13/13	-
3	ADP	I	1298	4	-	1/12/32/32	0/3/3/3
3	ADP	H	1297	4	-	4/12/32/32	0/3/3/3
2	NLG	I	1300	-	-	1/13/13/13	-
2	NLG	F	1300	-	-	0/13/13/13	-
2	NLG	G	1301	-	-	1/13/13/13	-
2	NLG	H	1299	-	-	1/13/13/13	-
2	NLG	D	1302	-	-	1/13/13/13	-

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1299	NLG	C8-C7	-10.23	1.29	1.50
2	G	1301	NLG	C8-C7	-10.02	1.29	1.50
2	B	1302	NLG	C8-C7	-9.63	1.30	1.50
2	D	1302	NLG	C8-C7	-9.61	1.30	1.50
2	K	1298	NLG	C8-C7	-9.57	1.30	1.50

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1298	NLG	OXT-C-O	-10.48	100.31	124.09
2	G	1301	NLG	OXT-C-O	-10.39	100.50	124.09
2	H	1299	NLG	OXT-C-O	-10.33	100.63	124.09
2	F	1300	NLG	OXT-C-O	-10.32	100.65	124.09
2	A	1302	NLG	OXT-C-O	-10.32	100.66	124.09

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1300	ADP	PA-O3A-PB-O3B
3	C	1300	ADP	C4'-C5'-O5'-PA
3	J	1298	ADP	PA-O3A-PB-O3B
3	J	1298	ADP	C4'-C5'-O5'-PA
2	H	1299	NLG	CA-CB-CG-CD

There are no ring outliers.

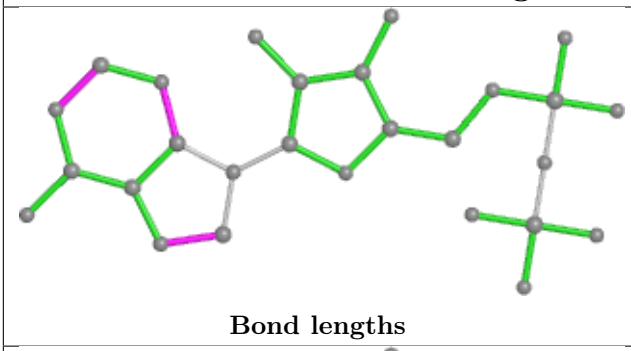
15 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1299	ADP	1	0
3	F	1299	ADP	2	0
3	J	1298	ADP	13	0
3	C	1300	ADP	2	0
2	L	1302	NLG	3	0
3	B	1300	ADP	2	0
3	E	1299	ADP	3	0
3	L	1300	ADP	3	0
2	K	1298	NLG	4	0
3	H	1297	ADP	5	0
2	I	1300	NLG	1	0
2	F	1300	NLG	3	0
2	G	1301	NLG	4	0
2	H	1299	NLG	6	0
2	D	1302	NLG	1	0

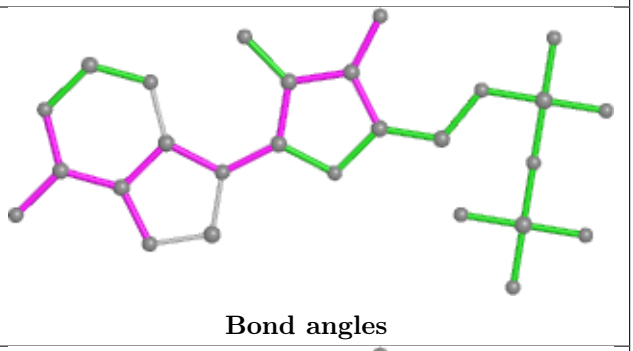
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

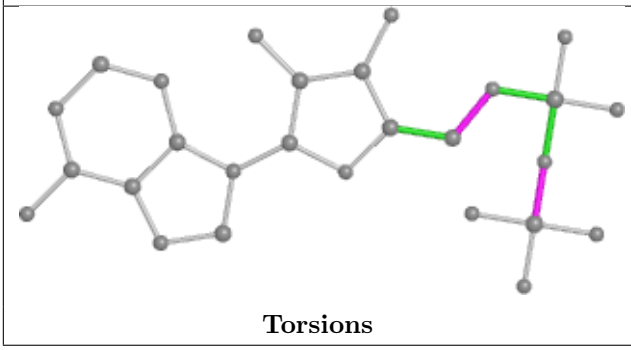
Ligand ADP D 1300



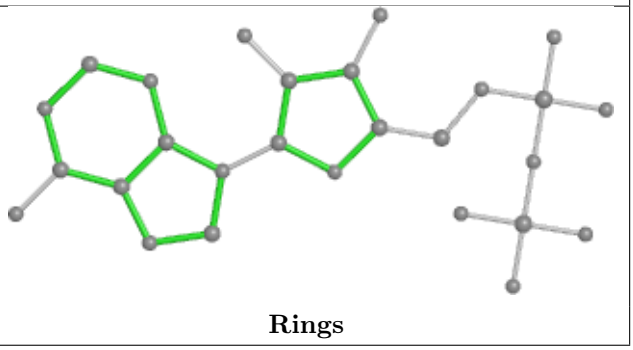
Bond lengths



Bond angles

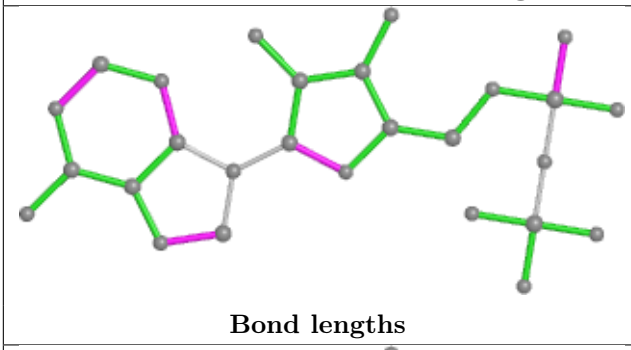


Torsions



Rings

Ligand ADP G 1299



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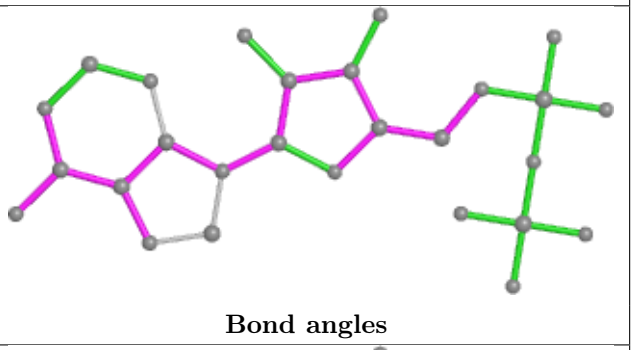

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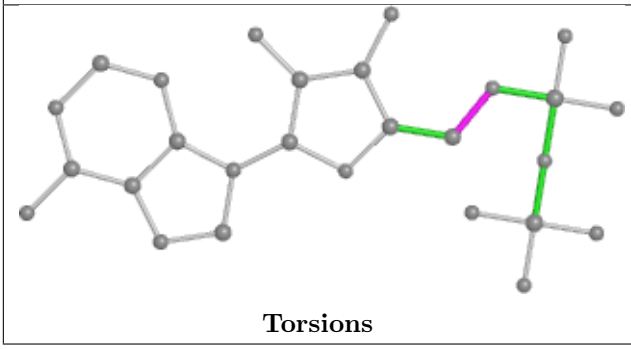

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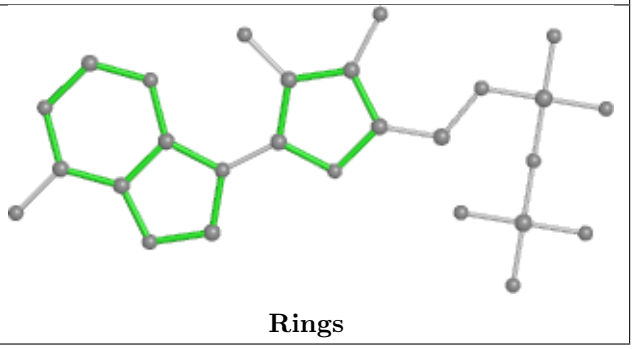
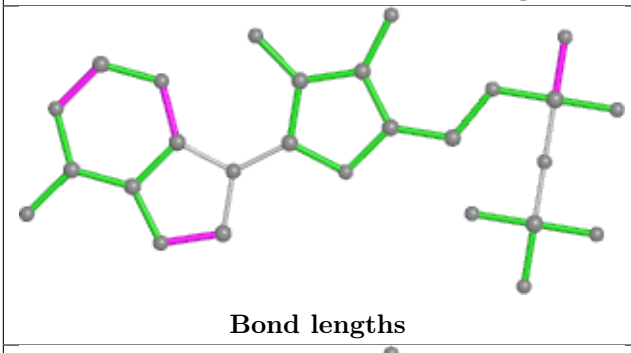
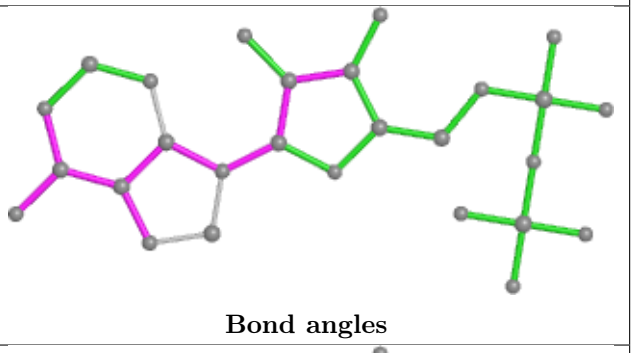


Rings

Ligand ADP F 1299



Bond lengths



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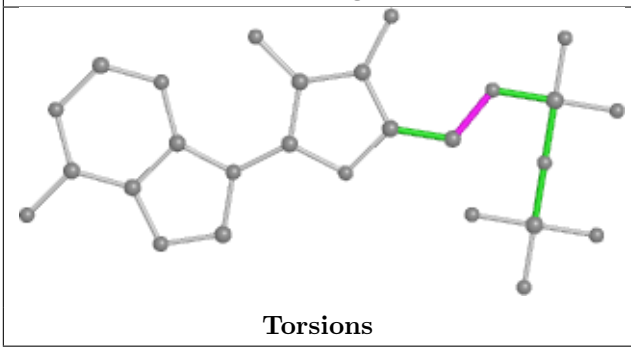

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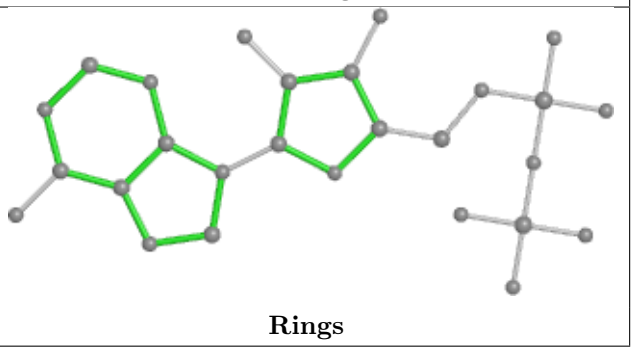
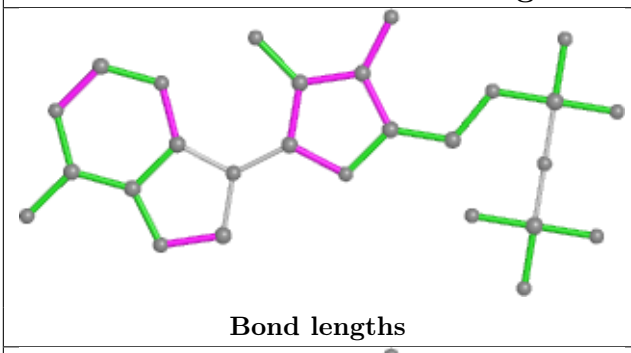


Rings

Ligand ADP J 1298



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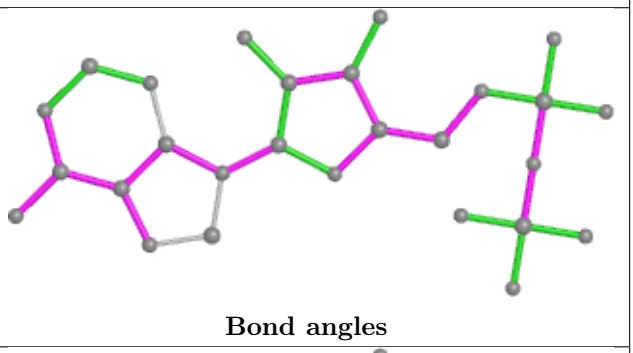
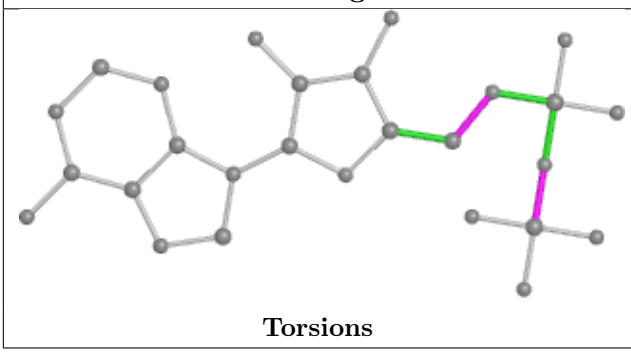


Bond angles



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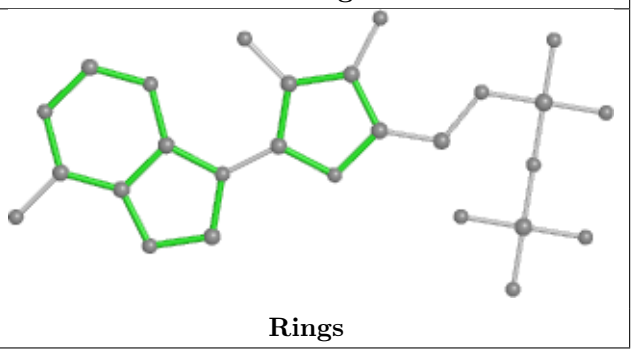
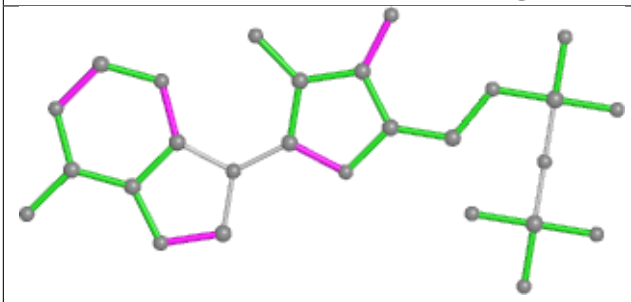
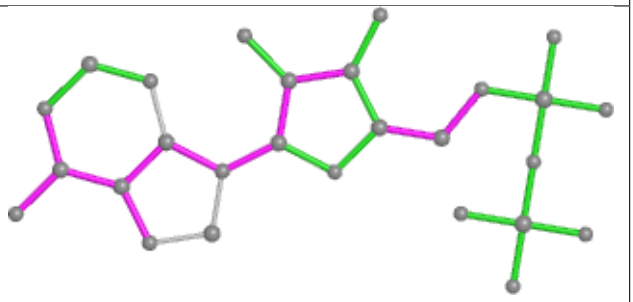


Rings

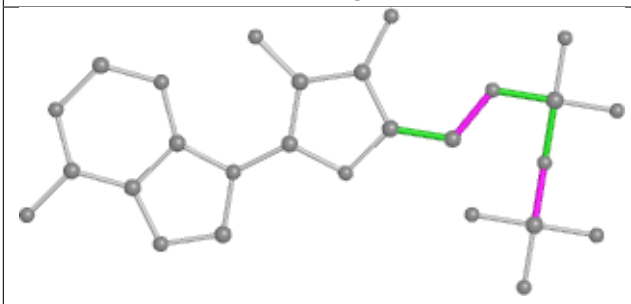
Ligand ADP C 1300



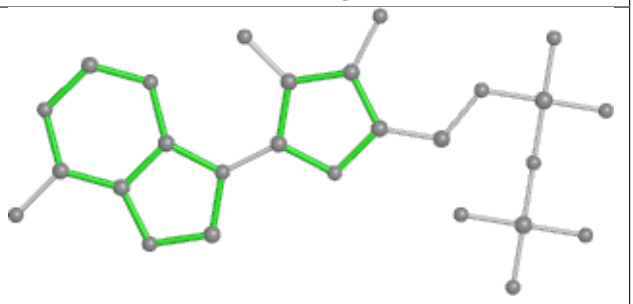
Bond lengths



Bond angles

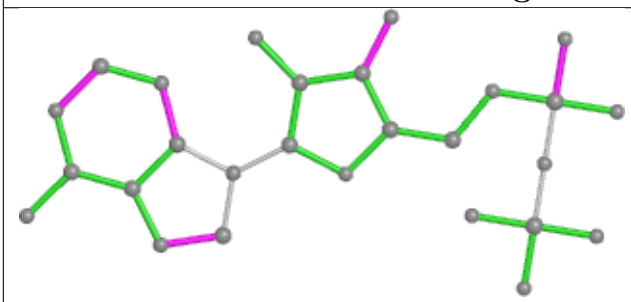


Torsions

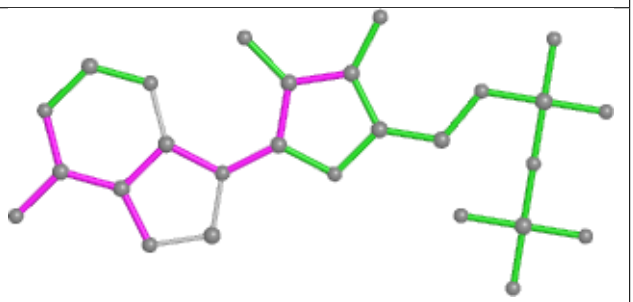


Rings

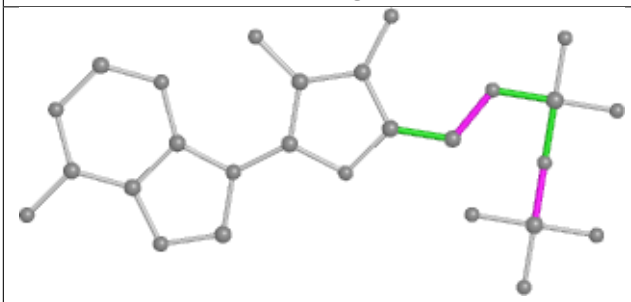
Ligand ADP B 1300



Bond lengths



Bond angles



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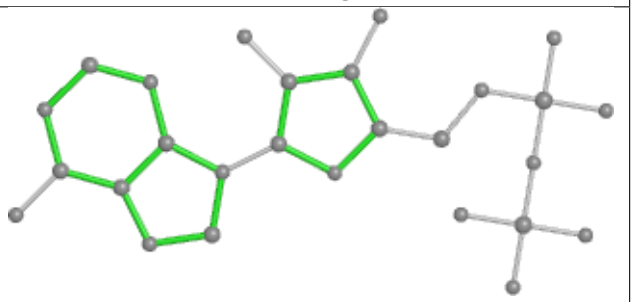
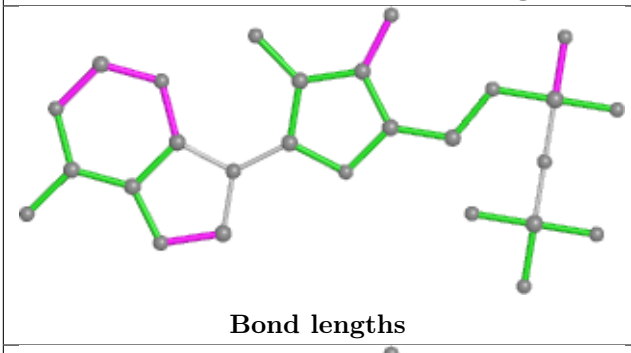
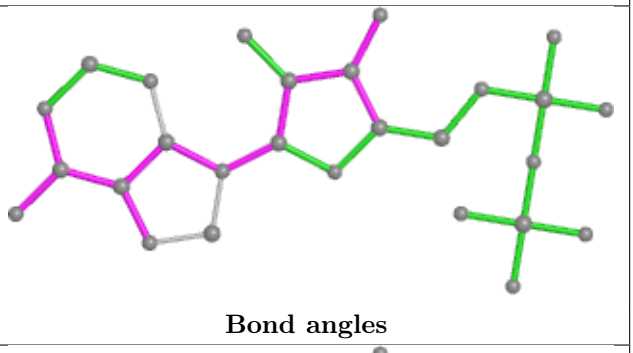


Rings

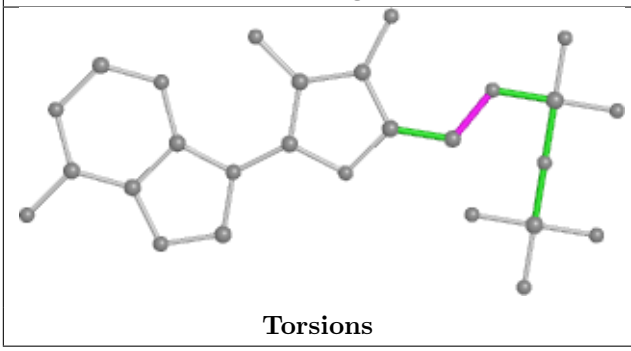
Ligand ADP E 1299



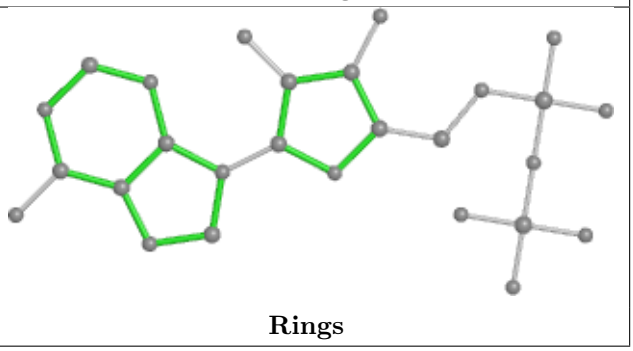
Bond lengths



Bond angles

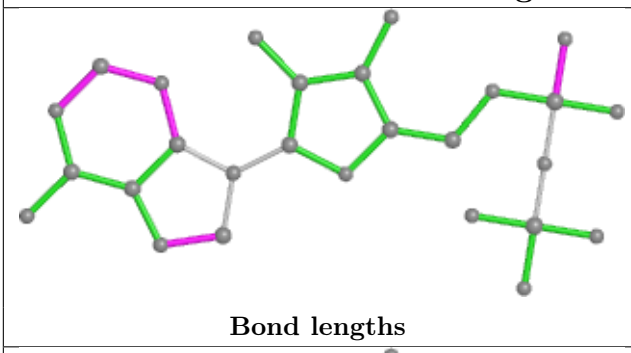


Torsions

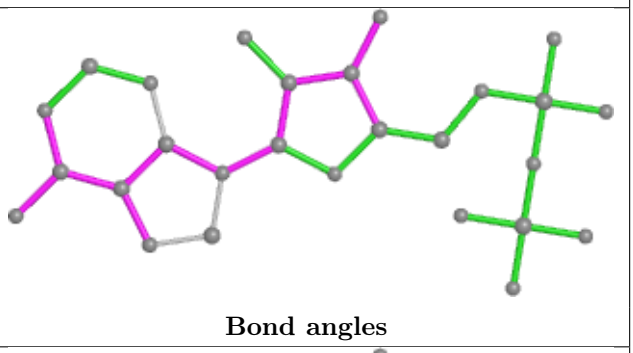


Rings

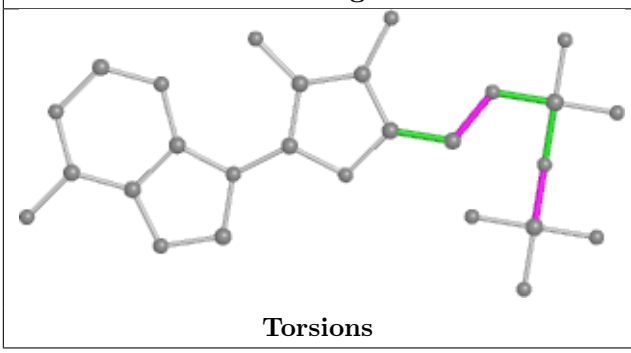
Ligand ADP L 1300



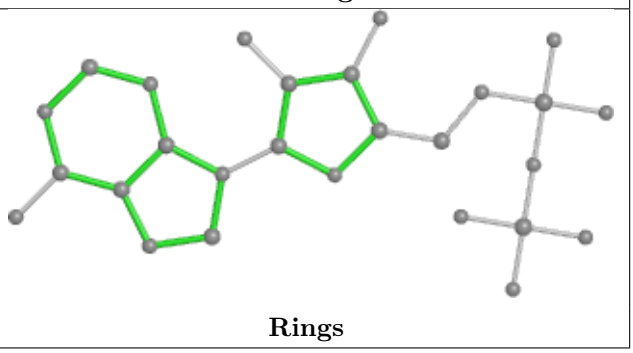
Bond lengths



Bond angles

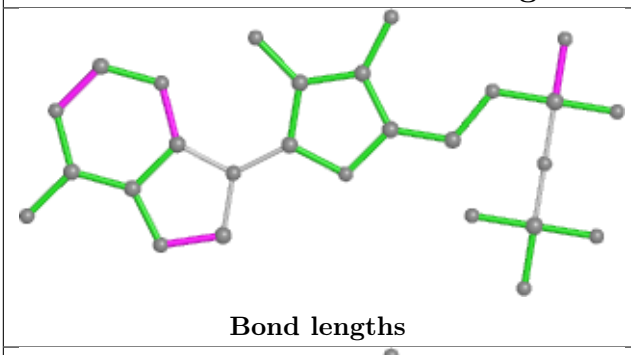


Torsions

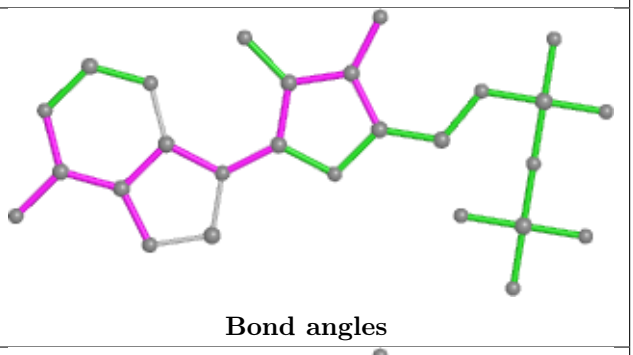


Rings

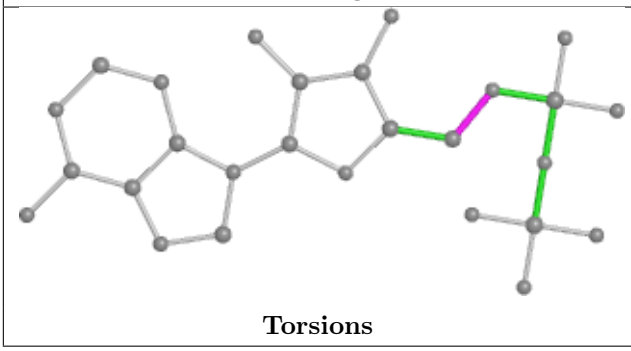
Ligand ADP I 1298



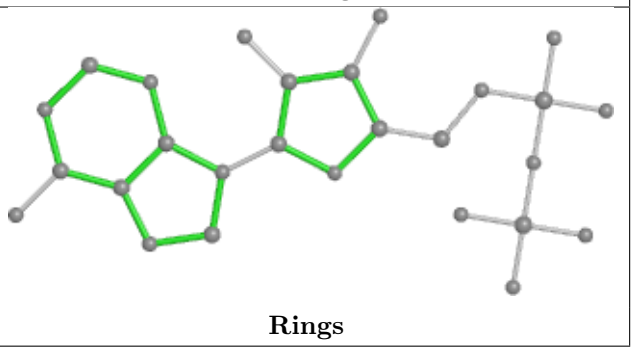
Bond lengths



Bond angles

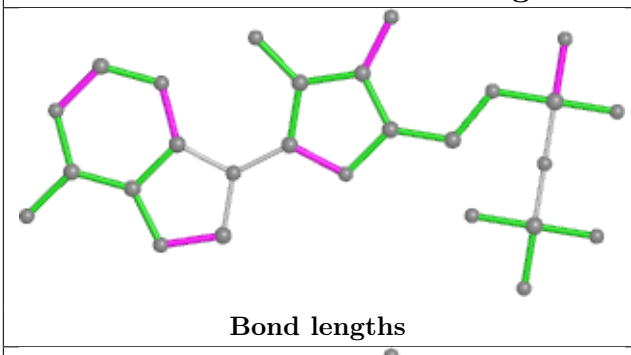


Torsions

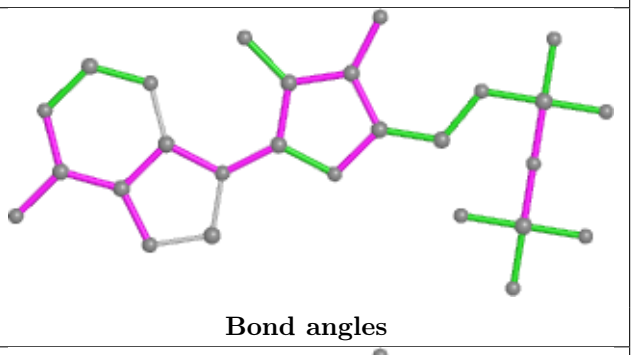


Rings

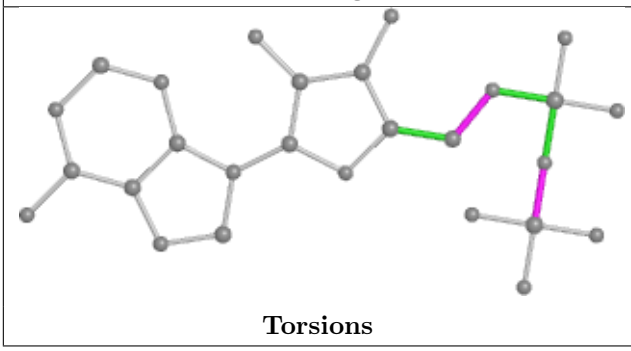
Ligand ADP H 1297



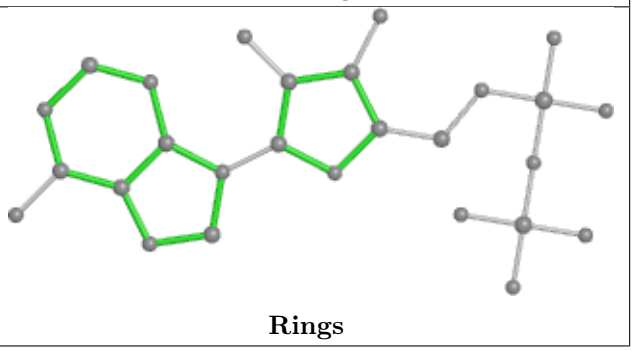
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

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, 95^{th} 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	292/300 (97%)	0.29	8 (2%) 54 38	28, 67, 120, 133	0
1	B	297/300 (99%)	0.27	8 (2%) 54 38	31, 63, 103, 130	0
1	C	299/300 (99%)	0.16	1 (0%) 94 87	21, 47, 92, 115	0
1	D	295/300 (98%)	0.20	1 (0%) 94 87	17, 46, 88, 132	0
1	E	288/300 (96%)	0.44	16 (5%) 24 15	52, 82, 128, 158	0
1	F	292/300 (97%)	0.54	22 (7%) 14 8	45, 90, 139, 157	0
1	G	298/300 (99%)	0.54	25 (8%) 11 6	49, 87, 124, 155	0
1	H	296/300 (98%)	0.74	36 (12%) 4 2	53, 106, 135, 142	0
1	I	289/300 (96%)	0.45	14 (4%) 30 19	45, 84, 123, 147	0
1	J	280/300 (93%)	1.28	74 (26%) 0 0	80, 126, 157, 164	0
1	K	274/300 (91%)	1.93	108 (39%) 0 0	106, 140, 161, 167	0
1	L	294/300 (98%)	0.82	33 (11%) 5 3	69, 102, 131, 151	0
All	All	3494/3600 (97%)	0.63	346 (9%) 7 4	17, 85, 147, 167	0

The worst 5 of 346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	2	THR	10.4
1	K	293	THR	10.3
1	K	3	LEU	10.2
1	K	213	LYS	9.7
1	K	68	GLY	8.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
2	NLG	F	1300	13/13	0.38	1.05	119,119,120,120	13
2	NLG	K	1298	13/13	0.57	0.97	100,101,102,103	13
2	NLG	H	1299	13/13	0.64	0.51	115,116,118,118	13
3	ADP	J	1298	27/27	0.64	0.37	123,124,125,125	27
3	ADP	H	1297	27/27	0.67	0.42	120,121,122,122	27
5	CL	L	1303	1/1	0.67	0.26	100,100,100,100	0
5	CL	G	1302	1/1	0.71	0.22	92,92,92,92	0
2	NLG	L	1302	13/13	0.71	0.35	108,110,112,112	0
2	NLG	G	1301	13/13	0.75	0.30	91,95,99,99	13
4	MG	H	1298	1/1	0.78	0.13	94,94,94,94	0
5	CL	H	1300	1/1	0.80	0.10	97,97,97,97	0
4	MG	C	1301	1/1	0.82	0.28	110,110,110,110	0
4	MG	I	1299	1/1	0.85	0.17	74,74,74,74	0
4	MG	L	1301	1/1	0.86	0.27	68,68,68,68	0
4	MG	E	1300	1/1	0.86	0.29	69,69,69,69	0
3	ADP	C	1300	27/27	0.88	0.28	70,90,117,118	0
3	ADP	G	1299	27/27	0.88	0.25	83,93,120,120	0
2	NLG	I	1300	13/13	0.88	0.37	93,95,96,96	0
2	NLG	E	1301	13/13	0.90	0.34	79,83,86,86	0
2	NLG	A	1302	13/13	0.91	0.26	75,78,82,82	0
3	ADP	F	1299	27/27	0.91	0.18	103,109,124,125	0
5	CL	D	1303	1/1	0.91	0.24	86,86,86,86	0
2	NLG	D	1302	13/13	0.92	0.34	56,58,61,64	0
3	ADP	L	1300	27/27	0.93	0.19	68,76,90,92	0
5	CL	B	1303	1/1	0.93	0.18	82,82,82,82	0
3	ADP	E	1299	27/27	0.94	0.20	55,64,77,77	0
2	NLG	B	1302	13/13	0.94	0.24	57,64,66,68	0
3	ADP	I	1298	27/27	0.94	0.20	48,53,82,84	0
4	MG	D	1301	1/1	0.95	0.21	56,56,56,56	0
3	ADP	B	1300	27/27	0.96	0.18	62,68,71,72	0
3	ADP	D	1300	27/27	0.97	0.18	43,48,58,59	0
5	CL	C	1302	1/1	0.97	0.12	84,84,84,84	0

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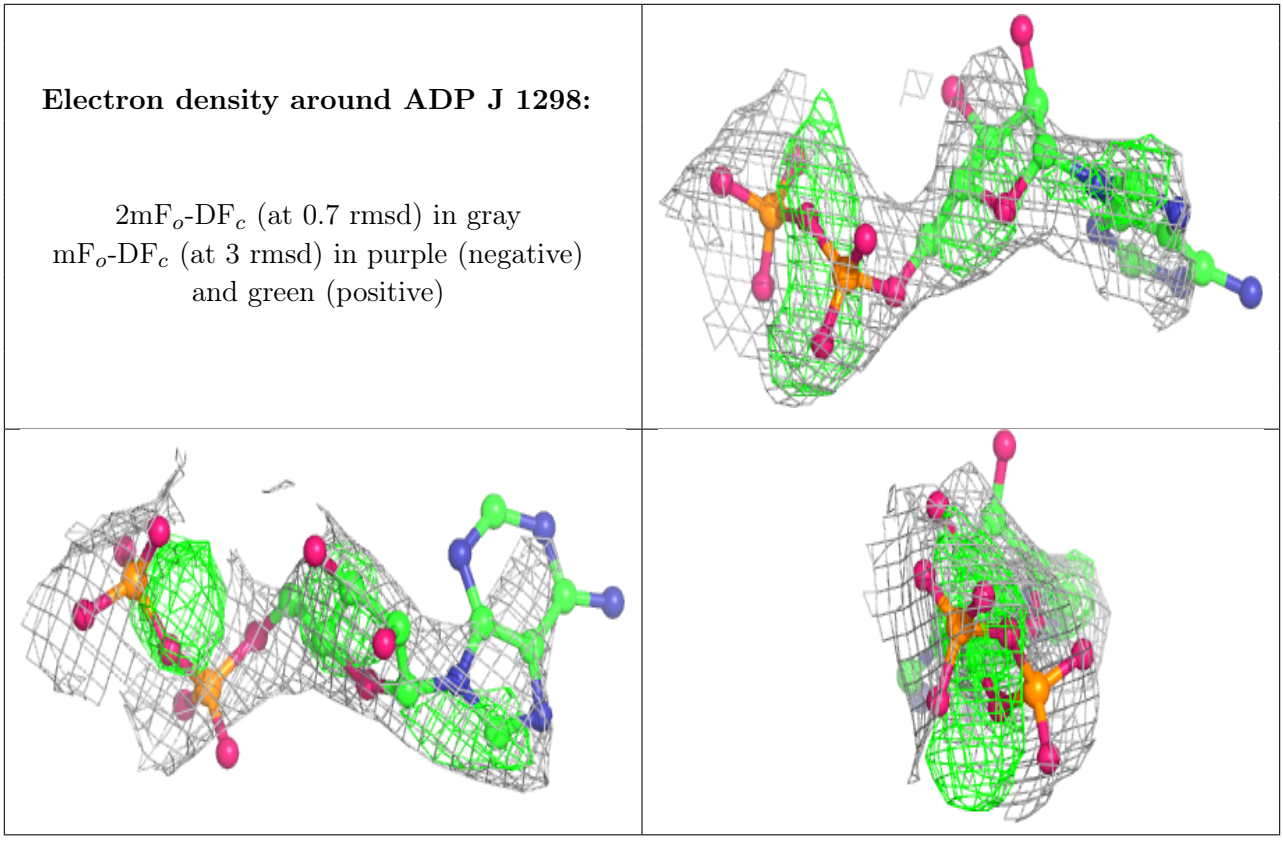
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	G	1300	1/1	0.98	0.20	85,85,85,85	0
4	MG	B	1301	1/1	0.98	0.32	50,50,50,50	0

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.

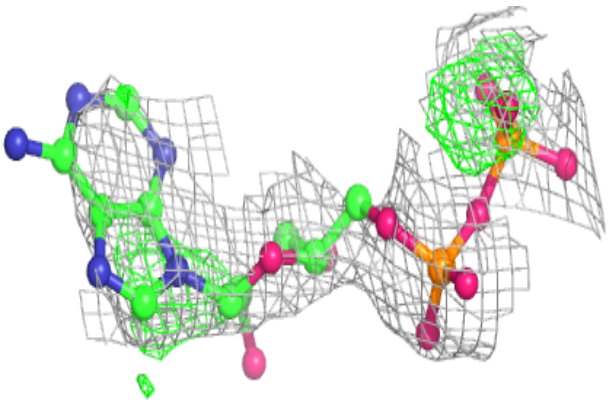
Electron density around ADP J 1298:

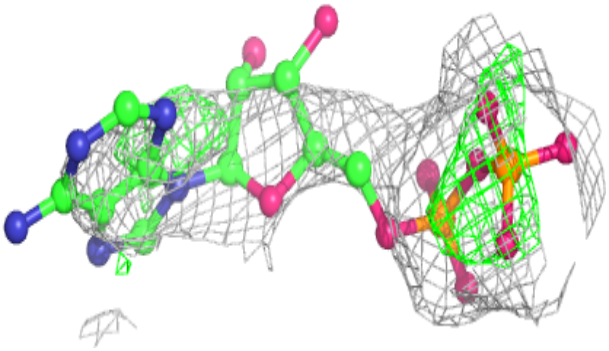
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

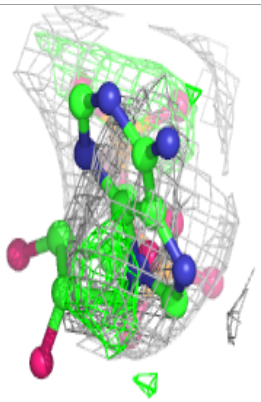


Electron density around ADP H 1297:

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

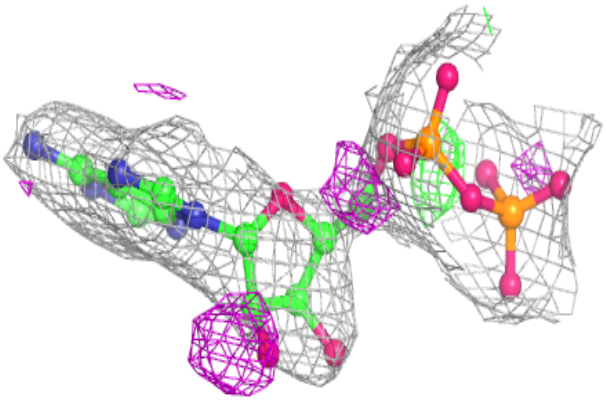


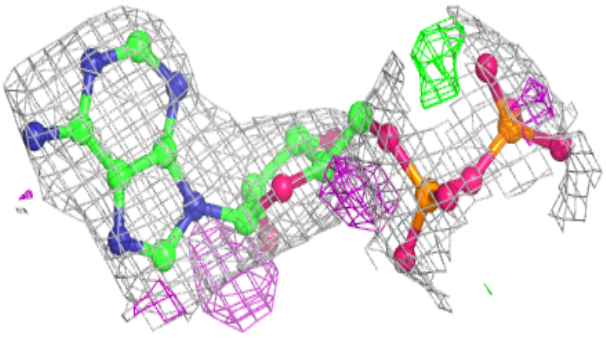


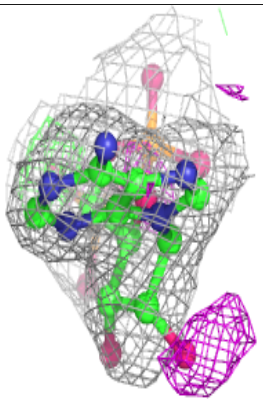


Electron density around ADP C 1300:

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

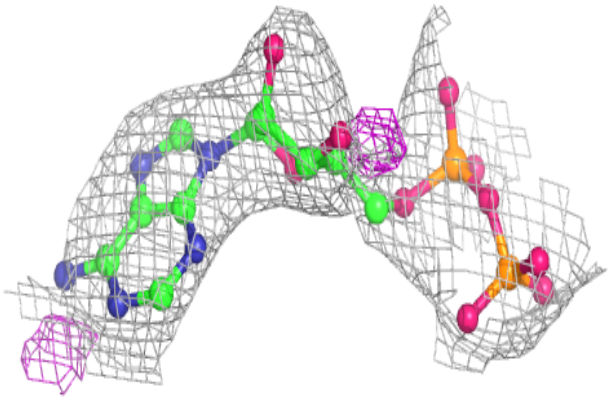


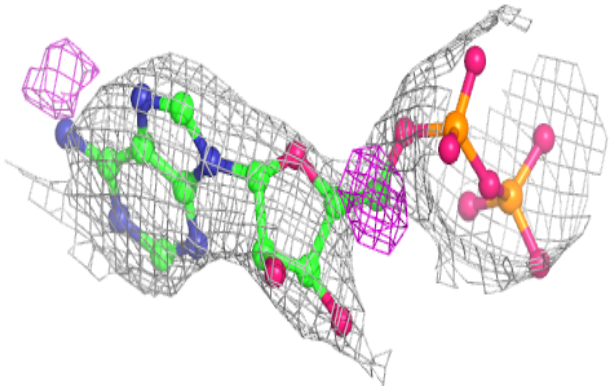


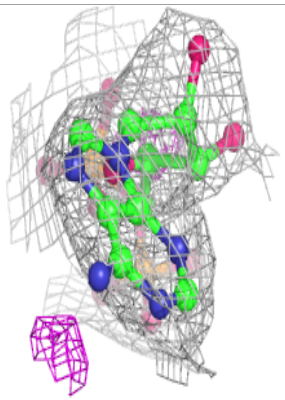


Electron density around ADP G 1299:

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

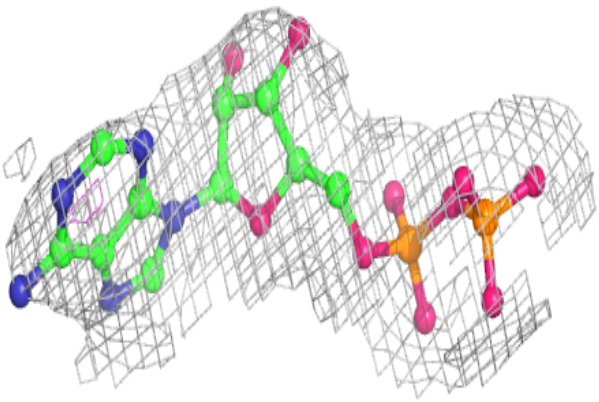


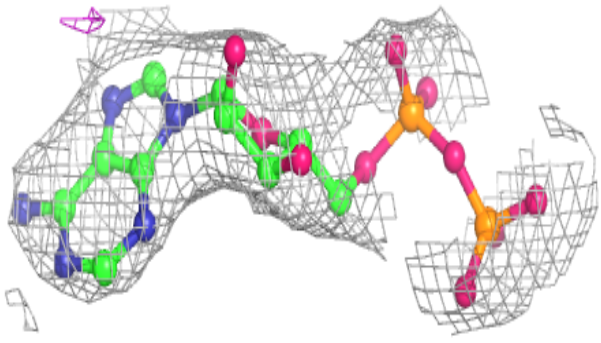


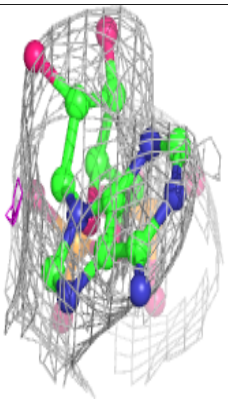


Electron density around ADP F 1299:

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

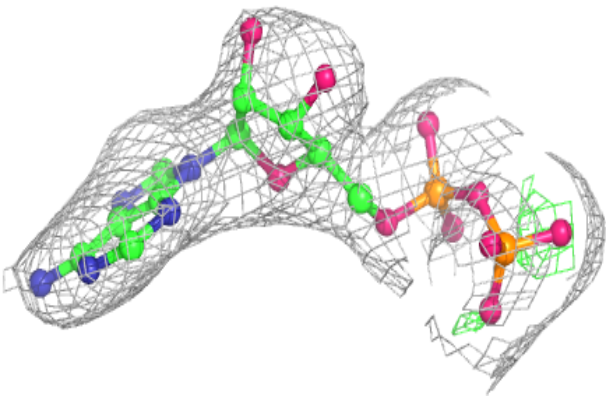


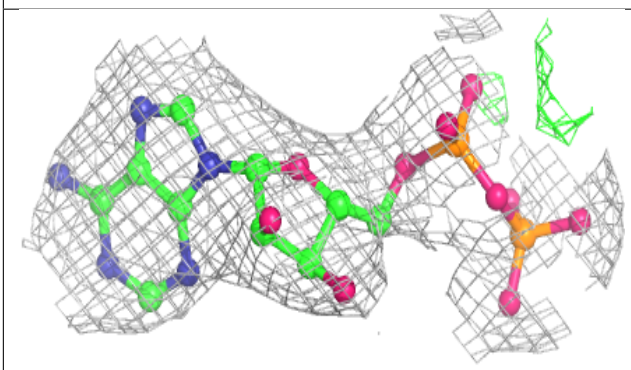


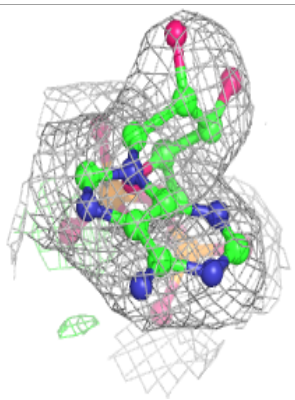


Electron density around ADP L 1300:

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

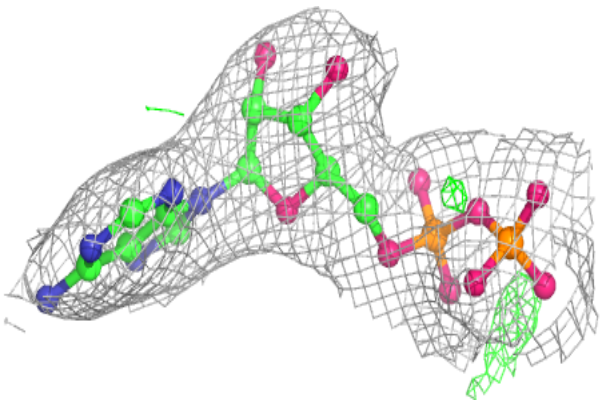


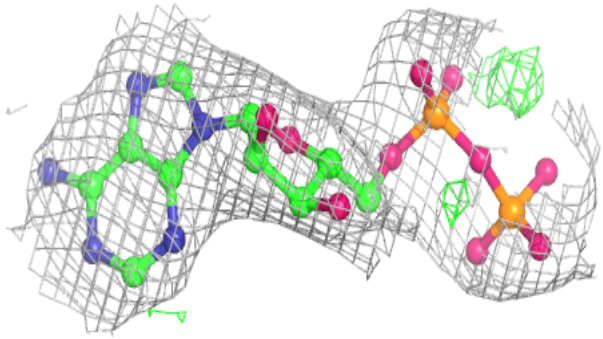


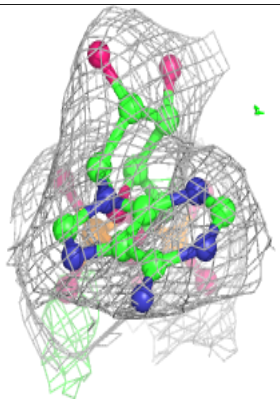


Electron density around ADP E 1299:

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

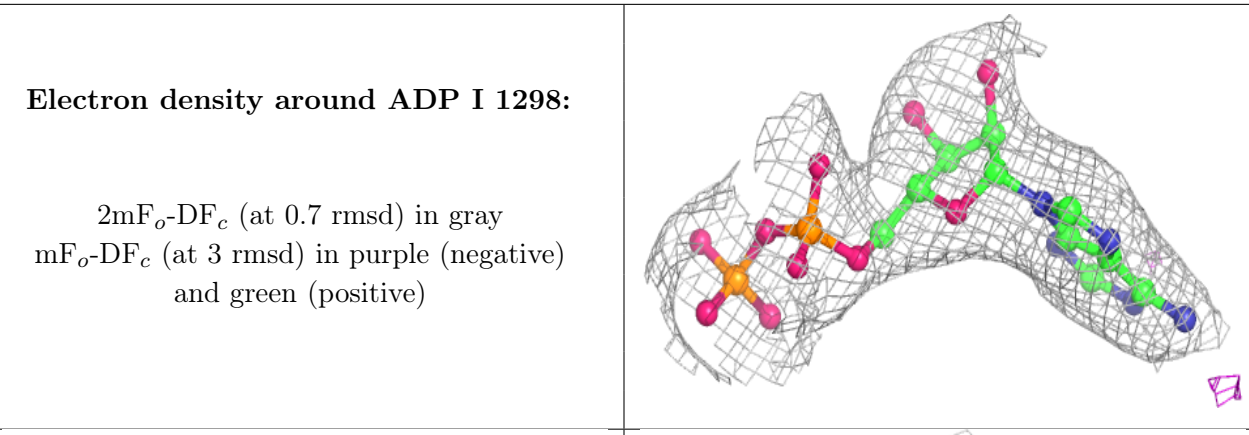






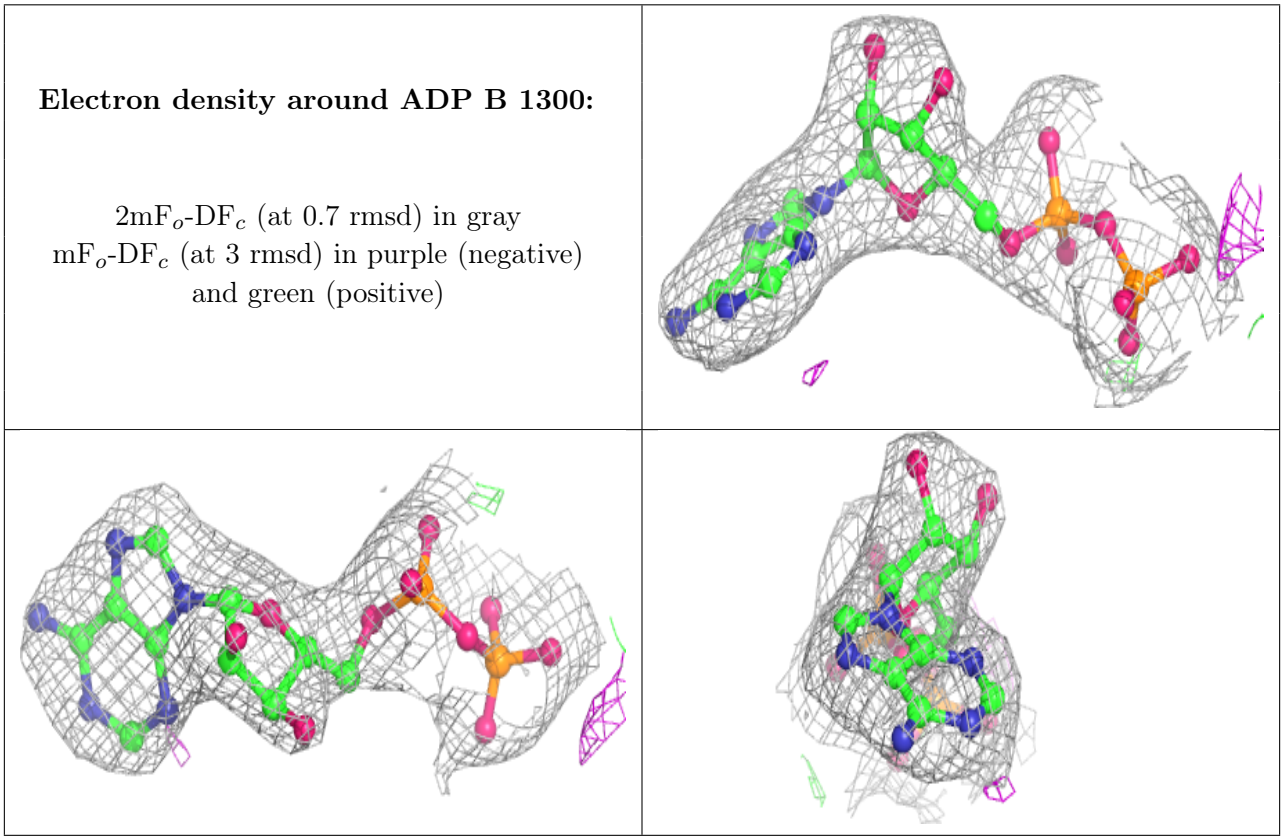
Electron density around ADP I 1298:

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



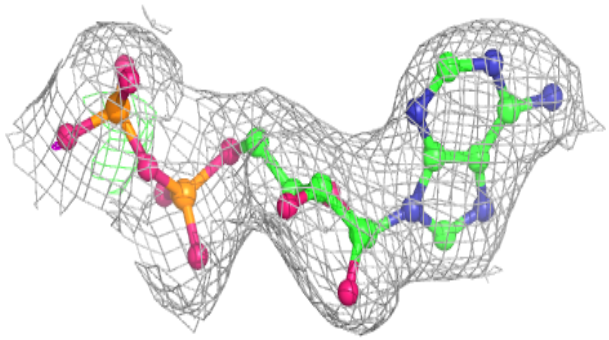
Electron density around ADP B 1300:

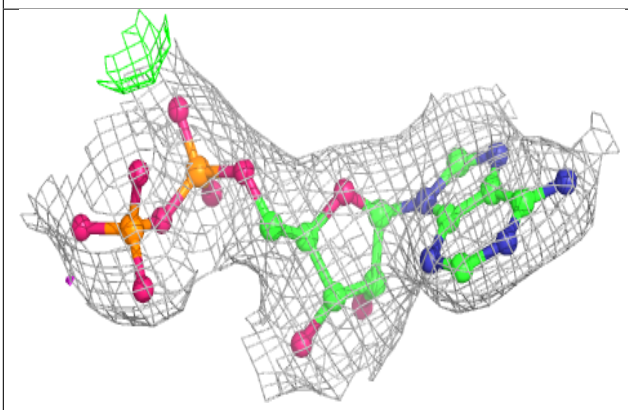
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

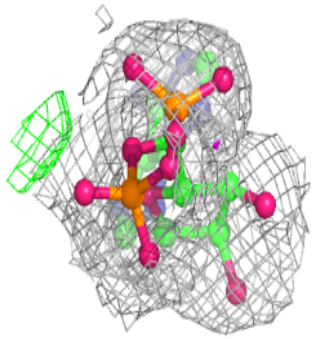


Electron density around ADP D 1300:

$2mF_o$-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.