Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 09:17 AM EST

PDB ID	:	4FBP
Title	:	CONFORMATIONAL TRANSITION OF FRUCTOSE-1,6-BISPHOSPHATASE: STRUCTURE COMPARISON BETWEEN THE AMP COMPLEX (T FORM) AND THE FRUCTOSE 6-PHOSPHATE COMPLEX (R FORM)
Authors	:	Ke, H.; Zhang, Y.; Liang, J.-Y.; Lipscomb, W.N.
Deposited on	:	1991-02-11
Resolution	:	2.50 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 (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 (1)) were used in the production of this report:

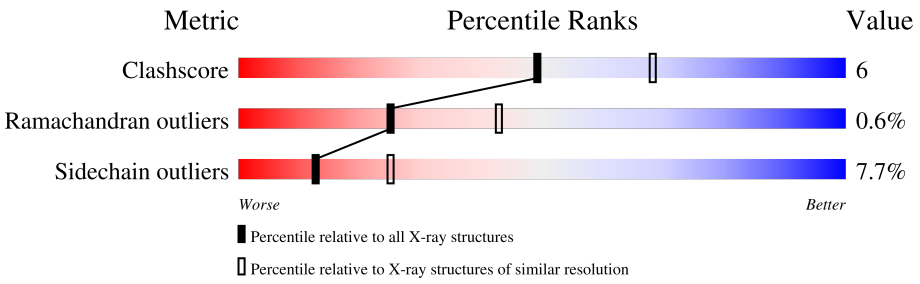
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	335	75% 18% • • 5%
1	B	335	73% 18% • • 5%
1	C	335	70% 20% • 5%
1	D	335	71% 21% • • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12988 atoms, of which 2840 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.

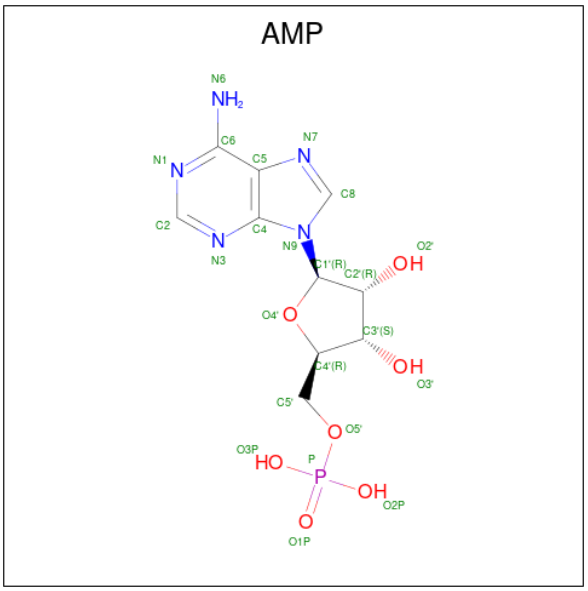
- Molecule 1 is a protein called FRUCTOSE 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	318	2963	1546	536	410	456	15	0	0	1
1	B	318	2963	1546	536	410	456	15	0	0	1
1	C	318	2963	1546	536	410	456	15	0	0	1
1	D	318	2963	1546	536	410	456	15	0	0	1

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	conflict	UNP P00636
A	96	THR	SER	conflict	UNP P00636
A	199	ASN	ASP	conflict	UNP P00636
B	20	GLN	GLU	conflict	UNP P00636
B	96	THR	SER	conflict	UNP P00636
B	199	ASN	ASP	conflict	UNP P00636
C	20	GLN	GLU	conflict	UNP P00636
C	96	THR	SER	conflict	UNP P00636
C	199	ASN	ASP	conflict	UNP P00636
D	20	GLN	GLU	conflict	UNP P00636
D	96	THR	SER	conflict	UNP P00636
D	199	ASN	ASP	conflict	UNP P00636

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
2	B	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
2	C	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
2	D	1	23	10	5	7	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	A	98	294	196	98	0	0
			Total	H	O		
3	B	81	243	162	81	0	0
			Total	H	O		
3	C	81	243	162	81	0	0
			Total	H	O		
3	D	88	264	176	88	0	0

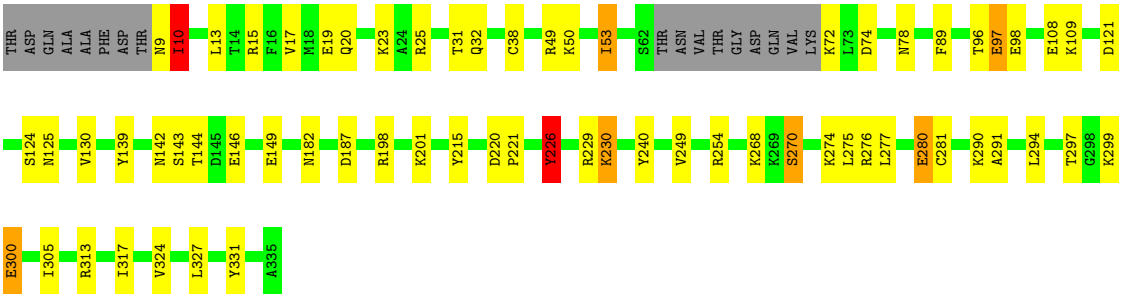
3 Residue-property plots (i)

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.

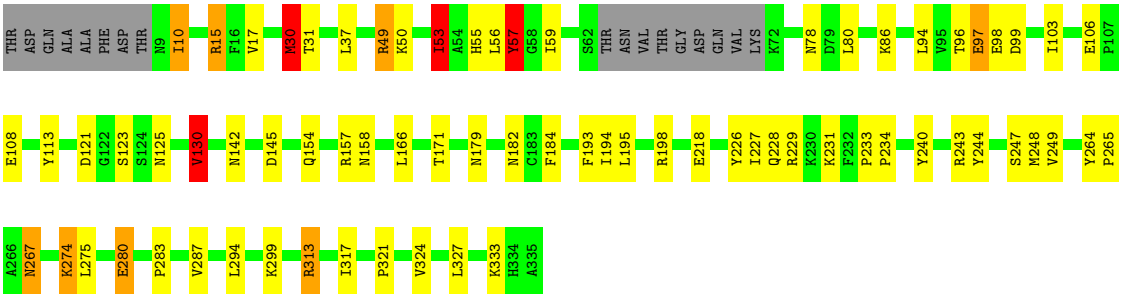
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain A:



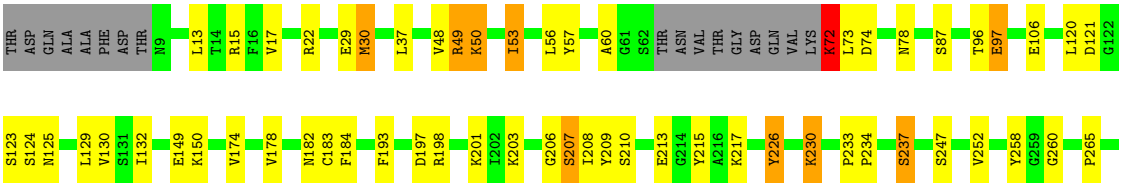
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain B:



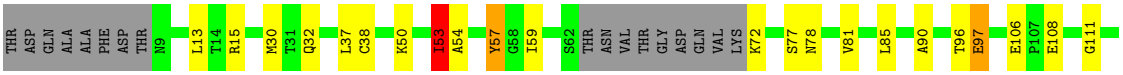
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain C:



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain D:



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	78.50Å 88.50Å 211.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12988	wwPDB-VP
Average B, all atoms ($Å^2$)	17.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP

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	0.74	0/2468	1.41	15/3337 (0.4%)
1	B	0.74	0/2468	1.43	18/3337 (0.5%)
1	C	0.73	0/2468	1.40	16/3337 (0.5%)
1	D	0.70	0/2468	1.35	18/3337 (0.5%)
All	All	0.73	0/9872	1.40	67/13348 (0.5%)

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	A	0	3
1	B	0	5
1	C	0	4
1	D	0	4
All	All	0	16

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	254	ARG	NE-CZ-NH2	-15.13	112.73	120.30
1	C	49	ARG	NE-CZ-NH2	-13.95	113.33	120.30
1	B	49	ARG	NE-CZ-NH2	-13.62	113.49	120.30
1	B	313	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	C	15	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	A	254	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	D	254	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	D	254	ARG	NE-CZ-NH1	9.15	124.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	313	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	C	72	LYS	CA-CB-CG	8.17	131.38	113.40
1	A	215	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	B	49	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	C	30	MET	CG-SD-CE	-7.95	87.48	100.20
1	B	30	MET	CG-SD-CE	-7.89	87.58	100.20
1	D	243	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	D	15	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	B	15	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	49	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	229	ARG	CB-CG-CD	-6.85	93.79	111.60
1	C	215	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	A	15	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	280	GLU	OE1-CD-OE2	-6.60	115.38	123.30
1	A	229	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	C	30	MET	CA-CB-CG	-6.40	102.42	113.30
1	B	53	ILE	CB-CA-C	-6.32	98.96	111.60
1	A	49	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	249	VAL	CG1-CB-CG2	-6.24	100.92	110.90
1	A	19	GLU	CA-CB-CG	-6.22	99.72	113.40
1	D	106	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	D	198	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	217	LYS	CA-CB-CG	6.12	126.86	113.40
1	D	240	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	149	GLU	CA-CB-CG	5.99	126.58	113.40
1	C	217	LYS	CA-CB-CG	5.98	126.56	113.40
1	A	331	TYR	CB-CG-CD1	-5.86	117.49	121.00
1	D	53	ILE	CB-CA-C	-5.85	99.90	111.60
1	C	22	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	247	SER	N-CA-C	-5.74	95.51	111.00
1	D	140	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	49	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	130	VAL	CA-CB-CG2	-5.65	102.42	110.90
1	A	226	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	B	229	ARG	N-CA-CB	-5.59	100.54	110.60
1	A	10	ILE	CA-CB-CG2	-5.59	99.73	110.90
1	A	249	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	C	322	GLU	CA-CB-CG	-5.55	101.19	113.40
1	A	280	GLU	OE1-CD-OE2	-5.53	116.66	123.30
1	D	72	LYS	CB-CG-CD	-5.48	97.35	111.60
1	B	243	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	29	GLU	OE1-CD-OE2	-5.37	116.85	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	72	LYS	CA-CB-CG	5.36	125.19	113.40
1	D	197	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	22	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	17	VAL	CG1-CB-CG2	-5.23	102.54	110.90
1	B	267	ASN	CA-C-N	5.22	128.69	117.20
1	D	268	LYS	CA-C-N	-5.21	105.73	117.20
1	B	157	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	57	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	C	53	ILE	CB-CA-C	-5.18	101.23	111.60
1	D	215	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	B	228	GLN	CA-CB-CG	5.09	124.59	113.40
1	B	333	LYS	CA-CB-CG	5.06	124.53	113.40
1	C	15	ARG	CG-CD-NE	-5.06	101.18	111.80
1	D	30	MET	CA-CB-CG	-5.05	104.71	113.30
1	C	120	LEU	CA-CB-CG	5.03	126.87	115.30
1	A	300	GLU	CA-CB-CG	5.02	124.45	113.40
1	D	258	TYR	CB-CG-CD1	-5.01	117.99	121.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
1	A	226	TYR	Sidechain
1	A	240	TYR	Sidechain
1	B	226	TYR	Sidechain
1	B	240	TYR	Sidechain
1	B	244	TYR	Sidechain
1	B	264	TYR	Sidechain
1	B	57	TYR	Sidechain
1	C	209	TYR	Sidechain
1	C	226	TYR	Sidechain
1	C	258	TYR	Sidechain
1	C	57	TYR	Sidechain
1	D	215	TYR	Sidechain
1	D	258	TYR	Sidechain
1	D	264	TYR	Sidechain
1	D	57	TYR	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	2427	536	2486	27	0
1	B	2427	536	2486	34	0
1	C	2427	536	2486	33	0
1	D	2427	536	2486	33	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	98	196	0	0	0
3	B	81	162	0	0	0
3	C	81	162	0	2	0
3	D	88	176	0	2	0
All	All	10148	2840	9992	117	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 6.

All (117) 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:125:ASN:HB3	1:B:130:VAL:HG12	1.57	0.85
1:D:126:ILE:HG12	1:D:132:ILE:HD13	1.70	0.73
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.70	0.72
1:B:274:LYS:HD3	1:B:275:LEU:HD23	1.74	0.69
1:B:78:ASN:OD1	1:B:96:THR:HG21	1.94	0.68
1:B:218:GLU:HB3	1:B:267:ASN:HB2	1.74	0.68
1:A:17:VAL:HG12	1:A:31:THR:HG23	1.80	0.63
1:C:125:ASN:HB3	1:C:130:VAL:HB	1.79	0.63
1:B:184:PHE:HB3	1:B:193:PHE:HB3	1.81	0.62
1:D:125:ASN:HB3	1:D:130:VAL:HB	1.82	0.61
1:C:206:GLY:HA3	1:C:260:GLY:HA2	1.85	0.59
1:A:277:LEU:HA	1:A:281:CYS:HB2	1.85	0.59
1:D:270:SER:HB2	1:D:272:LYS:HG3	1.85	0.58
1:C:203:LYS:O	1:C:320:SER:HB3	2.03	0.58
1:D:37:LEU:HD13	1:D:85:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASN:HD22	1:B:198:ARG:HA	1.70	0.57
1:C:182:ASN:HD22	1:C:198:ARG:HA	1.70	0.56
1:C:97:GLU:HG2	1:C:279:TYR:CE1	2.41	0.56
1:A:13:LEU:HD23	1:A:38:CYS:SG	2.46	0.56
1:C:72:LYS:HB2	1:C:74:ASP:OD1	2.05	0.56
1:B:317:ILE:HG21	1:B:327:LEU:HD23	1.88	0.55
1:C:252:VAL:HG11	1:C:284:MET:SD	2.47	0.55
1:A:10:ILE:HG23	1:B:57:TYR:HB3	1.90	0.54
1:B:294:LEU:HB2	1:B:324:VAL:HG11	1.89	0.53
1:D:294:LEU:HD12	1:D:324:VAL:HB	1.90	0.53
1:C:213:GLU:HB3	1:D:231:LYS:HZ2	1.74	0.53
1:D:97:GLU:HG2	1:D:279:TYR:CE1	2.44	0.52
1:A:10:ILE:CG2	1:B:57:TYR:HB3	2.39	0.52
1:A:50:LYS:HB3	1:A:53:ILE:HG12	1.92	0.52
1:C:78:ASN:OD1	1:C:96:THR:HG21	2.10	0.51
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.10	0.51
1:C:297:THR:HG21	1:C:305:ILE:HD11	1.93	0.51
1:A:317:ILE:HG21	1:A:327:LEU:HD23	1.92	0.50
1:D:184:PHE:HB3	1:D:193:PHE:HB3	1.93	0.50
1:C:213:GLU:HB3	1:D:231:LYS:NZ	2.27	0.50
1:B:17:VAL:HG12	1:B:31:THR:HG23	1.94	0.50
1:A:297:THR:HG21	1:A:305:ILE:HD11	1.94	0.50
1:C:13:LEU:HB2	1:C:193:PHE:HB2	1.93	0.49
1:C:326:GLU:O	1:C:329:GLU:HG3	2.12	0.49
1:D:78:ASN:OD1	1:D:96:THR:HG21	2.11	0.49
1:C:268:LYS:NZ	3:C:517:HOH:O	2.45	0.49
1:B:50:LYS:O	1:B:53:ILE:HG13	2.12	0.49
1:B:294:LEU:HG	1:B:321:PRO:HA	1.94	0.49
1:B:283:PRO:O	1:B:287:VAL:HG23	2.13	0.49
1:D:201:LYS:HG2	1:D:291:ALA:O	2.13	0.49
1:C:184:PHE:HB3	1:C:193:PHE:HB3	1.94	0.49
1:C:129:LEU:HD11	1:D:172:MET:HB2	1.94	0.48
1:C:230:LYS:HD2	1:C:230:LYS:N	2.28	0.48
1:C:97:GLU:HG2	1:C:279:TYR:HE1	1.78	0.48
1:D:226:TYR:HB2	1:D:327:LEU:HD13	1.94	0.48
1:D:297:THR:HG23	1:D:315:PRO:HD2	1.95	0.47
1:A:96:THR:HG22	1:A:98:GLU:H	1.79	0.47
1:A:187:ASP:HB2	1:B:53:ILE:HD12	1.96	0.47
1:D:268:LYS:N	1:D:268:LYS:HD2	2.30	0.47
1:A:276:ARG:HA	1:A:313:ARG:HA	1.97	0.47
1:D:276:ARG:HB2	1:D:280:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:CZ	1:A:230:LYS:HD3	2.50	0.47
1:A:274:LYS:HD3	1:A:275:LEU:HD23	1.96	0.47
1:B:154:GLN:HE21	1:B:158:ASN:HD22	1.63	0.47
1:B:294:LEU:HD12	1:B:324:VAL:HB	1.97	0.46
1:D:77:SER:O	1:D:81:VAL:HG23	2.16	0.46
1:D:172:MET:HG3	1:D:184:PHE:O	2.15	0.46
1:D:204:LYS:NZ	1:D:322:GLU:OE2	2.49	0.46
1:C:233:PRO:HA	1:C:234:PRO:HD3	1.77	0.46
1:B:80:LEU:HG	1:C:60:ALA:HB2	1.97	0.46
1:D:13:LEU:HD23	1:D:38:CYS:SG	2.56	0.46
1:C:48:VAL:HA	1:C:73:LEU:HD21	1.98	0.46
1:A:96:THR:HG22	1:A:97:GLU:N	2.31	0.45
1:B:10:ILE:HD11	1:B:194:ILE:HG12	1.98	0.45
1:B:55:HIS:HA	1:B:59:ILE:HG22	1.98	0.45
1:A:23:LYS:O	1:A:25:ARG:NH1	2.49	0.45
1:B:94:LEU:HB2	1:B:103:ILE:HB	1.99	0.45
1:A:10:ILE:HD11	1:B:59:ILE:HB	1.98	0.45
1:D:50:LYS:NZ	3:D:514:HOH:O	2.49	0.45
1:A:182:ASN:HD22	1:A:198:ARG:HA	1.81	0.45
1:B:166:LEU:O	1:B:171:THR:HA	2.17	0.45
1:D:146:GLU:HA	1:D:147:PRO:HD2	1.78	0.45
1:C:276:ARG:HB2	1:C:280:GLU:OE1	2.17	0.45
1:A:276:ARG:HD3	1:A:280:GLU:OE1	2.17	0.44
1:B:96:THR:HG22	1:B:98:GLU:H	1.81	0.44
1:A:32:GLN:HE21	1:A:32:GLN:HA	1.81	0.44
1:A:294:LEU:HD12	1:A:324:VAL:HB	1.98	0.44
1:D:201:LYS:HG3	3:D:482:HOH:O	2.15	0.44
1:C:206:GLY:HA3	1:C:260:GLY:CA	2.48	0.44
1:D:288:MET:HG3	1:D:318:LEU:HB2	1.99	0.44
1:C:201:LYS:HA	1:C:291:ALA:O	2.17	0.43
1:C:269:LYS:O	1:C:270:SER:HB2	2.18	0.43
1:D:54:ALA:HB1	1:D:59:ILE:HD12	1.99	0.43
1:B:30:MET:HG3	1:B:113:TYR:CZ	2.54	0.43
1:C:294:LEU:HD12	1:C:321:PRO:HA	2.00	0.43
1:A:89:PHE:HA	1:A:109:LYS:O	2.19	0.43
1:B:227:ILE:HG22	1:B:231:LYS:HE3	2.00	0.43
1:C:328:LEU:HD23	1:C:328:LEU:HA	1.87	0.43
1:B:15:ARG:HA	1:D:32:GLN:HE22	1.84	0.43
1:B:96:THR:HB	1:B:99:ASP:H	1.84	0.42
1:A:9:ASN:HD22	1:C:87:SER:HA	1.84	0.42
1:B:248:MET:SD	1:B:280:GLU:HB3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LYS:HZ3	1:B:106:GLU:CD	2.22	0.42
1:C:50:LYS:NZ	3:C:405:HOH:O	2.49	0.42
1:C:174:VAL:HG22	1:C:183:CYS:SG	2.60	0.42
1:B:96:THR:HG22	1:B:97:GLU:N	2.34	0.42
1:D:114:VAL:HB	1:D:139:TYR:HB2	2.00	0.42
1:C:125:ASN:HD22	1:C:247:SER:HB3	1.85	0.42
1:D:97:GLU:HG2	1:D:279:TYR:HE1	1.85	0.42
1:B:195:LEU:HD21	1:B:198:ARG:HG2	2.01	0.42
1:B:50:LYS:HB3	1:B:53:ILE:HG12	2.02	0.41
1:D:53:ILE:O	1:D:57:TYR:HD1	2.04	0.41
1:C:226:TYR:HB2	1:C:327:LEU:HD13	2.02	0.41
1:A:220:ASP:HB2	1:A:221:PRO:HD2	2.02	0.41
1:B:233:PRO:HA	1:B:234:PRO:HD3	1.72	0.41
1:D:90:ALA:HA	1:D:111:GLY:HA3	2.03	0.41
1:D:306:VAL:HA	1:D:307:PRO:HD3	1.93	0.40
1:A:201:LYS:HA	1:A:291:ALA:O	2.22	0.40
1:C:282:ASN:HD22	1:C:303:LEU:HD23	1.86	0.40
1:D:233:PRO:HA	1:D:234:PRO:HD2	1.93	0.40
1:A:290:LYS:HD3	1:A:290:LYS:HA	1.88	0.40
1:D:166:LEU:HD13	1:D:249:VAL:HG12	2.03	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	314/335 (94%)	297 (95%)	15 (5%)	2 (1%)	25 43
1	B	314/335 (94%)	302 (96%)	12 (4%)	0	100 100
1	C	314/335 (94%)	294 (94%)	16 (5%)	4 (1%)	12 21
1	D	314/335 (94%)	295 (94%)	17 (5%)	2 (1%)	25 43
All	All	1256/1340 (94%)	1188 (95%)	60 (5%)	8 (1%)	25 43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	270	SER
1	C	237	SER
1	A	268	LYS
1	C	207	SER
1	C	178	VAL
1	D	270	SER
1	D	271	PRO
1	A	270	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	263/278 (95%)	246 (94%)	17 (6%)	17 33
1	B	263/278 (95%)	244 (93%)	19 (7%)	14 28
1	C	263/278 (95%)	235 (89%)	28 (11%)	6 13
1	D	263/278 (95%)	246 (94%)	17 (6%)	17 33
All	All	1052/1112 (95%)	971 (92%)	81 (8%)	13 25

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	20	GLN
1	A	53	ILE
1	A	72	LYS
1	A	74	ASP
1	A	97	GLU
1	A	108	GLU
1	A	121	ASP
1	A	124	SER
1	A	142	ASN
1	A	143	SER
1	A	144	THR

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Mol	Chain	Res	Type
1	A	146	GLU
1	A	230	LYS
1	A	270	SER
1	A	299	LYS
1	A	300	GLU
1	B	10	ILE
1	B	30	MET
1	B	37	LEU
1	B	49	ARG
1	B	53	ILE
1	B	56	LEU
1	B	97	GLU
1	B	108	GLU
1	B	121	ASP
1	B	123	SER
1	B	130	VAL
1	B	142	ASN
1	B	145	ASP
1	B	179	ASN
1	B	247	SER
1	B	265	PRO
1	B	274	LYS
1	B	299	LYS
1	B	313	ARG
1	C	30	MET
1	C	37	LEU
1	C	49	ARG
1	C	50	LYS
1	C	53	ILE
1	C	56	LEU
1	C	72	LYS
1	C	97	GLU
1	C	106	GLU
1	C	121	ASP
1	C	123	SER
1	C	124	SER
1	C	132	ILE
1	C	149	GLU
1	C	150	LYS
1	C	197	ASP
1	C	207	SER
1	C	208	ILE

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Mol	Chain	Res	Type
1	C	210	SER
1	C	230	LYS
1	C	237	SER
1	C	265	PRO
1	C	269	LYS
1	C	276	ARG
1	C	300	GLU
1	C	313	ARG
1	C	320	SER
1	C	329	GLU
1	D	53	ILE
1	D	97	GLU
1	D	108	GLU
1	D	121	ASP
1	D	123	SER
1	D	127	ASP
1	D	142	ASN
1	D	179	ASN
1	D	199	ASN
1	D	230	LYS
1	D	247	SER
1	D	265	PRO
1	D	270	SER
1	D	276	ARG
1	D	297	THR
1	D	300	GLU
1	D	332	GLN

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	9	ASN
1	A	32	GLN
1	A	35	ASN
1	A	142	ASN
1	A	154	GLN
1	A	182	ASN
1	A	236	ASN
1	A	282	ASN
1	B	32	GLN
1	B	35	ASN
1	B	154	GLN

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	182	ASN
1	B	282	ASN
1	C	125	ASN
1	C	154	GLN
1	C	182	ASN
1	C	282	ASN
1	D	32	GLN
1	D	35	ASN
1	D	142	ASN
1	D	182	ASN
1	D	282	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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AMP	D	338	-	22,25,25	1.14	3 (13%)	25,38,38	1.64	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AMP	C	338	-	22,25,25	1.19	3 (13%)	25,38,38	1.32	3 (12%)
2	AMP	B	338	-	22,25,25	1.08	1 (4%)	25,38,38	1.22	3 (12%)
2	AMP	A	338	-	22,25,25	1.10	1 (4%)	25,38,38	1.37	3 (12%)

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	AMP	D	338	-	-	1/6/26/26	0/3/3/3
2	AMP	C	338	-	-	0/6/26/26	0/3/3/3
2	AMP	B	338	-	-	0/6/26/26	0/3/3/3
2	AMP	A	338	-	-	0/6/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	338	AMP	C2-N3	3.45	1.37	1.32
2	C	338	AMP	C2-N3	3.33	1.37	1.32
2	A	338	AMP	C2-N3	3.26	1.37	1.32
2	B	338	AMP	C2-N3	3.21	1.37	1.32
2	C	338	AMP	C5'-C4'	-2.31	1.44	1.51
2	C	338	AMP	C2-N1	2.26	1.38	1.33
2	D	338	AMP	C2-N1	2.14	1.37	1.33
2	D	338	AMP	C5'-C4'	-2.06	1.45	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	338	AMP	N3-C2-N1	-5.12	120.68	128.68
2	A	338	AMP	N3-C2-N1	-3.73	122.86	128.68
2	C	338	AMP	N3-C2-N1	-3.52	123.18	128.68
2	D	338	AMP	C5-C6-N1	-3.47	112.49	120.35
2	B	338	AMP	O2P-P-O5'	3.31	115.53	106.73
2	D	338	AMP	C5-C6-N6	3.00	124.91	120.35
2	B	338	AMP	N3-C2-N1	-2.96	124.05	128.68
2	A	338	AMP	C5-C6-N1	-2.90	113.77	120.35
2	D	338	AMP	O2P-P-O5'	2.74	114.04	106.73
2	A	338	AMP	O2P-P-O5'	2.63	113.73	106.73
2	C	338	AMP	C5-C6-N1	-2.62	114.40	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	338	AMP	C5-C6-N1	-2.19	115.38	120.35
2	C	338	AMP	O2P-P-O5'	2.18	112.53	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

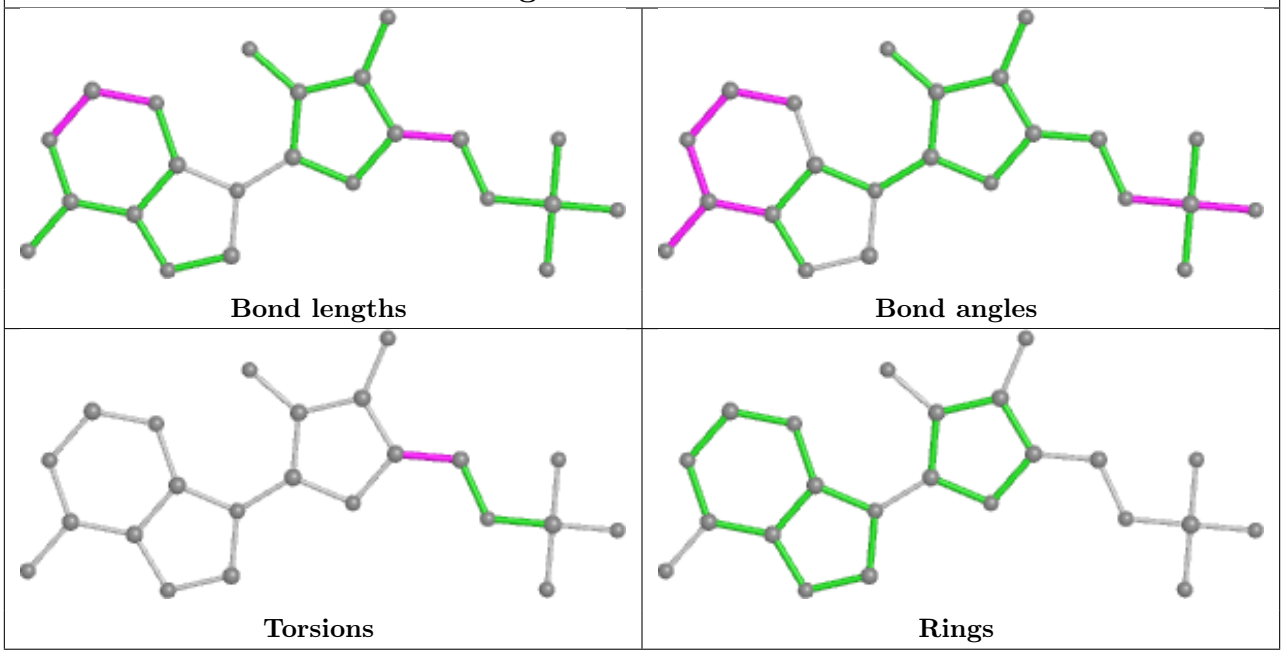
Mol	Chain	Res	Type	Atoms
2	D	338	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

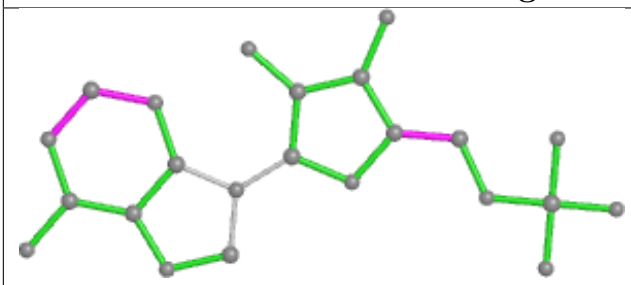
No monomer is involved in short contacts.

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.

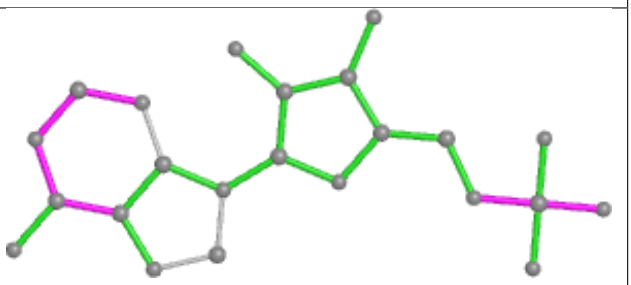
Ligand AMP D 338



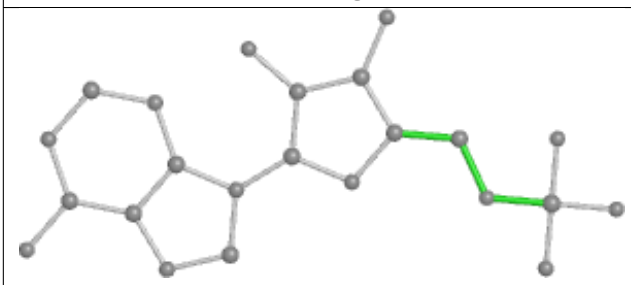
Ligand AMP C 338



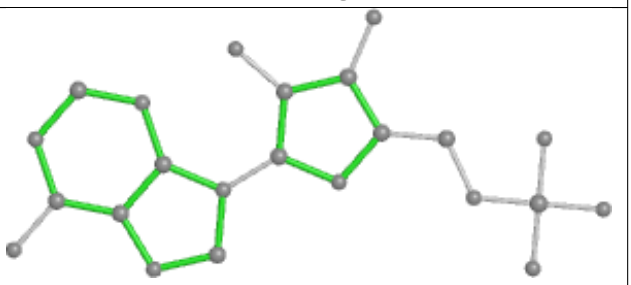
Bond lengths



Bond angles

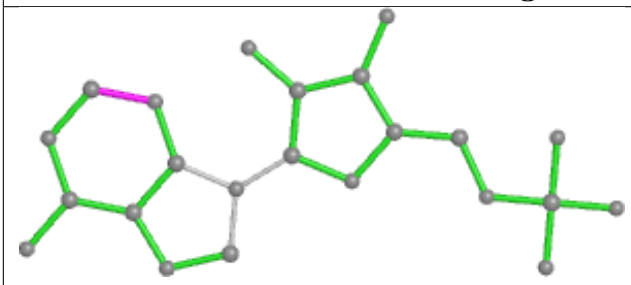


Torsions

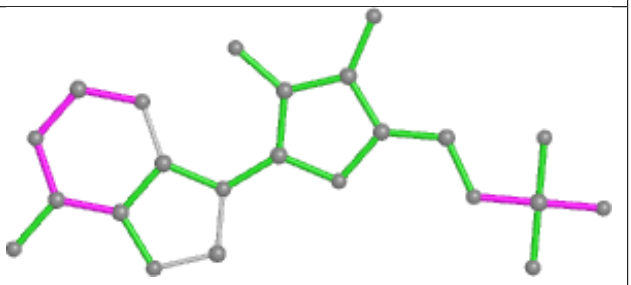


Rings

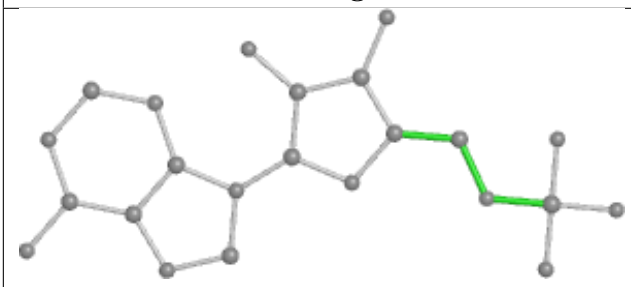
Ligand AMP B 338



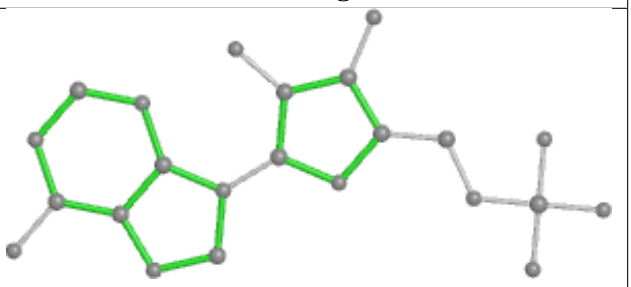
Bond lengths



Bond angles

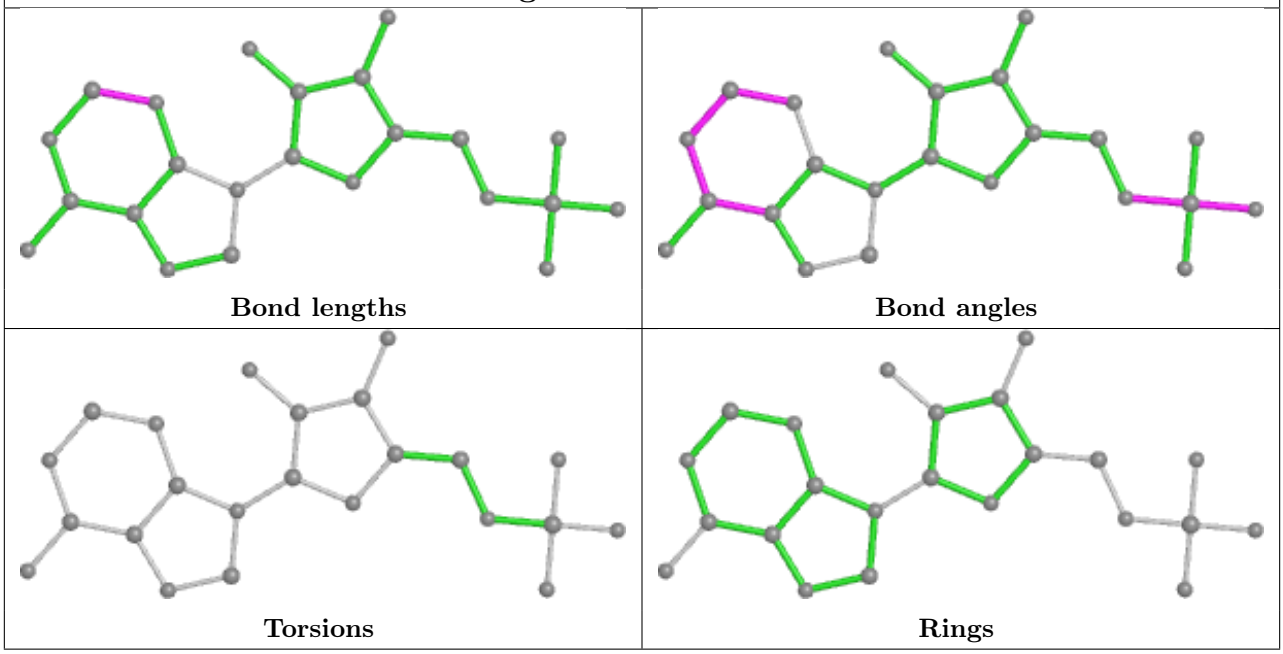


Torsions



Rings

Ligand AMP A 338



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.