WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:27 PM GMT

PDB ID : 1FPF
Title : STRUCTURAL ASPECTS OF THE ALLOSTERIC INHIBITION OF FRU
CTOSE-1,6-BISPHOSPHATASE BY AMP: THE BINDING OF BOTH
THE SUBSTRATE ANALOGUE 2,5-ANHYDRO-D-GLUCITOL-1,6-BISP
HOSPHATE AND CATALYTIC METAL IONS MONITORED BY X-RAY
CRYSTALLOGRAPHY
Authors : Villeret, V.; Huang, S.; Zhang, Y.; Lipscomb, W.N.
Deposited on : 1994-12-15
Resolution : 2.10 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.10 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.
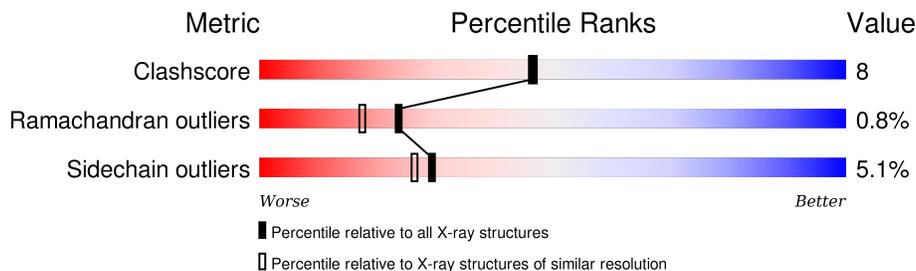
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	77% 14% •• 5%
1	B	335	76% 16% •• 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6500 atoms, of which 1404 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
1	A	317	Total	C	H	N	O	S	0	0	0
			2962	1546	536	409	456	15			
1	B	317	Total	C	H	N	O	S	0	0	0
			2962	1546	536	409	456	15			

There are 6 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

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is 2,5-ANHYDROGLUCITOL-1,6-BIPHOSPHATE (three-letter code: AHG) (formula: $C_6H_{14}O_{11}P_2$).
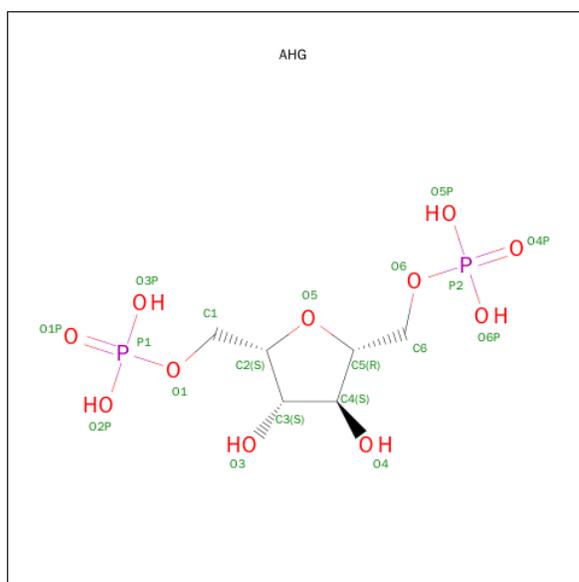
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			29	6	10	11	2		
3	B	1	Total	C	H	O	P	0	0
			29	6	10	11	2		

• Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).
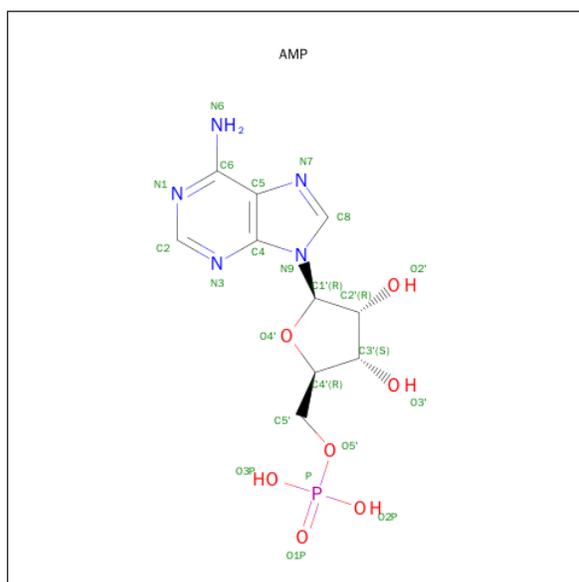
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	84	Total 252	H 168	O 84	0	0
5	B	72	Total 216	H 144	O 72	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain A:

- Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain B:
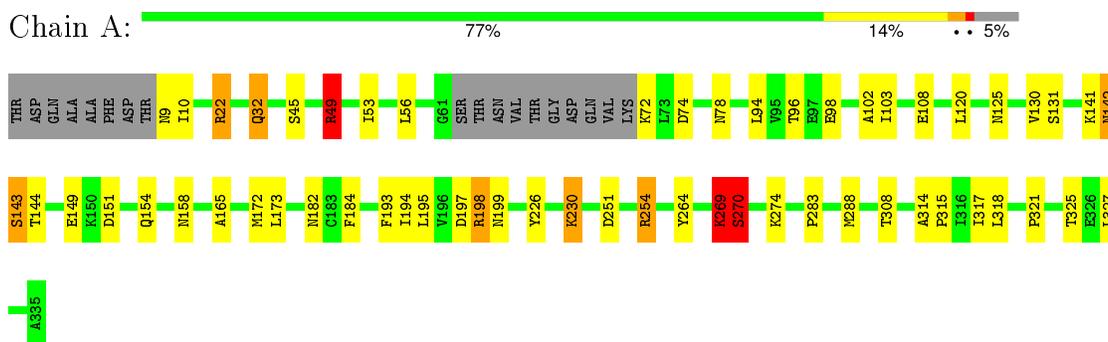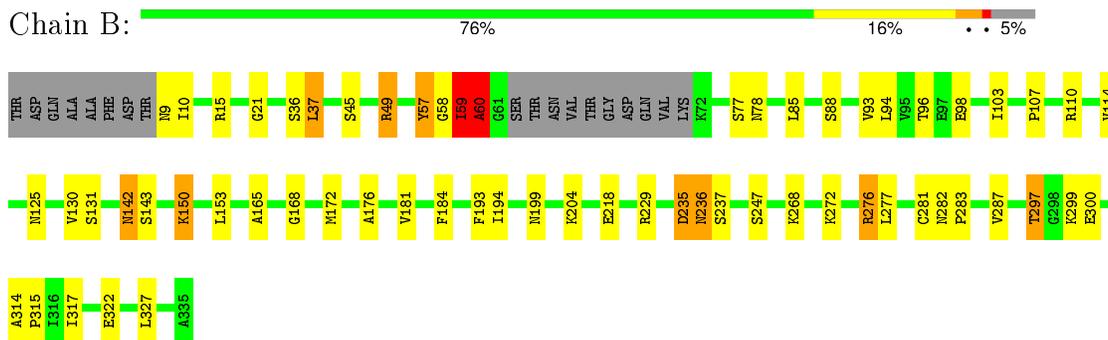
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	61.10Å　　166.60Å　　80.10Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	8.00　–　2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183　,　(Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6500	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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, MN, AHG

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	0.76	3/2467 (0.1%)	0.75	2/3335 (0.1%)
1	B	0.74	2/2467 (0.1%)	0.78	3/3335 (0.1%)
All	All	0.75	5/4934 (0.1%)	0.76	5/6670 (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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	SER	CA-CB	6.62	1.62	1.52
1	B	131	SER	CA-CB	-6.12	1.43	1.52
1	A	131	SER	CA-CB	-5.65	1.44	1.52
1	B	77	SER	CA-CB	-5.60	1.44	1.52
1	A	269	LYS	CA-CB	5.00	1.65	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	59	ILE	N-CA-C	-5.48	96.20	111.00
1	B	235	ASP	N-CA-C	-5.36	96.52	111.00
1	A	49	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	254	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	60	ALA	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	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	2426	536	2486	40	0
1	B	2426	536	2486	36	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	19	10	10	0	0
3	B	19	10	10	0	0
4	A	23	0	10	1	0
4	B	23	0	10	1	0
5	A	84	168	0	1	0
5	B	72	144	0	0	0
All	All	5096	1404	5012	76	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 8.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:HG22	1:A:98:GLU:H	1.42	0.85
1:B:37:LEU:HD13	1:B:85:LEU:HD21	1.64	0.80
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.46	0.79
1:A:78:ASN:OD1	1:A:96:THR:HG21	1.86	0.76
1:B:96:THR:HG22	1:B:98:GLU:H	1.52	0.75
1:B:78:ASN:OD1	1:B:96:THR:HG21	1.87	0.74
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.71	0.72
1:A:142:ASN:O	1:A:143:SER:HB3	1.89	0.72
1:B:125:ASN:HB3	1:B:130:VAL:HB	1.72	0.71
1:A:182:ASN:HD22	1:A:198:ARG:HA	1.54	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:O	1:A:325:THR:HG23	1.94	0.68
1:B:107:PRO:HA	1:B:110:ARG:HG3	1.79	0.65
1:B:10:ILE:HD11	1:B:194:ILE:HD12	1.79	0.65
1:A:269:LYS:HD2	1:A:274:LYS:HB2	1.79	0.63
1:A:269:LYS:HD3	1:A:269:LYS:O	1.99	0.62
1:A:45:SER:O	1:A:49:ARG:HG2	1.99	0.61
1:A:32:GLN:HE21	1:A:32:GLN:HA	1.65	0.61
4:A:339:AMP:H8	4:A:339:AMP:O5'	1.85	0.59
1:B:297:THR:HG22	1:B:299:LYS:H	1.66	0.58
1:B:142:ASN:H	1:B:142:ASN:ND2	2.01	0.58
1:B:283:PRO:O	1:B:287:VAL:HG23	2.05	0.57
1:A:32:GLN:HA	1:A:32:GLN:NE2	2.21	0.56
1:A:10:ILE:HD11	1:A:194:ILE:HD12	1.89	0.55
1:A:182:ASN:ND2	1:A:199:ASN:H	2.06	0.54
1:B:58:GLY:C	1:B:60:ALA:H	2.10	0.53
1:A:102:ALA:CB	1:A:149:GLU:HG3	2.39	0.53
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.92	0.52
1:A:226:TYR:CZ	1:A:230:LYS:HD3	2.45	0.51
1:A:94:LEU:HB2	1:A:103:ILE:HB	1.93	0.51
1:B:150:LYS:HD3	1:B:153:LEU:HD12	1.93	0.51
1:B:235:ASP:O	1:B:237:SER:N	2.44	0.50
1:A:165:ALA:HA	1:A:172:MET:O	2.12	0.50
1:A:102:ALA:HB2	1:A:149:GLU:HG3	1.92	0.50
1:B:49:ARG:NH2	1:B:168:GLY:O	2.42	0.49
1:B:142:ASN:ND2	1:B:143:SER:H	2.11	0.49
1:B:317:ILE:HG21	1:B:327:LEU:HD23	1.94	0.49
1:A:195:LEU:HD21	1:A:198:ARG:HG3	1.94	0.49
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.94	0.48
1:B:36:SER:OG	1:B:88:SER:HB3	2.13	0.48
1:B:184:PHE:HB3	1:B:193:PHE:HB3	1.95	0.48
1:A:22:ARG:NH1	1:A:22:ARG:HG2	2.22	0.47
1:A:182:ASN:ND2	1:A:198:ARG:HA	2.23	0.47
1:B:58:GLY:C	1:B:60:ALA:N	2.67	0.47
1:A:9:ASN:ND2	1:A:9:ASN:O	2.47	0.47
1:A:53:ILE:CD1	1:A:56:LEU:HD12	2.45	0.47
1:B:142:ASN:HD22	1:B:143:SER:H	1.62	0.47
1:A:269:LYS:C	1:A:269:LYS:HD3	2.35	0.46
1:A:10:ILE:HB	1:B:57:TYR:O	2.15	0.46
1:A:154:GLN:HE21	1:A:158:ASN:HD22	1.64	0.46
1:B:218:GLU:OE2	1:B:268:LYS:HG2	2.16	0.46
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LYS:HE2	1:B:322:GLU:OE2	2.16	0.46
1:B:276:ARG:HD3	1:B:276:ARG:N	2.30	0.46
1:A:142:ASN:ND2	1:A:142:ASN:O	2.44	0.45
1:A:254:ARG:HD2	5:A:348:HOH:O	2.15	0.45
1:B:9:ASN:OD1	1:B:9:ASN:N	2.49	0.45
1:B:314:ALA:HA	1:B:315:PRO:HD3	1.80	0.45
1:B:176:ALA:HB2	1:B:181:VAL:HG22	2.00	0.44
1:B:94:LEU:HB2	1:B:103:ILE:HB	2.00	0.43
1:B:59:ILE:O	1:B:59:ILE:HG23	2.18	0.43
1:A:251:ASP:OD1	1:A:254:ARG:NH2	2.47	0.43
1:A:141:LYS:HZ2	1:A:151:ASP:CG	2.22	0.43
1:B:21:GLY:HA2	4:B:339:AMP:C5	2.54	0.43
1:A:314:ALA:HA	1:A:315:PRO:HD3	1.87	0.42
1:A:269:LYS:HD2	1:A:274:LYS:CB	2.49	0.42
1:A:317:ILE:HG21	1:A:327:LEU:HD23	2.01	0.42
1:B:297:THR:HB	1:B:300:GLU:O	2.20	0.42
1:A:96:THR:HG22	1:A:98:GLU:N	2.23	0.42
1:A:53:ILE:HD12	1:A:56:LEU:HD12	2.02	0.42
1:B:272:LYS:HB2	1:B:272:LYS:HE3	1.76	0.41
1:A:288:MET:HG3	1:A:318:LEU:HB2	2.02	0.41
1:A:269:LYS:O	1:A:270:SER:O	2.38	0.41
1:B:93:VAL:HB	1:B:114:VAL:HG13	2.02	0.41
1:B:45:SER:O	1:B:49:ARG:HD2	2.21	0.41
1:B:165:ALA:HA	1:B:172:MET:O	2.21	0.41
1:B:282:ASN:HA	1:B:282:ASN:HD22	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	313/335 (93%)	301 (96%)	10 (3%)	2 (1%)	30	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	313/335 (93%)	300 (96%)	10 (3%)	3 (1%)	19	13
All	All	626/670 (93%)	601 (96%)	20 (3%)	5 (1%)	24	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	SER
1	B	60	ALA
1	A	270	SER
1	B	236	ASN
1	B	59	ILE

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%)	247 (94%)	16 (6%)	23	19
1	B	263/278 (95%)	252 (96%)	11 (4%)	36	35
All	All	526/556 (95%)	499 (95%)	27 (5%)	29	26

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	32	GLN
1	A	49	ARG
1	A	72	LYS
1	A	74	ASP
1	A	108	GLU
1	A	142	ASN
1	A	144	THR
1	A	173	LEU
1	A	197	ASP
1	A	198	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	230	LYS
1	A	264	TYR
1	A	269	LYS
1	A	283	PRO
1	A	308	THR
1	B	15	ARG
1	B	37	LEU
1	B	49	ARG
1	B	142	ASN
1	B	150	LYS
1	B	199	ASN
1	B	229	ARG
1	B	236	ASN
1	B	247	SER
1	B	276	ARG
1	B	297	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	35	ASN
1	A	154	GLN
1	A	182	ASN
1	A	228	GLN
1	A	282	ASN
1	A	334	HIS
1	B	9	ASN
1	B	35	ASN
1	B	142	ASN
1	B	154	GLN
1	B	182	ASN
1	B	228	GLN
1	B	236	ASN
1	B	282	ASN
1	B	332	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
3	AHG	A	338	2	19,19,19	1.16	3 (15%)	27,29,29	1.77	7 (25%)
4	AMP	A	339	-	20,25,25	2.27	4 (20%)	22,38,38	3.18	9 (40%)
3	AHG	B	338	2	19,19,19	1.40	3 (15%)	27,29,29	1.93	5 (18%)
4	AMP	B	339	-	20,25,25	2.30	2 (10%)	22,38,38	2.82	6 (27%)

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	AHG	A	338	2	-	0/12/28/28	0/1/1/1
4	AMP	A	339	-	-	0/6/26/26	0/3/3/3
3	AHG	B	338	2	-	0/12/28/28	0/1/1/1
4	AMP	B	339	-	-	0/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	339	AMP	O3'-C3'	-7.11	1.25	1.43
4	A	339	AMP	O3'-C3'	-6.98	1.26	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	339	AMP	O2'-C2'	-5.99	1.28	1.43
4	A	339	AMP	O2'-C2'	-4.98	1.31	1.43
3	B	338	AHG	O5-C5	-2.86	1.38	1.45
4	A	339	AMP	P-O2P	-2.55	1.45	1.54
3	A	338	AHG	O1-C1	-2.34	1.35	1.44
3	A	338	AHG	P2-O6P	-2.12	1.47	1.54
3	A	338	AHG	O3-C3	2.41	1.48	1.43
3	B	338	AHG	C4-C3	2.53	1.60	1.53
3	B	338	AHG	O3-C3	2.67	1.49	1.43
4	A	339	AMP	C2-N3	3.53	1.38	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	339	AMP	N3-C2-N1	-11.59	120.02	128.89
4	B	339	AMP	N3-C2-N1	-10.77	120.65	128.89
4	A	339	AMP	C4-C5-N7	-4.05	105.76	109.48
3	B	338	AHG	O4-C4-C5	-3.37	100.93	111.05
3	A	338	AHG	O4-C4-C3	-3.22	101.35	111.83
3	A	338	AHG	O5-C5-C4	-3.21	98.68	105.15
3	B	338	AHG	O3-C3-C4	-3.20	101.42	111.83
3	B	338	AHG	O5-C2-C1	-2.84	99.17	109.32
4	B	339	AMP	O2'-C2'-C3'	-2.66	103.17	111.83
4	A	339	AMP	C4'-O4'-C1'	-2.57	106.89	109.72
4	A	339	AMP	O2'-C2'-C3'	-2.43	103.91	111.83
3	A	338	AHG	O6P-P2-O6	-2.33	99.84	106.56
3	A	338	AHG	O6P-P2-O5P	2.10	115.37	107.38
4	B	339	AMP	O4'-C1'-N9	2.13	112.56	108.10
4	A	339	AMP	O3'-C3'-C4'	2.16	117.54	111.05
4	A	339	AMP	O3'-C3'-C2'	2.30	119.30	111.83
4	B	339	AMP	C2-N1-C6	2.45	123.14	118.77
3	A	338	AHG	O6-P2-O4P	2.58	113.70	107.14
4	A	339	AMP	O2P-P-O5'	2.62	114.11	106.56
3	A	338	AHG	O1-P1-O1P	2.97	114.71	107.14
3	B	338	AHG	O3-C3-C2	3.42	121.30	111.05
4	A	339	AMP	C2-N1-C6	3.48	124.98	118.77
4	B	339	AMP	C2'-C1'-N9	3.63	119.84	114.29
4	B	339	AMP	O2P-P-O5'	3.85	117.65	106.56
4	A	339	AMP	C2'-C1'-N9	4.09	120.54	114.29
3	A	338	AHG	O4-C4-C5	4.22	123.72	111.05
3	B	338	AHG	O4-C4-C3	5.35	129.22	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	339	AMP	1	0
4	B	339	AMP	1	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.