



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:42 PM BST

PDB ID : 4GX6  
Title : AMP Complexes of Porcine Liver Fructose-1,6-bisphosphatase with Mutation E192Q  
Authors : Gao, Y.; Honzatko, R.B.  
Deposited on : 2012-09-03  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

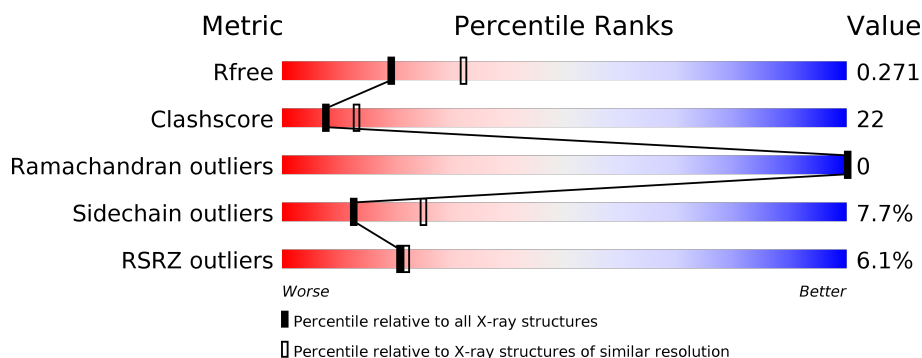
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	337	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>• •</div> </div> </div>
1	B	337	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>31%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5304 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.

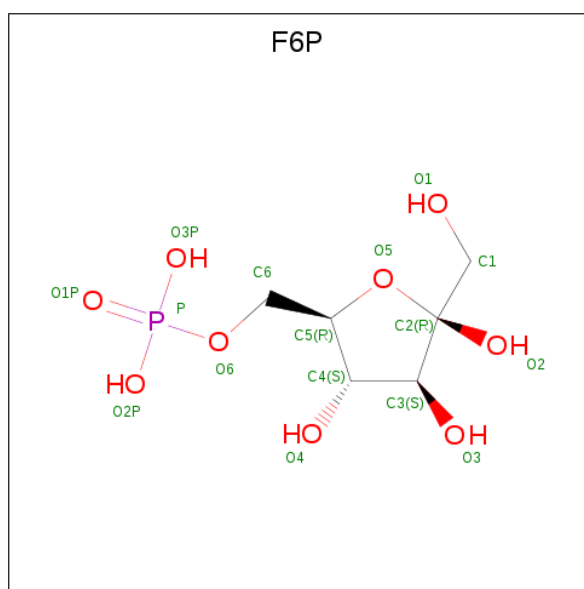
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2496	1587	421	473	15			
1	B	327	Total	C	N	O	S	0	0	0
			2496	1587	421	473	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLN	GLU	engineered mutation	UNP P00636
B	192	GLN	GLU	engineered mutation	UNP P00636

- Molecule 2 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula:  $C_6H_{13}O_9P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		

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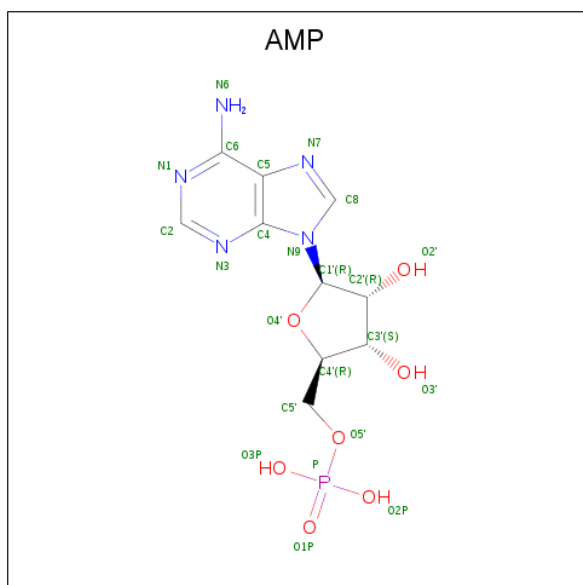
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



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 PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total	O	0	0
			111	111		
6	B	109	Total	O	0	0
			109	109		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.92Å 165.34Å 79.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 2.50 38.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.2 (39.56-2.50) 92.3 (38.47-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.211 , 0.273 0.211 , 0.271	Depositor DCC
$R_{free}$ test set	1312 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: AMP, PO4, MG, F6P

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	1.01	0/2538	0.87	1/3434 (0.0%)
1	B	1.10	4/2538 (0.2%)	0.90	3/3434 (0.1%)
All	All	1.06	4/5076 (0.1%)	0.88	4/6868 (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	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	GLU	CD-OE1	7.83	1.34	1.25
1	B	48	VAL	CB-CG1	-5.40	1.41	1.52
1	B	279	TYR	CE2-CZ	-5.34	1.31	1.38
1	B	160	VAL	CB-CG2	-5.24	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	SER	N-CA-C	6.80	129.36	111.00
1	B	67	GLY	N-CA-C	-5.42	99.54	113.10
1	A	199	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	199	ASP	CB-CG-OD2	5.18	122.96	118.30



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	ASN	Peptide
1	B	142	ASN	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2496	0	2554	97	0
1	B	2496	0	2554	128	0
2	A	16	0	11	0	0
2	B	16	0	11	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	23	0	12	1	0
4	B	23	0	12	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	111	0	0	16	0
6	B	109	0	0	24	0
All	All	5304	0	5154	223	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 22.

All (223) 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:13:LEU:HD23	1:A:38:CYS:SG	1.69	1.32
1:B:135:ILE:HD11	1:B:249:VAL:CG2	1.68	1.23
1:A:13:LEU:CD2	1:A:38:CYS:SG	2.39	1.10
1:B:135:ILE:HD11	1:B:249:VAL:HG22	1.25	1.10
1:B:299:LYS:HE2	6:B:602:HOH:O	1.50	1.06
1:A:15:ARG:HD2	6:A:597:HOH:O	1.55	1.06
1:A:316:ILE:HD12	1:A:317:ILE:N	1.77	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:HG13	1:B:56:LEU:HD12	1.48	0.94
1:B:157:ARG:HG3	1:B:157:ARG:HH11	1.31	0.94
1:A:19:GLU:HG3	6:A:598:HOH:O	1.66	0.93
1:B:228:GLN:HA	1:B:228:GLN:OE1	1.71	0.90
1:B:135:ILE:CD1	1:B:249:VAL:HG22	2.02	0.86
1:B:65:VAL:HG13	1:B:69:GLN:HB2	1.58	0.85
1:B:53:ILE:CG1	1:B:56:LEU:HD12	2.06	0.85
1:A:70:VAL:HG22	6:A:578:HOH:O	1.76	0.83
1:B:302:VAL:HG21	1:B:316:ILE:HD13	1.61	0.82
1:B:157:ARG:HG3	1:B:157:ARG:NH1	1.94	0.80
1:A:123:SER:HA	1:A:126:ILE:HG12	1.62	0.80
1:B:157:ARG:CG	1:B:157:ARG:HH11	1.95	0.79
1:A:204:LYS:O	1:A:321:PRO:HD2	1.83	0.79
1:B:120:LEU:HD11	1:B:132:ILE:HD12	1.63	0.79
1:A:139:TYR:CZ	1:A:159:LEU:HG	2.21	0.76
1:B:72:LYS:HB3	6:B:529:HOH:O	1.85	0.76
1:A:139:TYR:CZ	1:A:159:LEU:CD2	2.69	0.76
1:A:38:CYS:SG	1:A:193:PHE:CD2	2.79	0.76
1:B:135:ILE:CD1	1:B:249:VAL:CG2	2.60	0.75
1:B:330:ILE:HD13	1:B:330:ILE:N	2.03	0.73
1:B:218:GLU:HG2	1:B:268:LYS:HE3	1.71	0.72
1:B:70:VAL:HG12	1:B:71:LYS:N	2.05	0.71
1:A:318:LEU:HD12	1:A:318:LEU:C	2.11	0.71
1:B:65:VAL:CG1	1:B:69:GLN:HB2	2.21	0.70
1:B:267:ASN:HA	6:B:596:HOH:O	1.91	0.69
1:A:65:VAL:CG1	1:A:65:VAL:O	2.39	0.69
1:B:330:ILE:CD1	6:B:518:HOH:O	2.40	0.69
1:A:221:PRO:HB2	1:A:334:HIS:CE1	2.28	0.69
1:B:63:THR:HG22	1:B:63:THR:O	1.92	0.69
1:B:321:PRO:O	1:B:325:THR:HG23	1.93	0.68
1:A:58:GLY:HA2	6:A:610:HOH:O	1.94	0.68
1:B:70:VAL:CG1	1:B:71:LYS:N	2.57	0.68
1:B:267:ASN:CA	6:B:596:HOH:O	2.44	0.66
1:B:68:ASP:O	1:B:69:GLN:NE2	2.29	0.65
1:A:316:ILE:HD12	1:A:317:ILE:H	1.58	0.65
1:A:254:ARG:HD2	6:A:515:HOH:O	1.96	0.65
1:B:86:LYS:HE2	6:B:505:HOH:O	1.96	0.65
1:B:204:LYS:O	1:B:320:SER:HB3	1.97	0.64
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.32	0.64
1:B:65:VAL:HG13	1:B:69:GLN:CB	2.28	0.64
1:A:139:TYR:CE2	1:A:159:LEU:HD21	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLY:CA	6:A:610:HOH:O	2.47	0.63
1:B:146:GLU:HG2	1:B:147:PRO:HD2	1.79	0.62
1:A:139:TYR:CE1	1:A:159:LEU:HG	2.34	0.62
1:B:142:ASN:ND2	6:B:508:HOH:O	2.32	0.62
2:B:401:F6P:H11	6:B:551:HOH:O	1.99	0.62
1:B:135:ILE:HD11	1:B:249:VAL:HG21	1.78	0.61
1:A:65:VAL:O	1:A:65:VAL:HG13	2.01	0.61
1:B:321:PRO:HB2	6:B:606:HOH:O	2.01	0.60
1:A:32:GLN:OE1	1:A:32:GLN:HA	2.00	0.60
1:B:268:LYS:HA	6:B:588:HOH:O	2.00	0.60
1:A:48:VAL:HA	1:A:73:LEU:HD21	1.84	0.60
1:A:9:ASN:N	6:A:609:HOH:O	2.35	0.60
1:A:38:CYS:SG	1:A:193:PHE:CE2	2.95	0.60
1:B:120:LEU:HD11	1:B:132:ILE:CD1	2.32	0.60
1:A:139:TYR:CE2	1:A:159:LEU:CD2	2.85	0.59
1:A:139:TYR:OH	1:A:156:GLY:HA2	2.02	0.59
1:A:139:TYR:CZ	1:A:159:LEU:CG	2.85	0.59
1:B:217:LYS:O	1:B:217:LYS:CG	2.50	0.59
1:B:157:ARG:NE	1:B:304:ASP:OD2	2.34	0.59
1:B:65:VAL:HG11	1:B:69:GLN:O	2.01	0.59
1:A:19:GLU:OE2	1:A:22:ARG:NH2	2.36	0.58
1:B:97:GLU:HB2	1:B:279:TYR:CE1	2.37	0.58
1:A:333:LYS:HG2	1:A:333:LYS:O	2.02	0.58
1:B:194:ILE:O	1:B:196:VAL:HG13	2.03	0.58
1:A:142:ASN:N	1:A:142:ASN:OD1	2.30	0.58
1:B:275:LEU:HD12	1:B:316:ILE:HG21	1.86	0.58
1:A:139:TYR:OH	1:A:159:LEU:HG	2.03	0.58
1:A:316:ILE:HD11	1:A:318:LEU:HB3	1.84	0.58
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.85	0.58
1:A:29:GLU:OE1	1:A:112:LYS:HG2	2.04	0.58
1:A:10:ILE:HG12	1:B:57:TYR:O	2.04	0.58
1:B:29:GLU:OE1	1:B:112:LYS:HG2	2.03	0.58
1:B:173:LEU:HD23	1:B:173:LEU:C	2.24	0.57
1:A:165:ALA:HA	1:A:172:MET:O	2.03	0.57
1:B:179:ASN:HB2	6:B:533:HOH:O	2.03	0.57
1:A:224:THR:HB	6:A:603:HOH:O	2.04	0.57
1:A:58:GLY:N	6:A:610:HOH:O	2.37	0.57
1:B:37:LEU:HD12	1:B:85:LEU:HD21	1.87	0.56
1:A:139:TYR:CZ	1:A:159:LEU:HD21	2.39	0.56
1:B:218:GLU:HG2	1:B:268:LYS:HG3	1.86	0.56
1:B:13:LEU:HD23	1:B:184:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:HG13	1:B:56:LEU:CD1	2.30	0.55
1:A:227:ILE:HG22	1:A:231:LYS:HE3	1.88	0.55
1:B:22:ARG:HH11	1:B:22:ARG:HG2	1.72	0.55
1:A:208:ILE:CD1	6:A:552:HOH:O	2.55	0.54
1:A:10:ILE:CD1	1:A:194:ILE:HG13	2.36	0.54
1:A:82:ILE:O	1:A:86:LYS:HG3	2.08	0.54
1:B:157:ARG:HD2	1:B:304:ASP:OD2	2.08	0.54
1:B:251:ASP:OD1	1:B:254:ARG:NH2	2.41	0.54
1:A:21:GLY:HA3	6:A:596:HOH:O	2.08	0.54
1:B:173:LEU:HD23	1:B:174:VAL:N	2.23	0.53
1:B:299:LYS:CE	6:B:602:HOH:O	2.26	0.53
1:B:66:THR:O	1:B:67:GLY:C	2.44	0.53
1:B:309:ASP:C	1:B:309:ASP:OD2	2.47	0.53
1:A:96:SER:HB2	1:A:117:PHE:CZ	2.43	0.53
1:A:13:LEU:HD21	1:A:38:CYS:HB2	1.92	0.52
1:B:198:ARG:HH11	1:B:198:ARG:CG	2.23	0.52
1:A:316:ILE:HD12	1:A:316:ILE:C	2.31	0.51
1:B:177:MET:HB3	6:B:521:HOH:O	2.10	0.51
1:B:271:PRO:HD2	6:B:597:HOH:O	2.10	0.51
1:B:157:ARG:HE	1:B:304:ASP:CG	2.13	0.51
1:A:332:GLN:O	1:A:335:ALA:N	2.44	0.51
1:B:218:GLU:CG	1:B:268:LYS:HG3	2.41	0.51
1:B:223:ILE:HG13	6:B:591:HOH:O	2.10	0.50
1:B:53:ILE:HG12	1:B:56:LEU:HD12	1.92	0.50
1:B:157:ARG:CD	1:B:304:ASP:OD2	2.59	0.50
1:B:330:ILE:CD1	1:B:330:ILE:N	2.74	0.50
1:A:218:GLU:HB2	1:A:267:ASN:HB2	1.91	0.50
2:B:401:F6P:C1	6:B:551:HOH:O	2.57	0.50
1:A:218:GLU:OE1	1:A:269:LYS:HB2	2.10	0.50
1:A:204:LYS:C	1:A:321:PRO:HD2	2.32	0.50
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.92	0.50
1:A:141:LYS:HE3	1:A:151:ASP:OD1	2.12	0.49
1:B:261:ILE:HD12	1:B:318:LEU:O	2.12	0.49
1:B:198:ARG:HH11	1:B:198:ARG:HG2	1.77	0.49
1:B:216:ALA:HA	1:B:219:PHE:CD2	2.48	0.49
1:B:22:ARG:HG2	1:B:22:ARG:NH1	2.28	0.49
1:B:102:ALA:HB3	1:B:149:GLU:HG2	1.95	0.49
1:A:18:MET:O	1:A:22:ARG:HG3	2.13	0.48
1:A:37:LEU:HD21	1:A:136:PHE:CE2	2.49	0.48
1:B:82:ILE:HD12	1:B:103:ILE:HD13	1.94	0.48
1:B:221:PRO:HB2	1:B:334:HIS:ND1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:HD12	1:B:318:LEU:C	2.34	0.48
1:B:226:TYR:HB2	1:B:327:LEU:HD13	1.95	0.48
1:B:63:THR:O	1:B:63:THR:CG2	2.60	0.48
1:A:208:ILE:HD12	6:A:552:HOH:O	2.13	0.48
1:B:270:SER:HB3	1:B:273:GLY:O	2.14	0.48
1:B:261:ILE:HD11	1:B:317:ILE:CG2	2.43	0.47
1:A:78:ASN:OD1	1:A:119:PRO:HG3	2.14	0.47
1:B:40:ALA:O	1:B:44:ILE:HG13	2.13	0.47
1:B:267:ASN:C	6:B:596:HOH:O	2.51	0.47
1:B:45:SER:O	1:B:49:ARG:HD3	2.14	0.47
1:A:38:CYS:SG	1:A:193:PHE:HD2	2.35	0.47
1:A:49:ARG:O	1:A:50:LYS:HB2	2.14	0.47
1:B:218:GLU:CD	1:B:268:LYS:HG3	2.34	0.47
1:B:299:LYS:HG2	6:B:604:HOH:O	2.14	0.47
1:B:275:LEU:HD12	1:B:316:ILE:CG2	2.45	0.47
1:A:123:SER:HA	1:A:126:ILE:CG1	2.40	0.46
1:A:62:SER:OG	1:A:62:SER:O	2.31	0.46
1:B:299:LYS:HB2	6:B:577:HOH:O	2.15	0.46
1:B:217:LYS:O	1:B:217:LYS:HG2	2.15	0.46
1:A:45:SER:O	1:A:49:ARG:HD3	2.15	0.46
1:B:36:SER:OG	1:B:88:SER:HB3	2.15	0.46
1:A:147:PRO:HA	1:A:151:ASP:OD1	2.16	0.46
6:A:527:HOH:O	1:B:217:LYS:HB3	2.15	0.46
1:B:330:ILE:HD13	1:B:330:ILE:H	1.76	0.46
1:A:276:ARG:NH1	1:A:311:HIS:O	2.45	0.46
1:A:218:GLU:CB	1:A:267:ASN:HB2	2.46	0.46
1:B:206:GLY:HA3	1:B:260:GLY:N	2.31	0.46
1:A:232:PHE:CE1	1:B:217:LYS:HB2	2.51	0.46
1:A:66:THR:HG23	1:A:67:GLY:N	2.31	0.45
1:B:72:LYS:CB	6:B:529:HOH:O	2.54	0.45
1:A:106:GLU:OE1	1:A:109:LYS:NZ	2.31	0.45
1:A:70:VAL:HA	6:A:578:HOH:O	2.16	0.45
1:A:10:ILE:HD11	1:A:194:ILE:HG13	1.99	0.45
1:A:148:SER:OG	1:A:150:LYS:HG2	2.16	0.45
1:B:217:LYS:HG2	1:B:218:GLU:HG3	1.99	0.45
1:A:156:GLY:HA3	1:A:303:LEU:HD22	1.97	0.45
1:B:37:LEU:HD21	1:B:136:PHE:CD2	2.52	0.45
1:B:13:LEU:HB2	1:B:193:PHE:HB2	1.98	0.45
1:B:220:ASP:HB2	1:B:221:PRO:HD2	1.99	0.45
1:A:70:VAL:CG1	1:A:71:LYS:N	2.80	0.44
1:B:10:ILE:O	1:B:10:ILE:HG23	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:HIS:O	1:A:335:ALA:C	2.56	0.44
1:B:93:VAL:HG22	1:B:104:ILE:CD1	2.47	0.44
1:A:199:ASP:O	1:A:199:ASP:OD1	2.35	0.44
1:A:227:ILE:CG2	1:A:231:LYS:HE3	2.47	0.44
1:A:230:LYS:HD3	1:A:230:LYS:HA	1.68	0.44
1:A:70:VAL:HG12	1:A:71:LYS:N	2.32	0.44
1:A:218:GLU:HB2	1:A:267:ASN:CB	2.47	0.44
1:B:267:ASN:O	1:B:270:SER:C	2.57	0.44
1:B:302:VAL:HA	1:B:305:ILE:HD12	2.00	0.43
1:B:64:ASN:OD1	1:B:64:ASN:O	2.36	0.43
1:A:166:LEU:O	1:A:171:THR:HA	2.18	0.43
1:B:204:LYS:HA	1:B:321:PRO:HD2	2.00	0.43
1:B:330:ILE:HD11	6:B:518:HOH:O	2.14	0.43
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.85	0.43
1:B:36:SER:HB3	1:B:84:VAL:HG12	2.00	0.43
1:B:123:SER:HA	1:B:126:ILE:CD1	2.49	0.43
1:B:233:PRO:HA	1:B:234:PRO:HD2	1.90	0.43
1:A:187:ASP:HB2	1:B:53:ILE:HG22	1.99	0.43
1:A:179:ASN:HB2	6:A:576:HOH:O	2.19	0.43
1:A:96:SER:HB2	1:A:117:PHE:CE2	2.54	0.43
1:B:330:ILE:HD13	6:B:518:HOH:O	2.14	0.43
1:A:10:ILE:CG1	1:B:57:TYR:O	2.67	0.43
1:B:261:ILE:CD1	1:B:324:VAL:HG22	2.49	0.43
1:B:270:SER:HA	6:B:597:HOH:O	2.19	0.43
1:A:121:ASP:N	1:A:133:GLY:O	2.46	0.42
1:A:157:ARG:HA	1:A:157:ARG:HD3	1.85	0.42
1:B:205:LYS:HE2	1:B:240:TYR:OH	2.19	0.42
1:B:198:ARG:NH1	1:B:198:ARG:CG	2.81	0.42
1:B:231:LYS:HD2	6:B:515:HOH:O	2.19	0.42
1:B:13:LEU:HD12	1:B:38:CYS:SG	2.60	0.42
1:B:143:SER:O	1:B:144:THR:OG1	2.30	0.42
1:B:13:LEU:HD23	1:B:184:PHE:CE2	2.55	0.42
1:B:22:ARG:NH1	1:B:22:ARG:CG	2.79	0.42
1:A:216:ALA:HA	1:A:219:PHE:CE2	2.54	0.41
1:A:267:ASN:OD1	1:A:269:LYS:HB3	2.20	0.41
1:A:88:SER:O	1:A:89:PHE:HB2	2.20	0.41
1:B:242:ALA:O	1:B:243:ARG:HG2	2.20	0.41
1:A:139:TYR:CE1	1:A:159:LEU:N	2.88	0.41
1:A:251:ASP:HA	1:A:254:ARG:NH2	2.35	0.41
1:B:216:ALA:HA	1:B:219:PHE:CE2	2.55	0.41
1:B:65:VAL:CG1	1:B:66:THR:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LYS:HD3	1:B:204:LYS:HA	1.77	0.41
1:A:225:GLU:HA	6:A:591:HOH:O	2.20	0.41
1:A:81:VAL:HG11	1:A:117:PHE:CD2	2.56	0.41
1:A:59:ILE:HB	1:B:10:ILE:HD13	2.01	0.41
1:B:186:LEU:HB2	1:B:193:PHE:CE1	2.56	0.41
1:A:199:ASP:O	1:A:199:ASP:CG	2.58	0.40
1:B:17:VAL:HG11	1:B:34:LEU:HB2	2.02	0.40
1:B:199:ASP:O	1:B:199:ASP:OD1	2.39	0.40
1:B:229:ARG:HG2	1:B:234:PRO:HD2	2.03	0.40
1:B:128:CYS:O	1:B:129:LEU:HB2	2.21	0.40
4:A:404:AMP:O5'	4:A:404:AMP:H8	2.05	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	325/337 (96%)	323 (99%)	2 (1%)	0	100	100
1	B	325/337 (96%)	318 (98%)	7 (2%)	0	100	100
All	All	650/674 (96%)	641 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	248 (91%)	24 (9%)	10	19
1	B	272/279 (98%)	254 (93%)	18 (7%)	16	32
All	All	544/558 (98%)	502 (92%)	42 (8%)	13	25

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	ARG
1	A	22	ARG
1	A	30	MET
1	A	32	GLN
1	A	62	SER
1	A	65	VAL
1	A	69	GLN
1	A	100	LYS
1	A	112	LYS
1	A	140	ARG
1	A	143	SER
1	A	145	ASP
1	A	150	LYS
1	A	157	ARG
1	A	190	ILE
1	A	197	ASP
1	A	218	GLU
1	A	264	TYR
1	A	267	ASN
1	A	272	LYS
1	A	277	LEU
1	A	310	ILE
1	A	316	ILE
1	B	13	LEU
1	B	38	CYS
1	B	71	LYS
1	B	99	ASP
1	B	100	LYS
1	B	143	SER
1	B	157	ARG
1	B	160	VAL
1	B	190	ILE
1	B	198	ARG
1	B	217	LYS

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Mol	Chain	Res	Type
1	B	228	GLN
1	B	264	TYR
1	B	269	LYS
1	B	272	LYS
1	B	277	LEU
1	B	316	ILE
1	B	330	ILE

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

Mol	Chain	Res	Type
1	A	334	HIS
1	B	142	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	F6P	A	401	3	15,16,16	1.09	1 (6%)	17,25,25	1.31	2 (11%)
4	AMP	A	404	-	22,25,25	1.07	2 (9%)	25,38,38	1.47	5 (20%)
2	F6P	B	401	3	15,16,16	0.95	1 (6%)	17,25,25	1.35	3 (17%)
4	AMP	B	404	-	22,25,25	1.14	2 (9%)	25,38,38	1.70	3 (12%)
5	PO4	A	405	3	4,4,4	0.91	0	6,6,6	1.72	1 (16%)
5	PO4	B	405	3	4,4,4	0.87	0	6,6,6	1.57	1 (16%)

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	F6P	A	401	3	-	2/9/28/28	0/1/1/1
2	F6P	B	401	3	-	1/9/28/28	0/1/1/1
4	AMP	B	404	-	-	0/6/26/26	0/3/3/3
4	AMP	A	404	-	-	0/6/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	F6P	O2-C2	3.53	1.46	1.40
2	B	401	F6P	O2-C2	3.04	1.45	1.40
4	B	404	AMP	C5-C4	2.75	1.48	1.40
4	A	404	AMP	C5-C4	2.27	1.46	1.40
4	A	404	AMP	O4'-C1'	2.19	1.44	1.41
4	B	404	AMP	C8-N7	2.03	1.38	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	AMP	O2P-P-O5'	-3.87	96.44	106.73
4	A	404	AMP	N3-C2-N1	-3.58	123.09	128.68
4	B	404	AMP	N3-C2-N1	-3.54	123.14	128.68
5	B	405	PO4	O4-P-O2	3.35	118.72	107.97
5	A	405	PO4	O3-P-O2	3.28	118.49	107.97
2	A	401	F6P	O1-C1-C2	-3.03	105.42	111.86
4	B	404	AMP	C2-N1-C6	3.02	123.92	118.75
2	B	401	F6P	O1-C1-C2	-2.91	105.67	111.86
4	A	404	AMP	C3'-C2'-C1'	2.82	105.22	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	AMP	C2-N1-C6	2.68	123.34	118.75
4	A	404	AMP	C4-C5-N7	-2.68	106.61	109.40
2	A	401	F6P	O4-C4-C5	-2.36	104.23	111.05
2	B	401	F6P	O2P-P-O6	-2.26	100.72	106.73
2	B	401	F6P	O3P-P-O2P	2.14	115.83	107.64
4	A	404	AMP	O3P-P-O1P	2.04	118.65	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	F6P	C6-O6-P-O1P
2	A	401	F6P	C6-O6-P-O2P
2	B	401	F6P	C4-C5-C6-O6

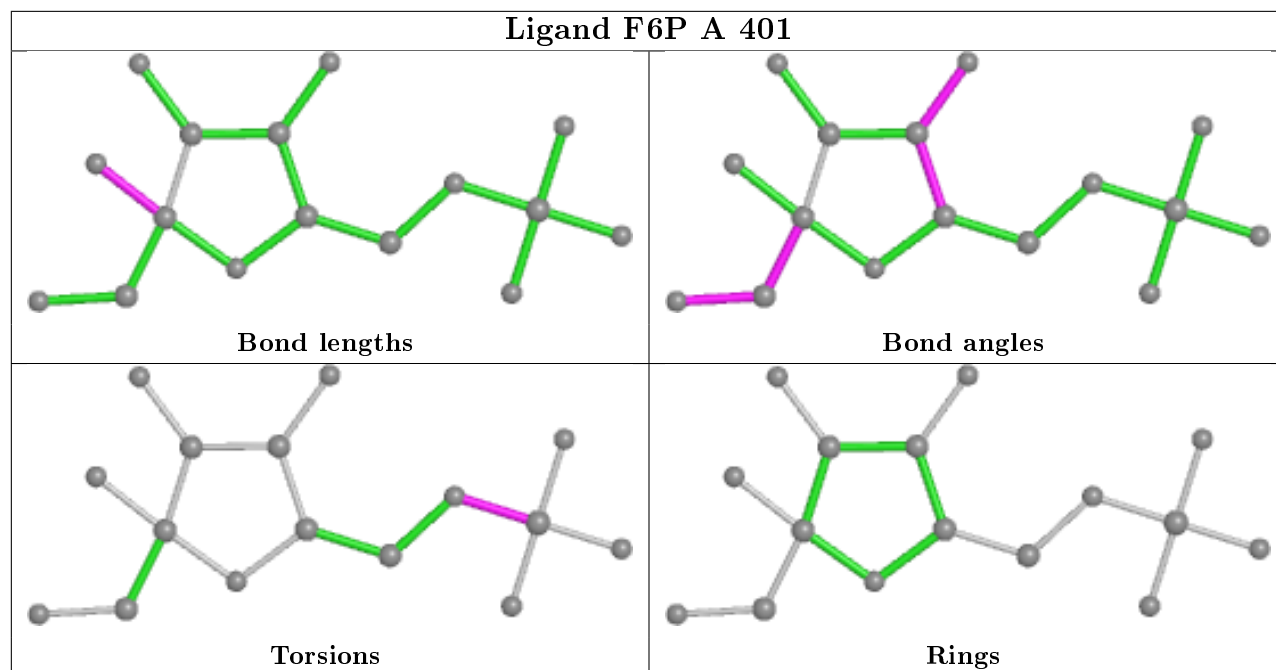
There are no ring outliers.

2 monomers are involved in 3 short contacts:

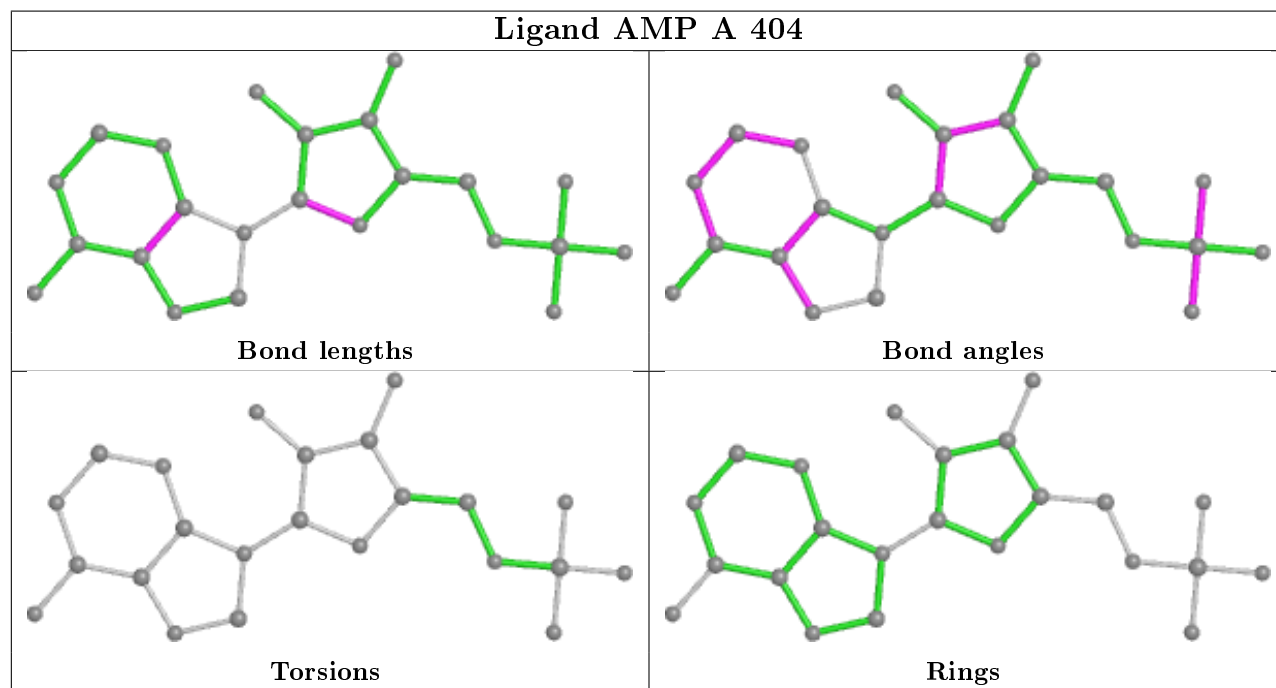
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	AMP	1	0
2	B	401	F6P	2	0

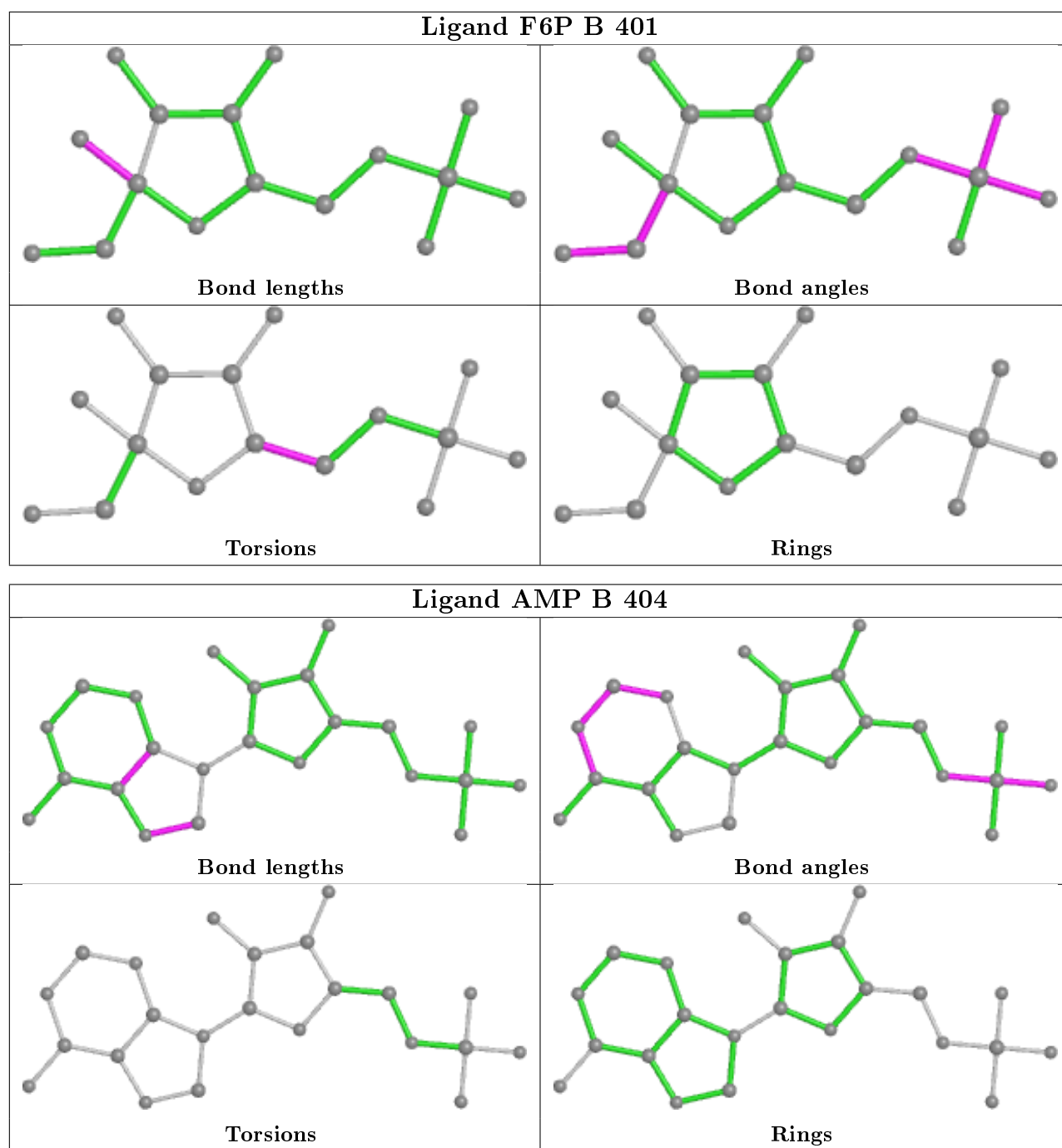
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand F6P A 401



## Ligand AMP A 404





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	327/337 (97%)	0.19	23 (7%) 16 16	13, 24, 51, 86	0
1	B	327/337 (97%)	0.10	17 (5%) 27 29	13, 23, 45, 86	0
All	All	654/674 (97%)	0.14	40 (6%) 21 22	13, 24, 51, 86	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	VAL	12.0
1	A	67	GLY	10.3
1	B	66	THR	9.4
1	A	63	THR	9.2
1	A	70	VAL	9.0
1	A	66	THR	8.9
1	B	67	GLY	8.5
1	B	70	VAL	8.2
1	A	64	ASN	8.2
1	A	65	VAL	7.4
1	B	68	ASP	6.7
1	B	69	GLN	6.7
1	B	64	ASN	6.4
1	A	68	ASP	5.8
1	A	69	GLN	5.6
1	B	63	THR	4.9
1	B	56	LEU	4.2
1	B	62	SER	4.0
1	B	142	ASN	4.0
1	A	269	LYS	3.8
1	B	144	THR	3.5
1	A	56	LEU	3.5
1	A	62	SER	3.4
1	A	268	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	270	SER	2.9
1	A	143	SER	2.9
1	A	142	ASN	2.7
1	A	71	LYS	2.7
1	A	108	GLU	2.6
1	A	61	GLY	2.6
1	B	71	LYS	2.5
1	A	38	CYS	2.4
1	B	143	SER	2.4
1	A	335	ALA	2.2
1	A	146	GLU	2.1
1	A	144	THR	2.1
1	B	199	ASP	2.1
1	B	269	LYS	2.1
1	A	332	GLN	2.0
1	B	108	GLU	2.0

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MG	B	402	1/1	0.94	0.13	5,5,5,5	0
3	MG	A	402	1/1	0.95	0.14	10,10,10,10	0
2	F6P	B	401	16/16	0.95	0.13	11,21,23,27	0
5	PO4	B	405	5/5	0.95	0.14	39,40,42,43	0
5	PO4	A	405	5/5	0.96	0.13	44,45,48,49	0
3	MG	A	403	1/1	0.96	0.17	19,19,19,19	0
3	MG	B	403	1/1	0.97	0.17	9,9,9,9	0

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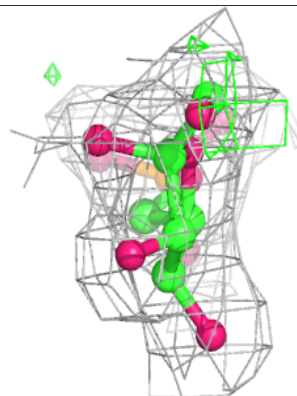
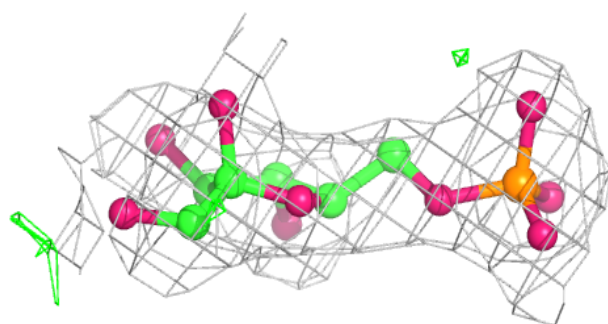
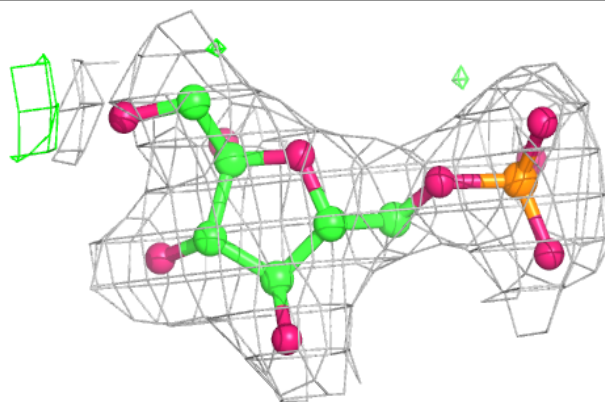
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	AMP	B	404	23/23	0.97	0.11	20,25,29,30	0
4	AMP	A	404	23/23	0.97	0.11	18,25,28,29	0
2	F6P	A	401	16/16	0.97	0.12	19,23,25,26	0

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 F6P B 401:**

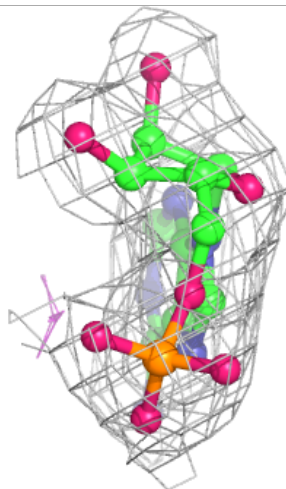
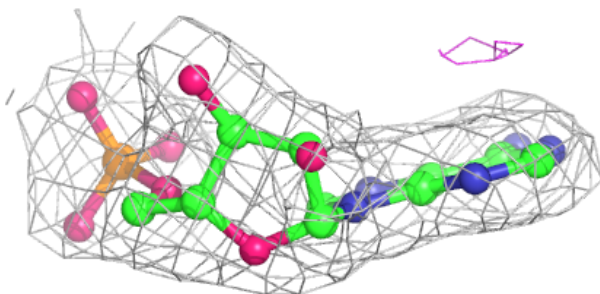
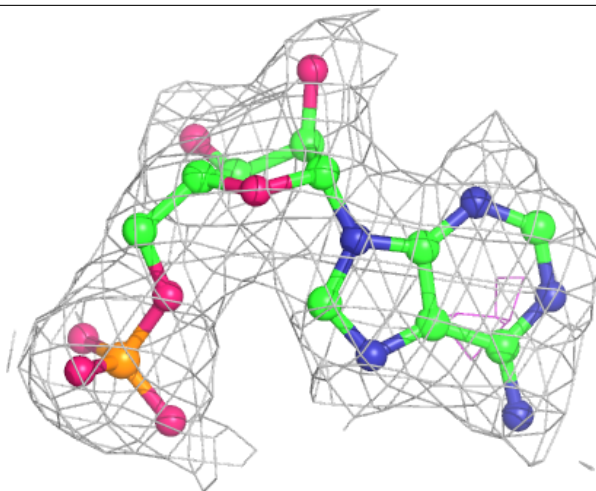
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





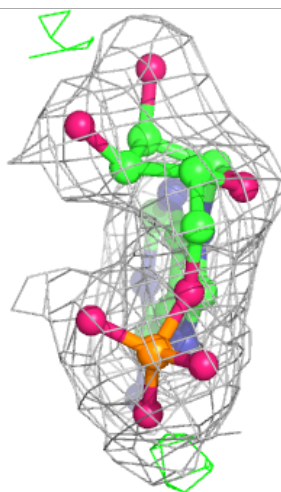
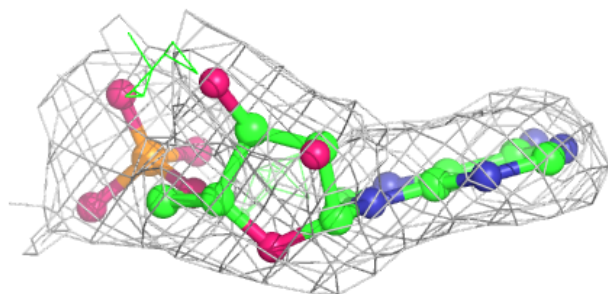
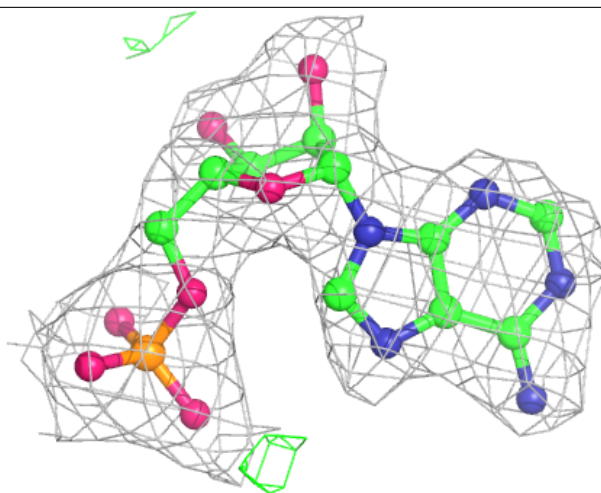
**Electron density around AMP B 404:**

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



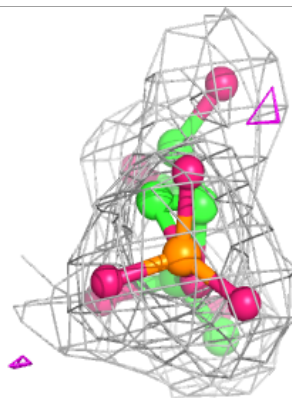
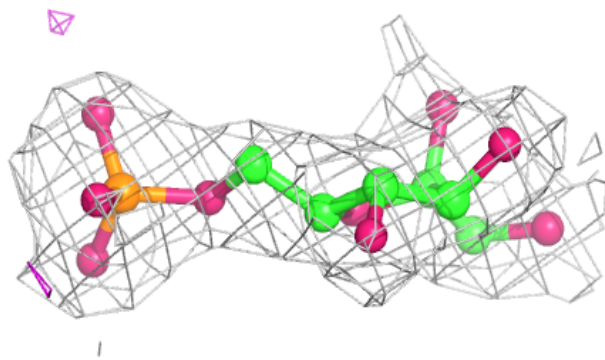
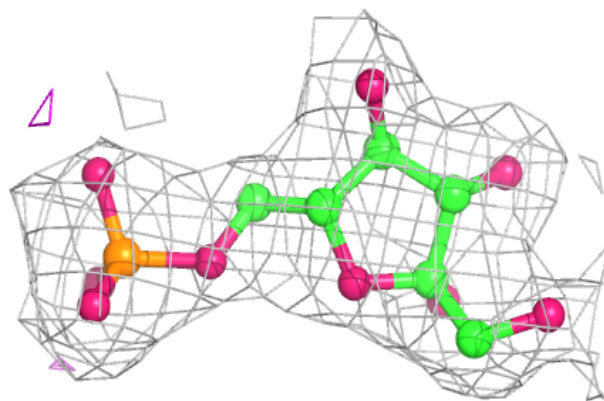
**Electron density around AMP A 404:**

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



**Electron density around F6P A 401:**

$2mF_o - DF_c$  (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.