



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:43 AM BST

PDB ID : 1NV7  
Title : Fructose-1,6-Bisphosphatase Complex With AMP, Magnesium, Fructose-6-Phosphate, Phosphate and Thallium (20 mM)  
Authors : Choe, J.; Iancu, C.V.; Fromm, H.J.; Honzatko, R.B.  
Deposited on : 2003-02-02  
Resolution : 2.15 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.

---

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

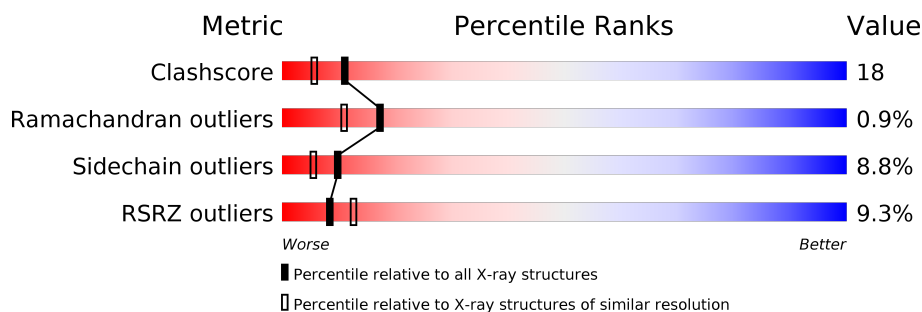
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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>9%</div> <div>67%</div> <div>25%</div> <div>6%</div> <div>.</div> </div>
1	B	337	<div> <div>9%</div> <div>72%</div> <div>20%</div> <div>5%</div> <div>.</div> </div>

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
4	PO4	A	3434	-	-	-	X
4	PO4	B	4434	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TL	A	3354	-	-	-	X
6	TL	B	4353	-	-	-	X
6	TL	B	4354	-	-	-	X

## 2 Entry composition [i](#)

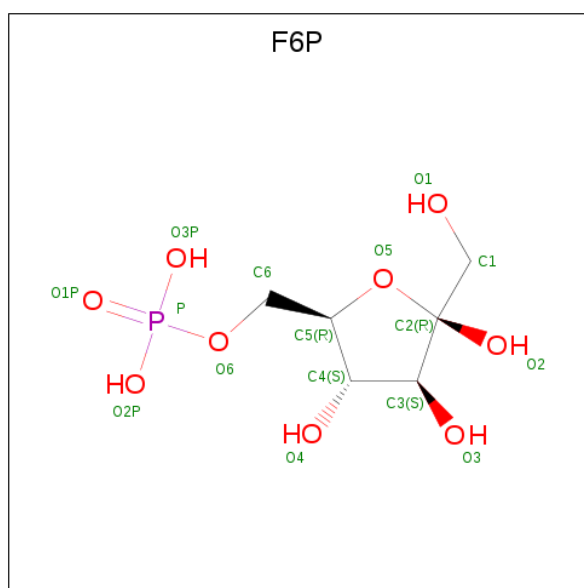
There are 7 unique types of molecules in this entry. The entry contains 5515 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2496	1587	420	474	15			
1	B	327	Total	C	N	O	S	0	0	0
			2496	1587	420	474	15			

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

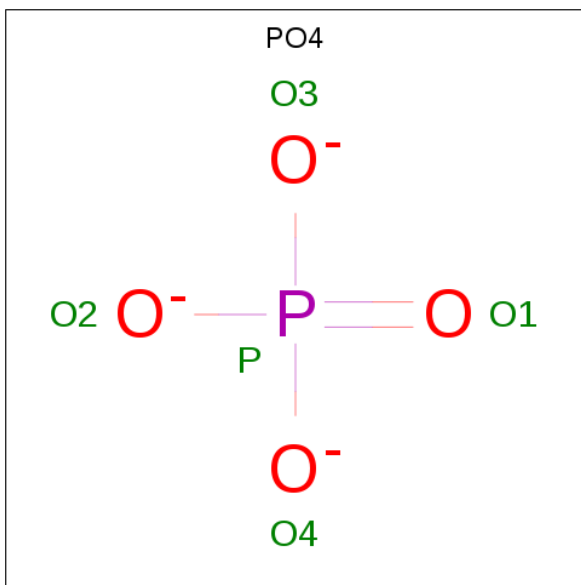


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

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

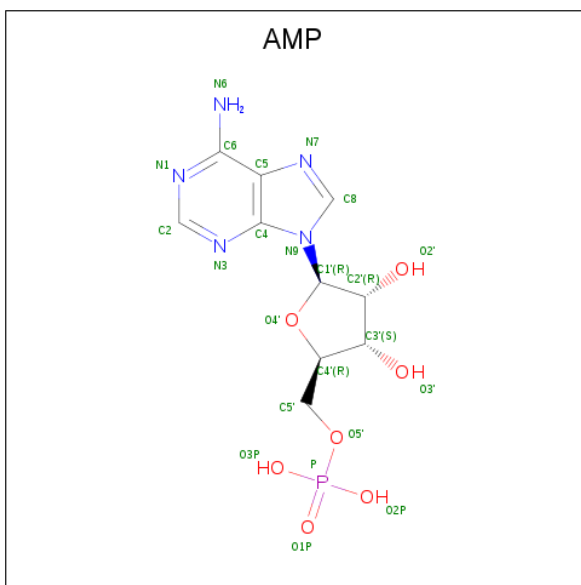
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



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

- Molecule 6 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Tl	0	0
			4	4		
6	A	4	Total	Tl	0	0
			4	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	204	Total	O	0	0
			204	204		
7	B	221	Total	O	0	0
			221	221		

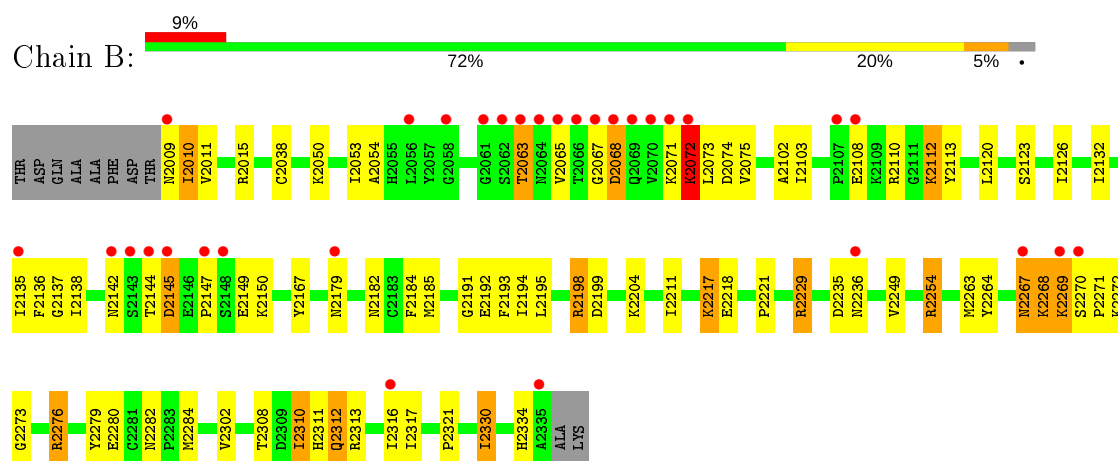
### 3 Residue-property plots [i](#)

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: Fructose-1,6-Bisphosphatase



#### • Molecule 1: Fructose-1,6-Bisphosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.95Å 166.15Å 79.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.15 32.43 – 2.04	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.15) 88.9 (32.43-2.04)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.05Å)	Xtriage
Refinement program	CNS, SHELXL-97	Depositor
R, $R_{free}$	0.182 , 0.251 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 75.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.14% 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, MG, F6P, PO4, TL

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	0.32	0/2538	0.91	4/3434 (0.1%)
1	B	0.36	0/2538	0.98	6/3434 (0.2%)
All	All	0.34	0/5076	0.95	10/6868 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2254	ARG	CD-NE-CZ	18.36	149.31	123.60
1	B	2254	ARG	NE-CZ-NH1	11.49	126.04	120.30
1	A	1254	ARG	CD-NE-CZ	9.48	136.87	123.60
1	A	1254	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	B	2254	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	A	1254	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	B	2276	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	2276	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	1025	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	2229	ARG	NE-CZ-NH1	5.24	122.92	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2552	106	0
1	B	2496	0	2552	81	0
2	A	16	0	10	0	0
2	B	16	0	9	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	23	0	12	1	0
5	B	23	0	12	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	204	0	0	15	0
7	B	221	0	0	11	0
All	All	5515	0	5147	184	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 18.

All (184) 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:2135:ILE:HD11	1:B:2249:VAL:CG2	1.79	1.10
1:B:2135:ILE:HD11	1:B:2249:VAL:HG22	1.12	1.08
1:B:2302:VAL:HG21	1:B:2316:ILE:HD13	1.42	1.01
1:A:1223:ILE:CD1	7:A:5109:HOH:O	2.11	0.97
1:A:1044:ILE:HD11	1:A:1077:SER:HA	1.46	0.97
1:A:1223:ILE:HD12	7:A:5109:HOH:O	1.66	0.95
1:A:1211:ILE:CD1	7:A:5026:HOH:O	2.18	0.91
1:A:1302:VAL:HG21	1:A:1316:ILE:HD13	1.50	0.90
1:A:1044:ILE:CD1	1:A:1077:SER:HA	2.01	0.89
1:A:1211:ILE:HD12	1:A:1212:ASN:H	1.37	0.89
1:A:1211:ILE:HD13	1:A:1263:MET:O	1.77	0.85
1:A:1326:GLU:O	1:A:1330:ILE:HD13	1.75	0.84
1:A:1044:ILE:HD13	1:A:1080:LEU:HD12	1.60	0.83
1:A:1249:VAL:HG12	7:A:5225:HOH:O	1.78	0.83
1:B:2120:LEU:HD11	1:B:2132:ILE:HD13	1.61	0.82
1:B:2010:ILE:HD13	1:B:2011:VAL:N	1.95	0.82
1:B:2108:GLU:HG2	7:B:5307:HOH:O	1.79	0.82
1:A:1058:GLY:HA3	1:A:1063:THR:HB	1.63	0.80
1:A:1211:ILE:HD12	7:A:5026:HOH:O	1.78	0.80
1:B:2126:ILE:HD13	1:B:2132:ILE:HG21	1.64	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:ILE:HD12	1:A:1317:ILE:H	1.46	0.80
1:A:1010:ILE:HD13	1:A:1011:VAL:N	1.96	0.80
1:A:1146:GLU:OE2	1:A:1147:PRO:HD2	1.83	0.79
1:B:2310:ILE:CD1	7:B:5124:HOH:O	2.30	0.79
1:B:2135:ILE:CD1	1:B:2249:VAL:HG22	2.06	0.79
1:B:2204:LYS:HD3	7:B:5313:HOH:O	1.83	0.77
1:B:2132:ILE:HD12	1:B:2167:TYR:HD2	1.49	0.77
1:A:1115:VAL:HG13	1:A:1138:ILE:HD13	1.67	0.76
1:A:1302:VAL:CG2	1:A:1316:ILE:HD13	2.17	0.75
1:A:1218:GLU:OE2	7:A:5392:HOH:O	2.04	0.74
1:A:1102:ALA:HB2	1:A:1149:GLU:HG3	1.68	0.73
1:B:2310:ILE:HD12	7:B:5124:HOH:O	1.88	0.73
1:B:2316:ILE:HD12	1:B:2317:ILE:H	1.53	0.73
1:B:2010:ILE:CD1	1:B:2194:ILE:HD12	2.19	0.73
1:A:1261:ILE:HD12	1:A:1318:LEU:O	1.87	0.72
1:A:1211:ILE:HD12	1:A:1212:ASN:N	2.05	0.72
1:A:1194:ILE:HD11	1:B:2054:ALA:HB2	1.71	0.71
1:A:1142:ASN:H	1:A:1142:ASN:HD22	1.36	0.71
1:B:2310:ILE:HD13	1:B:2310:ILE:H	1.55	0.70
1:A:1044:ILE:CD1	1:A:1080:LEU:HD12	2.21	0.70
1:A:1010:ILE:HD11	1:A:1194:ILE:HG23	1.72	0.70
1:B:2302:VAL:CG2	1:B:2316:ILE:HD13	2.18	0.70
1:A:1229:ARG:NH1	1:A:1330:ILE:HD11	2.06	0.69
1:A:1044:ILE:HD13	1:A:1080:LEU:CD1	2.20	0.69
1:A:1103:ILE:HD13	7:A:5193:HOH:O	1.93	0.68
1:A:1050:LYS:HD2	1:A:1053:ILE:HD12	1.75	0.68
1:B:2269:LYS:HG3	1:B:2269:LYS:O	1.91	0.68
1:B:2010:ILE:HD11	1:B:2194:ILE:HG23	1.75	0.67
1:B:2010:ILE:HD11	1:B:2194:ILE:HD12	1.76	0.67
1:A:1182:ASN:HD22	1:A:1198:ARG:HA	1.58	0.67
1:A:1120:LEU:HD11	1:A:1132:ILE:HD12	1.75	0.67
1:B:2010:ILE:HD13	1:B:2011:VAL:H	1.60	0.67
1:B:2126:ILE:CD1	1:B:2132:ILE:HG21	2.25	0.65
1:A:1316:ILE:HD12	1:A:1317:ILE:N	2.12	0.64
1:A:1328:LEU:O	1:A:1332:GLN:HG3	1.98	0.64
1:B:2310:ILE:HD13	7:B:5124:HOH:O	1.97	0.63
1:A:1115:VAL:HG13	1:A:1138:ILE:CD1	2.28	0.62
1:A:1330:ILE:CD1	7:A:5160:HOH:O	2.48	0.61
1:A:1308:THR:H	1:A:1312:GLN:HE22	1.49	0.61
1:A:1308:THR:H	1:A:1312:GLN:NE2	1.98	0.61
1:A:1065:VAL:O	1:A:1065:VAL:HG23	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2102:ALA:HB2	1:B:2149:GLU:HG3	1.83	0.60
1:A:1096:SER:HB2	1:A:1117:PHE:CZ	2.38	0.59
1:A:1142:ASN:HD22	1:A:1142:ASN:N	2.00	0.59
1:B:2072:LYS:HB3	1:B:2074:ASP:OD2	2.03	0.59
1:B:2229:ARG:NH1	1:B:2330:ILE:HD11	2.18	0.58
1:A:1033:LEU:HD21	1:A:1138:ILE:HD12	1.84	0.58
1:B:2065:VAL:HG12	1:B:2067:GLY:O	2.03	0.57
1:A:1182:ASN:ND2	1:A:1198:ARG:HG3	2.19	0.57
1:A:1261:ILE:CD1	1:A:1324:VAL:HG22	2.35	0.56
1:B:2137:GLY:C	1:B:2138:ILE:HD12	2.25	0.56
1:A:1086:LYS:HE2	1:A:1106:GLU:OE2	2.06	0.56
1:B:2279:TYR:OH	1:B:2311:HIS:HD2	1.89	0.56
1:A:1080:LEU:O	1:A:1084:VAL:HG23	2.05	0.55
1:A:1102:ALA:CB	1:A:1149:GLU:HG3	2.37	0.55
1:B:2310:ILE:H	1:B:2310:ILE:CD1	2.20	0.55
1:A:1133:GLY:HA3	1:A:1249:VAL:HG11	1.89	0.55
1:B:2065:VAL:CG1	1:B:2067:GLY:O	2.55	0.55
1:A:1211:ILE:HD13	7:A:5026:HOH:O	1.95	0.54
1:A:1269:LYS:O	1:A:1271:PRO:HD3	2.07	0.54
1:A:1204:LYS:HD3	7:A:5277:HOH:O	2.07	0.54
1:A:1307:PRO:HA	1:A:1312:GLN:HE22	1.72	0.54
1:A:1059:ILE:HD12	1:B:2010:ILE:HG21	1.90	0.54
1:B:2182:ASN:ND2	1:B:2199:ASP:H	2.05	0.54
1:B:2218:GLU:OE1	1:B:2267:ASN:HB2	2.08	0.53
1:B:2010:ILE:HD12	1:B:2194:ILE:HD12	1.88	0.53
1:B:2229:ARG:CZ	1:B:2330:ILE:HD11	2.38	0.53
1:B:2182:ASN:HD22	1:B:2198:ARG:HA	1.74	0.53
1:A:1263:MET:HB3	1:A:1317:ILE:CD1	2.39	0.53
1:A:1044:ILE:HD12	1:A:1077:SER:OG	2.09	0.53
1:A:1036:SER:O	1:A:1084:VAL:HG11	2.09	0.53
1:B:2072:LYS:HE2	1:B:2074:ASP:OD2	2.08	0.53
1:A:1142:ASN:H	1:A:1142:ASN:ND2	2.05	0.52
1:B:2009:ASN:HA	7:B:5190:HOH:O	2.08	0.52
1:A:1269:LYS:O	1:A:1269:LYS:HE2	2.09	0.52
1:B:2073:LEU:HG	1:B:2120:LEU:HD21	1.92	0.51
1:A:1112:LYS:NZ	5:A:3337:AMP:O1P	2.40	0.51
1:A:1052:GLY:HA2	7:B:5311:HOH:O	2.09	0.51
1:A:1263:MET:HG2	1:A:1317:ILE:HD12	1.93	0.51
1:B:2120:LEU:CD1	1:B:2132:ILE:HD13	2.37	0.51
1:A:1142:ASN:ND2	1:A:1143:SER:H	2.09	0.51
1:A:1063:THR:HG23	1:A:1063:THR:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:SER:HB2	1:A:1117:PHE:CE2	2.46	0.50
1:A:1179:ASN:HB2	7:A:5200:HOH:O	2.11	0.50
1:A:1010:ILE:HD13	1:A:1011:VAL:H	1.76	0.50
1:A:1069:GLN:OE1	1:A:1069:GLN:O	2.30	0.50
1:B:2191:GLY:HA2	7:B:5085:HOH:O	2.12	0.50
1:A:1149:GLU:OE1	1:A:1310:ILE:HD12	2.11	0.50
1:A:1092:CYS:HA	1:A:1105:VAL:HB	1.94	0.50
1:A:1182:ASN:ND2	1:A:1199:ASP:H	2.09	0.50
1:B:2135:ILE:HD12	1:B:2284:MET:CE	2.41	0.49
1:B:2235:ASP:O	1:B:2236:ASN:HB3	2.11	0.49
1:A:1044:ILE:HD12	1:A:1077:SER:CB	2.43	0.49
1:B:2316:ILE:HD12	1:B:2317:ILE:N	2.25	0.48
1:A:1267:ASN:HD22	1:A:1269:LYS:H	1.61	0.48
1:A:1223:ILE:HD11	1:A:1265:PRO:HB2	1.94	0.48
1:B:2270:SER:HB3	1:B:2273:GLY:C	2.34	0.48
1:A:1068:ASP:N	1:A:1068:ASP:OD1	2.47	0.48
1:B:2268:LYS:O	1:B:2271:PRO:HD3	2.13	0.47
1:A:1268:LYS:HE3	7:A:5206:HOH:O	2.14	0.47
1:B:2135:ILE:HD12	1:B:2284:MET:HE1	1.97	0.47
1:B:2103:ILE:HD12	1:B:2103:ILE:N	2.29	0.47
1:B:2068:ASP:N	1:B:2068:ASP:OD1	2.47	0.47
1:B:2254:ARG:HD2	7:B:5056:HOH:O	2.14	0.47
1:B:2195:LEU:HD21	1:B:2198:ARG:HG3	1.98	0.46
1:A:1128:CYS:O	1:A:1129:LEU:HB2	2.14	0.46
1:A:1044:ILE:HD12	1:A:1077:SER:HA	1.90	0.46
1:B:2123:SER:HB3	7:B:5310:HOH:O	2.16	0.46
1:B:2310:ILE:N	1:B:2310:ILE:HD13	2.25	0.46
1:A:1082:ILE:CD1	1:A:1117:PHE:HZ	2.29	0.46
1:A:1218:GLU:OE1	1:A:1268:LYS:HB2	2.15	0.46
1:B:2145:ASP:N	1:B:2145:ASP:OD1	2.49	0.46
1:A:1044:ILE:CD1	1:A:1077:SER:CA	2.86	0.46
1:B:2102:ALA:CB	1:B:2149:GLU:HG3	2.46	0.45
1:B:2204:LYS:HD2	1:B:2321:PRO:HG2	1.98	0.45
1:A:1036:SER:HB3	1:A:1084:VAL:HG12	1.99	0.45
1:A:1029:GLU:OE1	1:A:1112:LYS:HG2	2.16	0.45
1:A:1269:LYS:HB2	7:A:5393:HOH:O	2.17	0.45
1:B:2308:THR:H	1:B:2312:GLN:HE22	1.64	0.44
1:B:2074:ASP:OD2	1:B:2075:VAL:N	2.50	0.44
1:A:1126:ILE:HG23	7:A:5381:HOH:O	2.18	0.44
1:B:2010:ILE:O	1:B:2015:ARG:NH2	2.50	0.44
1:A:1157:ARG:NH1	1:A:1289:GLU:OE2	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:ILE:HG21	1:A:1327:LEU:HD23	1.98	0.44
1:A:1143:SER:OG	1:A:1150:LYS:NZ	2.48	0.43
1:A:1233:PRO:HA	1:A:1234:PRO:HD3	1.91	0.43
1:A:1013:LEU:HD22	1:A:1017:VAL:HG23	2.00	0.43
1:A:1276:ARG:O	1:A:1280:GLU:HB2	2.18	0.43
1:B:2135:ILE:HD11	1:B:2249:VAL:HG21	1.83	0.43
1:A:1053:ILE:HD13	1:B:2185:MET:HG2	2.00	0.43
1:A:1141:LYS:HE3	1:A:1151:ASP:OD2	2.18	0.43
1:A:1092:CYS:HB3	1:A:1111:GLY:O	2.18	0.43
1:B:2270:SER:HB3	1:B:2273:GLY:O	2.19	0.43
1:B:2269:LYS:O	1:B:2269:LYS:NZ	2.52	0.43
1:B:2112:LYS:HG2	1:B:2113:TYR:CE2	2.53	0.43
1:B:2218:GLU:CD	1:B:2268:LYS:HB2	2.39	0.43
1:B:2268:LYS:HB3	1:B:2269:LYS:H	1.68	0.43
1:B:2221:PRO:HB2	1:B:2334:HIS:CE1	2.54	0.43
1:B:2136:PHE:HD1	1:B:2138:ILE:CD1	2.31	0.42
1:B:2308:THR:H	1:B:2312:GLN:NE2	2.17	0.42
1:A:1204:LYS:HA	1:A:1204:LYS:HD3	1.77	0.42
1:A:1310:ILE:HD12	7:A:5197:HOH:O	2.18	0.42
1:A:1261:ILE:HD13	1:A:1324:VAL:HG22	2.01	0.42
1:A:1146:GLU:CD	1:A:1147:PRO:HD2	2.39	0.42
1:B:2276:ARG:O	1:B:2280:GLU:HB2	2.20	0.42
1:B:2050:LYS:HD2	1:B:2053:ILE:HD12	2.02	0.42
1:B:2229:ARG:NH2	1:B:2330:ILE:CD1	2.83	0.42
1:B:2184:PHE:HB3	1:B:2193:PHE:HB3	2.01	0.41
1:B:2217:LYS:HE2	1:B:2217:LYS:HB2	1.59	0.41
1:B:2229:ARG:HH22	1:B:2330:ILE:HD12	1.85	0.41
1:A:1106:GLU:OE1	1:A:1109:LYS:HD2	2.21	0.41
1:A:1082:ILE:HD11	1:A:1117:PHE:HZ	1.84	0.41
1:A:1141:LYS:HE3	1:A:1151:ASP:CG	2.40	0.41
1:A:1115:VAL:HG22	1:A:1138:ILE:CD1	2.51	0.41
1:A:1106:GLU:CD	1:A:1106:GLU:H	2.24	0.41
1:B:2110:ARG:HD3	1:B:2147:PRO:HG3	2.02	0.41
1:B:2132:ILE:HD12	1:B:2167:TYR:CD2	2.40	0.41
1:A:1019:GLU:HA	1:A:1019:GLU:OE2	2.21	0.41
1:B:2211:ILE:HD12	1:B:2263:MET:HB2	2.03	0.41
1:B:2276:ARG:NH2	1:B:2313:ARG:NH2	2.69	0.41
1:A:1143:SER:HB2	1:A:1145:ASP:OD1	2.21	0.40
1:B:2138:ILE:HD12	1:B:2138:ILE:N	2.36	0.40
1:A:1126:ILE:HA	7:B:5084:HOH:O	2.20	0.40
1:A:1184:PHE:HB3	1:A:1193:PHE:HB3	2.04	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%)	310 (95%)	12 (4%)	3 (1%)	17	11
1	B	325/337 (96%)	314 (97%)	8 (2%)	3 (1%)	17	11
All	All	650/674 (96%)	624 (96%)	20 (3%)	6 (1%)	17	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2268	LYS
1	A	1069	GLN
1	B	2072	LYS
1	A	1071	LYS
1	B	2063	THR
1	A	1065	VAL

### 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%)	247 (91%)	25 (9%)	9	5
1	B	272/279 (98%)	249 (92%)	23 (8%)	10	6
All	All	544/558 (98%)	496 (91%)	48 (9%)	10	5

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	ILE
1	A	1013	LEU
1	A	1015	ARG
1	A	1062	SER
1	A	1064	ASN
1	A	1066	THR
1	A	1068	ASP
1	A	1071	LYS
1	A	1074	ASP
1	A	1141	LYS
1	A	1142	ASN
1	A	1145	ASP
1	A	1146	GLU
1	A	1157	ARG
1	A	1197	ASP
1	A	1211	ILE
1	A	1229	ARG
1	A	1264	TYR
1	A	1267	ASN
1	A	1269	LYS
1	A	1277	LEU
1	A	1310	ILE
1	A	1316	ILE
1	A	1330	ILE
1	A	1332	GLN
1	B	2010	ILE
1	B	2038	CYS
1	B	2063	THR
1	B	2068	ASP
1	B	2071	LYS
1	B	2072	LYS
1	B	2112	LYS
1	B	2142	ASN
1	B	2144	THR
1	B	2145	ASP
1	B	2150	LYS
1	B	2179	ASN
1	B	2192	GLU
1	B	2198	ARG
1	B	2217	LYS
1	B	2264	TYR
1	B	2267	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	2269	LYS
1	B	2272	LYS
1	B	2282	ASN
1	B	2310	ILE
1	B	2312	GLN
1	B	2330	ILE

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	1035	ASN
1	A	1064	ASN
1	A	1142	ASN
1	A	1154	GLN
1	A	1158	ASN
1	A	1182	ASN
1	A	1267	ASN
1	A	1311	HIS
1	A	1312	GLN
1	B	2154	GLN
1	B	2158	ASN
1	B	2182	ASN
1	B	2267	ASN
1	B	2282	ASN
1	B	2311	HIS
1	B	2312	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 10 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
5	AMP	B	4337	-	22,25,25	0.67	0	25,38,38	0.67	1 (4%)
5	AMP	A	3337	-	22,25,25	0.67	0	25,38,38	0.70	1 (4%)
2	F6P	A	3336	6	15,16,16	0.60	0	17,25,25	0.68	0
2	F6P	B	4336	6	15,16,16	0.52	0	17,25,25	0.62	0
4	PO4	A	3434	3,6	4,4,4	1.66	0	6,6,6	0.44	0
4	PO4	B	4434	3,6	4,4,4	1.64	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	F6P	A	3336	6	-	0/9/28/28	0/1/1/1
2	F6P	B	4336	6	-	5/9/28/28	0/1/1/1
5	AMP	B	4337	-	-	0/6/26/26	0/3/3/3
5	AMP	A	3337	-	-	0/6/26/26	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3337	AMP	C5-C6-N6	2.29	123.83	120.35
5	B	4337	AMP	C5-C6-N6	2.15	123.62	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

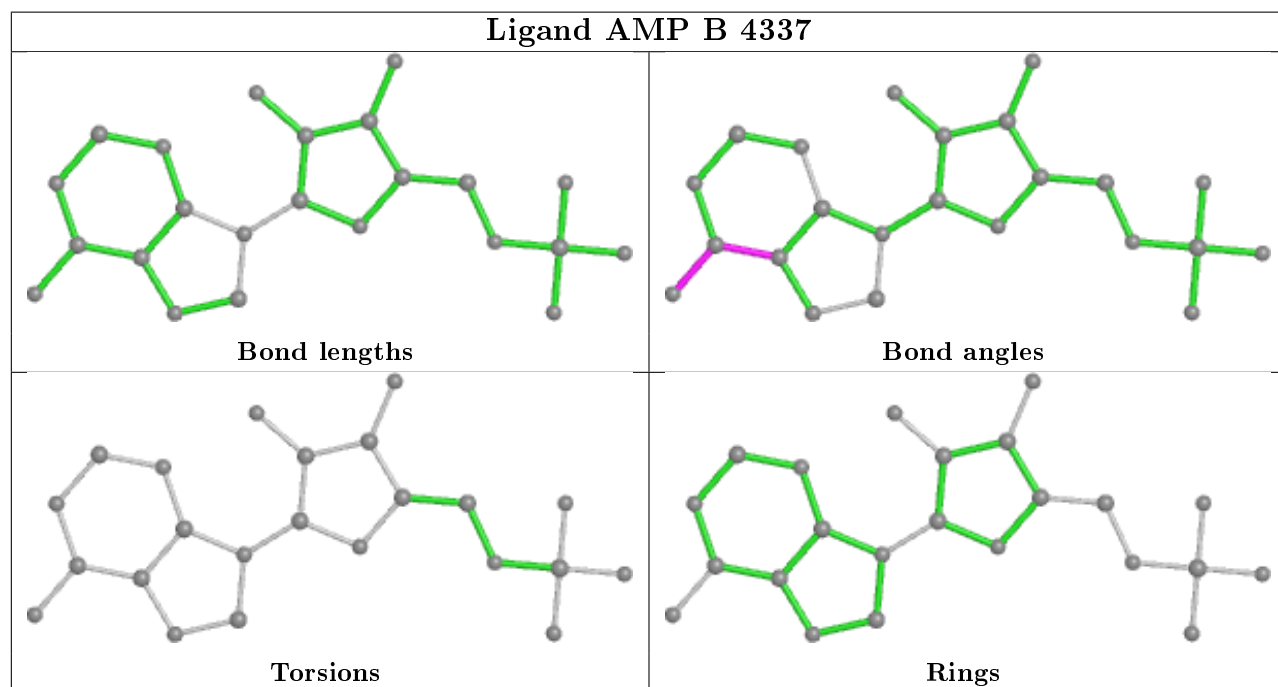
Mol	Chain	Res	Type	Atoms
2	B	4336	F6P	O1-C1-C2-O2
2	B	4336	F6P	O1-C1-C2-C3
2	B	4336	F6P	C6-O6-P-O1P
2	B	4336	F6P	O1-C1-C2-O5
2	B	4336	F6P	C6-O6-P-O2P

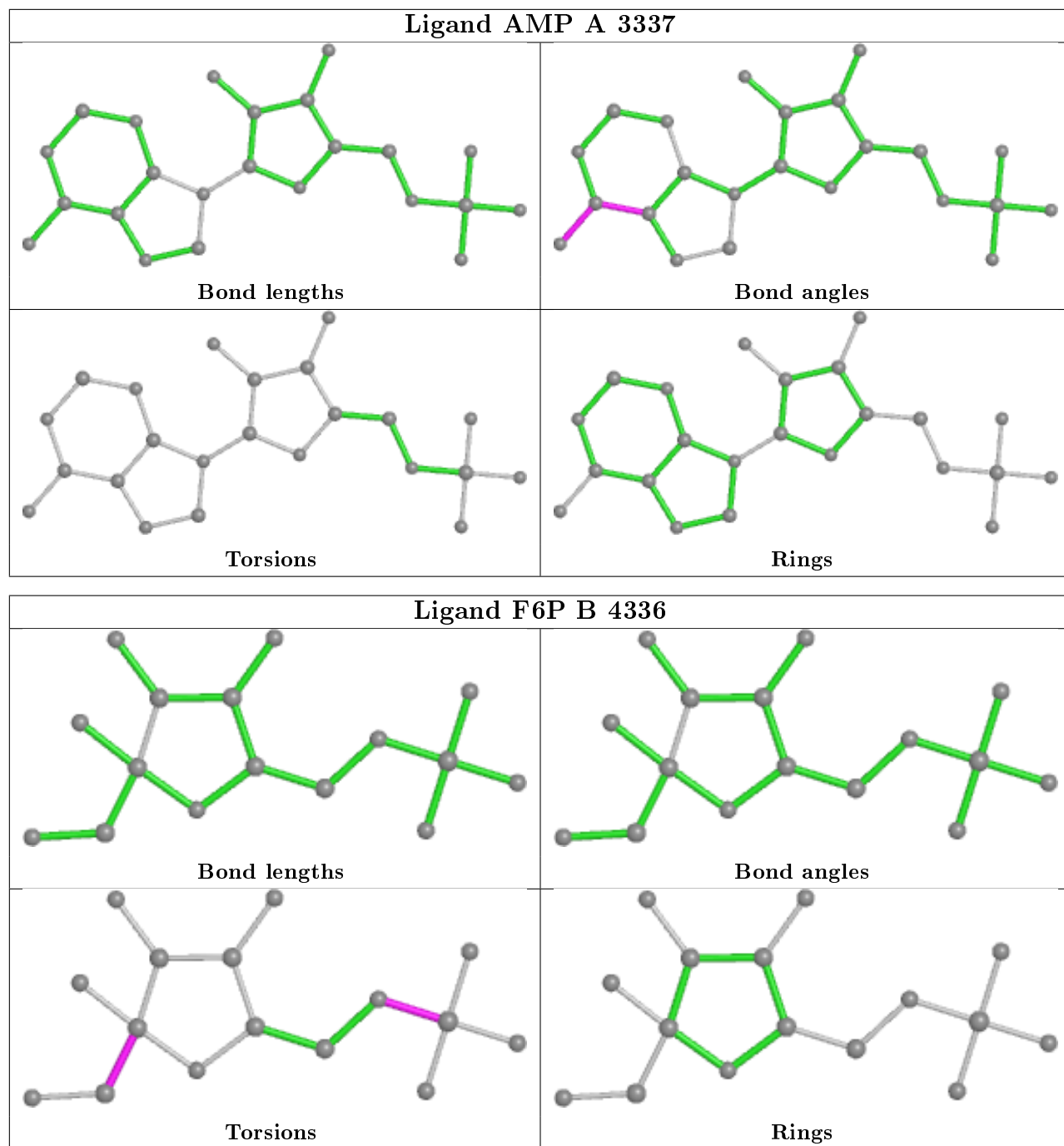
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3337	AMP	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 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.





## 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%)	0.67	30 (9%)	9 13	8, 21, 50, 108	0
1	B	327/337 (97%)	0.61	31 (9%)	8 12	7, 19, 48, 119	1 (0%)
All	All	654/674 (97%)	0.64	61 (9%)	8 13	7, 20, 50, 119	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2067	GLY	19.2
1	B	2065	VAL	15.5
1	A	1063	THR	15.4
1	B	2066	THR	13.5
1	A	1067	GLY	13.3
1	B	2068	ASP	12.9
1	A	1066	THR	11.8
1	B	2070	VAL	11.5
1	A	1064	ASN	11.1
1	B	2064	ASN	10.8
1	A	1070	VAL	9.6
1	A	1068	ASP	9.3
1	B	2069	GLN	9.1
1	A	1335	ALA	8.9
1	B	2063	THR	8.4
1	A	1065	VAL	7.9
1	A	1069	GLN	7.5
1	B	2142	ASN	6.1
1	A	1143	SER	5.6
1	A	1144	THR	5.4
1	B	2267	ASN	5.3
1	A	1062	SER	4.7
1	B	2179	ASN	4.6
1	A	1268	LYS	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	2269	LYS	4.1
1	B	2144	THR	4.1
1	A	1142	ASN	4.1
1	B	2107	PRO	3.7
1	B	2145	ASP	3.7
1	B	2143	SER	3.7
1	B	2062	SER	3.6
1	B	2270	SER	3.6
1	B	2236	ASN	3.6
1	A	1145	ASP	3.5
1	A	1269	LYS	3.5
1	B	2061	GLY	3.4
1	B	2009	ASN	3.4
1	A	1270	SER	3.2
1	A	1332	GLN	3.2
1	A	1236	ASN	3.1
1	A	1330	ILE	3.0
1	B	2072	LYS	2.9
1	B	2108	GLU	2.8
1	B	2071	LYS	2.7
1	A	1009	ASN	2.6
1	A	1061	GLY	2.6
1	A	1108	GLU	2.5
1	A	1037	LEU	2.4
1	B	2135	ILE	2.4
1	A	1179	ASN	2.3
1	B	2056	LEU	2.3
1	B	2148	SER	2.3
1	A	1334	HIS	2.3
1	B	2335	ALA	2.3
1	A	1071	LYS	2.3
1	B	2058	GLY	2.3
1	B	2147	PRO	2.2
1	A	1263	MET	2.1
1	A	1147	PRO	2.0
1	A	1033	LEU	2.0
1	B	2316	ILE	2.0

## 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

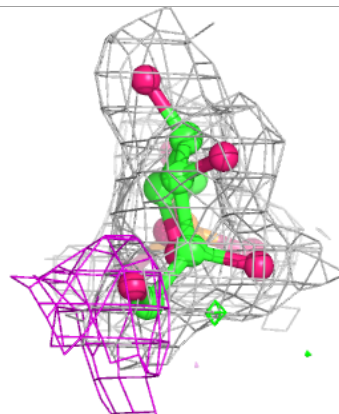
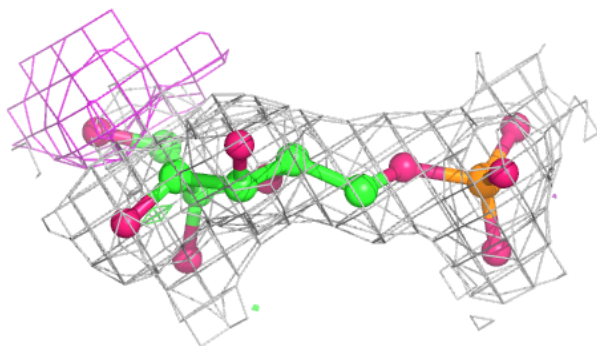
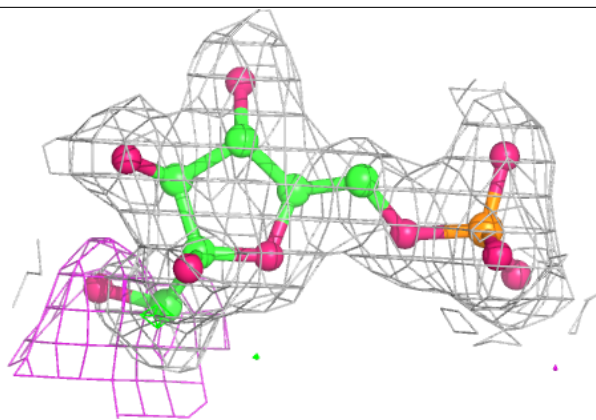
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
6	TL	B	4353	1/1	0.53	0.49	117,117,117,117	0
6	TL	B	4354	1/1	0.53	0.40	126,126,126,126	0
6	TL	A	3352	1/1	0.61	0.39	135,135,135,135	0
4	PO4	A	3434	5/5	0.68	0.43	35,35,35,35	0
6	TL	B	4351	1/1	0.69	0.40	111,111,111,111	0
6	TL	A	3354	1/1	0.70	0.41	118,118,118,118	0
3	MG	A	3341	1/1	0.70	0.26	29,29,29,29	0
4	PO4	B	4434	5/5	0.78	0.49	33,33,33,33	0
6	TL	A	3353	1/1	0.85	0.44	129,129,129,129	0
3	MG	B	4341	1/1	0.87	0.38	24,24,24,24	0
2	F6P	B	4336	16/16	0.88	0.15	16,17,17,19	0
6	TL	B	4352	1/1	0.90	0.34	95,95,95,95	0
2	F6P	A	3336	16/16	0.90	0.15	16,17,17,19	0
5	AMP	B	4337	23/23	0.92	0.15	22,23,23,24	0
5	AMP	A	3337	23/23	0.94	0.14	23,23,24,25	0
6	TL	A	3351	1/1	0.97	0.51	132,132,132,132	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 4336:**

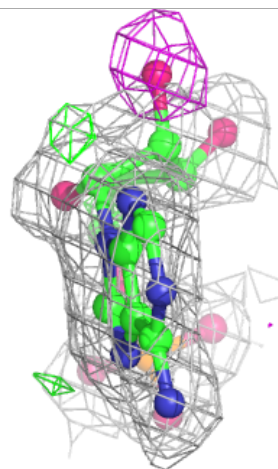
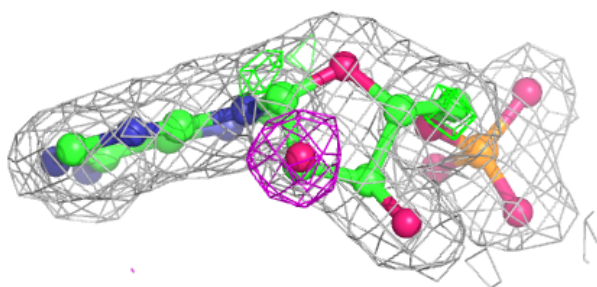
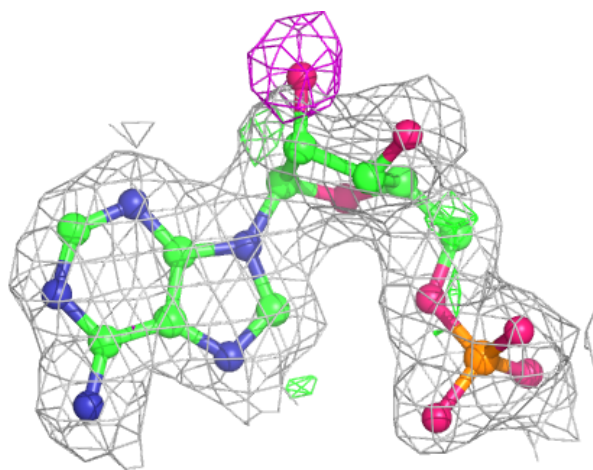
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





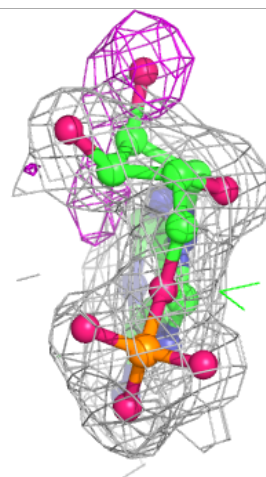
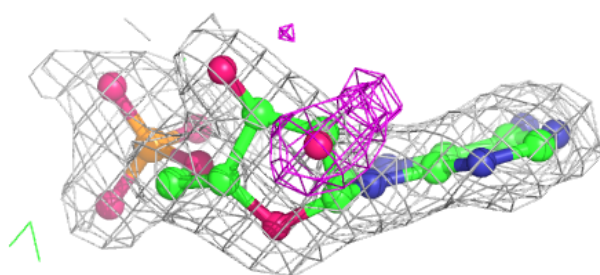
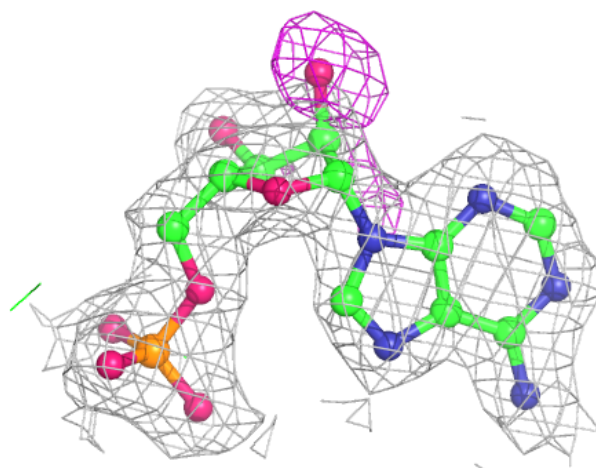
**Electron density around AMP B 4337:**

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



**Electron density around AMP A 3337:**

$2mF_o-DF_c$  (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.