



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:56 AM BST

PDB ID : 3IFC  
Title : Human muscle fructose-1,6-bisphosphatase E69Q mutant in complex with AMP and alpha fructose-6-phosphate  
Authors : Kolodziejczyk, R.; Zarzycki, M.; Jaskolski, M.; Dzugaj, A.  
Deposited on : 2009-07-24  
Resolution : 1.97 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

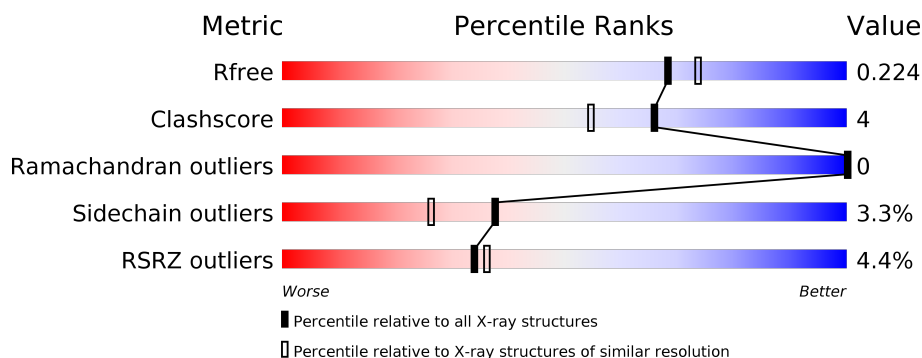
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	338	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>•</div> </div> </div>
1	B	338	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>•</div> <div>5%</div> </div> </div>
1	C	338	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	D	338	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	C	343	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10790 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.

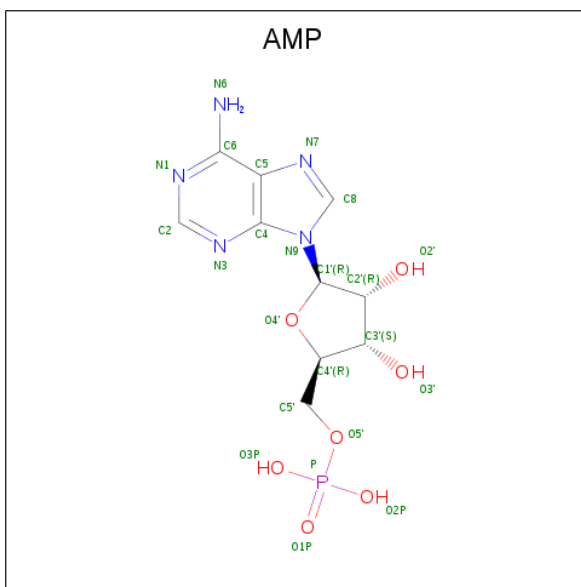
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	36	4	0
			2473	1574	411	475	13			
1	B	320	Total	C	N	O	S	59	5	0
			2471	1575	409	475	12			
1	C	321	Total	C	N	O	S	47	3	0
			2466	1568	411	475	12			
1	D	319	Total	C	N	O	S	65	3	0
			2441	1555	406	467	13			

There are 8 discrepancies between the modelled and reference sequences:

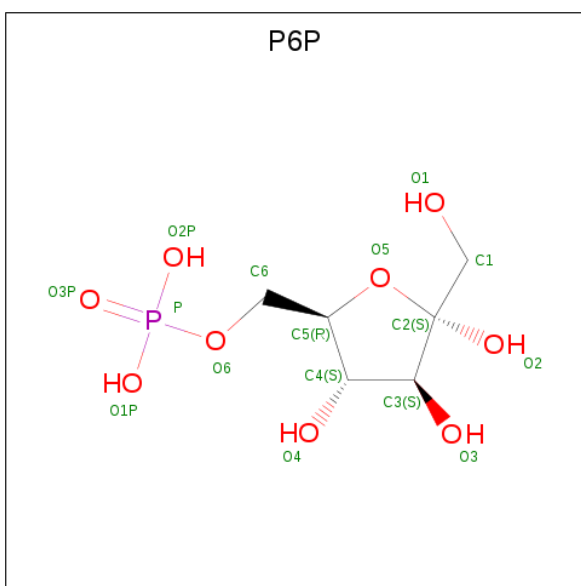
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLN	GLU	engineered mutation	UNP O00757
A	85	LEU	VAL	SEE REMARK 999	UNP O00757
B	69	GLN	GLU	engineered mutation	UNP O00757
B	85	LEU	VAL	SEE REMARK 999	UNP O00757
C	69	GLN	GLU	engineered mutation	UNP O00757
C	85	LEU	VAL	SEE REMARK 999	UNP O00757
D	69	GLN	GLU	engineered mutation	UNP O00757
D	85	LEU	VAL	SEE REMARK 999	UNP O00757

- Molecule 2 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).



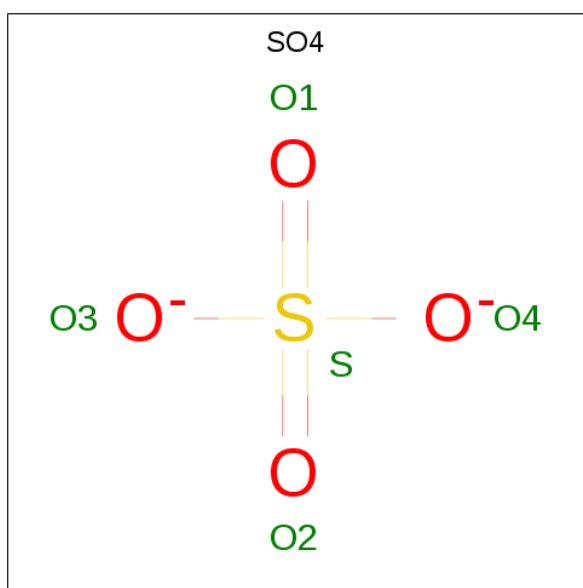
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is 6-O-phosphono-alpha-D-fructofuranose (three-letter code: P6P) (formula:  $C_6H_{13}O_9P$ ).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	218	Total	O	0	0
			218	218		
6	B	163	Total	O	0	0
			163	163		

*Continued on next page...*

*Continued from previous page...*

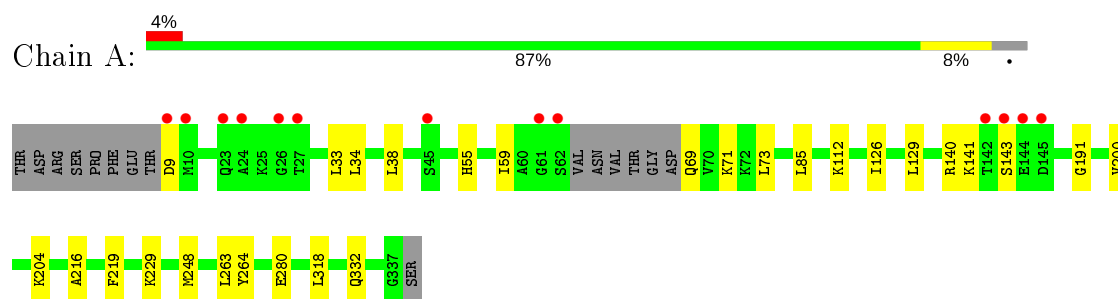
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	183	Total 183	O 183	0	0
6	D	138	Total 138	O 138	0	0



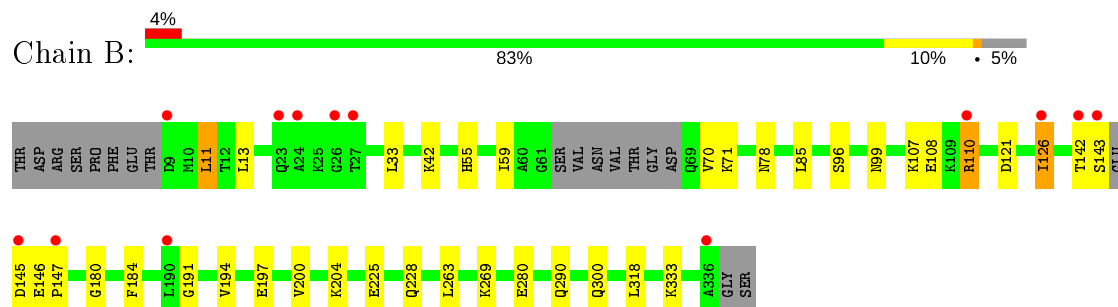
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

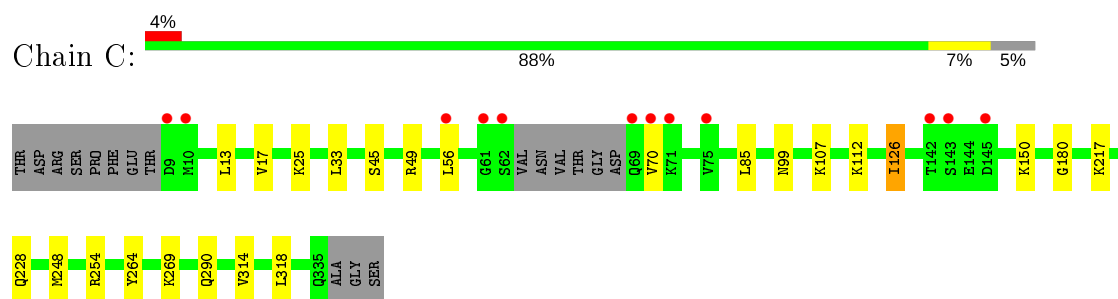
- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2



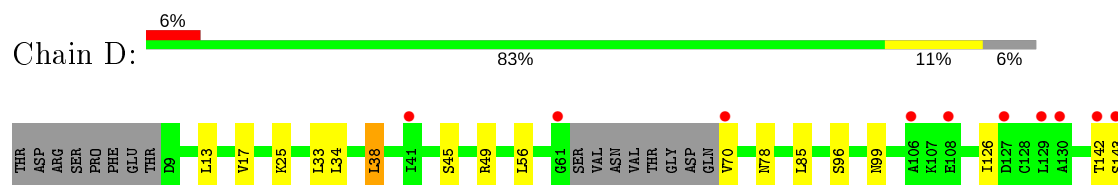
- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

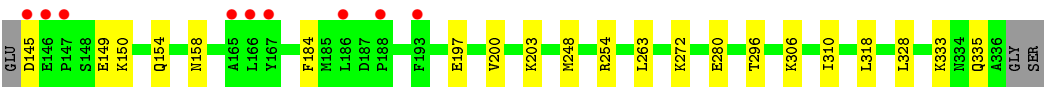


- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2



- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.14Å 234.54Å 71.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.97 49.90 – 1.97	Depositor EDS
% Data completeness (in resolution range)	91.8 (50.00-1.97) 91.7 (49.90-1.97)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.167 , 0.197 0.194 , 0.224	Depositor DCC
$R_{free}$ test set	1334 reflections (1.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10790	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: P6P, GOL, SO4, 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	0.98	0/2523	0.81	0/3409
1	B	0.87	0/2520	0.81	1/3403 (0.0%)
1	C	0.96	3/2510 (0.1%)	0.86	4/3391 (0.1%)
1	D	0.92	2/2487 (0.1%)	0.78	1/3359 (0.0%)
All	All	0.94	5/10040 (0.0%)	0.82	6/13562 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	LYS	CG-CD	-5.96	1.32	1.52
1	D	272	LYS	CG-CD	-5.26	1.34	1.52
1	C	314	VAL	CB-CG2	-5.16	1.42	1.52
1	C	25	LYS	CG-CD	-5.14	1.34	1.52
1	D	25	LYS	CG-CD	-5.08	1.35	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	LYS	CG-CD-CE	-5.97	93.99	111.90
1	C	248	MET	CG-SD-CE	-5.95	90.67	100.20
1	D	254	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	254	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	110	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	112	LYS	N-CA-CB	-5.02	101.56	110.60

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	2473	0	2538	17	0
1	B	2471	0	2534	28	0
1	C	2466	0	2523	8	0
1	D	2441	0	2506	25	0
2	A	23	0	12	1	0
2	B	23	0	12	1	0
2	C	23	0	12	0	0
2	D	23	0	12	1	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	18	0	23	1	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
5	D	6	0	8	0	0
6	A	218	0	0	3	0
6	B	163	0	0	2	0
6	C	183	0	0	1	0
6	D	138	0	0	2	0
All	All	10790	0	10240	79	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 4.

All (79) 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:332:GLN:HG2	6:A:616:HOH:O	1.81	0.80
1:D:78:ASN:HD21	1:D:99:ASN:HD21	1.30	0.79
1:D:203:LYS:HE3	6:D:663:HOH:O	1.85	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASN:HD21	1:B:99:ASN:HD21	1.33	0.76
1:D:197:GLU:HG2	1:D:200:VAL:CG1	2.18	0.73
1:B:146:GLU:HG3	1:B:147:PRO:HD2	1.72	0.71
1:A:248:MET:HE1	1:A:280:GLU:CD	2.15	0.66
1:B:145:ASP:OD2	1:B:146:GLU:N	2.30	0.65
1:B:146:GLU:HG3	1:B:147:PRO:CD	2.26	0.65
1:C:99:ASN:HD22	5:C:343:GOL:H2	1.61	0.65
1:B:143:SER:HB2	1:B:145:ASP:HB2	1.81	0.63
1:B:96:SER:HB3	1:B:99:ASN:HD22	1.63	0.63
1:A:248:MET:HE1	1:A:280:GLU:OE2	1.99	0.63
1:D:197:GLU:HG2	1:D:200:VAL:HG12	1.79	0.62
1:B:143:SER:HB2	1:B:145:ASP:CB	2.31	0.61
1:D:142:THR:O	1:D:143:SER:CB	2.49	0.60
1:D:197:GLU:CG	1:D:200:VAL:HG12	2.33	0.59
1:B:180:GLY:H	1:B:290:GLN:NE2	2.01	0.58
1:B:11:LEU:HD22	1:B:194:VAL:HG13	1.85	0.58
1:D:96:SER:HB3	1:D:99:ASN:HD22	1.69	0.58
1:D:126:ILE:HA	6:D:508:HOH:O	2.03	0.57
1:B:126:ILE:HA	6:B:485:HOH:O	2.05	0.56
1:B:318:LEU:HD12	1:B:318:LEU:C	2.26	0.56
1:D:154:GLN:HE21	1:D:158:ASN:HD22	1.54	0.56
1:B:142:THR:O	1:B:143:SER:CB	2.55	0.55
1:D:142:THR:O	1:D:143:SER:OG	2.20	0.55
1:A:248:MET:CE	1:A:280:GLU:OE2	2.56	0.54
1:B:33[A]:LEU:HD11	1:B:85:LEU:HD22	1.88	0.54
1:D:197:GLU:CG	1:D:200:VAL:CG1	2.86	0.54
1:C:33:LEU:HD11	1:C:85:LEU:HD22	1.90	0.53
1:C:180:GLY:H	1:C:290:GLN:NE2	2.09	0.51
1:B:300:GLN:NE2	6:B:659:HOH:O	2.36	0.50
1:D:197:GLU:HG2	1:D:200:VAL:HG13	1.93	0.49
1:A:140:ARG:NH1	2:A:339:AMP:O3'	2.46	0.48
1:B:33[A]:LEU:CD1	1:B:85:LEU:HD22	2.43	0.48
1:B:11:LEU:CD2	1:B:194:VAL:HG13	2.43	0.48
1:D:248:MET:HE1	1:D:280:GLU:CD	2.34	0.47
1:D:318:LEU:C	1:D:318:LEU:HD12	2.34	0.47
1:D:33:LEU:HD11	1:D:85:LEU:HD22	1.95	0.47
1:A:126:ILE:HA	6:A:394:HOH:O	2.14	0.47
1:B:197:GLU:CD	1:B:200:VAL:HG12	2.35	0.47
1:A:33:LEU:HD11	1:A:85:LEU:HD22	1.96	0.47
1:D:13:LEU:HD12	1:D:17:VAL:HG23	1.96	0.47
1:B:55:HIS:HA	1:B:59:ILE:HG22	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:HD13	1:D:184:PHE:CE1	2.49	0.47
1:A:33:LEU:CD1	1:A:85:LEU:HD22	2.44	0.47
1:D:296:THR:HG21	1:D:328:LEU:HD21	1.97	0.46
1:D:248:MET:HE2	1:D:248:MET:HB2	1.77	0.46
1:C:45:SER:O	1:C:49:ARG:HD3	2.16	0.46
1:B:180:GLY:H	1:B:290:GLN:HE21	1.64	0.46
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.51	0.45
1:A:191:GLY:HA3	1:B:191:GLY:HA3	1.98	0.45
1:D:33:LEU:CD1	1:D:85:LEU:HD22	2.47	0.45
1:A:204:LYS:HB2	5:A:344:GOL:H31	1.99	0.45
1:B:225:GLU:OE1	1:B:333:LYS:HE3	2.17	0.45
1:A:55:HIS:HA	1:A:59:ILE:HG22	2.00	0.44
1:C:33:LEU:CD1	1:C:85:LEU:HD22	2.48	0.44
1:B:121:ASP:OD1	1:B:280[A]:GLU:OE2	2.36	0.43
1:A:248:MET:HE1	1:A:280:GLU:CG	2.48	0.43
1:B:42:LYS:NZ	1:B:191:GLY:O	2.44	0.43
1:B:142:THR:O	1:B:143:SER:HB3	2.18	0.43
1:A:229:LYS:HG3	6:A:562:HOH:O	2.18	0.42
1:D:143:SER:C	1:D:145:ASP:N	2.71	0.42
1:C:13:LEU:HD12	1:C:17:VAL:HG23	2.02	0.42
2:D:339:AMP:H8	2:D:339:AMP:O5'	2.01	0.42
1:D:45:SER:O	1:D:49:ARG:HD3	2.20	0.42
1:B:13:LEU:HD13	1:B:184:PHE:CZ	2.55	0.41
1:D:13:LEU:HD13	1:D:184:PHE:CZ	2.55	0.41
1:B:143:SER:C	1:B:145:ASP:N	2.73	0.41
2:B:339:AMP:O5'	2:B:339:AMP:H8	2.03	0.41
1:A:141:LYS:NZ	1:A:143:SER:O	2.50	0.41
1:C:126:ILE:HA	6:C:487:HOH:O	2.21	0.41
1:D:34:LEU:O	1:D:38:LEU:HD22	2.22	0.40
1:A:318:LEU:C	1:A:318:LEU:HD12	2.41	0.40
1:A:34:LEU:O	1:A:38:LEU:HD23	2.21	0.40
1:D:149:GLU:HG3	1:D:310:ILE:HG21	2.04	0.40
1:C:318:LEU:HD12	1:C:318:LEU:C	2.42	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	323/338 (96%)	318 (98%)	5 (2%)	0	100	100
1	B	319/338 (94%)	312 (98%)	7 (2%)	0	100	100
1	C	320/338 (95%)	312 (98%)	8 (2%)	0	100	100
1	D	316/338 (94%)	309 (98%)	7 (2%)	0	100	100
All	All	1278/1352 (94%)	1251 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	269/279 (96%)	259 (96%)	10 (4%)	34	22
1	B	268/279 (96%)	257 (96%)	11 (4%)	30	18
1	C	268/279 (96%)	260 (97%)	8 (3%)	41	29
1	D	265/279 (95%)	257 (97%)	8 (3%)	41	29
All	All	1070/1116 (96%)	1033 (96%)	37 (4%)	38	24

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	69	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	71	LYS
1	A	73	LEU
1	A	112	LYS
1	A	129	LEU
1	A	200[A]	VAL
1	A	200[B]	VAL
1	A	263	LEU
1	A	264	TYR
1	B	11	LEU
1	B	70	VAL
1	B	71	LYS
1	B	107	LYS
1	B	108	GLU
1	B	110	ARG
1	B	126	ILE
1	B	204	LYS
1	B	228	GLN
1	B	263	LEU
1	B	269	LYS
1	C	56	LEU
1	C	70	VAL
1	C	126	ILE
1	C	217	LYS
1	C	228[A]	GLN
1	C	228[B]	GLN
1	C	264	TYR
1	C	269	LYS
1	D	38	LEU
1	D	56	LEU
1	D	70	VAL
1	D	150	LYS
1	D	263	LEU
1	D	306	LYS
1	D	333	LYS
1	D	335	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	325	GLN
1	B	99	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	158	ASN
1	B	290	GLN
1	C	158	ASN
1	C	290	GLN
1	D	99	ASN
1	D	154	GLN
1	D	300	GLN

### 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 ⓘ

23 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
4	SO4	B	341	-	4,4,4	0.16	0	6,6,6	0.71	0
2	AMP	D	339	-	22,25,25	1.39	4 (18%)	25,38,38	1.37	3 (12%)
5	GOL	A	346	-	5,5,5	0.42	0	5,5,5	0.88	0
2	AMP	B	339	-	22,25,25	1.34	3 (13%)	25,38,38	1.36	3 (12%)
5	GOL	B	343	-	5,5,5	0.79	0	5,5,5	1.87	2 (40%)
4	SO4	A	341	-	4,4,4	0.28	0	6,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	D	342	-	4,4,4	0.32	0	6,6,6	0.47	0
3	P6P	D	340	-	15,16,16	1.33	1 (6%)	17,25,25	1.31	2 (11%)
4	SO4	A	343	-	4,4,4	0.26	0	6,6,6	0.56	0
2	AMP	A	339	-	22,25,25	1.37	4 (18%)	25,38,38	1.71	8 (32%)
2	AMP	C	339	-	22,25,25	1.06	2 (9%)	25,38,38	1.45	5 (20%)
5	GOL	C	343	-	5,5,5	0.77	0	5,5,5	2.68	3 (60%)
5	GOL	D	343	-	5,5,5	0.60	0	5,5,5	1.01	0
3	P6P	A	340	-	15,16,16	1.36	2 (13%)	17,25,25	1.24	1 (5%)
5	GOL	A	345	-	5,5,5	1.17	1 (20%)	5,5,5	1.88	1 (20%)
4	SO4	D	341	-	4,4,4	0.18	0	6,6,6	0.29	0
4	SO4	C	342	-	4,4,4	0.25	0	6,6,6	0.73	0
4	SO4	C	341	-	4,4,4	0.15	0	6,6,6	0.32	0
3	P6P	C	340	-	15,16,16	1.29	1 (6%)	17,25,25	0.99	1 (5%)
3	P6P	B	340	-	15,16,16	1.56	2 (13%)	17,25,25	1.31	4 (23%)
5	GOL	A	344	-	5,5,5	0.37	0	5,5,5	1.17	0
4	SO4	A	342	-	4,4,4	0.26	0	6,6,6	0.42	0
4	SO4	B	342	-	4,4,4	0.27	0	6,6,6	0.64	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
5	GOL	D	343	-	-	4/4/4/4	-
2	AMP	D	339	-	-	0/6/26/26	0/3/3/3
5	GOL	B	343	-	-	2/4/4/4	-
5	GOL	A	345	-	-	1/4/4/4	-
5	GOL	A	346	-	-	4/4/4/4	-
2	AMP	A	339	-	-	0/6/26/26	0/3/3/3
2	AMP	C	339	-	-	0/6/26/26	0/3/3/3
5	GOL	C	343	-	-	3/4/4/4	-
5	GOL	A	344	-	-	2/4/4/4	-
2	AMP	B	339	-	-	0/6/26/26	0/3/3/3
3	P6P	D	340	-	-	6/9/28/28	0/1/1/1
3	P6P	A	340	-	-	4/9/28/28	0/1/1/1
3	P6P	C	340	-	-	1/9/28/28	0/1/1/1
3	P6P	B	340	-	-	5/9/28/28	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	340	P6P	O2-C2	4.98	1.49	1.40
3	C	340	P6P	O2-C2	4.43	1.48	1.40
3	D	340	P6P	O2-C2	4.09	1.47	1.40
2	B	339	AMP	O4'-C1'	3.46	1.45	1.41
2	D	339	AMP	C2-N3	3.45	1.37	1.32
3	A	340	P6P	O2-C2	3.39	1.46	1.40
2	A	339	AMP	C5-C4	3.22	1.49	1.40
2	A	339	AMP	O4'-C1'	3.18	1.45	1.41
2	B	339	AMP	C5-C4	3.06	1.49	1.40
2	B	339	AMP	C2-N3	2.81	1.36	1.32
2	D	339	AMP	C5-C4	2.81	1.48	1.40
2	A	339	AMP	C2-N3	2.63	1.36	1.32
3	A	340	P6P	O3-C3	2.59	1.47	1.42
5	A	345	GOL	O2-C2	-2.51	1.35	1.43
2	C	339	AMP	C5-C4	2.48	1.47	1.40
2	D	339	AMP	O4'-C1'	2.48	1.44	1.41
2	C	339	AMP	C2-N3	2.40	1.36	1.32
2	D	339	AMP	C2-N1	2.28	1.38	1.33
3	B	340	P6P	C1-C2	2.10	1.55	1.52
2	A	339	AMP	C2-N1	2.04	1.37	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	339	AMP	N3-C2-N1	-3.52	123.18	128.68
5	C	343	GOL	C3-C2-C1	3.52	125.38	111.70
5	C	343	GOL	O2-C2-C3	-3.43	94.02	109.12
2	B	339	AMP	N3-C2-N1	-3.27	123.57	128.68
2	A	339	AMP	O3P-P-O2P	3.21	119.89	107.64
2	D	339	AMP	N3-C2-N1	-3.19	123.69	128.68
2	C	339	AMP	N3-C2-N1	-3.19	123.70	128.68
3	C	340	P6P	O2P-P-O6	2.99	114.69	106.73
5	B	343	GOL	O3-C3-C2	-2.98	95.92	110.20
2	B	339	AMP	C2-N1-C6	2.93	123.76	118.75
2	A	339	AMP	N6-C6-N1	2.87	124.54	118.57
2	D	339	AMP	N6-C6-N1	2.81	124.41	118.57
5	A	345	GOL	O2-C2-C3	-2.77	96.92	109.12
2	C	339	AMP	O5'-P-O1P	-2.77	98.71	106.47
2	A	339	AMP	O2P-P-O5'	-2.73	99.46	106.73
2	A	339	AMP	O5'-P-O1P	-2.58	99.23	106.47
5	C	343	GOL	O3-C3-C2	-2.53	98.09	110.20
2	A	339	AMP	C2-N1-C6	2.49	123.01	118.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	339	AMP	N6-C6-N1	2.48	123.71	118.57
2	D	339	AMP	C1'-N9-C4	-2.42	122.39	126.64
3	B	340	P6P	O2-C2-O5	2.37	114.08	109.50
2	B	339	AMP	N6-C6-N1	2.34	123.44	118.57
2	C	339	AMP	C1'-N9-C4	-2.34	122.53	126.64
3	A	340	P6P	P-O6-C6	2.34	124.73	118.30
3	D	340	P6P	O2P-P-O1P	2.31	116.46	107.64
3	B	340	P6P	O2P-P-O3P	-2.25	101.86	110.68
2	A	339	AMP	O4'-C1'-C2'	-2.22	103.69	106.93
2	A	339	AMP	O3P-P-O5'	2.21	112.63	106.73
5	B	343	GOL	O2-C2-C3	-2.14	99.70	109.12
3	B	340	P6P	O1P-P-O6	2.14	112.42	106.73
3	D	340	P6P	P-O6-C6	2.12	124.14	118.30
3	B	340	P6P	O3-C3-C4	2.03	120.32	113.32
2	C	339	AMP	O3P-P-O2P	2.00	115.28	107.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	346	GOL	O1-C1-C2-C3
5	A	346	GOL	C1-C2-C3-O3
5	B	343	GOL	C1-C2-C3-O3
3	D	340	P6P	C6-O6-P-O1P
3	D	340	P6P	C6-O6-P-O2P
3	D	340	P6P	O1-C1-C2-O2
3	D	340	P6P	O1-C1-C2-C3
5	C	343	GOL	C1-C2-C3-O3
5	D	343	GOL	O1-C1-C2-O2
5	D	343	GOL	C1-C2-C3-O3
3	A	340	P6P	O1-C1-C2-O2
3	A	340	P6P	O1-C1-C2-C3
3	A	340	P6P	O1-C1-C2-O5
3	B	340	P6P	C6-O6-P-O1P
3	B	340	P6P	C6-O6-P-O2P
5	A	344	GOL	O1-C1-C2-O2
5	A	344	GOL	O1-C1-C2-C3
5	D	343	GOL	O2-C2-C3-O3
3	D	340	P6P	O1-C1-C2-O5
5	D	343	GOL	O1-C1-C2-C3
5	A	346	GOL	O1-C1-C2-O2
5	A	346	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	340	P6P	C6-O6-P-O3P
3	B	340	P6P	C6-O6-P-O3P
5	B	343	GOL	O2-C2-C3-O3
5	C	343	GOL	O2-C2-C3-O3
3	B	340	P6P	O1-C1-C2-C3
3	B	340	P6P	O1-C1-C2-O2
3	A	340	P6P	C6-O6-P-O1P
3	C	340	P6P	O1-C1-C2-C3
5	C	343	GOL	O1-C1-C2-C3
5	A	345	GOL	O1-C1-C2-C3

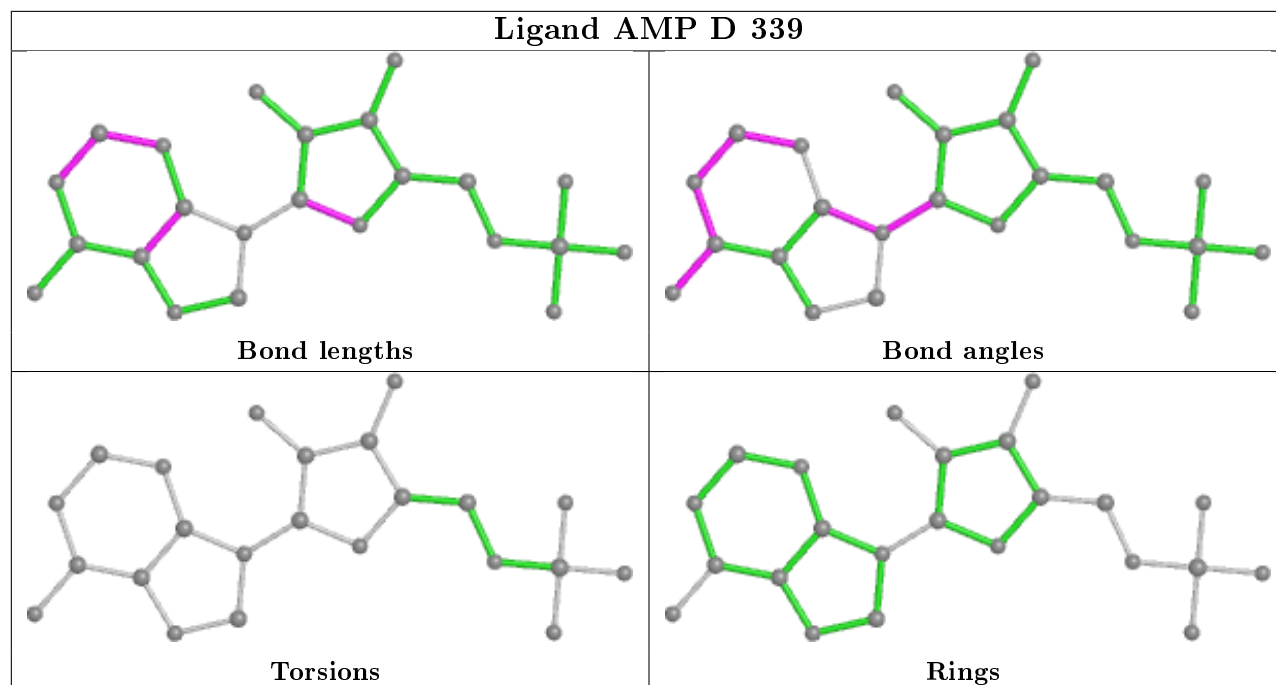
There are no ring outliers.

5 monomers are involved in 5 short contacts:

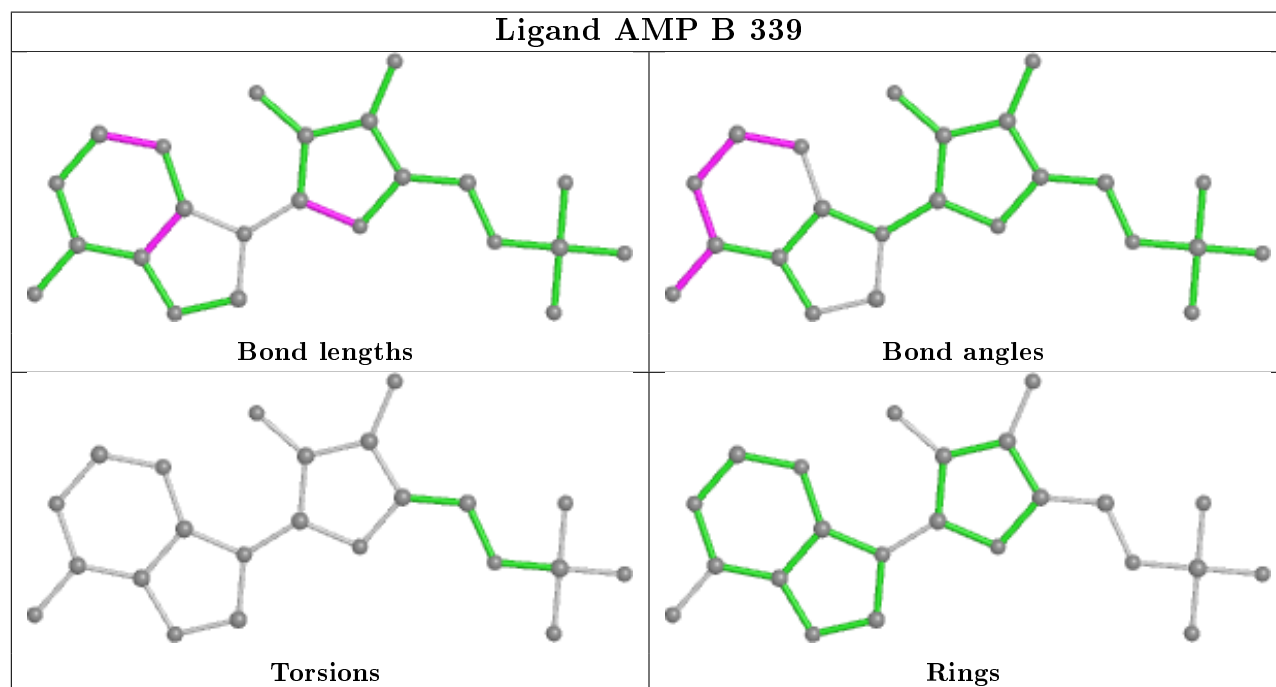
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	339	AMP	1	0
2	B	339	AMP	1	0
2	A	339	AMP	1	0
5	C	343	GOL	1	0
5	A	344	GOL	1	0

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.

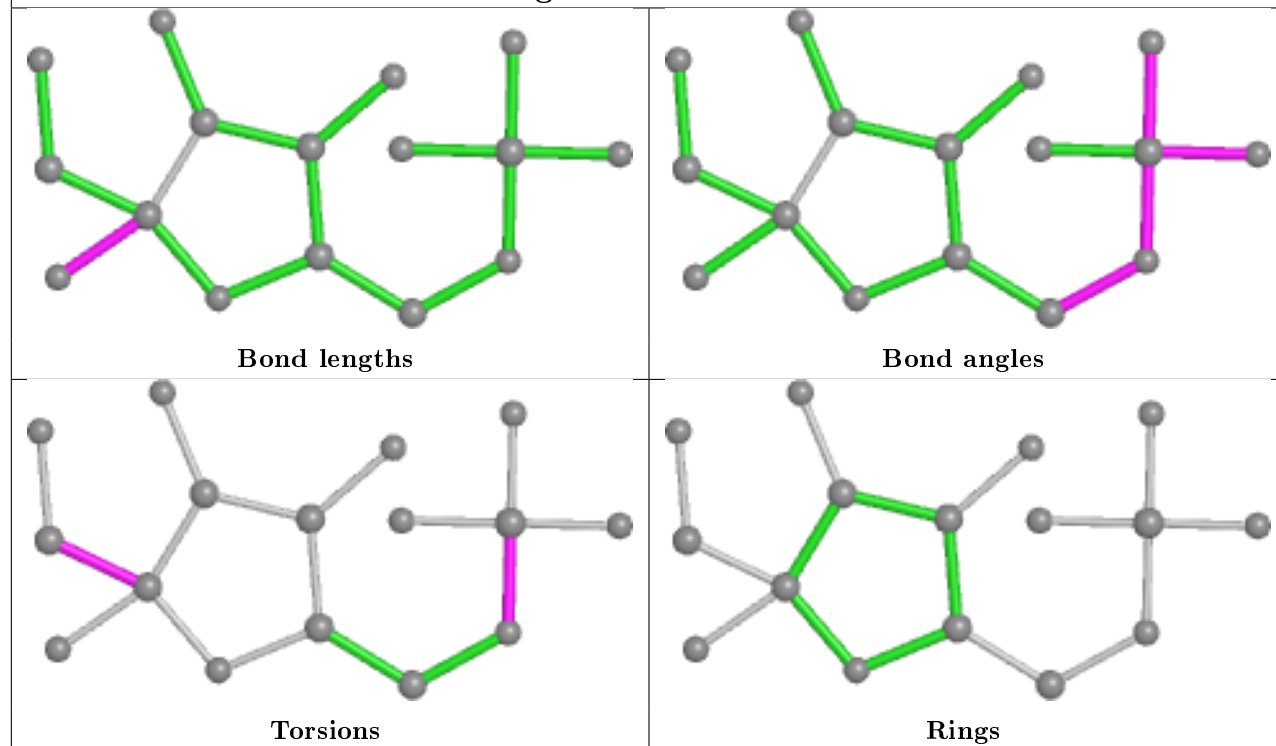
## Ligand AMP D 339



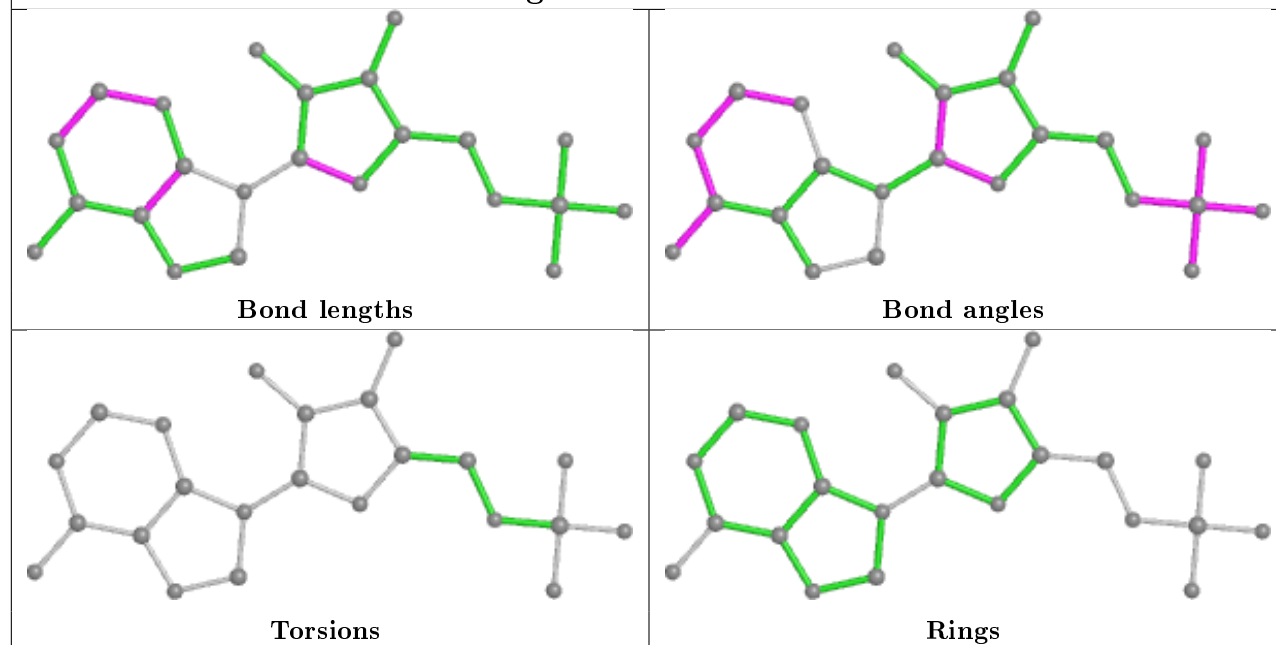
## Ligand AMP B 339



## Ligand P6P D 340

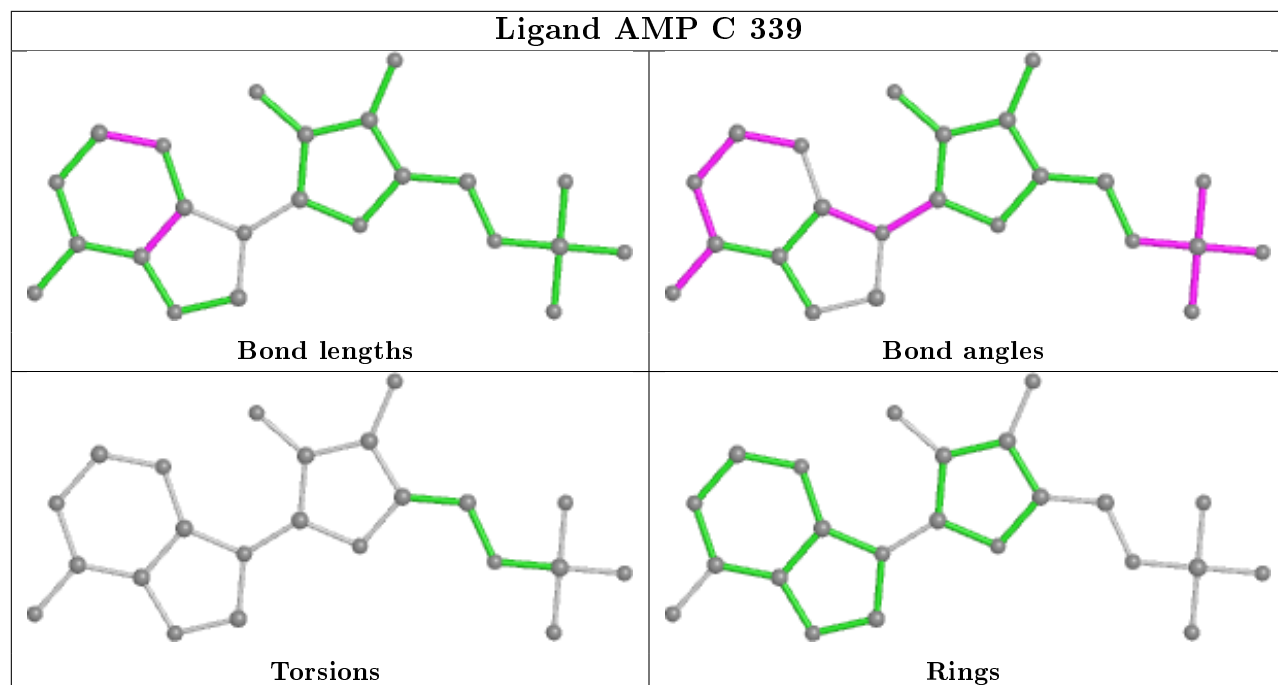


## Ligand AMP A 339

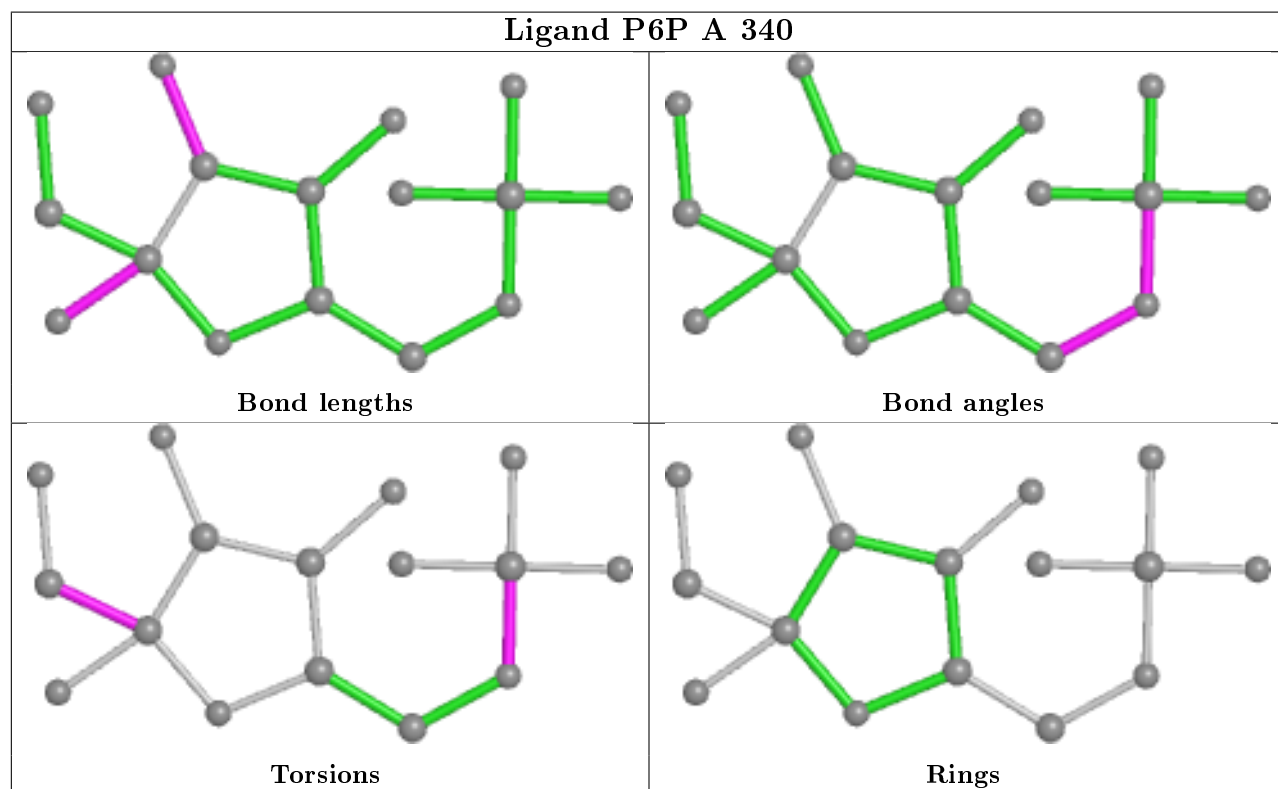


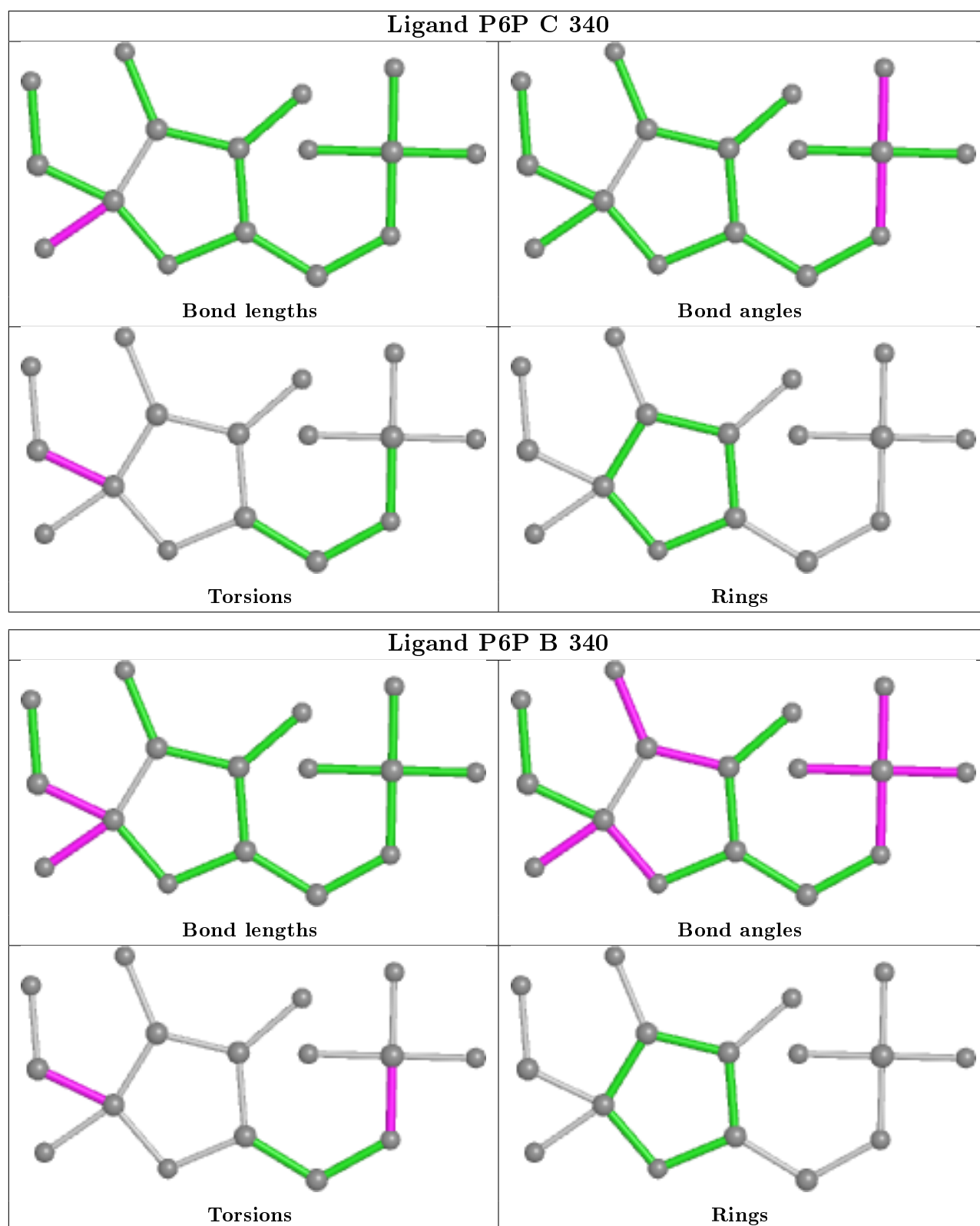


## Ligand AMP C 339



## Ligand P6P A 340





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	323/338 (95%)	0.24	13 (4%)	38 40	16, 26, 51, 82	12 (3%)
1	B	320/338 (94%)	0.27	13 (4%)	37 39	21, 32, 58, 79	19 (5%)
1	C	321/338 (94%)	0.30	12 (3%)	41 44	18, 28, 52, 74	14 (4%)
1	D	319/338 (94%)	0.41	19 (5%)	21 23	21, 32, 56, 74	21 (6%)
All	All	1283/1352 (94%)	0.30	57 (4%)	34 36	16, 30, 55, 82	66 (5%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	142	THR	7.3
1	C	70	VAL	7.2
1	B	142	THR	5.2
1	A	142	THR	4.8
1	D	145	ASP	4.5
1	A	144	GLU	4.3
1	C	71	LYS	4.2
1	C	142	THR	4.2
1	A	62	SER	4.1
1	D	70	VAL	4.0
1	C	69	GLN	3.8
1	A	10	MET	3.7
1	A	24	ALA	3.7
1	B	145	ASP	3.6
1	B	27	THR	3.5
1	C	62	SER	3.3
1	D	129	LEU	3.3
1	A	61	GLY	3.2
1	D	61	GLY	3.1
1	B	336	ALA	3.1
1	B	26	GLY	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	145	ASP	3.1
1	D	143	SER	2.9
1	A	143	SER	2.8
1	D	108	GLU	2.8
1	B	143	SER	2.8
1	B	9	ASP	2.7
1	D	147	PRO	2.6
1	A	26	GLY	2.6
1	D	106	ALA	2.6
1	D	193	PHE	2.6
1	D	166	LEU	2.6
1	D	130	ALA	2.5
1	B	110	ARG	2.5
1	C	9	ASP	2.4
1	D	188	PRO	2.4
1	B	126	ILE	2.3
1	D	186	LEU	2.3
1	A	23	GLN	2.3
1	B	147	PRO	2.3
1	D	167	TYR	2.2
1	C	75	VAL	2.2
1	A	27	THR	2.2
1	D	146	GLU	2.2
1	D	41	ILE	2.2
1	B	24	ALA	2.2
1	B	190	LEU	2.1
1	C	143	SER	2.1
1	C	56	LEU	2.1
1	D	127	ASP	2.1
1	A	9	ASP	2.1
1	C	61	GLY	2.1
1	C	145	ASP	2.0
1	D	165	ALA	2.0
1	B	23	GLN	2.0
1	A	45	SER	2.0
1	C	10	MET	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 ⓘ

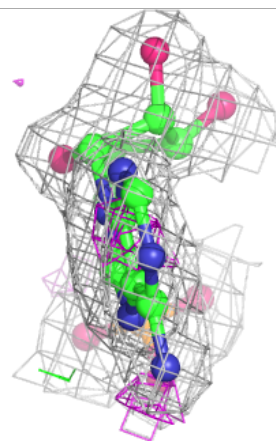
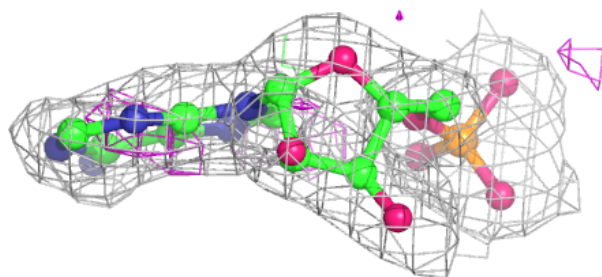
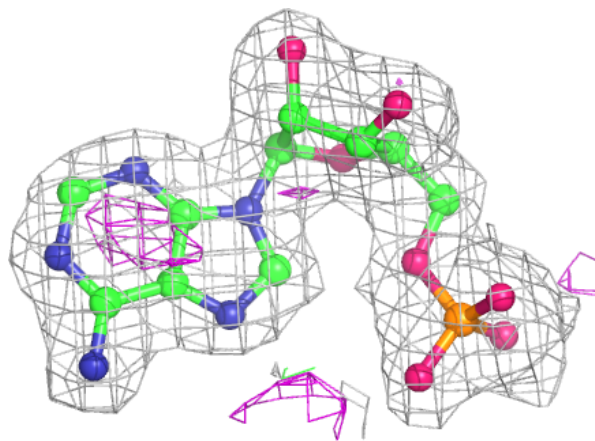
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	D	343	6/6	0.88	0.16	51,56,56,57	0
5	GOL	A	344	6/6	0.88	0.24	36,42,45,48	0
5	GOL	A	345	6/6	0.89	0.15	38,42,44,45	0
5	GOL	A	346	6/6	0.89	0.14	55,57,59,59	0
5	GOL	B	343	6/6	0.92	0.12	42,46,49,50	0
5	GOL	C	343	6/6	0.93	0.15	40,41,45,45	0
4	SO4	B	342	5/5	0.93	0.10	42,44,45,46	5
2	AMP	D	339	23/23	0.94	0.13	36,42,43,45	0
2	AMP	B	339	23/23	0.94	0.22	37,40,43,44	0
4	SO4	B	341	5/5	0.95	0.10	44,44,49,51	5
3	P6P	D	340	16/16	0.95	0.15	33,46,50,53	0
4	SO4	A	343	5/5	0.95	0.18	41,44,46,47	5
4	SO4	C	341	5/5	0.95	0.13	41,43,45,46	5
3	P6P	B	340	16/16	0.95	0.15	30,44,52,56	0
2	AMP	A	339	23/23	0.95	0.17	31,35,38,38	0
2	AMP	C	339	23/23	0.95	0.13	30,36,40,40	0
3	P6P	A	340	16/16	0.96	0.12	27,38,43,45	0
3	P6P	C	340	16/16	0.97	0.13	28,36,45,51	0
4	SO4	D	341	5/5	0.97	0.11	40,43,45,45	5
4	SO4	C	342	5/5	0.97	0.11	36,37,39,39	5
4	SO4	A	342	5/5	0.97	0.10	40,42,43,46	5
4	SO4	D	342	5/5	0.97	0.10	38,43,44,45	5
4	SO4	A	341	5/5	0.98	0.07	42,43,44,46	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.

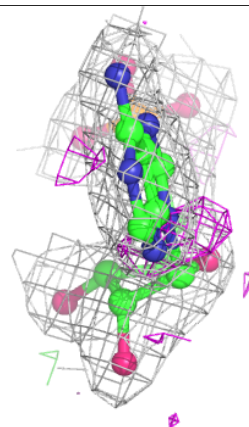
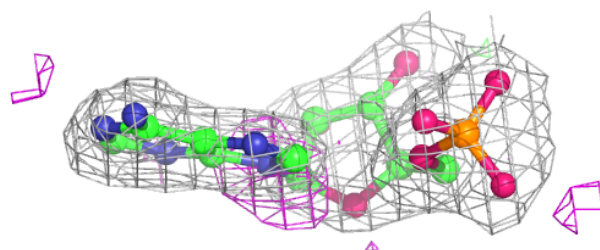
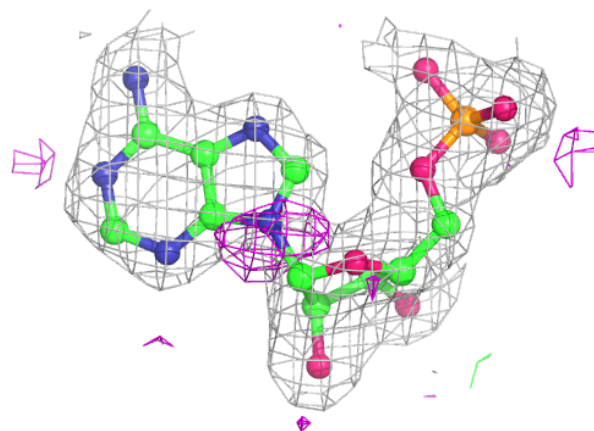
**Electron density around AMP D 339:**

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

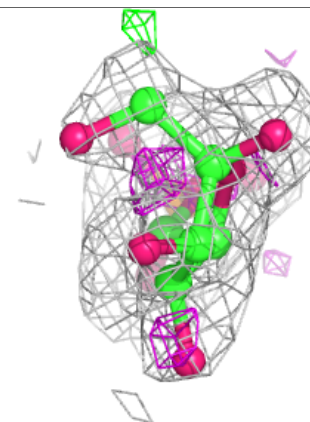
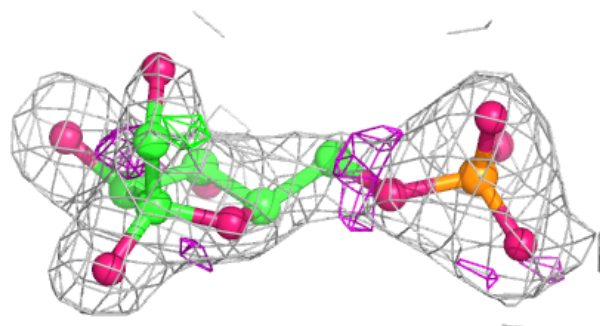
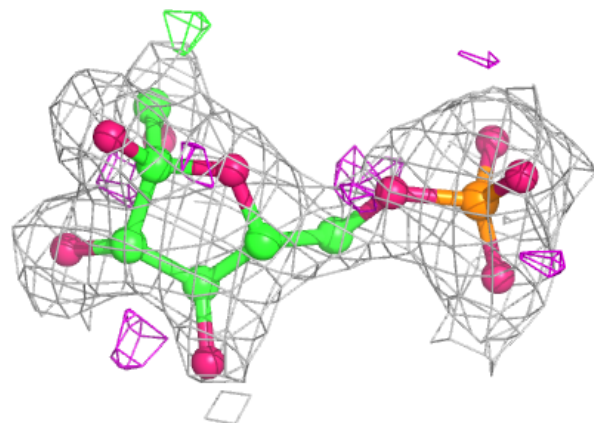


**Electron density around AMP B 339:**

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

**Electron density around P6P D 340:**

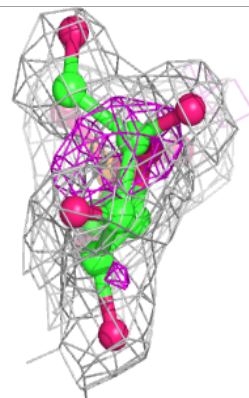
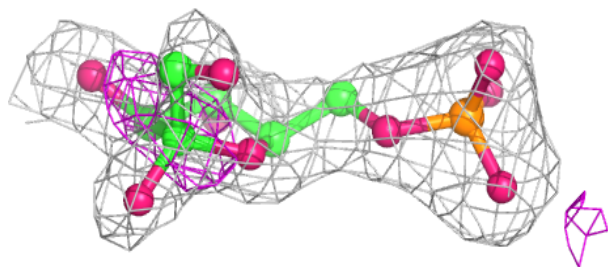
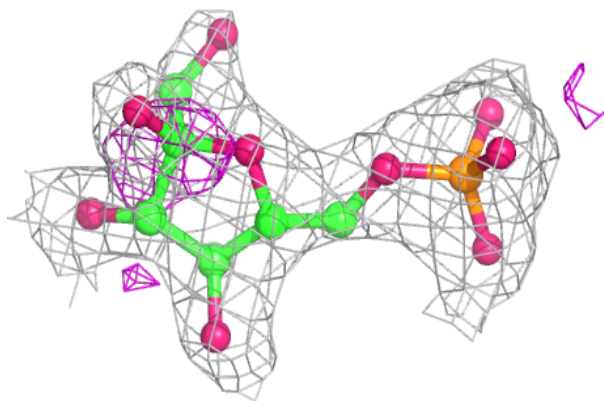
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





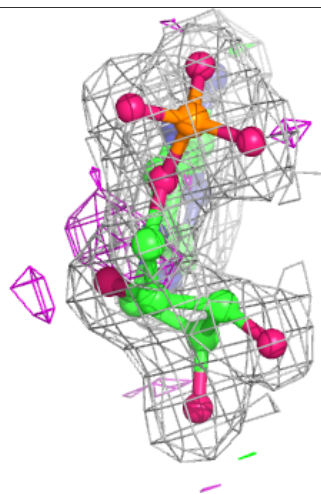
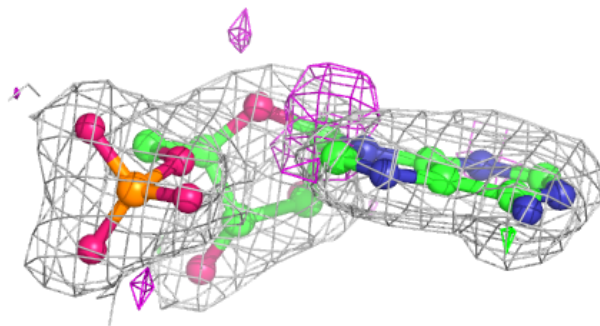
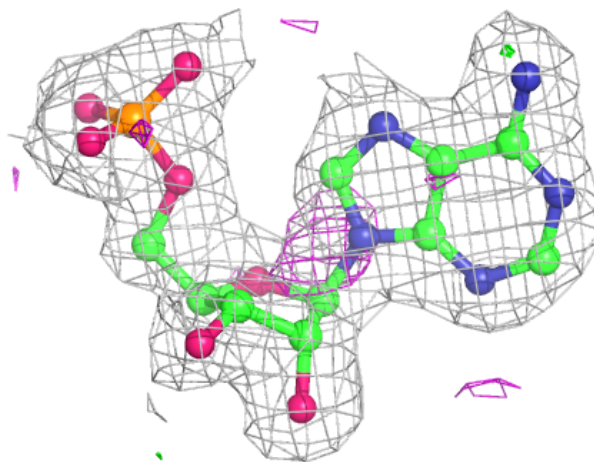
**Electron density around P6P B 340:**

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



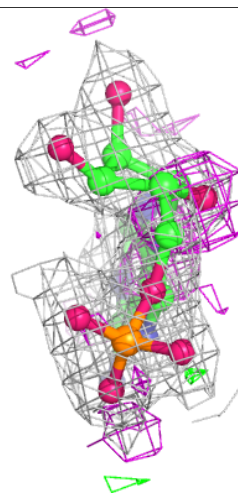
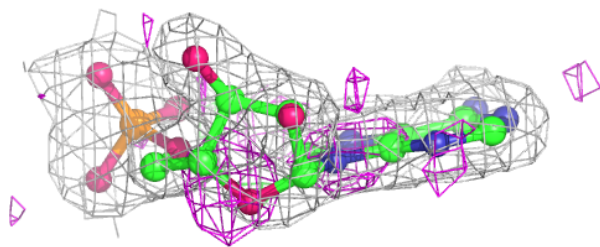
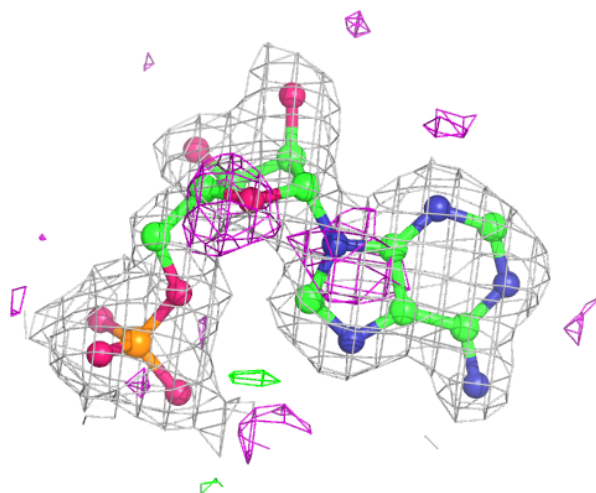
**Electron density around AMP A 339:**

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



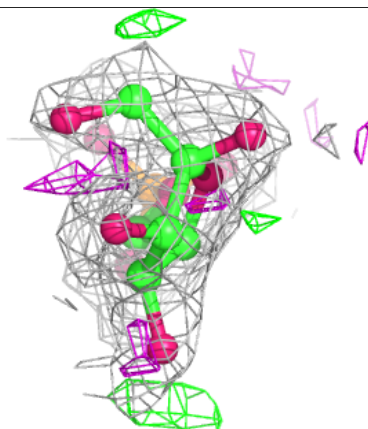
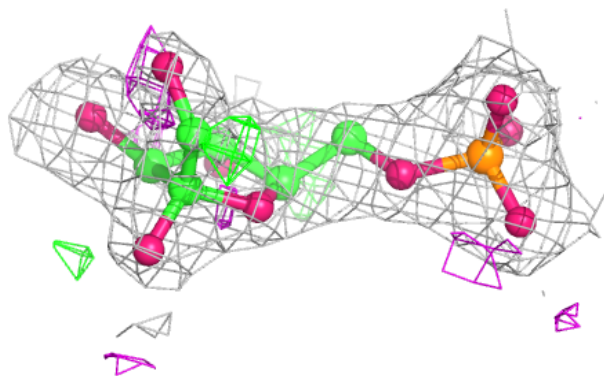
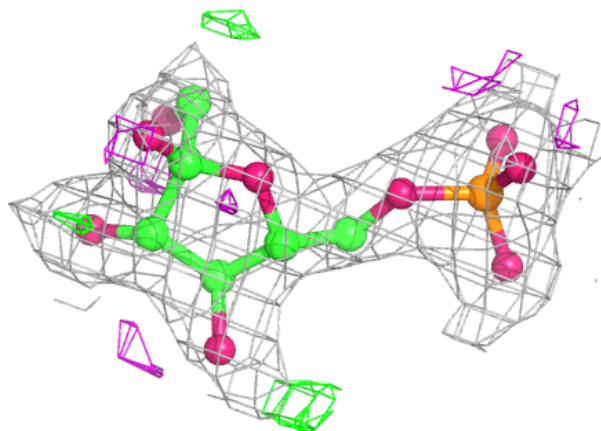
**Electron density around AMP C 339:**

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



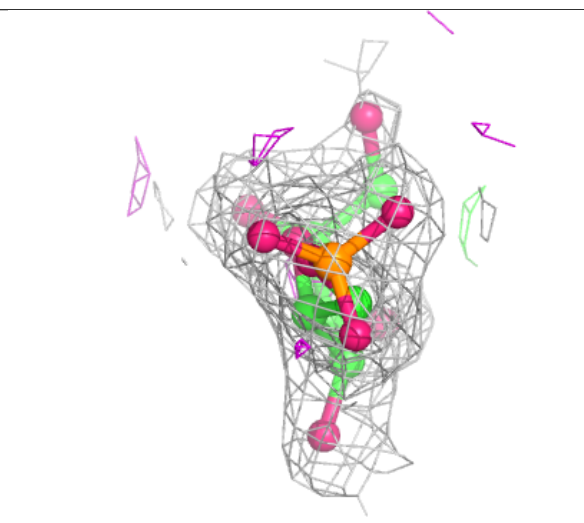
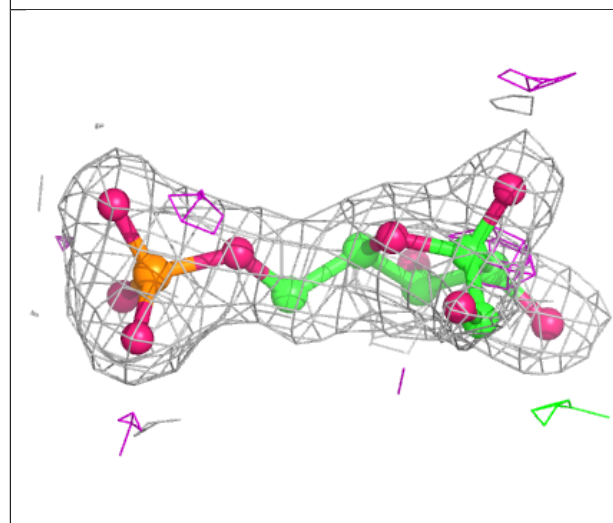
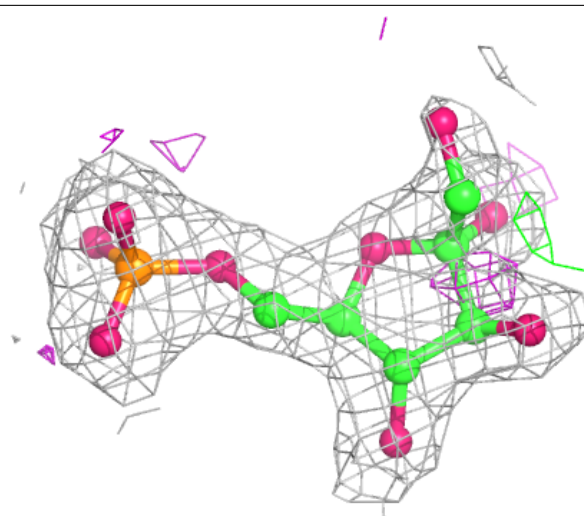
**Electron density around P6P A 340:**

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



**Electron density around P6P C 340:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.