



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 01:57 AM EDT

PDB ID : 3IFA
Title : Human muscle fructose-1,6-bisphosphatase E69Q mutant in complex with AMP
Authors : Kolodziejczyk, R.; Zarzycki, M.; Jaskolski, M.; Dzugaj, A.
Deposited on : 2009-07-24
Resolution : 1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.36
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) : 2.36

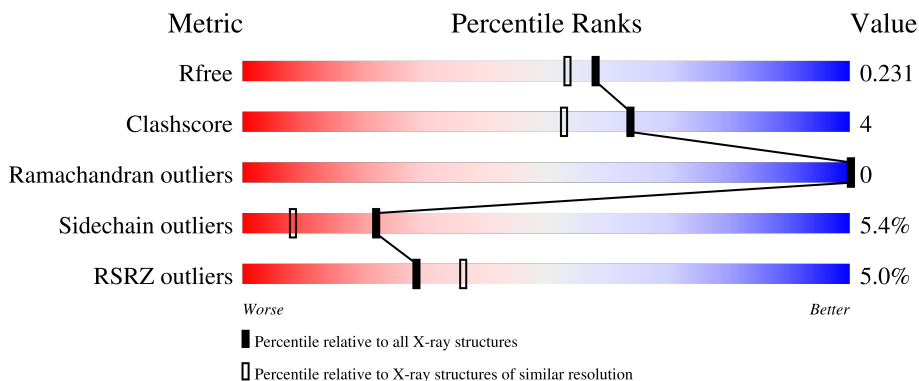
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


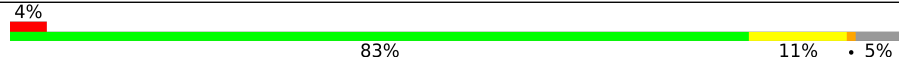
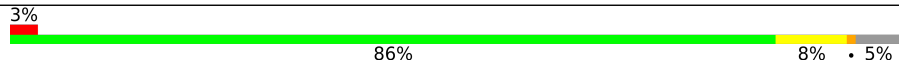

The reported resolution of this entry is 1.93 Å.

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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 6% 86% 9%
1	B	338	 4% 83% 11% 5%
1	C	338	 3% 86% 8% 5%
1	D	338	 6% 82% 12% 5%

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	GOL	A	344	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10752 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.

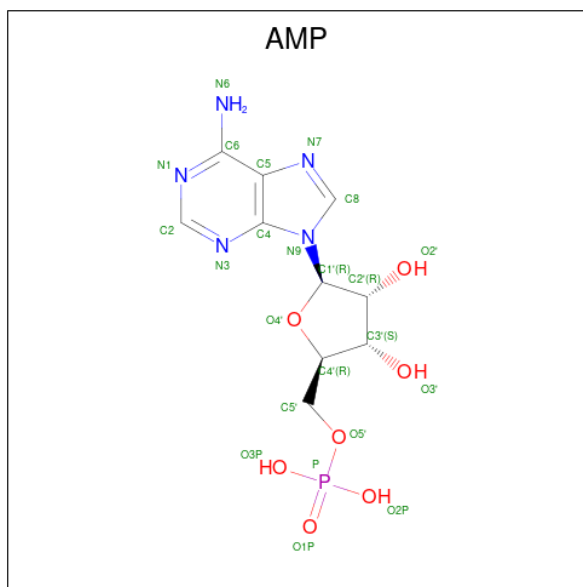
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	2505	1594	418	480	13	35	5	0
1	B	321	2476	1576	410	477	13	54	5	0
1	C	321	2464	1568	411	473	12	33	3	0
1	D	322	2464	1570	410	470	14	60	4	0

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: C₁₀H₁₄N₅O₇P).



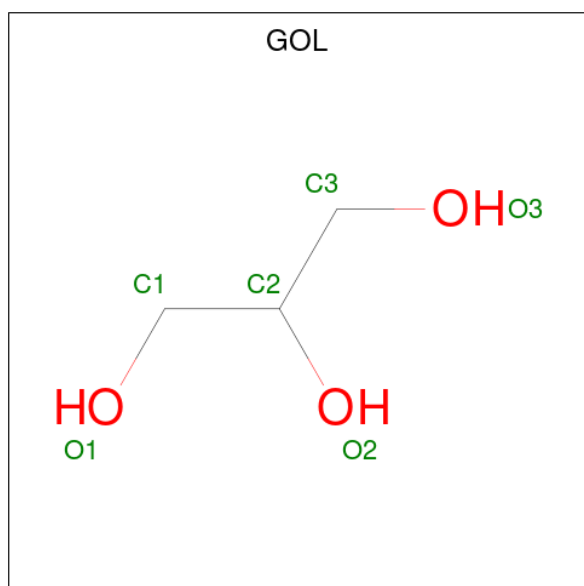
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

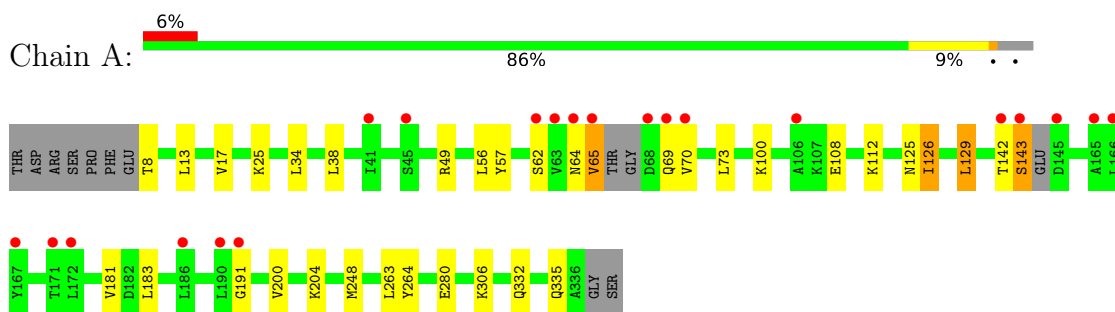
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	137	Total	O	0	0
			137	137		
5	C	184	Total	O	0	0
			184	184		
5	D	114	Total	O	0	0
			114	114		

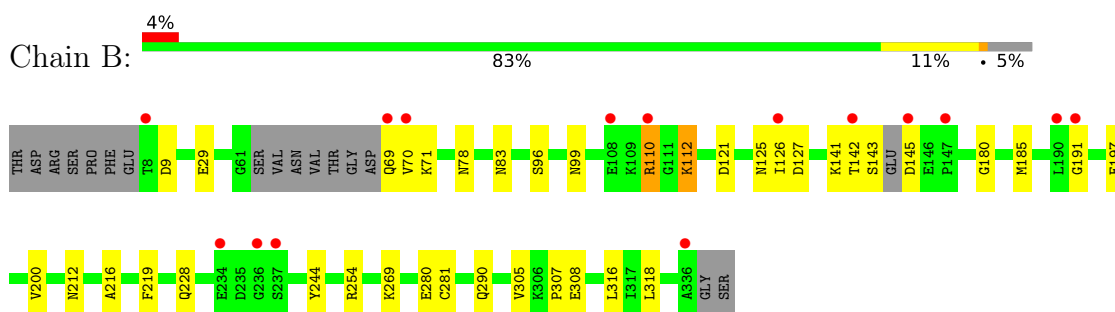
3 Residue-property plots [i](#)

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.

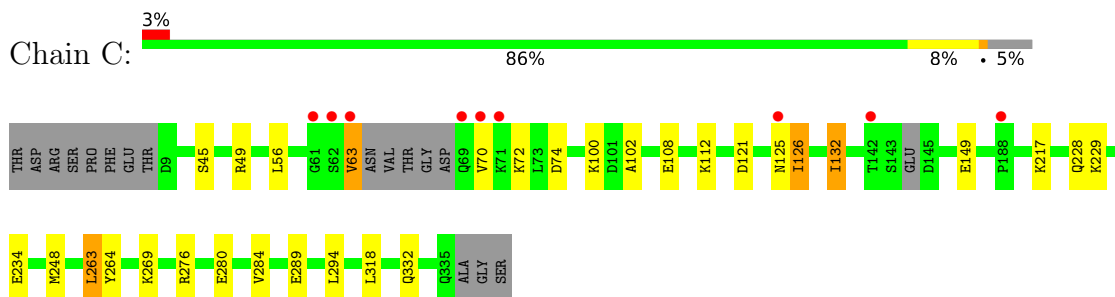
- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2



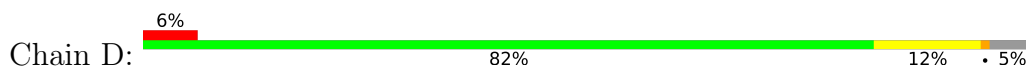
- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2

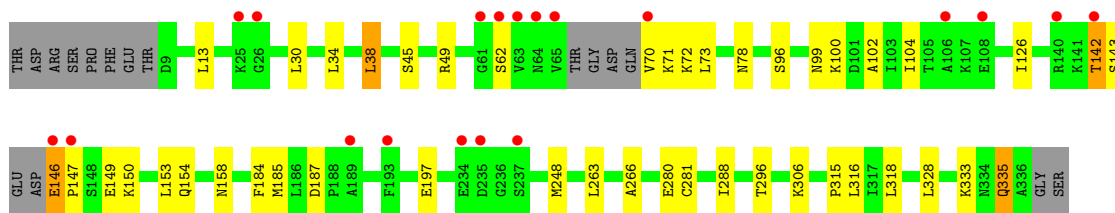


- Molecule 1: Fructose-1,6-bisphosphatase isozyme 2



- 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, α , β , γ	218.11Å 234.26Å 71.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.93 49.43 – 1.93	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-1.93) 92.0 (49.43-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.92Å)	Xtrriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.168 , 0.199 0.207 , 0.231	Depositor DCC
R_{free} test set	1289 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.608	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10752	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AMP, SO4

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	1.00	0/2557	0.83	1/3455 (0.0%)
1	B	0.88	1/2525 (0.0%)	0.80	2/3410 (0.1%)
1	C	0.99	1/2507 (0.0%)	0.83	3/3386 (0.1%)
1	D	0.85	1/2513 (0.0%)	0.76	3/3395 (0.1%)
All	All	0.93	3/10102 (0.0%)	0.81	9/13646 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	ASN	CA-CB	-5.28	1.39	1.53
1	D	150	LYS	CG-CD	-5.25	1.34	1.52
1	C	289	GLU	CD-OE1	5.21	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	276	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	187	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	110	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	187	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	263	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	49	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	335	GLN	CA-CB-CG	-5.17	102.02	113.40
1	C	74	ASP	CB-CG-OD1	-5.03	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2576	21	0
1	B	2476	0	2535	21	0
1	C	2464	0	2525	10	0
1	D	2464	0	2536	31	0
2	A	23	0	12	0	0
2	B	23	0	12	1	0
2	C	23	0	12	0	0
2	D	23	0	12	1	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	18	0	24	3	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	3	0
5	A	215	0	0	3	0
5	B	137	0	0	0	0
5	C	184	0	0	2	0
5	D	114	0	0	0	0
All	All	10752	0	10268	83	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 (83) 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:D:78:ASN:HD21	1:D:99:ASN:HD21	1.17	0.91
1:D:100:LYS:H	4:D:343:GOL:H31	1.39	0.85
1:B:78:ASN:HD21	1:B:99:ASN:HD21	1.26	0.81
1:D:100:LYS:N	4:D:343:GOL:H31	1.99	0.78
1:B:143:SER:HB2	1:B:145:ASP:HB3	1.68	0.75
1:D:73:LEU:HD23	1:D:126:ILE:CD1	2.19	0.71
1:D:142:THR:O	1:D:143:SER:HB3	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD23	1:A:126:ILE:CD1	2.20	0.71
1:B:142:THR:O	1:B:143:SER:CB	2.44	0.66
1:B:305:VAL:O	1:B:307:PRO:HD3	1.97	0.65
1:D:281[B]:CYS:SG	1:D:316:LEU:HD22	2.38	0.64
1:B:96:SER:HB3	1:B:99:ASN:HD22	1.62	0.63
1:D:100:LYS:H	4:D:343:GOL:C3	2.13	0.61
1:D:142:THR:O	1:D:143:SER:CB	2.50	0.59
1:B:180:GLY:H	1:B:290:GLN:NE2	2.01	0.59
1:D:154:GLN:HE21	1:D:158:ASN:HD22	1.52	0.58
1:D:34:LEU:O	1:D:38:LEU:HD22	2.03	0.58
1:D:153:LEU:O	1:D:306:LYS:HE3	2.04	0.58
1:D:146:GLU:HG3	1:D:147:PRO:HD2	1.86	0.57
1:D:318:LEU:HD12	1:D:318:LEU:C	2.25	0.57
1:B:143:SER:HB2	1:B:145:ASP:CB	2.34	0.56
1:B:141:LYS:NZ	1:B:145:ASP:O	2.39	0.56
1:D:73:LEU:CD2	1:D:126:ILE:CD1	2.85	0.55
1:B:318:LEU:C	1:B:318:LEU:HD12	2.28	0.54
1:A:34:LEU:O	1:A:38:LEU:HD23	2.07	0.54
1:A:142:THR:O	1:A:143:SER:HB3	2.07	0.54
1:B:316:LEU:HD11	1:B:318:LEU:HD23	1.89	0.54
1:A:126:ILE:HA	5:A:412:HOH:O	2.06	0.53
1:B:180:GLY:H	1:B:290:GLN:HE21	1.56	0.53
1:D:102:ALA:HB2	1:D:149:GLU:HG3	1.92	0.52
1:A:142:THR:O	1:A:143:SER:CB	2.58	0.52
1:B:29:GLU:OE1	1:B:112:LYS:HE3	2.10	0.51
1:D:73:LEU:HD23	1:D:126:ILE:HD13	1.93	0.51
1:D:13:LEU:HD13	1:D:184:PHE:CE1	2.45	0.51
1:A:100:LYS:H	4:A:344:GOL:H11	1.76	0.51
1:A:183:LEU:HG	1:A:200[B]:VAL:HG11	1.92	0.50
1:B:143:SER:CB	1:B:145:ASP:HB3	2.41	0.50
1:C:102:ALA:HB2	1:C:149:GLU:HG3	1.93	0.50
1:D:70:VAL:HG12	1:D:126:ILE:CG2	2.41	0.50
1:C:248:MET:HE2	1:C:284:VAL:HG21	1.93	0.49
1:C:63:VAL:N	5:C:349:HOH:O	2.33	0.49
1:B:142:THR:O	1:B:143:SER:HB3	2.11	0.49
1:D:288:ILE:HG13	1:D:318:LEU:HD13	1.94	0.49
1:D:73:LEU:CD2	1:D:126:ILE:HD11	2.42	0.49
1:A:248:MET:HE1	1:A:280:GLU:HB3	1.95	0.49
1:C:318:LEU:C	1:C:318:LEU:HD12	2.33	0.48
1:D:13:LEU:HD13	1:D:184:PHE:CZ	2.49	0.48
1:D:296:THR:HG21	1:D:328:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:AMP:O5'	2:B:339:AMP:H8	1.97	0.48
1:A:335:GLN:NE2	5:A:396:HOH:O	2.37	0.48
1:A:248:MET:HE1	1:A:280:GLU:CD	2.35	0.47
1:D:104:ILE:HD12	1:D:104:ILE:N	2.30	0.47
1:A:13:LEU:HD12	1:A:17:VAL:HG23	1.96	0.47
1:D:96:SER:HB3	1:D:99:ASN:HD22	1.78	0.46
1:D:146:GLU:HG3	1:D:147:PRO:CD	2.45	0.46
1:A:191:GLY:HA3	1:B:191:GLY:HA3	1.98	0.46
1:D:45:SER:O	1:D:49:ARG:HD3	2.16	0.45
1:A:125:ASN:HA	5:A:623:HOH:O	2.16	0.45
1:D:248:MET:HE1	1:D:280:GLU:HB3	1.98	0.45
2:D:339:AMP:H8	2:D:339:AMP:O5'	1.99	0.45
1:B:142:THR:O	1:B:143:SER:OG	2.33	0.45
1:D:248:MET:CE	1:D:280:GLU:HB3	2.47	0.44
1:A:204:LYS:H	4:A:346:GOL:H32	1.83	0.44
1:A:248:MET:CE	1:A:280:GLU:OE2	2.65	0.44
1:D:266:ALA:HB2	1:D:315:PRO:HG3	2.00	0.44
1:D:70:VAL:HG12	1:D:126:ILE:HG21	2.00	0.43
1:A:181:VAL:HB	1:A:200[B]:VAL:HG22	2.01	0.43
1:C:126:ILE:HD11	1:C:132:ILE:CD1	2.48	0.43
1:D:318:LEU:HD12	1:D:318:LEU:O	2.18	0.43
1:C:121:ASP:OD2	1:C:280:GLU:OE2	2.37	0.42
1:C:234:GLU:HA	1:C:234:GLU:OE1	2.19	0.42
1:B:212:ASN:HB2	1:B:244:TYR:CE2	2.54	0.42
1:A:57:TYR:CE1	1:A:65:VAL:HG21	2.55	0.42
1:C:45:SER:O	1:C:49:ARG:HD3	2.20	0.42
1:B:121:ASP:OD1	1:B:280[A]:GLU:OE2	2.38	0.42
1:A:248:MET:HB2	1:A:248:MET:HE2	1.79	0.42
1:A:204:LYS:H	4:A:346:GOL:C3	2.33	0.42
1:C:125:ASN:HB2	5:C:608:HOH:O	2.18	0.42
1:A:332:GLN:HG3	1:C:294:LEU:CD2	2.50	0.41
1:B:281[B]:CYS:SG	1:B:316:LEU:HD22	2.60	0.41
1:B:197:GLU:CD	1:B:200:VAL:HG12	2.41	0.41
1:A:129:LEU:HD12	1:A:129:LEU:HA	1.96	0.40
1:B:216:ALA:HA	1:B:219:PHE:CD2	2.57	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	325/338 (96%)	320 (98%)	5 (2%)	0	100	100
1	B	320/338 (95%)	314 (98%)	6 (2%)	0	100	100
1	C	318/338 (94%)	311 (98%)	7 (2%)	0	100	100
1	D	320/338 (95%)	313 (98%)	7 (2%)	0	100	100
All	All	1283/1352 (95%)	1258 (98%)	25 (2%)	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	274/279 (98%)	258 (94%)	16 (6%)	20	7
1	B	269/279 (96%)	256 (95%)	13 (5%)	25	10
1	C	268/279 (96%)	251 (94%)	17 (6%)	18	5
1	D	269/279 (96%)	257 (96%)	12 (4%)	27	12
All	All	1080/1116 (97%)	1022 (95%)	58 (5%)	22	8

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	25	LYS

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Mol	Chain	Res	Type
1	A	56	LEU
1	A	62	SER
1	A	64	ASN
1	A	65	VAL
1	A	69	GLN
1	A	70	VAL
1	A	108	GLU
1	A	112	LYS
1	A	126	ILE
1	A	129	LEU
1	A	143	SER
1	A	263	LEU
1	A	264	TYR
1	A	306	LYS
1	B	9	ASP
1	B	69	GLN
1	B	70	VAL
1	B	71	LYS
1	B	83	ASN
1	B	110	ARG
1	B	112	LYS
1	B	126	ILE
1	B	127	ASP
1	B	185	MET
1	B	228	GLN
1	B	269	LYS
1	B	308	GLU
1	C	56	LEU
1	C	63	VAL
1	C	70	VAL
1	C	72	LYS
1	C	100	LYS
1	C	108	GLU
1	C	112	LYS
1	C	126	ILE
1	C	132	ILE
1	C	217	LYS
1	C	228[A]	GLN
1	C	228[B]	GLN
1	C	229	LYS
1	C	263	LEU
1	C	264	TYR

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Mol	Chain	Res	Type
1	C	269	LYS
1	C	332	GLN
1	D	30	LEU
1	D	38	LEU
1	D	62	SER
1	D	71	LYS
1	D	72	LYS
1	D	142	THR
1	D	146	GLU
1	D	185	MET
1	D	197	GLU
1	D	263	LEU
1	D	333	LYS
1	D	335	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	B	35	ASN
1	B	99	ASN
1	B	268	GLN
1	B	290	GLN
1	C	125	ASN
1	C	154	GLN
1	D	99	ASN
1	D	154	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

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
3	SO4	B	341	-	4,4,4	0.16	0	6,6,6	0.32	0
3	SO4	C	342	-	4,4,4	0.16	0	6,6,6	0.45	0
2	AMP	B	339	-	22,25,25	1.37	3 (13%)	25,38,38	1.71	6 (24%)
3	SO4	D	342	-	4,4,4	0.24	0	6,6,6	0.37	0
4	GOL	A	345	-	5,5,5	0.36	0	5,5,5	1.97	2 (40%)
3	SO4	C	341	-	4,4,4	0.35	0	6,6,6	0.66	0
3	SO4	A	343	-	4,4,4	0.25	0	6,6,6	0.59	0
3	SO4	D	341	-	4,4,4	0.08	0	6,6,6	0.42	0
3	SO4	D	340	-	4,4,4	0.18	0	6,6,6	0.94	0
4	GOL	C	343	-	5,5,5	0.79	0	5,5,5	0.98	0
3	SO4	A	341	-	4,4,4	0.21	0	6,6,6	0.65	0
2	AMP	C	339	-	22,25,25	1.06	1 (4%)	25,38,38	1.47	3 (12%)
3	SO4	B	340	-	4,4,4	0.31	0	6,6,6	0.66	0
4	GOL	B	343	-	5,5,5	0.72	0	5,5,5	1.89	2 (40%)
3	SO4	C	340	-	4,4,4	0.20	0	6,6,6	0.41	0
3	SO4	A	342	-	4,4,4	0.27	0	6,6,6	0.26	0
2	AMP	A	339	-	22,25,25	1.18	3 (13%)	25,38,38	1.62	5 (20%)
4	GOL	A	344	-	5,5,5	1.12	1 (20%)	5,5,5	2.27	2 (40%)
3	SO4	A	340	-	4,4,4	0.47	0	6,6,6	0.60	0
3	SO4	B	342	-	4,4,4	0.20	0	6,6,6	0.59	0
4	GOL	A	346	-	5,5,5	0.32	0	5,5,5	1.60	1 (20%)
2	AMP	D	339	-	22,25,25	1.38	3 (13%)	25,38,38	1.49	4 (16%)
4	GOL	D	343	-	5,5,5	0.58	0	5,5,5	1.14	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
4	GOL	A	344	-	-	3/4/4/4	-
4	GOL	A	345	-	-	0/4/4/4	-
4	GOL	B	343	-	-	1/4/4/4	-
2	AMP	B	339	-	-	0/6/26/26	0/3/3/3
4	GOL	C	343	-	-	1/4/4/4	-
4	GOL	A	346	-	-	2/4/4/4	-
2	AMP	D	339	-	-	0/6/26/26	0/3/3/3
2	AMP	C	339	-	-	0/6/26/26	0/3/3/3
2	AMP	A	339	-	-	1/6/26/26	0/3/3/3
4	GOL	D	343	-	-	0/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	339	AMP	O4'-C1'	3.74	1.46	1.41
2	B	339	AMP	O4'-C1'	3.36	1.45	1.41
2	B	339	AMP	C2-N3	3.35	1.37	1.32
2	B	339	AMP	C5-C4	2.87	1.48	1.40
2	A	339	AMP	C5-C4	2.74	1.48	1.40
2	D	339	AMP	C2-N3	2.74	1.36	1.32
2	C	339	AMP	C5-C4	2.64	1.47	1.40
2	A	339	AMP	O4'-C1'	2.54	1.44	1.41
2	D	339	AMP	C5-C4	2.41	1.47	1.40
2	A	339	AMP	C2-N3	2.37	1.35	1.32
4	A	344	GOL	O2-C2	-2.08	1.37	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	339	AMP	N3-C2-N1	-4.01	122.41	128.68
2	A	339	AMP	O2P-P-O5'	-3.90	96.35	106.73
2	B	339	AMP	N3-C2-N1	-3.78	122.76	128.68
2	C	339	AMP	O3P-P-O5'	3.67	116.50	106.73
2	A	339	AMP	O3P-P-O2P	3.60	121.40	107.64
2	A	339	AMP	N3-C2-N1	-3.44	123.30	128.68
2	C	339	AMP	N3-C2-N1	-3.41	123.35	128.68
4	A	344	GOL	O2-C2-C1	-3.39	94.21	109.12
2	B	339	AMP	O2P-P-O5'	-3.03	98.67	106.73
4	A	345	GOL	O3-C3-C2	-3.02	95.71	110.20
2	B	339	AMP	N6-C6-N1	2.97	124.73	118.57
4	A	344	GOL	O3-C3-C2	-2.87	96.46	110.20
2	D	339	AMP	N6-C6-N1	2.76	124.30	118.57
2	B	339	AMP	O2P-P-O1P	2.63	120.99	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	343	GOL	C3-C2-C1	2.63	121.93	111.70
2	C	339	AMP	N6-C6-N1	2.51	123.77	118.57
4	A	346	GOL	C3-C2-C1	-2.49	102.01	111.70
4	B	343	GOL	O3-C3-C2	-2.39	98.75	110.20
2	A	339	AMP	N6-C6-N1	2.29	123.32	118.57
2	D	339	AMP	C2-N1-C6	2.25	122.61	118.75
2	B	339	AMP	C3'-C2'-C1'	2.20	104.29	100.98
2	D	339	AMP	O2'-C2'-C3'	2.19	118.92	111.82
4	A	345	GOL	C3-C2-C1	2.19	120.23	111.70
2	B	339	AMP	C2-N1-C6	2.19	122.50	118.75
2	A	339	AMP	O3'-C3'-C2'	2.01	118.32	111.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	344	GOL	O1-C1-C2-C3
4	A	344	GOL	C1-C2-C3-O3
4	A	346	GOL	O1-C1-C2-C3
2	A	339	AMP	C5'-O5'-P-O1P
4	A	344	GOL	O2-C2-C3-O3
4	A	346	GOL	O1-C1-C2-O2
4	C	343	GOL	C1-C2-C3-O3
4	B	343	GOL	O2-C2-C3-O3

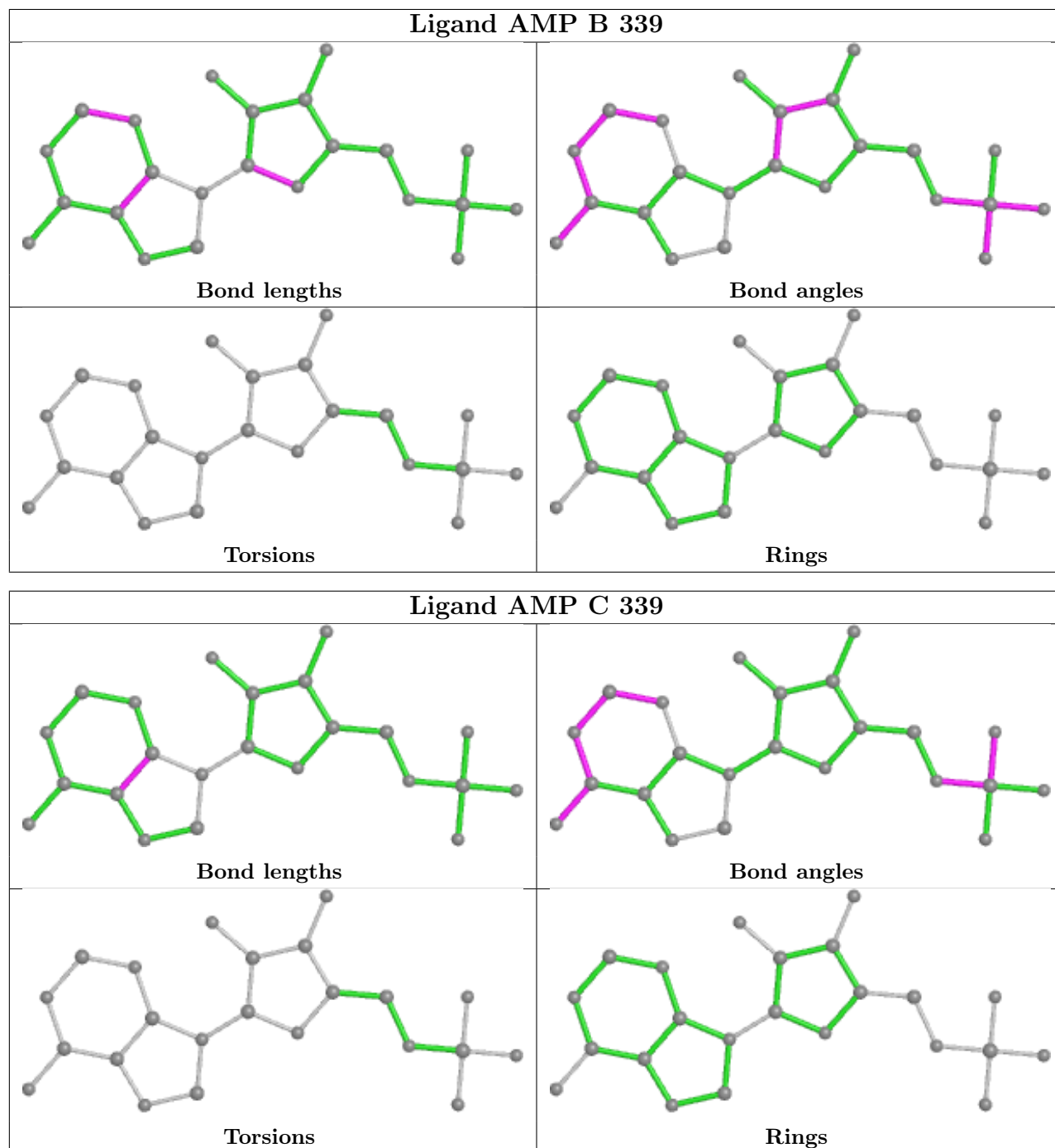
There are no ring outliers.

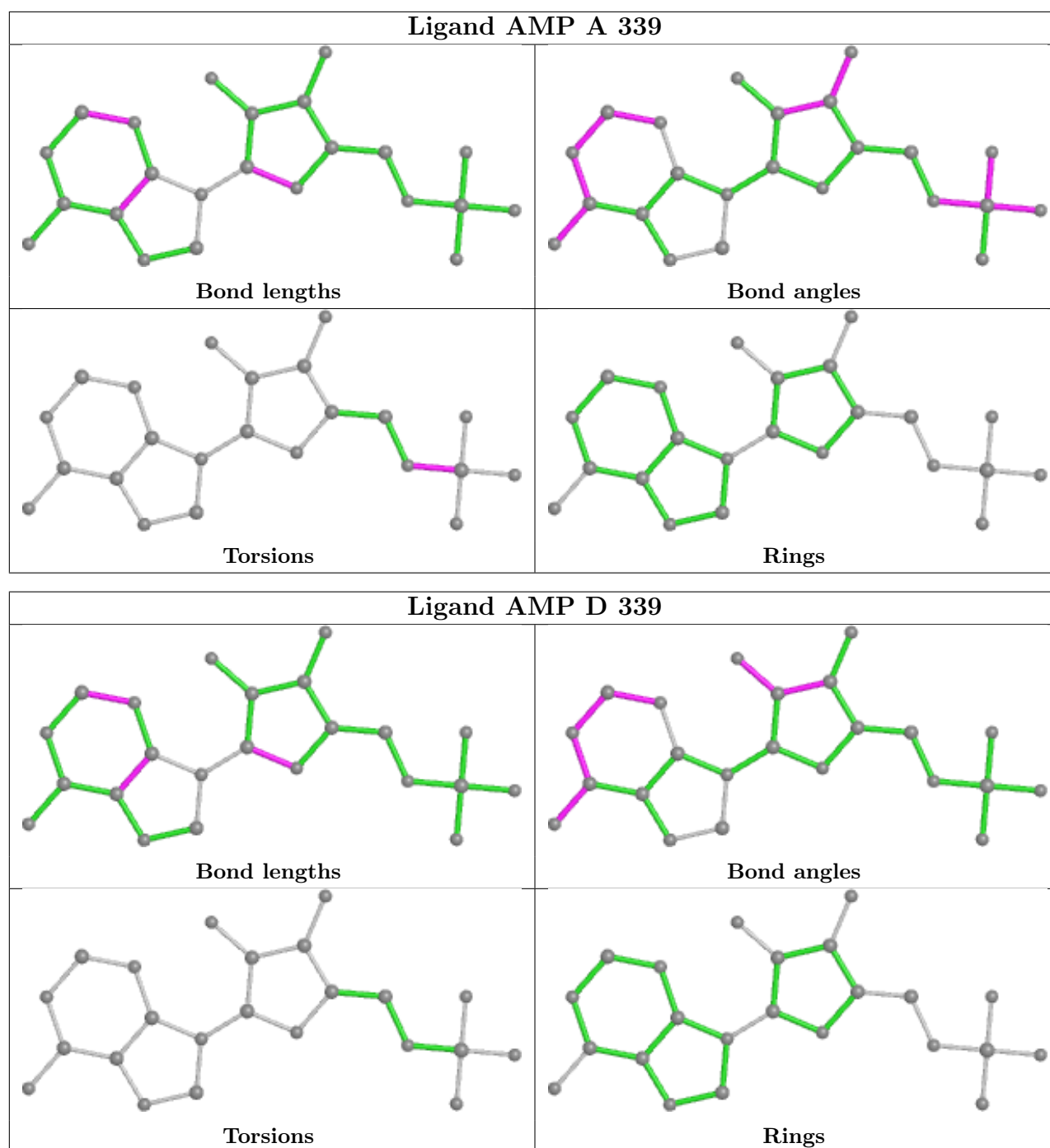
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	339	AMP	1	0
4	A	344	GOL	1	0
4	A	346	GOL	2	0
2	D	339	AMP	1	0
4	D	343	GOL	3	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, 95th 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 ²)	Q<0.9
1	A	326/338 (96%)	0.43	21 (6%) 19 26	17, 28, 52, 76	10 (3%)
1	B	321/338 (94%)	0.38	15 (4%) 31 39	23, 37, 59, 76	16 (4%)
1	C	321/338 (94%)	0.32	9 (2%) 53 60	19, 30, 52, 72	11 (3%)
1	D	322/338 (95%)	0.45	19 (5%) 22 28	26, 38, 60, 76	17 (5%)
All	All	1290/1352 (95%)	0.39	64 (4%) 28 36	17, 34, 58, 76	54 (4%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	VAL	9.2
1	A	63	VAL	9.2
1	D	142	THR	6.6
1	B	142	THR	6.1
1	D	63	VAL	6.1
1	A	64	ASN	5.6
1	A	65	VAL	5.4
1	C	62	SER	5.4
1	A	142	THR	5.4
1	C	70	VAL	5.3
1	A	62	SER	5.1
1	D	62	SER	4.6
1	D	65	VAL	4.4
1	B	145	ASP	4.4
1	C	69	GLN	4.0
1	A	145	ASP	4.0
1	B	236	GLY	3.9
1	D	64	ASN	3.8
1	A	70	VAL	3.7
1	B	70	VAL	3.3
1	D	108	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	8	THR	3.3
1	B	336	ALA	3.2
1	A	68	ASP	3.1
1	D	70	VAL	3.1
1	D	147	PRO	3.0
1	B	190	LEU	3.0
1	A	190	LEU	2.9
1	D	106	ALA	2.8
1	B	191	GLY	2.7
1	B	126	ILE	2.6
1	C	61	GLY	2.6
1	C	125	ASN	2.6
1	C	142	THR	2.6
1	A	69	GLN	2.6
1	D	140	ARG	2.5
1	A	41	ILE	2.5
1	D	235	ASP	2.5
1	A	191	GLY	2.4
1	A	171	THR	2.4
1	B	108	GLU	2.4
1	A	143	SER	2.3
1	B	147	PRO	2.3
1	C	188	PRO	2.3
1	A	45	SER	2.2
1	C	71	LYS	2.2
1	D	193	PHE	2.2
1	B	237	SER	2.2
1	A	172	LEU	2.2
1	D	26	GLY	2.2
1	A	165	ALA	2.1
1	B	110	ARG	2.1
1	A	166	LEU	2.1
1	D	25	LYS	2.1
1	D	61	GLY	2.1
1	D	189	ALA	2.1
1	D	237	SER	2.1
1	D	234	GLU	2.1
1	D	146	GLU	2.0
1	A	186	LEU	2.0
1	B	234	GLU	2.0
1	B	69	GLN	2.0
1	A	167	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	106	ALA	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, 95th 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.

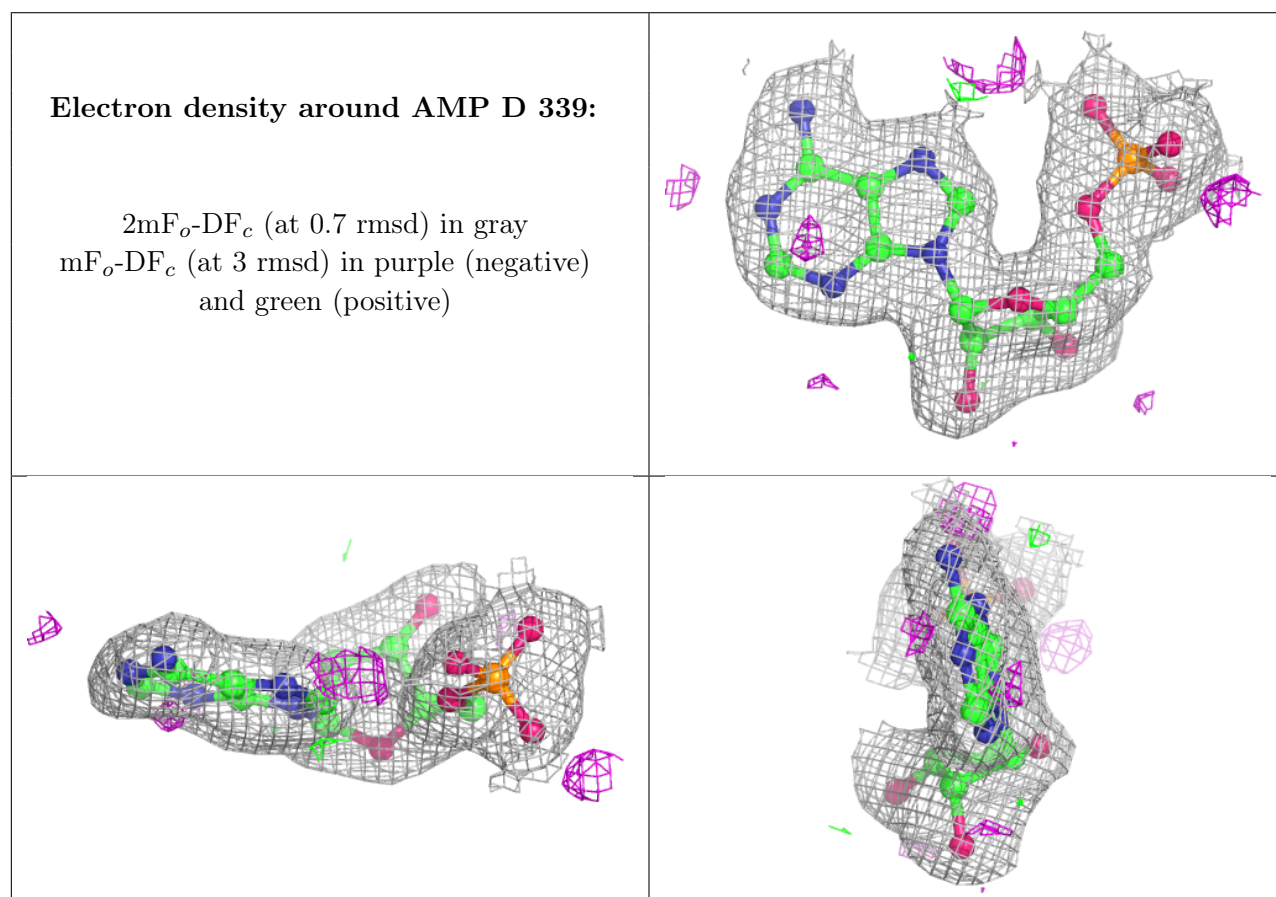
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	D	343	6/6	0.77	0.18	52,55,56,58	0
4	GOL	C	343	6/6	0.82	0.22	43,45,48,50	0
4	GOL	A	345	6/6	0.83	0.17	50,51,53,53	0
4	GOL	A	346	6/6	0.88	0.22	41,45,49,51	0
3	SO4	B	342	5/5	0.90	0.15	44,45,50,50	5
3	SO4	D	341	5/5	0.90	0.12	49,52,56,56	5
4	GOL	A	344	6/6	0.91	0.15	39,41,42,47	0
4	GOL	B	343	6/6	0.91	0.10	46,49,51,54	0
2	AMP	D	339	23/23	0.93	0.11	34,38,40,43	0
3	SO4	A	343	5/5	0.93	0.22	44,47,51,51	5
2	AMP	B	339	23/23	0.94	0.12	34,36,39,41	0
3	SO4	C	340	5/5	0.95	0.12	45,46,47,48	5
2	AMP	C	339	23/23	0.96	0.10	28,33,35,37	0
3	SO4	B	340	5/5	0.96	0.10	30,33,36,37	5
3	SO4	C	342	5/5	0.96	0.10	49,50,52,53	5
3	SO4	D	340	5/5	0.96	0.11	37,38,40,42	5
3	SO4	B	341	5/5	0.96	0.11	43,43,46,47	5
3	SO4	D	342	5/5	0.96	0.09	43,44,46,46	5
2	AMP	A	339	23/23	0.97	0.08	27,31,33,35	0
3	SO4	A	340	5/5	0.97	0.08	29,30,37,39	0
3	SO4	A	341	5/5	0.97	0.10	40,43,44,44	5
3	SO4	A	342	5/5	0.98	0.08	41,42,45,46	5

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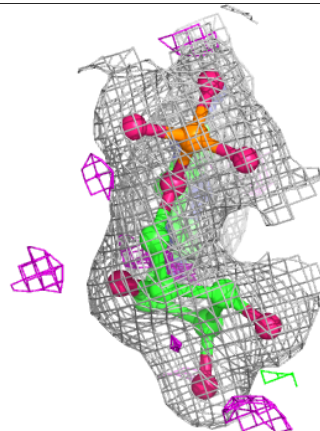
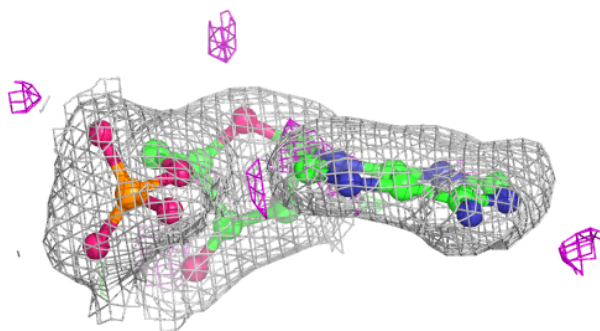
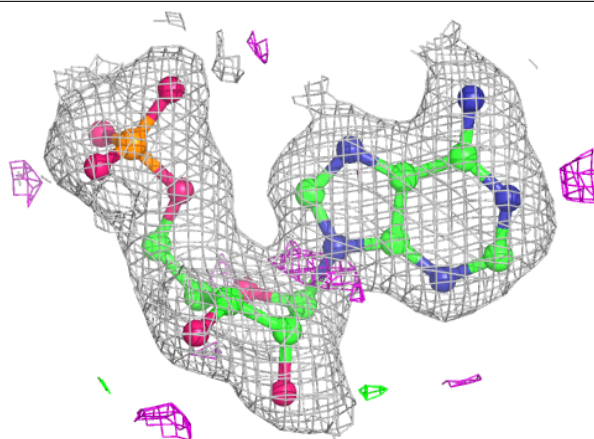
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	C	341	5/5	0.98	0.13	27,29,30,30	5

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.



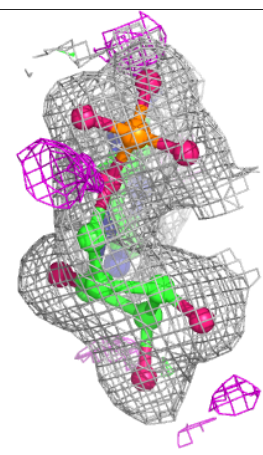
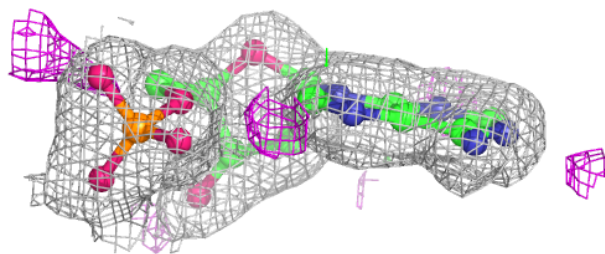
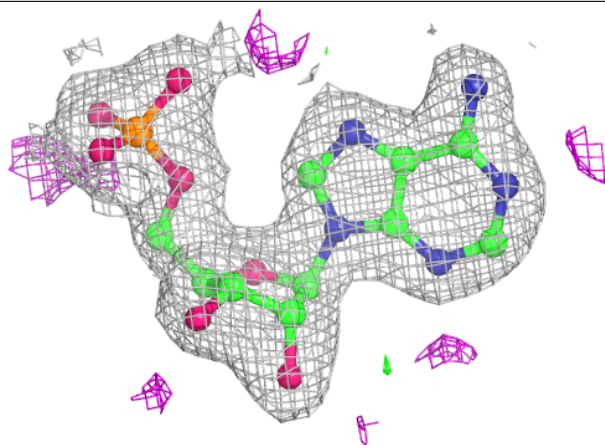
Electron density around AMP B 339:

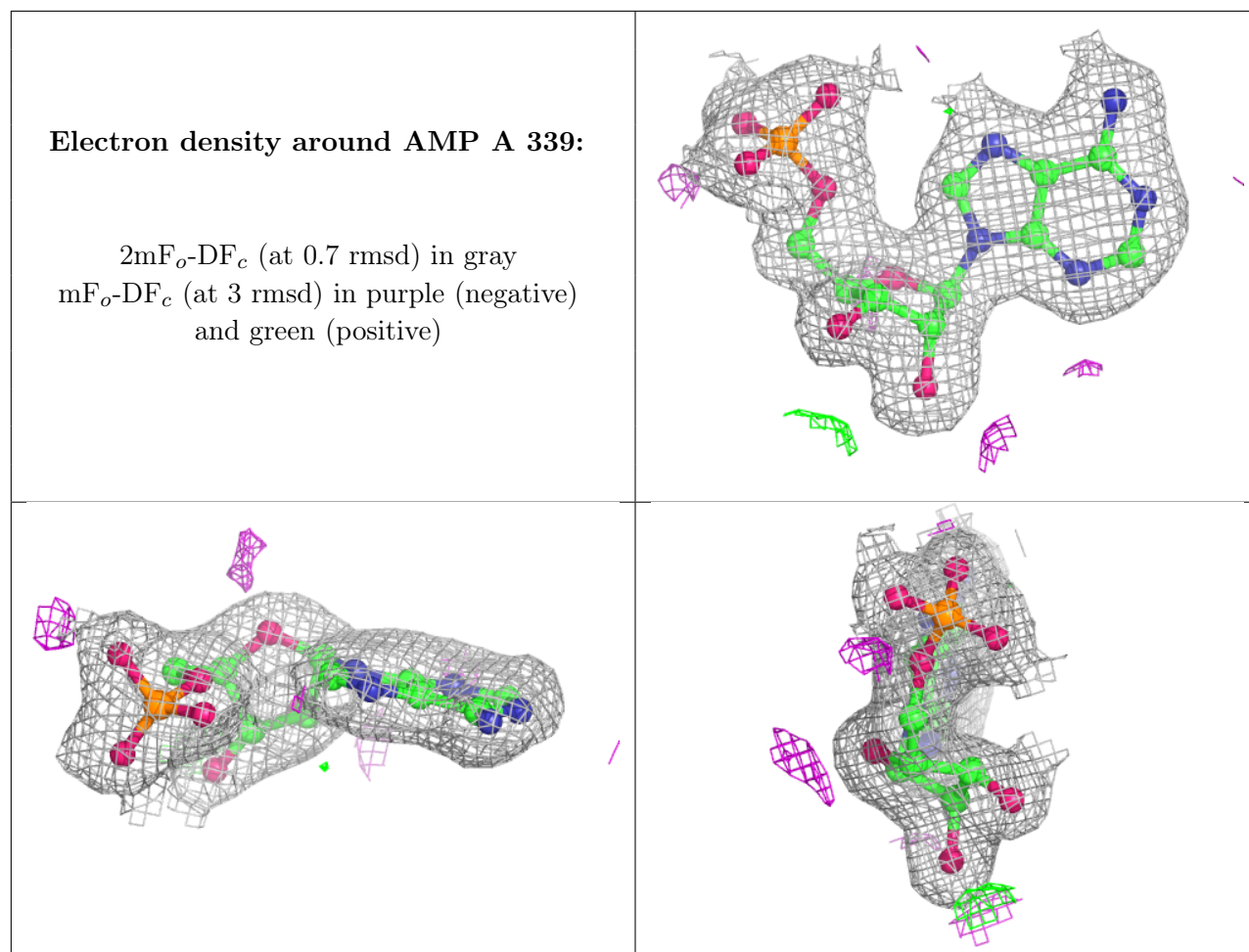
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.