



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2021 – 04:11 PM EDT

PDB ID : 7MJ0
Title : LarB, a carboxylase/hydrolase involved in synthesis of the cofactor for lactate racemase, in complex with adenosine monophosphate AMP
Authors : Chatterjee, S.; Rankin, J.A.; Lagishetty, S.; Hu, J.; Hausinger, R.P.
Deposited on : 2021-04-19
Resolution : 3.01 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 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 : 2.23.1
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) : 2.23.1

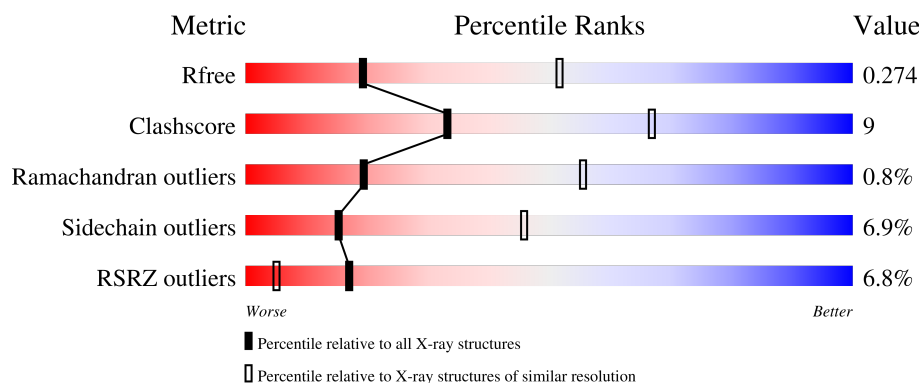
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	256	
1	B	256	
1	C	256	
1	D	256	
1	E	256	

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Mol	Chain	Length	Quality of chain
1	F	256	<p>14% 57% 20% 9%</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8549 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 Pyridinium-3,5-biscarboxylic acid mononucleotide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1418	897	241	273	7			
1	B	202	Total	C	N	O	S	0	0	0
			1404	889	241	266	8			
1	C	207	Total	C	N	O	S	0	0	0
			1453	918	248	279	8			
1	D	203	Total	C	N	O	S	0	0	0
			1425	904	243	270	8			
1	E	198	Total	C	N	O	S	0	0	0
			1382	871	235	268	8			
1	F	201	Total	C	N	O	S	0	0	0
			1419	901	243	268	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ALA	-	expression tag	UNP F9UST0
A	248	SER	-	expression tag	UNP F9UST0
A	249	TRP	-	expression tag	UNP F9UST0
A	250	SER	-	expression tag	UNP F9UST0
A	251	HIS	-	expression tag	UNP F9UST0
A	252	PRO	-	expression tag	UNP F9UST0
A	253	GLN	-	expression tag	UNP F9UST0
A	254	PHE	-	expression tag	UNP F9UST0
A	255	GLU	-	expression tag	UNP F9UST0
A	256	LYS	-	expression tag	UNP F9UST0
B	247	ALA	-	expression tag	UNP F9UST0
B	248	SER	-	expression tag	UNP F9UST0
B	249	TRP	-	expression tag	UNP F9UST0
B	250	SER	-	expression tag	UNP F9UST0
B	251	HIS	-	expression tag	UNP F9UST0
B	252	PRO	-	expression tag	UNP F9UST0
B	253	GLN	-	expression tag	UNP F9UST0

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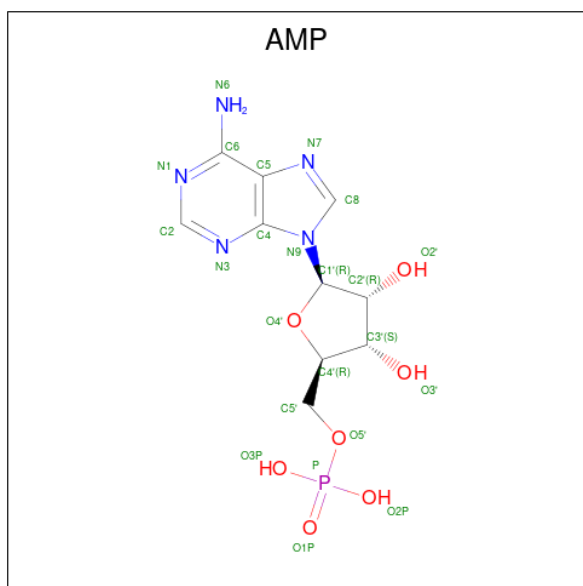
Chain	Residue	Modelled	Actual	Comment	Reference
B	254	PHE	-	expression tag	UNP F9UST0
B	255	GLU	-	expression tag	UNP F9UST0
B	256	LYS	-	expression tag	UNP F9UST0
C	247	ALA	-	expression tag	UNP F9UST0
C	248	SER	-	expression tag	UNP F9UST0
C	249	TRP	-	expression tag	UNP F9UST0
C	250	SER	-	expression tag	UNP F9UST0
C	251	HIS	-	expression tag	UNP F9UST0
C	252	PRO	-	expression tag	UNP F9UST0
C	253	GLN	-	expression tag	UNP F9UST0
C	254	PHE	-	expression tag	UNP F9UST0
C	255	GLU	-	expression tag	UNP F9UST0
C	256	LYS	-	expression tag	UNP F9UST0
D	247	ALA	-	expression tag	UNP F9UST0
D	248	SER	-	expression tag	UNP F9UST0
D	249	TRP	-	expression tag	UNP F9UST0
D	250	SER	-	expression tag	UNP F9UST0
D	251	HIS	-	expression tag	UNP F9UST0
D	252	PRO	-	expression tag	UNP F9UST0
D	253	GLN	-	expression tag	UNP F9UST0
D	254	PHE	-	expression tag	UNP F9UST0
D	255	GLU	-	expression tag	UNP F9UST0
D	256	LYS	-	expression tag	UNP F9UST0
E	247	ALA	-	expression tag	UNP F9UST0
E	248	SER	-	expression tag	UNP F9UST0
E	249	TRP	-	expression tag	UNP F9UST0
E	250	SER	-	expression tag	UNP F9UST0
E	251	HIS	-	expression tag	UNP F9UST0
E	252	PRO	-	expression tag	UNP F9UST0
E	253	GLN	-	expression tag	UNP F9UST0
E	254	PHE	-	expression tag	UNP F9UST0
E	255	GLU	-	expression tag	UNP F9UST0
E	256	LYS	-	expression tag	UNP F9UST0
F	247	ALA	-	expression tag	UNP F9UST0
F	248	SER	-	expression tag	UNP F9UST0
F	249	TRP	-	expression tag	UNP F9UST0
F	250	SER	-	expression tag	UNP F9UST0
F	251	HIS	-	expression tag	UNP F9UST0
F	252	PRO	-	expression tag	UNP F9UST0
F	253	GLN	-	expression tag	UNP F9UST0
F	254	PHE	-	expression tag	UNP F9UST0
F	255	GLU	-	expression tag	UNP F9UST0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	256	LYS	-	expression tag	UNP F9UST0

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	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		

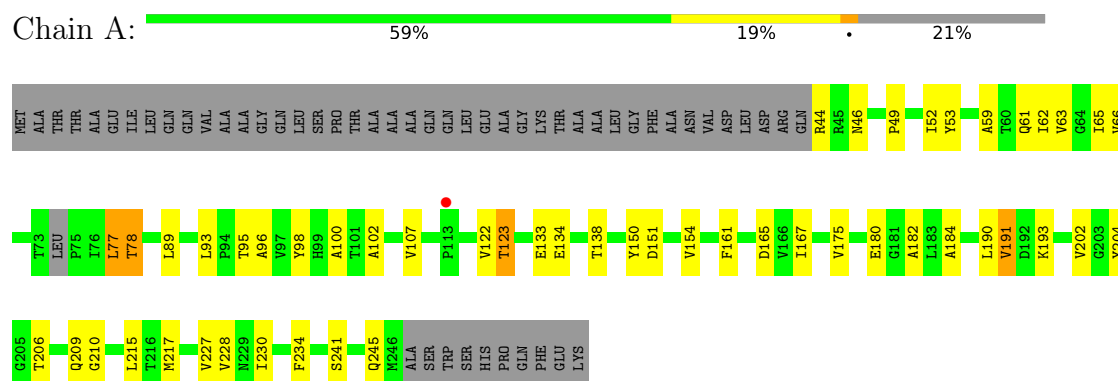
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

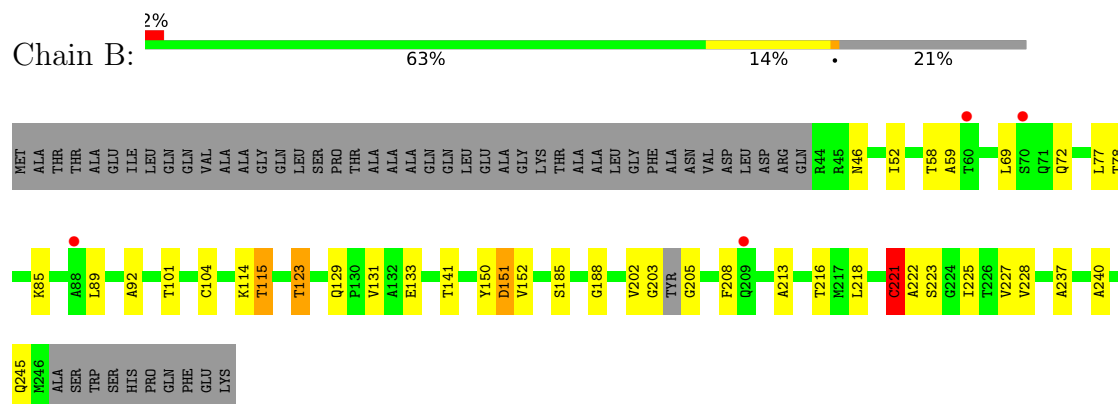
3 Residue-property plots [i](#)

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.

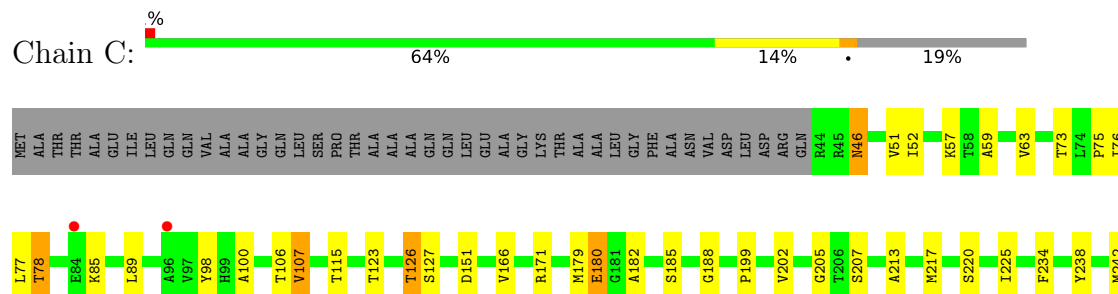
- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



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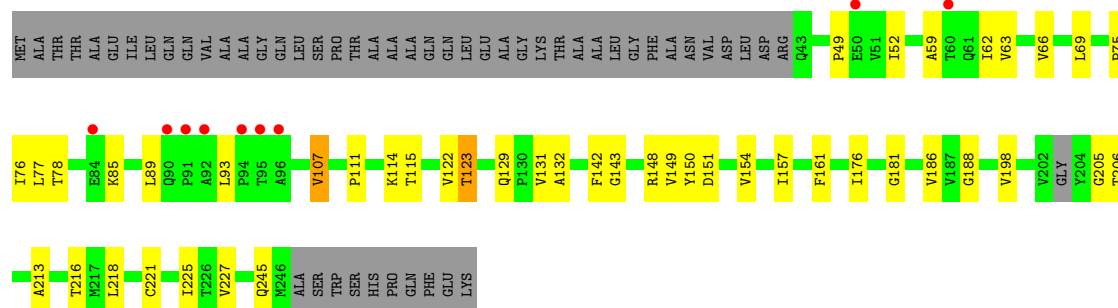


- Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

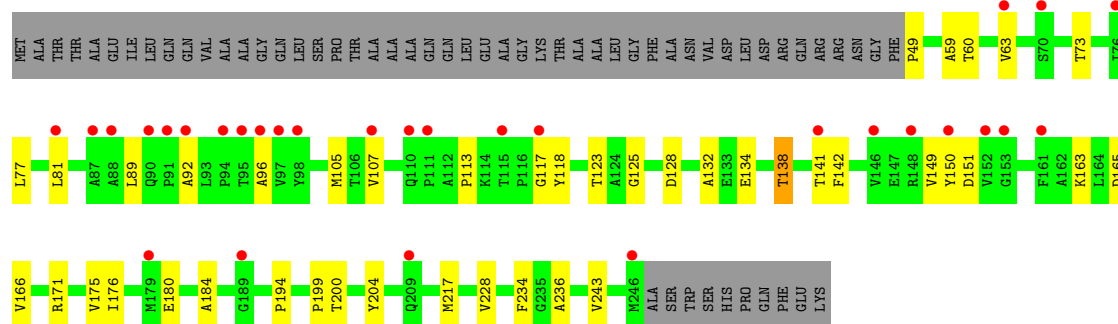




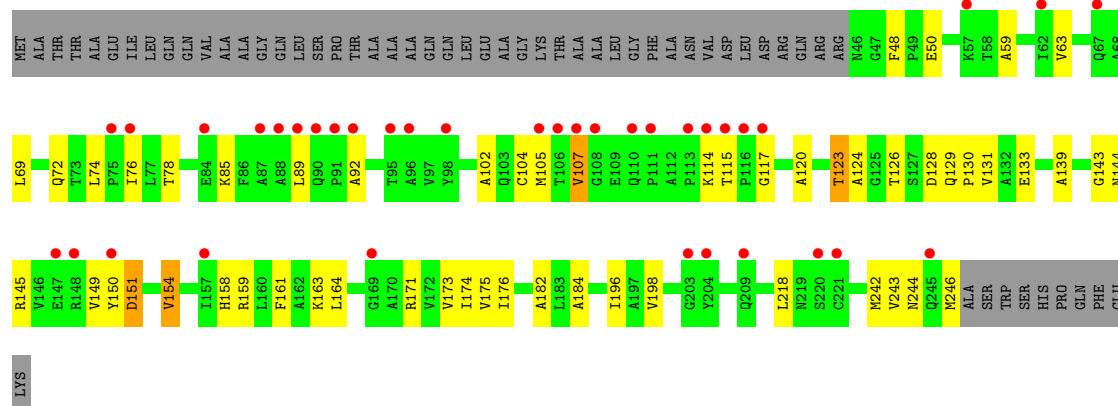
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



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• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.28Å 121.28Å 213.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.79 – 3.01 39.79 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.79-3.01) 100.0 (39.79-3.01)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.235 , 0.275 0.235 , 0.274	Depositor DCC
R_{free} test set	1675 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8549	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.08% 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

5.1 Standard geometry

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

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	0.52	0/1440	0.73	1/1968 (0.1%)
1	B	0.55	0/1424	0.74	2/1947 (0.1%)
1	C	0.58	0/1476	0.74	2/2018 (0.1%)
1	D	0.49	0/1446	0.62	1/1978 (0.1%)
1	E	0.32	0/1402	0.50	0/1918
1	F	0.30	0/1441	0.50	0/1970
All	All	0.48	0/8629	0.65	6/11799 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	CYS	CB-CA-C	-11.96	86.48	110.40
1	C	249	TRP	CB-CA-C	-7.39	95.62	110.40
1	B	221	CYS	N-CA-C	6.34	128.12	111.00
1	A	77	LEU	CA-CB-CG	6.08	129.28	115.30
1	D	221	CYS	CA-CB-SG	5.48	123.86	114.00
1	C	250	SER	N-CA-CB	5.32	118.48	110.50

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	1418	0	1406	28	0
1	B	1404	0	1399	20	0
1	C	1453	0	1447	20	0
1	D	1425	0	1419	28	0
1	E	1382	0	1382	21	0
1	F	1419	0	1432	32	0
2	A	23	0	12	1	0
2	C	23	0	12	0	0
3	A	2	0	0	0	0
All	All	8549	0	8509	146	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 9.

All (146) 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:123:THR:HG22	1:B:151:ASP:H	1.39	0.87
1:E:149:VAL:HG13	1:E:163:LYS:HD2	1.55	0.87
1:A:180:GLU:HG2	1:A:182:ALA:H	1.47	0.80
1:E:63:VAL:HG11	1:E:92:ALA:HB1	1.66	0.78
1:A:77:LEU:HD11	1:A:138:THR:HG22	1.72	0.72
1:B:69:LEU:HD22	1:B:72:GLN:HE21	1.57	0.70
1:D:154:VAL:HG11	1:D:186:VAL:HG21	1.74	0.70
1:E:134:GLU:O	1:E:138:THR:OG1	2.11	0.69
1:C:76:ILE:HB	1:C:107:VAL:HG13	1.74	0.69
1:F:123:THR:HG22	1:F:151:ASP:H	1.56	0.69
1:E:132:ALA:HA	1:E:176:ILE:HD13	1.75	0.67
1:D:129:GLN:HA	1:D:132:ALA:HB3	1.78	0.65
1:C:126:THR:HG22	1:C:151:ASP:OD2	1.98	0.64
1:F:117:GLY:HA3	1:F:171:ARG:HG3	1.80	0.64
1:F:161:PHE:HA	1:F:164:LEU:HB2	1.80	0.63
1:A:191:VAL:HG23	1:A:193:LYS:H	1.62	0.63
1:B:222:ALA:O	1:B:223:SER:C	2.38	0.63
1:A:63:VAL:HA	1:A:93:LEU:HD11	1.81	0.62
1:C:52:ILE:HB	1:C:78:THR:HG23	1.81	0.62
1:A:123:THR:HG22	1:A:151:ASP:H	1.63	0.62
1:A:123:THR:HB	1:A:150:TYR:HA	1.81	0.62
1:E:81:LEU:HD22	1:E:105:MET:HB2	1.80	0.62
1:D:76:ILE:HB	1:D:107:VAL:HG23	1.82	0.61
1:B:221:CYS:O	1:B:223:SER:N	2.32	0.61
1:A:138:THR:HG21	1:A:234:PHE:HD1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:ALA:HB1	1:F:144:ASN:HB2	1.83	0.60
1:B:59:ALA:HB1	1:B:89:LEU:HD21	1.85	0.58
1:E:228:VAL:HG21	1:E:236:ALA:HB2	1.85	0.58
1:E:118:TYR:OH	1:E:166:VAL:O	2.20	0.57
1:D:123:THR:HG22	1:D:150:TYR:HA	1.87	0.57
1:D:63:VAL:HG23	1:D:89:LEU:HD13	1.86	0.57
1:F:76:ILE:HB	1:F:107:VAL:HG13	1.85	0.56
1:D:213:ALA:HA	1:D:216:THR:HG22	1.87	0.56
1:C:59:ALA:HB1	1:C:89:LEU:HD21	1.88	0.55
1:E:243:VAL:HG13	1:F:243:VAL:HG13	1.87	0.55
1:B:213:ALA:O	1:B:216:THR:HG22	2.07	0.54
1:A:52:ILE:HB	1:A:78:THR:HG22	1.88	0.54
1:A:98:TYR:CE2	1:A:100:ALA:HA	2.42	0.54
1:F:63:VAL:HG23	1:F:89:LEU:HD22	1.90	0.54
1:B:52:ILE:HB	1:B:78:THR:HG23	1.90	0.53
1:E:117:GLY:HA3	1:E:171:ARG:HG3	1.90	0.53
1:E:123:THR:HG23	1:E:128:ASP:HB2	1.91	0.53
1:E:138:THR:HG21	1:E:234:PHE:HD1	1.73	0.53
1:F:175:VAL:HG11	1:F:184:ALA:HA	1.91	0.53
1:A:210:GLY:HA3	1:A:230:ILE:HD13	1.91	0.53
1:B:227:VAL:HG12	1:B:228:VAL:O	2.09	0.52
1:E:96:ALA:HB2	1:E:107:VAL:HG12	1.92	0.52
1:B:115:THR:HG21	1:B:245:GLN:HG2	1.90	0.52
1:D:52:ILE:N	1:D:77:LEU:O	2.33	0.52
1:E:199:PRO:HD3	1:E:217:MET:HE1	1.91	0.51
1:A:122:VAL:HG21	1:A:167:ILE:HD13	1.92	0.51
1:B:115:THR:CG2	1:B:245:GLN:HG2	2.41	0.51
1:F:50:GLU:HG3	1:F:69:LEU:HD13	1.93	0.51
1:F:59:ALA:HB1	1:F:89:LEU:HD21	1.93	0.51
1:A:102:ALA:HB2	1:A:133:GLU:HB3	1.93	0.50
1:A:63:VAL:HG23	1:A:89:LEU:HD22	1.94	0.50
1:E:59:ALA:HB1	1:E:89:LEU:HD21	1.93	0.50
1:E:77:LEU:HB2	1:E:141:THR:HG21	1.93	0.50
1:C:46:ASN:O	1:C:46:ASN:ND2	2.44	0.50
1:A:165:ASP:OD1	1:A:165:ASP:N	2.45	0.50
1:D:148:ARG:HG2	1:D:150:TYR:CZ	2.48	0.49
1:D:188:GLY:HA3	1:D:225:ILE:HD11	1.95	0.49
1:F:120:ALA:HB3	1:F:173:VAL:HG22	1.95	0.49
1:D:62:ILE:O	1:D:66:VAL:HG23	2.14	0.48
1:B:133:GLU:OE1	1:B:150:TYR:OH	2.24	0.48
1:C:98:TYR:CE2	1:C:100:ALA:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:LEU:HD23	1:D:227:VAL:HG21	1.95	0.48
1:D:69:LEU:HD12	1:D:76:ILE:HD13	1.95	0.48
1:D:75:PRO:HG2	1:D:111:PRO:HD3	1.96	0.48
1:A:175:VAL:HG11	1:A:184:ALA:HA	1.96	0.48
1:E:49:PRO:HD2	1:E:142:PHE:CE2	2.49	0.48
1:F:85:LYS:O	1:F:89:LEU:HG	2.13	0.47
1:F:123:THR:HG22	1:F:150:TYR:HA	1.95	0.47
1:B:77:LEU:HB2	1:B:141:THR:HG21	1.96	0.47
1:F:159:ARG:O	1:F:163:LYS:NZ	2.43	0.47
1:C:76:ILE:O	1:C:106:THR:HA	2.15	0.47
1:F:154:VAL:HG21	1:F:182:ALA:HB3	1.96	0.47
1:B:114:LYS:HE3	1:C:249:TRP:CE2	2.50	0.47
1:B:203:GLY:C	1:B:205:GLY:HA3	2.36	0.47
1:C:63:VAL:HG23	1:C:89:LEU:HD22	1.98	0.46
1:C:188:GLY:HA3	1:C:225:ILE:HD11	1.96	0.46
1:B:78:THR:O	1:B:104:CYS:HA	2.14	0.46
1:D:114:LYS:HD2	1:D:245:GLN:OE1	2.16	0.46
1:F:78:THR:HB	1:F:105:MET:HB3	1.98	0.46
1:D:122:VAL:HG22	1:D:149:VAL:HB	1.98	0.46
1:F:114:LYS:HG3	1:F:143:GLY:HA3	1.98	0.46
1:D:218:LEU:HD23	1:D:227:VAL:CG2	2.46	0.45
1:F:63:VAL:CG2	1:F:89:LEU:HD22	2.45	0.45
1:D:59:ALA:HB1	1:D:89:LEU:HD21	1.99	0.45
1:F:63:VAL:HG11	1:F:92:ALA:HB1	1.99	0.45
1:A:96:ALA:HB2	1:A:107:VAL:HG12	1.97	0.45
1:D:49:PRO:HG2	1:D:142:PHE:CE1	2.52	0.45
1:D:181:GLY:HA3	1:D:216:THR:HG21	1.99	0.45
1:F:174:ILE:HA	1:F:196:ILE:O	2.16	0.45
1:A:59:ALA:HB1	1:A:89:LEU:HD21	1.99	0.44
1:E:175:VAL:HG11	1:E:184:ALA:HA	2.00	0.44
1:F:123:THR:CG2	1:F:151:ASP:H	2.27	0.44
1:E:138:THR:HG21	1:E:234:PHE:CD1	2.52	0.44
1:A:241:SER:O	1:A:245:GLN:HG3	2.17	0.44
1:F:72:GLN:C	1:F:74:LEU:H	2.21	0.44
1:D:114:LYS:HE3	1:D:143:GLY:HA3	2.00	0.44
1:B:85:LYS:O	1:B:89:LEU:HG	2.18	0.44
1:B:188:GLY:HA3	1:B:225:ILE:HD11	1.99	0.44
1:F:128:ASP:HB3	1:F:176:ILE:HG22	2.00	0.44
1:A:217:MET:HB3	1:A:217:MET:HE3	1.79	0.43
1:C:51:VAL:HG11	1:C:234:PHE:CZ	2.53	0.43
1:D:176:ILE:HG13	1:D:198:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PHE:HE1	1:A:190:LEU:HD11	1.84	0.43
1:C:199:PRO:HD3	1:C:217:MET:HE1	2.01	0.43
1:F:78:THR:O	1:F:104:CYS:HA	2.18	0.43
1:E:194:PRO:HD3	1:F:242:MET:HB3	1.99	0.43
1:A:62:ILE:O	1:A:66:VAL:HG23	2.18	0.43
1:A:204:TYR:OH	2:A:301:AMP:C2	2.71	0.43
1:C:85:LYS:O	1:C:89:LEU:HG	2.19	0.43
1:C:57:LYS:O	1:C:85:LYS:NZ	2.52	0.43
1:D:157:ILE:HG12	1:D:161:PHE:CE2	2.54	0.43
1:E:125:GLY:HA2	1:E:151:ASP:OD1	2.18	0.43
1:F:129:GLN:HB3	1:F:130:PRO:HD3	2.00	0.43
1:A:227:VAL:HG12	1:A:228:VAL:O	2.20	0.42
1:D:52:ILE:HB	1:D:78:THR:HA	2.02	0.42
1:B:89:LEU:O	1:B:92:ALA:N	2.52	0.42
1:D:213:ALA:O	1:D:216:THR:HG22	2.20	0.42
1:A:134:GLU:O	1:A:138:THR:HG23	2.19	0.42
1:C:213:ALA:O	1:C:217:MET:HG3	2.20	0.42
1:D:63:VAL:HG22	1:D:93:LEU:HD11	2.02	0.42
1:F:124:ALA:O	1:F:151:ASP:HA	2.20	0.42
1:F:69:LEU:HB2	1:F:76:ILE:HD11	2.02	0.41
1:A:52:ILE:HB	1:A:78:THR:CG2	2.49	0.41
1:D:148:ARG:HG2	1:D:150:TYR:OH	2.20	0.41
1:C:238:TYR:HE1	1:C:242:MET:HE3	1.86	0.41
1:F:102:ALA:HB2	1:F:133:GLU:HB3	2.03	0.41
1:F:158:HIS:CD2	1:F:159:ARG:HG3	2.56	0.41
1:F:176:ILE:HG12	1:F:198:VAL:HB	2.01	0.41
1:C:63:VAL:CG2	1:C:89:LEU:HD22	2.51	0.40
1:D:85:LYS:O	1:D:89:LEU:HG	2.21	0.40
1:A:215:LEU:HA	1:A:215:LEU:HD23	1.74	0.40
1:B:129:GLN:O	1:B:133:GLU:HB2	2.22	0.40
1:B:237:ALA:HA	1:B:240:ALA:HB3	2.04	0.40
1:D:52:ILE:HB	1:D:78:THR:HG23	2.02	0.40
1:C:171:ARG:HH12	1:C:248:SER:HB3	1.86	0.40
1:F:149:VAL:HG13	1:F:163:LYS:HD2	2.04	0.40
1:A:61:GLN:O	1:A:65:ILE:HG13	2.20	0.40
1:E:123:THR:HB	1:E:150:TYR:HA	2.03	0.40
1:A:44:ARG:O	1:A:46:ASN:ND2	2.54	0.40
1:C:180:GLU:HG2	1:C:182:ALA:H	1.86	0.40
1:C:202:VAL:O	1:C:202:VAL:CG2	2.69	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	198/256 (77%)	183 (92%)	12 (6%)	3 (2%)	10	40
1	B	198/256 (77%)	183 (92%)	15 (8%)	0	100	100
1	C	205/256 (80%)	184 (90%)	18 (9%)	3 (2%)	10	40
1	D	199/256 (78%)	179 (90%)	19 (10%)	1 (0%)	29	66
1	E	196/256 (77%)	172 (88%)	21 (11%)	3 (2%)	10	40
1	F	199/256 (78%)	180 (90%)	19 (10%)	0	100	100
All	All	1195/1536 (78%)	1081 (90%)	104 (9%)	10 (1%)	19	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	75	PRO
1	E	204	TYR
1	E	73	THR
1	A	53	TYR
1	A	206	THR
1	C	249	TRP
1	C	205	GLY
1	D	205	GLY
1	E	113	PRO
1	A	49	PRO

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	142/191 (74%)	135 (95%)	7 (5%)	25	60
1	B	139/191 (73%)	126 (91%)	13 (9%)	8	31
1	C	146/191 (76%)	130 (89%)	16 (11%)	6	24
1	D	142/191 (74%)	136 (96%)	6 (4%)	30	65
1	E	140/191 (73%)	135 (96%)	5 (4%)	35	69
1	F	143/191 (75%)	131 (92%)	12 (8%)	11	37
All	All	852/1146 (74%)	793 (93%)	59 (7%)	15	46

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR
1	A	95	THR
1	A	123	THR
1	A	154	VAL
1	A	191	VAL
1	A	202	VAL
1	A	209	GLN
1	B	46	ASN
1	B	58	THR
1	B	101	THR
1	B	115	THR
1	B	123	THR
1	B	131	VAL
1	B	151	ASP
1	B	152	VAL
1	B	185	SER
1	B	202	VAL
1	B	208	PHE
1	B	218	LEU
1	B	221	CYS
1	C	46	ASN
1	C	73	THR
1	C	77	LEU
1	C	78	THR
1	C	107	VAL
1	C	115	THR
1	C	123	THR
1	C	126	THR
1	C	127	SER
1	C	166	VAL

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Mol	Chain	Res	Type
1	C	179	MET
1	C	180	GLU
1	C	185	SER
1	C	207	SER
1	C	220	SER
1	C	249	TRP
1	D	107	VAL
1	D	115	THR
1	D	123	THR
1	D	131	VAL
1	D	151	ASP
1	D	206	THR
1	E	60	THR
1	E	138	THR
1	E	165	ASP
1	E	180	GLU
1	E	200	THR
1	F	48	PHE
1	F	107	VAL
1	F	115	THR
1	F	123	THR
1	F	126	THR
1	F	131	VAL
1	F	145	ARG
1	F	151	ASP
1	F	154	VAL
1	F	218	LEU
1	F	244	ASN
1	F	246	MET

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

Mol	Chain	Res	Type
1	A	46	ASN
1	B	72	GLN

5.3.3 RNA ⓘ

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 [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AMP	A	301	3	22,25,25	0.71	1 (4%)	25,38,38	0.72	1 (4%)
2	AMP	C	301	-	22,25,25	0.72	1 (4%)	25,38,38	0.79	1 (4%)

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	AMP	A	301	3	-	5/6/26/26	0/3/3/3
2	AMP	C	301	-	-	4/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	AMP	C8-N7	-2.25	1.30	1.34
2	A	301	AMP	C8-N7	-2.09	1.31	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	AMP	C5-C6-N6	2.08	123.51	120.35
2	C	301	AMP	C5-C6-N6	2.07	123.50	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

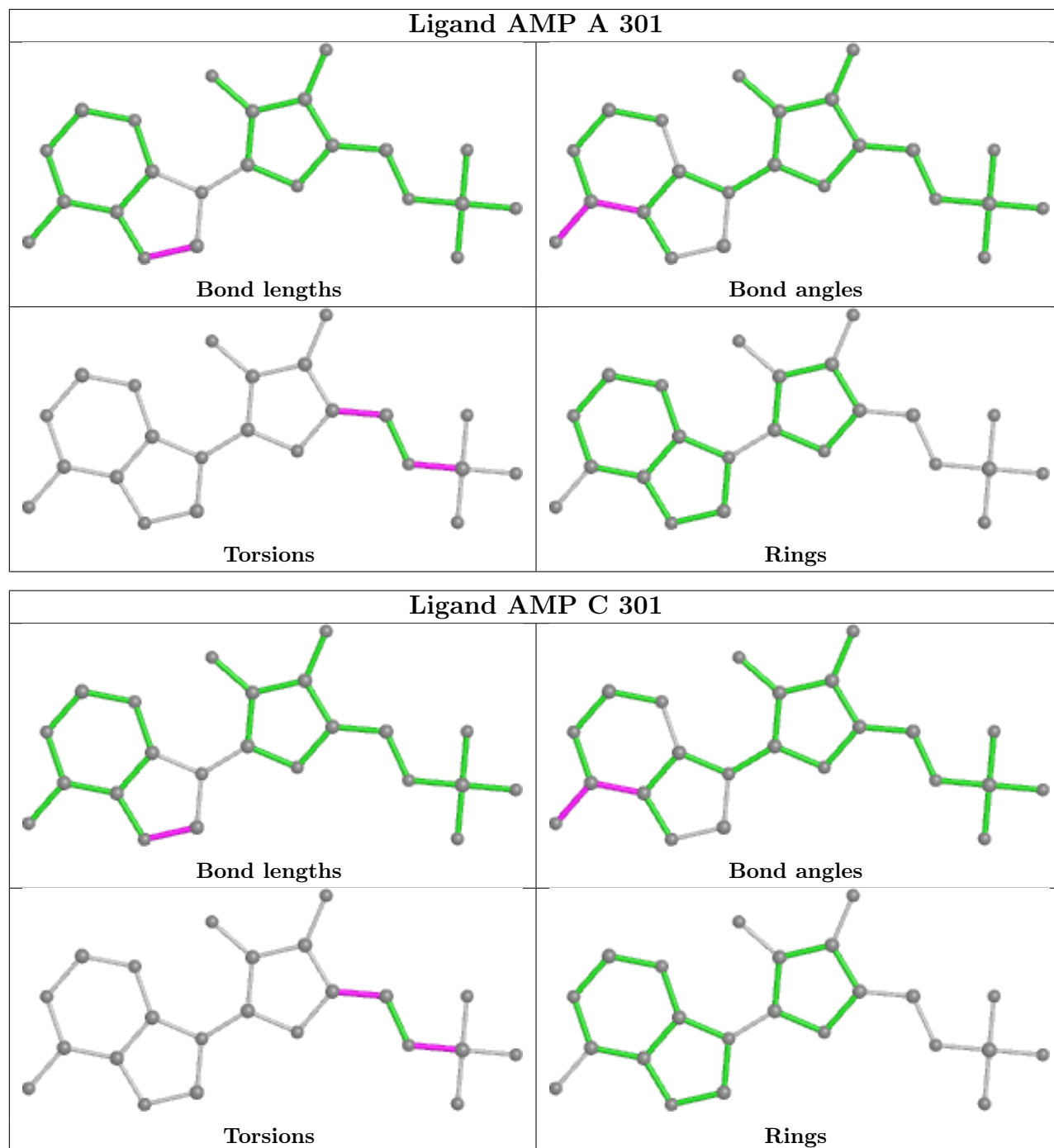
Mol	Chain	Res	Type	Atoms
2	A	301	AMP	C5'-O5'-P-O1P
2	A	301	AMP	C5'-O5'-P-O2P
2	A	301	AMP	C5'-O5'-P-O3P
2	A	301	AMP	C3'-C4'-C5'-O5'
2	C	301	AMP	C5'-O5'-P-O2P
2	C	301	AMP	C5'-O5'-P-O3P
2	A	301	AMP	O4'-C4'-C5'-O5'
2	C	301	AMP	C3'-C4'-C5'-O5'
2	C	301	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	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, 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	202/256 (78%)	-0.24	1 (0%) 91 75	25, 62, 145, 222	0
1	B	202/256 (78%)	-0.19	4 (1%) 65 36	23, 66, 132, 197	0
1	C	207/256 (80%)	-0.29	2 (0%) 82 58	29, 60, 135, 205	0
1	D	203/256 (79%)	0.03	9 (4%) 34 13	35, 80, 153, 219	0
1	E	198/256 (77%)	0.77	30 (15%) 2 1	122, 164, 219, 263	0
1	F	201/256 (78%)	1.06	37 (18%) 1 0	138, 172, 234, 303	0
All	All	1213/1536 (78%)	0.18	83 (6%) 17 5	23, 101, 204, 303	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	96	ALA	16.9
1	F	115	THR	7.4
1	E	96	ALA	6.8
1	E	153	GLY	6.8
1	D	91	PRO	5.7
1	E	115	THR	5.4
1	F	110	GLN	5.3
1	F	87	ALA	5.1
1	E	91	PRO	5.0
1	F	92	ALA	5.0
1	E	117	GLY	4.9
1	F	107	VAL	4.6
1	E	90	GLN	4.4
1	F	111	PRO	4.2
1	D	92	ALA	4.1
1	F	106	THR	4.1
1	F	148	ARG	4.0
1	F	220	SER	4.0
1	E	94	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	67	GLN	3.7
1	E	87	ALA	3.7
1	F	113	PRO	3.7
1	E	141	THR	3.6
1	F	105	MET	3.6
1	F	209	GLN	3.6
1	F	91	PRO	3.6
1	F	95	THR	3.5
1	F	204	TYR	3.5
1	D	60	THR	3.4
1	E	95	THR	3.4
1	E	152	VAL	3.4
1	F	114	LYS	3.4
1	F	57	LYS	3.3
1	E	70	SER	3.3
1	E	146	VAL	3.2
1	F	76	ILE	3.2
1	B	60	THR	3.2
1	F	150	TYR	3.2
1	D	84	GLU	3.2
1	F	157	ILE	3.1
1	F	62	ILE	3.1
1	F	221	CYS	3.1
1	E	189	GLY	3.0
1	E	150	TYR	3.0
1	E	76	ILE	2.9
1	E	81	LEU	2.9
1	E	246	MET	2.8
1	E	110	GLN	2.8
1	D	94	PRO	2.8
1	F	89	LEU	2.7
1	E	88	ALA	2.7
1	F	116	PRO	2.7
1	E	107	VAL	2.7
1	D	95	THR	2.7
1	C	84	GLU	2.7
1	F	203	GLY	2.6
1	D	90	GLN	2.6
1	D	50	GLU	2.6
1	E	111	PRO	2.6
1	F	108	GLY	2.6
1	F	98	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	96	ALA	2.5
1	E	63	VAL	2.4
1	E	161	PHE	2.4
1	F	75	PRO	2.4
1	E	92	ALA	2.4
1	B	209	GLN	2.4
1	E	179	MET	2.3
1	E	98	TYR	2.3
1	E	97	VAL	2.2
1	F	84	GLU	2.2
1	F	88	ALA	2.2
1	F	245	GLN	2.2
1	F	117	GLY	2.1
1	E	209	GLN	2.1
1	B	88	ALA	2.1
1	F	169	GLY	2.1
1	B	70	SER	2.1
1	F	147	GLU	2.1
1	F	90	GLN	2.1
1	A	113	PRO	2.0
1	C	96	ALA	2.0
1	E	148	ARG	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.

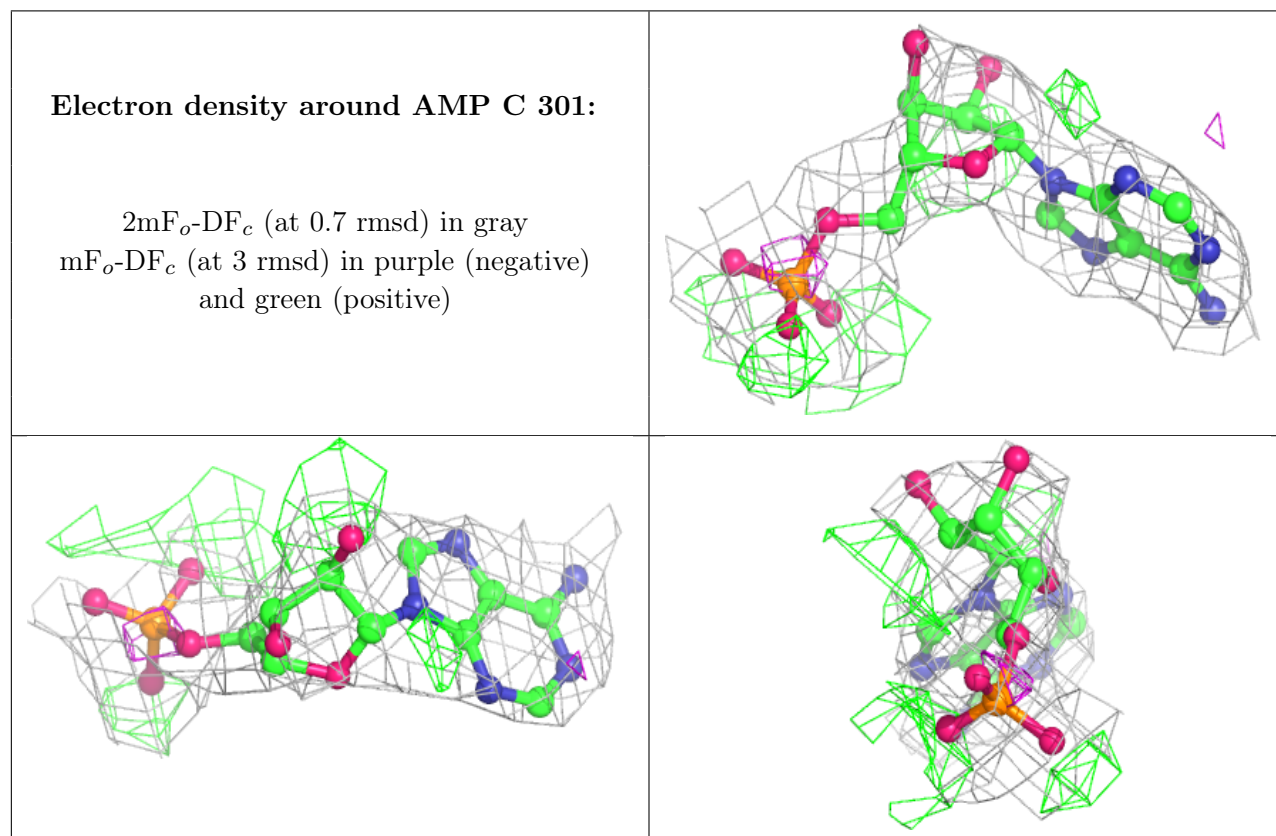
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AMP	C	301	23/23	0.76	0.35	55,59,61,62	23

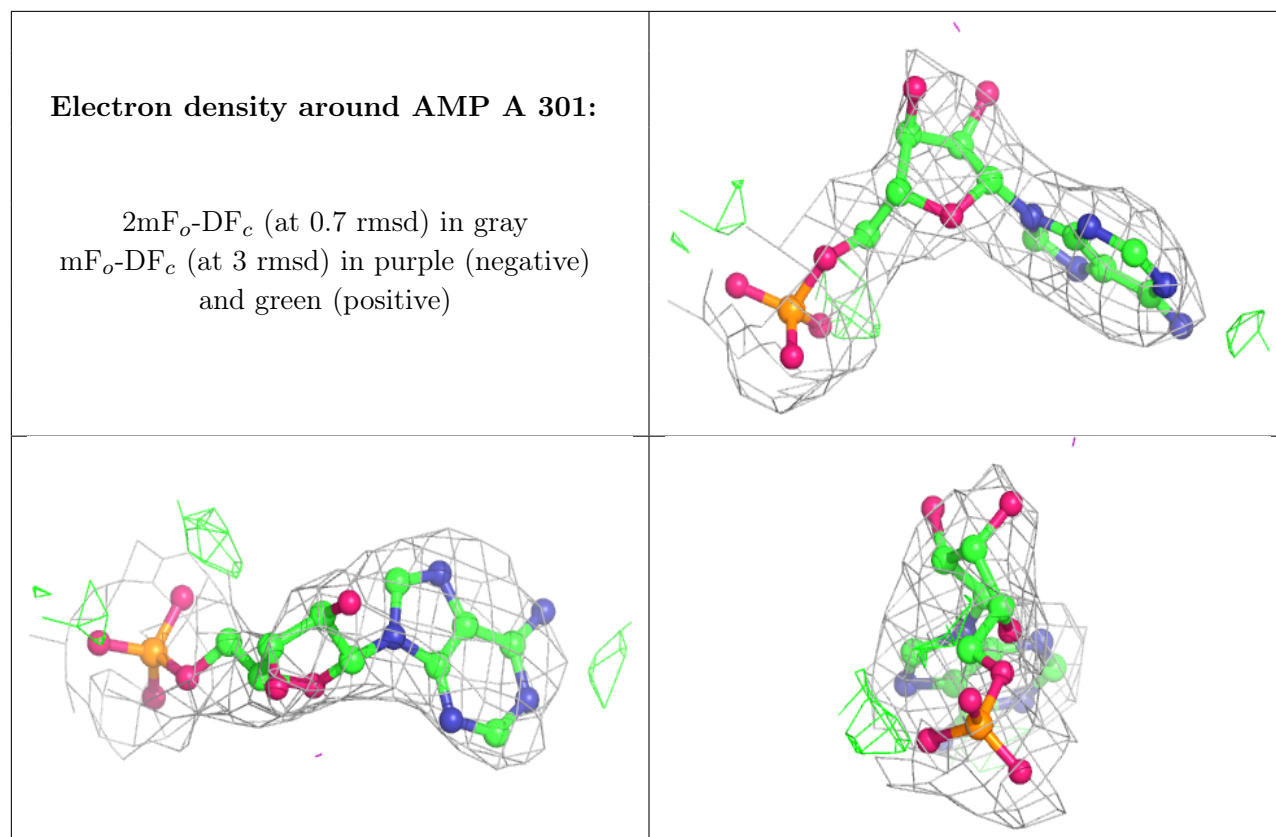
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	303	1/1	0.80	0.36	24,24,24,24	1
2	AMP	A	301	23/23	0.81	0.24	48,78,86,88	23
3	MG	A	302	1/1	0.84	0.18	24,24,24,24	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.