



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2021 – 12:07 PM EDT

PDB ID : 7JIJ  
Title : ATP-bound AMP-activated protein kinase  
Authors : Yan, Y.; Zhou, X.E.; Powell, K.; Xu, T.; Brunzelle, J.S.; Xu, H.X.; Melcher, K.  
Deposited on : 2020-07-23  
Resolution : 5.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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

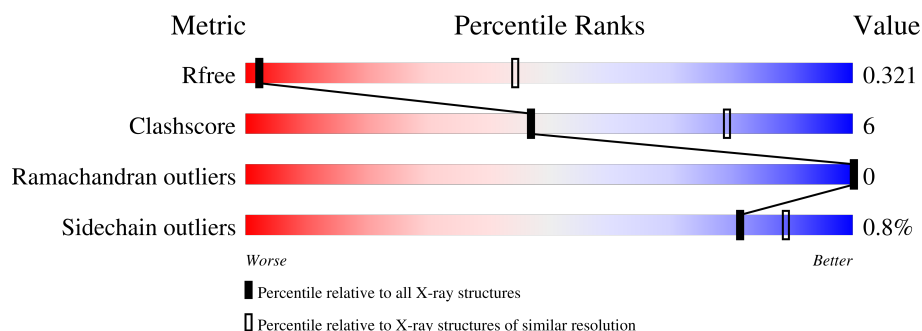
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	M	373	<div> <div style="width: 85%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
2	A	484	<div> <div style="width: 67%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 16%; background-color: grey;"></div> </div>
3	B	198	<div> <div style="width: 37%; background-color: green;"></div> <div style="width: 7%; background-color: yellow;"></div> <div style="width: 56%; background-color: grey;"></div> </div>
4	G	306	<div> <div style="width: 82%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
5	C	2	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 50%; background-color: yellow;"></div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9372 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 Maltose/maltodextrin ABC transporter substrate-binding protein MalE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	M	367	Total	C	N	O	S		0	0	0
			2834	1826	460	542	6				

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MET	-	initiating methionine	UNP A0A6D0N546
M	84	ALA	ASP	conflict	UNP A0A6D0N546
M	85	ALA	LYS	conflict	UNP A0A6D0N546
M	241	ALA	LYS	conflict	UNP A0A6D0N546
M	369	ASN	-	expression tag	UNP A0A6D0N546
M	370	ALA	-	expression tag	UNP A0A6D0N546
M	371	ALA	-	expression tag	UNP A0A6D0N546
M	372	GLU	-	expression tag	UNP A0A6D0N546
M	373	PHE	-	expression tag	UNP A0A6D0N546

- Molecule 2 is a protein called 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	407	Total	C	N	O	P	S	0	0	0
			3319	2127	581	591	1	19			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	472	LEU	ILE	conflict	UNP Q13131
A	528	PRO	GLU	conflict	UNP Q13131
A	?	-	ALA	deletion	UNP Q13131
A	?	-	LYS	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	GLY	deletion	UNP Q13131

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q13131
A	?	-	ALA	deletion	UNP Q13131
A	?	-	THR	deletion	UNP Q13131
A	?	-	PRO	deletion	UNP Q13131
A	?	-	GLN	deletion	UNP Q13131
A	530	PRO	SER	conflict	UNP Q13131
A	?	-	VAL	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	ASN	deletion	UNP Q13131
A	?	-	TYR	deletion	UNP Q13131
A	?	-	ARG	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	CYS	deletion	UNP Q13131
A	?	-	GLN	deletion	UNP Q13131
A	?	-	ARG	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	ASP	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	ASP	deletion	UNP Q13131
A	?	-	ALA	deletion	UNP Q13131
A	?	-	GLU	deletion	UNP Q13131
A	?	-	ALA	deletion	UNP Q13131
A	?	-	GLN	deletion	UNP Q13131
A	?	-	GLY	deletion	UNP Q13131
A	?	-	LYS	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	GLU	deletion	UNP Q13131
A	?	-	VAL	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	LEU	deletion	UNP Q13131
A	?	-	THR	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	VAL	deletion	UNP Q13131
A	?	-	THR	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	LEU	deletion	UNP Q13131
A	?	-	ASP	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131
A	?	-	PRO	deletion	UNP Q13131

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP Q13131
A	?	-	ASP	deletion	UNP Q13131
A	?	-	LEU	deletion	UNP Q13131
A	?	-	THR	deletion	UNP Q13131
A	?	-	PRO	deletion	UNP Q13131
A	?	-	ARG	deletion	UNP Q13131
A	?	-	PRO	deletion	UNP Q13131
A	?	-	GLY	deletion	UNP Q13131
A	?	-	SER	deletion	UNP Q13131

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	87	Total	C	N	O	S	0	0	0
			695	455	117	119	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	75	MET	-	initiating methionine	UNP O43741
B	199	ALA	GLU	conflict	UNP O43741
B	200	ALA	GLU	conflict	UNP O43741

- Molecule 4 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	300	Total	C	N	O	S	0	0	0
			2420	1574	402	437	7			

There are 3 discrepancies between the modelled and reference sequences:

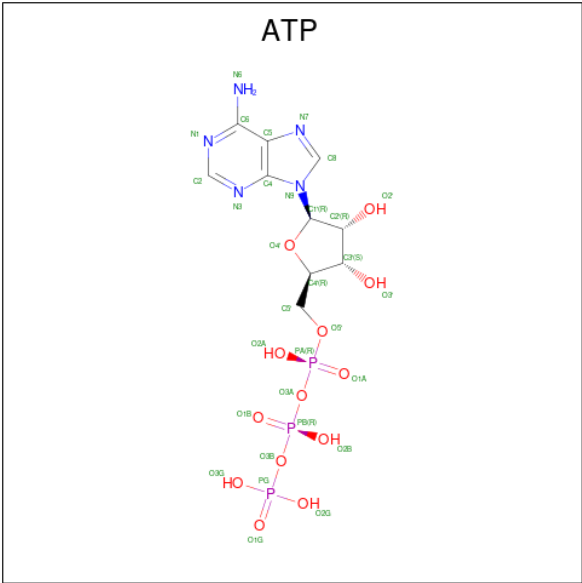
Chain	Residue	Modelled	Actual	Comment	Reference
G	22	MET	-	initiating methionine	UNP P54619
G	23	GLY	-	expression tag	UNP P54619
G	31	PHE	SER	conflict	UNP P54619

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



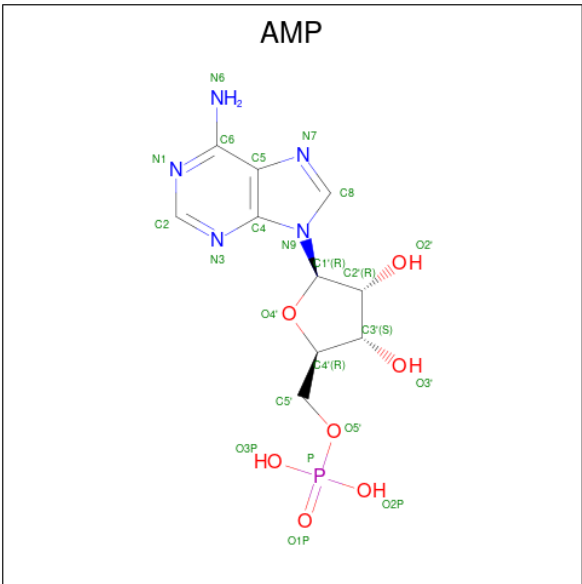
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



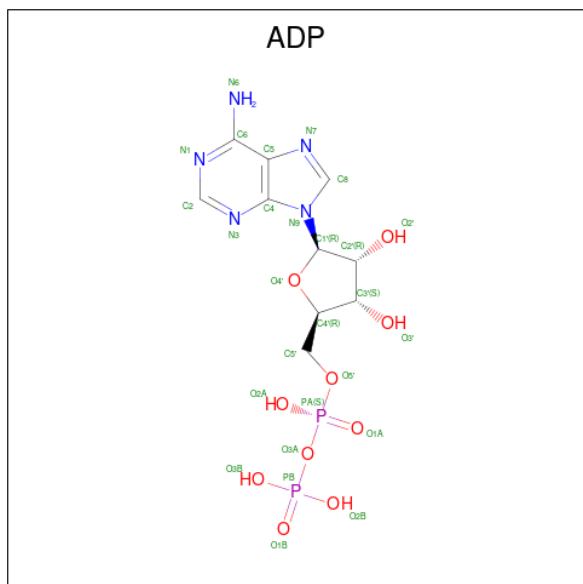
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



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

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

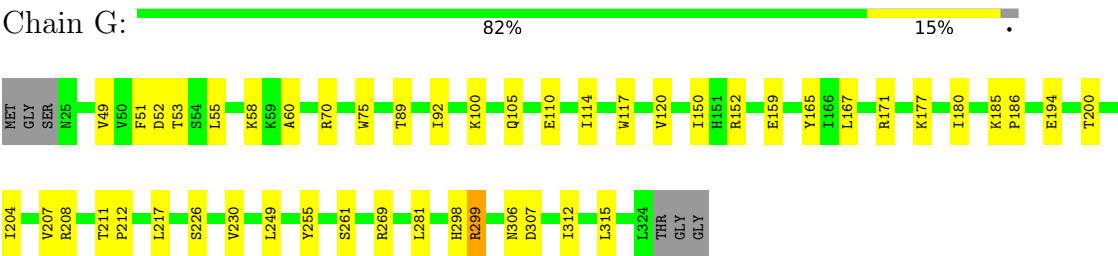


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		





● Molecule 4: 5'-AMP-activated protein kinase subunit gamma-1



● Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.69Å 126.69Å 332.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.90 – 5.50 49.45 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.90-5.50) 85.6 (49.45-4.50)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.249 , 0.323 0.249 , 0.321	Depositor DCC
$R_{free}$ test set	821 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	188.7	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 313.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.147 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	9372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	429.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, ATP, ADP, AMP, TPO

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	M	0.27	0/2904	0.46	0/3947
2	A	0.29	1/3387 (0.0%)	0.50	0/4573
3	B	0.26	0/716	0.51	0/975
4	G	0.33	0/2472	0.48	0/3356
All	All	0.29	1/9479 (0.0%)	0.48	0/12851

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	94	VAL	CB-CG2	-5.33	1.41	1.52

There are no bond angle outliers.

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	M	2834	0	2792	31	0
2	A	3319	0	3335	57	0
3	B	695	0	722	9	0
4	G	2420	0	2479	28	0
5	C	23	0	21	0	0
6	G	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	23	0	12	1	0
8	G	27	0	12	1	0
All	All	9372	0	9385	117	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 6.

All (117) 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)
2:A:221:VAL:HG23	2:A:222:PRO:HD3	1.58	0.84
2:A:260:THR:HG22	2:A:261:ILE:H	1.49	0.77
3:B:241:LEU:HD11	3:B:253:LEU:HD12	1.66	0.77
2:A:82:TYR:HD2	2:A:94:VAL:HG21	1.55	0.71
2:A:260:THR:HG22	2:A:261:ILE:N	2.06	0.70
2:A:84:VAL:HG12	2:A:93:MET:HG2	1.75	0.68
1:M:47:GLU:HB3	2:A:55:ARG:HH22	1.61	0.66
2:A:82:TYR:HD2	2:A:94:VAL:CG2	2.08	0.66
4:G:226:SER:OG	4:G:299:ARG:NH2	2.32	0.62
2:A:336:MET:HG2	2:A:340:LYS:HD2	1.80	0.62
2:A:32:VAL:HG12	2:A:47:LYS:HA	1.84	0.59
2:A:196:GLU:HB2	2:A:258:ARG:HD2	1.84	0.59
2:A:76:PRO:O	2:A:156:LYS:NZ	2.34	0.59
4:G:58:LYS:HG3	4:G:110:GLU:HA	1.85	0.59
1:M:93:PRO:HD2	1:M:305:ALA:HB1	1.85	0.59
2:A:46:VAL:HG12	2:A:94:VAL:HG12	1.85	0.58
4:G:194:GLU:HB2	4:G:281:LEU:HB3	1.84	0.58
1:M:93:PRO:HG2	1:M:94:PHE:CD1	2.38	0.58
2:A:24:LEU:HB2	2:A:32:VAL:HG23	1.84	0.58
2:A:82:TYR:CD2	2:A:94:VAL:HG21	2.37	0.58
2:A:138:VAL:HG11	2:A:194:GLY:HA3	1.85	0.58
2:A:23:THR:OG1	2:A:33:LYS:NZ	2.36	0.58
4:G:249:LEU:HD23	4:G:255:TYR:HA	1.84	0.58
2:A:107:ILE:HD11	2:A:209:LEU:HD23	1.86	0.57
2:A:65:ARG:O	2:A:69:ASN:ND2	2.38	0.56
4:G:100:LYS:HB2	4:G:105:GLN:HG2	1.86	0.56
3:B:225:CYS:SG	3:B:226:ASP:N	2.78	0.56
2:A:168:ASP:OD1	3:B:258:ARG:NH1	2.39	0.56
4:G:152:ARG:NH2	6:G:401:ATP:O3G	2.40	0.55
1:M:323:MET:O	1:M:327:GLN:HG3	2.07	0.55
2:A:98:VAL:HB	2:A:150:ASP:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:124:LEU:HD11	1:M:141:LEU:HD11	1.90	0.54
3:B:267:LEU:HB2	4:G:49:VAL:HG12	1.90	0.54
1:M:74:GLN:OE1	1:M:101:TYR:OH	2.26	0.53
2:A:260:THR:CG2	2:A:261:ILE:H	2.18	0.53
1:M:131:TRP:HB2	1:M:252:PHE:HD1	1.72	0.53
4:G:208:ARG:HB3	4:G:211:THR:HG23	1.91	0.53
1:M:99:VAL:HG23	1:M:105:LEU:HD22	1.91	0.52
2:A:112:ARG:HD2	2:A:112:ARG:H	1.75	0.52
4:G:212:PRO:HA	4:G:261:SER:HA	1.90	0.52
1:M:64:TRP:HE1	1:M:68:ARG:HD2	1.74	0.52
1:M:11:ILE:HG12	1:M:61:ILE:HB	1.91	0.52
1:M:231:PRO:HB2	1:M:299:LYS:HD3	1.91	0.52
1:M:194:LEU:HD23	1:M:359:VAL:HG13	1.93	0.51
2:A:82:TYR:HB3	2:A:94:VAL:HG23	1.92	0.51
4:G:89:THR:OG1	8:G:403:ADP:O2B	2.29	0.51
2:A:218:ASP:OD2	2:A:223:THR:OG1	2.29	0.50
2:A:260:THR:CG2	2:A:261:ILE:N	2.74	0.50
2:A:83:GLN:O	2:A:94:VAL:HG22	2.12	0.49
1:M:93:PRO:HG2	1:M:94:PHE:HD1	1.76	0.49
3:B:246:ILE:HG22	3:B:251:MET:HA	1.94	0.49
1:M:256:PRO:HG3	1:M:328:LYS:HD2	1.94	0.49
2:A:126:LEU:HA	2:A:129:VAL:HG22	1.95	0.48
4:G:200:THR:OG1	7:G:402:AMP:O2'	2.26	0.48
3:B:208:LEU:HD12	3:B:209:PRO:HD2	1.94	0.48
2:A:90:ASP:N	2:A:90:ASP:OD1	2.46	0.48
2:A:176:CYS:SG	2:A:177:GLY:N	2.84	0.47
1:M:111:ALA:HB2	1:M:301:LEU:HD13	1.97	0.47
2:A:15:ILE:HG21	2:A:85:ILE:HD13	1.96	0.47
1:M:124:LEU:HD21	1:M:141:LEU:HD11	1.97	0.47
3:B:252:VAL:HG12	3:B:269:TYR:CD1	2.50	0.47
1:M:56:GLY:HA2	1:M:270:ALA:HB3	1.97	0.46
1:M:302:GLY:HA3	1:M:319:ILE:HD12	1.98	0.46
4:G:204:ILE:HD12	4:G:312:ILE:HG12	1.98	0.46
2:A:201:SER:HA	2:A:204:VAL:HG22	1.97	0.46
4:G:55:LEU:HB3	4:G:114:ILE:HD12	1.97	0.46
1:M:295:VAL:HG22	1:M:301:LEU:HD12	1.97	0.46
2:A:210:LEU:HD13	2:A:239:LEU:HD22	1.98	0.46
2:A:343:TYR:HE2	2:A:362:HIS:HE2	1.64	0.46
2:A:340:LYS:HB3	4:G:171:ARG:HH22	1.80	0.46
2:A:528:PRO:HA	4:G:159:GLU:HG3	1.97	0.46
2:A:252:GLN:HG3	2:A:254:ASP:H	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:443:THR:HG22	2:A:444:SER:H	1.80	0.45
2:A:20:LEU:HD13	2:A:33:LYS:HD2	1.98	0.45
2:A:75:HIS:HB3	2:A:78:ILE:HB	1.98	0.45
1:M:233:ALA:O	1:M:237:ILE:HG13	2.16	0.45
1:M:71:GLY:HA2	1:M:336:PRO:HB3	1.99	0.45
2:A:139:HIS:HA	2:A:163:SER:HA	1.98	0.44
3:B:209:PRO:HA	3:B:210:PRO:HD3	1.88	0.44
2:A:465:PHE:HE2	2:A:545:ILE:HD11	1.83	0.44
1:M:316:ASP:HB3	1:M:319:ILE:HG12	1.98	0.44
2:A:415:VAL:HG22	2:A:548:LEU:HD21	1.99	0.44
4:G:92:ILE:HG23	4:G:217:LEU:HD22	2.00	0.44
2:A:349:PRO:HG2	2:A:352:PHE:HB2	2.01	0.43
2:A:464:ASP:OD2	3:B:240:HIS:ND1	2.44	0.43
2:A:220:HIS:CE1	2:A:222:PRO:HD2	2.54	0.43
1:M:135:PRO:HG3	1:M:196:PHE:HZ	1.82	0.43
2:A:535:ILE:HG21	4:G:75:TRP:CE2	2.54	0.43
2:A:242:SER:O	2:A:245:SER:OG	2.32	0.43
2:A:79:ILE:HD11	2:A:156:LYS:HB3	2.01	0.43
4:G:207:VAL:HG23	4:G:230:VAL:HG12	2.01	0.43
2:A:51:ARG:HG3	2:A:55:ARG:NE	2.34	0.42
4:G:150:ILE:HG22	4:G:152:ARG:H	1.83	0.42
4:G:306:ASN:O	4:G:307:ASP:HB2	2.19	0.42
1:M:92:TYR:HE2	1:M:96:TRP:HB3	1.84	0.42
1:M:99:VAL:HG21	1:M:109:PRO:HD3	2.00	0.42
1:M:47:GLU:HB3	2:A:55:ARG:NH2	2.32	0.42
1:M:123:LEU:HD23	1:M:124:LEU:HG	2.01	0.42
4:G:185:LYS:HA	4:G:186:PRO:HD3	1.94	0.42
4:G:117:TRP:HA	4:G:120:VAL:HG22	2.02	0.42
2:A:82:TYR:CD2	2:A:94:VAL:CG2	2.94	0.41
4:G:165:TYR:HD2	4:G:167:LEU:HD22	1.85	0.41
4:G:177:LYS:O	4:G:180:ILE:HG22	2.20	0.41
1:M:88:GLN:HG3	1:M:92:TYR:CE2	2.55	0.41
2:A:21:GLY:N	2:A:34:VAL:O	2.48	0.41
2:A:49:LEU:HB2	2:A:91:ILE:HB	2.03	0.41
1:M:246:VAL:HB	1:M:318:ARG:HG2	2.03	0.41
2:A:241:PRO:HA	2:A:244:ILE:HD12	2.03	0.41
4:G:298:HIS:O	4:G:315:LEU:HG	2.20	0.41
4:G:70:ARG:HD3	4:G:152:ARG:NH2	2.36	0.40
2:A:363:PRO:HB2	6:G:401:ATP:H5'1	2.03	0.40
2:A:141:ASP:HB2	2:A:162:LEU:HD22	2.02	0.40
4:G:52:ASP:OD1	4:G:53:THR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:LEU:HD21	1:M:228:ILE:HD12	2.03	0.40
2:A:239:LEU:HD13	2:A:243:VAL:HB	2.04	0.40
4:G:51:PHE:CE2	4:G:60:ALA:HB1	2.56	0.40
1:M:9:LEU:HB2	1:M:37:VAL:HG22	2.03	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	M	365/373 (98%)	351 (96%)	14 (4%)	0	100	100
2	A	398/484 (82%)	376 (94%)	22 (6%)	0	100	100
3	B	85/198 (43%)	77 (91%)	8 (9%)	0	100	100
4	G	298/306 (97%)	289 (97%)	9 (3%)	0	100	100
All	All	1146/1361 (84%)	1093 (95%)	53 (5%)	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	M	289/294 (98%)	289 (100%)	0	100	100
2	A	368/439 (84%)	362 (98%)	6 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	79/181 (44%)	79 (100%)	0	100	100
4	G	274/279 (98%)	272 (99%)	2 (1%)	84	90
All	All	1010/1193 (85%)	1002 (99%)	8 (1%)	81	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	50	ASN
2	A	110	ASN
2	A	112	ARG
2	A	221	VAL
2	A	237	GLN
2	A	438	ARG
4	G	269	ARG
4	G	299	ARG

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

Mol	Chain	Res	Type
2	A	69	ASN
2	A	110	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
2	TPO	A	174	2	8,10,11	1.10	0	10,14,16	1.98	1 (10%)

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	TPO	A	174	2	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	174	TPO	P-OG1-CB	-5.58	106.36	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

2 monosaccharides 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	$\# Z  > 2$
5	GLC	C	1	5	12,12,12	0.64	0	17,17,17	0.90	1 (5%)
5	GLC	C	2	5	11,11,12	0.47	0	15,15,17	0.92	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	GLC	C	1	5	-	0/2/22/22	0/1/1/1
5	GLC	C	2	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	GLC	C1-O5-C5	-2.37	109.19	113.66

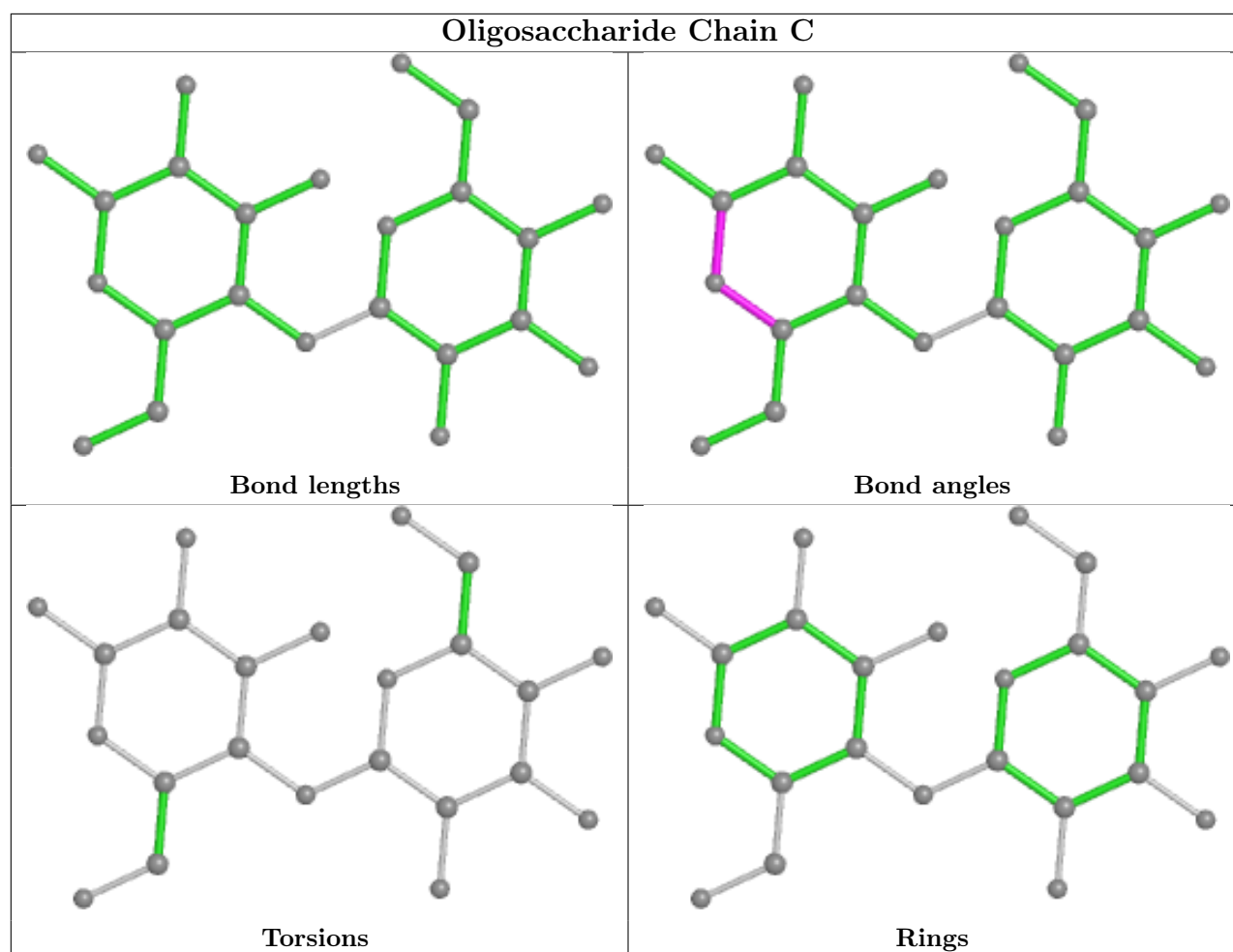
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
7	AMP	G	402	-	22,25,25	1.31	2 (9%)	25,38,38	1.49	4 (16%)
6	ATP	G	401	-	26,33,33	0.95	1 (3%)	31,52,52	1.57	5 (16%)
8	ADP	G	403	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)

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
7	AMP	G	402	-	-	3/6/26/26	0/3/3/3
6	ATP	G	401	-	-	3/18/38/38	0/3/3/3
8	ADP	G	403	-	-	3/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	402	AMP	C6-N6	4.10	1.49	1.34
6	G	401	ATP	C5-C4	2.58	1.47	1.40
8	G	403	ADP	C5-C4	2.45	1.47	1.40
7	G	402	AMP	P-O1P	-2.38	1.42	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	401	ATP	C3'-C2'-C1'	3.63	106.44	100.98
6	G	401	ATP	PB-O3B-PG	-3.41	121.11	132.83
8	G	403	ADP	C3'-C2'-C1'	3.30	105.95	100.98
7	G	402	AMP	N3-C2-N1	-3.25	123.60	128.68
6	G	401	ATP	N3-C2-N1	-3.22	123.65	128.68
8	G	403	ADP	PA-O3A-PB	-3.10	122.19	132.83
8	G	403	ADP	N3-C2-N1	-3.09	123.85	128.68
7	G	402	AMP	C3'-C2'-C1'	2.92	105.38	100.98
6	G	401	ATP	PA-O3A-PB	-2.87	122.96	132.83
6	G	401	ATP	C4-C5-N7	-2.87	106.40	109.40
8	G	403	ADP	C4-C5-N7	-2.75	106.53	109.40
7	G	402	AMP	O3P-P-O2P	2.61	117.62	107.64
7	G	402	AMP	C2'-C3'-C4'	2.40	107.31	102.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	401	ATP	C5'-O5'-PA-O1A
6	G	401	ATP	C5'-O5'-PA-O2A
6	G	401	ATP	C5'-O5'-PA-O3A
7	G	402	AMP	C5'-O5'-P-O3P
7	G	402	AMP	O4'-C4'-C5'-O5'

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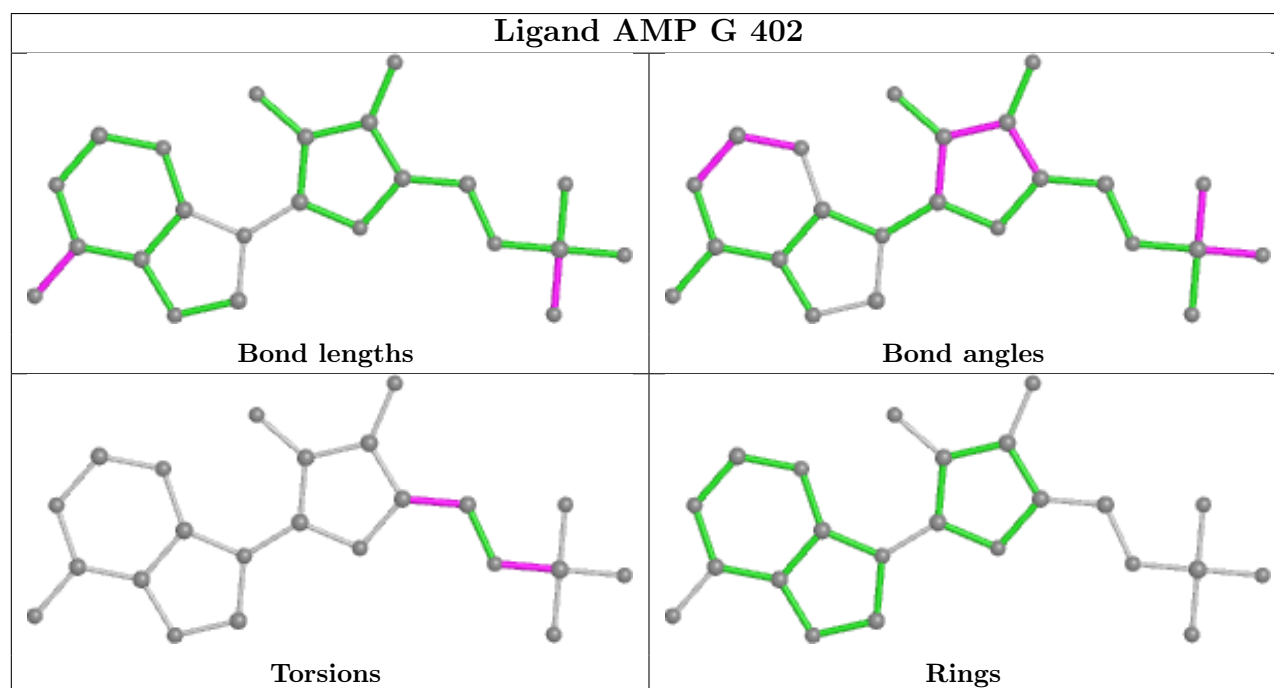
Mol	Chain	Res	Type	Atoms
7	G	402	AMP	C3'-C4'-C5'-O5'
8	G	403	ADP	PB-O3A-PA-O1A
8	G	403	ADP	PB-O3A-PA-O2A
8	G	403	ADP	C5'-O5'-PA-O3A

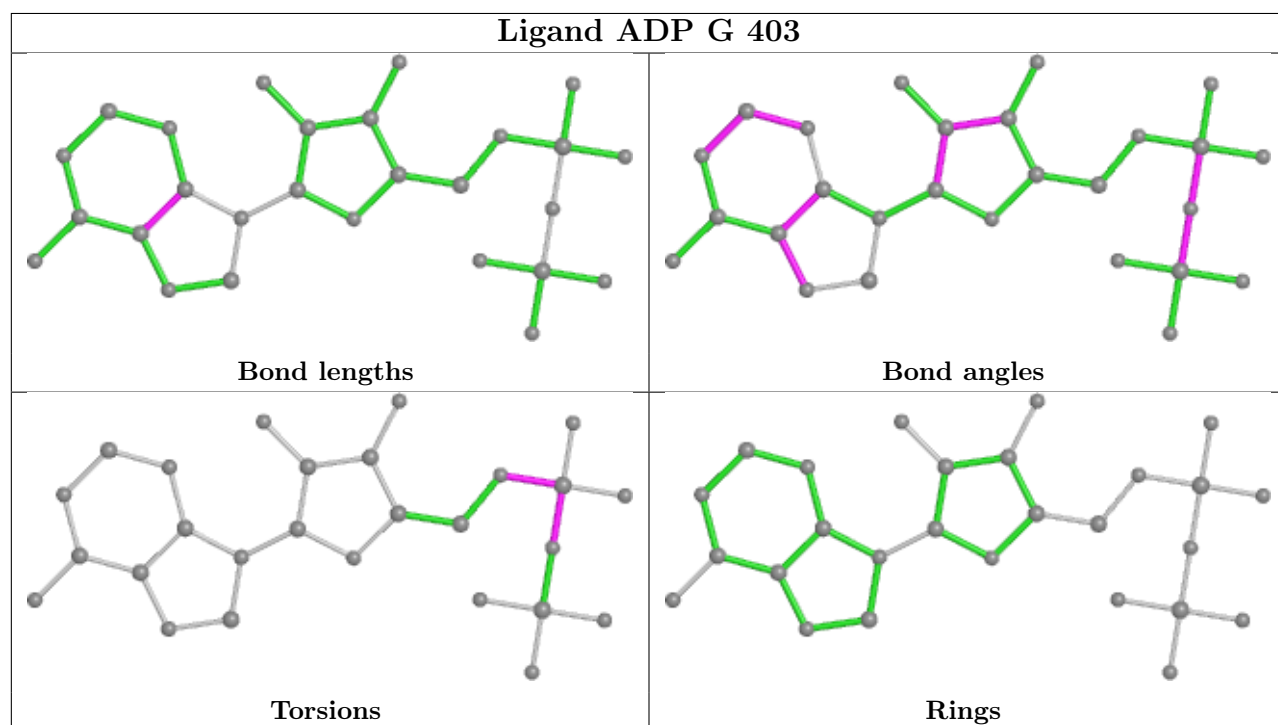
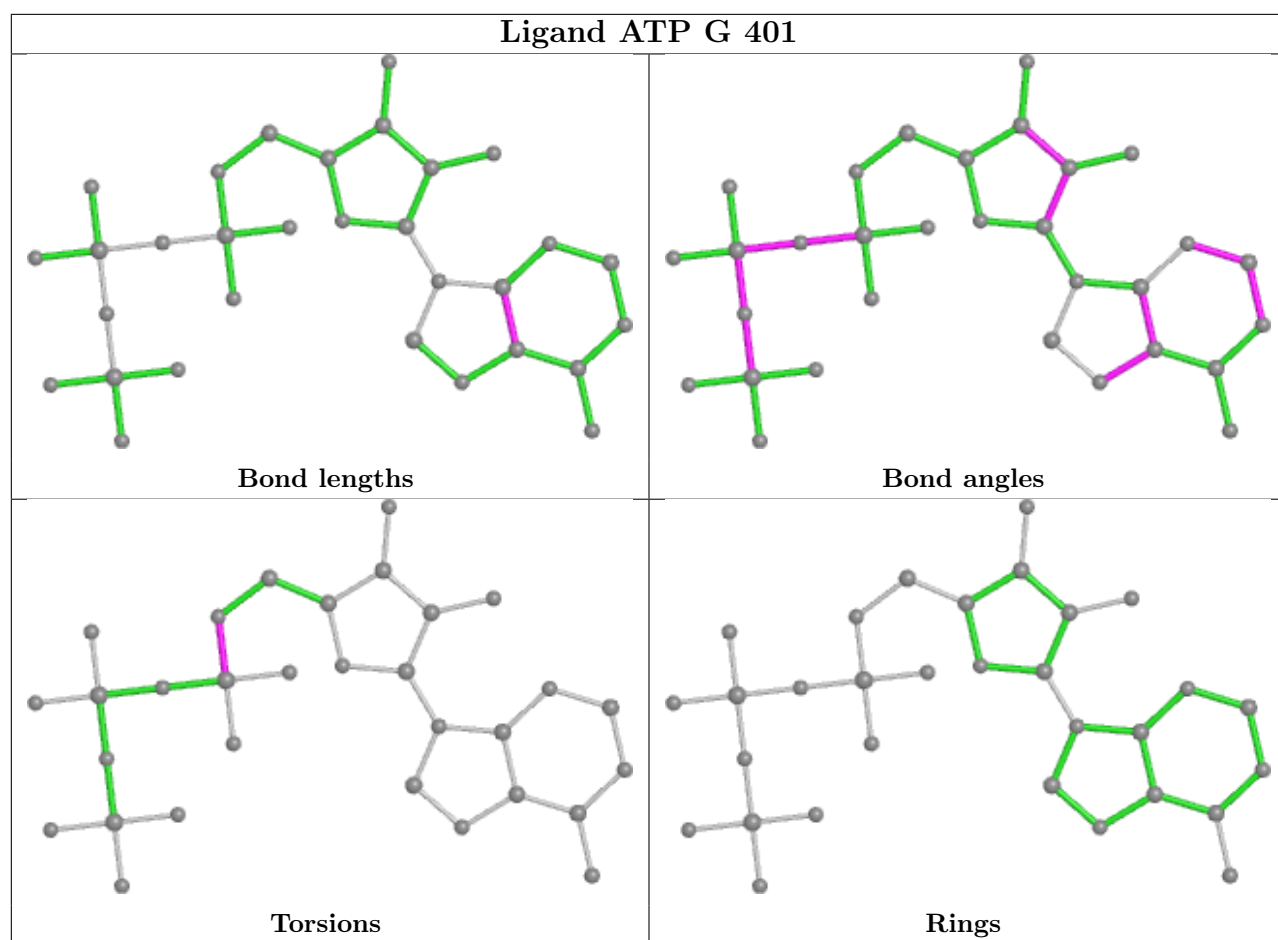
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	402	AMP	1	0
6	G	401	ATP	2	0
8	G	403	ADP	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

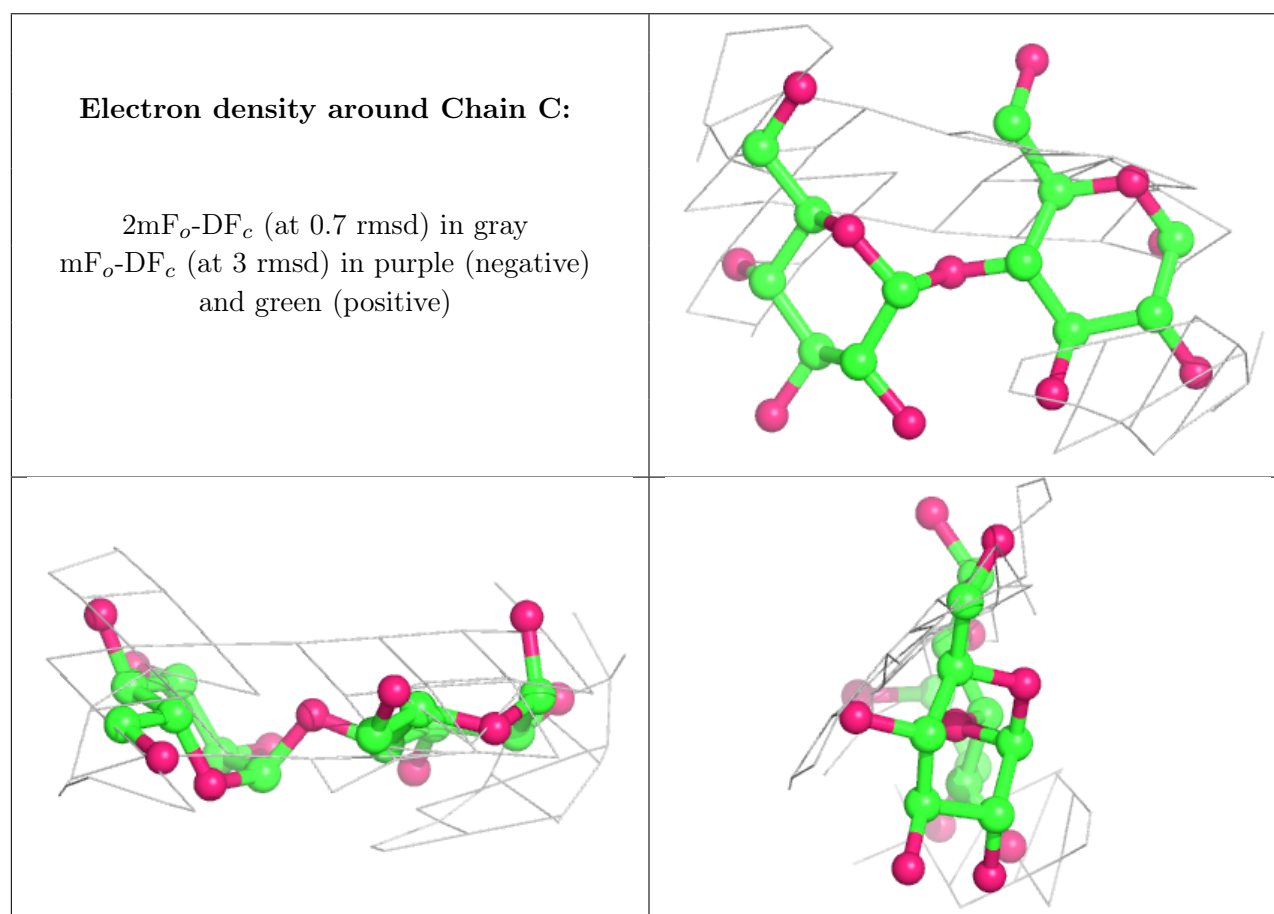
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

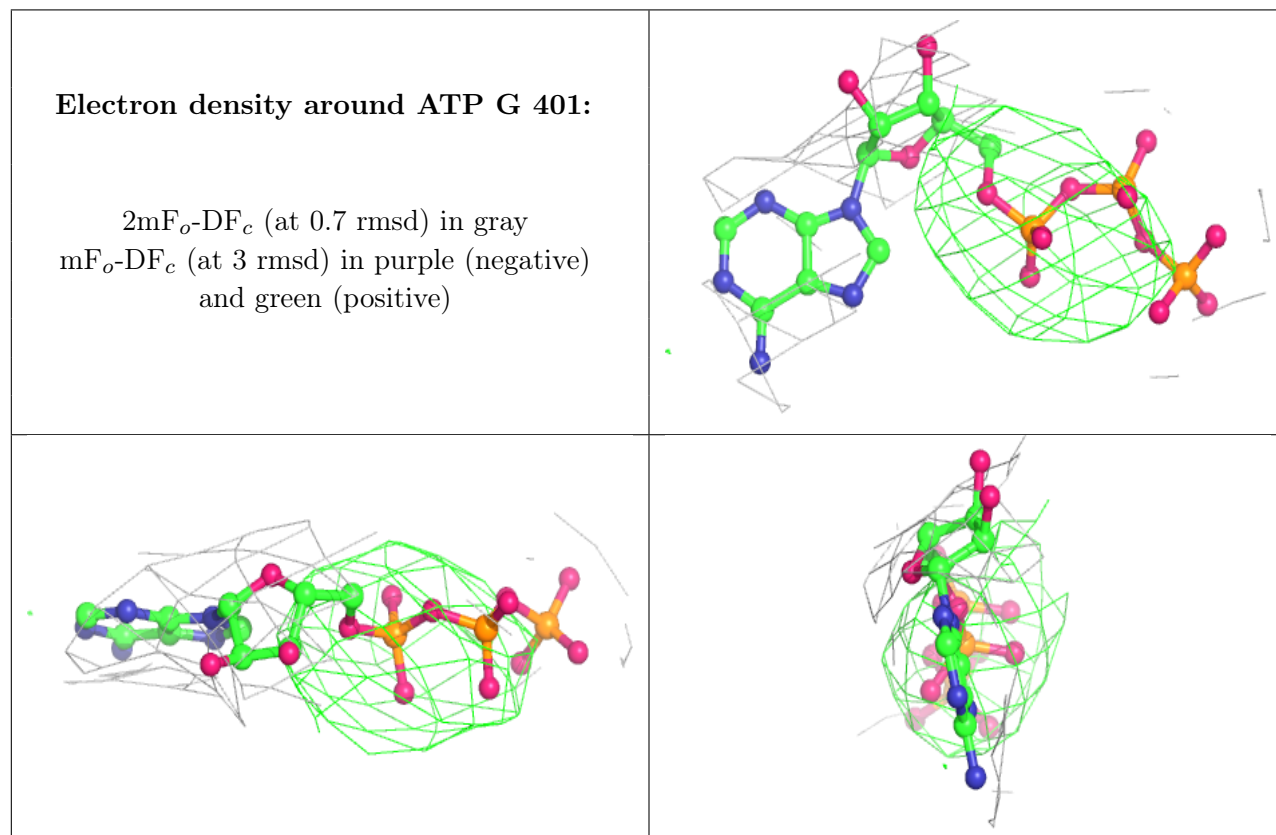


### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

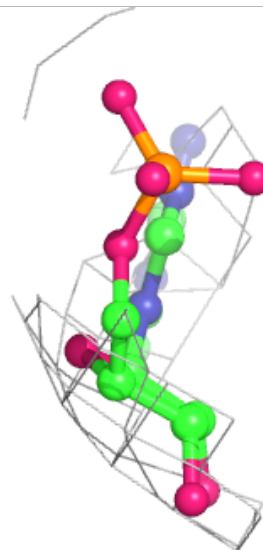
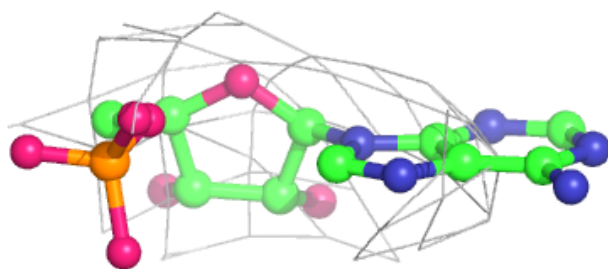
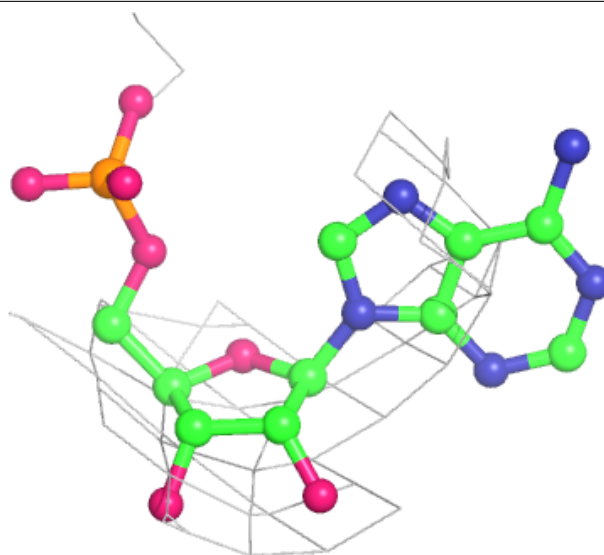


The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



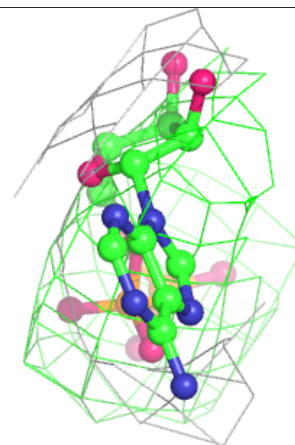
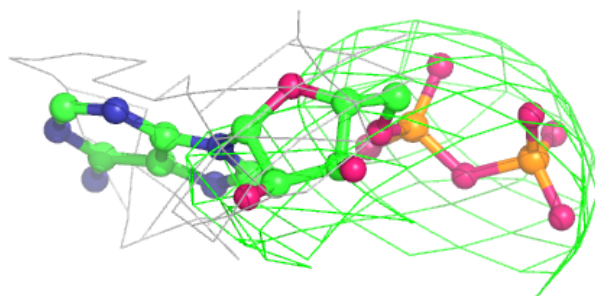
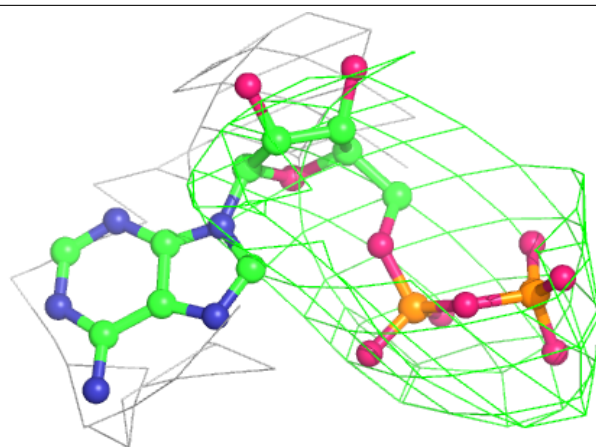
**Electron density around AMP G 402:**

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



**Electron density around ADP G 403:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.