



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:20 PM UTC

PDB ID : 7JIJ / pdb_00007jjj
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

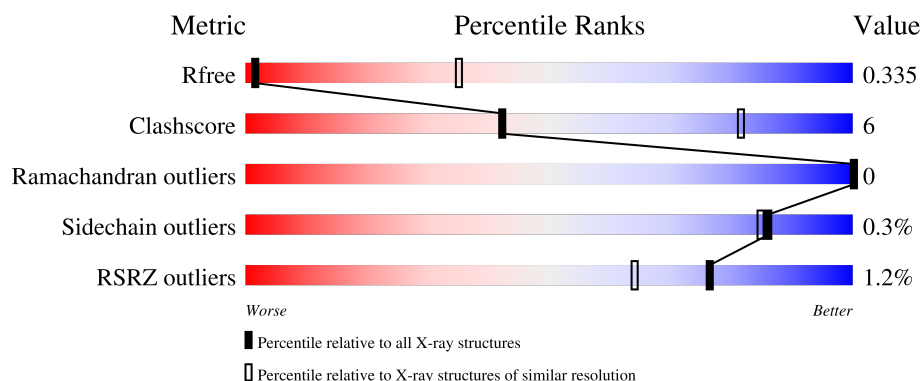
1 Overall quality at a glance

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}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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	M	373	2% 85% 13% .
2	A	484	67% 17% 16%
3	B	198	36% 8% 56%
4	G	306	2% 83% 15% .
5	C	2	50% 50%

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
			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:

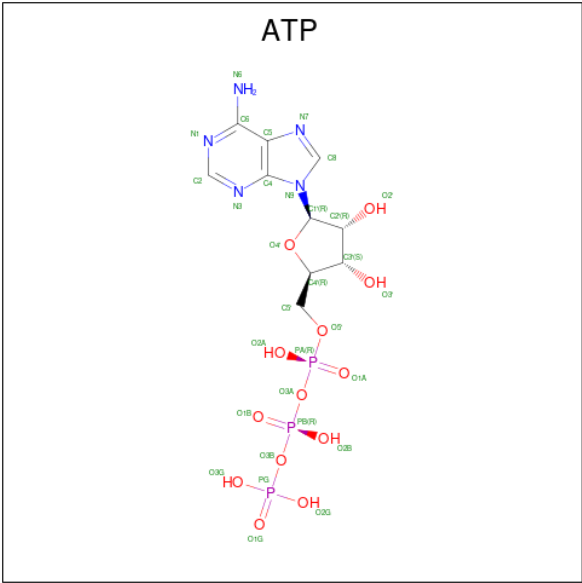
Chain	Residue	Modelled	Actual	Comment	Reference
G	22	MET	-	initiating methionine	UNP P54619
G	23	GLY	-	expression tag	UNP P54619
G	31	PHE	SER	conflict	UNP P54619

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



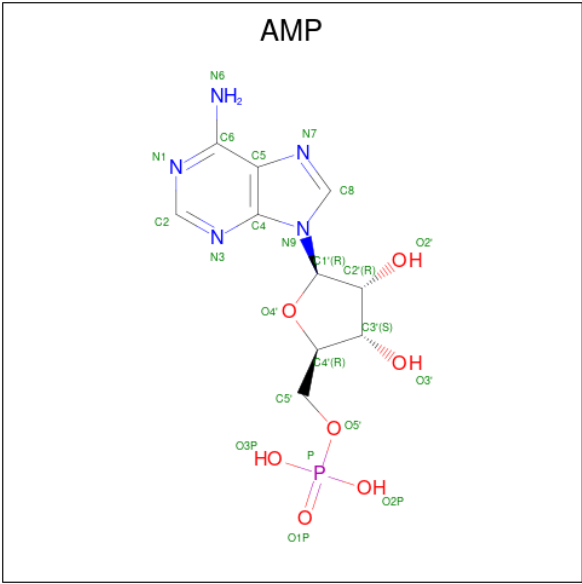
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



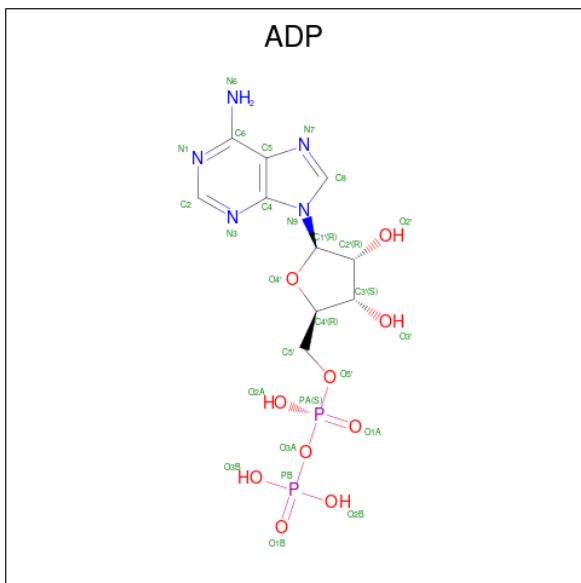
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

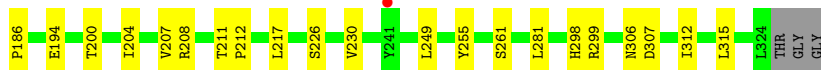
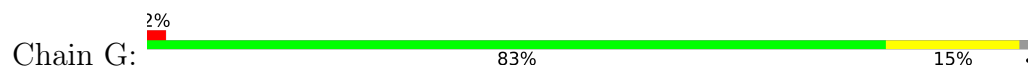
- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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, α , β , γ	126.69Å 126.69Å 332.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.90 – 5.50 24.90 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.90-5.50) 97.9 (24.90-5.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.249 , 0.323 0.257 , 0.335	Depositor DCC
R_{free} test set	823 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	188.7	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 261.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.147 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9372	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: AMP, ADP, GLC, ATP, 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	0.15	0/2904	0.38	0/3947
2	A	0.19	0/3387	0.47	0/4573
3	B	0.16	0/716	0.41	0/975
4	G	0.25	0/2472	0.39	0/3356
All	All	0.20	0/9479	0.42	0/12851

There are no bond length outliers.

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	59	0
3	B	695	0	722	10	0
4	G	2420	0	2479	28	0
5	C	23	0	21	0	0
6	G	31	0	12	2	0
7	G	23	0	12	1	0
8	G	27	0	12	1	0
All	All	9372	0	9385	119	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 (119) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:336:MET:HE1	3:B:262:LYS:HE2	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:124:GLN:O	2:A:127:SER:OG	2.37	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
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%)	365 (99%)	3 (1%)	73	79
3	B	79/181 (44%)	79 (100%)	0	100	100
4	G	274/279 (98%)	274 (100%)	0	100	100
All	All	1010/1193 (85%)	1007 (100%)	3 (0%)	86	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	19	ILE
2	A	221	VAL
2	A	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	51	GLN
1	M	220	ASN
1	M	369	ASN
2	A	77	HIS
2	A	110	ASN
2	A	135	HIS
2	A	146	ASN
4	G	105	GLN

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	1.13	0	10,14,16	2.19	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	-	1/9/11/13	-

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	-6.24	106.36	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	174	TPO	N-CA-CB-CG2

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	0.88	1 (5%)
5	GLC	C	2	5	11,11,12	0.46	0	15,15,17	0.82	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-2.31	109.19	113.65

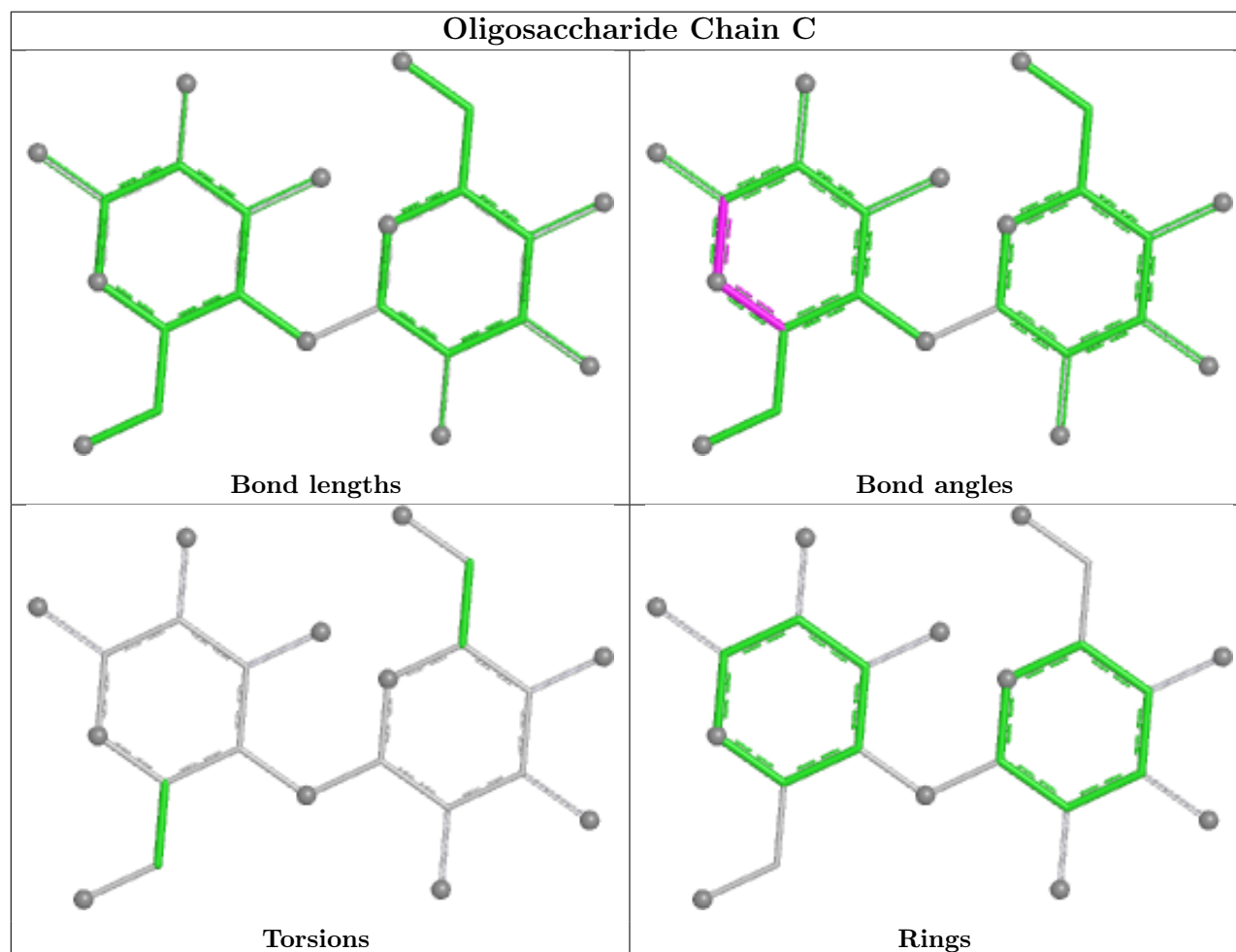
There are no chirality outliers.

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

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
8	ADP	G	403	-	28,29,29	1.41	4 (14%)	43,45,45	1.91	10 (23%)
6	ATP	G	401	-	32,33,33	1.40	4 (12%)	48,52,52	1.81	9 (18%)
7	AMP	G	402	-	25,25,25	1.56	4 (16%)	37,38,38	2.02	13 (35%)

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
8	ADP	G	403	-	-	2/16/32/32	0/3/3/3
6	ATP	G	401	-	-	3/22/38/38	0/3/3/3
7	AMP	G	402	-	-	3/10/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	402	AMP	C6-N6	5.81	1.49	1.34
6	G	401	ATP	C5-C4	4.86	1.47	1.39
8	G	403	ADP	C5-C4	4.66	1.47	1.39
6	G	401	ATP	C5-C6	2.84	1.48	1.41
8	G	403	ADP	C5-C6	2.75	1.48	1.41
7	G	402	AMP	P-O1P	-2.45	1.42	1.50
6	G	401	ATP	C8-N7	2.44	1.36	1.31
8	G	403	ADP	C5-N7	-2.29	1.34	1.39
8	G	403	ADP	C8-N7	2.25	1.36	1.31
6	G	401	ATP	C5-N7	-2.12	1.35	1.39
7	G	402	AMP	C8-N7	2.11	1.35	1.31
7	G	402	AMP	C5-N7	-2.10	1.35	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	401	ATP	C5-C4-N3	-6.20	118.18	126.72
8	G	403	ADP	C5-C4-N3	-5.96	118.50	126.72
7	G	402	AMP	C5-C4-N3	-5.90	118.59	126.72
8	G	403	ADP	N3-C4-N9	4.88	135.46	127.17
6	G	401	ATP	N3-C4-N9	4.81	135.34	127.17
7	G	402	AMP	N3-C4-N9	4.24	134.38	127.17
6	G	401	ATP	C2-N3-C4	3.86	121.27	111.83
8	G	403	ADP	C2-N3-C4	3.72	120.91	111.83
6	G	401	ATP	C4-C5-N7	-3.65	106.40	110.58
8	G	403	ADP	C4-C5-N7	-3.54	106.53	110.58
7	G	402	AMP	N3-C2-N1	-3.29	123.60	128.58
6	G	401	ATP	N3-C2-N1	-3.26	123.65	128.58
8	G	403	ADP	N3-C2-N1	-3.13	123.85	128.58
7	G	402	AMP	C2-N3-C4	3.10	119.40	111.83
8	G	403	ADP	C4-N9-C8	3.00	108.88	105.74
7	G	402	AMP	N9-C8-N7	-2.98	109.71	113.94
8	G	403	ADP	C5-N7-C8	2.71	107.71	103.45
6	G	401	ATP	C5-N7-C8	2.67	107.64	103.45
7	G	402	AMP	C5-N7-C8	2.64	107.60	103.45
6	G	401	ATP	C3'-C2'-C1'	2.63	106.44	101.46
7	G	402	AMP	O3P-P-O2P	2.62	117.62	107.80
7	G	402	AMP	C4-C5-N7	-2.54	107.68	110.58
7	G	402	AMP	C6-C5-C4	2.43	120.50	117.18
7	G	402	AMP	C2'-C3'-C4'	2.43	107.31	102.61
7	G	402	AMP	O4'-C1'-N9	2.38	112.67	108.09
8	G	403	ADP	C3'-C2'-C1'	2.37	105.95	101.46
6	G	401	ATP	C4-N9-C8	2.37	108.22	105.74
8	G	403	ADP	N9-C8-N7	-2.19	110.83	113.94
7	G	402	AMP	C4-N9-C8	2.13	107.98	105.74
6	G	401	ATP	C6-C5-N7	2.13	136.19	132.09
8	G	403	ADP	C6-C5-N7	2.08	136.10	132.09
7	G	402	AMP	C3'-C2'-C1'	2.07	105.38	101.46

There are no chirality outliers.

All (8) 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
7	G	402	AMP	C5'-O5'-P-O3P
7	G	402	AMP	O4'-C4'-C5'-O5'

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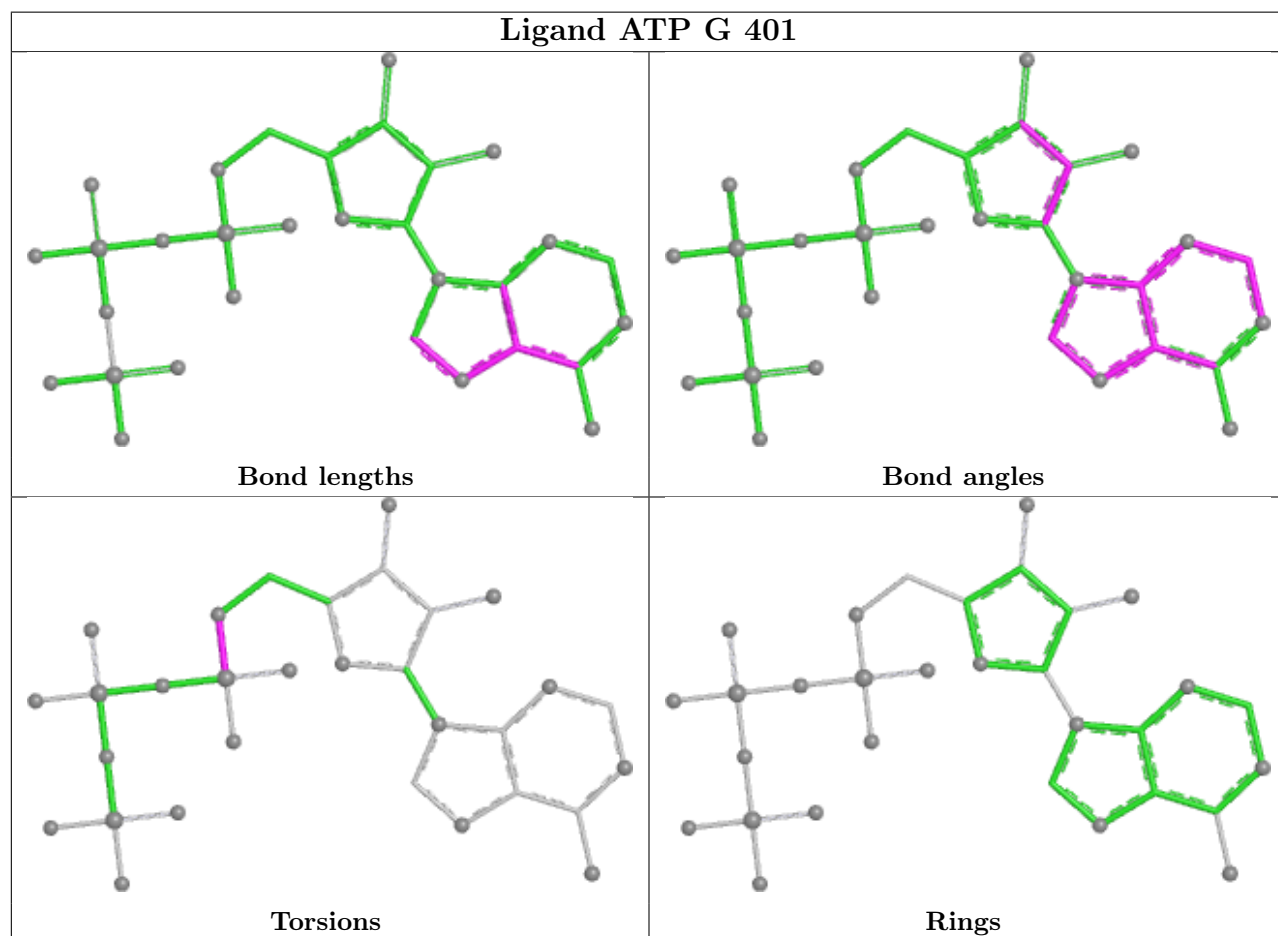
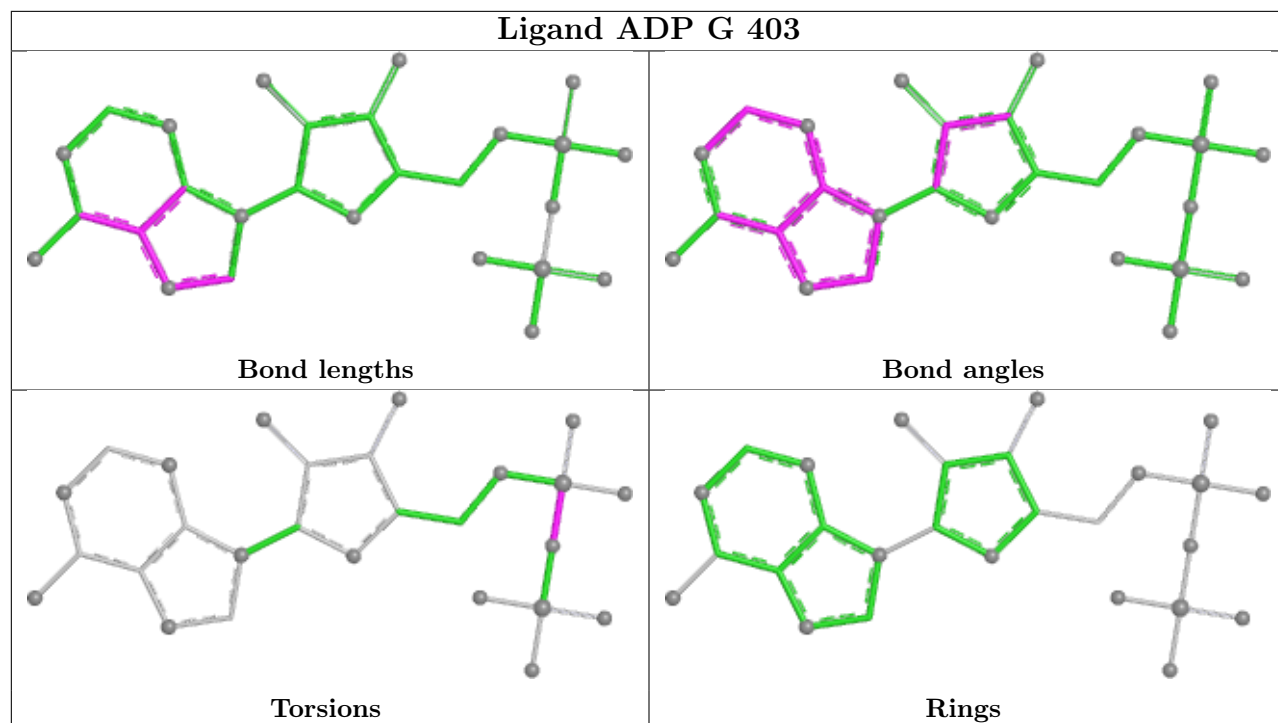
Mol	Chain	Res	Type	Atoms
7	G	402	AMP	C3'-C4'-C5'-O5'
8	G	403	ADP	PB-O3A-PA-O1A
6	G	401	ATP	C5'-O5'-PA-O3A
8	G	403	ADP	PB-O3A-PA-O2A

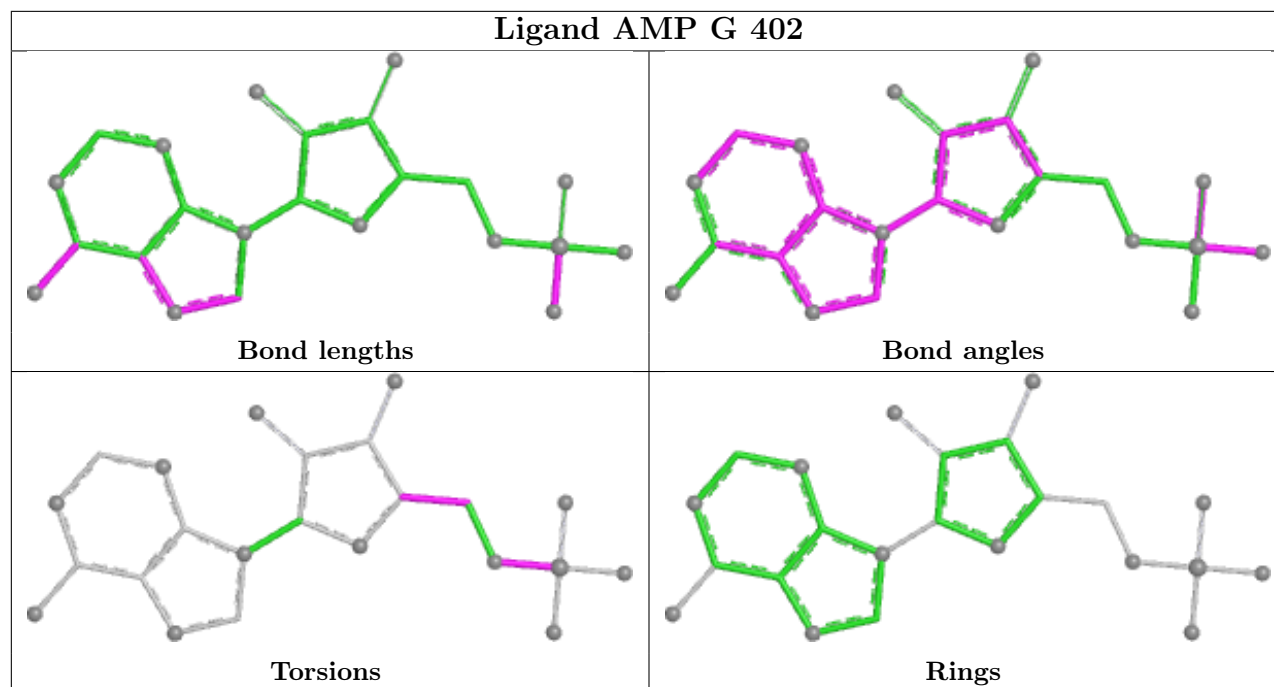
There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

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

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	M	367/373 (98%)	-0.16	7 (1%) 66 55	248, 482, 655, 873	0
2	A	406/484 (83%)	-0.18	2 (0%) 87 77	226, 393, 553, 645	0
3	B	87/198 (43%)	-0.25	0 100 100	261, 397, 569, 605	0
4	G	300/306 (98%)	-0.17	5 (1%) 69 58	210, 386, 524, 634	0
All	All	1160/1361 (85%)	-0.17	14 (1%) 76 64	210, 418, 603, 873	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	150	MET	3.9
4	G	71	ALA	3.8
1	M	266	ALA	3.6
1	M	110	ILE	3.3
4	G	241	TYR	3.2
1	M	338	MET	2.8
1	M	370	ALA	2.7
1	M	341	PHE	2.6
4	G	173	LEU	2.6
2	A	404	SER	2.4
2	A	93	MET	2.4
4	G	86	LEU	2.3
4	G	91	PHE	2.1
1	M	373	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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.

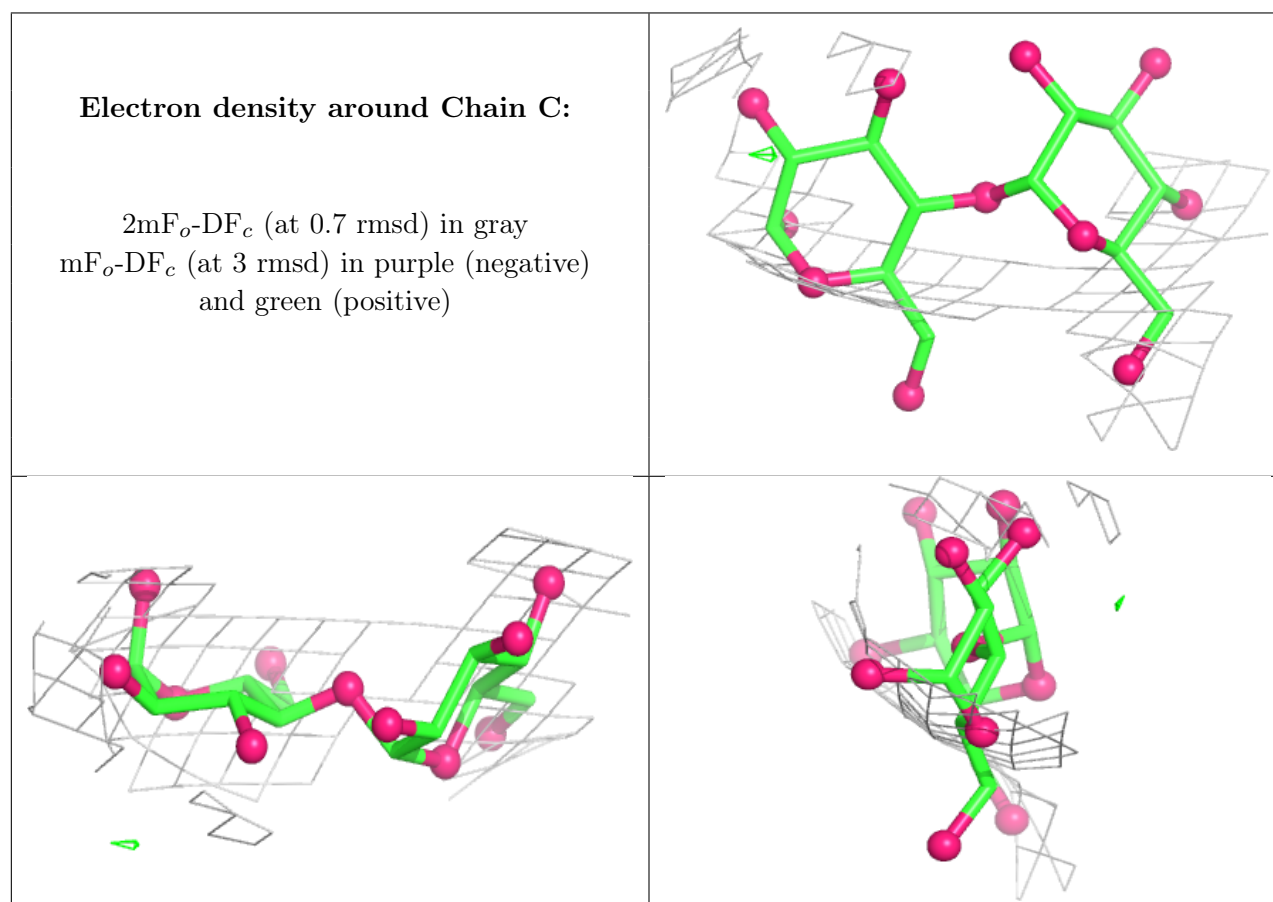
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TPO	A	174	11/12	0.93	0.06	292,330,362,391	0

6.3 Carbohydrates [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($\text{\AA}^2$)	Q<0.9
5	GLC	C	1	12/12	-	-	294,379,379,379	0
5	GLC	C	2	11/12	-	-	237,333,379,379	0

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.

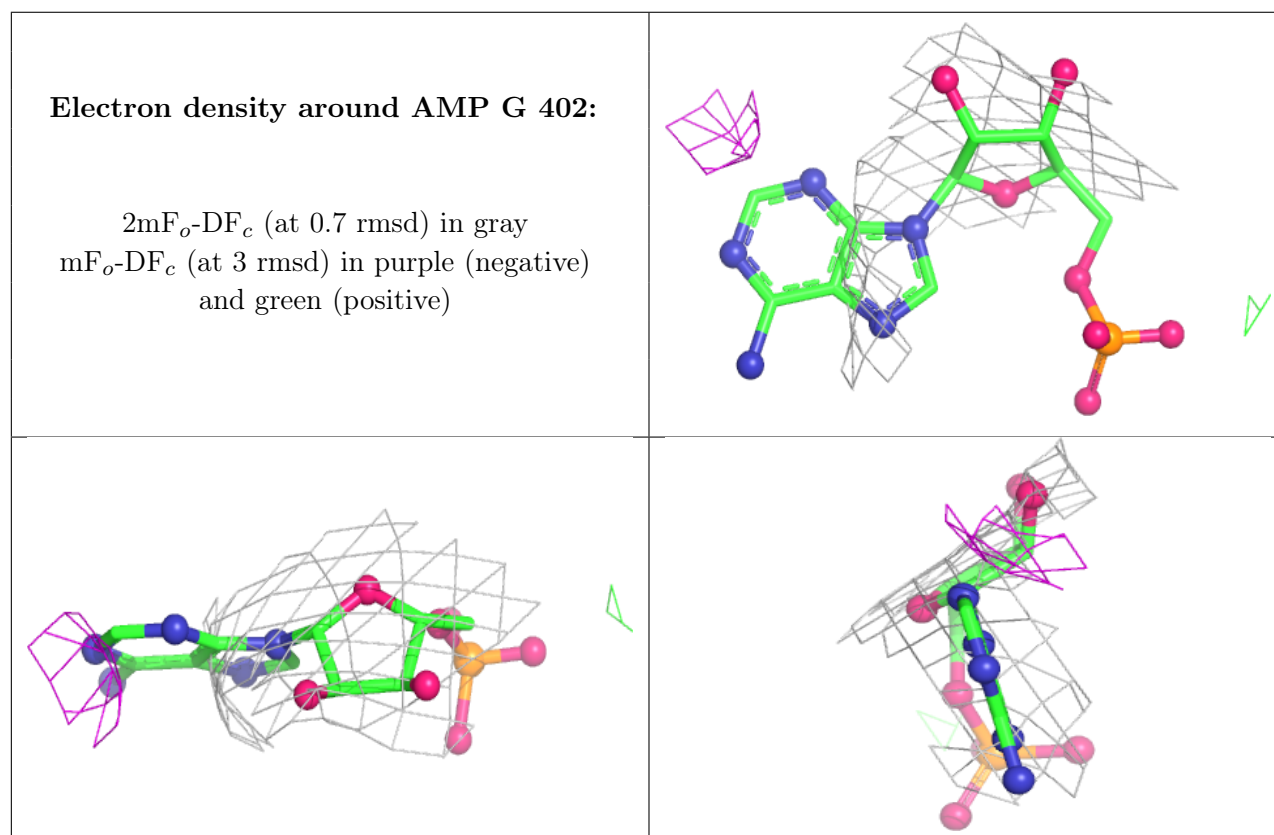


6.4 Ligands ⓘ

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.

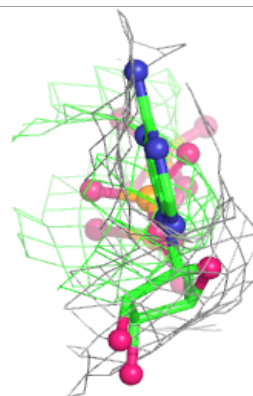
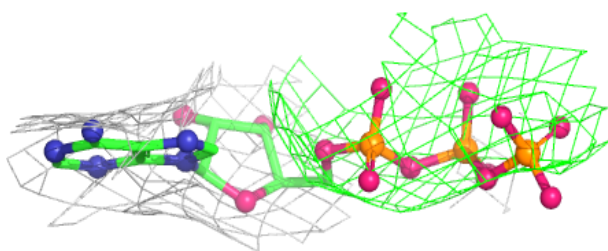
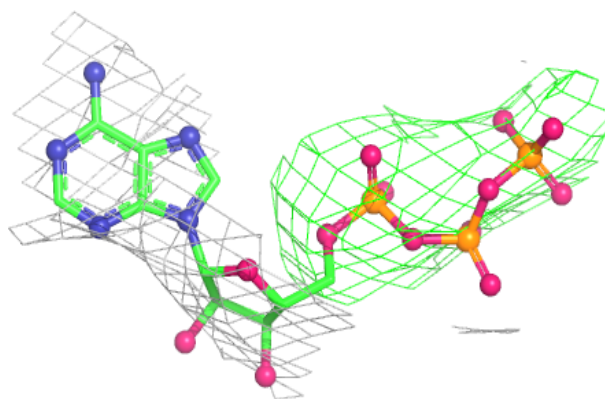
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	AMP	G	402	23/23	0.71	0.12	342,342,394,394	0
6	ATP	G	401	31/31	0.88	0.12	377,379,379,379	0
8	ADP	G	403	27/27	0.91	0.09	355,379,379,379	0

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

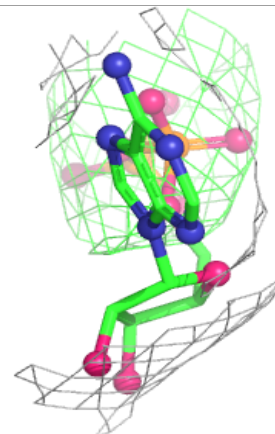
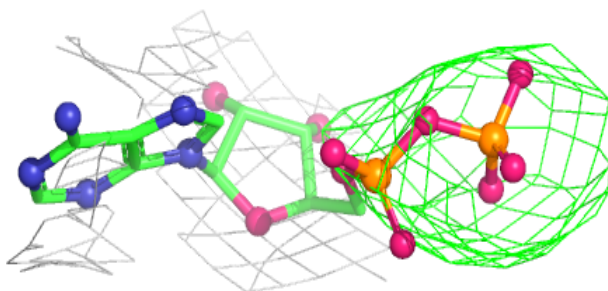
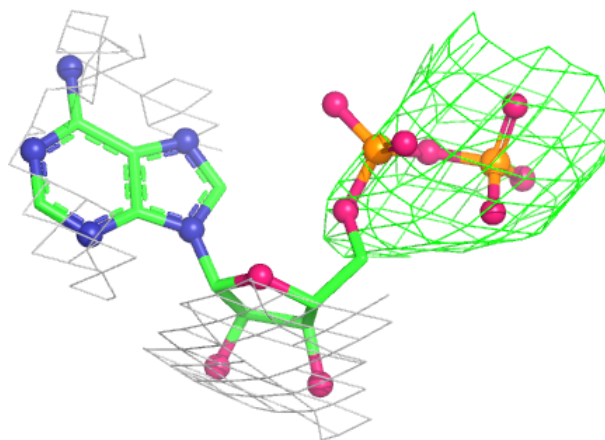


Electron density around ATP G 401:

$2mF_o-DF_c$ (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](#)

There are no such residues in this entry.