



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:57 AM UTC

PDB ID : 4EOJ / pdb\_00004eoj  
Title : Thr 160 phosphorylated CDK2 H84S, Q85M, K89D - human cyclin A3 complex with ATP  
Authors : Echalier, A.; Cot, E.; Camasses, A.; Hodimont, E.; Hoh, F.; Sheinerman, F.; Krasinska, L.; Fisher, D.  
Deposited on : 2012-04-14  
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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)  
Xtrriage (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

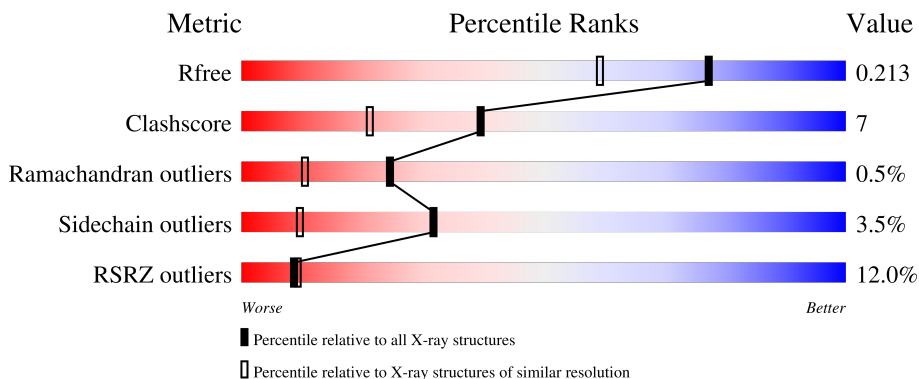
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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  $\leq 5\%$ . 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	302	 11% 82% 14% 6%
1	C	302	 20% 76% 15% 6%
2	B	258	 8% 92% 7% 5%
2	D	258	 8% 91% 8% 5%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9679 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	296	Total	C	N	O	P	S	0	9	0
			2442	1580	416	435	1	10			
1	C	283	Total	C	N	O	P	S	0	4	0
			2293	1484	386	414	1	8			

There are 14 discrepancies between the modelled and reference sequences:

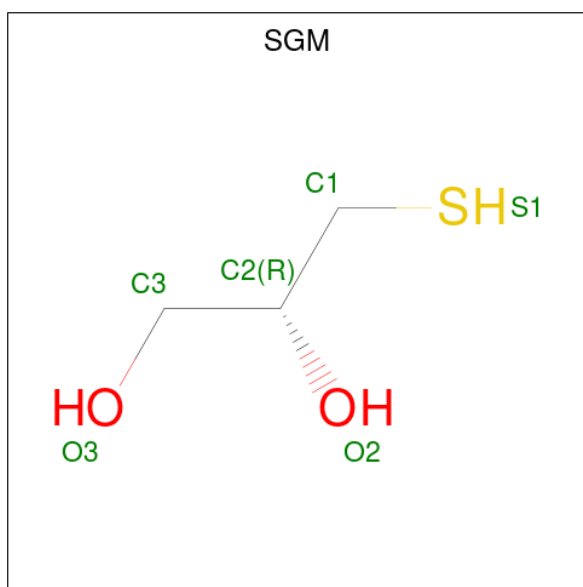
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
A	84	SER	HIS	engineered mutation	UNP P24941
A	85	MET	GLN	engineered mutation	UNP P24941
A	89	ASP	LYS	engineered mutation	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	LEU	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941
C	84	SER	HIS	engineered mutation	UNP P24941
C	85	MET	GLN	engineered mutation	UNP P24941
C	89	ASP	LYS	engineered mutation	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	257	Total	C	N	O	S	10	2	0
			2092	1354	342	385	11			
2	D	256	Total	C	N	O	S	0	4	0
			2106	1361	347	386	12			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			6	3	2	1		
5	B	1	Total	C	O	S	0	0
			6	3	2	1		

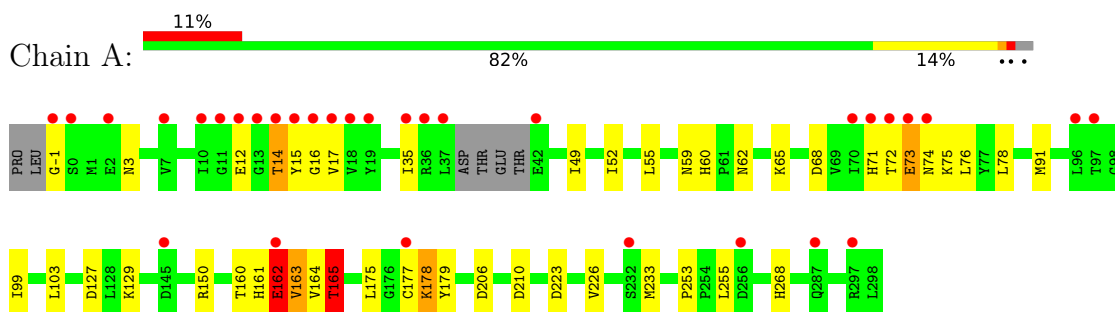
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	229	Total	O	0	0
			229	229		
6	B	177	Total	O	0	0
			177	177		
6	C	135	Total	O	0	0
			135	135		
6	D	129	Total	O	0	0
			129	129		

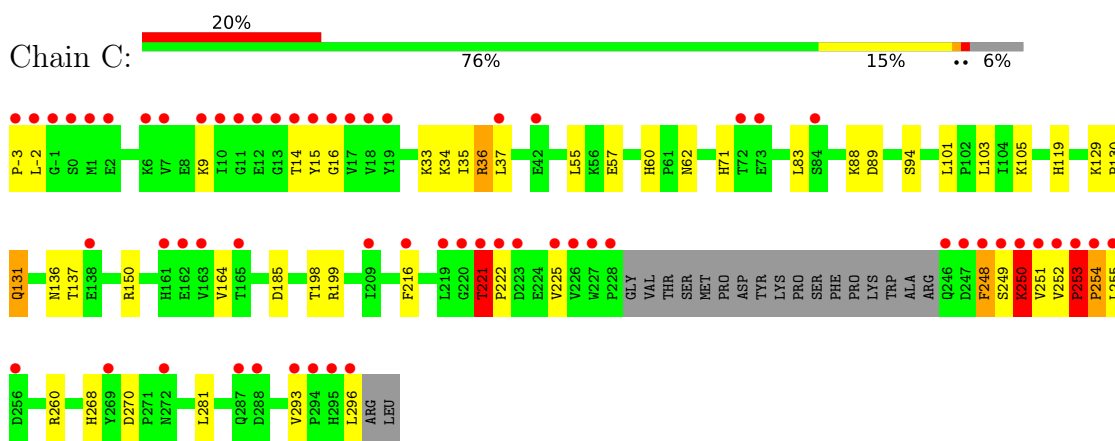
### 3 Residue-property plots [i](#)

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.

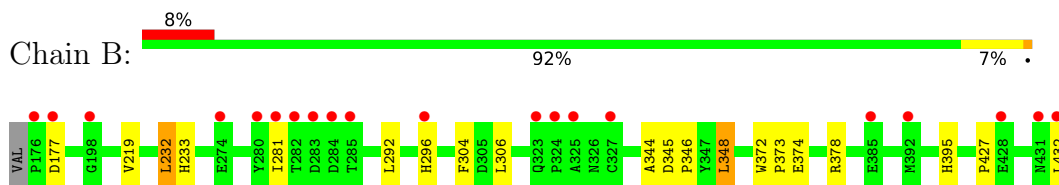
- Molecule 1: Cyclin-dependent kinase 2



- Molecule 1: Cyclin-dependent kinase 2

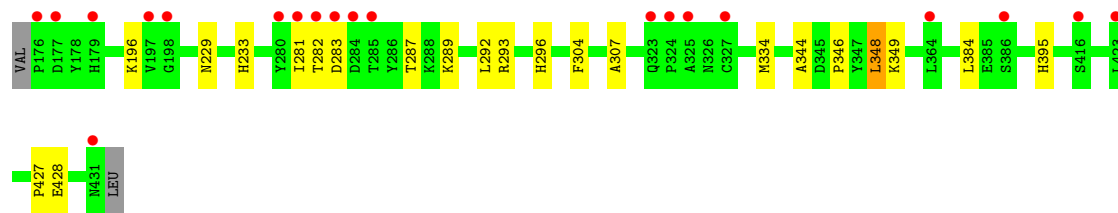


- Molecule 2: Cyclin-A2



- Molecule 2: Cyclin-A2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.56Å 133.85Å 149.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.65 30.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-1.65) 99.1 (30.00-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.65Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.196 , 0.215 0.196 , 0.213	Depositor DCC
$R_{free}$ test set	8773 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: ATP, SGM, TPO, 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	0.60	1/2491 (0.0%)	0.80	3/3377 (0.1%)
1	C	0.62	3/2336 (0.1%)	0.96	10/3168 (0.3%)
2	B	0.54	2/2143 (0.1%)	0.71	0/2909
2	D	0.44	0/2157	0.75	1/2926 (0.0%)
All	All	0.56	6/9127 (0.1%)	0.81	14/12380 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	ASP	C-N	-7.99	1.23	1.33
1	C	253	PRO	CA-C	-7.79	1.45	1.52
2	B	373	PRO	C-O	-6.13	1.17	1.23
1	A	75	LYS	C-O	-5.75	1.16	1.23
1	C	221	THR	CA-CB	5.18	1.61	1.52
2	B	372	TRP	C-O	-5.11	1.17	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	PRO	N-CA-C	-13.48	94.25	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	SER	N-CA-C	-11.43	86.45	110.80
1	A	163	VAL	N-CA-C	7.45	118.17	110.05
2	D	282	THR	N-CA-C	-7.26	104.86	113.21
1	C	250	LYS	CA-C-N	6.89	134.09	121.70
1	C	250	LYS	C-N-CA	6.89	134.09	121.70
1	C	249	SER	CB-CA-C	6.72	123.80	110.42
1	C	221	THR	CA-C-N	6.55	126.50	119.76
1	C	221	THR	C-N-CA	6.55	126.50	119.76
1	C	248	PHE	N-CA-C	6.15	119.39	107.71
1	C	221	THR	N-CA-CB	6.13	118.26	110.23
1	A	253	PRO	N-CA-C	5.44	117.34	110.70
1	A	165	THR	N-CA-CB	5.27	117.79	109.83
1	C	250	LYS	N-CA-C	-5.01	96.97	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLU	Peptide
1	C	250	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2442	0	2474	49	0
1	C	2293	0	2327	53	0
2	B	2092	0	2108	12	0
2	D	2106	0	2121	18	0
3	A	31	0	12	0	0
3	C	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	12	0	15	0	0
6	A	229	0	0	4	0
6	B	177	0	0	2	0
6	C	135	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	129	0	0	4	0
All	All	9679	0	9069	121	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 7.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177[A]:CYS:SG	1:A:233:MET:HE3	1.41	1.57
1:A:72:THR:HG22	1:A:73:GLU:CD	1.71	1.15
1:A:177[A]:CYS:SG	1:A:233:MET:CE	2.35	1.12
1:A:72:THR:HG22	1:A:73:GLU:OE1	1.58	1.01
1:C:36:ARG:HG2	1:C:36:ARG:HH21	1.28	0.98
1:C:252:VAL:C	1:C:253:PRO:O	2.01	0.95
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.86	0.94
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.05	0.94
1:C:252:VAL:O	1:C:253:PRO:O	1.87	0.92
1:A:177[A]:CYS:HG	1:A:233:MET:HE3	1.35	0.89
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.92	0.86
1:C:255:LEU:O	1:C:260:ARG:NH1	2.11	0.84
1:A:60:HIS:HD2	1:A:62:ASN:H	1.26	0.83
1:A:72:THR:CG2	1:A:73:GLU:OE1	2.29	0.81
1:A:60:HIS:CD2	1:A:62:ASN:H	1.99	0.80
1:C:250:LYS:HB3	1:C:252:VAL:H	1.48	0.79
1:A:71:HIS:HE2	2:B:304:PHE:HE2	1.30	0.77
1:A:72:THR:HG22	1:A:73:GLU:OE2	1.86	0.75
1:A:268:HIS:CE1	6:A:492:HOH:O	2.40	0.74
1:C:14:THR:C	1:C:16:GLY:H	1.97	0.73
1:C:33:LYS:HE3	6:C:510:HOH:O	1.88	0.73
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.72	0.71
1:C:60:HIS:HD2	1:C:62:ASN:H	1.39	0.70
1:A:12:GLU:OE2	1:A:17:VAL:HG22	1.94	0.68
2:D:281:ILE:C	2:D:283:ASP:H	2.00	0.67
1:A:210:ASP:OD2	6:A:539:HOH:O	2.12	0.67
1:C:250:LYS:HG2	1:C:252:VAL:HG23	1.76	0.67
1:C:250:LYS:HB3	1:C:252:VAL:HG23	1.78	0.65
2:D:346:PRO:O	2:D:349:LYS:HG2	1.96	0.65
1:C:60:HIS:CD2	1:C:62:ASN:H	2.15	0.65
1:C:268:HIS:HD2	1:C:270:ASP:H	1.44	0.65
1:A:71:HIS:NE2	2:B:304:PHE:HE2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:PRO:O	1:C:255:LEU:C	2.36	0.63
1:C:36:ARG:HG2	1:C:36:ARG:NH2	2.04	0.63
1:C:216:PHE:HB3	1:C:221:THR:HB	1.81	0.62
2:B:374:GLU:OE2	2:B:378:ARG:HD2	2.00	0.61
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.77	0.61
1:C:250:LYS:CB	1:C:252:VAL:HG23	2.31	0.61
1:A:129:LYS:NZ	1:A:165:THR:HG21	2.16	0.60
1:C:252:VAL:O	1:C:253:PRO:C	2.41	0.60
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.85	0.59
1:A:73:GLU:CD	1:A:73:GLU:H	2.09	0.59
1:A:14:THR:C	1:A:16:GLY:H	2.11	0.58
1:A:72:THR:CG2	1:A:73:GLU:CD	2.63	0.58
2:D:289:LYS:O	2:D:293[B]:ARG:HG3	2.04	0.57
2:B:374:GLU:CD	2:B:378:ARG:HD2	2.29	0.57
1:A:127:ASP:OD1	1:A:165:THR:HG23	2.04	0.57
1:C:253:PRO:O	1:C:255:LEU:N	2.39	0.56
2:D:395:HIS:HE1	2:D:427:PRO:O	1.88	0.56
1:A:73:GLU:OE2	1:A:74:ASN:N	2.30	0.55
2:B:395:HIS:HE1	2:B:427:PRO:O	1.89	0.55
1:A:73:GLU:CD	1:A:73:GLU:N	2.65	0.54
1:A:14:THR:O	1:A:15:TYR:CB	2.54	0.54
1:A:71:HIS:NE2	2:B:304:PHE:CE2	2.73	0.53
1:C:119:HIS:HD2	6:D:501:HOH:O	1.90	0.53
1:A:3:ASN:OD1	2:D:293[B]:ARG:NH2	2.39	0.53
2:D:229:ASN:HD22	2:D:334[B]:MET:HE2	1.74	0.53
1:A:60:HIS:HE1	6:A:419:HOH:O	1.92	0.52
1:C:14:THR:C	1:C:16:GLY:N	2.60	0.52
1:C:94:SER:O	1:C:199:ARG:HD3	2.09	0.52
1:C:250:LYS:CG	1:C:252:VAL:HG23	2.38	0.52
1:A:72:THR:CG2	1:A:73:GLU:OE2	2.55	0.52
1:C:15:TYR:CG	1:C:35:ILE:HG12	2.45	0.52
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.91	0.51
2:B:233:HIS:HE1	6:B:647:HOH:O	1.92	0.51
1:A:12:GLU:OE2	1:A:17:VAL:CG2	2.57	0.51
1:A:175:LEU:HB2	1:A:233:MET:HE2	1.92	0.51
1:C:222:PRO:HB2	1:C:225:VAL:HG23	1.93	0.51
1:C:253:PRO:CB	1:C:254:PRO:CD	2.89	0.51
2:D:233:HIS:HE1	6:D:576:HOH:O	1.94	0.51
1:C:36:ARG:NH2	1:C:36:ARG:CG	2.73	0.50
2:D:233:HIS:HD2	6:D:504:HOH:O	1.95	0.50
2:B:233:HIS:HD2	6:B:603:HOH:O	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:N	1:C:253:PRO:CD	2.74	0.50
1:C:83:LEU:HD12	1:C:136:ASN:HB3	1.94	0.50
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.95	0.49
1:A:14:THR:C	1:A:16:GLY:N	2.70	0.48
1:A:103:LEU:HD22	6:A:569:HOH:O	2.13	0.48
1:C:137:THR:O	1:C:293:VAL:HG13	2.13	0.48
1:C:33:LYS:CE	6:C:510:HOH:O	2.53	0.48
1:C:57:GLU:OE2	2:D:307:ALA:HB3	2.14	0.48
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.95	0.48
1:A:71:HIS:O	1:A:72:THR:OG1	2.30	0.47
1:C:131:GLN:NE2	1:C:131:GLN:H	2.12	0.47
1:C:198:THR:HG22	1:C:253:PRO:HG2	1.96	0.47
1:A:14:THR:O	1:A:15:TYR:HB2	2.14	0.47
1:C:-3:PRO:HA	1:C:-2:LEU:HA	1.72	0.47
1:A:162:GLU:HG2	1:A:163:VAL:HG12	1.95	0.47
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.97	0.47
1:A:35:ILE:HB	1:A:76:LEU:HB3	1.96	0.47
1:C:221:THR:HA	1:C:222:PRO:HD3	1.53	0.47
1:A:71:HIS:C	1:A:72:THR:OG1	2.57	0.46
1:A:223:ASP:H	1:A:226[A]:VAL:HG12	1.81	0.46
1:A:178:LYS:HE3	1:A:179:TYR:CZ	2.51	0.45
1:A:161[A]:HIS:CD2	1:A:161[A]:HIS:C	2.94	0.45
1:A:162:GLU:HG2	1:A:163:VAL:CG1	2.47	0.45
1:C:253:PRO:O	1:C:254:PRO:C	2.60	0.45
1:C:137:THR:HG22	1:C:296:LEU:HD13	1.99	0.45
1:C:250:LYS:HB3	1:C:252:VAL:N	2.22	0.44
1:A:59[B]:ASN:HD21	1:A:65:LYS:HE2	1.81	0.44
1:C:251:VAL:O	1:C:251:VAL:HG12	2.17	0.43
6:C:450:HOH:O	2:D:296:HIS:HD2	2.01	0.43
1:A:60:HIS:HD2	1:A:62:ASN:N	2.06	0.43
1:C:129:LYS:HG3	1:C:131:GLN:HG2	2.00	0.43
1:A:73:GLU:HG2	1:A:74:ASN:OD1	2.18	0.43
1:A:127:ASP:OD1	1:A:165:THR:CG2	2.67	0.43
1:C:252:VAL:N	1:C:253:PRO:HD2	2.34	0.43
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.02	0.42
1:A:91:MET:HG2	1:A:99:ILE:HD11	2.02	0.42
1:C:222:PRO:HB2	1:C:225:VAL:CG2	2.50	0.42
1:C:250:LYS:HG2	1:C:252:VAL:CG2	2.46	0.42
2:B:345:ASP:HA	2:B:346:PRO:HA	1.89	0.42
1:A:-1:GLY:HA3	1:A:68:ASP:OD2	2.20	0.42
1:C:105:LYS:HB2	1:C:105:LYS:HE2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:PRO:HB3	1:C:254:PRO:HD3	2.01	0.41
2:D:229:ASN:HD22	2:D:334[B]:MET:CE	2.34	0.41
1:A:162:GLU:HG3	1:A:163:VAL:HA	2.03	0.41
1:A:72:THR:HG22	1:A:73:GLU:H	1.86	0.41
1:C:222:PRO:CB	1:C:225:VAL:HG23	2.51	0.41
1:C:71:HIS:NE2	2:D:304:PHE:HE2	2.19	0.40
2:D:287:THR:HB	6:D:515:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/302 (99%)	292 (97%)	6 (2%)	2 (1%)	18	6
1	C	282/302 (93%)	266 (94%)	13 (5%)	3 (1%)	11	2
2	B	257/258 (100%)	256 (100%)	1 (0%)	0	100	100
2	D	258/258 (100%)	255 (99%)	3 (1%)	0	100	100
All	All	1097/1120 (98%)	1069 (97%)	23 (2%)	5 (0%)	24	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL
1	A	162	GLU
1	C	253	PRO
1	C	254	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/265 (101%)	259 (97%)	9 (3%)	32	10
1	C	252/265 (95%)	238 (94%)	14 (6%)	19	3
2	B	233/232 (100%)	226 (97%)	7 (3%)	36	13
2	D	234/232 (101%)	229 (98%)	5 (2%)	47	24
All	All	987/994 (99%)	952 (96%)	35 (4%)	32	10

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	55	LEU
1	A	73	GLU
1	A	150	ARG
1	A	165	THR
1	A	178	LYS
1	A	206[A]	ASP
1	A	206[B]	ASP
1	A	255	LEU
2	B	177	ASP
2	B	232	LEU
2	B	281	ILE
2	B	292	LEU
2	B	296	HIS
2	B	348	LEU
2	B	432	LEU
1	C	9	LYS
1	C	34	LYS
1	C	36	ARG
1	C	37	LEU
1	C	55	LEU
1	C	101	LEU
1	C	103	LEU
1	C	131	GLN

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Mol	Chain	Res	Type
1	C	150	ARG
1	C	221	THR
1	C	248	PHE
1	C	250	LYS
1	C	253	PRO
1	C	281	LEU
2	D	196	LYS
2	D	292	LEU
2	D	348	LEU
2	D	384	LEU
2	D	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	265	GLN
2	B	228	GLN
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	313	GLN
2	B	395	HIS
2	B	425	ASN
1	C	59	ASN
1	C	60	HIS
1	C	71	HIS
1	C	119	HIS
1	C	131	GLN
1	C	246	GLN
1	C	265	GLN
1	C	268	HIS
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	313	GLN
2	D	323	GLN
2	D	395	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TPO	A	160	1	8,10,11	1.02	1 (12%)	10,14,16	0.98	0
1	TPO	C	160	1	8,10,11	0.76	0	10,14,16	1.08	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
1	TPO	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-OG1	2.05	1.63	1.59

There are no bond angle outliers.

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](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
5	SGM	B	503	-	5,5,5	0.34	0	5,5,5	0.49	0
3	ATP	A	301	4	32,33,33	1.49	6 (18%)	48,52,52	1.81	11 (22%)
3	ATP	C	301	-	32,33,33	1.45	4 (12%)	48,52,52	1.71	9 (18%)
5	SGM	B	502	-	5,5,5	0.47	0	5,5,5	0.56	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	SGM	B	503	-	-	0/4/4/4	-
3	ATP	A	301	4	-	3/22/38/38	0/3/3/3
3	ATP	C	301	-	-	0/22/38/38	0/3/3/3
5	SGM	B	502	-	-	3/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	ATP	C5-C4	4.90	1.47	1.39
3	A	301	ATP	C5-C4	4.74	1.47	1.39
3	A	301	ATP	C5-C6	2.92	1.49	1.41
3	C	301	ATP	C5-C6	2.89	1.49	1.41
3	A	301	ATP	PB-O3A	2.66	1.62	1.59
3	A	301	ATP	C8-N7	2.58	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	ATP	PA-O3A	2.47	1.62	1.59
3	C	301	ATP	C8-N7	2.42	1.36	1.31
3	A	301	ATP	C5-N7	-2.36	1.34	1.39
3	C	301	ATP	C5-N7	-2.24	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	ATP	C5-C4-N3	-6.07	118.36	126.72
3	C	301	ATP	C5-C4-N3	-5.81	118.72	126.72
3	C	301	ATP	N3-C4-N9	4.61	135.01	127.17
3	A	301	ATP	N3-C4-N9	4.57	134.94	127.17
3	A	301	ATP	C2-N3-C4	3.91	121.37	111.83
3	C	301	ATP	C2-N3-C4	3.64	120.72	111.83
3	A	301	ATP	C4-C5-N7	-3.53	106.55	110.58
3	C	301	ATP	C4-C5-N7	-3.48	106.60	110.58
3	A	301	ATP	N3-C2-N1	-3.19	123.76	128.58
3	C	301	ATP	N3-C2-N1	-3.05	123.96	128.58
3	A	301	ATP	C2'-C1'-N9	-2.68	106.64	113.30
3	C	301	ATP	C4-N9-C8	2.65	108.52	105.74
3	C	301	ATP	C5-N7-C8	2.59	107.52	103.45
3	A	301	ATP	C3'-C2'-C1'	2.57	106.33	101.46
3	A	301	ATP	C5-N7-C8	2.55	107.45	103.45
3	A	301	ATP	O4'-C1'-N9	2.39	112.68	108.09
3	A	301	ATP	C6-C5-N7	2.17	136.27	132.09
3	C	301	ATP	C6-C5-N7	2.07	136.08	132.09
3	A	301	ATP	C4-N9-C8	2.01	107.85	105.74
3	C	301	ATP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

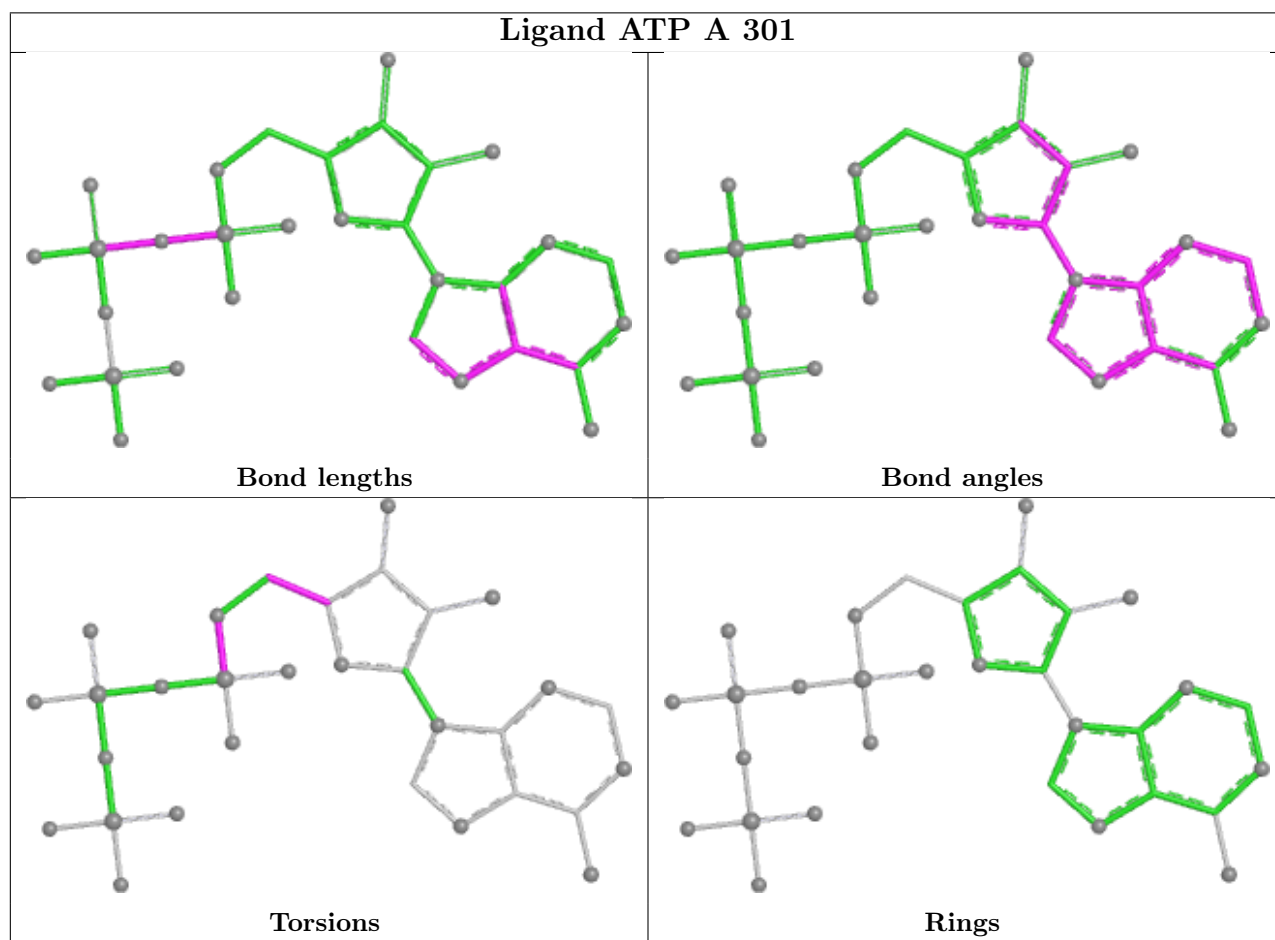
All (6) torsion outliers are listed below:

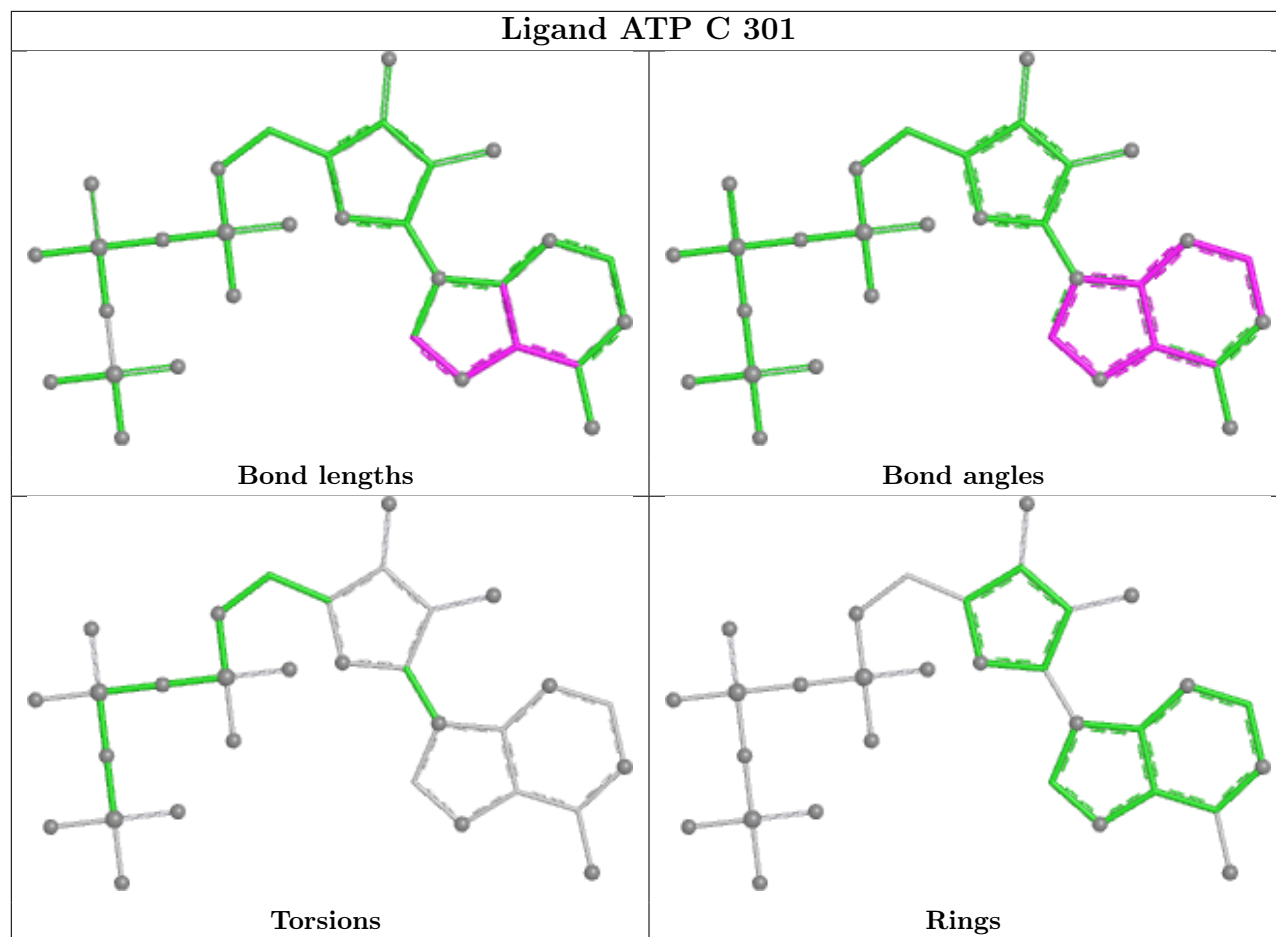
Mol	Chain	Res	Type	Atoms
3	A	301	ATP	O4'-C4'-C5'-O5'
5	B	502	SGM	S1-C1-C2-O2
3	A	301	ATP	C3'-C4'-C5'-O5'
5	B	502	SGM	O2-C2-C3-O3
3	A	301	ATP	C5'-O5'-PA-O1A
5	B	502	SGM	S1-C1-C2-C3

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 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	295/302 (97%)	0.41	32 (10%) 11 11	6, 19, 41, 53	9 (3%)
1	C	282/302 (93%)	1.10	59 (20%) 2 3	11, 26, 55, 75	4 (1%)
2	B	256/258 (99%)	0.36	20 (7%) 19 22	12, 22, 36, 48	1 (0%)
2	D	256/258 (99%)	0.60	20 (7%) 19 22	12, 26, 44, 58	4 (1%)
All	All	1089/1120 (97%)	0.62	131 (12%) 9 9	6, 24, 45, 75	18 (1%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	VAL	11.9
1	C	-3	PRO	10.5
1	C	14	THR	7.9
1	C	17	VAL	7.5
1	C	295[A]	HIS	7.0
1	A	73	GLU	7.0
2	B	284	ASP	6.9
2	B	283	ASP	6.9
2	B	176	PRO	6.9
1	C	251	VAL	6.7
2	B	432	LEU	6.7
2	D	284	ASP	6.0
1	A	15	TYR	5.9
2	B	285	THR	5.8
1	A	14	THR	5.6
1	C	227	TRP	5.6
1	A	72	THR	5.5
1	A	12	GLU	5.5
1	C	13	GLY	5.2
1	C	254	PRO	5.1
1	C	249	SER	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	256	ASP	5.0
1	C	162	GLU	5.0
1	A	71	HIS	5.0
1	A	37	LEU	4.9
1	C	-2	LEU	4.9
2	D	283	ASP	4.9
2	B	323	GLN	4.9
2	D	285	THR	4.8
1	A	96	LEU	4.8
1	C	253	PRO	4.8
1	C	228	PRO	4.6
2	B	431	ASN	4.6
1	A	17	VAL	4.4
1	A	-1	GLY	4.4
1	A	13	GLY	4.4
2	D	431	ASN	4.3
1	A	97	THR	4.2
2	D	176	PRO	4.2
1	C	15	TYR	4.1
1	A	162	GLU	4.1
1	A	36	ARG	4.1
1	C	247	ASP	4.1
2	D	179[A]	HIS	4.0
2	B	282	THR	4.0
1	C	246	GLN	4.0
2	D	177	ASP	4.0
1	C	226	VAL	4.0
1	C	220	GLY	4.0
1	C	248	PHE	3.9
1	C	287	GLN	3.8
1	C	0	SER	3.7
2	B	198	GLY	3.7
1	C	296	LEU	3.7
1	A	287	GLN	3.7
1	A	2	GLU	3.6
1	C	219	LEU	3.6
1	C	10	ILE	3.6
2	D	198	GLY	3.5
1	C	2	GLU	3.5
1	C	19	TYR	3.5
1	A	35	ILE	3.5
2	D	324	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	281	ILE	3.3
1	C	9	LYS	3.2
1	C	225	VAL	3.1
2	D	323	GLN	3.1
1	C	250	LYS	3.1
2	B	177	ASP	3.1
1	C	11	GLY	3.1
2	B	327	CYS	3.1
1	A	19	TYR	3.0
1	C	294	PRO	2.9
1	C	72	THR	2.9
1	A	16	GLY	2.9
1	A	297	ARG	2.9
1	C	73	GLU	2.9
2	B	324	PRO	2.8
1	A	42	GLU	2.8
1	C	12	GLU	2.8
1	C	-1	GLY	2.8
1	C	84	SER	2.7
1	C	16	GLY	2.7
1	C	272	ASN	2.7
1	A	74	ASN	2.7
2	D	386	SER	2.6
1	C	165[A]	THR	2.6
1	C	269	TYR	2.6
1	C	161	HIS	2.6
2	D	423	LEU	2.6
1	A	18	VAL	2.6
1	C	293	VAL	2.6
1	A	232	SER	2.5
1	C	163	VAL	2.5
1	A	145	ASP	2.5
1	A	256	ASP	2.5
2	D	280	TYR	2.5
1	C	223	ASP	2.5
2	B	428	GLU	2.4
1	A	7	VAL	2.4
1	C	209	ILE	2.4
1	C	138	GLU	2.4
1	C	222	PRO	2.4
1	A	0	SER	2.4
1	C	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	327	CYS	2.4
2	D	364	LEU	2.4
2	D	197	VAL	2.4
2	B	274	GLU	2.3
1	C	255	LEU	2.3
1	A	11	GLY	2.3
1	C	7	VAL	2.3
1	C	288	ASP	2.3
2	D	282	THR	2.2
2	D	416	SER	2.2
1	A	10	ILE	2.2
1	C	221	THR	2.2
2	D	325	ALA	2.2
1	C	6	LYS	2.2
1	C	37	LEU	2.2
2	B	392	MET	2.2
2	B	385	GLU	2.2
2	B	296	HIS	2.2
2	B	280	TYR	2.2
2	B	281	ILE	2.1
1	C	216	PHE	2.1
1	C	42	GLU	2.0
1	C	18	VAL	2.0
1	A	70	ILE	2.0
2	B	325	ALA	2.0
1	A	177[A]	CYS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	A	160	11/12	0.98	0.05	14,17,18,19	0
1	TPO	C	160	11/12	0.98	0.05	17,19,22,22	0

## 6.3 Carbohydrates [\(i\)](#)

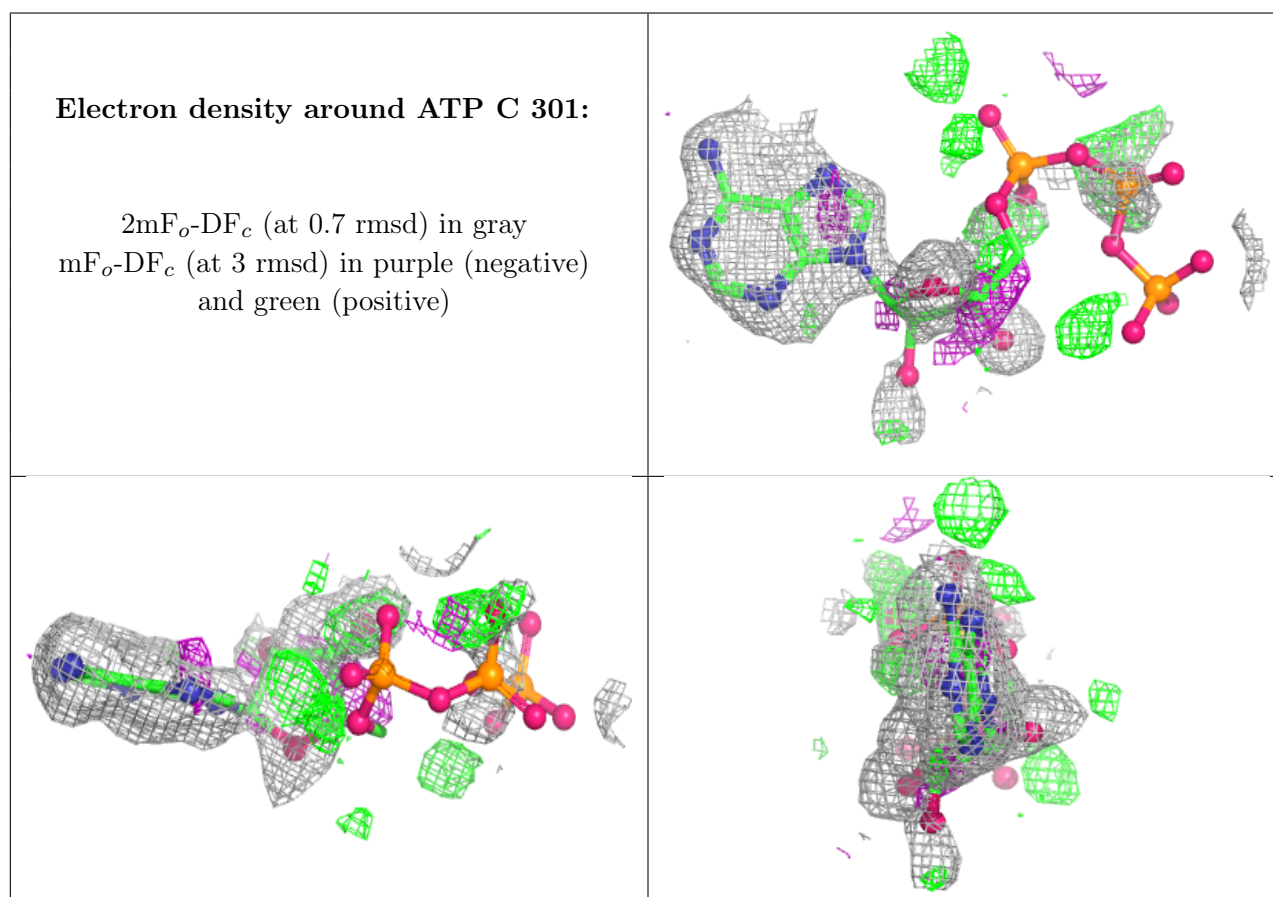
There are no oligosaccharides in this entry.

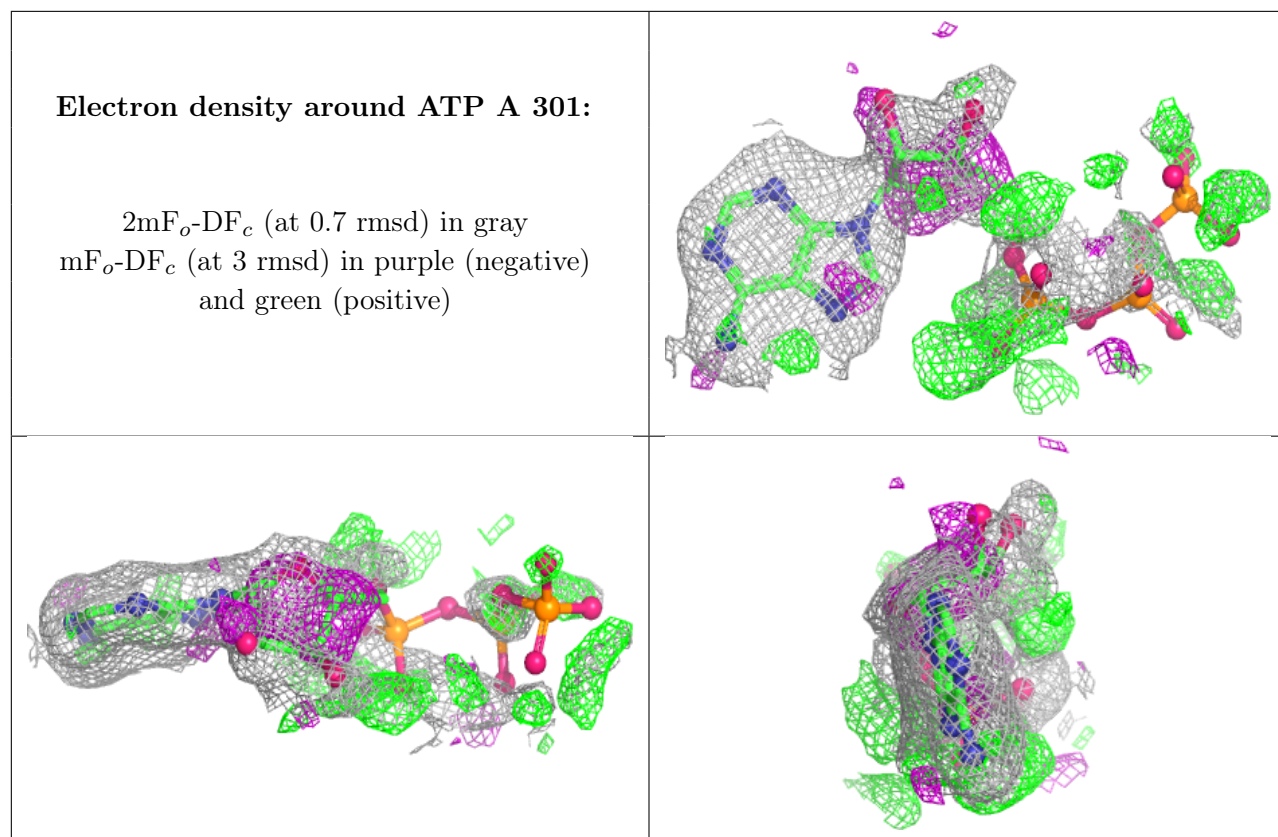
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	C	301	31/31	0.64	0.33	46,54,55,55	14
4	MG	A	302	1/1	0.65	0.18	51,51,51,51	0
5	SGM	B	503	6/6	0.72	0.21	71,71,71,71	0
3	ATP	A	301	31/31	0.74	0.27	30,46,47,47	13
5	SGM	B	502	6/6	0.88	0.17	36,40,41,43	0
4	MG	B	501	1/1	0.94	0.07	30,30,30,30	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.