Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:00 PM BST

PDB ID	:	4EOQ
Title	:	Thr 160 phosphorylated CDK2 WT - 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	:	2.15 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

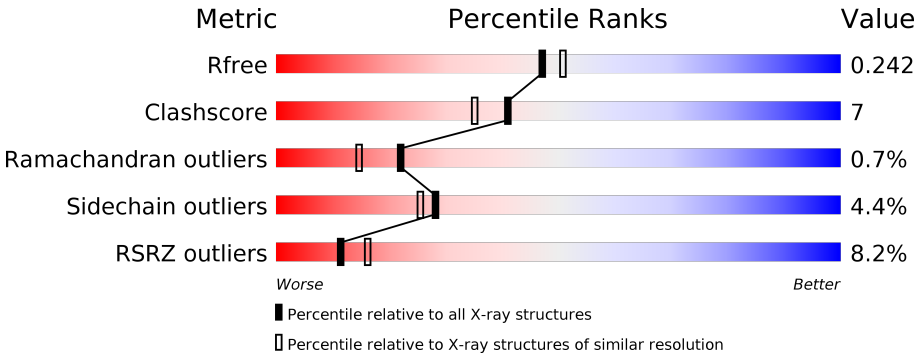
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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 <=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	301	5% 85% 11%
1	C	301	16% 74% 14% 8%
2	B	258	5% 88% 11%
2	D	258	6% 85% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9271 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
1	A	296	Total	C	N	O	P	S	0	3	0
			2405	1559	412	425	1	8			
1	C	276	Total	C	N	O	P	S	0	1	0
			2220	1438	379	395	1	7			

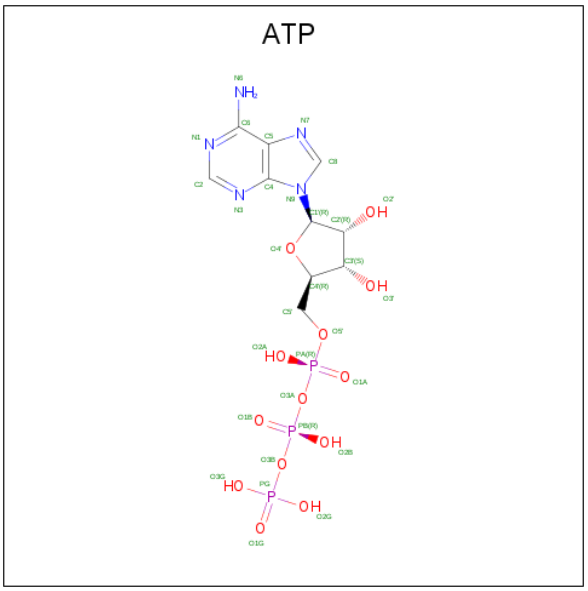
There are 8 discrepancies between the modelled and reference sequences:

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
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

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	0	0
			2076	1345	338	382	11			
2	D	254	Total	C	N	O	S	0	1	0
			2063	1335	338	379	11			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

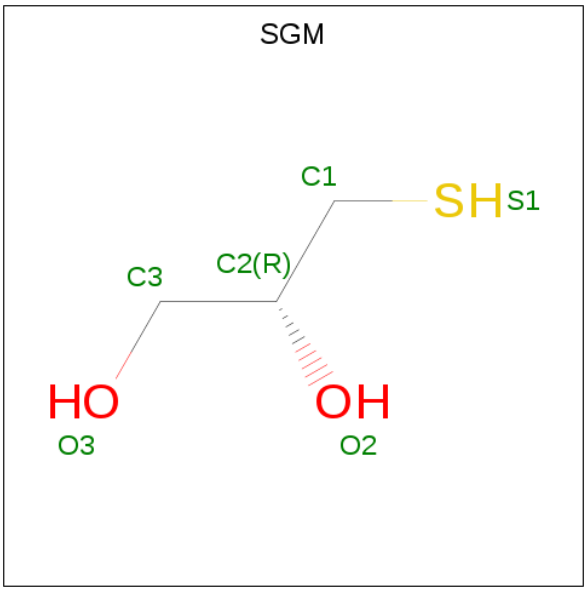


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



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

- Molecule 6 is water.

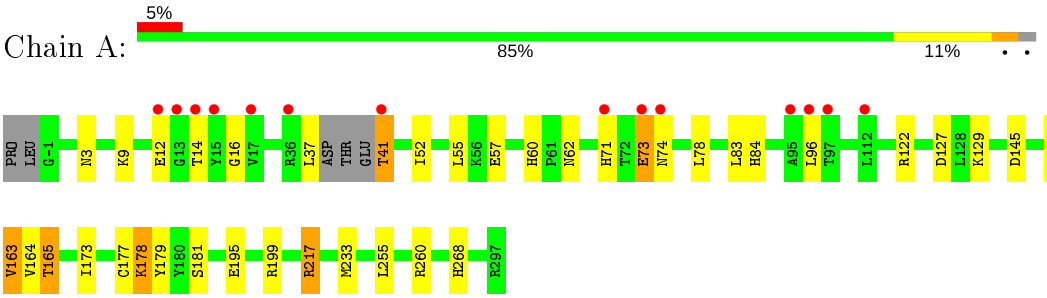
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	148	Total O 148 148	0	0
6	B	121	Total O 121 121	0	0
6	C	82	Total O 82 82	0	0
6	D	80	Total O 80 80	0	0

3 Residue-property plots

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.

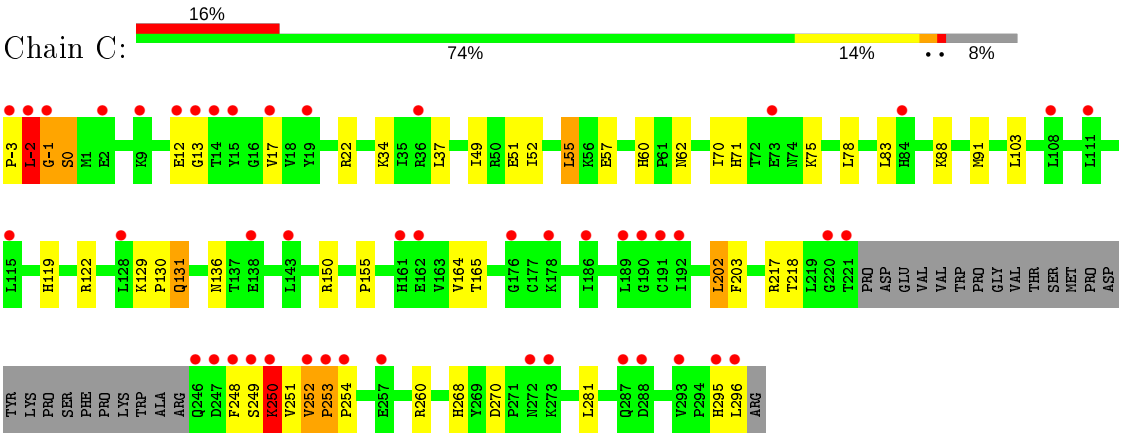
- Molecule 1: Cyclin-dependent kinase 2

Chain A:



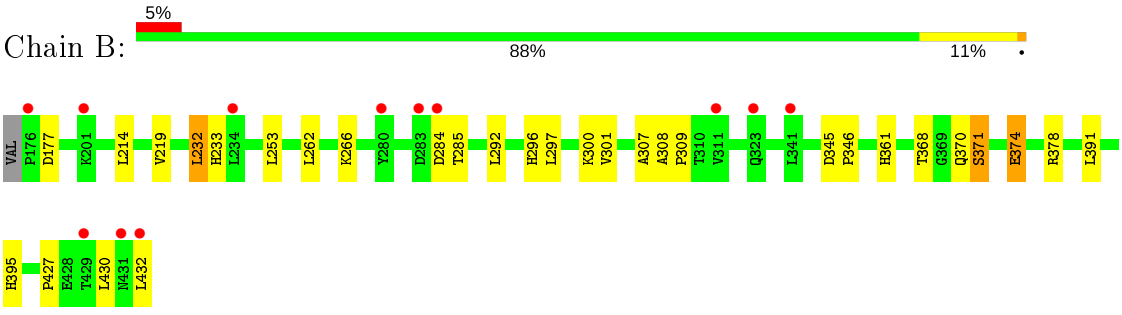
- Molecule 1: Cyclin-dependent kinase 2

Chain C:



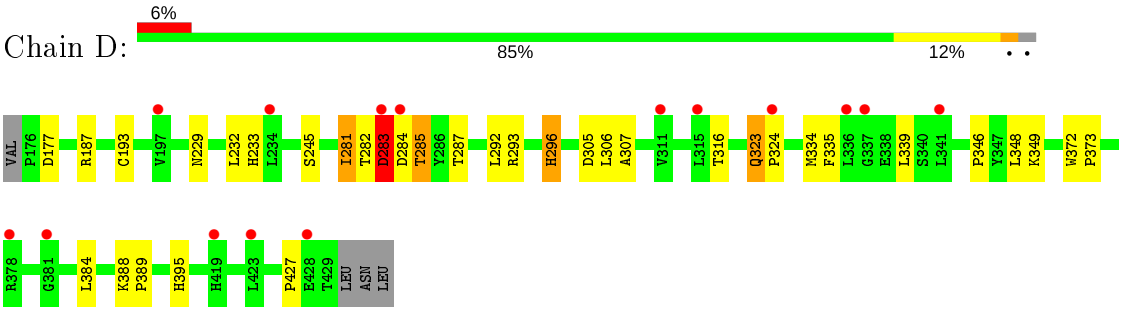
- Molecule 2: Cyclin-A2

Chain B:



- Molecule 2: Cyclin-A2

Chain D:


6%
85%
12%
VAL P176 D177 R187 C193 V197 N229 L232 H233 L234 S245 I281 T282 D283 D284 T285 Y286 T287 L292 R293 H296 D305 L306 A307 V311 L315 T316 Q323 P324 M334 F335 L336 G337 E338 L339 S340 L341 P346 Y347 L348 K349 W372 P373
R378 G381 L384 K388 P389 H395 H419 L423 P427 E428 T429 LEU ASN LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.72Å 134.19Å 149.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 29.91 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.15) 99.3 (29.91-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.234 0.207 , 0.242	Depositor DCC
R_{free} test set	4042 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9271	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.61	0/2455	0.64	1/3328 (0.0%)
1	C	0.48	0/2260	0.66	5/3059 (0.2%)
2	B	0.54	1/2126 (0.0%)	0.56	0/2886
2	D	0.48	0/2113	0.57	0/2867
All	All	0.53	1/8954 (0.0%)	0.61	6/12140 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	371	SER	CB-OG	-5.52	1.35	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	0	SER	N-CA-C	-8.94	86.85	111.00
1	C	-1	GLY	N-CA-C	6.08	128.29	113.10
1	C	-2	LEU	CA-CB-CG	-6.07	101.35	115.30
1	C	250	LYS	N-CA-CB	5.51	120.52	110.60
1	C	248	PHE	N-CA-C	5.38	125.52	111.00
1	A	217	ARG	NE-CZ-NH1	-5.09	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2405	0	2442	42	1
1	C	2220	0	2269	51	0
2	B	2076	0	2098	31	0
2	D	2063	0	2083	25	0
3	A	31	0	12	1	0
3	C	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	6	0	7	0	0
5	D	6	0	8	2	0
6	A	148	0	0	5	1
6	B	121	0	0	2	0
6	C	82	0	0	3	0
6	D	80	0	0	5	0
All	All	9271	0	8931	127	1

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 (127) 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:9:LYS:CE	1:A:12:GLU:HG3	1.68	1.23
1:C:-2:LEU:N	1:C:-2:LEU:HD23	1.67	1.03
1:A:9:LYS:HE3	1:A:12:GLU:HG3	1.40	1.03
2:B:301:VAL:CG2	1:C:-2:LEU:HD11	1.88	1.03
1:A:9:LYS:HE3	1:A:12:GLU:CG	1.91	1.00
1:A:9:LYS:NZ	1:A:12:GLU:CD	2.17	0.97
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.03	0.97
1:A:9:LYS:CE	1:A:12:GLU:CG	2.44	0.96
2:D:193:CYS:SG	5:D:501:SGM:S1	2.53	0.95
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.88	0.92
1:C:-3:PRO:HG2	6:C:466:HOH:O	1.70	0.91
1:C:-3:PRO:C	1:C:-2:LEU:HD23	1.90	0.91
2:B:301:VAL:HG23	1:C:-2:LEU:HD11	1.54	0.90
1:A:9:LYS:HZ2	1:A:12:GLU:CD	1.76	0.86
2:B:301:VAL:HG23	1:C:-2:LEU:CD1	2.05	0.85
1:A:9:LYS:HE2	1:A:12:GLU:HG3	1.58	0.84
1:C:-2:LEU:N	1:C:-2:LEU:CD2	2.30	0.84
1:A:71:HIS:CE1	2:B:296:HIS:CD2	2.65	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.93	0.83
2:B:361:HIS:HE1	2:B:371:SER:HB3	1.42	0.82
2:B:301:VAL:HG22	1:C:-2:LEU:HD11	1.61	0.81
2:B:361:HIS:CE1	2:B:371:SER:HB3	2.16	0.81
1:C:12:GLU:HG3	1:C:13:GLY:H	1.50	0.76
2:D:229:ASN:HD22	2:D:334:MET:HE2	1.53	0.72
1:C:-3:PRO:CG	6:C:466:HOH:O	2.30	0.71
2:D:285:THR:N	6:D:670:HOH:O	2.24	0.70
1:A:60:HIS:HD2	1:A:62:ASN:H	1.40	0.70
1:A:9:LYS:NZ	1:A:12:GLU:OE2	2.22	0.70
2:B:300:LYS:HB3	1:C:-2:LEU:HD13	1.77	0.67
1:A:71:HIS:ND1	2:B:300:LYS:HE3	2.10	0.66
1:A:177:CYS:HB2	1:A:233:MET:CE	2.25	0.66
1:A:181:SER:HB3	6:A:487:HOH:O	1.95	0.66
2:B:361:HIS:CE1	2:B:371:SER:CB	2.78	0.65
1:A:71:HIS:HE1	2:B:296:HIS:CD2	2.13	0.65
2:B:361:HIS:HE1	2:B:371:SER:CB	2.10	0.65
1:A:60:HIS:CD2	1:A:62:ASN:H	2.15	0.64
1:C:60:HIS:CD2	1:C:62:ASN:H	2.16	0.64
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.33	0.63
2:D:229:ASN:HD22	2:D:334:MET:CE	2.10	0.63
1:A:260:ARG:HD3	6:A:408:HOH:O	1.99	0.63
2:B:374:GLU:OE1	2:B:378:ARG:HD3	1.99	0.63
2:D:346:PRO:O	2:D:349:LYS:HG2	1.99	0.62
2:D:395:HIS:HE1	2:D:427:PRO:O	1.82	0.62
1:A:9:LYS:NZ	1:A:12:GLU:CG	2.61	0.62
1:A:145:ASP:OD2	3:A:301:ATP:O1B	2.17	0.62
2:B:300:LYS:CB	1:C:-2:LEU:HD13	2.30	0.61
1:C:60:HIS:HD2	1:C:62:ASN:H	1.48	0.59
1:A:161[B]:HIS:O	1:A:162:GLU:O	2.20	0.59
1:A:9:LYS:NZ	1:A:12:GLU:HG3	2.17	0.59
1:C:249:SER:N	1:C:250:LYS:HB3	2.16	0.59
1:A:9:LYS:HZ1	1:A:12:GLU:CD	2.03	0.56
2:B:368:THR:OG1	2:B:370:GLN:HG3	2.06	0.56
1:C:252:VAL:HG13	1:C:253:PRO:HD2	1.89	0.55
1:A:9:LYS:CE	1:A:12:GLU:CD	2.74	0.55
1:A:96:LEU:O	1:A:96:LEU:HG	2.07	0.54
2:B:395:HIS:HE1	2:B:427:PRO:O	1.90	0.54
1:C:88:LYS:HA	1:C:91:MET:HE2	1.88	0.54
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.79	0.54
1:C:250:LYS:C	1:C:250:LYS:HE3	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.08	0.53
2:B:300:LYS:HB3	1:C:-2:LEU:HB3	1.91	0.53
1:C:51:GLU:O	1:C:55:LEU:HB2	2.09	0.53
1:C:83:LEU:HD12	1:C:136:ASN:HB3	1.90	0.53
1:A:127:ASP:OD1	1:A:165:THR:CG2	2.58	0.51
1:A:127:ASP:OD1	1:A:165:THR:HG23	2.10	0.51
1:C:129:LYS:NZ	1:C:165:THR:HG21	2.25	0.51
1:A:163:VAL:HA	6:A:421:HOH:O	2.11	0.51
1:C:12:GLU:HG3	1:C:13:GLY:N	2.22	0.51
2:B:301:VAL:CG2	1:C:-2:LEU:CD1	2.68	0.51
2:D:287:THR:HB	6:D:617:HOH:O	2.11	0.50
2:B:233:HIS:HE1	6:B:652:HOH:O	1.93	0.50
1:C:57:GLU:OE2	2:D:307:ALA:HB3	2.11	0.50
1:A:129:LYS:NZ	1:A:165:THR:HG21	2.27	0.49
1:C:-1:GLY:CA	1:C:70:ILE:HG12	2.43	0.48
1:C:250:LYS:HG3	1:C:251:VAL:HG23	1.95	0.48
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.95	0.48
1:A:41:THR:OG1	1:A:41:THR:O	2.29	0.48
2:B:395:HIS:HB2	2:B:430:LEU:HD11	1.95	0.48
1:C:295[B]:HIS:CG	1:C:296:LEU:N	2.82	0.48
3:C:301:ATP:O5'	3:C:301:ATP:H8	1.96	0.47
1:C:268:HIS:HD2	1:C:270:ASP:H	1.61	0.47
1:A:178:LYS:HE3	1:A:179:TYR:CZ	2.49	0.47
1:C:119:HIS:HD2	6:D:603:HOH:O	1.97	0.46
1:C:252:VAL:HG13	1:C:253:PRO:CD	2.45	0.46
2:D:283:ASP:HB3	2:D:284:ASP:H	1.37	0.46
1:C:-1:GLY:HA3	1:C:70:ILE:HG12	1.96	0.46
1:A:3:ASN:OD1	2:D:293[B]:ARG:NH2	2.42	0.45
1:C:34:LYS:HD3	1:C:75:LYS:HD2	1.99	0.45
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.99	0.45
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.99	0.45
2:D:281:ILE:H	2:D:281:ILE:HG13	1.48	0.45
2:D:305:ASP:HB3	5:D:501:SGM:H12	1.99	0.45
1:A:14:THR:C	1:A:16:GLY:H	2.19	0.44
1:A:37:LEU:HD13	2:B:296:HIS:HE1	1.81	0.44
2:D:233:HIS:HE1	6:D:646:HOH:O	2.00	0.43
2:D:372:TRP:HA	2:D:373:PRO:HD3	1.88	0.43
2:B:345:ASP:HA	2:B:346:PRO:HA	1.88	0.43
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.90	0.42
2:B:391:LEU:HD23	2:B:432:LEU:HD22	2.01	0.42
2:B:300:LYS:HB3	1:C:-2:LEU:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161[B]:HIS:HE1	1:A:173:ILE:O	2.02	0.42
1:C:249:SER:HB3	1:C:260:ARG:HD3	2.01	0.42
1:A:9:LYS:CE	1:A:12:GLU:OE2	2.68	0.42
1:C:218:THR:HG23	1:C:250:LYS:CD	2.49	0.42
2:B:262:LEU:HD11	2:B:266:LYS:HE3	2.01	0.42
1:C:218:THR:CG2	1:C:250:LYS:HD3	2.49	0.42
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.02	0.42
1:C:130:PRO:HD2	1:C:131:GLN:NE2	2.34	0.42
1:A:73:GLU:CG	1:A:74:ASN:H	2.33	0.42
1:C:253:PRO:HA	1:C:254:PRO:HA	1.54	0.42
2:B:219:VAL:HG22	2:B:232:LEU:HD11	2.03	0.41
6:C:452:HOH:O	2:D:296:HIS:HD2	2.03	0.41
1:A:60:HIS:HE1	6:A:471:HOH:O	2.03	0.41
1:A:268:HIS:CE1	6:A:475:HOH:O	2.73	0.41
2:B:297:LEU:HD12	1:C:-2:LEU:HD12	2.02	0.41
1:A:195:GLU:O	1:A:199:ARG:N	2.52	0.41
2:B:214:LEU:HD22	2:B:253:LEU:HG	2.02	0.41
2:B:177:ASP:HB2	6:B:720:HOH:O	2.20	0.41
1:C:155:PRO:HD2	2:D:316:THR:HB	2.02	0.41
2:D:187:ARG:HD3	6:D:606:HOH:O	2.20	0.41
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.55	0.41
1:C:-3:PRO:H3	1:C:-1:GLY:H	1.69	0.41
2:D:323:GLN:HA	2:D:324:PRO:HA	1.86	0.40
1:C:131:GLN:H	1:C:131:GLN:NE2	2.20	0.40
1:A:14:THR:C	1:A:16:GLY:N	2.75	0.40
1:A:84:HIS:CD2	1:A:84:HIS:H	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:NH1	6:A:515:HOH:O[4_445]	2.11	0.09

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	294/301 (98%)	281 (96%)	10 (3%)	3 (1%)	15 9
1	C	272/301 (90%)	254 (93%)	15 (6%)	3 (1%)	14 8
2	B	255/258 (99%)	251 (98%)	4 (2%)	0	100 100
2	D	253/258 (98%)	250 (99%)	2 (1%)	1 (0%)	34 29
All	All	1074/1118 (96%)	1036 (96%)	31 (3%)	7 (1%)	22 15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
2	D	283	ASP
1	A	163	VAL
1	C	253	PRO
1	A	164	VAL
1	C	164	VAL
1	C	250	LYS

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	262/264 (99%)	251 (96%)	11 (4%)	30 28
1	C	242/264 (92%)	227 (94%)	15 (6%)	18 14
2	B	231/232 (100%)	226 (98%)	5 (2%)	52 55
2	D	229/232 (99%)	217 (95%)	12 (5%)	23 19
All	All	964/992 (97%)	921 (96%)	43 (4%)	28 24

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR

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Mol	Chain	Res	Type
1	A	55	LEU
1	A	73	GLU
1	A	83	LEU
1	A	122	ARG
1	A	150	ARG
1	A	161[A]	HIS
1	A	161[B]	HIS
1	A	165	THR
1	A	178	LYS
1	A	255	LEU
2	B	232	LEU
2	B	284	ASP
2	B	285	THR
2	B	292	LEU
2	B	374	GLU
1	C	-2	LEU
1	C	0	SER
1	C	17	VAL
1	C	22	ARG
1	C	37	LEU
1	C	55	LEU
1	C	103	LEU
1	C	122	ARG
1	C	131	GLN
1	C	150	ARG
1	C	202	LEU
1	C	217	ARG
1	C	250	LYS
1	C	252	VAL
1	C	281	LEU
2	D	177	ASP
2	D	232	LEU
2	D	245	SER
2	D	281	ILE
2	D	282	THR
2	D	283	ASP
2	D	285	THR
2	D	292	LEU
2	D	296	HIS
2	D	323	GLN
2	D	348	LEU
2	D	384	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	84	HIS
1	A	272	ASN
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
1	C	59	ASN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	85	GLN
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	395	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	C	160	1	8,10,11	0.88	0	10,14,16	0.93	0
1	TPO	A	160	1	8,10,11	0.90	0	10,14,16	0.97	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	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	D	501	-	5,5,5	0.36	0	5,5,5	0.63	0
3	ATP	C	301	-	26,33,33	0.95	1 (3%)	31,52,52	1.33	3 (9%)
3	ATP	A	301	4	26,33,33	1.04	3 (11%)	31,52,52	1.28	4 (12%)
5	SGM	B	502	-	5,5,5	0.48	0	5,5,5	0.55	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	D	501	-	-	0/4/4/4	-
3	ATP	C	301	-	-	3/18/38/38	0/3/3/3
3	ATP	A	301	4	-	0/18/38/38	0/3/3/3
5	SGM	B	502	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	ATP	C5-C4	2.70	1.48	1.40
3	C	301	ATP	C5-C4	2.51	1.47	1.40
3	A	301	ATP	O4'-C1'	2.29	1.44	1.41
3	A	301	ATP	C2-N3	2.02	1.35	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	ATP	N3-C2-N1	-3.34	123.45	128.68
3	A	301	ATP	N3-C2-N1	-2.86	124.21	128.68
3	A	301	ATP	PB-O3B-PG	-2.80	123.21	132.83
3	C	301	ATP	C3'-C2'-C1'	2.65	104.97	100.98
3	A	301	ATP	C4-C5-N7	-2.65	106.64	109.40
3	C	301	ATP	PA-O3A-PB	-2.02	125.91	132.83
3	A	301	ATP	PA-O3A-PB	-2.01	125.92	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	502	SGM	S1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	301	ATP	PB-O3B-PG-O1G
3	C	301	ATP	PA-O3A-PB-O2B
3	C	301	ATP	C5'-O5'-PA-O1A

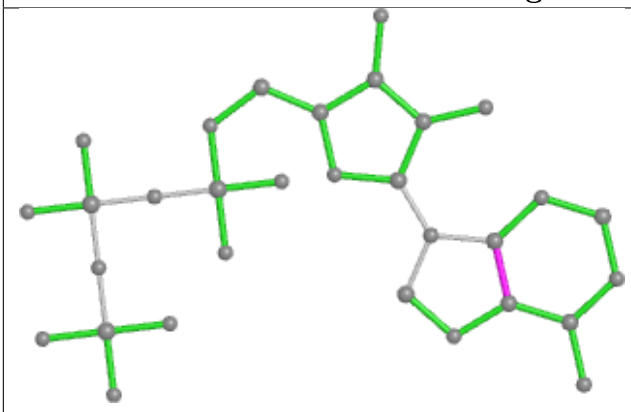
There are no ring outliers.

3 monomers are involved in 4 short contacts:

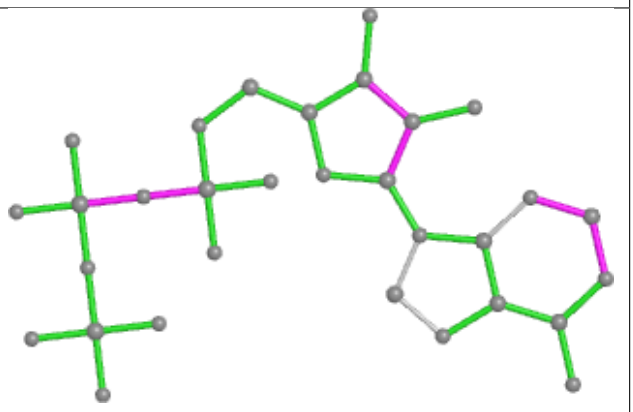
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	SGM	2	0
3	C	301	ATP	1	0
3	A	301	ATP	1	0

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 then 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.

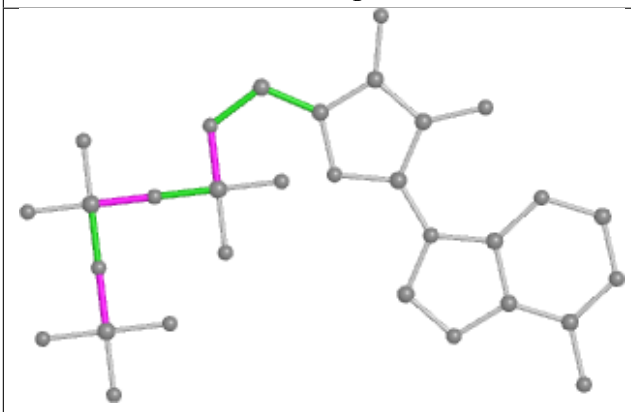
Ligand ATP C 301



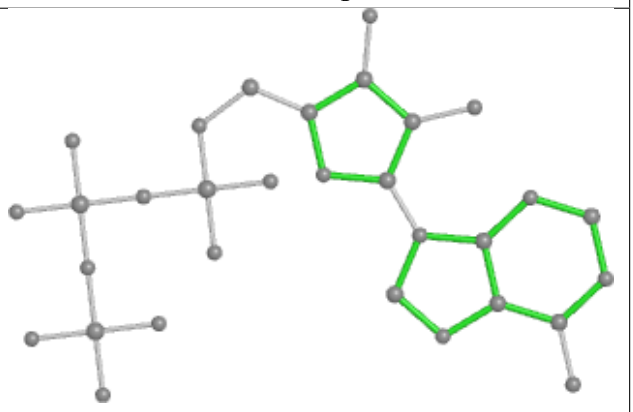
Bond lengths



Bond angles

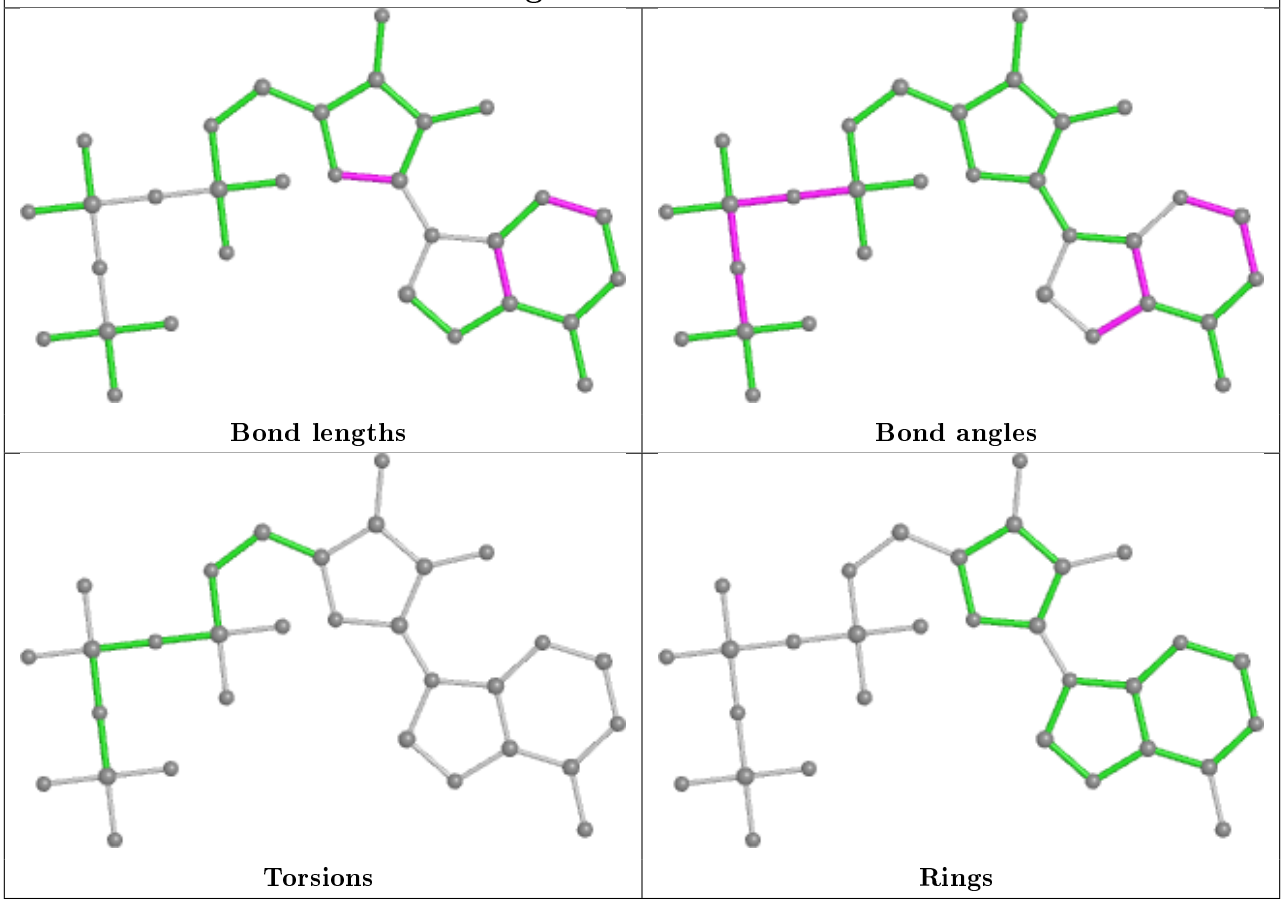


Torsions



Rings

Ligand ATP A 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	295/301 (98%)	0.19	15 (5%) 28 36	11, 21, 50, 59	0
1	C	275/301 (91%)	0.82	47 (17%) 1 1	19, 33, 65, 87	0
2	B	257/258 (99%)	0.21	12 (4%) 31 41	12, 24, 40, 56	0
2	D	254/258 (98%)	0.46	15 (5%) 22 30	16, 35, 68, 80	0
All	All	1081/1118 (96%)	0.42	89 (8%) 11 16	11, 28, 61, 87	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	TYR	11.1
1	C	14	THR	8.0
1	A	96	LEU	7.8
1	C	247	ASP	7.5
1	C	253	PRO	6.8
1	C	13	GLY	6.3
1	C	295[A]	HIS	6.1
2	D	283	ASP	5.4
1	C	-1	GLY	5.4
1	C	246	GLN	5.4
1	C	254	PRO	5.2
1	A	15	TYR	5.0
1	C	17	VAL	4.9
1	C	189	LEU	4.8
1	C	248	PHE	4.7
2	B	283	ASP	4.7
2	D	378	ARG	4.6
1	C	296	LEU	4.4
1	A	12	GLU	4.3
2	B	432	LEU	4.2
2	B	323	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	-2	LEU	4.1
1	A	95	ALA	4.0
1	C	12	GLU	4.0
1	C	293	VAL	3.8
2	B	284	ASP	3.7
1	C	221	THR	3.6
1	C	128	LEU	3.6
1	C	273	LYS	3.6
1	A	17	VAL	3.5
1	A	97	THR	3.5
1	A	71	HIS	3.5
2	B	280	TYR	3.5
1	C	287	GLN	3.4
1	C	192	ILE	3.4
1	C	19	TYR	3.2
2	B	176	PRO	3.2
1	C	220	GLY	3.2
1	C	36	ARG	3.2
1	A	41	THR	3.2
1	C	-3	PRO	3.2
2	D	311	VAL	3.1
2	D	324	PRO	3.1
1	C	252	VAL	3.1
1	A	74	ASN	3.1
1	C	9	LYS	3.0
2	B	431	ASN	3.0
1	C	288	ASP	2.9
1	A	73	GLU	2.9
1	A	36	ARG	2.9
1	C	115	LEU	2.8
1	C	186	ILE	2.8
1	C	111	LEU	2.8
2	D	315	LEU	2.8
2	D	284	ASP	2.8
1	C	191	CYS	2.7
2	B	311	VAL	2.6
2	B	201	LYS	2.6
2	D	337	GLY	2.6
2	D	381	GLY	2.6
1	C	2	GLU	2.6
1	C	138	GLU	2.5
1	C	250	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	73	GLU	2.4
2	D	419	HIS	2.4
2	B	341	LEU	2.4
2	D	336	LEU	2.4
1	A	14	THR	2.3
1	C	162	GLU	2.3
1	C	176	GLY	2.3
2	D	234	LEU	2.3
2	D	423	LEU	2.3
1	C	143	LEU	2.3
1	A	162	GLU	2.2
1	A	112	LEU	2.2
1	C	178	LYS	2.2
2	D	197	VAL	2.2
2	D	341	LEU	2.2
1	C	84	HIS	2.1
1	C	161	HIS	2.1
1	C	249	SER	2.1
2	B	429	THR	2.1
1	C	257	GLU	2.1
2	D	428	GLU	2.1
1	A	13	GLY	2.1
1	C	190	GLY	2.1
1	C	272	ASN	2.1
2	B	234	LEU	2.0
1	C	108	LEU	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^{th} 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
1	TPO	C	160	11/12	0.98	0.08	22,24,27,28	0
1	TPO	A	160	11/12	0.98	0.10	19,20,21,21	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

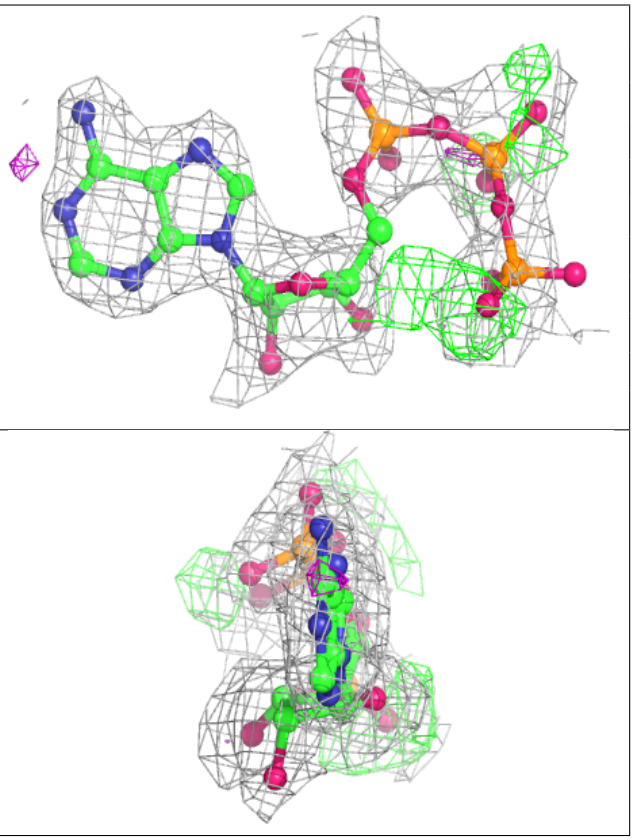
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

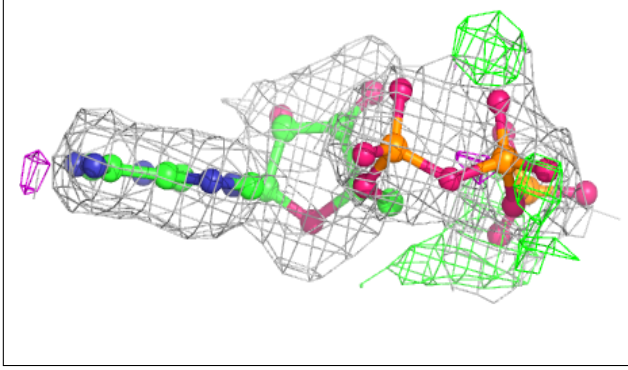
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SGM	D	501	6/6	0.79	0.25	62,64,65,67	0
3	ATP	C	301	31/31	0.81	0.17	39,49,52,53	14
4	MG	A	302	1/1	0.85	0.09	41,41,41,41	0
5	SGM	B	502	6/6	0.88	0.17	42,45,46,47	0
3	ATP	A	301	31/31	0.90	0.15	31,43,54,55	9
4	MG	B	501	1/1	0.98	0.05	29,29,29,29	0

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 C 301:

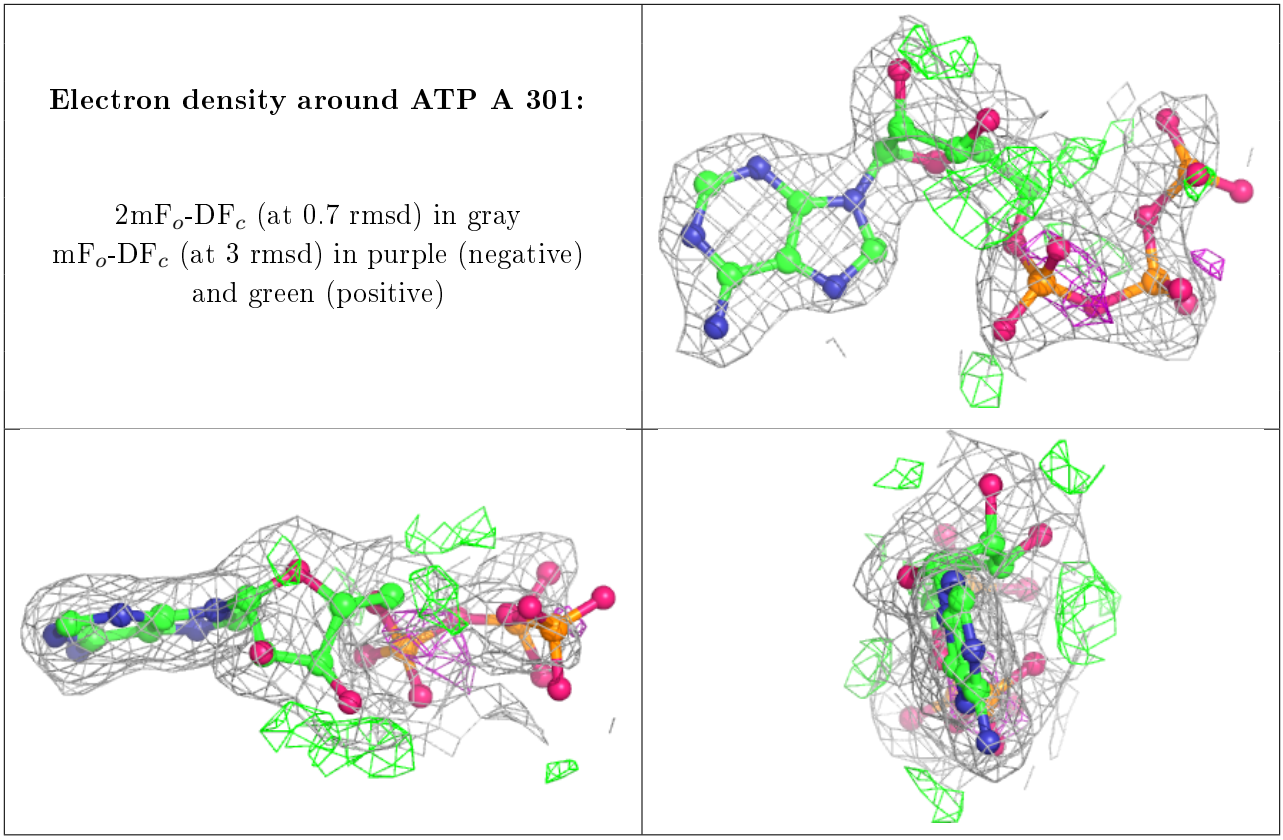
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around ATP A 301:

$2mF_o$-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.