Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:27 am BST

PDB ID	:	4EOM
Title	:	Thr 160 phosphorylated CDK2 H84S, Q85M, Q131E - 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	:	2.10 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:

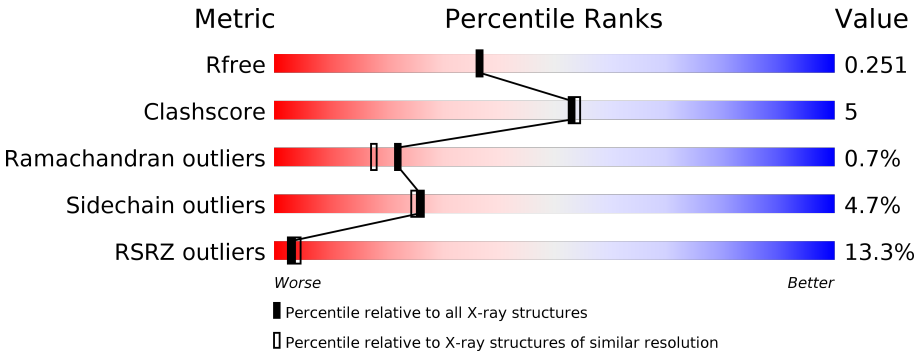
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	8% 85% 12%
1	C	301	19% 75% 15% 8%
2	B	258	7% 90% 9%
2	D	258	18% 85% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8958 atoms, of which 8 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	297	Total	C	N	O	P	S	0	3	0
			2403	1558	409	426	1	9			
1	C	276	Total	C	N	O	P	S	0	1	0
			2215	1435	375	396	1	8			

There are 14 discrepancies between the modelled and reference sequences:

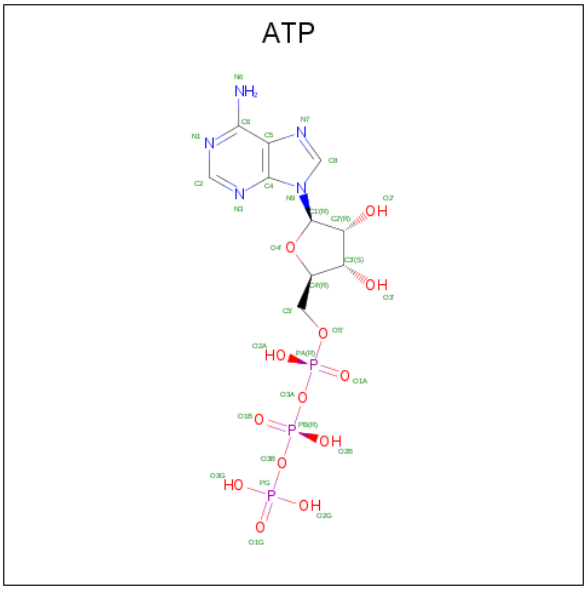
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PRO	-	EXPRESSION TAG	UNP P24941
A	-2	LEU	-	EXPRESSION TAG	UNP P24941
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	SER	-	EXPRESSION TAG	UNP P24941
A	84	SER	HIS	ENGINEERED MUTATION	UNP P24941
A	85	MET	GLN	ENGINEERED MUTATION	UNP P24941
A	131	GLU	GLN	ENGINEERED 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	131	GLU	GLN	ENGINEERED MUTATION	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	H	N	O	P	0	0
			35	10	4	5	13	3		
3	C	1	Total	C	H	N	O	P	0	0
			35	10	4	5	13	3		

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

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

- Molecule 5 is water.

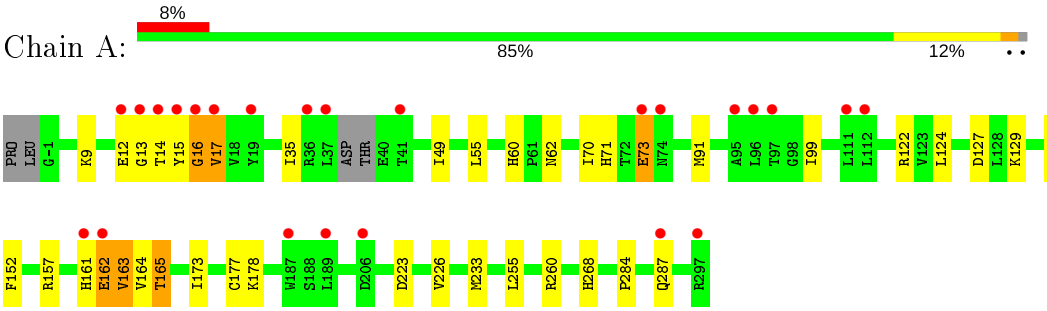
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	41	Total	O	0	0
			41	41		
5	C	16	Total	O	0	0
			16	16		
5	D	6	Total	O	0	0
			6	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

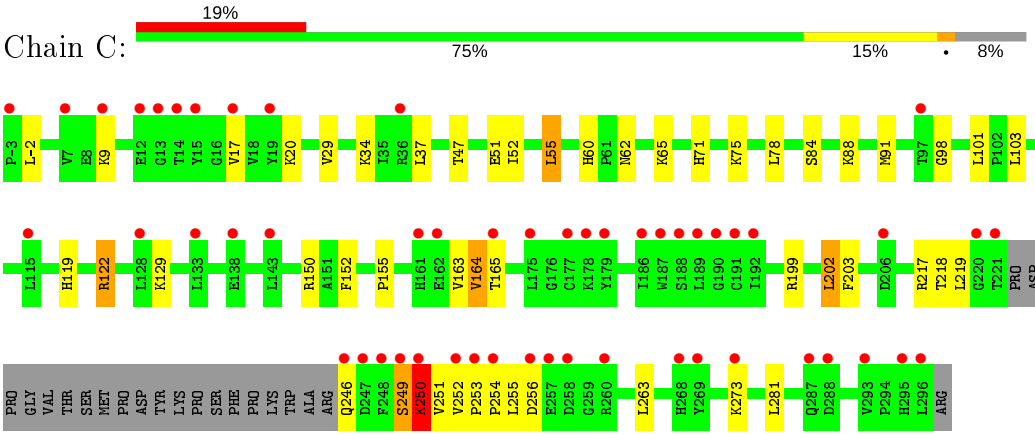
- Molecule 1: Cyclin-dependent kinase 2

Chain A:



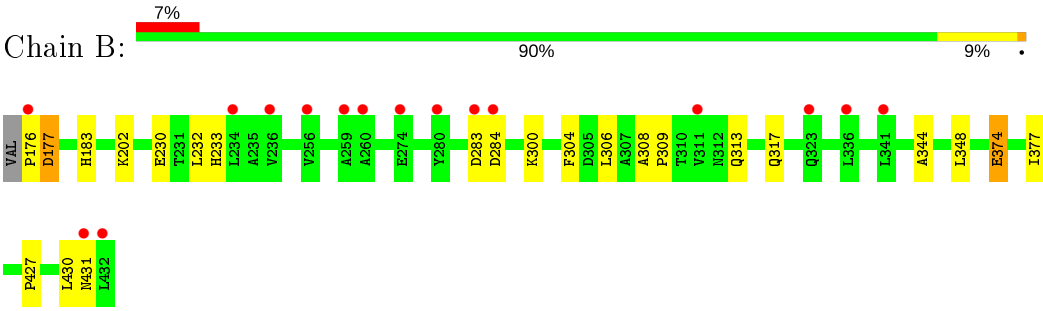
- Molecule 1: Cyclin-dependent kinase 2

Chain C:



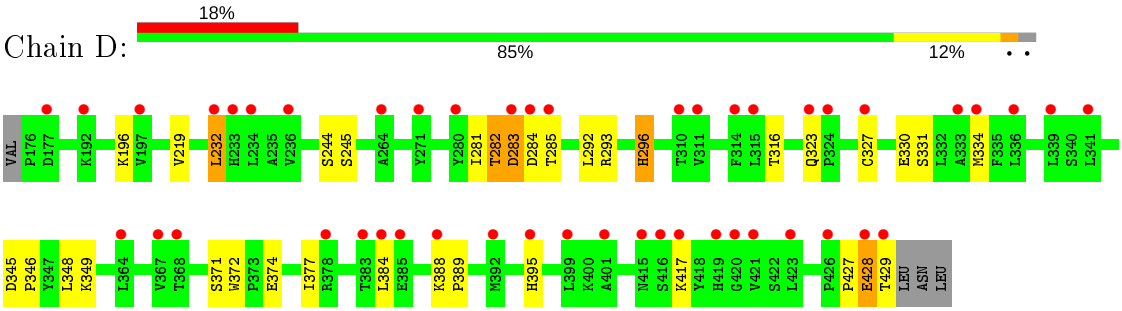
- Molecule 2: Cyclin-A2

Chain B:



- Molecule 2: Cyclin-A2

Chain D:


18%
85%
12%
VAL P176 D177 K192 K196 V197 V219 L232 H233 L234 A235 V236 S244 S245 A264 Y271 Y280 I281 T282 D283 D284 T285 L292 R293 H296 T310 V311 F314 L315 T316 Q323 P324 C327 E330 S331 L332 A333 M334 F335 L336 L339 S340 L341
D345 P346 Y347 L348 K349 L364 V367 T368 S371 W372 P373 E374 I377 R378 T383 L384 E385 K388 P389 M392 H395 L399 K400 A401 N415 S416 K417 Y418 H419 G420 V421 S422 L423 P426 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	74.02Å 134.04Å 149.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.10) 97.5 (29.91-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.208 , 0.243 0.218 , 0.251	Depositor DCC
R_{free} test set	4236 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8958	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, 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	0.68	0/2452	0.70	0/3323
1	C	0.49	0/2254	0.64	2/3050 (0.1%)
2	B	0.56	0/2126	0.64	0/2886
2	D	0.47	0/2113	0.60	0/2867
All	All	0.56	0/8945	0.65	2/12126 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	250	LYS	N-CA-CB	8.39	125.71	110.60
1	C	249	SER	N-CA-C	5.27	125.22	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ILE	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	2403	0	2436	42	0
1	C	2215	0	2266	31	0
2	B	2076	0	2099	15	0
2	D	2063	0	2083	18	0
3	A	31	4	12	3	0
3	C	31	4	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	65	0	0	4	1
5	B	41	0	0	2	0
5	C	16	0	0	2	0
5	D	6	0	0	0	0
All	All	8950	8	8908	96	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 5.

All (96) 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:14:THR:C	1:A:16:GLY:HA2	1.64	1.18
1:A:9:LYS:HE3	1:A:12:GLU:HG3	1.30	1.07
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.02	0.95
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.87	0.91
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.87	0.91
1:A:161[B]:HIS:O	1:A:162:GLU:O	1.91	0.88
2:D:293[B]:ARG:HB3	2:D:293[B]:ARG:HH21	1.40	0.87
1:A:177:CYS:HB2	1:A:233:MET:CE	2.07	0.85
1:A:60:HIS:HD2	1:A:62:ASN:H	1.31	0.79
1:A:284:PRO:O	1:A:287:GLN:HG2	1.86	0.76
1:A:9:LYS:HE3	1:A:12:GLU:CG	2.14	0.75
1:A:15:TYR:N	1:A:16:GLY:HA2	2.03	0.73
1:A:14:THR:C	1:A:16:GLY:CA	2.54	0.71
1:A:60:HIS:CD2	1:A:62:ASN:H	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLY:HA2	1:C:199:ARG:HD3	1.76	0.68
1:A:129:LYS:NZ	1:A:165:THR:HG21	2.08	0.68
1:A:15:TYR:N	1:A:16:GLY:CA	2.58	0.66
1:A:14:THR:CA	1:A:16:GLY:HA2	2.25	0.66
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.72	0.65
1:A:71:HIS:CE1	2:B:300:LYS:HE3	2.32	0.65
1:A:12:GLU:HG2	1:A:17:VAL:HG12	1.79	0.64
1:A:14:THR:O	1:A:15:TYR:HB2	1.97	0.64
1:C:129:LYS:NZ	1:C:165:THR:HG21	2.12	0.64
1:A:71:HIS:CD2	2:B:304:PHE:HE2	2.18	0.62
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.35	0.62
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.35	0.61
1:A:177:CYS:HB2	1:A:233:MET:HE2	1.81	0.61
1:A:260:ARG:HD3	5:A:435:HOH:O	2.00	0.61
1:C:60:HIS:HD2	1:C:62:ASN:H	1.49	0.60
1:A:15:TYR:HB3	1:A:35:ILE:HA	1.85	0.59
1:A:13:GLY:HA3	3:A:301:ATP:O2B	2.02	0.59
1:A:145:ASP:OD2	3:A:301:ATP:O1B	2.22	0.58
1:C:60:HIS:CD2	1:C:62:ASN:H	2.23	0.57
2:B:233:HIS:HE1	5:B:504:HOH:O	1.87	0.56
1:C:88:LYS:HA	1:C:91:MET:HE2	1.87	0.56
2:D:346:PRO:O	2:D:349:LYS:HG2	2.06	0.56
1:C:250:LYS:HG3	1:C:251:VAL:HG23	1.87	0.56
1:C:218:THR:HG23	1:C:250:LYS:HD3	1.89	0.55
2:D:282:THR:O	2:D:283:ASP:HB2	2.07	0.55
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.88	0.55
1:A:223:ASP:OD1	1:A:226:VAL:HG12	2.07	0.54
1:C:251:VAL:HG21	1:C:263:LEU:HD21	1.89	0.54
1:A:162:GLU:O	1:A:163:VAL:HG22	2.09	0.53
1:A:14:THR:OG1	1:A:15:TYR:N	2.43	0.52
1:C:155:PRO:HD2	2:D:316:THR:HB	1.91	0.52
2:D:293[B]:ARG:CB	2:D:293[B]:ARG:HH21	2.19	0.52
2:D:395:HIS:HE1	2:D:427:PRO:O	1.93	0.51
1:A:14:THR:O	1:A:16:GLY:HA2	2.05	0.51
2:B:430:LEU:O	2:B:431:ASN:HB2	2.10	0.51
2:D:196:LYS:HD3	2:D:244:SER:HB3	1.93	0.51
2:B:230:GLU:OE2	2:B:313:GLN:NE2	2.43	0.51
2:B:202:LYS:HE3	1:C:65:LYS:NZ	2.26	0.50
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.94	0.50
1:C:163:VAL:HG23	1:C:164:VAL:HG23	1.94	0.50
1:A:14:THR:O	1:A:15:TYR:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:ND1	2:B:300:LYS:HE3	2.28	0.48
2:B:176:PRO:HA	5:B:501:HOH:O	2.13	0.48
1:C:34:LYS:HD3	1:C:75:LYS:HD2	1.95	0.48
1:A:157:ARG:HB2	5:A:447:HOH:O	2.14	0.47
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.96	0.47
1:C:129:LYS:HZ3	1:C:165:THR:HG21	1.80	0.47
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.80	0.46
1:A:13:GLY:HA3	3:A:301:ATP:PB	2.56	0.46
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.99	0.46
1:C:20:LYS:HE3	1:C:29:VAL:HG11	1.98	0.46
1:A:129:LYS:HZ3	1:A:165:THR:HG21	1.81	0.45
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.98	0.45
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.85	0.45
1:A:161[B]:HIS:HE1	1:A:173:ILE:O	2.00	0.44
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.52	0.44
2:B:395:HIS:HE1	2:B:427:PRO:O	2.01	0.44
1:A:268:HIS:HD2	5:A:453:HOH:O	1.99	0.44
2:D:374:GLU:HA	2:D:377:ILE:HD12	2.00	0.44
1:C:47:THR:HG23	5:C:416:HOH:O	2.18	0.44
1:A:127:ASP:OD1	1:A:165:THR:CG2	2.66	0.43
1:C:250:LYS:HG3	1:C:251:VAL:H	1.83	0.43
1:A:161[B]:HIS:O	1:A:162:GLU:C	2.55	0.43
1:C:218:THR:HG22	1:C:219:LEU:HD23	2.00	0.43
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.99	0.43
1:A:129:LYS:HZ2	1:A:165:THR:HG21	1.81	0.43
1:C:250:LYS:HG3	1:C:251:VAL:N	2.34	0.43
2:D:371:SER:O	2:D:372:TRP:C	2.57	0.43
1:C:98:GLY:HA2	1:C:199:ARG:CD	2.47	0.42
1:A:73:GLU:H	1:A:73:GLU:CD	2.22	0.42
1:A:60:HIS:HE1	5:A:411:HOH:O	2.02	0.42
2:D:345:ASP:HA	2:D:346:PRO:HA	1.81	0.42
1:C:119:HIS:HD2	5:C:415:HOH:O	2.03	0.41
1:C:51:GLU:O	1:C:55:LEU:HB2	2.20	0.41
2:D:330:GLU:O	2:D:334:MET:HG3	2.20	0.41
2:B:374:GLU:HA	2:B:377:ILE:HD12	2.02	0.41
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.90	0.41
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.97	0.41
1:C:249:SER:HA	1:C:250:LYS:C	2.40	0.41
2:D:428:GLU:O	2:D:429:THR:C	2.60	0.40
2:B:176:PRO:HB2	2:B:177:ASP:H	1.62	0.40
1:C:101:LEU:HD12	1:C:254:PRO:HG2	2.03	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)
5:A:462:HOH:O	5:A:463:HOH:O[4_545]	1.57	0.63

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	295/301 (98%)	281 (95%)	10 (3%)	4 (1%)	11 6
1	C	272/301 (90%)	253 (93%)	17 (6%)	2 (1%)	22 18
2	B	255/258 (99%)	250 (98%)	5 (2%)	0	100 100
2	D	253/258 (98%)	247 (98%)	5 (2%)	1 (0%)	34 32
All	All	1075/1118 (96%)	1031 (96%)	37 (3%)	7 (1%)	22 18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	A	163	VAL
1	A	164	VAL
1	C	164	VAL
2	D	283	ASP
1	C	253	PRO
1	A	16	GLY

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	261/264 (99%)	253 (97%)	8 (3%)	40 43
1	C	242/264 (92%)	225 (93%)	17 (7%)	15 12
2	B	231/232 (100%)	226 (98%)	5 (2%)	52 57
2	D	229/232 (99%)	214 (93%)	15 (7%)	16 14
All	All	963/992 (97%)	918 (95%)	45 (5%)	26 25

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	55	LEU
1	A	73	GLU
1	A	122	ARG
1	A	150	ARG
1	A	165	THR
1	A	178	LYS
1	A	255	LEU
2	B	177	ASP
2	B	232	LEU
2	B	283	ASP
2	B	284	ASP
2	B	374	GLU
1	C	-2	LEU
1	C	9	LYS
1	C	17	VAL
1	C	37	LEU
1	C	55	LEU
1	C	84	SER
1	C	103	LEU
1	C	122	ARG
1	C	150	ARG
1	C	202	LEU
1	C	217	ARG
1	C	246	GLN
1	C	250	LYS
1	C	252	VAL
1	C	256	ASP
1	C	273	LYS
1	C	281	LEU
2	D	232	LEU

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Mol	Chain	Res	Type
2	D	245	SER
2	D	281	ILE
2	D	282	THR
2	D	284	ASP
2	D	285	THR
2	D	292	LEU
2	D	296	HIS
2	D	323	GLN
2	D	327	CYS
2	D	331	SER
2	D	348	LEU
2	D	384	LEU
2	D	417	LYS
2	D	428	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	119	HIS
1	C	246	GLN
2	D	254	GLN
2	D	296	HIS
2	D	323	GLN
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 (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	1.01	0	10,14,16	1.02	0
1	TPO	C	160	1	8,10,11	0.85	0	10,14,16	0.91	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	-

There are no bond length outliers.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	C	301	4	26,33,33	1.03	2 (7%)	31,52,52	1.25	3 (9%)
3	ATP	A	301	4	26,33,33	1.01	2 (7%)	31,52,52	1.36	5 (16%)

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
3	ATP	C	301	4	-	2/18/38/38	0/3/3/3
3	ATP	A	301	4	-	1/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	ATP	C5-C4	2.81	1.48	1.40
3	A	301	ATP	C5-C4	2.76	1.48	1.40
3	C	301	ATP	C2-N3	2.22	1.35	1.32
3	A	301	ATP	O4'-C1'	2.02	1.43	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	ATP	C4-C5-N7	-3.18	106.09	109.40
3	A	301	ATP	N3-C2-N1	-3.12	123.81	128.68
3	C	301	ATP	N3-C2-N1	-3.03	123.94	128.68
3	A	301	ATP	C3'-C2'-C1'	2.57	104.85	100.98
3	A	301	ATP	PB-O3B-PG	-2.48	124.32	132.83
3	C	301	ATP	C4-C5-N7	-2.07	107.24	109.40
3	A	301	ATP	PA-O3A-PB	-2.04	125.81	132.83
3	C	301	ATP	C3'-C2'-C1'	2.03	104.03	100.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	ATP	O4'-C4'-C5'-O5'
3	C	301	ATP	C3'-C4'-C5'-O5'
3	A	301	ATP	PG-O3B-PB-O2B

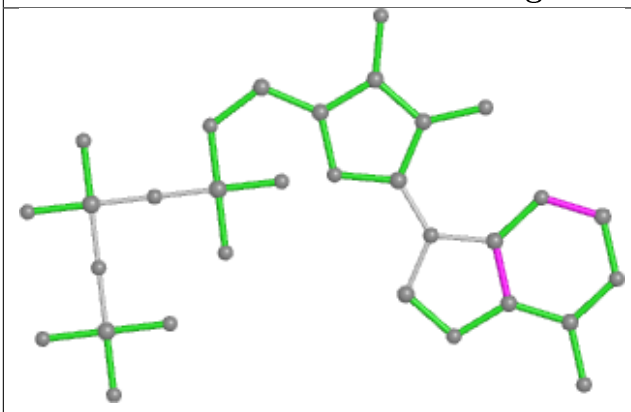
There are no ring outliers.

1 monomer is involved in 3 short contacts:

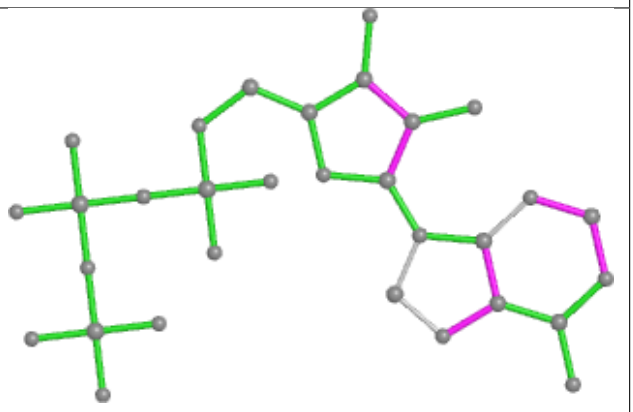
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	ATP	3	0

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.

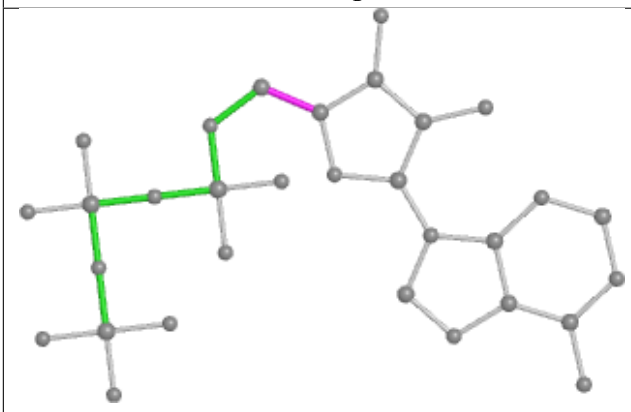
Ligand ATP C 301



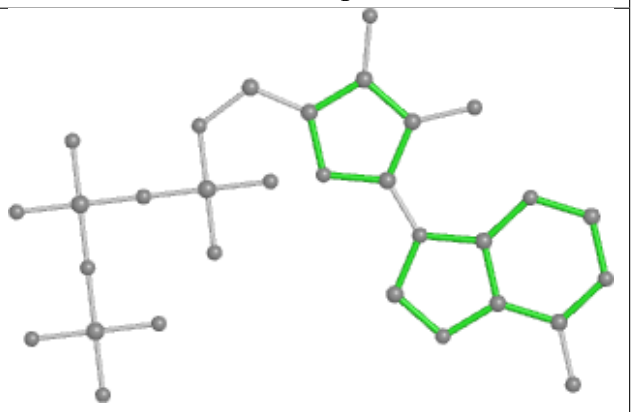
Bond lengths



Bond angles

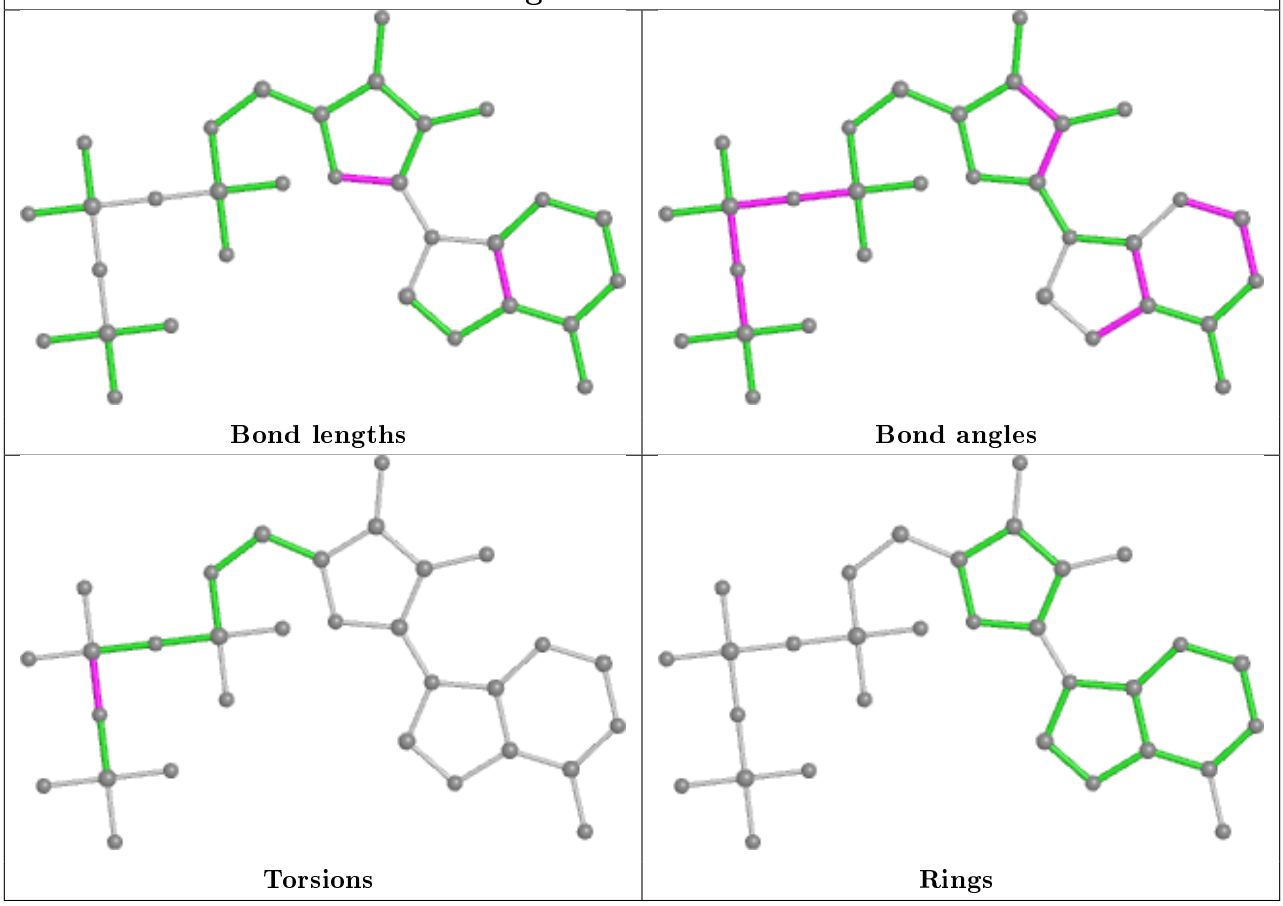


Torsions



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	296/301 (98%)	0.45	24 (8%) 12 15	17, 30, 61, 72	0
1	C	275/301 (91%)	1.21	56 (20%) 1 1	32, 51, 82, 115	0
2	B	257/258 (99%)	0.46	17 (6%) 18 23	17, 33, 51, 66	0
2	D	254/258 (98%)	0.95	47 (18%) 1 1	29, 54, 94, 111	0
All	All	1082/1118 (96%)	0.76	144 (13%) 3 4	17, 41, 82, 115	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	TYR	8.6
1	C	296	LEU	7.8
1	C	253	PRO	7.6
1	A	96	LEU	7.0
2	D	423	LEU	7.0
1	C	254	PRO	6.7
2	B	432	LEU	6.7
1	C	273	LYS	6.6
1	C	189	LEU	6.5
1	A	15	TYR	6.1
1	C	295[A]	HIS	6.1
1	C	220	GLY	5.9
1	C	14	THR	5.5
1	C	13	GLY	5.2
1	C	247	ASP	5.1
1	A	12	GLU	4.9
1	C	12	GLU	4.8
1	C	248	PHE	4.8
1	C	250	LYS	4.8
2	D	378	ARG	4.6
1	C	17	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	287	GLN	4.5
2	D	336	LEU	4.4
2	B	431	ASN	4.4
2	D	419	HIS	4.3
1	C	192	ILE	4.3
1	C	252	VAL	4.3
1	C	246	GLN	4.2
1	C	288	ASP	4.2
2	D	283	ASP	4.2
2	B	323	GLN	4.1
1	C	186	ILE	4.1
1	C	256	ASP	4.1
2	B	176	PRO	4.1
1	C	221	THR	4.0
2	D	284	ASP	4.0
1	A	95	ALA	4.0
2	B	283	ASP	3.9
1	C	111	LEU	3.9
2	D	315	LEU	3.9
1	C	258	ASP	3.8
2	D	392	MET	3.8
1	C	175	LEU	3.8
1	C	249	SER	3.8
1	C	128	LEU	3.8
1	C	97	THR	3.7
2	D	323	GLN	3.7
1	A	36	ARG	3.7
2	D	311	VAL	3.7
1	A	97	THR	3.6
1	A	162	GLU	3.6
1	A	73	GLU	3.6
2	D	415	ASN	3.5
2	D	327	CYS	3.5
2	D	420	GLY	3.5
1	C	108	LEU	3.3
2	D	384	LEU	3.2
2	D	197	VAL	3.2
2	D	416	SER	3.2
2	B	284	ASP	3.2
2	D	399	LEU	3.2
1	C	293	VAL	3.2
1	C	36	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	13	GLY	3.1
2	D	401	ALA	3.1
2	B	341	LEU	3.0
1	C	19	TYR	3.0
2	D	280	TYR	3.0
1	C	260	ARG	2.9
1	C	162	GLU	2.9
1	C	179	TYR	2.9
1	C	7	VAL	2.9
1	C	188	SER	2.9
2	D	232	LEU	2.9
1	C	138	GLU	2.9
1	C	-3	PRO	2.9
1	C	177	CYS	2.8
1	A	41	THR	2.8
2	D	285	THR	2.8
2	D	417	LYS	2.8
1	C	143	LEU	2.8
1	A	112	LEU	2.7
2	D	333	ALA	2.7
1	C	161	HIS	2.7
1	A	19	TYR	2.7
2	D	429	THR	2.7
1	C	269	TYR	2.7
1	C	206	ASP	2.7
1	C	178	LYS	2.7
2	B	311	VAL	2.6
1	C	190	GLY	2.6
1	C	112	LEU	2.6
2	D	341	LEU	2.6
2	D	395	HIS	2.5
1	C	187	TRP	2.5
1	A	111	LEU	2.5
2	D	233	HIS	2.5
1	C	133	LEU	2.5
2	B	403	GLN	2.5
2	D	368	THR	2.5
2	D	421	VAL	2.5
2	B	280	TYR	2.5
2	D	385	GLU	2.5
2	D	428	GLU	2.5
1	A	37	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	17	VAL	2.4
1	A	74	ASN	2.4
2	D	264	ALA	2.4
2	D	388	LYS	2.4
2	D	192	LYS	2.3
2	B	274	GLU	2.3
1	C	191	CYS	2.3
2	D	334	MET	2.3
1	C	115	LEU	2.2
2	B	260	ALA	2.2
2	D	234	LEU	2.2
2	D	314	PHE	2.2
1	A	187	TRP	2.2
1	C	9	LYS	2.2
2	D	339	LEU	2.2
2	B	256	VAL	2.2
2	D	367	VAL	2.2
1	A	14	THR	2.2
1	A	189	LEU	2.2
1	C	257	GLU	2.2
2	D	310	THR	2.2
2	D	383	THR	2.2
1	A	16	GLY	2.2
2	B	336	LEU	2.2
2	D	324	PRO	2.2
2	D	426	PRO	2.2
2	D	271	TYR	2.2
1	A	206[A]	ASP	2.2
2	B	259	ALA	2.2
2	B	234	LEU	2.1
1	A	161[A]	HIS	2.1
2	B	236	VAL	2.1
1	C	268	HIS	2.1
2	D	177	ASP	2.1
1	A	297	ARG	2.1
2	D	236	VAL	2.1
2	D	364	LEU	2.0
1	C	165	THR	2.0
1	A	287	GLN	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	0.96	0.13	35,40,42,44	0
1	TPO	A	160	11/12	0.99	0.10	22,23,25,27	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

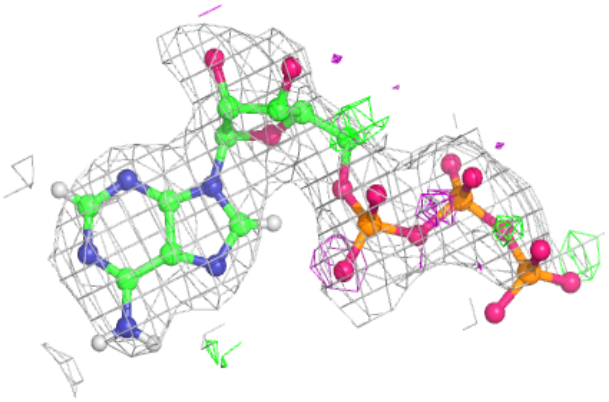
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

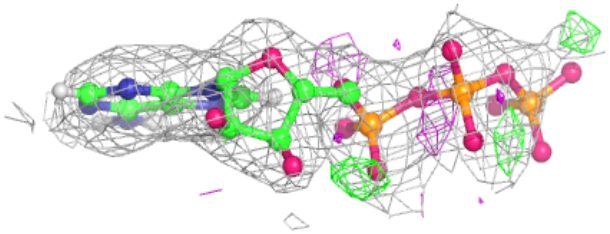
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	302	1/1	0.81	0.09	38,38,38,38	0
4	MG	D	501	1/1	0.82	0.09	51,51,51,51	0
4	MG	C	302	1/1	0.83	0.09	62,62,62,62	0
3	ATP	C	301	31/31	0.92	0.13	45,55,67,68	4
3	ATP	A	301	31/31	0.94	0.11	36,39,52,52	4

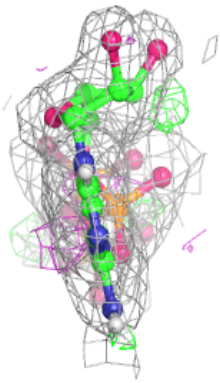
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

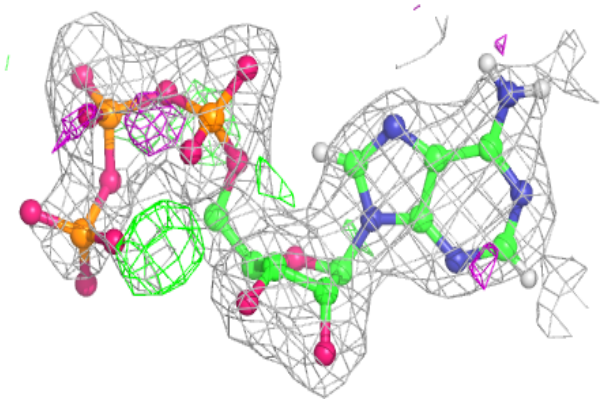


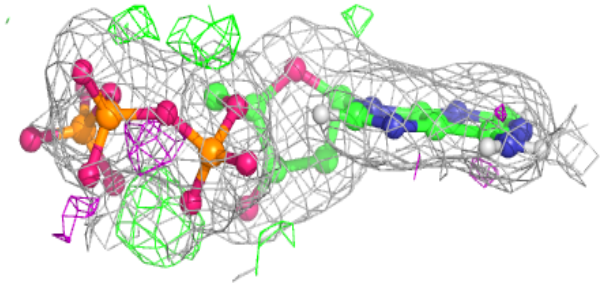


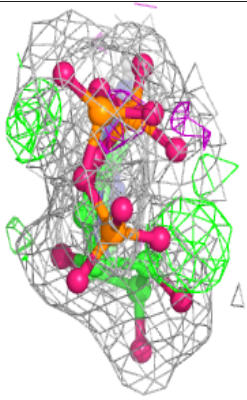


Electron density around ATP A 301:

$2mF_o$-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.