



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:24 PM UTC

PDB ID : 4EEO / pdb_00004eoo
Title : Thr 160 phosphorylated CDK2 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

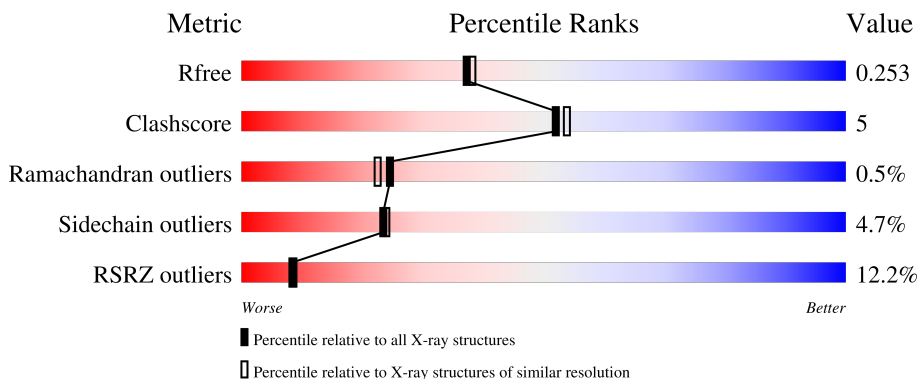
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	299	 7% 83% 15% ..
1	C	299	 22% 82% 15% .
2	B	258	 5% 86% 12% .
2	D	258	 13% 84% 12% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9456 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	295	Total	C	N	O	P	S	0	3	0
			2398	1555	410	424	1	8			
1	C	298	Total	C	N	O	P	S	0	1	0
			2402	1558	407	428	1	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
A	131	GLU	GLN	engineered mutation	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	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
			Total	C	N	O	S			
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	254	Total	C	N	O	S	0	1	0
			2063	1335	338	379	11			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued from previous page...

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

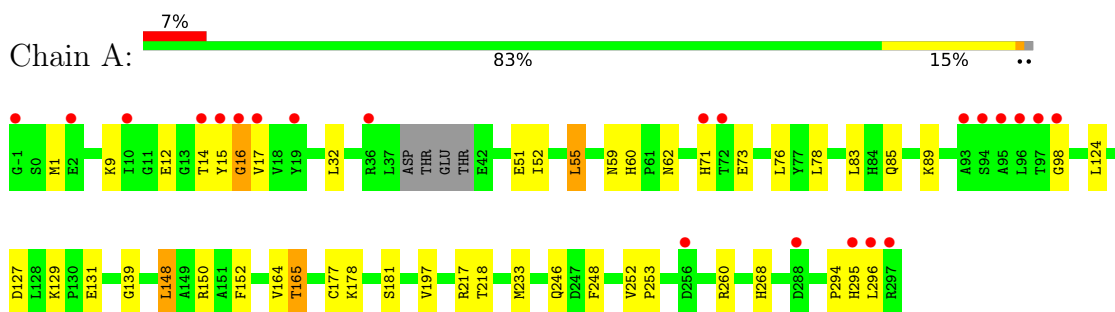
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	154	Total 154	O 154	0	0
6	B	118	Total 118	O 118	0	0
6	C	82	Total 82	O 82	0	0
6	D	79	Total 79	O 79	0	0

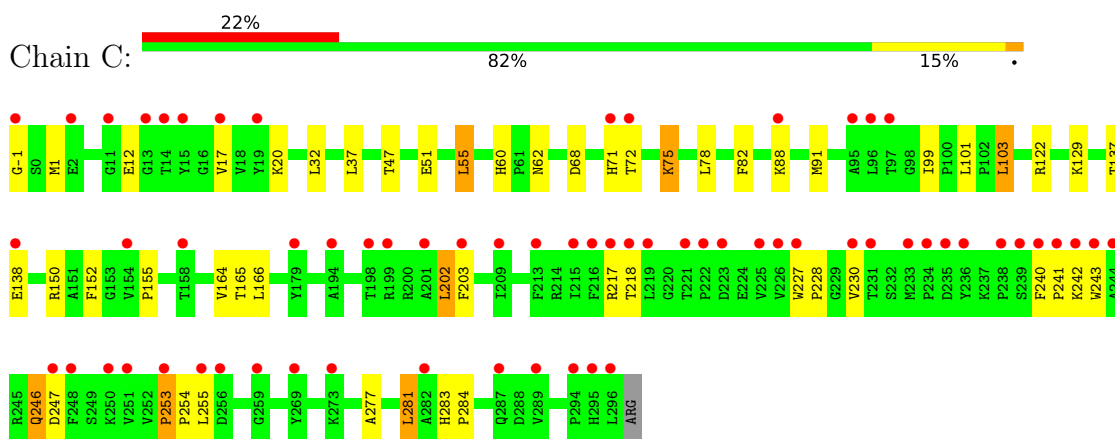
3 Residue-property plots [i](#)

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.

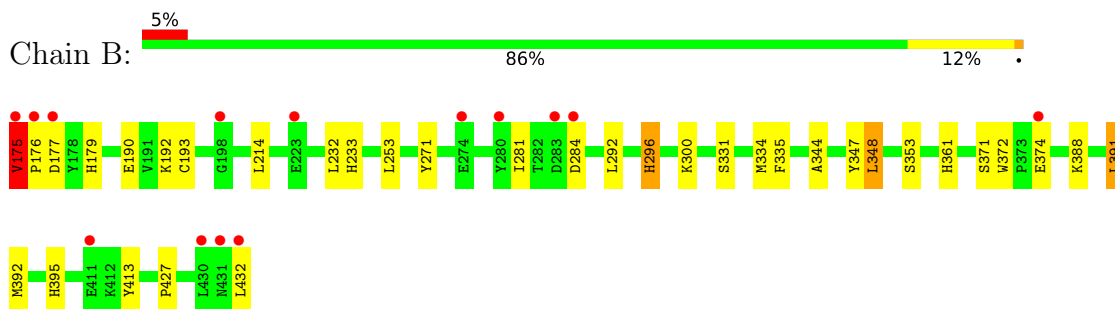
- Molecule 1: Cyclin-dependent kinase 2




- Molecule 1: Cyclin-dependent kinase 2

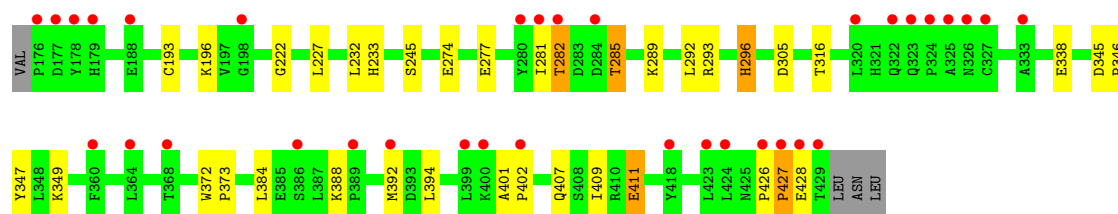


- Molecule 2: Cyclin-A2



- Molecule 2: Cyclin-A2

Chain D:  13% 84% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.11Å 134.49Å 148.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.10 29.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.79-2.10) 98.5 (29.79-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.253 0.214 , 0.253	Depositor DCC
R_{free} test set	4381 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9456	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SGM, 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	0.72	0/2448	0.86	2/3318 (0.1%)
1	C	0.65	0/2453	0.83	2/3328 (0.1%)
2	B	0.67	0/2133	0.88	5/2897 (0.2%)
2	D	0.62	0/2113	0.81	1/2867 (0.0%)
All	All	0.67	0/9147	0.84	10/12410 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	VAL	CA-C-N	-7.81	111.36	120.11
2	B	175	VAL	C-N-CA	-7.81	111.36	120.11
1	A	98	GLY	N-CA-C	6.34	123.83	112.22
2	B	271	TYR	CA-C-N	-6.01	115.33	119.66
2	B	271	TYR	C-N-CA	-6.01	115.33	119.66
2	D	285	THR	N-CA-C	5.42	117.62	111.11
1	C	166	LEU	N-CA-C	5.39	117.57	111.11
2	B	347	TYR	N-CA-C	5.13	118.80	112.54
1	A	253	PRO	N-CA-C	5.08	116.90	110.70
1	C	253	PRO	N-CA-C	5.02	116.83	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2398	0	2433	31	1
1	C	2402	0	2437	28	0
2	B	2083	0	2107	19	0
2	D	2063	0	2083	21	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	31	0	12	2	0
4	C	31	0	12	0	0
5	B	6	0	8	2	0
5	D	6	0	8	2	0
6	A	154	0	0	7	1
6	B	118	0	0	1	0
6	C	82	0	0	1	0
6	D	79	0	0	1	0
All	All	9456	0	9100	93	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 (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:CYS:SG	5:B:502:SGM:S1	2.34	0.87
2:B:176:PRO:HD2	2:B:179:HIS:CE1	2.13	0.84
2:D:274:GLU:HG2	2:D:277:GLU:HG3	1.62	0.82
1:C:71:HIS:HD2	2:D:296:HIS:CE1	2.03	0.76
1:A:148:LEU:HG	6:A:422:HOH:O	1.84	0.76
1:A:15:TYR:N	1:A:16:GLY:HA3	2.01	0.76
2:D:193:CYS:SG	5:D:501:SGM:S1	2.64	0.74
1:A:60:HIS:HD2	1:A:62:ASN:H	1.37	0.70
1:C:60:HIS:HD2	1:C:62:ASN:H	1.37	0.70
1:C:218:THR:HA	1:C:246:GLN:NE2	2.08	0.69
1:A:60:HIS:CD2	1:A:62:ASN:H	2.10	0.69
1:C:60:HIS:CD2	1:C:62:ASN:H	2.11	0.68
2:B:175:VAL:HB	2:B:176:PRO:CD	2.25	0.67
2:D:407:GLN:O	2:D:411:GLU:HG2	1.97	0.65
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.66	0.64
2:B:175:VAL:HB	2:B:176:PRO:HD2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:N	1:A:16:GLY:CA	2.63	0.61
2:B:176:PRO:HD2	2:B:179:HIS:NE2	2.16	0.61
1:A:127:ASP:OD1	1:A:165:THR:HG23	2.02	0.60
1:C:227:TRP:O	1:C:230:VAL:HG23	2.01	0.60
1:A:252:VAL:HB	6:A:408:HOH:O	2.01	0.59
1:A:260:ARG:HD3	6:A:409:HOH:O	2.01	0.59
1:C:51:GLU:O	1:C:55:LEU:HB2	2.02	0.59
1:A:268:HIS:HD2	6:A:519:HOH:O	1.85	0.58
1:A:15:TYR:H	1:A:16:GLY:HA3	1.68	0.58
1:C:72:THR:HB	1:C:75:LYS:H	1.69	0.57
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.86	0.57
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.87	0.56
1:C:88:LYS:HA	1:C:91:MET:HE2	1.88	0.56
1:A:15:TYR:H	1:A:16:GLY:CA	2.19	0.55
1:A:129:LYS:NZ	1:A:165:THR:HG21	2.22	0.55
2:B:233:HIS:HE1	6:B:651:HOH:O	1.88	0.55
1:A:83:LEU:O	4:A:302:ATP:H2	1.90	0.54
1:A:85:GLN:HG3	1:A:89:LYS:HE3	1.91	0.53
1:A:177:CYS:HB2	1:A:233:MET:CE	2.37	0.53
1:A:131:GLU:HG3	6:A:550:HOH:O	2.08	0.52
1:A:9:LYS:NZ	1:A:12:GLU:OE2	2.41	0.52
1:A:218:THR:HA	1:A:246:GLN:HE21	1.74	0.52
1:C:47:THR:HG23	6:C:467:HOH:O	2.10	0.52
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.92	0.52
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.46	0.51
1:C:129:LYS:NZ	1:C:165:THR:HG21	2.26	0.51
1:A:268:HIS:CE1	6:A:476:HOH:O	2.63	0.50
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.42	0.50
1:C:241:PRO:HB2	1:C:243:TRP:NE1	2.26	0.50
1:C:-1:GLY:HA3	1:C:68:ASP:OD2	2.11	0.50
2:D:289:LYS:O	2:D:293[B]:ARG:HG3	2.12	0.50
1:A:181:SER:HB3	6:A:489:HOH:O	2.11	0.49
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.58	0.49
4:A:302:ATP:O3B	4:A:302:ATP:H5'2	2.12	0.49
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.49	0.48
1:A:9:LYS:HE2	1:A:12:GLU:HG3	1.96	0.48
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.49	0.47
2:B:176:PRO:HB2	2:B:177:ASP:O	2.14	0.47
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.97	0.46
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.94	0.46
2:D:347:TYR:OH	2:D:394:LEU:HA	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ALA:O	1:C:281:LEU:HD22	2.16	0.45
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.51	0.45
1:A:1:MET:HE1	1:A:32:LEU:HD13	1.98	0.45
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.51	0.45
2:B:388:LYS:O	2:B:392:MET:HG2	2.17	0.44
1:C:12:GLU:HA	1:C:17:VAL:HG12	1.99	0.44
1:C:253:PRO:HG2	1:C:254:PRO:HD3	2.00	0.44
1:C:71:HIS:CD2	2:D:296:HIS:HE1	2.35	0.43
2:B:371:SER:O	2:B:372:TRP:C	2.61	0.43
2:D:372:TRP:HA	2:D:373:PRO:HD3	1.86	0.43
2:D:345:ASP:HA	2:D:346:PRO:HA	1.85	0.43
1:C:155:PRO:HD2	2:D:316:THR:HB	2.01	0.43
1:A:51:GLU:O	1:A:55:LEU:HB2	2.19	0.43
2:B:331:SER:HA	2:B:334:MET:HE3	2.01	0.43
2:D:282:THR:O	2:D:282:THR:OG1	2.35	0.43
1:C:217:ARG:O	1:C:246:GLN:NE2	2.37	0.42
2:D:426:PRO:HA	2:D:427:PRO:HD3	1.86	0.42
2:B:395:HIS:HE1	2:B:427:PRO:O	2.03	0.42
1:C:240:PHE:HA	1:C:241:PRO:HD3	1.92	0.42
1:C:99:ILE:HG23	1:C:103:LEU:HD12	2.03	0.41
2:D:233:HIS:HE1	6:D:644:HOH:O	2.03	0.41
2:D:338:GLU:HG2	2:D:409:ILE:HD13	2.03	0.41
1:C:1:MET:HE1	1:C:32:LEU:HD13	2.03	0.41
1:C:20:LYS:HE3	1:C:82:PHE:CZ	2.56	0.41
1:C:129:LYS:HZ2	1:C:165:THR:HG21	1.85	0.41
2:D:305:ASP:HB3	5:D:501:SGM:H12	2.03	0.41
2:D:388:LYS:O	2:D:392:MET:HG2	2.21	0.41
1:A:71:HIS:HD1	2:B:300:LYS:HG3	1.86	0.41
2:B:190:GLU:OE2	2:B:353:SER:OG	2.37	0.40
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.56	0.40
1:C:283:HIS:HA	1:C:284:PRO:HD2	1.91	0.40
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.03	0.40
1:A:139:GLY:HA2	1:A:294:PRO:HD3	2.03	0.40
2:B:192:LYS:HB3	5:B:502:SGM:H31	2.04	0.40
1:A:295:HIS:CD2	1:A:296:LEU:HG	2.57	0.40
2:D:346:PRO:O	2:D:349:LYS:HG2	2.22	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:516:HOH:O[4_445]	2.06	0.14

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	293/299 (98%)	279 (95%)	12 (4%)	2 (1%)	18	15
1	C	296/299 (99%)	283 (96%)	11 (4%)	2 (1%)	18	15
2	B	256/258 (99%)	252 (98%)	4 (2%)	0	100	100
2	D	253/258 (98%)	246 (97%)	6 (2%)	1 (0%)	30	28
All	All	1098/1114 (99%)	1060 (96%)	33 (3%)	5 (0%)	24	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	A	164	VAL
1	A	16	GLY
2	D	427	PRO
1	C	228	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	261/262 (100%)	250 (96%)	11 (4%)	26	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	262/262 (100%)	247 (94%)	15 (6%)	18	17
2	B	232/232 (100%)	222 (96%)	10 (4%)	26	27
2	D	229/232 (99%)	218 (95%)	11 (5%)	23	23
All	All	984/988 (100%)	937 (95%)	47 (5%)	23	23

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	17	VAL
1	A	55	LEU
1	A	59[A]	ASN
1	A	59[B]	ASN
1	A	73	GLU
1	A	148	LEU
1	A	150	ARG
1	A	165	THR
1	A	178	LYS
1	A	248	PHE
2	B	175	VAL
2	B	232	LEU
2	B	281	ILE
2	B	284	ASP
2	B	292	LEU
2	B	296	HIS
2	B	348	LEU
2	B	374	GLU
2	B	391	LEU
2	B	432	LEU
1	C	37	LEU
1	C	55	LEU
1	C	75	LYS
1	C	78	LEU
1	C	101	LEU
1	C	103	LEU
1	C	137	THR
1	C	138	GLU
1	C	150	ARG
1	C	202	LEU
1	C	242	LYS
1	C	246	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	247	ASP
1	C	255	LEU
1	C	281	LEU
2	D	196	LYS
2	D	232	LEU
2	D	245	SER
2	D	281	ILE
2	D	282	THR
2	D	285	THR
2	D	292	LEU
2	D	296	HIS
2	D	384	LEU
2	D	411	GLU
2	D	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	246	GLN
1	A	265	GLN
2	B	254	GLN
2	B	296	HIS
2	B	395	HIS
1	C	59	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	85	GLN
2	D	179	HIS
2	D	228	GLN
2	D	254	GLN
2	D	296	HIS
2	D	419	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	C	160	1	8,10,11	0.81	0	10,14,16	1.10	0
1	TPO	A	160	1	8,10,11	0.92	0	10,14,16	1.11	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	-	0/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

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	A	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 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
4	ATP	C	301	3	32,33,33	1.66	7 (21%)	48,52,52	1.77	8 (16%)
5	SGM	D	501	-	5,5,5	0.41	0	5,5,5	0.40	0
5	SGM	B	502	-	5,5,5	0.47	0	5,5,5	0.39	0
4	ATP	A	302	3	32,33,33	1.62	7 (21%)	48,52,52	1.74	8 (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
4	ATP	C	301	3	-	2/22/38/38	0/3/3/3
5	SGM	D	501	-	-	1/4/4/4	-
5	SGM	B	502	-	-	2/4/4/4	-
4	ATP	A	302	3	-	0/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	ATP	C5-C4	4.93	1.47	1.39
4	A	302	ATP	C5-C4	4.75	1.47	1.39
4	C	301	ATP	PB-O3A	3.55	1.63	1.59
4	A	302	ATP	PB-O3A	3.49	1.63	1.59
4	C	301	ATP	PA-O3A	3.35	1.63	1.59
4	A	302	ATP	PA-O3A	3.10	1.62	1.59
4	A	302	ATP	C5-C6	2.78	1.48	1.41
4	C	301	ATP	C5-N7	-2.68	1.34	1.39
4	C	301	ATP	PB-O3B	2.67	1.62	1.59
4	A	302	ATP	PB-O3B	2.63	1.62	1.59
4	C	301	ATP	C5-C6	2.59	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	ATP	C5-N7	-2.32	1.34	1.39
4	C	301	ATP	C8-N7	2.24	1.36	1.31
4	A	302	ATP	C8-N7	2.01	1.35	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	ATP	C5-C4-N3	-6.17	118.22	126.72
4	A	302	ATP	C5-C4-N3	-5.67	118.91	126.72
4	C	301	ATP	N3-C4-N9	5.03	135.72	127.17
4	A	302	ATP	N3-C4-N9	4.54	134.90	127.17
4	C	301	ATP	C2-N3-C4	3.84	121.20	111.83
4	A	302	ATP	C2-N3-C4	3.63	120.70	111.83
4	C	301	ATP	N3-C2-N1	-3.44	123.38	128.58
4	A	302	ATP	C4-C5-N7	-3.38	106.72	110.58
4	A	302	ATP	N3-C2-N1	-3.19	123.75	128.58
4	A	302	ATP	C2'-C1'-N9	-3.16	105.44	113.30
4	C	301	ATP	C4-C5-N7	-3.09	107.05	110.58
4	A	302	ATP	C5-N7-C8	2.50	107.38	103.45
4	A	302	ATP	C4-N9-C8	2.48	108.34	105.74
4	C	301	ATP	C5-N7-C8	2.46	107.32	103.45
4	C	301	ATP	C2'-C1'-N9	-2.29	107.61	113.30
4	C	301	ATP	C4-N9-C8	2.22	108.07	105.74

There are no chirality outliers.

All (5) torsion outliers are listed below:

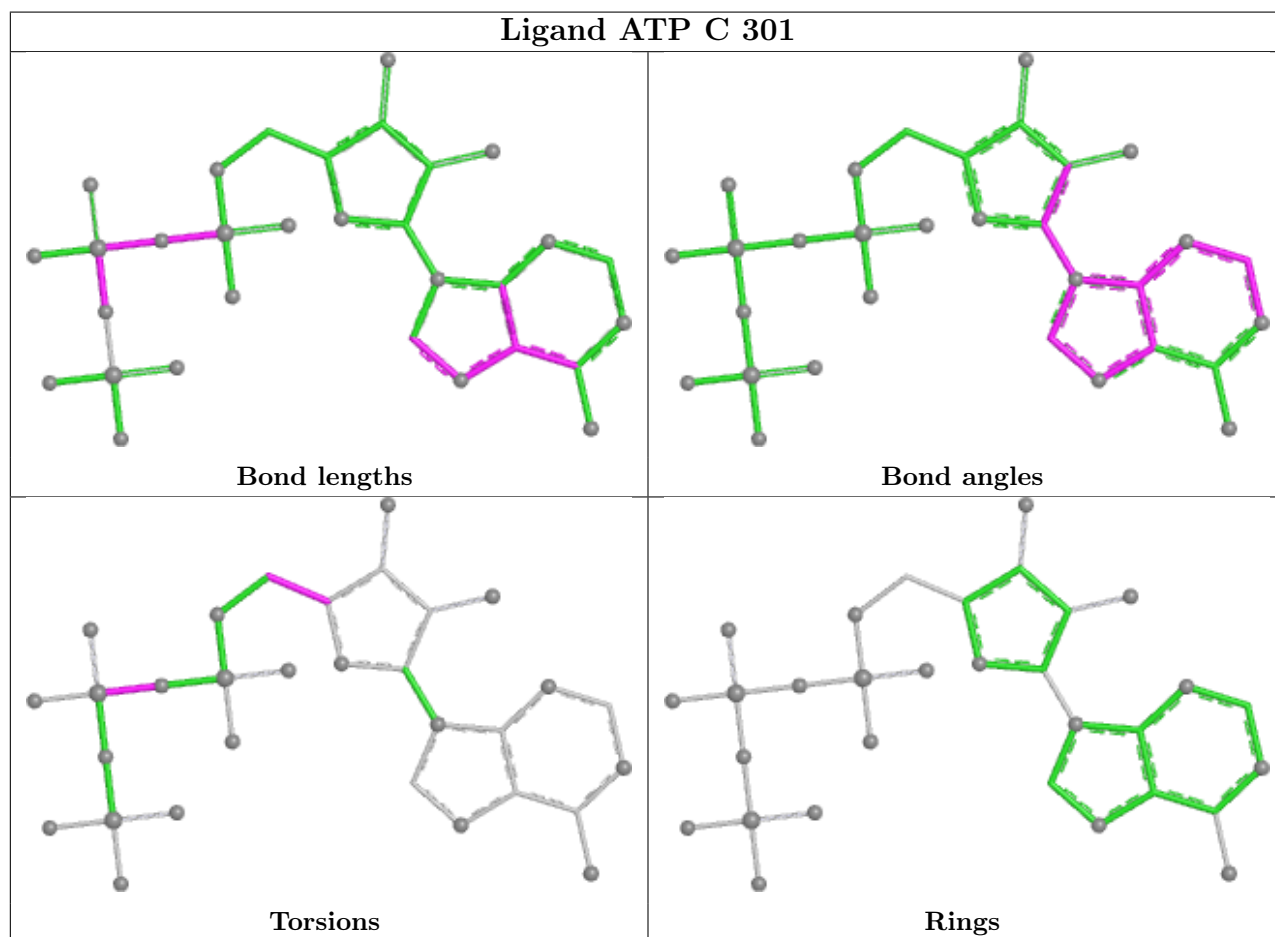
Mol	Chain	Res	Type	Atoms
5	B	502	SGM	S1-C1-C2-O2
4	C	301	ATP	PA-O3A-PB-O3B
5	B	502	SGM	O2-C2-C3-O3
5	D	501	SGM	S1-C1-C2-O2
4	C	301	ATP	O4'-C4'-C5'-O5'

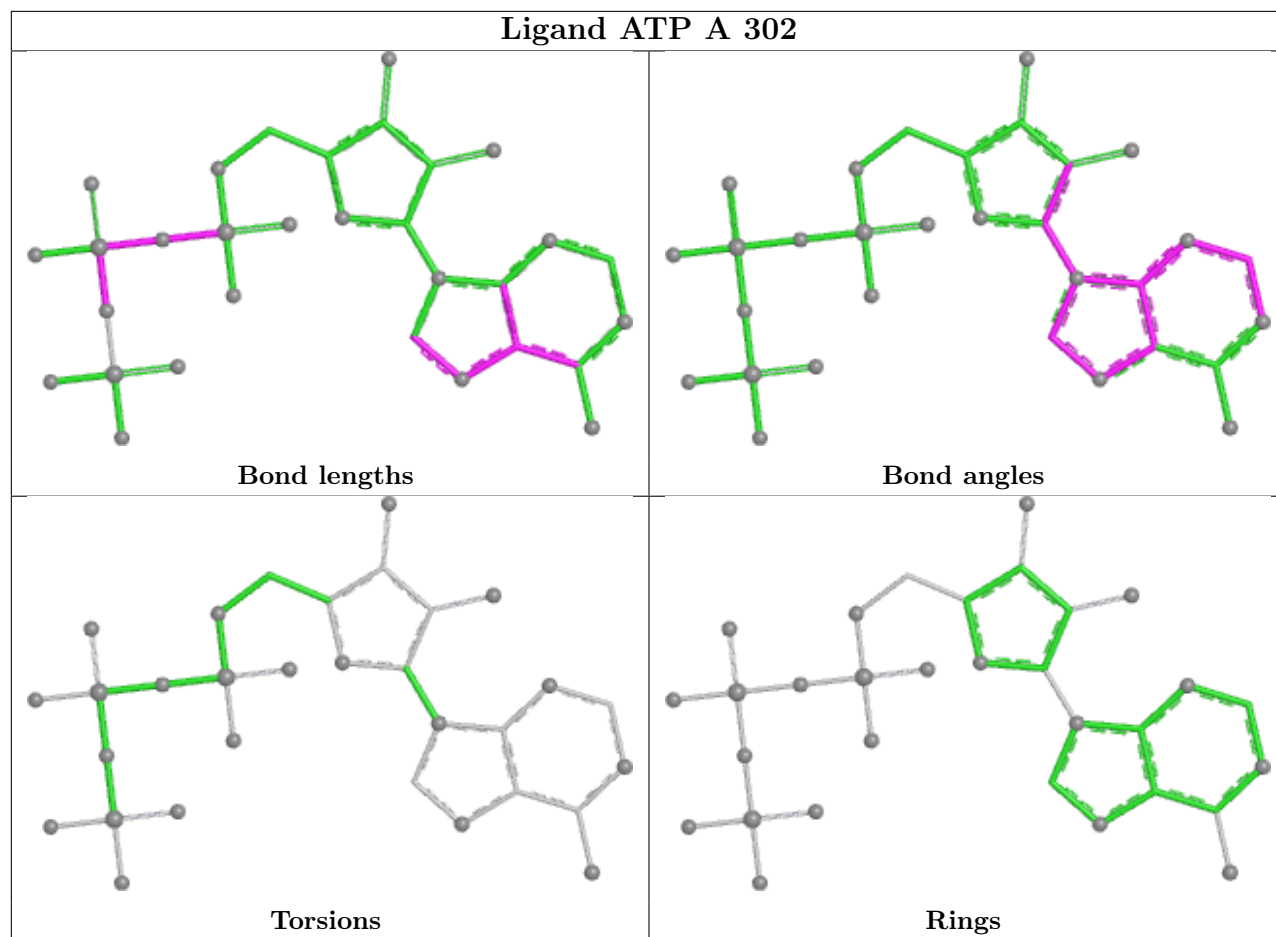
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	SGM	2	0
5	B	502	SGM	2	0
4	A	302	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	294/299 (98%)	0.18	22 (7%) 20 21	15, 28, 62, 80	3 (1%)
1	C	297/299 (99%)	1.20	65 (21%) 2 2	31, 53, 98, 116	1 (0%)
2	B	258/258 (100%)	0.22	14 (5%) 31 33	19, 32, 51, 78	0
2	D	254/258 (98%)	0.86	34 (13%) 7 7	18, 50, 82, 96	1 (0%)
All	All	1103/1114 (99%)	0.62	135 (12%) 8 8	15, 40, 81, 116	5 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	243	TRP	5.8
2	B	175	VAL	5.6
1	C	241	PRO	5.4
1	A	95	ALA	5.4
1	C	295[A]	HIS	5.4
1	C	256	ASP	5.0
1	A	96	LEU	5.0
2	D	428	GLU	4.8
1	C	213	PHE	4.6
1	C	226	VAL	4.6
2	D	429	THR	4.6
1	C	244	ALA	4.6
1	A	296	LEU	4.5
1	C	230	VAL	4.4
1	C	15	TYR	4.4
1	C	236	TYR	4.4
2	B	176	PRO	4.3
1	C	248	PHE	4.2
1	A	15	TYR	4.2
1	C	253	PRO	4.1
1	C	296	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	176	PRO	3.9
1	C	17	VAL	3.9
1	C	14	THR	3.8
1	A	295	HIS	3.8
1	C	234	PRO	3.6
1	C	227	TRP	3.5
2	D	423	LEU	3.5
1	C	-1	GLY	3.4
1	A	97	THR	3.4
2	D	399	LEU	3.3
2	D	392	MET	3.3
1	C	19	TYR	3.3
1	C	251	VAL	3.3
1	C	240	PHE	3.2
1	C	231	THR	3.2
1	C	209	ILE	3.1
1	C	235	ASP	3.1
1	A	71	HIS	3.1
1	C	259	GLY	3.0
2	D	326	ASN	3.0
2	D	402	PRO	3.0
1	C	2	GLU	2.9
1	C	96	LEU	2.9
1	C	287	GLN	2.9
1	C	194	ALA	2.9
1	C	282	ALA	2.9
2	B	432	LEU	2.9
1	C	233	MET	2.9
1	C	238	PRO	2.9
2	D	325	ALA	2.9
1	A	93	ALA	2.8
1	C	201	ALA	2.7
1	C	179	TYR	2.7
1	C	247	ASP	2.7
2	B	177	ASP	2.7
1	A	-1	GLY	2.7
2	D	426	PRO	2.7
2	D	418	TYR	2.6
1	C	88	LYS	2.6
1	A	16	GLY	2.6
1	C	11	GLY	2.6
2	D	178	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	97	THR	2.6
1	C	255	LEU	2.6
2	B	284	ASP	2.6
2	D	280	TYR	2.6
2	B	430	LEU	2.6
2	B	411	GLU	2.5
1	C	198	THR	2.5
2	D	177	ASP	2.5
2	D	320	LEU	2.5
1	A	36	ARG	2.5
2	D	284	ASP	2.5
2	D	179	HIS	2.5
2	B	431	ASN	2.5
1	A	256	ASP	2.5
2	D	323	GLN	2.5
1	C	222	PRO	2.5
1	C	225	VAL	2.4
1	A	288	ASP	2.4
2	B	283	ASP	2.4
1	C	203	PHE	2.4
1	A	2	GLU	2.4
2	B	280	TYR	2.4
1	C	218	THR	2.4
2	D	324	PRO	2.4
2	D	322	GLN	2.4
1	A	17	VAL	2.4
1	C	289	VAL	2.4
1	C	242	LYS	2.4
1	C	250	LYS	2.4
1	A	19	TYR	2.4
2	B	198	GLY	2.4
2	D	360	PHE	2.4
1	C	215	ILE	2.4
1	C	199	ARG	2.4
1	C	217	ARG	2.3
1	A	72	THR	2.3
2	D	386	SER	2.3
1	A	14	THR	2.3
2	D	282	THR	2.3
1	C	223	ASP	2.3
1	A	94	SER	2.3
1	C	13	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	223	GLU	2.2
2	D	368	THR	2.2
2	B	374	GLU	2.2
1	C	216	PHE	2.2
1	A	10	ILE	2.2
1	C	72	THR	2.2
1	C	221	THR	2.2
2	B	274	GLU	2.2
1	C	219	LEU	2.2
2	D	424	LEU	2.2
1	C	269	TYR	2.2
2	D	188	GLU	2.1
2	D	198	GLY	2.1
2	D	364	LEU	2.1
1	A	98	GLY	2.1
1	C	154	VAL	2.1
2	D	427	PRO	2.1
1	A	297	ARG	2.1
2	D	281	ILE	2.1
2	D	333	ALA	2.1
2	D	327	CYS	2.1
1	C	71	HIS	2.1
2	D	400	LYS	2.1
1	C	95	ALA	2.1
1	C	158	THR	2.0
1	C	294	PRO	2.0
1	C	138	GLU	2.0
1	C	239	SER	2.0
1	C	273	LYS	2.0
2	D	389	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.96	0.08	41,45,51,51	0
1	TPO	A	160	11/12	0.99	0.04	22,22,23,24	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

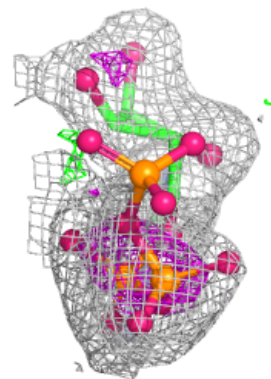
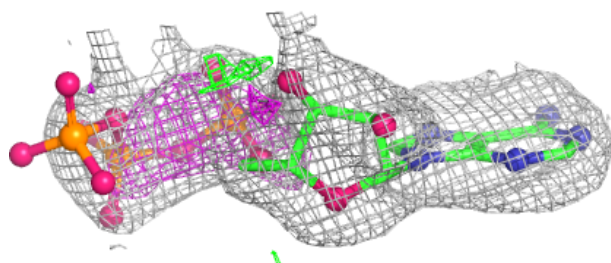
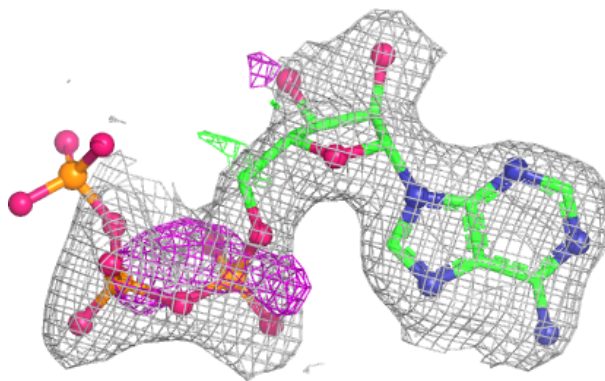
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SGM	D	501	6/6	0.80	0.14	59,61,64,65	0
3	MG	C	302	1/1	0.86	0.10	57,57,57,57	0
4	ATP	C	301	31/31	0.87	0.12	43,54,58,59	4
5	SGM	B	502	6/6	0.92	0.13	48,50,52,57	0
4	ATP	A	302	31/31	0.92	0.10	29,36,52,52	4
3	MG	A	301	1/1	0.95	0.05	37,37,37,37	0
3	MG	B	501	1/1	0.96	0.05	40,40,40,40	0

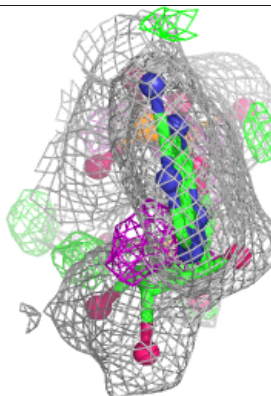
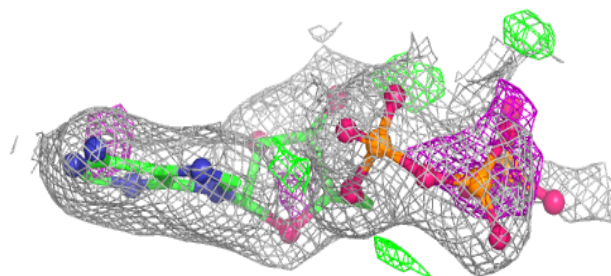
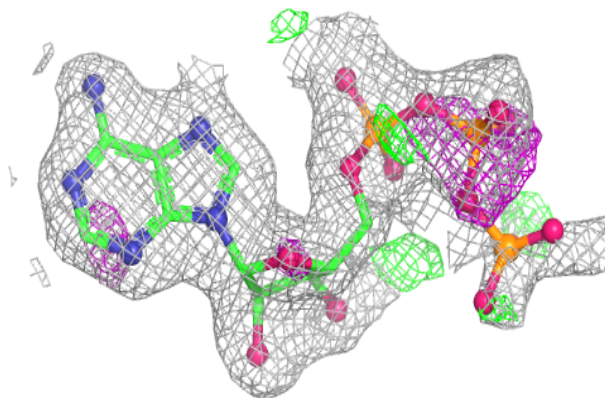
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 302:**

$2mF_o-DF_c$ (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.