Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 08:07 AM EDT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

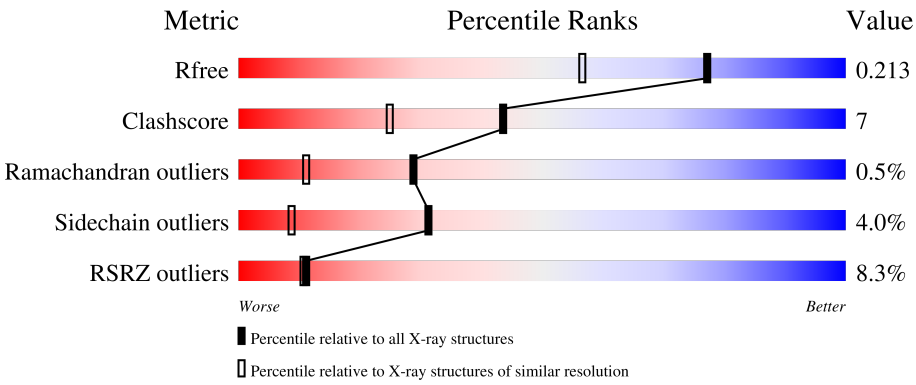
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	302	7% 82% 14% • •
1	C	302	13% 76% 15% • • 6%
2	B	258	5% 93% 6% •
2	D	258	7% 91% 7% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9679 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyclin-dependent kinase 2.

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

There are 14 discrepancies between the modelled and reference sequences:

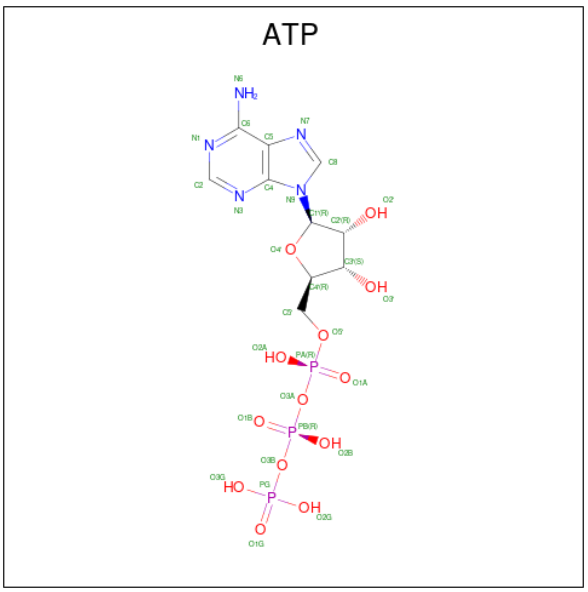
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PRO	-	EXPRESSION TAG	UNP P24941
A	-2	LEU	-	EXPRESSION TAG	UNP P24941
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	SER	-	EXPRESSION TAG	UNP P24941
A	84	SER	HIS	ENGINEERED MUTATION	UNP P24941
A	85	MET	GLN	ENGINEERED MUTATION	UNP P24941
A	89	ASP	LYS	ENGINEERED MUTATION	UNP P24941
C	-3	PRO	-	EXPRESSION TAG	UNP P24941
C	-2	LEU	-	EXPRESSION TAG	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941
C	84	SER	HIS	ENGINEERED MUTATION	UNP P24941
C	85	MET	GLN	ENGINEERED MUTATION	UNP P24941
C	89	ASP	LYS	ENGINEERED MUTATION	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$).

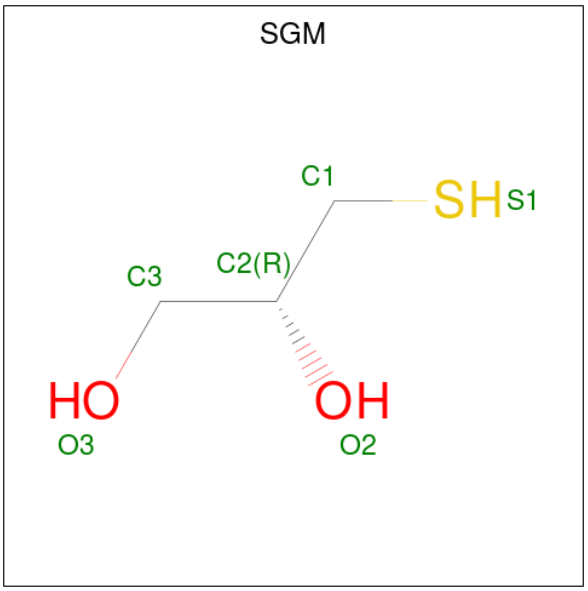


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

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

- Molecule 6 is water.

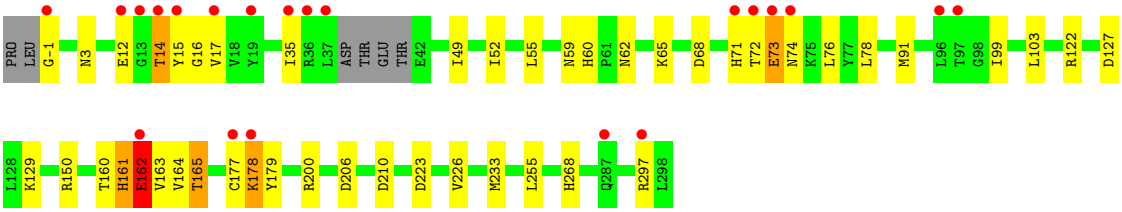
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	229	229	229	0	0
			Total	O		
6	B	177	177	177	0	0
			Total	O		
6	C	135	135	135	0	0
			Total	O		
6	D	129	129	129	0	0

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.

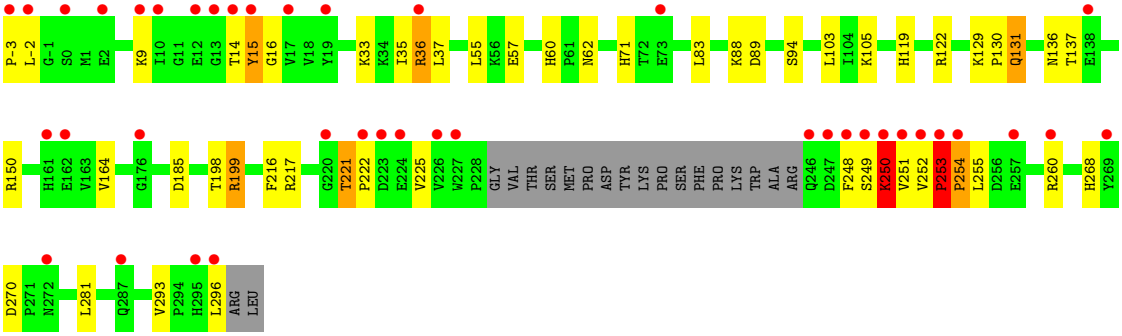
- Molecule 1: Cyclin-dependent kinase 2

Chain A:



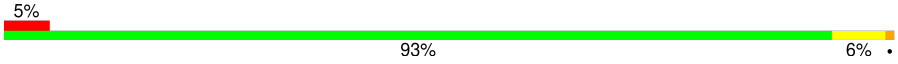
- Molecule 1: Cyclin-dependent kinase 2

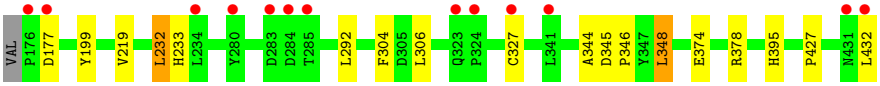
Chain C:



- Molecule 2: Cyclin-A2

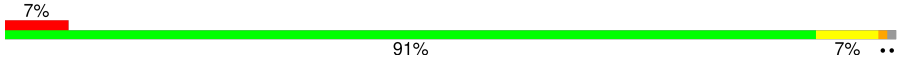
Chain B:

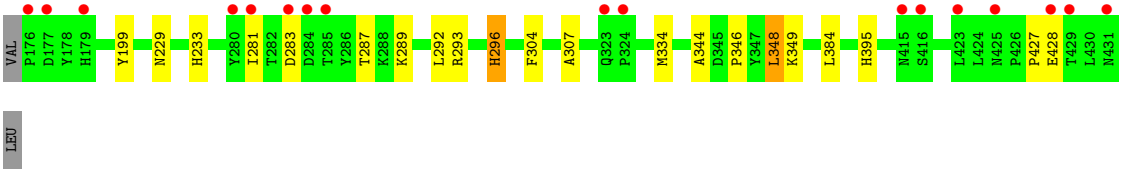




- Molecule 2: Cyclin-A2

Chain D:




VAL
P176
D177
Y178
H179
Y199
N229
H233
Y280
I281
T282
D283
D284
T285
Y286
T287
K288
K289
L292
R293
H296
F304
A307
Q323
P324
M334
A344
D345
P346
Y347
L348
K349
L384
H395
N415
S416
L423
L424
N425
P426
P427
E428
T429
L430
N431
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	73.56Å 133.85Å 149.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.65 37.26 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-1.65) 99.1 (37.26-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.196 , 0.215 0.196 , 0.213	Depositor DCC
R_{free} test set	8773 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9679	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.50	0/2491	0.63	0/3377
1	C	0.49	0/2336	0.72	6/3168 (0.2%)
2	B	0.45	0/2143	0.56	0/2909
2	D	0.36	0/2157	0.53	0/2926
All	All	0.46	0/9127	0.62	6/12380 (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
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	249	SER	N-CA-C	-9.09	86.45	111.00
1	C	249	SER	CB-CA-C	7.21	123.80	110.10
1	C	253	PRO	N-CA-C	-6.87	94.25	112.10
1	C	250	LYS	N-CA-C	-5.20	96.97	111.00
1	C	89	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	199	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2442	0	2474	47	0
1	C	2293	0	2327	52	0
2	B	2092	0	2108	13	0
2	D	2106	0	2121	18	0
3	A	31	0	12	0	0
3	C	31	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	12	0	15	1	0
6	A	229	0	0	4	0
6	B	177	0	0	2	0
6	C	135	0	0	3	0
6	D	129	0	0	4	0
All	All	9679	0	9069	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177[A]:CYS:SG	1:A:233:MET:HE3	1.51	1.48
1:A:177[A]:CYS:SG	1:A:233:MET:CE	2.35	1.12
1:A:72:THR:HG22	1:A:73:GLU:CD	1.71	1.10
1:A:72:THR:HG22	1:A:73:GLU:OE1	1.58	1.01
1:C:36:ARG:HG2	1:C:36:ARG:HH21	1.28	0.98
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.86	0.94
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.05	0.94
1:C:252:VAL:O	1:C:253:PRO:O	1.87	0.92
1:C:252:VAL:C	1:C:253:PRO:O	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:ATP:H5'2	3:C:301:ATP:O3B	1.74	0.87
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.92	0.86
1:C:255:LEU:O	1:C:260:ARG:NH1	2.11	0.84
1:A:60:HIS:HD2	1:A:62:ASN:H	1.26	0.83
1:A:72:THR:CG2	1:A:73:GLU:OE1	2.29	0.81
1:A:60:HIS:CD2	1:A:62:ASN:H	1.99	0.80
1:C:250:LYS:HB3	1:C:252:VAL:H	1.48	0.79
1:A:71:HIS:HE2	2:B:304:PHE:HE2	1.30	0.77
1:A:72:THR:HG22	1:A:73:GLU:OE2	1.86	0.75
1:A:268:HIS:CE1	6:A:492:HOH:O	2.40	0.74
1:C:33:LYS:HE3	6:C:510:HOH:O	1.88	0.73
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.72	0.71
1:C:60:HIS:HD2	1:C:62:ASN:H	1.39	0.70
1:C:14:THR:C	1:C:16:GLY:H	1.97	0.68
1:A:12:GLU:OE2	1:A:17:VAL:HG22	1.94	0.68
1:A:210:ASP:OD2	6:A:539:HOH:O	2.12	0.67
1:C:250:LYS:HG2	1:C:252:VAL:HG23	1.76	0.67
1:C:250:LYS:HB3	1:C:252:VAL:HG23	1.78	0.65
2:D:346:PRO:O	2:D:349:LYS:HG2	1.96	0.65
1:C:60:HIS:CD2	1:C:62:ASN:H	2.15	0.65
2:D:281:ILE:C	2:D:283:ASP:H	2.00	0.65
1:C:268:HIS:HD2	1:C:270:ASP:H	1.44	0.65
1:A:71:HIS:NE2	2:B:304:PHE:HE2	1.95	0.64
1:C:36:ARG:HG2	1:C:36:ARG:NH2	2.04	0.63
1:C:216:PHE:HB3	1:C:221:THR:HB	1.81	0.62
2:B:374:GLU:OE2	2:B:378:ARG:HD2	2.00	0.61
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.77	0.61
1:C:250:LYS:CB	1:C:252:VAL:HG23	2.31	0.61
1:A:129:LYS:NZ	1:A:165:THR:HG21	2.16	0.60
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.85	0.59
1:C:254:PRO:O	1:C:255:LEU:C	2.36	0.59
1:C:252:VAL:O	1:C:253:PRO:C	2.41	0.59
2:D:289:LYS:O	2:D:293[B]:ARG:HG3	2.04	0.57
1:A:127:ASP:OD1	1:A:165:THR:HG23	2.04	0.57
1:C:253:PRO:O	1:C:255:LEU:N	2.39	0.56
2:D:395:HIS:HE1	2:D:427:PRO:O	1.88	0.56
1:A:73:GLU:OE2	1:A:74:ASN:N	2.30	0.55
2:B:395:HIS:HE1	2:B:427:PRO:O	1.89	0.55
1:C:14:THR:C	1:C:16:GLY:N	2.60	0.55
1:A:73:GLU:CD	1:A:73:GLU:H	2.09	0.54
1:A:14:THR:C	1:A:16:GLY:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:O	1:A:15:TYR:CB	2.54	0.54
1:A:71:HIS:NE2	2:B:304:PHE:CE2	2.73	0.53
1:C:119:HIS:HD2	6:D:501:HOH:O	1.90	0.53
1:A:3:ASN:OD1	2:D:293[B]:ARG:NH2	2.39	0.53
1:A:60:HIS:HE1	6:A:419:HOH:O	1.92	0.52
1:C:94:SER:O	1:C:199:ARG:HD3	2.09	0.52
1:C:250:LYS:CG	1:C:252:VAL:HG23	2.38	0.52
2:B:374:GLU:CD	2:B:378:ARG:HD2	2.29	0.52
1:A:72:THR:CG2	1:A:73:GLU:OE2	2.55	0.52
1:C:15:TYR:CG	1:C:35:ILE:HG12	2.45	0.52
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.91	0.51
2:B:233:HIS:HE1	6:B:647:HOH:O	1.92	0.51
1:A:12:GLU:OE2	1:A:17:VAL:CG2	2.57	0.51
1:C:222:PRO:HB2	1:C:225:VAL:HG23	1.93	0.51
1:C:253:PRO:CB	1:C:254:PRO:CD	2.89	0.51
2:D:233:HIS:HE1	6:D:576:HOH:O	1.94	0.51
1:C:36:ARG:NH2	1:C:36:ARG:CG	2.73	0.50
2:D:233:HIS:HD2	6:D:504:HOH:O	1.95	0.50
1:A:73:GLU:CD	1:A:73:GLU:N	2.65	0.50
2:B:233:HIS:HD2	6:B:603:HOH:O	1.93	0.50
1:C:252:VAL:N	1:C:253:PRO:CD	2.74	0.50
1:C:83:LEU:HD12	1:C:136:ASN:HB3	1.94	0.50
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.95	0.49
1:A:103:LEU:HD22	6:A:569:HOH:O	2.13	0.48
1:C:137:THR:O	1:C:293:VAL:HG13	2.13	0.48
1:C:33:LYS:CE	6:C:510:HOH:O	2.53	0.48
1:C:57:GLU:OE2	2:D:307:ALA:HB3	2.14	0.48
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.95	0.48
1:A:71:HIS:O	1:A:72:THR:OG1	2.30	0.47
1:C:131:GLN:NE2	1:C:131:GLN:H	2.12	0.47
1:C:198:THR:HG22	1:C:253:PRO:HG2	1.96	0.47
1:A:14:THR:O	1:A:15:TYR:HB2	2.14	0.47
1:C:-3:PRO:HA	1:C:-2:LEU:HA	1.72	0.47
1:A:162:GLU:HG2	1:A:163:VAL:HG12	1.95	0.47
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.97	0.47
1:A:35:ILE:HB	1:A:76:LEU:HB3	1.96	0.47
1:C:221:THR:HA	1:C:222:PRO:HD3	1.53	0.47
1:A:223:ASP:H	1:A:226[A]:VAL:HG12	1.81	0.46
1:A:178:LYS:HE3	1:A:179:TYR:CZ	2.51	0.45
1:A:162:GLU:HG2	1:A:163:VAL:CG1	2.47	0.45
1:C:137:THR:HG22	1:C:296:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LYS:HB3	1:C:252:VAL:N	2.22	0.44
1:A:59[B]:ASN:HD21	1:A:65:LYS:HE2	1.81	0.44
1:A:14:THR:C	1:A:16:GLY:N	2.70	0.44
1:A:177[A]:CYS:SG	1:A:233:MET:HE2	2.47	0.43
1:C:251:VAL:O	1:C:251:VAL:HG12	2.17	0.43
2:D:334[B]:MET:HE3	2:D:334[B]:MET:HB3	1.86	0.43
6:C:450:HOH:O	2:D:296:HIS:HD2	2.01	0.43
1:A:60:HIS:HD2	1:A:62:ASN:N	2.06	0.43
1:C:129:LYS:HG3	1:C:131:GLN:HG2	2.00	0.43
1:A:73:GLU:HG2	1:A:74:ASN:OD1	2.18	0.43
1:A:127:ASP:OD1	1:A:165:THR:CG2	2.67	0.43
1:C:252:VAL:N	1:C:253:PRO:HD2	2.34	0.43
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.02	0.42
1:A:91:MET:HG2	1:A:99:ILE:HD11	2.02	0.42
1:C:222:PRO:HB2	1:C:225:VAL:CG2	2.50	0.42
1:C:250:LYS:HG2	1:C:252:VAL:CG2	2.46	0.42
2:B:345:ASP:HA	2:B:346:PRO:HA	1.89	0.42
1:A:-1:GLY:HA3	1:A:68:ASP:OD2	2.20	0.42
3:C:301:ATP:O2G	3:C:301:ATP:O2B	2.38	0.42
2:B:327:CYS:SG	5:B:503:SGM:S1	3.13	0.42
1:C:105:LYS:HB2	1:C:105:LYS:HE2	1.88	0.42
1:A:71:HIS:C	1:A:72:THR:OG1	2.57	0.41
1:C:253:PRO:HB3	1:C:254:PRO:HD3	2.01	0.41
2:D:229:ASN:HD22	2:D:334[B]:MET:CE	2.34	0.41
1:A:162:GLU:HG3	1:A:163:VAL:HA	2.03	0.41
1:A:72:THR:HG22	1:A:73:GLU:H	1.86	0.41
1:C:222:PRO:CB	1:C:225:VAL:HG23	2.51	0.41
1:A:161[A]:HIS:CD2	1:A:161[A]:HIS:C	2.94	0.40
1:C:71:HIS:NE2	2:D:304:PHE:HE2	2.19	0.40
2:D:287:THR:HB	6:D:515:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/302 (99%)	292 (97%)	6 (2%)	2 (1%)	22	6
1	C	282/302 (93%)	266 (94%)	13 (5%)	3 (1%)	14	2
2	B	257/258 (100%)	256 (100%)	1 (0%)	0	100	100
2	D	258/258 (100%)	255 (99%)	3 (1%)	0	100	100
All	All	1097/1120 (98%)	1069 (97%)	23 (2%)	5 (0%)	29	11

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/265 (101%)	254 (95%)	14 (5%)	23	5
1	C	252/265 (95%)	237 (94%)	15 (6%)	19	3
2	B	233/232 (100%)	227 (97%)	6 (3%)	46	21
2	D	234/232 (101%)	228 (97%)	6 (3%)	46	21
All	All	987/994 (99%)	946 (96%)	41 (4%)	31	8

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	55	LEU
1	A	73	GLU

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Mol	Chain	Res	Type
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	200	ARG
1	A	206[A]	ASP
1	A	206[B]	ASP
1	A	255	LEU
1	A	297	ARG
2	B	177	ASP
2	B	199	TYR
2	B	232	LEU
2	B	292	LEU
2	B	348	LEU
2	B	432	LEU
1	C	9	LYS
1	C	15	TYR
1	C	36	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	217	ARG
1	C	221	THR
1	C	248	PHE
1	C	250	LYS
1	C	253	PRO
1	C	281	LEU
2	D	199	TYR
2	D	292	LEU
2	D	296	HIS
2	D	348	LEU
2	D	384	LEU
2	D	428	GLU

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

Mol	Chain	Res	Type
1	A	60	HIS
2	B	233	HIS
2	B	254	GLN
2	B	312	ASN
2	B	395	HIS
2	B	425	ASN
1	C	60	HIS
1	C	71	HIS
1	C	119	HIS
1	C	131	GLN
1	C	246	GLN
1	C	265	GLN
1	C	268	HIS
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	323	GLN
2	D	395	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	C	160	1	8,10,11	0.76	0	10,14,16	1.08	0
1	TPO	A	160	1	8,10,11	1.02	1 (12%)	10,14,16	0.98	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	-	0/9/11/13	-

All (1) bond length outliers are listed below:

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

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
3	ATP	C	301	-	28,33,33	1.03	2 (7%)	34,52,52	1.09	2 (5%)
3	ATP	A	301	4	28,33,33	1.14	4 (14%)	34,52,52	1.21	3 (8%)
5	SGM	B	502	-	5,5,5	0.47	0	5,5,5	0.56	0
5	SGM	B	503	-	5,5,5	0.34	0	5,5,5	0.49	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
3	ATP	C	301	-	-	0/18/38/38	0/3/3/3
3	ATP	A	301	4	-	3/18/38/38	0/3/3/3
5	SGM	B	502	-	-	3/4/4/4	-
5	SGM	B	503	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	ATP	PB-O3A	2.66	1.62	1.59
3	A	301	ATP	O4'-C1'	2.56	1.44	1.40
3	A	301	ATP	PA-O3A	2.47	1.62	1.59
3	C	301	ATP	O4'-C1'	2.22	1.43	1.40
3	A	301	ATP	C2-N3	2.07	1.35	1.32
3	C	301	ATP	C2-N3	2.00	1.35	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	ATP	N3-C2-N1	-3.62	123.76	128.67
3	C	301	ATP	N3-C2-N1	-3.47	123.96	128.67
3	A	301	ATP	O4'-C1'-N9	2.97	112.68	108.75
3	A	301	ATP	C4-C5-N7	-2.64	106.55	109.34
3	C	301	ATP	C4-C5-N7	-2.59	106.60	109.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

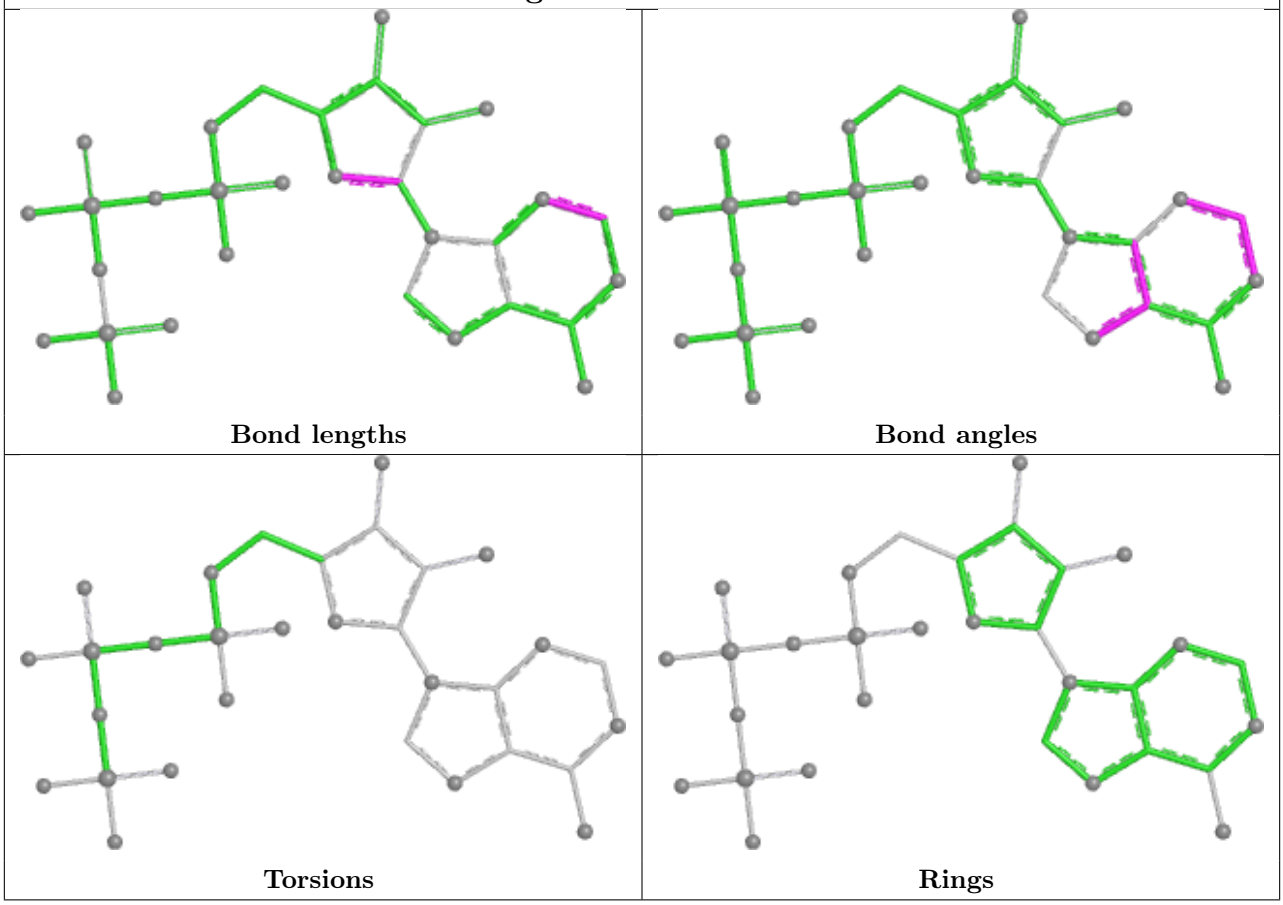
There are no ring outliers.

2 monomers are involved in 3 short contacts:

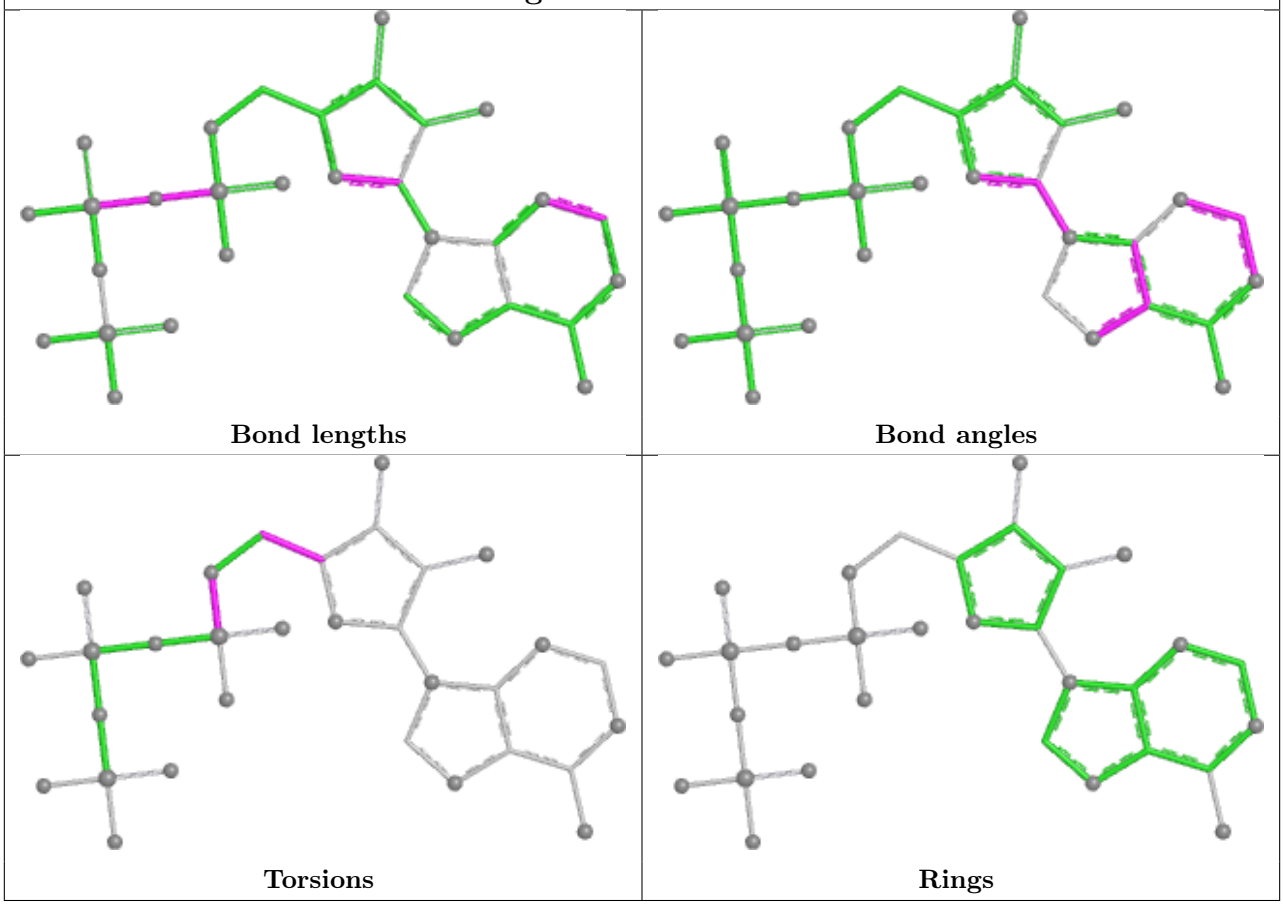
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	ATP	2	0
5	B	503	SGM	1	0

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



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 (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	295/302 (97%)	0.35	21 (7%)	16	15	11, 19, 41, 53	0
1	C	282/302 (93%)	0.63	40 (14%)	2	2	16, 26, 55, 75	0
2	B	257/258 (99%)	0.26	13 (5%)	28	27	12, 22, 36, 48	0
2	D	256/258 (99%)	0.31	17 (6%)	18	17	14, 26, 44, 58	0
All	All	1090/1120 (97%)	0.39	91 (8%)	11	11	11, 24, 45, 75	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	246	GLN	9.6
1	C	252	VAL	9.5
2	B	432	LEU	9.3
1	C	14	THR	9.0
1	C	-3	PRO	8.7
1	C	17	VAL	8.1
1	C	295[A]	HIS	7.4
1	C	247	ASP	6.7
1	A	96	LEU	6.5
2	D	284	ASP	6.5
2	B	283	ASP	6.2
1	A	15	TYR	5.9
2	B	284	ASP	5.9
1	A	36	ARG	5.9
2	D	283	ASP	5.5
1	C	15	TYR	5.4
2	B	323	GLN	5.4
1	C	223	ASP	5.0
1	C	254	PRO	5.0
1	A	73	GLU	4.7
1	C	249	SER	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	176	PRO	4.6
1	C	248	PHE	4.6
2	B	285	THR	4.6
1	C	296	LEU	4.3
1	A	12	GLU	4.3
1	A	71	HIS	4.2
1	C	-2	LEU	4.2
2	D	176	PRO	4.2
1	C	19	TYR	4.1
2	D	431	ASN	4.0
1	A	37	LEU	4.0
1	C	12	GLU	4.0
1	C	253	PRO	4.0
2	D	323	GLN	3.9
1	A	17	VAL	3.8
1	C	9	LYS	3.7
1	A	19	TYR	3.6
1	C	220	GLY	3.6
1	A	72	THR	3.6
2	B	431	ASN	3.5
1	C	226	VAL	3.4
2	B	280	TYR	3.3
1	C	222	PRO	3.3
2	D	177	ASP	3.3
1	C	162	GLU	3.2
1	A	-1	GLY	3.2
1	C	10	ILE	3.2
1	C	36	ARG	3.2
1	C	250	LYS	3.2
2	D	324	PRO	3.1
1	C	73	GLU	3.1
1	C	0	SER	3.0
1	A	162	GLU	3.0
2	D	179[A]	HIS	3.0
1	C	224	GLU	3.0
1	C	13	GLY	3.0
2	D	285	THR	2.9
1	A	177[A]	CYS	2.8
2	B	324	PRO	2.8
1	A	74	ASN	2.7
1	A	35	ILE	2.7
2	D	428	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	97	THR	2.7
2	D	280	TYR	2.6
1	C	227	TRP	2.6
1	C	269	TYR	2.5
2	B	341	LEU	2.5
1	C	260	ARG	2.5
1	C	2	GLU	2.5
1	A	287	GLN	2.5
1	C	287	GLN	2.4
1	C	272	ASN	2.3
2	D	416	SER	2.3
2	B	234	LEU	2.3
1	A	297	ARG	2.3
1	A	14	THR	2.2
2	D	425	ASN	2.2
1	A	13	GLY	2.2
2	D	423	LEU	2.2
1	C	138	GLU	2.2
1	A	178	LYS	2.2
2	B	327	CYS	2.2
1	C	161	HIS	2.1
1	C	251	VAL	2.1
2	D	281	ILE	2.1
1	C	257	GLU	2.1
2	D	429	THR	2.0
1	C	176	GLY	2.0
2	B	177	ASP	2.0
2	D	415	ASN	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	A	160	11/12	0.99	0.06	14,17,18,19	0
1	TPO	C	160	11/12	0.99	0.06	17,19,22,22	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

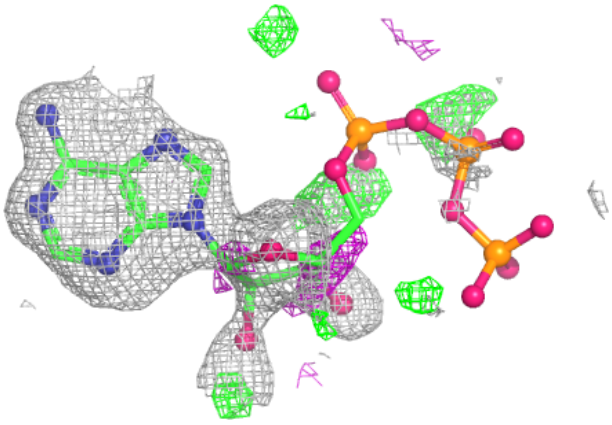
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

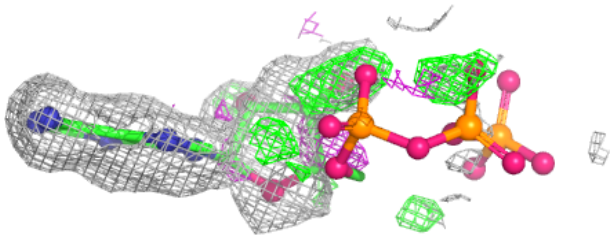
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	302	1/1	0.60	0.19	51,51,51,51	0
5	SGM	B	503	6/6	0.64	0.23	71,71,71,71	0
3	ATP	C	301	31/31	0.79	0.28	46,54,55,55	14
3	ATP	A	301	31/31	0.81	0.27	30,46,47,47	13
5	SGM	B	502	6/6	0.85	0.17	36,40,41,43	0
4	MG	B	501	1/1	0.97	0.06	30,30,30,30	0

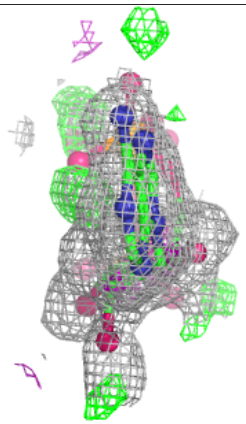
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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)

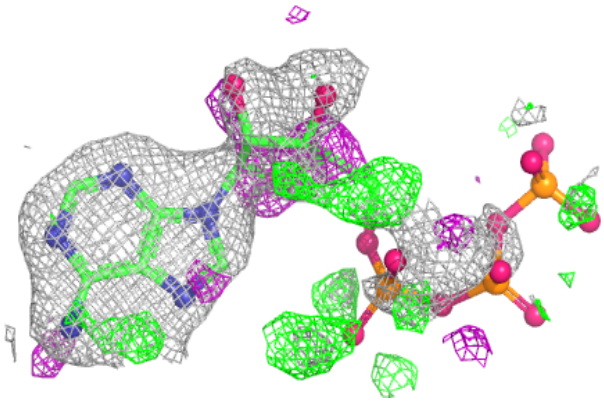


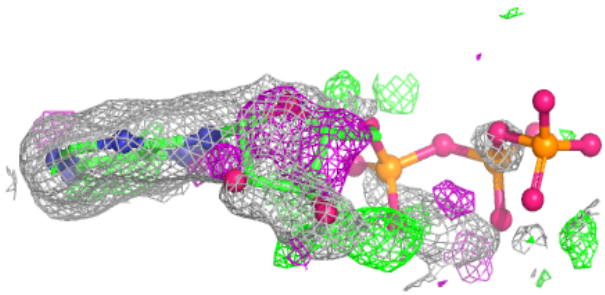


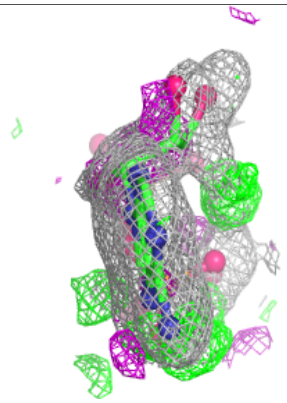


Electron density around ATP A 301:

$2mF_o$-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.