



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:31 PM BST

PDB ID : 4O0M  
Title : Crystal structure of T. Elongatus BP-1 Clock Protein KaiC  
Authors : Pattanayek, R.; Egli, M.  
Deposited on : 2013-12-13  
Resolution : 2.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

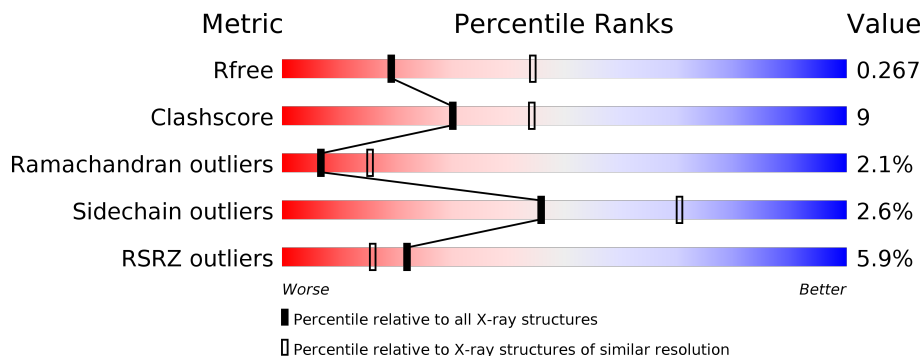
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	524	 6% 73% 20% • 6%
1	B	524	 5% 67% 24% • 6%
1	C	524	 5% 72% 20% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	804	-	-	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11943 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	494	3873	2439	670	751	2	11	0	0	0
1	B	490	3841	2419	665	744	2	11	0	0	0
1	C	490	3832	2413	665	741	2	11	0	0	0

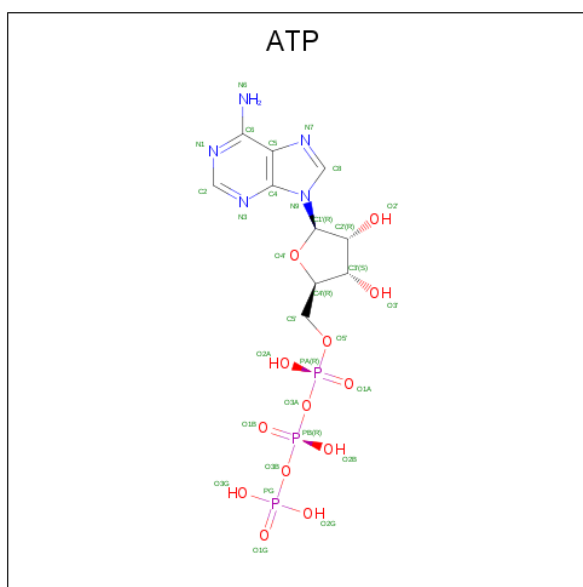
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	519	HIS	-	EXPRESSION TAG	UNP Q79V60
A	520	HIS	-	EXPRESSION TAG	UNP Q79V60
A	521	HIS	-	EXPRESSION TAG	UNP Q79V60
A	522	HIS	-	EXPRESSION TAG	UNP Q79V60
A	523	HIS	-	EXPRESSION TAG	UNP Q79V60
A	524	HIS	-	EXPRESSION TAG	UNP Q79V60
B	519	HIS	-	EXPRESSION TAG	UNP Q79V60
B	520	HIS	-	EXPRESSION TAG	UNP Q79V60
B	521	HIS	-	EXPRESSION TAG	UNP Q79V60
B	522	HIS	-	EXPRESSION TAG	UNP Q79V60
B	523	HIS	-	EXPRESSION TAG	UNP Q79V60
B	524	HIS	-	EXPRESSION TAG	UNP Q79V60
C	519	HIS	-	EXPRESSION TAG	UNP Q79V60
C	520	HIS	-	EXPRESSION TAG	UNP Q79V60
C	521	HIS	-	EXPRESSION TAG	UNP Q79V60
C	522	HIS	-	EXPRESSION TAG	UNP Q79V60
C	523	HIS	-	EXPRESSION TAG	UNP Q79V60
C	524	HIS	-	EXPRESSION TAG	UNP Q79V60

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	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 31 10 5 13 3	0	0
3	A	1	Total C N O P 31 10 5 13 3	0	0
3	B	1	Total C N O P 31 10 5 13 3	0	0
3	B	1	Total C N O P 31 10 5 13 3	0	0
3	C	1	Total C N O P 31 10 5 13 3	0	0
3	C	1	Total C N O P 31 10 5 13 3	0	0

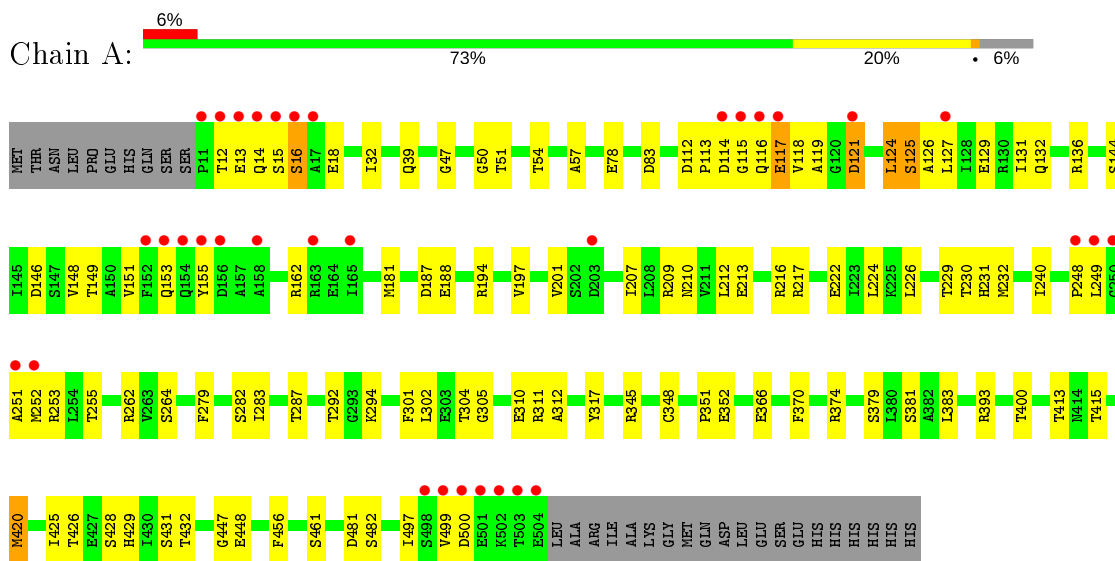
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	80	Total 80	O 80	0	0
4	B	66	Total 66	O 66	0	0
4	C	59	Total 59	O 59	0	0

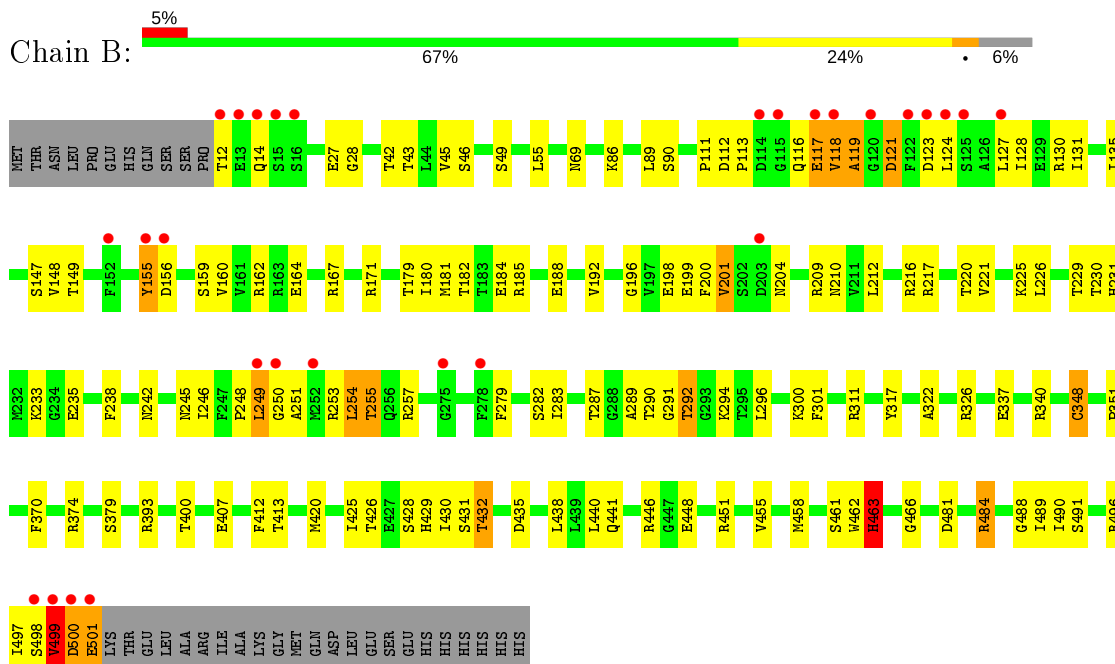
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

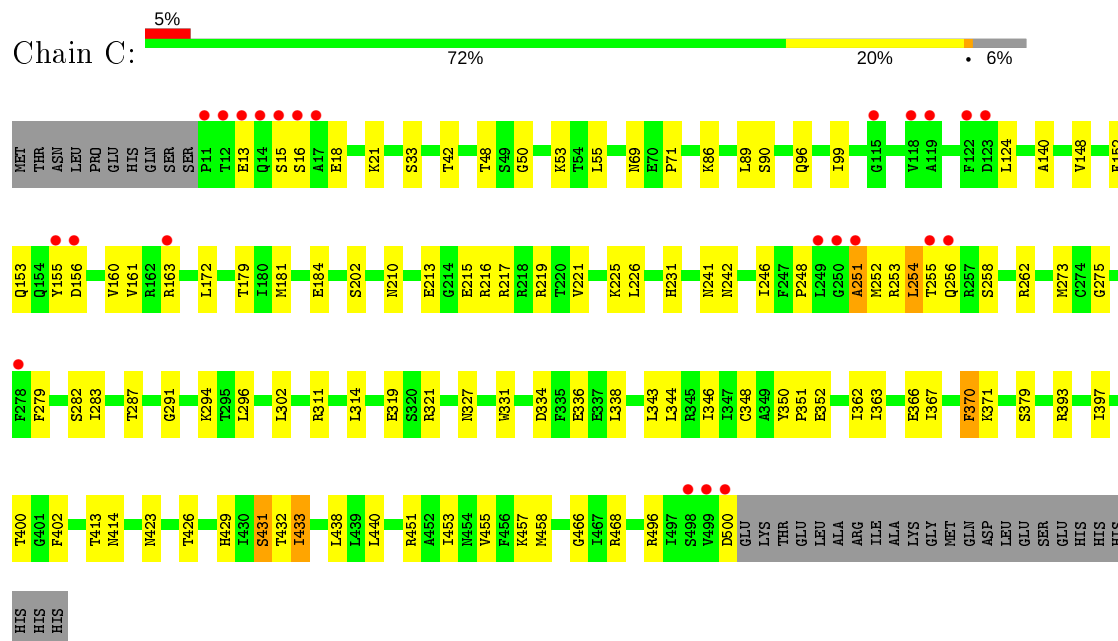
- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.81Å 195.29Å 136.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.99 – 2.84 68.32 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.4 (58.99-2.84) 94.6 (68.32-2.84)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.225 , 0.270 0.227 , 0.267	Depositor DCC
$R_{free}$ test set	2079 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtrriage
Anisotropy	0.687	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.26	0/3915	0.45	0/5279
1	B	0.27	0/3882	0.44	0/5235
1	C	0.24	0/3873	0.41	0/5223
All	All	0.26	0/11670	0.43	0/15737

There are no bond length outliers.

There are no bond angle outliers.

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	3873	0	3858	72	0
1	B	3841	0	3824	92	0
1	C	3832	0	3820	69	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	62	0	24	0	0
3	B	62	0	24	2	0
3	C	62	0	24	3	0
4	A	80	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	66	0	0	3	0
4	C	59	0	0	4	0
All	All	11943	0	11574	217	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 9.

All (217) 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:C:438:LEU:CD2	1:C:455:VAL:HG22	1.78	1.13
1:C:438:LEU:HD21	1:C:455:VAL:HG22	1.57	0.86
1:A:116:GLN:HB2	1:A:117:GLU:HB2	1.58	0.85
1:B:379:SER:H	1:B:413:THR:HB	1.43	0.83
1:A:415:THR:HG21	1:B:432:TPO:HG21	1.60	0.82
1:B:112:ASP:HB3	1:B:113:PRO:HD2	1.65	0.78
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.65	0.78
1:C:248:PRO:HB2	1:C:251:ALA:HB3	1.68	0.75
1:C:393:ARG:HH21	1:C:429:HIS:HB2	1.50	0.74
1:A:209:ARG:NH2	1:A:222:GLU:OE1	2.23	0.72
1:B:124:LEU:HD21	1:B:167:ARG:HD3	1.74	0.70
1:B:42:THR:HG22	1:B:179:THR:HB	1.74	0.69
1:A:126:ALA:HB2	1:A:129:GLU:HB2	1.74	0.69
1:C:438:LEU:HD22	1:C:455:VAL:HG22	1.72	0.68
1:A:194:ARG:NH2	1:B:196:GLY:O	2.27	0.68
1:B:253:ARG:O	1:B:255:THR:N	2.27	0.68
1:A:125:SER:O	1:A:129:GLU:N	2.28	0.67
1:B:86:LYS:HA	1:B:89:LEU:HD12	1.76	0.67
1:B:248:PRO:O	1:B:251:ALA:N	2.24	0.66
1:C:156:ASP:HB3	1:C:160:VAL:HG21	1.77	0.66
1:B:294:LYS:HG3	1:B:440:LEU:HD12	1.78	0.66
1:B:28:GLY:HA2	1:B:248:PRO:HG3	1.77	0.65
1:A:57:ALA:HB1	1:A:144:SER:HB3	1.78	0.65
1:C:283:ILE:HG13	1:C:400:THR:HG23	1.77	0.65
1:C:241:ASN:OD1	1:C:242:ASN:N	2.29	0.64
1:A:117:GLU:H	1:A:118:VAL:HG22	1.62	0.64
1:B:45:VAL:HG23	1:B:180:ILE:HD11	1.80	0.64
1:A:124:LEU:O	1:A:126:ALA:N	2.32	0.62
1:B:69:ASN:ND2	4:B:720:HOH:O	2.31	0.62
1:C:253:ARG:O	1:C:255:THR:N	2.33	0.62
1:B:121:ASP:C	1:B:123:ASP:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:HA	1:B:130:ARG:HB2	1.80	0.62
1:B:426:THR:HG22	1:B:428:SER:H	1.65	0.62
1:A:210:ASN:O	1:A:217:ARG:NH1	2.33	0.61
1:C:202:SER:O	1:C:225:LYS:NZ	2.31	0.61
1:A:118:VAL:H	1:A:121:ASP:HA	1.65	0.61
1:A:352:GLU:HB3	1:B:249:LEU:HD21	1.83	0.61
1:C:21:LYS:NZ	1:C:33:SER:O	2.29	0.61
1:C:397:ILE:HD11	1:C:433:ILE:HD13	1.82	0.61
1:A:345:ARG:NH1	1:A:366:GLU:OE1	2.32	0.61
1:A:426:THR:HG22	1:A:428:SER:H	1.65	0.61
1:A:226:LEU:HD12	1:A:231:HIS:HB3	1.83	0.61
1:C:50:GLY:O	1:C:219:ARG:NH2	2.34	0.61
1:B:221:VAL:HG23	1:B:238:PHE:CD1	2.36	0.61
1:C:15:SER:HB2	1:C:16:SER:HA	1.82	0.61
1:C:438:LEU:HD23	1:C:455:VAL:HA	1.82	0.60
1:A:216:ARG:NH2	1:B:235:GLU:O	2.34	0.60
1:A:393:ARG:NH2	1:A:428:SER:O	2.35	0.60
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.83	0.60
1:B:498:SER:HA	1:B:499:VAL:C	2.23	0.59
1:B:317:TYR:HB3	1:B:351:PRO:HG3	1.85	0.59
1:B:124:LEU:HD11	1:B:167:ARG:HB2	1.84	0.59
1:A:481:ASP:OD1	1:A:482:SER:N	2.36	0.59
1:B:162:ARG:HH12	1:B:200:PHE:HB2	1.69	0.58
1:B:326:ARG:HD3	1:C:258:SER:HB3	1.85	0.58
1:C:338:LEU:HB3	1:C:344:LEU:HB3	1.85	0.58
1:B:118:VAL:O	1:B:119:ALA:C	2.42	0.58
1:A:287:THR:HG21	1:A:425:ILE:HG23	1.85	0.58
1:A:148:VAL:HG21	1:A:181:MET:HG2	1.84	0.57
1:C:69:ASN:ND2	4:C:729:HOH:O	2.37	0.57
1:B:438:LEU:HD23	1:B:455:VAL:HA	1.87	0.57
1:C:311:ARG:HG2	1:C:343:LEU:HA	1.86	0.57
1:B:337:GLU:OE2	1:B:340:ARG:NH1	2.38	0.57
1:B:446:ARG:HH21	1:B:496:ARG:HH12	1.49	0.57
1:C:287:THR:HG22	1:C:414:ASN:HB3	1.87	0.57
1:B:116:GLN:OE1	1:B:116:GLN:N	2.38	0.57
1:A:127:LEU:HD23	1:A:127:LEU:H	1.70	0.56
1:B:246:ILE:O	1:B:248:PRO:HD3	2.05	0.56
1:C:321:ARG:HD3	1:C:346:ILE:HG21	1.86	0.56
1:C:311:ARG:NH1	1:C:370:PHE:O	2.38	0.55
1:A:47:GLY:HA3	1:A:51:THR:HG21	1.88	0.55
1:A:229:THR:OG1	1:A:230:THR:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.87	0.55
1:C:379:SER:H	1:C:413:THR:HG1	1.53	0.55
1:A:302:LEU:HD22	1:A:312:ALA:HB1	1.88	0.55
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.90	0.54
1:A:153:GLN:O	1:B:159:SER:HB3	2.07	0.54
1:B:462:TRP:O	1:B:463:HIS:ND1	2.40	0.54
1:B:121:ASP:OD1	1:B:123:ASP:HB2	2.08	0.54
1:A:240:ILE:HG12	4:A:967:HOH:O	2.08	0.54
1:C:311:ARG:HH22	1:C:371:LYS:HB2	1.72	0.53
1:B:481:ASP:HB3	1:B:484:ARG:NH2	2.24	0.53
1:A:305:GLY:O	1:A:310:GLU:HG2	2.08	0.53
1:B:149:THR:HG21	1:B:184:GLU:H	1.74	0.53
1:B:90:SER:OG	3:B:604:ATP:N6	2.38	0.53
1:B:198:GLU:N	1:B:198:GLU:OE1	2.39	0.52
1:B:438:LEU:CD2	1:B:455:VAL:HG22	2.39	0.52
1:C:262:ARG:NH1	1:C:275:GLY:O	2.40	0.52
1:B:301:PHE:O	1:B:374:ARG:NH1	2.42	0.52
1:A:351:PRO:HB3	1:A:383:LEU:HD23	1.92	0.52
1:B:127:LEU:O	1:B:131:ILE:N	2.41	0.52
1:A:127:LEU:HD12	1:A:131:ILE:HD11	1.92	0.52
1:A:117:GLU:H	1:A:118:VAL:CG2	2.23	0.51
1:C:334:ASP:OD1	1:C:336:GLU:HG2	2.11	0.51
1:B:160:VAL:O	1:B:164:GLU:HG3	2.10	0.51
1:C:319:GLU:OE1	1:C:327:ASN:ND2	2.44	0.51
1:C:90:SER:OG	3:C:603:ATP:N6	2.32	0.50
1:A:112:ASP:O	1:A:114:ASP:N	2.40	0.50
1:A:216:ARG:NH1	1:B:233:LYS:O	2.44	0.50
1:B:117:GLU:C	1:B:119:ALA:H	2.15	0.50
1:B:311:ARG:HB3	1:B:370:PHE:CE2	2.46	0.50
1:C:184:GLU:OE2	4:C:756:HOH:O	2.20	0.50
1:C:251:ALA:O	1:C:253:ARG:N	2.45	0.50
1:A:116:GLN:CB	1:A:117:GLU:HB2	2.38	0.50
1:B:279:PHE:HB2	1:B:282:SER:HB3	1.94	0.50
1:B:283:ILE:N	1:B:435:ASP:OD2	2.41	0.50
1:B:287:THR:HG21	1:B:425:ILE:HG23	1.94	0.49
1:C:221:VAL:HG11	1:C:246:ILE:HD13	1.93	0.49
1:C:291:GLY:O	1:C:451:ARG:NH1	2.40	0.49
1:A:162:ARG:HB2	1:A:197:VAL:HG11	1.95	0.48
1:A:301:PHE:O	1:A:374:ARG:NH1	2.44	0.48
1:B:128:ILE:HD11	1:B:171:ARG:HB2	1.96	0.48
1:A:125:SER:O	1:A:129:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:N	1:A:118:VAL:HA	2.27	0.48
1:B:488:GLY:O	1:B:491:SER:OG	2.28	0.48
1:A:32:ILE:HA	1:A:232:MET:SD	2.54	0.48
1:B:112:ASP:HB3	1:B:113:PRO:CD	2.41	0.48
1:B:156:ASP:O	4:B:732:HOH:O	2.20	0.48
1:C:279:PHE:HB2	1:C:282:SER:HB2	1.95	0.48
1:A:78:GLU:HG3	1:B:162:ARG:HH21	1.78	0.47
1:C:160:VAL:HG22	1:C:163:ARG:HH12	1.79	0.47
1:C:172:LEU:HD13	1:C:179:THR:HG21	1.96	0.47
1:C:371:LYS:NZ	4:C:757:HOH:O	2.30	0.47
1:A:132:GLN:HE21	1:A:136:ARG:NH2	2.12	0.47
1:B:147:SER:H	1:B:182:THR:HB	1.79	0.47
1:B:27:GLU:HG2	1:B:245:ASN:HA	1.97	0.47
1:B:248:PRO:O	1:B:250:GLY:N	2.47	0.47
1:C:42:THR:HG21	1:C:181:MET:SD	2.54	0.47
1:C:215:GLU:HB2	1:C:216:ARG:NH1	2.29	0.47
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.50	0.47
1:B:441:GLN:NE2	1:B:490:ILE:O	2.33	0.47
1:B:348:CYS:HB3	1:C:254:LEU:HB2	1.97	0.46
1:C:362:ILE:O	1:C:366:GLU:HG2	2.16	0.46
1:C:153:GLN:C	1:C:155:TYR:H	2.17	0.46
1:B:212:LEU:HD12	1:B:216:ARG:O	2.15	0.46
1:C:226:LEU:HD12	1:C:231:HIS:HB3	1.97	0.46
1:A:381:SER:OG	1:A:415:THR:HG22	2.15	0.46
1:A:112:ASP:C	1:A:114:ASP:H	2.18	0.46
1:A:114:ASP:OD1	1:A:115:GLY:N	2.49	0.46
1:A:279:PHE:HB2	1:A:282:SER:HB3	1.98	0.46
1:C:210:ASN:O	1:C:217:ARG:NH1	2.48	0.46
1:A:262:ARG:HH22	1:A:461:SER:HB2	1.81	0.46
1:B:499:VAL:O	1:B:500:ASP:HB2	2.15	0.46
1:A:162:ARG:HG3	1:A:201:VAL:HG21	1.98	0.46
1:A:13:GLU:HG2	1:A:14:GLN:H	1.79	0.45
1:C:367:ILE:HG21	1:C:402:PHE:HE2	1.81	0.45
1:B:291:GLY:O	1:B:451:ARG:NH1	2.31	0.45
1:A:12:THR:H	1:A:13:GLU:HA	1.82	0.45
1:C:273:MET:SD	1:C:468:ARG:HD3	2.57	0.45
1:A:499:VAL:HA	1:A:500:ASP:C	2.35	0.45
1:C:86:LYS:HA	1:C:89:LEU:HD12	1.99	0.45
1:B:185:ARG:NH1	1:B:188:GLU:O	2.49	0.45
1:C:55:LEU:HG	3:C:603:ATP:O1A	2.17	0.45
1:C:367:ILE:O	1:C:371:LYS:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:HA	1:B:204:ASN:HB2	1.99	0.44
1:B:426:THR:HG21	1:B:430:ILE:HG12	1.99	0.44
1:A:50:GLY:HA3	1:B:225:LYS:HB3	1.98	0.44
1:B:123:ASP:HA	1:B:127:LEU:H	1.83	0.44
1:C:338:LEU:HB3	1:C:344:LEU:CB	2.47	0.44
1:C:294:LYS:HG3	1:C:440:LEU:HD12	1.99	0.44
1:B:55:LEU:HG	3:B:604:ATP:O1A	2.17	0.44
1:C:296:LEU:HD13	1:C:331:TRP:CD2	2.52	0.44
1:B:162:ARG:HG3	1:B:201:VAL:CG2	2.48	0.44
1:A:54:THR:HG23	1:A:146:ASP:OD2	2.18	0.43
1:C:217:ARG:NH2	4:C:741:HOH:O	2.52	0.43
1:C:363:ILE:O	1:C:367:ILE:HG12	2.18	0.43
1:C:48:THR:O	1:C:53:LYS:NZ	2.51	0.43
1:A:115:GLY:HA3	1:A:116:GLN:HA	1.66	0.43
1:B:121:ASP:C	1:B:123:ASP:N	2.72	0.43
1:B:123:ASP:O	1:B:127:LEU:N	2.51	0.43
1:C:152:PHE:CE2	1:C:161:VAL:HG13	2.53	0.43
1:A:149:THR:HG21	1:A:194:ARG:HD2	2.00	0.43
1:B:210:ASN:O	1:B:217:ARG:NH1	2.51	0.43
1:B:248:PRO:HG2	1:B:251:ALA:HB2	2.00	0.43
1:A:448:GLU:HG2	1:B:466:GLY:HA2	1.99	0.43
1:B:148:VAL:HG21	1:B:181:MET:SD	2.58	0.43
1:C:148:VAL:HG21	1:C:181:MET:HE3	2.00	0.43
1:A:207:ILE:HD11	1:A:224:LEU:HD22	2.00	0.43
1:A:425:ILE:HD11	1:A:456:PHE:CE2	2.53	0.43
1:B:448:GLU:HG2	1:C:466:GLY:HA2	2.01	0.43
1:A:15:SER:HB3	1:A:16:SER:HA	2.01	0.43
1:A:253:ARG:O	1:A:255:THR:N	2.48	0.43
1:C:426:THR:OG1	1:C:431:SEP:O1P	2.25	0.43
1:B:209:ARG:NH1	4:B:737:HOH:O	2.51	0.42
1:B:458:MET:HG2	1:B:461:SER:HB3	1.99	0.42
1:A:447:GLY:HA2	1:B:489:ILE:HD12	2.02	0.42
1:C:90:SER:HG	3:C:603:ATP:HN61	1.59	0.42
1:B:283:ILE:HD12	1:B:412:PHE:HE2	1.84	0.42
1:A:117:GLU:HB3	1:A:118:VAL:HA	2.01	0.42
1:B:322:ALA:HB3	1:C:256:GLN:O	2.19	0.42
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.94	0.42
1:C:302:LEU:HD11	1:C:314:LEU:HD13	2.02	0.42
1:C:71:PRO:HB2	1:C:140:ALA:HA	2.01	0.42
1:B:226:LEU:HD12	1:B:231:HIS:HB3	2.01	0.42
1:C:423:ASN:OD1	1:C:423:ASN:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:MET:HE2	1:A:420:MET:HB2	1.93	0.42
1:B:497:ILE:O	1:B:500:ASP:N	2.53	0.41
1:A:379:SER:N	1:A:413:THR:OG1	2.35	0.41
1:B:499:VAL:O	1:B:501:GLU:HA	2.20	0.41
1:A:126:ALA:HA	1:A:129:GLU:H	1.85	0.41
1:A:348:CYS:HB3	1:B:254:LEU:HB3	2.02	0.41
1:A:294:LYS:HE2	1:A:294:LYS:HB2	1.84	0.41
1:B:257:ARG:HH21	1:B:407:GLU:HG2	1.86	0.41
1:C:216:ARG:NH2	1:C:352:GLU:OE1	2.53	0.41
1:C:350:TYR:HA	1:C:351:PRO:HD3	1.94	0.41
1:C:458:MET:HB3	1:C:458:MET:HE3	1.97	0.41
1:A:264:SER:OG	1:A:304:THR:HG21	2.21	0.41
1:A:393:ARG:HH21	1:A:429:HIS:HB2	1.85	0.41
1:B:393:ARG:NH2	1:B:429:HIS:HB2	2.36	0.41
1:A:187:ASP:OD1	1:A:188:GLU:N	2.53	0.41
1:B:289:ALA:O	1:B:292:THR:OG1	2.25	0.41
1:B:43:THR:O	1:B:180:ILE:HD12	2.20	0.41
1:B:296:LEU:O	1:B:300:LYS:HG2	2.20	0.41
1:B:290:THR:OG1	1:C:457:LYS:NZ	2.35	0.40
1:C:96:GLN:HA	1:C:99:ILE:HD12	2.03	0.40
1:B:229:THR:OG1	1:B:230:THR:N	2.54	0.40
1:C:438:LEU:HD23	1:C:455:VAL:HG22	1.87	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	490/524 (94%)	455 (93%)	24 (5%)	11 (2%)	<b>6</b>   <b>14</b>
1	B	486/524 (93%)	443 (91%)	31 (6%)	12 (2%)	<b>5</b>   <b>12</b>
1	C	486/524 (93%)	447 (92%)	32 (7%)	7 (1%)	<b>11</b>   <b>24</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1462/1572 (93%)	1345 (92%)	87 (6%)	30 (2%)	<b>7</b> <b>15</b>

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ALA
1	B	117	GLU
1	B	118	VAL
1	B	500	ASP
1	C	254	LEU
1	A	18	GLU
1	A	117	GLU
1	A	155	TYR
1	A	212	LEU
1	B	119	ALA
1	B	121	ASP
1	B	249	LEU
1	B	254	LEU
1	C	251	ALA
1	C	252	MET
1	A	213	GLU
1	A	420	MET
1	B	420	MET
1	C	13	GLU
1	C	124	LEU
1	B	155	TYR
1	B	348	CYS
1	B	463	HIS
1	B	499	VAL
1	C	18	GLU
1	C	348	CYS
1	A	113	PRO
1	A	125	SER
1	A	252	MET
1	A	121	ASP

### 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	418/445 (94%)	410 (98%)	8 (2%)	57	77
1	B	414/445 (93%)	396 (96%)	18 (4%)	29	54
1	C	413/445 (93%)	407 (98%)	6 (2%)	65	82
All	All	1245/1335 (93%)	1213 (97%)	32 (3%)	46	70

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	39	GLN
1	A	83	ASP
1	A	124	LEU
1	A	151	VAL
1	A	249	LEU
1	A	292	THR
1	A	497	ILE
1	B	12	THR
1	B	14	GLN
1	B	46	SER
1	B	49	SER
1	B	111	PRO
1	B	135	ILE
1	B	155	TYR
1	B	192	VAL
1	B	199	GLU
1	B	201	VAL
1	B	220	THR
1	B	242	ASN
1	B	255	THR
1	B	292	THR
1	B	463	HIS
1	B	484	ARG
1	B	499	VAL
1	B	501	GLU
1	C	213	GLU
1	C	370	PHE
1	C	433	ILE
1	C	453	ILE
1	C	496	ARG

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Mol	Chain	Res	Type
1	C	500	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	323	GLN
1	B	361	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 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	432	1	8,10,11	1.10	0	10,14,16	1.85	2 (20%)
1	SEP	C	431	1	8,9,10	1.54	1 (12%)	8,12,14	1.51	2 (25%)
1	SEP	A	431	1	8,9,10	1.53	1 (12%)	8,12,14	1.47	2 (25%)
1	TPO	B	432	1	8,10,11	1.16	0	10,14,16	2.17	2 (20%)
1	SEP	B	431	1	8,9,10	1.54	1 (12%)	8,12,14	1.51	2 (25%)
1	TPO	A	432	1	8,10,11	1.06	0	10,14,16	1.98	2 (20%)

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	432	1	-	1/9/11/13	-
1	SEP	C	431	1	-	3/5/8/10	-
1	SEP	A	431	1	-	4/5/8/10	-
1	TPO	B	432	1	-	1/9/11/13	-
1	SEP	B	431	1	-	3/5/8/10	-
1	TPO	A	432	1	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	431	SEP	P-O1P	3.37	1.61	1.50
1	A	431	SEP	P-O1P	3.36	1.61	1.50
1	B	431	SEP	P-O1P	3.34	1.61	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	TPO	P-OG1-CB	-5.39	106.94	123.21
1	B	432	TPO	P-OG1-CB	-5.05	107.97	123.21
1	C	432	TPO	P-OG1-CB	-4.73	108.93	123.21
1	B	432	TPO	CG2-CB-CA	-4.18	104.91	113.16
1	A	431	SEP	OG-CB-CA	2.78	110.85	108.14
1	C	431	SEP	OG-CB-CA	2.76	110.83	108.14
1	C	432	TPO	CG2-CB-CA	-2.67	107.90	113.16
1	B	431	SEP	OG-CB-CA	2.64	110.72	108.14
1	B	431	SEP	P-OG-CB	-2.58	111.19	118.30
1	C	431	SEP	P-OG-CB	-2.53	111.33	118.30
1	A	432	TPO	CG2-CB-CA	-2.51	108.22	113.16
1	A	431	SEP	P-OG-CB	-2.30	111.96	118.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	432	TPO	CB-OG1-P-O1P
1	C	431	SEP	CB-OG-P-O1P
1	C	431	SEP	CB-OG-P-O2P
1	C	431	SEP	CB-OG-P-O3P
1	A	431	SEP	CB-OG-P-O2P
1	A	431	SEP	CB-OG-P-O3P
1	B	431	SEP	CB-OG-P-O2P

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Mol	Chain	Res	Type	Atoms
1	B	431	SEP	CB-OG-P-O3P
1	A	431	SEP	CB-OG-P-O1P
1	B	431	SEP	CB-OG-P-O1P
1	A	431	SEP	CA-CB-OG-P
1	B	432	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	431	SEP	1	0
1	B	432	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	602	2	26,33,33	0.92	1 (3%)	31,52,52	1.51	5 (16%)
3	ATP	A	803	-	26,33,33	0.93	1 (3%)	31,52,52	1.48	5 (16%)
3	ATP	C	603	2	26,33,33	0.94	1 (3%)	31,52,52	1.46	5 (16%)
3	ATP	A	802	2	26,33,33	0.95	1 (3%)	31,52,52	1.49	5 (16%)
3	ATP	B	602	2	26,33,33	0.91	1 (3%)	31,52,52	1.56	5 (16%)
3	ATP	B	604	2	26,33,33	0.92	1 (3%)	31,52,52	1.46	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	602	2	-	8/18/38/38	0/3/3/3
3	ATP	A	803	-	-	7/18/38/38	0/3/3/3
3	ATP	C	603	2	-	8/18/38/38	0/3/3/3
3	ATP	A	802	2	-	7/18/38/38	0/3/3/3
3	ATP	B	602	2	-	6/18/38/38	0/3/3/3
3	ATP	B	604	2	-	9/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	ATP	C5-C4	2.49	1.47	1.40
3	C	602	ATP	C5-C4	2.44	1.47	1.40
3	B	602	ATP	C5-C4	2.43	1.47	1.40
3	C	603	ATP	C5-C4	2.41	1.47	1.40
3	A	803	ATP	C5-C4	2.39	1.47	1.40
3	B	604	ATP	C5-C4	2.35	1.47	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ATP	PB-O3B-PG	-3.91	119.42	132.83
3	C	602	ATP	PB-O3B-PG	-3.61	120.44	132.83
3	A	802	ATP	PB-O3B-PG	-3.56	120.61	132.83
3	A	802	ATP	C3'-C2'-C1'	3.46	106.18	100.98
3	B	602	ATP	C3'-C2'-C1'	3.38	106.07	100.98
3	C	602	ATP	C3'-C2'-C1'	3.34	106.01	100.98
3	A	803	ATP	N3-C2-N1	-3.25	123.60	128.68
3	C	603	ATP	N3-C2-N1	-3.20	123.68	128.68
3	B	602	ATP	N3-C2-N1	-3.20	123.68	128.68
3	B	604	ATP	N3-C2-N1	-3.18	123.70	128.68
3	A	803	ATP	PB-O3B-PG	-3.17	121.93	132.83
3	C	602	ATP	N3-C2-N1	-3.15	123.76	128.68
3	B	604	ATP	PB-O3B-PG	-3.11	122.16	132.83
3	B	604	ATP	C3'-C2'-C1'	3.07	105.60	100.98
3	C	603	ATP	C3'-C2'-C1'	3.03	105.55	100.98
3	A	803	ATP	C3'-C2'-C1'	3.03	105.53	100.98
3	B	602	ATP	PA-O3A-PB	-2.96	122.66	132.83
3	C	602	ATP	PA-O3A-PB	-2.96	122.66	132.83
3	C	603	ATP	PA-O3A-PB	-2.89	122.92	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	ATP	N3-C2-N1	-2.89	124.17	128.68
3	C	603	ATP	PB-O3B-PG	-2.87	122.97	132.83
3	A	803	ATP	PA-O3A-PB	-2.82	123.16	132.83
3	B	604	ATP	C4-C5-N7	-2.72	106.56	109.40
3	A	803	ATP	C4-C5-N7	-2.72	106.56	109.40
3	A	802	ATP	PA-O3A-PB	-2.69	123.58	132.83
3	C	603	ATP	C4-C5-N7	-2.69	106.59	109.40
3	A	802	ATP	C4-C5-N7	-2.54	106.75	109.40
3	C	602	ATP	C4-C5-N7	-2.42	106.88	109.40
3	B	602	ATP	C4-C5-N7	-2.42	106.88	109.40
3	B	604	ATP	PA-O3A-PB	-2.24	125.14	132.83

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	ATP	PB-O3A-PA-O5'
3	C	602	ATP	C5'-O5'-PA-O1A
3	C	602	ATP	C5'-O5'-PA-O2A
3	A	803	ATP	C5'-O5'-PA-O1A
3	A	803	ATP	C5'-O5'-PA-O2A
3	C	603	ATP	C5'-O5'-PA-O1A
3	C	603	ATP	C5'-O5'-PA-O2A
3	A	802	ATP	PB-O3B-PG-O2G
3	A	802	ATP	C5'-O5'-PA-O1A
3	A	802	ATP	C5'-O5'-PA-O2A
3	B	602	ATP	PB-O3B-PG-O2G
3	B	602	ATP	PB-O3A-PA-O5'
3	B	602	ATP	C5'-O5'-PA-O1A
3	B	602	ATP	C5'-O5'-PA-O2A
3	B	604	ATP	C5'-O5'-PA-O2A
3	A	802	ATP	PA-O3A-PB-O1B
3	A	802	ATP	PB-O3A-PA-O5'
3	B	604	ATP	PB-O3A-PA-O5'
3	A	803	ATP	PB-O3B-PG-O1G
3	B	604	ATP	PB-O3B-PG-O1G
3	B	604	ATP	C5'-O5'-PA-O3A
3	A	803	ATP	PA-O3A-PB-O2B
3	C	603	ATP	PA-O3A-PB-O1B
3	B	604	ATP	C5'-O5'-PA-O1A
3	B	604	ATP	C3'-C4'-C5'-O5'
3	C	602	ATP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	A	802	ATP	PA-O3A-PB-O2B
3	B	602	ATP	PA-O3A-PB-O2B
3	C	602	ATP	PB-O3B-PG-O1G
3	C	603	ATP	PA-O3A-PB-O2B
3	C	603	ATP	PB-O3B-PG-O1G
3	C	602	ATP	PB-O3B-PG-O2G
3	A	803	ATP	PB-O3B-PG-O2G
3	A	803	ATP	PB-O3B-PG-O3G
3	C	603	ATP	PB-O3B-PG-O2G
3	C	603	ATP	PB-O3B-PG-O3G
3	B	604	ATP	PB-O3B-PG-O2G
3	B	604	ATP	PB-O3B-PG-O3G
3	C	602	ATP	C5'-O5'-PA-O3A
3	A	803	ATP	C5'-O5'-PA-O3A
3	C	603	ATP	C5'-O5'-PA-O3A
3	A	802	ATP	C5'-O5'-PA-O3A
3	B	602	ATP	C5'-O5'-PA-O3A
3	C	602	ATP	C3'-C4'-C5'-O5'
3	B	604	ATP	PB-O3A-PA-O2A

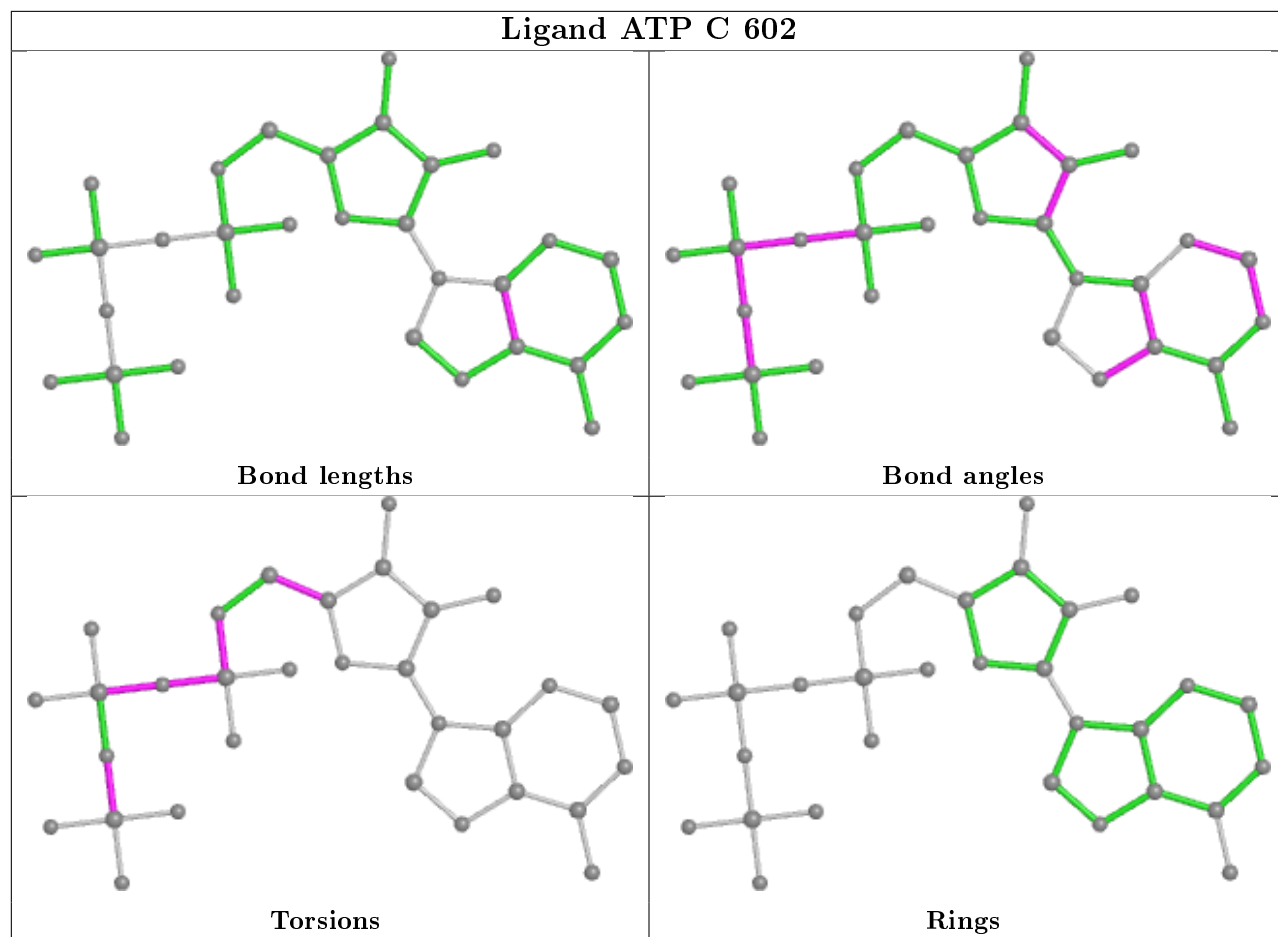
There are no ring outliers.

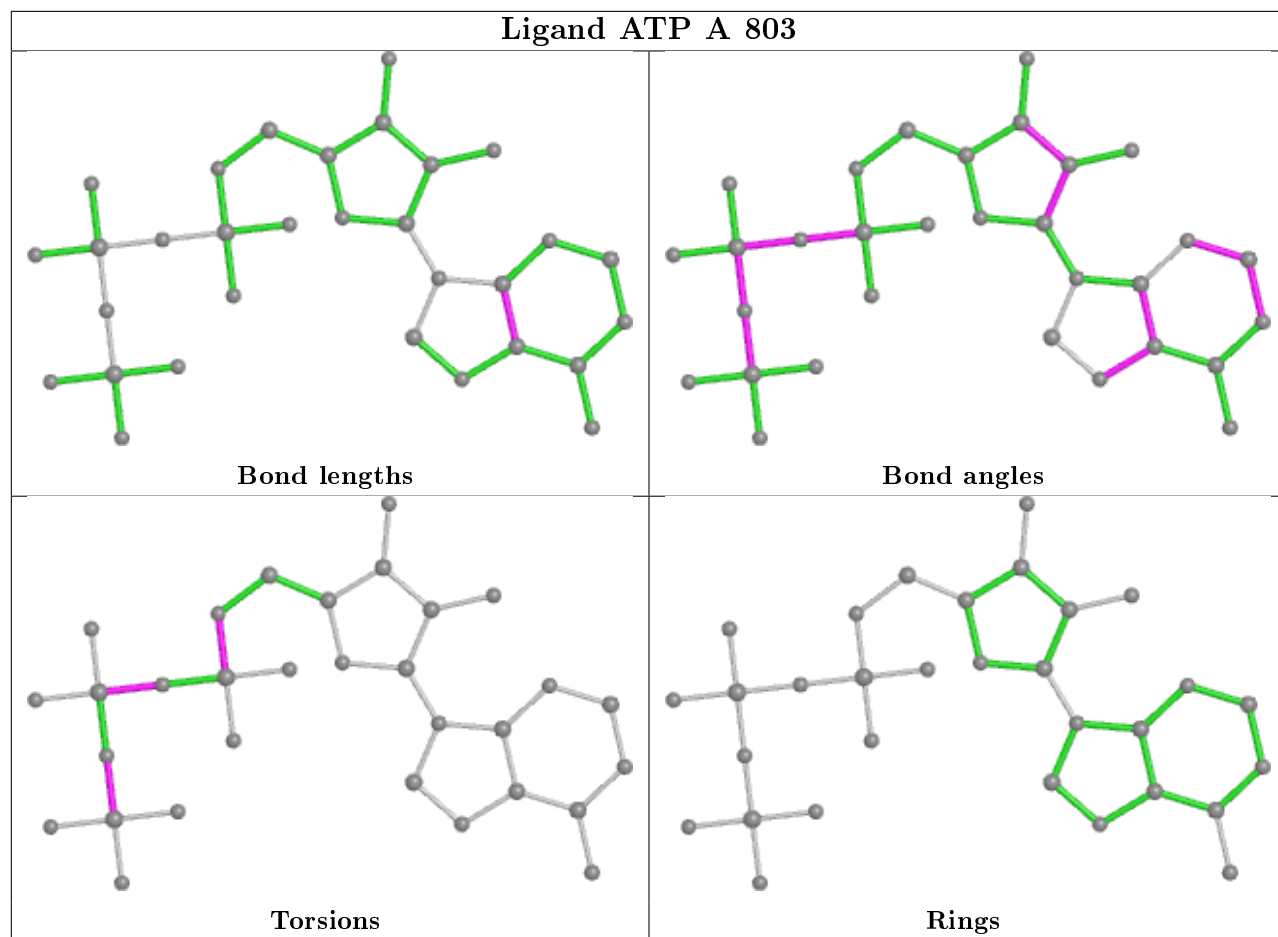
2 monomers are involved in 5 short contacts:

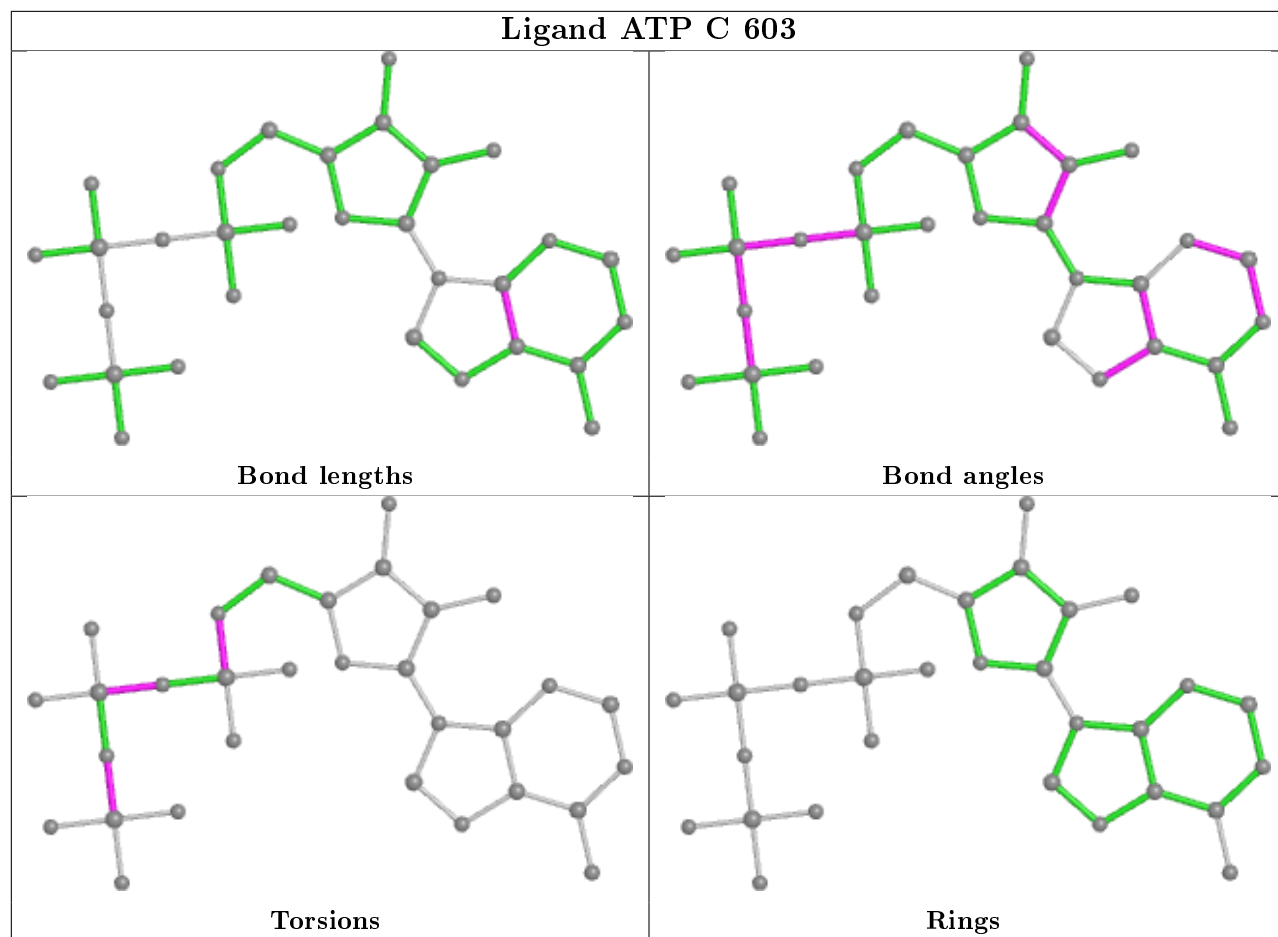
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	ATP	3	0
3	B	604	ATP	2	0

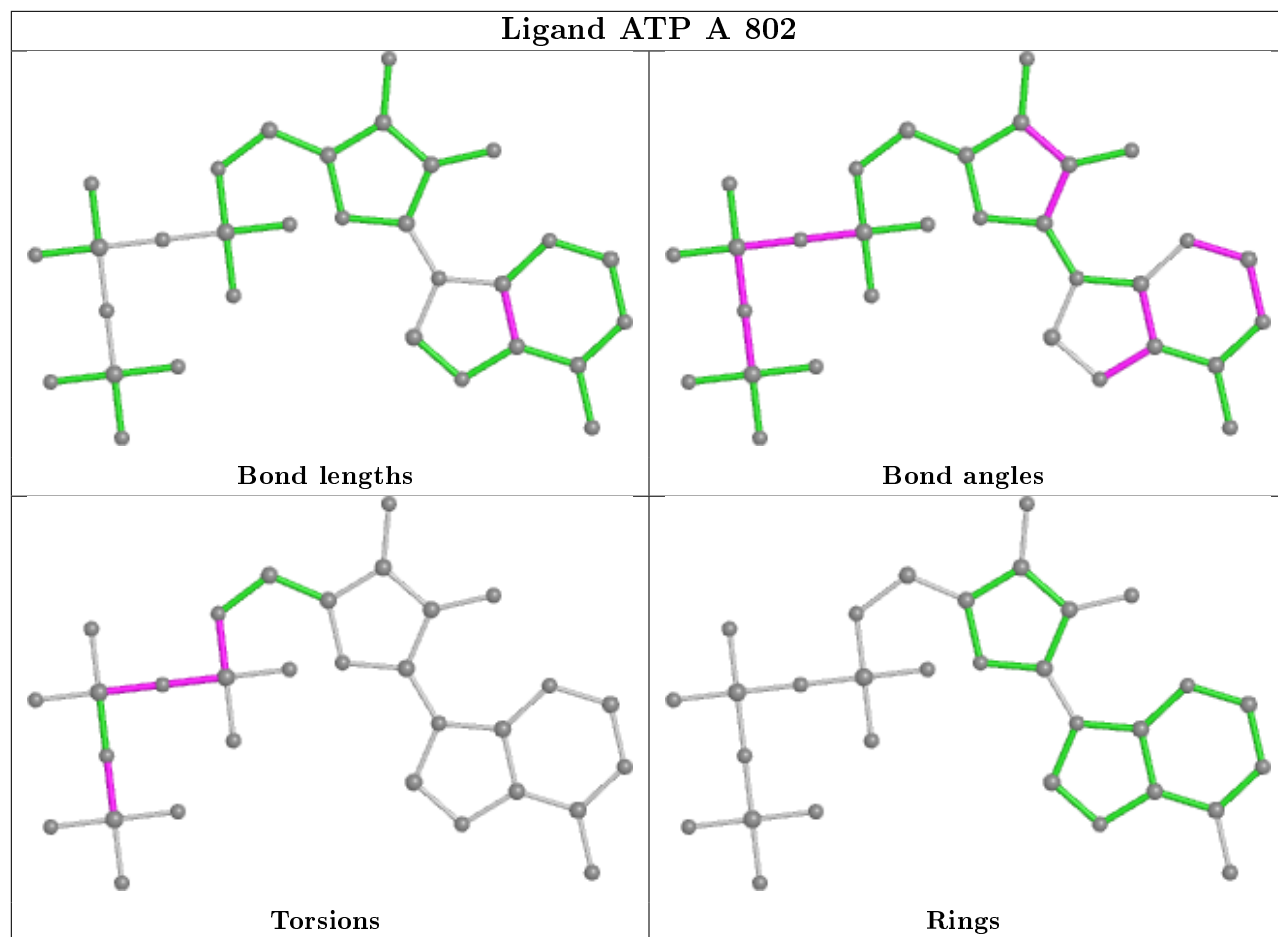
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

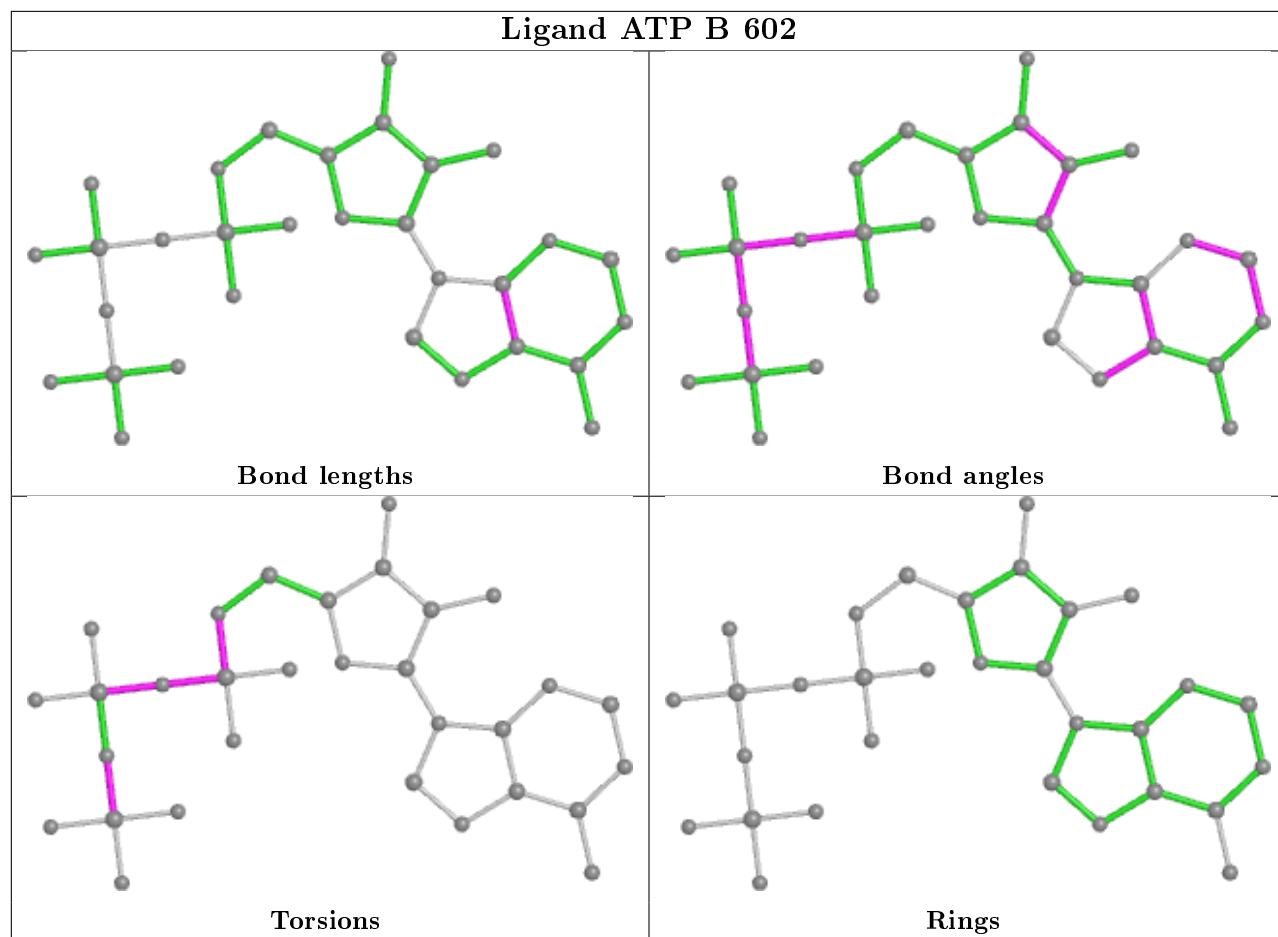


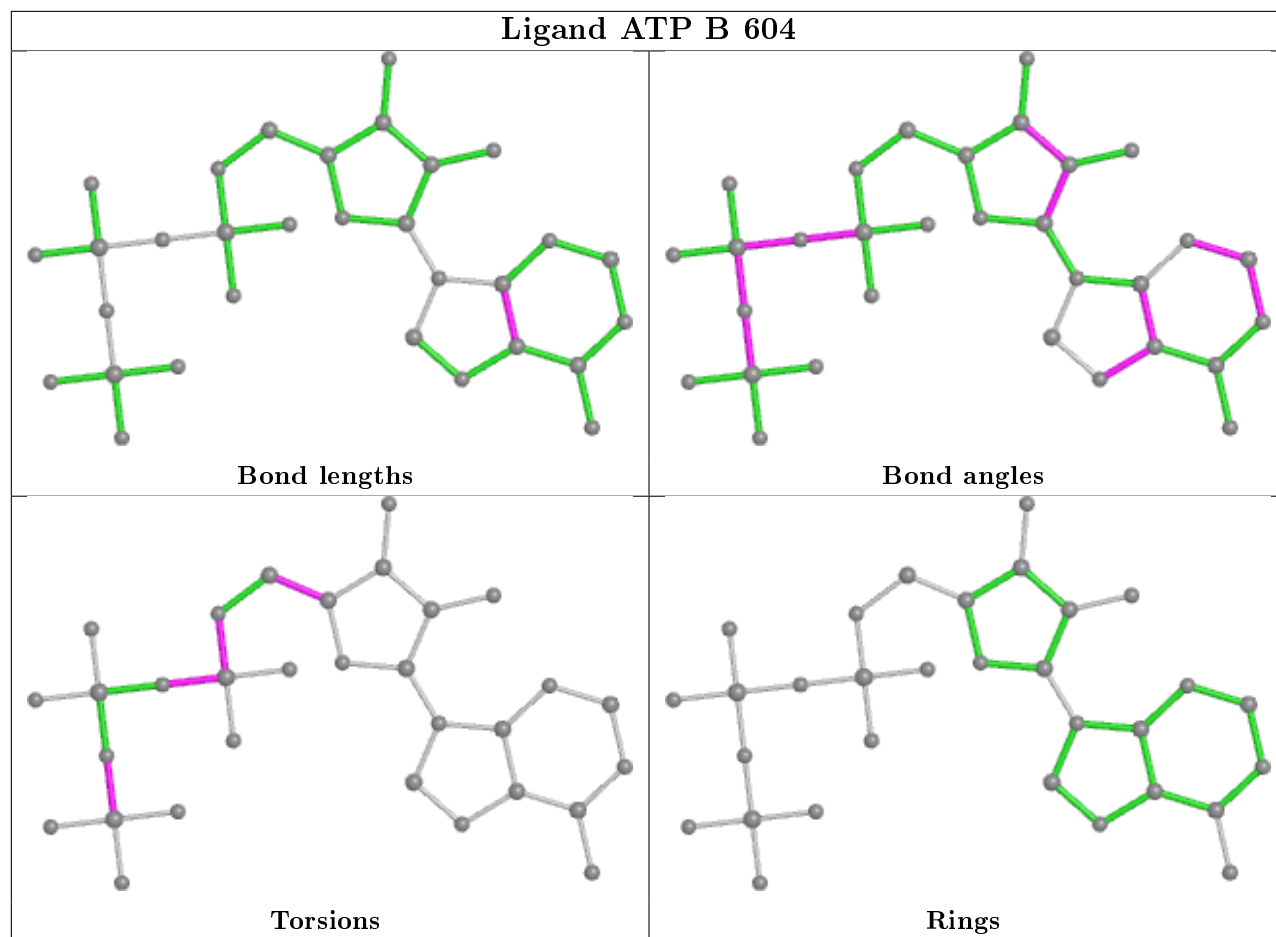












## 5.7 Other polymers [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	492/524 (93%)	0.31	34 (6%) 16 11	24, 44, 109, 151	0
1	B	488/524 (93%)	0.31	28 (5%) 23 17	25, 45, 99, 141	0
1	C	488/524 (93%)	0.34	24 (4%) 29 22	23, 51, 106, 143	0
All	All	1468/1572 (93%)	0.32	86 (5%) 22 16	23, 47, 107, 151	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	TYR	12.4
1	C	500	ASP	8.6
1	C	15	SER	8.3
1	A	15	SER	7.7
1	A	503	THR	7.5
1	B	155	TYR	7.0
1	B	15	SER	6.9
1	B	124	LEU	6.9
1	A	504	GLU	6.8
1	C	250	GLY	6.5
1	C	13	GLU	6.3
1	A	250	GLY	6.2
1	C	498	SER	6.0
1	A	154	GLN	5.7
1	A	114	ASP	5.5
1	B	500	ASP	5.4
1	C	499	VAL	5.2
1	A	14	GLN	5.2
1	C	11	PRO	5.1
1	B	14	GLN	5.0
1	B	498	SER	5.0
1	B	123	ASP	5.0
1	B	252	MET	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	251	ALA	4.9
1	B	13	GLU	4.8
1	B	501	GLU	4.8
1	B	117	GLU	4.7
1	A	501	GLU	4.7
1	A	502	LYS	4.7
1	C	278	PHE	4.5
1	A	12	THR	4.5
1	B	16	SER	4.4
1	A	153	GLN	4.4
1	A	249	LEU	4.4
1	A	17	ALA	4.3
1	C	12	THR	4.2
1	A	11	PRO	4.2
1	C	14	GLN	4.2
1	B	499	VAL	4.2
1	A	203	ASP	4.1
1	B	12	THR	4.1
1	A	121	ASP	4.0
1	A	13	GLU	4.0
1	B	115	GLY	3.7
1	B	122	PHE	3.7
1	C	255	THR	3.7
1	C	17	ALA	3.4
1	C	119	ALA	3.4
1	C	155	TYR	3.3
1	A	16	SER	3.3
1	A	156	ASP	3.3
1	C	249	LEU	3.1
1	A	500	ASP	3.1
1	A	117	GLU	3.0
1	A	499	VAL	3.0
1	B	120	GLY	3.0
1	A	251	ALA	3.0
1	B	152	PHE	2.9
1	C	123	ASP	2.9
1	C	16	SER	2.9
1	B	156	ASP	2.8
1	B	118	VAL	2.8
1	C	256	GLN	2.8
1	B	114	ASP	2.7
1	B	249	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	2.7
1	B	275	GLY	2.7
1	A	115	GLY	2.7
1	A	163	ARG	2.7
1	C	118	VAL	2.7
1	C	115	GLY	2.6
1	A	152	PHE	2.6
1	A	498	SER	2.6
1	C	156	ASP	2.6
1	A	165	ILE	2.5
1	B	278	PHE	2.4
1	C	122	PHE	2.3
1	B	203	ASP	2.3
1	A	252	MET	2.3
1	A	248	PRO	2.3
1	B	127	LEU	2.2
1	B	125	SER	2.2
1	A	158	ALA	2.1
1	C	163	ARG	2.1
1	A	116	GLN	2.0
1	B	250	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	C	431	10/11	0.84	0.21	56,60,78,92	0
1	TPO	C	432	11/12	0.88	0.23	59,67,78,85	0
1	SEP	B	431	10/11	0.88	0.22	43,50,79,90	0
1	SEP	A	431	10/11	0.92	0.18	47,54,67,76	0
1	TPO	B	432	11/12	0.95	0.17	44,47,64,69	0
1	TPO	A	432	11/12	0.96	0.14	51,53,65,66	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

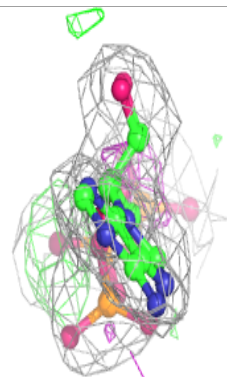
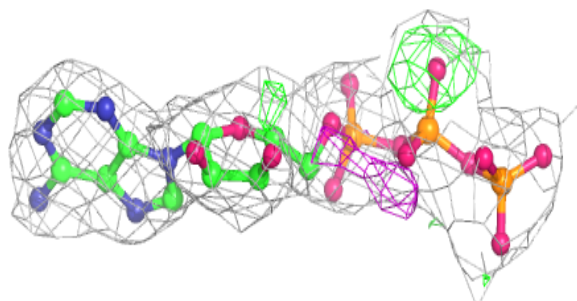
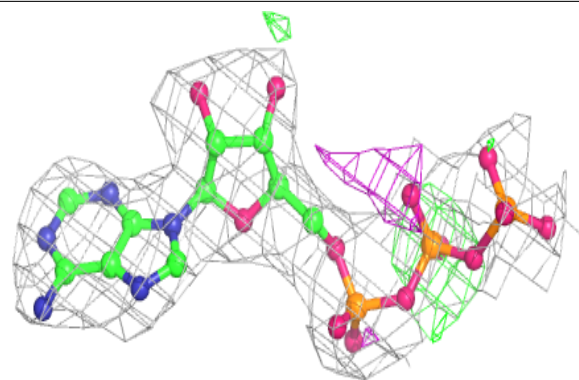
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	804	1/1	0.25	0.49	64,64,64,64	0
2	MG	C	604	1/1	0.70	0.13	45,45,45,45	0
2	MG	B	601	1/1	0.80	0.17	47,47,47,47	0
2	MG	A	801	1/1	0.89	0.26	32,32,32,32	0
2	MG	B	603	1/1	0.90	0.26	41,41,41,41	0
2	MG	C	601	1/1	0.91	0.26	44,44,44,44	0
3	ATP	B	604	31/31	0.92	0.20	28,37,61,67	0
3	ATP	A	803	31/31	0.93	0.19	24,32,63,74	0
3	ATP	C	602	31/31	0.94	0.21	31,36,58,77	0
3	ATP	C	603	31/31	0.94	0.18	26,37,59,68	0
3	ATP	B	602	31/31	0.94	0.19	32,41,63,75	0
3	ATP	A	802	31/31	0.96	0.16	26,33,47,65	0

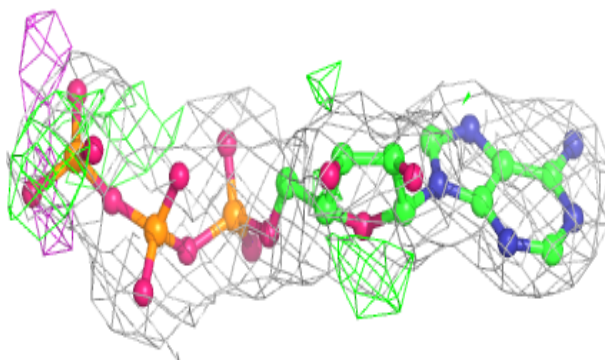
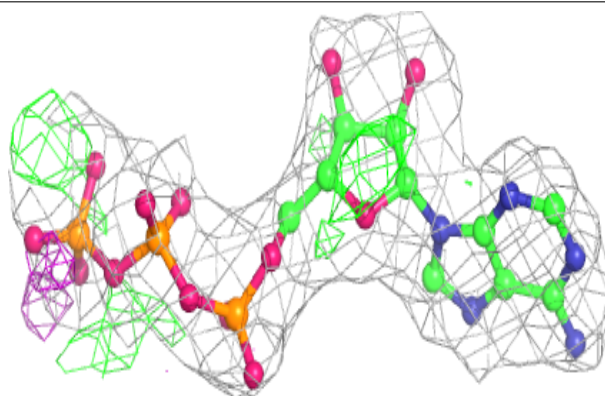
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 604:**

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

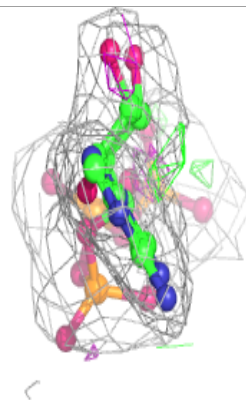
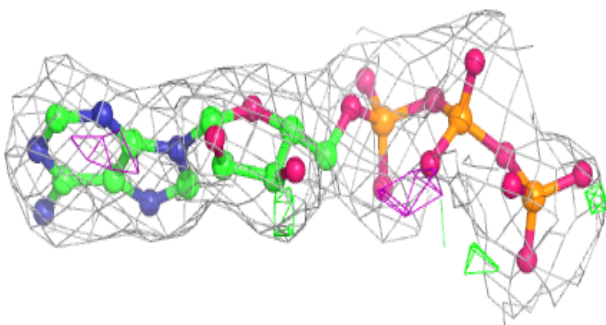
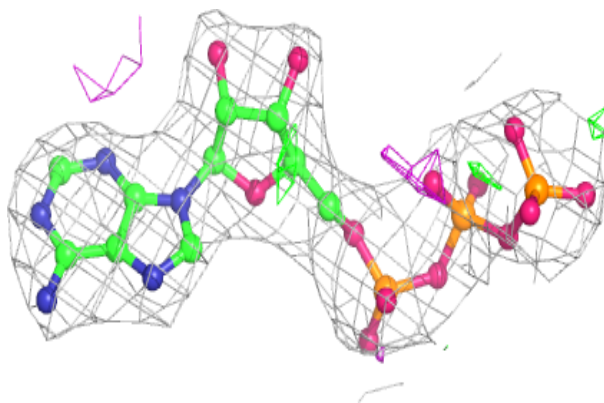
**Electron density around ATP A 803:**

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

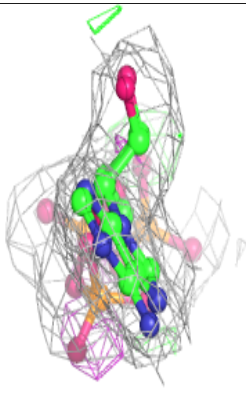
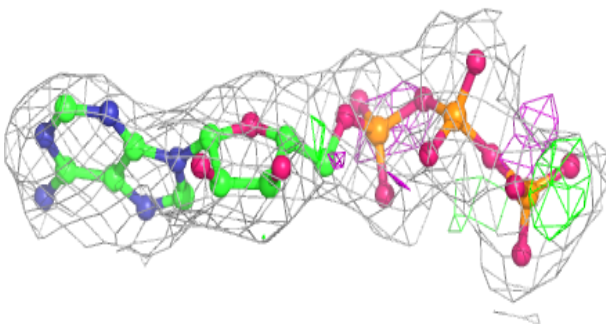
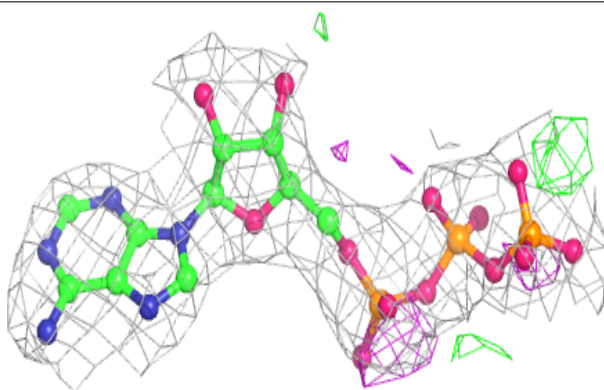


**Electron density around ATP C 602:**

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

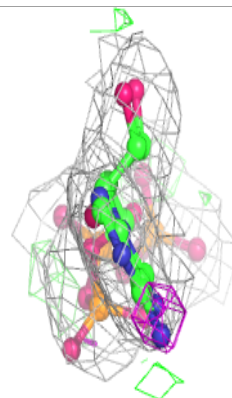
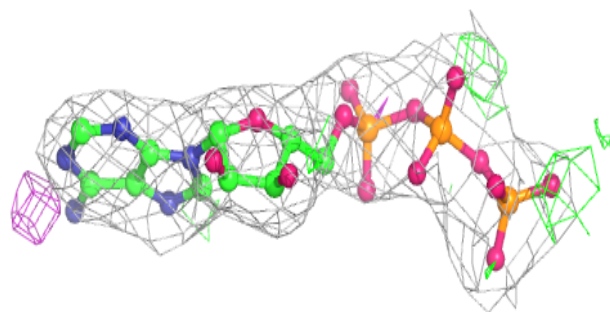
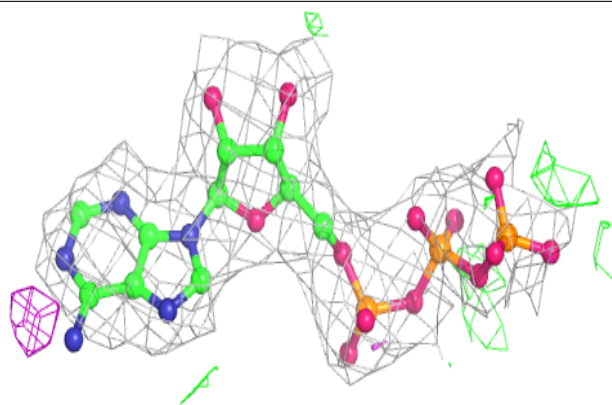
**Electron density around ATP C 603:**

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

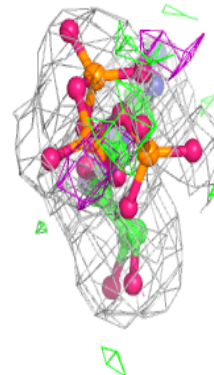
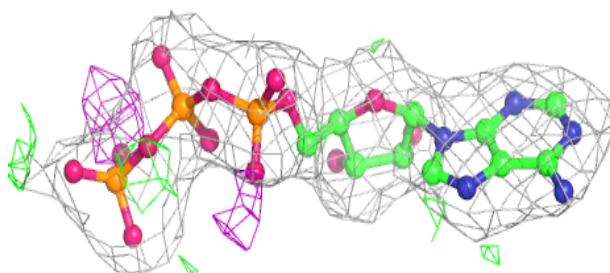
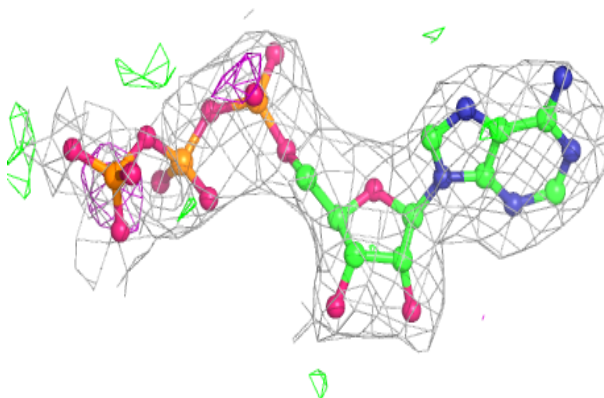


**Electron density around ATP B 602:**

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

**Electron density around ATP A 802:**

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



## 6.5 Other polymers

There are no such residues in this entry.