



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:54 pm BST

PDB ID : 3IN5  
Title : Structure of human DNA polymerase kappa inserting dATP opposite an 8-oxoG DNA lesion  
Authors : Silverstein, T.D.; Vasquez-Del Carpio, R.; Aggarwal, A.K.  
Deposited on : 2009-08-11  
Resolution : 3.20 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	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

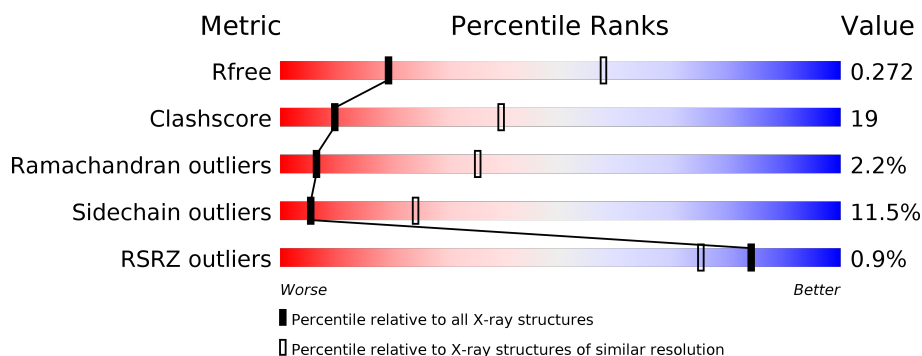
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	508	<div> <div>8%</div> <div>52%</div> <div>30%</div> <div>14%</div> </div>
1	B	508	<div> <div>54%</div> <div>27%</div> <div>5%</div> <div>14%</div> </div>
2	P	13	<div> <div>8%</div> <div>54%</div> <div>31%</div> <div>15%</div> </div>
2	Q	13	<div> <div>38%</div> <div>31%</div> <div>23%</div> <div>8%</div> </div>
3	T	18	<div> <div>22%</div> <div>33%</div> <div>28%</div> <div>17%</div> </div>
3	U	18	<div> <div>6%</div> <div>44%</div> <div>28%</div> <div>6%</div> <div>22%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7894 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 DNA polymerase kappa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	1	0
			3410	2148	598	643	21			
1	B	437	Total	C	N	O	S	0	0	0
			3346	2106	585	633	22			

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*G\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*CP\*TP\*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	0	0	0
			227	108	48	61	10			
2	Q	12	Total	C	N	O	P	0	0	0
			249	118	53	67	11			

- Molecule 3 is a DNA chain called DNA (5'-D(\*C\*CP\*TP\*AP\*(8OG)P\*GP\*AP\*GP\*TP\*C P\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	N	O	P	0	0	0
			300	144	51	91	14			
3	U	14	Total	C	N	O	P	0	0	0
			280	134	49	84	13			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
4	B	1	Total 30	C 10	N 5	O 12	P 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mg 2 2	0	0
5	A	2	Total Mg 2 2	0	0

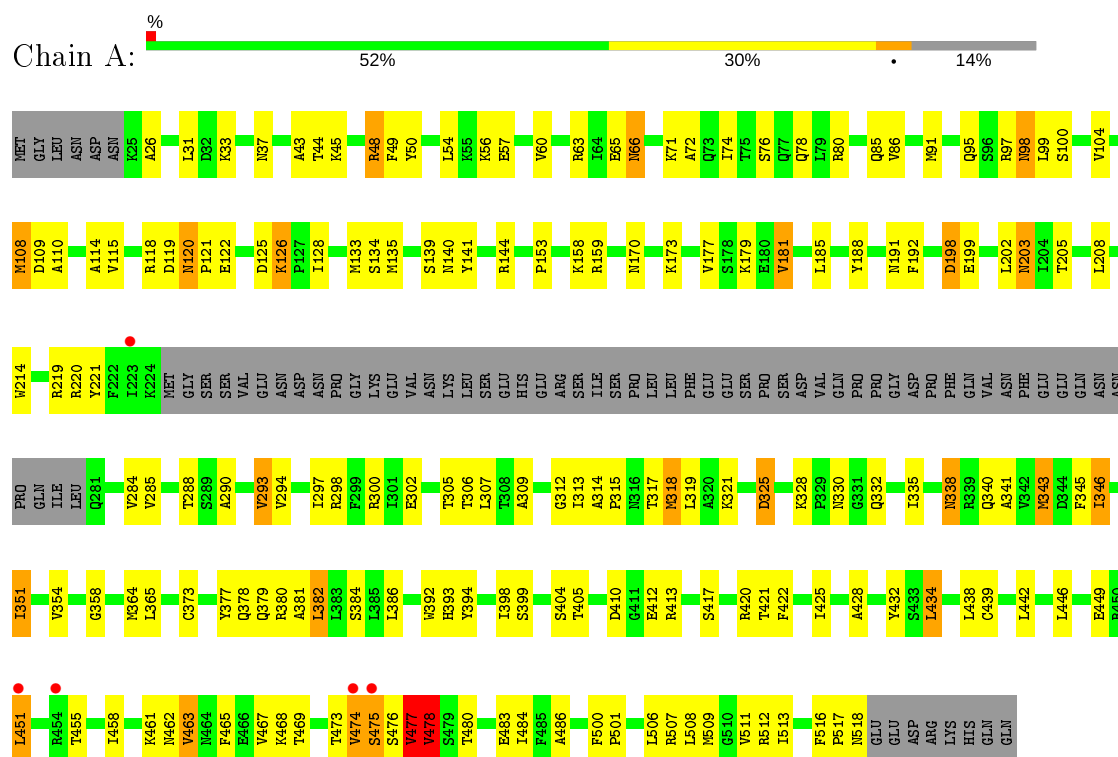
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total O 10 10	0	0
6	B	7	Total O 7 7	0	0
6	U	1	Total O 1 1	0	0

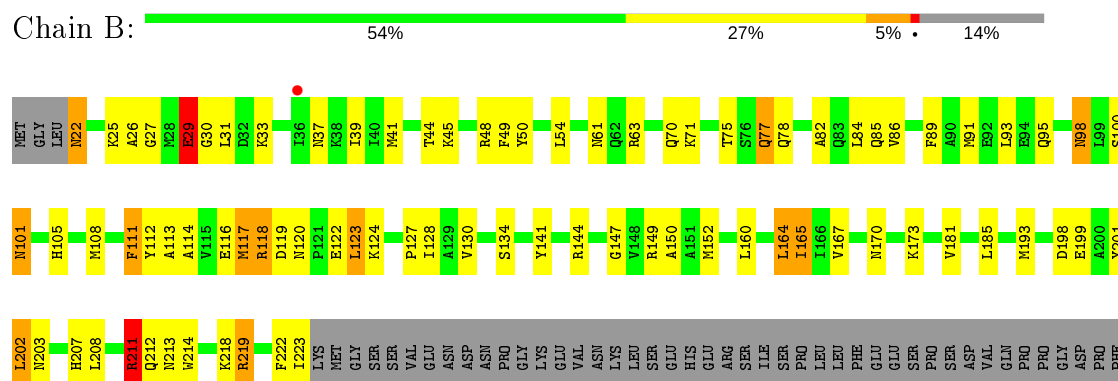
### 3 Residue-property plots [i](#)

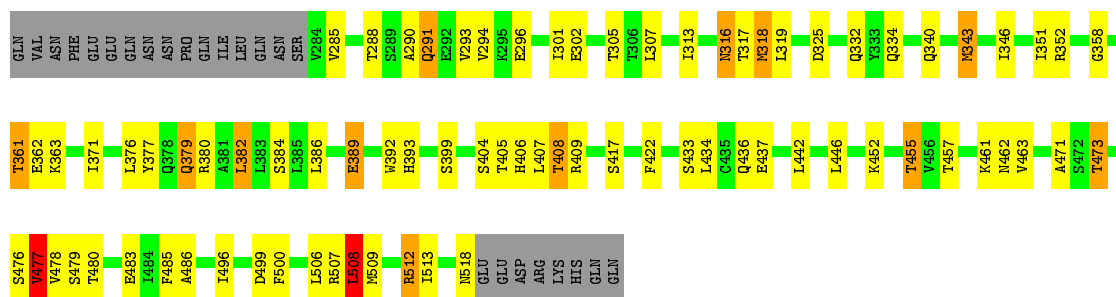
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: DNA polymerase kappa

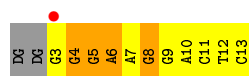


- Molecule 1: DNA polymerase kappa





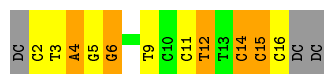
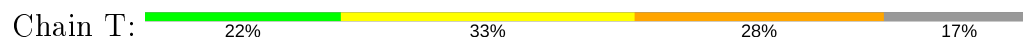
- Molecule 2: DNA (5'-D(\*GP\*G\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*CP\*TP\*(DOC))-3')



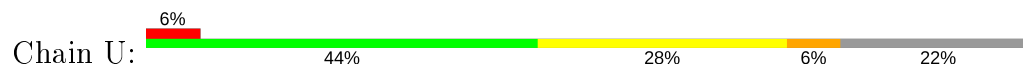
- Molecule 2: DNA (5'-D(\*GP\*G\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*CP\*TP\*(DOC))-3')



- Molecule 3: DNA (5'-D(\*C\*CP\*TP\*AP\*(8OG)P\*GP\*AP\*GP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3')



- Molecule 3: DNA (5'-D(\*C\*CP\*TP\*AP\*(8OG)P\*GP\*AP\*GP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.85Å 154.48Å 217.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.12 – 3.20 47.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.12-3.20) 99.9 (47.12-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.225 , 0.274 0.223 , 0.272	Depositor DCC
$R_{free}$ test set	1640 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: 8OG, MG, ATP, DOC

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	0.60	0/3465	0.70	0/4677
1	B	0.59	1/3397 (0.0%)	0.70	3/4591 (0.1%)
2	P	1.22	1/236 (0.4%)	1.77	6/364 (1.6%)
2	Q	1.17	2/261 (0.8%)	1.80	8/403 (2.0%)
3	T	1.17	0/307	2.08	14/468 (3.0%)
3	U	1.12	1/285 (0.4%)	1.88	6/434 (1.4%)
All	All	0.70	5/7951 (0.1%)	0.98	37/10937 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389	GLU	CD-OE2	7.81	1.34	1.25
2	P	12	DT	C3'-O3'	-5.93	1.36	1.44
3	U	12	DT	C1'-N1	5.90	1.56	1.49
2	Q	12	DT	C3'-O3'	-5.62	1.36	1.44
2	Q	11	DC	C3'-O3'	-5.01	1.37	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	4	DA	O4'-C4'-C3'	-13.94	97.64	106.00
3	T	2	DC	O4'-C1'-N1	12.30	116.61	108.00
3	U	12	DT	O4'-C1'-N1	11.27	115.89	108.00
3	T	12	DT	O4'-C1'-N1	11.26	115.88	108.00
3	U	8	DG	O4'-C1'-N9	10.41	115.29	108.00
2	Q	2	DG	P-O3'-C3'	9.01	130.52	119.70
2	P	4	DG	O4'-C1'-N9	8.47	113.93	108.00
3	T	6	DG	O4'-C4'-C3'	-8.17	101.10	106.00
3	T	15	DC	O4'-C1'-N1	7.95	113.57	108.00
3	T	6	DG	O4'-C1'-N9	-7.77	102.56	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	2	DC	P-O3'-C3'	7.61	128.83	119.70
3	T	12	DT	N3-C4-O4	7.39	124.33	119.90
2	Q	6	DA	O4'-C4'-C3'	-7.35	101.56	104.50
2	P	3	DG	P-O3'-C3'	7.33	128.50	119.70
3	T	2	DC	O4'-C1'-C2'	-7.02	100.28	105.90
3	T	9	DT	N3-C4-O4	6.42	123.75	119.90
3	U	13	DT	N3-C4-O4	6.38	123.73	119.90
2	P	12	DT	O4'-C1'-N1	6.30	112.41	108.00
1	B	211	ARG	NE-CZ-NH1	6.23	123.41	120.30
2	P	8	DG	O4'-C1'-N9	-6.23	103.64	108.00
2	P	6	DA	O4'-C1'-N9	6.18	112.33	108.00
2	P	5	DG	O4'-C1'-N9	6.12	112.28	108.00
3	T	2	DC	C4'-C3'-C2'	-5.83	97.85	103.10
3	U	9	DT	N3-C4-O4	5.82	123.39	119.90
2	Q	12	DT	N3-C4-O4	5.72	123.33	119.90
3	T	12	DT	C5-C4-O4	-5.72	120.90	124.90
1	B	508	LEU	CA-CB-CG	5.69	128.38	115.30
3	T	14	DC	O4'-C1'-N1	5.65	111.96	108.00
3	T	4	DA	N1-C6-N6	5.59	121.96	118.60
2	Q	7	DA	O4'-C4'-C3'	-5.59	102.27	104.50
3	U	13	DT	C5-C4-O4	-5.47	121.07	124.90
1	B	512	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	Q	7	DA	O4'-C1'-N9	-5.40	104.22	108.00
3	T	3	DT	C5-C4-O4	-5.39	121.13	124.90
2	Q	12	DT	O4'-C1'-N1	5.30	111.71	108.00
2	Q	12	DT	C5-C4-O4	-5.30	121.19	124.90
2	Q	9	DG	N1-C6-O6	5.16	123.00	119.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3410	0	3394	148	0
1	B	3346	0	3281	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	227	0	124	15	0
2	Q	249	0	135	6	0
3	T	300	0	171	6	0
3	U	280	0	159	2	0
4	A	30	0	10	4	0
4	B	30	0	10	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	10	0	0	1	0
6	B	7	0	0	0	0
6	U	1	0	0	0	0
All	All	7894	0	7284	292	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 19.

All (292) 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:B:351:ILE:HD11	1:B:376:LEU:HD22	1.15	1.11
1:B:361:THR:HG22	2:Q:11:DC:OP1	1.50	1.09
1:B:351:ILE:CD1	1:B:376:LEU:HD22	2.00	0.90
1:B:408:THR:HG23	1:B:408:THR:O	1.71	0.88
1:A:128:ILE:HG12	1:A:140:ASN:ND2	1.90	0.86
1:A:185:LEU:HD13	1:A:202:LEU:HD11	1.57	0.86
1:A:108:MET:HE3	1:A:309:ALA:HB2	1.58	0.85
1:B:29:GLU:OE2	1:B:31:LEU:HD12	1.79	0.82
2:P:5:DG:H2''	2:P:6:DA:C5'	2.11	0.81
1:A:108:MET:CE	1:A:309:ALA:HB2	2.09	0.81
1:B:408:THR:O	1:B:408:THR:CG2	2.29	0.80
1:A:203:ASN:ND2	1:A:205:THR:HG22	1.97	0.80
1:B:294:VAL:HG12	1:B:332:GLN:OE1	1.83	0.79
1:B:185:LEU:HD22	1:B:202:LEU:HD21	1.66	0.78
2:P:4:DG:H2''	2:P:5:DG:O5'	1.84	0.77
1:A:305:THR:O	1:A:306:THR:HB	1.83	0.77
1:B:214:TRP:O	1:B:219:ARG:NH2	2.18	0.76
1:A:128:ILE:HG12	1:A:140:ASN:HD22	1.50	0.75
2:P:5:DG:H2''	2:P:6:DA:H5'	1.68	0.75
1:B:39:ILE:HG21	1:B:160:LEU:HD12	1.67	0.75
1:A:170:ASN:HD22	1:A:173:LYS:HE2	1.53	0.73
1:A:394:TYR:O	1:A:398:ILE:HD12	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:THR:HG22	1:A:50:TYR:HB2	1.71	0.73
1:A:48:ARG:HD3	1:A:463:VAL:HG13	1.73	0.71
1:B:457:THR:HG23	1:B:471:ALA:HB2	1.72	0.71
1:A:141:TYR:HA	1:A:144:ARG:HD3	1.74	0.70
1:A:120:ASN:C	1:A:120:ASN:HD22	1.95	0.70
1:A:455:THR:OG1	1:A:473:THR:HB	1.93	0.69
1:A:338:ASN:ND2	1:A:341:ALA:H	1.91	0.69
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.57	0.69
2:P:5:DG:C2'	2:P:6:DA:H5'	2.24	0.68
1:A:480:THR:HG22	1:A:483:GLU:HG2	1.74	0.67
1:A:43:ALA:HB2	1:A:159:ARG:HH11	1.59	0.67
1:B:33:LYS:HG2	1:B:37:ASN:HD21	1.59	0.67
1:A:43:ALA:HB2	1:A:159:ARG:NH1	2.10	0.67
1:A:473:THR:HG22	2:P:6:DA:OP1	1.96	0.66
1:B:26:ALA:HB1	1:B:144:ARG:NH2	2.11	0.66
1:A:328:LYS:HE2	4:A:1:ATP:PG	2.35	0.66
2:P:5:DG:H2''	2:P:6:DA:H5''	1.76	0.66
1:B:483:GLU:O	1:B:486:ALA:HB3	1.96	0.65
1:B:211:ARG:CG	1:B:211:ARG:HH11	2.09	0.65
1:A:208:LEU:HD11	1:A:290:ALA:HB2	1.78	0.65
1:A:108:MET:HE3	1:A:309:ALA:CB	2.26	0.65
1:A:177:VAL:O	1:A:181:VAL:HG13	1.96	0.65
1:A:318:MET:CE	1:A:319:LEU:HD23	2.27	0.64
1:A:473:THR:HG22	2:P:6:DA:P	2.37	0.64
1:B:446:LEU:HD22	1:B:513:ILE:HG21	1.78	0.64
1:B:352:ARG:HD3	1:B:362:GLU:CD	2.18	0.64
1:B:29:GLU:HG2	1:B:30:GLY:H	1.63	0.63
1:A:338:ASN:HD21	1:A:341:ALA:H	1.44	0.63
1:A:76:SER:O	1:A:80:ARG:HG3	1.99	0.63
1:A:480:THR:CG2	1:A:483:GLU:HG2	2.29	0.62
1:A:461:LYS:HB3	1:A:508:LEU:HB3	1.82	0.62
1:A:50:TYR:CE2	1:A:54:LEU:HD22	2.34	0.62
1:B:316:ASN:ND2	1:B:319:LEU:H	1.96	0.62
1:B:71:LYS:HD2	1:B:382:LEU:HD11	1.81	0.61
1:B:455:THR:HG23	1:B:473:THR:HB	1.81	0.61
1:A:214:TRP:O	1:A:219:ARG:NH1	2.34	0.61
1:B:316:ASN:HD21	1:B:319:LEU:H	1.49	0.61
1:B:101:ASN:N	1:B:101:ASN:HD22	1.99	0.61
1:B:77:GLN:HG2	1:B:78:GLN:N	2.14	0.61
1:A:91:MET:SD	1:B:91:MET:CE	2.89	0.60
1:A:335:ILE:HD11	1:A:345:PHE:CG	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:CG2	1:B:160:LEU:HD12	2.32	0.60
1:A:91:MET:SD	1:B:91:MET:HE1	2.42	0.60
1:B:478:VAL:HG13	1:B:483:GLU:HB2	1.82	0.60
1:B:480:THR:HG23	1:B:483:GLU:OE1	2.02	0.59
1:A:203:ASN:ND2	1:A:205:THR:CG2	2.65	0.59
1:A:335:ILE:HD11	1:A:345:PHE:CD2	2.38	0.59
1:B:291:GLN:NE2	1:B:334:GLN:OE1	2.36	0.58
1:B:219:ARG:O	1:B:285:VAL:HA	2.03	0.58
1:B:478:VAL:HG13	1:B:483:GLU:CB	2.33	0.58
1:A:305:THR:O	1:A:306:THR:CB	2.52	0.58
1:B:316:ASN:HD22	1:B:316:ASN:C	2.06	0.58
1:B:41:MET:HE2	1:B:41:MET:HA	1.85	0.57
1:B:507:ARG:NH1	3:U:5:8OG:OP1	2.37	0.57
1:A:108:MET:HA	1:A:108:MET:HE3	1.86	0.57
1:B:98:ASN:HD22	1:B:98:ASN:C	2.07	0.57
1:B:211:ARG:NH2	1:B:296:GLU:OE2	2.36	0.57
1:B:208:LEU:HD11	1:B:290:ALA:HB2	1.86	0.57
1:B:291:GLN:HE22	1:B:334:GLN:HB3	1.69	0.57
1:A:318:MET:HE1	1:A:319:LEU:HD23	1.85	0.57
2:Q:7:DA:H2"	2:Q:8:DG:OP2	2.05	0.57
1:A:306:THR:O	1:A:306:THR:HG22	2.05	0.57
1:B:105:HIS:CE1	1:B:199:GLU:HG2	2.40	0.57
3:T:5:8OG:H2'	3:T:6:DG:H5'	1.87	0.57
1:A:170:ASN:ND2	1:A:173:LYS:HB2	2.20	0.56
1:B:508:LEU:HD13	1:B:509:MET:N	2.19	0.56
1:A:420:ARG:O	1:A:508:LEU:HD22	2.05	0.56
1:B:480:THR:OG1	1:B:483:GLU:HG3	2.05	0.56
1:A:65:GLU:OE2	1:A:65:GLU:HA	2.06	0.56
1:A:26:ALA:HB1	1:A:325:ASP:OD2	2.06	0.56
1:B:455:THR:HG23	1:B:473:THR:CB	2.36	0.56
1:A:203:ASN:CG	1:A:205:THR:HG22	2.25	0.55
1:B:26:ALA:HB1	1:B:144:ARG:HH21	1.71	0.55
1:B:211:ARG:HH11	1:B:211:ARG:HG3	1.70	0.55
1:A:379:GLN:HG2	1:B:340:GLN:NE2	2.22	0.55
1:A:413:ARG:NH2	1:A:449:GLU:OE1	2.40	0.55
1:B:119:ASP:OD2	1:B:173:LYS:NZ	2.39	0.55
1:B:185:LEU:CD2	1:B:202:LEU:HD21	2.36	0.55
1:B:318:MET:HE2	1:B:319:LEU:HA	1.87	0.55
1:B:114:ALA:HA	1:B:117:MET:HG3	1.88	0.55
1:B:202:LEU:N	1:B:202:LEU:HD12	2.22	0.55
1:A:351:ILE:CD1	1:A:365:LEU:HD12	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLN:HE22	1:B:334:GLN:CB	2.20	0.54
1:A:474:VAL:O	1:A:475:SER:HB3	2.07	0.54
1:A:86:VAL:HG11	1:A:380:ARG:HB2	1.89	0.54
1:B:114:ALA:HB1	1:B:307:LEU:HD22	1.88	0.54
1:A:220:ARG:HB2	1:A:285:VAL:HG12	1.87	0.54
1:A:516:PHE:HB3	1:A:517:PRO:HD2	1.89	0.54
1:B:384:SER:HA	1:B:392:TRP:CD1	2.43	0.54
1:B:417:SER:HB3	1:B:512:ARG:HG3	1.90	0.54
1:B:113:ALA:O	1:B:117:MET:HG2	2.07	0.53
1:A:108:MET:HE1	1:A:309:ALA:HB2	1.87	0.53
1:A:451:LEU:HD23	1:A:516:PHE:CE2	2.43	0.53
1:A:294:VAL:HG12	1:A:332:GLN:OE1	2.07	0.53
1:B:48:ARG:NH1	1:B:463:VAL:HG11	2.24	0.53
1:A:115:VAL:HG22	1:A:177:VAL:HG21	1.91	0.53
1:A:306:THR:CG2	1:A:306:THR:O	2.56	0.53
1:B:108:MET:HB2	1:B:198:ASP:HB2	1.90	0.53
1:B:117:MET:HE2	1:B:124:LYS:HA	1.90	0.53
1:A:500:PHE:CG	1:A:501:PRO:HA	2.44	0.53
3:T:4:DA:H2"	3:T:5:8OG:OP2	2.10	0.52
1:B:39:ILE:CG2	1:B:160:LEU:CD1	2.88	0.52
1:B:111:PHE:O	1:B:112:TYR:C	2.47	0.52
1:B:201:TYR:C	1:B:202:LEU:HD12	2.30	0.52
1:A:144:ARG:NH2	4:A:1:ATP:O2G	2.43	0.52
1:A:477:VAL:O	1:A:478:VAL:HB	2.09	0.52
1:B:193:MET:HE1	1:B:408:THR:C	2.31	0.52
1:A:56:LYS:O	1:A:60:VAL:HG23	2.10	0.51
1:A:420:ARG:HH11	1:A:420:ARG:HG3	1.75	0.51
1:B:128:ILE:HG22	1:B:165:ILE:HG23	1.93	0.51
1:B:105:HIS:HD2	1:B:201:TYR:CE1	2.29	0.51
1:A:318:MET:HE2	1:A:319:LEU:HD23	1.92	0.51
1:A:298:ARG:HH21	1:A:330:ASN:ND2	2.09	0.51
1:A:135:MET:HA	1:A:153:PRO:HA	1.92	0.51
1:A:382:LEU:HD22	1:A:386:LEU:HG	1.92	0.50
1:A:97:ARG:HG2	1:A:99:LEU:CD1	2.41	0.50
1:B:382:LEU:HD22	1:B:386:LEU:HG	1.92	0.50
1:A:108:MET:HB2	1:A:198:ASP:HB2	1.93	0.50
1:A:302:GLU:HA	1:A:307:LEU:O	2.12	0.50
1:B:111:PHE:CD2	1:B:198:ASP:HB3	2.46	0.50
1:A:422:PHE:CE2	1:A:434:LEU:HD11	2.48	0.49
1:A:473:THR:N	2:P:6:DA:OP1	2.42	0.49
1:A:483:GLU:O	1:A:486:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:ND2	1:A:100:SER:H	2.10	0.49
1:A:422:PHE:HE2	1:A:434:LEU:HD11	1.78	0.49
1:A:199:GLU:OE2	1:A:321:LYS:NZ	2.46	0.49
1:A:477:VAL:O	1:A:478:VAL:CB	2.60	0.49
1:A:97:ARG:CD	1:A:99:LEU:HD11	2.43	0.49
1:A:314:ALA:HB1	1:A:315:PRO:HD2	1.95	0.49
1:B:117:MET:CE	1:B:124:LYS:HA	2.42	0.49
1:A:384:SER:HA	1:A:392:TRP:CD1	2.48	0.48
1:B:476:SER:O	1:B:477:VAL:HB	2.12	0.48
1:B:111:PHE:O	1:B:114:ALA:N	2.46	0.48
1:B:98:ASN:C	1:B:98:ASN:ND2	2.67	0.48
1:B:44:THR:HG22	1:B:50:TYR:HB2	1.94	0.48
1:A:120:ASN:HD21	1:A:122:GLU:HG3	1.79	0.48
1:A:325:ASP:HA	1:A:328:LYS:HG3	1.96	0.48
1:B:433:SER:O	1:B:437:GLU:HG3	2.14	0.47
1:B:211:ARG:HH22	1:B:296:GLU:CD	2.17	0.47
1:B:343:MET:O	1:B:346:ILE:HG22	2.14	0.47
1:B:29:GLU:CG	1:B:30:GLY:H	2.28	0.47
1:A:108:MET:HA	1:A:108:MET:CE	2.44	0.47
1:A:364:MET:HE1	6:A:9:HOH:O	2.14	0.47
1:B:422:PHE:CE2	1:B:434:LEU:HD11	2.49	0.47
1:B:316:ASN:HD21	1:B:319:LEU:HG	1.78	0.47
1:A:434:LEU:HD22	1:A:438:LEU:HG	1.97	0.47
1:A:340:GLN:HE22	1:B:379:GLN:HG2	1.80	0.47
1:B:123:LEU:HD23	1:B:165:ILE:HD13	1.97	0.47
1:B:141:TYR:OH	4:B:2:ATP:O3G	2.09	0.46
1:B:417:SER:HA	1:B:442:LEU:HD13	1.98	0.46
1:A:318:MET:HE2	1:A:319:LEU:N	2.31	0.46
1:B:317:THR:HG21	1:B:404:SER:HB2	1.98	0.46
1:B:377:TYR:HB2	1:B:399:SER:HB2	1.98	0.46
1:B:294:VAL:HG11	1:B:313:ILE:HD11	1.96	0.46
1:A:474:VAL:HG23	1:A:475:SER:H	1.81	0.45
1:B:100:SER:HB2	1:B:101:ASN:HD22	1.81	0.45
1:B:317:THR:CG2	1:B:404:SER:HB2	2.45	0.45
1:A:328:LYS:HE2	4:A:1:ATP:O1G	2.16	0.45
1:A:422:PHE:CE1	1:A:425:ILE:HD12	2.51	0.45
1:A:461:LYS:HD3	1:A:467:VAL:HG22	1.98	0.45
1:A:442:LEU:CD2	1:A:511:VAL:HG12	2.47	0.45
2:P:8:DG:H1'	2:P:9:DG:H5''	1.97	0.45
1:A:377:TYR:HB2	1:A:399:SER:HB2	1.98	0.45
1:B:86:VAL:HG11	1:B:380:ARG:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MET:HE1	1:A:158:LYS:HD2	1.98	0.45
1:A:478:VAL:HG22	1:A:483:GLU:HG3	1.98	0.45
1:B:49:PHE:CE2	3:U:4:DA:C5	3.04	0.45
1:A:434:LEU:HD13	1:A:509:MET:SD	2.56	0.45
1:B:389:GLU:HG3	1:B:393:HIS:CE1	2.52	0.45
1:A:317:THR:HG23	1:A:404:SER:HB2	1.98	0.45
1:B:436:GLN:HA	1:B:485:PHE:CD1	2.52	0.45
1:A:438:LEU:O	1:A:439:CYS:C	2.55	0.45
1:B:147:GLY:O	1:B:152:MET:CE	2.65	0.45
1:B:473:THR:HB	2:Q:6:DA:OP2	2.17	0.45
1:B:446:LEU:CD2	1:B:513:ILE:HG21	2.47	0.45
1:B:61:ASN:OD1	1:B:363:LYS:NZ	2.50	0.45
1:A:192:PHE:C	1:A:192:PHE:CD1	2.89	0.45
1:A:177:VAL:HG11	1:A:307:LEU:HD12	1.99	0.45
1:B:512:ARG:NH1	1:B:512:ARG:HG3	2.27	0.44
1:A:74:ILE:HG23	1:A:78:GLN:HE21	1.83	0.44
1:B:75:THR:HG1	1:B:78:GLN:H	1.65	0.44
1:A:134:SER:O	1:A:135:MET:HB2	2.18	0.44
1:A:314:ALA:HB1	1:A:315:PRO:CD	2.48	0.44
3:T:14:DC:C4	3:T:15:DC:N4	2.85	0.44
1:B:112:TYR:HB3	1:B:130:VAL:HG21	1.99	0.44
1:B:25:LYS:O	1:B:26:ALA:HB3	2.18	0.44
1:A:290:ALA:HA	1:A:293:VAL:HG13	2.00	0.44
1:A:177:VAL:HG11	1:A:307:LEU:CD1	2.48	0.44
1:A:417:SER:HB2	1:A:512:ARG:NH1	2.32	0.44
1:B:22:ASN:HD22	1:B:22:ASN:N	2.16	0.44
1:B:358:GLY:HA3	2:Q:11:DC:O5'	2.17	0.44
1:A:421:THR:N	3:T:6:DG:OP1	2.38	0.44
1:A:294:VAL:HG21	1:A:313:ILE:HG12	1.99	0.44
1:A:63:ARG:HH12	2:P:10:DA:H5''	1.81	0.44
1:B:317:THR:HG22	1:B:404:SER:H	1.83	0.44
2:P:6:DA:C6	2:P:7:DA:N6	2.86	0.44
1:A:48:ARG:HD3	1:A:463:VAL:CG1	2.45	0.44
1:A:358:GLY:HA3	2:P:11:DC:O5'	2.18	0.43
1:A:382:LEU:HD22	1:A:386:LEU:CD1	2.47	0.43
1:A:54:LEU:HD12	1:A:57:GLU:OE2	2.18	0.43
1:B:141:TYR:HA	1:B:144:ARG:HD3	2.00	0.43
1:B:147:GLY:O	1:B:152:MET:HE3	2.18	0.43
3:T:15:DC:H2''	3:T:16:DC:C5	2.53	0.43
1:A:343:MET:CE	1:A:343:MET:HA	2.48	0.43
1:A:461:LYS:HD3	1:A:467:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ARG:HG3	1:B:150:ALA:O	2.17	0.43
1:A:346:ILE:HG23	1:A:373:CYS:HB3	2.00	0.43
1:A:428:ALA:O	1:A:432:TYR:HD1	2.02	0.43
1:A:66:ASN:ND2	1:A:66:ASN:N	2.66	0.43
1:A:97:ARG:HG2	1:A:99:LEU:HD11	2.00	0.43
1:B:452:LYS:HG2	1:B:479:SER:HB3	2.01	0.43
1:A:354:VAL:HG11	1:A:398:ILE:HG12	2.00	0.43
1:B:116:GLU:OE2	1:B:167:VAL:HG11	2.18	0.43
1:B:207:HIS:NE2	1:B:211:ARG:NH1	2.66	0.43
1:B:288:THR:O	1:B:288:THR:HG22	2.17	0.43
1:B:358:GLY:HA3	2:Q:11:DC:P	2.59	0.43
1:A:480:THR:HG22	1:A:483:GLU:CG	2.44	0.43
1:A:120:ASN:C	1:A:120:ASN:ND2	2.68	0.43
1:A:98:ASN:HD22	1:A:99:LEU:N	2.16	0.43
1:A:203:ASN:HD21	1:A:205:THR:CG2	2.31	0.43
1:B:118:ARG:HD3	1:B:119:ASP:OD1	2.19	0.43
1:A:120:ASN:HA	1:A:121:PRO:HD2	1.80	0.42
1:A:478:VAL:HG23	1:A:483:GLU:HB2	2.01	0.42
1:B:39:ILE:HB	1:B:160:LEU:HD11	2.00	0.42
3:T:11:DC:H2"	3:T:12:DT:H71	2.01	0.42
4:A:1:ATP:C8	2:P:13:DOC:H2'	2.54	0.42
1:B:120:ASN:OD1	1:B:122:GLU:N	2.52	0.42
1:B:202:LEU:CD1	1:B:202:LEU:N	2.82	0.42
2:P:6:DA:C6	2:P:7:DA:C6	3.07	0.42
1:B:316:ASN:C	1:B:316:ASN:ND2	2.72	0.42
1:B:318:MET:HE2	1:B:319:LEU:CA	2.49	0.42
1:A:49:PHE:HA	1:A:465:PHE:CE1	2.53	0.42
1:A:74:ILE:HA	1:A:78:GLN:NE2	2.35	0.42
1:A:346:ILE:HG23	1:A:373:CYS:CB	2.48	0.42
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.89	0.42
1:B:461:LYS:HB3	1:B:508:LEU:HB3	2.02	0.42
1:A:104:VAL:HA	1:A:312:GLY:O	2.20	0.42
1:A:109:ASP:O	1:A:110:ALA:C	2.58	0.42
1:A:346:ILE:O	1:A:373:CYS:HB2	2.19	0.42
1:A:71:LYS:HG3	1:A:382:LEU:HD21	2.02	0.42
1:A:125:ASP:HB3	1:A:126:LYS:NZ	2.34	0.42
1:B:499:ASP:O	1:B:500:PHE:C	2.59	0.42
1:A:318:MET:HE2	1:A:319:LEU:CA	2.50	0.41
1:A:98:ASN:HD22	1:A:98:ASN:C	2.22	0.41
1:A:80:ARG:NH2	1:B:95:GLN:O	2.49	0.41
2:P:5:DG:C6	2:P:6:DA:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378[A]:GLN:OE1	1:A:378[A]:GLN:HA	2.21	0.41
1:A:139:SER:O	1:A:144:ARG:HD2	2.20	0.41
1:A:446:LEU:CD2	1:A:513:ILE:HD13	2.50	0.41
1:B:181:VAL:HG13	1:B:301:ILE:CD1	2.50	0.41
1:B:352:ARG:HD3	1:B:362:GLU:OE1	2.20	0.41
1:B:212:GLN:HG3	1:B:213:ASN:N	2.34	0.41
1:B:508:LEU:C	1:B:508:LEU:HD13	2.40	0.41
2:Q:8:DG:OP2	2:Q:8:DG:H2'	2.21	0.41
1:B:222:PHE:O	1:B:223:ILE:CB	2.69	0.41
1:A:188:TYR:CE1	1:A:297:ILE:HG12	2.55	0.41
1:B:70:GLN:O	1:B:71:LYS:C	2.58	0.41
1:A:33:LYS:O	1:A:37:ASN:HB2	2.21	0.41
1:B:101:ASN:ND2	1:B:101:ASN:N	2.67	0.41
1:A:221:TYR:CE2	1:A:300:ARG:HD2	2.56	0.41
1:B:193:MET:HE3	1:B:407:LEU:HB3	2.02	0.41
1:A:340:GLN:NE2	1:B:379:GLN:HG2	2.35	0.41
1:B:82:ALA:O	1:B:86:VAL:HG23	2.20	0.41
1:B:89:PHE:HE2	1:B:93:LEU:HD11	1.85	0.41
1:A:208:LEU:HD11	1:A:290:ALA:CB	2.50	0.40
1:A:219:ARG:O	1:A:285:VAL:HA	2.21	0.40
1:B:127:PRO:C	1:B:164:LEU:HD12	2.41	0.40
1:B:105:HIS:CD2	1:B:201:TYR:CE1	3.09	0.40
1:A:114:ALA:HB1	1:A:307:LEU:HD22	2.02	0.40
1:A:43:ALA:CB	1:A:159:ARG:NH1	2.84	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	435/508 (86%)	390 (90%)	33 (8%)	12 (3%)	<b>5</b> 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	433/508 (85%)	385 (89%)	41 (10%)	7 (2%)	9	43
All	All	868/1016 (85%)	775 (89%)	74 (8%)	19 (2%)	6	35

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	SER
1	A	477	VAL
1	B	29	GLU
1	B	45	LYS
1	B	111	PHE
1	B	477	VAL
1	A	478	VAL
1	B	409	ARG
1	A	410	ASP
1	B	27	GLY
1	B	462	ASN
1	A	72	ALA
1	A	346	ILE
1	A	412	GLU
1	A	476	SER
1	A	45	LYS
1	A	381	ALA
1	A	462	ASN
1	A	474	VAL

### 5.3.2 Protein sidechains ⓘ

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	365/454 (80%)	326 (89%)	39 (11%)	6	27
1	B	350/454 (77%)	307 (88%)	43 (12%)	4	21
All	All	715/908 (79%)	633 (88%)	82 (12%)	5	24

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	48	ARG
1	A	66	ASN
1	A	85	GLN
1	A	95	GLN
1	A	98	ASN
1	A	108	MET
1	A	118	ARG
1	A	119	ASP
1	A	120	ASN
1	A	126	LYS
1	A	179	LYS
1	A	181	VAL
1	A	191	ASN
1	A	198	ASP
1	A	203	ASN
1	A	284	VAL
1	A	288	THR
1	A	293	VAL
1	A	318	MET
1	A	325	ASP
1	A	338	ASN
1	A	343	MET
1	A	351	ILE
1	A	382	LEU
1	A	393	HIS
1	A	405	THR
1	A	434	LEU
1	A	451	LEU
1	A	458	ILE
1	A	463	VAL
1	A	468	LYS
1	A	469	THR
1	A	477	VAL
1	A	478	VAL
1	A	484	ILE
1	A	506	LEU
1	A	507	ARG
1	A	518	ASN
1	B	22	ASN
1	B	29	GLU
1	B	54	LEU
1	B	63	ARG

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Mol	Chain	Res	Type
1	B	77	GLN
1	B	84	LEU
1	B	85	GLN
1	B	98	ASN
1	B	101	ASN
1	B	117	MET
1	B	118	ARG
1	B	123	LEU
1	B	134	SER
1	B	164	LEU
1	B	165	ILE
1	B	170	ASN
1	B	202	LEU
1	B	203	ASN
1	B	211	ARG
1	B	218	LYS
1	B	219	ARG
1	B	291	GLN
1	B	293	VAL
1	B	302	GLU
1	B	305	THR
1	B	316	ASN
1	B	318	MET
1	B	325	ASP
1	B	343	MET
1	B	361	THR
1	B	371	ILE
1	B	379	GLN
1	B	382	LEU
1	B	405	THR
1	B	406	HIS
1	B	408	THR
1	B	455	THR
1	B	473	THR
1	B	477	VAL
1	B	496	ILE
1	B	506	LEU
1	B	508	LEU
1	B	518	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	66	ASN
1	A	77	GLN
1	A	78	GLN
1	A	83	GLN
1	A	98	ASN
1	A	120	ASN
1	A	170	ASN
1	A	203	ASN
1	A	327	ASN
1	A	330	ASN
1	A	338	ASN
1	A	340	GLN
1	A	379	GLN
1	B	22	ASN
1	B	37	ASN
1	B	66	ASN
1	B	69	GLN
1	B	77	GLN
1	B	98	ASN
1	B	101	ASN
1	B	213	ASN
1	B	291	GLN
1	B	316	ASN
1	B	330	ASN
1	B	334	GLN
1	B	338	ASN
1	B	340	GLN
1	B	379	GLN
1	B	397	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
2	DOC	Q	13	3,2	14,19,20	0.78	0	13,26,29	2.08	4 (30%)
3	8OG	U	5	3	18,25,26	1.28	1 (5%)	21,37,40	2.03	6 (28%)
2	DOC	P	13	3,2	14,19,20	0.96	1 (7%)	13,26,29	2.17	5 (38%)
3	8OG	T	5	3	18,25,26	1.36	2 (11%)	21,37,40	1.85	5 (23%)

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
2	DOC	Q	13	3,2	-	3/4/18/19	0/2/2/2
3	8OG	U	5	3	-	1/3/21/22	0/3/3/3
2	DOC	P	13	3,2	-	3/4/18/19	0/2/2/2
3	8OG	T	5	3	-	2/3/21/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	5	8OG	O6-C6	4.49	1.35	1.24
3	U	5	8OG	O6-C6	4.48	1.35	1.24
3	T	5	8OG	C6-C5	-2.53	1.37	1.41
2	P	13	DOC	C6-N1	-2.12	1.33	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	5	8OG	N3-C2-N1	-5.31	120.14	127.22
2	Q	13	DOC	C2-N3-C4	4.98	121.39	116.34
2	P	13	DOC	C2-N3-C4	4.89	121.30	116.34
3	T	5	8OG	C2-N3-C4	4.57	120.57	115.36
3	U	5	8OG	C2-N3-C4	4.49	120.48	115.36
3	T	5	8OG	N3-C2-N1	-4.48	121.25	127.22
3	U	5	8OG	C6-N1-C2	3.38	121.30	115.93
2	P	13	DOC	C3'-C2'-C1'	3.10	106.36	102.78
2	P	13	DOC	N4-C4-N3	2.66	120.70	116.49
2	P	13	DOC	C5-C4-N3	-2.66	118.65	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	5	8OG	C6-C5-C4	-2.58	118.33	120.80
3	T	5	8OG	C5-C6-N1	-2.54	119.96	123.43
2	Q	13	DOC	C5-C4-N3	-2.52	118.82	121.72
3	U	5	8OG	C5-C6-N1	-2.41	120.13	123.43
2	P	13	DOC	C2'-C1'-N1	-2.37	108.01	112.48
3	T	5	8OG	C6-N1-C2	2.36	119.67	115.93
2	Q	13	DOC	C3'-C2'-C1'	2.30	105.43	102.78
3	U	5	8OG	N2-C2-N3	2.21	121.39	117.79
3	T	5	8OG	C8-N9-C1'	2.11	129.53	125.90
2	Q	13	DOC	N4-C4-N3	2.08	119.78	116.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	13	DOC	O4'-C1'-N1-C6
2	Q	13	DOC	O4'-C4'-C5'-O5'
2	P	13	DOC	O4'-C1'-N1-C6
2	P	13	DOC	O4'-C4'-C5'-O5'
3	U	5	8OG	O4'-C4'-C5'-O5'
3	T	5	8OG	O4'-C4'-C5'-O5'
3	T	5	8OG	C3'-C4'-C5'-O5'
2	Q	13	DOC	C3'-C4'-C5'-O5'
2	P	13	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	5	8OG	1	0
2	P	13	DOC	1	0
3	T	5	8OG	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	ATP	A	1	5	26,32,33	0.76	0	30,50,52	1.71	5 (16%)
4	ATP	B	2	5	26,32,33	0.87	1 (3%)	30,50,52	1.61	6 (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
4	ATP	A	1	5	-	4/18/34/38	0/3/3/3
4	ATP	B	2	5	-	5/18/34/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	ATP	C5-C4	2.19	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	ATP	N3-C2-N1	-4.83	121.13	128.68
4	A	1	ATP	C2'-C1'-N9	-4.33	104.28	114.27
4	B	2	ATP	N3-C2-N1	-3.94	122.52	128.68
4	A	1	ATP	PB-O3B-PG	-3.24	121.71	132.83
4	B	2	ATP	PA-O3A-PB	-3.16	121.98	132.83
4	B	2	ATP	PB-O3B-PG	-2.80	123.21	132.83
4	A	1	ATP	C2-N1-C6	2.77	123.48	118.75
4	B	2	ATP	C2'-C1'-N9	-2.57	108.34	114.27
4	B	2	ATP	C4-C5-N7	-2.19	107.12	109.40
4	A	1	ATP	PA-O3A-PB	-2.17	125.37	132.83
4	B	2	ATP	C2-N1-C6	2.06	122.28	118.75

There are no chirality outliers.



All (9) torsion outliers are listed below:

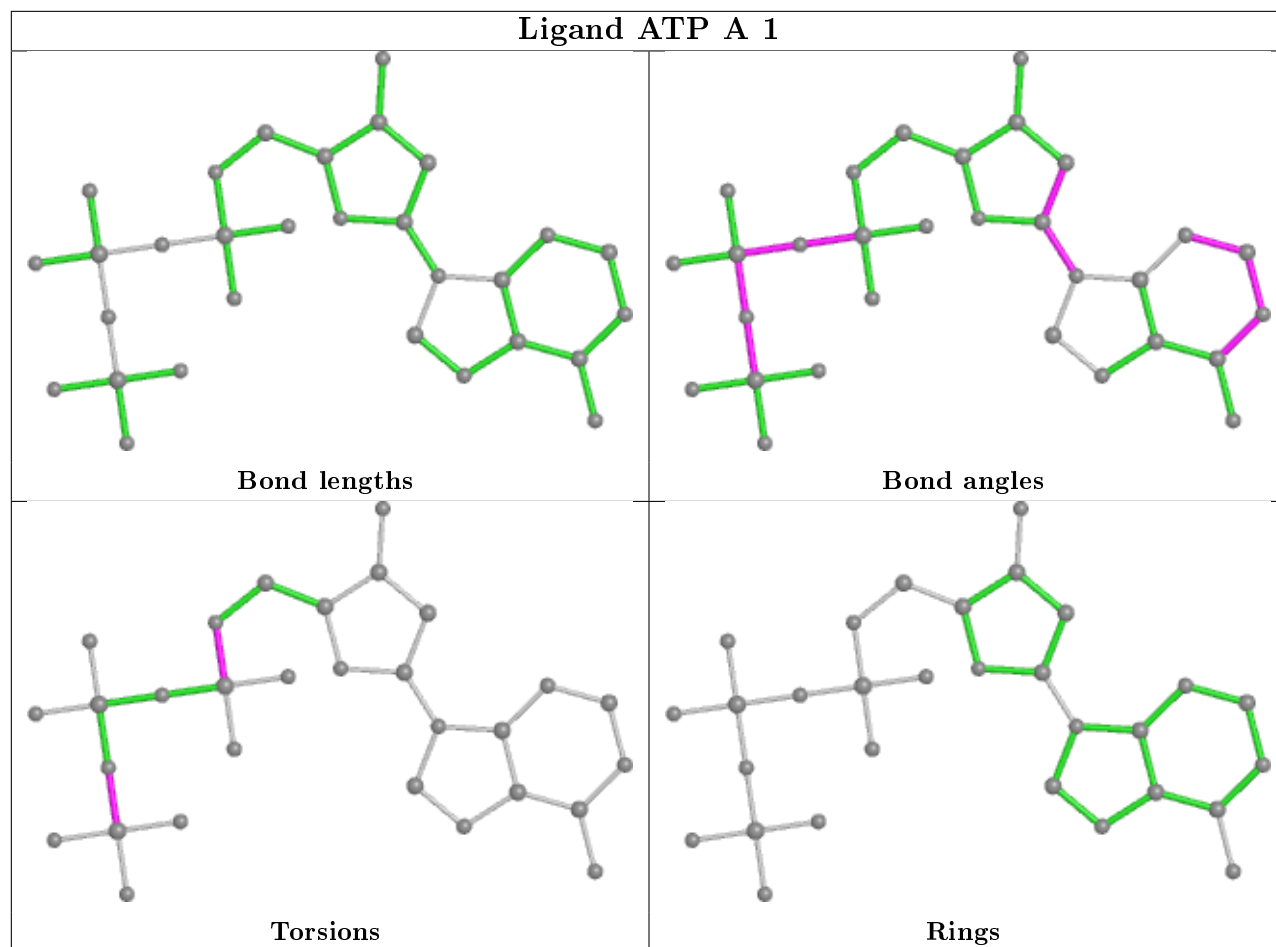
Mol	Chain	Res	Type	Atoms
4	B	2	ATP	C5'-O5'-PA-O1A
4	B	2	ATP	C5'-O5'-PA-O2A
4	B	2	ATP	O4'-C4'-C5'-O5'
4	A	1	ATP	PB-O3B-PG-O1G
4	A	1	ATP	C5'-O5'-PA-O3A
4	B	2	ATP	C5'-O5'-PA-O3A
4	B	2	ATP	C3'-C4'-C5'-O5'
4	A	1	ATP	PB-O3B-PG-O2G
4	A	1	ATP	PB-O3B-PG-O3G

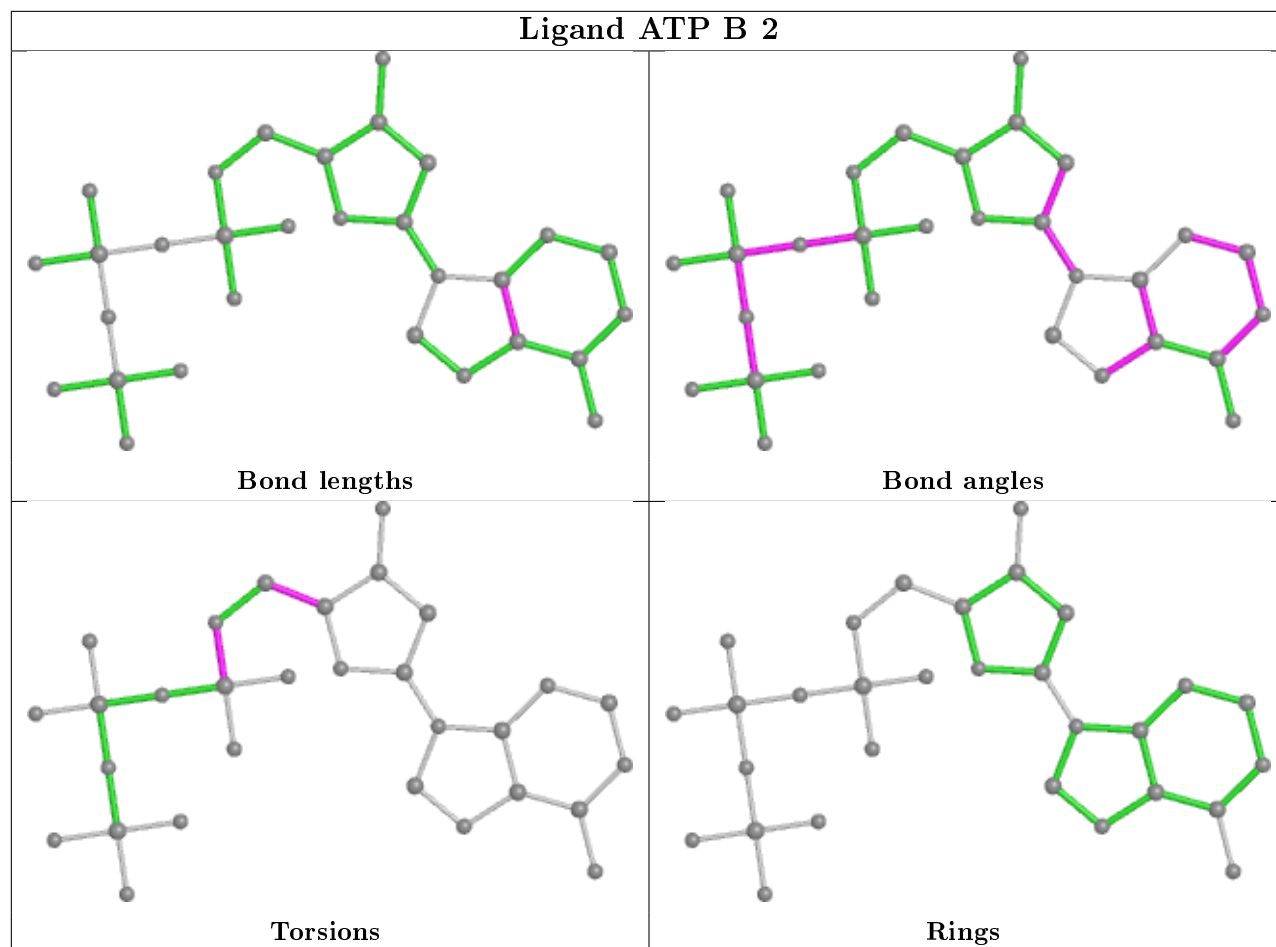
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	ATP	4	0
4	B	2	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 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	438/508 (86%)	-0.15	5 (1%) 80 69	27, 47, 75, 89	0
1	B	437/508 (86%)	-0.13	1 (0%) 95 94	33, 55, 84, 97	0
2	P	10/13 (76%)	0.40	1 (10%) 7 4	42, 63, 98, 116	0
2	Q	11/13 (84%)	0.02	0 100 100	48, 59, 91, 102	0
3	T	14/18 (77%)	0.27	0 100 100	43, 79, 129, 133	0
3	U	13/18 (72%)	0.18	1 (7%) 13 7	49, 66, 100, 109	0
All	All	923/1078 (85%)	-0.12	8 (0%) 84 75	27, 52, 81, 133	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	474	VAL	3.1
1	A	223	ILE	3.0
2	P	3	DG	2.9
3	U	17	DC	2.6
1	A	475	SER	2.3
1	B	36	ILE	2.3
1	A	451	LEU	2.3
1	A	454	ARG	2.1

### 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
2	DOC	Q	13	18/19	0.96	0.17	51,54,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	8OG	U	5	23/24	0.97	0.16	39,42,46,47	0
2	DOC	P	13	18/19	0.97	0.18	38,39,44,44	0
3	8OG	T	5	23/24	0.97	0.17	38,40,42,43	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

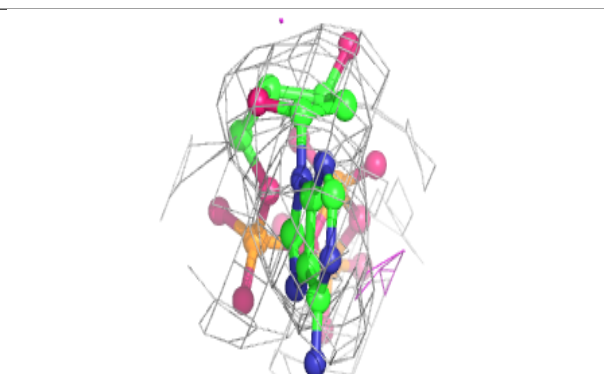
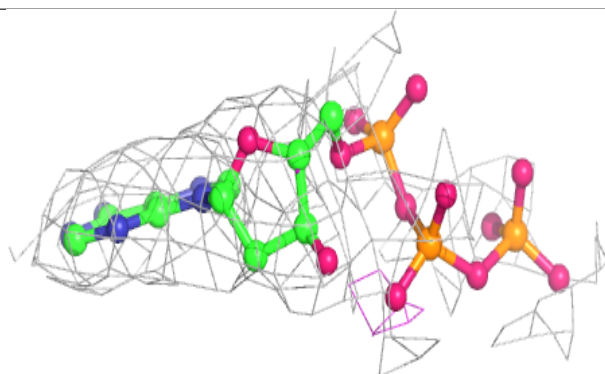
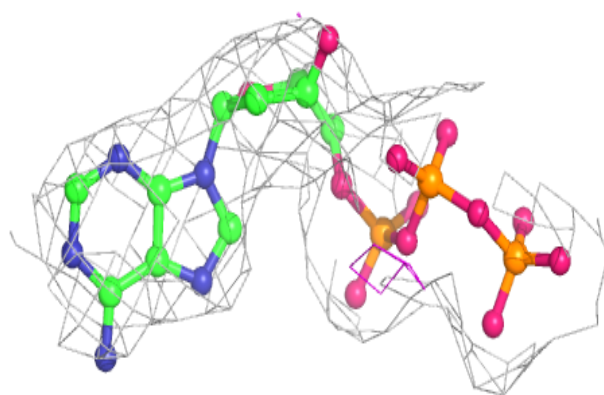
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	4	1/1	0.57	0.32	57,57,57,57	0
5	MG	A	3	1/1	0.74	0.20	41,41,41,41	0
4	ATP	B	2	30/31	0.96	0.18	49,55,59,60	0
5	MG	A	2	1/1	0.98	0.12	26,26,26,26	0
4	ATP	A	1	30/31	0.98	0.16	29,33,35,35	0
5	MG	B	1	1/1	0.98	0.13	37,37,37,37	0

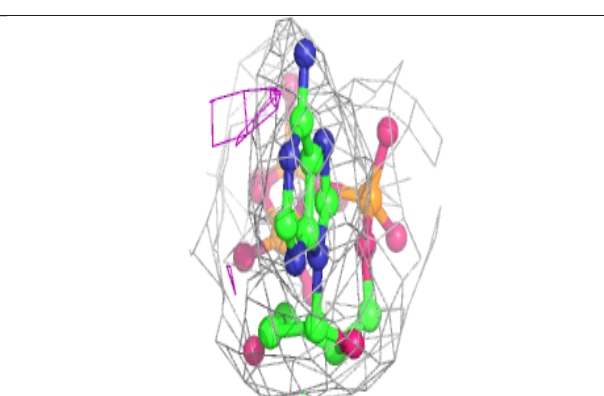
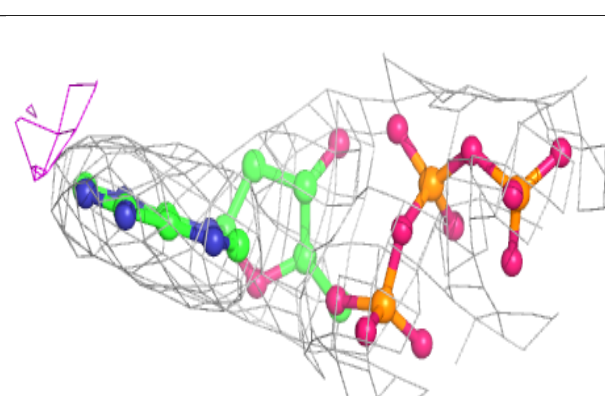
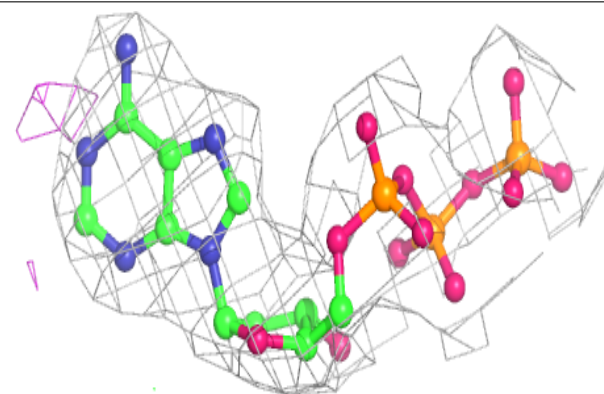
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 2:**

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

**Electron density around ATP A 1:**

$2mF_o-DF_c$  (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.