



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:53 pm BST

PDB ID : 1MB9  
Title : BETA-LACTAM SYNTHETASE COMPLEXED WITH ATP  
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Deposited on : 2002-08-02  
Resolution : 2.11 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

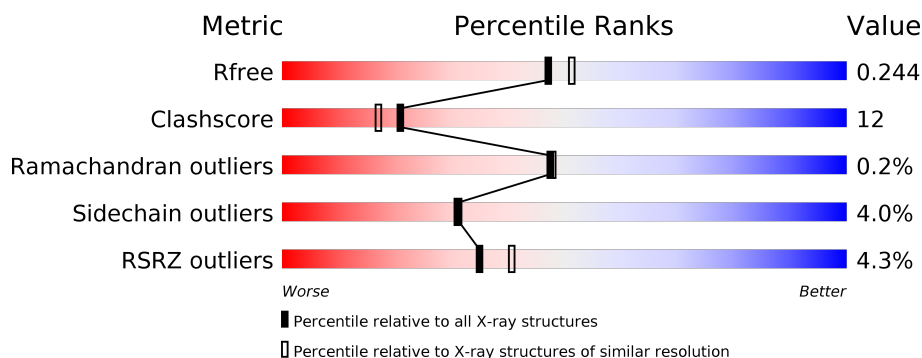
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	513	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	B	513	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>

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
4	AMP	A	706[B]	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7960 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.

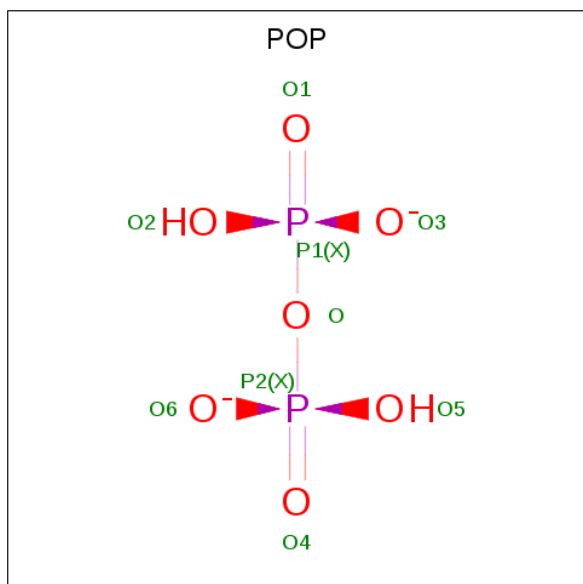
- Molecule 1 is a protein called BETA-LACTAM SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3653	2283	670	692	8			
1	B	497	Total	C	N	O	S	0	0	0
			3739	2334	688	709	8			

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

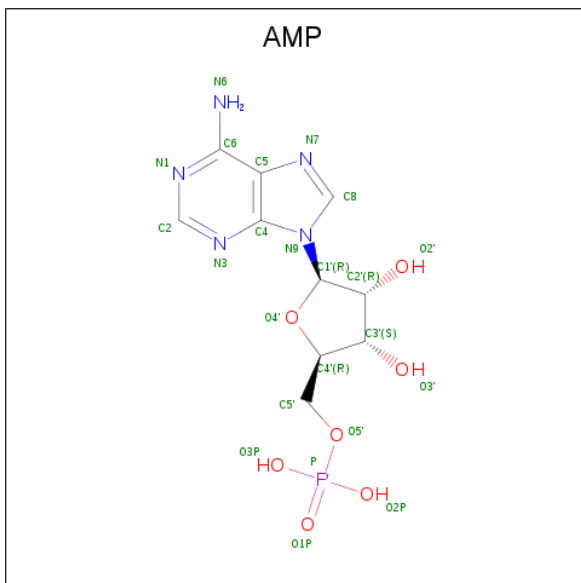
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



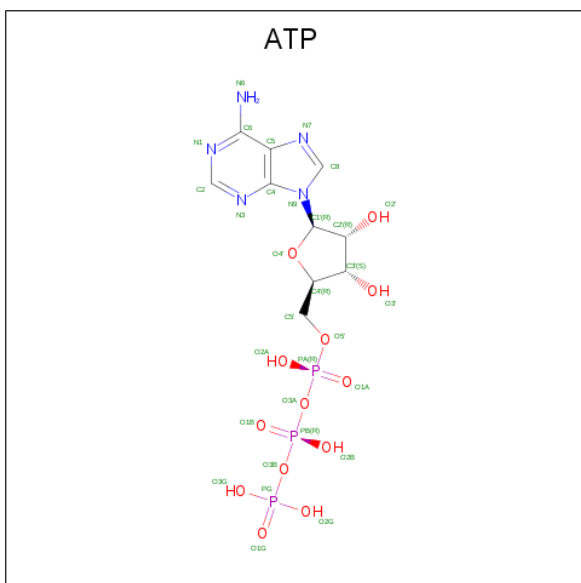
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	1
			9	7	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0
			23	10	5	7	1	1

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

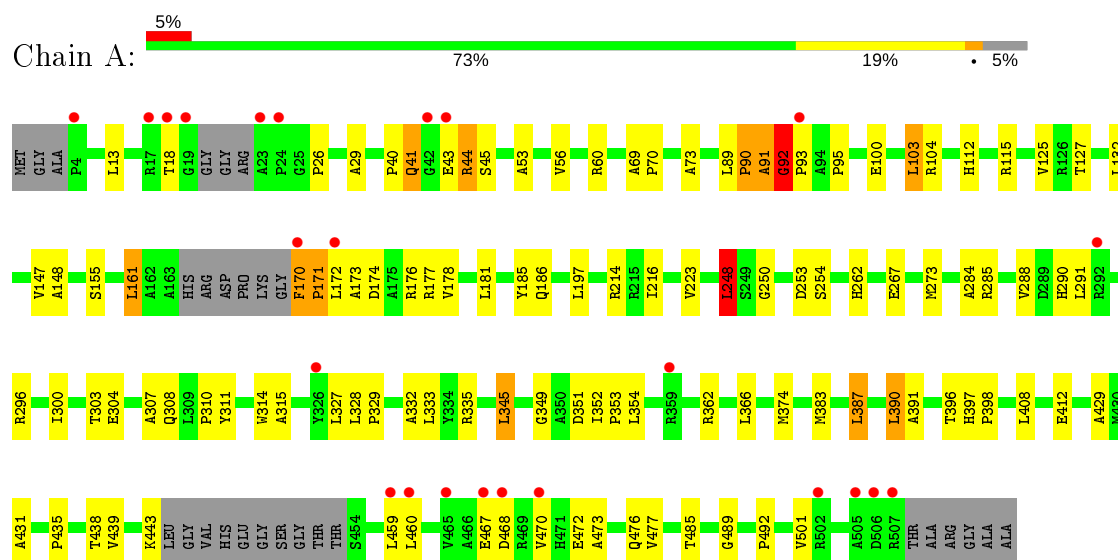
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	222	Total 222	O 222	0	0
6	B	248	Total 248	O 248	0	0

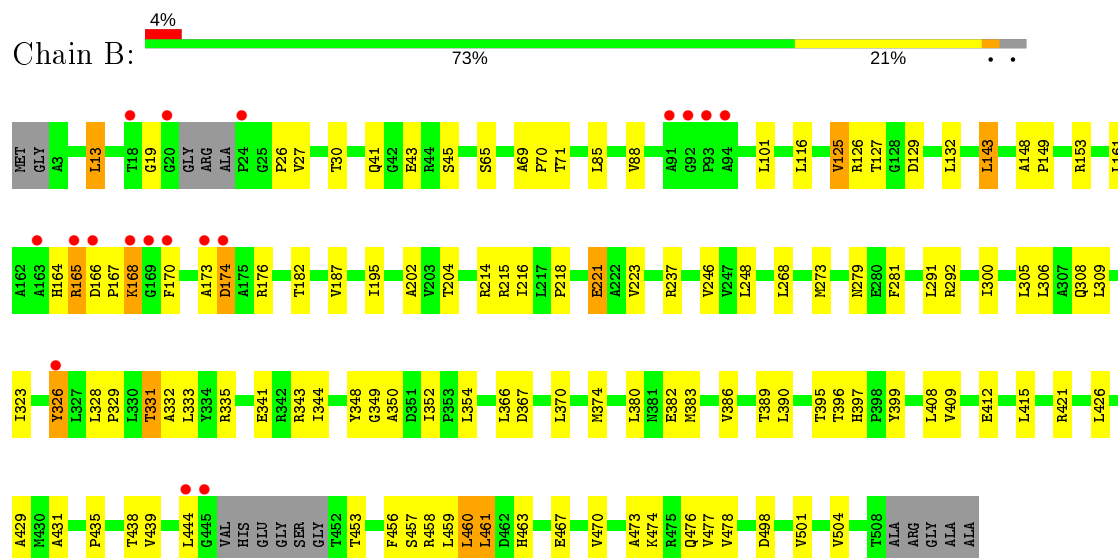
### 3 Residue-property plots [i](#)

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: BETA-LACTAM SYNTHETASE



#### • Molecule 1: BETA-LACTAM SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.25Å 97.57Å 81.31Å 90.00° 90.69° 90.00°	Depositor
Resolution (Å)	24.78 – 2.11 48.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (24.78-2.11) 96.2 (48.79-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.251 0.204 , 0.244	Depositor DCC
$R_{free}$ test set	4774 reflections (7.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.45	2/3725 (0.1%)	0.79	10/5082 (0.2%)
1	B	0.35	0/3814	0.69	1/5204 (0.0%)
All	All	0.40	2/7539 (0.0%)	0.74	11/10286 (0.1%)

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	1	6
1	B	0	2
All	All	1	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	PHE	C-N	5.56	1.44	1.34
1	A	92	GLY	CA-C	-5.34	1.43	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ALA	C-N-CD	11.23	151.99	128.40
1	A	91	ALA	C-N-CA	11.14	145.70	122.30
1	B	174	ASP	CB-CG-OD2	9.28	126.65	118.30
1	A	170	PHE	C-N-CD	8.69	146.65	128.40
1	A	171	PRO	CA-N-CD	-7.19	101.44	111.50
1	A	70	PRO	CA-N-CD	-7.10	101.56	111.50
1	A	91	ALA	N-CA-CB	6.03	118.54	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ASP	C-N-CA	5.71	135.97	121.70
1	A	248	LEU	CA-CB-CG	5.48	127.89	115.30
1	A	468	ASP	O-C-N	5.47	131.45	122.70
1	A	91	ALA	N-CA-C	5.24	125.14	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	91	ALA	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	LEU	Mainchain
1	A	90	PRO	Mainchain,Peptide
1	A	91	ALA	Mainchain,Peptide
1	A	92	GLY	Mainchain
1	B	174	ASP	Mainchain
1	B	460	LEU	Mainchain

## 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	3653	0	3645	90	0
1	B	3739	0	3732	91	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	0	1	0
4	A	23	0	9	4	0
5	A	31	0	10	0	0
5	B	31	0	11	1	0
6	A	222	0	0	1	0
6	B	248	0	0	3	0
All	All	7960	0	7407	182	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 12.

All (182) 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)
5:B:702:ATP:C1'	5:B:702:ATP:O4'	1.77	1.31
1:A:467:GLU:HG3	1:A:470:VAL:HG11	1.25	1.14
1:A:467:GLU:HG3	1:A:470:VAL:CG1	1.86	1.06
4:A:706[B]:AMP:C4'	4:A:706[B]:AMP:C8	2.52	0.92
1:B:456:PHE:O	1:B:460:LEU:HD23	1.71	0.90
1:B:173:ALA:O	1:B:204:THR:OG1	1.90	0.90
1:B:459:LEU:HD11	1:B:501:VAL:HG11	1.51	0.90
1:A:41:GLN:HB2	1:A:45:SER:HB2	1.53	0.89
4:A:706[B]:AMP:C4'	4:A:706[B]:AMP:H8	1.87	0.85
1:A:112:HIS:HD2	1:A:115:ARG:HE	1.32	0.77
1:A:248:LEU:HD22	1:A:250:GLY:H	1.50	0.77
1:B:306:LEU:HD13	1:B:459:LEU:HD23	1.66	0.76
1:A:472:GLU:HG3	1:A:476:GLN:HE21	1.53	0.74
1:A:216:ILE:HD12	1:B:88:VAL:HG11	1.71	0.72
1:B:383:MET:HE3	1:B:397:HIS:HB2	1.71	0.72
1:A:148:ALA:HB1	1:A:170:PHE:CE2	2.26	0.70
1:B:195:ILE:HG12	1:B:202:ALA:HB2	1.74	0.70
1:B:459:LEU:CD1	1:B:501:VAL:HG11	2.21	0.70
1:B:153:ARG:HH12	1:B:168:LYS:HD3	1.56	0.69
1:B:153:ARG:HH22	1:B:168:LYS:HD3	1.56	0.68
1:B:323:ILE:HD12	1:B:382:GLU:HG2	1.75	0.67
1:A:327:LEU:HD22	1:A:387:LEU:HD21	1.76	0.66
1:B:431:ALA:HA	1:B:439:VAL:HG11	1.77	0.66
1:B:374:MET:HE3	1:B:409:VAL:HG22	1.78	0.66
1:B:69:ALA:HB1	1:B:70:PRO:HD2	1.77	0.65
1:A:390:LEU:HD12	1:A:391:ALA:N	2.12	0.64
1:B:309:LEU:HA	1:B:328:LEU:HD21	1.79	0.64
1:B:218:PRO:HG2	1:B:221:GLU:HB2	1.78	0.64
1:B:125:VAL:HG13	1:B:132:LEU:HB2	1.79	0.64
1:A:467:GLU:HG3	1:A:470:VAL:HG12	1.80	0.63
1:B:476:GLN:NE2	1:B:504:VAL:HG13	2.13	0.62
1:A:216:ILE:HD11	1:B:116:LEU:HD22	1.81	0.62
1:B:476:GLN:HE21	1:B:504:VAL:HG13	1.66	0.61
1:A:352:ILE:HG22	1:A:374:MET:CE	2.32	0.59
1:A:254:SER:HB3	4:A:706[B]:AMP:O2'	2.02	0.59
1:A:148:ALA:CB	1:A:170:PHE:CD2	2.86	0.59
1:A:308:GLN:HE22	1:A:335:ARG:HH11	1.51	0.59
1:A:285:ARG:O	1:A:288:VAL:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLN:HG2	1:B:45:SER:OG	2.03	0.58
1:A:13:LEU:HD22	1:A:26:PRO:HB3	1.84	0.58
1:A:176:ARG:HG2	1:A:176:ARG:HH11	1.69	0.58
1:A:345:LEU:HD22	1:A:396:THR:CG2	2.34	0.58
1:A:73:ALA:HB2	1:A:103:LEU:HD13	1.86	0.57
1:B:165:ARG:HD3	1:B:166:ASP:N	2.19	0.57
1:A:148:ALA:CB	1:A:170:PHE:CE2	2.88	0.57
1:B:308:GLN:HG3	1:B:332:ALA:HB2	1.87	0.57
1:A:383:MET:HB2	1:A:397:HIS:CD2	2.39	0.56
1:A:147:VAL:O	1:A:170:PHE:HB2	2.05	0.56
1:A:95:PRO:HB3	1:A:100:GLU:HG2	1.88	0.56
1:B:467:GLU:HG3	6:B:734:HOH:O	2.05	0.55
1:B:435:PRO:HG2	1:B:438:THR:OG1	2.07	0.55
1:B:458:ARG:NH2	1:B:461:LEU:HD23	2.22	0.55
4:A:706[B]:AMP:H8	4:A:706[B]:AMP:C5'	2.20	0.54
1:A:214:ARG:HB2	1:B:116:LEU:HD23	1.89	0.54
1:B:13:LEU:HD12	1:B:26:PRO:HB3	1.89	0.54
1:B:19:GLY:HA2	1:B:43:GLU:OE2	2.08	0.54
1:A:173:ALA:O	1:A:174:ASP:HB2	2.07	0.54
1:A:95:PRO:HG3	1:A:104:ARG:HG3	1.90	0.54
1:A:40:PRO:HG2	1:A:41:GLN:NE2	2.23	0.54
1:A:435:PRO:HG2	1:A:438:THR:OG1	2.07	0.54
1:B:459:LEU:HD12	1:B:460:LEU:HD22	1.89	0.53
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.72	0.53
1:B:153:ARG:NH2	1:B:168:LYS:HD3	2.24	0.53
1:B:453:THR:HG23	1:B:457:SER:HB2	1.91	0.53
1:B:326:TYR:OH	1:B:382:GLU:HB3	2.10	0.52
1:B:386:VAL:HA	1:B:389:THR:OG1	2.09	0.52
1:B:461:LEU:HD11	1:B:467:GLU:HG2	1.90	0.52
1:A:300:ILE:HG13	1:A:300:ILE:O	2.10	0.52
1:A:308:GLN:HE22	1:A:335:ARG:HD3	1.75	0.52
1:B:453:THR:CG2	1:B:457:SER:HB2	2.40	0.51
1:A:176:ARG:NH1	1:A:176:ARG:HG2	2.25	0.51
1:A:18:THR:HB	1:A:197:LEU:HG	1.90	0.51
1:A:315:ALA:HB2	1:A:390:LEU:HD23	1.91	0.51
1:B:214:ARG:NH1	1:B:367:ASP:OD1	2.44	0.51
1:B:65:SER:HB2	1:B:71:THR:HB	1.92	0.51
1:B:467:GLU:HA	1:B:470:VAL:HG23	1.93	0.51
1:B:348:TYR:C	1:B:348:TYR:CD1	2.84	0.50
1:B:326:TYR:OH	1:B:348:TYR:CE2	2.61	0.50
1:A:460:LEU:HD23	1:A:501:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ASN:HD22	1:B:281:PHE:H	1.59	0.50
1:A:352:ILE:HG22	1:A:374:MET:HE2	1.94	0.50
1:A:148:ALA:HB2	1:A:170:PHE:CD2	2.47	0.49
1:B:352:ILE:HG22	1:B:374:MET:HE2	1.94	0.49
1:B:354:LEU:HD21	1:B:408:LEU:HD22	1.93	0.49
1:A:351:ASP:OD2	1:A:443:LYS:HE2	2.12	0.49
1:A:307:ALA:O	1:A:310:PRO:HD2	2.12	0.49
1:B:27:VAL:O	1:B:27:VAL:HG13	2.11	0.49
1:B:273:MET:HB2	1:B:333:LEU:HD13	1.93	0.49
1:B:85:LEU:O	1:B:88:VAL:HG22	2.12	0.49
1:A:285:ARG:HA	1:A:288:VAL:HG22	1.95	0.49
1:B:153:ARG:NH1	1:B:168:LYS:HD3	2.23	0.49
1:B:335:ARG:HD2	6:B:736:HOH:O	2.13	0.49
1:A:308:GLN:NE2	1:A:335:ARG:HH11	2.11	0.48
1:A:308:GLN:HB2	1:A:328:LEU:HD22	1.95	0.48
1:A:352:ILE:HG22	1:A:374:MET:HE1	1.96	0.48
1:A:92:GLY:N	1:A:93:PRO:HD2	2.28	0.48
1:A:300:ILE:HD13	1:A:332:ALA:HB1	1.95	0.48
1:B:176:ARG:HB2	1:B:176:ARG:NH2	2.29	0.48
1:B:459:LEU:HD13	1:B:463:HIS:HD2	1.77	0.48
1:B:350:ALA:HB2	1:B:399:TYR:CD1	2.49	0.48
1:B:167:PRO:HG2	1:B:182:THR:OG1	2.14	0.48
1:A:125:VAL:HG13	1:A:132:LEU:HB2	1.96	0.48
1:A:290:HIS:CG	1:A:435:PRO:HD3	2.49	0.48
1:A:73:ALA:HB2	1:A:103:LEU:CD1	2.43	0.48
1:B:352:ILE:HG22	1:B:374:MET:CE	2.44	0.48
1:B:473:ALA:O	1:B:477:VAL:HG23	2.13	0.48
1:A:127:THR:HG23	1:A:127:THR:O	2.14	0.48
1:A:314:TRP:CD1	1:A:485:THR:HB	2.49	0.48
1:B:309:LEU:CD2	1:B:328:LEU:HD11	2.43	0.47
1:A:349:GLY:O	1:A:353:PRO:HD2	2.14	0.47
1:B:165:ARG:HD2	1:B:168:LYS:NZ	2.29	0.47
1:A:285:ARG:HD3	1:A:288:VAL:CG2	2.44	0.47
1:A:181:LEU:N	1:A:181:LEU:HD12	2.30	0.47
1:B:143:LEU:HD13	1:B:187:VAL:HG21	1.95	0.47
1:B:237:ARG:O	1:B:343:ARG:HD3	2.15	0.47
1:A:354:LEU:HD21	1:A:408:LEU:HD22	1.97	0.47
1:B:125:VAL:CG1	1:B:132:LEU:HB2	2.43	0.46
1:A:53:ALA:O	1:A:56:VAL:HG12	2.15	0.46
1:A:60:ARG:HG3	6:A:783:HOH:O	2.14	0.46
1:B:215:ARG:HG3	1:B:216:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HA	1:B:164:HIS:CE1	2.51	0.46
1:B:366:LEU:O	1:B:366:LEU:HD23	2.16	0.46
1:B:366:LEU:C	1:B:366:LEU:HD23	2.36	0.46
1:B:71:THR:OG1	1:B:127:THR:HG23	2.15	0.46
1:B:458:ARG:HH21	1:B:461:LEU:HB3	1.81	0.46
1:A:112:HIS:CD2	1:A:115:ARG:HE	2.22	0.45
1:A:173:ALA:O	1:A:174:ASP:CB	2.65	0.45
1:B:380:LEU:HB3	1:B:382:GLU:HG3	1.97	0.45
1:A:284:ALA:O	1:A:288:VAL:HG13	2.17	0.45
1:A:176:ARG:NH2	1:A:186:GLN:HG2	2.32	0.45
1:A:383:MET:HB2	1:A:397:HIS:NE2	2.31	0.45
1:A:273:MET:HB2	1:A:333:LEU:HD22	1.99	0.45
1:A:308:GLN:HG3	1:A:332:ALA:HB2	1.99	0.44
1:A:43:GLU:CD	1:A:43:GLU:H	2.19	0.44
1:B:129:ASP:HB3	6:B:926:HOH:O	2.17	0.44
1:B:223:VAL:HG13	1:B:429:ALA:HA	1.99	0.44
1:A:366:LEU:HD23	1:A:366:LEU:C	2.38	0.44
1:B:344:ILE:HB	1:B:395:THR:HG22	2.00	0.44
1:A:328:LEU:HB2	1:A:329:PRO:HD3	2.00	0.44
1:B:153:ARG:HH22	1:B:168:LYS:CD	2.29	0.44
1:A:273:MET:HE1	1:A:329:PRO:HB3	2.00	0.44
1:A:171:PRO:HA	1:A:185:TYR:OH	2.18	0.43
1:A:155:SER:HB3	1:A:161:LEU:CD2	2.47	0.43
1:B:474:LYS:O	1:B:478:VAL:HG23	2.18	0.43
1:B:149:PRO:HD3	1:B:170:PHE:CE2	2.54	0.43
1:B:148:ALA:HA	1:B:170:PHE:CE2	2.54	0.43
1:B:246:VAL:HG23	1:B:268:LEU:HD11	2.01	0.43
1:A:311:TYR:CZ	1:A:492:PRO:HB2	2.54	0.43
1:B:149:PRO:HD3	1:B:170:PHE:HE2	1.83	0.43
1:A:155:SER:HB3	1:A:161:LEU:HD21	2.01	0.43
1:B:30:THR:HG23	1:B:389:THR:HB	2.01	0.43
1:A:472:GLU:O	1:A:476:GLN:HG3	2.19	0.43
1:B:456:PHE:CD2	1:B:474:LYS:HD2	2.54	0.43
1:B:237:ARG:HB3	1:B:396:THR:HG21	2.01	0.43
1:A:178:VAL:HG12	1:A:181:LEU:HD13	2.01	0.42
1:B:292:ARG:HD3	1:B:292:ARG:HA	1.83	0.42
1:A:29:ALA:HA	1:A:314:TRP:CH2	2.54	0.42
1:A:397:HIS:HA	1:A:398:PRO:HD2	1.93	0.42
1:B:305:LEU:HD11	1:B:329:PRO:HA	2.00	0.42
1:A:253:ASP:HB2	3:A:705[B]:POP:O2	2.18	0.42
1:A:431:ALA:HA	1:A:439:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:HG3	1:A:185:TYR:CE2	2.55	0.42
1:A:262:HIS:CE1	1:A:267:GLU:HA	2.54	0.42
1:A:296:ARG:HH21	1:A:296:ARG:HG2	1.84	0.42
1:B:195:ILE:HG12	1:B:202:ALA:CB	2.47	0.42
1:B:348:TYR:CE1	1:B:383:MET:HG3	2.55	0.42
1:B:461:LEU:HD12	1:B:461:LEU:HA	1.80	0.42
1:A:73:ALA:CB	1:A:103:LEU:HD13	2.49	0.42
1:B:328:LEU:HB2	1:B:329:PRO:HD3	2.00	0.42
1:A:44:ARG:HG3	1:A:44:ARG:NH1	2.34	0.41
1:A:473:ALA:O	1:A:477:VAL:HG23	2.19	0.41
1:A:366:LEU:HD23	1:A:366:LEU:O	2.20	0.41
1:B:383:MET:HG2	1:B:397:HIS:CD2	2.56	0.41
1:A:89:LEU:HA	1:A:90:PRO:HD3	1.59	0.41
1:B:300:ILE:HG13	1:B:300:ILE:O	2.18	0.41
1:A:303:THR:HG23	1:A:304:GLU:N	2.36	0.41
1:B:348:TYR:CG	1:B:349:GLY:N	2.88	0.41
1:A:92:GLY:N	1:A:93:PRO:CD	2.83	0.41
1:A:223:VAL:HG13	1:A:429:ALA:HA	2.02	0.40
1:B:331:THR:O	1:B:335:ARG:HG3	2.21	0.40
1:B:335:ARG:HG2	1:B:390:LEU:HD11	2.03	0.40
1:B:71:THR:HA	1:B:126:ARG:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	477/513 (93%)	459 (96%)	17 (4%)	1 (0%)	47	48
1	B	491/513 (96%)	472 (96%)	18 (4%)	1 (0%)	47	48
All	All	968/1026 (94%)	931 (96%)	35 (4%)	2 (0%)	47	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	444	LEU
1	A	489	GLY

### 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	379/395 (96%)	367 (97%)	12 (3%)	39	40
1	B	388/395 (98%)	369 (95%)	19 (5%)	25	22
All	All	767/790 (97%)	736 (96%)	31 (4%)	31	31

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	44	ARG
1	A	103	LEU
1	A	161	LEU
1	A	248	LEU
1	A	291	LEU
1	A	345	LEU
1	A	362	ARG
1	A	387	LEU
1	A	390	LEU
1	A	412	GLU
1	A	459	LEU
1	B	13	LEU
1	B	101	LEU
1	B	125	VAL
1	B	143	LEU
1	B	165	ARG
1	B	168	LYS
1	B	221	GLU
1	B	248	LEU
1	B	291	LEU

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Mol	Chain	Res	Type
1	B	326	TYR
1	B	331	THR
1	B	341	GLU
1	B	370	LEU
1	B	412	GLU
1	B	415	LEU
1	B	421	ARG
1	B	426	LEU
1	B	461	LEU
1	B	498	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	112	HIS
1	A	236	GLN
1	A	290	HIS
1	A	308	GLN
1	A	358	HIS
1	A	440	ASN
1	A	476	GLN
1	A	491	HIS
1	B	41	GLN
1	B	279	ASN
1	B	463	HIS
1	B	476	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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$
5	ATP	A	701[A]	2	26,33,33	2.18	4 (15%)	31,52,52	2.66	12 (38%)
4	AMP	A	706[B]	2	22,25,25	3.48	6 (27%)	25,38,38	4.28	10 (40%)
5	ATP	B	702	2	26,33,33	6.10	13 (50%)	31,52,52	3.29	15 (48%)
3	POP	A	705[B]	2	6,8,8	1.16	0	13,13,13	1.91	2 (15%)

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
5	ATP	A	701[A]	2	-	9/18/38/38	0/3/3/3
4	AMP	A	706[B]	2	1/1/5/5	3/6/26/26	0/3/3/3
5	ATP	B	702	2	-	7/18/38/38	0/3/3/3
3	POP	A	705[B]	2	-	0/6/6/6	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	702	ATP	O4'-C1'	25.87	1.77	1.41
4	A	706[B]	AMP	C2'-C1'	11.65	1.71	1.53
5	B	702	ATP	PA-O5'	-8.95	1.23	1.59
5	B	702	ATP	C4-N3	6.37	1.44	1.35
5	A	701[A]	ATP	O5'-C5'	-6.18	1.21	1.44
4	A	706[B]	AMP	C3'-C4'	6.06	1.68	1.53
5	B	702	ATP	PA-O1A	5.76	1.71	1.50
4	A	706[B]	AMP	O4'-C1'	-5.58	1.33	1.41
5	A	701[A]	ATP	C4-N3	5.58	1.43	1.35
4	A	706[B]	AMP	C5'-C4'	-5.39	1.34	1.51
5	B	702	ATP	C2-N1	5.37	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	702	ATP	O4'-C4'	5.09	1.56	1.45
5	B	702	ATP	C5'-C4'	4.99	1.67	1.51
5	A	701[A]	ATP	C2-N1	4.33	1.42	1.33
5	B	702	ATP	C2'-C1'	4.18	1.60	1.53
4	A	706[B]	AMP	C2'-C3'	3.26	1.62	1.53
4	A	706[B]	AMP	O5'-C5'	-3.18	1.32	1.44
5	A	701[A]	ATP	C6-N6	-3.13	1.22	1.34
5	B	702	ATP	PB-O2B	-2.84	1.42	1.55
5	B	702	ATP	C6-N6	-2.58	1.24	1.34
5	B	702	ATP	C2-N3	2.48	1.36	1.32
5	B	702	ATP	C8-N7	-2.38	1.30	1.34
5	B	702	ATP	O3'-C3'	-2.13	1.38	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	706[B]	AMP	O5'-C5'-C4'	12.52	152.08	108.99
5	B	702	ATP	O4'-C1'-C2'	-10.41	91.72	106.93
4	A	706[B]	AMP	P-O5'-C5'	10.20	146.40	118.30
5	B	702	ATP	C3'-C2'-C1'	8.37	113.58	100.98
4	A	706[B]	AMP	O4'-C4'-C5'	7.40	133.72	109.37
4	A	706[B]	AMP	O3'-C3'-C4'	7.39	132.41	111.05
5	A	701[A]	ATP	PA-O5'-C5'	6.73	161.17	121.68
5	A	701[A]	ATP	C3'-C2'-C1'	6.21	110.33	100.98
5	B	702	ATP	O4'-C4'-C5'	4.82	125.22	109.37
5	B	702	ATP	N3-C2-N1	-4.76	121.24	128.68
5	B	702	ATP	C2-N1-C6	4.69	126.78	118.75
5	A	701[A]	ATP	N3-C2-N1	-4.65	121.42	128.68
5	A	701[A]	ATP	C2-N1-C6	4.64	126.69	118.75
3	A	705[B]	POP	P2-O-P1	4.55	148.44	132.83
4	A	706[B]	AMP	O2'-C2'-C1'	4.38	127.04	110.85
5	A	701[A]	ATP	PA-O3A-PB	-4.24	118.27	132.83
4	A	706[B]	AMP	C4-C5-N7	4.23	113.81	109.40
3	A	705[B]	POP	O6-P2-O	-4.01	91.20	104.64
5	B	702	ATP	O2'-C2'-C1'	3.48	123.69	110.85
4	A	706[B]	AMP	N6-C6-N1	3.46	125.75	118.57
5	B	702	ATP	C5'-C4'-C3'	3.35	127.74	115.18
5	A	701[A]	ATP	C5-C6-N1	-3.35	112.77	120.35
5	A	701[A]	ATP	PB-O3B-PG	-3.32	121.42	132.83
5	B	702	ATP	C5-C6-N1	-3.30	112.86	120.35
5	B	702	ATP	O2B-PB-O1B	2.87	126.44	112.24
4	A	706[B]	AMP	C1'-N9-C4	2.83	131.61	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701[A]	ATP	C5-C6-N6	2.80	124.61	120.35
4	A	706[B]	AMP	C2-N1-C6	2.58	123.16	118.75
5	A	701[A]	ATP	O5'-C5'-C4'	2.50	117.60	108.99
5	A	701[A]	ATP	C1'-N9-C4	2.46	130.96	126.64
5	B	702	ATP	PB-O3B-PG	-2.45	124.41	132.83
5	A	701[A]	ATP	O5'-PA-O1A	-2.38	99.77	109.07
5	B	702	ATP	C5-C6-N6	2.34	123.92	120.35
5	B	702	ATP	C1'-N9-C4	2.34	130.75	126.64
5	B	702	ATP	PA-O5'-C5'	2.33	135.33	121.68
4	A	706[B]	AMP	C5-C6-N1	-2.31	115.13	120.35
5	B	702	ATP	N6-C6-N1	2.24	123.22	118.57
5	B	702	ATP	O3'-C3'-C2'	2.24	119.06	111.82
5	A	701[A]	ATP	O4'-C1'-C2'	-2.17	103.75	106.93

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	706[B]	AMP	C4'

All (19) torsion outliers are listed below:

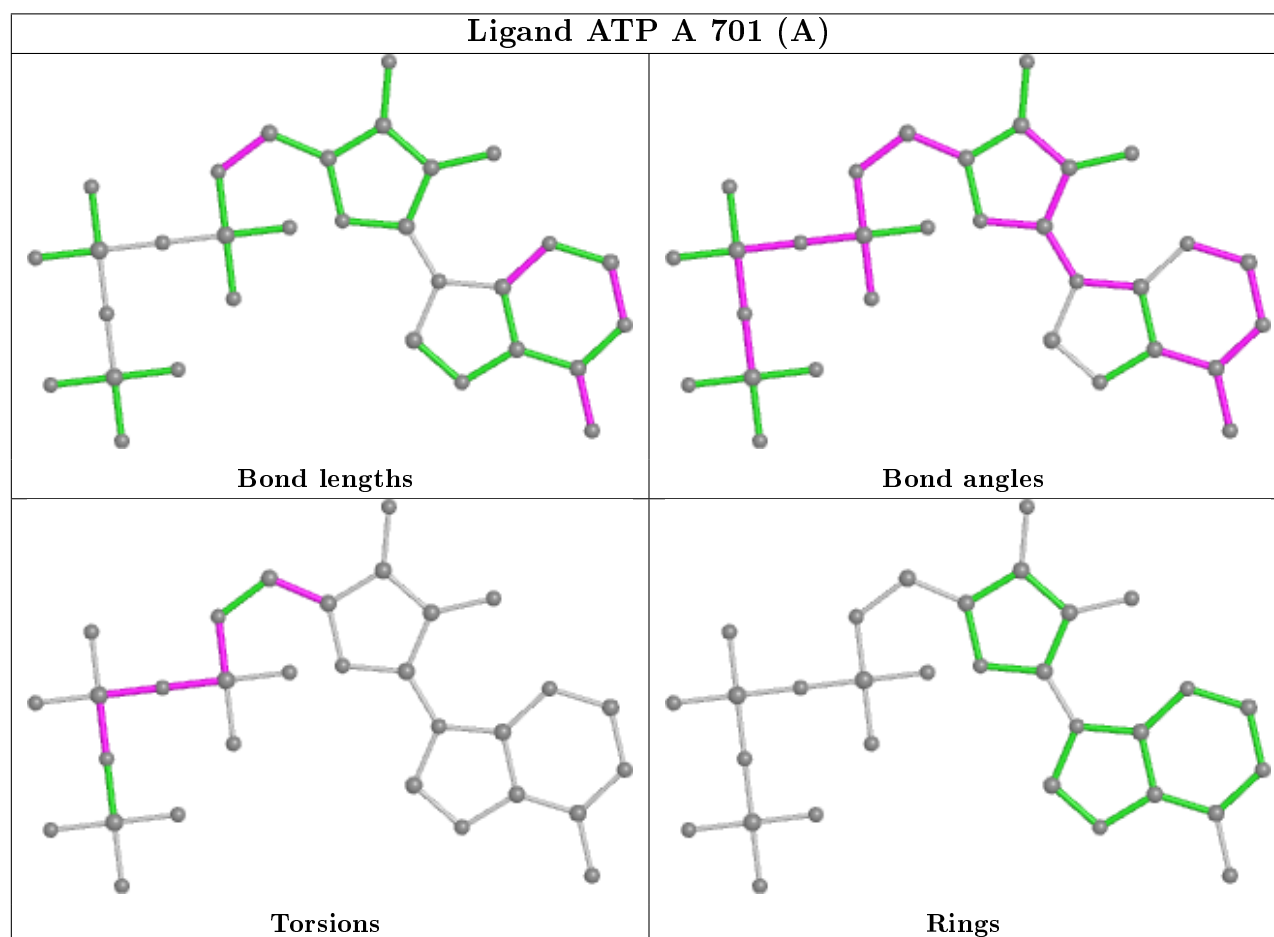
Mol	Chain	Res	Type	Atoms
5	B	702	ATP	C5'-O5'-PA-O2A
5	A	701[A]	ATP	C5'-O5'-PA-O1A
5	A	701[A]	ATP	C5'-O5'-PA-O2A
5	A	701[A]	ATP	O4'-C4'-C5'-O5'
5	B	702	ATP	O4'-C4'-C5'-O5'
4	A	706[B]	AMP	C4'-C5'-O5'-P
4	A	706[B]	AMP	C3'-C4'-C5'-O5'
5	A	701[A]	ATP	C3'-C4'-C5'-O5'
5	A	701[A]	ATP	PB-O3A-PA-O5'
5	B	702	ATP	C3'-C4'-C5'-O5'
5	B	702	ATP	C5'-O5'-PA-O3A
5	A	701[A]	ATP	PA-O3A-PB-O2B
5	B	702	ATP	C5'-O5'-PA-O1A
5	B	702	ATP	PA-O3A-PB-O1B
5	B	702	ATP	PA-O3A-PB-O2B
5	A	701[A]	ATP	PG-O3B-PB-O1B
5	A	701[A]	ATP	C5'-O5'-PA-O3A
5	A	701[A]	ATP	PA-O3A-PB-O1B
4	A	706[B]	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

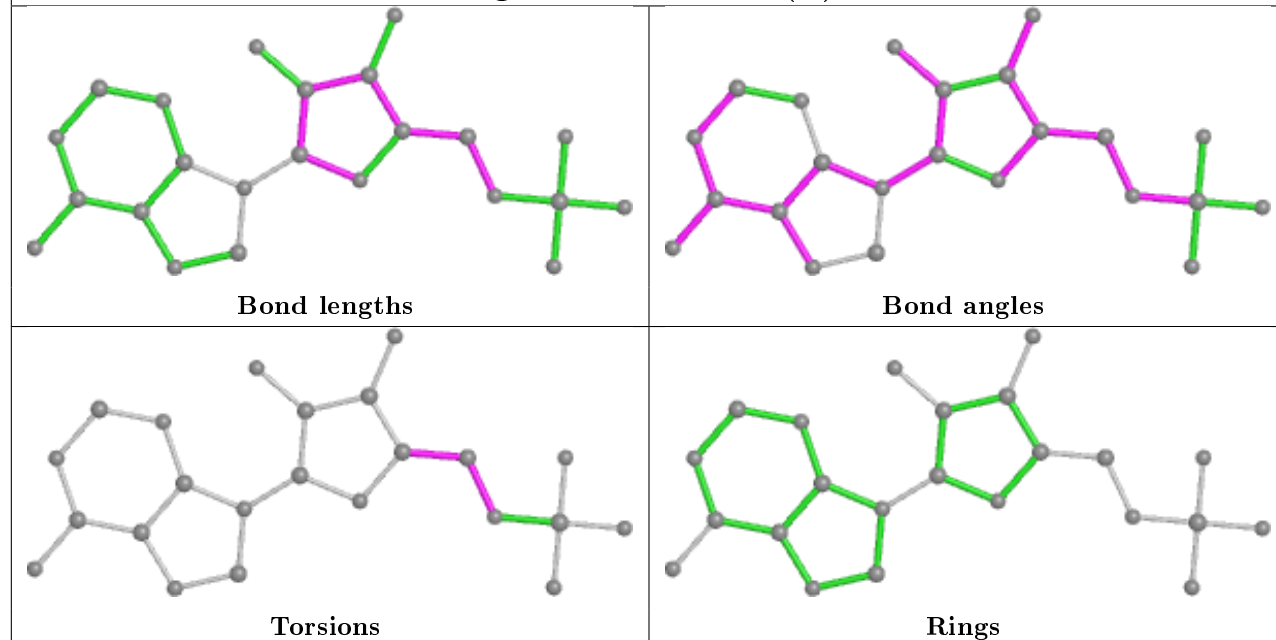
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706[B]	AMP	4	0
5	B	702	ATP	1	0
3	A	705[B]	POP	1	0

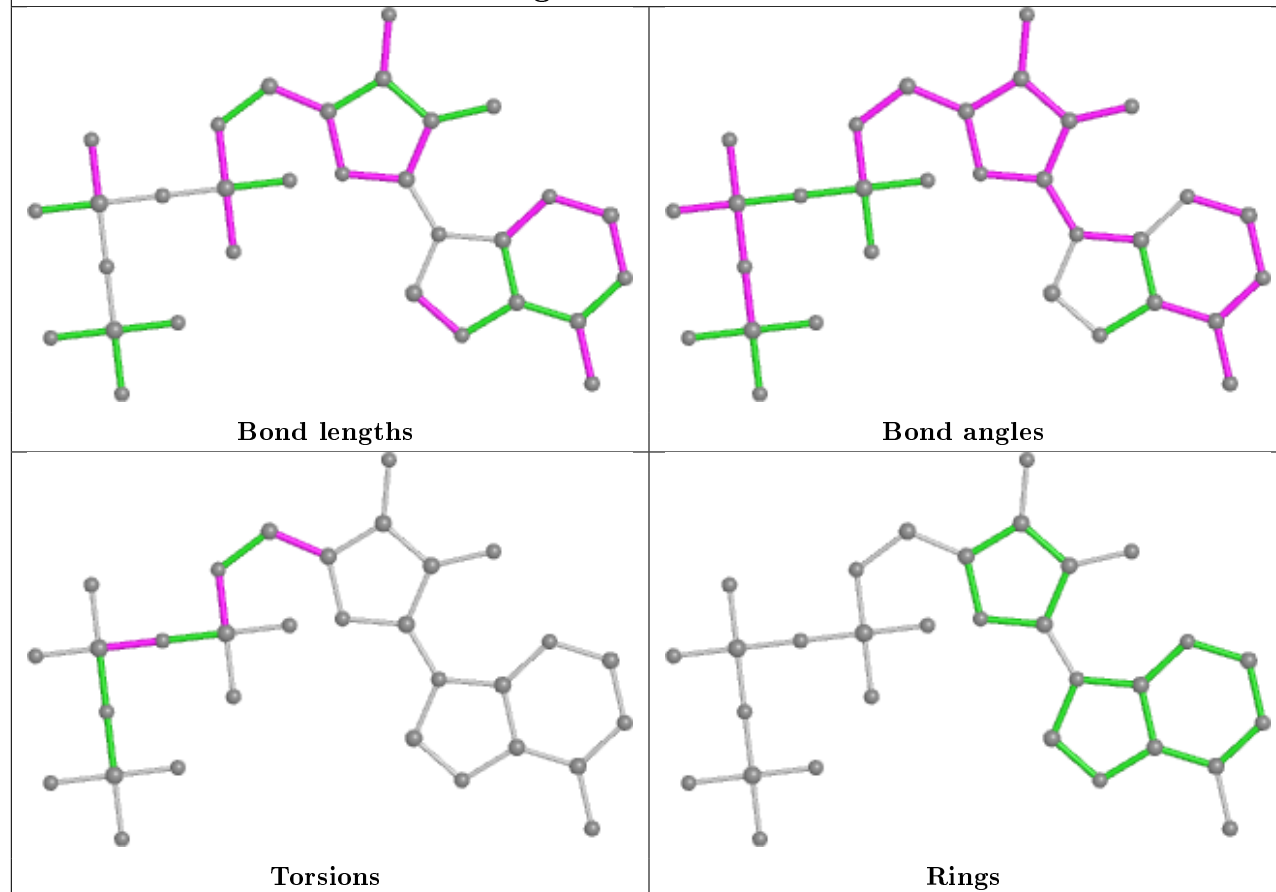
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand AMP A 706 (B)



## Ligand ATP B 702



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	485/513 (94%)	0.07	24 (4%)	29 35	6, 19, 48, 62	0
1	B	497/513 (96%)	0.00	18 (3%)	42 49	8, 20, 41, 62	0
All	All	982/1026 (95%)	0.03	42 (4%)	35 41	6, 20, 46, 62	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	PHE	5.8
1	A	18	THR	5.5
1	B	165	ARG	5.5
1	A	470	VAL	5.0
1	B	92	GLY	4.5
1	B	93	PRO	4.4
1	A	42	GLY	4.1
1	B	91	ALA	3.8
1	A	93	PRO	3.8
1	A	467	GLU	3.7
1	A	4	PRO	3.6
1	A	468	ASP	3.6
1	B	94	ALA	3.4
1	A	459	LEU	3.4
1	A	19	GLY	3.2
1	A	359	ARG	3.2
1	B	166	ASP	3.2
1	B	444	LEU	3.0
1	A	507	ARG	2.9
1	B	326	TYR	2.8
1	A	43	GLU	2.8
1	A	23	ALA	2.8
1	A	465	VAL	2.7
1	B	173	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	326	TYR	2.5
1	A	502	ARG	2.4
1	B	445	GLY	2.4
1	A	17	ARG	2.3
1	A	24	PRO	2.3
1	B	163	ALA	2.3
1	A	506	ASP	2.3
1	B	24	PRO	2.2
1	A	460	LEU	2.2
1	B	170	PHE	2.2
1	B	174	ASP	2.2
1	B	168	LYS	2.1
1	A	292	ARG	2.1
1	A	505	ALA	2.1
1	B	18	THR	2.1
1	B	20	GLY	2.1
1	B	169	GLY	2.1
1	A	172	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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
4	AMP	A	706[B]	23/23	0.82	0.19	20,23,28,29	23
5	ATP	B	702	31/31	0.88	0.15	12,27,33,34	0
2	MG	A	604	1/1	0.89	0.08	18,18,18,18	0
2	MG	A	603	1/1	0.90	0.13	26,26,26,26	0
5	ATP	A	701[A]	31/31	0.92	0.16	16,23,24,25	31

*Continued on next page...*

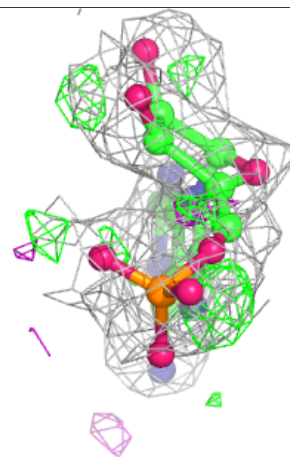
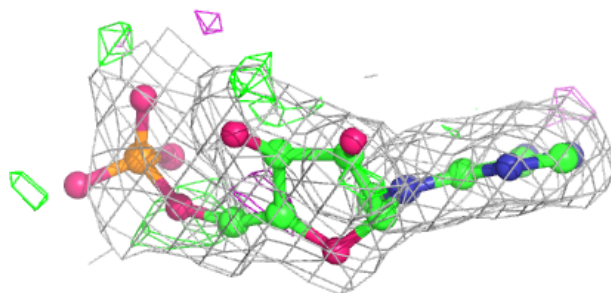
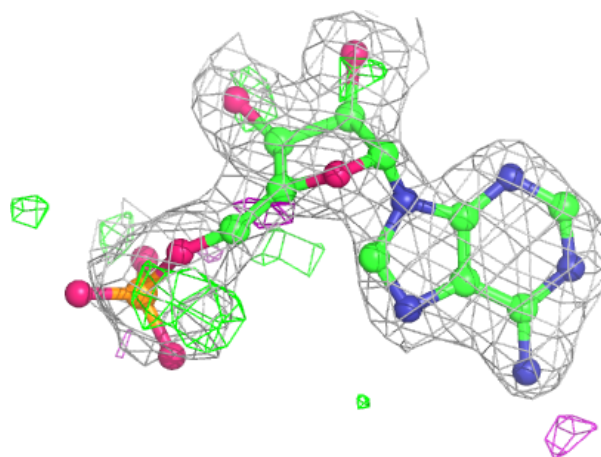
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	602	1/1	0.93	0.05	18,18,18,18	0
2	MG	B	601	1/1	0.94	0.07	17,17,17,17	0
3	POP	A	705[B]	9/9	0.96	0.11	4,7,8,11	9

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.

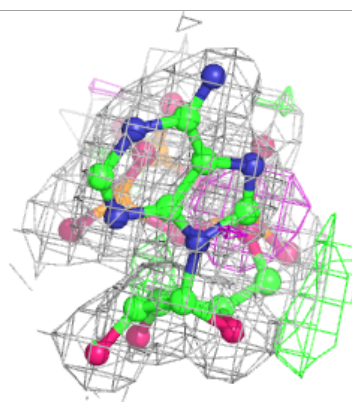
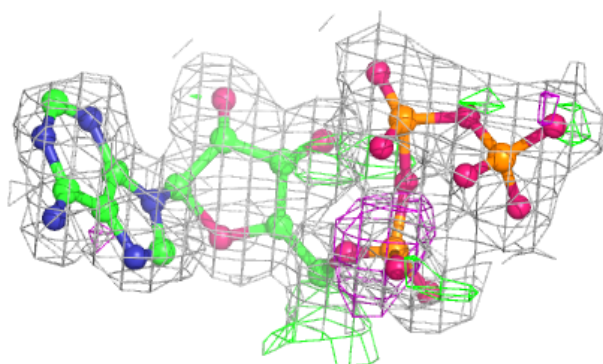
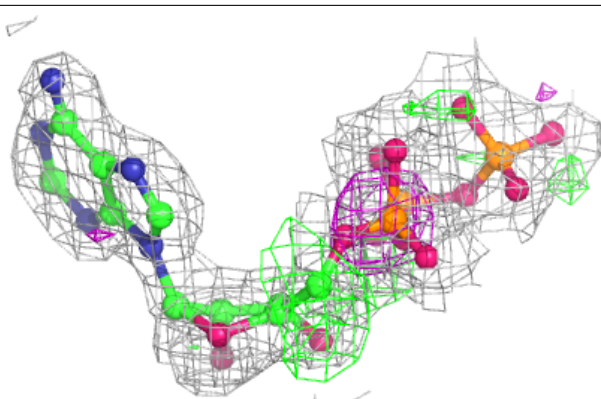
**Electron density around AMP A 706 (B):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

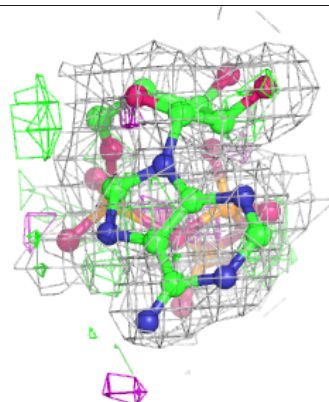
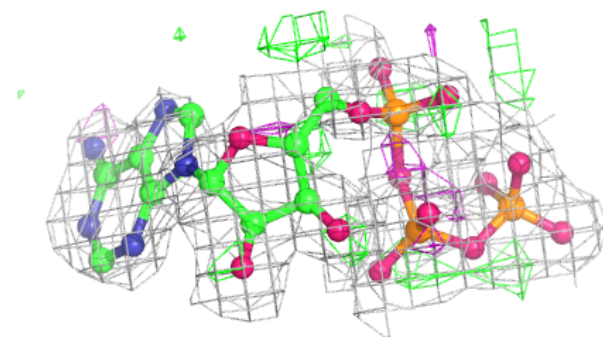
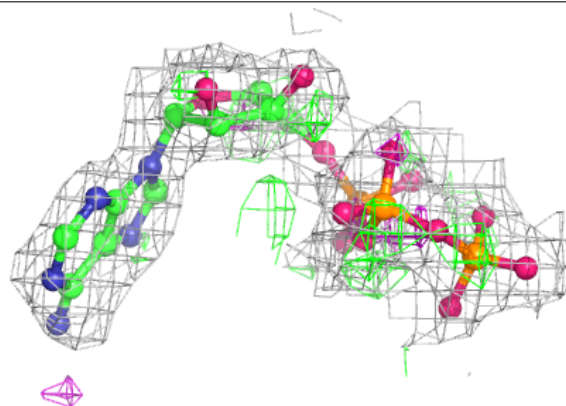


**Electron density around ATP B 702:**

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

**Electron density around ATP A 701 (A):**

$2mF_o-DF_c$  (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.