



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:25 AM UTC

PDB ID : 2HS0 / pdb_00002hs0
Title : T. maritima PurL complexed with ATP
Authors : Ealick, S.E.; Morar, M.
Deposited on : 2006-07-20
Resolution : 2.52 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

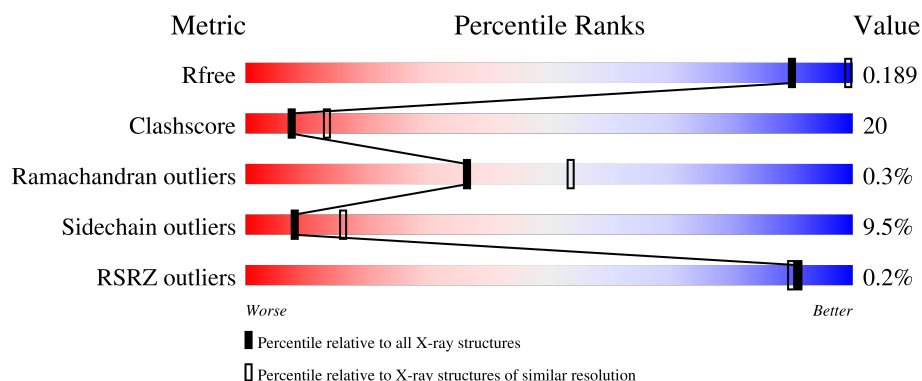
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	603	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4755 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.

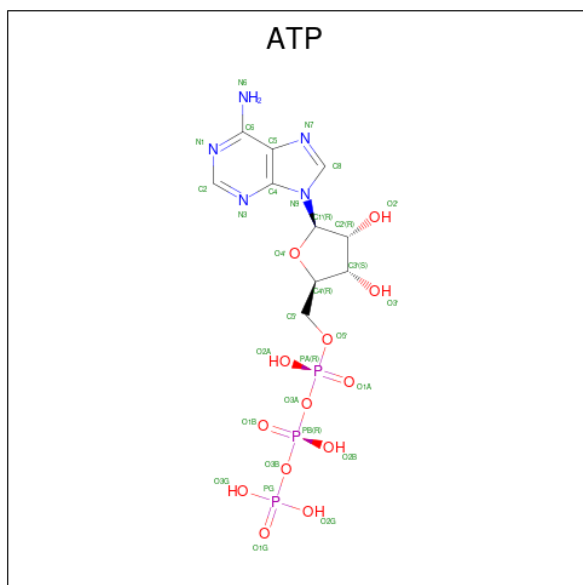
- Molecule 1 is a protein called Phosphoribosylformylglycinamidine synthase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4473	2849	764	842	18			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	1
			45	11	5	23	6		

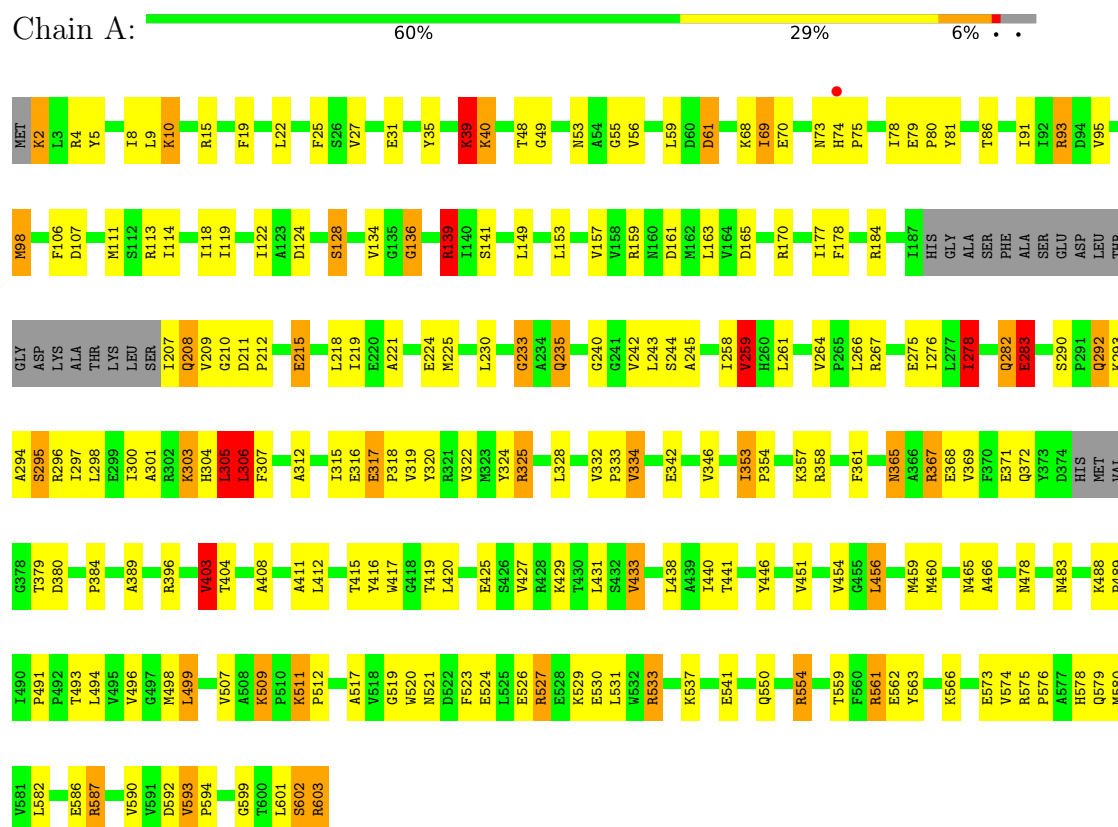
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total 204	O 204	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: Phosphoribosylformylglycinamide synthase II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.87Å 71.53Å 137.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.73 – 2.52 31.73 – 2.52	Depositor EDS
% Data completeness (in resolution range)	(Not available) (31.73-2.52) 92.9 (31.73-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.253 0.183 , 0.189	Depositor DCC
R_{free} test set	940 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4755	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.91	0/4562	1.67	77/6190 (1.2%)

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	0

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	HIS	N-CA-C	14.78	130.75	113.02
1	A	304	HIS	CA-C-N	12.87	144.87	121.70
1	A	304	HIS	C-N-CA	12.87	144.87	121.70
1	A	139	ARG	NE-CZ-NH2	-9.79	110.39	119.20
1	A	304	HIS	O-C-N	-9.17	110.56	122.39
1	A	403	VAL	CB-CA-C	-8.95	95.08	111.18
1	A	305	LEU	N-CA-CB	-8.57	95.93	110.50
1	A	98	MET	N-CA-C	-8.03	103.05	113.17
1	A	136	GLY	N-CA-C	-8.03	99.74	110.58
1	A	491	PRO	CA-C-N	-7.98	110.42	120.23
1	A	491	PRO	C-N-CA	-7.98	110.42	120.23
1	A	267	ARG	N-CA-C	-7.84	103.85	113.41
1	A	507	VAL	CB-CA-C	7.35	120.03	110.91
1	A	419	THR	N-CA-C	7.20	118.77	111.07
1	A	509	LYS	CA-C-N	-7.12	112.43	119.76
1	A	509	LYS	C-N-CA	-7.12	112.43	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	LYS	N-CA-C	7.05	119.82	111.71
1	A	333	PRO	CA-C-N	6.96	130.35	120.53
1	A	333	PRO	C-N-CA	6.96	130.35	120.53
1	A	306	LEU	N-CA-C	6.95	125.61	110.80
1	A	211	ASP	CA-C-N	6.86	127.14	119.32
1	A	211	ASP	C-N-CA	6.86	127.14	119.32
1	A	61	ASP	N-CA-CB	6.64	121.71	110.49
1	A	19	PHE	N-CA-C	6.55	118.97	111.11
1	A	157	VAL	N-CA-C	6.52	117.68	108.36
1	A	353	ILE	CA-C-N	6.40	126.35	120.21
1	A	353	ILE	C-N-CA	6.40	126.35	120.21
1	A	210	GLY	N-CA-C	-6.35	104.63	111.93
1	A	297	ILE	CB-CA-C	-6.33	103.78	111.88
1	A	441	THR	CA-C-N	-6.33	111.85	122.29
1	A	441	THR	C-N-CA	-6.33	111.85	122.29
1	A	282	GLN	N-CA-C	6.32	118.18	110.41
1	A	211	ASP	N-CA-C	6.31	119.48	109.64
1	A	278	ILE	CB-CA-C	6.29	117.42	110.62
1	A	412	LEU	N-CA-C	6.28	118.92	111.33
1	A	53	ASN	N-CA-C	6.23	118.33	108.67
1	A	128	SER	N-CA-C	6.21	120.12	112.54
1	A	9	LEU	CA-C-N	6.14	128.83	120.54
1	A	9	LEU	C-N-CA	6.14	128.83	120.54
1	A	283	GLU	CA-CB-CG	6.07	126.24	114.10
1	A	602	SER	N-CA-C	5.97	117.61	108.42
1	A	55	GLY	N-CA-C	-5.92	106.92	115.27
1	A	417	TRP	N-CA-C	5.88	118.17	111.11
1	A	25	PHE	N-CA-C	5.87	117.67	111.28
1	A	529	LYS	N-CA-C	5.80	118.39	111.71
1	A	31	GLU	N-CA-C	-5.65	105.27	111.82
1	A	9	LEU	N-CA-C	-5.60	105.25	111.36
1	A	49	GLY	N-CA-C	-5.57	99.98	113.18
1	A	592	ASP	N-CA-C	-5.57	107.07	112.97
1	A	554	ARG	N-CA-C	-5.51	105.36	111.36
1	A	139	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	A	283	GLU	CB-CG-CD	5.49	121.94	112.60
1	A	59	LEU	CB-CG-CD2	-5.46	94.31	110.70
1	A	587	ARG	CB-CG-CD	5.45	123.84	111.30
1	A	98	MET	CG-SD-CE	5.44	112.87	100.90
1	A	233	GLY	N-CA-C	-5.42	100.33	113.18
1	A	219	ILE	N-CA-C	5.40	115.84	110.23
1	A	283	GLU	N-CA-C	5.38	118.82	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	THR	N-CA-C	5.38	116.83	111.07
1	A	550	GLN	N-CA-C	-5.38	104.98	112.30
1	A	328	LEU	CA-C-N	-5.29	117.53	122.66
1	A	328	LEU	C-N-CA	-5.29	117.53	122.66
1	A	61	ASP	N-CA-C	5.27	122.03	110.80
1	A	136	GLY	CA-C-O	-5.26	117.28	120.91
1	A	599	GLY	N-CA-C	5.23	117.08	110.38
1	A	478	ASN	N-CA-CB	-5.23	103.30	111.56
1	A	283	GLU	CB-CA-C	5.20	119.28	111.89
1	A	318	PRO	CA-C-N	-5.13	116.78	122.27
1	A	318	PRO	C-N-CA	-5.13	116.78	122.27
1	A	40	LYS	N-CA-C	5.12	116.86	111.28
1	A	563	TYR	N-CA-C	-5.09	106.85	113.16
1	A	451	VAL	N-CA-C	5.08	115.31	110.53
1	A	354	PRO	N-CA-C	5.07	118.31	111.22
1	A	517	ALA	CA-C-N	-5.05	116.93	123.19
1	A	517	ALA	C-N-CA	-5.05	116.93	123.19
1	A	259	VAL	CB-CA-C	5.03	118.07	110.63
1	A	499	LEU	CA-CB-CG	5.00	133.81	116.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	61	ASP	CA

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	4473	0	4511	184	0
2	A	2	0	0	0	0
3	A	76	0	18	2	0
4	A	204	0	0	8	0
All	All	4755	0	4529	184	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 20.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HE21	1:A:208:GLN:HA	1.12	1.13
1:A:427:VAL:O	1:A:431:LEU:HD23	1.49	1.10
1:A:561:ARG:HG2	1:A:561:ARG:HH11	0.98	1.09
1:A:593:VAL:HG13	1:A:594:PRO:HD2	1.31	1.08
1:A:561:ARG:HG2	1:A:561:ARG:NH1	1.56	1.06
1:A:365:ASN:HD21	1:A:367:ARG:CB	1.71	1.01
1:A:40:LYS:HE3	1:A:342:GLU:OE1	1.62	0.98
1:A:602:SER:HB2	1:A:603:ARG:HD2	1.46	0.97
1:A:561:ARG:HH11	1:A:561:ARG:CG	1.76	0.97
1:A:365:ASN:HD21	1:A:367:ARG:HB2	1.30	0.97
1:A:601:LEU:N	1:A:601:LEU:HD23	1.81	0.94
1:A:208:GLN:HE21	1:A:208:GLN:CA	1.81	0.93
1:A:431:LEU:HD22	1:A:431:LEU:N	1.79	0.93
1:A:208:GLN:HA	1:A:208:GLN:NE2	1.86	0.90
1:A:601:LEU:HD23	1:A:601:LEU:H	1.33	0.90
1:A:593:VAL:HG13	1:A:594:PRO:CD	2.03	0.88
1:A:431:LEU:N	1:A:431:LEU:CD2	2.39	0.86
1:A:261:LEU:HD21	1:A:322:VAL:HG13	1.58	0.84
1:A:420:LEU:HD12	1:A:466:ALA:HB2	1.60	0.82
1:A:243:LEU:HD22	1:A:278:ILE:HD11	1.62	0.82
1:A:170:ARG:HD2	4:A:1120:HOH:O	1.80	0.81
1:A:379:THR:HG22	1:A:380:ASP:H	1.45	0.81
1:A:79:GLU:OE2	1:A:207:ILE:HG12	1.80	0.80
1:A:208:GLN:NE2	1:A:209:VAL:H	1.79	0.80
1:A:243:LEU:CD2	1:A:278:ILE:HD11	2.12	0.80
1:A:379:THR:HG22	1:A:380:ASP:N	1.97	0.80
1:A:261:LEU:CD2	1:A:322:VAL:HG13	2.14	0.77
1:A:488:LYS:HD3	1:A:489:PRO:HD2	1.68	0.75
1:A:358:ARG:NH2	1:A:576:PRO:HA	2.03	0.73
1:A:384:PRO:HD3	4:A:1111:HOH:O	1.87	0.72
1:A:320:TYR:HB2	1:A:334:VAL:HG23	1.70	0.72
1:A:261:LEU:HD12	1:A:276:ILE:HG22	1.71	0.71
1:A:365:ASN:C	1:A:365:ASN:HD22	1.98	0.71
1:A:431:LEU:CD2	1:A:431:LEU:H	2.03	0.71
1:A:379:THR:CG2	1:A:380:ASP:H	2.04	0.70
1:A:165:ASP:O	1:A:233:GLY:HA2	1.90	0.70
1:A:365:ASN:HD21	1:A:367:ARG:HB3	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLU:H	1:A:579:GLN:NE2	1.91	0.69
1:A:527:ARG:HE	1:A:579:GLN:NE2	1.92	0.67
1:A:294:ALA:O	1:A:298:LEU:HG	1.95	0.67
1:A:365:ASN:ND2	1:A:367:ARG:CB	2.52	0.67
1:A:184:ARG:NH1	1:A:275:GLU:OE1	2.27	0.66
1:A:520:TRP:CH2	1:A:593:VAL:HG22	2.30	0.66
1:A:367:ARG:HG3	1:A:367:ARG:HH11	1.60	0.66
1:A:601:LEU:N	1:A:601:LEU:CD2	2.58	0.65
1:A:379:THR:CG2	1:A:380:ASP:N	2.62	0.61
1:A:425:GLU:O	1:A:429:LYS:HG3	1.99	0.61
1:A:431:LEU:HD23	1:A:431:LEU:H	1.65	0.61
1:A:574:VAL:HG22	1:A:578:HIS:HB3	1.82	0.61
1:A:365:ASN:C	1:A:365:ASN:ND2	2.57	0.61
1:A:139:ARG:HG3	1:A:361:PHE:CD2	2.37	0.60
1:A:208:GLN:HE21	1:A:209:VAL:H	1.49	0.59
1:A:159:ARG:NH2	1:A:161:ASP:OD2	2.32	0.59
1:A:416:TYR:OH	1:A:465:ASN:ND2	2.24	0.59
1:A:4:ARG:HE	1:A:5:TYR:HE2	1.50	0.59
1:A:404:THR:HA	1:A:496:VAL:O	2.04	0.58
1:A:295:SER:HB3	4:A:1253:HOH:O	2.04	0.57
1:A:320:TYR:HB2	1:A:334:VAL:CG2	2.34	0.57
1:A:488:LYS:HD3	1:A:489:PRO:CD	2.33	0.57
1:A:367:ARG:HG3	1:A:367:ARG:NH1	2.18	0.57
1:A:511:LYS:HZ3	1:A:586:GLU:HG3	1.70	0.57
1:A:208:GLN:HE21	1:A:209:VAL:N	2.01	0.57
1:A:511:LYS:NZ	1:A:586:GLU:HG3	2.19	0.57
1:A:106:PHE:HB2	1:A:153:LEU:HB3	1.87	0.56
1:A:264:VAL:O	1:A:266:LEU:CD1	2.53	0.56
1:A:208:GLN:NE2	1:A:209:VAL:N	2.50	0.56
1:A:561:ARG:NH1	1:A:561:ARG:CG	2.40	0.56
1:A:221:ALA:O	1:A:225:MET:HG3	2.06	0.55
1:A:389:ALA:HA	1:A:403:VAL:HG13	1.88	0.55
1:A:139:ARG:HG2	1:A:361:PHE:HE2	1.71	0.55
1:A:243:LEU:HD22	1:A:278:ILE:CD1	2.32	0.55
1:A:261:LEU:HD12	1:A:276:ILE:CG2	2.35	0.55
1:A:139:ARG:HG2	1:A:361:PHE:CE2	2.42	0.55
1:A:224:GLU:OE2	1:A:303:LYS:NZ	2.38	0.55
1:A:521:ASN:HA	1:A:574:VAL:HG23	1.88	0.55
1:A:593:VAL:CG1	1:A:594:PRO:CD	2.81	0.54
1:A:80:PRO:HB3	1:A:118:ILE:HG13	1.87	0.54
1:A:264:VAL:O	1:A:266:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:O	1:A:39:LYS:HG2	2.07	0.54
1:A:527:ARG:HE	1:A:579:GLN:HE22	1.55	0.54
1:A:139:ARG:HD3	4:A:1067:HOH:O	2.07	0.54
1:A:15:ARG:HH11	1:A:15:ARG:HG2	1.74	0.53
1:A:261:LEU:HD21	1:A:322:VAL:CG1	2.36	0.53
1:A:603:ARG:NE	4:A:1127:HOH:O	2.42	0.53
1:A:290:SER:HB3	1:A:292:GLN:OE1	2.08	0.53
1:A:261:LEU:CD2	1:A:322:VAL:CG1	2.87	0.52
1:A:524:GLU:H	1:A:579:GLN:HE22	1.57	0.52
1:A:56:VAL:HG11	1:A:163:LEU:HD22	1.92	0.52
1:A:118:ILE:O	1:A:122:ILE:HG12	2.10	0.52
1:A:177:ILE:HD13	1:A:242:VAL:HG22	1.91	0.52
1:A:365:ASN:ND2	1:A:367:ARG:HB3	2.21	0.52
1:A:86:THR:O	1:A:86:THR:HG22	2.11	0.51
1:A:317:GLU:O	1:A:319:VAL:N	2.43	0.51
1:A:603:ARG:NE	1:A:603:ARG:HA	2.26	0.51
1:A:243:LEU:HD23	1:A:278:ILE:HD11	1.88	0.51
1:A:139:ARG:HG2	4:A:1069:HOH:O	2.12	0.50
1:A:40:LYS:HG3	4:A:1113:HOH:O	2.12	0.50
1:A:128:SER:CB	1:A:212:PRO:HB2	2.42	0.50
1:A:68:LYS:HE2	3:A:1066[A]:ATP:O1B	2.11	0.49
1:A:74:HIS:HB3	1:A:75:PRO:HD3	1.94	0.49
1:A:114:ILE:HG23	1:A:119:ILE:HD12	1.93	0.49
1:A:159:ARG:HH21	1:A:161:ASP:CG	2.19	0.49
1:A:208:GLN:CA	1:A:208:GLN:NE2	2.55	0.49
1:A:389:ALA:HB2	1:A:403:VAL:HG13	1.93	0.49
1:A:27:VAL:HG11	1:A:240:GLY:HA2	1.94	0.49
1:A:537:LYS:NZ	1:A:541:GLU:OE2	2.31	0.49
1:A:78:ILE:HG22	1:A:79:GLU:HG3	1.94	0.49
1:A:367:ARG:HH11	1:A:367:ARG:CG	2.26	0.48
1:A:114:ILE:CG2	1:A:119:ILE:HD12	2.43	0.48
1:A:2:LYS:O	1:A:2:LYS:HG3	2.14	0.48
1:A:533:ARG:HH11	1:A:533:ARG:HG2	1.77	0.48
1:A:258:ILE:CD1	1:A:315:ILE:HG21	2.44	0.48
1:A:440:ILE:HD11	1:A:498:MET:HE2	1.94	0.48
1:A:10:LYS:HE2	1:A:10:LYS:HB2	1.79	0.48
1:A:70:GLU:OE2	3:A:1066[A]:ATP:O1G	2.31	0.48
1:A:365:ASN:ND2	1:A:367:ARG:HB2	2.13	0.48
1:A:128:SER:HB2	1:A:212:PRO:HB2	1.94	0.47
1:A:389:ALA:CA	1:A:403:VAL:HG13	2.44	0.47
1:A:69:ILE:O	1:A:69:ILE:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:HB	1:A:312:ALA:HB2	1.96	0.47
1:A:70:GLU:HB2	1:A:91:ILE:HD13	1.95	0.47
1:A:81:TYR:OH	1:A:124:ASP:OD2	2.27	0.47
1:A:365:ASN:ND2	1:A:367:ARG:H	2.12	0.47
1:A:530:GLU:OE2	1:A:533:ARG:HD3	2.15	0.47
1:A:521:ASN:ND2	4:A:1201:HOH:O	2.47	0.47
1:A:184:ARG:HH11	1:A:275:GLU:CD	2.22	0.46
1:A:365:ASN:ND2	1:A:367:ARG:N	2.63	0.46
1:A:389:ALA:CB	1:A:403:VAL:HG13	2.44	0.46
1:A:93:ARG:HD3	1:A:215:GLU:OE1	2.16	0.46
1:A:139:ARG:CG	1:A:361:PHE:CE2	2.98	0.46
1:A:261:LEU:HD23	1:A:322:VAL:HG13	1.97	0.46
1:A:353:ILE:HG23	1:A:353:ILE:O	2.15	0.46
1:A:459:MET:HE1	1:A:493:THR:N	2.31	0.45
1:A:208:GLN:HE21	1:A:208:GLN:C	2.24	0.45
1:A:561:ARG:HH22	1:A:566:LYS:HG2	1.82	0.45
1:A:559:THR:O	1:A:562:GLU:HB2	2.17	0.45
1:A:119:ILE:HD13	1:A:369:VAL:CG1	2.47	0.45
1:A:139:ARG:HG3	1:A:361:PHE:HD2	1.81	0.45
1:A:128:SER:HB2	1:A:212:PRO:CB	2.46	0.45
1:A:459:MET:HE2	1:A:494:LEU:HB2	1.99	0.45
1:A:230:LEU:HA	1:A:293:LYS:HD3	1.99	0.45
1:A:575:ARG:O	1:A:576:PRO:C	2.60	0.45
1:A:134:VAL:O	1:A:134:VAL:CG1	2.65	0.45
1:A:533:ARG:HH11	1:A:533:ARG:CG	2.30	0.44
1:A:114:ILE:HG23	1:A:119:ILE:CD1	2.47	0.44
1:A:368:GLU:OE2	1:A:554:ARG:NH2	2.51	0.44
1:A:111:MET:HB3	1:A:113:ARG:O	2.17	0.44
1:A:95:VAL:HA	1:A:98:MET:HE3	2.00	0.44
1:A:324:TYR:O	1:A:325:ARG:HB2	2.18	0.44
1:A:244:SER:O	1:A:245:ALA:C	2.60	0.44
1:A:446:TYR:O	1:A:483:ASN:HB2	2.17	0.44
1:A:574:VAL:HG22	1:A:578:HIS:CB	2.47	0.44
1:A:300:ILE:O	1:A:301:ALA:C	2.60	0.44
1:A:433:VAL:O	1:A:433:VAL:HG13	2.18	0.44
1:A:531:LEU:HD22	1:A:579:GLN:HB3	1.98	0.43
1:A:261:LEU:HD22	1:A:261:LEU:N	2.32	0.43
1:A:91:ILE:HD12	1:A:91:ILE:HA	1.81	0.43
1:A:235:GLN:HG2	1:A:245:ALA:HA	2.00	0.43
1:A:15:ARG:HG2	1:A:15:ARG:NH1	2.34	0.43
1:A:527:ARG:HH21	1:A:579:GLN:HE21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:NH1	1:A:275:GLU:CD	2.78	0.42
1:A:178:PHE:CE2	1:A:218:LEU:HD12	2.54	0.42
1:A:240:GLY:O	1:A:243:LEU:HB3	2.20	0.42
1:A:456:LEU:HD22	1:A:460:MET:HG2	2.01	0.42
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.78	0.42
1:A:282:GLN:HB2	1:A:283:GLU:OE2	2.20	0.41
1:A:346:VAL:HG11	1:A:454:VAL:HG22	2.02	0.41
1:A:519:GLY:HA2	1:A:593:VAL:CG1	2.50	0.41
1:A:306:LEU:H	1:A:306:LEU:HG	1.56	0.41
1:A:4:ARG:O	1:A:8:ILE:HG13	2.19	0.41
1:A:69:ILE:HA	1:A:153:LEU:HA	2.02	0.41
1:A:73:ASN:OD1	1:A:149:LEU:HA	2.20	0.41
1:A:580:MET:HE3	1:A:580:MET:HB2	1.87	0.41
1:A:107:ASP:O	1:A:136:GLY:HA3	2.21	0.41
1:A:305:LEU:N	1:A:305:LEU:CD1	2.83	0.41
1:A:27:VAL:HG11	1:A:240:GLY:CA	2.51	0.41
1:A:590:VAL:O	1:A:590:VAL:HG12	2.21	0.41
1:A:178:PHE:HA	1:A:307:PHE:O	2.21	0.41
1:A:511:LYS:HB2	1:A:512:PRO:HD2	2.02	0.41
1:A:582:LEU:HA	1:A:582:LEU:HD23	1.80	0.41
1:A:367:ARG:NH2	1:A:562:GLU:OE2	2.55	0.40
1:A:134:VAL:O	1:A:134:VAL:HG12	2.22	0.40
1:A:523:PHE:CD1	1:A:523:PHE:C	2.99	0.40
1:A:408:ALA:HA	1:A:411:ALA:HB3	2.04	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	574/603 (95%)	541 (94%)	31 (5%)	2 (0%)	36 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	325	ARG

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	484/502 (96%)	438 (90%)	46 (10%)	8 16

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	10	LYS
1	A	22	LEU
1	A	39	LYS
1	A	48	THR
1	A	61	ASP
1	A	69	ILE
1	A	93	ARG
1	A	139	ARG
1	A	141	SER
1	A	208	GLN
1	A	215	GLU
1	A	235	GLN
1	A	259	VAL
1	A	278	ILE
1	A	283	GLU
1	A	292	GLN
1	A	295	SER
1	A	296	ARG
1	A	303	LYS
1	A	305	LEU
1	A	316	GLU
1	A	317	GLU

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Mol	Chain	Res	Type
1	A	332	VAL
1	A	334	VAL
1	A	357	LYS
1	A	365	ASN
1	A	367	ARG
1	A	371	GLU
1	A	372	GLN
1	A	396	ARG
1	A	403	VAL
1	A	433	VAL
1	A	438	LEU
1	A	456	LEU
1	A	499	LEU
1	A	509	LYS
1	A	511	LYS
1	A	526	GLU
1	A	527	ARG
1	A	533	ARG
1	A	561	ARG
1	A	573	GLU
1	A	587	ARG
1	A	593	VAL
1	A	603	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	208	GLN
1	A	365	ASN
1	A	465	ASN
1	A	486	GLN
1	A	579	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	A	1066[A]	-	32,33,33	1.54	7 (21%)	48,52,52	2.32	12 (25%)
3	ATP	A	1066[B]	2	32,33,33	1.52	7 (21%)	48,52,52	2.42	17 (35%)
3	ATP	A	1065	2	32,33,33	1.55	6 (18%)	48,52,52	1.79	10 (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
3	ATP	A	1066[A]	-	-	6/22/38/38	0/3/3/3
3	ATP	A	1066[B]	2	-	2/22/38/38	0/3/3/3
3	ATP	A	1065	2	-	3/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1066[A]	ATP	C5-C4	4.78	1.47	1.39
3	A	1066[B]	ATP	C5-C4	4.78	1.47	1.39
3	A	1065	ATP	C5-C4	4.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1065	ATP	PB-O3B	3.26	1.63	1.59
3	A	1066[A]	ATP	PA-O3A	2.96	1.62	1.59
3	A	1066[B]	ATP	PB-O3A	2.83	1.62	1.59
3	A	1066[A]	ATP	PB-O3B	2.81	1.62	1.59
3	A	1065	ATP	PA-O3A	2.72	1.62	1.59
3	A	1065	ATP	PB-O3A	2.64	1.62	1.59
3	A	1066[A]	ATP	C5-C6	2.59	1.48	1.41
3	A	1066[B]	ATP	C5-C6	2.59	1.48	1.41
3	A	1066[A]	ATP	PB-O3A	2.45	1.62	1.59
3	A	1066[B]	ATP	PB-O3B	2.40	1.62	1.59
3	A	1065	ATP	C8-N7	2.39	1.36	1.31
3	A	1066[B]	ATP	PA-O3A	2.38	1.62	1.59
3	A	1065	ATP	C5-N7	-2.31	1.34	1.39
3	A	1066[A]	ATP	C5-N7	-2.29	1.34	1.39
3	A	1066[B]	ATP	C5-N7	-2.29	1.34	1.39
3	A	1066[A]	ATP	C8-N9	-2.08	1.34	1.37
3	A	1066[B]	ATP	C8-N9	-2.08	1.34	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1066[A]	ATP	C5-C4-N3	-7.37	116.57	126.72
3	A	1066[B]	ATP	C5-C4-N3	-7.37	116.57	126.72
3	A	1066[A]	ATP	C4-C5-N7	-7.19	102.36	110.58
3	A	1066[B]	ATP	C4-C5-N7	-7.19	102.36	110.58
3	A	1066[A]	ATP	C5-N7-C8	5.71	112.42	103.45
3	A	1066[B]	ATP	C5-N7-C8	5.71	112.42	103.45
3	A	1065	ATP	C5-C4-N3	-5.32	119.39	126.72
3	A	1066[A]	ATP	N3-C4-N9	4.88	135.47	127.17
3	A	1066[B]	ATP	N3-C4-N9	4.88	135.47	127.17
3	A	1065	ATP	N3-C4-N9	4.33	134.52	127.17
3	A	1066[A]	ATP	N9-C8-N7	-4.17	108.02	113.94
3	A	1066[B]	ATP	N9-C8-N7	-4.17	108.02	113.94
3	A	1065	ATP	C2-N1-C6	4.12	125.50	118.73
3	A	1065	ATP	N3-C2-N1	-3.54	123.22	128.58
3	A	1066[A]	ATP	C4-N9-C8	3.34	109.25	105.74
3	A	1066[B]	ATP	C4-N9-C8	3.34	109.25	105.74
3	A	1065	ATP	N6-C6-N1	3.15	125.38	118.38
3	A	1066[A]	ATP	C2-N3-C4	3.02	119.20	111.83
3	A	1066[B]	ATP	C2-N3-C4	3.02	119.20	111.83
3	A	1066[A]	ATP	C6-C5-N7	2.86	137.60	132.09
3	A	1066[B]	ATP	C6-C5-N7	2.86	137.60	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1065	ATP	C2-N3-C4	2.86	118.81	111.83
3	A	1066[B]	ATP	O5'-C5'-C4'	-2.81	99.42	108.99
3	A	1066[B]	ATP	O2G-PG-O3B	-2.72	95.53	104.64
3	A	1065	ATP	O2B-PB-O1B	2.69	124.95	112.44
3	A	1066[B]	ATP	O3G-PG-O2G	2.49	117.12	107.80
3	A	1065	ATP	O2'-C2'-C1'	2.48	118.66	110.10
3	A	1066[A]	ATP	O2'-C2'-C1'	2.27	117.92	110.10
3	A	1066[B]	ATP	O2'-C2'-C1'	2.27	117.92	110.10
3	A	1065	ATP	C4-C5-N7	-2.15	108.13	110.58
3	A	1065	ATP	C2'-C1'-N9	-2.14	107.99	113.30
3	A	1066[B]	ATP	O2A-PA-O1A	2.12	122.29	112.44
3	A	1066[B]	ATP	O2B-PB-O3B	-2.11	101.58	107.27
3	A	1066[A]	ATP	C2'-C1'-N9	-2.10	108.08	113.30
3	A	1066[B]	ATP	C2'-C1'-N9	-2.10	108.08	113.30
3	A	1066[B]	ATP	O2B-PB-O1B	2.10	122.20	112.44
3	A	1066[A]	ATP	O3A-PA-O1A	-2.04	104.57	110.70
3	A	1066[A]	ATP	C6-C5-C4	2.01	119.92	117.18
3	A	1066[B]	ATP	C6-C5-C4	2.01	119.92	117.18

There are no chirality outliers.

All (11) torsion outliers are listed below:

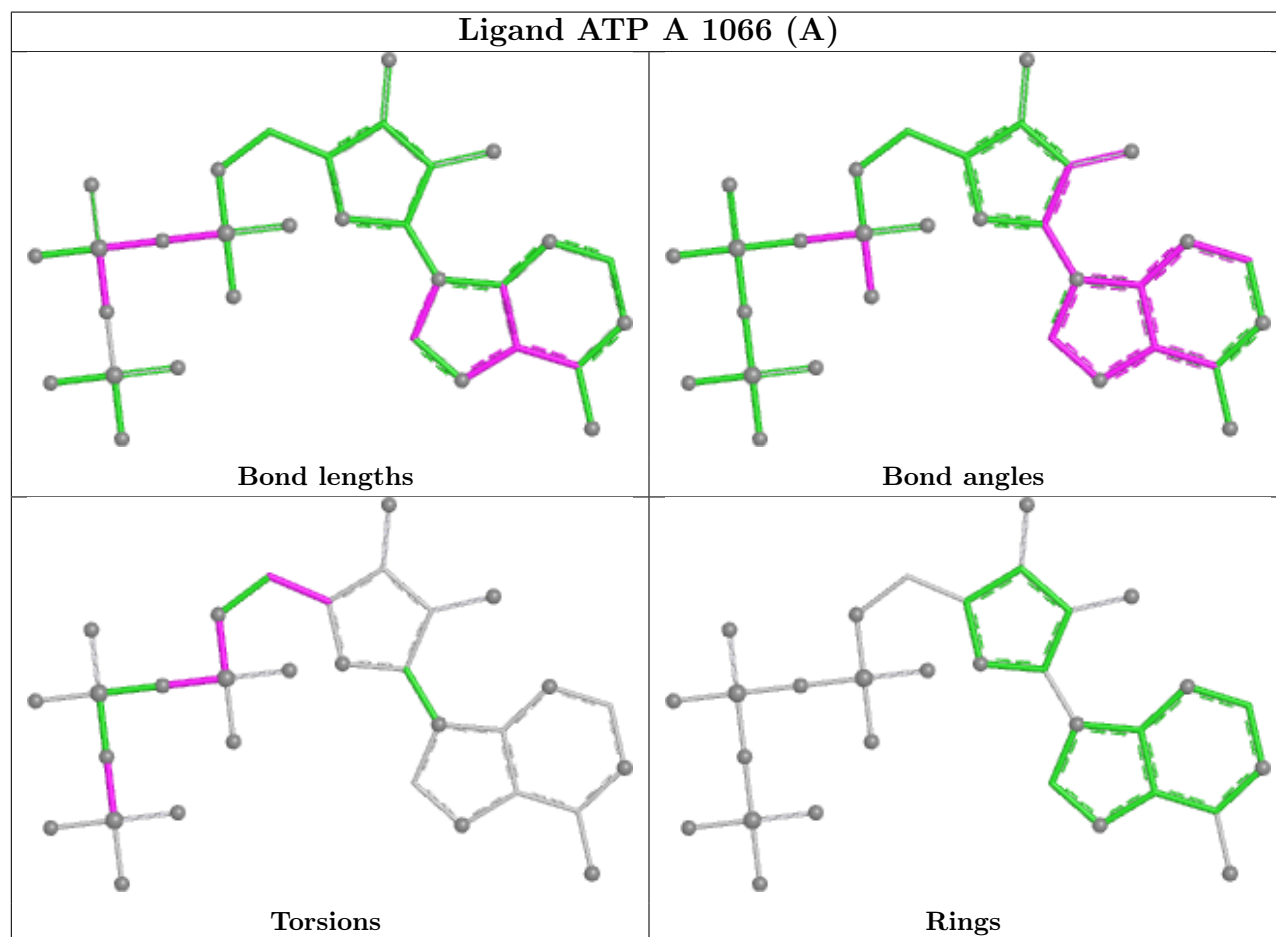
Mol	Chain	Res	Type	Atoms
3	A	1065	ATP	PB-O3B-PG-O2G
3	A	1066[A]	ATP	PB-O3B-PG-O3G
3	A	1066[A]	ATP	C5'-O5'-PA-O1A
3	A	1066[B]	ATP	PB-O3B-PG-O3G
3	A	1066[A]	ATP	C3'-C4'-C5'-O5'
3	A	1066[A]	ATP	O4'-C4'-C5'-O5'
3	A	1066[A]	ATP	PB-O3A-PA-O5'
3	A	1065	ATP	PB-O3B-PG-O3G
3	A	1066[B]	ATP	PB-O3B-PG-O1G
3	A	1066[A]	ATP	PB-O3A-PA-O2A
3	A	1065	ATP	PB-O3B-PG-O1G

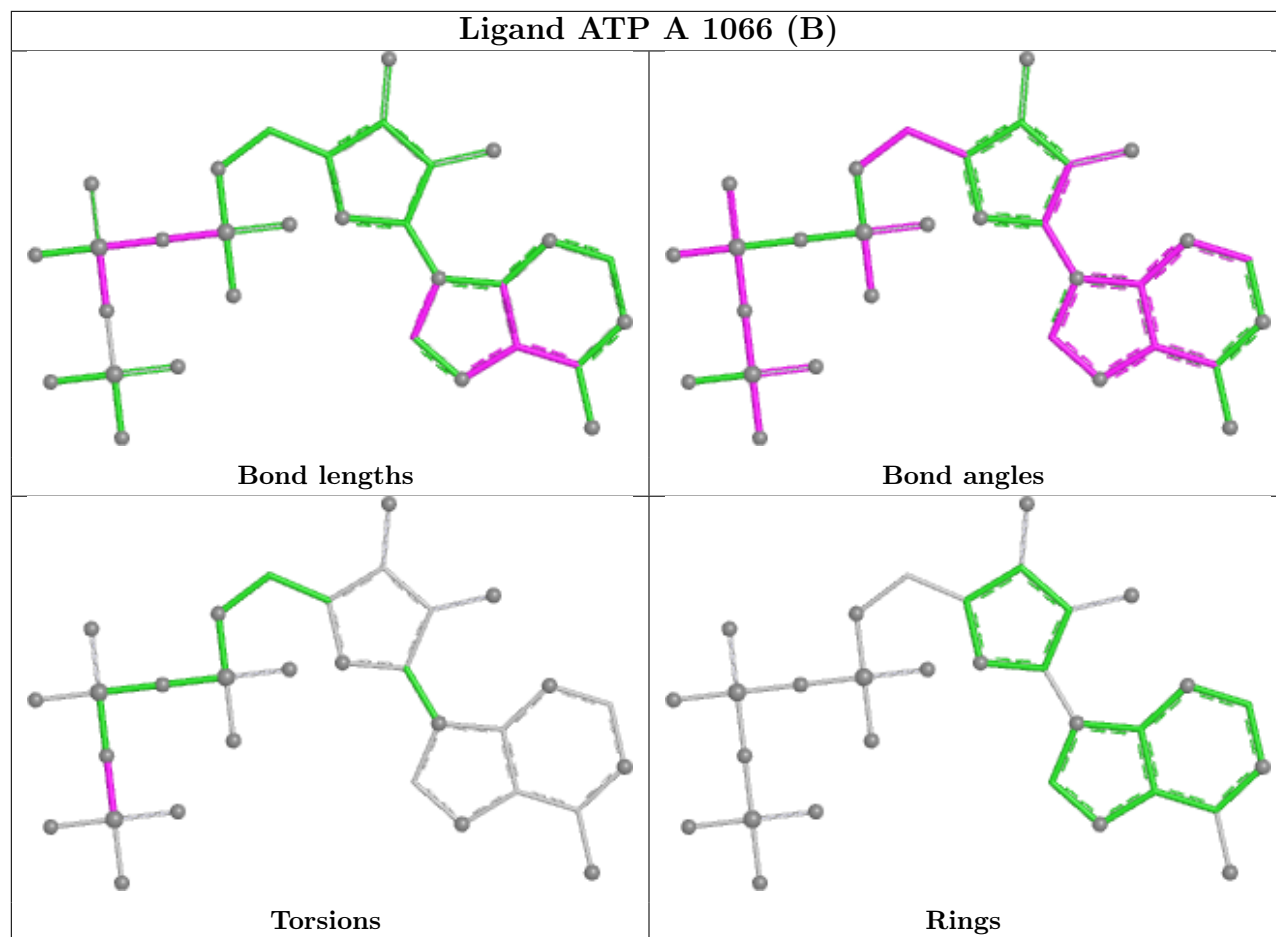
There are no ring outliers.

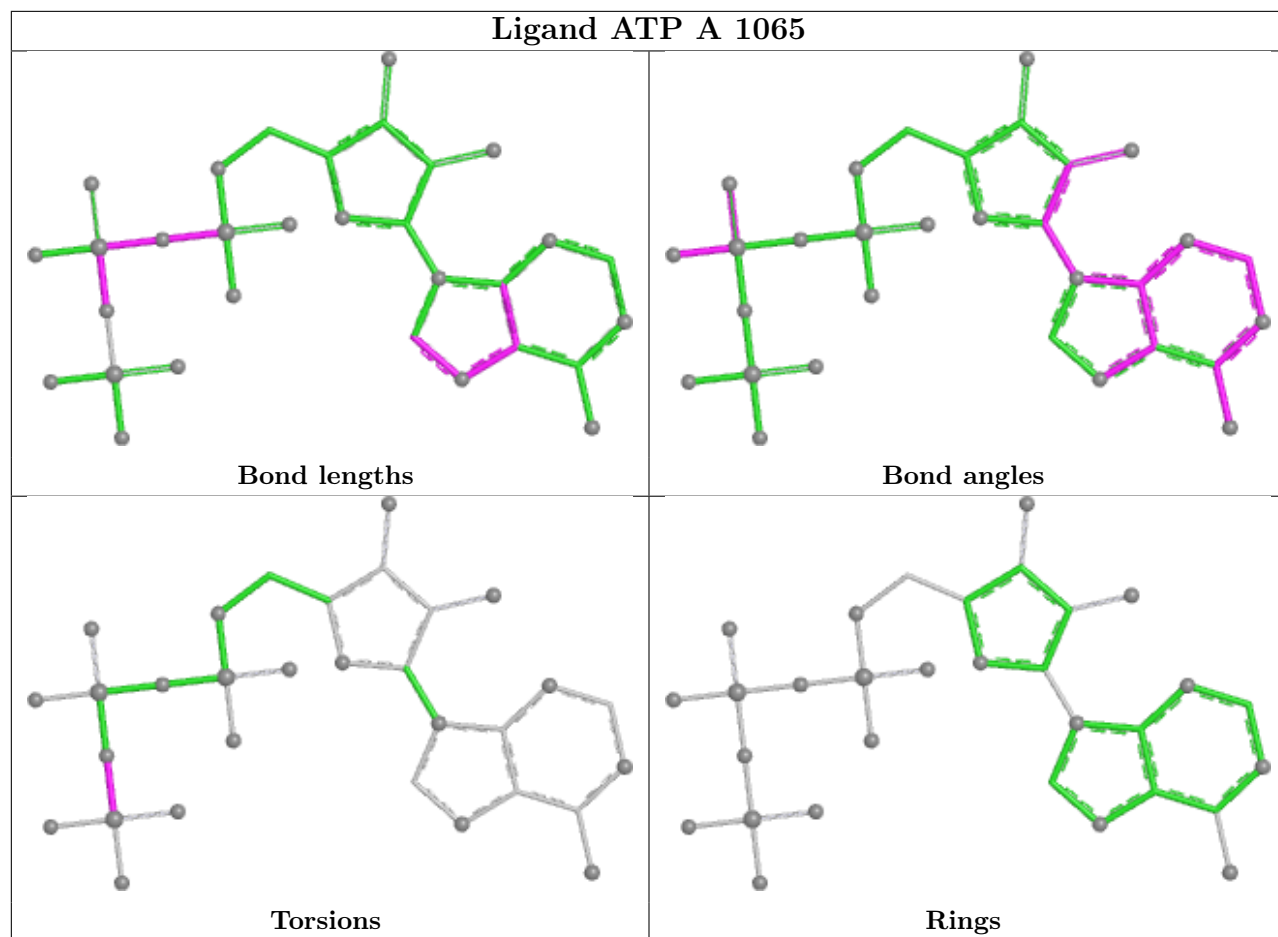
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1066[A]	ATP	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	580/603 (96%)	-0.48	1 (0%) 91 90	21, 38, 62, 89	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	HIS	2.3

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

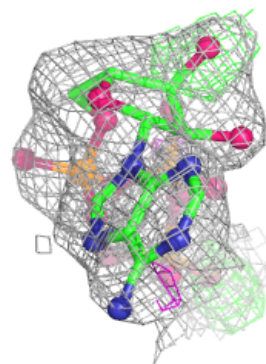
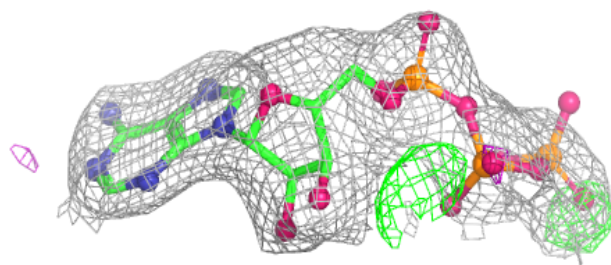
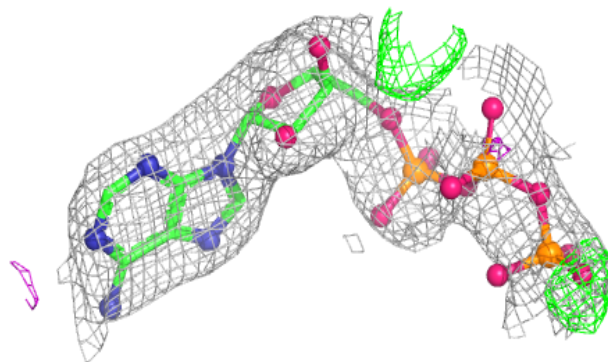
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	903	1/1	0.87	0.10	29,29,29,29	0
2	MG	A	904	1/1	0.88	0.12	54,54,54,54	0
3	ATP	A	1066[A]	31/31	0.90	0.09	34,49,67,68	14
3	ATP	A	1066[B]	31/31	0.90	0.09	34,49,56,57	14
3	ATP	A	1065	31/31	0.98	0.05	26,30,33,34	0

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.

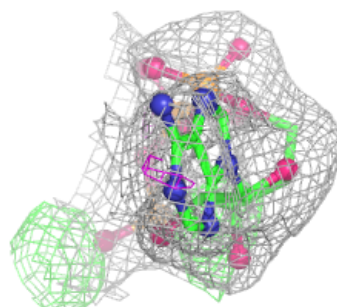
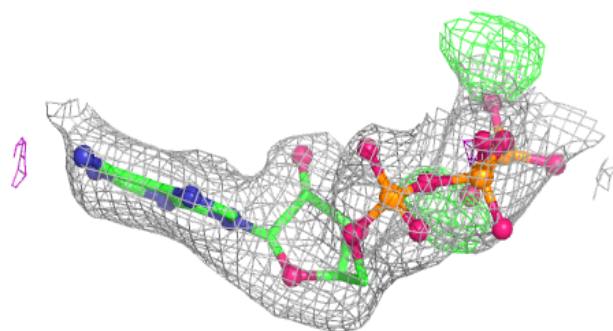
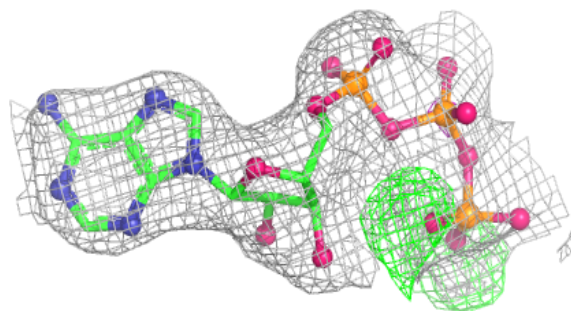
Electron density around ATP A 1066 (A):

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

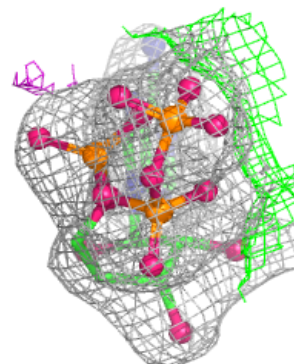
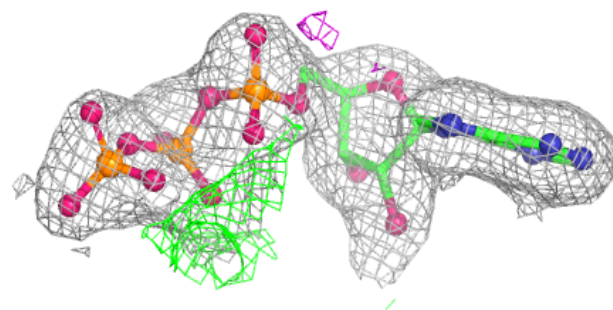
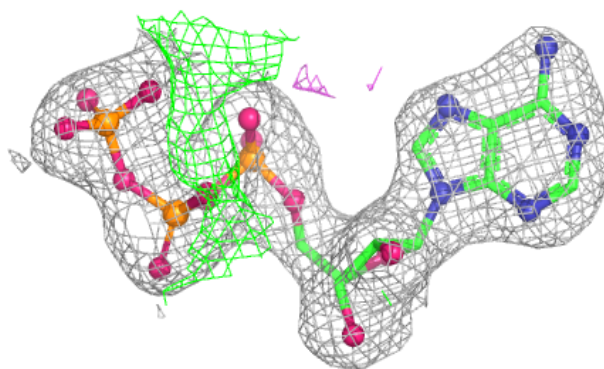


Electron density around ATP A 1066 (B):

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

**Electron density around ATP A 1065:**

$2mF_o-DF_c$ (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.