



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:45 PM GMT

PDB ID : 2HS0
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

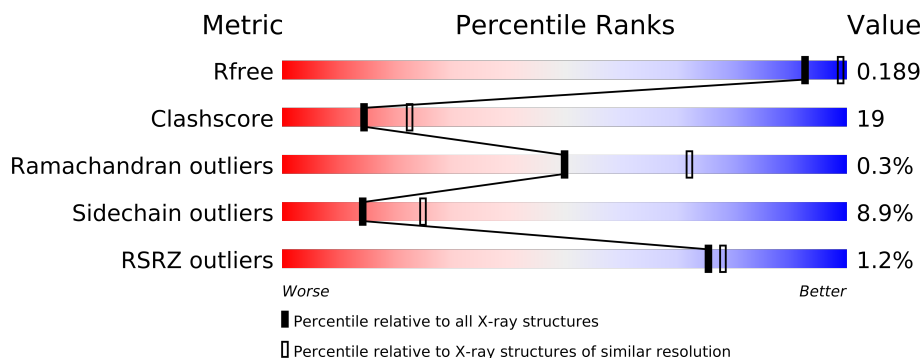
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


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}	66092	3240 (2.54-2.50)
Clashscore	79885	4080 (2.54-2.50)
Ramachandran outliers	78287	3990 (2.54-2.50)
Sidechain outliers	78261	3992 (2.54-2.50)
RSRZ outliers	66119	3241 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	603	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	904	-	X
3	ATP	A	1066[A]	-	X
3	ATP	A	1066[B]	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4755 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

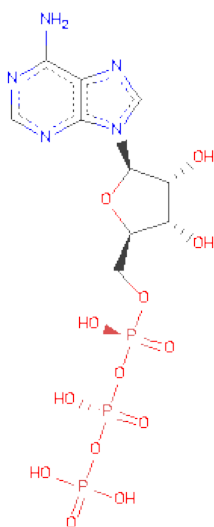
- Molecule 1 is a protein called Phosphoribosylformylglycinamidinesynthase II.

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 (three-letter code: MG) (formula: Mg).

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

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

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 31.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (31.73-2.52) 92.7 (31.72-2.50)	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 1.1	Depositor
R, R_{free}	0.200 , 0.253 0.184 , 0.189	Depositor DCC
R_{free} test set	896 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19320 reflections	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.

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	0.73	0/4562	1.34	43/6190 (0.7%)

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 (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH2	-19.83	110.39	120.30
1	A	139	ARG	NE-CZ-NH1	13.40	127.00	120.30
1	A	59	LEU	CB-CG-CD2	-9.82	94.31	111.00
1	A	304	HIS	C-N-CA	9.27	144.87	121.70
1	A	403	VAL	CB-CA-C	-8.59	95.08	111.40
1	A	601	LEU	CB-CG-CD2	-8.48	96.59	111.00
1	A	304	HIS	CA-C-N	8.22	135.29	117.20
1	A	94	ASP	CB-CG-OD1	8.18	125.66	118.30
1	A	499	LEU	CA-CB-CG	8.05	133.81	115.30
1	A	98	MET	CG-SD-CE	7.92	112.87	100.20
1	A	325	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	304	HIS	O-C-N	-7.59	110.56	122.70
1	A	304	HIS	N-CA-C	7.32	130.75	111.00
1	A	305	LEU	N-CA-CB	-7.24	95.93	110.40
1	A	428	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	60	ASP	CB-CG-OD1	7.11	124.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	LEU	CB-CG-CD2	-6.74	99.55	111.00
1	A	61	ASP	N-CA-CB	6.17	121.71	110.60
1	A	420	LEU	CB-CG-CD1	-6.17	100.51	111.00
1	A	296	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	A	420	LEU	CB-CG-CD2	-5.90	100.97	111.00
1	A	283	GLU	CA-CB-CG	5.84	126.24	113.40
1	A	494	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	A	161	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	431	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	A	565	LEU	CB-CG-CD2	-5.67	101.35	111.00
1	A	159	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	403	VAL	CG1-CB-CG2	5.56	119.80	110.90
1	A	305	LEU	CB-CG-CD1	5.54	120.42	111.00
1	A	43	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	216	LYS	CD-CE-NZ	5.47	124.27	111.70
1	A	306	LEU	N-CA-C	5.41	125.61	111.00
1	A	337	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	136	GLY	N-CA-C	-5.34	99.74	113.10
1	A	125	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	49	GLY	N-CA-C	-5.25	99.98	113.10
1	A	101	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	185	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	4	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	56	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	A	263	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	233	GLY	N-CA-C	-5.11	100.33	113.10
1	A	61	ASP	CB-CG-OD1	-5.02	113.78	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	61	ASP	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4473	0	4510	176	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	4528	176	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (176) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:GLN:HA	1:A:208:GLN:HE21	1.12	1.13
1:A:427:VAL:O	1:A:431:LEU:HD23	1.49	1.10
1:A:561:ARG:HH11	1:A:561:ARG:HG2	0.98	1.09
1:A:593:VAL:HG13	1:A:594:PRO:HD2	1.31	1.08
1:A:561:ARG:NH1	1:A:561:ARG:HG2	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:HD23	1:A:601:LEU:N	1.81	0.94
1:A:208:GLN:HE21	1:A:208:GLN:CA	1.81	0.93
1:A:431:LEU:N	1:A:431:LEU:HD22	1.79	0.93
1:A:208:GLN:HA	1:A:208:GLN:NE2	1.86	0.90
1:A:601:LEU:H	1:A:601:LEU:HD23	1.33	0.90
1:A:593:VAL:HG13	1:A:594:PRO:CD	2.03	0.88
1:A:431:LEU:CD2	1:A:431:LEU:N	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
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:365:ASN:HD22	1:A:365:ASN:C	1.98	0.66
1:A:367:ARG:HG3	1:A:367:ARG:HH11	1.60	0.66
1:A:601:LEU:CD2	1:A:601:LEU:N	2.58	0.65
1:A:379:THR:CG2	1:A:380:ASP:N	2.62	0.61
1:A:431:LEU:H	1:A:431:LEU:HD23	1.65	0.61
1:A:425:GLU:O	1:A:429:LYS:HG3	1.99	0.61
1:A:574:VAL:HG22	1:A:578:HIS:HB3	1.82	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:488:LYS:HD3	1:A:489:PRO:CD	2.33	0.57
1:A:320:TYR:HB2	1:A:334:VAL:CG2	2.34	0.57
1:A:367:ARG:NH1	1:A:367:ARG:HG3	2.18	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:365:ASN:ND2	1:A:365:ASN:C	2.57	0.56
1:A:561:ARG:CG	1:A:561:ARG:NH1	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:527:ARG:HE	1:A:579:GLN:HE22	1.55	0.54
1:A:35:TYR:O	1:A:39:LYS:HG2	2.07	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:603:ARG:NE	4:A:1127:HOH:O	2.42	0.53
1:A:261:LEU:HD21	1:A:322:VAL:CG1	2.36	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:365:ASN:ND2	1:A:367:ARG:HB3	2.21	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: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:HA	1:A:603:ARG:NE	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: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: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:27:VAL:HG11	1:A:240:GLY:HA2	1.94	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:533:ARG:HH11	1:A:533:ARG:HG2	1.77	0.48
1:A:2:LYS:O	1:A:2:LYS:HG3	2.14	0.48
1:A:258:ILE:CD1	1:A:315:ILE:HG21	2.44	0.48
1:A:10:LYS:HE2	1:A:10:LYS:HB2	1.79	0.48
1:A:365:ASN:ND2	1:A:367:ARG:HB2	2.13	0.48
1:A:70:GLU:OE2	3:A:1066[A]:ATP:O1G	2.31	0.48
1:A:128:SER:HB2	1:A:212:PRO:HB2	1.94	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:259:VAL:HB	1:A:312:ALA:HB2	1.96	0.47
1:A:365:ASN:ND2	1:A:367:ARG:H	2.12	0.47
1:A:70:GLU:HB2	1:A:91:ILE:HD13	1.95	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: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:261:LEU:HD23	1:A:322:VAL:HG13	1.97	0.46
1:A:139:ARG:CG	1:A:361:PHE:CE2	2.98	0.46
1:A:353:ILE:O	1:A:353:ILE:HG23	2.15	0.46
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:139:ARG:HG3	1:A:361:PHE:HD2	1.81	0.45
1:A:119:ILE:HD13	1:A:369:VAL:CG1	2.47	0.45
1:A:81:TYR:OH	1:A:124:ASP:OD2	2.27	0.45
1:A:159:ARG:HH21	1:A:161:ASP:CG	2.19	0.45
1:A:128:SER:HB2	1:A:212:PRO:CB	2.46	0.45
1:A:230:LEU:HA	1:A:293:LYS:HD3	1.99	0.45
1:A:134:VAL:CG1	1:A:134:VAL:O	2.65	0.45
1:A:511:LYS:HZ1	1:A:586:GLU:HG3	1.83	0.44
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:324:TYR:O	1:A:325:ARG:HB2	2.18	0.44
1:A:537:LYS:NZ	1:A:541:GLU:OE2	2.31	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:433:VAL:HG13	1:A:433:VAL:O	2.18	0.44
1:A:531:LEU:HD22	1:A:579:GLN:HB3	1.98	0.43
1:A:261:LEU:N	1:A:261:LEU:HD22	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:511:LYS:HZ3	1:A:586:GLU:HG3	1.84	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.78	0.42
1:A:184:ARG:HH11	1:A:275:GLU:CD	2.22	0.42
1:A:346:VAL:HG11	1:A:454:VAL:HG22	2.02	0.41
1:A:282:GLN:HB2	1:A:283:GLU:OE2	2.20	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:107:ASP:O	1:A:136:GLY:HA3	2.21	0.41
1:A:305:LEU:CD1	1:A:305:LEU:N	2.83	0.41
1:A:208:GLN:HE21	1:A:208:GLN:C	2.24	0.41
1:A:27:VAL:HG11	1:A:240:GLY:CA	2.51	0.41
1:A:590:VAL:HG12	1:A:590:VAL:O	2.21	0.41
1:A:511:LYS:HB2	1:A:512:PRO:HD2	2.02	0.41
1:A:178:PHE:HA	1:A:307:PHE:O	2.21	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:575:ARG:O	1:A:576:PRO:C	2.60	0.40
1:A:134:VAL:HG12	1:A:134:VAL:O	2.22	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

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	574/603 (95%)	541 (94%)	31 (5%)	2 (0%)	50 72

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%)	441 (91%)	43 (9%)	14	25

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	4	ARG
1	A	22	LEU
1	A	48	THR
1	A	61	ASP
1	A	67	PHE
1	A	69	ILE
1	A	93	ARG
1	A	116	ASP
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	317	GLU
1	A	332	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

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Mol	Chain	Res	Type
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	587	ARG
1	A	603	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	127	ASN
1	A	208	GLN
1	A	339	ASN
1	A	365	ASN
1	A	465	ASN
1	A	486	GLN
1	A	579	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 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	1065	2	33,33,33	1.14	3 (9%)	52,52,52	1.78	10 (19%)
3	ATP	A	1066[A]	-	12,13,33	0.84	0	20,21,52	1.31	2 (10%)
3	ATP	A	1066[B]	2	12,13,33	0.77	0	20,21,52	1.79	5 (25%)

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	1065	2	-	0/22/38/38	0/1/3/3
3	ATP	A	1066[A]	-	-	0/15/15/38	0/0/0/3
3	ATP	A	1066[B]	2	-	0/15/15/38	0/0/0/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1065	ATP	C5-C4	2.95	1.47	1.40
3	A	1065	ATP	C4-N9	-2.38	1.34	1.37
3	A	1065	ATP	PG-O3B	2.29	1.64	1.60

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1065	ATP	N3-C2-N1	-6.56	123.22	128.71
3	A	1066[B]	ATP	PA-O3A-PB	-5.41	115.81	131.68
3	A	1065	ATP	N3-C4-N9	5.04	134.52	125.43
3	A	1065	ATP	C2-N1-C6	3.73	125.50	118.77
3	A	1065	ATP	O4'-C1'-N9	3.31	111.52	108.44
3	A	1066[A]	ATP	O5'-PA-O3A	3.18	112.46	102.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1065	ATP	N6-C6-N1	3.06	125.38	119.36
3	A	1066[A]	ATP	PB-O3B-PG	-3.00	122.89	131.68
3	A	1065	ATP	C5-C4-N3	-2.90	119.39	125.70
3	A	1065	ATP	O2'-C2'-C1'	2.46	118.66	111.23
3	A	1066[B]	ATP	O3G-PG-O2G	2.44	117.12	107.61
3	A	1065	ATP	O2B-PB-O1B	2.28	124.95	112.21
3	A	1066[B]	ATP	O3G-PG-O1G	2.16	117.50	110.44
3	A	1065	ATP	O4'-C1'-C2'	-2.16	103.46	106.77
3	A	1065	ATP	C2'-C1'-N9	-2.06	107.99	113.27
3	A	1066[B]	ATP	O3A-PB-O3B	2.05	105.84	101.66
3	A	1066[B]	ATP	O2G-PG-O3B	-2.03	95.53	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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%)	-0.29	7 (1%) 75 78	21, 38, 62, 89	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ILE	3.9
1	A	74	HIS	2.9
1	A	209	VAL	2.6
1	A	603	ARG	2.5
1	A	3	LEU	2.4
1	A	13	LEU	2.3
1	A	563	TYR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	904	1/1	0.32	13.29	54,54,54,54	0
3	ATP	A	1066[B]	14/31	0.18	3.84	50,54,56,57	14
2	MG	A	903	1/1	0.24	1.43	29,29,29,29	0
3	ATP	A	1066[A]	14/31	0.18	1.14	54,65,68,68	14
3	ATP	A	1065	31/31	0.15	-0.06	26,30,33,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.