



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:47 PM GMT

PDB ID : 1GC5
Title : CRYSTAL STRUCTURE OF A NOVEL ADP-DEPENDENT GLUCOKINASE FROM THERMOCOCCUS LITORALIS
Authors : Ito, S.; Fushinobu, S.; Yoshioka, I.; Koga, S.; Matsuzawa, H.; Wakagi, T.
Deposited on : 2000-07-20
Resolution : 2.30 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>

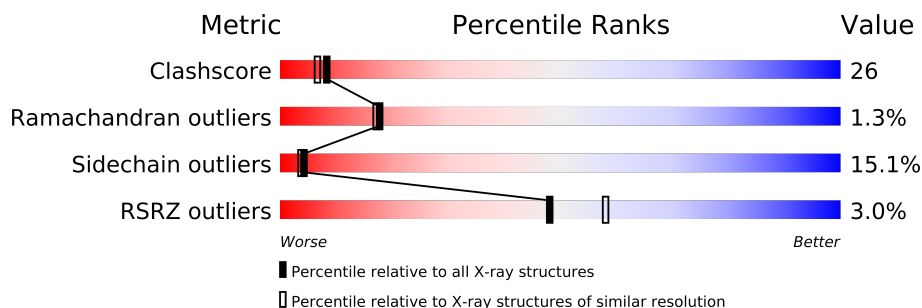
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	467	

2 Entry composition i

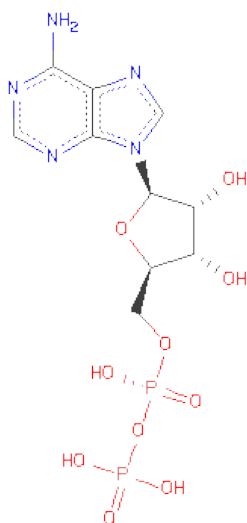
There are 3 unique types of molecules in this entry. The entry contains 3884 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ADP-DEPENDENT GLUCOKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	3780	2418	642	710	10	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	77	Total 77 O 77	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.80Å 109.80Å 129.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.30 47.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 77.3 (47.54-2.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.252 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.6	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35911 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3884	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: ADP

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	0.38	0/3852	0.61	1/5202 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ALA	N-CA-C	5.09	124.74	111.00

There are no chirality outliers.

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	3780	0	3787	200	0
2	A	27	0	12	0	0
3	A	77	0	0	5	0
All	All	3884	0	3799	200	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 26.

All (200) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:338:ASN:ND2	1:A:430:ARG:HE	1.55	1.03
1:A:40:ASN:HA	1:A:148:GLN:HE22	1.32	0.93
1:A:78:ILE:HD12	1:A:78:ILE:H	1.31	0.92
1:A:31:LYS:HB2	1:A:235:GLU:HG3	1.52	0.91
1:A:56:VAL:HB	1:A:196:PHE:CZ	2.11	0.84
1:A:216:ARG:HD3	3:A:570:HOH:O	1.76	0.84
1:A:40:ASN:HA	1:A:148:GLN:NE2	1.93	0.83
1:A:293:VAL:HG21	1:A:315:ILE:HD11	1.61	0.81
1:A:148:GLN:HG3	3:A:566:HOH:O	1.83	0.77
1:A:87:ARG:HE	1:A:95:MET:HE1	1.51	0.76
1:A:338:ASN:ND2	1:A:430:ARG:NE	2.34	0.75
1:A:277:HIS:HD2	1:A:301:SER:OG	1.69	0.75
1:A:190:PRO:HA	1:A:203:GLU:HG2	1.67	0.75
1:A:56:VAL:HB	1:A:196:PHE:HZ	1.49	0.75
1:A:365:GLY:H	1:A:431:GLN:HE22	1.34	0.75
1:A:127:ASN:HD21	1:A:153:VAL:H	1.36	0.70
1:A:338:ASN:HD21	1:A:430:ARG:HE	1.35	0.70
1:A:101:SER:OG	1:A:104:VAL:HG23	1.92	0.70
1:A:306:GLU:HB2	3:A:509:HOH:O	1.90	0.70
1:A:313:MET:O	1:A:316:ILE:HG22	1.93	0.69
1:A:5:LEU:O	1:A:5:LEU:HD12	1.93	0.68
1:A:59:LYS:HZ1	1:A:78:ILE:HG21	1.59	0.67
1:A:427:MET:HB2	1:A:430:ARG:O	1.95	0.67
1:A:50:ASP:O	1:A:54:LYS:HD3	1.94	0.67
1:A:163:GLU:O	1:A:166:LYS:HB2	1.95	0.66
1:A:415:LYS:HE2	1:A:416:GLU:HG2	1.78	0.65
1:A:59:LYS:NZ	1:A:78:ILE:HG21	2.12	0.65
1:A:95:MET:HE2	1:A:97:TRP:HE1	1.60	0.64
1:A:163:GLU:HB2	1:A:168:LYS:HG3	1.79	0.64
1:A:385:LYS:HD2	1:A:393:GLN:NE2	2.13	0.64
1:A:415:LYS:CE	1:A:416:GLU:HG2	2.28	0.63
1:A:59:LYS:HD2	1:A:78:ILE:HB	1.80	0.63
1:A:61:LYS:HB2	1:A:61:LYS:HZ3	1.64	0.63
1:A:430:ARG:CG	1:A:430:ARG:HH11	2.11	0.63
1:A:415:LYS:HD3	1:A:416:GLU:N	2.14	0.63
1:A:61:LYS:NZ	1:A:61:LYS:HB2	2.13	0.63
1:A:24:LEU:HD21	1:A:391:ILE:HG12	1.81	0.63
1:A:466:LYS:O	1:A:467:ARG:HB2	1.97	0.63
1:A:338:ASN:HD22	1:A:430:ARG:HE	1.39	0.63
1:A:78:ILE:HD12	1:A:78:ILE:N	2.10	0.62
1:A:316:ILE:HD13	1:A:316:ILE:O	1.98	0.62
1:A:195:VAL:HG12	1:A:196:PHE:CD1	2.34	0.62
1:A:72:PRO:HD2	1:A:97:TRP:CZ3	2.34	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:290:GLU:O	1:A:294:GLU:HG3	1.99	0.62
1:A:360:LEU:HD11	1:A:430:ARG:HD3	1.82	0.61
1:A:31:LYS:HB2	1:A:235:GLU:CG	2.27	0.61
1:A:127:ASN:ND2	1:A:153:VAL:H	1.98	0.61
1:A:330:ILE:O	1:A:334:ILE:HG13	1.99	0.61
1:A:60:GLY:C	1:A:62:GLU:H	2.02	0.61
1:A:314:GLU:HG2	1:A:315:ILE:N	2.16	0.61
1:A:386:GLY:HA2	1:A:445:SER:HB3	1.82	0.61
1:A:189:PHE:O	1:A:203:GLU:HG2	2.02	0.60
1:A:52:LEU:O	1:A:56:VAL:HG23	2.02	0.59
1:A:53:GLU:HA	1:A:196:PHE:CZ	2.37	0.59
1:A:74:LYS:HD2	1:A:98:PHE:HB3	1.83	0.59
1:A:41:ILE:HD11	1:A:148:GLN:HG2	1.84	0.59
1:A:465:ARG:C	1:A:467:ARG:N	2.55	0.59
1:A:430:ARG:NH1	1:A:430:ARG:HG2	2.16	0.59
1:A:338:ASN:HD21	1:A:430:ARG:NE	1.99	0.58
1:A:446:THR:HG23	1:A:446:THR:O	2.01	0.58
1:A:23:ALA:O	1:A:27:ILE:HG12	2.03	0.58
1:A:247:GLU:HG3	1:A:287:ARG:HB2	1.85	0.57
1:A:74:LYS:HB3	1:A:98:PHE:O	2.04	0.57
1:A:302:VAL:CG2	1:A:346:ILE:HD13	2.35	0.57
1:A:11:LEU:HD21	1:A:422:ASN:OD1	2.05	0.56
1:A:236:LEU:HD21	1:A:462:PHE:CG	2.42	0.55
1:A:423:GLY:O	1:A:433:ALA:HA	2.06	0.55
1:A:72:PRO:HG3	1:A:80:GLU:HG2	1.88	0.55
1:A:11:LEU:HA	1:A:14:ARG:NH1	2.22	0.55
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.70	0.55
1:A:141:VAL:O	1:A:220:ARG:HD2	2.06	0.54
1:A:56:VAL:HG21	1:A:196:PHE:HE1	1.72	0.54
1:A:289:ARG:O	1:A:293:VAL:HG23	2.08	0.54
1:A:71:PRO:HG3	1:A:87:ARG:CZ	2.37	0.54
1:A:348:ARG:HG3	1:A:361:THR:HG22	1.90	0.54
1:A:384:MET:O	1:A:444:LYS:HD2	2.09	0.53
1:A:95:MET:HE2	1:A:97:TRP:NE1	2.24	0.53
1:A:312:ILE:O	1:A:315:ILE:HG13	2.08	0.53
1:A:5:LEU:O	1:A:9:ILE:HG13	2.08	0.53
1:A:60:GLY:O	1:A:62:GLU:N	2.41	0.53
1:A:366:GLU:HG3	1:A:424:LEU:HD11	1.90	0.53
1:A:130:GLY:O	1:A:134:ARG:HA	2.08	0.53
1:A:190:PRO:HA	1:A:203:GLU:CG	2.37	0.53
1:A:162:PHE:CE1	1:A:167:LEU:HD23	2.43	0.53
1:A:71:PRO:HG3	1:A:87:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:HIS:CE1	1:A:211:ASP:HB2	2.43	0.53
1:A:340:LEU:HD23	1:A:349:ILE:HD13	1.91	0.53
1:A:56:VAL:HG12	1:A:61:LYS:HB3	1.91	0.52
1:A:157:ILE:O	1:A:171:HIS:HD2	1.92	0.52
1:A:347:GLU:HA	1:A:362:GLN:HG3	1.91	0.52
1:A:163:GLU:N	1:A:166:LYS:O	2.40	0.52
1:A:162:PHE:HD2	1:A:221:ARG:HD3	1.73	0.52
1:A:320:GLU:O	1:A:324:GLU:HG2	2.09	0.52
1:A:86:LEU:O	1:A:89:ILE:HB	2.10	0.51
1:A:348:ARG:HD2	1:A:363:TYR:OH	2.11	0.51
1:A:56:VAL:HG13	1:A:64:VAL:HG11	1.91	0.51
1:A:368:VAL:O	1:A:372:LEU:HG	2.11	0.51
1:A:53:GLU:HG3	1:A:196:PHE:CE2	2.45	0.50
1:A:162:PHE:CD1	1:A:167:LEU:HD23	2.46	0.50
1:A:384:MET:HE2	1:A:385:LYS:HE2	1.93	0.50
1:A:313:MET:HA	1:A:316:ILE:HG22	1.93	0.50
1:A:21:GLU:OE1	1:A:395:ARG:NH2	2.45	0.49
1:A:365:GLY:H	1:A:431:GLN:NE2	2.06	0.49
1:A:162:PHE:CD2	1:A:221:ARG:HD3	2.47	0.49
1:A:40:ASN:CA	1:A:148:GLN:HE22	2.13	0.49
1:A:87:ARG:HE	1:A:95:MET:CE	2.24	0.48
1:A:37:TYR:HA	1:A:140:HIS:ND1	2.28	0.48
1:A:199:GLN:HG2	1:A:200:ALA:N	2.27	0.48
1:A:236:LEU:HD23	1:A:275:LYS:HB2	1.95	0.48
1:A:465:ARG:C	1:A:467:ARG:H	2.17	0.48
1:A:430:ARG:HB3	1:A:430:ARG:HH11	1.79	0.48
1:A:78:ILE:H	1:A:78:ILE:CD1	2.08	0.48
1:A:108:LEU:HD13	1:A:185:TYR:CD1	2.49	0.48
1:A:286:ARG:NH1	1:A:314:GLU:OE2	2.47	0.47
1:A:11:LEU:HD21	1:A:422:ASN:CG	2.34	0.47
1:A:60:GLY:C	1:A:62:GLU:N	2.68	0.47
1:A:65:PHE:HA	1:A:68:ILE:HG12	1.96	0.47
1:A:31:LYS:O	1:A:136:PRO:HG2	2.15	0.47
1:A:191:ARG:NH2	1:A:442:SER:N	2.62	0.47
1:A:56:VAL:HG21	1:A:196:PHE:CE1	2.49	0.47
1:A:191:ARG:NH2	1:A:442:SER:H	2.12	0.47
1:A:217:VAL:HG12	1:A:217:VAL:O	2.15	0.47
1:A:36:ALA:HB3	1:A:239:ILE:HD13	1.96	0.47
1:A:430:ARG:CG	1:A:430:ARG:NH1	2.72	0.46
1:A:293:VAL:HG21	1:A:315:ILE:CD1	2.40	0.46
1:A:360:LEU:HD11	1:A:430:ARG:CD	2.45	0.46
1:A:135:ILE:HD13	1:A:459:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:HIS:HE1	1:A:211:ASP:OD1	1.99	0.46
1:A:195:VAL:O	1:A:197:ASP:N	2.48	0.46
1:A:334:ILE:HD13	1:A:432:LEU:HD21	1.97	0.46
1:A:86:LEU:HD21	1:A:195:VAL:HG11	1.97	0.46
1:A:89:ILE:HG23	1:A:200:ALA:HB2	1.98	0.46
1:A:87:ARG:HG2	1:A:95:MET:SD	2.56	0.46
1:A:444:LYS:HE3	1:A:444:LYS:CA	2.45	0.45
1:A:146:LYS:O	1:A:150:GLU:HG2	2.16	0.45
1:A:72:PRO:HD2	1:A:97:TRP:CH2	2.52	0.45
1:A:366:GLU:HG3	1:A:424:LEU:CD1	2.45	0.45
1:A:256:LYS:HA	1:A:256:LYS:HD2	1.49	0.45
1:A:143:GLN:OE1	1:A:179:GLU:HB3	2.17	0.45
1:A:56:VAL:CB	1:A:196:PHE:CZ	2.93	0.45
1:A:331:PHE:CE2	1:A:416:GLU:HG3	2.51	0.45
1:A:11:LEU:HA	1:A:14:ARG:HH12	1.81	0.45
1:A:255:TYR:CD1	1:A:259:LEU:HD12	2.52	0.45
1:A:462:PHE:HB2	3:A:516:HOH:O	2.16	0.44
1:A:90:LYS:C	1:A:92:GLY:N	2.71	0.44
1:A:94:ALA:HB2	1:A:204:ASN:HD21	1.82	0.44
1:A:74:LYS:HB2	1:A:100:GLU:OE1	2.18	0.44
1:A:104:VAL:O	1:A:107:TYR:HB3	2.18	0.43
1:A:37:TYR:HA	1:A:140:HIS:HD1	1.83	0.43
1:A:195:VAL:O	1:A:198:VAL:HG13	2.17	0.43
1:A:264:SER:O	1:A:268:ILE:HG13	2.19	0.43
1:A:255:TYR:CE1	1:A:259:LEU:HD12	2.53	0.43
1:A:246:LYS:O	1:A:255:TYR:HB3	2.19	0.43
1:A:430:ARG:CB	1:A:430:ARG:HH11	2.31	0.43
1:A:116:LEU:C	1:A:117:ARG:HG2	2.35	0.43
1:A:317:GLY:HA2	1:A:319:GLU:OE1	2.19	0.43
1:A:386:GLY:HA2	1:A:445:SER:H	1.83	0.43
1:A:190:PRO:CA	1:A:203:GLU:HG2	2.42	0.42
1:A:68:ILE:H	1:A:68:ILE:HG12	1.61	0.42
1:A:335:ASP:O	1:A:339:VAL:HG23	2.19	0.42
1:A:222:GLU:OE2	1:A:222:GLU:N	2.48	0.42
1:A:324:GLU:HA	1:A:327:GLU:HB2	2.01	0.42
1:A:266:LEU:HD21	1:A:299:PHE:CZ	2.55	0.42
1:A:362:GLN:HE21	1:A:362:GLN:HB3	1.50	0.42
1:A:90:LYS:O	1:A:92:GLY:N	2.53	0.42
1:A:117:ARG:HE	1:A:117:ARG:HB3	1.57	0.42
1:A:8:ARG:CZ	1:A:411:GLU:HG2	2.48	0.42
1:A:159:VAL:HG22	3:A:517:HOH:O	2.20	0.42
1:A:145:PRO:HD2	1:A:148:GLN:HB2	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:383:ALA:HB1	1:A:443:PRO:HB3	2.01	0.42
1:A:321:LEU:O	1:A:325:VAL:HG23	2.19	0.42
1:A:269:LEU:HD22	1:A:274:VAL:HG11	2.02	0.42
1:A:90:LYS:C	1:A:92:GLY:H	2.23	0.42
1:A:41:ILE:HG23	1:A:151:LEU:HD11	2.01	0.42
1:A:446:THR:CG2	1:A:446:THR:O	2.68	0.42
1:A:65:PHE:HA	1:A:68:ILE:CG1	2.50	0.41
1:A:136:PRO:HA	1:A:156:PRO:HB2	2.02	0.41
1:A:5:LEU:HD12	1:A:9:ILE:HG13	2.02	0.41
1:A:6:LYS:O	1:A:10:ARG:HG3	2.21	0.41
1:A:117:ARG:NH2	1:A:387:ASN:ND2	2.68	0.41
1:A:34:LEU:HD11	1:A:223:PHE:HE2	1.86	0.41
1:A:71:PRO:HA	1:A:72:PRO:HD3	1.95	0.41
1:A:444:LYS:HE3	1:A:444:LYS:N	2.35	0.41
1:A:10:ARG:O	1:A:13:LYS:HB2	2.21	0.41
1:A:129:LEU:HD12	1:A:133:TYR:CD2	2.56	0.41
1:A:386:GLY:HA3	1:A:444:LYS:HB3	2.04	0.40
1:A:390:ARG:O	1:A:393:GLN:HG3	2.21	0.40
1:A:131:GLY:HA3	1:A:153:VAL:HG11	2.02	0.40
1:A:40:ASN:HB2	1:A:182:LEU:O	2.20	0.40
1:A:277:HIS:CD2	1:A:301:SER:OG	2.59	0.40
1:A:313:MET:HA	1:A:316:ILE:CG2	2.51	0.40
1:A:415:LYS:HD3	1:A:416:GLU:HG2	2.04	0.40
1:A:247:GLU:OE2	1:A:287:ARG:NH1	2.55	0.40
1:A:419:GLU:HA	1:A:424:LEU:O	2.22	0.40
1:A:43:ALA:HA	1:A:116:LEU:HD23	2.03	0.40
1:A:193:PHE:CE2	1:A:195:VAL:CG2	3.05	0.40
1:A:199:GLN:HB3	1:A:199:GLN:HE21	1.54	0.40
1:A:11:LEU:HD11	1:A:422:ASN:ND2	2.36	0.40
1:A:184:HIS:CE1	1:A:211:ASP:CB	3.04	0.40
1:A:34:LEU:HD11	1:A:223:PHE:CE2	2.56	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	465/467 (100%)	437 (94%)	22 (5%)	6 (1%)	18	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	196	PHE
1	A	90	LYS
1	A	37	TYR
1	A	445	SER
1	A	197	ASP

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	403/403 (100%)	342 (85%)	61 (15%)	4	4

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	5	LEU
1	A	11	LEU
1	A	21	GLU
1	A	45	LYS
1	A	47	LEU
1	A	53	GLU
1	A	55	ARG
1	A	61	LYS
1	A	69	GLU
1	A	73	GLU
1	A	74	LYS
1	A	78	ILE
1	A	87	ARG
1	A	88	SER
1	A	91	LEU

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Mol	Chain	Res	Type
1	A	93	LYS
1	A	101	SER
1	A	103	GLU
1	A	117	ARG
1	A	118	ILE
1	A	129	LEU
1	A	134	ARG
1	A	147	LEU
1	A	159	VAL
1	A	162	PHE
1	A	173	LYS
1	A	188	GLU
1	A	198	VAL
1	A	199	GLN
1	A	202	ARG
1	A	204	ASN
1	A	205	ARG
1	A	242	LEU
1	A	247	GLU
1	A	256	LYS
1	A	263	GLU
1	A	280	PHE
1	A	290	GLU
1	A	304	LEU
1	A	314	GLU
1	A	316	ILE
1	A	318	ASP
1	A	321	LEU
1	A	324	GLU
1	A	327	GLU
1	A	332	SER
1	A	354	TYR
1	A	362	GLN
1	A	366	GLU
1	A	385	LYS
1	A	395	ARG
1	A	409	LEU
1	A	415	LYS
1	A	418	THR
1	A	430	ARG
1	A	435	VAL
1	A	442	SER

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Mol	Chain	Res	Type
1	A	444	LYS
1	A	446	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	25	ASN
1	A	127	ASN
1	A	144	ASN
1	A	148	GLN
1	A	171	HIS
1	A	199	GLN
1	A	277	HIS
1	A	338	ASN
1	A	352	HIS
1	A	362	GLN
1	A	387	ASN
1	A	393	GLN
1	A	431	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 ⓘ

1 ligand is 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	ADP	A	470	-	29,29,29	1.29	4 (13%)	45,45,45	2.33	6 (13%)

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	ADP	A	470	-	-	0/16/32/32	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	470	ADP	C4-N9	-3.78	1.32	1.37
2	A	470	ADP	PB-O2B	2.40	1.63	1.54
2	A	470	ADP	C5-N7	-2.27	1.31	1.40
2	A	470	ADP	O4'-C1'	2.24	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	470	ADP	N3-C2-N1	-11.97	118.70	128.71
2	A	470	ADP	O4'-C1'-N9	4.90	113.00	108.44
2	A	470	ADP	N3-C4-N9	4.37	133.33	125.43
2	A	470	ADP	C2-N3-C4	3.25	123.28	114.01
2	A	470	ADP	C4-C5-N7	-3.07	106.89	109.52
2	A	470	ADP	C5-C4-N3	-2.95	119.28	125.70

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	467/467 (100%)	-0.34	14 (2%) 48 58	14, 31, 75, 93	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	PHE	5.1
1	A	467	ARG	4.3
1	A	166	LYS	3.4
1	A	194	GLN	3.4
1	A	64	VAL	3.3
1	A	163	GLU	3.0
1	A	198	VAL	2.8
1	A	165	ASN	2.7
1	A	164	GLY	2.3
1	A	191	ARG	2.2
1	A	195	VAL	2.2
1	A	66	GLU	2.1
1	A	197	ASP	2.1
1	A	59	LYS	2.1

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(Å ²)	Q<0.9
2	ADP	A	470	27/27	0.14	0.85	40,50,86,88	0

6.5 Other polymers

There are no such residues in this entry.