



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:42 AM GMT

PDB ID : 3UBO  
Title : The crystal structure of adenosine kinase from Sinorhizobium meliloti  
Authors : Zhang, Z.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2011-10-24  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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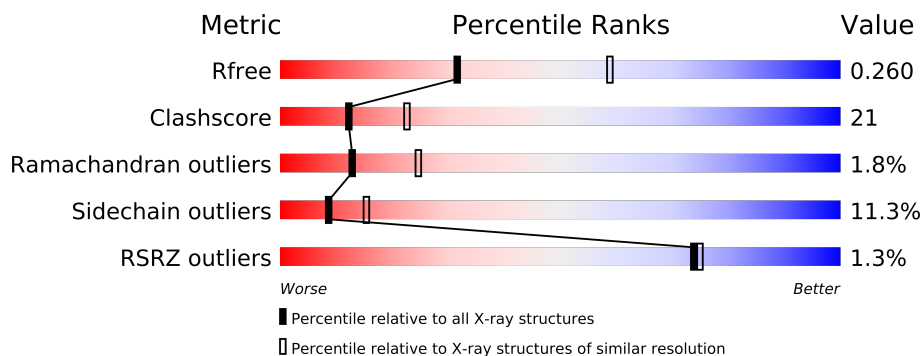
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. 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	354	
1	B	354	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5120 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 adenosine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	Se	0	0	0
			2538	1585	448	494	5	6			
1	B	327	Total	C	N	O	S	Se	0	0	0
			2444	1524	430	479	5	6			

There are 48 discrepancies between the modelled and reference sequences:

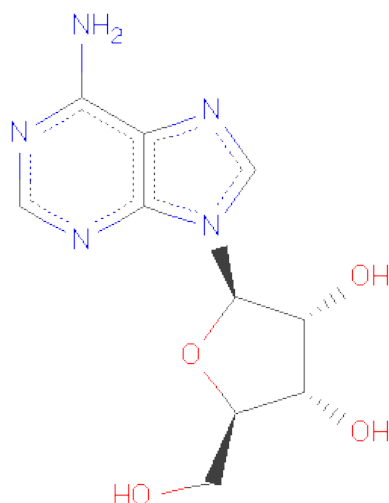
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	EXPRESSION TAG	UNP Q92T17
A	0	VAL	-	EXPRESSION TAG	UNP Q92T17
A	331	ALA	-	EXPRESSION TAG	UNP Q92T17
A	332	GLU	-	EXPRESSION TAG	UNP Q92T17
A	333	ASN	-	EXPRESSION TAG	UNP Q92T17
A	334	LEU	-	EXPRESSION TAG	UNP Q92T17
A	335	TYR	-	EXPRESSION TAG	UNP Q92T17
A	336	PHE	-	EXPRESSION TAG	UNP Q92T17
A	337	GLN	-	EXPRESSION TAG	UNP Q92T17
A	338	SER	-	EXPRESSION TAG	UNP Q92T17
A	339	HIS	-	EXPRESSION TAG	UNP Q92T17
A	340	HIS	-	EXPRESSION TAG	UNP Q92T17
A	341	HIS	-	EXPRESSION TAG	UNP Q92T17
A	342	HIS	-	EXPRESSION TAG	UNP Q92T17
A	343	HIS	-	EXPRESSION TAG	UNP Q92T17
A	344	HIS	-	EXPRESSION TAG	UNP Q92T17
A	345	TRP	-	EXPRESSION TAG	UNP Q92T17
A	346	SER	-	EXPRESSION TAG	UNP Q92T17
A	347	HIS	-	EXPRESSION TAG	UNP Q92T17
A	348	PRO	-	EXPRESSION TAG	UNP Q92T17
A	349	GLN	-	EXPRESSION TAG	UNP Q92T17
A	350	PHE	-	EXPRESSION TAG	UNP Q92T17
A	351	GLU	-	EXPRESSION TAG	UNP Q92T17
A	352	LYS	-	EXPRESSION TAG	UNP Q92T17
B	-1	MSE	-	EXPRESSION TAG	UNP Q92T17

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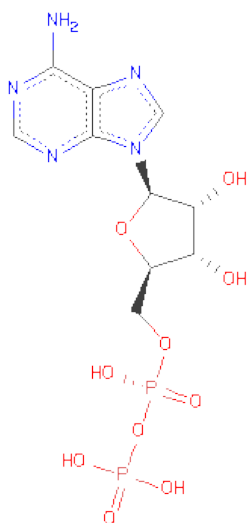
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	VAL	-	EXPRESSION TAG	UNP Q92T17
B	331	ALA	-	EXPRESSION TAG	UNP Q92T17
B	332	GLU	-	EXPRESSION TAG	UNP Q92T17
B	333	ASN	-	EXPRESSION TAG	UNP Q92T17
B	334	LEU	-	EXPRESSION TAG	UNP Q92T17
B	335	TYR	-	EXPRESSION TAG	UNP Q92T17
B	336	PHE	-	EXPRESSION TAG	UNP Q92T17
B	337	GLN	-	EXPRESSION TAG	UNP Q92T17
B	338	SER	-	EXPRESSION TAG	UNP Q92T17
B	339	HIS	-	EXPRESSION TAG	UNP Q92T17
B	340	HIS	-	EXPRESSION TAG	UNP Q92T17
B	341	HIS	-	EXPRESSION TAG	UNP Q92T17
B	342	HIS	-	EXPRESSION TAG	UNP Q92T17
B	343	HIS	-	EXPRESSION TAG	UNP Q92T17
B	344	HIS	-	EXPRESSION TAG	UNP Q92T17
B	345	TRP	-	EXPRESSION TAG	UNP Q92T17
B	346	SER	-	EXPRESSION TAG	UNP Q92T17
B	347	HIS	-	EXPRESSION TAG	UNP Q92T17
B	348	PRO	-	EXPRESSION TAG	UNP Q92T17
B	349	GLN	-	EXPRESSION TAG	UNP Q92T17
B	350	PHE	-	EXPRESSION TAG	UNP Q92T17
B	351	GLU	-	EXPRESSION TAG	UNP Q92T17
B	352	LYS	-	EXPRESSION TAG	UNP Q92T17

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 4 is water.

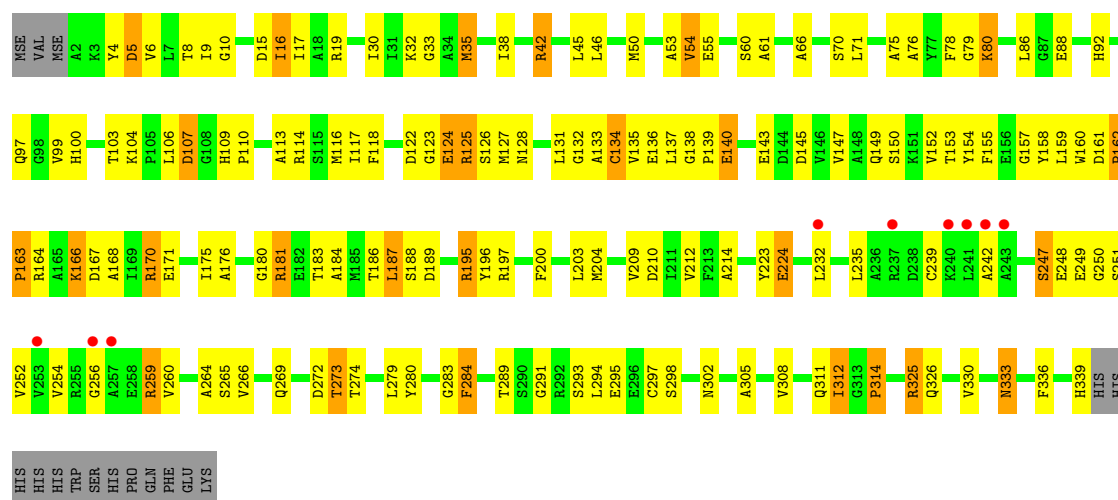
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	25	Total	O	0	0
			25	25		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

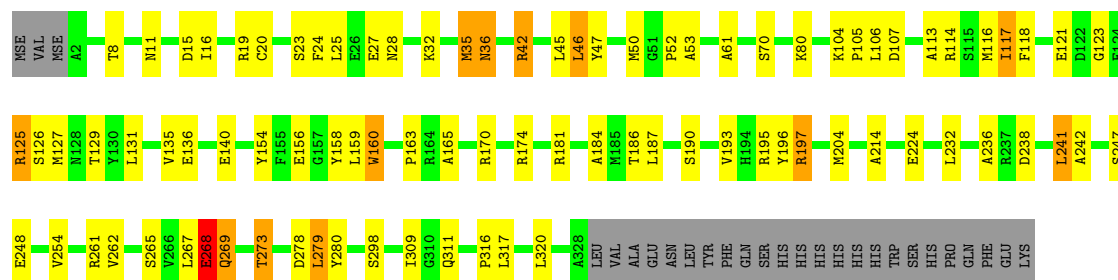
#### • Molecule 1: adenosine kinase

Chain A: 



#### • Molecule 1: adenosine kinase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.31 Å   156.31 Å   89.08 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	45.12 – 2.60 45.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.12-2.60) 100.0 (45.12-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.65 (at 2.61 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.235 , 0.267 0.230 , 0.260	Depositor DCC
$R_{free}$ test set	1940 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.0	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 38776 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: ADN, 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	1.12	2/2573 (0.1%)	1.04	5/3476 (0.1%)
1	B	0.98	0/2476	0.96	2/3344 (0.1%)
All	All	1.06	2/5049 (0.0%)	1.00	7/6820 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	ARG	CG-CD	5.66	1.66	1.51
1	A	336	PHE	CE2-CZ	5.47	1.47	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	LEU	CA-CB-CG	-5.77	102.03	115.30
1	A	5	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	B	241	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	A	189	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	15	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	189	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	312	ILE	N-CA-C	-5.20	96.97	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	2538	0	2482	136	0
1	B	2444	0	2391	79	0
2	A	19	0	13	5	0
2	B	19	0	12	6	0
3	A	27	0	12	4	0
3	B	27	0	12	3	0
4	A	21	0	0	3	0
4	B	25	0	0	1	0
All	All	5120	0	4922	213	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 21.

All (213) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:MSE:O	1:A:35:MSE:HG3	1.39	1.14
1:A:116:MSE:HA	1:A:116:MSE:HE3	1.32	1.09
1:A:50:MSE:HE3	1:A:53:ALA:HB2	1.12	1.08
1:A:50:MSE:CE	1:A:53:ALA:HB2	1.90	1.02
1:B:50:MSE:HE3	1:B:53:ALA:HB2	1.42	0.98
1:A:106:LEU:HD21	1:A:136:GLU:HG3	1.48	0.92
1:A:50:MSE:HE3	1:A:53:ALA:CB	2.03	0.87
1:A:71:LEU:CD1	1:A:283:GLY:HA2	2.05	0.86
1:A:180:GLY:HA2	4:A:367:HOH:O	1.78	0.84
1:A:250:GLY:HA2	1:A:264:ALA:HB2	1.60	0.83
1:B:278:ASP:OD2	2:B:353:ADN:H5'1	1.79	0.83
1:A:117:ILE:HG12	1:A:127:MSE:HG2	1.62	0.81
1:A:106:LEU:O	1:A:107:ASP:HB2	1.78	0.81
1:A:187:LEU:HD22	1:A:214:ALA:HB2	1.63	0.81
1:B:311:GLN:HE22	1:B:317:LEU:H	1.29	0.81
1:B:268:GLU:HA	1:B:268:GLU:OE2	1.79	0.81
1:B:311:GLN:HE22	1:B:316:PRO:HA	1.45	0.80
1:B:50:MSE:CE	1:B:53:ALA:HB2	2.12	0.79
1:B:35:MSE:HE2	1:B:36:ASN:N	1.98	0.79
1:A:254:VAL:HG22	1:A:259:ARG:NH1	1.98	0.79
1:B:50:MSE:HG3	1:B:118:PHE:CE1	2.18	0.78
1:A:5:ASP:HB3	1:A:289:THR:OG1	1.84	0.77
1:B:123:GLY:O	1:B:273:THR:HB	1.86	0.75
1:A:232:LEU:HD22	1:A:254:VAL:HG21	1.68	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:ILE:HB	1:A:116:MSE:HE1	1.67	0.75
1:A:259:ARG:HH11	1:A:259:ARG:HG2	1.53	0.74
1:B:311:GLN:NE2	1:B:317:LEU:H	1.86	0.73
1:B:106:LEU:HD11	1:B:136:GLU:HG3	1.69	0.73
1:A:50:MSE:CE	1:A:53:ALA:CB	2.66	0.73
1:B:35:MSE:HG2	1:B:158:TYR:CE2	2.25	0.72
1:B:121:GLU:HG3	4:B:358:HOH:O	1.90	0.71
1:A:150:SER:O	1:A:181:ARG:HG3	1.93	0.69
1:A:176:ALA:O	1:A:181:ARG:HB2	1.93	0.68
1:A:305:ALA:HB1	3:A:354:ADP:O4'	1.93	0.68
1:A:16:ILE:HG22	1:A:50:MSE:HE1	1.75	0.67
1:A:92:HIS:NE2	1:B:47:TYR:O	2.27	0.67
1:B:117:ILE:HD13	1:B:127:MSE:HG2	1.78	0.66
1:A:33:GLY:O	1:A:125:ARG:NH1	2.28	0.66
1:A:106:LEU:CD2	1:A:136:GLU:HG3	2.24	0.65
1:A:4:TYR:HB2	1:A:150:SER:OG	1.97	0.65
1:A:50:MSE:HG3	1:A:118:PHE:HE1	1.61	0.65
1:A:210:ASP:O	1:A:239:CYS:HB2	1.96	0.65
1:A:50:MSE:SE	1:A:116:MSE:HE2	2.47	0.65
1:B:279:LEU:CD1	1:B:316:PRO:HD3	2.28	0.64
1:A:326:GLN:O	1:A:330:VAL:HG23	1.97	0.64
1:B:159:LEU:O	1:B:165:ALA:HB3	1.99	0.62
1:A:80:LYS:HB3	1:A:134:CYS:HA	1.81	0.62
1:B:187:LEU:HD22	1:B:214:ALA:HB2	1.81	0.62
1:B:50:MSE:HG3	1:B:118:PHE:HE1	1.65	0.61
1:A:145:ASP:O	1:A:149:GLN:HG3	2.00	0.61
1:A:147:VAL:HG12	1:A:176:ALA:HB2	1.83	0.61
1:A:80:LYS:HG2	1:A:137:LEU:HB2	1.82	0.61
1:B:28:ASN:O	1:B:42:ARG:NH2	2.34	0.61
1:B:279:LEU:HD11	1:B:316:PRO:HD3	1.81	0.60
1:A:123:GLY:O	1:A:273:THR:HB	2.00	0.60
1:B:106:LEU:HD21	1:B:136:GLU:HG3	1.84	0.59
1:A:66:ALA:CB	1:A:97:GLN:HG3	2.33	0.59
1:A:153:THR:O	1:A:184:ALA:N	2.30	0.59
1:A:106:LEU:O	1:A:107:ASP:CB	2.48	0.59
1:A:116:MSE:HA	1:A:116:MSE:CE	2.21	0.59
1:B:269:GLN:HE21	1:B:269:GLN:HA	1.68	0.58
1:B:35:MSE:HG2	1:B:158:TYR:HE2	1.67	0.58
1:B:160:TRP:HB3	1:B:196:TYR:CE1	2.38	0.58
1:A:16:ILE:HB	1:A:116:MSE:CE	2.34	0.58
1:B:156:GLU:CD	2:B:353:ADN:H2	2.24	0.58
1:A:284:PHE:C	1:A:284:PHE:CD1	2.78	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:THR:HA	1:A:154:TYR:O	2.04	0.57
1:B:241:LEU:HD12	1:B:242:ALA:N	2.20	0.57
1:A:239:CYS:SG	1:A:242:ALA:HB2	2.45	0.57
1:A:106:LEU:HD21	1:A:136:GLU:CG	2.30	0.57
1:A:170:ARG:CG	1:A:171:GLU:N	2.68	0.57
1:B:204:MSE:HE2	1:B:238:ASP:HB2	1.87	0.57
1:A:122:ASP:OD1	1:A:124:GLU:HB2	2.04	0.57
1:A:251:SER:CB	1:A:280:TYR:OH	2.52	0.56
1:B:35:MSE:O	1:B:35:MSE:HG3	2.04	0.56
1:B:45:LEU:C	1:B:45:LEU:HD23	2.25	0.56
1:A:259:ARG:NH1	1:A:259:ARG:HG2	2.17	0.56
1:B:113:ALA:HB2	1:B:131:LEU:O	2.05	0.56
1:A:35:MSE:O	1:A:35:MSE:CG	2.30	0.56
1:B:267:LEU:HD12	3:B:354:ADP:C2	2.40	0.56
1:A:183:THR:OG1	1:A:209:VAL:HA	2.06	0.56
1:A:160:TRP:HB3	1:A:196:TYR:CE1	2.41	0.56
1:A:250:GLY:CA	1:A:264:ALA:HB2	2.33	0.55
1:A:254:VAL:HG22	1:A:259:ARG:HH11	1.70	0.55
1:B:241:LEU:HD12	1:B:242:ALA:H	1.72	0.55
1:A:50:MSE:HG3	1:A:118:PHE:CE1	2.40	0.55
1:B:23:SER:O	1:B:27:GLU:HG3	2.08	0.54
1:A:113:ALA:HB2	1:A:131:LEU:O	2.08	0.54
1:A:204:MSE:HE3	1:A:212:VAL:HG21	1.89	0.54
1:A:71:LEU:HD13	1:A:283:GLY:HA2	1.86	0.54
1:A:30:ILE:HD13	1:A:128:ASN:HD21	1.72	0.53
1:A:272:ASP:HB3	1:A:311:GLN:O	2.07	0.53
1:B:262:VAL:HG21	1:B:298:SER:HB2	1.90	0.53
1:A:106:LEU:HD11	1:A:136:GLU:HG3	1.91	0.53
1:B:204:MSE:HE2	1:B:238:ASP:CB	2.39	0.53
1:B:311:GLN:HE22	1:B:317:LEU:N	2.01	0.53
1:A:139:PRO:HG3	1:A:167:ASP:O	2.09	0.52
1:B:104:LYS:HG2	1:B:105:PRO:HD2	1.91	0.52
1:B:8:THR:HA	1:B:154:TYR:O	2.09	0.52
1:A:6:VAL:O	1:A:75:ALA:HA	2.10	0.52
1:A:9:ILE:O	1:A:155:PHE:HA	2.08	0.52
1:A:138:GLY:C	1:A:168:ALA:HB2	2.29	0.52
1:A:247:SER:HB2	1:A:248:GLU:OE2	2.09	0.52
1:A:45:LEU:HD23	1:A:45:LEU:C	2.29	0.52
3:A:354:ADP:O5'	3:A:354:ADP:H8	1.93	0.52
1:A:143:GLU:O	1:A:147:VAL:HG23	2.10	0.51
1:A:171:GLU:O	1:A:175:ILE:HG13	2.10	0.51
1:A:235:LEU:HD21	1:A:242:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:TRP:HE3	1:A:160:TRP:N	2.09	0.50
1:B:35:MSE:C	1:B:35:MSE:HE2	2.32	0.50
1:A:127:MSE:SE	2:A:353:ADN:H8	2.61	0.50
1:A:259:ARG:HB2	4:A:359:HOH:O	2.12	0.49
1:A:160:TRP:N	1:A:160:TRP:CE3	2.80	0.49
1:A:223:TYR:O	1:A:224:GLU:C	2.49	0.49
1:B:156:GLU:OE2	2:B:353:ADN:H2	2.12	0.49
1:A:135:VAL:HA	1:A:162:PRO:HB3	1.94	0.49
1:A:180:GLY:CA	4:A:367:HOH:O	2.49	0.49
1:A:97:GLN:NE2	1:B:52:PRO:CG	2.76	0.49
1:B:174:ARG:HG2	1:B:174:ARG:HH11	1.78	0.49
1:B:106:LEU:HD21	1:B:136:GLU:CG	2.43	0.48
1:A:75:ALA:HB3	1:A:99:VAL:HG22	1.95	0.48
1:A:260:VAL:HG21	1:A:294:LEU:HB2	1.95	0.48
1:A:79:GLY:O	1:A:103:THR:HG21	2.14	0.48
1:B:50:MSE:CE	1:B:53:ALA:CB	2.89	0.48
1:A:180:GLY:C	1:A:181:ARG:HD3	2.35	0.48
1:B:280:TYR:C	1:B:280:TYR:CD1	2.86	0.48
1:A:80:LYS:HG2	1:A:137:LEU:CA	2.44	0.47
1:B:193:VAL:O	1:B:197:ARG:N	2.47	0.47
1:A:32:LYS:HA	1:A:126:SER:OG	2.14	0.47
1:A:152:VAL:HG12	1:A:153:THR:N	2.27	0.47
1:B:16:ILE:HG22	1:B:50:MSE:HE1	1.97	0.47
1:A:154:TYR:HA	1:A:184:ALA:O	2.14	0.47
1:B:267:LEU:CD1	3:B:354:ADP:C2	2.97	0.47
1:A:161:ASP:HA	1:A:196:TYR:OH	2.14	0.47
1:A:160:TRP:HB3	1:A:196:TYR:CZ	2.50	0.47
1:B:24:PHE:C	1:B:24:PHE:CD1	2.89	0.46
1:B:268:GLU:OE2	1:B:268:GLU:CA	2.53	0.46
1:A:116:MSE:HB2	1:A:128:ASN:HB2	1.98	0.46
1:B:311:GLN:NE2	1:B:316:PRO:HA	2.23	0.46
1:A:158:TYR:CE2	1:A:188:SER:HB3	2.50	0.46
1:A:92:HIS:CD2	1:B:47:TYR:O	2.69	0.46
1:A:274:THR:HG22	1:A:314:PRO:HB3	1.98	0.46
1:B:8:THR:HB	1:B:61:ALA:HB1	1.98	0.45
1:A:9:ILE:HD11	1:A:78:PHE:CD2	2.51	0.45
1:B:8:THR:HG22	1:B:154:TYR:HB3	1.97	0.45
1:A:252:VAL:O	1:A:252:VAL:HG13	2.16	0.45
1:A:106:LEU:HA	1:A:106:LEU:HD12	1.61	0.45
1:A:80:LYS:CB	1:A:134:CYS:HA	2.46	0.45
1:A:35:MSE:SE	2:A:353:ADN:HN61	2.50	0.45
1:A:147:VAL:CG1	1:A:176:ALA:HB2	2.45	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:HIS:HA	1:A:110:PRO:C	2.37	0.44
1:B:70:SER:HB3	1:B:320:LEU:HD12	2.00	0.44
1:A:333:ASN:C	1:A:333:ASN:OD1	2.56	0.44
1:B:125:ARG:O	1:B:125:ARG:HD2	2.16	0.44
1:B:35:MSE:HE1	1:B:129:THR:HB	1.99	0.44
1:A:163:PRO:HB2	1:A:164:ARG:HG3	2.00	0.44
1:B:236:ALA:HB2	1:B:254:VAL:HG13	1.99	0.44
1:A:4:TYR:O	1:A:150:SER:HA	2.18	0.43
1:B:273:THR:HA	1:B:309:ILE:HG12	1.99	0.43
1:B:135:VAL:HG12	1:B:163:PRO:HD3	1.99	0.43
1:B:309:ILE:HG21	1:B:309:ILE:HD13	1.71	0.43
1:A:38:ILE:HB	1:A:42:ARG:HG2	2.00	0.43
1:B:32:LYS:HA	1:B:126:SER:OG	2.18	0.43
1:A:9:ILE:CD1	1:A:78:PHE:HD2	2.30	0.43
1:A:35:MSE:CE	2:A:353:ADN:N6	2.82	0.43
1:A:76:ALA:HA	1:A:99:VAL:HG13	1.99	0.43
1:B:19:ARG:HG3	1:B:20:CYS:N	2.34	0.43
1:B:190:SER:O	1:B:193:VAL:HB	2.18	0.43
1:A:9:ILE:HD11	1:A:78:PHE:HD2	1.83	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.71	0.42
1:A:187:LEU:HD22	1:A:214:ALA:CB	2.43	0.42
1:A:157:GLY:HA3	1:A:200:PHE:CZ	2.54	0.42
1:A:284:PHE:C	1:A:284:PHE:HD1	2.20	0.42
1:A:140:GLU:H	1:A:140:GLU:HG3	1.32	0.42
1:A:139:PRO:HG3	1:A:167:ASP:C	2.40	0.42
1:B:25:LEU:HD13	1:B:32:LYS:HB2	2.01	0.42
1:A:187:LEU:O	1:A:188:SER:HB2	2.20	0.42
1:B:45:LEU:HD23	1:B:46:LEU:N	2.35	0.42
1:A:157:GLY:CA	1:A:200:PHE:CZ	3.03	0.42
1:A:251:SER:HB2	1:A:280:TYR:OH	2.19	0.42
1:A:80:LYS:HA	1:A:80:LYS:HD3	1.40	0.42
1:A:302:ASN:HA	3:A:354:ADP:O2'	2.19	0.42
1:A:99:VAL:CG1	1:A:100:HIS:N	2.82	0.42
1:A:60:SER:N	2:A:353:ADN:H1'	2.35	0.42
1:B:15:ASP:OD1	2:B:353:ADN:O2'	2.30	0.42
1:A:170:ARG:HG3	1:A:171:GLU:N	2.29	0.42
1:B:279:LEU:HD13	1:B:316:PRO:HD3	1.98	0.41
1:B:154:TYR:HA	1:B:184:ALA:O	2.21	0.41
1:A:80:LYS:NZ	1:A:104:LYS:O	2.54	0.41
1:A:17:ILE:HB	1:A:54:VAL:HG12	2.02	0.41
1:A:88:GLU:HG2	1:A:88:GLU:O	2.20	0.41
1:A:80:LYS:HG2	1:A:137:LEU:CB	2.47	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:232:LEU:HD22	1:B:254:VAL:HG21	2.02	0.41
1:A:247:SER:HA	3:A:354:ADP:C8	2.55	0.41
1:B:247:SER:HA	3:B:354:ADP:C8	2.56	0.41
1:A:157:GLY:C	1:A:159:LEU:H	2.24	0.41
1:B:269:GLN:CA	1:B:269:GLN:HE21	2.34	0.41
1:B:248:GLU:N	1:B:248:GLU:OE2	2.49	0.41
1:B:158:TYR:HB3	2:B:353:ADN:N1	2.35	0.41
1:B:195:ARG:HG2	1:B:196:TYR:CE2	2.56	0.41
1:A:110:PRO:HB2	1:A:133:ALA:N	2.35	0.41
1:B:11:ASN:HB2	2:B:353:ADN:C2	2.51	0.40
1:A:247:SER:HB2	1:A:248:GLU:H	1.59	0.40
1:B:196:TYR:O	1:B:197:ARG:C	2.58	0.40
1:A:116:MSE:CA	1:A:116:MSE:HE3	2.21	0.40
1:A:30:ILE:HD13	1:A:128:ASN:ND2	2.36	0.40
1:A:10:GLY:HA3	1:A:61:ALA:HB3	2.04	0.40
1:A:35:MSE:CE	2:A:353:ADN:HN61	2.35	0.40
1:B:35:MSE:HB2	1:B:127:MSE:HE3	2.02	0.40
1:A:297:CYS:O	1:A:298:SER:C	2.58	0.40
1:A:195:ARG:HG2	1:A:196:TYR:CE2	2.56	0.40
1:A:110:PRO:HB2	1:A:132:GLY:C	2.41	0.40
1:A:325:ARG:HB3	1:A:325:ARG:HE	1.78	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	336/354 (95%)	293 (87%)	35 (10%)	8 (2%)	9	16
1	B	325/354 (92%)	304 (94%)	17 (5%)	4 (1%)	19	39
All	All	661/708 (93%)	597 (90%)	52 (8%)	12 (2%)	13	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLY
1	A	134	CYS
1	B	197	ARG
1	B	224	GLU
1	A	224	GLU
1	B	268	GLU
1	A	163	PRO
1	A	107	ASP
1	A	166	LYS
1	B	107	ASP
1	A	256	GLY
1	A	162	PRO

### 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	257/268 (96%)	219 (85%)	38 (15%)	4	8
1	B	247/268 (92%)	228 (92%)	19 (8%)	18	35
All	All	504/536 (94%)	447 (89%)	57 (11%)	9	15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	19	ARG
1	A	35	MSE
1	A	42	ARG
1	A	46	LEU
1	A	54	VAL
1	A	55	GLU
1	A	70	SER
1	A	80	LYS
1	A	86	LEU
1	A	114	ARG
1	A	124	GLU
1	A	125	ARG
1	A	140	GLU

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Mol	Chain	Res	Type
1	A	166	LYS
1	A	170	ARG
1	A	181	ARG
1	A	186	THR
1	A	187	LEU
1	A	197	ARG
1	A	203	LEU
1	A	247	SER
1	A	249	GLU
1	A	259	ARG
1	A	265	SER
1	A	266	VAL
1	A	269	GLN
1	A	273	THR
1	A	279	LEU
1	A	284	PHE
1	A	293	SER
1	A	295	GLU
1	A	308	VAL
1	A	312	ILE
1	A	314	PRO
1	A	325	ARG
1	A	333	ASN
1	A	339	HIS
1	B	35	MSE
1	B	36	ASN
1	B	42	ARG
1	B	46	LEU
1	B	80	LYS
1	B	114	ARG
1	B	116	MSE
1	B	117	ILE
1	B	125	ARG
1	B	140	GLU
1	B	160	TRP
1	B	170	ARG
1	B	181	ARG
1	B	186	THR
1	B	261	ARG
1	B	265	SER
1	B	268	GLU
1	B	269	GLN

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Mol	Chain	Res	Type
1	B	273	THR

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

Mol	Chain	Res	Type
1	A	97	GLN
1	A	177	HIS
1	A	302	ASN
1	B	269	GLN
1	B	302	ASN
1	B	311	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 ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ADN	A	353	-	21,21,21	2.71	9 (42%)	31,31,31	2.38	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	A	354	-	29,29,29	3.30	14 (48%)	45,45,45	2.44	14 (31%)
2	ADN	B	353	-	21,21,21	3.34	11 (52%)	31,31,31	2.59	10 (32%)
3	ADP	B	354	-	29,29,29	2.73	13 (44%)	45,45,45	2.44	11 (24%)

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	ADN	A	353	-	-	0/6/22/22	0/1/3/3
3	ADP	A	354	-	-	0/16/32/32	0/1/3/3
2	ADN	B	353	-	-	0/6/22/22	0/1/3/3
3	ADP	B	354	-	-	0/16/32/32	0/1/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	354	ADP	C4-N9	8.28	1.49	1.37
2	B	353	ADN	C2-N3	6.58	1.45	1.32
3	A	354	ADP	C2-N3	6.37	1.44	1.32
2	B	353	ADN	C2-N1	6.12	1.45	1.33
2	B	353	ADN	C4-N3	6.04	1.44	1.35
3	A	354	ADP	C8-N7	5.90	1.46	1.34
3	B	354	ADP	C4-N9	5.87	1.46	1.37
3	B	354	ADP	C2-N3	5.36	1.42	1.32
3	A	354	ADP	PA-O3A	5.19	1.69	1.59
2	A	353	ADN	C2-N3	5.02	1.42	1.32
2	A	353	ADN	C2-N1	5.00	1.43	1.33
2	B	353	ADN	C2'-C1'	-4.85	1.46	1.53
3	B	354	ADP	PB-O1B	4.73	1.67	1.51
3	B	354	ADP	C2'-C1'	-4.61	1.46	1.53
3	A	354	ADP	PB-O1B	4.53	1.66	1.51
3	B	354	ADP	C8-N7	4.46	1.43	1.34
2	B	353	ADN	C8-N7	4.44	1.43	1.34
3	A	354	ADP	PB-O3A	4.33	1.67	1.60
2	A	353	ADN	C8-N9	4.25	1.42	1.36
2	A	353	ADN	C4-N3	4.16	1.42	1.35
3	A	354	ADP	C6-N6	4.02	1.48	1.35
2	A	353	ADN	C8-N7	4.00	1.42	1.34
2	B	353	ADN	C8-N9	3.94	1.42	1.36
2	A	353	ADN	C2'-C1'	-3.73	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	354	ADP	PB-O2B	3.69	1.68	1.54
3	B	354	ADP	C2-N1	3.67	1.41	1.33
3	B	354	ADP	PA-O1A	3.64	1.65	1.51
3	A	354	ADP	PA-O1A	3.62	1.65	1.51
3	A	354	ADP	C2-N1	3.62	1.41	1.33
3	A	354	ADP	C3'-C4'	3.44	1.62	1.53
3	B	354	ADP	PB-O2B	3.42	1.67	1.54
2	B	353	ADN	C6-N6	3.36	1.45	1.35
3	B	354	ADP	C6-N6	3.31	1.45	1.35
2	A	353	ADN	C3'-C4'	3.31	1.62	1.53
3	B	354	ADP	PB-O3A	3.12	1.65	1.60
2	B	353	ADN	C4-N9	3.00	1.42	1.37
2	A	353	ADN	C6-N6	2.86	1.44	1.35
2	B	353	ADN	C3'-C4'	2.83	1.60	1.53
3	A	354	ADP	C4-N3	2.68	1.39	1.35
3	B	354	ADP	PA-O3A	2.68	1.64	1.59
2	B	353	ADN	C5-C4	2.60	1.46	1.40
2	A	353	ADN	C5-C4	2.58	1.46	1.40
3	A	354	ADP	O4'-C4'	2.57	1.51	1.45
2	B	353	ADN	C2'-C3'	2.30	1.59	1.53
3	B	354	ADP	C4-N3	2.27	1.39	1.35
3	B	354	ADP	C3'-C4'	2.07	1.58	1.53
3	A	354	ADP	PA-O5'	2.05	1.68	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	354	ADP	N3-C2-N1	-12.16	118.54	128.71
3	A	354	ADP	N3-C2-N1	-9.97	120.38	128.71
2	B	353	ADN	C5'-C4'-C3'	7.95	134.53	115.06
2	B	353	ADN	N3-C2-N1	-7.50	122.44	128.71
3	A	354	ADP	O4'-C1'-N9	7.00	114.95	108.44
2	A	353	ADN	N3-C2-N1	-6.32	123.43	128.71
2	A	353	ADN	C4'-O4'-C1'	-6.09	103.14	109.75
2	A	353	ADN	C5'-C4'-C3'	4.97	127.22	115.06
2	A	353	ADN	O3'-C3'-C4'	4.70	124.94	111.08
3	B	354	ADP	N3-C4-N9	4.17	132.96	125.43
2	B	353	ADN	C4-C5-N7	-3.94	106.15	109.52
2	A	353	ADN	C1'-N9-C4	-3.88	119.94	126.64
2	B	353	ADN	O4'-C4'-C5'	3.78	117.23	109.15
3	A	354	ADP	N3-C4-N9	3.46	131.69	125.43
3	B	354	ADP	C8-N9-C4	3.36	109.46	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	354	ADP	O4'-C1'-N9	3.31	111.52	108.44
3	B	354	ADP	O2A-PA-O3A	3.14	120.04	105.14
3	A	354	ADP	O3'-C3'-C4'	3.05	120.06	111.08
3	A	354	ADP	O3A-PA-O5'	2.97	116.67	103.41
3	B	354	ADP	O2'-C2'-C3'	2.92	121.34	111.83
2	B	353	ADN	N3-C4-N9	2.92	130.71	125.43
3	A	354	ADP	O2'-C2'-C3'	2.81	120.99	111.83
3	A	354	ADP	O3'-C3'-C2'	2.80	120.94	111.83
3	A	354	ADP	O3A-PB-O1B	-2.78	91.98	111.00
2	A	353	ADN	C8-N9-C1'	2.76	131.81	126.38
3	B	354	ADP	O3A-PA-O5'	-2.65	91.56	103.41
2	B	353	ADN	O3'-C3'-C4'	2.65	118.89	111.08
2	B	353	ADN	C6-C5-C4	2.63	122.07	117.25
2	B	353	ADN	N7-C8-N9	-2.58	107.06	114.36
3	A	354	ADP	C5-C4-N3	-2.49	120.29	125.70
3	A	354	ADP	O4'-C4'-C5'	2.44	118.07	109.36
2	A	353	ADN	O4'-C1'-C2'	2.41	110.47	106.77
3	B	354	ADP	O3'-C3'-C2'	2.40	119.65	111.83
3	A	354	ADP	O4'-C4'-C3'	-2.27	100.56	105.17
3	A	354	ADP	O2'-C2'-C1'	2.27	118.08	111.23
2	B	353	ADN	C8-N7-C5	2.16	110.27	103.58
2	B	353	ADN	C5-C4-N3	-2.15	121.02	125.70
3	B	354	ADP	N6-C6-N1	2.14	123.58	119.36
3	A	354	ADP	O3A-PA-O1A	-2.13	95.99	111.28
3	B	354	ADP	C5-C6-N6	-2.09	115.98	120.72
3	A	354	ADP	O3B-PB-O3A	2.04	114.84	105.14
3	B	354	ADP	N7-C8-N9	-2.02	108.64	114.36

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, 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	338/354 (95%)	-0.08	9 (2%) 52 49	44, 63, 82, 95	0
1	B	327/354 (92%)	-0.16	0 100 100	46, 63, 82, 92	0
All	All	665/708 (93%)	-0.12	9 (1%) 74 72	44, 63, 82, 95	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	ALA	3.6
1	A	241	LEU	3.3
1	A	232	LEU	2.7
1	A	243	ALA	2.7
1	A	253	VAL	2.6
1	A	237	ARG	2.2
1	A	257	ALA	2.2
1	A	240	LYS	2.0
1	A	256	GLY	2.0

### 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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADN	A	353	19/19	0.21	1.65	55,59,62,62	0
3	ADP	A	354	27/27	0.16	0.90	67,70,75,78	0
3	ADP	B	354	27/27	0.16	0.33	62,69,74,75	0
2	ADN	B	353	19/19	0.16	0.10	56,63,65,65	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.