



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:33 PM GMT

PDB ID : 1TZ3  
Title : crystal structure of aminoimidazole riboside kinase complexed with aminoimidazole riboside  
Authors : Zhang, Y.; Dougherty, M.; Downs, D.M.; Ealick, S.E.  
Deposited on : 2004-07-09  
Resolution : 2.90 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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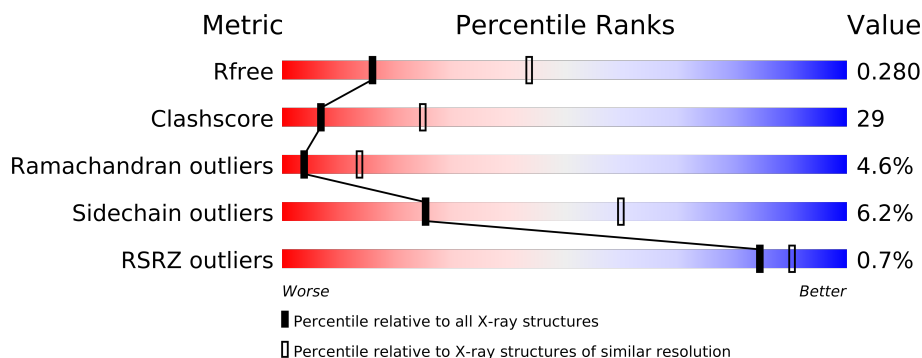
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	339	
1	B	339	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	AIS	A	402	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4485 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 putative sugar kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	Se	0	0	0
			2221	1407	377	423	10	4			
1	B	298	Total	C	N	O	S	Se	0	0	0
			2204	1393	376	421	10	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-18	GLY	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-17	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-16	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-15	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-14	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-13	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-12	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-11	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-10	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-9	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-8	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-7	GLY	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-6	LEU	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-5	VAL	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-4	PRO	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-3	ARG	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-2	GLY	-	CLONING ARTIFACT	UNP Q8ZKR2
A	-1	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
A	0	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
A	148	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKR2
A	165	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKR2
A	286	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKR2
A	294	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKR2
B	-19	MET	-	CLONING ARTIFACT	UNP Q8ZKR2

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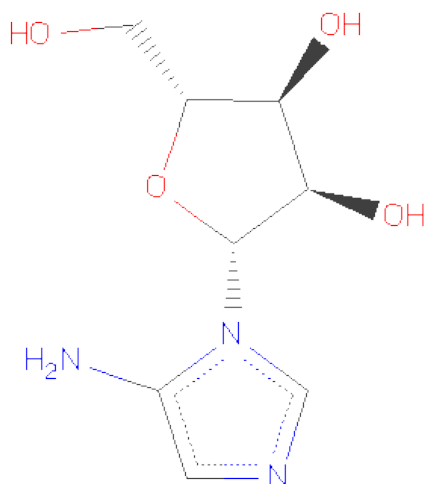
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-17	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-16	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-15	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-14	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-13	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-12	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-11	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-10	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-9	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-8	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-7	GLY	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-6	LEU	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-5	VAL	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-4	PRO	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-3	ARG	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-2	GLY	-	CLONING ARTIFACT	UNP Q8ZKR2
B	-1	SER	-	CLONING ARTIFACT	UNP Q8ZKR2
B	0	HIS	-	CLONING ARTIFACT	UNP Q8ZKR2
B	148	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKR2
B	165	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKR2
B	286	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKR2
B	294	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKR2

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 3 is 5-AMINOIMIDAZOLE RIBONUCLEOSIDE (three-letter code: AIS) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	21	Total	O	0	0
			21	21		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.85Å 54.10Å 89.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.77 – 2.90 46.34 – 2.68	Depositor EDS
% Data completeness (in resolution range)	91.1 (28.77-2.90) 90.2 (46.34-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.275 0.221 , 0.280	Depositor DCC
$R_{free}$ test set	1366 reflections (10.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.8	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 35272 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: K, AIS

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	0.39	0/2264	0.65	0/3077
1	B	0.39	0/2247	0.63	0/3055
All	All	0.39	0/4511	0.64	0/6132

There are no bond length outliers.

There are no bond angle outliers.

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	2221	0	2131	120	0
1	B	2204	0	2098	136	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	15	0	13	3	0
4	A	20	0	0	3	0
4	B	21	0	0	3	0
All	All	4485	0	4242	251	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 29.

All (251) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:GLN:H	1:A:203:GLN:NE2	1.43	1.14
1:A:35:ASN:HD22	1:A:294:MSE:HE2	1.15	1.04
1:A:104:HIS:HB2	1:A:105:PRO:HD3	1.36	1.04
1:A:194:CYS:HA	1:A:199:ALA:HB3	1.45	0.97
1:A:203:GLN:H	1:A:203:GLN:HE21	1.05	0.94
1:B:21:LYS:HD3	1:B:22:GLN:N	1.81	0.94
1:A:160:ASN:ND2	1:A:162:ARG:HH12	1.66	0.91
1:A:156:LEU:HG	4:A:618:HOH:O	1.70	0.91
1:B:294:MSE:HA	1:B:297:LEU:HD13	1.53	0.90
1:A:203:GLN:N	1:A:203:GLN:HE21	1.71	0.89
1:B:203:GLN:H	1:B:203:GLN:HE21	0.88	0.88
1:B:156:LEU:HG	4:B:622:HOH:O	1.74	0.88
1:B:203:GLN:HE21	1:B:203:GLN:N	1.72	0.87
1:A:104:HIS:HB2	1:A:105:PRO:CD	2.08	0.82
1:A:303:LEU:O	1:A:307:LEU:HG	1.79	0.82
1:B:203:GLN:H	1:B:203:GLN:NE2	1.74	0.80
1:B:102:LEU:N	1:B:102:LEU:HD12	1.97	0.79
1:A:35:ASN:HD22	1:A:294:MSE:CE	1.95	0.78
1:A:104:HIS:HD1	1:A:105:PRO:HD2	1.48	0.78
1:B:264:ARG:HA	1:B:264:ARG:HE	1.48	0.78
1:A:35:ASN:ND2	1:A:294:MSE:HE2	1.96	0.78
1:A:203:GLN:N	1:A:203:GLN:NE2	2.26	0.74
1:A:285:ALA:O	1:A:288:VAL:HG22	1.88	0.74
1:A:35:ASN:OD1	1:A:293:ALA:HB1	1.89	0.72
1:B:207:TYR:HB2	4:B:611:HOH:O	1.90	0.71
1:B:83:THR:O	1:B:107:ALA:HB2	1.92	0.70
1:B:162:ARG:HG2	1:B:164:LYS:HZ1	1.57	0.69
1:A:264:ARG:HE	1:A:264:ARG:HA	1.57	0.69
1:A:90:ASN:HB2	1:A:98:SER:OG	1.93	0.69
1:A:175:LEU:O	1:A:179:SER:HB2	1.93	0.69
1:B:244:VAL:HA	1:B:288:VAL:CG1	2.24	0.68
1:B:21:LYS:HD3	1:B:22:GLN:H	1.57	0.68
1:B:244:VAL:HA	1:B:288:VAL:HG11	1.75	0.68
1:A:21:LYS:O	1:A:23:ASN:N	2.28	0.67
1:B:120:ARG:O	1:B:123:GLU:HB2	1.95	0.66
1:B:164:LYS:HD3	1:B:164:LYS:H	1.60	0.66
1:B:228:LEU:HD11	1:B:230:THR:HG23	1.77	0.66
1:B:145:ALA:HB3	1:B:182:LEU:HD13	1.76	0.66
1:A:161:LEU:HD13	1:A:163:SER:H	1.59	0.66
1:A:229:ILE:HG12	1:A:234:GLU:HG3	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:216:THR:HB	1:B:230:THR:HG22	1.77	0.65
1:B:109:THR:O	1:B:136:PRO:HB2	1.96	0.64
1:A:286:MSE:O	1:A:289:THR:HG23	1.99	0.63
1:B:294:MSE:HG3	1:B:297:LEU:HD22	1.80	0.63
1:B:247:THR:HA	1:B:288:VAL:HG22	1.81	0.63
1:B:216:THR:HG21	1:B:268:TRP:HH2	1.64	0.63
1:A:104:HIS:CB	1:A:105:PRO:HD3	2.21	0.62
1:B:104:HIS:C	1:B:106:GLY:H	2.03	0.62
1:A:42:ARG:NH1	1:A:297:LEU:HB2	2.14	0.62
1:B:172:ILE:HB	1:B:173:PRO:HD3	1.82	0.62
1:A:261:THR:HG21	1:A:276:ALA:HA	1.82	0.61
1:A:32:ALA:HA	1:A:252:ASP:OD2	2.00	0.61
1:B:132:LEU:HD22	1:B:138:ARG:HG3	1.83	0.61
1:A:169:THR:O	1:A:169:THR:HG22	1.99	0.61
1:A:104:HIS:CB	1:A:105:PRO:CD	2.78	0.60
1:B:209:LEU:H	1:B:209:LEU:HD22	1.68	0.59
1:B:65:VAL:HG11	1:B:294:MSE:HE1	1.83	0.59
1:B:104:HIS:C	1:B:106:GLY:N	2.56	0.59
1:A:135:ARG:CB	1:A:136:PRO:HD3	2.32	0.59
1:A:246:ASP:HB3	1:A:290:ALA:O	2.03	0.59
1:B:224:ASP:O	1:B:236:HIS:HE1	1.84	0.59
1:B:75:PHE:CZ	1:B:117:PRO:HB3	2.38	0.58
1:B:299:PHE:HB3	1:B:300:PRO:HD2	1.85	0.58
1:A:158:ASP:HB2	4:A:618:HOH:O	2.03	0.58
1:A:104:HIS:HD1	1:A:105:PRO:CD	2.16	0.58
1:A:199:ALA:HB2	4:A:619:HOH:O	2.03	0.58
1:A:196:LEU:HB3	1:A:208:TYR:CE2	2.38	0.58
1:A:162:ARG:HE	3:A:402:AIS:H2	1.68	0.58
1:B:32:ALA:HA	1:B:252:ASP:OD2	2.03	0.58
1:B:42:ARG:O	1:B:43:LEU:HD12	2.03	0.58
1:B:87:LEU:HB3	1:B:100:THR:O	2.05	0.57
1:B:53:LEU:HD12	1:B:76:LEU:HD11	1.86	0.57
1:B:161:LEU:O	1:B:162:ARG:HG3	2.04	0.57
1:A:35:ASN:HA	1:A:294:MSE:HE2	1.87	0.57
1:B:187:LYS:HE2	1:B:220:SER:HB2	1.86	0.57
1:A:225:GLY:HA3	1:A:237:PHE:O	2.04	0.56
1:A:148:MSE:SE	1:A:153:GLY:HA3	2.55	0.56
1:B:102:LEU:N	1:B:102:LEU:CD1	2.68	0.56
1:B:123:GLU:HB3	1:B:148:MSE:HE1	1.86	0.56
1:A:75:PHE:CE2	1:A:117:PRO:HB3	2.41	0.56
1:B:14:SER:HB2	1:B:85:ALA:O	2.05	0.56
1:B:14:SER:C	1:B:62:LEU:HD11	2.26	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:240:PRO:HB3	1:A:310:HIS:CD2	2.41	0.56
1:A:218:ILE:HD12	1:A:258:LEU:HD21	1.88	0.55
1:B:108:ASP:N	1:B:108:ASP:OD1	2.38	0.55
1:B:17:LEU:HB3	1:B:25:TYR:HB3	1.88	0.55
1:B:169:THR:O	1:B:169:THR:HG22	2.07	0.55
1:B:264:ARG:HA	1:B:264:ARG:NE	2.19	0.55
1:B:75:PHE:CE2	1:B:117:PRO:HB3	2.41	0.55
1:A:55:ASP:HB3	1:A:80:ALA:HB2	1.87	0.55
1:A:101:TYR:HE1	3:A:402:AS:N3	2.04	0.55
1:A:161:LEU:CD1	1:A:163:SER:H	2.20	0.55
1:B:261:THR:HG21	1:B:276:ALA:HA	1.89	0.55
1:A:228:LEU:HD11	1:A:273:LEU:HD13	1.89	0.54
1:B:123:GLU:HB3	1:B:148:MSE:CE	2.38	0.54
1:B:169:THR:HG23	1:B:172:ILE:HD12	1.90	0.54
1:B:65:VAL:CG1	1:B:294:MSE:HE1	2.38	0.54
1:B:285:ALA:O	1:B:288:VAL:N	2.41	0.54
1:A:224:ASP:O	1:A:238:PRO:HA	2.08	0.53
1:B:188:VAL:HG11	1:B:193:LEU:HD21	1.90	0.53
1:B:10:ILE:HG21	1:B:125:PHE:CZ	2.43	0.53
1:B:38:VAL:HG21	1:B:294:MSE:SE	2.59	0.53
1:A:145:ALA:HB3	1:A:182:LEU:HD13	1.90	0.53
1:A:64:GLN:NE2	1:A:64:GLN:HA	2.25	0.52
1:A:264:ARG:HA	1:A:264:ARG:NE	2.24	0.52
1:B:46:GLU:HG2	4:B:635:HOH:O	2.09	0.52
1:A:38:VAL:HG21	1:A:294:MSE:SE	2.60	0.52
1:A:35:ASN:ND2	1:A:294:MSE:CE	2.65	0.52
1:A:261:THR:HG21	1:A:276:ALA:CA	2.39	0.52
1:A:210:ARG:C	1:A:212:LEU:H	2.12	0.52
1:B:42:ARG:HG2	1:B:42:ARG:O	2.10	0.52
1:B:148:MSE:SE	1:B:153:GLY:HA3	2.59	0.52
1:B:18:VAL:HG23	1:B:28:CYS:SG	2.50	0.52
1:A:42:ARG:HH11	1:A:297:LEU:HB2	1.75	0.52
1:B:194:CYS:O	1:B:198:GLY:N	2.43	0.52
1:B:79:ASP:OD1	1:B:80:ALA:N	2.43	0.52
1:B:155:VAL:HB	1:B:183:ALA:HA	1.91	0.52
1:B:162:ARG:CG	1:B:164:LYS:HZ1	2.22	0.51
1:B:135:ARG:HH11	1:B:138:ARG:HH11	1.56	0.51
1:A:193:LEU:O	1:A:196:LEU:HB2	2.10	0.51
1:B:15:VAL:HG22	1:B:62:LEU:HG	1.91	0.51
1:B:18:VAL:CG2	1:B:28:CYS:SG	2.99	0.51
1:A:9:VAL:HG11	1:A:33:SER:O	2.10	0.51
1:A:10:ILE:HG22	1:A:126:TYR:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:PHE:HB2	1:B:148:MSE:HG2	1.92	0.51
1:B:216:THR:HG21	1:B:268:TRP:CH2	2.46	0.51
1:B:210:ARG:HH11	1:B:210:ARG:HG3	1.75	0.51
1:A:208:TYR:O	1:A:212:LEU:HD12	2.10	0.51
1:A:89:VAL:HG22	1:A:99:PHE:HE1	1.76	0.51
1:B:41:ALA:C	1:B:43:LEU:H	2.14	0.51
1:A:24:SER:N	1:B:27:LYS:HD3	2.26	0.50
1:A:53:LEU:O	1:A:78:LEU:HA	2.11	0.50
1:A:160:ASN:ND2	1:A:162:ARG:NH1	2.47	0.50
1:A:121:GLN:HG2	1:A:122:TYR:CD2	2.47	0.50
1:A:190:ALA:HB2	1:A:221:LEU:HD23	1.94	0.49
1:B:88:ILE:O	1:B:88:ILE:HG13	2.12	0.49
1:B:228:LEU:HD11	1:B:230:THR:CG2	2.42	0.49
1:B:126:TYR:CE2	1:B:255:VAL:HG11	2.47	0.49
1:A:108:ASP:O	1:A:111:VAL:HG23	2.13	0.49
1:B:162:ARG:HG2	1:B:164:LYS:NZ	2.27	0.49
1:B:221:LEU:HB2	1:B:225:GLY:O	2.12	0.49
1:A:225:GLY:HA2	1:A:281:ASN:ND2	2.28	0.49
1:A:87:LEU:HD21	3:A:402:AIS:O2'	2.13	0.49
1:B:210:ARG:NH1	1:B:210:ARG:HG3	2.28	0.49
1:A:269:ASP:OD1	1:A:271:ALA:HB3	2.13	0.49
1:B:284:GLY:O	1:B:287:ALA:HB3	2.12	0.48
1:A:125:PHE:HB2	1:A:148:MSE:HG2	1.95	0.48
1:A:54:GLY:C	1:A:56:ASP:H	2.15	0.48
1:B:225:GLY:HA2	1:B:239:ALA:HB2	1.94	0.48
1:A:113:PRO:O	1:A:116:LEU:HB2	2.13	0.48
1:B:287:ALA:HA	1:B:296:ALA:HB1	1.94	0.48
1:B:121:GLN:HG2	1:B:122:TYR:CD1	2.49	0.48
1:A:197:SER:O	1:A:198:GLY:C	2.52	0.48
1:B:101:TYR:C	1:B:102:LEU:HD12	2.34	0.48
1:B:168:ASN:C	1:B:170:ASP:H	2.17	0.48
1:A:104:HIS:CD2	1:A:104:HIS:H	2.24	0.48
1:B:135:ARG:NH1	1:B:138:ARG:HH11	2.12	0.48
1:B:135:ARG:N	1:B:136:PRO:HD3	2.29	0.48
1:A:126:TYR:C	1:A:126:TYR:CD1	2.88	0.48
1:B:9:VAL:HG13	1:B:33:SER:HB3	1.95	0.48
1:B:86:VAL:O	1:B:102:LEU:HD13	2.14	0.47
1:B:10:ILE:HG22	1:B:126:TYR:O	2.14	0.47
1:A:168:ASN:C	1:A:170:ASP:H	2.17	0.47
1:B:126:TYR:C	1:B:126:TYR:CD1	2.87	0.47
1:B:52:CYS:O	1:B:108:ASP:HA	2.14	0.47
1:A:175:LEU:HD22	1:A:175:LEU:H	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:GLU:HA	1:A:143:GLU:OE1	2.15	0.47
1:B:86:VAL:C	1:B:87:LEU:HD23	2.35	0.46
1:A:210:ARG:HA	1:A:214:CYS:O	2.15	0.46
1:A:79:ASP:C	1:A:81:ASP:H	2.18	0.46
1:A:188:VAL:HG22	1:A:189:SER:N	2.30	0.46
1:A:188:VAL:O	1:A:219:ILE:HA	2.16	0.46
1:B:6:LYS:HD3	1:B:8:TRP:CZ2	2.50	0.46
1:B:21:LYS:C	1:B:21:LYS:HD3	2.32	0.46
1:A:225:GLY:HA2	1:A:281:ASN:HD21	1.81	0.45
1:A:121:GLN:O	1:A:122:TYR:HB2	2.14	0.45
1:A:135:ARG:CB	1:A:136:PRO:CD	2.93	0.45
1:B:56:ASP:N	1:B:56:ASP:OD1	2.44	0.45
1:B:261:THR:HG21	1:B:276:ALA:CA	2.46	0.45
1:A:124:TRP:CD2	1:A:154:TYR:HB2	2.52	0.45
1:A:221:LEU:O	1:A:222:GLY:C	2.55	0.45
1:B:104:HIS:O	1:B:106:GLY:N	2.50	0.45
1:B:209:LEU:HD22	1:B:209:LEU:N	2.30	0.45
1:A:162:ARG:O	1:A:163:SER:C	2.54	0.45
1:B:168:ASN:ND2	1:B:170:ASP:HB2	2.31	0.45
1:B:133:THR:HG22	1:B:134:ASP:N	2.32	0.45
1:B:128:SER:HB2	1:B:160:ASN:HB2	1.99	0.45
1:B:54:GLY:O	1:B:59:GLY:HA3	2.18	0.44
1:A:14:SER:O	1:A:62:LEU:HD21	2.16	0.44
1:B:121:GLN:HG3	1:B:152:GLY:HA3	1.99	0.44
1:A:55:ASP:HB3	1:A:80:ALA:CB	2.46	0.44
1:A:172:ILE:HB	1:A:173:PRO:HD3	2.00	0.44
1:A:242:VAL:HG12	1:A:285:ALA:HB1	1.98	0.44
1:B:114:GLN:OE1	1:B:114:GLN:N	2.51	0.44
1:A:103:VAL:HG22	1:B:102:LEU:HB3	1.99	0.44
1:B:120:ARG:CB	1:B:123:GLU:OE2	2.66	0.44
1:B:228:LEU:HD22	1:B:273:LEU:HD22	1.99	0.44
1:B:243:ASP:O	1:B:244:VAL:CB	2.66	0.44
1:A:132:LEU:HD13	1:A:175:LEU:HB3	1.99	0.44
1:A:286:MSE:HG2	1:A:306:PHE:CD2	2.53	0.44
1:B:303:LEU:O	1:B:307:LEU:HG	2.18	0.43
1:B:178:ARG:HD3	1:B:178:ARG:HA	1.81	0.43
1:A:82:LEU:HB3	1:A:107:ALA:HB2	2.00	0.43
1:B:122:TYR:CD2	1:B:266:ASN:HB3	2.53	0.43
1:B:135:ARG:HH11	1:B:138:ARG:NH1	2.17	0.43
1:A:102:LEU:HD13	1:B:86:VAL:HG11	2.01	0.43
1:B:82:LEU:N	1:B:82:LEU:HD12	2.34	0.43
1:A:53:LEU:HD12	1:A:76:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:ALA:HB1	1:A:202:TRP:CD1	2.53	0.43
1:B:174:GLU:OE1	1:B:174:GLU:HA	2.19	0.43
1:A:109:THR:HB	1:A:134:ASP:HB2	2.01	0.43
1:B:210:ARG:HD2	1:B:210:ARG:C	2.38	0.43
1:B:171:GLU:HB3	1:B:175:LEU:HD21	2.01	0.43
1:A:135:ARG:O	1:A:136:PRO:C	2.57	0.42
1:B:61:PHE:O	1:B:65:VAL:HG23	2.19	0.42
1:A:223:ALA:O	1:A:239:ALA:HB3	2.18	0.42
1:B:19:PRO:HG3	1:B:25:TYR:HE1	1.85	0.42
1:A:5:ASN:OD1	1:A:122:TYR:HB3	2.19	0.42
1:A:207:TYR:HB3	1:A:211:ASP:OD2	2.20	0.42
1:A:162:ARG:O	1:A:165:MSE:HG2	2.20	0.42
1:A:286:MSE:HG2	1:A:306:PHE:CE2	2.54	0.42
1:A:75:PHE:CZ	1:A:117:PRO:HB3	2.55	0.42
1:B:135:ARG:N	1:B:136:PRO:CD	2.82	0.41
1:A:55:ASP:HB3	1:A:80:ALA:CA	2.49	0.41
1:A:156:LEU:HD21	1:A:255:VAL:HG13	2.02	0.41
1:A:294:MSE:HA	1:A:297:LEU:HG	2.01	0.41
1:A:87:LEU:HD12	1:A:87:LEU:C	2.41	0.41
1:B:261:THR:O	1:B:264:ARG:HB2	2.20	0.41
1:A:43:LEU:O	1:A:260:PHE:CE1	2.73	0.41
1:A:86:VAL:HB	1:B:102:LEU:HD23	2.02	0.41
1:B:9:VAL:HG11	1:B:33:SER:O	2.21	0.41
1:B:101:TYR:HB2	1:B:104:HIS:CE1	2.55	0.41
1:A:19:PRO:HG3	1:A:25:TYR:HE1	1.84	0.41
1:B:101:TYR:N	1:B:101:TYR:CD1	2.88	0.41
1:B:188:VAL:HG22	1:B:189:SER:N	2.35	0.41
1:B:307:LEU:C	1:B:309:SER:H	2.24	0.41
1:B:306:PHE:O	1:B:309:SER:HB3	2.19	0.41
1:A:186:CYS:HB3	1:A:209:LEU:HD13	2.03	0.41
1:B:246:ASP:O	1:B:288:VAL:HA	2.21	0.41
1:A:104:HIS:ND1	1:A:105:PRO:HD2	2.24	0.41
1:A:104:HIS:CD2	1:B:105:PRO:HD3	2.56	0.41
1:B:260:PHE:O	1:B:264:ARG:HD2	2.21	0.41
1:A:273:LEU:O	1:A:277:ILE:HG13	2.20	0.41
1:A:54:GLY:O	1:A:59:GLY:HA3	2.20	0.41
1:B:143:GLU:HA	1:B:143:GLU:OE1	2.20	0.41
1:B:20:GLU:HG3	1:B:21:LYS:H	1.86	0.41
1:B:161:LEU:O	1:B:162:ARG:CG	2.68	0.40
1:A:168:ASN:O	1:A:170:ASP:N	2.54	0.40
1:B:100:THR:HG22	1:B:101:TYR:N	2.36	0.40
1:B:207:TYR:CD1	1:B:210:ARG:NH2	2.89	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:218:ILE:HD12	1:B:258:LEU:HD21	2.02	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	295/339 (87%)	241 (82%)	36 (12%)	18 (6%)	2	7
1	B	294/339 (87%)	260 (88%)	25 (8%)	9 (3%)	7	26
All	All	589/678 (87%)	501 (85%)	61 (10%)	27 (5%)	4	14

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	23	ASN
1	A	104	HIS
1	A	135	ARG
1	A	196	LEU
1	A	198	GLY
1	B	20	GLU
1	B	22	GLN
1	B	245	VAL
1	A	169	THR
1	A	222	GLY
1	B	244	VAL
1	A	244	VAL
1	A	248	THR
1	A	287	ALA
1	B	42	ARG
1	B	107	ALA
1	A	102	LEU
1	B	135	ARG

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Mol	Chain	Res	Type
1	B	169	THR
1	A	80	ALA
1	A	163	SER
1	A	164	LYS
1	B	163	SER
1	A	136	PRO
1	A	309	SER
1	A	106	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/263 (86%)	210 (93%)	16 (7%)	21	52
1	B	222/263 (84%)	210 (95%)	12 (5%)	31	69
All	All	448/526 (85%)	420 (94%)	28 (6%)	25	60

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	CYS
1	A	83	THR
1	A	104	HIS
1	A	108	ASP
1	A	116	LEU
1	A	129	SER
1	A	149	ARG
1	A	160	ASN
1	A	161	LEU
1	A	203	GLN
1	A	215	ASP
1	A	217	THR
1	A	234	GLU
1	A	243	ASP
1	A	264	ARG
1	A	281	ASN
1	B	52	CYS

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Mol	Chain	Res	Type
1	B	86	VAL
1	B	87	LEU
1	B	102	LEU
1	B	114	GLN
1	B	149	ARG
1	B	160	ASN
1	B	165	MSE
1	B	203	GLN
1	B	216	THR
1	B	217	THR
1	B	264	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	35	ASN
1	A	64	GLN
1	A	67	GLN
1	A	160	ASN
1	A	168	ASN
1	A	195	GLN
1	A	203	GLN
1	A	281	ASN
1	A	302	GLN
1	A	310	HIS
1	B	35	ASN
1	B	64	GLN
1	B	104	HIS
1	B	121	GLN
1	B	160	ASN
1	B	168	ASN
1	B	195	GLN
1	B	203	GLN
1	B	236	HIS
1	B	281	ASN

### 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, 4 are monoatomic - leaving 1 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	AIS	A	402	-	16,16,16	1.08	2 (12%)	23,23,23	2.47	4 (17%)

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	AIS	A	402	-	-	0/6/22/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	AIS	C4-C5	-2.86	1.33	1.37
3	A	402	AIS	C2-N1	-2.05	1.33	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	AIS	C4'-O4'-C1'	-7.30	101.82	109.75
3	A	402	AIS	C4-C5-N1	6.80	109.99	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	AIS	O4'-C1'-C2'	-3.79	100.97	106.77
3	A	402	AIS	O4'-C1'-N1	2.77	113.93	108.08

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	299/339 (88%)	-0.03	2 (0%) 84 90	30, 52, 75, 99	0
1	B	298/339 (87%)	-0.07	2 (0%) 84 90	32, 53, 77, 91	0
All	All	597/678 (88%)	-0.05	4 (0%) 84 90	30, 52, 76, 99	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	VAL	3.4
1	A	205	ALA	2.2
1	B	104	HIS	2.1
1	B	165	MSE	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
3	AIS	A	402	15/15	0.33	3.70	75,75,75,75	0
2	K	A	405	1/1	0.10	-1.76	69,69,69,69	0
2	K	A	404	1/1	0.07	-2.28	52,52,52,52	0
2	K	B	407	1/1	0.08	-2.60	52,52,52,52	0
2	K	B	406	1/1	0.07	-2.83	64,64,64,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.