Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:01 AM GMT

PDB ID	:	1TYY
Title	:	Crystal structure of aminoimidazole riboside kinase from Salmonella enterica
Authors	:	Zhang, Y.; Dougherty, M.; Downs, D.M.; Ealick, S.E.
Deposited on	:	2004-07-08
Resolution	:	2.60 Å(reported)

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	Percentile Ranks	Value
Rfree		0.304
Clashscore		21
Ramachandran outliers		2.1%
Sidechain outliers		6.8%
RSRZ outliers		1.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
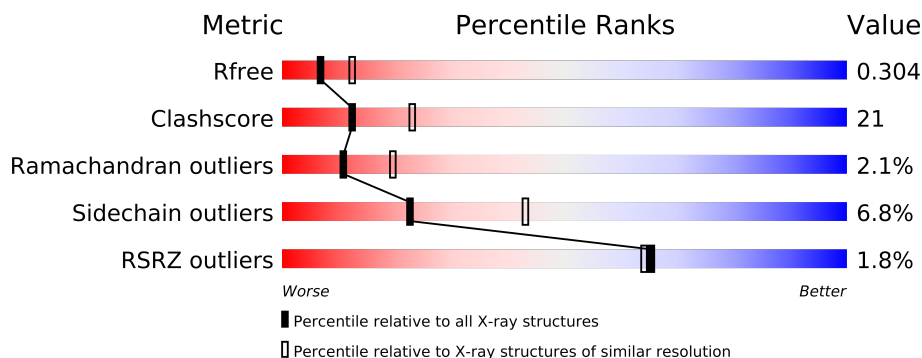
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 >=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	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4429 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	297	Total	C	N	O	S	Se	0	0	0
			2195	1392	371	418	10	4			
1	B	296	Total	C	N	O	S	Se	0	0	0
			2176	1373	370	420	10	3			

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	-	EXPRESSION TAG	UNP Q8ZKR2
A	-14	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
A	-13	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
A	-12	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
A	-11	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
A	-10	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
A	-9	SER	-	EXPRESSION TAG	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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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	-	EXPRESSION TAG	UNP Q8ZKR2
B	-14	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
B	-13	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
B	-12	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
B	-11	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
B	-10	HIS	-	EXPRESSION TAG	UNP Q8ZKR2
B	-9	SER	-	EXPRESSION TAG	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 2	K 2	0	0
2	A	2	Total 2	K 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total 26	O 26	0	0
3	B	28	Total 28	O 28	0	0

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.
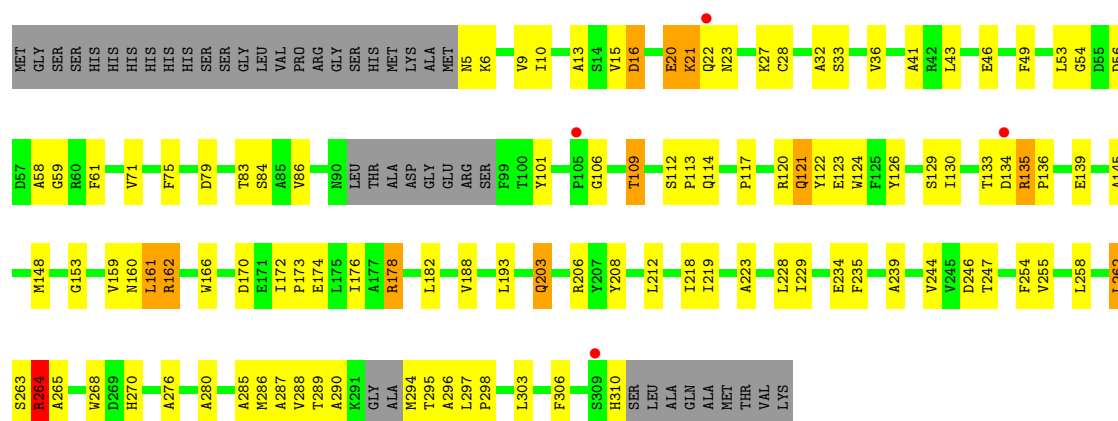
• Molecule 1: putative sugar kinase

Chain A:
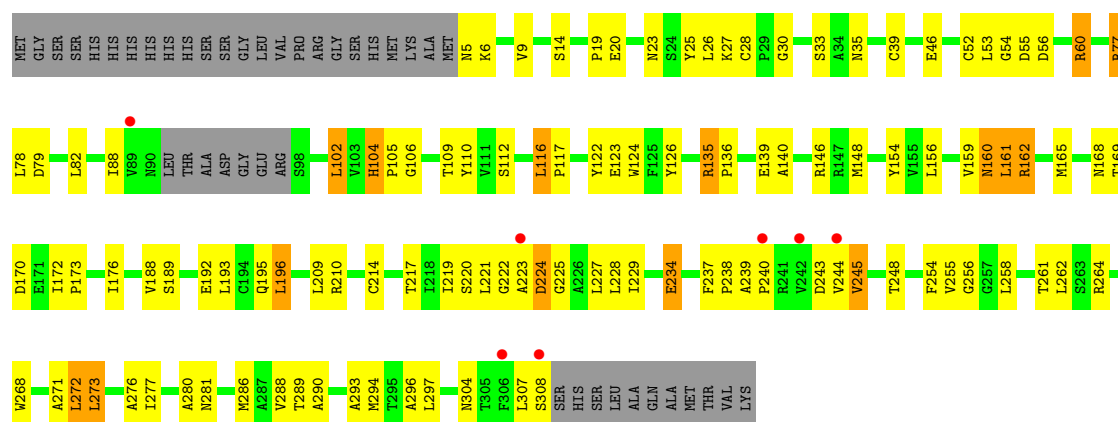
• Molecule 1: putative sugar kinase

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.43Å 53.99Å 89.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.01 – 2.60 46.23 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.8 (32.01-2.60) 82.7 (46.23-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.293 0.234 , 0.304	Depositor DCC
R_{free} test set	1726 reflections (9.86%)	DCC
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.31$	Xtriage
Outliers	0 of 38124 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4429	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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

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	0.47	0/2236	0.67	1/3039 (0.0%)
1	B	0.45	0/2216	0.63	1/3015 (0.0%)
All	All	0.46	0/4452	0.65	2/6054 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	135	ARG	N-CA-C	5.86	126.83	111.00
1	A	135	ARG	N-CA-C	5.01	124.53	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	2195	0	2105	88	0
1	B	2176	0	2060	95	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	0	1	0
All	All	4429	0	4165	181	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 (181) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:ASN:HD21	1:A:293:ALA:HB1	1.36	0.88
1:B:219:ILE:HD11	1:B:229:ILE:HD11	1.57	0.86
1:B:264:ARG:HE	1:B:264:ARG:HA	1.39	0.85
1:B:203:GLN:H	1:B:203:GLN:NE2	1.74	0.85
1:B:6:LYS:HG3	1:B:46:GLU:HG2	1.58	0.83
1:B:246:ASP:O	1:B:288:VAL:HA	1.83	0.79
1:A:229:ILE:HG12	1:A:234:GLU:HG3	1.66	0.76
1:B:106:GLY:O	1:B:109:THR:HG22	1.85	0.76
1:B:15:VAL:CG2	1:B:86:VAL:HG22	2.18	0.74
1:B:258:LEU:HD12	1:B:276:ALA:HB1	1.70	0.74
1:B:203:GLN:H	1:B:203:GLN:HE21	1.34	0.73
1:B:159:VAL:HG23	1:B:176:ILE:HD12	1.72	0.72
1:A:210:ARG:HA	1:A:214:CYS:O	1.90	0.72
1:B:20:GLU:HG2	1:B:21:LYS:H	1.54	0.70
1:A:53:LEU:O	1:A:78:LEU:HA	1.91	0.70
1:B:54:GLY:O	1:B:59:GLY:HA3	1.93	0.68
1:A:104:HIS:CB	1:A:105:PRO:HD3	2.23	0.68
1:B:287:ALA:HA	1:B:296:ALA:CB	2.23	0.68
1:A:82:LEU:HD11	1:A:110:TYR:CE2	2.30	0.67
1:B:9:VAL:HG11	1:B:33:SER:O	1.95	0.67
1:B:123:GLU:HB3	1:B:148:MSE:HE1	1.77	0.66
1:A:244:VAL:HA	1:A:288:VAL:HG12	1.76	0.66
1:B:287:ALA:HA	1:B:296:ALA:HB1	1.78	0.65
1:A:9:VAL:HG11	1:A:33:SER:O	1.97	0.65
1:B:159:VAL:HG13	1:B:188:VAL:HG23	1.80	0.64
1:A:54:GLY:HA2	1:A:79:ASP:O	1.98	0.64
1:A:159:VAL:HG23	1:A:176:ILE:HD12	1.78	0.64
1:A:26:LEU:HD12	1:A:28:CYS:SG	2.39	0.63
1:A:159:VAL:CG1	1:A:188:VAL:HG23	2.29	0.63
1:A:79:ASP:HB3	1:A:82:LEU:HD23	1.80	0.62
1:A:159:VAL:HG13	1:A:188:VAL:HG23	1.81	0.62
1:B:244:VAL:HA	1:B:288:VAL:HG12	1.81	0.62
1:A:244:VAL:HG22	1:A:288:VAL:HG11	1.80	0.62
1:B:135:ARG:HB3	1:B:136:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:159:VAL:CG1	1:B:188:VAL:HG23	2.29	0.62
1:B:247:THR:HA	1:B:288:VAL:HG22	1.81	0.61
1:B:218:ILE:HD12	1:B:258:LEU:HD21	1.83	0.60
1:B:9:VAL:HG12	1:B:33:SER:HB3	1.84	0.59
1:A:123:GLU:HB2	1:A:148:MSE:HE1	1.84	0.59
1:A:14:SER:O	1:A:30:GLY:N	2.35	0.58
1:A:254:PHE:CD1	1:A:280:ALA:HB1	2.39	0.58
1:B:133:THR:HG23	1:B:134:ASP:OD1	2.03	0.58
1:B:219:ILE:HD11	1:B:229:ILE:CD1	2.32	0.58
1:B:13:ALA:O	1:B:53:LEU:HD21	2.04	0.57
1:A:35:ASN:HD21	1:A:293:ALA:CB	2.13	0.57
1:B:148:MSE:SE	1:B:153:GLY:HA3	2.53	0.57
1:B:109:THR:OG1	1:B:134:ASP:HB2	2.05	0.57
1:A:159:VAL:O	1:A:159:VAL:HG22	2.03	0.57
1:A:221:LEU:O	1:A:224:ASP:HB2	2.05	0.57
1:B:159:VAL:HG23	1:B:176:ILE:CD1	2.36	0.56
1:B:5:ASN:ND2	1:B:122:TYR:HB2	2.20	0.56
1:B:166:TRP:CG	1:B:172:ILE:HD11	2.42	0.55
1:A:168:ASN:C	1:A:170:ASP:H	2.10	0.55
1:A:168:ASN:O	1:A:170:ASP:N	2.40	0.55
1:B:20:GLU:O	1:B:21:LYS:O	2.24	0.54
1:B:75:PHE:CE2	1:B:117:PRO:HB3	2.43	0.54
1:A:195:GLN:HG2	1:A:195:GLN:O	2.08	0.54
1:B:145:ALA:HB3	1:B:182:LEU:HD13	1.90	0.54
1:A:172:ILE:O	1:A:176:ILE:HG12	2.08	0.54
1:A:35:ASN:ND2	1:A:293:ALA:HB1	2.14	0.54
1:A:6:LYS:HG3	1:A:46:GLU:HG2	1.90	0.54
1:B:188:VAL:HG13	1:B:219:ILE:HG23	1.89	0.53
1:B:170:ASP:O	1:B:173:PRO:HD2	2.09	0.53
1:B:159:VAL:HG22	1:B:159:VAL:O	2.08	0.53
1:A:156:LEU:HD21	1:A:255:VAL:HG13	1.90	0.53
1:B:263:SER:C	1:B:265:ALA:H	2.12	0.53
1:B:264:ARG:HA	1:B:264:ARG:NE	2.13	0.52
1:A:19:PRO:HG3	1:A:25:TYR:CE1	2.45	0.52
1:B:254:PHE:CD1	1:B:280:ALA:HB1	2.45	0.52
1:B:223:ALA:O	1:B:239:ALA:HB3	2.10	0.52
1:A:254:PHE:CE1	1:A:280:ALA:HB1	2.45	0.52
1:A:109:THR:O	1:A:136:PRO:HB2	2.10	0.51
1:B:13:ALA:HB2	1:B:49:PHE:CZ	2.45	0.51
1:A:220:SER:O	1:A:221:LEU:HD23	2.11	0.51
1:A:88:ILE:HD11	1:A:102:LEU:HD21	1.92	0.51
1:A:258:LEU:HD12	1:A:276:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:LYS:HB3	1:B:23:ASN:O	2.11	0.51
1:A:35:ASN:HA	1:A:294:MSE:HE2	1.93	0.51
1:B:75:PHE:CZ	1:B:117:PRO:HB3	2.45	0.51
1:A:162:ARG:HG2	1:A:165:MSE:SE	2.61	0.50
1:B:123:GLU:HB3	1:B:148:MSE:CE	2.41	0.50
1:A:104:HIS:CB	1:A:105:PRO:CD	2.89	0.50
1:A:261:THR:HG22	1:A:272:LEU:CD1	2.41	0.49
1:B:295:THR:C	1:B:297:LEU:H	2.15	0.49
1:A:294:MSE:HB2	1:A:297:LEU:HD12	1.95	0.49
1:A:25:TYR:CZ	1:B:27:LYS:HE3	2.47	0.49
1:A:159:VAL:HG23	1:A:176:ILE:CD1	2.42	0.49
1:B:206:ARG:O	1:B:229:ILE:HD13	2.12	0.48
1:B:285:ALA:O	1:B:289:THR:HG22	2.13	0.48
1:B:270:HIS:HB2	3:B:516:HOH:O	2.11	0.48
1:B:244:VAL:HG12	1:B:288:VAL:HG11	1.95	0.48
1:A:172:ILE:HB	1:A:173:PRO:HD3	1.95	0.48
1:B:172:ILE:O	1:B:176:ILE:HG12	2.14	0.48
1:B:106:GLY:O	1:B:109:THR:CG2	2.59	0.48
1:A:244:VAL:HG12	1:A:245:VAL:N	2.29	0.47
1:B:159:VAL:CG2	1:B:176:ILE:HD12	2.42	0.47
1:A:112:SER:HA	1:A:140:ALA:HB2	1.96	0.47
1:B:43:LEU:HD23	1:B:43:LEU:N	2.29	0.47
1:A:9:VAL:HG12	1:A:33:SER:HB3	1.97	0.47
1:A:135:ARG:O	1:A:136:PRO:C	2.52	0.47
1:B:228:LEU:O	1:B:234:GLU:HA	2.15	0.47
1:A:223:ALA:O	1:A:239:ALA:HB3	2.15	0.46
1:A:168:ASN:C	1:A:170:ASP:N	2.68	0.46
1:B:188:VAL:HG11	1:B:193:LEU:HD13	1.98	0.46
1:B:285:ALA:O	1:B:287:ALA:N	2.48	0.46
1:A:286:MSE:O	1:A:289:THR:HG23	2.15	0.46
1:A:192:GLU:O	1:A:196:LEU:HD23	2.15	0.46
1:B:289:THR:HG23	1:B:290:ALA:N	2.30	0.46
1:B:126:TYR:CD1	1:B:126:TYR:C	2.88	0.46
1:A:188:VAL:HG11	1:A:193:LEU:HD21	1.97	0.46
1:A:222:GLY:C	1:A:224:ASP:H	2.19	0.46
1:A:77:ARG:C	1:A:78:LEU:HD12	2.36	0.45
1:A:290:ALA:HB2	1:A:296:ALA:HB2	1.97	0.45
1:A:288:VAL:HG12	1:A:288:VAL:O	2.17	0.45
1:A:161:LEU:HD13	1:A:162:ARG:N	2.31	0.45
1:B:126:TYR:CE2	1:B:255:VAL:HG11	2.52	0.45
1:B:32:ALA:O	1:B:36:VAL:HG23	2.16	0.45
1:B:172:ILE:HB	1:B:173:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:58:ALA:O	1:B:61:PHE:N	2.50	0.44
1:B:208:TYR:O	1:B:212:LEU:HD13	2.17	0.44
1:A:225:GLY:HA3	1:A:237:PHE:O	2.18	0.44
1:A:304:ASN:HA	1:A:307:LEU:HD12	1.99	0.44
1:A:273:LEU:O	1:A:277:ILE:HG13	2.17	0.44
1:B:235:PHE:CD1	1:B:235:PHE:N	2.84	0.44
1:B:15:VAL:O	1:B:15:VAL:HG23	2.17	0.44
1:A:161:LEU:HD21	1:A:172:ILE:HG21	1.99	0.44
1:B:101:TYR:N	1:B:101:TYR:CD1	2.86	0.44
1:B:286:MSE:SE	1:B:298:PRO:HG3	2.67	0.44
1:B:123:GLU:CB	1:B:148:MSE:HE1	2.46	0.44
1:B:121:GLN:HG2	1:B:122:TYR:CD2	2.53	0.44
1:B:285:ALA:O	1:B:286:MSE:C	2.56	0.44
1:A:20:GLU:OE1	1:A:26:LEU:HB2	2.17	0.44
1:A:160:ASN:HD21	1:A:162:ARG:HH11	1.65	0.44
1:A:52:CYS:SG	1:A:77:ARG:CZ	3.06	0.43
1:B:306:PHE:HA	1:B:310:HIS:CB	2.48	0.43
1:A:188:VAL:HG22	1:A:189:SER:N	2.34	0.43
1:A:54:GLY:C	1:A:56:ASP:H	2.22	0.43
1:A:39:CYS:SG	1:A:256:GLY:HA3	2.59	0.43
1:B:161:LEU:HD13	1:B:162:ARG:N	2.34	0.43
1:B:130:ILE:O	1:B:133:THR:HG22	2.19	0.43
1:A:55:ASP:O	1:A:60:ARG:NH1	2.51	0.43
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.83	0.43
1:B:294:MSE:C	1:B:296:ALA:H	2.22	0.43
1:B:114:GLN:N	1:B:114:GLN:OE1	2.51	0.43
1:B:16:ASP:HB2	1:B:28:CYS:HB3	2.01	0.43
1:B:285:ALA:C	1:B:287:ALA:N	2.69	0.42
1:A:19:PRO:HG3	1:A:25:TYR:HE1	1.81	0.42
1:B:124:TRP:CZ2	1:B:262:LEU:HB3	2.54	0.42
1:A:161:LEU:HD12	1:A:195:GLN:NE2	2.34	0.42
1:B:129:SER:HB2	1:B:166:TRP:HZ2	1.84	0.42
1:A:227:LEU:HD11	1:A:234:GLU:HB3	2.01	0.42
1:A:126:TYR:C	1:A:126:TYR:CD1	2.92	0.42
1:B:20:GLU:HG2	1:B:21:LYS:N	2.28	0.42
1:A:281:ASN:HA	1:A:281:ASN:HD22	1.67	0.42
1:A:78:LEU:N	1:A:78:LEU:HD12	2.35	0.42
1:B:174:GLU:OE2	1:B:178:ARG:HD3	2.20	0.42
1:A:244:VAL:CG1	1:A:245:VAL:N	2.82	0.42
1:B:254:PHE:CE1	1:B:280:ALA:HB1	2.54	0.42
1:A:154:TYR:CE1	1:A:268:TRP:NE1	2.86	0.42
1:A:159:VAL:CG2	1:A:176:ILE:HD12	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:LEU:HD13	1:A:228:LEU:C	2.40	0.42
1:B:10:ILE:O	1:B:10:ILE:HG23	2.20	0.42
1:A:116:LEU:HA	1:A:117:PRO:HD3	1.84	0.41
1:A:261:THR:HG22	1:A:272:LEU:HD11	2.02	0.41
1:A:294:MSE:HB2	1:A:297:LEU:CD1	2.51	0.41
1:B:262:LEU:HD13	1:B:276:ALA:HB2	2.02	0.41
1:B:21:LYS:HB3	1:B:22:GLN:H	1.62	0.41
1:B:263:SER:O	1:B:265:ALA:N	2.54	0.41
1:B:15:VAL:HG23	1:B:86:VAL:HG22	2.01	0.41
1:A:161:LEU:HD13	1:A:161:LEU:C	2.41	0.41
1:A:237:PHE:HA	1:A:238:PRO:HD3	1.78	0.41
1:A:217:THR:HG22	1:A:219:ILE:HG13	2.02	0.41
1:B:303:LEU:O	1:B:306:PHE:HB3	2.21	0.40
1:A:248:THR:HG22	1:A:293:ALA:HB2	2.04	0.40
1:B:268:TRP:N	1:B:268:TRP:CD1	2.89	0.40
1:B:54:GLY:N	1:B:84:SER:OG	2.52	0.40
1:B:126:TYR:HE2	1:B:255:VAL:HG11	1.86	0.40
1:B:112:SER:HB2	1:B:113:PRO:HD2	2.03	0.40
1:A:5:ASN:ND2	1:A:122:TYR:HB2	2.37	0.40
1:B:41:ALA:HB2	1:B:71:VAL:HG22	2.03	0.40
1:A:124:TRP:CZ2	1:A:262:LEU:HB3	2.57	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	293/339 (86%)	256 (87%)	29 (10%)	8 (3%)	8	13
1	B	290/339 (86%)	254 (88%)	32 (11%)	4 (1%)	16	32
All	All	583/678 (86%)	510 (88%)	61 (10%)	12 (2%)	11	19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	LYS
1	A	23	ASN
1	A	169	THR
1	B	264	ARG
1	A	104	HIS
1	A	271	ALA
1	B	20	GLU
1	B	121	GLN
1	A	243	ASP
1	A	106	GLY
1	A	240	PRO
1	A	245	VAL

5.3.2   Protein sidechains (i)

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	221/263 (84%)	205 (93%)	16 (7%)	21	39
1	B	218/263 (83%)	204 (94%)	14 (6%)	25	47
All	All	439/526 (84%)	409 (93%)	30 (7%)	22	43

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	77	ARG
1	A	102	LEU
1	A	116	LEU
1	A	139	GLU
1	A	160	ASN
1	A	161	LEU
1	A	162	ARG
1	A	196	LEU
1	A	209	LEU
1	A	224	ASP
1	A	234	GLU
1	A	264	ARG
1	A	272	LEU

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Mol	Chain	Res	Type
1	A	273	LEU
1	A	308	SER
1	B	16	ASP
1	B	56	ASP
1	B	79	ASP
1	B	83	THR
1	B	109	THR
1	B	120	ARG
1	B	139	GLU
1	B	160	ASN
1	B	161	LEU
1	B	162	ARG
1	B	178	ARG
1	B	203	GLN
1	B	262	LEU
1	B	264	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	35	ASN
1	A	67	GLN
1	A	114	GLN
1	A	121	GLN
1	A	160	ASN
1	A	195	GLN
1	A	281	ASN
1	B	5	ASN
1	B	67	GLN
1	B	160	ASN
1	B	203	GLN
1	B	236	HIS
1	B	266	ASN
1	B	281	ASN

5.3.3 RNA (i)

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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(Å²)	Q<0.9
1	A	297/339 (87%)	0.07	7 (2%)	56	53	41, 67, 104, 143	0
1	B	296/339 (87%)	0.06	4 (1%)	72	72	44, 70, 108, 147	0
All	All	593/678 (87%)	0.07	11 (1%)	65	61	41, 68, 106, 147	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ALA	3.8
1	A	242	VAL	3.3
1	A	306	PHE	3.2
1	B	22	GLN	3.2
1	A	308	SER	2.8
1	A	244	VAL	2.5
1	A	89	VAL	2.2
1	B	309	SER	2.1
1	B	105	PRO	2.1
1	A	240	PRO	2.1
1	B	134	ASP	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	K	B	505	1/1	0.11	-1.38	78,78,78,78	0
2	K	A	404	1/1	0.07	-1.80	84,84,84,84	0
2	K	A	405	1/1	0.10	-1.91	78,78,78,78	0
2	K	B	504	1/1	0.06	-3.09	75,75,75,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.