



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 06:19 PM GMT

PDB ID : 1Q18  
Title : Crystal structure of E.coli glucokinase (Glk)  
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Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : 2003-07-18  
Resolution : 2.36 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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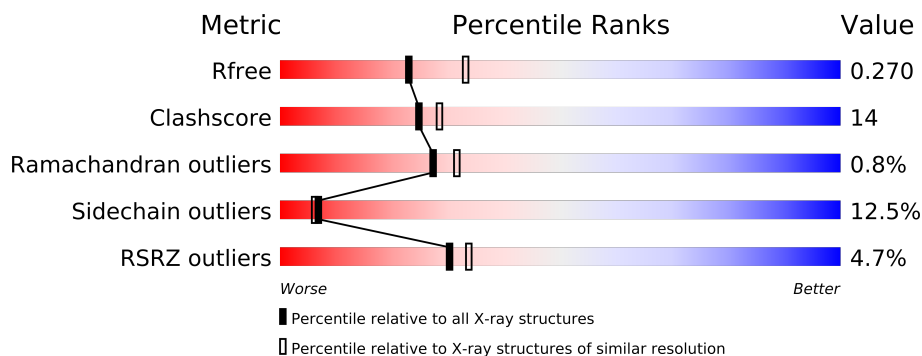
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.36 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	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	332	
1	B	332	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5295 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 Glucokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	Se	0	3	0
			2451	1570	423	446	7	5			
1	B	320	Total	C	N	O	S	Se	0	4	0
			2457	1574	426	445	6	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	modified residue	UNP P0A6V8
A	-9	GLY	-	CLONING ARTIFACT	UNP P0A6V8
A	-8	SER	-	CLONING ARTIFACT	UNP P0A6V8
A	-7	SER	-	CLONING ARTIFACT	UNP P0A6V8
A	-6	HIS	-	EXPRESSION TAG	UNP P0A6V8
A	-5	HIS	-	EXPRESSION TAG	UNP P0A6V8
A	-4	HIS	-	EXPRESSION TAG	UNP P0A6V8
A	-3	HIS	-	EXPRESSION TAG	UNP P0A6V8
A	-2	HIS	-	EXPRESSION TAG	UNP P0A6V8
A	-1	HIS	-	EXPRESSION TAG	UNP P0A6V8
A	11	GLY	-	CLONING ARTIFACT	UNP P0A6V8
A	1	SER	-	CLONING ARTIFACT	UNP P0A6V8
A	74	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
A	86	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
A	106	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
A	110	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
A	241	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
B	-10	MSE	-	modified residue	UNP P0A6V8
B	-9	GLY	-	CLONING ARTIFACT	UNP P0A6V8
B	-8	SER	-	CLONING ARTIFACT	UNP P0A6V8
B	-7	SER	-	CLONING ARTIFACT	UNP P0A6V8
B	-6	HIS	-	EXPRESSION TAG	UNP P0A6V8
B	-5	HIS	-	EXPRESSION TAG	UNP P0A6V8
B	-4	HIS	-	EXPRESSION TAG	UNP P0A6V8
B	-3	HIS	-	EXPRESSION TAG	UNP P0A6V8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP P0A6V8
B	-1	HIS	-	EXPRESSION TAG	UNP P0A6V8
B	11	GLY	-	CLONING ARTIFACT	UNP P0A6V8
B	1	SER	-	CLONING ARTIFACT	UNP P0A6V8
B	74	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
B	86	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
B	106	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
B	110	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8
B	241	MSE	MET	MODIFIED RESIDUE	UNP P0A6V8

- Molecule 2 is water.

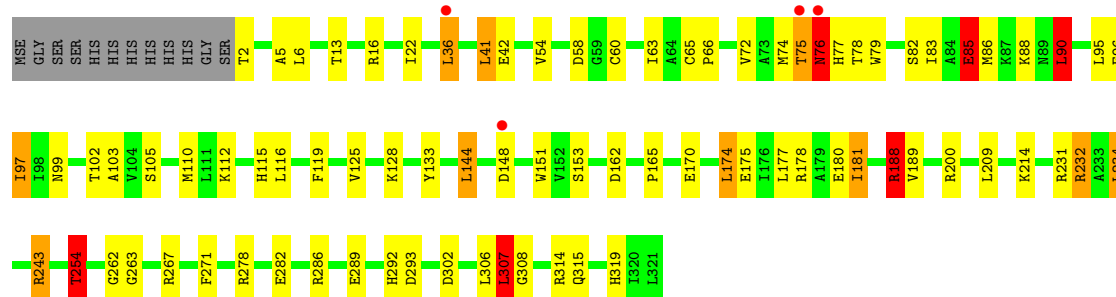
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	243	Total O 243 243	0	0
2	B	144	Total O 144 144	0	0

### 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.

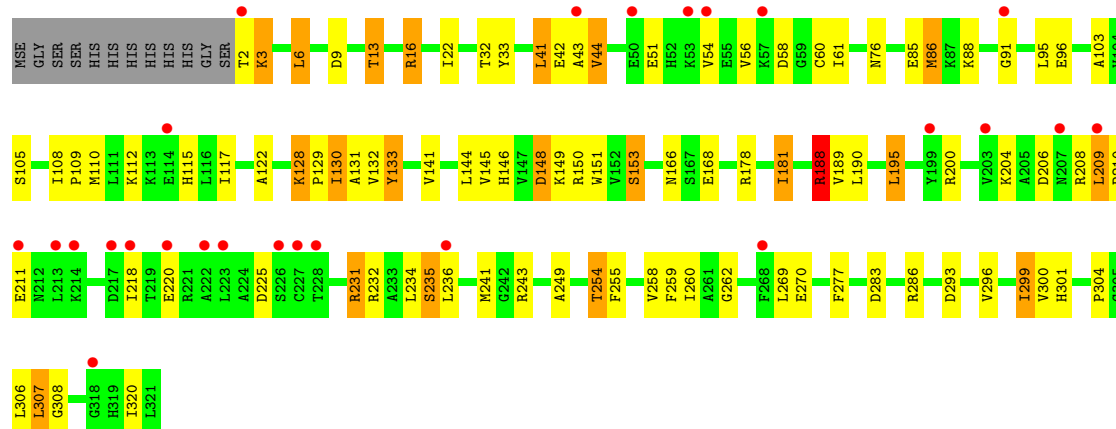
#### • Molecule 1: Glucokinase

Chain A: 



#### • Molecule 1: Glucokinase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.47Å 81.47Å 234.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.36 41.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (19.76-2.36) 96.3 (41.11-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.206 , 0.267 0.199 , 0.270	Depositor DCC
$R_{free}$ test set	1784 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34804 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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

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	0.93	1/2508 (0.0%)	1.00	11/3389 (0.3%)
1	B	0.77	1/2521 (0.0%)	0.89	7/3403 (0.2%)
All	All	0.85	2/5029 (0.0%)	0.95	18/6792 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLU	CG-CD	6.24	1.61	1.51
1	B	86	MSE	SE-CE	6.11	2.31	1.95

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	188	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	307	LEU	CA-CB-CG	7.72	133.05	115.30
1	A	90	LEU	C-N-CA	-6.91	107.78	122.30
1	B	148	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	58	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	36	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	132	VAL	CB-CA-C	-5.79	100.40	111.40
1	A	162	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	254	THR	N-CA-CB	-5.62	99.63	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	9	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	232	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	144	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	307	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	243	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	188	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	58	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	THR	Peptide
1	B	91	GLY	Peptide

## 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	2451	0	2460	74	0
1	B	2457	0	2473	64	0
2	A	243	0	0	25	0
2	B	144	0	0	16	0
All	All	5295	0	4933	137	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 14.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:MSE:CE	1:A:74:MSE:SE	2.19	1.38
1:B:86:MSE:CE	1:B:86:MSE:SE	2.31	1.28
1:A:293:ASP:HB2	2:A:541:HOH:O	1.24	1.26
1:A:153:SER:HB2	2:A:389:HOH:O	1.46	1.14

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:78:THR:HG22	2:A:502:HOH:O	1.62	0.99
1:A:65[B]:CYS:SG	1:A:66:PRO:HD2	2.07	0.94
1:A:175:GLU:HG2	1:B:168:GLU:HG3	1.47	0.94
1:A:151:TRP:H	1:A:315:GLN:HE22	1.10	0.89
1:A:65[B]:CYS:SG	2:A:382:HOH:O	2.30	0.89
1:A:65[B]:CYS:SG	2:A:377:HOH:O	2.32	0.87
1:A:42[A]:GLU:HG3	1:A:86:MSE:HE2	1.54	0.87
1:A:63:ILE:HG13	1:A:97[A]:ILE:HD12	1.56	0.85
1:A:175:GLU:HG3	2:A:451:HOH:O	1.74	0.85
1:A:282:GLU:OE1	1:A:292:HIS:HD2	1.59	0.83
1:A:75:THR:HA	2:A:532:HOH:O	1.78	0.82
1:B:2:THR:HA	1:B:3:LYS:HB2	1.62	0.82
1:B:43:ALA:C	2:B:397:HOH:O	2.17	0.81
1:A:292:HIS:HB3	2:A:342:HOH:O	1.78	0.81
1:A:112:LYS:H	1:A:115:HIS:HD2	1.30	0.79
1:B:117:ILE:HD12	1:B:300:VAL:HG11	1.67	0.76
1:B:112:LYS:H	1:B:115:HIS:HD2	1.35	0.75
1:B:148:ASP:O	1:B:149:LYS:HB2	1.87	0.75
1:A:178:ARG:O	1:A:181:ILE:O	2.06	0.74
1:A:231:ARG:CZ	2:A:512:HOH:O	2.35	0.74
1:B:44:VAL:N	2:B:397:HOH:O	2.22	0.72
1:B:188:ARG:HD3	2:B:350:HOH:O	1.91	0.71
1:A:82:SER:HB3	1:A:85:GLU:HB3	1.73	0.70
1:A:41:LEU:HB3	1:A:86:MSE:HE1	1.72	0.69
1:B:16:ARG:HD3	1:B:32:THR:OG1	1.92	0.68
1:B:190:LEU:HD22	1:B:241[B]:MSE:SE	2.44	0.68
1:A:42[A]:GLU:CG	1:A:86:MSE:HE2	2.23	0.68
1:A:254:THR:O	1:A:254:THR:CG2	2.41	0.68
1:A:234:LEU:HD13	1:A:271:PHE:CD2	2.31	0.66
1:B:43:ALA:CA	2:B:397:HOH:O	2.45	0.65
1:A:112:LYS:H	1:A:115:HIS:CD2	2.11	0.65
1:B:43:ALA:HA	2:B:397:HOH:O	1.97	0.65
1:B:178:ARG:O	1:B:181:ILE:O	2.15	0.64
1:A:282:GLU:OE1	1:A:292:HIS:CD2	2.48	0.64
1:A:65[B]:CYS:SG	1:A:66:PRO:CD	2.83	0.64
1:B:209:LEU:HD12	1:B:210:PRO:HD2	1.79	0.64
1:A:42[A]:GLU:HG3	1:A:86:MSE:HG3	1.81	0.63
1:A:74:MSE:HE3	2:A:504:HOH:O	1.97	0.63
1:A:170:GLU:OE2	1:A:243:ARG:NH2	2.32	0.62
1:B:130:ILE:HD13	1:B:144:LEU:HB3	1.81	0.62
1:B:112:LYS:H	1:B:115:HIS:CD2	2.16	0.61
1:B:130:ILE:HA	1:B:254[A]:THR:HG23	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:231:ARG:O	1:B:235:SER:HB2	2.02	0.60
1:B:243[A]:ARG:NH1	1:B:283:ASP:OD2	2.34	0.60
1:B:41:LEU:HB3	1:B:86:MSE:HE1	1.85	0.59
1:B:103:ALA:O	1:B:308:GLY:HA3	2.04	0.57
1:B:200:ARG:HD2	2:B:449:HOH:O	2.04	0.57
1:A:231:ARG:NH1	2:A:512:HOH:O	2.37	0.57
1:A:99:ASN:HD22	1:A:102:THR:H	1.52	0.57
1:A:188:ARG:HD3	2:A:333:HOH:O	2.04	0.56
1:B:195:LEU:HD22	1:B:218:ILE:HG21	1.87	0.56
1:A:180:GLU:HG3	2:A:454:HOH:O	2.05	0.55
1:B:2:THR:CA	1:B:3:LYS:HB2	2.36	0.55
1:A:86:MSE:HG2	1:A:90:LEU:HD22	1.89	0.54
1:A:165:PRO:HG3	1:A:174:LEU:HD12	1.90	0.54
1:A:151:TRP:N	1:A:315:GLN:HE22	1.92	0.54
1:B:128[B]:LYS:HG3	1:B:129:PRO:HD3	1.89	0.54
1:A:243:ARG:HD2	2:B:370:HOH:O	2.08	0.54
1:B:76:ASN:HB2	2:B:399:HOH:O	2.07	0.53
1:B:6:LEU:HD13	1:B:61:ILE:HD11	1.90	0.53
1:B:153:SER:HB2	2:B:363:HOH:O	2.07	0.53
1:A:63:ILE:HG13	1:A:97[A]:ILE:CD1	2.34	0.53
1:A:254:THR:HG22	1:A:254:THR:O	2.08	0.52
1:B:206:ASP:CB	1:B:208:ARG:HH21	2.22	0.52
1:B:166:ASN:HD22	1:B:243[A]:ARG:CZ	2.23	0.52
1:A:42[A]:GLU:OE2	1:A:85:GLU:OE1	2.28	0.52
1:B:115:HIS:HB3	1:B:301:HIS:HB2	1.92	0.52
1:B:22:ILE:CD1	2:B:343:HOH:O	2.57	0.51
1:A:105:SER:O	1:A:144:LEU:HD11	2.11	0.51
1:B:133:TYR:O	1:B:260:ILE:HA	2.10	0.51
1:B:206:ASP:HB3	1:B:208:ARG:HH21	1.75	0.51
1:A:200:ARG:NH2	2:A:454:HOH:O	2.42	0.51
1:A:234:LEU:HD13	1:A:271:PHE:CE2	2.46	0.51
1:A:119:PHE:O	1:A:278:ARG:HD3	2.12	0.50
1:B:299:ILE:HD11	1:B:304:PRO:HG3	1.94	0.50
1:A:72:VAL:HG21	1:A:97[A]:ILE:HD13	1.94	0.50
1:A:83:ILE:HG12	1:A:97[A]:ILE:HG21	1.94	0.50
1:A:88:LYS:HE3	2:A:546:HOH:O	2.11	0.50
1:A:42[A]:GLU:CG	1:A:86:MSE:HG3	2.41	0.49
1:A:293:ASP:CB	2:A:541:HOH:O	2.09	0.49
1:B:130:ILE:HG12	1:B:131:ALA:N	2.25	0.49
1:A:16:ARG:HG2	1:A:306:LEU:HD11	1.93	0.49
1:A:180:GLU:CG	2:A:454:HOH:O	2.60	0.49
1:B:13:THR:HG22	2:B:422:HOH:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:22:ILE:HD11	2:B:343:HOH:O	2.13	0.48
1:B:209:LEU:CD1	1:B:210:PRO:HD2	2.43	0.48
1:A:76:ASN:O	1:A:79:TRP:HB2	2.13	0.48
1:A:263:GLY:N	2:A:480:HOH:O	2.25	0.48
1:A:254:THR:O	1:A:254:THR:HG23	2.13	0.47
1:A:188:ARG:CD	2:A:333:HOH:O	2.61	0.47
1:B:105:SER:O	1:B:144:LEU:HD22	2.15	0.47
1:B:42:GLU:H	1:B:86:MSE:HE2	1.80	0.46
1:A:42[A]:GLU:HG3	1:A:86:MSE:CE	2.36	0.46
1:B:148:ASP:O	1:B:149:LYS:CB	2.61	0.46
1:B:243[B]:ARG:HG2	2:B:346:HOH:O	2.15	0.46
1:B:42:GLU:HB2	1:B:86:MSE:HE2	1.98	0.45
1:B:243[B]:ARG:HD2	2:B:329:HOH:O	2.16	0.45
1:B:43:ALA:O	1:B:44:VAL:HG23	2.17	0.45
1:A:103:ALA:O	1:A:308:GLY:HA3	2.16	0.45
1:B:320:ILE:HD12	2:B:459:HOH:O	2.16	0.45
1:B:259:PHE:N	1:B:259:PHE:CD1	2.85	0.45
1:A:60:CYS:HA	1:A:96:GLU:O	2.17	0.45
1:A:175:GLU:CG	2:A:451:HOH:O	2.50	0.45
1:B:153:SER:CB	2:B:363:HOH:O	2.63	0.45
1:A:83:ILE:HG12	1:A:97[B]:ILE:HG13	1.99	0.44
1:A:319:HIS:HE1	2:A:460:HOH:O	2.00	0.44
1:A:36:LEU:HG	2:A:507:HOH:O	2.16	0.44
1:B:128[B]:LYS:HG2	1:B:255:PHE:HB2	2.00	0.44
1:B:60:CYS:HA	1:B:96:GLU:O	2.18	0.43
1:A:170:GLU:CD	1:A:243:ARG:HH22	2.22	0.43
1:A:262:GLY:HA2	2:A:480:HOH:O	2.19	0.43
1:A:77:HIS:HD2	2:A:550:HOH:O	2.02	0.43
1:A:314:ARG:O	1:A:319:HIS:HB2	2.20	0.42
1:B:241[A]:MSE:HG2	1:B:277:PHE:HE1	1.85	0.42
1:B:129:PRO:HB3	1:B:145:VAL:HG12	2.02	0.41
1:A:302:ASP:HB3	2:A:494:HOH:O	2.20	0.41
1:B:258:VAL:O	1:B:296:VAL:HA	2.21	0.41
1:A:125:VAL:HG12	1:A:128:LYS:HD3	2.03	0.41
1:B:128[B]:LYS:HG3	1:B:129:PRO:CD	2.50	0.41
1:B:108:ILE:N	1:B:109:PRO:HD2	2.35	0.41
1:B:249:ALA:HA	1:B:254[B]:THR:OG1	2.21	0.41
1:B:16:ARG:HG2	1:B:306:LEU:HD11	2.03	0.41
1:B:33:TYR:CD1	1:B:33:TYR:N	2.89	0.41
1:A:110:MSE:HB2	1:A:307:LEU:HD13	2.02	0.40
1:A:5:ALA:HB2	1:A:22:ILE:HD11	2.04	0.40
1:A:125:VAL:CG1	1:A:128:LYS:HD3	2.52	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:146:HIS:HB2	1:B:151:TRP:CZ3	2.56	0.40
1:A:72:VAL:HG21	1:A:97[A]:ILE:CD1	2.51	0.40
1:A:177:LEU:O	1:A:181:ILE:HD13	2.22	0.40
1:A:151:TRP:H	1:A:315:GLN:NE2	1.94	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	321/332 (97%)	307 (96%)	13 (4%)	1 (0%)	50	62
1	B	322/332 (97%)	300 (93%)	18 (6%)	4 (1%)	19	19
All	All	643/664 (97%)	607 (94%)	31 (5%)	5 (1%)	27	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	ALA
1	A	76	ASN
1	B	3	LYS
1	B	262	GLY
1	B	44	VAL

### 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	256/257 (100%)	229 (90%)	27 (10%)	10	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	257/257 (100%)	218 (85%)	39 (15%)	4	4
All	All	513/514 (100%)	447 (87%)	66 (13%)	7	6

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	6	LEU
1	A	13	THR
1	A	41	LEU
1	A	54	VAL
1	A	76	ASN
1	A	85	GLU
1	A	90	LEU
1	A	95	LEU
1	A	97[A]	ILE
1	A	97[B]	ILE
1	A	116	LEU
1	A	133	TYR
1	A	148	ASP
1	A	174	LEU
1	A	181	ILE
1	A	188	ARG
1	A	189	VAL
1	A	209	LEU
1	A	214	LYS
1	A	232	ARG
1	A	234	LEU
1	A	254	THR
1	A	267	ARG
1	A	286	ARG
1	A	289	GLU
1	A	307	LEU
1	B	6	LEU
1	B	13	THR
1	B	16	ARG
1	B	41	LEU
1	B	51	GLU
1	B	54	VAL
1	B	56	VAL
1	B	85	GLU
1	B	88	LYS

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Mol	Chain	Res	Type
1	B	95	LEU
1	B	110	MSE
1	B	128[A]	LYS
1	B	128[B]	LYS
1	B	130	ILE
1	B	133	TYR
1	B	141	VAL
1	B	150	ARG
1	B	153	SER
1	B	181	ILE
1	B	188	ARG
1	B	189	VAL
1	B	195	LEU
1	B	204	LYS
1	B	209	LEU
1	B	211	GLU
1	B	220	GLU
1	B	225	ASP
1	B	231	ARG
1	B	232	ARG
1	B	234	LEU
1	B	235	SER
1	B	236	LEU
1	B	254[A]	THR
1	B	254[B]	THR
1	B	269	LEU
1	B	270	GLU
1	B	286	ARG
1	B	299	ILE
1	B	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	76	ASN
1	A	77	HIS
1	A	94	HIS
1	A	99	ASN
1	A	115	HIS
1	A	292	HIS
1	A	315	GLN

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Mol	Chain	Res	Type
1	B	77	HIS
1	B	115	HIS
1	B	247	ASN
1	B	251	ASN
1	B	312	HIS

### 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 ⓘ

There are no ligands in this entry.

### 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	320/332 (96%)	-0.08	4 (1%) 74 77	19, 29, 42, 58	0
1	B	320/332 (96%)	0.42	26 (8%) 12 14	21, 40, 66, 75	0
All	All	640/664 (96%)	0.17	30 (4%) 30 34	19, 34, 60, 75	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	LEU	5.7
1	B	2	THR	5.6
1	B	43	ALA	4.2
1	B	209	LEU	4.0
1	B	223	LEU	3.9
1	B	227	CYS	3.9
1	B	207	ASN	3.7
1	A	75	THR	3.6
1	B	222	ALA	3.1
1	B	214	LYS	3.1
1	B	220	GLU	2.9
1	B	228	THR	2.8
1	B	53	LYS	2.8
1	B	114	GLU	2.7
1	B	217	ASP	2.7
1	B	226	SER	2.6
1	A	36	LEU	2.5
1	B	211	GLU	2.5
1	B	50	GLU	2.4
1	B	54	VAL	2.4
1	B	268	PHE	2.4
1	B	57	LYS	2.3
1	A	76	ASN	2.3
1	B	91	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	199	TYR	2.2
1	A	148	ASP	2.1
1	B	236	LEU	2.1
1	B	218	ILE	2.1
1	B	318	GLY	2.0
1	B	203	VAL	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.