



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:54 PM GMT

PDB ID : 3ISP  
Title : Crystal structure of ArgP from Mycobacterium tuberculosis  
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Deposited on : 2009-08-27  
Resolution : 2.70 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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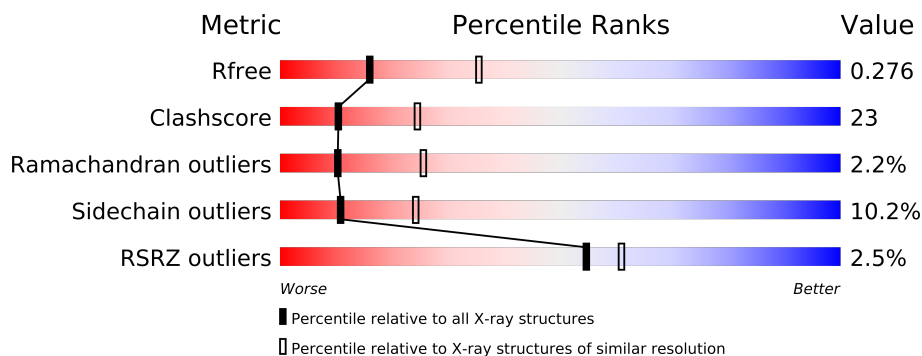
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	303	
1	B	303	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4267 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 HTH-type transcriptional regulator Rv1985c/MT2039.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2202	1387	404	401	10			
1	B	263	Total	C	N	O	S	0	0	0
			1988	1257	359	363	9			

- Molecule 2 is water.

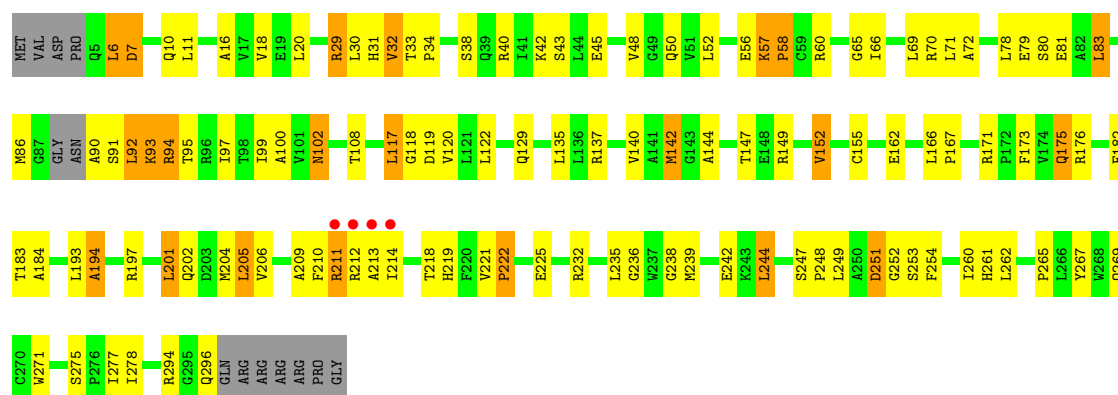
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	37	Total	O	0	0
			37	37		

### 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: HTH-type transcriptional regulator Rv1985c/MT2039

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.80Å 116.74Å 136.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.70 48.61 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.61-2.70) 89.4 (48.61-2.42)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 2.42Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.207 , 0.271 0.221 , 0.276	Depositor DCC
$R_{free}$ test set	1839 reflections (7.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26655 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	0.38	0/2245	0.57	0/3052
1	B	0.38	0/2028	0.54	0/2759
All	All	0.38	0/4273	0.56	0/5811

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	2202	0	2226	101	0
1	B	1988	0	1999	103	0
2	A	40	0	0	4	0
2	B	37	0	0	1	0
All	All	4267	0	4225	196	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 23.

All (196) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:ARG:HH11	1:A:94:ARG:HG3	1.24	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:LYS:HB3	1:A:58:PRO:HD3	1.38	1.01
1:A:57:LYS:HB3	1:A:58:PRO:CD	1.96	0.95
1:B:32:VAL:HG12	1:B:33:THR:H	1.32	0.92
1:B:8:GLY:H	1:B:9:PRO:HD2	1.37	0.90
1:B:8:GLY:H	1:B:9:PRO:CD	1.89	0.86
1:A:202:GLN:NE2	1:A:239:MET:H	1.74	0.85
1:A:97:ILE:HD12	1:A:142:MET:HG3	1.65	0.79
1:B:113:VAL:HG22	1:B:284:THR:HG22	1.64	0.78
1:B:186:ALA:HA	1:B:189:LYS:HB3	1.65	0.78
1:A:57:LYS:CB	1:A:58:PRO:HD3	2.12	0.77
1:A:171:ARG:HH21	1:A:252:GLY:HA2	1.47	0.76
1:A:205:LEU:O	1:A:206:VAL:HB	1.86	0.75
1:B:108:THR:HG22	1:B:109:TRP:H	1.52	0.75
1:B:108:THR:CG2	1:B:109:TRP:N	2.49	0.74
1:A:29:ARG:CG	1:A:29:ARG:HH11	2.01	0.74
1:B:173:PHE:CZ	1:B:191:PRO:HD2	2.23	0.73
1:B:182:PHE:O	1:B:182:PHE:CD2	2.42	0.73
1:A:251:ASP:HB3	1:A:253:SER:OG	1.89	0.72
1:B:24:ASP:O	1:B:28:GLU:HG3	1.89	0.72
1:B:171:ARG:HB2	1:B:172:PRO:HD3	1.72	0.71
1:A:204:MET:HB2	1:A:262:LEU:HD11	1.72	0.71
1:A:175:GLN:HA	1:A:175:GLN:HE21	1.55	0.70
1:A:94:ARG:NH1	1:A:94:ARG:HG3	1.99	0.69
1:A:81:GLU:OE2	1:A:277:ILE:HG13	1.92	0.69
1:B:152:VAL:HG13	1:B:153:PRO:HD2	1.73	0.69
1:B:66:ILE:HB	1:B:67:PRO:HD3	1.76	0.68
1:A:202:GLN:HE21	1:A:239:MET:H	1.41	0.67
1:A:95:THR:O	1:A:120:VAL:HG23	1.94	0.66
1:A:108:THR:HG22	1:A:244:LEU:HD13	1.76	0.66
1:B:248:PRO:HB2	1:B:254:PHE:CD2	2.31	0.66
1:B:108:THR:CG2	1:B:109:TRP:H	2.08	0.65
1:B:182:PHE:O	1:B:182:PHE:HD2	1.79	0.65
1:B:195:TRP:CD1	1:B:227:PHE:CE1	2.83	0.65
1:B:113:VAL:HG22	1:B:284:THR:CG2	2.27	0.64
1:B:225:GLU:C	1:B:228:THR:HG22	2.18	0.64
1:B:11:LEU:HD21	1:B:71:LEU:HD23	1.79	0.64
1:B:180:ASP:CG	1:B:181:GLY:H	2.01	0.63
1:A:92:LEU:HG	1:A:93:LYS:H	1.64	0.62
1:B:239:MET:HA	1:B:239:MET:HE2	1.81	0.62
1:A:10:GLN:HA	1:A:40:ARG:HG2	1.82	0.62
1:A:248:PRO:HB2	1:A:254:PHE:CD2	2.35	0.61
1:A:152:VAL:O	1:A:155:CYS:HB2	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:VAL:CG1	1:B:86:MET:HE1	2.30	0.60
1:A:197:ARG:N	1:A:197:ARG:HD3	2.16	0.60
1:A:97:ILE:CD1	1:A:142:MET:HG3	2.31	0.60
1:A:56:GLU:HG3	2:A:341:HOH:O	2.01	0.60
1:A:247:SER:HB3	1:A:248:PRO:HD3	1.83	0.59
1:B:104:ASP:O	1:B:108:THR:HB	2.03	0.59
1:B:32:VAL:HG12	1:B:33:THR:N	2.10	0.59
1:A:171:ARG:HG3	2:A:316:HOH:O	2.02	0.59
1:A:31:HIS:O	1:A:32:VAL:HG13	2.03	0.59
1:B:226:GLY:HA2	1:B:229:ALA:HB3	1.86	0.58
1:B:108:THR:HG23	1:B:109:TRP:N	2.18	0.58
1:A:102:ASN:H	1:A:102:ASN:HD22	1.51	0.58
1:A:29:ARG:O	1:A:30:LEU:HD23	2.04	0.57
1:B:108:THR:HG21	1:B:163:MET:HE1	1.85	0.57
1:A:202:GLN:HE21	1:A:238:GLY:HA2	1.69	0.57
1:A:117:LEU:HD22	1:A:122:LEU:HD22	1.85	0.57
1:B:180:ASP:CG	1:B:181:GLY:N	2.58	0.57
1:A:80:SER:HA	1:A:83:LEU:HD22	1.86	0.57
1:A:29:ARG:CG	1:A:29:ARG:NH1	2.66	0.56
1:B:106:MET:CE	1:B:124:VAL:HG11	2.35	0.56
1:B:167:PRO:HB2	1:B:257:VAL:HB	1.86	0.56
1:B:113:VAL:HG13	1:B:117:LEU:HD12	1.87	0.56
1:A:79:GLU:OE2	1:B:5:GLN:HA	2.06	0.55
1:B:189:LYS:O	1:B:189:LYS:HG3	2.06	0.55
1:B:41:ILE:O	1:B:45:GLU:HG2	2.05	0.55
1:A:175:GLN:HA	1:A:175:GLN:NE2	2.22	0.55
1:B:193:LEU:CD1	1:B:231:ALA:HB2	2.37	0.55
1:A:7:ASP:HA	1:A:10:GLN:HE21	1.72	0.54
1:B:113:VAL:CG2	1:B:284:THR:HG22	2.33	0.54
1:A:100:ALA:HB3	1:A:144:ALA:CB	2.38	0.54
1:B:119:ASP:OD2	1:B:280:ARG:NH2	2.35	0.54
1:B:195:TRP:HD1	1:B:227:PHE:CE1	2.25	0.54
1:B:38:SER:O	1:B:42:LYS:HG3	2.08	0.54
1:A:71:LEU:HD21	1:B:79:GLU:HG2	1.90	0.54
1:B:156:ARG:HH11	1:B:272:LYS:NZ	2.06	0.54
1:B:14:LEU:HA	1:B:41:ILE:HD11	1.90	0.54
1:B:156:ARG:HD3	1:B:272:LYS:HZ3	1.73	0.54
1:A:66:ILE:O	1:A:69:LEU:HB2	2.08	0.54
1:A:7:ASP:HA	1:A:10:GLN:NE2	2.22	0.54
1:A:173:PHE:CE1	1:A:236:GLY:HA2	2.43	0.54
1:A:202:GLN:HE21	1:A:238:GLY:CA	2.21	0.54
1:B:192:SER:O	1:B:218:THR:HA	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:HIS:NE2	1:A:235:LEU:HD22	2.23	0.53
1:A:102:ASN:N	1:A:102:ASN:HD22	2.06	0.53
1:B:193:LEU:HD12	1:B:231:ALA:HB2	1.90	0.53
1:A:202:GLN:HE21	1:A:239:MET:N	2.06	0.53
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.72	0.53
1:B:225:GLU:O	1:B:228:THR:HG22	2.08	0.53
1:B:283:ASP:OD1	1:B:286:ARG:NH2	2.40	0.53
1:B:150:ASN:H	1:B:150:ASN:ND2	2.06	0.53
1:B:97:ILE:HG13	1:B:97:ILE:O	2.07	0.53
1:A:210:PHE:O	1:A:212:ARG:N	2.42	0.53
1:A:204:MET:CB	1:A:262:LEU:HD11	2.37	0.53
1:B:173:PHE:HZ	1:B:191:PRO:HD2	1.70	0.52
1:A:45:GLU:HG2	1:A:50:GLN:O	2.09	0.52
1:A:162:GLU:HG2	1:A:265:PRO:HA	1.91	0.52
1:B:232:ARG:HD3	1:B:232:ARG:O	2.10	0.51
1:B:94:ARG:HB3	1:B:121:LEU:HD22	1.93	0.51
1:A:48:VAL:HG11	1:B:86:MET:HE1	1.91	0.51
1:B:182:PHE:O	1:B:184:ALA:N	2.43	0.51
1:B:7:ASP:HB3	1:B:8:GLY:CA	2.41	0.50
1:A:209:ALA:HB2	1:A:260:ILE:HD12	1.94	0.50
1:A:29:ARG:HG2	1:A:29:ARG:NH1	2.27	0.50
1:A:193:LEU:O	1:A:194:ALA:HB2	2.10	0.49
1:B:183:THR:O	1:B:185:ALA:N	2.45	0.49
1:A:92:LEU:HD23	1:A:92:LEU:N	2.26	0.49
1:A:48:VAL:HG13	1:B:86:MET:HE1	1.94	0.49
1:B:163:MET:HE3	1:B:266:LEU:HD11	1.94	0.49
1:B:54:VAL:O	1:B:59:CYS:HB3	2.13	0.48
1:A:275:SER:HB3	1:A:278:ILE:HG12	1.95	0.48
1:A:176:ARG:NH1	1:A:176:ARG:O	2.43	0.48
1:A:206:VAL:HG13	1:A:214:ILE:HG12	1.95	0.48
1:B:98:THR:HA	1:B:123:ASP:HB3	1.94	0.48
1:B:42:LYS:HA	1:B:45:GLU:CG	2.44	0.48
1:A:100:ALA:HB3	1:A:144:ALA:HB2	1.95	0.47
1:B:248:PRO:HB2	1:B:254:PHE:HB2	1.95	0.47
1:B:248:PRO:HB2	1:B:254:PHE:HD2	1.78	0.47
1:B:97:ILE:HD11	1:B:122:LEU:CD2	2.45	0.47
1:A:152:VAL:HG13	1:A:269:GLN:OE1	2.14	0.47
1:A:90:ALA:O	1:A:91:SER:HB2	2.15	0.47
1:A:260:ILE:HG22	1:A:261:HIS:N	2.29	0.47
1:B:49:GLY:O	1:B:50:GLN:HG3	2.14	0.47
1:B:93:LYS:HD3	2:B:317:HOH:O	2.14	0.46
1:B:282:THR:O	1:B:286:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:142:MET:HA	1:B:271:TRP:CE2	2.51	0.46
1:A:210:PHE:C	1:A:212:ARG:N	2.69	0.46
1:B:168:VAL:O	1:B:237:TRP:HA	2.15	0.46
1:B:108:THR:CG2	1:B:109:TRP:HD1	2.28	0.46
1:B:95:THR:HG21	1:B:277:ILE:HD12	1.97	0.46
1:A:149:ARG:HB2	1:A:267:TYR:CZ	2.51	0.46
1:A:57:LYS:CB	1:A:58:PRO:CD	2.76	0.45
1:B:117:LEU:HD13	1:B:122:LEU:HD21	1.98	0.45
1:B:108:THR:CG2	1:B:109:TRP:CD1	3.00	0.45
1:B:156:ARG:HH11	1:B:272:LYS:HZ3	1.63	0.45
1:A:129:GLN:HG3	1:A:147:THR:OG1	2.16	0.45
1:B:183:THR:C	1:B:185:ALA:H	2.18	0.45
1:B:7:ASP:HB3	1:B:8:GLY:HA3	1.99	0.45
1:A:183:THR:HG22	1:A:184:ALA:N	2.30	0.45
1:B:14:LEU:HA	1:B:41:ILE:CD1	2.47	0.45
1:A:142:MET:HB3	1:A:271:TRP:CZ3	2.52	0.44
1:A:232:ARG:NH2	1:A:248:PRO:HG3	2.31	0.44
1:B:54:VAL:HG13	1:B:54:VAL:O	2.18	0.44
1:A:78:LEU:HD13	1:B:74:GLN:HG3	1.99	0.44
1:B:97:ILE:HD12	1:B:281:ILE:HD13	2.00	0.44
1:B:6:LEU:HD12	1:B:6:LEU:C	2.37	0.44
1:A:94:ARG:HH11	1:A:94:ARG:CG	2.08	0.44
1:A:182:PHE:O	1:A:210:PHE:HZ	2.01	0.44
1:A:16:ALA:O	1:A:20:LEU:HB2	2.17	0.44
1:A:33:THR:O	1:A:34:PRO:C	2.56	0.44
1:A:57:LYS:CG	1:A:58:PRO:HD3	2.47	0.44
1:B:70:ARG:O	1:B:74:GLN:HG2	2.18	0.44
1:B:108:THR:CG2	1:B:163:MET:HE1	2.48	0.44
1:B:8:GLY:N	1:B:9:PRO:CD	2.62	0.43
1:A:50:GLN:HG3	1:B:86:MET:CE	2.48	0.43
1:B:97:ILE:O	1:B:97:ILE:CG1	2.66	0.43
1:A:92:LEU:O	1:A:93:LYS:O	2.37	0.43
1:A:18:VAL:HG11	1:A:69:LEU:HD11	2.00	0.43
1:B:20:LEU:HD11	1:B:29:ARG:HD2	2.00	0.43
1:A:60:ARG:NH1	2:A:336:HOH:O	2.51	0.43
1:B:235:LEU:O	1:B:235:LEU:HD23	2.19	0.43
1:A:201:LEU:HA	1:A:201:LEU:HD12	1.68	0.43
1:B:108:THR:HG22	1:B:109:TRP:CD1	2.54	0.43
1:B:183:THR:C	1:B:185:ALA:N	2.71	0.43
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.86	0.43
1:A:70:ARG:HB2	1:A:137:ARG:O	2.19	0.43
1:B:227:PHE:CE2	1:B:240:PHE:CE2	3.07	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:186:ALA:CA	1:B:189:LYS:HB3	2.44	0.42
1:B:45:GLU:H	1:B:45:GLU:HG2	1.72	0.42
1:A:92:LEU:H	1:A:92:LEU:HD23	1.84	0.42
1:B:268:TRP:CD1	1:B:282:THR:HG23	2.54	0.42
1:A:135:LEU:HD22	1:A:140:VAL:HG11	2.01	0.42
1:A:11:LEU:HB3	1:A:72:ALA:HB2	2.02	0.42
1:A:212:ARG:HG2	1:A:213:ALA:H	1.84	0.42
1:A:221:VAL:HA	1:A:222:PRO:HD3	1.77	0.42
1:A:52:LEU:HD22	1:A:65:GLY:HA2	2.02	0.42
2:A:337:HOH:O	1:B:134:ARG:HG3	2.20	0.41
1:A:6:LEU:O	1:A:7:ASP:HB2	2.19	0.41
1:A:86:MET:HE2	1:B:48:VAL:HB	2.03	0.41
1:A:166:LEU:HA	1:A:167:PRO:HD3	1.92	0.41
1:A:38:SER:O	1:A:42:LYS:HB2	2.21	0.41
1:A:210:PHE:C	1:A:212:ARG:H	2.24	0.41
1:B:32:VAL:HG12	1:B:36:ALA:HB3	2.03	0.41
1:B:11:LEU:HD12	1:B:11:LEU:HA	1.69	0.41
1:A:117:LEU:CD2	1:A:122:LEU:HD22	2.50	0.41
1:A:166:LEU:HD11	1:A:242:GLU:HG3	2.02	0.41
1:B:275:SER:HB3	1:B:278:ILE:HD12	2.02	0.41
1:B:247:SER:HB3	1:B:248:PRO:HD3	2.03	0.41
1:B:14:LEU:O	1:B:18:VAL:HG23	2.20	0.40
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.87	0.40
1:A:29:ARG:HG2	1:A:29:ARG:HH11	1.77	0.40
1:A:118:GLY:HA2	1:A:119:ASP:HA	1.86	0.40
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.71	0.40
1:B:227:PHE:HE2	1:B:240:PHE:CE2	2.39	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	286/303 (94%)	254 (89%)	26 (9%)	6 (2%)	11 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	255/303 (84%)	227 (89%)	22 (9%)	6 (2%)	9	22
All	All	541/606 (89%)	481 (89%)	48 (9%)	12 (2%)	10	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	93	LYS
1	A	7	ASP
1	A	251	ASP
1	B	183	THR
1	B	223	THR
1	B	222	PRO
1	A	194	ALA
1	A	211	ARG
1	B	184	ALA
1	B	8	GLY
1	B	80	SER

### 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	226/237 (95%)	202 (89%)	24 (11%)	10	22
1	B	204/237 (86%)	184 (90%)	20 (10%)	12	26
All	All	430/474 (91%)	386 (90%)	44 (10%)	11	24

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	29	ARG
1	A	32	VAL
1	A	43	SER
1	A	58	PRO
1	A	83	LEU

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Mol	Chain	Res	Type
1	A	92	LEU
1	A	94	ARG
1	A	99	ILE
1	A	102	ASN
1	A	117	LEU
1	A	142	MET
1	A	152	VAL
1	A	175	GLN
1	A	201	LEU
1	A	205	LEU
1	A	211	ARG
1	A	218	THR
1	A	222	PRO
1	A	225	GLU
1	A	244	LEU
1	A	249	LEU
1	A	294	ARG
1	A	296	GLN
1	B	39	GLN
1	B	55	ARG
1	B	59	CYS
1	B	81	GLU
1	B	93	LYS
1	B	94	ARG
1	B	108	THR
1	B	113	VAL
1	B	121	LEU
1	B	132	SER
1	B	135	LEU
1	B	140	VAL
1	B	150	ASN
1	B	171	ARG
1	B	232	ARG
1	B	251	ASP
1	B	254	PHE
1	B	277	ILE
1	B	292	LEU
1	B	294	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	102	ASN
1	A	129	GLN
1	A	131	HIS
1	A	158	HIS
1	A	175	GLN
1	A	202	GLN
1	B	5	GLN
1	B	39	GLN
1	B	150	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 ⓘ

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	290/303 (95%)	0.02	4 (1%) 72 77	44, 64, 100, 129	0
1	B	263/303 (86%)	0.11	10 (3%) 38 43	43, 75, 113, 127	0
All	All	553/606 (91%)	0.06	14 (2%) 54 61	43, 67, 108, 129	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	5.6
1	B	175	GLN	4.7
1	A	211	ARG	4.2
1	B	57	LYS	3.1
1	B	171	ARG	2.9
1	B	176	ARG	2.8
1	A	213	ALA	2.6
1	B	183	THR	2.4
1	B	49	GLY	2.4
1	B	60	ARG	2.3
1	A	214	ILE	2.2
1	B	177	HIS	2.1
1	B	59	CYS	2.1
1	A	212	ARG	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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.