



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:46 PM GMT

PDB ID : 3KD8  
Title : Cofactor-Independent Phosphoglycerate mutase from Thermoplasma Acidophilum DSM 1728  
Authors : Joachimiak, A.; Duke, N.E.C.; Marshall, N.; Buck, K.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2009-10-22  
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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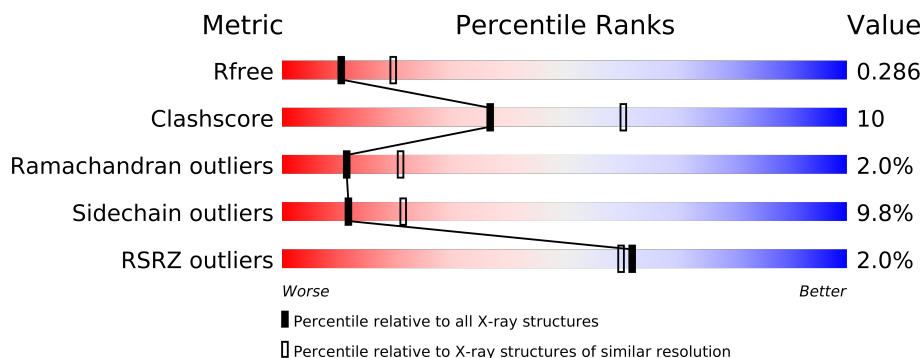
The following versions of software and data (see [references](#)) were used in the production of this report:

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	399	
1	B	399	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5761 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 2,3-bisphosphoglycerate-independent phosphoglycerate mutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	Se	0	0	0
			2817	1758	508	535	3	13			
1	B	365	Total	C	N	O	S	Se	0	0	0
			2799	1748	506	529	3	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9HL27
A	-1	ASN	-	expression tag	UNP Q9HL27
A	0	ALA	-	expression tag	UNP Q9HL27
B	-2	SER	-	expression tag	UNP Q9HL27
B	-1	ASN	-	expression tag	UNP Q9HL27
B	0	ALA	-	expression tag	UNP Q9HL27

- Molecule 2 is water.

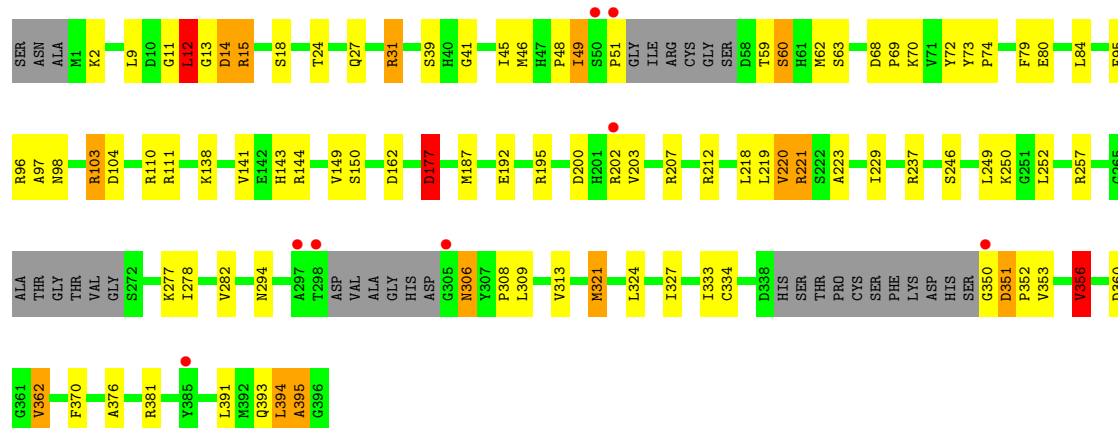
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		
2	B	70	Total	O	0	0
			70	70		

### 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 ( $\text{RSRZ} > 2$ ). 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.

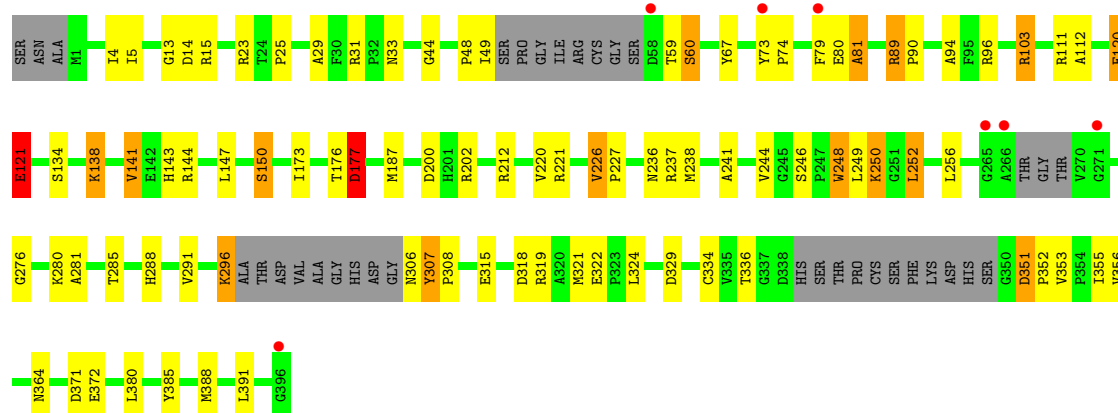
- Molecule 1: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase

Chain A: 



- Molecule 1: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.91Å 137.08Å 67.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.92 – 2.60 33.54 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (73.92-2.60) 99.9 (33.54-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.47 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.207 , 0.288 0.211 , 0.286	Depositor DCC
$R_{free}$ test set	1306 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 20.7	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 25666 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5761	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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	0.69	0/2856	0.82	5/3837 (0.1%)
1	B	0.69	1/2837 (0.0%)	0.80	1/3810 (0.0%)
All	All	0.69	1/5693 (0.0%)	0.81	6/7647 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356	VAL	CB-CG1	-6.00	1.40	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	195	ARG	CG-CD-NE	-5.64	99.97	111.80
1	A	356	VAL	CB-CA-C	-5.62	100.72	111.40
1	A	221	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	177	ASP	CB-CG-OD1	5.11	122.89	118.30
1	B	23	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	2817	0	2804	52	0
1	B	2799	0	2785	62	0
2	A	75	0	0	2	0
2	B	70	0	0	2	0
All	All	5761	0	5589	114	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 10.

All (114) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:80:GLU:HG3	1:B:96:ARG:HG2	1.41	1.03
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.23	1.02
1:A:149:VAL:HG21	1:A:187:MSE:HE1	1.42	1.00
1:A:80:GLU:HG3	1:A:96:ARG:HG2	1.44	0.96
1:A:14:ASP:O	1:A:15:ARG:HB2	1.66	0.94
1:B:103:ARG:HG3	1:B:103:ARG:HH11	1.32	0.91
1:B:120:GLU:O	1:B:121:GLU:HB2	1.72	0.90
1:B:249:LEU:O	1:B:250:LYS:HB2	1.71	0.89
1:A:278:ILE:O	1:A:282:VAL:HG23	1.74	0.88
1:B:249:LEU:O	1:B:250:LYS:CB	2.21	0.84
1:B:244:VAL:HG11	1:B:249:LEU:HB3	1.61	0.83
1:B:80:GLU:O	1:B:81:ALA:CB	2.29	0.81
1:B:244:VAL:HG11	1:B:249:LEU:CB	2.12	0.79
1:B:90:PRO:HA	1:B:226:VAL:HG22	1.65	0.78
1:A:80:GLU:HG3	1:A:96:ARG:CG	2.17	0.73
1:B:103:ARG:HD2	2:B:455:HOH:O	1.90	0.70
1:B:48:PRO:O	1:B:49:ILE:HB	1.90	0.69
1:B:80:GLU:HG3	1:B:96:ARG:CG	2.22	0.69
1:B:351:ASP:N	1:B:352:PRO:HD2	2.08	0.69
1:A:306:ASN:HD22	1:A:306:ASN:C	1.97	0.67
1:B:13:GLY:HA2	1:B:372:GLU:OE2	1.94	0.67
1:A:141:VAL:HG23	1:A:144:ARG:HH11	1.59	0.67
1:A:394:LEU:O	1:A:395:ALA:HB3	1.94	0.67
1:A:394:LEU:O	1:A:395:ALA:CB	2.43	0.67
1:B:238:MSE:HE1	1:B:388:MSE:SE	2.45	0.67
1:B:90:PRO:HB3	1:B:227:PRO:O	1.95	0.66
1:A:350:GLY:O	1:A:351:ASP:HB2	1.94	0.66
1:A:141:VAL:HG23	1:A:144:ARG:NH1	2.11	0.65
1:B:336:THR:HB	1:B:355:ILE:HG13	1.79	0.65
1:B:236:ASN:HB3	1:B:238:MSE:HE2	1.79	0.64
1:A:103:ARG:NH1	1:A:103:ARG:HG3	1.99	0.63
1:B:80:GLU:O	1:B:81:ALA:HB3	1.96	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:351:ASP:N	1:B:352:PRO:CD	2.63	0.62
1:A:149:VAL:CG2	1:A:187:MSE:HE1	2.24	0.61
1:A:321:MSE:HG2	1:A:324:LEU:HD12	1.84	0.60
1:B:319:ARG:NH1	2:B:432:HOH:O	2.37	0.57
1:A:31:ARG:NH1	1:A:370:PHE:O	2.37	0.57
1:B:241:ALA:HB2	1:B:288:HIS:CD2	2.40	0.56
1:B:244:VAL:HG11	1:B:249:LEU:HB2	1.85	0.56
1:B:334:CYS:HB2	1:B:391:LEU:HD21	1.87	0.56
1:B:176:THR:O	1:B:177:ASP:HB3	2.06	0.56
1:A:95:PHE:CD1	1:A:220:VAL:HG13	2.41	0.55
1:B:33:ASN:ND2	1:B:318:ASP:O	2.28	0.55
1:B:48:PRO:HB3	1:B:60:SER:OG	2.07	0.54
1:B:351:ASP:H	1:B:352:PRO:CD	2.22	0.53
1:B:296:LYS:CB	1:B:296:LYS:NZ	2.72	0.53
1:A:46:MSE:HE3	1:A:48:PRO:HG3	1.89	0.52
1:A:356:VAL:HG22	1:A:370:PHE:CE1	2.45	0.52
1:B:103:ARG:NH1	1:B:103:ARG:HG3	2.11	0.51
1:A:24:THR:OG1	1:A:27:GLN:HG3	2.10	0.51
1:A:59:THR:O	1:A:60:SER:HB2	2.10	0.51
1:A:98:ASN:OD1	1:A:221:ARG:NH2	2.43	0.51
1:A:324:LEU:HD22	1:A:333:ILE:HD12	1.92	0.51
1:A:327:ILE:HD11	1:A:333:ILE:HD11	1.91	0.51
1:A:277:LYS:NZ	1:A:294:ASN:O	2.43	0.51
1:B:173:ILE:HG13	1:B:187:MSE:HB3	1.92	0.51
1:B:5:ILE:HD12	1:B:281:ALA:HB1	1.94	0.50
1:A:2:LYS:HB2	1:A:395:ALA:HA	1.93	0.50
1:A:110:ARG:NH1	1:A:162:ASP:OD2	2.45	0.50
1:A:306:ASN:ND2	1:A:308:PRO:HD2	2.26	0.50
1:B:80:GLU:O	1:B:81:ALA:HB2	2.11	0.50
1:A:203:VAL:O	1:A:207:ARG:HG3	2.12	0.49
1:B:134:SER:OG	1:B:150:SER:HB2	2.12	0.49
1:B:385:TYR:O	1:B:385:TYR:CG	2.65	0.49
1:B:15:ARG:O	1:B:307:TYR:OH	2.24	0.49
1:B:94:ALA:HA	1:B:147:LEU:O	2.12	0.49
1:A:11:GLY:HA3	2:A:445:HOH:O	2.13	0.49
1:B:79:PHE:CE2	1:B:248:TRP:CD1	3.01	0.48
1:B:79:PHE:HE2	1:B:248:TRP:CD1	2.32	0.48
1:B:111:ARG:HD3	1:B:143:HIS:CE1	2.49	0.48
1:A:177:ASP:OD1	1:A:177:ASP:C	2.52	0.48
1:A:246:SER:HB2	1:A:249:LEU:HB2	1.97	0.47
1:B:5:ILE:HD13	1:B:291:VAL:HB	1.96	0.47
1:B:276:GLY:O	1:B:280:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:44:GLY:HA3	1:B:380:LEU:HB2	1.97	0.47
1:A:73:TYR:HA	1:A:74:PRO:HD3	1.71	0.47
1:A:104:ASP:N	2:A:463:HOH:O	2.28	0.46
1:A:95:PHE:CE1	1:A:223:ALA:HB2	2.51	0.46
1:B:138:LYS:HE2	1:B:138:LYS:HB2	1.75	0.46
1:B:296:LYS:HB3	1:B:296:LYS:HZ3	1.81	0.46
1:A:334:CYS:HB2	1:A:391:LEU:HD21	1.99	0.44
1:B:306:ASN:N	1:B:308:PRO:HD2	2.32	0.44
1:A:97:ALA:HB1	1:A:218:LEU:HD11	1.99	0.44
1:A:45:ILE:HG12	1:A:376:ALA:HA	2.00	0.44
1:A:68:ASP:HA	1:A:69:PRO:HD3	1.84	0.43
1:A:72:TYR:HD1	1:A:229:ILE:HD13	1.84	0.43
1:B:29:ALA:HB1	1:B:315:GLU:HG2	1.99	0.43
1:B:67:TYR:CZ	1:B:256:LEU:HD22	2.54	0.43
1:B:31:ARG:NH1	1:B:371:ASP:HB3	2.34	0.43
1:B:120:GLU:O	1:B:121:GLU:CB	2.55	0.43
1:A:391:LEU:O	1:A:394:LEU:O	2.36	0.43
1:A:306:ASN:ND2	1:A:306:ASN:C	2.69	0.42
1:A:111:ARG:HG2	1:A:143:HIS:CD2	2.54	0.42
1:B:252:LEU:HD22	1:B:256:LEU:HD11	2.02	0.42
1:A:80:GLU:CG	1:A:96:ARG:HE	2.33	0.42
1:B:226:VAL:HA	1:B:227:PRO:HD3	1.75	0.42
1:A:41:GLY:HA2	1:A:362:VAL:HG11	2.02	0.42
1:B:73:TYR:CD1	1:B:74:PRO:HD2	2.55	0.42
1:B:4:ILE:HD13	1:B:391:LEU:HB3	2.01	0.42
1:A:49:ILE:HD11	1:A:60:SER:HA	2.01	0.42
1:B:5:ILE:HD11	1:B:285:THR:CG2	2.51	0.41
1:A:12:LEU:HB3	1:A:13:GLY:H	1.74	0.41
1:A:351:ASP:N	1:A:352:PRO:HD2	2.35	0.41
1:A:203:VAL:O	1:A:207:ARG:CG	2.68	0.41
1:B:141:VAL:O	1:B:144:ARG:HB2	2.19	0.41
1:B:25:PRO:HD3	1:B:307:TYR:CE2	2.55	0.41
1:B:248:TRP:C	1:B:249:LEU:O	2.56	0.41
1:B:89:ARG:O	1:B:226:VAL:HG11	2.21	0.41
1:A:306:ASN:ND2	1:A:309:LEU:H	2.19	0.41
1:A:97:ALA:HA	1:A:219:LEU:O	2.21	0.41
1:B:73:TYR:HA	1:B:74:PRO:HD3	1.90	0.41
1:A:72:TYR:HB3	1:A:229:ILE:HD12	2.03	0.40
1:B:111:ARG:HG2	1:B:143:HIS:CD2	2.56	0.40
1:B:321:MSE:HB3	1:B:324:LEU:HD12	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	357/399 (90%)	334 (94%)	17 (5%)	6 (2%)	14	26
1	B	355/399 (89%)	334 (94%)	13 (4%)	8 (2%)	10	17
All	All	712/798 (89%)	668 (94%)	30 (4%)	14 (2%)	11	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	351	ASP
1	B	59	THR
1	B	81	ALA
1	B	121	GLU
1	A	12	LEU
1	A	49	ILE
1	A	395	ALA
1	A	15	ARG
1	B	112	ALA
1	B	250	LYS
1	B	14	ASP
1	B	177	ASP
1	B	351	ASP

### 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	307/318 (96%)	272 (89%)	35 (11%)	8	15
1	B	303/318 (95%)	278 (92%)	25 (8%)	16	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	610/636 (96%)	550 (90%)	60 (10%)	12	21

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	LEU
1	A	14	ASP
1	A	18	SER
1	A	31	ARG
1	A	39	SER
1	A	51	PRO
1	A	62	MSE
1	A	63	SER
1	A	70	LYS
1	A	79	PHE
1	A	84	LEU
1	A	103	ARG
1	A	138	LYS
1	A	150	SER
1	A	177	ASP
1	A	192	GLU
1	A	200	ASP
1	A	202	ARG
1	A	212	ARG
1	A	220	VAL
1	A	237	ARG
1	A	250	LYS
1	A	252	LEU
1	A	257	ARG
1	A	306	ASN
1	A	313	VAL
1	A	321	MSE
1	A	353	VAL
1	A	356	VAL
1	A	360	ASP
1	A	362	VAL
1	A	381	ARG
1	A	393	GLN
1	A	394	LEU
1	B	60	SER
1	B	89	ARG

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Mol	Chain	Res	Type
1	B	103	ARG
1	B	120	GLU
1	B	121	GLU
1	B	138	LYS
1	B	141	VAL
1	B	150	SER
1	B	177	ASP
1	B	200	ASP
1	B	202	ARG
1	B	212	ARG
1	B	220	VAL
1	B	221	ARG
1	B	226	VAL
1	B	237	ARG
1	B	246	SER
1	B	248	TRP
1	B	252	LEU
1	B	296	LYS
1	B	307	TYR
1	B	322	GLU
1	B	329	ASP
1	B	353	VAL
1	B	364	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	210	ASN
1	A	306	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	367/399 (91%)	-0.26	8 (2%) 59 56	17, 32, 48, 67	0
1	B	365/399 (91%)	-0.17	7 (1%) 64 61	17, 34, 50, 62	0
All	All	732/798 (91%)	-0.21	15 (2%) 62 60	17, 33, 49, 67	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	GLY	5.7
1	B	266	ALA	4.9
1	A	50	SER	4.6
1	B	396	GLY	3.5
1	A	51	PRO	3.3
1	B	265	GLY	3.3
1	B	79	PHE	3.2
1	A	202	ARG	2.9
1	A	305	GLY	2.8
1	A	298	THR	2.7
1	B	58	ASP	2.7
1	B	73	TYR	2.5
1	A	297	ALA	2.5
1	A	350	GLY	2.3
1	A	385	TYR	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.