



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 02:56 AM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

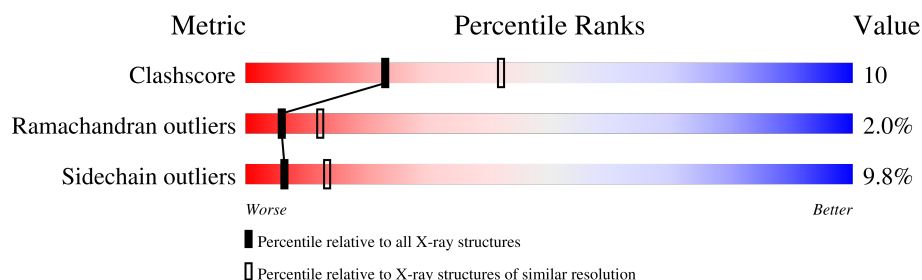
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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))
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS failed to run properly.

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 hydrogens and 0 are deuteriums.

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.

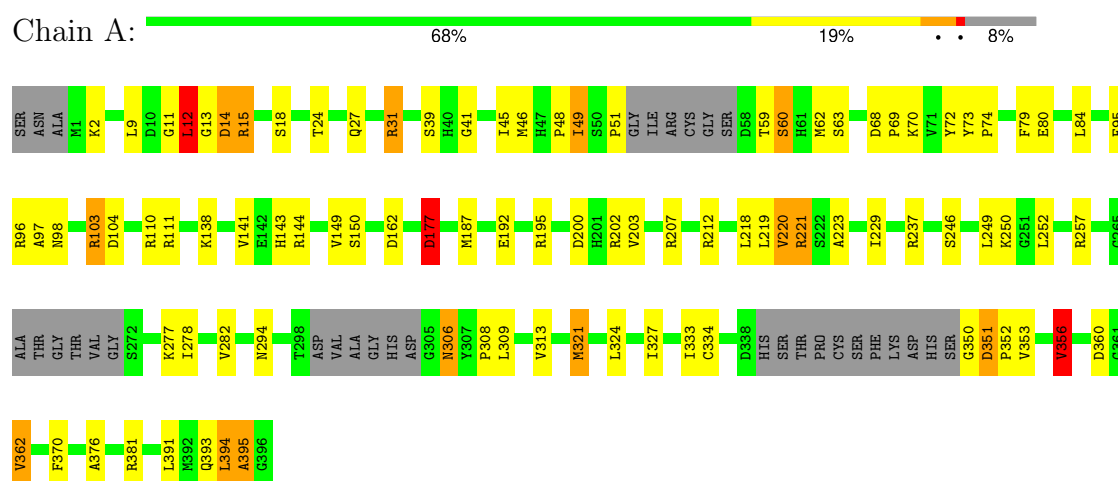
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		
2	B	70	Total	O	0	0
			70	70		

3 Residue-property plots

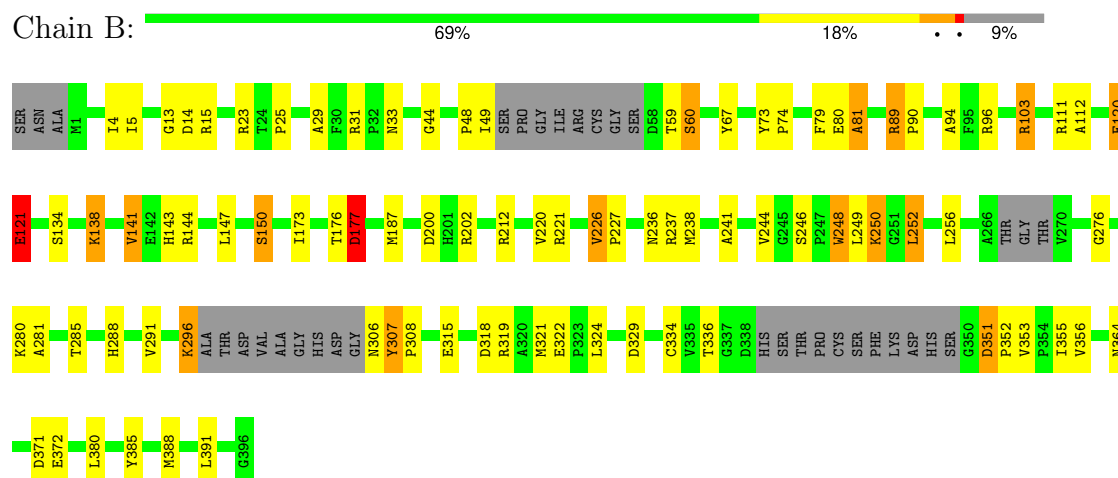
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

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



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



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.91Å 137.08Å 67.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.92 – 2.60	Depositor
% Data completeness (in resolution range)	99.8 (73.92-2.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.207 , 0.288	Depositor
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.523	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5761	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2817	0	2804	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:HH11	1:B:103:ARG:HG3	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:C	1:A:306:ASN:HD22	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:A:350:GLY:O	1:A:351:ASP:HB2	1.94	0.66
1:B:90:PRO:HB3	1:B:227:PRO:O	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HG3	1:A:103:ARG:NH1	1.99	0.63
1:B:80:GLU:O	1:B:81:ALA:HB3	1.96	0.63
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:HG3	1:B:103:ARG:NH1	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:CG	1:B:385:TYR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:GLY:HA3	1:B:380:LEU:HB2	1.97	0.47
1:B:276:GLY:O	1:B:280:LYS:HB2	2.15	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:HB2	1:B:138:LYS:HE2	1.75	0.46
1:B:296:LYS:HZ3	1:B:296:LYS:HB3	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:31:ARG:NH1	1:B:371:ASP:HB3	2.34	0.43
1:B:67:TYR:CZ	1:B:256:LEU:HD22	2.54	0.43
1:A:391:LEU:O	1:A:394:LEU:O	2.36	0.43
1:B:120:GLU:O	1:B:121:GLU:CB	2.55	0.43
1:A:306:ASN:C	1:A:306:ASN:ND2	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:A:12:LEU:HB3	1:A:13:GLY:H	1.74	0.41
1:B:5:ILE:HD11	1:B:285:THR:CG2	2.51	0.41
1:A:203:VAL:O	1:A:207:ARG:CG	2.68	0.41
1:A:351:ASP:N	1:A:352:PRO:HD2	2.35	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:A:97:ALA:HA	1:A:219:LEU:O	2.21	0.41
1:A:306:ASN:ND2	1:A:309:LEU:H	2.19	0.41
1:B:73:TYR:HA	1:B:74:PRO:HD3	1.90	0.41
1:B:89:ARG:O	1:B:226:VAL:HG11	2.21	0.41
1:A:72:TYR:HB3	1:A:229:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	7	16
1	B	355/399 (89%)	334 (94%)	13 (4%)	8 (2%)	5	10
All	All	712/798 (89%)	668 (94%)	30 (4%)	14 (2%)	6	12

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%)	4	9
1	B	303/318 (95%)	278 (92%)	25 (8%)	9	19
All	All	610/636 (96%)	550 (90%)	60 (10%)	6	13

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

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Mol	Chain	Res	Type
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
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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.