



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:39 PM GMT

PDB ID : 4A3S  
Title : Crystal structure of PFK from Bacillus subtilis  
Authors : Newman, J.A.; Hewitt, L.; Rodrigues, C.; Solovyova, A.S.; Harwood, C.R.;  
Lewis, R.J.  
Deposited on : 2011-10-04  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

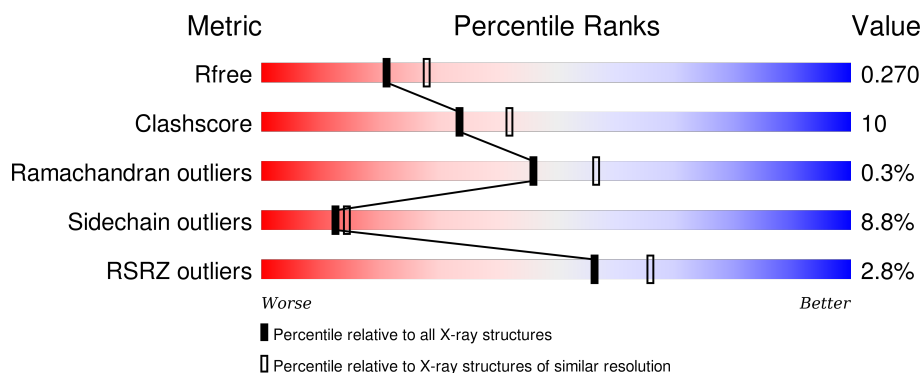
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	319	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 25%, green 72%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>72%</span> <span>25%</span> <span>.</span> </div> </div>
1	B	319	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 24%, green 74%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>74%</span> <span>24%</span> <span>.</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4992 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 6-PHOSPHOFRUCTOKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2407	1508	429	461	9			
1	B	319	Total	C	N	O	S	0	0	0
			2407	1508	429	461	9			

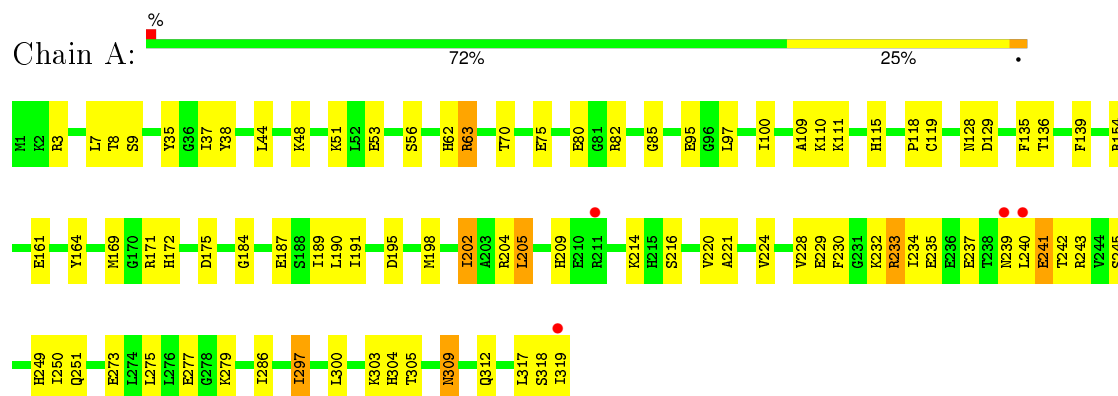
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	84	Total	O	0	0
			84	84		

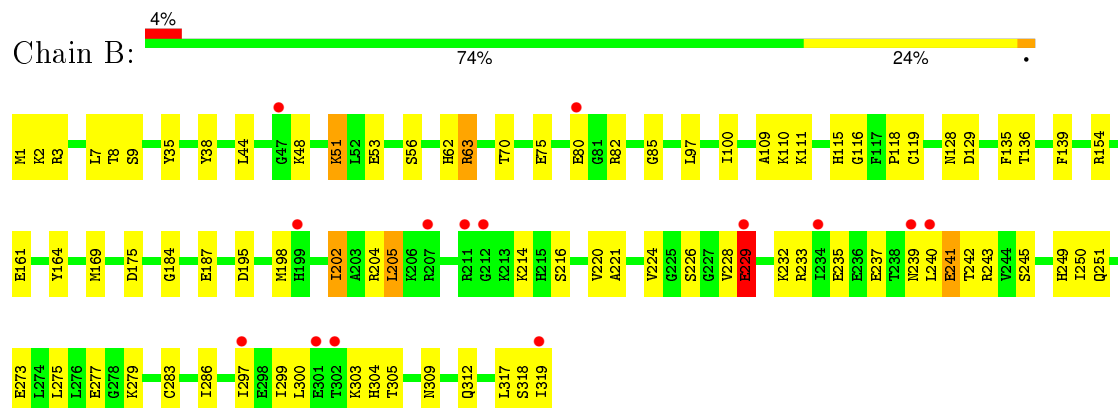
### 3 Residue-property plots

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: 6-PHOSPHOFRUCTOKINASE



#### • Molecule 1: 6-PHOSPHOFRUCTOKINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.43Å 77.01Å 101.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.74 – 2.30 45.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.74-2.30) 79.6 (45.74-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.229 , 0.276 0.223 , 0.270	Depositor DCC
$R_{free}$ test set	1814 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.878	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.3	EDS
Estimated twinning fraction	0.084 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 43601 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.64 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.3156e-03.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	0/2441	0.61	3/3286 (0.1%)
1	B	0.53	0/2441	0.63	3/3286 (0.1%)
All	All	0.51	0/4882	0.62	6/6572 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	205	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	63	ARG	CB-CG-CD	5.26	125.27	111.60
1	B	63	ARG	CB-CG-CD	5.21	125.13	111.60
1	B	229	GLU	CA-CB-CG	5.07	124.56	113.40
1	A	63	ARG	CG-CD-NE	-5.02	101.26	111.80

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	2407	0	2444	52	0
1	B	2407	0	2444	47	0
2	A	94	0	0	5	0
2	B	84	0	0	2	0
All	All	4992	0	4888	99	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 (99) 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:A:129:ASP:HA	1:A:304:HIS:CD2	2.03	0.94
1:B:129:ASP:HA	1:B:304:HIS:CD2	2.06	0.90
1:B:38:TYR:HB2	1:B:48:LYS:HG2	1.61	0.82
1:A:38:TYR:HB2	1:A:48:LYS:HG2	1.64	0.78
1:A:204:ARG:NH1	1:A:318:SER:OG	2.24	0.70
1:A:154:ARG:NH2	1:A:184:GLY:O	2.29	0.66
1:A:129:ASP:HA	1:A:304:HIS:HD2	1.60	0.65
1:A:161:GLU:OE2	1:A:214:LYS:HG3	1.96	0.65
1:B:161:GLU:OE2	1:B:214:LYS:HG3	1.97	0.65
1:B:154:ARG:NH2	1:B:184:GLY:O	2.30	0.65
1:B:204:ARG:NH1	1:B:318:SER:OG	2.31	0.64
1:B:169:MET:HE1	1:B:249:HIS:HA	1.81	0.62
1:A:171:ARG:HB3	2:A:2046:HOH:O	1.99	0.61
1:A:221:ALA:O	1:A:224:VAL:HG22	2.02	0.60
1:A:169:MET:HE1	1:A:249:HIS:HA	1.81	0.60
1:B:129:ASP:HA	1:B:304:HIS:HD2	1.65	0.60
1:A:129:ASP:HA	1:A:304:HIS:NE2	2.17	0.59
1:A:171:ARG:HD2	2:A:2046:HOH:O	2.02	0.58
1:A:309:ASN:HB2	2:A:2094:HOH:O	2.05	0.56
1:B:161:GLU:HB3	1:B:214:LYS:HB3	1.86	0.56
1:B:129:ASP:HA	1:B:304:HIS:NE2	2.21	0.56
1:B:128:ASN:OD1	1:B:135:PHE:HA	2.06	0.55
1:A:128:ASN:OD1	1:A:135:PHE:HA	2.06	0.55
1:A:9:SER:HA	1:A:70:THR:OG1	2.06	0.55
1:B:53:GLU:O	1:B:56:SER:HB2	2.07	0.55
1:A:161:GLU:HB3	1:A:214:LYS:HB3	1.89	0.54
1:B:221:ALA:O	1:B:224:VAL:HG22	2.08	0.53
1:B:9:SER:HA	1:B:70:THR:OG1	2.09	0.53
1:B:62:HIS:CE1	1:B:63:ARG:CZ	2.92	0.53
1:B:1:MET:N	2:B:2001:HOH:O	2.27	0.52
1:A:233:ARG:O	1:A:233:ARG:HG3	2.10	0.52
1:A:63:ARG:NH1	2:A:2027:HOH:O	2.44	0.51
1:B:128:ASN:HA	1:B:136:THR:OG1	2.10	0.51
1:A:129:ASP:CA	1:A:304:HIS:HD2	2.23	0.51
1:B:228:VAL:O	1:B:232:LYS:HG3	2.11	0.51
1:B:187:GLU:HG2	1:B:216:SER:HB3	1.91	0.51
1:A:7:LEU:C	1:A:7:LEU:HD12	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:HA	1:A:100:ILE:O	2.10	0.51
1:A:128:ASN:HB2	1:A:139:PHE:CD1	2.46	0.50
1:A:62:HIS:CE1	1:A:63:ARG:CZ	2.95	0.50
1:B:226:SER:O	1:B:229:GLU:HB2	2.12	0.49
1:A:209:HIS:HB2	2:A:2077:HOH:O	2.12	0.49
1:A:187:GLU:HG2	1:A:216:SER:HB3	1.95	0.48
1:A:164:TYR:CE2	1:A:243:ARG:HB2	2.49	0.48
1:A:128:ASN:HA	1:A:136:THR:OG1	2.14	0.48
1:A:35:TYR:CZ	1:A:51:LYS:HG3	2.49	0.48
1:B:233:ARG:HG3	1:B:233:ARG:O	2.13	0.47
1:A:228:VAL:O	1:A:232:LYS:HG3	2.15	0.47
1:B:82:ARG:CZ	1:B:115:HIS:HE1	2.28	0.47
1:A:273:GLU:O	1:A:277:GLU:HB2	2.15	0.47
1:B:35:TYR:CZ	1:B:51:LYS:HG3	2.50	0.47
1:B:2:LYS:HA	1:B:2:LYS:HD2	1.74	0.47
1:B:7:LEU:C	1:B:7:LEU:HD12	2.35	0.47
1:A:53:GLU:O	1:A:56:SER:HB2	2.15	0.46
1:B:202:ILE:O	1:B:205:LEU:HB3	2.15	0.46
1:B:44:LEU:O	1:B:85:GLY:HA2	2.16	0.46
1:A:202:ILE:O	1:A:205:LEU:HB3	2.16	0.46
1:A:82:ARG:CZ	1:A:115:HIS:HE1	2.28	0.46
1:B:8:THR:HA	1:B:100:ILE:O	2.16	0.46
1:B:128:ASN:HB2	1:B:139:PHE:CD1	2.51	0.45
1:A:95:GLU:O	1:A:118:PRO:HD2	2.17	0.45
1:B:3:ARG:HD3	1:B:35:TYR:CE1	2.51	0.45
1:A:275:LEU:C	1:A:277:GLU:H	2.19	0.45
1:B:129:ASP:CA	1:B:304:HIS:HD2	2.29	0.44
1:A:171:ARG:HB3	1:A:172:HIS:H	1.59	0.44
1:B:273:GLU:O	1:B:277:GLU:HB2	2.17	0.44
1:A:286:ILE:HG23	1:A:286:ILE:O	2.18	0.44
1:A:304:HIS:ND1	1:A:305:THR:N	2.65	0.44
1:A:202:ILE:HD12	1:A:237:GLU:HB2	2.00	0.44
1:B:198:MET:N	2:B:2062:HOH:O	2.41	0.44
1:A:250:ILE:HG13	1:A:251:GLN:N	2.32	0.43
1:B:164:TYR:CE2	1:B:243:ARG:HB2	2.52	0.43
1:A:97:LEU:HB2	1:A:119:CYS:SG	2.57	0.43
1:A:44:LEU:O	1:A:85:GLY:HA2	2.17	0.43
1:B:250:ILE:HG13	1:B:251:GLN:N	2.33	0.43
1:B:109:ALA:O	1:B:119:CYS:HB2	2.19	0.43
1:A:198:MET:O	1:A:202:ILE:HG12	2.19	0.42
1:B:304:HIS:ND1	1:B:305:THR:N	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:HIS:H	1:B:62:HIS:CD2	2.37	0.42
1:B:202:ILE:HD12	1:B:237:GLU:HB2	2.02	0.42
1:B:62:HIS:HE1	1:B:63:ARG:NH2	2.17	0.42
1:A:190:LEU:N	1:A:190:LEU:HD12	2.35	0.42
1:B:275:LEU:C	1:B:277:GLU:H	2.23	0.42
1:A:62:HIS:CD2	1:A:62:HIS:H	2.38	0.42
1:A:3:ARG:HD3	1:A:35:TYR:CE1	2.55	0.42
1:B:82:ARG:CZ	1:B:115:HIS:CE1	3.03	0.42
1:A:230:PHE:O	1:A:234:ILE:HG13	2.20	0.42
1:A:297:ILE:HD12	1:A:297:ILE:HA	1.74	0.42
1:B:97:LEU:HB2	1:B:119:CYS:SG	2.61	0.41
1:B:283:CYS:SG	1:B:299:ILE:HD11	2.60	0.41
1:B:286:ILE:HG23	1:B:286:ILE:O	2.21	0.41
1:A:7:LEU:HB3	1:A:37:ILE:HB	2.03	0.41
1:A:82:ARG:CZ	1:A:115:HIS:CE1	3.03	0.41
1:B:62:HIS:HE1	1:B:63:ARG:CZ	2.34	0.41
1:B:240:LEU:O	1:B:241:GLU:C	2.58	0.41
1:A:109:ALA:O	1:A:119:CYS:HB2	2.21	0.40
1:A:240:LEU:O	1:A:241:GLU:C	2.59	0.40
1:A:189:ILE:HG22	1:A:191:ILE:HG23	2.03	0.40
1:B:116:GLY:O	1:B:118:PRO:HD3	2.22	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	317/319 (99%)	301 (95%)	15 (5%)	1 (0%)	46	57
1	B	317/319 (99%)	299 (94%)	17 (5%)	1 (0%)	46	57
All	All	634/638 (99%)	600 (95%)	32 (5%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	GLU
1	B	241	GLU

### 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	251/251 (100%)	229 (91%)	22 (9%)	12	14
1	B	251/251 (100%)	229 (91%)	22 (9%)	12	14
All	All	502/502 (100%)	458 (91%)	44 (9%)	12	14

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

Mol	Chain	Res	Type
1	A	75	GLU
1	A	80	GLU
1	A	110	LYS
1	A	111	LYS
1	A	175	ASP
1	A	195	ASP
1	A	202	ILE
1	A	220	VAL
1	A	229	GLU
1	A	233	ARG
1	A	235	GLU
1	A	239	ASN
1	A	242	THR
1	A	245	SER
1	A	279	LYS
1	A	297	ILE
1	A	300	LEU
1	A	303	LYS
1	A	309	ASN
1	A	312	GLN
1	A	317	LEU

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Mol	Chain	Res	Type
1	A	319	ILE
1	B	51	LYS
1	B	75	GLU
1	B	80	GLU
1	B	110	LYS
1	B	111	LYS
1	B	175	ASP
1	B	195	ASP
1	B	202	ILE
1	B	220	VAL
1	B	229	GLU
1	B	235	GLU
1	B	239	ASN
1	B	242	THR
1	B	245	SER
1	B	279	LYS
1	B	297	ILE
1	B	300	LEU
1	B	303	LYS
1	B	309	ASN
1	B	312	GLN
1	B	317	LEU
1	B	319	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	115	HIS
1	A	287	GLN
1	A	308	GLN
1	A	312	GLN
1	B	62	HIS
1	B	115	HIS
1	B	172	HIS
1	B	287	GLN
1	B	308	GLN
1	B	312	GLN

### 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 carbohydrates 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	319/319 (100%)	0.06	4 (1%) 79 84	15, 34, 79, 96	0
1	B	319/319 (100%)	0.08	14 (4%) 38 47	18, 35, 79, 96	0
All	All	638/638 (100%)	0.07	18 (2%) 56 66	15, 35, 79, 96	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	LEU	6.9
1	A	319	ILE	6.3
1	B	212	GLY	4.3
1	B	240	LEU	3.7
1	B	199	HIS	3.6
1	A	239	ASN	3.4
1	B	234	ILE	3.1
1	B	80	GLU	3.1
1	B	319	ILE	2.8
1	B	229	GLU	2.5
1	A	211	ARG	2.5
1	B	207	ARG	2.4
1	B	211	ARG	2.4
1	B	239	ASN	2.2
1	B	47	GLY	2.2
1	B	301	GLU	2.2
1	B	297	ILE	2.0
1	B	302	THR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.