



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:34 PM GMT

PDB ID : 1BIA  
Title : THE E. COLI BIOTIN HOLOENZYME SYNTHETASE(SLASH)BIO RE-PRESSOR CRYSTAL STRUCTURE DELINEATES THE BIOTIN AND DNA-BINDING DOMAINS  
Authors : Wilson, K.P.; Shewchuk, L.M.; Matthews, B.W.  
Deposited on : 1992-07-06  
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

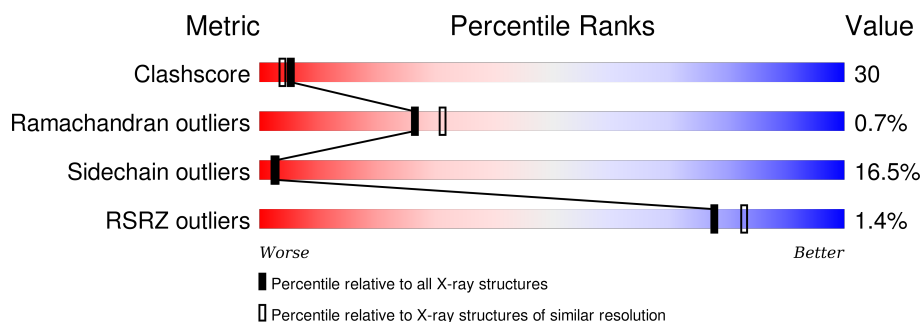
# 1 Overall quality at a glance

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))
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	321	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2244 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 BirA BIFUNCTIONAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2201	1411	381	401	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	43	Total	O	0	0
			43	43		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.00 Å 114.00 Å 60.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30 19.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 69.9 (19.45-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.30 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.190 , (Not available) 0.183 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 104.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 12667 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 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	0.99	13/2231 (0.6%)	1.38	23/3016 (0.8%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	GLU	CD-OE1	7.04	1.33	1.25
1	A	256	GLU	CD-OE2	6.52	1.32	1.25
1	A	313	GLU	CD-OE1	6.43	1.32	1.25
1	A	159	GLU	CD-OE1	6.25	1.32	1.25
1	A	251	GLU	CD-OE1	6.05	1.32	1.25
1	A	62	GLU	CD-OE2	6.01	1.32	1.25
1	A	190	GLU	CD-OE2	5.88	1.32	1.25
1	A	228	GLU	CD-OE2	5.86	1.32	1.25
1	A	110	GLU	CD-OE1	5.82	1.32	1.25
1	A	266	GLU	CD-OE1	5.77	1.31	1.25
1	A	254	GLU	CD-OE2	5.62	1.31	1.25
1	A	245	GLU	CD-OE1	5.44	1.31	1.25
1	A	23	GLU	CD-OE1	5.35	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	182	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	290	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	105	ASP	CB-CG-OD1	-7.15	111.87	118.30
1	A	170	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	269	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	49	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	282	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	96	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	A	269	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	167	ASP	CB-CG-OD2	-6.37	112.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	49	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	105	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	44	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	282	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	3	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	138	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	234	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	167	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	235	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	182	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	147	ILE	C-N-CA	-5.04	111.72	122.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2201	0	2257	134	0
2	A	43	0	0	6	0
All	All	2244	0	2257	134	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 30.

All (134) 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:53:VAL:HG13	1:A:56:LYS:HB2	1.34	1.09
1:A:276:VAL:HG21	1:A:314:ILE:HD11	1.37	1.02
1:A:23:GLU:HG3	1:A:33:ARG:HH21	1.21	0.99
1:A:277:LYS:HE3	1:A:284:GLU:HG2	1.49	0.92
1:A:301:GLU:HB2	1:A:306:ILE:HG12	1.55	0.88
1:A:53:VAL:CG1	1:A:56:LYS:HB2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.57	0.86
1:A:113:GLN:HE21	1:A:113:GLN:HA	1.39	0.85
1:A:316:LEU:HD12	1:A:317:ARG:N	1.92	0.85
1:A:70:LYS:HA	1:A:70:LYS:HE2	1.61	0.83
1:A:208:ASN:HB3	1:A:225:THR:HG22	1.62	0.81
1:A:316:LEU:HD12	1:A:317:ARG:H	1.44	0.80
1:A:317:ARG:HH11	1:A:317:ARG:HG2	1.47	0.78
1:A:65:GLN:HE22	1:A:234:ASP:HA	1.49	0.77
1:A:34:ALA:O	1:A:38:LYS:HG2	1.84	0.77
1:A:23:GLU:HG3	1:A:33:ARG:NH2	1.97	0.76
1:A:276:VAL:HG21	1:A:314:ILE:CD1	2.17	0.73
1:A:53:VAL:HG22	1:A:56:LYS:HG3	1.72	0.72
1:A:69:ALA:O	1:A:73:LEU:HD12	1.91	0.70
1:A:70:LYS:NZ	1:A:70:LYS:HB3	2.07	0.70
1:A:147:ILE:O	1:A:148:GLY:C	2.26	0.69
1:A:276:VAL:CG2	1:A:314:ILE:HD11	2.20	0.68
1:A:65:GLN:C	1:A:66:LEU:HD12	2.15	0.67
1:A:313:GLU:HA	2:A:335:HOH:O	1.95	0.67
1:A:182:ARG:NH1	1:A:223:TRP:O	2.27	0.67
1:A:23:GLU:N	1:A:23:GLU:OE1	2.28	0.66
1:A:146:ALA:O	1:A:149:LEU:N	2.30	0.65
1:A:280:ILE:HD12	1:A:311:GLY:O	1.97	0.64
1:A:42:THR:O	1:A:45:ASP:N	2.29	0.64
1:A:146:ALA:O	1:A:147:ILE:C	2.34	0.64
1:A:149:LEU:O	1:A:149:LEU:HD12	1.98	0.64
1:A:33:ARG:HB3	1:A:33:ARG:NH1	2.13	0.63
1:A:93:TYR:O	1:A:97:ARG:HD2	1.98	0.62
1:A:23:GLU:CG	1:A:33:ARG:HH21	2.06	0.62
1:A:33:ARG:HB3	1:A:33:ARG:HH11	1.65	0.61
1:A:153:ILE:HD11	1:A:250:LEU:HD11	1.82	0.60
1:A:277:LYS:HE3	1:A:284:GLU:CG	2.29	0.60
1:A:35:ALA:O	1:A:38:LYS:N	2.36	0.59
1:A:19:PHE:CE1	1:A:53:VAL:HG12	2.37	0.58
1:A:113:GLN:CA	1:A:113:GLN:HE21	2.04	0.58
1:A:8:LEU:O	1:A:11:ILE:HG22	2.04	0.58
1:A:53:VAL:CG2	1:A:56:LYS:HG3	2.35	0.57
1:A:23:GLU:H	1:A:23:GLU:CD	2.09	0.56
1:A:55:GLY:C	1:A:56:LYS:HG2	2.24	0.56
1:A:26:GLY:O	1:A:30:GLY:N	2.39	0.56
1:A:55:GLY:O	1:A:56:LYS:HG2	2.06	0.55
1:A:133:LEU:HD23	1:A:133:LEU:C	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HA	1:A:297:ALA:O	2.07	0.54
1:A:149:LEU:C	1:A:149:LEU:HD12	2.26	0.54
1:A:287:GLY:H	1:A:317:ARG:HH12	1.53	0.54
1:A:48:VAL:HG12	1:A:49:ASP:N	2.23	0.53
1:A:4:ASN:HB2	2:A:362:HOH:O	2.08	0.53
1:A:280:ILE:HG22	1:A:285:ILE:CD1	2.38	0.52
1:A:162:ARG:HH22	1:A:170:ARG:NH1	2.08	0.52
1:A:53:VAL:O	1:A:53:VAL:HG13	2.08	0.52
1:A:3:ASP:OD1	1:A:5:THR:OG1	2.28	0.51
1:A:280:ILE:HG22	1:A:285:ILE:HD13	1.92	0.51
1:A:264:ARG:O	1:A:265:TRP:C	2.48	0.51
1:A:162:ARG:NH2	1:A:170:ARG:NH1	2.59	0.51
1:A:271:PHE:HA	1:A:274:ARG:HD3	1.92	0.51
1:A:36:ILE:O	1:A:37:ASN:C	2.47	0.51
1:A:66:LEU:HD12	1:A:66:LEU:N	2.26	0.51
1:A:271:PHE:HB2	2:A:355:HOH:O	2.12	0.50
1:A:62:GLU:HG2	1:A:63:PRO:HD2	1.93	0.50
1:A:65:GLN:HE22	1:A:234:ASP:CA	2.22	0.50
1:A:70:LYS:HA	1:A:70:LYS:CE	2.38	0.49
1:A:18:GLU:O	1:A:59:SER:HB2	2.12	0.49
1:A:302:GLN:N	1:A:305:ILE:O	2.45	0.49
1:A:317:ARG:NH1	1:A:317:ARG:HG2	2.21	0.49
1:A:145:ALA:O	1:A:148:GLY:N	2.46	0.48
1:A:40:ILE:HG22	1:A:41:GLN:N	2.27	0.48
1:A:149:LEU:O	1:A:153:ILE:HG12	2.13	0.48
1:A:141:GLN:O	1:A:143:PRO:N	2.46	0.48
1:A:19:PHE:CE1	1:A:53:VAL:CG1	2.97	0.48
1:A:70:LYS:NZ	1:A:70:LYS:CB	2.77	0.47
1:A:8:LEU:HA	1:A:11:ILE:HG22	1.95	0.47
1:A:42:THR:O	1:A:43:LEU:C	2.51	0.47
1:A:19:PHE:CZ	1:A:53:VAL:HG11	2.50	0.47
1:A:33:ARG:CB	1:A:33:ARG:CZ	2.92	0.47
1:A:173:TRP:HA	1:A:174:PRO:HA	1.68	0.47
1:A:88:ASP:HB2	2:A:346:HOH:O	2.15	0.47
1:A:144:ALA:O	1:A:145:ALA:HB2	2.15	0.47
1:A:162:ARG:HH22	1:A:170:ARG:HH12	1.64	0.46
1:A:62:GLU:O	1:A:64:ILE:HG23	2.16	0.46
1:A:203:ILE:HG22	1:A:204:GLY:N	2.30	0.46
1:A:33:ARG:CZ	1:A:33:ARG:HB2	2.45	0.46
1:A:259:ALA:N	1:A:260:PRO:CD	2.79	0.46
1:A:4:ASN:O	1:A:7:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:CZ	1:A:53:VAL:CG1	3.00	0.45
1:A:286:PHE:N	1:A:286:PHE:CD1	2.83	0.45
1:A:171:VAL:HG21	1:A:265:TRP:CZ3	2.52	0.45
1:A:81:VAL:CG1	1:A:108:ILE:HD11	2.47	0.45
1:A:131:LEU:HD12	1:A:132:TYR:N	2.31	0.45
1:A:182:ARG:NH1	1:A:224:ILE:HG13	2.32	0.44
1:A:168:LYS:HB2	1:A:168:LYS:HE3	1.79	0.44
1:A:91:ASN:O	1:A:95:LEU:HG	2.18	0.44
1:A:168:LYS:NZ	1:A:180:GLN:HG3	2.32	0.44
1:A:65:GLN:NE2	1:A:234:ASP:OD1	2.50	0.44
1:A:168:LYS:HZ2	1:A:180:GLN:HG3	1.82	0.44
1:A:203:ILE:N	1:A:203:ILE:HD12	2.33	0.44
1:A:103:SER:HB3	1:A:137:TRP:CE3	2.53	0.44
1:A:317:ARG:NH1	1:A:317:ARG:CG	2.79	0.44
1:A:113:GLN:CA	1:A:113:GLN:NE2	2.77	0.44
1:A:280:ILE:CG2	1:A:285:ILE:HD13	2.48	0.44
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.84	0.43
1:A:92:GLN:HA	1:A:95:LEU:HB2	2.00	0.43
1:A:139:LEU:HD23	1:A:254:GLU:HG3	1.99	0.43
1:A:92:GLN:O	1:A:93:TYR:C	2.56	0.43
1:A:30:GLY:O	1:A:31:MET:HB3	2.18	0.43
1:A:48:VAL:CG1	1:A:49:ASP:N	2.79	0.43
1:A:134:SER:HA	1:A:203:ILE:O	2.18	0.43
1:A:5:THR:O	1:A:9:LYS:HG3	2.19	0.42
1:A:307:LYS:HB2	1:A:308:PRO:CD	2.50	0.42
1:A:244:ARG:HH11	1:A:244:ARG:HD3	1.72	0.42
1:A:1:MET:CG	1:A:2:LYS:N	2.82	0.42
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.34	0.42
1:A:89:SER:OG	1:A:92:GLN:HB2	2.20	0.42
1:A:36:ILE:HA	1:A:36:ILE:HD12	1.78	0.41
1:A:66:LEU:O	1:A:67:LEU:C	2.55	0.41
1:A:92:GLN:NE2	1:A:96:ASP:OD2	2.53	0.41
1:A:182:ARG:CZ	1:A:224:ILE:HG13	2.50	0.41
1:A:41:GLN:O	1:A:44:ARG:HB2	2.19	0.41
1:A:10:LEU:HD21	1:A:40:ILE:HD12	2.02	0.41
1:A:301:GLU:HG2	1:A:301:GLU:O	2.19	0.41
1:A:60:LEU:N	2:A:364:HOH:O	2.37	0.41
1:A:11:ILE:O	1:A:11:ILE:HG13	2.19	0.41
1:A:13:LEU:HA	1:A:13:LEU:HD23	1.68	0.41
1:A:49:ASP:HB3	1:A:61:PRO:CG	2.51	0.41
1:A:180:GLN:N	2:A:354:HOH:O	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HB2	1:A:308:PRO:HD2	2.03	0.40
1:A:280:ILE:CG2	1:A:285:ILE:CD1	2.99	0.40
1:A:97:ARG:O	1:A:98:ILE:C	2.57	0.40
1:A:103:SER:HB3	1:A:137:TRP:CD2	2.56	0.40
1:A:307:LYS:CB	1:A:308:PRO:CD	3.00	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	282/321 (88%)	259 (92%)	21 (7%)	2 (1%)	26	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	PRO
1	A	145	ALA

### 5.3.2 Protein sidechains [i](#)

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	224/258 (87%)	187 (84%)	37 (16%)	3	2

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	23	GLU
1	A	28	THR
1	A	33	ARG
1	A	36	ILE
1	A	38	LYS
1	A	40	ILE
1	A	49	ASP
1	A	52	THR
1	A	64	ILE
1	A	70	LYS
1	A	75	GLN
1	A	80	SER
1	A	89	SER
1	A	92	GLN
1	A	98	ILE
1	A	100	GLU
1	A	113	GLN
1	A	125	SER
1	A	149	LEU
1	A	150	SER
1	A	168	LYS
1	A	170	ARG
1	A	172	LYS
1	A	191	LEU
1	A	200	GLN
1	A	224	ILE
1	A	247	ARG
1	A	277	LYS
1	A	284	GLU
1	A	295	GLN
1	A	302	GLN
1	A	307	LYS
1	A	313	GLU
1	A	314	ILE
1	A	315	SER
1	A	317	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	92	GLN
1	A	113	GLN
1	A	200	GLN
1	A	302	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	292/321 (90%)	-0.39	4 (1%) 78 83	21, 48, 93, 100	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.3
1	A	78	GLY	2.1
1	A	16	ASN	2.1
1	A	53	VAL	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.