



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:01 PM GMT

PDB ID : 1TLQ  
Title : Crystal structure of protein ypjQ from Bacillus subtilis, Pfam DUF64  
Authors : Kniewel, R.; Rajashankar, K.R.; Solorzano, V.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2004-06-09  
Resolution : 2.40 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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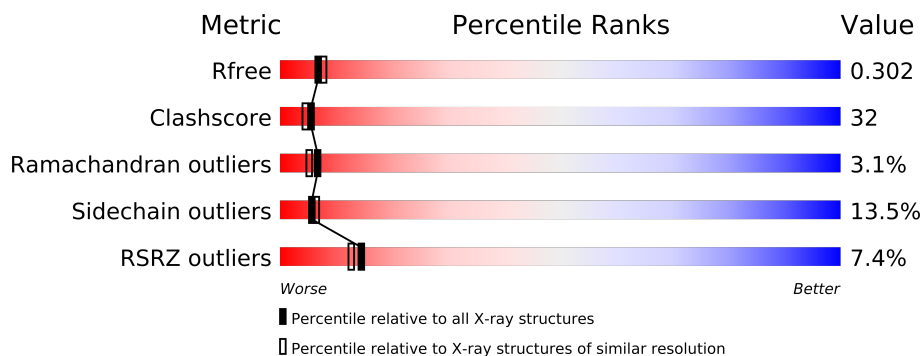
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	189	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1287 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 Hypothetical protein ypjQ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	Se	0	0	0
			1262	803	208	245	1	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CLONING ARTIFACT	UNP P54173
A	2	SER	-	CLONING ARTIFACT	UNP P54173
A	3	LEU	-	CLONING ARTIFACT	UNP P54173
A	8	MSE	MET	MODIFIED RESIDUE	UNP P54173
A	11	MSE	MET	MODIFIED RESIDUE	UNP P54173
A	18	MSE	MET	MODIFIED RESIDUE	UNP P54173
A	25	MSE	MET	MODIFIED RESIDUE	UNP P54173
A	50	MSE	MET	MODIFIED RESIDUE	UNP P54173
A	180	GLU	-	EXPRESSION TAG	UNP P54173
A	181	GLY	-	EXPRESSION TAG	UNP P54173
A	182	GLY	-	EXPRESSION TAG	UNP P54173
A	183	SER	-	EXPRESSION TAG	UNP P54173
A	184	HIS	-	EXPRESSION TAG	UNP P54173
A	185	HIS	-	EXPRESSION TAG	UNP P54173
A	186	HIS	-	EXPRESSION TAG	UNP P54173
A	187	HIS	-	EXPRESSION TAG	UNP P54173
A	188	HIS	-	EXPRESSION TAG	UNP P54173
A	189	HIS	-	EXPRESSION TAG	UNP P54173

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

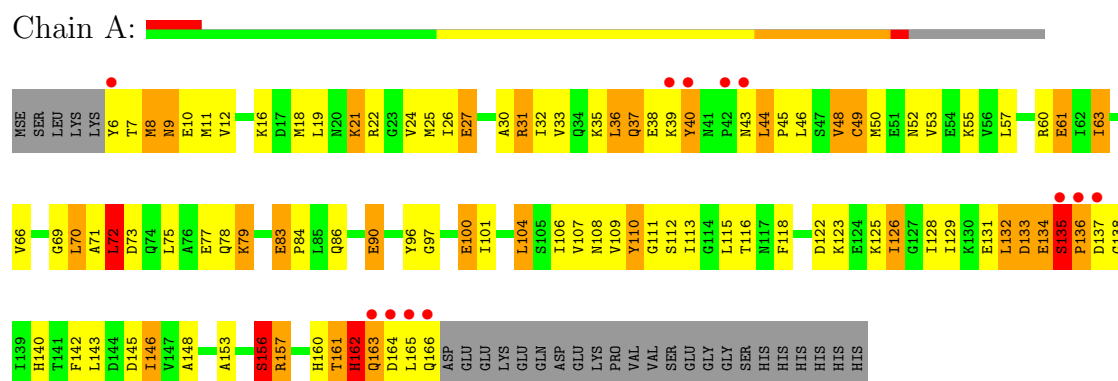
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	0	0

### 3 Residue-property plots i

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: Hypothetical protein ypjQ



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.11Å 118.11Å 65.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.40) 99.8 (19.69-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.34 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.232 , 0.295 0.250 , 0.302	Depositor DCC
$R_{free}$ test set	529 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 31.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 10999 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	1287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	2.04	35/1275 (2.7%)	1.74	26/1721 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CD-OE1	11.69	1.38	1.25
1	A	110	TYR	CE1-CZ	9.45	1.50	1.38
1	A	108	ASN	C-O	9.01	1.40	1.23
1	A	110	TYR	CD2-CE2	8.93	1.52	1.39
1	A	96	TYR	CG-CD2	7.58	1.49	1.39
1	A	100	GLU	CD-OE2	7.19	1.33	1.25
1	A	83	GLU	CD-OE1	6.87	1.33	1.25
1	A	25	MSE	CB-CG	6.70	1.72	1.52
1	A	48	VAL	CB-CG1	6.39	1.66	1.52
1	A	22	ARG	CZ-NH1	6.29	1.41	1.33
1	A	24	VAL	CB-CG2	6.23	1.66	1.52
1	A	31	ARG	CG-CD	6.13	1.67	1.51
1	A	118	PHE	CG-CD2	5.90	1.47	1.38
1	A	100	GLU	CD-OE1	5.80	1.32	1.25
1	A	112	SER	CA-C	-5.74	1.38	1.52
1	A	11	MSE	SE-CE	-5.67	1.61	1.95
1	A	156	SER	CA-CB	5.66	1.61	1.52
1	A	61	GLU	CD-OE2	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	LYS	CD-CE	5.58	1.65	1.51
1	A	109	VAL	CA-CB	-5.49	1.43	1.54
1	A	6	TYR	CD1-CE1	5.47	1.47	1.39
1	A	24	VAL	CA-CB	5.46	1.66	1.54
1	A	77	GLU	C-O	-5.42	1.13	1.23
1	A	77	GLU	CD-OE1	5.40	1.31	1.25
1	A	60	ARG	CZ-NH1	5.36	1.40	1.33
1	A	162	HIS	C-O	5.33	1.33	1.23
1	A	148	ALA	C-O	-5.31	1.13	1.23
1	A	106	ILE	CB-CG2	-5.27	1.36	1.52
1	A	21	LYS	CD-CE	5.25	1.64	1.51
1	A	101	ILE	CA-CB	5.20	1.66	1.54
1	A	90	GLU	CD-OE1	-5.18	1.20	1.25
1	A	6	TYR	CD2-CE2	5.16	1.47	1.39
1	A	22	ARG	NE-CZ	5.14	1.39	1.33
1	A	50	MSE	CG-SE	5.04	2.12	1.95
1	A	110	TYR	CG-CD2	5.01	1.45	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	A	60	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	A	22	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	A	133	ASP	CB-CG-OD2	11.74	128.87	118.30
1	A	157	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	A	25	MSE	CG-SE-CE	-8.72	79.72	98.90
1	A	60	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	145	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	8	MSE	CG-SE-CE	-7.55	82.29	98.90
1	A	157	ARG	CG-CD-NE	-7.39	96.28	111.80
1	A	18	MSE	CG-SE-CE	-7.07	83.35	98.90
1	A	133	ASP	CB-CG-OD1	-6.74	112.23	118.30
1	A	46	LEU	CB-CG-CD1	6.62	122.25	111.00
1	A	57	LEU	CB-CG-CD2	-6.34	100.21	111.00
1	A	122	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	146	ILE	CG1-CB-CG2	-5.94	98.34	111.40
1	A	49	CYS	CA-CB-SG	-5.91	103.37	114.00
1	A	11	MSE	CB-CG-SE	-5.90	94.99	112.70
1	A	72	LEU	CB-CG-CD2	5.88	121.00	111.00
1	A	116	THR	N-CA-CB	-5.66	99.55	110.30
1	A	73	ASP	CB-CG-OD2	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	MSE	CB-CG-SE	-5.39	96.53	112.70
1	A	157	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	44	LEU	CB-CA-C	5.30	120.27	110.20
1	A	19	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	A	104	LEU	CB-CA-C	-5.03	100.64	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	GLN	Peptide

## 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	1262	0	1289	82	0
2	A	1	0	0	0	0
3	A	24	0	0	8	0
All	All	1287	0	1289	82	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 32.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:THR:CG2	1:A:10:GLU:HG3	1.65	1.24
1:A:78:GLN:HG2	3:A:212:HOH:O	1.39	1.22
1:A:7:THR:HG22	1:A:10:GLU:CG	1.75	1.16
1:A:7:THR:HG22	1:A:10:GLU:HG3	1.10	1.08
1:A:113:ILE:HG22	1:A:156:SER:HB2	1.43	0.97
1:A:12:VAL:O	1:A:16:LYS:HG3	1.73	0.86
1:A:162:HIS:HA	1:A:165:LEU:HG	1.60	0.84
1:A:131:GLU:O	1:A:134:GLU:HB3	1.77	0.83
1:A:162:HIS:O	1:A:165:LEU:HB2	1.82	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:THR:HG23	1:A:10:GLU:H	1.45	0.79
1:A:12:VAL:HG22	1:A:63:ILE:HD11	1.64	0.79
1:A:134:GLU:HG3	3:A:203:HOH:O	1.85	0.76
1:A:136:PRO:C	1:A:138:GLY:H	1.87	0.76
1:A:79:LYS:HE2	3:A:206:HOH:O	1.86	0.76
1:A:78:GLN:CG	3:A:212:HOH:O	2.10	0.75
1:A:113:ILE:CG2	1:A:156:SER:HB2	2.16	0.75
1:A:79:LYS:HD3	1:A:79:LYS:N	2.03	0.74
1:A:8:MSE:O	1:A:12:VAL:HG23	1.90	0.72
1:A:71:ALA:O	1:A:75:LEU:HG	1.90	0.72
1:A:79:LYS:CD	1:A:79:LYS:N	2.54	0.70
1:A:104:LEU:HA	1:A:107:VAL:HG22	1.77	0.66
1:A:83:GLU:HA	1:A:83:GLU:OE2	1.96	0.65
1:A:134:GLU:C	1:A:134:GLU:OE1	2.35	0.64
1:A:70:LEU:HD11	1:A:143:LEU:HD13	1.79	0.64
1:A:157:ARG:HD2	3:A:202:HOH:O	1.98	0.64
1:A:136:PRO:C	1:A:138:GLY:N	2.53	0.62
1:A:7:THR:CG2	1:A:10:GLU:CG	2.50	0.62
1:A:40:TYR:HD1	1:A:40:TYR:O	1.84	0.60
1:A:126:ILE:O	1:A:129:ILE:HB	2.04	0.58
1:A:161:THR:HG22	1:A:162:HIS:N	2.20	0.57
1:A:7:THR:HG22	1:A:10:GLU:CD	2.24	0.57
1:A:86:GLN:NE2	1:A:90:GLU:HG3	2.20	0.55
1:A:135:SER:CB	1:A:136:PRO:CD	2.85	0.55
1:A:134:GLU:N	1:A:134:GLU:OE1	2.40	0.54
1:A:132:LEU:O	1:A:140:HIS:NE2	2.41	0.54
1:A:134:GLU:CA	1:A:134:GLU:OE1	2.55	0.54
1:A:32:ILE:HG23	1:A:126:ILE:HD11	1.91	0.53
1:A:104:LEU:HA	1:A:107:VAL:CG2	2.38	0.53
1:A:83:GLU:OE2	1:A:84:PRO:HA	2.09	0.53
1:A:161:THR:O	1:A:163:GLN:N	2.42	0.53
1:A:134:GLU:CG	1:A:134:GLU:O	2.54	0.52
1:A:79:LYS:CE	3:A:206:HOH:O	2.53	0.52
1:A:97:GLY:HA2	1:A:100:GLU:OE1	2.10	0.51
1:A:135:SER:HB3	1:A:136:PRO:HD3	1.92	0.51
1:A:40:TYR:CD1	1:A:40:TYR:C	2.85	0.51
1:A:86:GLN:O	1:A:90:GLU:HB2	2.10	0.50
1:A:40:TYR:HD1	1:A:40:TYR:C	2.14	0.50
1:A:30:ALA:HB1	1:A:49:CYS:HB2	1.94	0.48
1:A:9:ASN:HD22	1:A:9:ASN:H	1.62	0.48
1:A:12:VAL:HG22	1:A:63:ILE:CD1	2.40	0.48
1:A:134:GLU:OE1	1:A:135:SER:O	2.31	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:LYS:HG3	1:A:35:LYS:O	2.14	0.47
1:A:52:ASN:OD1	1:A:157:ARG:NH2	2.39	0.47
1:A:79:LYS:CD	1:A:79:LYS:H	2.27	0.47
1:A:128:ILE:O	1:A:132:LEU:HB2	2.15	0.47
1:A:86:GLN:HE21	1:A:90:GLU:HG3	1.79	0.47
1:A:36:LEU:C	1:A:37:GLN:HE21	2.17	0.47
1:A:161:THR:O	1:A:164:ASP:N	2.49	0.46
1:A:110:TYR:CD1	1:A:153:ALA:HB1	2.51	0.45
1:A:45:PRO:O	1:A:48:VAL:HB	2.16	0.45
1:A:113:ILE:HD12	1:A:160:HIS:CE1	2.52	0.45
1:A:72:LEU:HB3	1:A:142:PHE:CE1	2.53	0.44
1:A:7:THR:O	1:A:10:GLU:HB2	2.17	0.44
1:A:9:ASN:ND2	1:A:9:ASN:H	2.16	0.44
1:A:16:LYS:HE3	1:A:26:ILE:HD11	1.99	0.44
1:A:135:SER:CB	1:A:136:PRO:HD3	2.47	0.44
1:A:69:GLY:HA3	1:A:146:ILE:HD11	2.01	0.43
1:A:134:GLU:CG	3:A:203:HOH:O	2.55	0.43
1:A:66:VAL:CG1	1:A:70:LEU:HD22	2.49	0.43
1:A:43:ASN:O	1:A:45:PRO:HD3	2.18	0.43
1:A:61:GLU:HG3	3:A:205:HOH:O	2.18	0.43
1:A:66:VAL:HG12	1:A:70:LEU:HD22	2.00	0.42
1:A:111:GLY:O	1:A:115:LEU:HD13	2.20	0.42
1:A:79:LYS:HG2	1:A:79:LYS:HZ2	1.59	0.42
1:A:44:LEU:HA	1:A:45:PRO:HD3	1.64	0.41
1:A:30:ALA:HB1	1:A:49:CYS:CB	2.51	0.41
1:A:32:ILE:O	1:A:33:VAL:C	2.57	0.41
1:A:38:GLU:CG	1:A:39:LYS:N	2.84	0.41
1:A:70:LEU:CD1	1:A:143:LEU:HD13	2.48	0.40
1:A:131:GLU:C	1:A:133:ASP:N	2.74	0.40
1:A:44:LEU:HD12	1:A:45:PRO:HD2	2.02	0.40
1:A:27:GLU:HB2	1:A:31:ARG:NH2	2.37	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	159/189 (84%)	141 (89%)	13 (8%)	5 (3%)	<b>7</b> <b>5</b>

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	A	53	VAL
1	A	135	SER
1	A	137	ASP
1	A	136	PRO

### 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	141/161 (88%)	122 (86%)	19 (14%)	<b>6</b> <b>6</b>

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	21	LYS
1	A	27	GLU
1	A	36	LEU
1	A	37	GLN
1	A	40	TYR
1	A	55	LYS
1	A	63	ILE
1	A	70	LEU
1	A	72	LEU
1	A	79	LYS
1	A	123	LYS
1	A	126	ILE
1	A	132	LEU
1	A	134	GLU
1	A	135	SER
1	A	156	SER
1	A	161	THR

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Mol	Chain	Res	Type
1	A	166	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	37	GLN
1	A	86	GLN
1	A	87	HIS
1	A	108	ASN
1	A	117	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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	161/189 (85%)	0.15	12 (7%) 14 12	24, 40, 79, 87	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	TYR	6.2
1	A	137	ASP	4.7
1	A	135	SER	4.7
1	A	165	LEU	3.8
1	A	136	PRO	3.7
1	A	39	LYS	3.4
1	A	166	GLN	3.3
1	A	163	GLN	3.2
1	A	164	ASP	3.2
1	A	6	TYR	3.0
1	A	42	PRO	2.9
1	A	43	ASN	2.3

### 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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	190	1/1	0.02	-4.47	33,33,33,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.