



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:37 PM GMT

PDB ID : 3U3W
Title : Crystal Structure of Bacillus thuringiensis PlcR in complex with the peptide PapR7 and DNA
Authors : Grenha, R.; Slamti, L.; Bouillaut, L.; Lereclus, D.; Nessler, S.
Deposited on : 2011-10-06
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

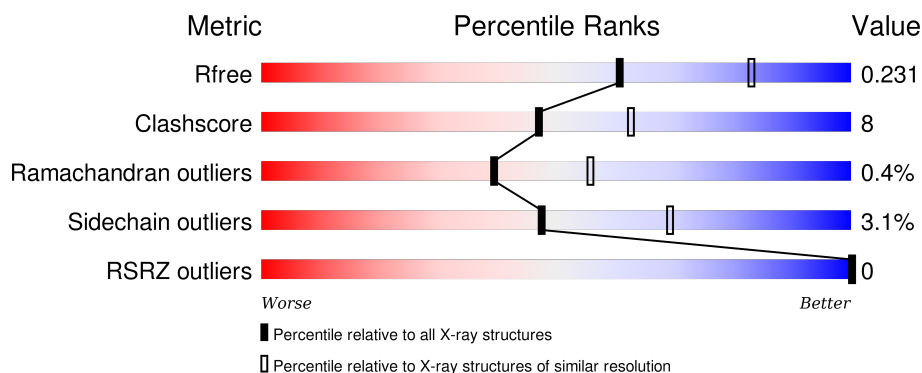
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



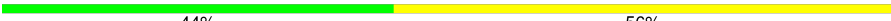
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 ≥ 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	293	<div> <div>80%</div> <div>14%</div> <div>• •</div> </div>
1	B	293	<div> <div>78%</div> <div>16%</div> <div>• •</div> </div>
2	P	7	<div> <div>100%</div> </div>
2	Q	7	<div> <div>100%</div> </div>
3	Y	18	<div> <div>78%</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
4	Z	18	 A horizontal bar chart showing the quality of chain Z. The bar is divided into two segments: a green segment on the left representing 44% and a yellow segment on the right representing 56%. The percentages are labeled below the bar.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5947 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 Transcriptional activator PlcR protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	8	0
			2413	1556	393	454	10			
1	B	280	Total	C	N	O	S	0	8	0
			2419	1558	395	456	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LEU	-	EXPRESSION TAG	UNP Q45782
A	287	GLU	-	EXPRESSION TAG	UNP Q45782
A	288	HIS	-	EXPRESSION TAG	UNP Q45782
A	289	HIS	-	EXPRESSION TAG	UNP Q45782
A	290	HIS	-	EXPRESSION TAG	UNP Q45782
A	291	HIS	-	EXPRESSION TAG	UNP Q45782
A	292	HIS	-	EXPRESSION TAG	UNP Q45782
A	293	HIS	-	EXPRESSION TAG	UNP Q45782
B	286	LEU	-	EXPRESSION TAG	UNP Q45782
B	287	GLU	-	EXPRESSION TAG	UNP Q45782
B	288	HIS	-	EXPRESSION TAG	UNP Q45782
B	289	HIS	-	EXPRESSION TAG	UNP Q45782
B	290	HIS	-	EXPRESSION TAG	UNP Q45782
B	291	HIS	-	EXPRESSION TAG	UNP Q45782
B	292	HIS	-	EXPRESSION TAG	UNP Q45782
B	293	HIS	-	EXPRESSION TAG	UNP Q45782

- Molecule 2 is a protein called C-terminus heptapeptide from PapR protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			60	41	7	12			
2	Q	7	Total	C	N	O	0	0	0
			60	41	7	12			

- Molecule 3 is a DNA chain called 5'-D(P*CP*TP*AP*TP*GP*CP*AP*AP*TP*AP*TP*T
P*TP*CP*AP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	18	Total	C	N	O	P	0	0	0
			365	177	60	110	18			

- Molecule 4 is a DNA chain called 5'-D(P*AP*TP*AP*TP*GP*AP*AP*AP*TP*AP*TP*
TP*GP*CP*AP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Z	18	Total	C	N	O	P	0	0	0
			373	179	70	106	18			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	112	Total	O	0	0
			112	112		
6	P	6	Total	O	0	0
			6	6		
6	Q	7	Total	O	0	0
			7	7		
6	Y	11	Total	O	0	0
			11	11		
6	Z	9	Total	O	0	0
			9	9		

- Molecule 4: 5'-D(P*AP*TP*AP*TP*GP*AP*AP*AP*TP*AP*TP*TP*GP*CP*AP*TP*AP*G)-3'

Chain Z:  44% 56%

A1	T2	A3	T4	G5	T11	T12	G13	T16	A17	G18
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.88Å 71.09Å 88.85Å 90.00° 115.53° 90.00°	Depositor
Resolution (Å)	53.19 – 2.40 53.19 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.9 (53.19-2.40) 96.3 (53.19-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.179 , 0.235 0.186 , 0.231	Depositor DCC
R_{free} test set	1913 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.2	EDS
Estimated twinning fraction	0.468 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 37992 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5947	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.41	0/2464	0.49	0/3312
1	B	0.41	0/2464	0.50	0/3312
2	P	0.36	0/62	0.48	0/82
2	Q	0.55	0/62	0.56	0/82
3	Y	0.59	0/407	1.25	0/625
4	Z	0.58	0/419	1.23	3/645 (0.5%)
All	All	0.44	0/5878	0.67	3/8058 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	16	DT	O4'-C1'-N1	7.55	113.28	108.00
4	Z	17	DA	O4'-C1'-N9	6.41	112.49	108.00
4	Z	16	DT	C1'-O4'-C4'	-5.01	105.09	110.10

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	2413	0	2405	39	0
1	B	2419	0	2403	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	60	0	50	0	0
2	Q	60	0	50	0	0
3	Y	365	0	207	4	0
4	Z	373	0	205	11	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	110	0	0	3	0
6	B	112	0	0	4	0
6	P	6	0	0	0	0
6	Q	7	0	0	0	0
6	Y	11	0	0	0	0
6	Z	9	0	0	0	0
All	All	5947	0	5320	83	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 8.

All (83) 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:273:HIS:HA	1:A:276:LYS:HD2	1.42	1.00
1:A:147:THR:HB	1:B:54:ALA:HB1	1.54	0.90
1:A:54:ALA:HB1	1:B:147:THR:HB	1.53	0.88
1:A:129:VAL:HG11	1:A:133:TYR:HD2	1.44	0.83
1:B:129:VAL:HG11	1:B:133:TYR:HD2	1.53	0.73
1:A:129:VAL:HG11	1:A:133:TYR:CD2	2.24	0.71
1:A:3:ALA:HB3	1:A:43:TYR:HE1	1.55	0.70
1:B:183:LYS:O	1:B:186:GLU:HG2	1.92	0.69
1:A:232:MET:HG3	1:B:232:MET:HG2	1.76	0.68
4:Z:11:DT:H2''	4:Z:12:DT:O5'	1.95	0.67
1:A:60:ILE:H	1:A:60:ILE:HD12	1.59	0.66
1:B:3:ALA:N	1:B:43:TYR:HE1	1.96	0.64
1:A:60:ILE:N	1:A:60:ILE:HD12	2.14	0.63
3:Y:11:DT:H2''	3:Y:12:DT:O5'	2.01	0.61
1:B:73[A]:GLU:HG3	1:B:77:GLN:HE21	1.64	0.61
1:A:84[B]:MET:O	1:A:88:GLN:HG3	2.03	0.59
1:A:232:MET:CG	1:B:232:MET:HG2	2.32	0.59
1:B:72:ILE:O	1:B:76:LYS:HG3	2.03	0.59
1:A:72:ILE:O	1:A:76:LYS:HG3	2.04	0.57
1:B:31:GLN:NE2	4:Z:3:DA:H62	2.04	0.56
1:B:3:ALA:N	1:B:43:TYR:CE1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:HG2	6:A:395:HOH:O	2.09	0.52
1:A:232:MET:HG3	1:B:232:MET:CG	2.38	0.52
1:A:262:LYS:HE3	1:B:269:ILE:HG22	1.90	0.52
1:A:60:ILE:CD1	1:A:60:ILE:H	2.23	0.52
3:Y:1:DC:H2"	3:Y:2:DT:H5"	1.91	0.52
1:A:84[A]:MET:O	1:A:88:GLN:HG3	2.10	0.52
4:Z:11:DT:H2'	4:Z:12:DT:C6	2.45	0.51
1:B:197:LYS:HA	1:B:234:LEU:CD1	2.41	0.51
1:A:3:ALA:HB3	1:A:43:TYR:CE1	2.43	0.51
1:A:242:ARG:O	1:A:246:LEU:HG	2.10	0.51
4:Z:1:DA:H2"	4:Z:2:DT:H5"	1.94	0.50
1:B:93:GLU:HG3	6:B:297:HOH:O	2.11	0.50
1:B:242:ARG:O	1:B:246:LEU:HG	2.11	0.50
1:B:86:CYS:N	1:B:94:ILE:HD11	2.27	0.49
3:Y:1:DC:H42	4:Z:18:DG:H1	1.60	0.49
1:A:90:ARG:O	1:A:94:ILE:HG13	2.12	0.49
4:Z:1:DA:H2"	4:Z:2:DT:C5'	2.43	0.49
1:A:242:ARG:NH1	6:A:315:HOH:O	2.45	0.49
1:A:269:ILE:HG22	1:B:262:LYS:HE3	1.95	0.48
1:A:200:TYR:CZ	1:A:237:GLN:HB3	2.48	0.48
1:B:36:ARG:NH2	4:Z:5:DG:O6	2.46	0.48
1:B:31:GLN:HE21	4:Z:3:DA:H62	1.61	0.47
1:B:197:LYS:HA	1:B:234:LEU:HD12	1.96	0.47
1:B:100:ASN:O	1:B:103:LYS:HG2	2.15	0.47
1:B:112[B]:GLN:O	1:B:116:GLN:HG3	2.15	0.47
1:A:275:TYR:HD1	1:A:275:TYR:H	1.62	0.47
1:B:192:GLU:HG3	6:B:403:HOH:O	2.14	0.47
3:Y:1:DC:H2"	3:Y:2:DT:C5'	2.46	0.46
1:A:197:LYS:HA	1:A:234:LEU:HD12	1.97	0.46
1:B:73[A]:GLU:HG3	1:B:77:GLN:NE2	2.30	0.46
1:A:81:GLN:HB3	1:A:97:LYS:HE2	1.97	0.45
1:A:86:CYS:N	1:A:94:ILE:HD11	2.30	0.45
1:B:129:VAL:HG11	1:B:133:TYR:CD2	2.43	0.45
4:Z:12:DT:H2"	4:Z:13:DG:C8	2.51	0.45
1:A:197:LYS:HA	1:A:234:LEU:CD1	2.46	0.45
1:B:200:TYR:HD1	1:B:238:LEU:HD23	1.82	0.45
1:A:43:TYR:HB3	6:A:399:HOH:O	2.16	0.45
1:B:239:TYR:CE1	1:B:262:LYS:HD3	2.52	0.45
1:A:147:THR:HB	1:B:54:ALA:CB	2.37	0.45
1:A:60:ILE:N	1:A:60:ILE:CD1	2.81	0.44
1:B:46:MET:O	1:B:50:GLN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:HD3	1:B:248:LYS:HA	1.69	0.44
1:A:129:VAL:CG1	1:A:133:TYR:CD2	2.98	0.44
1:A:11:LYS:O	1:A:15:VAL:HG23	2.17	0.44
1:A:248:LYS:HD3	1:A:248:LYS:HA	1.74	0.43
1:A:91:TYR:CD2	1:A:125:VAL:HG11	2.52	0.43
1:B:69:TYR:O	1:B:72:ILE:HD13	2.19	0.43
1:A:261:LYS:HB3	1:A:261:LYS:NZ	2.33	0.43
1:A:73[B]:GLU:CD	1:A:73[B]:GLU:H	2.22	0.43
1:B:129:VAL:CG1	1:B:133:TYR:HD2	2.26	0.43
1:B:14:ARG:HD3	1:B:24:LEU:HD22	2.01	0.43
4:Z:1:DA:H1'	4:Z:2:DT:H5''	2.01	0.43
1:B:219:VAL:HG11	1:B:242:ARG:HB2	2.01	0.42
1:B:112[A]:GLN:O	1:B:116:GLN:HG3	2.19	0.42
1:A:46:MET:O	1:A:50:GLN:HB3	2.20	0.42
4:Z:1:DA:C2'	4:Z:2:DT:H5''	2.50	0.42
1:B:87:LYS:HG2	6:B:393:HOH:O	2.19	0.42
1:B:11:LYS:O	1:B:15:VAL:HG23	2.19	0.42
1:B:273:HIS:HA	1:B:276:LYS:HD2	2.03	0.40
1:B:73[B]:GLU:CD	1:B:73[B]:GLU:H	2.23	0.40
1:A:262:LYS:HE3	1:B:269:ILE:CG2	2.52	0.40
1:B:154:ASN:HB2	6:B:352:HOH:O	2.21	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	286/293 (98%)	278 (97%)	7 (2%)	1 (0%)	46	63
1	B	286/293 (98%)	277 (97%)	8 (3%)	1 (0%)	46	63
2	P	5/7 (71%)	5 (100%)	0	0	100	100
2	Q	5/7 (71%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	582/600 (97%)	565 (97%)	15 (3%)	2 (0%)	39 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	THR
1	B	147	THR

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	260/265 (98%)	251 (96%)	9 (4%)	43 64
1	B	260/265 (98%)	253 (97%)	7 (3%)	52 73
2	P	6/6 (100%)	6 (100%)	0	100 100
2	Q	6/6 (100%)	6 (100%)	0	100 100
All	All	532/542 (98%)	516 (97%)	16 (3%)	47 70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	42	VAL
1	A	45	SER
1	A	103	LYS
1	A	221	LYS
1	A	242	ARG
1	A	275	TYR
1	A	277	GLU
1	A	282	LYS
1	B	71	ASP
1	B	72	ILE
1	B	87	LYS
1	B	146	LEU

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Mol	Chain	Res	Type
1	B	151	VAL
1	B	189	HIS
1	B	221	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	GLN
1	B	77	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 2 ligands modelled in this entry, 2 are 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.

No monomer is involved in short contacts.

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 [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, 95th 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 ²)	Q<0.9
1	A	280/293 (95%)	-0.40	0 100 100	22, 43, 69, 97	0
1	B	280/293 (95%)	-0.38	0 100 100	23, 43, 68, 98	0
2	P	7/7 (100%)	-0.48	0 100 100	26, 29, 58, 63	0
2	Q	7/7 (100%)	-0.66	0 100 100	26, 30, 60, 71	0
3	Y	18/18 (100%)	-0.80	0 100 100	54, 68, 88, 92	1 (5%)
4	Z	18/18 (100%)	-0.77	0 100 100	55, 69, 90, 96	0
All	All	610/636 (95%)	-0.42	0 100 100	22, 44, 74, 98	1 (0%)

There are no RSRZ outliers to report.

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](#)

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, 95th 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	B	1001	1/1	0.96	0.12	-	71,71,71,71	0
5	CA	A	1002	1/1	0.92	0.11	-	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.