



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:41 PM GMT

PDB ID : 1YAX  
Title : Crystal structure Analysis of S.typhimurium PhoQ sensor domain with Calcium  
Authors : Cho, U.S.; Xu, W.  
Deposited on : 2004-12-17  
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](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

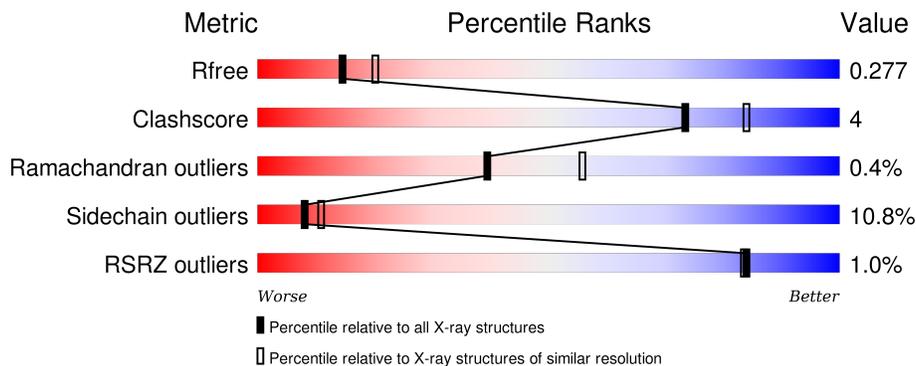
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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  $\geq 3$ , 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	153	 80% 17% ••
1	B	153	 71% 15% • 12%
1	C	153	 82% 15% ••
1	D	153	 69% 16% • 12%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4459 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 Virulence sensor protein phoQ, sensor domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1200	760	207	227	6	0	0	0
1	B	134	973	619	158	193	3	0	0	0
1	C	153	1196	759	206	225	6	0	0	0
1	D	134	976	620	158	195	3	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	INITIATING METHIONINE	UNP P14147
A	191	HIS	-	EXPRESSION TAG	UNP P14147
A	192	HIS	-	EXPRESSION TAG	UNP P14147
A	193	HIS	-	EXPRESSION TAG	UNP P14147
A	194	HIS	-	EXPRESSION TAG	UNP P14147
A	195	HIS	-	EXPRESSION TAG	UNP P14147
A	196	HIS	-	EXPRESSION TAG	UNP P14147
B	44	MET	-	INITIATING METHIONINE	UNP P14147
B	191	HIS	-	EXPRESSION TAG	UNP P14147
B	192	HIS	-	EXPRESSION TAG	UNP P14147
B	193	HIS	-	EXPRESSION TAG	UNP P14147
B	194	HIS	-	EXPRESSION TAG	UNP P14147
B	195	HIS	-	EXPRESSION TAG	UNP P14147
B	196	HIS	-	EXPRESSION TAG	UNP P14147
C	44	MET	-	INITIATING METHIONINE	UNP P14147
C	191	HIS	-	EXPRESSION TAG	UNP P14147
C	192	HIS	-	EXPRESSION TAG	UNP P14147
C	193	HIS	-	EXPRESSION TAG	UNP P14147
C	194	HIS	-	EXPRESSION TAG	UNP P14147
C	195	HIS	-	EXPRESSION TAG	UNP P14147
C	196	HIS	-	EXPRESSION TAG	UNP P14147

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Chain	Residue	Modelled	Actual	Comment	Reference
D	44	MET	-	INITIATING METHIONINE	UNP P14147
D	191	HIS	-	EXPRESSION TAG	UNP P14147
D	192	HIS	-	EXPRESSION TAG	UNP P14147
D	193	HIS	-	EXPRESSION TAG	UNP P14147
D	194	HIS	-	EXPRESSION TAG	UNP P14147
D	195	HIS	-	EXPRESSION TAG	UNP P14147
D	196	HIS	-	EXPRESSION TAG	UNP P14147

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	3	Total Ca 3 3	0	0
2	D	1	Total Ca 1 1	0	0
2	C	2	Total Ca 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	9	Total O 9 9	0	0
3	C	39	Total O 39 39	0	0
3	D	13	Total O 13 13	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.

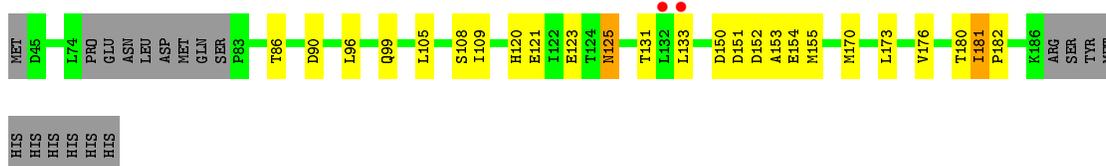
- Molecule 1: Virulence sensor protein phoQ, sensor domain

Chain A: 



- Molecule 1: Virulence sensor protein phoQ, sensor domain

Chain B: 



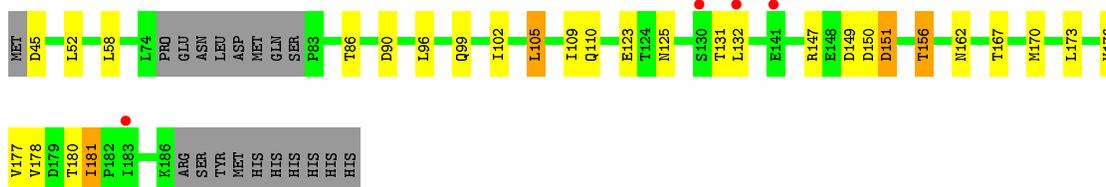
- Molecule 1: Virulence sensor protein phoQ, sensor domain

Chain C: 



- Molecule 1: Virulence sensor protein phoQ, sensor domain

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.08Å 134.87Å 58.44Å 90.00° 119.61° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 81.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.8 (50.00-2.40) 85.6 (81.69-2.20)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.242 , 0.280 0.246 , 0.277	Depositor DCC
$R_{free}$ test set	1514 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtrriage
Anisotropy	0.449	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.3	EDS
Estimated twinning fraction	0.487 for -h-2*1,-k,l	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Outliers	0 of 40169 reflections	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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 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	0.48	1/1230 (0.1%)	0.77	7/1682 (0.4%)
1	B	0.65	2/993 (0.2%)	0.69	2/1370 (0.1%)
1	C	0.48	0/1226	0.75	6/1677 (0.4%)
1	D	0.57	0/996	0.73	4/1374 (0.3%)
All	All	0.54	3/4445 (0.1%)	0.74	19/6103 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	ASP	CG-OD1	6.57	1.40	1.25
1	B	153	ALA	C-O	5.68	1.34	1.23
1	A	155	MET	SD-CE	-5.62	1.46	1.77

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ASP	CB-CG-OD2	7.14	124.73	118.30
1	A	90	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	150	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	149	ASP	CB-CG-OD2	6.34	124.00	118.30
1	B	150	ASP	CB-CG-OD2	6.23	123.91	118.30
1	C	149	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	151	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	179	ASP	CB-CG-OD2	5.94	123.65	118.30
1	D	150	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	45	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	151	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	127	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	127	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	45	ASP	CB-CG-OD2	5.32	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	179	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	149	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	151	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	151	ASP	CB-CG-OD2	5.05	122.85	118.30

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	1200	0	1128	8	0
1	B	973	0	862	9	0
1	C	1196	0	1121	7	0
1	D	976	0	864	11	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	46	0	0	0	0
3	B	9	0	0	1	0
3	C	39	0	0	1	0
3	D	13	0	0	1	0
All	All	4459	0	3975	34	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 4.

All (34) 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:109:ILE:HD12	1:B:176:VAL:HG11	1.74	0.69
1:D:109:ILE:HD12	1:D:176:VAL:HG11	1.77	0.66
1:C:90:ASP:HB3	1:C:96:LEU:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASP:HB3	1:B:96:LEU:HD11	1.85	0.58
1:D:102:ILE:HD13	1:D:132:LEU:HD12	1.85	0.57
1:B:86:THR:H	1:B:99:GLN:HE21	1.52	0.57
1:A:90:ASP:HB3	1:A:96:LEU:HD11	1.87	0.55
1:D:90:ASP:HB3	1:D:96:LEU:HD11	1.90	0.53
1:B:155:MET:SD	1:B:182:PRO:HG3	2.49	0.52
1:B:123:GLU:OE2	1:B:154:GLU:OE1	2.29	0.51
1:C:129:THR:OG1	1:C:157:HIS:HE1	1.94	0.50
1:D:151:ASP:OD2	3:D:1004:HOH:O	2.19	0.50
1:C:80:MET:HE3	3:C:1037:HOH:O	2.12	0.50
1:D:86:THR:H	1:D:99:GLN:HE21	1.60	0.49
1:B:120:HIS:HE1	3:B:1007:HOH:O	1.96	0.48
1:D:132:LEU:HD23	1:D:180:THR:HB	1.96	0.47
1:C:151:ASP:OD1	1:C:151:ASP:N	2.47	0.47
1:A:164:TYR:CE1	1:A:175:ILE:HD12	2.51	0.46
1:B:133:LEU:HD21	1:B:180:THR:O	2.16	0.46
1:A:52:LEU:HD21	1:A:179:ASP:HB2	1.98	0.45
1:D:105:LEU:HD21	1:D:178:VAL:HG21	1.99	0.44
1:D:52:LEU:HD22	1:D:177:VAL:HG12	2.00	0.43
1:D:123:GLU:HG2	1:D:156:THR:HB	2.00	0.43
1:C:133:LEU:HD22	1:C:137:HIS:ND1	2.34	0.43
1:A:128:ALA:O	1:A:131:THR:HB	2.18	0.43
1:B:125:ASN:C	1:B:125:ASN:HD22	2.22	0.43
1:B:181:ILE:HD12	1:B:182:PRO:O	2.19	0.42
1:A:78:LEU:HD12	1:A:78:LEU:C	2.38	0.42
1:A:81:GLN:HE21	1:A:81:GLN:HA	1.84	0.42
1:D:181:ILE:O	1:D:181:ILE:HG13	2.20	0.42
1:C:70:ILE:CG2	1:C:97:TRP:HB2	2.50	0.42
1:C:167:THR:HG21	1:D:58:LEU:HD13	2.01	0.42
1:A:155:MET:HE2	1:A:184:GLU:HB2	2.01	0.41
1:A:65:TRP:HZ2	1:A:68:ASN:HD22	1.67	0.41

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	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	B	130/153 (85%)	125 (96%)	5 (4%)	0	100	100
1	C	151/153 (99%)	146 (97%)	3 (2%)	2 (1%)	15	21
1	D	130/153 (85%)	123 (95%)	7 (5%)	0	100	100
All	All	562/612 (92%)	541 (96%)	19 (3%)	2 (0%)	39	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	151	ASP
1	C	79	ASP

### 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	128/143 (90%)	113 (88%)	15 (12%)	7	8
1	B	94/143 (66%)	86 (92%)	8 (8%)	13	20
1	C	126/143 (88%)	112 (89%)	14 (11%)	8	10
1	D	95/143 (66%)	84 (88%)	11 (12%)	7	9
All	All	443/572 (77%)	395 (89%)	48 (11%)	8	11

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	70	ILE
1	A	78	LEU
1	A	80	MET
1	A	81	GLN
1	A	114	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	116	THR
1	A	125	ASN
1	A	134	SER
1	A	141	GLU
1	A	155	MET
1	A	162	ASN
1	A	167	THR
1	A	173	LEU
1	A	186	LYS
1	B	105	LEU
1	B	108	SER
1	B	121	GLU
1	B	125	ASN
1	B	131	THR
1	B	170	MET
1	B	173	LEU
1	B	181	ILE
1	C	50	ARG
1	C	53	ARG
1	C	81	GLN
1	C	98	THR
1	C	101	ASN
1	C	114	LEU
1	C	134	SER
1	C	141	GLU
1	C	149	ASP
1	C	151	ASP
1	C	162	ASN
1	C	167	THR
1	C	169	ARG
1	C	173	LEU
1	D	105	LEU
1	D	110	GLN
1	D	125	ASN
1	D	131	THR
1	D	147	ARG
1	D	156	THR
1	D	162	ASN
1	D	167	THR
1	D	170	MET
1	D	173	LEU
1	D	181	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	81	GLN
1	A	125	ASN
1	A	157	HIS
1	A	162	ASN
1	B	99	GLN
1	B	125	ASN
1	B	137	HIS
1	B	140	GLN
1	C	125	ASN
1	C	157	HIS
1	C	162	ASN
1	D	99	GLN
1	D	110	GLN
1	D	125	ASN
1	D	140	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](#)

Of 7 ligands modelled in this entry, 7 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, 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	153/153 (100%)	-0.35	0 <b>100</b> <b>100</b>	9, 19, 37, 42	0
1	B	134/153 (87%)	-0.06	2 (1%) 76 75	26, 36, 49, 51	0
1	C	153/153 (100%)	-0.36	0 <b>100</b> <b>100</b>	10, 19, 37, 43	0
1	D	134/153 (87%)	-0.11	4 (2%) 54 53	27, 37, 50, 53	0
All	All	574/612 (93%)	-0.23	6 (1%) 84 83	9, 31, 47, 53	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	132	LEU	3.6
1	D	141	GLU	3.1
1	D	130	SER	2.3
1	B	132	LEU	2.2
1	B	133	LEU	2.1
1	D	183	ILE	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](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	1004	1/1	0.96	0.06	-2.60	49,49,49,49	0
2	CA	D	1001	1/1	0.97	0.07	-3.56	49,49,49,49	0
2	CA	A	1002	1/1	0.91	0.12	-	59,59,59,59	0
2	CA	C	1005	1/1	0.94	0.34	-	58,58,58,58	0
2	CA	A	1006	1/1	0.77	0.21	-	56,56,56,56	0
2	CA	C	1003	1/1	0.91	0.06	-	55,55,55,55	0
2	CA	A	1007	1/1	0.92	0.16	-	69,69,69,69	0

## 6.5 Other polymers

There are no such residues in this entry.