



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 06:20 AM GMT

PDB ID : 3QB2  
Title : The Crystal Structure of Immunity Factor for SPN (IFS)  
Authors : Smith, C.L.; Ellenberger, T.  
Deposited on : 2011-01-12  
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary 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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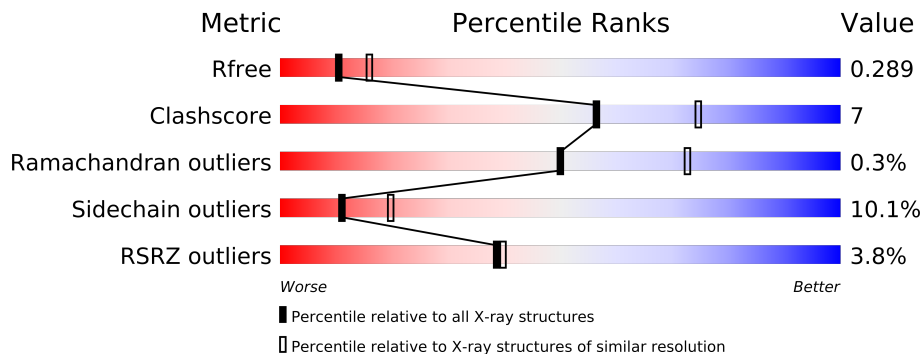
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	187	
1	B	187	
1	C	187	
1	D	187	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	190	-	X
2	SO4	D	188	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5085 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 Immunity factor for SPN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	Se	0	0	0
			1214	782	197	227	8			
1	B	173	Total	C	N	O	Se	0	0	0
			1338	857	213	260	8			
1	C	164	Total	C	N	O	Se	0	0	0
			1108	706	183	211	8			
1	D	159	Total	C	N	O	Se	0	0	0
			1240	797	199	236	8			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	PHE	-	SEE REMARK 999	UNP Q2VJ58
A	163	ARG	-	SEE REMARK 999	UNP Q2VJ58
A	164	SER	-	SEE REMARK 999	UNP Q2VJ58
A	165	PHE	-	SEE REMARK 999	UNP Q2VJ58
A	166	LEU	-	SEE REMARK 999	UNP Q2VJ58
A	167	GLU	-	SEE REMARK 999	UNP Q2VJ58
A	168	GLN	-	SEE REMARK 999	UNP Q2VJ58
A	169	LYS	-	SEE REMARK 999	UNP Q2VJ58
A	170	LEU	-	SEE REMARK 999	UNP Q2VJ58
A	171	ILE	-	SEE REMARK 999	UNP Q2VJ58
A	172	SER	-	SEE REMARK 999	UNP Q2VJ58
A	173	GLU	-	SEE REMARK 999	UNP Q2VJ58
A	174	GLU	-	SEE REMARK 999	UNP Q2VJ58
A	175	ASP	-	SEE REMARK 999	UNP Q2VJ58
A	176	LEU	-	SEE REMARK 999	UNP Q2VJ58
A	177	ASN	-	SEE REMARK 999	UNP Q2VJ58
A	178	SER	-	SEE REMARK 999	UNP Q2VJ58
A	179	ALA	-	SEE REMARK 999	UNP Q2VJ58
A	180	VAL	-	SEE REMARK 999	UNP Q2VJ58
A	181	ASP	-	SEE REMARK 999	UNP Q2VJ58
A	182	HIS	-	EXPRESSION TAG	UNP Q2VJ58

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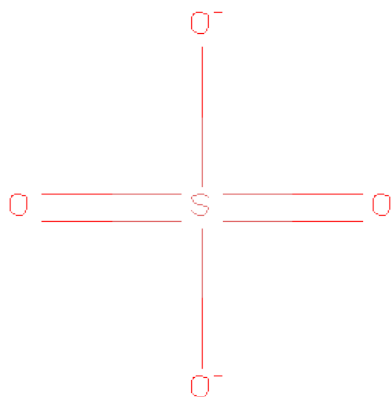
Chain	Residue	Modelled	Actual	Comment	Reference
A	183	HIS	-	EXPRESSION TAG	UNP Q2VJ58
A	184	HIS	-	EXPRESSION TAG	UNP Q2VJ58
A	185	HIS	-	EXPRESSION TAG	UNP Q2VJ58
A	186	HIS	-	EXPRESSION TAG	UNP Q2VJ58
A	187	HIS	-	EXPRESSION TAG	UNP Q2VJ58
B	162	PHE	-	SEE REMARK 999	UNP Q2VJ58
B	163	ARG	-	SEE REMARK 999	UNP Q2VJ58
B	164	SER	-	SEE REMARK 999	UNP Q2VJ58
B	165	PHE	-	SEE REMARK 999	UNP Q2VJ58
B	166	LEU	-	SEE REMARK 999	UNP Q2VJ58
B	167	GLU	-	SEE REMARK 999	UNP Q2VJ58
B	168	GLN	-	SEE REMARK 999	UNP Q2VJ58
B	169	LYS	-	SEE REMARK 999	UNP Q2VJ58
B	170	LEU	-	SEE REMARK 999	UNP Q2VJ58
B	171	ILE	-	SEE REMARK 999	UNP Q2VJ58
B	172	SER	-	SEE REMARK 999	UNP Q2VJ58
B	173	GLU	-	SEE REMARK 999	UNP Q2VJ58
B	174	GLU	-	SEE REMARK 999	UNP Q2VJ58
B	175	ASP	-	SEE REMARK 999	UNP Q2VJ58
B	176	LEU	-	SEE REMARK 999	UNP Q2VJ58
B	177	ASN	-	SEE REMARK 999	UNP Q2VJ58
B	178	SER	-	SEE REMARK 999	UNP Q2VJ58
B	179	ALA	-	SEE REMARK 999	UNP Q2VJ58
B	180	VAL	-	SEE REMARK 999	UNP Q2VJ58
B	181	ASP	-	SEE REMARK 999	UNP Q2VJ58
B	182	HIS	-	EXPRESSION TAG	UNP Q2VJ58
B	183	HIS	-	EXPRESSION TAG	UNP Q2VJ58
B	184	HIS	-	EXPRESSION TAG	UNP Q2VJ58
B	185	HIS	-	EXPRESSION TAG	UNP Q2VJ58
B	186	HIS	-	EXPRESSION TAG	UNP Q2VJ58
B	187	HIS	-	EXPRESSION TAG	UNP Q2VJ58
C	162	PHE	-	SEE REMARK 999	UNP Q2VJ58
C	163	ARG	-	SEE REMARK 999	UNP Q2VJ58
C	164	SER	-	SEE REMARK 999	UNP Q2VJ58
C	165	PHE	-	SEE REMARK 999	UNP Q2VJ58
C	166	LEU	-	SEE REMARK 999	UNP Q2VJ58
C	167	GLU	-	SEE REMARK 999	UNP Q2VJ58
C	168	GLN	-	SEE REMARK 999	UNP Q2VJ58
C	169	LYS	-	SEE REMARK 999	UNP Q2VJ58
C	170	LEU	-	SEE REMARK 999	UNP Q2VJ58
C	171	ILE	-	SEE REMARK 999	UNP Q2VJ58
C	172	SER	-	SEE REMARK 999	UNP Q2VJ58

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Chain	Residue	Modelled	Actual	Comment	Reference
C	173	GLU	-	SEE REMARK 999	UNP Q2VJ58
C	174	GLU	-	SEE REMARK 999	UNP Q2VJ58
C	175	ASP	-	SEE REMARK 999	UNP Q2VJ58
C	176	LEU	-	SEE REMARK 999	UNP Q2VJ58
C	177	ASN	-	SEE REMARK 999	UNP Q2VJ58
C	178	SER	-	SEE REMARK 999	UNP Q2VJ58
C	179	ALA	-	SEE REMARK 999	UNP Q2VJ58
C	180	VAL	-	SEE REMARK 999	UNP Q2VJ58
C	181	ASP	-	SEE REMARK 999	UNP Q2VJ58
C	182	HIS	-	EXPRESSION TAG	UNP Q2VJ58
C	183	HIS	-	EXPRESSION TAG	UNP Q2VJ58
C	184	HIS	-	EXPRESSION TAG	UNP Q2VJ58
C	185	HIS	-	EXPRESSION TAG	UNP Q2VJ58
C	186	HIS	-	EXPRESSION TAG	UNP Q2VJ58
C	187	HIS	-	EXPRESSION TAG	UNP Q2VJ58
D	162	PHE	-	SEE REMARK 999	UNP Q2VJ58
D	163	ARG	-	SEE REMARK 999	UNP Q2VJ58
D	164	SER	-	SEE REMARK 999	UNP Q2VJ58
D	165	PHE	-	SEE REMARK 999	UNP Q2VJ58
D	166	LEU	-	SEE REMARK 999	UNP Q2VJ58
D	167	GLU	-	SEE REMARK 999	UNP Q2VJ58
D	168	GLN	-	SEE REMARK 999	UNP Q2VJ58
D	169	LYS	-	SEE REMARK 999	UNP Q2VJ58
D	170	LEU	-	SEE REMARK 999	UNP Q2VJ58
D	171	ILE	-	SEE REMARK 999	UNP Q2VJ58
D	172	SER	-	SEE REMARK 999	UNP Q2VJ58
D	173	GLU	-	SEE REMARK 999	UNP Q2VJ58
D	174	GLU	-	SEE REMARK 999	UNP Q2VJ58
D	175	ASP	-	SEE REMARK 999	UNP Q2VJ58
D	176	LEU	-	SEE REMARK 999	UNP Q2VJ58
D	177	ASN	-	SEE REMARK 999	UNP Q2VJ58
D	178	SER	-	SEE REMARK 999	UNP Q2VJ58
D	179	ALA	-	SEE REMARK 999	UNP Q2VJ58
D	180	VAL	-	SEE REMARK 999	UNP Q2VJ58
D	181	ASP	-	SEE REMARK 999	UNP Q2VJ58
D	182	HIS	-	EXPRESSION TAG	UNP Q2VJ58
D	183	HIS	-	EXPRESSION TAG	UNP Q2VJ58
D	184	HIS	-	EXPRESSION TAG	UNP Q2VJ58
D	185	HIS	-	EXPRESSION TAG	UNP Q2VJ58
D	186	HIS	-	EXPRESSION TAG	UNP Q2VJ58
D	187	HIS	-	EXPRESSION TAG	UNP Q2VJ58

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	46	Total	O	0	0
			46	46		
3	C	13	Total	O	0	0
			13	13		
3	D	35	Total	O	0	0
			35	35		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.03Å 108.03Å 147.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.78 – 2.50 46.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.78-2.50) 98.8 (46.78-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.95 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.259 , 0.290 0.261 , 0.289	Depositor DCC
$R_{free}$ test set	1739 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.1	EDS
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 34514 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.56	0/1232	0.61	0/1660
1	B	0.48	0/1357	0.59	0/1832
1	C	0.39	0/1123	0.50	0/1531
1	D	0.48	0/1258	0.57	0/1695
All	All	0.48	0/4970	0.57	0/6718

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1214	0	1157	12	0
1	B	1338	0	1240	18	0
1	C	1108	0	871	16	0
1	D	1240	0	1176	15	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	61	0	0	5	0
3	B	46	0	0	2	0
3	C	13	0	0	0	0
3	D	35	0	0	2	0
All	All	5085	0	4444	61	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 7.

The worst 5 of 61 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:163:ARG:HG3	1:C:163:ARG:HH11	1.19	1.04
1:D:89:ILE:HG22	1:D:135:MSE:HE1	1.41	1.02
1:C:101:MSE:HE2	3:D:221:HOH:O	1.68	0.93
1:B:28:LEU:HB2	1:B:80:MSE:HE1	1.56	0.87
1:C:125:ALA:HB1	1:C:131:ILE:HD11	1.60	0.84

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	154/187 (82%)	151 (98%)	3 (2%)	0	100	100
1	B	171/187 (91%)	163 (95%)	8 (5%)	0	100	100
1	C	162/187 (87%)	146 (90%)	15 (9%)	1 (1%)	33	55
1	D	157/187 (84%)	151 (96%)	5 (3%)	1 (1%)	33	55
All	All	644/748 (86%)	611 (95%)	31 (5%)	2 (0%)	50	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	114	ASN

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Mol	Chain	Res	Type
1	D	46	ASP

### 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	121/159 (76%)	106 (88%)	15 (12%)	7	12
1	B	133/159 (84%)	123 (92%)	10 (8%)	19	34
1	C	79/159 (50%)	67 (85%)	12 (15%)	4	7
1	D	124/159 (78%)	115 (93%)	9 (7%)	20	36
All	All	457/636 (72%)	411 (90%)	46 (10%)	11	20

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	103	LEU
1	C	20	THR
1	D	109	LEU
1	B	109	LEU
1	B	151	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	ASN
1	B	121	ASN
1	C	97	ASN
1	B	100	ASN
1	C	91	GLN

### 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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	188	-	4,4,4	0.52	0	6,6,6	0.21	0
2	SO4	A	189	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	A	190	-	4,4,4	0.07	0	6,6,6	0.11	0
2	SO4	B	188	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	C	188	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	D	188	-	4,4,4	0.20	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	188	-	-	0/0/0/0	0/0/0/0
2	SO4	A	189	-	-	0/0/0/0	0/0/0/0
2	SO4	A	190	-	-	0/0/0/0	0/0/0/0
2	SO4	B	188	-	-	0/0/0/0	0/0/0/0
2	SO4	C	188	-	-	0/0/0/0	0/0/0/0
2	SO4	D	188	-	-	0/0/0/0	0/0/0/0

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	156/187 (83%)	-0.03	1 (0%) 86 88	20, 34, 51, 70	0
1	B	173/187 (92%)	-0.02	1 (0%) 86 88	26, 43, 65, 67	0
1	C	164/187 (87%)	0.61	23 (14%) 3 3	41, 68, 91, 93	0
1	D	159/187 (85%)	-0.11	0 100 100	24, 42, 53, 68	0
All	All	652/748 (87%)	0.11	25 (3%) 38 40	20, 44, 78, 93	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	116	GLN	8.7
1	C	120	ALA	5.0
1	C	115	ARG	4.9
1	C	126	LEU	4.8
1	C	131	ILE	3.5

### 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	190	5/5	0.21	6.45	78,78,79,80	0
2	SO4	D	188	5/5	0.17	3.21	90,91,91,91	0
2	SO4	A	189	5/5	0.13	0.68	85,85,86,86	0
2	SO4	B	188	5/5	0.14	0.19	75,75,76,76	0
2	SO4	C	188	5/5	0.22	-0.24	101,102,102,102	0
2	SO4	A	188	5/5	0.13	-0.55	44,45,47,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.