



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:43 am BST

PDB ID : 1B6D  
Title : BENICE JONES PROTEIN DEL: AN ENTIRE IMMUNOGLOBULIN  
KAPPA LIGHT-CHAIN DIMER  
Authors : Roussel, A.; Spinelli, S.; Deret, S.; Aucouturier, P.; Cambillau, C.  
Deposited on : 1999-01-13  
Resolution : 2.74 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

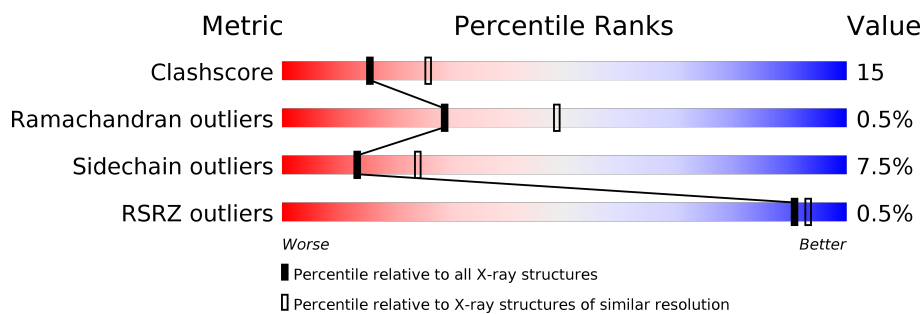
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.74 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	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 respectively. 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	212	 74% 23% •
1	B	212	 71% 25% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4305 atoms, of which 964 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 IMMUNOGLOBULIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	212	Total	C	H	N	O	S	8	0	0
			1995	1010	377	269	334	5			
1	B	212	Total	C	H	N	O	S	28	0	0
			1995	1010	377	269	334	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	ASN	CONFLICT	GB 4768677
A	31	SER	ASN	CONFLICT	GB 4768677
A	43	ALA	THR	CONFLICT	GB 4768677
A	49	HIS	TYR	CONFLICT	GB 4768677
A	50	ALA	GLY	CONFLICT	GB 4768677
A	53	SER	ASN	CONFLICT	GB 4768677
A	72	SER	ILE	CONFLICT	GB 4768677
A	83	LEU	ILE	CONFLICT	GB 4768677
A	93	SER	ASN	CONFLICT	GB 4768677
A	177	SER	ASN	CONFLICT	GB 4768677
B	30	SER	ASN	CONFLICT	GB 4768677
B	31	SER	ASN	CONFLICT	GB 4768677
B	43	ALA	THR	CONFLICT	GB 4768677
B	49	HIS	TYR	CONFLICT	GB 4768677
B	50	ALA	GLY	CONFLICT	GB 4768677
B	53	SER	ASN	CONFLICT	GB 4768677
B	72	SER	ILE	CONFLICT	GB 4768677
B	83	LEU	ILE	CONFLICT	GB 4768677
B	93	SER	ASN	CONFLICT	GB 4768677
B	177	SER	ASN	CONFLICT	GB 4768677

- Molecule 2 is water.

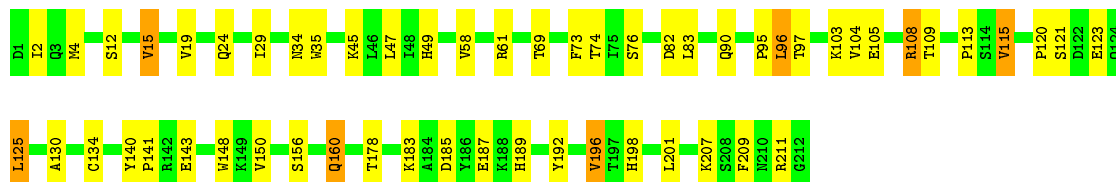
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	57	Total 171	H 114	O 57	0	0
2	B	48	Total 144	H 96	O 48	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

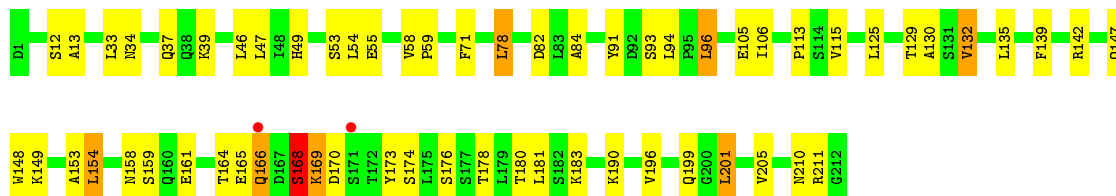
#### • Molecule 1: IMMUNOGLOBULIN

Chain A: 



#### • Molecule 1: IMMUNOGLOBULIN

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.60 Å   129.20 Å   86.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	6.00 – 2.74 19.57 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.4 (6.00-2.74) 94.4 (19.57-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.70 (at 2.75 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.207 ,      0.265 0.181 ,      (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.44	0/1652	0.69	0/2242
1	B	0.50	1/1652 (0.1%)	0.76	2/2242 (0.1%)
All	All	0.47	1/3304 (0.0%)	0.73	2/4484 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	GLU	C-N	-7.62	1.16	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	SER	O-C-N	5.32	131.22	122.70
1	B	170	ASP	O-C-N	5.21	131.03	122.70

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	1618	377	1569	42	0
1	B	1618	377	1568	52	0
2	A	57	114	0	10	1
2	B	48	96	0	1	0
All	All	3341	964	3137	93	1

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 15.

All (93) 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:34:ASN:ND2	1:A:49:HIS:HA	1.73	1.02
1:B:34:ASN:HD21	1:B:49:HIS:HD2	1.17	0.88
1:A:34:ASN:HD22	1:A:49:HIS:HA	1.40	0.86
1:B:34:ASN:HD21	1:B:49:HIS:CD2	1.95	0.85
1:B:34:ASN:ND2	1:B:49:HIS:HD2	1.75	0.84
1:B:54:LEU:HG	1:B:58:VAL:CG2	2.07	0.83
1:B:199:GLN:OE1	2:B:260:HOH:O	1.97	0.81
1:B:54:LEU:HG	1:B:58:VAL:HG23	1.62	0.79
1:A:34:ASN:HD21	1:A:49:HIS:CD2	2.03	0.76
1:B:166:GLN:NE2	1:B:173:TYR:CZ	2.54	0.74
1:B:166:GLN:NE2	1:B:173:TYR:CE2	2.54	0.74
1:A:115:VAL:HG11	1:A:196:VAL:HG11	1.70	0.73
1:B:34:ASN:ND2	1:B:49:HIS:CD2	2.56	0.71
1:A:183:LYS:O	1:A:187:GLU:HG2	1.94	0.67
1:A:34:ASN:HD21	1:A:49:HIS:HA	1.60	0.66
1:B:142:ARG:HB2	1:B:173:TYR:CZ	2.31	0.66
1:B:164:THR:HG22	1:B:174:SER:H	1.63	0.63
1:B:147:GLN:CG	1:B:154:LEU:HD21	2.31	0.61
1:B:201:LEU:HG	1:B:205:VAL:HG23	1.83	0.61
1:B:78:LEU:HD23	1:B:82:ASP:HB2	1.85	0.59
1:B:149:LYS:HA	1:B:153:ALA:O	2.04	0.57
1:A:15:VAL:HG13	2:A:255:HOH:O	2.04	0.57
1:B:132:VAL:HG22	1:B:148:TRP:CH2	2.40	0.57
1:A:49:HIS:HE1	2:A:233:HOH:O	1.88	0.56
1:A:61:ARG:HB2	1:A:76:SER:OG	2.04	0.56
1:B:190:LYS:NZ	1:B:211:ARG:NH2	2.54	0.55
1:A:95:PRO:O	1:A:97:THR:HG23	2.06	0.55
1:A:96:LEU:HD22	1:A:96:LEU:H	1.74	0.53
1:A:189:HIS:O	1:A:211:ARG:HD3	2.09	0.53
1:B:159:SER:HA	1:B:178:THR:O	2.09	0.52
1:A:24:GLN:HA	1:A:69:THR:O	2.11	0.51
1:B:142:ARG:HB2	1:B:173:TYR:CE2	2.45	0.51
1:B:33:LEU:HD22	1:B:71:PHE:CG	2.45	0.51
1:B:78:LEU:CD2	1:B:82:ASP:HB2	2.40	0.51
1:A:120:PRO:HG2	1:A:130:ALA:HB1	1.93	0.50
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.46	0.50
1:A:45:LYS:HE2	2:A:248:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:SER:HA	1:B:105:GLU:O	2.12	0.50
1:A:115:VAL:HG11	1:A:196:VAL:CG1	2.39	0.48
1:B:166:GLN:NE2	1:B:173:TYR:CD2	2.80	0.48
1:B:34:ASN:HB3	1:B:46:LEU:HD11	1.95	0.48
1:A:35:TRP:CE2	1:A:73:PHE:HB2	2.49	0.48
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.47	0.47
1:B:142:ARG:O	1:B:142:ARG:HG2	2.15	0.47
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.50	0.47
1:B:94:LEU:HD23	1:B:96:LEU:HD13	1.97	0.47
1:A:12:SER:HA	1:A:105:GLU:O	2.16	0.46
1:B:161:GLU:HA	1:B:176:SER:O	2.14	0.46
1:B:166:GLN:NE2	1:B:173:TYR:CE1	2.83	0.46
1:B:13:ALA:O	1:B:106:ILE:HD12	2.16	0.46
1:A:105:GLU:HG2	2:A:217:HOH:O	2.15	0.46
1:B:13:ALA:O	1:B:106:ILE:HA	2.16	0.46
1:B:34:ASN:OD1	1:B:91:TYR:CD2	2.69	0.46
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.97	0.45
1:B:49:HIS:O	1:B:53:SER:HB2	2.15	0.45
1:A:160:GLN:HG2	1:A:178:THR:HB	1.97	0.45
1:A:125:LEU:HD11	1:A:130:ALA:HB2	1.99	0.45
1:B:190:LYS:HZ3	1:B:211:ARG:NH2	2.16	0.44
1:A:34:ASN:HD21	1:A:49:HIS:CG	2.33	0.44
1:B:129:THR:HG22	1:B:130:ALA:N	2.31	0.44
1:A:4:MET:SD	1:A:90:GLN:HB3	2.57	0.44
1:A:134:CYS:HB2	1:A:148:TRP:CZ2	2.52	0.44
1:B:190:LYS:HZ1	1:B:211:ARG:NH2	2.15	0.44
1:B:39:LYS:HD3	1:B:84:ALA:HB2	2.00	0.43
1:A:108:ARG:HD3	1:A:109:THR:O	2.18	0.43
1:B:164:THR:O	1:B:164:THR:HG23	2.18	0.43
1:B:115:VAL:HA	1:B:135:LEU:O	2.19	0.43
1:A:143:GLU:HB2	2:A:229:HOH:O	2.17	0.43
1:B:113:PRO:HB3	1:B:139:PHE:HB3	2.00	0.43
1:B:34:ASN:HB3	1:B:46:LEU:CD1	2.49	0.43
1:A:108:ARG:HD2	1:A:140:TYR:CG	2.54	0.43
1:A:115:VAL:HG22	1:A:207:LYS:HG3	2.01	0.42
1:B:164:THR:HG22	1:B:174:SER:N	2.30	0.42
1:A:15:VAL:CG1	2:A:255:HOH:O	2.66	0.42
2:A:260:HOH:O	1:B:94:LEU:HD12	2.20	0.42
1:B:132:VAL:HG22	1:B:148:TRP:CZ3	2.54	0.41
1:B:125:LEU:O	1:B:183:LYS:HD2	2.20	0.41
1:B:58:VAL:HA	1:B:59:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLU:O	1:A:211:ARG:NH1	2.53	0.41
1:A:47:LEU:HA	1:A:58:VAL:HG21	2.02	0.41
1:A:19:VAL:O	1:A:74:THR:HA	2.20	0.41
1:B:147:GLN:HG2	1:B:154:LEU:HD21	2.01	0.41
1:B:55:GLU:O	1:B:58:VAL:HG22	2.20	0.41
1:A:49:HIS:CE1	2:A:233:HOH:O	2.69	0.41
2:A:260:HOH:O	1:B:94:LEU:CD1	2.68	0.41
1:A:34:ASN:HD21	1:A:49:HIS:HD2	1.60	0.41
1:A:96:LEU:HD22	1:B:46:LEU:HD22	2.03	0.41
1:B:201:LEU:HG	1:B:205:VAL:CG2	2.49	0.40
1:A:125:LEU:CD1	1:A:130:ALA:HB2	2.51	0.40
1:A:2:ILE:HD13	1:A:29:ILE:HG22	2.04	0.40
1:A:15:VAL:O	2:A:264:HOH:O	2.22	0.40
1:B:180:THR:O	1:B:181:LEU:HD23	2.22	0.40
1:A:141:PRO:O	1:A:198:HIS:HE1	2.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:263:HOH:H2	2:A:263:HOH:H2[3_655]	1.01	0.59

## 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	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
1	B	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	15	28
All	All	420/424 (99%)	396 (94%)	22 (5%)	2 (0%)	29	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	LYS
1	B	168	SER

### 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	186/186 (100%)	170 (91%)	16 (9%)	10	19
1	B	186/186 (100%)	174 (94%)	12 (6%)	17	30
All	All	372/372 (100%)	344 (92%)	28 (8%)	13	24

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	83	LEU
1	A	96	LEU
1	A	103	LYS
1	A	104	VAL
1	A	108	ARG
1	A	115	VAL
1	A	121	SER
1	A	123	GLU
1	A	125	LEU
1	A	150	VAL
1	A	156	SER
1	A	160	GLN
1	A	185	ASP
1	A	196	VAL
1	A	201	LEU
1	B	78	LEU
1	B	93	SER
1	B	96	LEU
1	B	132	VAL
1	B	154	LEU
1	B	158	ASN

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Mol	Chain	Res	Type
1	B	166	GLN
1	B	168	SER
1	B	169	LYS
1	B	196	VAL
1	B	201	LEU
1	B	210	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	34	ASN
1	A	49	HIS
1	A	89	GLN
1	A	137	ASN
1	A	189	HIS
1	A	198	HIS
1	B	34	ASN
1	B	49	HIS
1	B	89	GLN
1	B	155	GLN
1	B	158	ASN
1	B	166	GLN
1	B	199	GLN
1	B	210	ASN

### 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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	165:GLU	C	166:GLN	N	1.16

## 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	211/212 (99%)	-0.49	0	100   100	3, 18, 47, 57	4 (1%)
1	B	211/212 (99%)	-0.37	2 (0%)	84   88	3, 26, 49, 67	5 (2%)
All	All	422/424 (99%)	-0.43	2 (0%)	91   93	3, 22, 49, 67	9 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	GLN	3.2
1	B	171	SER	2.8

### 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.