



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 07:01 AM EDT

PDB ID : 7UC8  
Title : Pfs230 D1 domain in complex with 230AS-73  
Authors : Tang, W.K.; Tolia, N.H.  
Deposited on : 2022-03-16  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

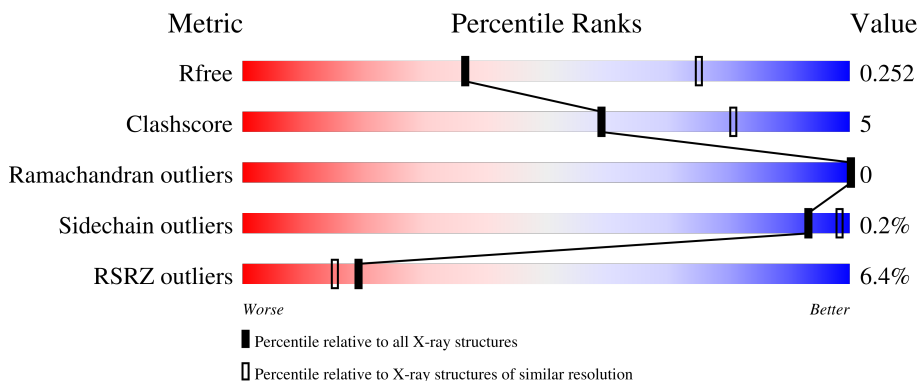
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of 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	345	
1	B	345	
1	C	345	
2	H	264	
2	I	264	

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Mol	Chain	Length	Quality of chain
2	J	264	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (7%), a large green segment (73%), a yellow segment (16%), and a small grey segment (11%).</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25072 atoms, of which 12487 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 Gametocyte surface protein P230.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	297	4802	1545	2407	373	465	12	0	0	0
1	B	296	4790	1541	2403	372	462	12	0	0	0
1	C	296	4790	1541	2403	372	462	12	0	0	0

- Molecule 2 is a protein called 230AS-73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	H	234	3555	1142	1758	305	345	5	0	0	0
2	I	234	3555	1142	1758	305	345	5	0	0	0
2	J	234	3555	1142	1758	305	345	5	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	9	Total	O	0	0
			9	9		

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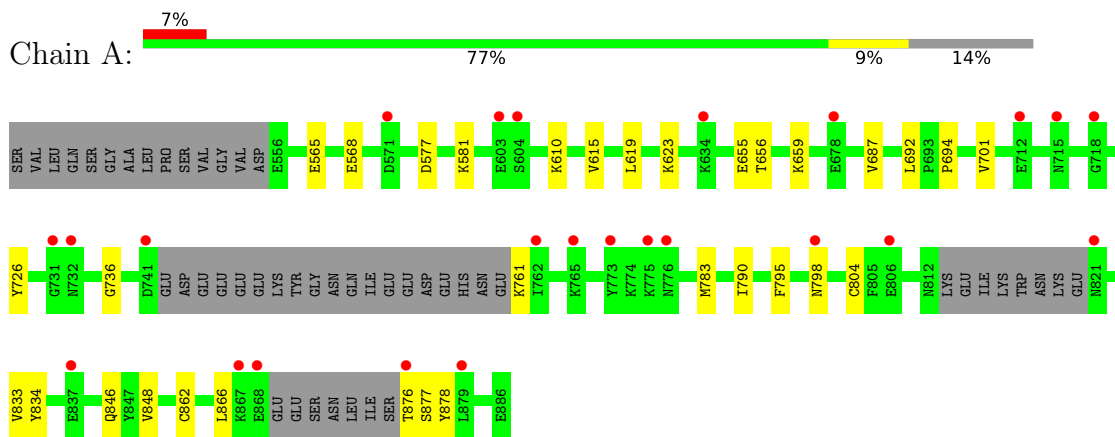
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total O 2 2	0	0
4	H	4	Total O 4 4	0	0
4	I	3	Total O 3 3	0	0

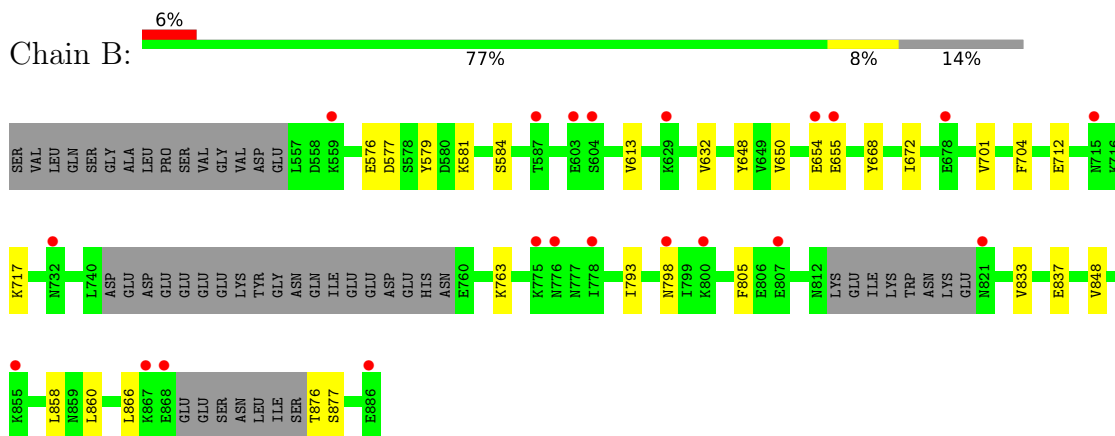
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

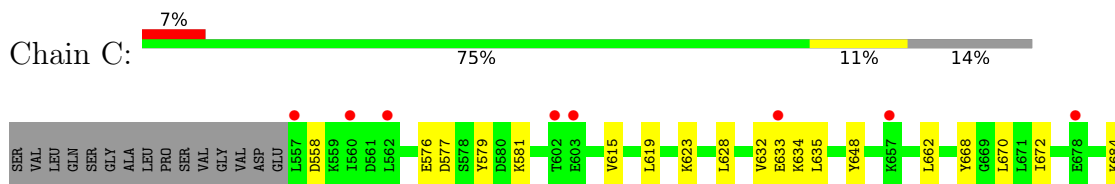
- Molecule 1: Gametocyte surface protein P230

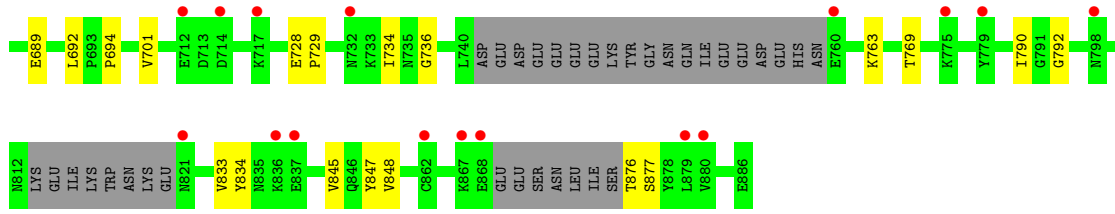


- Molecule 1: Gametocyte surface protein P230

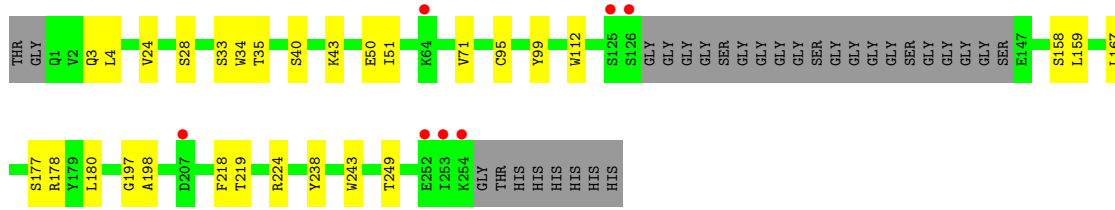
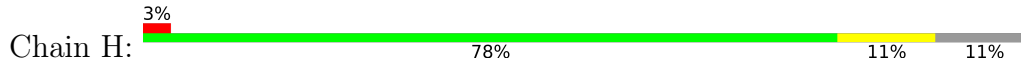


- Molecule 1: Gametocyte surface protein P230

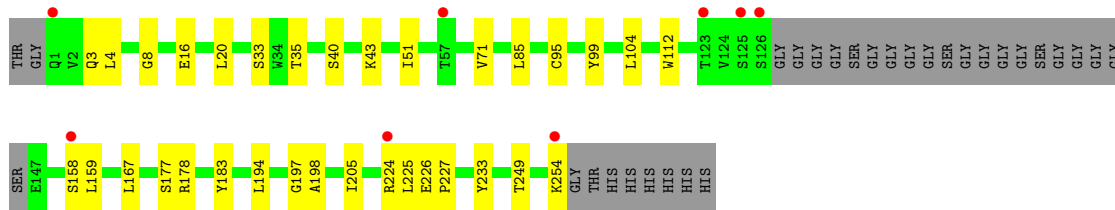
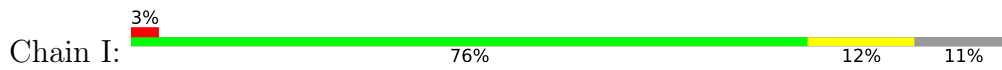




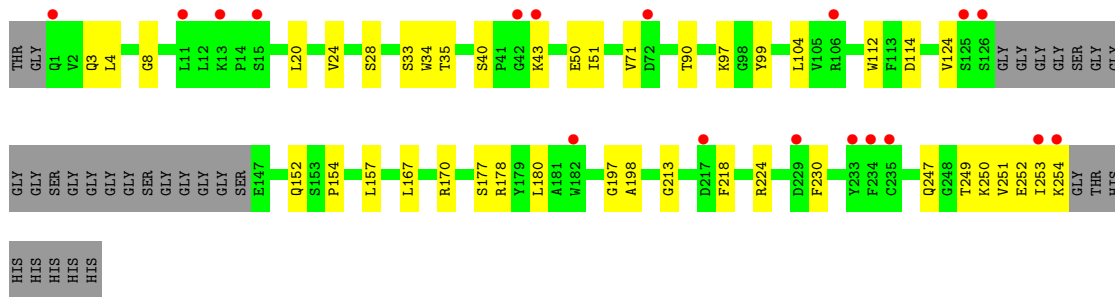
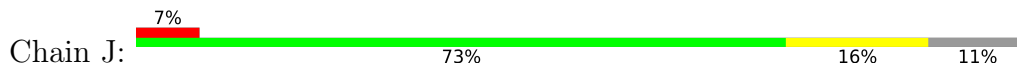
● Molecule 2: 230AS-73



● Molecule 2: 230AS-73



● Molecule 2: 230AS-73



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.46Å 89.46Å 225.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.90 19.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.85-2.90) 99.8 (19.85-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.88Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.215 , 0.252 0.215 , 0.252	Depositor DCC
$R_{free}$ test set	2024 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.044 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.51% 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](#)

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

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	0.28	0/2441	0.52	0/3295
1	B	0.28	0/2433	0.52	0/3284
1	C	0.28	0/2433	0.52	0/3284
2	H	0.30	0/1842	0.56	0/2505
2	I	0.28	0/1842	0.55	0/2505
2	J	0.28	0/1842	0.56	0/2505
All	All	0.28	0/12833	0.54	0/17378

There are no bond length outliers.

There are no bond angle outliers.

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	2395	2407	2406	24	0
1	B	2387	2403	2402	18	0
1	C	2387	2403	2402	23	0
2	H	1797	1758	1760	19	0
2	I	1797	1758	1760	20	0
2	J	1797	1758	1760	29	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	B	9	0	0	0	0
4	C	2	0	0	0	0
4	H	4	0	0	0	0
4	I	3	0	0	0	0
All	All	12585	12487	12490	117	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 5.

The worst 5 of 117 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:623:LYS:HE3	1:A:687:VAL:HG21	1.65	0.77
1:A:568:GLU:OE1	1:A:610:LYS:NZ	2.26	0.68
1:A:619:LEU:HD13	1:A:834:TYR:CE1	2.28	0.68
2:I:51:ILE:HD13	2:I:71:VAL:HG13	1.77	0.67
1:C:581:LYS:NZ	2:J:99:TYR:O	2.27	0.67

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	289/345 (84%)	277 (96%)	12 (4%)	0	100	100
1	B	288/345 (84%)	277 (96%)	11 (4%)	0	100	100
1	C	288/345 (84%)	279 (97%)	9 (3%)	0	100	100
2	H	230/264 (87%)	218 (95%)	12 (5%)	0	100	100
2	I	230/264 (87%)	220 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	230/264 (87%)	219 (95%)	11 (5%)	0	100	100
All	All	1555/1827 (85%)	1490 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	279/323 (86%)	279 (100%)	0	100	100
1	B	278/323 (86%)	278 (100%)	0	100	100
1	C	278/323 (86%)	278 (100%)	0	100	100
2	H	194/206 (94%)	193 (100%)	1 (0%)	88	96
2	I	194/206 (94%)	193 (100%)	1 (0%)	88	96
2	J	194/206 (94%)	193 (100%)	1 (0%)	88	96
All	All	1417/1587 (89%)	1414 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	224	ARG
2	I	224	ARG
2	J	224	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	297/345 (86%)	0.44	24 (8%) 12 9	25, 47, 88, 136	0
1	B	296/345 (85%)	0.39	21 (7%) 16 12	31, 52, 88, 127	0
1	C	296/345 (85%)	0.52	24 (8%) 12 9	38, 62, 97, 126	0
2	H	234/264 (88%)	0.12	7 (2%) 50 45	26, 38, 76, 120	0
2	I	234/264 (88%)	0.23	8 (3%) 45 40	29, 46, 77, 106	0
2	J	234/264 (88%)	0.40	18 (7%) 13 10	35, 56, 87, 122	0
All	All	1591/1827 (87%)	0.36	102 (6%) 19 15	25, 51, 88, 136	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	821	ASN	10.4
2	H	126	SER	9.6
1	B	821	ASN	8.4
1	C	712	GLU	7.3
2	J	126	SER	7.2

### 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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	C	901	1/1	0.71	0.27	65,65,65,65	0
3	NA	B	901	1/1	0.91	0.39	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.