



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2021 – 01:02 am BST

PDB ID : 6Y4A  
Title : Crystal structure of the M295I variant of Ssl1  
Authors : Mielenbrink, S.; Olbrich, A.; Urlacher, V.; Span, I.  
Deposited on : 2020-02-20  
Resolution : 1.78 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.

---

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	:	2.23.1
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)	:	2.23.1

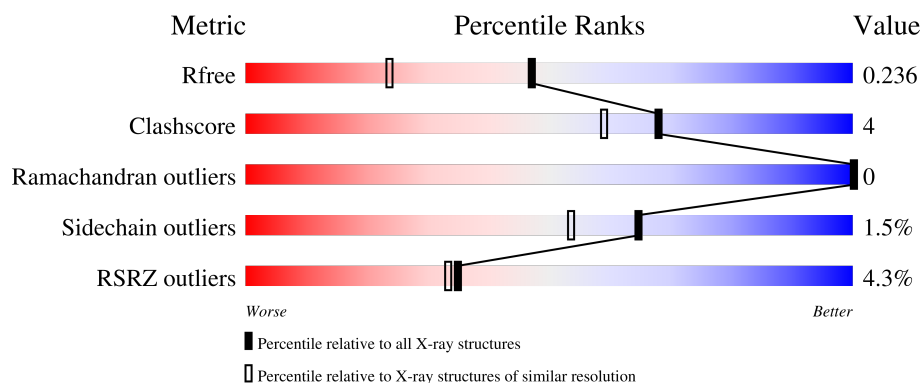
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	AAA	325	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 77%, yellow 77%, yellow 83%, grey 83%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>6%</span> <span>18%</span> </div> </div>
1	BBB	325	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, green 6%, green 75%, yellow 75%, yellow 83%, grey 83%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>75%</span> <span>8%</span> <span>18%</span> </div> </div>
1	CCC	325	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 74%, yellow 74%, yellow 83%, grey 83%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>74%</span> <span>9%</span> <span>17%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12879 atoms, of which 5977 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 Copper oxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	268	Total	C	H	N	O	S	105	0	0
			4060	1296	1985	381	389	9			
1	BBB	268	Total	C	H	N	O	S	105	0	0
			4060	1296	1985	381	389	9			
1	CCC	271	Total	C	H	N	O	S	106	0	0
			4110	1315	2007	384	395	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP B5HSR1
AAA	2	HIS	-	expression tag	UNP B5HSR1
AAA	3	HIS	-	expression tag	UNP B5HSR1
AAA	4	HIS	-	expression tag	UNP B5HSR1
AAA	5	HIS	-	expression tag	UNP B5HSR1
AAA	6	HIS	-	expression tag	UNP B5HSR1
AAA	7	HIS	-	expression tag	UNP B5HSR1
AAA	295	ILE	MET	engineered mutation	UNP B5HSR1
BBB	1	MET	-	initiating methionine	UNP B5HSR1
BBB	2	HIS	-	expression tag	UNP B5HSR1
BBB	3	HIS	-	expression tag	UNP B5HSR1
BBB	4	HIS	-	expression tag	UNP B5HSR1
BBB	5	HIS	-	expression tag	UNP B5HSR1
BBB	6	HIS	-	expression tag	UNP B5HSR1
BBB	7	HIS	-	expression tag	UNP B5HSR1
BBB	295	ILE	MET	engineered mutation	UNP B5HSR1
CCC	1	MET	-	initiating methionine	UNP B5HSR1
CCC	2	HIS	-	expression tag	UNP B5HSR1
CCC	3	HIS	-	expression tag	UNP B5HSR1
CCC	4	HIS	-	expression tag	UNP B5HSR1
CCC	5	HIS	-	expression tag	UNP B5HSR1
CCC	6	HIS	-	expression tag	UNP B5HSR1
CCC	7	HIS	-	expression tag	UNP B5HSR1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	295	ILE	MET	engineered mutation	UNP B5HSR1

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	3	Total Cu 3 3	0	0
2	BBB	3	Total Cu 3 3	0	0
2	CCC	3	Total Cu 3 3	0	0

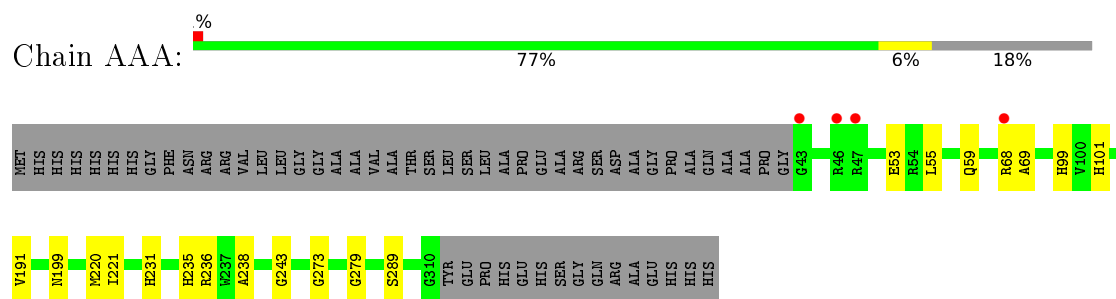
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	248	Total O 248 248	0	0
3	BBB	195	Total O 195 195	0	0
3	CCC	197	Total O 197 197	0	0

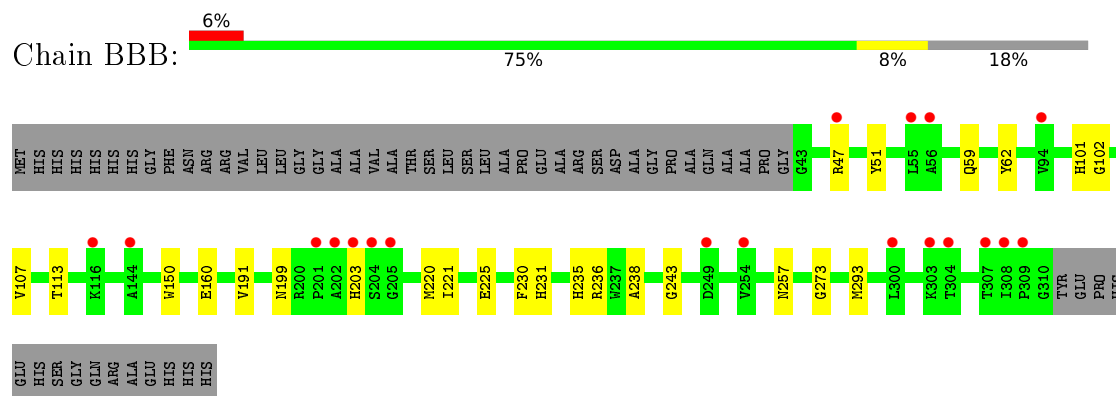
### 3 Residue-property plots [i](#)

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: Copper oxidase



- Molecule 1: Copper oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.38Å 104.32Å 162.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 1.78 48.03 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.08-1.78) 99.8 (48.03-1.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.186 , 0.228 0.196 , 0.236	Depositor DCC
$R_{free}$ test set	4262 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: CU

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	AAA	0.76	1/2132 (0.0%)	0.88	0/2893
1	BBB	0.74	0/2132	0.85	0/2893
1	CCC	0.74	0/2162	0.88	1/2935 (0.0%)
All	All	0.75	1/6426 (0.0%)	0.87	1/8721 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	53	GLU	CD-OE2	-5.83	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	241	ARG	NE-CZ-NH2	-5.86	117.37	120.30

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	AAA	2075	1985	1965	12	0
1	BBB	2075	1985	1965	21	0
1	CCC	2103	2007	1987	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AAA	3	0	0	0	0
2	BBB	3	0	0	0	0
2	CCC	3	0	0	0	0
3	AAA	248	0	0	0	0
3	BBB	195	0	0	0	0
3	CCC	197	0	0	2	0
All	All	6902	5977	5917	46	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 (46) 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:CCC:235:HIS:HE1	1:CCC:273:GLY:H	1.20	0.90
1:CCC:53:GLU:OE1	1:CCC:67:GLY:N	2.11	0.82
1:BBB:235:HIS:HE1	1:BBB:273:GLY:H	1.27	0.81
1:AAA:235:HIS:HE1	1:AAA:273:GLY:H	1.36	0.71
1:AAA:59:GLN:HE22	1:AAA:199:ASN:HB3	1.59	0.68
1:BBB:113:THR:OG1	1:BBB:160:GLU:OE1	2.08	0.68
1:CCC:203:HIS:HD2	1:CCC:293:MET:SD	2.16	0.68
1:BBB:59:GLN:HE22	1:BBB:199:ASN:HB3	1.66	0.60
1:BBB:203:HIS:CD2	1:BBB:293:MET:HE3	2.38	0.58
1:CCC:235:HIS:CE1	1:CCC:273:GLY:H	2.12	0.57
1:CCC:204:SER:HA	1:CCC:294:GLY:O	2.06	0.56
1:BBB:203:HIS:CE1	1:BBB:293:MET:HE2	2.41	0.55
1:AAA:55:LEU:HD21	1:AAA:69:ALA:HB3	1.89	0.54
1:CCC:46:ARG:NH1	1:CCC:82:ASP:OD2	2.41	0.53
1:BBB:203:HIS:CE1	1:BBB:293:MET:CE	2.92	0.52
1:CCC:102:GLY:HA3	1:CCC:150:TRP:CD2	2.45	0.52
1:BBB:231:HIS:CE1	1:CCC:101:HIS:CE1	2.98	0.51
1:CCC:191:VAL:HA	1:CCC:221:ILE:O	2.10	0.51
1:BBB:113:THR:CB	1:BBB:160:GLU:OE1	2.58	0.51
1:CCC:244:MET:CE	3:CCC:573:HOH:O	2.59	0.51
1:AAA:235:HIS:CE1	1:AAA:273:GLY:H	2.24	0.49
1:BBB:238:ALA:O	1:BBB:243:GLY:HA2	2.13	0.49
1:CCC:242:THR:HB	1:CCC:244:MET:HE2	1.95	0.48
1:BBB:203:HIS:CD2	1:BBB:293:MET:CE	2.97	0.48
1:CCC:244:MET:HE2	3:CCC:573:HOH:O	2.12	0.48
1:BBB:203:HIS:ND1	1:BBB:293:MET:HE2	2.29	0.48
1:BBB:102:GLY:HA3	1:BBB:150:TRP:CD2	2.49	0.47

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:47:ARG:HA	1:CCC:85:HIS:O	2.15	0.47
1:BBB:51:TYR:O	1:BBB:62:TYR:HA	2.16	0.45
1:BBB:203:HIS:CG	1:BBB:293:MET:HE2	2.52	0.45
1:AAA:289:SER:OG	1:BBB:225:GLU:OE1	2.31	0.45
1:BBB:191:VAL:HA	1:BBB:221:ILE:O	2.17	0.45
1:BBB:59:GLN:NE2	1:BBB:199:ASN:HB3	2.31	0.44
1:BBB:203:HIS:NE2	1:BBB:293:MET:CE	2.82	0.43
1:CCC:290:HIS:HB3	1:CCC:295:ILE:HD12	2.00	0.43
1:AAA:238:ALA:O	1:AAA:243:GLY:HA2	2.18	0.43
1:BBB:230:PHE:O	1:BBB:257:ASN:HA	2.19	0.43
1:AAA:279:GLY:HA3	1:BBB:107:VAL:HG11	2.01	0.42
1:AAA:191:VAL:HA	1:AAA:221:ILE:O	2.20	0.41
1:CCC:156:VAL:HG12	1:CCC:156:VAL:O	2.20	0.41
1:CCC:238:ALA:O	1:CCC:243:GLY:HA2	2.19	0.41
1:AAA:59:GLN:NE2	1:AAA:199:ASN:HD22	2.18	0.41
1:CCC:44:GLU:OE2	1:CCC:46:ARG:NH2	2.54	0.41
1:AAA:101:HIS:CE1	1:CCC:231:HIS:CE1	3.09	0.40
1:AAA:59:GLN:NE2	1:AAA:199:ASN:HB3	2.30	0.40
1:AAA:231:HIS:CE1	1:BBB:101:HIS:CE1	3.09	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	AAA	266/325 (82%)	260 (98%)	6 (2%)	0	100	100
1	BBB	266/325 (82%)	258 (97%)	8 (3%)	0	100	100
1	CCC	269/325 (83%)	263 (98%)	6 (2%)	0	100	100
All	All	801/975 (82%)	781 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	215/256 (84%)	211 (98%)	4 (2%)	57	43
1	BBB	215/256 (84%)	212 (99%)	3 (1%)	67	56
1	CCC	218/256 (85%)	215 (99%)	3 (1%)	67	56
All	All	648/768 (84%)	638 (98%)	10 (2%)	65	53

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	68	ARG
1	AAA	99	HIS
1	AAA	220	MET
1	AAA	236	ARG
1	BBB	47	ARG
1	BBB	220	MET
1	BBB	236	ARG
1	CCC	47	ARG
1	CCC	200	ARG
1	CCC	220	MET

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

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 ⓘ

### 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	AAA	268/325 (82%)	-0.03	4 (1%) 73 73	15, 23, 36, 58	14 (5%)
1	BBB	268/325 (82%)	0.42	19 (7%) 16 15	18, 29, 51, 73	14 (5%)
1	CCC	271/325 (83%)	0.34	12 (4%) 34 32	18, 28, 51, 89	14 (5%)
All	All	807/975 (82%)	0.24	35 (4%) 35 33	15, 26, 50, 89	42 (5%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	203	HIS	5.2
1	CCC	58	GLY	5.0
1	BBB	204	SER	5.0
1	CCC	203	HIS	4.5
1	CCC	202	ALA	4.5
1	CCC	57	ASP	4.3
1	BBB	56	ALA	4.1
1	AAA	43	GLY	3.7
1	BBB	47	ARG	3.7
1	CCC	204	SER	3.6
1	BBB	308	ILE	3.6
1	CCC	55	LEU	3.6
1	BBB	201	PRO	3.5
1	BBB	55	LEU	3.4
1	BBB	94	VAL	3.3
1	CCC	56	ALA	3.1
1	BBB	202	ALA	3.0
1	BBB	205	GLY	3.0
1	CCC	114	LEU	2.7
1	CCC	156	VAL	2.7
1	AAA	68	ARG	2.6
1	BBB	307	THR	2.6
1	AAA	47	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	BBB	303	LYS	2.5
1	BBB	249	ASP	2.5
1	BBB	116	LYS	2.5
1	BBB	254	VAL	2.5
1	BBB	304	THR	2.4
1	CCC	68	ARG	2.3
1	BBB	144	ALA	2.3
1	CCC	201	PRO	2.3
1	AAA	46	ARG	2.3
1	CCC	95	ARG	2.1
1	BBB	300	LEU	2.0
1	BBB	309	PRO	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 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
2	CU	BBB	402	1/1	0.98	0.07	37,37,37,37	0
2	CU	BBB	401	1/1	0.99	0.09	27,27,27,27	0
2	CU	AAA	402	1/1	0.99	0.06	30,30,30,30	0
2	CU	BBB	403	1/1	0.99	0.10	26,26,26,26	0
2	CU	CCC	402	1/1	0.99	0.07	30,30,30,30	0
2	CU	CCC	403	1/1	0.99	0.08	29,29,29,29	0
2	CU	CCC	401	1/1	1.00	0.10	23,23,23,23	0
2	CU	AAA	403	1/1	1.00	0.06	23,23,23,23	0
2	CU	AAA	401	1/1	1.00	0.09	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.