



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:19 AM BST

PDB ID : 6YH0  
Title : Marasmius oreades agglutinin (MOA) in complex with the truncated PVPRAHS synthetic substrate  
Authors : Cordara, G.; Manna, D.; Krengel, U.  
Deposited on : 2020-03-28  
Resolution : 1.56 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

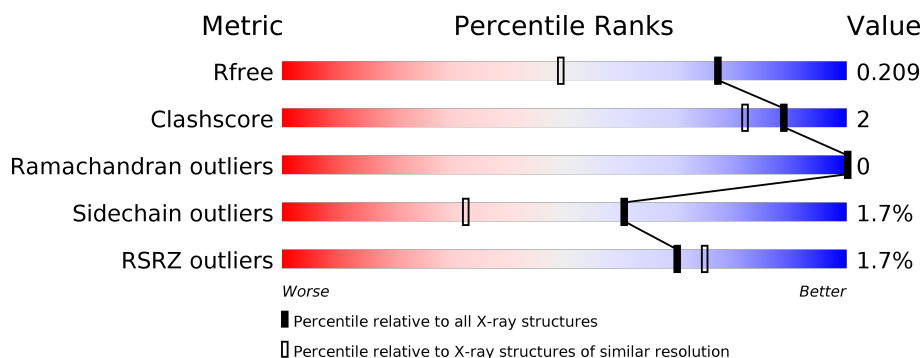
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

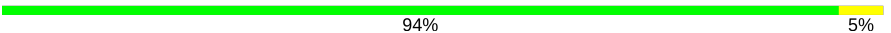

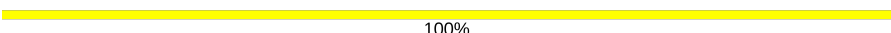
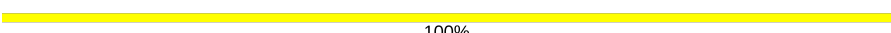
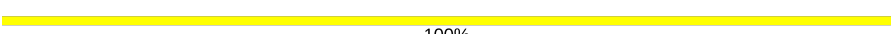
The reported resolution of this entry is 1.56 Å.

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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	AAA	293	 94% 5%
2	EEE	7	 57% 29% 14% 14% 43%
3	CCC	3	 100%
4	CcC	2	 100%
5	CeC	3	 100%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 2680 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 Agglutinin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	292	Total	As	C	N	O	S	2	13	0
			2351	2	1501	393	446	9			

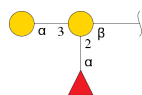
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	257	ALA	HIS	engineered mutation	UNP Q8X123

- Molecule 2 is a protein called PRO-VAL-PRO-ARG.

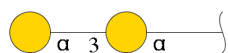
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	EEE	4	Total	C	N	O	0	0	0
			32	21	7	4			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose.



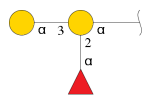
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	CCC	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 4 is an oligosaccharide called alpha-D-galactopyranose-(1-3)-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	CcC	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	CeC	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	2	Total	Ca	0	0
			2	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	2	Total	Na	0	0
			2	2		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	202	Total	O	0	0
			202	202		
9	EEE	1	Total	O	0	0
			1	1		

### 3 Residue-property plots


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.

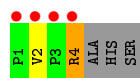
- Molecule 1: Agglutinin

Chain AAA: 



- Molecule 2: PRO-VAL-PRO-ARG

Chain EEE: 



- Molecule 3: alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain CCC: 

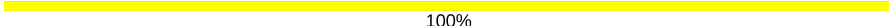


- Molecule 4: alpha-D-galactopyranose-(1-3)-alpha-D-galactopyranose

Chain CcC: 



- Molecule 5: alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]alpha-D-galactopyranose

Chain CeC: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.24Å 121.24Å 99.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.88 – 1.56 51.83 – 1.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.88-1.56) 100.0 (51.83-1.56)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.174 , 0.199 0.185 , 0.209	Depositor DCC
$R_{free}$ test set	3149 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2680	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: CZZ, CL, GLA, CA, GAL, FUC, 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	AAA	0.80	1/2440 (0.0%)	0.87	0/3315
2	EEE	0.58	0/33	1.15	0/44
All	All	0.80	1/2473 (0.0%)	0.87	0/3359

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	144	GLU	CD-OE1	5.12	1.31	1.25

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	AAA	2351	0	2235	8	1
2	EEE	32	0	38	1	0
3	CCC	33	0	29	0	0
4	CcC	23	0	21	0	0
5	CeC	33	0	30	0	0
6	AAA	2	0	0	0	0
7	AAA	2	0	0	0	0
8	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AAA	202	0	0	1	0
9	EEE	1	0	0	0	0
All	All	2680	0	2353	9	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 2.

All (9) 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:AAA:4[A]:ARG:NH2	1:AAA:162:GLU:OE2	2.26	0.68
2:EEE:2:VAL:O	2:EEE:4:ARG:NH2	2.30	0.65
1:AAA:4[A]:ARG:HD3	9:AAA:536:HOH:O	2.14	0.47
1:AAA:53:ILE:HG13	1:AAA:99:LEU:HD22	1.97	0.46
1:AAA:169[A]:ARG:HD2	1:AAA:268:ALA:O	2.17	0.45
1:AAA:169[B]:ARG:HD2	1:AAA:269:ASP:OD1	2.19	0.43
1:AAA:215[A]:CZZ:O1	1:AAA:276:GLN:NE2	2.48	0.43
1:AAA:169[A]:ARG:NH1	1:AAA:268:ALA:O	2.38	0.41
1:AAA:244:GLY:HA3	1:AAA:261:PHE:CE1	2.56	0.41

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)
1:AAA:55:ASN:ND2	1:AAA:55:ASN:ND2[8_555]	2.13	0.07

## 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	301/293 (103%)	293 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	EEE	2/7 (29%)	1 (50%)	1 (50%)	0	100	100
All	All	303/300 (101%)	294 (97%)	9 (3%)	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	243/232 (105%)	238 (98%)	5 (2%)	53	24
2	EEE	4/6 (67%)	3 (75%)	1 (25%)	0	0
All	All	247/238 (104%)	241 (98%)	6 (2%)	60	20

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	178[A]	ARG
1	AAA	178[B]	ARG
1	AAA	207[A]	LYS
1	AAA	207[B]	LYS
1	AAA	274	GLU
2	EEE	4	ARG

Some 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 ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CZZ	AAA	215[B]	1,2	3,7,8	1.11	0	0,7,9	0.00	-
1	CZZ	AAA	215[A]	1	3,7,8	1.23	1 (33%)	0,7,9	0.00	-

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
1	CZZ	AAA	215[B]	1,2	-	0/0/6/8	-
1	CZZ	AAA	215[A]	1	-	0/0/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	215[A]	CZZ	O-C	2.01	1.27	1.19

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	215[A]	CZZ	1	0

## 5.5 Carbohydrates

8 monosaccharides 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
3	GAL	CCC	1	3	12,12,12	1.46	1 (8%)	17,17,17	1.38	2 (11%)
3	FUC	CCC	2	3	10,10,11	0.98	0	14,14,16	1.13	1 (7%)
3	GLA	CCC	3	3	11,11,12	1.79	1 (9%)	15,15,17	1.51	2 (13%)
4	GLA	CcC	1	4	12,12,12	1.32	1 (8%)	17,17,17	1.45	3 (17%)
4	GLA	CcC	2	4	11,11,12	0.81	0	15,15,17	1.34	1 (6%)
5	GLA	CeC	1	5	12,12,12	1.03	1 (8%)	17,17,17	1.24	1 (5%)
5	FUC	CeC	2	5	10,10,11	0.73	0	14,14,16	1.33	2 (14%)
5	GLA	CeC	3	5	11,11,12	1.15	1 (9%)	15,15,17	1.43	2 (13%)

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
3	GAL	CCC	1	3	-	0/2/22/22	0/1/1/1
3	FUC	CCC	2	3	-	-	0/1/1/1
3	GLA	CCC	3	3	-	0/2/19/22	0/1/1/1
4	GLA	CcC	1	4	-	0/2/22/22	0/1/1/1
4	GLA	CcC	2	4	-	0/2/19/22	0/1/1/1
5	GLA	CeC	1	5	-	1/2/22/22	0/1/1/1
5	FUC	CeC	2	5	-	-	0/1/1/1
5	GLA	CeC	3	5	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	3	GLA	C2-C3	4.83	1.59	1.52
3	CCC	1	GAL	O3-C3	3.71	1.51	1.43
5	CeC	1	GLA	C1-C2	2.24	1.57	1.52
5	CeC	3	GLA	O3-C3	2.16	1.48	1.43
4	CcC	1	GLA	O2-C2	2.05	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	3	GLA	O2-C2-C1	3.45	116.21	109.15
5	CeC	3	GLA	O3-C3-C2	-3.42	103.44	109.99
4	CcC	2	GLA	O5-C1-C2	-3.28	105.70	110.77
5	CeC	2	FUC	O2-C2-C3	-2.97	104.19	110.14
3	CCC	1	GAL	O2-C2-C1	-2.94	102.33	109.16
4	CcC	1	GLA	O3-C3-C4	2.93	117.12	110.35
3	CCC	3	GLA	O2-C2-C3	-2.89	104.34	110.14
3	CCC	1	GAL	O3-C3-C4	2.64	116.44	110.35
5	CeC	1	GLA	C4-C3-C2	-2.57	106.34	110.82
4	CcC	1	GLA	O3-C3-C2	-2.28	105.08	110.35
4	CcC	1	GLA	C6-C5-C4	2.27	118.33	113.00
3	CCC	2	FUC	O3-C3-C2	-2.08	106.01	109.99
5	CeC	3	GLA	C1-O5-C5	2.05	114.97	112.19
5	CeC	2	FUC	O2-C2-C1	2.02	113.28	109.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CeC	1	GLA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 ⓘ

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	291/293 (99%)	-0.59	1 (0%) 94 95	20, 26, 39, 65	0
2	EEE	4/7 (57%)	3.68	4 (100%) 0 0	60, 62, 72, 74	4 (100%)
All	All	295/300 (98%)	-0.54	5 (1%) 70 75	20, 26, 41, 74	4 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	EEE	2	VAL	6.3
1	AAA	55	ASN	4.1
2	EEE	3	PRO	3.6
2	EEE	4	ARG	2.8
2	EEE	1	PRO	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains

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
1	CZZ	AAA	215[B]	8/9	0.95	0.07	25,28,52,53	8
1	CZZ	AAA	215[A]	8/9	0.95	0.07	21,24,41,51	8

### 6.3 Carbohydrates

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( $\text{\AA}^2$ )	Q<0.9
4	GLA	CcC	1	12/12	0.86	0.19	28,36,48,53	0
4	GLA	CcC	2	11/12	0.89	0.28	41,46,47,48	0
5	FUC	CeC	2	10/11	0.93	0.07	29,37,43,44	0
5	GLA	CeC	3	11/12	0.97	0.04	21,25,28,29	0
5	GLA	CeC	1	12/12	0.97	0.04	20,21,25,28	0
3	GAL	CCC	1	12/12	0.97	0.05	18,20,22,23	0
3	GLA	CCC	3	11/12	0.97	0.06	18,20,21,22	0
3	FUC	CCC	2	10/11	0.98	0.06	21,25,27,29	0

## 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( $\text{\AA}^2$ )	Q<0.9
7	NA	AAA	303	1/1	0.92	0.12	41,41,41,41	1
7	NA	AAA	304	1/1	0.95	0.08	32,32,32,32	1
8	CL	AAA	305	1/1	0.98	0.05	34,34,34,34	1
6	CA	AAA	302	1/1	1.00	0.04	25,25,25,25	0
6	CA	AAA	301	1/1	1.00	0.05	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.