



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:08 PM BST

PDB ID : 5DZW  
Title : Protocadherin alpha 4 extracellular cadherin domains 1-4  
Authors : Goodman, K.M.; Bahna, F.; Mannepalli, S.; Honig, B.; Shapiro, L.  
Deposited on : 2015-09-26  
Resolution : 2.43 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  
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

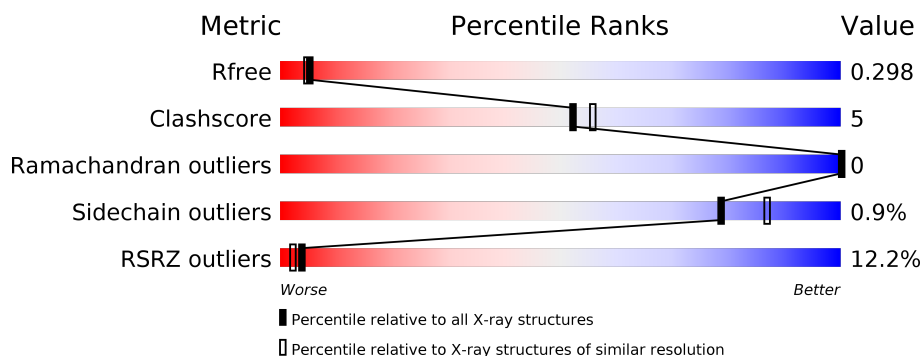
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	429	<div> <div>12%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3179 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.

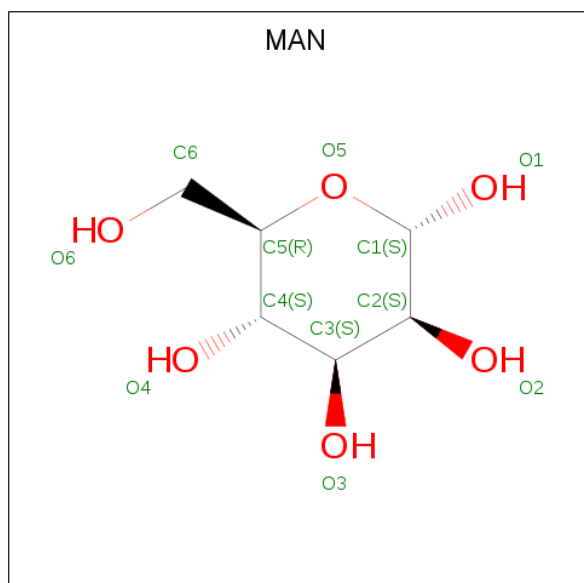
- Molecule 1 is a protein called Protocadherin alpha-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3113	1970	515	622	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

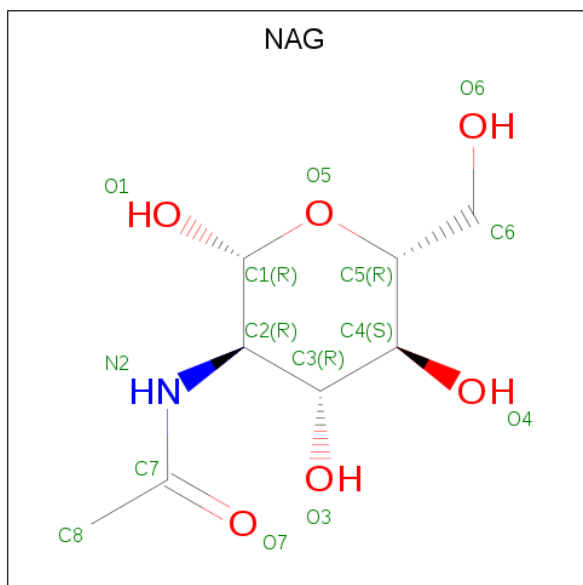
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	expression tag	UNP O88689
A	423	HIS	-	expression tag	UNP O88689
A	424	HIS	-	expression tag	UNP O88689
A	425	HIS	-	expression tag	UNP O88689
A	426	HIS	-	expression tag	UNP O88689
A	427	HIS	-	expression tag	UNP O88689
A	428	HIS	-	expression tag	UNP O88689
A	429	HIS	-	expression tag	UNP O88689

- Molecule 2 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	Ca	0	0
			9	9		

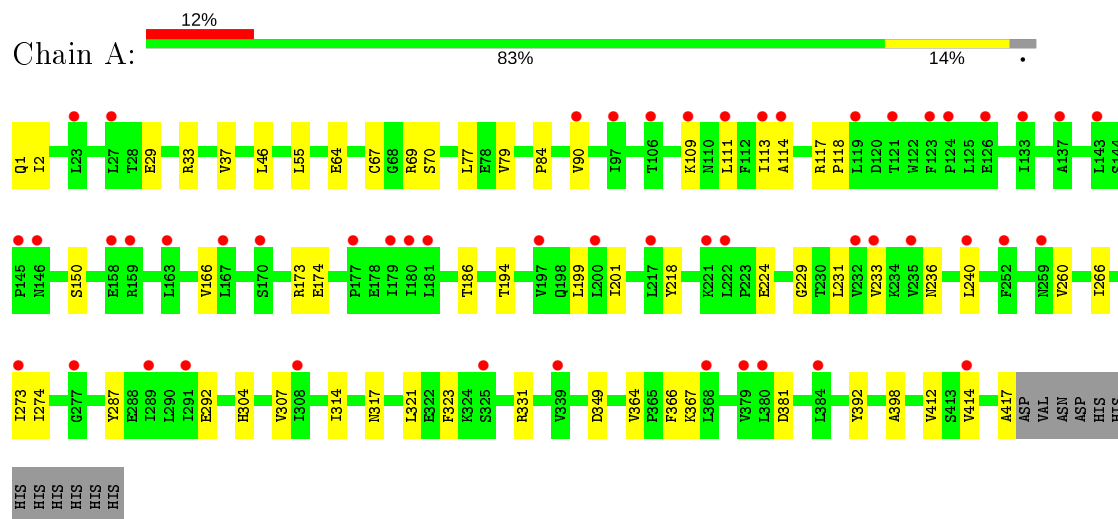
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		

### 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: Protocadherin alpha-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.48 Å   56.31 Å   173.67 Å 90.00°   99.05°   90.00°	Depositor
Resolution (Å)	29.57 – 2.43 44.71 – 2.43	Depositor EDS
% Data completeness (in resolution range)	54.9 (29.57-2.43) 55.3 (44.71-2.43)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.51 (at 2.42 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.266   ,   0.293 0.274   ,   0.298	Depositor DCC
$R_{free}$ test set	743 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	1.629	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	3179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, MAN

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	0.21	0/3169	0.38	0/4338

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

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	3113	0	3001	34	0
2	A	33	0	30	0	0
3	A	14	0	13	2	0
4	A	9	0	0	0	0
5	A	10	0	0	0	0
All	All	3179	0	3044	34	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.

All (34) 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:186:THR:HG22	1:A:194:THR:HG22	1.72	0.70
1:A:218:TYR:HB2	1:A:307:VAL:HG22	1.79	0.65
1:A:229:GLY:HA2	1:A:274:ILE:HD12	1.79	0.64
1:A:77:LEU:HB2	1:A:90:VAL:HG13	1.82	0.62
1:A:231:LEU:HA	1:A:274:ILE:HG22	1.87	0.57
1:A:113:ILE:HG23	1:A:117:ARG:HD2	1.87	0.57
1:A:174:GLU:HG2	1:A:240:LEU:HB3	1.85	0.56
1:A:317:ASN:ND2	1:A:349:ASP:OD1	2.39	0.54
1:A:111:LEU:HB2	1:A:201:ILE:HG12	1.88	0.54
1:A:236:ASN:HD22	3:A:504:NAG:H61	1.74	0.52
1:A:367:LYS:HB2	1:A:381:ASP:HB2	1.91	0.50
1:A:331:ARG:HA	1:A:417:ALA:HB3	1.93	0.50
1:A:392:TYR:HB2	1:A:414:VAL:HB	1.96	0.48
1:A:67:CYS:HB3	1:A:70:SER:HB2	1.95	0.48
1:A:292:GLU:HG2	1:A:304:HIS:ND1	2.29	0.48
1:A:37:VAL:HG22	1:A:79:VAL:HG22	1.96	0.47
1:A:114:ALA:HB3	1:A:117:ARG:HG3	1.97	0.47
1:A:266:ILE:HB	1:A:273:ILE:HG13	1.97	0.47
1:A:233:VAL:HG12	1:A:273:ILE:HB	1.98	0.45
1:A:33:ARG:NH2	1:A:84:PRO:O	2.39	0.45
1:A:150:SER:HB2	1:A:166:VAL:HG13	1.99	0.44
1:A:323:PHE:CE2	1:A:412:VAL:HB	2.53	0.44
1:A:2:ILE:HG23	1:A:90:VAL:HB	1.98	0.44
1:A:364:VAL:HG12	1:A:366:PHE:H	1.82	0.44
1:A:29:GLU:OE2	1:A:33:ARG:NH1	2.50	0.44
1:A:64:GLU:OE1	1:A:64:GLU:N	2.43	0.43
1:A:109:LYS:HB3	1:A:199:LEU:HD23	2.00	0.43
1:A:224:GLU:HB3	1:A:314:ILE:HG12	2.01	0.42
1:A:46:LEU:HB3	1:A:55:LEU:HD11	2.01	0.42
1:A:321:LEU:HD21	1:A:398:ALA:HB2	2.01	0.42
1:A:46:LEU:HD12	1:A:77:LEU:HD11	2.03	0.41
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.84	0.41
1:A:260:VAL:HG22	1:A:287:TYR:HD1	1.86	0.41
1:A:236:ASN:ND2	3:A:504:NAG:H61	2.36	0.40

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	415/429 (97%)	396 (95%)	19 (5%)	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	A	343/385 (89%)	340 (99%)	3 (1%)	78	87

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

Mol	Chain	Res	Type
1	A	1	GLN
1	A	69	ARG
1	A	173	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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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	MAN	A	501	1	11,11,12	0.70	0	15,15,17	1.11	2 (13%)
2	MAN	A	502	1	11,11,12	0.74	0	15,15,17	1.02	2 (13%)
2	MAN	A	503	1	11,11,12	0.62	0	15,15,17	1.23	2 (13%)
3	NAG	A	504	1	14,14,15	0.78	1 (7%)	17,19,21	0.97	1 (5%)

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	MAN	A	501	1	-	0/2/19/22	0/1/1/1
2	MAN	A	502	1	-	0/2/19/22	0/1/1/1
2	MAN	A	503	1	-	1/2/19/22	0/1/1/1
3	NAG	A	504	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	NAG	O5-C1	2.74	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	NAG	C1-O5-C5	3.76	117.29	112.19
2	A	503	MAN	C1-O5-C5	3.34	116.71	112.19
2	A	501	MAN	C1-O5-C5	2.46	115.53	112.19
2	A	503	MAN	O2-C2-C3	-2.38	105.38	110.14
2	A	501	MAN	O2-C2-C3	-2.19	105.75	110.14
2	A	502	MAN	O2-C2-C3	-2.19	105.75	110.14
2	A	502	MAN	C1-O5-C5	2.14	115.08	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	NAG	2	0

## 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	A	417/429 (97%)	0.87	51 (12%) 4 2	18, 53, 86, 113	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	LEU	6.7
1	A	259	ASN	5.3
1	A	181	LEU	5.0
1	A	179	ILE	4.8
1	A	167	LEU	4.4
1	A	325	SER	4.3
1	A	111	LEU	3.8
1	A	159	ARG	3.8
1	A	277	GLY	3.7
1	A	158	GLU	3.7
1	A	200	LEU	3.6
1	A	123	PHE	3.4
1	A	126	GLU	3.4
1	A	197	VAL	3.3
1	A	180	ILE	3.2
1	A	133	ILE	3.2
1	A	137	ALA	3.2
1	A	233	VAL	3.1
1	A	106	THR	3.0
1	A	273	ILE	3.0
1	A	380	LEU	3.0
1	A	384	LEU	2.9
1	A	119	LEU	2.8
1	A	121	THR	2.8
1	A	90	VAL	2.8
1	A	414	VAL	2.6
1	A	143	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	109	LYS	2.6
1	A	289	ILE	2.5
1	A	163	LEU	2.5
1	A	145	PRO	2.4
1	A	114	ALA	2.4
1	A	235	VAL	2.4
1	A	291	ILE	2.3
1	A	221	LYS	2.3
1	A	177	PRO	2.3
1	A	113	ILE	2.3
1	A	97	ILE	2.3
1	A	339	VAL	2.2
1	A	217	LEU	2.2
1	A	379	VAL	2.2
1	A	170	SER	2.2
1	A	146	ASN	2.2
1	A	252	PHE	2.2
1	A	240	LEU	2.2
1	A	124	PRO	2.2
1	A	232	VAL	2.1
1	A	27	LEU	2.1
1	A	23	LEU	2.1
1	A	308	ILE	2.0
1	A	368	LEU	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	504	14/15	0.67	0.25	69,76,82,84	0
2	MAN	A	502	11/12	0.84	0.22	49,61,68,70	0
4	CA	A	506	1/1	0.86	0.23	40,40,40,40	0
2	MAN	A	503	11/12	0.93	0.11	48,55,58,59	0
4	CA	A	511	1/1	0.94	0.18	35,35,35,35	0
4	CA	A	510	1/1	0.95	0.18	34,34,34,34	0
2	MAN	A	501	11/12	0.95	0.16	25,33,48,53	0
4	CA	A	509	1/1	0.96	0.09	44,44,44,44	0
4	CA	A	507	1/1	0.97	0.23	42,42,42,42	0
4	CA	A	508	1/1	0.98	0.13	21,21,21,21	0
4	CA	A	513	1/1	0.98	0.23	15,15,15,15	0
4	CA	A	512	1/1	0.98	0.29	32,32,32,32	0
4	CA	A	505	1/1	0.98	0.24	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.