



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:07 am GMT

PDB ID : 3L9R  
Title : Crystal structure of bovine CD1b3 with endogenously bound ligands  
Authors : Zajonc, D.M.; Girardi, E.  
Deposited on : 2010-01-05  
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

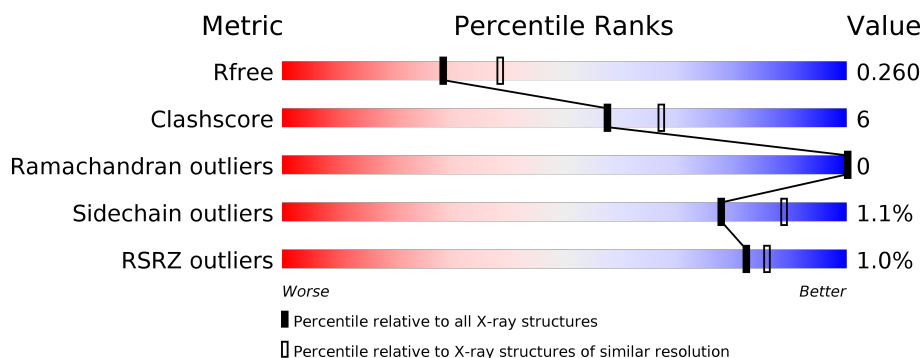
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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. 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	283	<div> <div style="width: 90%;"></div> <div style="width: 7%;"></div> <div style="width: 3%;"></div> </div> <div>90% 7% .</div>
1	C	283	<div> <div style="width: 85%;"></div> <div style="width: 11%;"></div> <div style="width: 4%;"></div> </div> <div>85% 11% .</div>
1	E	283	<div> <div style="width: 83%;"></div> <div style="width: 14%;"></div> <div style="width: 3%;"></div> </div> <div>83% 14% .</div>
1	G	283	<div> <div style="width: 86%;"></div> <div style="width: 11%;"></div> <div style="width: 3%;"></div> </div> <div>86% 11% .</div>
2	B	98	<div> <div style="width: 78%;"></div> <div style="width: 21%;"></div> <div style="width: 1%;"></div> </div> <div>78% 21% .</div>
2	D	98	<div> <div style="width: 92%;"></div> <div style="width: 8%;"></div> <div style="width: 0%;"></div> </div> <div>92% 8%</div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	98	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
2	H	98	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	L9R	A	284	-	-	-	X
5	L9R	E	285	-	-	-	X
6	GOL	C	285	-	-	-	X
8	L9Q	C	284	-	-	-	X
8	L9Q	G	289	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12721 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 CD1b3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2124	1355	364	395	10			
1	C	274	Total	C	N	O	S	0	0	0
			2114	1350	364	390	10			
1	E	275	Total	C	N	O	S	0	2	0
			2143	1364	367	401	11			
1	G	275	Total	C	N	O	S	0	0	0
			2125	1355	367	393	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	HIS	-	EXPRESSION TAG	UNP Q1L1H6
A	279	HIS	-	EXPRESSION TAG	UNP Q1L1H6
A	280	HIS	-	EXPRESSION TAG	UNP Q1L1H6
A	281	HIS	-	EXPRESSION TAG	UNP Q1L1H6
A	282	HIS	-	EXPRESSION TAG	UNP Q1L1H6
A	283	HIS	-	EXPRESSION TAG	UNP Q1L1H6
C	278	HIS	-	EXPRESSION TAG	UNP Q1L1H6
C	279	HIS	-	EXPRESSION TAG	UNP Q1L1H6
C	280	HIS	-	EXPRESSION TAG	UNP Q1L1H6
C	281	HIS	-	EXPRESSION TAG	UNP Q1L1H6
C	282	HIS	-	EXPRESSION TAG	UNP Q1L1H6
C	283	HIS	-	EXPRESSION TAG	UNP Q1L1H6
E	278	HIS	-	EXPRESSION TAG	UNP Q1L1H6
E	279	HIS	-	EXPRESSION TAG	UNP Q1L1H6
E	280	HIS	-	EXPRESSION TAG	UNP Q1L1H6
E	281	HIS	-	EXPRESSION TAG	UNP Q1L1H6
E	282	HIS	-	EXPRESSION TAG	UNP Q1L1H6
E	283	HIS	-	EXPRESSION TAG	UNP Q1L1H6
G	278	HIS	-	EXPRESSION TAG	UNP Q1L1H6
G	279	HIS	-	EXPRESSION TAG	UNP Q1L1H6
G	280	HIS	-	EXPRESSION TAG	UNP Q1L1H6

*Continued on next page...*

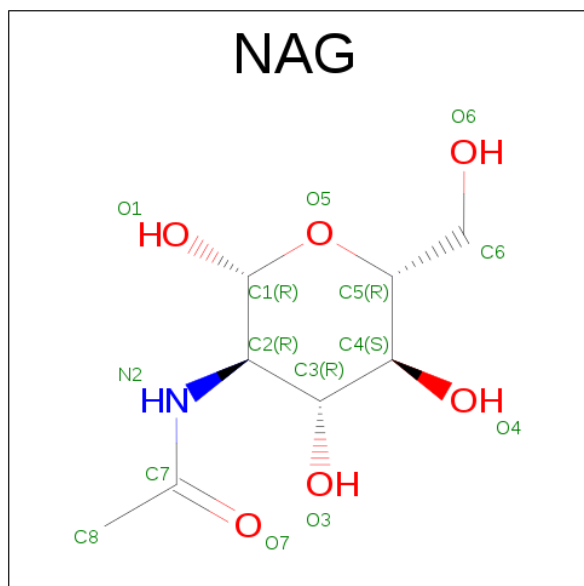
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	281	HIS	-	EXPRESSION TAG	UNP Q1L1H6
G	282	HIS	-	EXPRESSION TAG	UNP Q1L1H6
G	283	HIS	-	EXPRESSION TAG	UNP Q1L1H6

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			782	501	134	145	2			
2	D	98	Total	C	N	O	S	0	0	0
			780	500	134	144	2			
2	F	98	Total	C	N	O	S	0	0	0
			778	501	132	143	2			
2	H	98	Total	C	N	O	S	0	0	0
			786	504	134	146	2			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (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			
3	C	1	Total	C	N	O		0	0
			14	8	1	5			
3	E	1	Total	C	N	O		0	0
			14	8	1	5			

Continued on next page...

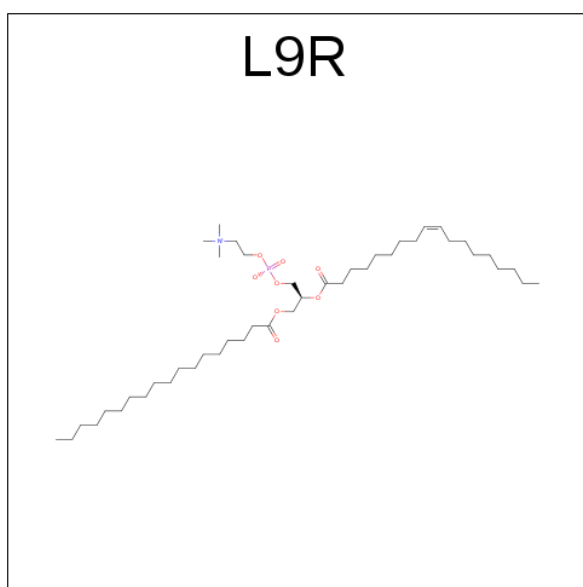
Continued from previous page...

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

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	6	Total	C	N	O	0	0
			70	40	2	28		

- Molecule 5 is (2S)-3-(OCTADECANOYLOXY)-2-[(9Z)-OCTADEC-9-ENOYLOXY]PROPYL 2-(TRIMETHYLAMMONIO)ETHYL PHOSPHATE (three-letter code: L9R) (formula:  $C_{44}H_{86}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
5	E	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

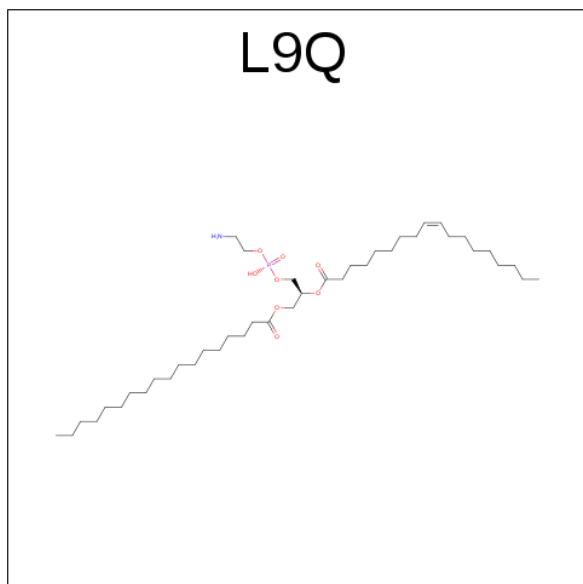


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	5	Total	C	N	O	0	0
			59	34	2	23		
7	E	5	Total	C	N	O	0	0
			59	34	2	23		
7	G	5	Total	C	N	O	0	0
			59	34	2	23		

- Molecule 8 is (1S)-2-{[(S)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(OCTADECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: L9Q) (formula: C<sub>41</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
8	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	1	Total	Cl	0	0
			1	1		
9	C	1	Total	Cl	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	93	Total	O	0	0
			93	93		
10	B	21	Total	O	0	0
			21	21		
10	C	90	Total	O	0	0
			90	90		
10	D	19	Total	O	0	0
			19	19		

*Continued on next page...*



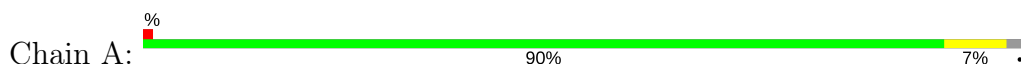
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	114	Total 114	O 114	0	0
10	F	27	Total 27	O 27	0	0
10	G	111	Total 111	O 111	0	0
10	H	31	Total 31	O 31	0	0

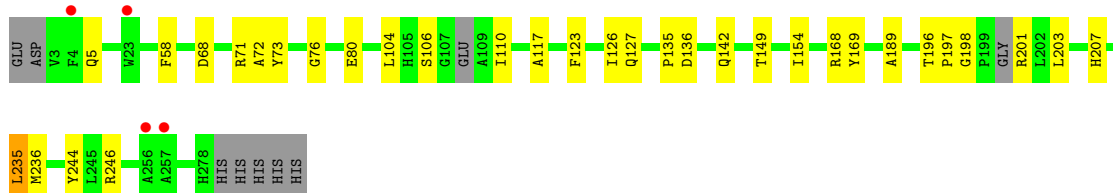
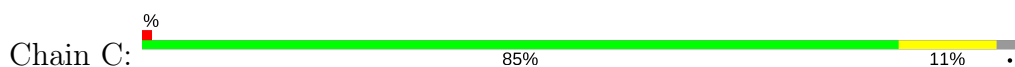
### 3 Residue-property plots [i](#)

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.

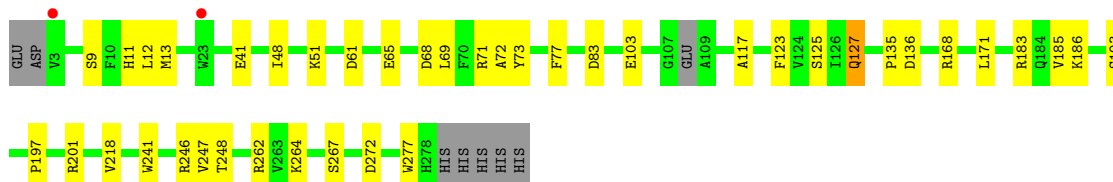
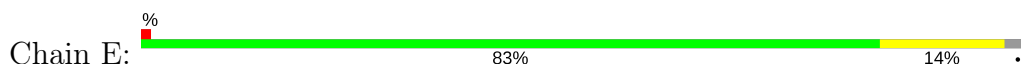
- Molecule 1: CD1b3



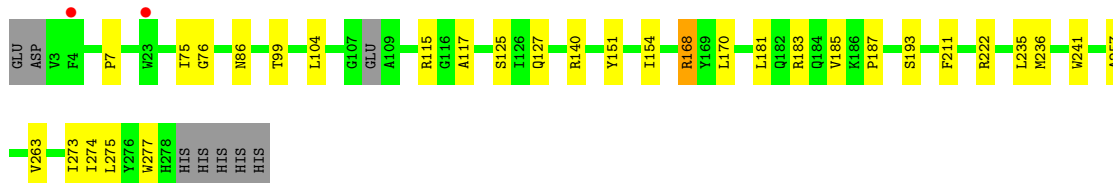
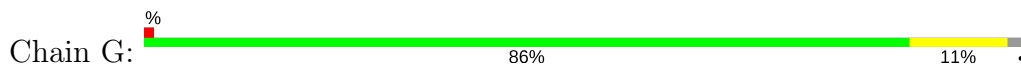
- Molecule 1: CD1b3



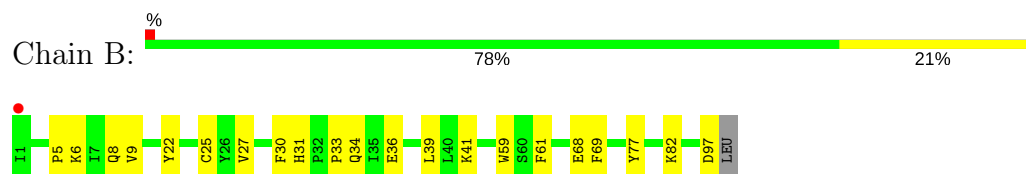
- Molecule 1: CD1b3



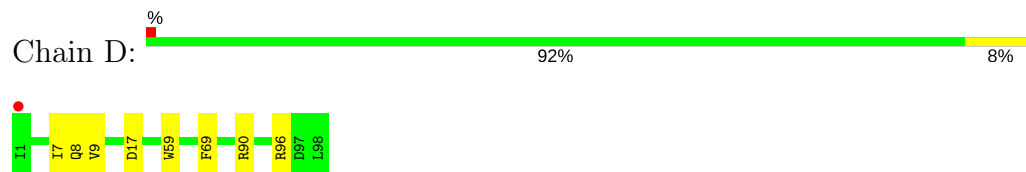
- Molecule 1: CD1b3



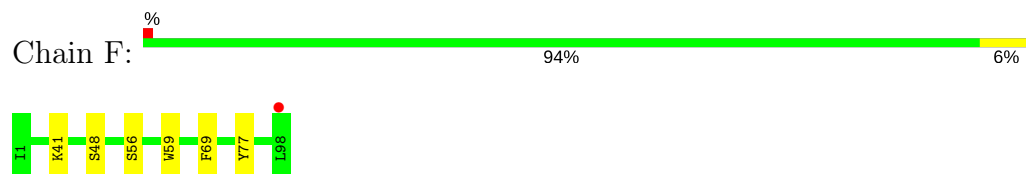
- Molecule 2: Beta-2-microglobulin



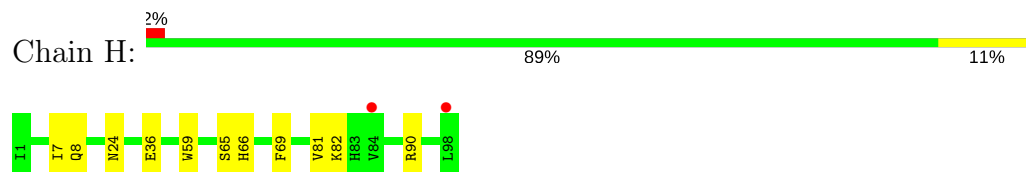
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.53Å 139.97Å 111.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.30 45.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.00-2.30) 99.4 (45.84-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.201 , 0.248 0.213 , 0.260	Depositor DCC
$R_{free}$ test set	4805 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 17.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.127 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12721	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: GOL, BMA, NAG, L9R, CL, L9Q, FUC, 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	0.61	0/2181	0.66	0/2969
1	C	0.61	0/2170	0.65	1/2953 (0.0%)
1	E	0.61	0/2199	0.67	2/2991 (0.1%)
1	G	0.64	0/2182	0.69	1/2970 (0.0%)
2	B	0.55	0/808	0.61	0/1104
2	D	0.50	0/806	0.58	0/1102
2	F	0.56	0/804	0.64	0/1100
2	H	0.54	0/812	0.61	0/1110
All	All	0.60	0/11962	0.65	4/16299 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	262	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	E	71	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	G	168	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	235	LEU	CA-CB-CG	-5.12	103.52	115.30

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	A	2124	0	2015	22	0
1	C	2114	0	2003	30	0
1	E	2143	0	2032	38	0
1	G	2125	0	2020	29	0
2	B	782	0	716	13	0
2	D	780	0	702	6	0
2	F	778	0	704	2	0
2	H	786	0	713	6	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	E	28	0	26	1	0
3	G	14	0	13	3	0
4	A	70	0	61	0	0
5	A	54	0	86	6	0
5	E	54	0	86	11	1
6	A	6	0	8	0	0
6	C	18	0	24	0	0
6	E	6	0	8	3	0
6	G	24	0	32	1	0
7	C	59	0	52	2	0
7	E	59	0	52	2	0
7	G	59	0	52	1	0
8	C	51	0	79	10	0
8	G	51	0	79	3	1
9	C	1	0	0	0	0
9	G	1	0	0	0	0
10	A	93	0	0	2	0
10	B	21	0	0	0	0
10	C	90	0	0	1	0
10	D	19	0	0	0	0
10	E	114	0	0	5	0
10	F	27	0	0	0	0
10	G	111	0	0	0	0
10	H	31	0	0	0	0
All	All	12721	0	11589	134	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 6.

The worst 5 of 134 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:E:103:GLU:HB2	6:E:284:GOL:H32	1.54	0.86
1:E:73:TYR:HB2	5:E:285:L9R:H32	1.59	0.82
1:A:73:TYR:HA	5:A:284:L9R:H3	1.62	0.81
1:E:72:ALA:CB	5:E:285:L9R:H5A	2.12	0.80
1:E:72:ALA:HB2	5:E:285:L9R:H5A	1.64	0.78

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)
5:E:285:L9R:O1P	8:G:289:L9Q:O31[3_554]	2.04	0.16

## 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	271/283 (96%)	261 (96%)	10 (4%)	0	100	100
1	C	268/283 (95%)	258 (96%)	10 (4%)	0	100	100
1	E	273/283 (96%)	269 (98%)	4 (2%)	0	100	100
1	G	271/283 (96%)	266 (98%)	5 (2%)	0	100	100
2	B	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
2	D	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	F	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	H	96/98 (98%)	96 (100%)	0	0	100	100
All	All	1466/1524 (96%)	1429 (98%)	37 (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	A	223/240 (93%)	223 (100%)	0	100	100
1	C	221/240 (92%)	219 (99%)	2 (1%)	82	91
1	E	226/240 (94%)	224 (99%)	2 (1%)	82	91
1	G	223/240 (93%)	221 (99%)	2 (1%)	82	91
2	B	84/94 (89%)	83 (99%)	1 (1%)	75	87
2	D	81/94 (86%)	80 (99%)	1 (1%)	75	87
2	F	81/94 (86%)	78 (96%)	3 (4%)	39	53
2	H	83/94 (88%)	81 (98%)	2 (2%)	54	72
All	All	1222/1336 (92%)	1209 (99%)	13 (1%)	78	89

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	127	GLN
2	F	48	SER
1	G	235	LEU
1	E	83	ASP
1	G	86	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	127	GLN
1	C	152	GLN
1	G	127	GLN
1	C	89	GLN
2	D	34	GLN

### 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 ⓘ

21 carbohydrates 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	$\# Z  > 2$
4	NAG	A	501	1,4	14,14,15	0.59	0	15,19,21	1.80	5 (33%)
4	NAG	A	502	4	14,14,15	0.76	0	15,19,21	1.00	0
4	BMA	A	503	4	11,11,12	0.76	0	13,15,17	1.44	2 (15%)
4	MAN	A	504	4	11,11,12	0.57	0	13,15,17	1.41	1 (7%)
4	FUC	A	506	4	9,10,11	0.72	0	13,14,16	0.97	1 (7%)
4	FUC	A	507	4	9,10,11	0.56	0	13,14,16	0.94	1 (7%)
7	NAG	C	501	1,7	14,14,15	0.83	1 (7%)	15,19,21	0.97	1 (6%)
7	NAG	C	502	7	14,14,15	0.76	0	15,19,21	1.07	1 (6%)
7	BMA	C	503	7	11,11,12	0.61	0	13,15,17	1.17	1 (7%)
7	FUC	C	506	7	9,10,11	0.61	0	13,14,16	0.70	0
7	FUC	C	507	7	9,10,11	0.62	0	13,14,16	0.60	0
7	NAG	E	501	1,7	14,14,15	0.77	1 (7%)	15,19,21	1.57	2 (13%)
7	NAG	E	502	7	14,14,15	0.77	0	15,19,21	1.31	2 (13%)
7	BMA	E	503	7	11,11,12	0.62	0	13,15,17	1.27	1 (7%)
7	FUC	E	506	7	9,10,11	0.77	0	13,14,16	1.00	1 (7%)
7	FUC	E	507	7	9,10,11	0.56	0	13,14,16	0.89	0
7	NAG	G	501	1,7	14,14,15	0.83	0	15,19,21	0.73	0
7	NAG	G	502	7	14,14,15	0.69	0	15,19,21	0.95	0
7	BMA	G	503	7	11,11,12	0.51	0	13,15,17	1.08	1 (7%)
7	FUC	G	506	7	9,10,11	0.82	0	13,14,16	0.79	0
7	FUC	G	507	7	9,10,11	0.73	0	13,14,16	1.10	1 (7%)

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
4	NAG	A	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	502	4	-	0/6/23/26	0/1/1/1
4	BMA	A	503	4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	4	-	0/2/19/22	0/1/1/1
4	FUC	A	506	4	-	0/0/17/20	0/1/1/1
4	FUC	A	507	4	-	0/0/17/20	0/1/1/1
7	NAG	C	501	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	502	7	-	0/6/23/26	0/1/1/1
7	BMA	C	503	7	-	0/2/19/22	0/1/1/1
7	FUC	C	506	7	-	0/0/17/20	0/1/1/1
7	FUC	C	507	7	-	0/0/17/20	0/1/1/1
7	NAG	E	501	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	502	7	-	0/6/23/26	0/1/1/1
7	BMA	E	503	7	-	0/2/19/22	0/1/1/1
7	FUC	E	506	7	-	0/0/17/20	0/1/1/1
7	FUC	E	507	7	-	0/0/17/20	0/1/1/1
7	NAG	G	501	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	502	7	-	0/6/23/26	0/1/1/1
7	BMA	G	503	7	-	0/2/19/22	0/1/1/1
7	FUC	G	506	7	-	0/0/17/20	0/1/1/1
7	FUC	G	507	7	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	501	NAG	O5-C1	-2.01	1.40	1.43
7	E	501	NAG	C1-C2	2.03	1.55	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	NAG	C2-N2-C7	-3.36	118.05	122.94
4	A	501	NAG	O4-C4-C3	-2.72	104.43	110.36
7	E	502	NAG	C2-N2-C7	-2.71	118.98	122.94
7	E	501	NAG	O7-C7-C8	-2.62	117.28	122.06
7	C	501	NAG	O5-C1-C2	-2.47	108.03	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	502	NAG	1	0
7	C	507	FUC	2	0
7	E	501	NAG	1	0
7	E	502	NAG	1	0
7	G	501	NAG	1	0

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z  > 2$
5	L9R	A	284	-	53,53,53	1.08	5 (9%)	58,61,61	1.36	5 (8%)
6	GOL	A	285	-	5,5,5	0.22	0	5,5,5	0.35	0
3	NAG	A	500	1	14,14,15	0.52	0	15,19,21	1.60	4 (26%)
8	L9Q	C	284	-	50,50,50	0.88	2 (4%)	52,55,55	0.83	2 (3%)
6	GOL	C	285	-	5,5,5	0.16	0	5,5,5	0.99	0
6	GOL	C	286	-	5,5,5	0.43	0	5,5,5	0.28	0
6	GOL	C	288	-	5,5,5	0.50	0	5,5,5	0.68	0
3	NAG	C	500	1	14,14,15	0.52	0	15,19,21	0.94	1 (6%)
6	GOL	E	284	-	5,5,5	0.34	0	5,5,5	0.24	0
5	L9R	E	285	-	53,53,53	1.27	5 (9%)	58,61,61	1.66	7 (12%)
3	NAG	E	500	1	14,14,15	0.43	0	15,19,21	2.32	5 (33%)
3	NAG	E	508	1	14,14,15	0.61	0	15,19,21	1.47	1 (6%)
6	GOL	G	284	-	5,5,5	0.22	0	5,5,5	0.33	0
6	GOL	G	285	-	5,5,5	0.24	0	5,5,5	0.33	0
6	GOL	G	286	-	5,5,5	0.36	0	5,5,5	0.34	0
6	GOL	G	287	-	5,5,5	0.34	0	5,5,5	0.44	0
8	L9Q	G	289	-	50,50,50	0.91	2 (4%)	52,55,55	1.05	2 (3%)
3	NAG	G	500	1	14,14,15	0.64	0	15,19,21	1.13	1 (6%)

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
5	L9R	A	284	-	-	0/57/57/57	0/0/0/0
6	GOL	A	285	-	-	0/4/4/4	0/0/0/0
3	NAG	A	500	1	-	0/6/23/26	0/1/1/1
8	L9Q	C	284	-	-	0/54/54/54	0/0/0/0
6	GOL	C	285	-	-	0/4/4/4	0/0/0/0
6	GOL	C	286	-	-	0/4/4/4	0/0/0/0
6	GOL	C	288	-	-	0/4/4/4	0/0/0/0
3	NAG	C	500	1	-	0/6/23/26	0/1/1/1
6	GOL	E	284	-	-	0/4/4/4	0/0/0/0
5	L9R	E	285	-	-	0/57/57/57	0/0/0/0
3	NAG	E	500	1	-	0/6/23/26	0/1/1/1
3	NAG	E	508	1	-	0/6/23/26	0/1/1/1
6	GOL	G	284	-	-	0/4/4/4	0/0/0/0
6	GOL	G	285	-	-	0/4/4/4	0/0/0/0
6	GOL	G	286	-	-	0/4/4/4	0/0/0/0
6	GOL	G	287	-	-	0/4/4/4	0/0/0/0
8	L9Q	G	289	-	-	0/54/54/54	0/0/0/0
3	NAG	G	500	1	-	0/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	284	L9Q	P-O4P	2.10	1.68	1.59
8	G	289	L9Q	C1-C2	2.11	1.56	1.50
5	E	285	L9R	C12-C11	2.13	1.56	1.50
8	C	284	L9Q	C12-C11	2.14	1.56	1.50
5	A	284	L9R	P-O4P	2.16	1.68	1.59

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	508	NAG	C3-C4-C5	-3.44	104.15	110.22
5	E	285	L9R	O3-C11-O11	-3.18	115.65	123.55
3	E	500	NAG	C4-C3-C2	-2.71	107.05	111.02
5	A	284	L9R	O3-C11-O11	-2.63	117.02	123.55
5	E	285	L9R	O2-C2-C1	-2.34	99.94	108.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	284	L9R	6	0
8	C	284	L9Q	10	0
6	E	284	GOL	3	0
5	E	285	L9R	11	1
3	E	508	NAG	1	0
6	G	286	GOL	1	0
8	G	289	L9Q	3	1
3	G	500	NAG	3	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 [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	275/283 (97%)	-0.01	2 (0%) 87 90	23, 39, 63, 73	0
1	C	274/283 (96%)	0.06	4 (1%) 74 78	21, 40, 65, 77	0
1	E	275/283 (97%)	-0.02	2 (0%) 87 90	21, 36, 58, 69	0
1	G	275/283 (97%)	-0.00	2 (0%) 87 90	21, 36, 60, 69	0
2	B	97/98 (98%)	0.03	1 (1%) 82 86	29, 54, 88, 124	0
2	D	98/98 (100%)	0.17	1 (1%) 82 86	31, 59, 91, 111	0
2	F	98/98 (100%)	-0.09	1 (1%) 82 86	27, 43, 66, 73	0
2	H	98/98 (100%)	0.00	2 (2%) 65 72	28, 51, 76, 95	0
All	All	1490/1524 (97%)	0.01	15 (1%) 82 86	21, 40, 71, 124	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	PHE	4.8
2	B	1	ILE	4.5
1	G	4	PHE	4.0
1	G	23	TRP	3.8
2	D	1	ILE	3.6

### 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	501	14/15	0.93	0.16	1.74	38,43,48,51	0
7	NAG	C	501	14/15	0.97	0.12	0.86	32,36,44,44	0
7	NAG	E	501	14/15	0.98	0.13	-0.07	31,35,40,42	0
7	NAG	G	501	14/15	0.98	0.11	-0.85	29,34,40,43	0
7	FUC	C	507	10/11	0.97	0.10	-	48,53,60,60	0
4	BMA	A	503	11/12	0.86	0.12	-	67,74,82,83	0
7	FUC	G	506	10/11	0.96	0.15	-	40,44,47,50	0
7	FUC	E	507	10/11	0.94	0.10	-	45,50,54,54	0
4	FUC	A	506	10/11	0.98	0.09	-	35,40,45,49	0
7	NAG	G	502	14/15	0.96	0.10	-	37,46,51,57	0
4	MAN	A	504	11/12	0.89	0.16	-	80,88,98,99	0
7	FUC	E	506	10/11	0.97	0.14	-	32,38,41,44	0
7	BMA	G	503	11/12	0.90	0.13	-	63,69,75,75	0
7	FUC	C	506	10/11	0.96	0.17	-	41,46,49,51	0
7	BMA	C	503	11/12	0.75	0.16	-	62,69,76,77	0
7	NAG	C	502	14/15	0.94	0.11	-	43,48,52,58	0
7	NAG	E	502	14/15	0.98	0.13	-	36,44,49,53	0
7	BMA	E	503	11/12	0.85	0.15	-	59,66,71,73	0
4	NAG	A	502	14/15	0.97	0.12	-	42,49,56,60	0
4	FUC	A	507	10/11	0.92	0.12	-	50,55,61,61	0
7	FUC	G	507	10/11	0.92	0.16	-	47,52,58,59	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	L9Q	G	289	51/51	0.69	0.30	7.12	34,51,81,83	0
8	L9Q	C	284	51/51	0.74	0.31	5.89	31,58,86,88	0
5	L9R	E	285	54/54	0.76	0.26	5.43	31,56,82,85	0
5	L9R	A	284	54/54	0.77	0.22	3.90	38,59,86,87	0
6	GOL	C	285	6/6	0.90	0.19	2.55	41,45,46,48	0
6	GOL	C	288	6/6	0.91	0.17	1.94	51,52,55,56	0
6	GOL	G	287	6/6	0.95	0.14	1.62	47,48,50,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	E	284	6/6	0.89	0.19	1.30	53,54,55,56	0
6	GOL	G	284	6/6	0.95	0.18	1.19	55,55,55,55	0
6	GOL	C	286	6/6	0.92	0.18	1.14	53,56,57,59	0
6	GOL	A	285	6/6	0.95	0.14	-0.27	56,56,57,58	0
9	CL	G	288	1/1	0.99	0.14	-0.40	30,30,30,30	0
6	GOL	G	285	6/6	0.91	0.12	-0.57	44,45,46,46	0
9	CL	C	287	1/1	0.98	0.12	-1.14	35,35,35,35	0
6	GOL	G	286	6/6	0.73	0.17	-	66,67,69,69	0
3	NAG	G	500	14/15	0.66	0.21	-	60,70,78,80	0
3	NAG	E	508	14/15	0.86	0.13	-	63,72,77,81	0
3	NAG	A	500	14/15	0.74	0.17	-	86,94,98,100	0
3	NAG	E	500	14/15	0.79	0.14	-	79,87,95,96	0
3	NAG	C	500	14/15	0.74	0.15	-	78,87,91,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.