



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2024 – 02:47 PM EDT

PDB ID : 4C1Y  
Title : Crystal Structure of Fucose binding lectin from *Aspergillus Fumigatus* (AFL) in complex with b-methylfucoside  
Authors : Houser, J.; Komarek, J.; Kostlanova, N.; Lahmann, M.; Cioci, G.; Varrot, A.; Imberty, A.; Wimmerova, M.  
Deposited on : 2013-08-14  
Resolution : 2.23 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 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

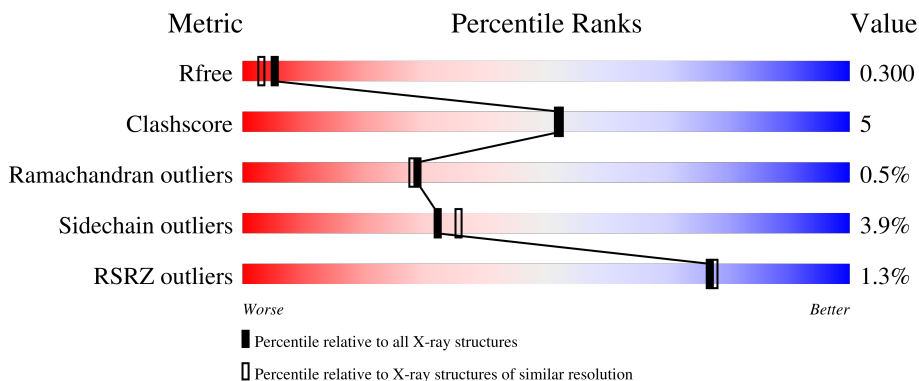
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	314	83% 15% .
2	B	314	84% 15% .
2	C	314	4% 82% 17% .
2	D	314	% 87% 13% .

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10093 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 FUCOSE-SPECIFIC LECTIN FLEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2439	1554	421	460	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	LEU	variant	UNP Q4WW81
A	111	CYS	ARG	variant	UNP Q4WW81

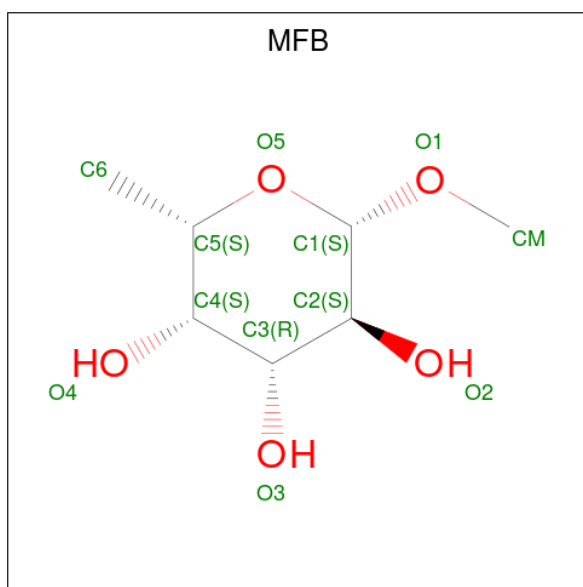
- Molecule 2 is a protein called FUCOSE-SPECIFIC LECTIN FLEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2443	1557	422	460	4			
2	C	314	Total	C	N	O	S	0	0	0
			2434	1553	418	459	4			
2	D	314	Total	C	N	O	S	0	0	0
			2438	1556	419	459	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	LEU	variant	UNP Q4WW81
B	111	CYS	ARG	variant	UNP Q4WW81
C	20	SER	LEU	variant	UNP Q4WW81
C	111	CYS	ARG	variant	UNP Q4WW81
D	20	SER	LEU	variant	UNP Q4WW81
D	111	CYS	ARG	variant	UNP Q4WW81

- Molecule 3 is methyl beta-L-fucopyranoside (three-letter code: MFB) (formula: C<sub>7</sub>H<sub>14</sub>O<sub>5</sub>).



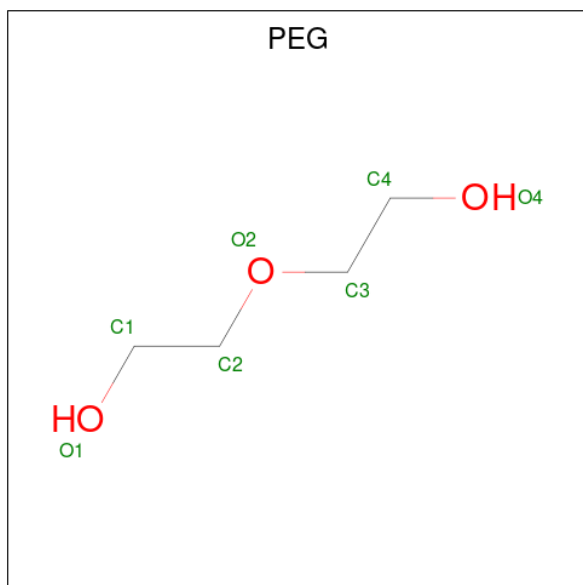
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	7	5		
3	A	1	Total	C	O	0	0
			12	7	5		
3	A	1	Total	C	O	0	0
			12	7	5		
3	B	1	Total	C	O	0	0
			12	7	5		
3	B	1	Total	C	O	0	0
			12	7	5		
3	B	1	Total	C	O	0	0
			12	7	5		
3	C	1	Total	C	O	0	0
			12	7	5		
3	C	1	Total	C	O	0	0
			12	7	5		
3	C	1	Total	C	O	0	0
			12	7	5		
3	C	1	Total	C	O	0	0
			12	7	5		
3	D	1	Total	C	O	0	0
			12	7	5		
3	D	1	Total	C	O	0	0
			12	7	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

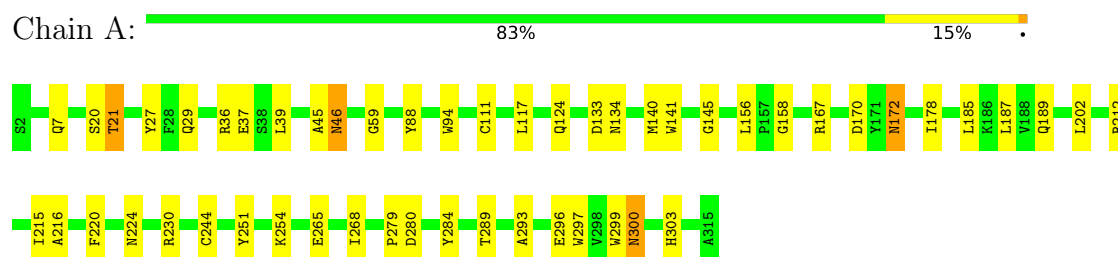
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	46	Total	O	0	0
			46	46		
7	C	19	Total	O	0	0
			19	19		
7	D	18	Total	O	0	0
			18	18		

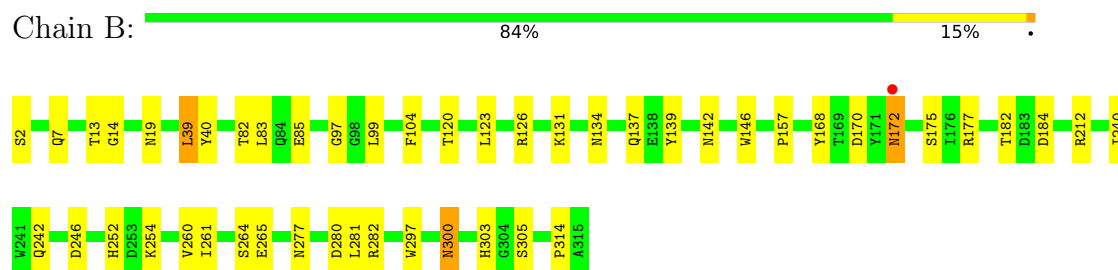
### 3 Residue-property plots

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.

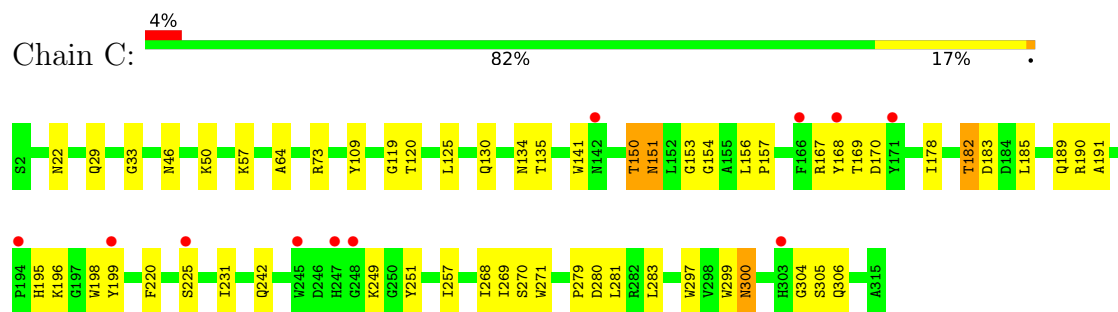
#### • Molecule 1: FUCOSE-SPECIFIC LECTIN FLEA



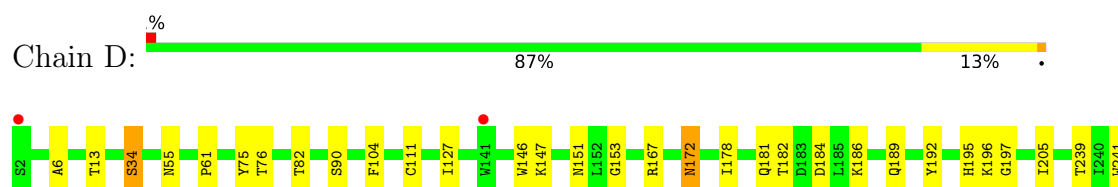
#### • Molecule 2: FUCOSE-SPECIFIC LECTIN FLEA

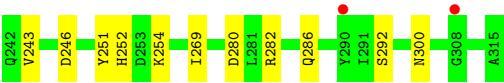


#### • Molecule 2: FUCOSE-SPECIFIC LECTIN FLEA



#### • Molecule 2: FUCOSE-SPECIFIC LECTIN FLEA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.21Å 90.33Å 189.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.23 48.14 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.14-2.23) 99.0 (48.14-2.23)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.243 , 0.313 0.230 , 0.300	Depositor DCC
$R_{free}$ test set	2993 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: PEG, CSX, CA, GOL, MFB

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	0.70	0/2502	0.82	1/3412 (0.0%)
2	B	0.68	0/2514	0.80	1/3427 (0.0%)
2	C	0.57	0/2505	0.73	0/3418
2	D	0.55	0/2509	0.71	0/3422
All	All	0.63	0/10030	0.77	2/13679 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	NE-CZ-NH2	-7.15	116.73	120.30
2	B	39	LEU	CA-CB-CG	5.89	128.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	19	ASN	Peptide

## 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	2439	0	2317	27	0
2	B	2443	0	2329	26	0
2	C	2434	0	2311	33	0
2	D	2438	0	2322	23	0
3	A	36	0	42	0	0
3	B	36	0	42	1	0
3	C	48	0	56	0	0
3	D	24	0	28	0	0
4	A	30	0	40	3	0
4	B	18	0	24	2	0
4	D	6	0	8	2	0
5	A	4	0	5	0	0
6	A	1	0	0	0	0
7	A	53	0	0	0	0
7	B	46	0	0	0	0
7	C	19	0	0	0	0
7	D	18	0	0	0	0
All	All	10093	0	9524	107	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 (107) 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:212:ARG:O	4:A:991:GOL:H2	1.75	0.84
2:B:212:ARG:O	4:B:990:GOL:O2	1.97	0.81
2:D:246:ASP:OD2	2:D:252:HIS:HE1	1.67	0.77
2:C:109:TYR:OH	2:C:134:ASN:OD1	2.06	0.71
2:B:300:ASN:ND2	2:B:303:HIS:H	1.93	0.66
2:D:146:TRP:HE1	4:D:920:GOL:HO3	1.44	0.66
2:D:195:HIS:CD2	2:D:196:LYS:HG3	2.35	0.62
2:B:246:ASP:OD2	2:B:252:HIS:HE1	1.83	0.61
2:B:182:THR:OG1	2:B:184:ASP:OD1	2.14	0.60
2:B:300:ASN:HD22	2:B:300:ASN:C	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:NH2	1:A:172:ASN:HA	2.18	0.59
2:C:242:GLN:CB	2:C:257:ILE:HD11	2.34	0.57
2:B:40:TYR:CE2	3:B:960:MFB:H62	2.40	0.56
1:A:189:GLN:NE2	1:A:251:TYR:OH	2.38	0.56
2:C:125:LEU:HB2	2:C:141:TRP:HB3	1.88	0.56
2:B:175:SER:HB3	2:B:177:ARG:HH12	1.71	0.56
2:B:212:ARG:O	4:B:990:GOL:C2	2.54	0.56
1:A:300:ASN:ND2	1:A:303:HIS:H	2.05	0.55
1:A:284:TYR:CE1	1:A:296:GLU:HG3	2.42	0.55
2:D:182:THR:OG1	2:D:184:ASP:OD1	2.17	0.55
2:B:300:ASN:HD21	2:B:303:HIS:H	1.54	0.54
2:C:300:ASN:HD22	2:C:300:ASN:C	2.11	0.54
1:A:170:ASP:OD1	1:A:224:ASN:HA	2.08	0.54
2:B:172:ASN:H	2:B:172:ASN:HD22	1.56	0.53
2:C:119:GLY:HA3	2:C:167:ARG:HD3	1.91	0.53
2:D:246:ASP:OD2	2:D:252:HIS:CE1	2.54	0.53
2:D:13:THR:HG22	2:D:286:GLN:NE2	2.23	0.52
2:C:135:THR:HA	2:C:154:GLY:HA2	1.91	0.52
2:C:242:GLN:HB3	2:C:257:ILE:HD11	1.91	0.52
2:D:61:PRO:O	2:D:76:THR:HG22	2.10	0.52
2:D:269:ILE:HG13	2:D:282:ARG:HB2	1.91	0.51
2:C:150:THR:HG21	2:C:198:TRP:CD1	2.46	0.51
2:B:14:GLY:HA2	2:B:265:GLU:HG3	1.92	0.51
2:B:126:ARG:HH12	2:B:142:ASN:HD21	1.58	0.50
1:A:230:ARG:NH2	4:A:950:GOL:O3	2.37	0.49
2:D:172:ASN:ND2	2:D:172:ASN:H	2.10	0.49
2:C:283:LEU:HB2	2:C:297:TRP:HB3	1.94	0.49
2:C:195:HIS:CG	2:C:196:LYS:H	2.31	0.49
1:A:117:LEU:HD12	1:A:124:GLN:HB3	1.95	0.48
1:A:289:THR:O	1:A:293:ALA:HB3	2.13	0.48
2:D:205:ILE:HB	2:D:243:VAL:HG11	1.94	0.48
2:C:190:ARG:NH2	2:C:199:TYR:O	2.42	0.48
2:C:182:THR:O	2:C:185:LEU:N	2.43	0.47
2:C:189:GLN:NE2	2:C:251:TYR:OH	2.47	0.47
1:A:300:ASN:C	1:A:300:ASN:HD22	2.16	0.47
2:C:29:GLN:OE1	2:C:33:GLY:O	2.32	0.47
1:A:29:GLN:HE22	1:A:59:GLY:H	1.62	0.47
2:C:242:GLN:HB2	2:C:257:ILE:HD11	1.96	0.47
2:B:131:LYS:HD2	2:B:137:GLN:HB2	1.95	0.47
2:C:191:ALA:O	2:C:198:TRP:CE3	2.67	0.47
2:D:167:ARG:NH2	2:D:172:ASN:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:HIS:CG	2:C:196:LYS:N	2.83	0.46
2:C:299:TRP:HA	2:C:304:GLY:O	2.15	0.46
1:A:265:GLU:OE2	4:A:991:GOL:H12	2.15	0.46
1:A:27:TYR:CE1	1:A:37:GLU:HG3	2.50	0.46
2:C:191:ALA:O	2:C:198:TRP:HE3	1.98	0.46
2:D:75:TYR:CZ	2:D:127:ILE:HD11	2.51	0.46
1:A:220:PHE:CE2	1:A:279:PRO:HG3	2.51	0.46
2:D:151:ASN:ND2	2:D:153:GLY:H	2.14	0.46
2:B:168:TYR:HB3	2:B:170:ASP:OD1	2.16	0.45
1:A:133:ASP:O	1:A:134:ASN:HB2	2.15	0.45
1:A:216:ALA:HB1	1:A:268:ILE:HG22	1.99	0.45
2:B:2:SER:HB3	2:B:7:GLN:HE21	1.82	0.45
2:D:34:SER:OG	2:D:55:ASN:ND2	2.49	0.45
2:C:297:TRP:CH2	2:C:299:TRP:HB2	2.52	0.45
2:D:82:THR:HA	2:D:104:PHE:O	2.17	0.45
2:D:146:TRP:C	2:D:147:LYS:HG2	2.37	0.45
2:D:192:TYR:CE2	2:D:197:GLY:HA2	2.52	0.45
2:B:240:ILE:HG13	2:B:260:VAL:HG11	1.99	0.45
2:C:231:ILE:HD12	2:C:231:ILE:N	2.32	0.44
2:B:82:THR:HA	2:B:104:PHE:O	2.17	0.44
1:A:45:ALA:O	1:A:46:ASN:HB2	2.16	0.44
2:D:181:GLN:HA	2:D:186:LYS:O	2.17	0.44
2:D:6:ALA:O	2:D:292:SER:OG	2.32	0.44
2:C:64:ALA:HA	2:C:73:ARG:O	2.19	0.43
2:C:156:LEU:C	2:C:156:LEU:HD23	2.39	0.43
2:C:151:ASN:ND2	2:C:153:GLY:H	2.17	0.43
2:B:261:ILE:HG12	2:B:264:SER:HB2	2.01	0.43
2:C:168:TYR:C	2:C:170:ASP:H	2.22	0.43
1:A:202:LEU:HD12	1:A:202:LEU:N	2.34	0.43
2:B:99:LEU:HD13	2:B:146:TRP:CD2	2.53	0.42
2:C:130:GLN:HA	2:C:135:THR:O	2.19	0.42
1:A:141:TRP:CZ3	1:A:145:GLY:HA2	2.54	0.42
2:B:242:GLN:O	2:B:254:LYS:HA	2.19	0.42
2:D:146:TRP:NE1	4:D:920:GOL:O3	2.38	0.42
1:A:20:SER:O	1:A:21:THR:C	2.57	0.42
2:D:239:THR:OG1	2:D:241:TRP:CD1	2.72	0.42
2:C:268:ILE:HG13	2:C:269:ILE:N	2.34	0.42
2:D:189:GLN:NE2	2:D:251:TYR:OH	2.53	0.42
2:D:151:ASN:HD22	2:D:153:GLY:H	1.68	0.42
2:C:22:ASN:HB3	2:C:271:TRP:CZ2	2.55	0.42
2:C:283:LEU:HD12	2:C:297:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:LEU:O	2:B:282:ARG:HD3	2.21	0.41
2:C:270:SER:HB3	2:C:281:LEU:HD23	2.01	0.41
1:A:158:GLY:HA3	1:A:212:ARG:NE	2.35	0.41
2:C:220:PHE:CE2	2:C:279:PRO:HG3	2.55	0.41
1:A:7:GLN:NE2	2:B:134:ASN:HD21	2.19	0.41
1:A:187:LEU:HD22	1:A:215:ILE:HD11	2.02	0.41
2:B:282:ARG:HA	2:B:297:TRP:O	2.20	0.41
1:A:156:LEU:HD12	1:A:185:LEU:HD23	2.03	0.41
1:A:7:GLN:HE22	2:B:134:ASN:HD21	1.69	0.41
1:A:88:TYR:HB2	1:A:94:TRP:CD2	2.56	0.41
2:B:85:GLU:OE1	2:B:97:GLY:HA3	2.20	0.41
2:B:83:LEU:HD11	2:B:139:TYR:CE2	2.56	0.41
2:C:151:ASN:HD22	2:C:153:GLY:H	1.69	0.40
1:A:297:TRP:CH2	1:A:299:TRP:HB2	2.57	0.40
2:C:156:LEU:HA	2:C:157:PRO:HD3	1.99	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	311/314 (99%)	298 (96%)	11 (4%)	2 (1%)	25	23
2	B	312/314 (99%)	292 (94%)	19 (6%)	1 (0%)	41	44
2	C	312/314 (99%)	282 (90%)	27 (9%)	3 (1%)	15	11
2	D	312/314 (99%)	302 (97%)	10 (3%)	0	100	100
All	All	1247/1256 (99%)	1174 (94%)	67 (5%)	6 (0%)	29	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
2	C	46	ASN
2	C	183	ASP
2	C	169	THR
1	A	21	THR
2	B	157	PRO

### 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	247/248 (100%)	239 (97%)	8 (3%)	39	44
2	B	249/249 (100%)	239 (96%)	10 (4%)	31	34
2	C	247/249 (99%)	234 (95%)	13 (5%)	22	21
2	D	248/249 (100%)	240 (97%)	8 (3%)	39	44
All	All	991/995 (100%)	952 (96%)	39 (4%)	32	35

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	111	CYS
1	A	140	MET
1	A	172	ASN
1	A	178	ILE
1	A	254	LYS
1	A	280	ASP
1	A	300	ASN
2	B	13	THR
2	B	39	LEU
2	B	120	THR
2	B	123	LEU
2	B	172	ASN
2	B	277	ASN
2	B	280	ASP
2	B	300	ASN

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Mol	Chain	Res	Type
2	B	305	SER
2	B	314	PRO
2	C	50	LYS
2	C	57	LYS
2	C	120	THR
2	C	150	THR
2	C	151	ASN
2	C	178	ILE
2	C	182	THR
2	C	225	SER
2	C	249	LYS
2	C	280	ASP
2	C	300	ASN
2	C	305	SER
2	C	306	GLN
2	D	34	SER
2	D	90	SER
2	D	111	CYS
2	D	172	ASN
2	D	178	ILE
2	D	254	LYS
2	D	280	ASP
2	D	300	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	29	GLN
1	A	46	ASN
1	A	55	ASN
1	A	151	ASN
1	A	172	ASN
1	A	189	GLN
1	A	242	GLN
1	A	276	ASN
1	A	300	ASN
2	B	7	GLN
2	B	46	ASN
2	B	55	ASN
2	B	142	ASN
2	B	151	ASN

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Mol	Chain	Res	Type
2	B	172	ASN
2	B	189	GLN
2	B	252	HIS
2	B	300	ASN
2	C	7	GLN
2	C	29	GLN
2	C	46	ASN
2	C	55	ASN
2	C	151	ASN
2	C	189	GLN
2	C	242	GLN
2	C	277	ASN
2	C	300	ASN
2	C	303	HIS
2	C	306	GLN
2	D	7	GLN
2	D	23	HIS
2	D	29	GLN
2	D	55	ASN
2	D	151	ASN
2	D	172	ASN
2	D	189	GLN
2	D	252	HIS
2	D	276	ASN
2	D	300	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	CSX	A	244	1	3,6,7	0.72	0	1,6,8	2.32	1 (100%)

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	CSX	A	244	1	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	CSX	CA-CB-SG	-2.32	108.28	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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
4	GOL	A	990	-	5,5,5	0.85	0	5,5,5	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MFB	B	910	-	12,12,12	0.87	1 (8%)	17,17,17	0.86	1 (5%)
3	MFB	A	930	-	12,12,12	0.83	0	17,17,17	1.15	2 (11%)
5	PEG	A	992	-	3,3,6	0.78	0	2,2,5	0.18	0
3	MFB	C	950	-	12,12,12	0.84	0	17,17,17	0.78	0
3	MFB	C	930	-	12,12,12	0.85	1 (8%)	17,17,17	1.19	2 (11%)
4	GOL	B	990	-	5,5,5	0.79	0	5,5,5	1.12	0
3	MFB	A	960	-	12,12,12	0.68	0	17,17,17	0.98	1 (5%)
3	MFB	D	960	-	12,12,12	0.80	1 (8%)	17,17,17	1.02	1 (5%)
4	GOL	B	920	-	5,5,5	0.50	0	5,5,5	0.75	0
3	MFB	D	930	-	12,12,12	0.77	0	17,17,17	1.10	1 (5%)
3	MFB	A	910	-	12,12,12	0.87	1 (8%)	17,17,17	0.90	1 (5%)
4	GOL	A	950	-	5,5,5	0.51	0	5,5,5	0.99	0
3	MFB	C	960	-	12,12,12	0.58	0	17,17,17	1.04	0
3	MFB	B	930	-	12,12,12	0.81	0	17,17,17	1.25	2 (11%)
4	GOL	A	920	-	5,5,5	0.60	0	5,5,5	0.25	0
3	MFB	B	960	-	12,12,12	0.94	1 (8%)	17,17,17	1.55	4 (23%)
3	MFB	C	910	-	12,12,12	0.95	1 (8%)	17,17,17	0.93	0
4	GOL	A	940	-	5,5,5	0.49	0	5,5,5	0.46	0
4	GOL	D	920	-	5,5,5	0.53	0	5,5,5	0.51	0
4	GOL	A	991	-	5,5,5	0.27	0	5,5,5	0.49	0
4	GOL	B	950	-	5,5,5	0.50	0	5,5,5	0.40	0

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	GOL	A	990	-	-	2/4/4/4	-
3	MFB	B	910	-	-	0/2/22/22	0/1/1/1
3	MFB	A	930	-	-	0/2/22/22	0/1/1/1
5	PEG	A	992	-	-	1/1/1/4	-
3	MFB	C	950	-	-	0/2/22/22	0/1/1/1
3	MFB	C	930	-	-	2/2/22/22	0/1/1/1
4	GOL	B	990	-	-	2/4/4/4	-
3	MFB	A	960	-	-	0/2/22/22	0/1/1/1
3	MFB	D	960	-	-	0/2/22/22	0/1/1/1
4	GOL	B	920	-	-	2/4/4/4	-
3	MFB	D	930	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MFB	A	910	-	-	0/2/22/22	0/1/1/1
4	GOL	A	950	-	-	4/4/4/4	-
3	MFB	C	960	-	-	0/2/22/22	0/1/1/1
3	MFB	B	930	-	-	0/2/22/22	0/1/1/1
4	GOL	A	920	-	-	0/4/4/4	-
3	MFB	B	960	-	-	0/2/22/22	0/1/1/1
3	MFB	C	910	-	-	0/2/22/22	0/1/1/1
4	GOL	A	940	-	-	2/4/4/4	-
4	GOL	D	920	-	-	2/4/4/4	-
4	GOL	A	991	-	-	2/4/4/4	-
4	GOL	B	950	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	960	MFB	O1-C1	2.59	1.44	1.40
3	A	910	MFB	O1-C1	2.48	1.44	1.40
3	C	930	MFB	O1-C1	2.46	1.44	1.40
3	C	910	MFB	O1-C1	2.37	1.44	1.40
3	B	910	MFB	O1-C1	2.22	1.44	1.40
3	D	960	MFB	O1-C1	2.01	1.43	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	930	MFB	O1-C1-C2	3.02	111.69	108.15
3	B	960	MFB	C1-C2-C3	2.93	116.09	110.00
3	B	960	MFB	O5-C5-C6	2.87	112.90	106.70
3	B	930	MFB	C1-O5-C5	-2.79	108.87	113.67
3	B	960	MFB	C3-C4-C5	-2.66	105.63	109.77
3	B	910	MFB	O1-C1-C2	2.59	111.18	108.15
3	C	930	MFB	O1-C1-C2	2.56	111.15	108.15
3	A	930	MFB	O3-C3-C2	-2.42	104.75	110.35
3	A	910	MFB	C1-C2-C3	2.23	114.63	110.00
3	A	930	MFB	C1-O5-C5	-2.16	109.95	113.67
3	B	930	MFB	O1-C1-C2	2.10	110.62	108.15
3	D	960	MFB	O3-C3-C4	2.05	115.10	110.35
3	A	960	MFB	C1-O5-C5	-2.04	110.16	113.67
3	B	960	MFB	C1-O5-C5	-2.03	110.17	113.67
3	C	930	MFB	O5-C5-C6	2.00	111.03	106.70

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	950	GOL	O1-C1-C2-C3
4	A	990	GOL	C1-C2-C3-O3
4	A	991	GOL	O1-C1-C2-C3
4	B	950	GOL	O1-C1-C2-C3
4	B	950	GOL	C1-C2-C3-O3
3	C	930	MFB	O5-C1-O1-CM
3	C	930	MFB	C2-C1-O1-CM
4	A	940	GOL	C1-C2-C3-O3
4	A	950	GOL	C1-C2-C3-O3
4	B	990	GOL	O1-C1-C2-C3
4	D	920	GOL	O1-C1-C2-C3
4	A	940	GOL	O2-C2-C3-O3
4	A	990	GOL	O2-C2-C3-O3
4	B	950	GOL	O2-C2-C3-O3
4	D	920	GOL	O1-C1-C2-O2
4	A	950	GOL	O2-C2-C3-O3
4	B	950	GOL	O1-C1-C2-O2
4	B	920	GOL	C1-C2-C3-O3
4	A	950	GOL	O1-C1-C2-O2
4	A	991	GOL	O1-C1-C2-O2
4	B	990	GOL	O1-C1-C2-O2
5	A	992	PEG	O1-C1-C2-O2
4	B	920	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	990	GOL	2	0
4	A	950	GOL	1	0
3	B	960	MFB	1	0
4	D	920	GOL	2	0
4	A	991	GOL	2	0

## 5.7 Other polymers

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 [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	313/314 (99%)	-0.35	0 <span>100</span> <span>100</span>	8, 19, 35, 62	0
2	B	314/314 (100%)	-0.36	1 (0%) <span>94</span> <span>94</span>	10, 19, 35, 47	0
2	C	314/314 (100%)	0.26	11 (3%) <span>44</span> <span>43</span>	14, 34, 56, 74	0
2	D	314/314 (100%)	0.01	4 (1%) <span>77</span> <span>78</span>	17, 31, 48, 70	0
All	All	1255/1256 (99%)	-0.11	16 (1%) <span>77</span> <span>78</span>	8, 25, 49, 74	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2	SER	4.3
2	C	225	SER	3.4
2	C	199	TYR	3.4
2	D	141	TRP	2.9
2	C	171	TYR	2.8
2	C	248	GLY	2.7
2	C	194	PRO	2.5
2	C	166	PHE	2.4
2	C	142	ASN	2.4
2	D	290	TYR	2.4
2	B	172	ASN	2.4
2	C	245	TRP	2.4
2	C	303	HIS	2.3
2	D	308	GLY	2.3
2	C	247	HIS	2.2
2	C	168	TYR	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSX	A	244	7/8	0.94	0.11	21,23,27,27	0

### 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
4	GOL	A	990	6/6	0.76	0.20	21,25,27,30	0
4	GOL	D	920	6/6	0.77	0.18	25,30,33,33	0
5	PEG	A	992	4/7	0.77	0.23	34,35,36,36	0
4	GOL	A	950	6/6	0.80	0.16	25,27,30,30	0
4	GOL	B	990	6/6	0.80	0.14	29,31,32,33	0
4	GOL	A	991	6/6	0.81	0.16	36,37,39,39	0
4	GOL	A	920	6/6	0.83	0.15	28,31,32,33	0
3	MFB	C	950	12/12	0.84	0.22	33,39,43,44	0
3	MFB	C	930	12/12	0.84	0.20	54,56,59,60	0
4	GOL	B	950	6/6	0.85	0.15	37,40,40,41	0
4	GOL	A	940	6/6	0.87	0.14	35,38,39,43	0
3	MFB	B	910	12/12	0.88	0.17	27,35,43,44	0
3	MFB	A	910	12/12	0.89	0.14	23,28,32,33	0
3	MFB	C	910	12/12	0.90	0.13	28,33,37,37	0
3	MFB	D	960	12/12	0.91	0.16	31,35,37,37	0
3	MFB	B	930	12/12	0.93	0.11	24,28,34,36	0
3	MFB	D	930	12/12	0.93	0.22	35,38,40,42	0
3	MFB	B	960	12/12	0.94	0.19	24,29,31,34	0
3	MFB	A	930	12/12	0.94	0.12	23,25,27,27	0
3	MFB	A	960	12/12	0.94	0.10	18,20,23,24	0
4	GOL	B	920	6/6	0.95	0.13	19,20,21,22	0
3	MFB	C	960	12/12	0.96	0.13	20,22,26,27	0
6	CA	A	1316	1/1	0.98	0.17	26,26,26,26	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.