Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 11:11 am GMT

PDB ID	:	6TRT
Title	:	Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) double cysteine mutant S180C/T742C.
Authors	:	Roversi, P.; Zitzmann, N.; Ibba, R.; Hensen, M.
Deposited on	:	2019-12-19
Resolution	:	4.58 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*
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:

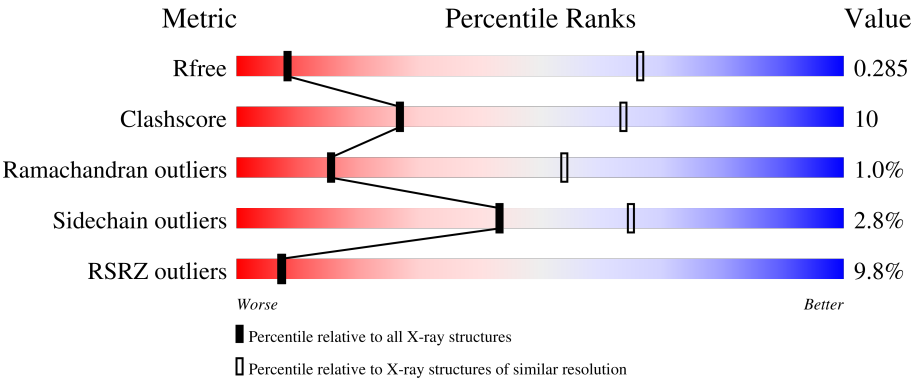
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.58 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	1060 (5.30-3.80)
Clashscore	141614	1128 (5.30-3.80)
Ramachandran outliers	138981	1072 (5.30-3.80)
Sidechain outliers	138945	1053 (5.30-3.80)
RSRZ outliers	127900	1102 (5.46-3.70)

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 >=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 <=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	1494	9% 70% 20% 8%
2	B	3	100%
2	D	3	100%
3	C	8	75% 25%

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
2	NAG	D	1	-	-	-	X
2	NAG	D	2	-	-	-	X
3	MAN	C	4	-	-	-	X
3	MAN	C	5	-	-	-	X
5	NAG	A	1607	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11210 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.

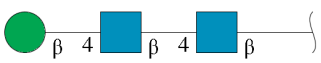
- Molecule 1 is a protein called UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1369	11007	7045	1875	2053	34	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	180	CYS	SER	engineered mutation	UNP G0SB58
A	742	CYS	THR	engineered mutation	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



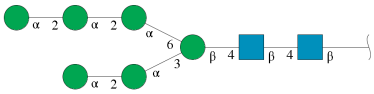
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

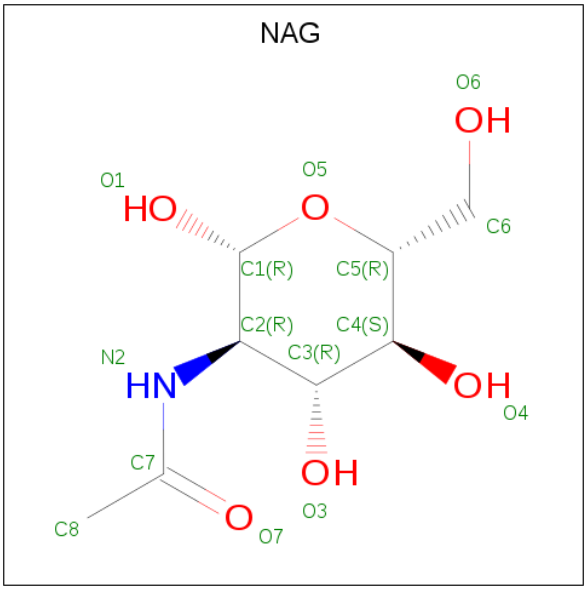


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 4 is TERBIUM(III) ION (three-letter code: TB) (formula: Tb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Tb	0	0
			3	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



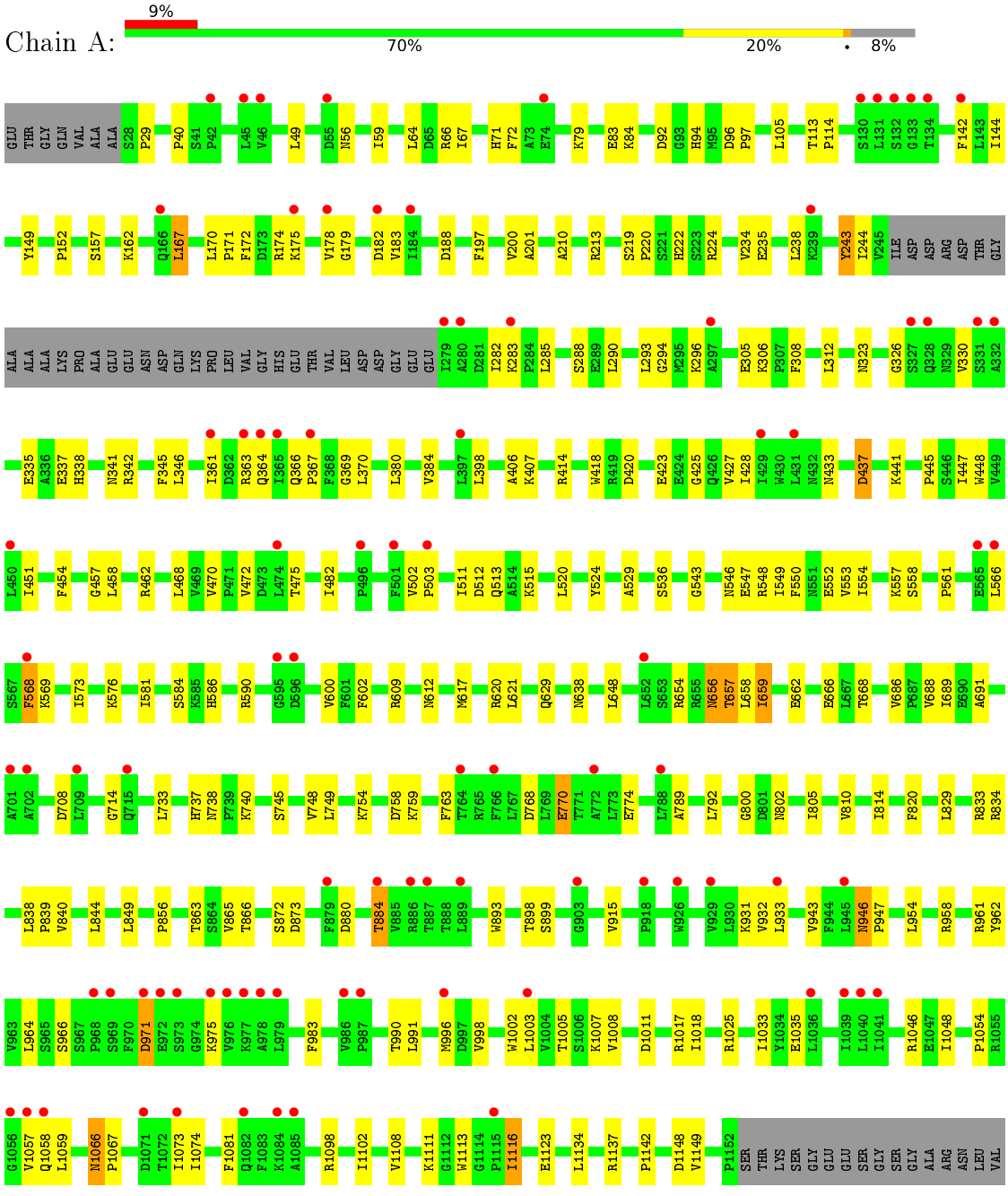
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

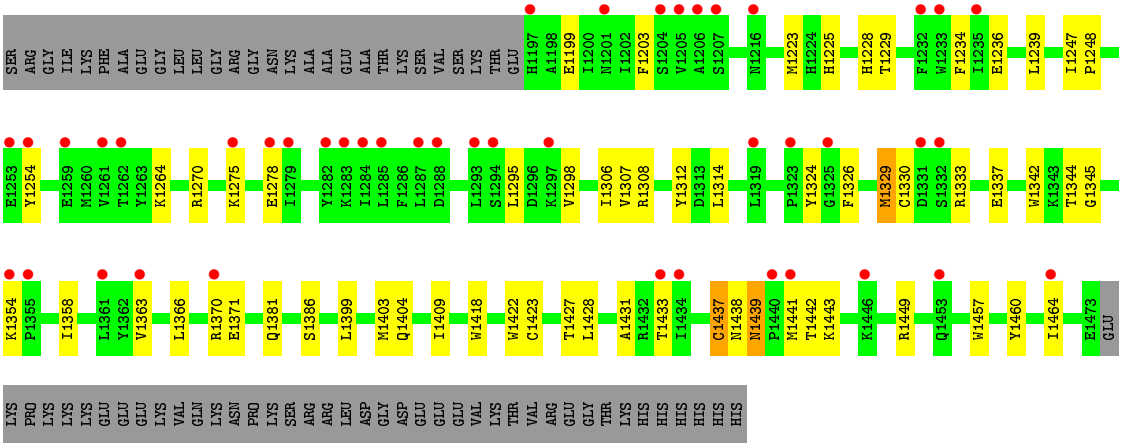
3 Residue-property plots (i)

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: UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain A:



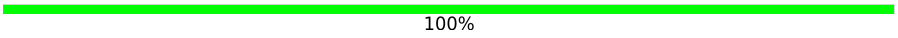


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

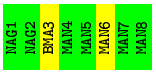
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	148.80Å 148.80Å 235.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	128.86 – 4.58 128.86 – 4.56	Depositor EDS
% Data completeness (in resolution range)	54.9 (128.86-4.58) 54.9 (128.86-4.56)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 4.47Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.291 , 0.297 0.281 , 0.285	Depositor DCC
R_{free} test set	418 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å^2)	263.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 177.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.083 for -h,-k,l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	11210	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, TB, 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	0.29	0/11272	0.61	3/15289 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	305	GLU	C-N-CA	6.93	139.03	121.70
1	A	243	TYR	C-N-CA	5.82	136.25	121.70
1	A	568	PHE	C-N-CA	5.43	135.28	121.70

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	11007	0	10875	225	6
2	B	39	0	34	0	0
2	D	39	0	34	0	0
3	C	94	0	79	3	0
4	A	3	0	0	0	0
5	A	28	0	26	0	0
All	All	11210	0	11048	228	6

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 10.

All (228) 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:1225:HIS:ND1	1:A:1308:ARG:HA	1.64	1.11
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.24	1.02
3:C:3:BMA:H4	3:C:6:MAN:H61	1.44	0.97
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	1.95	0.94
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	2.05	0.91
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.56	0.88
1:A:67:ILE:HG22	1:A:72:PHE:CD2	2.12	0.84
1:A:1329:MET:HG2	1:A:1358:ILE:HD11	1.61	0.82
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.12	0.82
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.60	0.82
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.42	0.82
1:A:149:TYR:CE1	1:A:157:SER:HB3	2.16	0.80
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	1.64	0.79
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.82	0.78
1:A:338:HIS:O	1:A:341:ASN:HB2	1.81	0.78
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.66	0.78
1:A:72:PHE:CE1	1:A:84:LYS:HG3	2.20	0.77
1:A:59:ILE:HD13	1:A:94:HIS:ND1	2.00	0.76
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.66	0.76
1:A:244:ILE:HA	1:A:285:LEU:HB3	1.67	0.76
1:A:554:ILE:HG21	1:A:568:PHE:HE1	1.50	0.75
1:A:686:VAL:O	1:A:754:LYS:HE2	1.87	0.74
1:A:59:ILE:HD13	1:A:94:HIS:CG	2.22	0.74
1:A:380:LEU:HG	1:A:865:VAL:HG13	1.70	0.72
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.54	0.72
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.71	0.72
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	2.07	0.71
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.71	0.71
1:A:407:LYS:NZ	1:A:884:THR:HB	2.04	0.71
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.57	0.70
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.75	0.69
1:A:244:ILE:HD11	1:A:954:LEU:HD13	1.75	0.69
1:A:1098:ARG:HH21	1:A:1102:ILE:HD11	1.58	0.68
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.75	0.68
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.76	0.68
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.59	0.68
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.25	0.67
1:A:243:TYR:O	1:A:285:LEU:HG	1.95	0.67
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.77	0.67
1:A:244:ILE:HG12	1:A:285:LEU:HD12	1.75	0.67
1:A:433:ASN:O	1:A:437:ASP:HB2	1.95	0.66
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.78	0.65
1:A:475:THR:HA	1:A:543:GLY:HA3	1.79	0.65
3:C:3:BMA:C4	3:C:6:MAN:H61	2.25	0.65
1:A:554:ILE:HG23	1:A:558:SER:HB2	1.79	0.64
1:A:1354:LYS:HD2	1:A:1404:GLN:HG3	1.79	0.64
1:A:243:TYR:HD1	1:A:285:LEU:HD23	1.63	0.64
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.79	0.64
1:A:188:ASP:OD1	1:A:219:SER:HB3	1.98	0.63
1:A:546:ASN:HB3	1:A:549:ILE:CG2	2.28	0.63
1:A:72:PHE:HE1	1:A:84:LYS:HG3	1.64	0.63
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.30	0.62
1:A:238:LEU:HD13	1:A:283:LYS:HE2	1.80	0.62
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.81	0.62
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.81	0.62
1:A:67:ILE:CG2	1:A:72:PHE:HD2	2.12	0.62
1:A:451:ILE:HA	1:A:629:GLN:HG2	1.81	0.61
1:A:447:ILE:HG23	1:A:448:TRP:CD1	2.36	0.61
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.52	0.60
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.31	0.60
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.84	0.60
1:A:66:ARG:O	1:A:71:HIS:HB3	2.02	0.59
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.33	0.59
1:A:1428:LEU:HD12	1:A:1431:ALA:HB3	1.85	0.59
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.86	0.58
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.89	0.58
1:A:1366:LEU:O	1:A:1370:ARG:HG3	2.04	0.57
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.85	0.57
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.85	0.57
1:A:174:ARG:O	1:A:213:ARG:HB3	2.05	0.57
1:A:1422:TRP:HZ3	1:A:1437:CYS:HB2	1.68	0.57
1:A:40:PRO:HB3	1:A:224:ARG:HD2	1.86	0.57
3:C:3:BMA:H4	3:C:6:MAN:C6	2.28	0.57
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.68	0.56
1:A:243:TYR:CD1	1:A:285:LEU:HD23	2.40	0.56
1:A:834:ARG:O	1:A:839:PRO:HD3	2.06	0.56
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.41	0.56
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.86	0.56
1:A:554:ILE:O	1:A:558:SER:HB2	2.06	0.55
1:A:554:ILE:O	1:A:558:SER:CB	2.55	0.55
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.87	0.55
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.88	0.54
1:A:407:LYS:HZ2	1:A:884:THR:HB	1.69	0.54
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.37	0.54
1:A:805:ILE:HG12	1:A:810:VAL:HG22	1.89	0.54
1:A:1438:ASN:HA	1:A:1449:ARG:HH22	1.71	0.54
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.34	0.54
1:A:296:LYS:HE2	1:A:330:VAL:HG13	1.90	0.54
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.89	0.54
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.43	0.54
1:A:656:ASN:O	1:A:657:THR:O	2.25	0.54
1:A:338:HIS:HD2	1:A:898:THR:CG2	2.11	0.53
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.73	0.53
1:A:554:ILE:HG21	1:A:568:PHE:CE1	2.38	0.53
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.91	0.53
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.73	0.53
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.21	0.52
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.27	0.52
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.39	0.52
1:A:1003:LEU:HD21	1:A:1264:LYS:HB2	1.92	0.52
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.92	0.51
1:A:872:SER:HB2	1:A:884:THR:OG1	2.10	0.51
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.92	0.51
1:A:546:ASN:CB	1:A:549:ILE:HG22	2.36	0.51
1:A:657:THR:HG23	1:A:659:ILE:HG22	1.92	0.51
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.93	0.51
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.75	0.50
1:A:899:SER:HA	1:A:943:VAL:O	2.11	0.50
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.94	0.50
1:A:283:LYS:NZ	1:A:285:LEU:HD21	2.27	0.49
1:A:524:TYR:CE2	1:A:558:SER:HA	2.47	0.49
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.13	0.49
1:A:174:ARG:O	1:A:213:ARG:CB	2.60	0.49
1:A:546:ASN:O	1:A:549:ILE:HG22	2.13	0.49
1:A:235:GLU:HB2	1:A:958:ARG:HD2	1.95	0.49
1:A:1111:LYS:HB2	1:A:1116:ILE:HG13	1.94	0.49
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.94	0.49
1:A:656:ASN:HD21	1:A:662:GLU:H	1.61	0.48
1:A:178:VAL:HG22	1:A:789:ALA:CB	2.42	0.48
1:A:294:GLY:HA3	1:A:947:PRO:HB3	1.93	0.48
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.78	0.48
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.95	0.48
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.96	0.48
1:A:1329:MET:SD	1:A:1342:TRP:CH2	3.07	0.48
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.96	0.48
1:A:56:ASN:HB3	1:A:59:ILE:HG22	1.95	0.48
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.34	0.47
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.96	0.47
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.49	0.47
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.97	0.47
1:A:840:VAL:HG21	1:A:863:THR:HA	1.96	0.47
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.79	0.47
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.16	0.47
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.45	0.47
1:A:79:LYS:O	1:A:83:GLU:HG2	2.15	0.47
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.96	0.47
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.97	0.47
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.50	0.47
1:A:366:GLN:HG2	1:A:369:GLY:H	1.80	0.47
1:A:1199:GLU:OE1	1:A:1228:HIS:ND1	2.48	0.46
1:A:536:SER:HA	1:A:549:ILE:HD13	1.96	0.46
1:A:668:THR:HG23	1:A:810:VAL:HB	1.97	0.46
1:A:472:VAL:O	1:A:503:PRO:HA	2.15	0.46
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.16	0.46
1:A:144:ILE:HB	1:A:149:TYR:HE2	1.79	0.46
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.50	0.46
1:A:654:ARG:HE	1:A:657:THR:HB	1.80	0.46
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	1.98	0.46
1:A:428:ILE:HA	1:A:502:VAL:HG12	1.97	0.46
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.34	0.46
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.56	0.46
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.50	0.46
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.97	0.46
1:A:829:LEU:O	1:A:833:ARG:HB2	2.15	0.45
1:A:737:HIS:NE2	1:A:749:LEU:HD12	2.31	0.45
1:A:458:LEU:HD21	1:A:621:LEU:HD21	1.99	0.45
1:A:553:VAL:O	1:A:557:LYS:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.95	0.45
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.46	0.45
1:A:326:GLY:CA	1:A:330:VAL:HG11	2.43	0.45
1:A:573:ILE:HB	1:A:576:LYS:CB	2.47	0.45
1:A:740:LYS:HB2	1:A:800:GLY:HA3	1.98	0.45
1:A:745:SER:O	1:A:748:VAL:HG22	2.17	0.44
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.17	0.44
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.64	0.44
1:A:367:PRO:HD3	1:A:962:TYR:OH	2.18	0.44
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.51	0.44
1:A:656:ASN:ND2	1:A:662:GLU:H	2.16	0.44
1:A:691:ALA:HB3	1:A:856:PRO:HG2	2.00	0.44
1:A:105:LEU:HD13	1:A:966:SER:HA	1.99	0.43
1:A:179:GLY:HA3	1:A:210:ALA:HA	2.00	0.43
1:A:1116:ILE:HD13	1:A:1116:ILE:H	1.84	0.43
1:A:548:ARG:O	1:A:552:GLU:OE2	2.36	0.43
1:A:561:PRO:CG	1:A:566:LEU:HD23	2.49	0.43
1:A:64:LEU:HD12	1:A:67:ILE:HD11	1.99	0.43
1:A:802:ASN:HB2	1:A:814:ILE:HB	2.00	0.43
1:A:1098:ARG:HG3	1:A:1148:ASP:OD1	2.19	0.43
1:A:441:LYS:HA	1:A:462:ARG:HD3	2.01	0.43
1:A:586:HIS:O	1:A:590:ARG:HB2	2.18	0.43
1:A:335:GLU:HA	1:A:337:GLU:HG2	2.00	0.43
1:A:468:LEU:HD22	1:A:617:MET:SD	2.58	0.43
1:A:282:ILE:HG13	1:A:990:THR:CG2	2.47	0.43
1:A:1399:LEU:HD12	1:A:1399:LEU:HA	1.95	0.43
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.19	0.43
1:A:113:THR:OG1	1:A:114:PRO:HD3	2.19	0.43
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	3.06	0.43
1:A:283:LYS:HZ3	1:A:285:LEU:HD11	1.84	0.43
1:A:1295:LEU:CD2	1:A:1298:VAL:CG2	2.84	0.43
1:A:370:LEU:HD13	1:A:933:LEU:HD11	2.00	0.43
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.94	0.42
1:A:234:VAL:HG22	1:A:996:MET:CE	2.49	0.42
1:A:770:GLU:OE2	1:A:774:GLU:OE2	2.37	0.42
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.47	0.42
1:A:445:PRO:HG3	1:A:462:ARG:NH2	2.35	0.42
1:A:1295:LEU:HD21	1:A:1298:VAL:HG23	1.90	0.42
1:A:283:LYS:HZ2	1:A:285:LEU:HD21	1.84	0.42
1:A:971:ASP:HB2	1:A:975:LYS:O	2.20	0.42
1:A:361:ILE:HG13	1:A:364:GLN:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:VAL:CG2	1:A:584:SER:HA	2.49	0.42
1:A:554:ILE:HD13	1:A:568:PHE:CE1	2.55	0.42
1:A:561:PRO:HG3	1:A:566:LEU:HD23	2.02	0.42
1:A:219:SER:HA	1:A:220:PRO:HD3	1.95	0.42
1:A:447:ILE:CG2	1:A:448:TRP:CD1	3.02	0.42
1:A:468:LEU:HD11	1:A:600:VAL:HG12	2.02	0.42
1:A:1247:ILE:CG1	1:A:1248:PRO:HD3	2.50	0.42
1:A:689:ILE:HD12	1:A:733:LEU:HD23	2.02	0.42
1:A:1074:ILE:HD13	1:A:1081:PHE:HB3	2.02	0.41
1:A:482:ILE:HD12	1:A:609:ARG:HH22	1.86	0.41
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	2.02	0.41
1:A:296:LYS:HD3	1:A:326:GLY:HA2	2.02	0.41
1:A:423:GLU:OE1	1:A:590:ARG:NH1	2.53	0.41
1:A:686:VAL:O	1:A:688:VAL:HG23	2.20	0.41
1:A:178:VAL:HG22	1:A:789:ALA:HB2	2.02	0.41
1:A:167:LEU:HD11	1:A:182:ASP:HB3	2.01	0.41
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.86	0.41
1:A:482:ILE:HD12	1:A:609:ARG:NH2	2.36	0.41
1:A:1460:TYR:O	1:A:1464:ILE:HG12	2.21	0.41
1:A:654:ARG:HH11	1:A:657:THR:H	1.68	0.41
1:A:708:ASP:O	1:A:714:GLY:HA3	2.21	0.41
1:A:1098:ARG:HG2	1:A:1148:ASP:HA	2.03	0.41
1:A:763:PHE:HD1	1:A:768:ASP:CB	2.34	0.40
1:A:1295:LEU:HD21	1:A:1298:VAL:HG21	1.94	0.40
1:A:1275:LYS:O	1:A:1278:GLU:HB2	2.21	0.40
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.37	0.40
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.37	0.40

All (6) 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:A:1442:THR:OG1	1:A:1442:THR:CG2[5_554]	1.39	0.81
1:A:1442:THR:CB	1:A:1442:THR:CB[5_554]	1.39	0.81
1:A:1442:THR:CB	1:A:1442:THR:CG2[5_554]	1.49	0.71
1:A:1442:THR:CG2	1:A:1442:THR:CG2[5_554]	1.51	0.69
1:A:1442:THR:CB	1:A:1442:THR:OG1[5_554]	1.55	0.65
1:A:1441:MET:CG	1:A:1441:MET:SD[5_554]	1.90	0.30

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	1363/1494 (91%)	1284 (94%)	65 (5%)	14 (1%)	15 54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	SER
1	A	569	LYS
1	A	656	ASN
1	A	657	THR
1	A	659	ILE
1	A	1439	ASN
1	A	454	PHE
1	A	162	LYS
1	A	666	GLU
1	A	1337	GLU
1	A	658	LEU
1	A	1142	PRO
1	A	306	LYS
1	A	457	GLY

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	1196/1297 (92%)	1163 (97%)	33 (3%)	43 65

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	167	LEU
1	A	175	LYS
1	A	222	HIS
1	A	308	PHE
1	A	323	ASN
1	A	342	ARG
1	A	363	ARG
1	A	414	ARG
1	A	437	ASP
1	A	513	GLN
1	A	612	ASN
1	A	620	ARG
1	A	638	ASN
1	A	758	ASP
1	A	759	LYS
1	A	770	GLU
1	A	820	PHE
1	A	873	ASP
1	A	880	ASP
1	A	884	THR
1	A	946	ASN
1	A	971	ASP
1	A	1066	ASN
1	A	1116	ILE
1	A	1123	GLU
1	A	1203	PHE
1	A	1312	TYR
1	A	1329	MET
1	A	1330	CYS
1	A	1437	CYS
1	A	1439	ASN
1	A	1443	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	GLN
1	A	656	ASN
1	A	1305	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

14 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

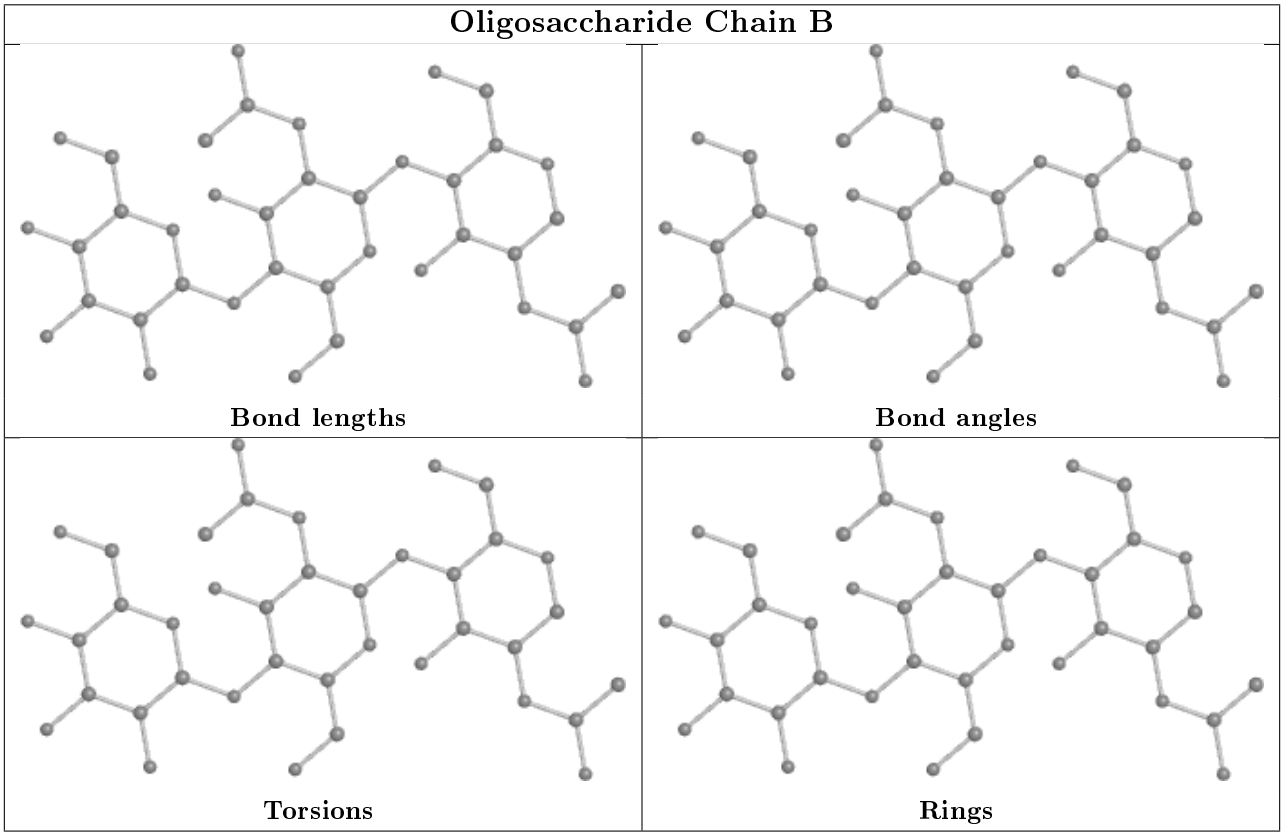
There are no chirality outliers.

There are no torsion outliers.

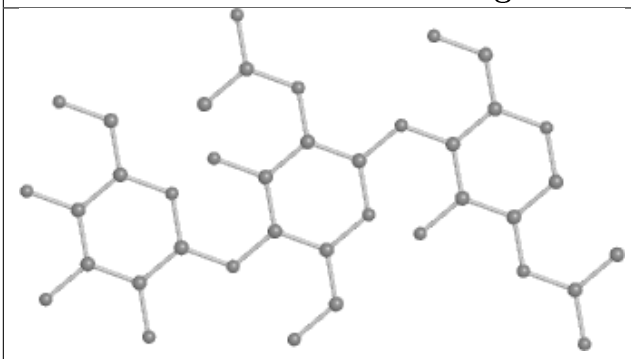
There are no ring outliers.

No monomer is involved in short contacts.

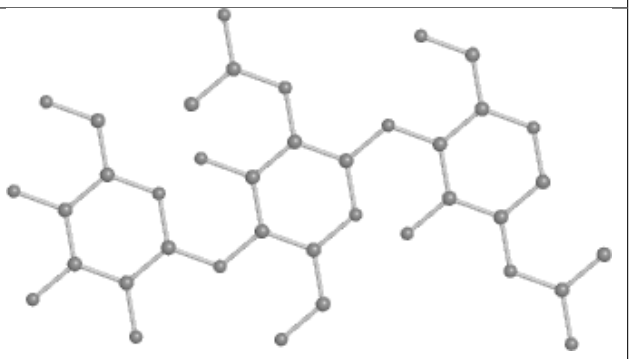
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



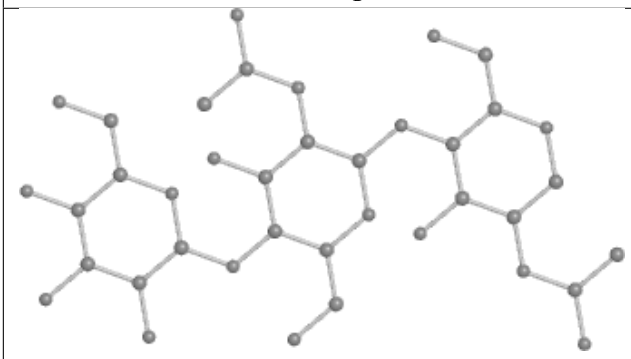
Oligosaccharide Chain D



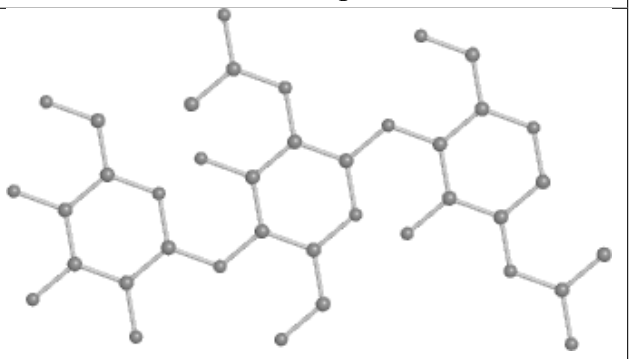
Bond lengths



Bond angles

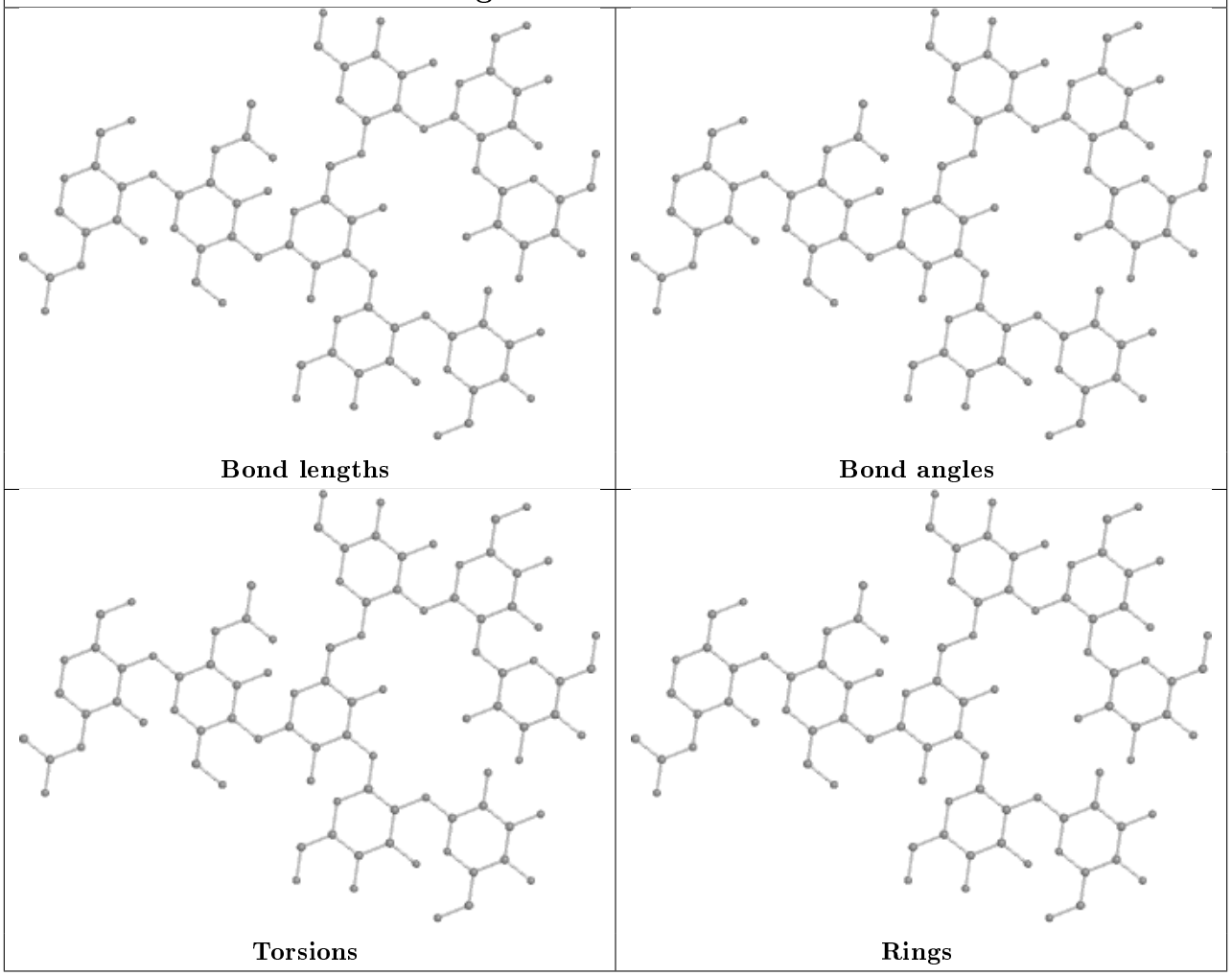


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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

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^{th} 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^2)	Q<0.9
1	A	1369/1494 (91%)	0.54	134 (9%) 7 7	54, 128, 265, 300	1 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	SER	14.0
1	A	133	GLY	11.2
1	A	1084	LYS	6.0
1	A	279	ILE	5.8
1	A	1205	VAL	5.7
1	A	1197	HIS	5.5
1	A	134	THR	5.0
1	A	978	ALA	4.8
1	A	1206	ALA	4.5
1	A	1282	TYR	4.4
1	A	131	LEU	4.3
1	A	175	LYS	4.2
1	A	565	GLU	4.1
1	A	566	LEU	3.9
1	A	1355	PRO	3.9
1	A	968	PRO	3.9
1	A	1464	ILE	3.8
1	A	1283	LYS	3.8
1	A	1058	GLN	3.8
1	A	887	THR	3.8
1	A	367	PRO	3.8
1	A	1233	TRP	3.7
1	A	595	GLY	3.6
1	A	1204	SER	3.6
1	A	503	PRO	3.5
1	A	297	ALA	3.5
1	A	933	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	652	LEU	3.4
1	A	1041	ILE	3.3
1	A	879	PHE	3.3
1	A	884	THR	3.3
1	A	1259	GLU	3.3
1	A	1293	LEU	3.3
1	A	979	LEU	3.2
1	A	1201	ASN	3.2
1	A	363	ARG	3.2
1	A	1361	LEU	3.2
1	A	1284	ILE	3.1
1	A	364	GLN	3.1
1	A	1071	ASP	3.0
1	A	45	LEU	3.0
1	A	972	GLU	3.0
1	A	596	ASP	3.0
1	A	1040	LEU	2.9
1	A	977	LYS	2.9
1	A	996	MET	2.9
1	A	1056	GLY	2.9
1	A	1332	SER	2.9
1	A	332	ALA	2.9
1	A	280	ALA	2.9
1	A	886	ARG	2.9
1	A	1207	SER	2.9
1	A	328	GLN	2.8
1	A	1262	THR	2.8
1	A	1285	LEU	2.8
1	A	42	PRO	2.8
1	A	945	LEU	2.8
1	A	283	LYS	2.8
1	A	365	ILE	2.8
1	A	568	PHE	2.8
1	A	1073	ILE	2.8
1	A	701	ALA	2.7
1	A	1363	VAL	2.7
1	A	496	PRO	2.7
1	A	973	SER	2.7
1	A	1354	LYS	2.7
1	A	55	ASP	2.7
1	A	986	VAL	2.6
1	A	1085	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1370	ARG	2.6
1	A	1331	ASP	2.6
1	A	1453	GLN	2.6
1	A	715	GLN	2.6
1	A	975	LYS	2.6
1	A	1446	LYS	2.6
1	A	1441	MET	2.5
1	A	709	LEU	2.5
1	A	429	ILE	2.5
1	A	1434	ILE	2.5
1	A	1275	LYS	2.5
1	A	1325	GLY	2.5
1	A	327	SER	2.5
1	A	474	LEU	2.5
1	A	1319	LEU	2.5
1	A	1235	ILE	2.5
1	A	74	GLU	2.5
1	A	976	VAL	2.5
1	A	1294	SER	2.5
1	A	361	ILE	2.4
1	A	1287	LEU	2.4
1	A	1288	ASP	2.4
1	A	969	SER	2.4
1	A	1323	PRO	2.4
1	A	766	PHE	2.4
1	A	431	LEU	2.4
1	A	1003	LEU	2.4
1	A	1115	PRO	2.4
1	A	772	ALA	2.3
1	A	926	TRP	2.3
1	A	1253	GLU	2.3
1	A	1254	TYR	2.3
1	A	1057	VAL	2.3
1	A	450	LEU	2.3
1	A	130	SER	2.2
1	A	1039	ILE	2.2
1	A	1297	LYS	2.2
1	A	1232	PHE	2.2
1	A	184	ILE	2.2
1	A	46	VAL	2.2
1	A	764	THR	2.2
1	A	1261	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	239	LYS	2.2
1	A	1036	LEU	2.2
1	A	788	LEU	2.2
1	A	178	VAL	2.2
1	A	918	PRO	2.2
1	A	971	ASP	2.1
1	A	1082	GLN	2.1
1	A	501	PHE	2.1
1	A	182	ASP	2.1
1	A	331	SER	2.1
1	A	142	PHE	2.1
1	A	1440	PRO	2.1
1	A	397	LEU	2.1
1	A	903	GLY	2.1
1	A	1216	ASN	2.1
1	A	1278	GLU	2.1
1	A	702	ALA	2.1
1	A	1433	THR	2.1
1	A	889	LEU	2.1
1	A	987	PRO	2.0
1	A	1279	ILE	2.0
1	A	929	VAL	2.0
1	A	166	GLN	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)

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^{th} 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^2)	Q<0.9
3	MAN	C	4	11/12	0.13	0.49	300,300,300,300	0
3	BMA	C	3	11/12	0.32	0.36	291,296,298,298	0
3	MAN	C	5	11/12	0.48	0.55	300,300,300,300	0
2	BMA	D	3	11/12	0.57	0.36	291,292,292,293	0
2	NAG	D	2	14/15	0.58	0.81	290,292,295,296	0

Continued on next page...

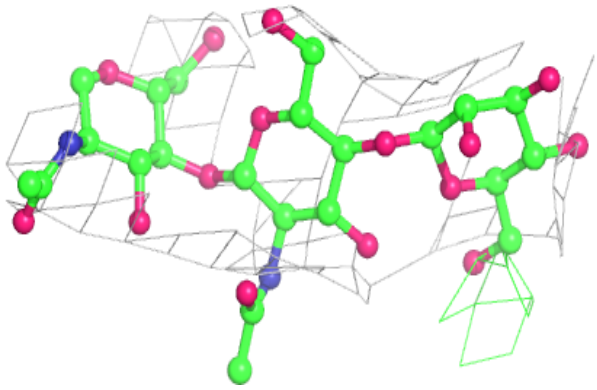
Continued from previous page...

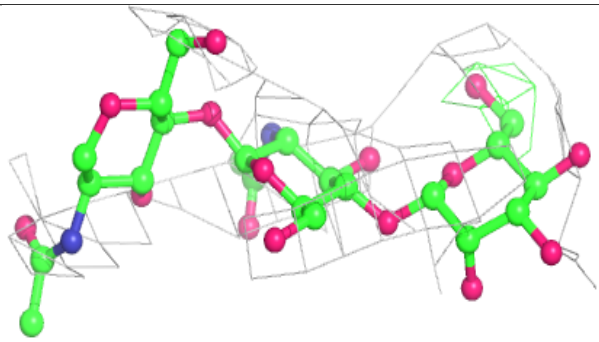
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	C	6	11/12	0.60	0.30	300,300,300,300	0
2	BMA	B	3	11/12	0.60	0.39	167,261,296,297	0
3	MAN	C	8	11/12	0.71	0.27	298,298,299,299	0
2	NAG	D	1	14/15	0.72	0.74	286,292,293,294	0
3	MAN	C	7	11/12	0.83	0.23	297,298,299,299	0
3	NAG	C	2	14/15	0.89	0.33	191,214,266,286	0
2	NAG	B	1	14/15	0.91	0.27	95,109,135,138	0
2	NAG	B	2	14/15	0.92	0.22	113,153,272,293	0
3	NAG	C	1	14/15	0.93	0.41	132,156,192,273	0

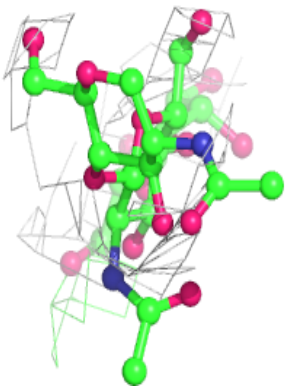
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

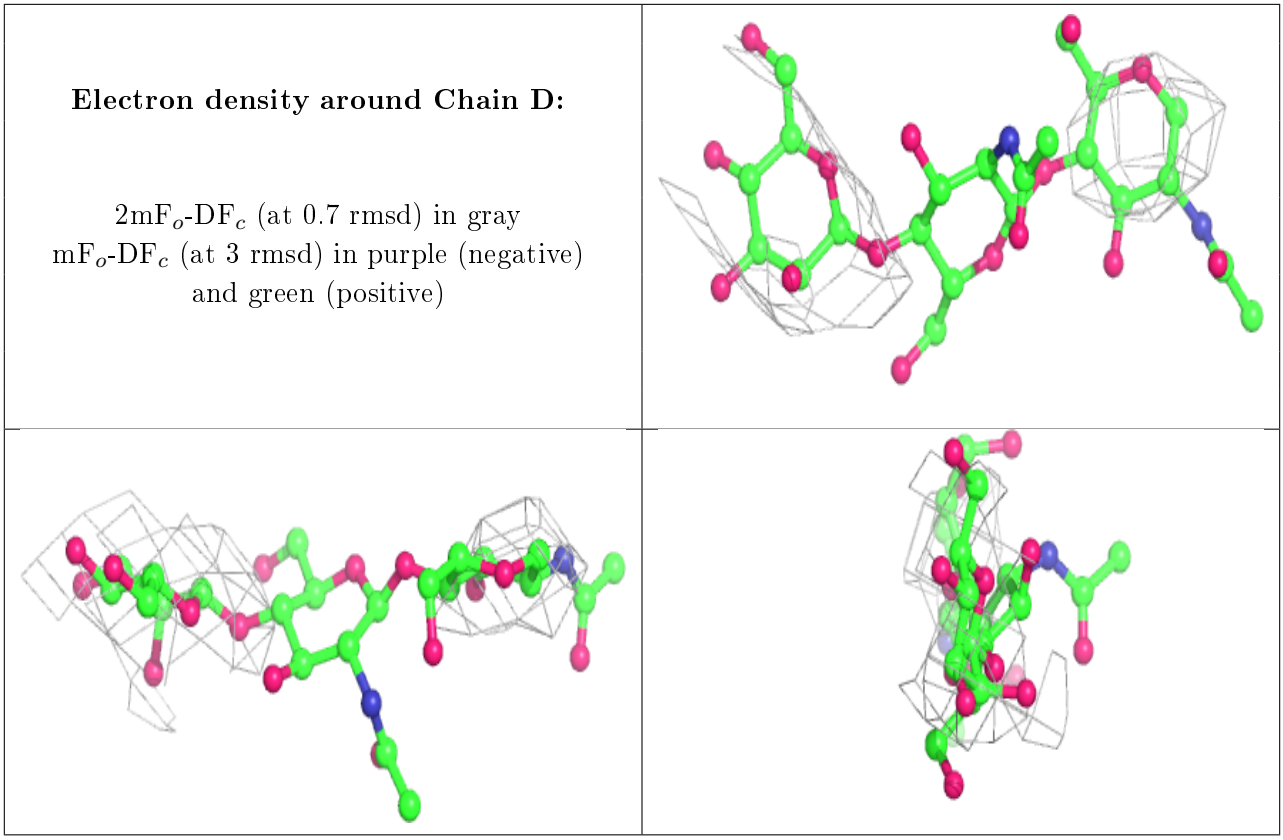






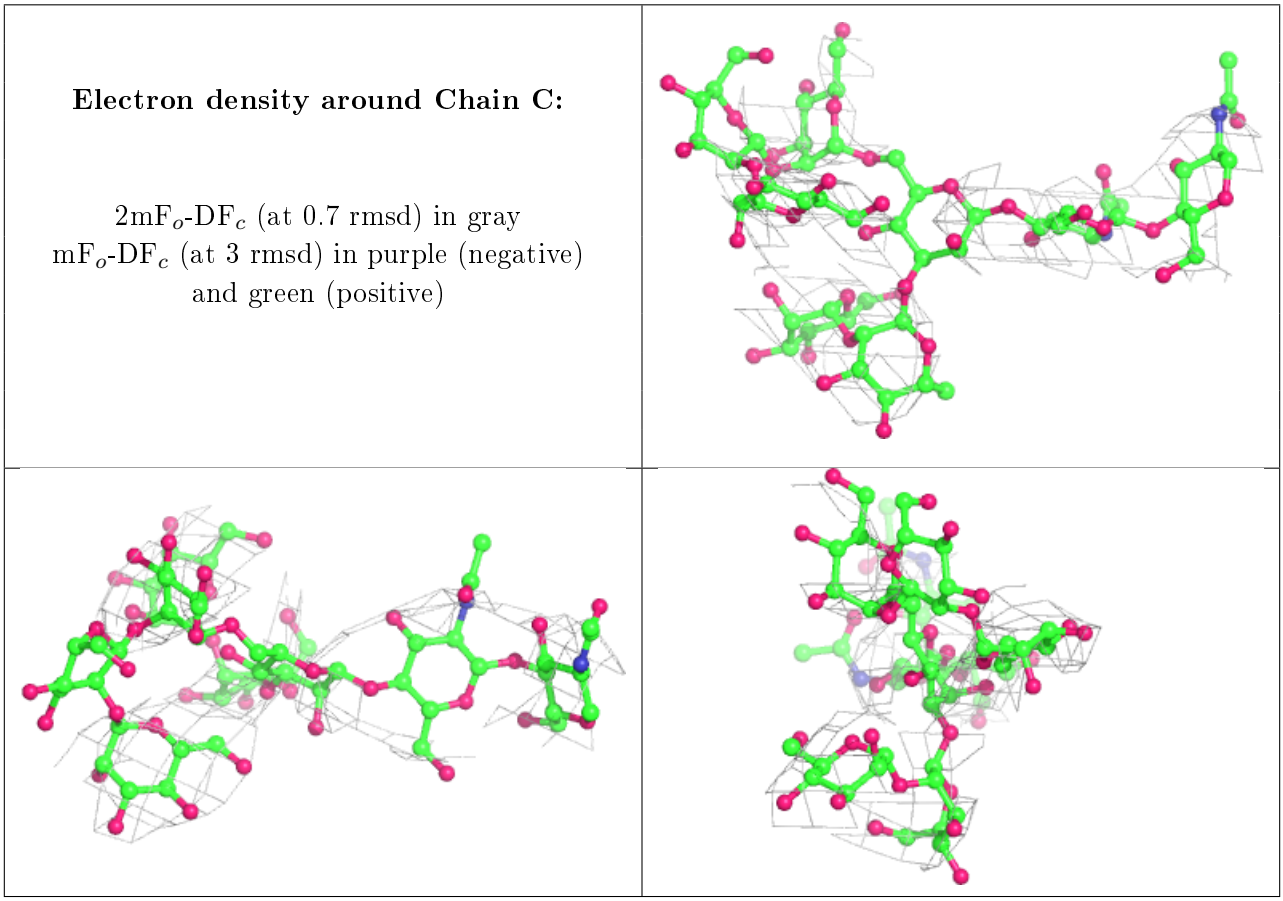
Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

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^{th} 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^2)	Q<0.9
5	NAG	A	1607	14/15	0.39	0.52	114,191,280,293	0
4	TB	A	1601	1/1	0.73	0.36	213,213,213,213	0
5	NAG	A	1619	14/15	0.87	0.56	289,290,291,291	0
4	TB	A	1602	1/1	0.99	0.28	166,166,166,166	0
4	TB	A	1603	1/1	0.99	0.31	83,83,83,83	0

6.5 Other polymers

There are no such residues in this entry.