wwPDB X-ray Structure Validation Summary Report (i)

Dec 7, 2023 – 01:44 pm GMT

PDB ID	:	1UR9
Title	:	Interactions of a family 18 chitinase with the designed inhibitor HM508, and its degradation product, chitobiono-delta-lactone
Authors	:	Vaaje-Kolstad, G.; Vasella, A.; Peter, M.G.; Netter, C.; Houston, D.R.; Westereng, B.; Synstad, B.; Eijsink, V.G.H.; Van Aalten, D.M.F.
Deposited on	:	2003-10-27
Resolution	:	1.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

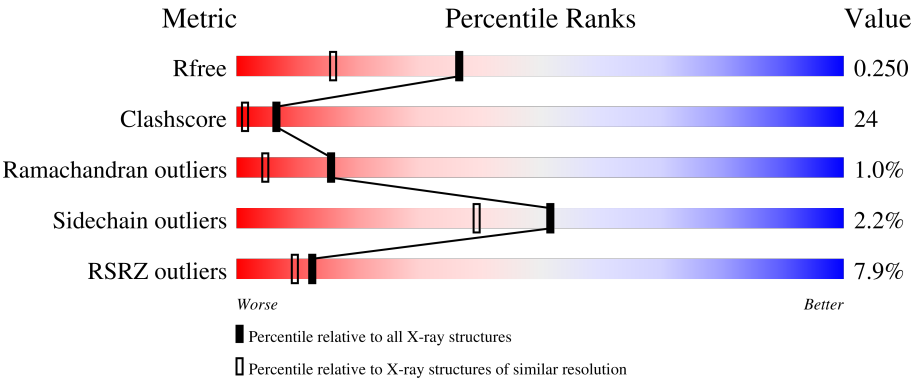
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	499	8% 75% 23%
1	B	499	7% 74% 24%
2	C	2	50% 50%
2	D	2	100%

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
3	GOL	A	1500	-	-	X	-
3	GOL	A	1502	-	-	X	-
3	GOL	A	1505	-	-	X	-
3	GOL	A	1507	-	-	X	-
3	GOL	A	1509	-	-	X	-
3	GOL	A	1511	-	-	-	X
3	GOL	A	1512	-	-	X	X
3	GOL	A	1513	-	-	X	X
3	GOL	A	1517	-	-	X	-
3	GOL	A	1521	-	-	X	-
3	GOL	A	1525	-	-	X	-
3	GOL	A	1527	-	-	X	-
3	GOL	A	1528	-	-	X	X
3	GOL	B	1500	-	-	X	-
3	GOL	B	1503	-	-	X	-
3	GOL	B	1505	-	-	X	-
3	GOL	B	1508	-	-	X	-
3	GOL	B	1511	-	-	X	-
3	GOL	B	1514	-	-	X	-
3	GOL	B	1515	-	-	X	-
3	GOL	B	1516	-	-	X	-
3	GOL	B	1521	-	-	X	-
3	GOL	B	1522	-	-	X	-
3	GOL	B	1527	-	-	X	-
3	GOL	B	1528	-	-	-	X
3	GOL	B	1529	-	-	X	-
3	GOL	B	1531	-	-	X	-
4	SO4	A	1533	-	-	X	-
5	PHJ	A	2503	-	-	X	-
5	PHJ	B	2503	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9198 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 CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	2	1
			3904	2498	658	733	15			
1	B	498	Total	C	N	O	S	0	7	0
			3933	2513	664	741	15			

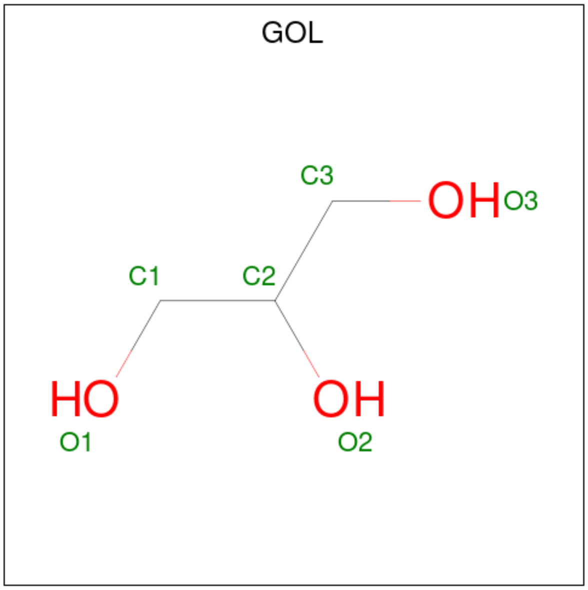
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ASN	ASP	engineered mutation	UNP Q54276
B	142	ASN	ASP	engineered mutation	UNP Q54276
A	499	ARG	ALA	conflict	UNP Q54276
B	499	ARG	ALA	conflict	UNP Q54276

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-(acetylamido)-2-deoxy-D-glucono-1,5-lactone.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

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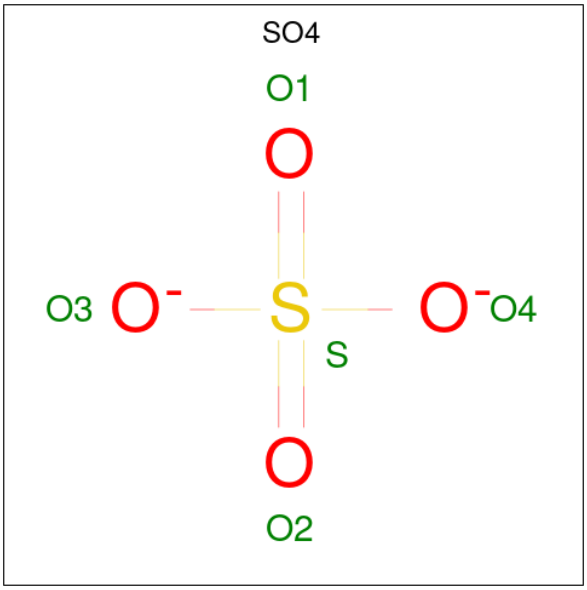
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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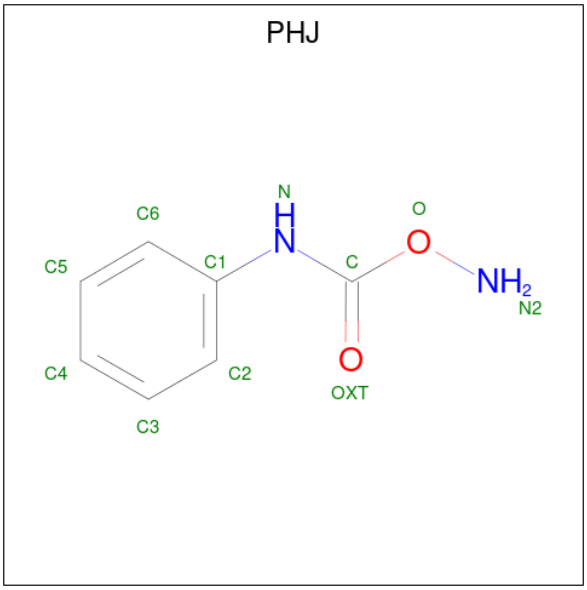
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is N-[(AMINOOXY)CARBONYL]-N-PHENYLAMINE (three-letter code: PHJ) (formula: $C_7H_8N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 11 7 2 2	0	0
5	B	1	Total C N O 11 7 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	413	Total O 413 413	0	0

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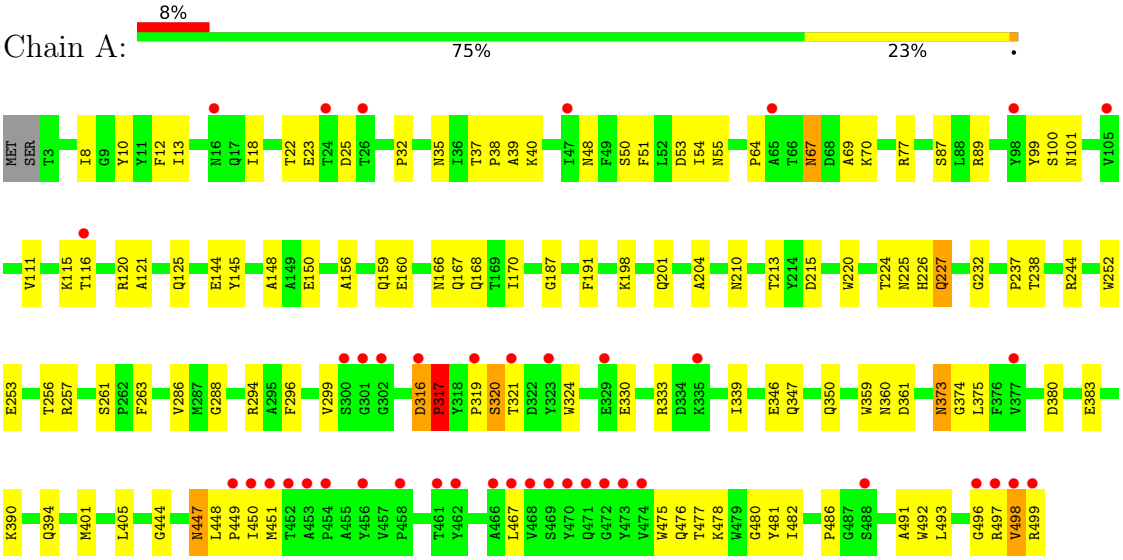
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	441	Total	O	0	0
			441	441		

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.

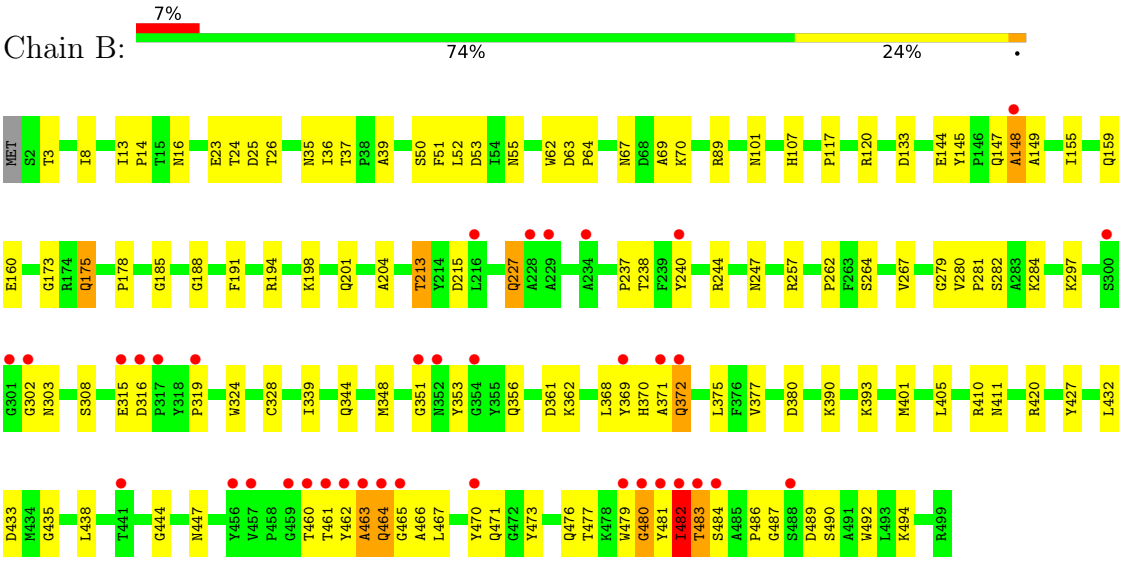
• Molecule 1: CHITINASE B

Chain A:



• Molecule 1: CHITINASE B

Chain B:

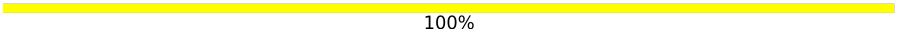


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-(acetylamido)-2-deoxy-D-gluco no-1,5-lactone

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-(acetylamido)-2-deoxy-D-gluco no-1,5-lactone

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.52Å 104.18Å 185.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 1.80 24.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (24.88-1.80) 97.0 (24.87-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 1.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.255 0.199 , 0.250	Depositor DCC
R_{free} test set	983 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: GOL, PHJ, GDL, SO4, NAG

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	0.50	0/4023	0.78	4/5486 (0.1%)
1	B	0.50	0/4078	0.71	1/5558 (0.0%)
All	All	0.50	0/8101	0.75	5/11044 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	ASP	C-N-CD	-20.42	75.67	120.60
1	A	316	ASP	C-N-CA	13.40	178.27	122.00
1	B	482	ILE	N-CA-C	6.82	129.41	111.00
1	A	317	PRO	CA-N-CD	-5.73	103.48	111.50
1	A	100	SER	N-CA-C	5.17	124.97	111.00

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	3904	0	3729	159	0
1	B	3933	0	3745	198	0
2	C	28	0	20	1	0
2	D	28	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	186	0	248	99	0
3	B	198	0	264	109	0
4	A	30	0	0	4	0
4	B	15	0	0	2	0
5	A	11	0	7	5	0
5	B	11	0	7	7	0
6	A	413	0	0	17	0
6	B	441	0	0	25	0
All	All	9198	0	8040	388	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 24.

The worst 5 of 388 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:51:PHE:H	3:A:1524:GOL:H2	1.08	1.08
1:B:64:PRO:HD3	3:B:1511:GOL:H2	1.33	1.07
1:B:23:GLU:H	3:B:1510:GOL:H31	1.13	1.06
1:A:168:GLN:HE22	3:A:1521:GOL:H11	1.20	1.04
1:A:361:ASP:H	3:A:1517:GOL:H32	1.19	1.01

There are no symmetry-related clashes.

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	497/499 (100%)	480 (97%)	14 (3%)	3 (1%)	25 12
1	B	503/499 (101%)	482 (96%)	14 (3%)	7 (1%)	11 3
All	All	1000/998 (100%)	962 (96%)	28 (3%)	10 (1%)	15 5

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	PRO
1	B	148	ALA
1	B	372	GLN
1	B	483	THR
1	B	463	ALA

5.3.2 Protein sidechains (i)

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	403/406 (99%)	396 (98%)	7 (2%)	60	51
1	B	408/406 (100%)	396 (97%)	12 (3%)	42	29
All	All	811/812 (100%)	792 (98%)	19 (2%)	52	37

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	339	ILE
1	B	464	GLN
1	B	482	ILE
1	B	411	ASN
1	B	175	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	GLN
1	B	350	GLN
1	B	347	GLN
1	B	372	GLN
1	A	347	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

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GDL	C	1	2,5	14,14,15	1.44	2 (14%)	17,19,21	2.17	2 (11%)
2	NAG	C	2	2	14,14,15	0.91	0	17,19,21	0.72	0
2	GDL	D	1	2,5	14,14,15	1.43	3 (21%)	17,19,21	2.10	2 (11%)
2	NAG	D	2	2	14,14,15	1.08	1 (7%)	17,19,21	0.63	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
2	GDL	C	1	2,5	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	GDL	D	1	2,5	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	GDL	O5-C1	-3.63	1.37	1.43
2	D	1	GDL	O5-C1	-3.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.52	1.56	1.52
2	D	1	GDL	C1-C2	2.29	1.55	1.52
2	C	1	GDL	C2-N2	2.22	1.50	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	GDL	O5-C1-C2	7.35	122.89	111.29
2	D	1	GDL	O5-C1-C2	7.09	122.48	111.29
2	D	1	GDL	C1-O5-C5	3.54	116.99	112.19
2	C	1	GDL	C1-O5-C5	3.44	116.85	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	GDL	C1-C2-N2-C7
2	D	1	GDL	C1-C2-N2-C7

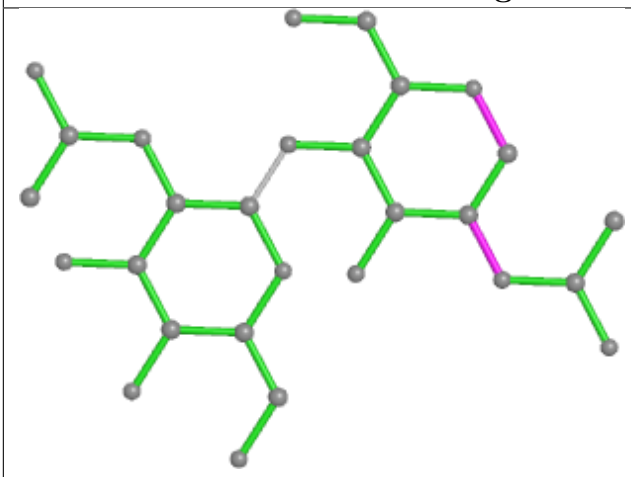
There are no ring outliers.

1 monomer is involved in 1 short contact:

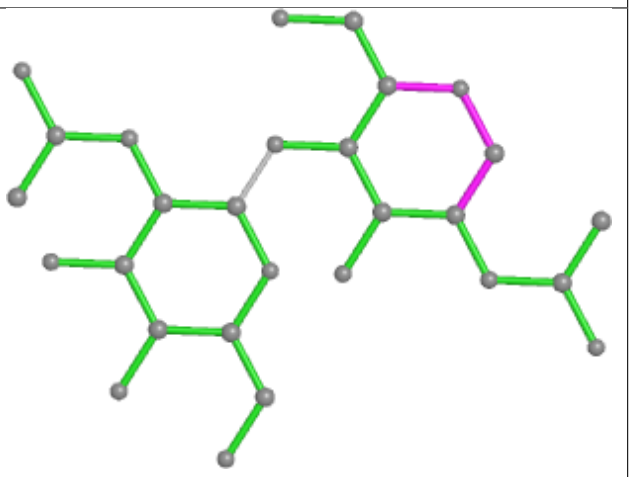
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GDL	1	0

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

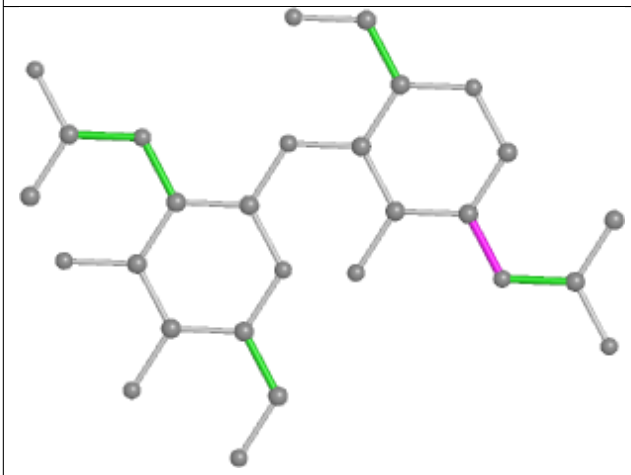
Oligosaccharide Chain C



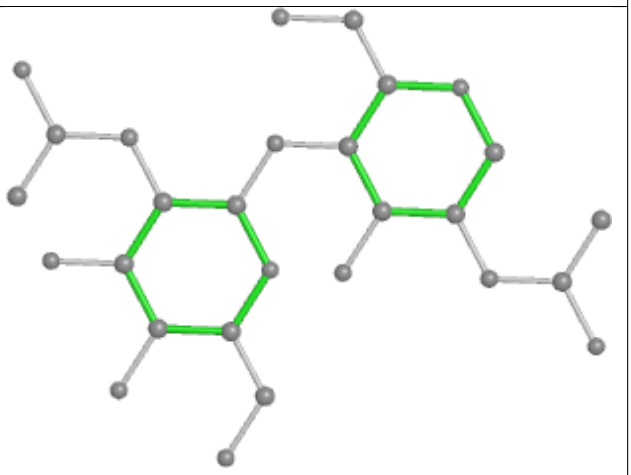
Bond lengths



Bond angles

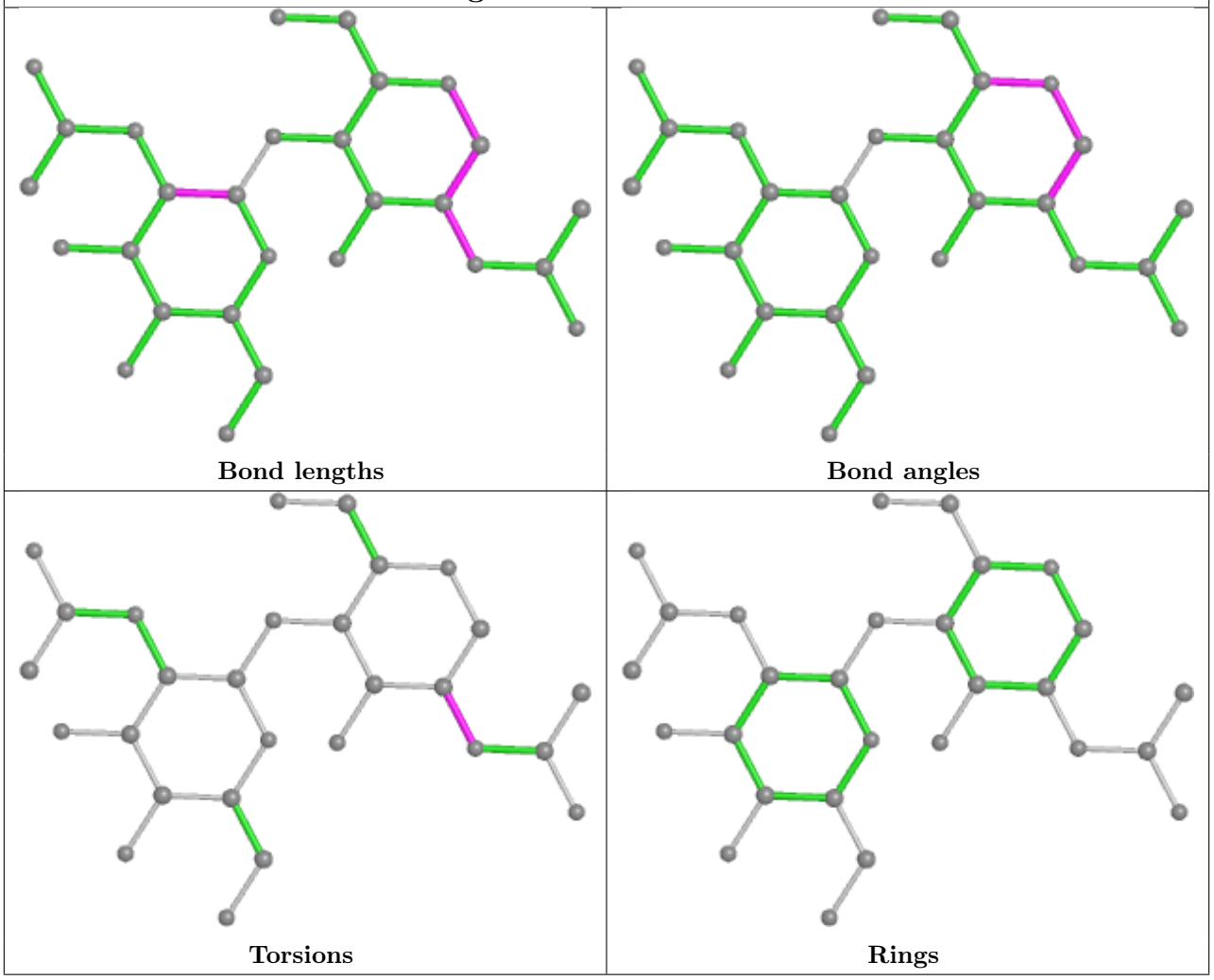


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

75 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	1512	-	5,5,5	0.43	0	5,5,5	0.31	0
3	GOL	B	1511	-	5,5,5	0.32	0	5,5,5	0.26	0
3	GOL	B	1513	-	5,5,5	0.31	0	5,5,5	0.31	0
4	SO4	B	1534	-	4,4,4	0.27	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	1515	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	A	1513	-	5,5,5	0.22	0	5,5,5	0.31	0
3	GOL	B	1526	-	5,5,5	0.41	0	5,5,5	0.19	0
3	GOL	B	1531	-	5,5,5	0.24	0	5,5,5	0.29	0
3	GOL	B	1523	-	5,5,5	0.41	0	5,5,5	0.16	0
3	GOL	B	1501	-	5,5,5	0.35	0	5,5,5	0.21	0
3	GOL	A	1523	-	5,5,5	0.33	0	5,5,5	0.18	0
3	GOL	B	1520	-	5,5,5	0.27	0	5,5,5	0.31	0
3	GOL	B	1537	-	5,5,5	0.15	0	5,5,5	0.31	0
4	SO4	A	1533	-	4,4,4	0.23	0	6,6,6	0.11	0
3	GOL	B	1504	-	5,5,5	0.31	0	5,5,5	0.27	0
3	GOL	A	1528	-	5,5,5	0.26	0	5,5,5	0.31	0
3	GOL	A	1504	-	5,5,5	0.33	0	5,5,5	0.20	0
3	GOL	A	1511	-	5,5,5	0.32	0	5,5,5	0.35	0
3	GOL	B	1521	-	5,5,5	0.30	0	5,5,5	0.31	0
3	GOL	B	1525	-	5,5,5	0.27	0	5,5,5	0.28	0
3	GOL	A	1525	-	5,5,5	0.23	0	5,5,5	0.25	0
3	GOL	A	1526	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	B	1508	-	5,5,5	0.41	0	5,5,5	0.19	0
3	GOL	A	1502	-	5,5,5	0.23	0	5,5,5	0.42	0
3	GOL	A	1503	-	5,5,5	0.19	0	5,5,5	0.37	0
3	GOL	B	1509	-	5,5,5	0.26	0	5,5,5	0.26	0
3	GOL	B	1514	-	5,5,5	0.30	0	5,5,5	0.26	0
4	SO4	B	1535	-	4,4,4	0.25	0	6,6,6	0.08	0
3	GOL	A	1505	-	5,5,5	0.21	0	5,5,5	0.20	0
3	GOL	A	1510	-	5,5,5	0.36	0	5,5,5	0.18	0
3	GOL	B	1517	-	5,5,5	0.50	0	5,5,5	0.43	0
5	PHJ	A	2503	2	9,11,11	1.70	2 (22%)	12,13,13	0.94	1 (8%)
3	GOL	A	1518	-	5,5,5	0.28	0	5,5,5	0.26	0
3	GOL	A	1506	-	5,5,5	0.59	0	5,5,5	0.14	0
3	GOL	A	1501	-	5,5,5	0.37	0	5,5,5	0.33	0
3	GOL	A	1524	-	5,5,5	0.23	0	5,5,5	0.33	0
3	GOL	B	1507	-	5,5,5	0.29	0	5,5,5	0.32	0
3	GOL	B	1519	-	5,5,5	0.28	0	5,5,5	0.31	0
4	SO4	A	1535	-	4,4,4	0.24	0	6,6,6	0.10	0
3	GOL	A	1514	-	5,5,5	0.28	0	5,5,5	0.24	0
4	SO4	A	1536	-	4,4,4	0.26	0	6,6,6	0.11	0
3	GOL	A	1538	-	5,5,5	0.28	0	5,5,5	0.33	0
4	SO4	A	1532	-	4,4,4	0.26	0	6,6,6	0.26	0
3	GOL	B	1505	-	5,5,5	0.43	0	5,5,5	0.24	0
3	GOL	A	1520	-	5,5,5	0.29	0	5,5,5	0.29	0
3	GOL	A	1508	-	5,5,5	0.26	0	5,5,5	0.31	0
3	GOL	A	1507	-	5,5,5	0.41	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	1519	-	5,5,5	0.34	0	5,5,5	0.31	0
3	GOL	B	1510	-	5,5,5	0.33	0	5,5,5	0.32	0
3	GOL	A	1509	-	5,5,5	0.33	0	5,5,5	0.35	0
3	GOL	B	1528	-	5,5,5	0.40	0	5,5,5	0.20	0
4	SO4	A	1537	-	4,4,4	0.28	0	6,6,6	0.04	0
5	PHJ	B	2503	2	9,11,11	1.73	2 (22%)	12,13,13	1.08	2 (16%)
3	GOL	B	1518	-	5,5,5	0.44	0	5,5,5	0.15	0
3	GOL	B	1530	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	B	1503	-	5,5,5	0.25	0	5,5,5	0.21	0
3	GOL	B	1502	-	5,5,5	0.20	0	5,5,5	0.43	0
3	GOL	B	1500	-	5,5,5	0.21	0	5,5,5	0.25	0
3	GOL	B	1506	-	5,5,5	0.37	0	5,5,5	0.33	0
3	GOL	A	1500	-	5,5,5	0.22	0	5,5,5	0.36	0
3	GOL	B	1512	-	5,5,5	0.44	0	5,5,5	0.29	0
3	GOL	B	1529	-	5,5,5	0.42	0	5,5,5	0.23	0
3	GOL	A	1521	-	5,5,5	0.29	0	5,5,5	0.31	0
3	GOL	A	1529	-	5,5,5	0.33	0	5,5,5	0.30	0
3	GOL	B	1522	-	5,5,5	0.31	0	5,5,5	0.36	0
3	GOL	A	1517	-	5,5,5	0.34	0	5,5,5	0.21	0
3	GOL	A	1522	-	5,5,5	0.28	0	5,5,5	0.32	0
3	GOL	B	1516	-	5,5,5	0.28	0	5,5,5	0.31	0
4	SO4	A	1534	-	4,4,4	0.34	0	6,6,6	0.20	0
3	GOL	A	1515	-	5,5,5	0.30	0	5,5,5	0.26	0
3	GOL	A	1516	-	5,5,5	0.52	0	5,5,5	0.16	0
3	GOL	B	1524	-	5,5,5	0.23	0	5,5,5	0.33	0
4	SO4	B	1536	-	4,4,4	0.27	0	6,6,6	0.07	0
3	GOL	B	1527	-	5,5,5	0.32	0	5,5,5	0.23	0
3	GOL	A	1527	-	5,5,5	0.27	0	5,5,5	0.23	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
3	GOL	A	1512	-	-	0/4/4/4	-
3	GOL	B	1511	-	-	0/4/4/4	-
3	GOL	B	1513	-	-	0/4/4/4	-
3	GOL	B	1515	-	-	0/4/4/4	-
3	GOL	A	1513	-	-	0/4/4/4	-
3	GOL	B	1526	-	-	0/4/4/4	-
3	GOL	B	1531	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1523	-	-	0/4/4/4	-
3	GOL	B	1501	-	-	0/4/4/4	-
3	GOL	A	1523	-	-	0/4/4/4	-
3	GOL	B	1520	-	-	0/4/4/4	-
3	GOL	B	1537	-	-	0/4/4/4	-
3	GOL	B	1504	-	-	0/4/4/4	-
3	GOL	A	1528	-	-	0/4/4/4	-
3	GOL	A	1504	-	-	0/4/4/4	-
3	GOL	A	1511	-	-	0/4/4/4	-
3	GOL	B	1521	-	-	0/4/4/4	-
3	GOL	B	1525	-	-	0/4/4/4	-
3	GOL	A	1525	-	-	0/4/4/4	-
3	GOL	A	1526	-	-	0/4/4/4	-
3	GOL	B	1508	-	-	0/4/4/4	-
3	GOL	A	1502	-	-	0/4/4/4	-
3	GOL	A	1503	-	-	0/4/4/4	-
3	GOL	B	1509	-	-	0/4/4/4	-
3	GOL	B	1514	-	-	0/4/4/4	-
3	GOL	A	1505	-	-	0/4/4/4	-
3	GOL	A	1510	-	-	0/4/4/4	-
3	GOL	B	1517	-	-	0/4/4/4	-
5	PHJ	A	2503	2	-	0/4/6/6	0/1/1/1
3	GOL	A	1518	-	-	0/4/4/4	-
3	GOL	A	1506	-	-	0/4/4/4	-
3	GOL	A	1501	-	-	0/4/4/4	-
3	GOL	A	1524	-	-	0/4/4/4	-
3	GOL	B	1507	-	-	0/4/4/4	-
3	GOL	B	1519	-	-	0/4/4/4	-
3	GOL	A	1514	-	-	0/4/4/4	-
3	GOL	A	1538	-	-	0/4/4/4	-
3	GOL	B	1505	-	-	0/4/4/4	-
3	GOL	A	1520	-	-	0/4/4/4	-
3	GOL	A	1508	-	-	0/4/4/4	-
3	GOL	A	1507	-	-	0/4/4/4	-
3	GOL	A	1519	-	-	0/4/4/4	-
3	GOL	B	1510	-	-	0/4/4/4	-
3	GOL	A	1509	-	-	0/4/4/4	-
3	GOL	B	1528	-	-	0/4/4/4	-
5	PHJ	B	2503	2	-	0/4/6/6	0/1/1/1
3	GOL	B	1518	-	-	0/4/4/4	-
3	GOL	B	1530	-	-	0/4/4/4	-
3	GOL	B	1503	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1502	-	-	0/4/4/4	-
3	GOL	B	1500	-	-	0/4/4/4	-
3	GOL	B	1506	-	-	0/4/4/4	-
3	GOL	A	1500	-	-	0/4/4/4	-
3	GOL	B	1512	-	-	0/4/4/4	-
3	GOL	B	1529	-	-	0/4/4/4	-
3	GOL	A	1521	-	-	0/4/4/4	-
3	GOL	A	1529	-	-	0/4/4/4	-
3	GOL	B	1522	-	-	0/4/4/4	-
3	GOL	A	1517	-	-	0/4/4/4	-
3	GOL	A	1522	-	-	0/4/4/4	-
3	GOL	B	1516	-	-	0/4/4/4	-
3	GOL	A	1515	-	-	0/4/4/4	-
3	GOL	A	1516	-	-	0/4/4/4	-
3	GOL	B	1524	-	-	0/4/4/4	-
3	GOL	B	1527	-	-	0/4/4/4	-
3	GOL	A	1527	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2503	PHJ	C1-N	-3.26	1.35	1.41
5	B	2503	PHJ	C1-N	-3.21	1.35	1.41
5	A	2503	PHJ	OXT-C	2.38	1.26	1.21
5	B	2503	PHJ	OXT-C	2.37	1.26	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2503	PHJ	O-C-N	2.68	117.42	110.35
5	A	2503	PHJ	O-C-N	2.54	117.03	110.35
5	B	2503	PHJ	OXT-C-N	-2.03	121.68	126.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

66 monomers are involved in 219 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1512	GOL	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1511	GOL	11	0
4	B	1534	SO4	1	0
3	B	1515	GOL	6	0
3	A	1513	GOL	8	0
3	B	1526	GOL	1	0
3	B	1531	GOL	6	0
3	B	1523	GOL	2	0
3	B	1501	GOL	1	0
3	A	1523	GOL	1	0
3	B	1537	GOL	2	0
4	A	1533	SO4	2	0
3	B	1504	GOL	1	0
3	A	1528	GOL	5	0
3	A	1504	GOL	2	0
3	B	1521	GOL	4	0
3	B	1525	GOL	3	0
3	A	1525	GOL	5	0
3	A	1526	GOL	3	0
3	B	1508	GOL	8	0
3	A	1502	GOL	7	0
3	A	1503	GOL	2	0
3	B	1509	GOL	3	0
3	B	1514	GOL	5	0
3	A	1505	GOL	4	0
3	A	1510	GOL	3	0
3	B	1517	GOL	1	0
5	A	2503	PHJ	5	0
3	A	1518	GOL	2	0
3	A	1506	GOL	3	0
3	A	1501	GOL	2	0
3	A	1524	GOL	3	0
3	B	1507	GOL	1	0
3	B	1519	GOL	1	0
4	A	1536	SO4	1	0
3	A	1538	GOL	1	0
3	B	1505	GOL	4	0
3	A	1520	GOL	2	0
3	A	1508	GOL	1	0
3	A	1507	GOL	7	0
3	A	1519	GOL	1	0
3	B	1510	GOL	3	0
3	A	1509	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1528	GOL	3	0
4	A	1537	SO4	1	0
5	B	2503	PHJ	7	0
3	B	1518	GOL	3	0
3	B	1530	GOL	2	0
3	B	1503	GOL	5	0
3	B	1502	GOL	2	0
3	B	1500	GOL	6	0
3	B	1506	GOL	3	0
3	A	1500	GOL	6	0
3	B	1512	GOL	3	0
3	B	1529	GOL	4	0
3	A	1521	GOL	4	0
3	A	1529	GOL	2	0
3	B	1522	GOL	4	0
3	A	1517	GOL	5	0
3	B	1516	GOL	4	0
3	A	1515	GOL	1	0
3	A	1516	GOL	1	0
3	B	1524	GOL	3	0
4	B	1536	SO4	1	0
3	B	1527	GOL	4	0
3	A	1527	GOL	5	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

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	497/499 (99%)	0.38	42 (8%)	10	8	16, 32, 52, 63	0
1	B	498/499 (99%)	0.31	37 (7%)	14	11	20, 30, 51, 73	0
All	All	995/998 (99%)	0.34	79 (7%)	12	9	16, 30, 52, 73	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	VAL	7.3
1	B	481	TYR	6.4
1	A	472	GLY	5.6
1	B	463	ALA	5.1
1	B	483	THR	5.1

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

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

6.3 Carbohydrates

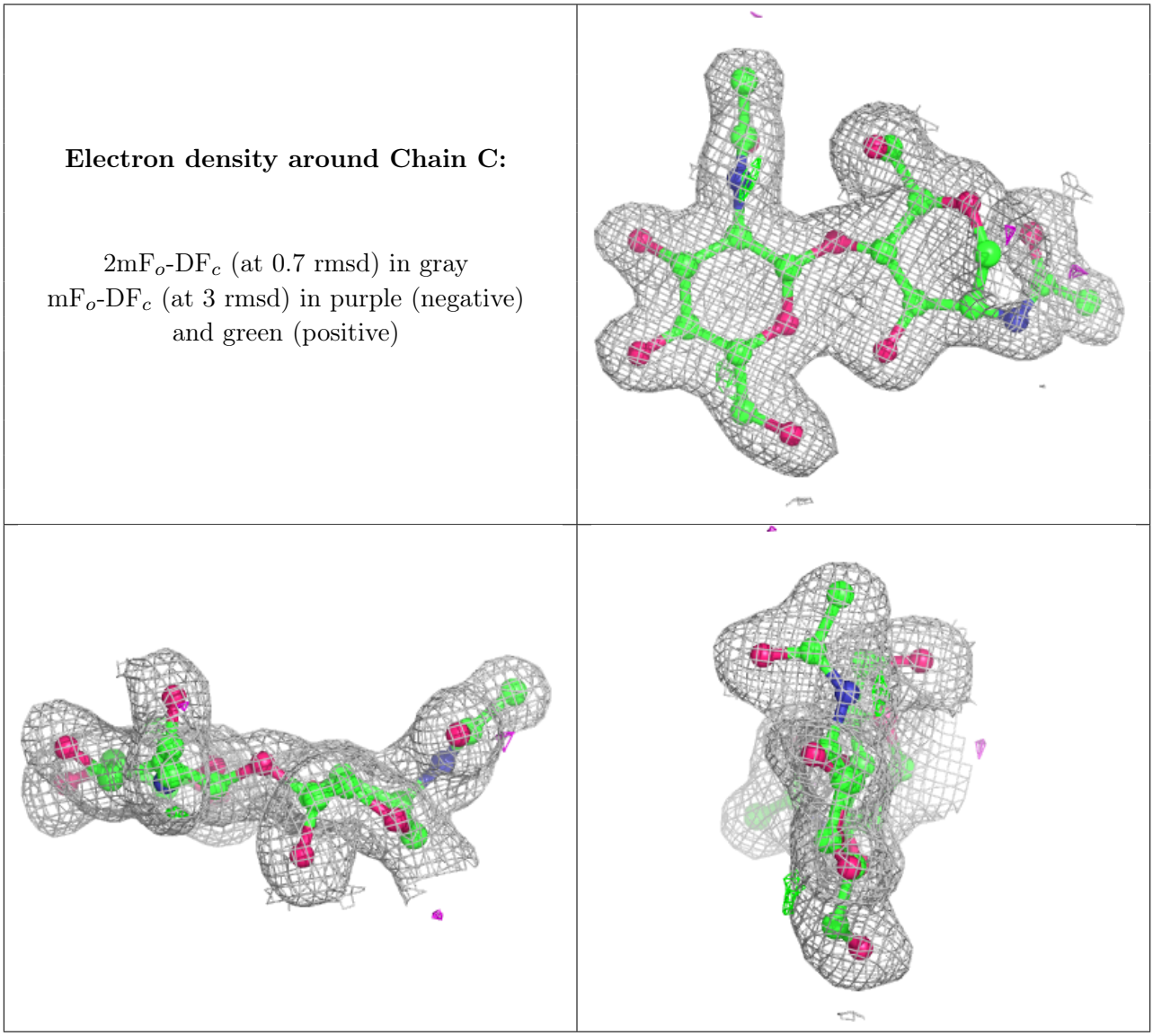
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAG	C	2	14/15	0.90	0.10	26,28,32,34	0
2	GDL	C	1	14/15	0.94	0.09	21,23,27,27	0
2	GDL	D	1	14/15	0.95	0.08	20,23,25,25	0
2	NAG	D	2	14/15	0.96	0.07	21,24,27,28	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.

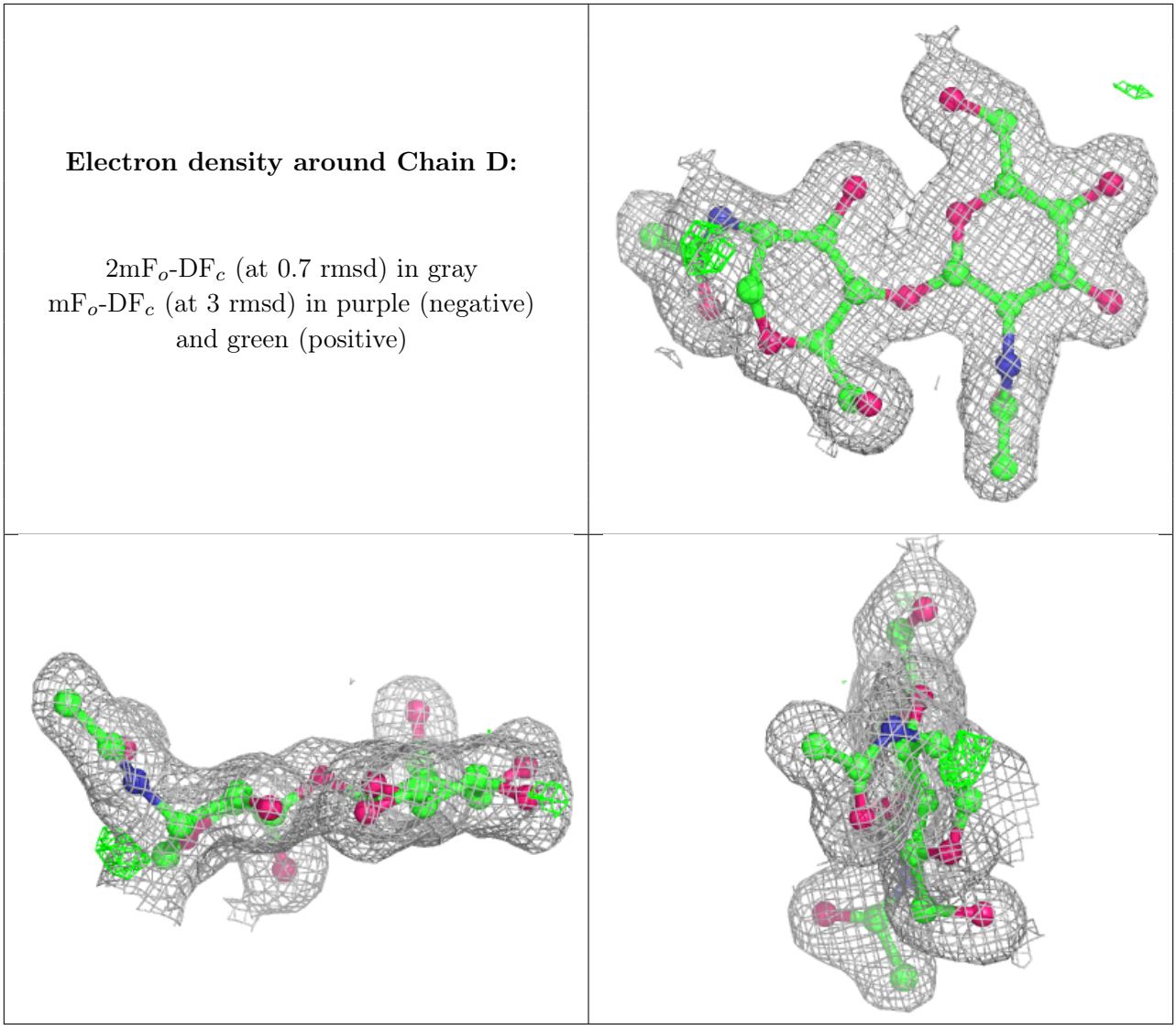
Electron density around Chain C:

$2mF_o$-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)



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
3	GOL	B	1518	6/6	0.48	0.28	63,65,65,67	0
3	GOL	B	1512	6/6	0.53	0.34	44,51,52,55	0
3	GOL	A	1511	6/6	0.53	0.41	78,79,79,79	0
3	GOL	A	1516	6/6	0.55	0.26	47,52,53,53	0
3	GOL	B	1528	6/6	0.58	0.42	69,70,71,71	0
3	GOL	B	1514	6/6	0.61	0.37	71,73,73,75	0
3	GOL	B	1529	6/6	0.61	0.35	66,66,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	1517	6/6	0.62	0.24	51,53,54,54	0
3	GOL	B	1522	6/6	0.62	0.34	64,66,67,68	0
3	GOL	A	1529	6/6	0.63	0.26	60,62,62,63	0
3	GOL	B	1508	6/6	0.64	0.21	58,59,59,60	0
3	GOL	A	1510	6/6	0.65	0.16	63,64,65,65	0
3	GOL	B	1507	6/6	0.65	0.23	55,57,58,58	0
3	GOL	B	1515	6/6	0.66	0.28	57,59,60,61	0
3	GOL	A	1538	6/6	0.66	0.33	66,67,68,70	0
3	GOL	A	1501	6/6	0.67	0.25	64,65,66,68	0
3	GOL	A	1509	6/6	0.68	0.36	58,61,63,65	0
3	GOL	A	1523	6/6	0.68	0.21	66,69,69,71	0
3	GOL	A	1512	6/6	0.69	0.45	58,60,61,62	0
3	GOL	B	1505	6/6	0.70	0.23	47,55,56,59	0
3	GOL	B	1519	6/6	0.71	0.32	69,70,71,72	0
3	GOL	B	1511	6/6	0.72	0.32	52,53,54,55	0
3	GOL	A	1528	6/6	0.72	0.50	74,75,77,77	0
3	GOL	A	1517	6/6	0.73	0.32	60,62,62,62	0
3	GOL	A	1527	6/6	0.73	0.36	69,70,70,71	0
3	GOL	B	1526	6/6	0.74	0.17	58,59,60,62	0
3	GOL	A	1514	6/6	0.74	0.23	74,74,75,75	0
3	GOL	A	1519	6/6	0.74	0.19	57,60,61,64	0
3	GOL	A	1520	6/6	0.75	0.36	58,60,61,63	0
3	GOL	B	1521	6/6	0.77	0.35	65,66,67,67	0
3	GOL	A	1513	6/6	0.78	0.40	68,70,70,72	0
3	GOL	A	1508	6/6	0.78	0.31	57,61,63,65	0
3	GOL	B	1506	6/6	0.79	0.29	49,54,55,55	0
3	GOL	A	1522	6/6	0.80	0.33	72,73,75,75	0
3	GOL	A	1515	6/6	0.80	0.18	68,69,69,70	0
3	GOL	B	1502	6/6	0.81	0.23	46,49,50,52	0
3	GOL	B	1523	6/6	0.81	0.31	51,53,53,53	0
3	GOL	B	1503	6/6	0.81	0.22	55,56,58,62	0
3	GOL	A	1525	6/6	0.81	0.41	35,39,42,46	0
3	GOL	B	1510	6/6	0.81	0.14	68,69,70,70	0
3	GOL	B	1530	6/6	0.81	0.32	60,62,62,63	0
3	GOL	A	1506	6/6	0.82	0.21	40,44,46,46	0
3	GOL	B	1524	6/6	0.82	0.28	72,72,73,73	0
3	GOL	B	1504	6/6	0.82	0.19	41,47,51,54	0
3	GOL	A	1521	6/6	0.83	0.20	58,59,61,62	0
3	GOL	B	1520	6/6	0.83	0.21	65,66,66,67	0
3	GOL	B	1516	6/6	0.83	0.33	62,64,64,65	0
3	GOL	A	1500	6/6	0.83	0.27	42,46,49,52	0
3	GOL	A	1526	6/6	0.83	0.34	49,52,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1518	6/6	0.84	0.27	82,82,83,83	0
3	GOL	A	1504	6/6	0.84	0.22	39,42,43,47	0
3	GOL	B	1527	6/6	0.84	0.24	63,64,64,66	0
3	GOL	B	1500	6/6	0.85	0.26	60,61,64,64	0
3	GOL	B	1513	6/6	0.85	0.16	65,67,67,67	0
3	GOL	A	1507	6/6	0.85	0.17	48,49,51,53	0
3	GOL	B	1531	6/6	0.85	0.33	69,69,70,71	0
3	GOL	B	1501	6/6	0.86	0.33	53,55,58,58	0
3	GOL	B	1525	6/6	0.86	0.26	80,80,81,81	0
3	GOL	B	1537	6/6	0.86	0.21	56,57,59,59	0
3	GOL	A	1505	6/6	0.87	0.20	43,50,53,55	0
3	GOL	A	1524	6/6	0.87	0.31	56,57,58,61	0
3	GOL	B	1509	6/6	0.88	0.25	49,49,50,50	0
3	GOL	A	1503	6/6	0.88	0.25	37,39,45,48	0
3	GOL	A	1502	6/6	0.90	0.23	36,42,42,45	0
4	SO4	B	1536	5/5	0.91	0.18	92,92,92,92	0
5	PHJ	A	2503	11/11	0.91	0.14	28,34,42,43	0
4	SO4	A	1535	5/5	0.93	0.13	82,82,83,83	0
4	SO4	B	1535	5/5	0.93	0.23	71,72,73,73	0
5	PHJ	B	2503	11/11	0.93	0.12	25,34,37,38	0
4	SO4	A	1536	5/5	0.94	0.21	78,79,79,80	0
4	SO4	A	1537	5/5	0.94	0.36	92,93,93,93	0
4	SO4	A	1534	5/5	0.95	0.15	46,46,49,49	0
4	SO4	A	1532	5/5	0.98	0.12	42,44,46,46	0
4	SO4	A	1533	5/5	0.99	0.19	49,53,53,54	0
4	SO4	B	1534	5/5	0.99	0.14	53,54,54,56	0

6.5 Other polymers (i)

There are no such residues in this entry.