wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2024 – 11:38 PM EDT

PDB ID	:	1YWH
Title	:	crystal structure of urokinase plasminogen activator receptor
Authors	:	Llinas, P.; Le Du, M.H.; Gardsvoll, H.; Dano, K.; Ploug, M.; Gilquin, B.; Stura, E.A.; Menez, A.
Deposited on	:	2005-02-18
Resolution	:	2.70 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:

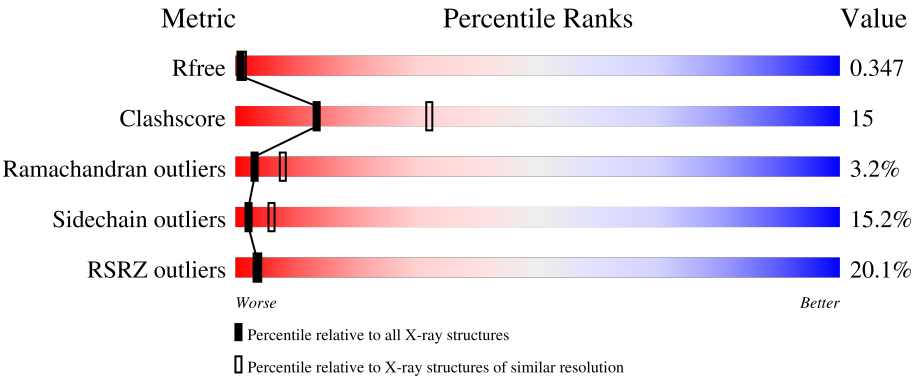
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	313	20% 51% 26% 6% • 14%
1	C	313	16% 51% 25% 6% • 17%
1	E	313	16% 53% 25% 5% 16%
1	G	313	13% 50% 27% 6% 18%
1	I	313	16% 47% 29% 9% 16%

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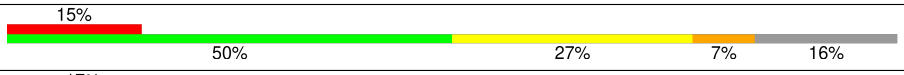
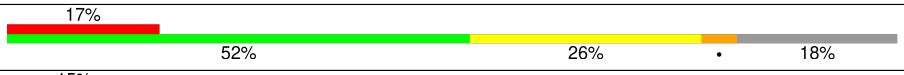
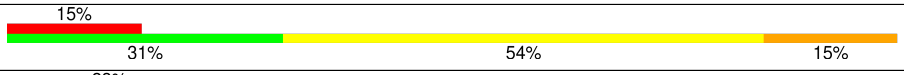
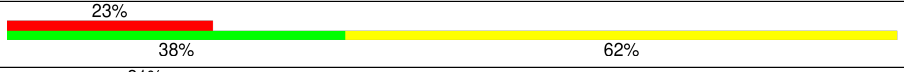
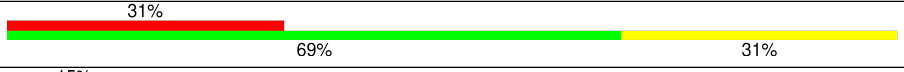
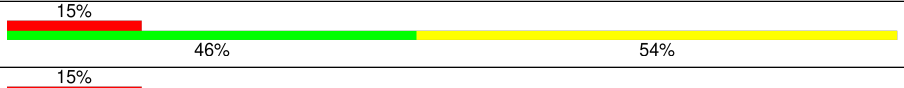
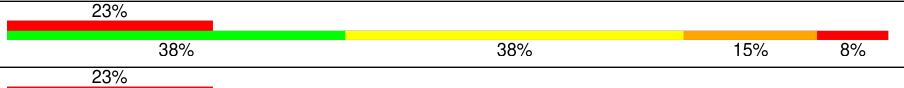
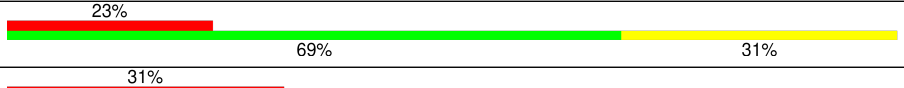
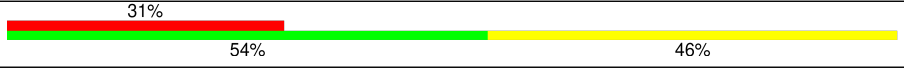
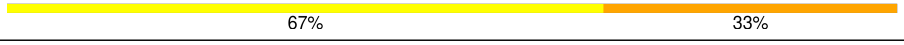
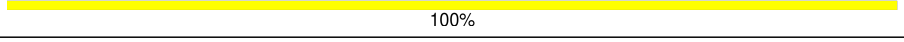
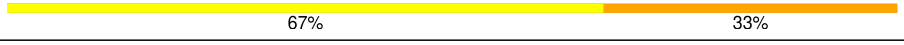
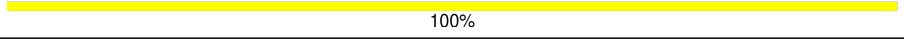
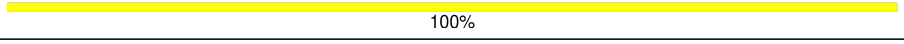
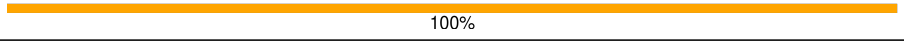
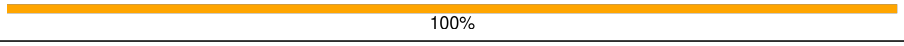
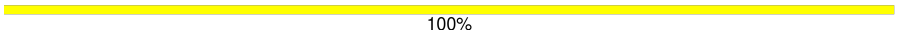
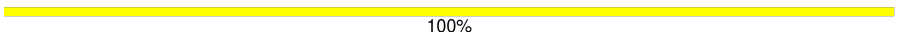
Mol	Chain	Length	Quality of chain
1	K	313	
1	M	313	
1	O	313	
2	B	13	
2	D	13	
2	F	13	
2	H	13	
2	J	13	
2	L	13	
2	N	13	
2	P	13	
3	Q	3	
3	S	3	
3	T	3	
3	b	3	
4	R	2	
4	U	2	
4	V	2	
4	X	2	
4	Y	2	
4	a	2	
4	d	2	
4	g	2	
5	W	2	
5	f	2	

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Mol	Chain	Length	Quality of chain
6	Z	5	20% 80%
6	c	5	100%
6	e	5	100%
6	h	5	20% 80%

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	FUC	Q	3	X	-	-	-
3	NAG	S	1	X	-	-	-
3	FUC	S	3	X	-	-	-
3	FUC	T	3	X	-	-	-
3	FUC	b	3	X	-	-	-
4	FUC	R	2	X	-	-	-
4	FUC	U	2	X	-	-	-
4	FUC	V	2	X	-	-	-
4	NAG	X	1	X	-	-	-
4	FUC	X	2	X	-	-	-
4	FUC	Y	2	X	-	-	-
4	FUC	a	2	X	-	-	-
4	FUC	d	2	X	-	-	-
4	FUC	g	2	X	-	-	-
6	NAG	Z	1	X	-	-	-
6	NAG	c	1	X	-	-	-
6	NAG	e	1	X	-	-	-
6	NAG	h	1	X	-	-	-
7	NAG	A	317	X	-	-	-
7	NAG	A	321	X	-	-	-
7	NAG	C	316	X	-	-	-
7	NAG	C	321	X	-	-	-
7	NAG	K	331	X	-	-	-
7	NAG	O	321	X	-	-	-
8	SO4	K	810	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 18552 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 Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2040	1222	377	407	34			
1	C	259	Total	C	N	O	S	0	0	0
			1985	1188	368	395	34			
1	E	262	Total	C	N	O	S	0	0	0
			2006	1202	370	400	34			
1	G	258	Total	C	N	O	S	0	0	0
			1978	1186	363	395	34			
1	I	264	Total	C	N	O	S	0	0	0
			2008	1201	372	401	34			
1	K	257	Total	C	N	O	S	0	0	0
			1969	1180	363	392	34			
1	M	263	Total	C	N	O	S	0	0	0
			2016	1204	374	404	34			
1	O	258	Total	C	N	O	S	0	0	0
			1970	1180	362	394	34			

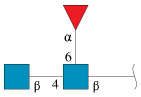
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLN	ASN	conflict	UNP Q9UMV0
C	200	GLN	ASN	conflict	UNP Q9UMV0
E	200	GLN	ASN	conflict	UNP Q9UMV0
G	200	GLN	ASN	conflict	UNP Q9UMV0
I	200	GLN	ASN	conflict	UNP Q9UMV0
K	200	GLN	ASN	conflict	UNP Q9UMV0
M	200	GLN	ASN	conflict	UNP Q9UMV0
O	200	GLN	ASN	conflict	UNP Q9UMV0

- Molecule 2 is a protein called antagonist peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	D	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	F	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	H	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	J	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	L	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	N	13	Total	C	N	O	0	0	0
			116	78	17	21			
2	P	13	Total	C	N	O	0	0	0
			116	78	17	21			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	S	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	T	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	b	3	Total	C	N	O	0	0	0
			38	22	2	14			

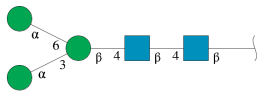
- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	R	2	Total C N O 24 14 1 9	0	0	0
4	U	2	Total C N O 24 14 1 9	0	0	0
4	V	2	Total C N O 24 14 1 9	0	0	0
4	X	2	Total C N O 24 14 1 9	0	0	0
4	Y	2	Total C N O 24 14 1 9	0	0	0
4	a	2	Total C N O 24 14 1 9	0	0	0
4	d	2	Total C N O 24 14 1 9	0	0	0
4	g	2	Total C N O 24 14 1 9	0	0	0

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

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

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
6	Z	5	Total C N O 61 34 2 25	0	0	0
6	c	5	Total C N O 61 34 2 25	0	0	0

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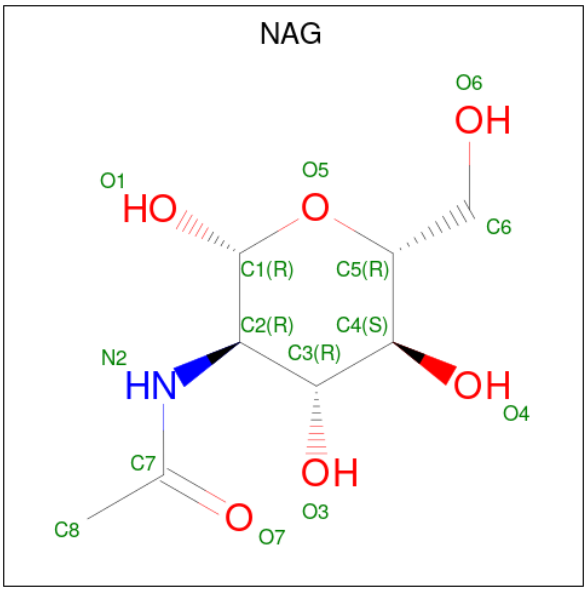
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	e	5	Total C N O 61 34 2 25	0	0	0
6	h	5	Total C N O 61 34 2 25	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0
7	K	1	Total C N O 14 8 1 5	0	0
7	K	1	Total C N O 14 8 1 5	0	0

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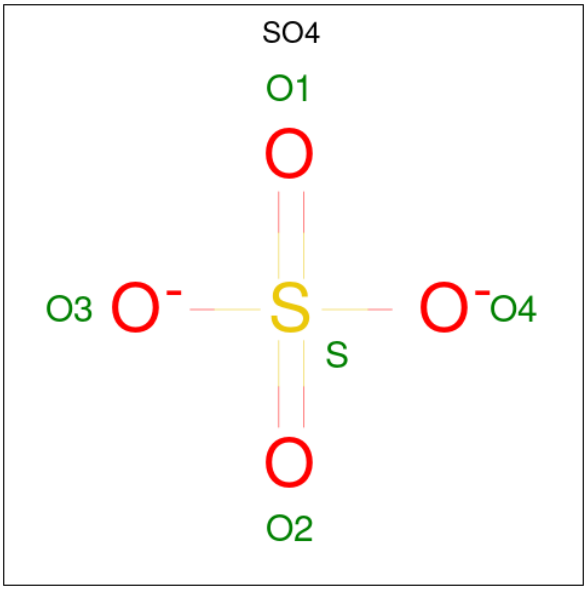
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	K	1	Total O S 5 4 1	0	0
8	K	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	O	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	81	Total O 81 81	0	0
9	B	5	Total O 5 5	0	0
9	C	85	Total O 85 85	0	0
9	D	2	Total O 2 2	0	0
9	E	98	Total O 98 98	0	0
9	F	8	Total O 8 8	0	0
9	G	88	Total O 88 88	0	0

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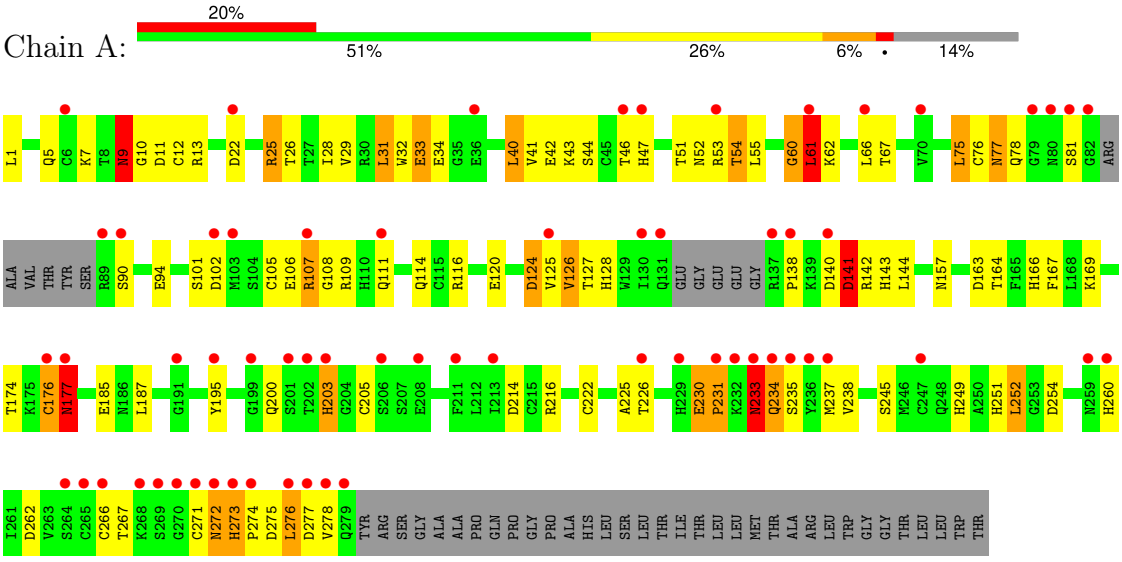
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	4	Total O 4 4	0	0
9	I	87	Total O 87 87	0	0
9	J	3	Total O 3 3	0	0
9	K	83	Total O 83 83	0	0
9	L	2	Total O 2 2	0	0
9	M	91	Total O 91 91	0	0
9	N	1	Total O 1 1	0	0
9	O	106	Total O 106 106	0	0
9	P	5	Total O 5 5	0	0

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.

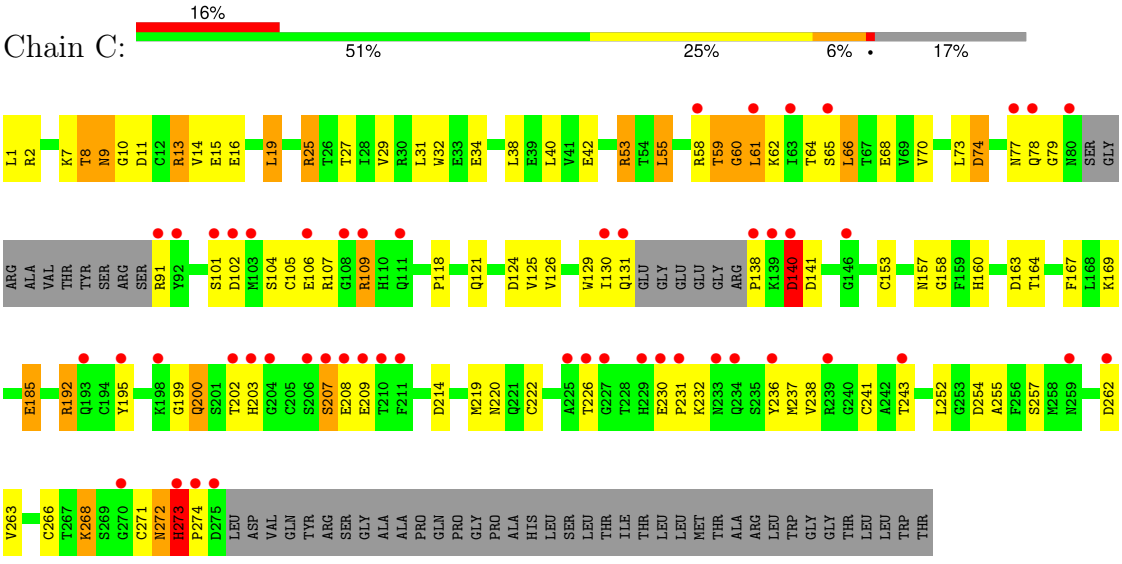
• Molecule 1: Urokinase plasminogen activator surface receptor

Chain A:



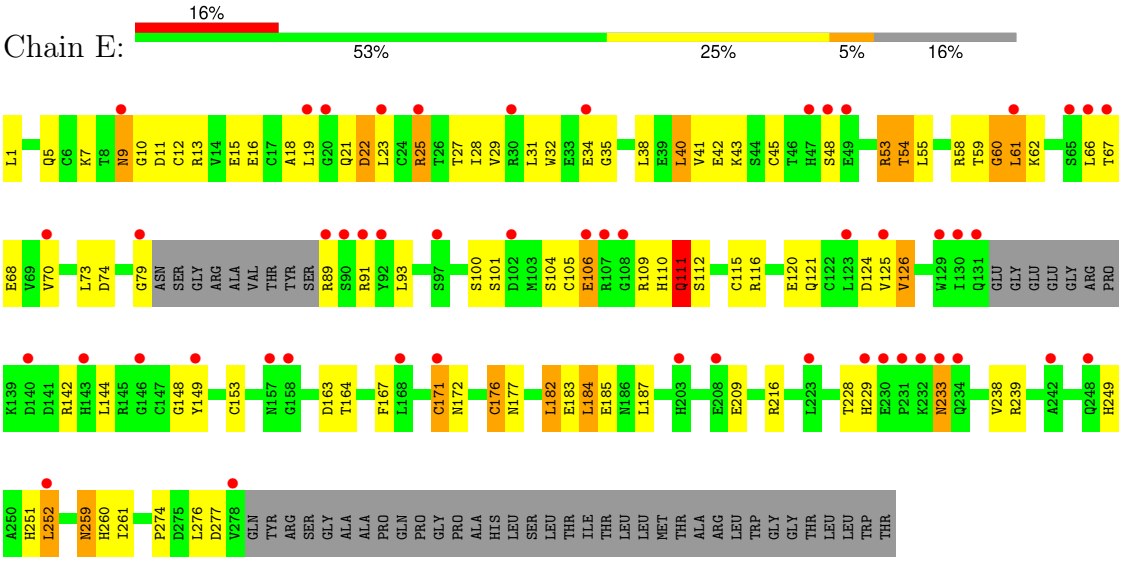
• Molecule 1: Urokinase plasminogen activator surface receptor

Chain C:



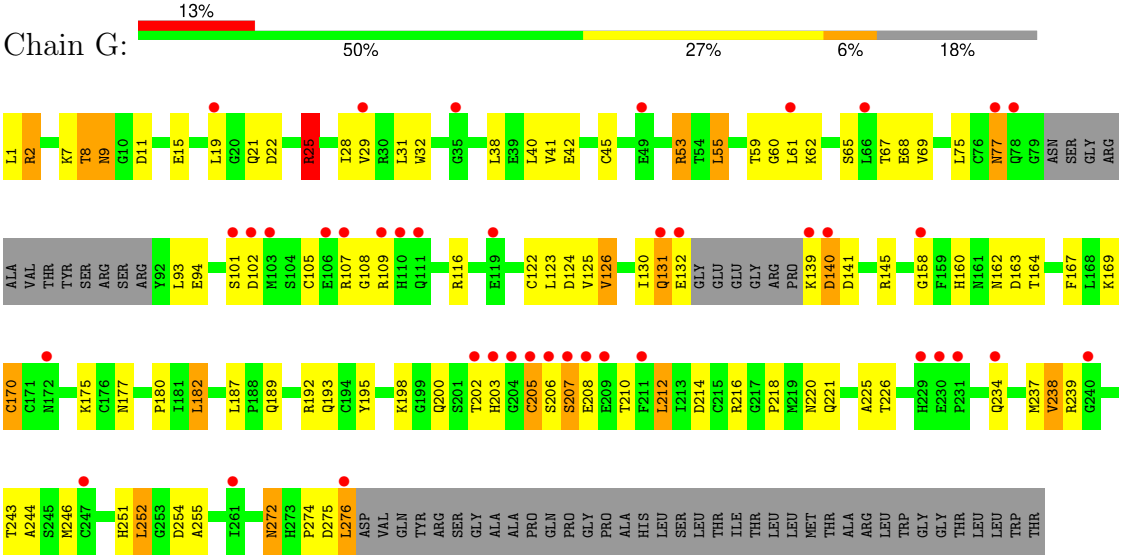
• Molecule 1: Urokinase plasminogen activator surface receptor

Chain E:



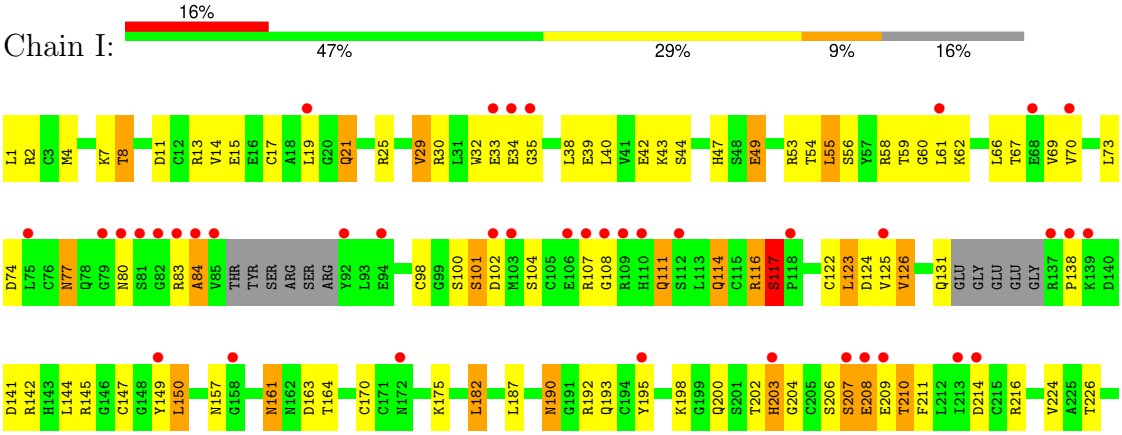
• Molecule 1: Urokinase plasminogen activator surface receptor

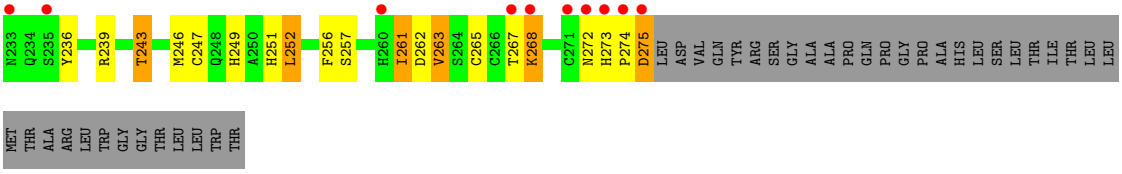
Chain G:



• Molecule 1: Urokinase plasminogen activator surface receptor

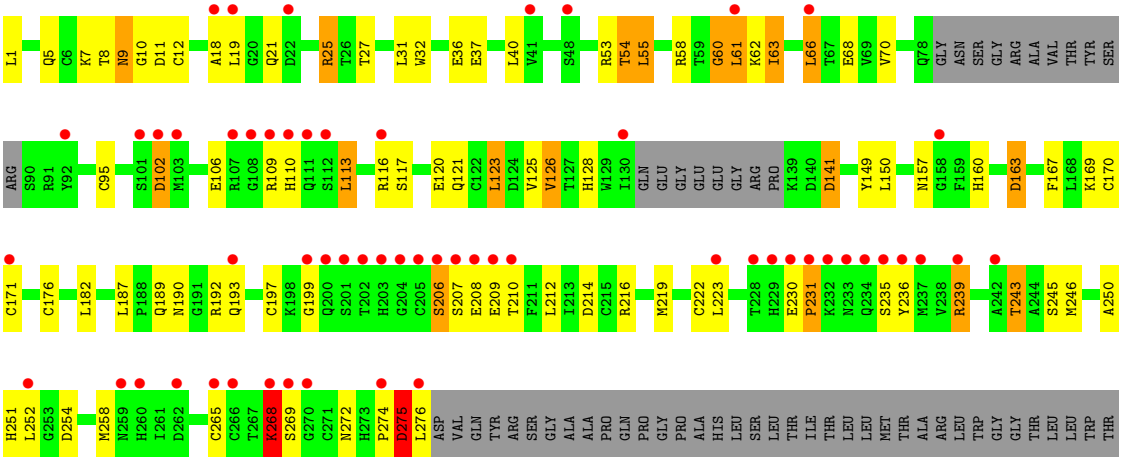
Chain I:





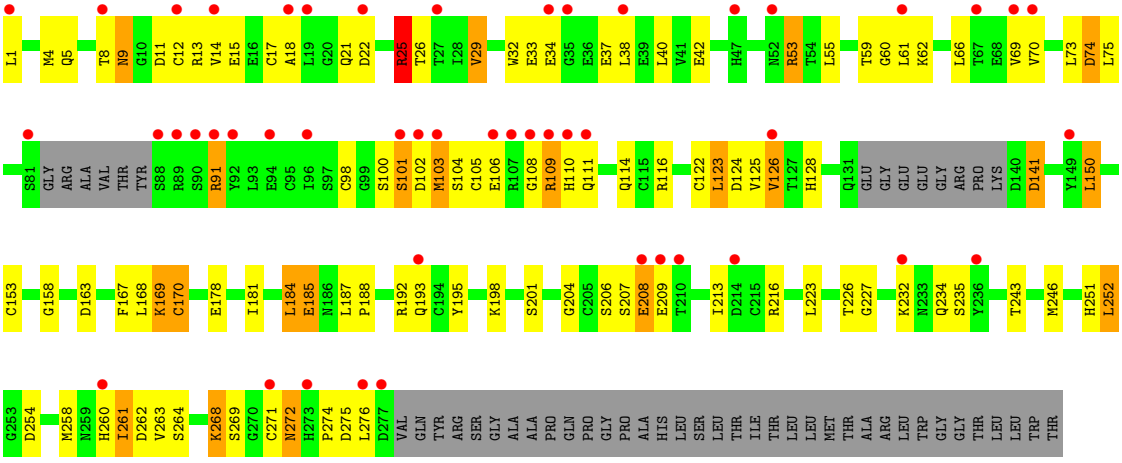
• Molecule 1: Urokinase plasminogen activator surface receptor

Chain K:



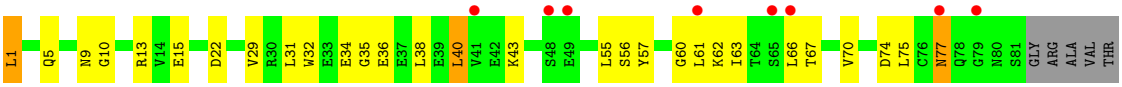
• Molecule 1: Urokinase plasminogen activator surface receptor

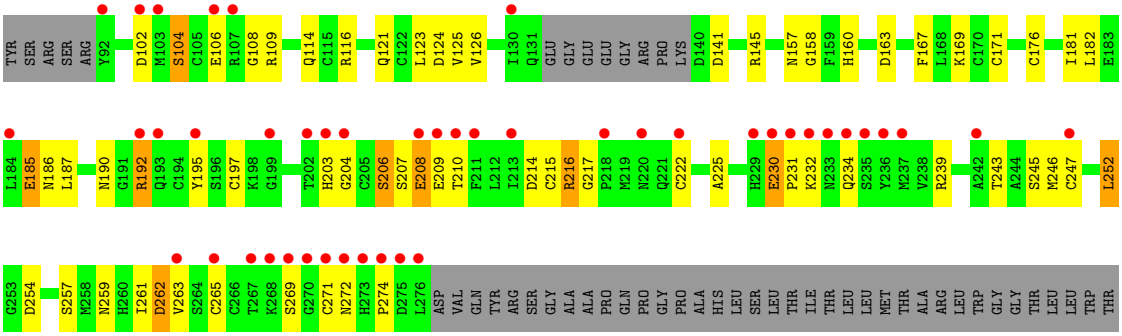
Chain M:



• Molecule 1: Urokinase plasminogen activator surface receptor

Chain O:



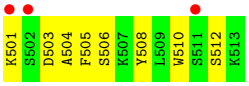


• Molecule 2: antagonist peptide

Chain B:

• Molecule 2: antagonist peptide

Chain D:

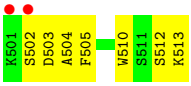


• Molecule 2: antagonist peptide

Chain F:

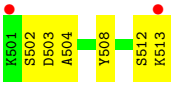
• Molecule 2: antagonist peptide

Chain H:



• Molecule 2: antagonist peptide

Chain J:



• Molecule 2: antagonist peptide

Chain L:

• Molecule 2: antagonist peptide

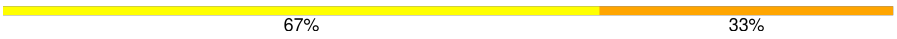
Chain N:

• Molecule 2: antagonist peptide

Chain P:

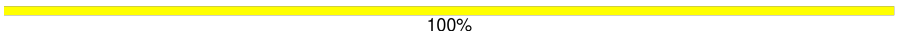
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain S:

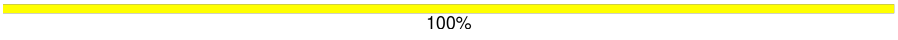


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

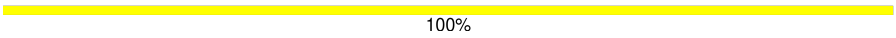
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

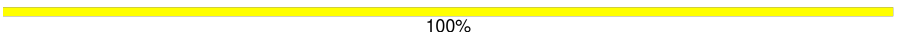
Chain X:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

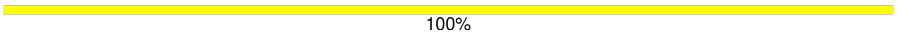
Chain g:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

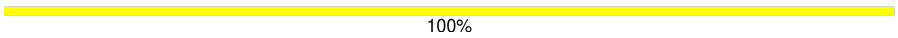


• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

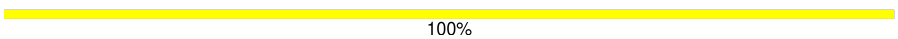
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



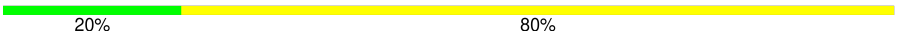
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



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

Chain h:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.93Å 136.83Å 140.54Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	24.85 – 2.70 24.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.85-2.70) 97.1 (24.85-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.245 , 0.315 0.281 , 0.347	Depositor DCC
R_{free} test set	5335 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	18552	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.00% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, ALC, DLY, BMA, SO4, FUC, DSN

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	0.55	2/2072 (0.1%)	0.87	11/2791 (0.4%)
1	C	0.62	3/2016 (0.1%)	0.87	10/2713 (0.4%)
1	E	0.54	0/2037	0.85	4/2742 (0.1%)
1	G	0.54	0/2009	0.90	10/2704 (0.4%)
1	I	0.53	1/2039 (0.0%)	0.85	9/2746 (0.3%)
1	K	0.60	1/2000 (0.1%)	0.85	6/2693 (0.2%)
1	M	0.52	0/2047	0.87	7/2755 (0.3%)
1	O	0.50	0/2001	0.82	7/2695 (0.3%)
2	B	0.63	0/91	0.86	1/116 (0.9%)
2	D	0.56	0/91	0.82	1/116 (0.9%)
2	F	0.61	0/91	0.82	0/116
2	H	0.67	0/91	0.88	1/116 (0.9%)
2	J	0.71	0/91	0.96	1/116 (0.9%)
2	L	0.54	0/91	0.86	0/116
2	N	0.56	0/91	0.92	1/116 (0.9%)
2	P	0.49	0/91	0.84	0/116
All	All	0.55	7/16949 (0.0%)	0.86	69/22767 (0.3%)

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
1	A	0	3
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	2
All	All	0	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	268	LYS	CE-NZ	14.47	1.85	1.49
1	C	273	HIS	CE1-NE2	13.68	1.64	1.32
1	C	273	HIS	CG-ND1	11.19	1.63	1.38
1	A	233	ASN	CG-ND2	6.80	1.49	1.32
1	I	268	LYS	CE-NZ	5.75	1.63	1.49

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	141	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	102	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	262	ASP	CB-CG-OD2	6.68	124.31	118.30
1	I	141	ASP	CB-CG-OD2	6.54	124.19	118.30
2	H	503	ASP	CB-CG-OD2	6.45	124.10	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	GLU	Peptide
1	A	272	ASN	Peptide
1	A	61	LEU	Peptide
1	E	61	LEU	Peptide
1	G	208	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2040	0	1885	59	0
1	C	1985	0	1840	72	0
1	E	2006	0	1864	66	0
1	G	1978	0	1836	62	0
1	I	2008	0	1850	67	0
1	K	1969	0	1825	65	0
1	M	2016	0	1868	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1970	0	1823	55	0
2	B	116	0	112	9	0
2	D	116	0	112	7	0
2	F	116	0	112	3	0
2	H	116	0	112	3	0
2	J	116	0	112	2	0
2	L	116	0	112	7	0
2	N	116	0	112	2	0
2	P	116	0	112	6	0
3	Q	38	0	34	0	0
3	S	38	0	34	0	0
3	T	38	0	34	0	0
3	b	38	0	34	0	0
4	R	24	0	22	0	0
4	U	24	0	22	1	0
4	V	24	0	22	0	0
4	X	24	0	22	0	0
4	Y	24	0	22	1	0
4	a	24	0	22	0	0
4	d	24	0	22	0	0
4	g	24	0	22	0	0
5	W	28	0	25	2	0
5	f	28	0	25	0	0
6	Z	61	0	52	0	0
6	c	61	0	52	0	0
6	e	61	0	52	0	0
6	h	61	0	52	0	0
7	A	28	0	26	0	0
7	C	28	0	26	0	0
7	E	14	0	13	0	0
7	G	14	0	13	0	0
7	I	14	0	13	0	0
7	K	28	0	26	0	0
7	M	14	0	13	0	0
7	O	14	0	13	0	0
8	A	15	0	0	1	0
8	C	15	0	0	1	0
8	E	15	0	0	0	0
8	G	20	0	0	1	0
8	I	15	0	0	1	0
8	K	10	0	0	3	0
8	M	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	5	0	0	0	0
9	A	81	0	0	2	0
9	B	5	0	0	0	0
9	C	85	0	0	1	0
9	D	2	0	0	1	0
9	E	98	0	0	4	0
9	F	8	0	0	1	0
9	G	88	0	0	3	0
9	H	4	0	0	0	0
9	I	87	0	0	1	0
9	J	3	0	0	0	0
9	K	83	0	0	4	0
9	L	2	0	0	1	0
9	M	91	0	0	3	0
9	N	1	0	0	0	0
9	O	106	0	0	4	0
9	P	5	0	0	1	0
All	All	18552	0	16400	495	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 15.

The worst 5 of 495 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:K:268:LYS:CE	1:K:268:LYS:NZ	1.85	1.38
1:C:273:HIS:HB3	1:C:274:PRO:HD3	1.11	1.10
1:C:273:HIS:HB3	1:C:274:PRO:CD	1.86	1.05
1:C:55:LEU:HB3	1:C:66:LEU:HD23	1.35	1.04
1:G:55:LEU:HD23	1:G:123:LEU:HD12	1.46	0.97

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	262/313 (84%)	231 (88%)	16 (6%)	15 (6%)	1 2
1	C	253/313 (81%)	226 (89%)	16 (6%)	11 (4%)	2 4
1	E	256/313 (82%)	229 (90%)	22 (9%)	5 (2%)	6 16
1	G	252/313 (80%)	233 (92%)	16 (6%)	3 (1%)	11 28
1	I	258/313 (82%)	228 (88%)	23 (9%)	7 (3%)	4 10
1	K	251/313 (80%)	227 (90%)	20 (8%)	4 (2%)	8 21
1	M	257/313 (82%)	230 (90%)	15 (6%)	12 (5%)	2 4
1	O	252/313 (80%)	223 (88%)	20 (8%)	9 (4%)	3 6
2	B	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	D	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	F	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	H	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	J	8/13 (62%)	7 (88%)	0	1 (12%)	0 0
2	L	8/13 (62%)	7 (88%)	0	1 (12%)	0 0
2	N	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	P	8/13 (62%)	8 (100%)	0	0	100 100
All	All	2105/2608 (81%)	1884 (90%)	153 (7%)	68 (3%)	3 8

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	A	231	PRO
1	A	276	LEU
1	C	208	GLU
1	C	273	HIS

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	234/273 (86%)	208 (89%)	26 (11%)	5 12
1	C	229/273 (84%)	192 (84%)	37 (16%)	2 5
1	E	232/273 (85%)	200 (86%)	32 (14%)	3 7
1	G	229/273 (84%)	188 (82%)	41 (18%)	1 4
1	I	230/273 (84%)	183 (80%)	47 (20%)	1 3
1	K	228/273 (84%)	194 (85%)	34 (15%)	2 6
1	M	234/273 (86%)	196 (84%)	38 (16%)	2 5
1	O	228/273 (84%)	198 (87%)	30 (13%)	3 8
2	B	10/10 (100%)	8 (80%)	2 (20%)	1 3
2	D	10/10 (100%)	10 (100%)	0	100 100
2	F	10/10 (100%)	10 (100%)	0	100 100
2	H	10/10 (100%)	8 (80%)	2 (20%)	1 3
2	J	10/10 (100%)	9 (90%)	1 (10%)	6 16
2	L	10/10 (100%)	8 (80%)	2 (20%)	1 3
2	N	10/10 (100%)	10 (100%)	0	100 100
2	P	10/10 (100%)	10 (100%)	0	100 100
All	All	1924/2264 (85%)	1632 (85%)	292 (15%)	2 6

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	53	ARG
1	O	216	ARG
1	M	103	MET
1	M	268	LYS
1	G	1	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	190	ASN
1	O	77	ASN
1	K	221	GLN
1	M	128	HIS
1	O	189	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues 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	ALC	H	504	2	9,11,12	0.60	0	11,13,15	1.84	3 (27%)
2	ALC	N	504	2	9,11,12	0.52	0	11,13,15	1.89	4 (36%)
2	ALC	P	504	2	9,11,12	0.59	0	11,13,15	0.97	0
2	ALC	F	504	2	9,11,12	0.50	0	11,13,15	1.44	2 (18%)
2	ALC	D	504	2	9,11,12	0.59	0	11,13,15	1.52	2 (18%)
2	ALC	B	504	2	9,11,12	0.48	0	11,13,15	1.69	3 (27%)
2	ALC	L	504	2	9,11,12	0.62	0	11,13,15	1.14	1 (9%)
2	ALC	J	504	2	9,11,12	0.53	0	11,13,15	1.99	4 (36%)

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	ALC	H	504	2	-	0/5/14/16	0/1/1/1
2	ALC	N	504	2	-	0/5/14/16	0/1/1/1
2	ALC	P	504	2	-	0/5/14/16	0/1/1/1
2	ALC	F	504	2	-	2/5/14/16	0/1/1/1
2	ALC	D	504	2	-	0/5/14/16	0/1/1/1
2	ALC	B	504	2	-	3/5/14/16	0/1/1/1
2	ALC	L	504	2	-	0/5/14/16	0/1/1/1
2	ALC	J	504	2	-	0/5/14/16	0/1/1/1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	504	ALC	CB-CG-CD1	-4.25	101.82	111.71
2	J	504	ALC	CD1-CG-CD2	3.46	117.76	109.29
2	J	504	ALC	CB-CG-CD1	-3.36	103.90	111.71
2	B	504	ALC	CG-CB-CA	3.32	118.98	114.52
2	N	504	ALC	CB-CG-CD1	-3.23	104.18	111.71

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	504	ALC	O-C-CA-CB
2	F	504	ALC	C-CA-CB-CG
2	B	504	ALC	CA-CB-CG-CD1
2	B	504	ALC	CA-CB-CG-CD2
2	B	504	ALC	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	504	ALC	1	0
2	B	504	ALC	2	0
2	L	504	ALC	1	0

5.5 Carbohydrates (i)

52 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	$\#\|Z\| > 2$
3	NAG	Q	1	3,1	14,14,15	0.56	0	17,19,21	1.36	3 (17%)
3	NAG	Q	2	3	14,14,15	0.64	0	17,19,21	1.76	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FUC	Q	3	3	10,10,11	0.65	0	14,14,16	1.08	1 (7%)
4	NAG	R	1	4,1	14,14,15	0.54	0	17,19,21	1.60	2 (11%)
4	FUC	R	2	4	10,10,11	0.58	0	14,14,16	0.73	0
3	NAG	S	1	3,1	14,14,15	0.53	0	17,19,21	2.43	4 (23%)
3	NAG	S	2	3	14,14,15	0.70	1 (7%)	17,19,21	1.49	3 (17%)
3	FUC	S	3	3	10,10,11	0.62	0	14,14,16	0.92	0
3	NAG	T	1	3,1	14,14,15	0.57	0	17,19,21	1.72	4 (23%)
3	NAG	T	2	3	14,14,15	0.58	0	17,19,21	1.39	1 (5%)
3	FUC	T	3	3	10,10,11	0.71	0	14,14,16	1.35	2 (14%)
4	NAG	U	1	4,1	14,14,15	0.57	0	17,19,21	1.84	4 (23%)
4	FUC	U	2	4	10,10,11	0.86	0	14,14,16	1.84	3 (21%)
4	NAG	V	1	4,1	14,14,15	0.55	0	17,19,21	1.66	3 (17%)
4	FUC	V	2	4	10,10,11	0.57	0	14,14,16	1.06	1 (7%)
5	NAG	W	1	5,1	14,14,15	0.67	0	17,19,21	1.06	2 (11%)
5	NAG	W	2	5	14,14,15	0.60	0	17,19,21	1.27	2 (11%)
4	NAG	X	1	4,1	14,14,15	0.58	0	17,19,21	1.50	2 (11%)
4	FUC	X	2	4	10,10,11	0.67	0	14,14,16	1.30	1 (7%)
4	NAG	Y	1	4,1	14,14,15	0.42	0	17,19,21	1.62	2 (11%)
4	FUC	Y	2	4	10,10,11	0.75	0	14,14,16	1.59	2 (14%)
6	NAG	Z	1	6,1	14,14,15	0.45	0	17,19,21	1.09	1 (5%)
6	NAG	Z	2	6	14,14,15	0.60	0	17,19,21	1.07	0
6	BMA	Z	3	6	11,11,12	0.48	0	15,15,17	2.91	5 (33%)
6	MAN	Z	4	6	11,11,12	0.62	0	15,15,17	1.90	3 (20%)
6	MAN	Z	5	6	11,11,12	0.71	0	15,15,17	1.10	1 (6%)
4	NAG	a	1	4,1	14,14,15	0.48	0	17,19,21	1.69	2 (11%)
4	FUC	a	2	4	10,10,11	0.59	0	14,14,16	1.08	0
3	NAG	b	1	3,1	14,14,15	0.62	0	17,19,21	1.57	3 (17%)
3	NAG	b	2	3	14,14,15	0.64	0	17,19,21	2.53	4 (23%)
3	FUC	b	3	3	10,10,11	0.61	0	14,14,16	0.87	0
6	NAG	c	1	6,1	14,14,15	0.66	0	17,19,21	1.61	5 (29%)
6	NAG	c	2	6	14,14,15	0.68	0	17,19,21	1.17	2 (11%)
6	BMA	c	3	6	11,11,12	0.90	1 (9%)	15,15,17	1.70	3 (20%)
6	MAN	c	4	6	11,11,12	0.73	0	15,15,17	1.83	4 (26%)
6	MAN	c	5	6	11,11,12	0.68	0	15,15,17	1.24	3 (20%)
4	NAG	d	1	4,1	14,14,15	0.42	0	17,19,21	1.90	5 (29%)
4	FUC	d	2	4	10,10,11	0.67	0	14,14,16	0.95	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	e	1	6,1	14,14,15	0.60	0	17,19,21	1.64	1 (5%)
6	NAG	e	2	6	14,14,15	0.59	0	17,19,21	1.15	1 (5%)
6	BMA	e	3	6	11,11,12	0.56	0	15,15,17	1.81	3 (20%)
6	MAN	e	4	6	11,11,12	0.76	0	15,15,17	2.52	6 (40%)
6	MAN	e	5	6	11,11,12	0.63	0	15,15,17	1.30	1 (6%)
5	NAG	f	1	5,1	14,14,15	0.68	0	17,19,21	1.31	1 (5%)
5	NAG	f	2	5	14,14,15	0.54	0	17,19,21	1.71	3 (17%)
4	NAG	g	1	4,1	14,14,15	0.52	0	17,19,21	1.32	2 (11%)
4	FUC	g	2	4	10,10,11	0.68	0	14,14,16	1.33	2 (14%)
6	NAG	h	1	6,1	14,14,15	0.68	0	17,19,21	1.79	4 (23%)
6	NAG	h	2	6	14,14,15	0.53	0	17,19,21	0.82	0
6	BMA	h	3	6	11,11,12	0.92	1 (9%)	15,15,17	1.49	2 (13%)
6	MAN	h	4	6	11,11,12	0.75	0	15,15,17	1.49	2 (13%)
6	MAN	h	5	6	11,11,12	0.62	0	15,15,17	1.73	2 (13%)

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	NAG	Q	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	5/6/23/26	0/1/1/1
3	FUC	Q	3	3	2/2/4/5	-	0/1/1/1
4	NAG	R	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	R	2	4	2/2/4/5	-	0/1/1/1
3	NAG	S	1	3,1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	FUC	S	3	3	2/2/4/5	-	0/1/1/1
3	NAG	T	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	FUC	T	3	3	2/2/4/5	-	0/1/1/1
4	NAG	U	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	U	2	4	2/2/4/5	-	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	V	2	4	2/2/4/5	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	W	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	W	2	5	-	3/6/23/26	0/1/1/1
4	NAG	X	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1
4	FUC	X	2	4	2/2/4/5	-	0/1/1/1
4	NAG	Y	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	Y	2	4	2/2/4/5	-	0/1/1/1
6	NAG	Z	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	5	6	-	2/2/19/22	1/1/1/1
4	NAG	a	1	4,1	-	5/6/23/26	0/1/1/1
4	FUC	a	2	4	2/2/4/5	-	0/1/1/1
3	NAG	b	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	b	2	3	-	4/6/23/26	0/1/1/1
3	FUC	b	3	3	2/2/4/5	-	0/1/1/1
6	NAG	c	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	c	2	6	-	4/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
6	MAN	c	4	6	-	2/2/19/22	0/1/1/1
6	MAN	c	5	6	-	0/2/19/22	0/1/1/1
4	NAG	d	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	d	2	4	2/2/4/5	-	0/1/1/1
6	NAG	e	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	BMA	e	3	6	-	0/2/19/22	0/1/1/1
6	MAN	e	4	6	-	2/2/19/22	1/1/1/1
6	MAN	e	5	6	-	1/2/19/22	0/1/1/1
5	NAG	f	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	3/6/23/26	0/1/1/1
4	NAG	g	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	g	2	4	2/2/4/5	-	0/1/1/1
6	NAG	h	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	h	2	6	-	2/6/23/26	0/1/1/1
6	BMA	h	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	h	4	6	-	1/2/19/22	0/1/1/1
6	MAN	h	5	6	-	2/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	3	BMA	O5-C1	-2.30	1.39	1.43
6	c	3	BMA	O5-C1	-2.14	1.40	1.43
3	S	2	NAG	C1-C2	2.01	1.55	1.52

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	3	BMA	C1-O5-C5	8.96	124.20	112.19
3	b	2	NAG	C1-O5-C5	8.60	123.71	112.19
3	S	1	NAG	C1-O5-C5	7.70	122.51	112.19
6	e	4	MAN	C1-C2-C3	-6.47	100.22	109.64
6	e	1	NAG	C1-O5-C5	5.78	119.94	112.19

5 of 30 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	Q	3	FUC	C5
3	Q	3	FUC	C1
3	S	1	NAG	C1
3	S	3	FUC	C5
3	S	3	FUC	C1

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	h	5	MAN	C1-C2-C3-C4-C5-O5

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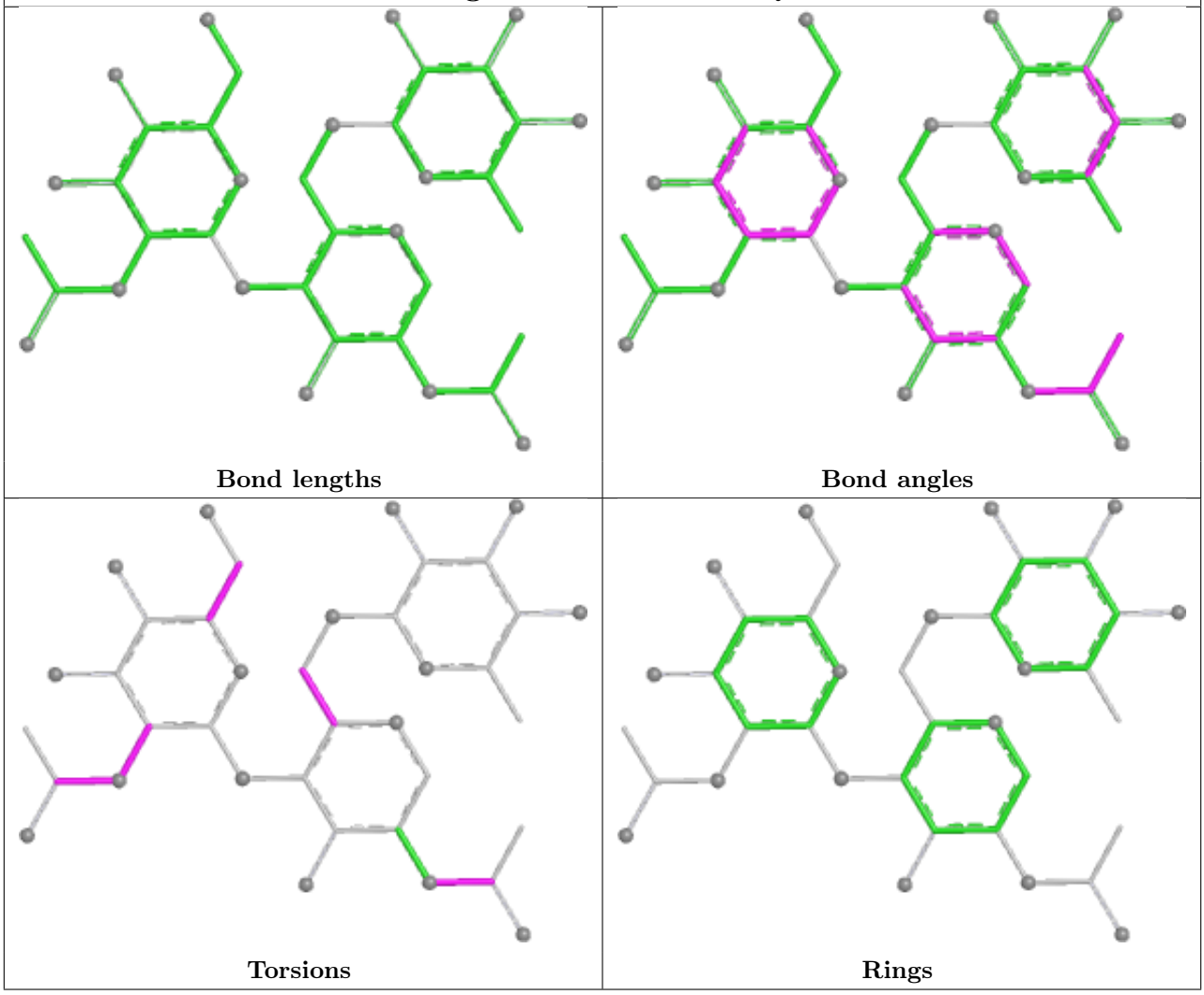
Mol	Chain	Res	Type	Atoms
6	e	4	MAN	C1-C2-C3-C4-C5-O5
6	Z	5	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

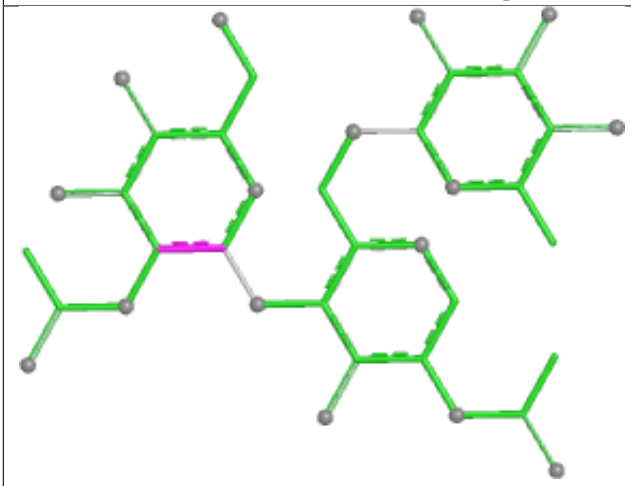
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	1	NAG	1	0
5	W	2	NAG	1	0
4	U	1	NAG	1	0
5	W	1	NAG	2	0

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

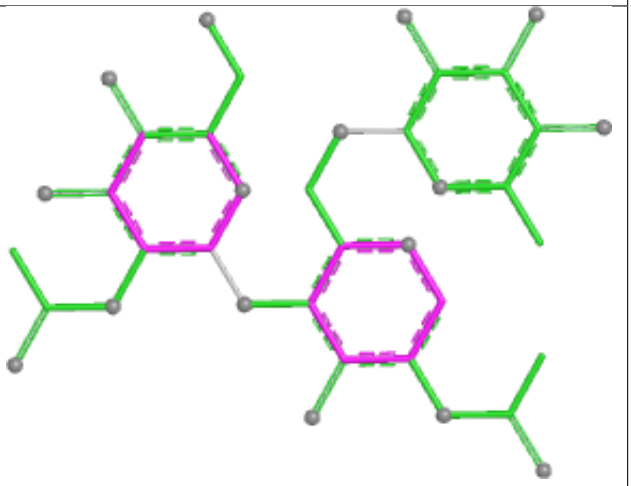
Oligosaccharide Chain Q



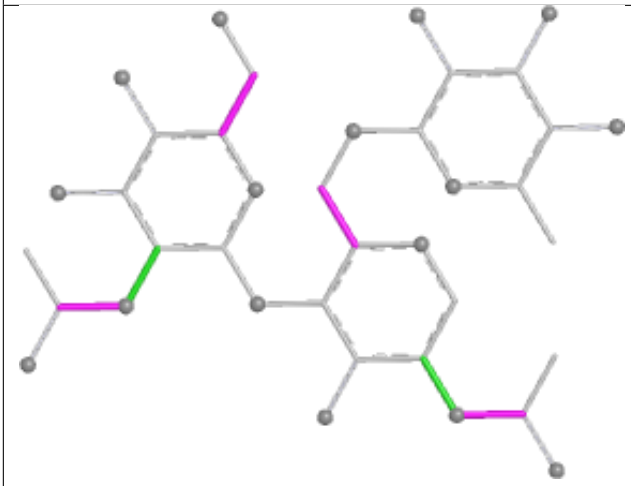
Oligosaccharide Chain S



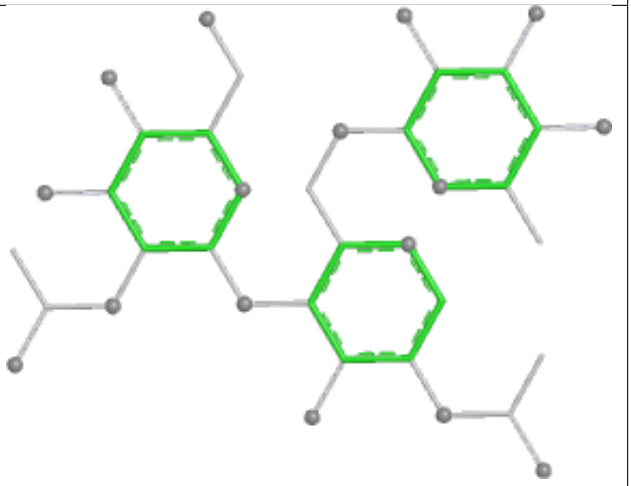
Bond lengths



Bond angles

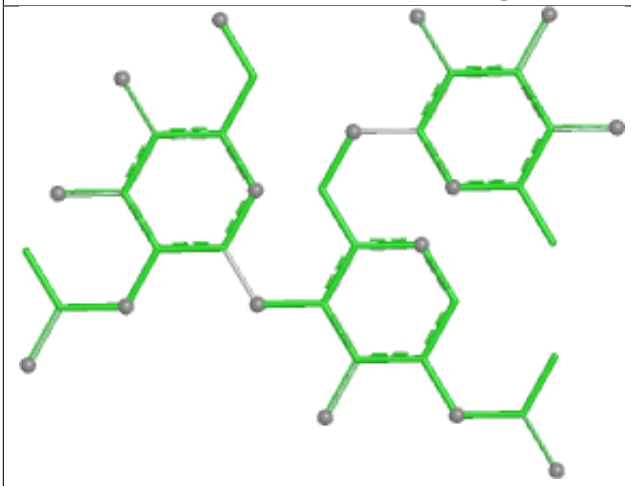


Torsions

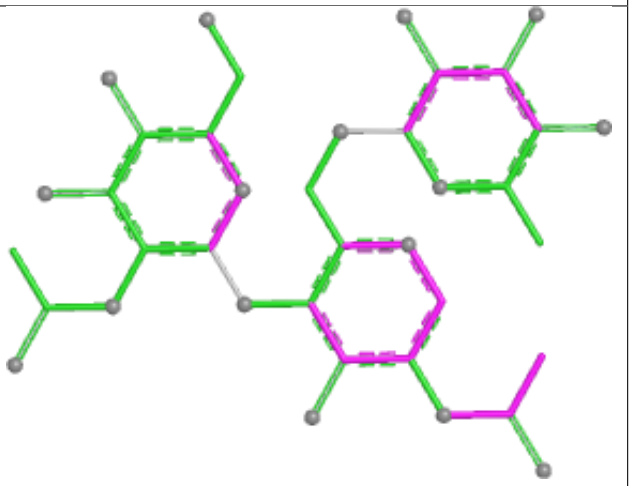


Rings

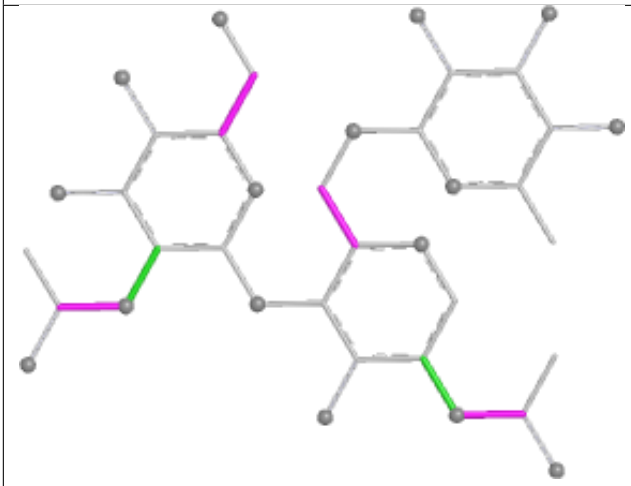
Oligosaccharide Chain T



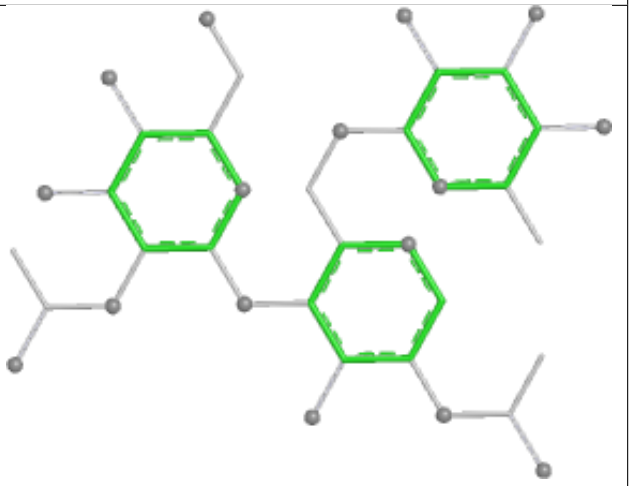
Bond lengths



Bond angles

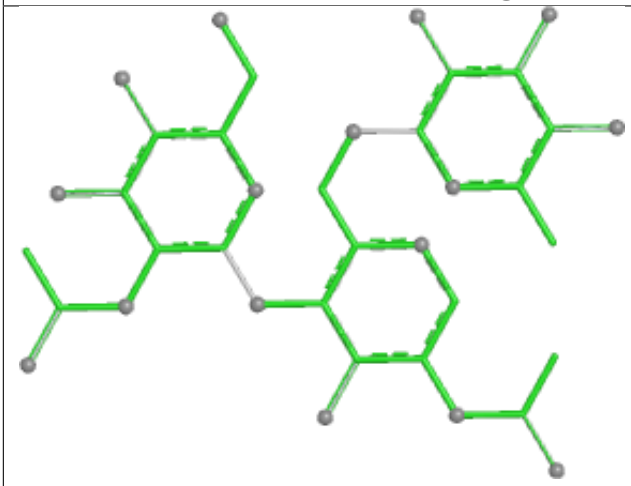


Torsions

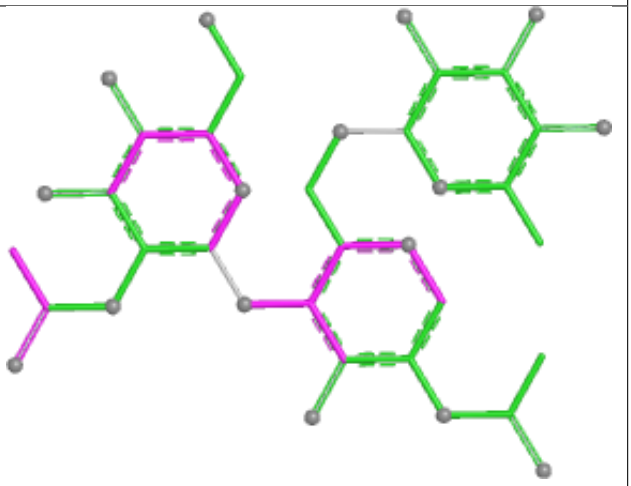


Rings

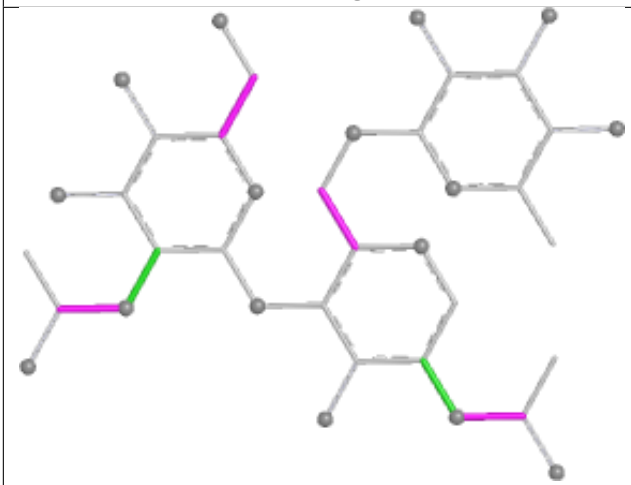
Oligosaccharide Chain b



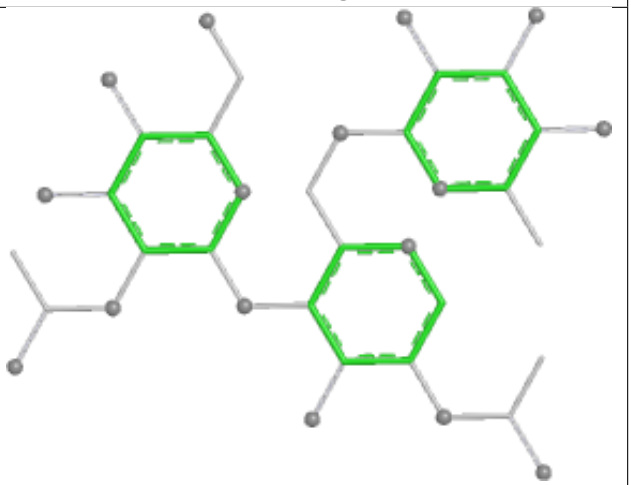
Bond lengths



Bond angles

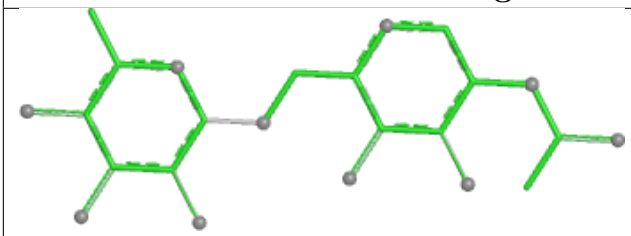


Torsions

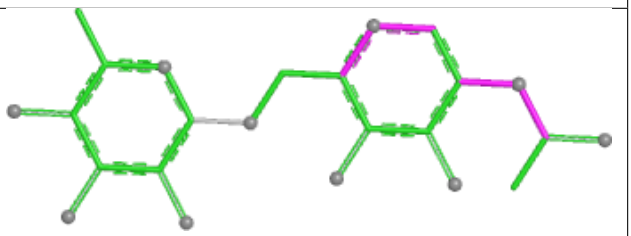


Rings

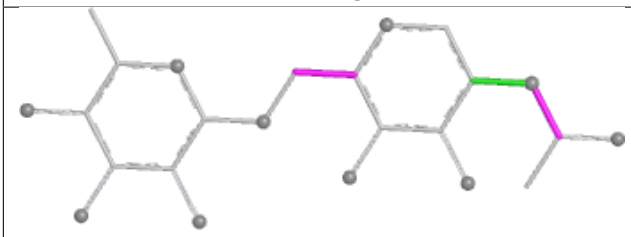
Oligosaccharide Chain R



Bond lengths



Bond angles



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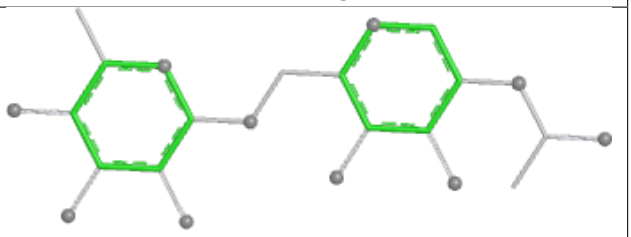
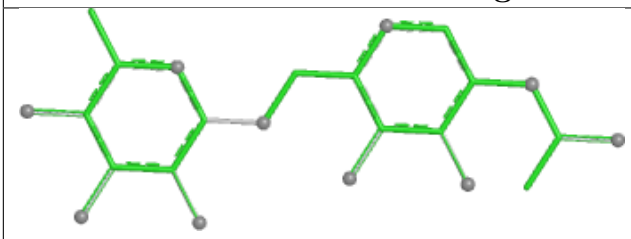


Rings

Oligosaccharide Chain U



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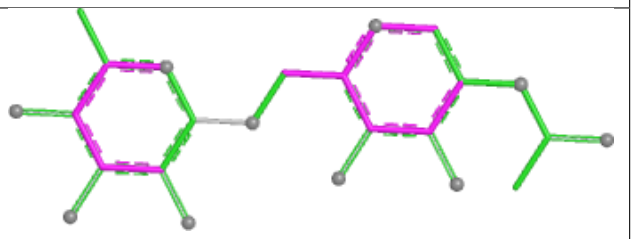
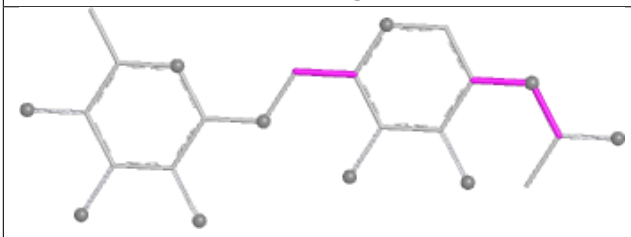


Bond angles



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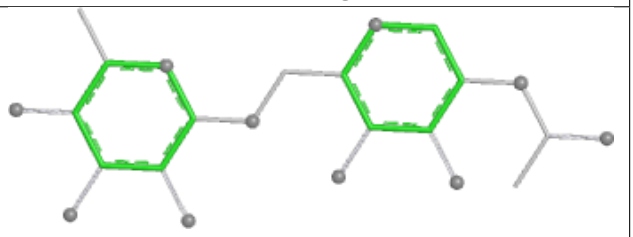
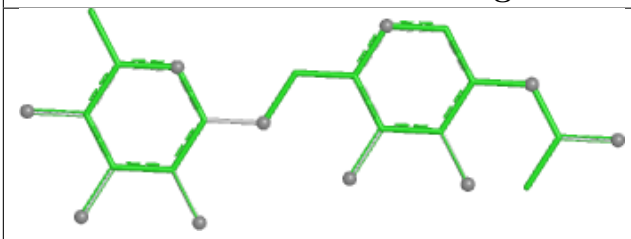
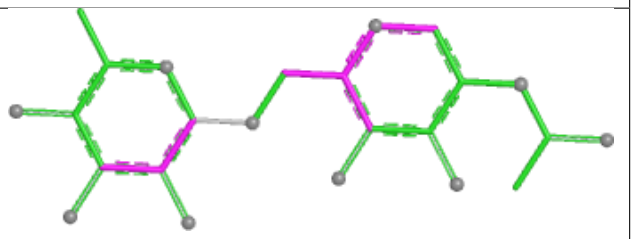


Rings

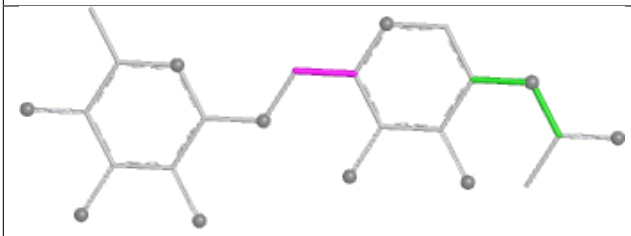
Oligosaccharide Chain V



Bond lengths



Bond angles



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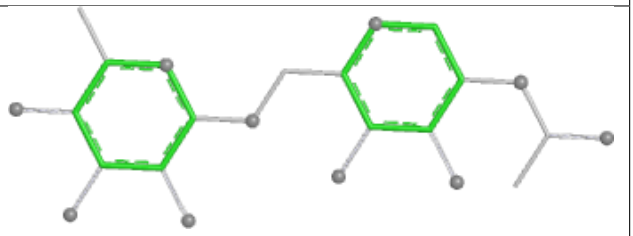
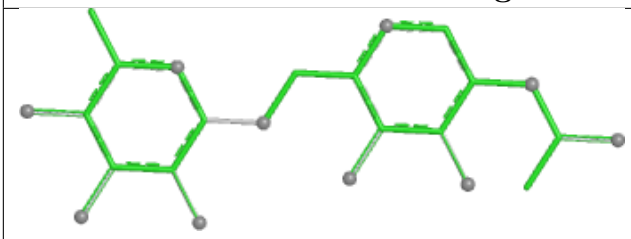
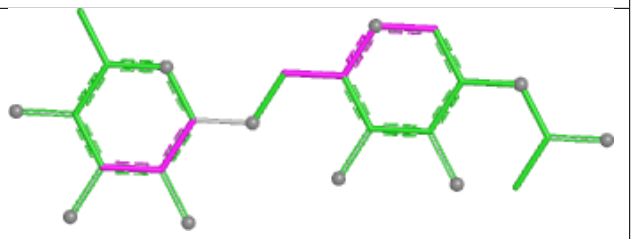


Rings

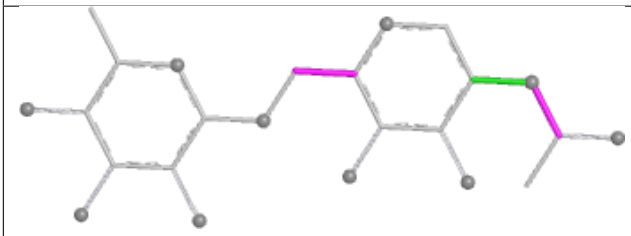
Oligosaccharide Chain X



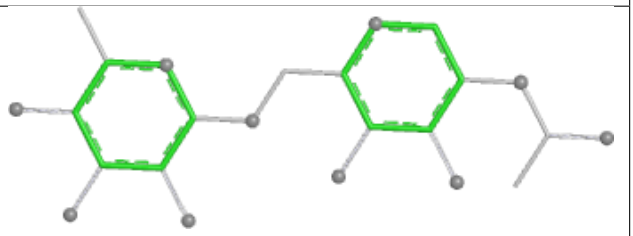
Bond lengths



Bond angles

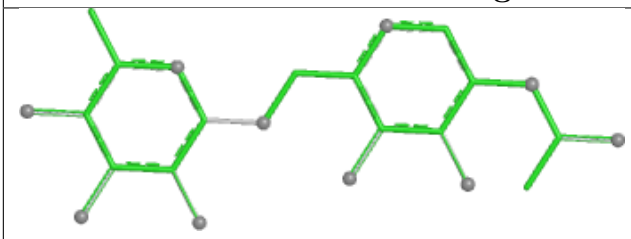


Torsions

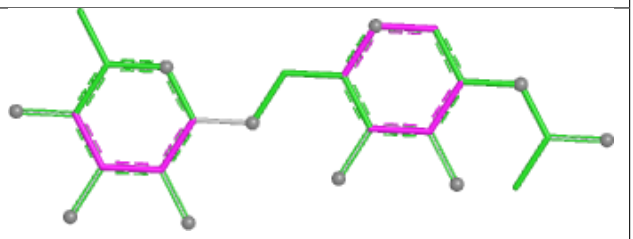


Rings

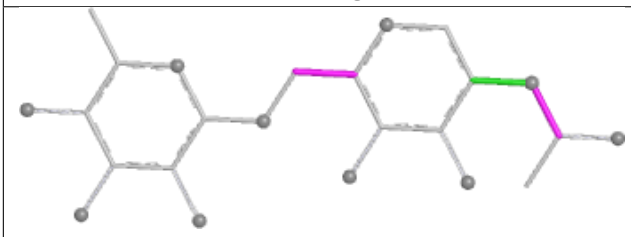
Oligosaccharide Chain Y



Bond lengths



Bond angles



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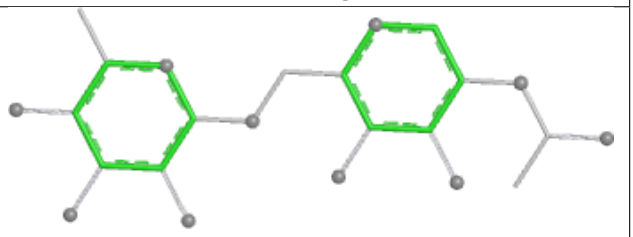
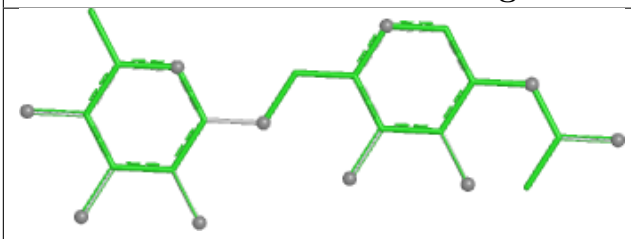
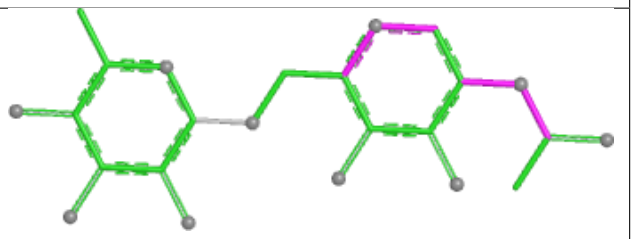


Rings

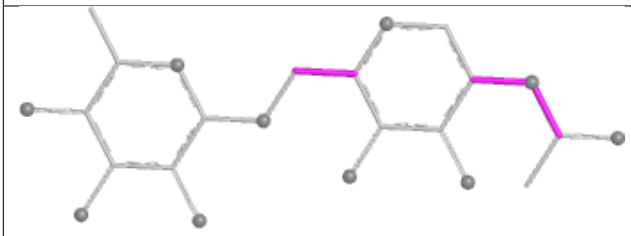
Oligosaccharide Chain a



Bond lengths



Bond angles



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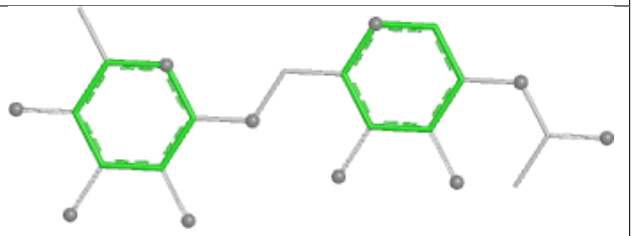
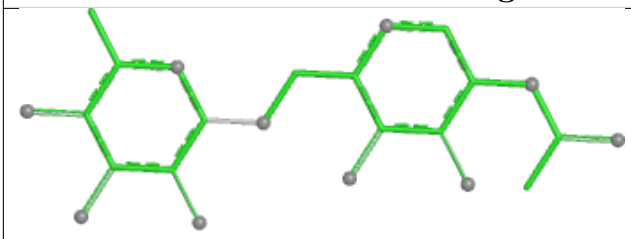
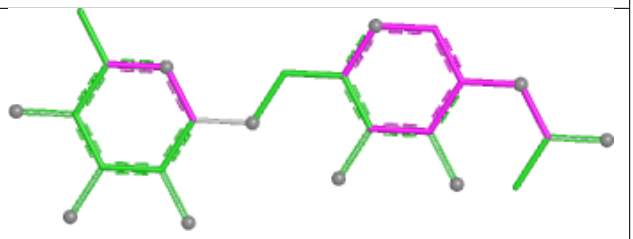


Rings

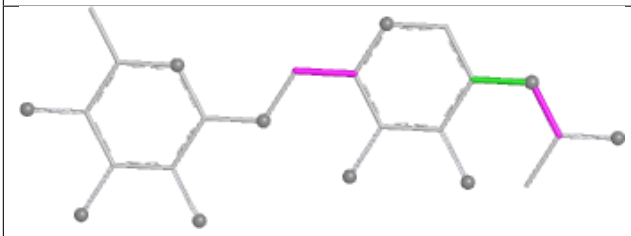
Oligosaccharide Chain d



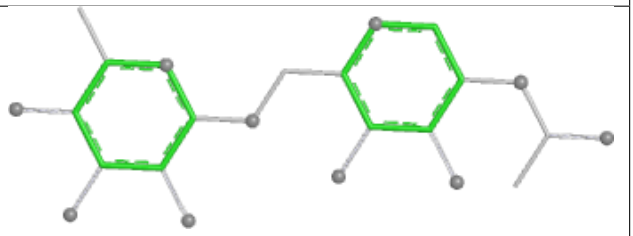
Bond lengths



Bond angles

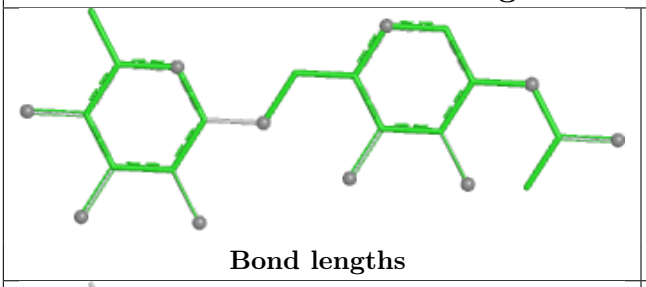


Torsions

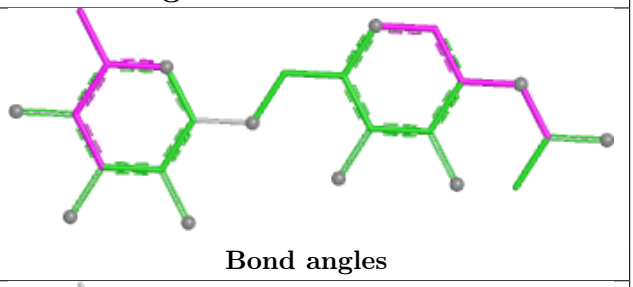


Rings

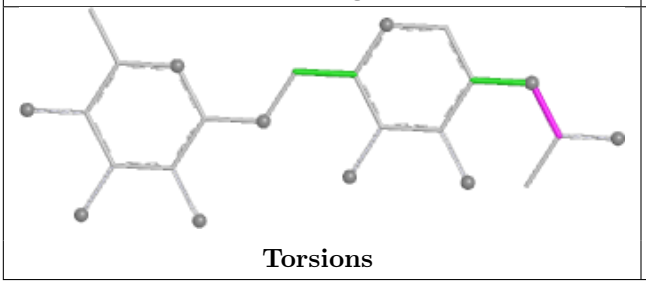
Oligosaccharide Chain g



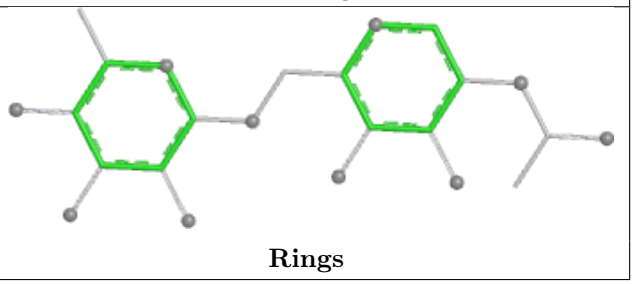
Bond lengths



Bond angles

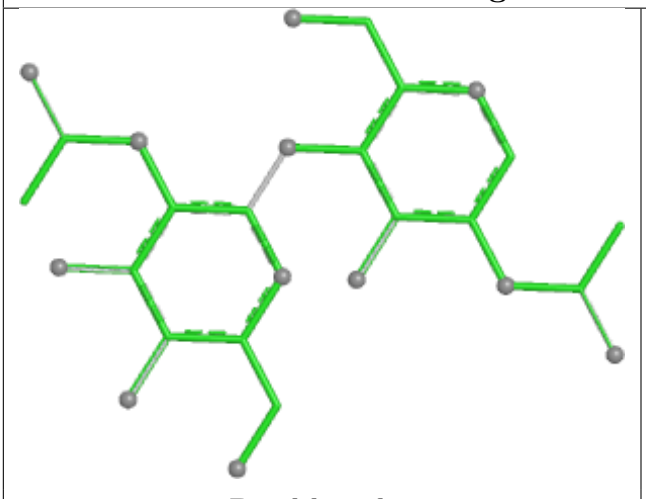


Torsions

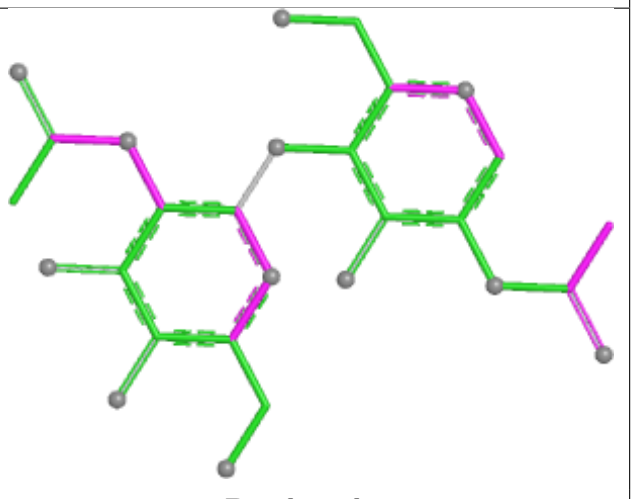


Rings

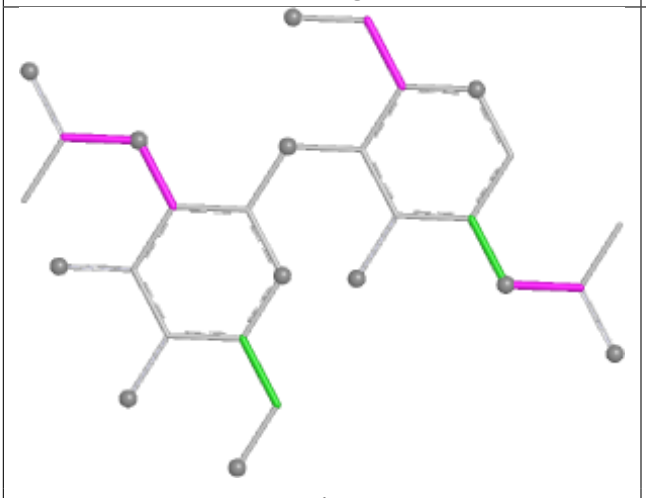
Oligosaccharide Chain W



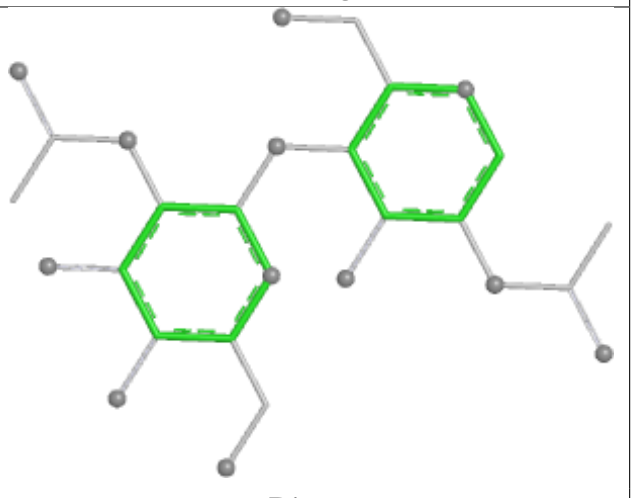
Bond lengths



Bond angles

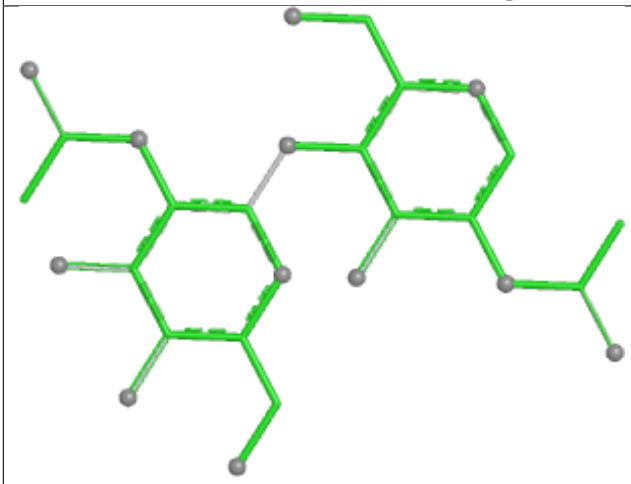


Torsions

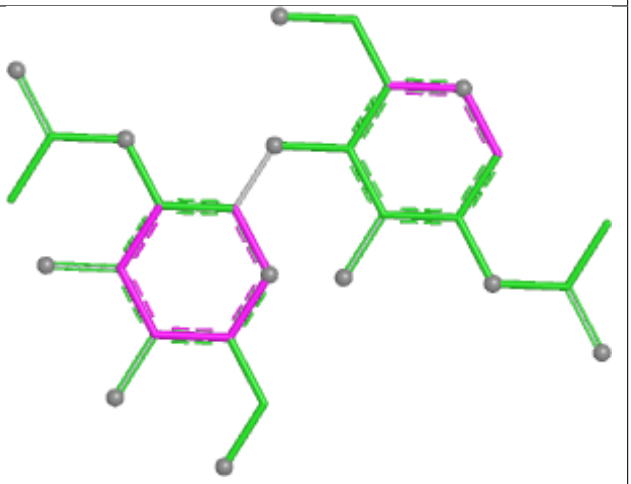


Rings

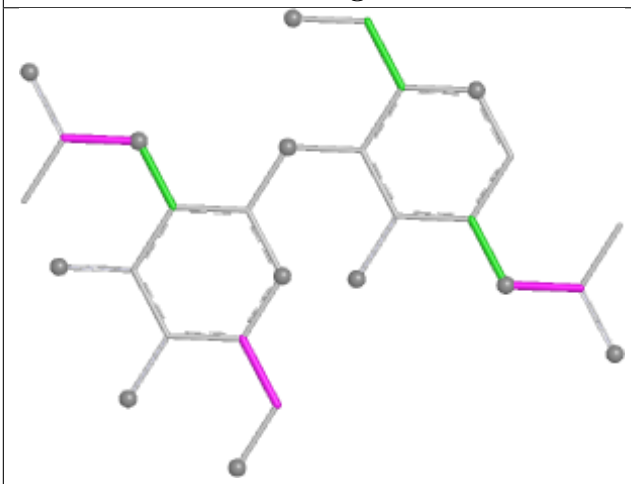
Oligosaccharide Chain f



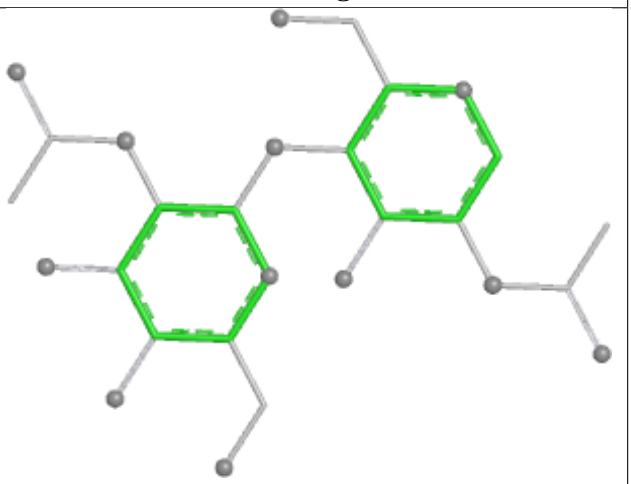
Bond lengths



Bond angles

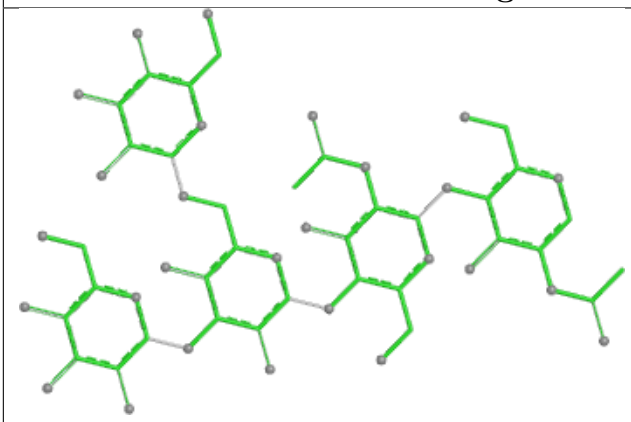


Torsions

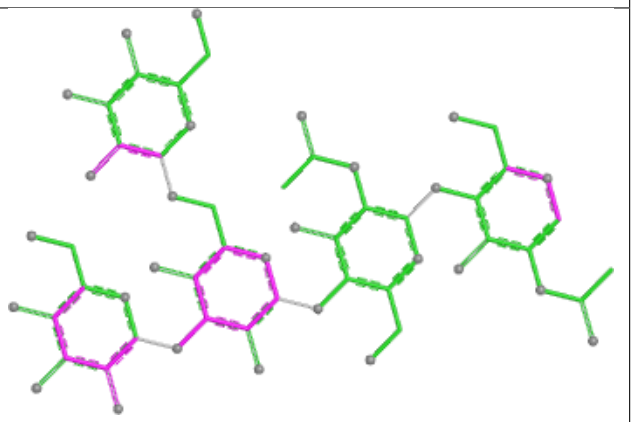


Rings

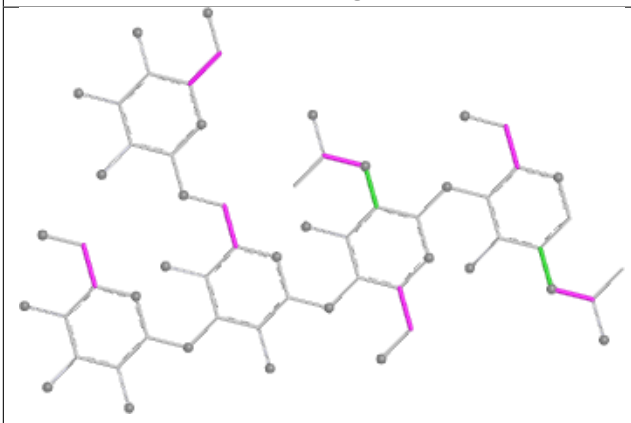
Oligosaccharide Chain Z



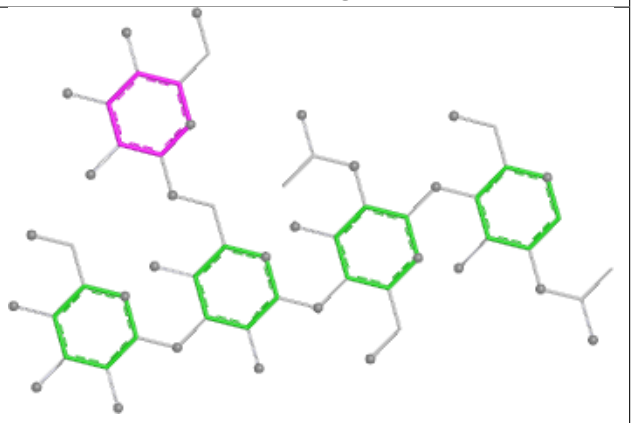
Bond lengths



Bond angles

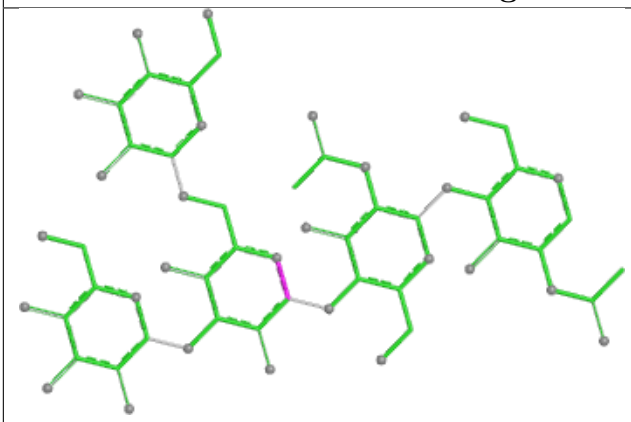


Torsions

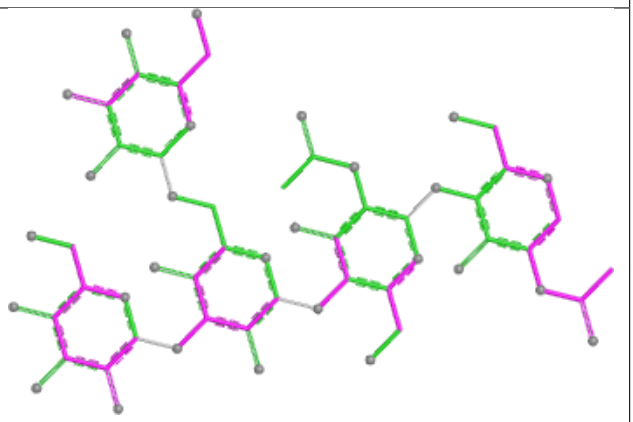


Rings

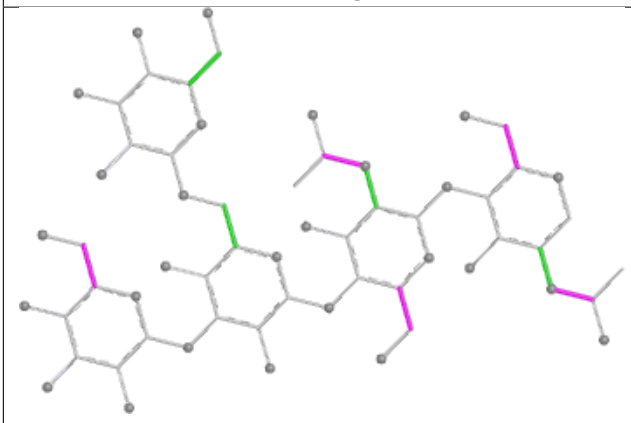
Oligosaccharide Chain c



Bond lengths



Bond angles



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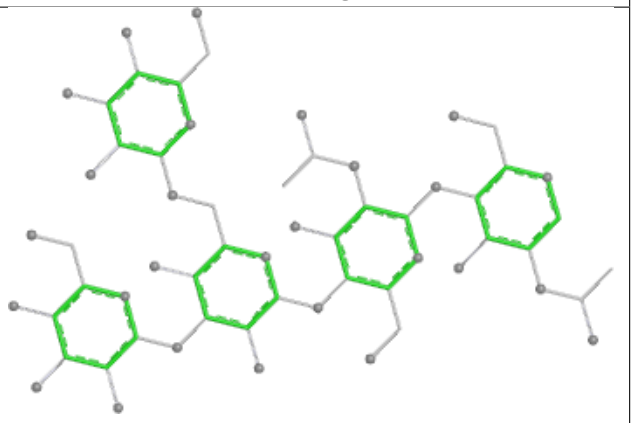
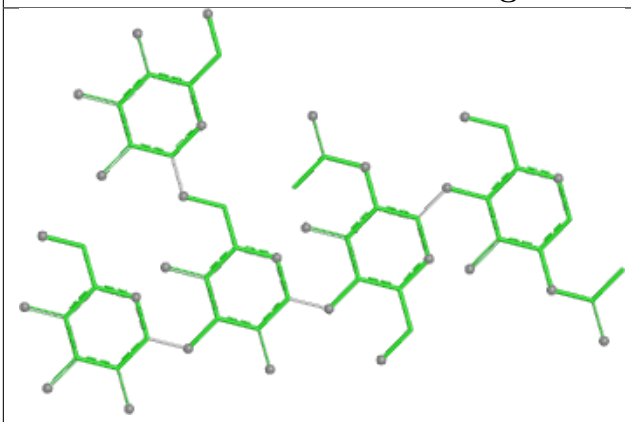
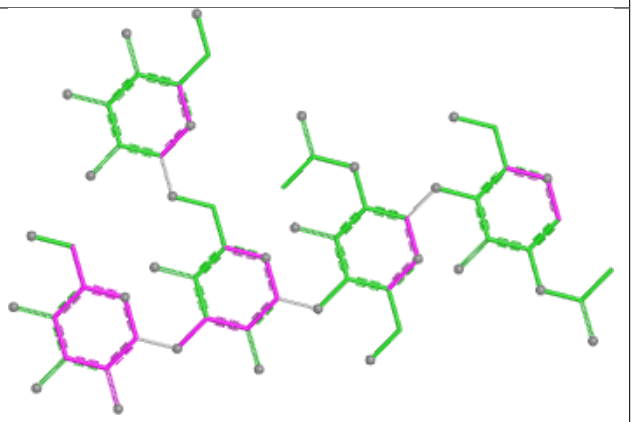


Rings

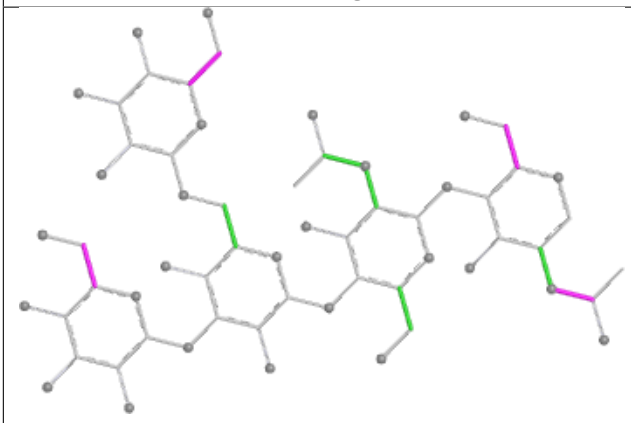
Oligosaccharide Chain e



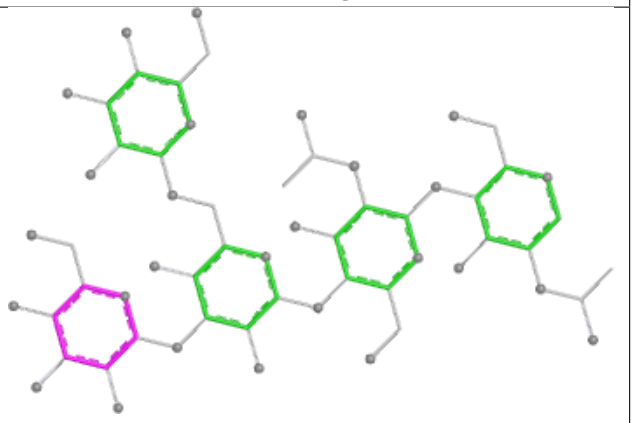
Bond lengths



Bond angles

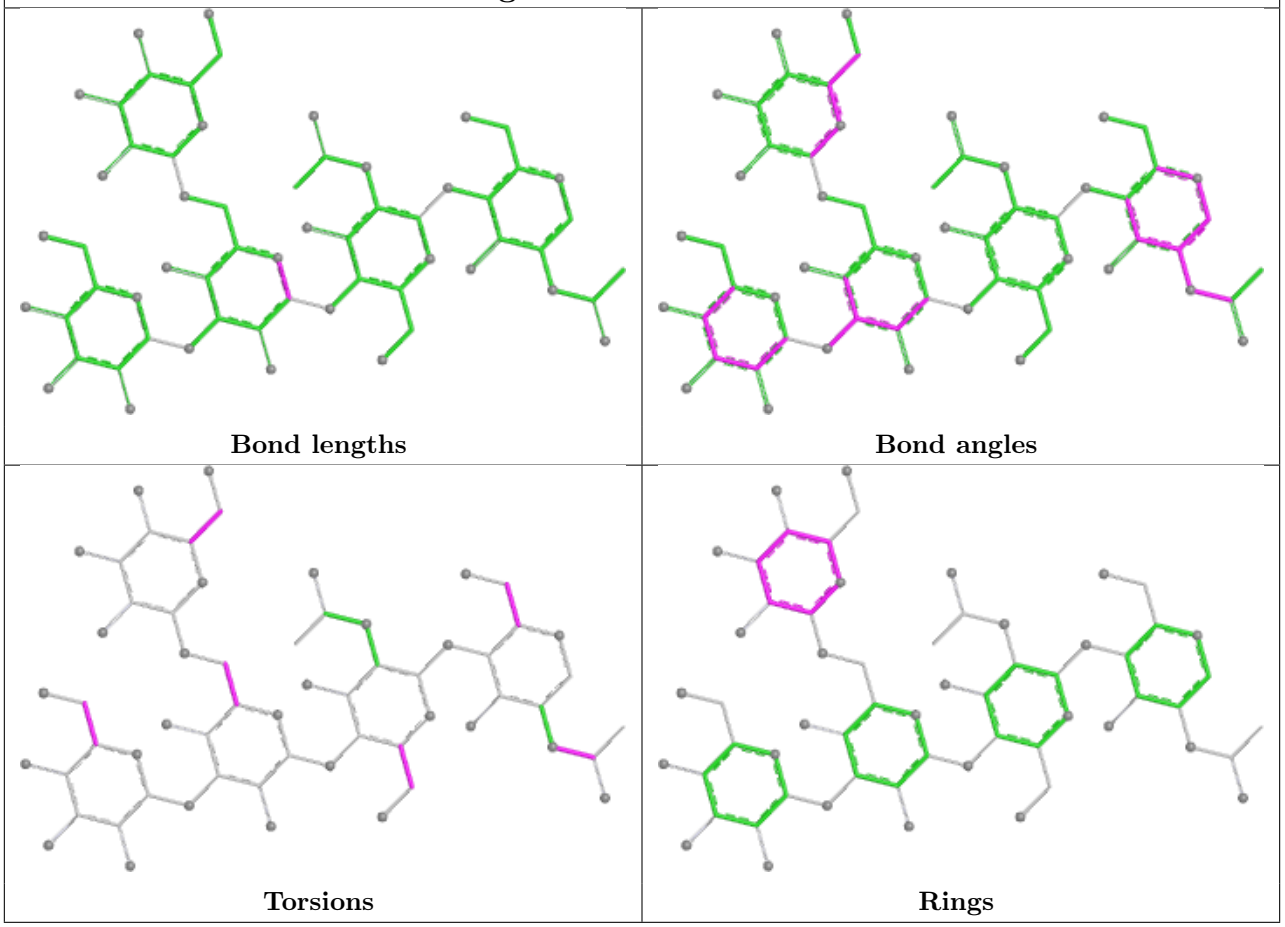


Torsions



Rings

Oligosaccharide Chain h



5.6 Ligand geometry (i)

32 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	$\#\|Z\| > 2$
8	SO4	E	815	-	4,4,4	0.28	0	6,6,6	0.61	0
8	SO4	C	814	-	4,4,4	0.27	0	6,6,6	0.37	0
7	NAG	K	322	1	14,14,15	0.85	0	17,19,21	1.35	2 (11%)
8	SO4	I	821	-	4,4,4	0.26	0	6,6,6	0.14	0
8	SO4	E	820	-	4,4,4	0.31	0	6,6,6	0.14	0
8	SO4	A	801	-	4,4,4	0.30	0	6,6,6	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	C	316	1	14,14,15	0.43	0	17,19,21	1.15	1 (5%)
8	SO4	G	816	-	4,4,4	0.25	0	6,6,6	0.58	0
8	SO4	K	803	-	4,4,4	0.27	0	6,6,6	0.17	0
7	NAG	O	321	1	14,14,15	0.72	0	17,19,21	0.89	1 (5%)
7	NAG	M	331	1	14,14,15	0.41	0	17,19,21	1.57	1 (5%)
7	NAG	K	331	1	14,14,15	0.54	0	17,19,21	1.63	3 (17%)
7	NAG	G	321	1	14,14,15	0.69	0	17,19,21	1.23	2 (11%)
8	SO4	G	802	-	4,4,4	0.26	0	6,6,6	0.32	0
8	SO4	C	806	-	4,4,4	0.24	0	6,6,6	0.29	0
7	NAG	E	317	1	14,14,15	0.58	0	17,19,21	1.40	1 (5%)
8	SO4	C	818	-	4,4,4	0.21	0	6,6,6	0.22	0
8	SO4	I	804	-	4,4,4	0.26	0	6,6,6	0.27	0
7	NAG	I	321	1	14,14,15	0.72	1 (7%)	17,19,21	1.08	0
8	SO4	I	809	-	4,4,4	0.28	0	6,6,6	0.09	0
8	SO4	K	810	-	4,4,4	0.27	0	6,6,6	0.14	0
8	SO4	M	819	-	4,4,4	0.28	0	6,6,6	0.04	0
8	SO4	M	811	-	4,4,4	0.29	0	6,6,6	0.28	0
8	SO4	G	817	-	4,4,4	0.22	0	6,6,6	0.19	0
8	SO4	G	808	-	4,4,4	0.25	0	6,6,6	0.30	0
7	NAG	C	321	1	14,14,15	0.65	0	17,19,21	0.94	1 (5%)
7	NAG	A	321	1	14,14,15	0.69	0	17,19,21	2.16	5 (29%)
8	SO4	A	813	-	4,4,4	0.21	0	6,6,6	0.46	0
7	NAG	A	317	1	14,14,15	0.48	0	17,19,21	1.69	2 (11%)
8	SO4	A	805	-	4,4,4	0.23	0	6,6,6	0.11	0
8	SO4	E	807	-	4,4,4	0.23	0	6,6,6	0.17	0
8	SO4	O	812	-	4,4,4	0.31	0	6,6,6	0.16	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
7	NAG	O	321	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	M	331	1	-	4/6/23/26	0/1/1/1
7	NAG	C	321	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	321	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	I	321	1	-	2/6/23/26	0/1/1/1
7	NAG	K	331	1	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	321	1	-	5/6/23/26	0/1/1/1
7	NAG	A	317	1	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	K	322	1	-	5/6/23/26	0/1/1/1
7	NAG	E	317	1	-	4/6/23/26	0/1/1/1
7	NAG	C	316	1	1/1/5/7	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	321	NAG	C1-C2	2.17	1.55	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	321	NAG	C1-O5-C5	6.60	121.03	112.19
7	M	331	NAG	C1-O5-C5	5.85	120.02	112.19
7	A	317	NAG	C1-O5-C5	5.32	119.32	112.19
7	E	317	NAG	C1-O5-C5	3.82	117.30	112.19
7	K	331	NAG	C1-O5-C5	3.76	117.23	112.19

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	317	NAG	C1
7	A	321	NAG	C1
7	C	316	NAG	C1
7	C	321	NAG	C1
7	K	331	NAG	C1

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	321	NAG	C8-C7-N2-C2
7	A	321	NAG	O7-C7-N2-C2
7	C	316	NAG	C8-C7-N2-C2
7	C	316	NAG	O7-C7-N2-C2
7	C	321	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	801	SO4	1	0
8	K	803	SO4	1	0
8	C	818	SO4	1	0
8	I	804	SO4	1	0
8	K	810	SO4	2	0
8	M	811	SO4	1	0
8	G	817	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	268/313 (85%)	1.47	63 (23%) 2 3	45, 57, 69, 98	0
1	C	259/313 (82%)	1.29	51 (19%) 3 4	48, 58, 66, 76	0
1	E	262/313 (83%)	1.26	51 (19%) 4 4	46, 56, 64, 72	0
1	G	258/313 (82%)	1.24	40 (15%) 6 6	46, 57, 66, 69	0
1	I	264/313 (84%)	1.31	50 (18%) 4 4	44, 58, 69, 89	0
1	K	257/313 (82%)	1.41	58 (22%) 3 3	45, 58, 67, 78	0
1	M	263/313 (84%)	1.35	48 (18%) 4 4	43, 57, 66, 83	0
1	O	258/313 (82%)	1.37	53 (20%) 3 3	47, 58, 68, 87	0
2	B	10/13 (76%)	1.77	2 (20%) 3 4	53, 60, 69, 71	0
2	D	10/13 (76%)	1.48	3 (30%) 1 2	50, 57, 64, 66	0
2	F	10/13 (76%)	2.03	4 (40%) 1 1	51, 63, 71, 71	0
2	H	10/13 (76%)	1.43	2 (20%) 3 4	52, 56, 65, 69	0
2	J	10/13 (76%)	1.51	2 (20%) 3 4	47, 54, 64, 70	0
2	L	10/13 (76%)	1.88	3 (30%) 1 2	50, 56, 72, 75	0
2	N	10/13 (76%)	1.83	3 (30%) 1 2	49, 55, 66, 71	0
2	P	10/13 (76%)	1.75	4 (40%) 1 1	52, 58, 72, 74	0
All	All	2169/2608 (83%)	1.35	437 (20%) 3 4	43, 57, 67, 98	0

The worst 5 of 437 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	274	PRO	7.4
1	E	231	PRO	6.4
1	G	202	THR	6.3
1	A	278	VAL	6.3
1	G	208	GLU	6.0

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^{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	DLY	P	507	9/10	0.84	0.17	54,55,61,63	0
2	DLY	B	507	9/10	0.88	0.15	53,54,58,58	0
2	ALC	J	504	11/12	0.92	0.18	55,56,57,57	0
2	ALC	H	504	11/12	0.92	0.20	54,56,61,61	0
2	DLY	F	507	9/10	0.93	0.13	51,52,57,57	0
2	DSN	D	506	6/7	0.93	0.10	51,52,52,52	0
2	ALC	F	504	11/12	0.93	0.16	54,54,56,58	0
2	DSN	J	506	6/7	0.93	0.12	52,52,52,54	0
2	DLY	L	507	9/10	0.93	0.14	51,52,59,61	0
2	DSN	P	506	6/7	0.93	0.10	56,56,56,57	0
2	DSN	F	506	6/7	0.93	0.14	49,50,50,50	0
2	ALC	D	504	11/12	0.94	0.15	53,54,55,56	0
2	ALC	N	504	11/12	0.94	0.16	55,56,57,58	0
2	DSN	N	506	6/7	0.94	0.13	51,51,52,53	0
2	DLY	N	507	9/10	0.94	0.17	47,50,50,51	0
2	DSN	B	506	6/7	0.94	0.10	52,54,54,54	0
2	DLY	D	507	9/10	0.94	0.16	51,52,53,53	0
2	ALC	B	504	11/12	0.95	0.15	56,57,58,60	0
2	DLY	J	507	9/10	0.95	0.15	49,50,50,51	0
2	ALC	L	504	11/12	0.96	0.14	60,61,63,63	0
2	DSN	L	506	6/7	0.96	0.09	53,54,54,55	0
2	ALC	P	504	11/12	0.96	0.18	59,60,61,63	0
2	DLY	H	507	9/10	0.96	0.13	50,50,51,51	0
2	DSN	H	506	6/7	0.96	0.09	48,50,50,50	0

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

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^{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
7	NAG	A	321	14/15	0.40	0.21	75,78,80,80	0
7	NAG	K	331	14/15	0.40	0.23	84,86,88,88	0
7	NAG	K	322	14/15	0.57	0.18	76,79,80,81	0
7	NAG	G	321	14/15	0.57	0.21	76,80,82,83	0
7	NAG	I	321	14/15	0.63	0.18	76,79,80,80	0
7	NAG	C	316	14/15	0.66	0.16	77,80,84,84	0
7	NAG	E	317	14/15	0.66	0.15	72,75,80,80	0
7	NAG	A	317	14/15	0.67	0.18	78,82,85,85	0
7	NAG	C	321	14/15	0.71	0.16	78,82,83,84	0
7	NAG	O	321	14/15	0.71	0.17	78,82,82,83	0
7	NAG	M	331	14/15	0.74	0.15	72,75,76,76	0
8	SO4	A	805	5/5	0.85	0.18	132,132,133,133	0
8	SO4	C	806	5/5	0.86	0.16	79,80,81,81	0
8	SO4	E	807	5/5	0.89	0.21	125,125,125,125	0
8	SO4	E	820	5/5	0.89	0.22	86,87,87,87	0
8	SO4	C	814	5/5	0.90	0.15	65,67,68,69	0
8	SO4	K	810	5/5	0.90	0.13	84,85,86,86	0
8	SO4	O	812	5/5	0.90	0.17	79,79,80,80	0
8	SO4	A	801	5/5	0.91	0.10	70,70,72,72	0
8	SO4	C	818	5/5	0.92	0.15	75,75,76,77	0
8	SO4	I	821	5/5	0.92	0.22	71,72,72,73	0
8	SO4	G	816	5/5	0.93	0.11	61,62,63,63	0
8	SO4	M	819	5/5	0.93	0.20	79,79,80,80	0
8	SO4	A	813	5/5	0.93	0.10	64,66,66,67	0
8	SO4	G	802	5/5	0.94	0.09	56,57,58,58	0
8	SO4	E	815	5/5	0.94	0.10	56,57,58,58	0
8	SO4	K	803	5/5	0.95	0.07	61,61,61,62	0
8	SO4	I	804	5/5	0.95	0.11	58,58,59,60	0
8	SO4	I	809	5/5	0.95	0.11	64,65,65,65	0
8	SO4	G	817	5/5	0.95	0.12	67,69,69,70	0
8	SO4	G	808	5/5	0.96	0.10	58,58,60,60	0
8	SO4	M	811	5/5	0.97	0.06	63,63,63,64	0

6.5 Other polymers (i)

There are no such residues in this entry.