Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 12:53 am GMT

PDB ID	:	8OS6
Title	:	Structure of a GFRA1/GDNF LICAM complex
Authors	:	Houghton, F.M.; Adams, S.E.; Briggs, D.C.; McDonald, N.Q.
Deposited on	:	2023-04-18
Resolution	:	2.66 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

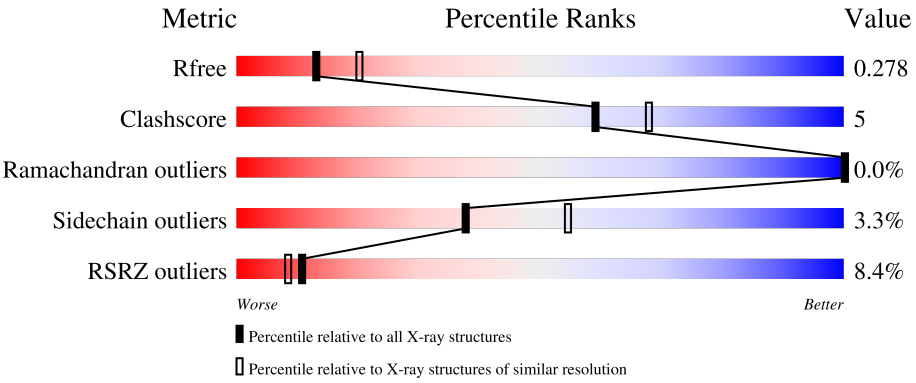
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	260	8% 72% 8% 20%
1	C	260	6% 71% 7% 22%
1	E	260	7% 71% 8% 21%
1	G	260	7% 70% 8% 22%
1	I	260	3% 69% 8% 23%

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Mol	Chain	Length	Quality of chain
1	K	260	8% 69% 8% 22%
1	M	260	7% 71% 7% 22%
1	O	260	5% 67% 12% 21%
1	Q	260	7% 71% 7% 22%
1	S	260	7% 69% 8% 22%
2	B	99	12% 84% 13%
2	D	99	11% 88% 11%
2	F	99	7% 90% 9%
2	H	99	5% 88% 9%
2	J	99	4% 84% 15%
2	L	99	8% 79% 18%
2	N	99	7% 85% 10%
2	P	99	7% 84% 12%
2	R	99	12% 90% 6%
2	T	99	10% 78% 17%
3	U	2	100%
3	Y	2	50% 50%
3	Z	2	50% 50%
3	b	2	100%
4	V	3	100%
4	W	3	100%
4	X	3	100%
5	a	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 46489 atoms, of which 22664 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 GDNF family receptor alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	207	Total	C	H	N	O	S	0	0	0
			3128	981	1530	285	310	22			
1	C	204	Total	C	H	N	O	S	0	0	0
			3071	967	1496	281	305	22			
1	E	205	Total	C	H	N	O	S	0	0	0
			3087	971	1507	281	306	22			
1	G	204	Total	C	H	N	O	S	0	0	0
			3073	969	1495	281	306	22			
1	I	201	Total	C	H	N	O	S	0	0	0
			3055	958	1498	278	299	22			
1	K	202	Total	C	H	N	O	S	0	0	0
			3043	959	1483	278	301	22			
1	M	204	Total	C	H	N	O	S	0	0	0
			3086	967	1511	281	305	22			
1	O	205	Total	C	H	N	O	S	0	0	0
			3084	968	1509	282	303	22			
1	Q	203	Total	C	H	N	O	S	0	0	0
			3061	962	1494	279	304	22			
1	S	203	Total	C	H	N	O	S	0	0	0
			3060	964	1491	280	303	22			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	GLY	-	expression tag	UNP Q98TT9
A	354	SER	-	expression tag	UNP Q98TT9
A	355	GLU	-	expression tag	UNP Q98TT9
C	353	GLY	-	expression tag	UNP Q98TT9
C	354	SER	-	expression tag	UNP Q98TT9
C	355	GLU	-	expression tag	UNP Q98TT9
E	353	GLY	-	expression tag	UNP Q98TT9
E	354	SER	-	expression tag	UNP Q98TT9
E	355	GLU	-	expression tag	UNP Q98TT9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	353	GLY	-	expression tag	UNP Q98TT9
G	354	SER	-	expression tag	UNP Q98TT9
G	355	GLU	-	expression tag	UNP Q98TT9
I	353	GLY	-	expression tag	UNP Q98TT9
I	354	SER	-	expression tag	UNP Q98TT9
I	355	GLU	-	expression tag	UNP Q98TT9
K	353	GLY	-	expression tag	UNP Q98TT9
K	354	SER	-	expression tag	UNP Q98TT9
K	355	GLU	-	expression tag	UNP Q98TT9
M	353	GLY	-	expression tag	UNP Q98TT9
M	354	SER	-	expression tag	UNP Q98TT9
M	355	GLU	-	expression tag	UNP Q98TT9
O	353	GLY	-	expression tag	UNP Q98TT9
O	354	SER	-	expression tag	UNP Q98TT9
O	355	GLU	-	expression tag	UNP Q98TT9
Q	353	GLY	-	expression tag	UNP Q98TT9
Q	354	SER	-	expression tag	UNP Q98TT9
Q	355	GLU	-	expression tag	UNP Q98TT9
S	353	GLY	-	expression tag	UNP Q98TT9
S	354	SER	-	expression tag	UNP Q98TT9
S	355	GLU	-	expression tag	UNP Q98TT9

- Molecule 2 is a protein called Glial cell line-derived neurotrophic factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	97	Total	C	H	N	O	S	0	0	0
			1481	473	720	132	149	7			
2	D	98	Total	C	H	N	O	S	0	0	0
			1535	485	752	138	153	7			
2	F	98	Total	C	H	N	O	S	0	0	0
			1522	485	741	136	153	7			
2	H	96	Total	C	H	N	O	S	0	0	0
			1500	478	732	133	150	7			
2	J	98	Total	C	H	N	O	S	0	0	0
			1518	483	741	135	152	7			
2	L	96	Total	C	H	N	O	S	0	0	0
			1493	475	729	132	150	7			
2	N	95	Total	C	H	N	O	S	0	0	0
			1502	475	739	132	149	7			
2	P	95	Total	C	H	N	O	S	0	0	0
			1487	472	728	131	149	7			
2	R	95	Total	C	H	N	O	S	0	0	0
			1502	475	739	132	149	7			

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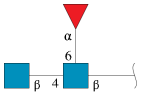
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	T	95	Total	C	H	N	O	S	0	1	0
			1503	475	740	132	149	7			

- Molecule 3 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
3	U	2	Total	C	H	N	O	0	0	0
			40	16	12	2	10			
3	Y	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
3	Z	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
3	b	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 4 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.

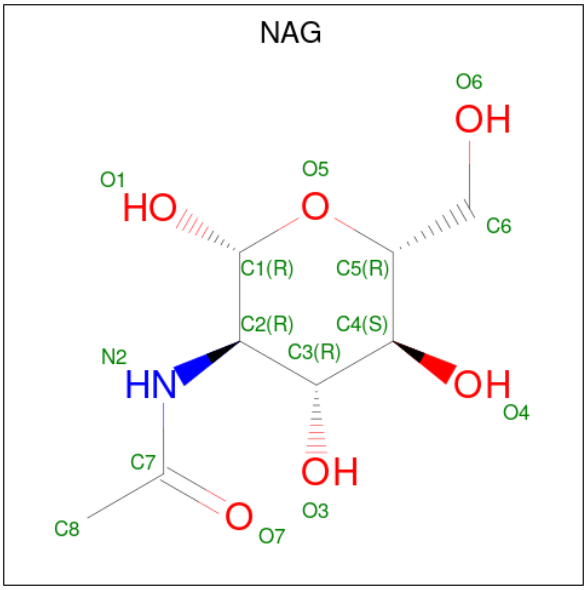


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	V	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			
4	W	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			
4	X	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	a	2	Total C H N O 46 14 22 1 9	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C H N O 27 8 13 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C H N O 27 8 13 1 5	0	0
6	I	1	Total C N O 14 8 1 5	0	0
6	K	1	Total C H N O 27 8 13 1 5	0	0
6	L	1	Total C H N O 27 8 13 1 5	0	0
6	M	1	Total C N O 14 8 1 5	0	0
6	R	1	Total C H N O 27 8 13 1 5	0	0
6	S	1	Total C H N O 27 8 13 1 5	0	0
6	T	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

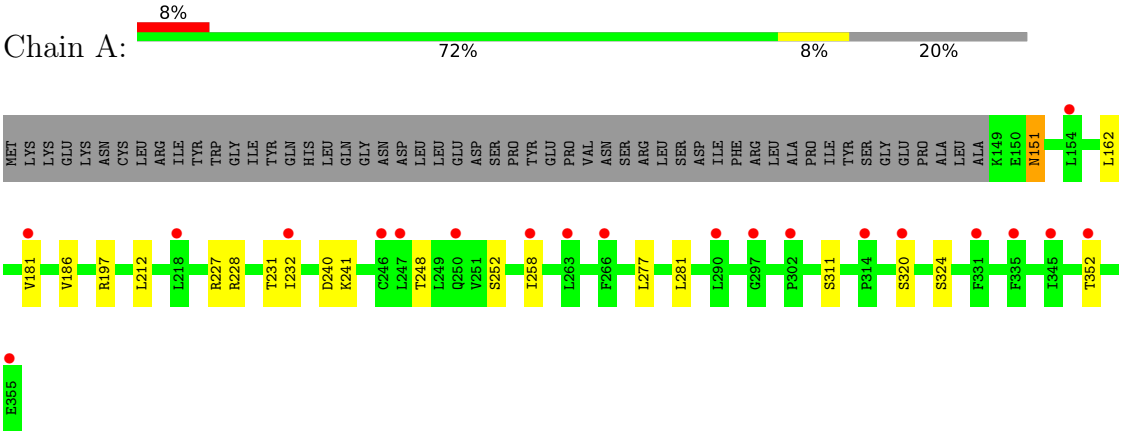
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	C	2	Total O 2 2	0	0
7	E	3	Total O 3 3	0	0
7	G	2	Total O 2 2	0	0
7	I	1	Total O 1 1	0	0
7	K	2	Total O 2 2	0	0
7	M	1	Total O 1 1	0	0
7	O	1	Total O 1 1	0	0
7	Q	2	Total O 2 2	0	0
7	S	2	Total O 2 2	0	0

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.

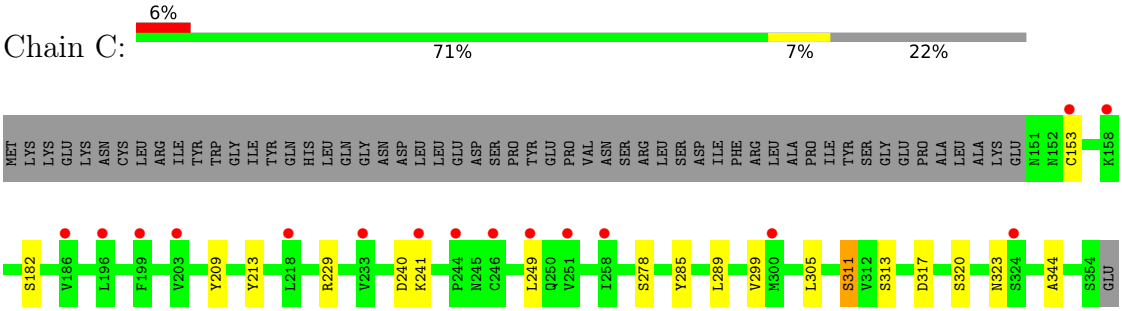
• Molecule 1: GDNF family receptor alpha

Chain A:



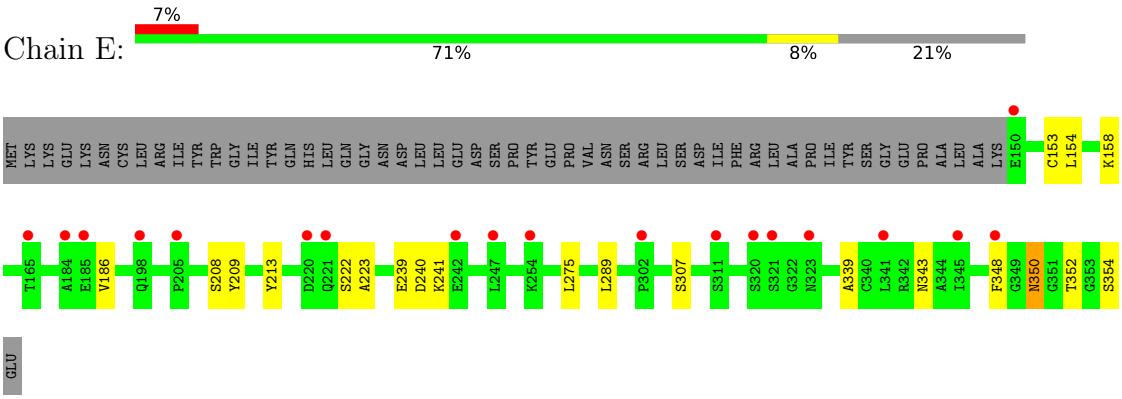
• Molecule 1: GDNF family receptor alpha

Chain C:



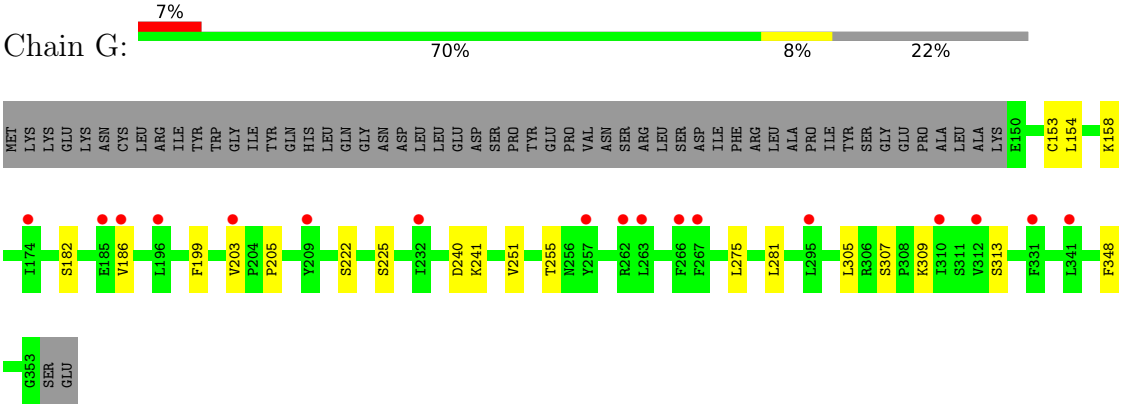
• Molecule 1: GDNF family receptor alpha

Chain E:



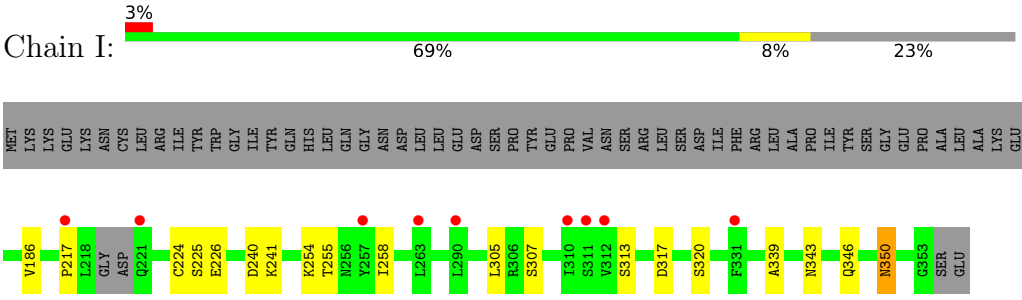
• Molecule 1: GDNF family receptor alpha

Chain G:



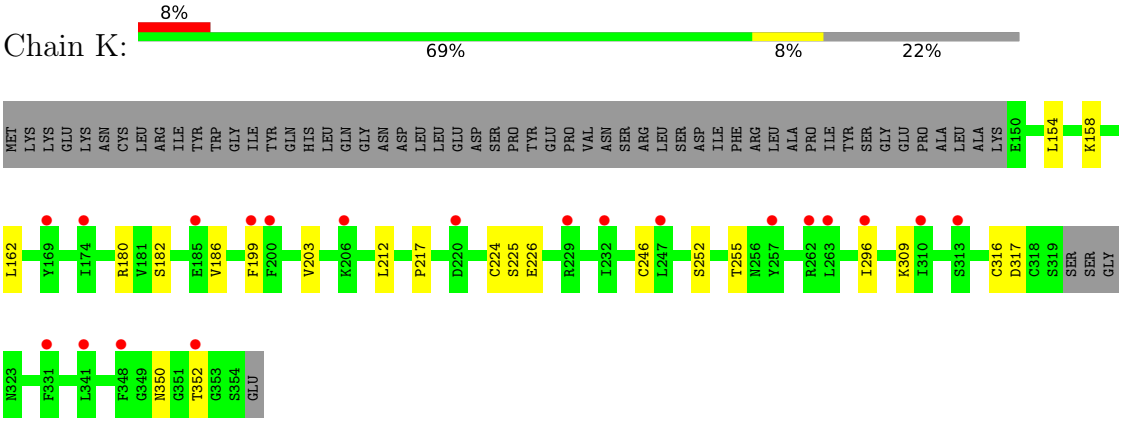
• Molecule 1: GDNF family receptor alpha

Chain I:



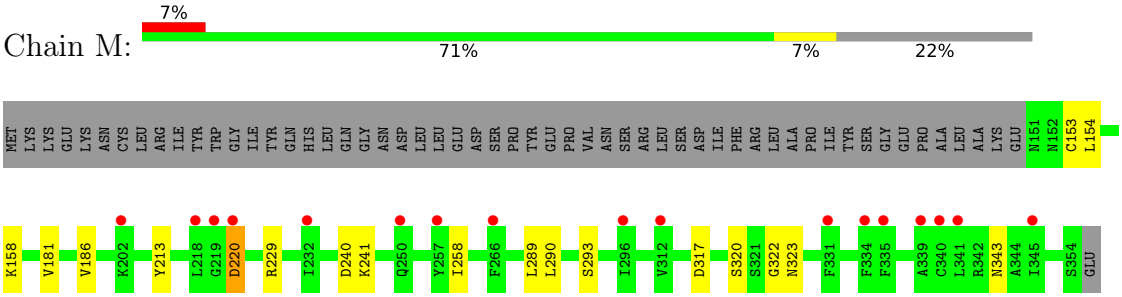
• Molecule 1: GDNF family receptor alpha

Chain K:

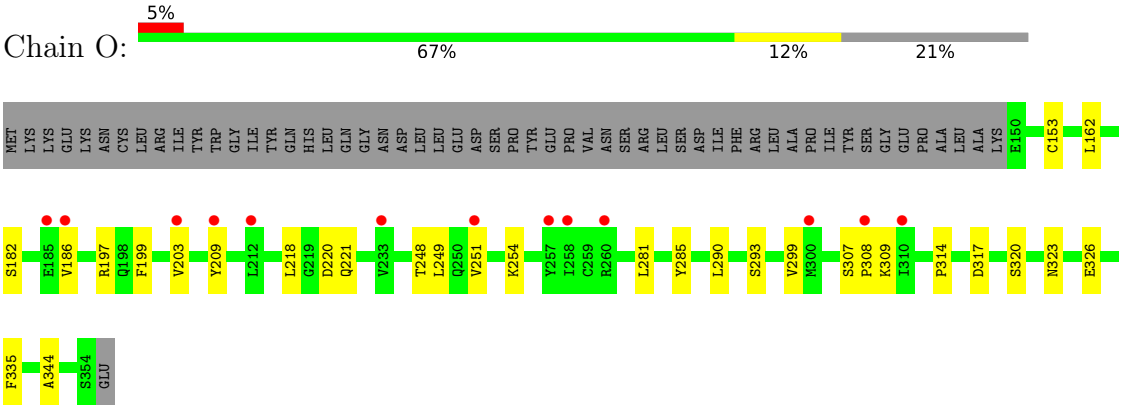


• Molecule 1: GDNF family receptor alpha

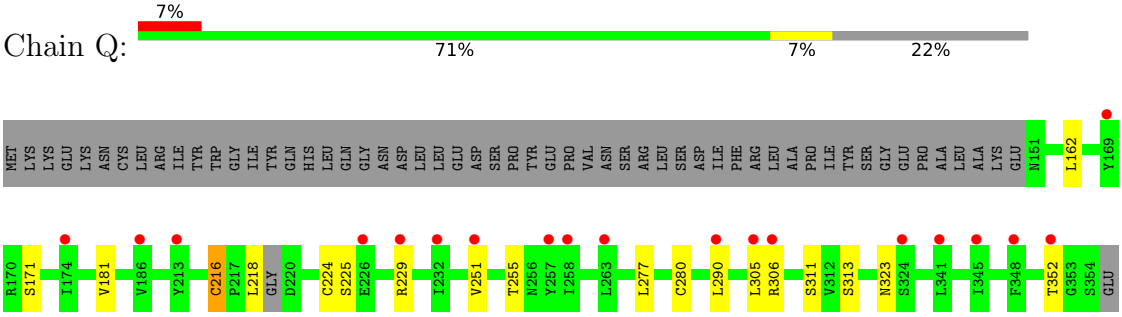
Chain M:



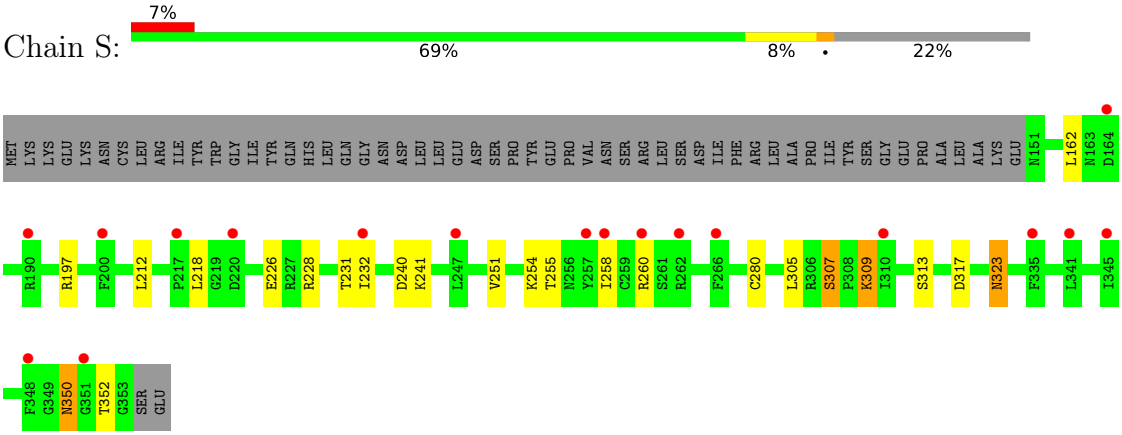
• Molecule 1: GDNF family receptor alpha



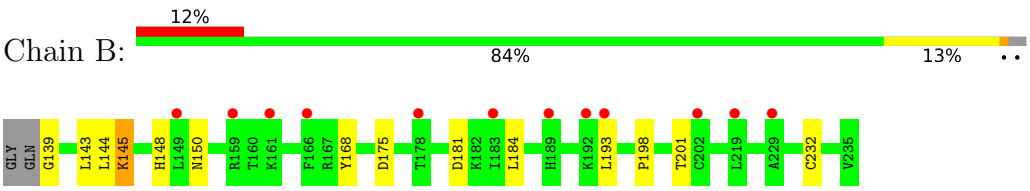
• Molecule 1: GDNF family receptor alpha



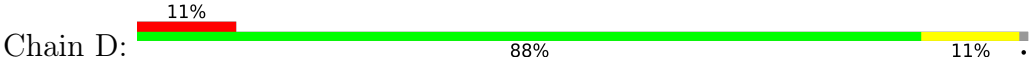
• Molecule 1: GDNF family receptor alpha

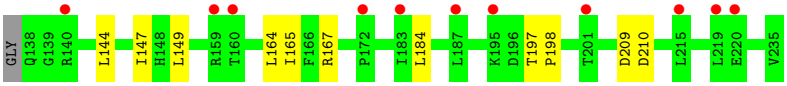


• Molecule 2: Glial cell line-derived neurotrophic factor



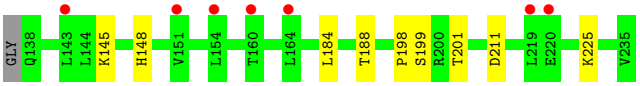
• Molecule 2: Glial cell line-derived neurotrophic factor





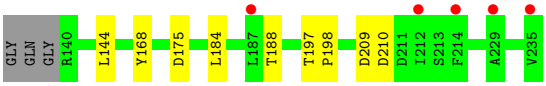
• Molecule 2: Glial cell line-derived neurotrophic factor

Chain F:



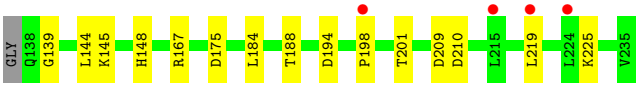
• Molecule 2: Glial cell line-derived neurotrophic factor

Chain H:



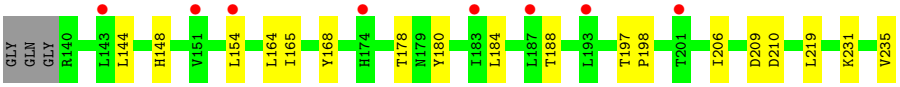
• Molecule 2: Glial cell line-derived neurotrophic factor

Chain J:



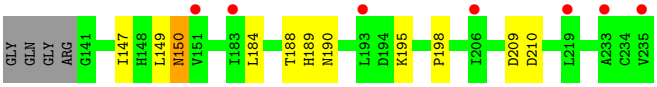
• Molecule 2: Glial cell line-derived neurotrophic factor

Chain L:



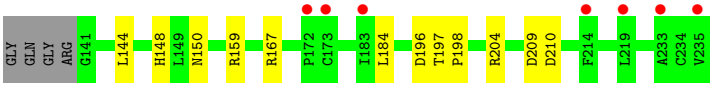
• Molecule 2: Glial cell line-derived neurotrophic factor

Chain N:



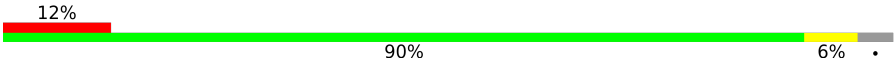
• Molecule 2: Glial cell line-derived neurotrophic factor

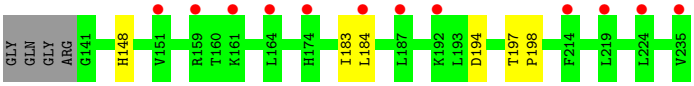
Chain P:



• Molecule 2: Glial cell line-derived neurotrophic factor

Chain R:



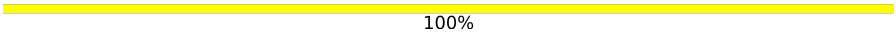


• Molecule 2: Glial cell line-derived neurotrophic factor

Chain T:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

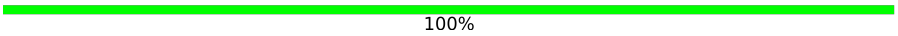
Chain Y:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

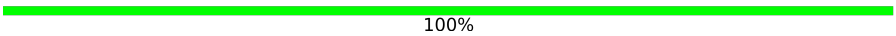
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

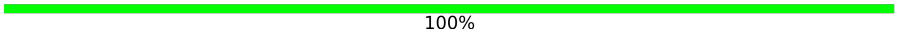


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



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

Chain W: 

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

Chain X: 

• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	114.14Å 170.04Å 130.79Å 90.00° 96.17° 90.00°	Depositor
Resolution (Å)	90.45 – 2.66 130.03 – 2.66	Depositor EDS
% Data completeness (in resolution range)	88.1 (90.45-2.66) 88.3 (130.03-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.244 , 0.283 0.248 , 0.278	Depositor DCC
R_{free} test set	3852 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	46489	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: FUC, 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	0.25	0/1628	0.47	0/2196
1	C	0.26	0/1605	0.47	0/2166
1	E	0.25	0/1610	0.47	0/2173
1	G	0.25	0/1608	0.47	0/2170
1	I	0.26	0/1586	0.47	0/2139
1	K	0.25	0/1589	0.47	0/2145
1	M	0.26	0/1605	0.47	0/2166
1	O	0.26	0/1605	0.48	0/2166
1	Q	0.26	0/1596	0.49	0/2154
1	S	0.26	0/1599	0.48	0/2158
2	B	0.26	0/775	0.52	2/1046 (0.2%)
2	D	0.24	0/797	0.47	0/1073
2	F	0.23	0/795	0.46	0/1070
2	H	0.24	0/782	0.47	0/1053
2	J	0.24	0/791	0.47	0/1065
2	L	0.23	0/778	0.46	0/1049
2	N	0.23	0/777	0.46	0/1046
2	P	0.24	0/773	0.47	0/1042
2	R	0.23	0/777	0.46	0/1046
2	T	0.24	0/784	0.46	0/1056
All	All	0.25	0/23860	0.47	2/32179 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	145	LYS	CA-CB-CG	5.36	125.20	113.40
2	B	145	LYS	CB-CA-C	5.19	120.78	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1598	1530	1533	13	0
1	C	1575	1496	1511	7	0
1	E	1580	1507	1510	13	0
1	G	1578	1495	1512	12	0
1	I	1557	1498	1498	13	0
1	K	1560	1483	1488	13	0
1	M	1575	1511	1511	12	0
1	O	1575	1509	1507	16	0
1	Q	1567	1494	1497	12	0
1	S	1569	1491	1506	20	0
2	B	761	720	720	9	0
2	D	783	752	752	7	0
2	F	781	741	752	7	0
2	H	768	732	741	4	0
2	J	777	741	746	10	0
2	L	764	729	730	17	0
2	N	763	739	739	9	0
2	P	759	728	728	9	0
2	R	763	739	739	6	0
2	T	763	740	732	11	0
3	U	28	12	25	1	0
3	Y	28	25	25	4	0
3	Z	28	25	25	2	0
3	b	28	25	25	0	0
4	V	38	34	34	0	0
4	W	38	34	34	0	0
4	X	38	34	34	7	0
5	a	24	22	22	0	0
6	B	14	13	13	0	0
6	E	14	0	13	1	0
6	G	14	13	13	1	0
6	I	14	0	13	4	0
6	K	14	13	13	1	0
6	L	14	13	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	14	0	13	6	0
6	R	14	13	13	1	0
6	S	14	13	13	4	0
6	T	14	0	13	2	0
7	A	3	0	0	0	0
7	C	2	0	0	0	0
7	E	3	0	0	0	0
7	G	2	0	0	0	0
7	I	1	0	0	0	0
7	K	2	0	0	0	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
7	Q	2	0	0	0	0
7	S	2	0	0	0	0
All	All	23825	22664	22806	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (218) 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)
6:I:401:NAG:H83	1:S:323:ASN:HB2	1.18	1.10
6:I:401:NAG:O3	6:I:401:NAG:H82	1.70	0.90
6:I:401:NAG:H83	1:S:323:ASN:CB	2.03	0.89
6:M:401:NAG:H3	6:M:401:NAG:H83	1.55	0.89
6:I:401:NAG:C8	1:S:323:ASN:HB2	2.02	0.88
4:X:2:NAG:H83	4:X:2:NAG:H3	1.63	0.81
1:S:254:LYS:O	1:S:260:ARG:NH2	2.19	0.75
1:S:350:ASN:ND2	6:S:401:NAG:H83	2.05	0.72
6:T:301:NAG:O3	6:T:301:NAG:H82	1.90	0.71
1:S:251:VAL:O	1:S:255:THR:HG23	1.92	0.69
1:C:213:TYR:CE2	1:C:289:LEU:HD22	2.28	0.69
2:D:184:LEU:HD22	2:D:198:PRO:CG	2.24	0.68
1:I:162:LEU:HD21	2:J:148:HIS:NE2	2.10	0.66
1:K:226:GLU:HB3	2:L:219:LEU:HD21	1.78	0.66
1:S:307:SER:OG	1:S:309:LYS:O	2.14	0.65
2:D:184:LEU:HD22	2:D:198:PRO:HG2	1.78	0.65
2:F:184:LEU:O	2:F:188:THR:HG23	1.96	0.65
2:F:184:LEU:HD22	2:F:198:PRO:HG3	1.78	0.65
2:F:184:LEU:HD22	2:F:198:PRO:CG	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:350:ASN:OD1	1:I:350:ASN:N	2.28	0.64
3:Y:2:NAG:C1	3:Y:2:NAG:H82	2.27	0.63
1:I:240:ASP:OD1	1:I:241:LYS:N	2.31	0.62
2:T:148:HIS:ND1	6:T:301:NAG:O7	2.32	0.62
2:L:144:LEU:HD12	2:L:168:TYR:O	2.00	0.62
2:T:144:LEU:HD12	2:T:168:TYR:O	2.00	0.62
2:F:145:LYS:NZ	2:P:196:ASP:OD2	2.32	0.61
1:S:240:ASP:OD1	1:S:241:LYS:N	2.33	0.61
1:E:213:TYR:CE2	1:E:289:LEU:HD22	2.36	0.61
4:X:1:NAG:H82	4:X:1:NAG:C1	2.31	0.60
1:A:151:ASN:OD1	1:A:151:ASN:N	2.34	0.60
1:A:212:LEU:HD12	1:A:231:THR:HG21	1.83	0.59
1:M:323:ASN:CB	6:S:401:NAG:H82	2.33	0.59
2:L:148:HIS:CD2	6:L:301:NAG:H83	2.38	0.59
1:A:231:THR:HG23	1:A:232:ILE:HG23	1.85	0.59
1:K:224:CYS:SG	1:K:225:SER:N	2.76	0.58
1:G:240:ASP:OD1	1:G:241:LYS:N	2.36	0.58
6:M:401:NAG:H3	6:M:401:NAG:C8	2.31	0.58
1:M:154:LEU:HD21	1:M:158:LYS:HE3	1.85	0.58
6:R:301:NAG:O7	6:R:301:NAG:O3	2.21	0.57
2:P:184:LEU:HD22	2:P:198:PRO:CG	2.35	0.57
2:D:164:LEU:HD12	2:D:165:ILE:N	2.19	0.57
1:M:213:TYR:CE2	1:M:289:LEU:HD22	2.40	0.57
1:A:240:ASP:OD1	1:A:241:LYS:N	2.37	0.56
2:T:160:THR:OG1	2:T:161:LYS:N	2.39	0.56
1:M:323:ASN:HB2	6:S:401:NAG:H82	1.88	0.56
2:T:184:LEU:HD22	2:T:198:PRO:CG	2.36	0.56
1:I:346:GLN:O	1:I:350:ASN:OD1	2.24	0.56
1:A:320:SER:HB3	1:A:324:SER:OG	2.06	0.56
1:M:240:ASP:OD1	1:M:241:LYS:N	2.39	0.55
1:Q:162:LEU:HD21	2:R:148:HIS:HE2	1.71	0.55
2:L:209:ASP:OD1	2:L:210:ASP:N	2.40	0.55
3:Y:2:NAG:C1	3:Y:2:NAG:C8	2.84	0.55
1:C:240:ASP:OD1	1:C:241:LYS:N	2.39	0.55
1:O:326:GLU:OE1	1:O:326:GLU:N	2.39	0.55
2:P:197:THR:HG23	2:P:197:THR:O	2.07	0.55
2:L:184:LEU:HD22	2:L:198:PRO:CG	2.37	0.55
2:L:206:ILE:HD11	2:L:231:LYS:HE2	1.88	0.55
3:Y:1:NAG:O7	3:Y:1:NAG:O3	2.21	0.55
4:X:2:NAG:H82	4:X:3:FUC:C1	2.38	0.54
2:N:147:ILE:CD1	2:N:149:LEU:HD21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:184:LEU:HD22	2:N:198:PRO:CG	2.37	0.54
2:D:209:ASP:OD1	2:D:210:ASP:N	2.39	0.54
6:M:401:NAG:H82	6:M:401:NAG:C1	2.36	0.54
2:B:144:LEU:HD12	2:B:168:TYR:O	2.08	0.54
1:S:162:LEU:HD21	2:T:148:HIS:NE2	2.22	0.54
1:Q:218:LEU:H	1:Q:218:LEU:HD23	1.74	0.53
1:A:248:THR:HG22	1:G:348:PHE:CE1	2.44	0.53
1:S:231:THR:HG23	1:S:232:ILE:HG23	1.89	0.53
1:G:305:LEU:HD21	1:G:313:SER:HB3	1.90	0.53
2:N:150:ASN:OD1	3:Z:1:NAG:N2	2.41	0.53
4:X:1:NAG:C1	4:X:1:NAG:C8	2.86	0.53
1:G:154:LEU:HD21	1:G:158:LYS:HE3	1.91	0.52
2:R:197:THR:HG23	2:R:197:THR:O	2.09	0.52
1:G:307:SER:OG	1:G:309:LYS:O	2.27	0.52
2:J:144:LEU:HD21	2:J:167:ARG:HB3	1.90	0.52
2:L:184:LEU:O	2:L:188:THR:HG23	2.09	0.52
1:K:352:THR:HG22	1:K:352:THR:O	2.09	0.52
2:B:181:ASP:OD2	2:B:201:THR:OG1	2.28	0.52
2:D:144:LEU:HD21	2:D:167:ARG:HD3	1.92	0.52
2:P:209:ASP:OD1	2:P:210:ASP:N	2.42	0.52
2:J:209:ASP:OD1	2:J:210:ASP:N	2.41	0.51
2:L:164:LEU:HD12	2:L:165:ILE:N	2.25	0.51
4:X:1:NAG:H61	4:X:2:NAG:H82	1.92	0.51
4:X:2:NAG:H3	4:X:2:NAG:C8	2.36	0.51
2:J:139:GLY:HA2	2:J:175:ASP:OD2	2.11	0.51
1:Q:352:THR:O	1:Q:352:THR:HG22	2.10	0.51
2:J:184:LEU:HD22	2:J:198:PRO:CG	2.40	0.51
1:I:258:ILE:H	1:I:258:ILE:HD12	1.76	0.51
4:X:1:NAG:H3	4:X:1:NAG:H83	1.92	0.51
1:K:154:LEU:HD21	1:K:158:LYS:HE3	1.91	0.50
1:E:354:SER:O	6:E:401:NAG:H82	2.11	0.50
1:I:217:PRO:HD2	1:I:224:CYS:SG	2.52	0.50
2:T:144:LEU:HD11	2:T:167:ARG:HB3	1.93	0.49
2:N:150:ASN:OD1	2:N:150:ASN:N	2.44	0.49
2:J:144:LEU:HD23	2:J:145:LYS:N	2.27	0.49
1:S:305:LEU:HD11	1:S:313:SER:CB	2.43	0.49
1:O:162:LEU:HD21	2:P:148:HIS:CE1	2.48	0.49
1:E:240:ASP:OD1	1:E:241:LYS:N	2.46	0.49
2:L:197:THR:HG23	2:L:197:THR:O	2.13	0.48
1:I:254:LYS:HB2	1:O:290:LEU:HD11	1.95	0.48
2:T:209:ASP:OD1	2:T:210:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:144:LEU:HD11	2:P:167:ARG:HB3	1.95	0.48
1:S:212:LEU:HD12	1:S:231:THR:HG21	1.96	0.48
2:H:144:LEU:HD12	2:H:168:TYR:O	2.14	0.48
1:O:186:VAL:HG12	1:O:186:VAL:O	2.13	0.47
1:K:162:LEU:HD21	2:L:148:HIS:CE1	2.49	0.47
1:A:258:ILE:HD12	1:A:258:ILE:H	1.80	0.47
2:L:235:VAL:HG23	2:L:235:VAL:OXT	2.15	0.47
1:S:352:THR:O	1:S:352:THR:HG22	2.14	0.47
1:K:199:PHE:CE1	1:K:203:VAL:HG21	2.50	0.47
2:P:184:LEU:HD22	2:P:198:PRO:HG3	1.97	0.47
1:Q:216:CYS:SG	1:Q:225:SER:N	2.88	0.47
1:S:305:LEU:HD21	1:S:313:SER:HB3	1.97	0.47
1:S:226:GLU:HB3	2:T:219:LEU:HD21	1.97	0.47
2:F:201:THR:HG22	2:P:204:ARG:NH2	2.30	0.46
1:K:350:ASN:HD22	6:K:401:NAG:H83	1.79	0.46
1:S:305:LEU:HD11	1:S:313:SER:HB3	1.96	0.46
2:N:184:LEU:HD22	2:N:198:PRO:HG2	1.97	0.46
1:O:209:TYR:HE2	1:O:293:SER:HG	1.62	0.46
1:E:350:ASN:N	1:E:350:ASN:OD1	2.49	0.46
1:G:251:VAL:O	1:G:255:THR:HG23	2.16	0.46
2:B:139:GLY:N	2:B:175:ASP:OD1	2.48	0.46
1:S:228:ARG:O	1:S:231:THR:HG22	2.15	0.46
1:K:180:ARG:HH22	1:K:186:VAL:HG22	1.80	0.46
2:L:206:ILE:HD11	2:L:231:LYS:CE	2.46	0.45
2:B:193:LEU:HD11	2:T:168:TYR:OH	2.16	0.45
2:H:209:ASP:OD1	2:H:210:ASP:N	2.48	0.45
1:O:323:ASN:ND2	1:Q:277:LEU:HD21	2.32	0.45
1:O:307:SER:OG	1:O:309:LYS:O	2.34	0.45
2:P:184:LEU:HD22	2:P:198:PRO:HG2	1.97	0.45
2:B:184:LEU:HD22	2:B:198:PRO:CG	2.47	0.45
2:B:184:LEU:HD22	2:B:198:PRO:HG2	1.99	0.45
2:N:209:ASP:OD1	2:N:210:ASP:N	2.48	0.45
1:M:220:ASP:OD1	1:M:220:ASP:N	2.50	0.45
3:U:2:NAG:O7	3:U:2:NAG:H3	2.16	0.45
2:F:184:LEU:HD22	2:F:198:PRO:HG2	1.99	0.45
1:Q:277:LEU:C	1:Q:277:LEU:HD23	2.38	0.44
1:G:281:LEU:C	1:G:281:LEU:HD23	2.38	0.44
1:I:226:GLU:HB3	2:J:219:LEU:HD21	1.99	0.44
1:A:252:SER:HA	1:G:205:PRO:HG3	2.00	0.44
1:K:217:PRO:HD2	1:K:224:CYS:SG	2.57	0.44
1:M:258:ILE:HD12	1:M:258:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:401:NAG:C8	6:M:401:NAG:C1	2.95	0.44
1:A:228:ARG:O	1:A:231:THR:HG22	2.18	0.44
1:M:186:VAL:HG12	1:M:186:VAL:O	2.17	0.44
2:L:164:LEU:HD12	2:L:165:ILE:C	2.39	0.43
1:C:305:LEU:HD12	1:C:311:SER:HB3	1.99	0.43
1:E:186:VAL:O	1:E:186:VAL:HG12	2.18	0.43
1:O:314:PRO:HD3	1:O:335:PHE:CG	2.53	0.43
1:S:350:ASN:CG	6:S:401:NAG:H83	2.38	0.43
1:C:285:TYR:HD1	1:C:344:ALA:HB2	1.83	0.43
1:E:154:LEU:C	1:E:154:LEU:HD23	2.39	0.43
2:D:164:LEU:HD12	2:D:165:ILE:C	2.38	0.43
1:M:154:LEU:C	1:M:154:LEU:HD23	2.39	0.43
1:A:162:LEU:HD21	2:B:148:HIS:NE2	2.34	0.43
2:J:184:LEU:HD22	2:J:198:PRO:HG3	2.00	0.43
2:D:147:ILE:CD1	2:D:149:LEU:HD21	2.49	0.43
2:J:184:LEU:HD22	2:J:198:PRO:HG2	2.01	0.43
1:K:252:SER:O	1:K:255:THR:HG22	2.18	0.43
1:A:324:SER:H	6:G:401:NAG:H81	1.84	0.43
1:E:275:LEU:N	1:E:275:LEU:HD12	2.34	0.43
2:F:211:ASP:OD2	2:F:225:LYS:NZ	2.52	0.43
2:N:184:LEU:HD22	2:N:198:PRO:HG3	2.01	0.43
1:O:218:LEU:N	1:O:218:LEU:HD22	2.34	0.43
2:L:180:TYR:CZ	2:L:184:LEU:HD11	2.54	0.42
1:C:249:LEU:HD11	1:C:299:VAL:HG22	2.02	0.42
1:G:275:LEU:HD12	1:G:275:LEU:N	2.34	0.42
1:M:258:ILE:HD12	1:M:258:ILE:N	2.34	0.42
1:I:339:ALA:O	1:I:343:ASN:ND2	2.52	0.42
2:R:184:LEU:HD22	2:R:198:PRO:CG	2.49	0.42
1:G:199:PHE:CE1	1:G:203:VAL:HG21	2.53	0.42
2:H:197:THR:HG23	2:H:197:THR:O	2.20	0.42
1:O:285:TYR:HD1	1:O:344:ALA:HB2	1.84	0.42
1:O:281:LEU:HD23	1:O:281:LEU:C	2.39	0.42
3:Y:2:NAG:H3	3:Y:2:NAG:H83	2.01	0.42
1:I:305:LEU:HD11	1:I:313:SER:HB3	2.00	0.42
2:L:154:LEU:HD22	2:R:183:ILE:HG23	2.02	0.42
1:Q:162:LEU:HD21	2:R:148:HIS:NE2	2.32	0.42
2:B:168:TYR:CZ	2:T:193:LEU:HD22	2.54	0.42
2:N:147:ILE:HD11	2:N:149:LEU:HD21	2.02	0.42
2:T:180:TYR:CZ	2:T:184:LEU:HD11	2.55	0.42
2:H:184:LEU:HD22	2:H:198:PRO:HB2	2.02	0.42
1:K:154:LEU:C	1:K:154:LEU:HD23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:290:LEU:HD21	1:Q:251:VAL:HG13	2.01	0.42
1:E:222:SER:OG	1:E:223:ALA:N	2.53	0.41
1:E:339:ALA:O	1:E:343:ASN:ND2	2.53	0.41
6:M:401:NAG:HN2	1:Q:323:ASN:HB2	1.85	0.41
1:E:154:LEU:HD21	1:E:158:LYS:HE3	2.03	0.41
1:E:208:SER:HG	1:E:209:TYR:HD1	1.64	0.41
2:N:150:ASN:OD1	3:Z:1:NAG:C2	2.68	0.41
2:L:184:LEU:HD22	2:L:198:PRO:HG3	2.02	0.41
1:O:199:PHE:CD1	1:O:203:VAL:HG21	2.56	0.41
1:C:305:LEU:HD11	1:C:313:SER:CB	2.51	0.41
1:E:154:LEU:HD23	1:E:154:LEU:O	2.20	0.41
1:M:343:ASN:HB3	1:Q:323:ASN:HD21	1.84	0.41
1:O:254:LYS:HB2	1:Q:290:LEU:HD11	2.02	0.41
2:B:144:LEU:HD13	2:B:232:CYS:SG	2.60	0.41
1:O:220:ASP:HA	1:O:308:PRO:HA	2.02	0.41
1:S:258:ILE:HD12	1:S:258:ILE:H	1.86	0.41
1:G:199:PHE:CD1	1:G:203:VAL:HG21	2.55	0.41
2:J:194:ASP:N	2:J:194:ASP:OD1	2.54	0.41
1:O:249:LEU:HD11	1:O:299:VAL:HG12	2.03	0.41
1:Q:305:LEU:HD21	1:Q:313:SER:HB3	2.03	0.41
1:E:348:PHE:O	1:E:352:THR:HG23	2.21	0.41
1:G:186:VAL:HG12	1:G:186:VAL:O	2.20	0.41
1:K:212:LEU:HD21	1:K:296:ILE:HD11	2.03	0.41
2:L:184:LEU:HD22	2:L:198:PRO:HG2	2.03	0.41
1:O:248:THR:O	1:O:251:VAL:HG22	2.20	0.41
2:R:194:ASP:N	2:R:194:ASP:OD1	2.54	0.41
1:S:218:LEU:HD23	1:S:218:LEU:H	1.85	0.41
1:A:186:VAL:HG12	1:A:186:VAL:O	2.20	0.41
1:I:224:CYS:SG	1:I:225:SER:N	2.94	0.41
1:I:186:VAL:O	1:I:186:VAL:HG12	2.22	0.40
6:M:401:NAG:H83	6:M:401:NAG:C3	2.39	0.40
1:C:209:TYR:N	1:C:209:TYR:CD1	2.89	0.40
1:I:305:LEU:HD11	1:I:313:SER:CB	2.51	0.40
1:A:277:LEU:C	1:A:277:LEU:HD23	2.42	0.40
1:K:296:ILE:O	1:K:296:ILE:HG22	2.22	0.40

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	205/260 (79%)	194 (95%)	11 (5%)	0	100	100
1	C	202/260 (78%)	191 (95%)	11 (5%)	0	100	100
1	E	203/260 (78%)	198 (98%)	5 (2%)	0	100	100
1	G	202/260 (78%)	193 (96%)	9 (4%)	0	100	100
1	I	197/260 (76%)	193 (98%)	4 (2%)	0	100	100
1	K	198/260 (76%)	194 (98%)	4 (2%)	0	100	100
1	M	202/260 (78%)	198 (98%)	3 (2%)	1 (0%)	29	43
1	O	203/260 (78%)	194 (96%)	9 (4%)	0	100	100
1	Q	199/260 (76%)	194 (98%)	5 (2%)	0	100	100
1	S	201/260 (77%)	195 (97%)	6 (3%)	0	100	100
2	B	95/99 (96%)	93 (98%)	2 (2%)	0	100	100
2	D	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
2	F	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	H	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
2	J	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
2	L	94/99 (95%)	90 (96%)	4 (4%)	0	100	100
2	N	93/99 (94%)	88 (95%)	5 (5%)	0	100	100
2	P	93/99 (94%)	89 (96%)	4 (4%)	0	100	100
2	R	93/99 (94%)	87 (94%)	6 (6%)	0	100	100
2	T	94/99 (95%)	91 (97%)	3 (3%)	0	100	100
All	All	2956/3590 (82%)	2852 (96%)	103 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	322	GLY

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	184/232 (79%)	177 (96%)	7 (4%)	33	49
1	C	182/232 (78%)	174 (96%)	8 (4%)	28	43
1	E	181/232 (78%)	177 (98%)	4 (2%)	52	70
1	G	182/232 (78%)	178 (98%)	4 (2%)	52	70
1	I	180/232 (78%)	174 (97%)	6 (3%)	38	54
1	K	179/232 (77%)	174 (97%)	5 (3%)	43	61
1	M	182/232 (78%)	175 (96%)	7 (4%)	33	49
1	O	180/232 (78%)	174 (97%)	6 (3%)	38	54
1	Q	181/232 (78%)	172 (95%)	9 (5%)	24	38
1	S	181/232 (78%)	174 (96%)	7 (4%)	32	48
2	B	85/90 (94%)	82 (96%)	3 (4%)	36	52
2	D	89/90 (99%)	88 (99%)	1 (1%)	73	85
2	F	89/90 (99%)	87 (98%)	2 (2%)	52	70
2	H	88/90 (98%)	86 (98%)	2 (2%)	50	68
2	J	88/90 (98%)	85 (97%)	3 (3%)	37	53
2	L	87/90 (97%)	86 (99%)	1 (1%)	73	85
2	N	88/90 (98%)	83 (94%)	5 (6%)	20	31
2	P	87/90 (97%)	85 (98%)	2 (2%)	50	68
2	R	88/90 (98%)	88 (100%)	0	100	100
2	T	89/90 (99%)	83 (93%)	6 (7%)	16	25
All	All	2690/3220 (84%)	2602 (97%)	88 (3%)	38	54

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	181	VAL
1	A	197	ARG

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Mol	Chain	Res	Type
1	A	227	ARG
1	A	281	LEU
1	A	311	SER
1	A	352	THR
2	B	143	LEU
2	B	145	LYS
2	B	150	ASN
1	C	153	CYS
1	C	182	SER
1	C	229	ARG
1	C	278	SER
1	C	311	SER
1	C	317	ASP
1	C	320	SER
1	C	323	ASN
2	D	197	THR
1	E	153	CYS
1	E	239	GLU
1	E	307	SER
1	E	350	ASN
2	F	148	HIS
2	F	199	SER
1	G	153	CYS
1	G	182	SER
1	G	222	SER
1	G	225	SER
2	H	175	ASP
2	H	188	THR
1	I	153	CYS
1	I	255	THR
1	I	307	SER
1	I	317	ASP
1	I	320	SER
1	I	350	ASN
2	J	188	THR
2	J	201	THR
2	J	225	LYS
1	K	182	SER
1	K	246	CYS
1	K	309	LYS
1	K	316	CYS
1	K	317	ASP

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Mol	Chain	Res	Type
2	L	178	THR
1	M	153	CYS
1	M	181	VAL
1	M	220	ASP
1	M	229	ARG
1	M	293	SER
1	M	317	ASP
1	M	320	SER
2	N	150	ASN
2	N	188	THR
2	N	189	HIS
2	N	190	ASN
2	N	195	LYS
1	O	153	CYS
1	O	182	SER
1	O	197	ARG
1	O	221	GLN
1	O	317	ASP
1	O	320	SER
2	P	150	ASN
2	P	159	ARG
1	Q	171	SER
1	Q	181	VAL
1	Q	216	CYS
1	Q	224	CYS
1	Q	229	ARG
1	Q	255	THR
1	Q	280	CYS
1	Q	306	ARG
1	Q	311	SER
1	S	197	ARG
1	S	280	CYS
1	S	307	SER
1	S	309	LYS
1	S	317	ASP
1	S	323	ASN
1	S	350	ASN
2	T	150	ASN
2	T	160	THR
2	T	177	GLU
2	T	188	THR
2	T	189	HIS

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Mol	Chain	Res	Type
2	T	218	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	152	ASN
1	C	323	ASN
1	E	343	ASN
2	F	227	HIS
2	H	227	HIS
1	I	343	ASN
2	L	148	HIS
1	M	152	ASN
2	P	148	HIS
1	Q	221	GLN
1	Q	323	ASN
1	Q	350	ASN
1	S	323	ASN

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

19 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	U	1	1,3	14,14,15	0.93	2 (14%)	17,19,21	1.25	2 (11%)
3	NAG	U	2	3	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	V	1	2,4	14,14,15	0.26	0	17,19,21	0.37	0
4	NAG	V	2	4	14,14,15	0.25	0	17,19,21	0.53	0
4	FUC	V	3	4	10,10,11	0.72	0	14,14,16	0.84	0
4	NAG	W	1	2,4	14,14,15	0.21	0	17,19,21	0.34	0
4	NAG	W	2	4	14,14,15	0.20	0	17,19,21	0.43	0
4	FUC	W	3	4	10,10,11	0.83	0	14,14,16	0.88	0
4	NAG	X	1	2,4	14,14,15	0.39	0	17,19,21	0.91	1 (5%)
4	NAG	X	2	4	14,14,15	0.33	0	17,19,21	1.03	2 (11%)
4	FUC	X	3	4	10,10,11	0.98	1 (10%)	14,14,16	0.82	0
3	NAG	Y	1	2,3	14,14,15	0.43	0	17,19,21	0.46	0
3	NAG	Y	2	3	14,14,15	0.36	0	17,19,21	0.82	1 (5%)
3	NAG	Z	1	2,3	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	Z	2	3	14,14,15	0.21	0	17,19,21	0.52	0
5	NAG	a	1	1,5	14,14,15	0.30	0	17,19,21	0.56	0
5	FUC	a	2	5	10,10,11	0.84	0	14,14,16	0.87	0
3	NAG	b	1	2,3	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	b	2	3	14,14,15	0.30	0	17,19,21	0.56	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	NAG	U	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
4	NAG	V	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	FUC	V	3	4	-	-	0/1/1/1
4	NAG	W	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	FUC	W	3	4	-	-	0/1/1/1
4	NAG	X	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	X	2	4	-	3/6/23/26	0/1/1/1
4	FUC	X	3	4	-	-	0/1/1/1
3	NAG	Y	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Z	1	2,3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	a	2	5	-	-	0/1/1/1
3	NAG	b	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1	NAG	O5-C1	2.57	1.47	1.43
3	U	1	NAG	C1-C2	2.22	1.55	1.52
4	X	3	FUC	C1-C2	2.03	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1	NAG	C1-O5-C5	3.63	117.11	112.19
4	X	2	NAG	C2-N2-C7	2.78	126.86	122.90
3	Y	2	NAG	C2-N2-C7	2.48	126.43	122.90
4	X	1	NAG	C2-N2-C7	2.39	126.31	122.90
4	X	2	NAG	C1-O5-C5	2.32	115.33	112.19
3	U	1	NAG	O4-C4-C5	2.23	114.84	109.30

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Y	1	NAG	C1-C2-N2-C7
5	a	1	NAG	C4-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
3	b	1	NAG	C8-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
3	U	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C1-C2-N2-C7
3	U	1	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
4	X	1	NAG	C1-C2-N2-C7
3	U	2	NAG	C3-C2-N2-C7
3	Y	1	NAG	C3-C2-N2-C7
3	b	2	NAG	C3-C2-N2-C7
4	X	2	NAG	C3-C2-N2-C7
3	Z	1	NAG	C1-C2-N2-C7

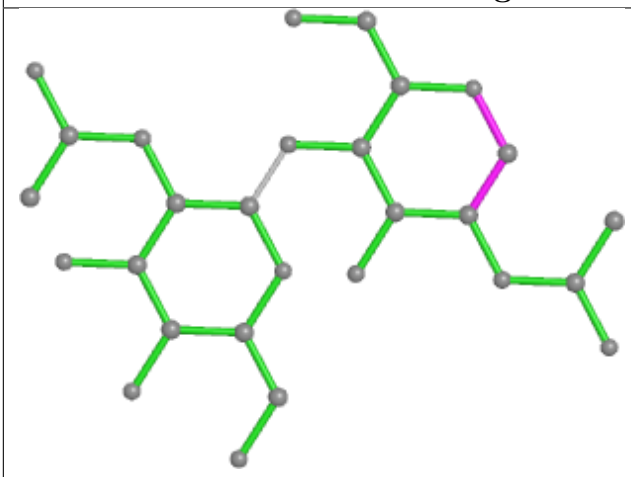
There are no ring outliers.

7 monomers are involved in 14 short contacts:

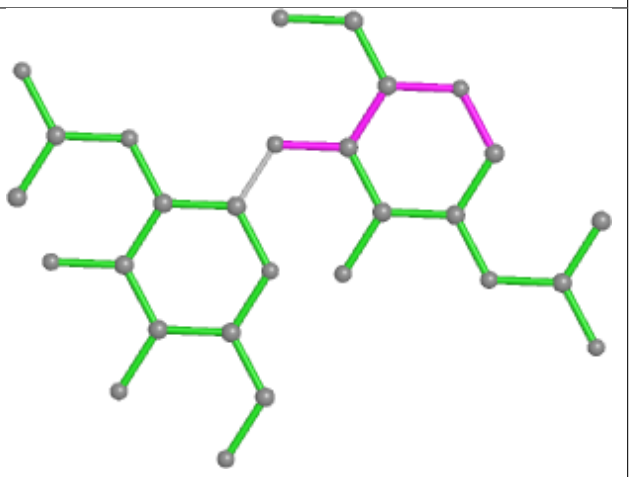
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	1	NAG	2	0
4	X	1	NAG	4	0
3	U	2	NAG	1	0
3	Y	1	NAG	1	0
3	Y	2	NAG	3	0
4	X	2	NAG	4	0
4	X	3	FUC	1	0

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

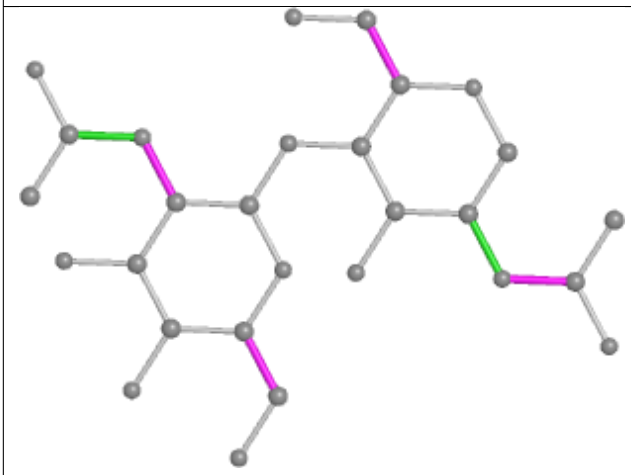
Oligosaccharide Chain U



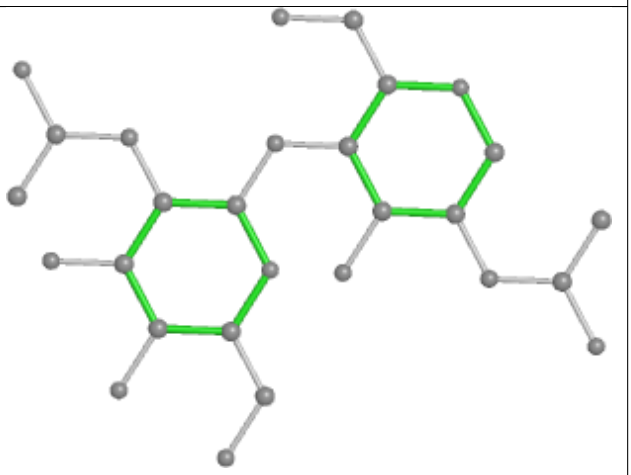
Bond lengths



Bond angles

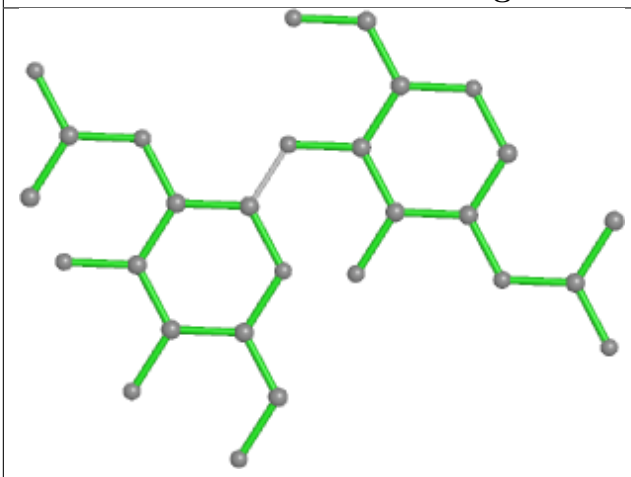


Torsions

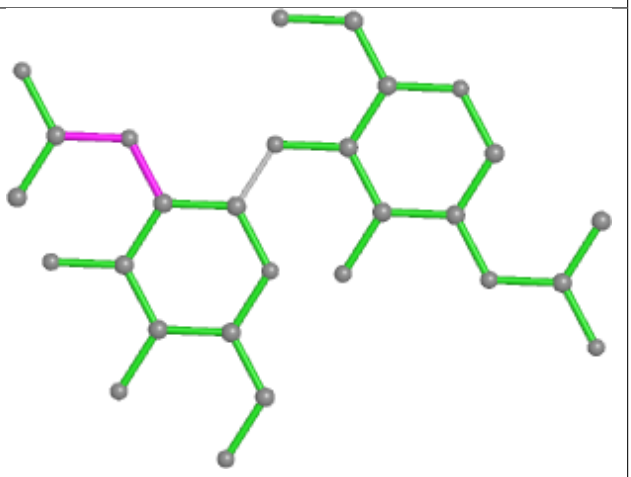


Rings

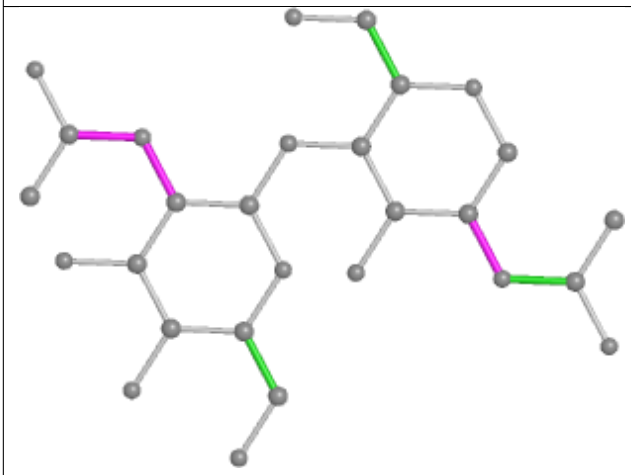
Oligosaccharide Chain Y



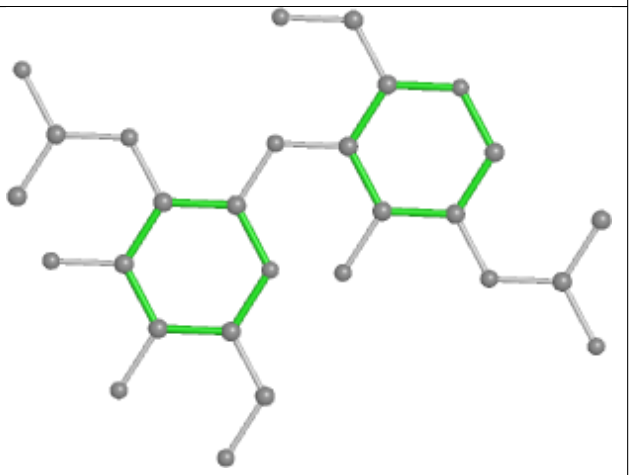
Bond lengths



Bond angles

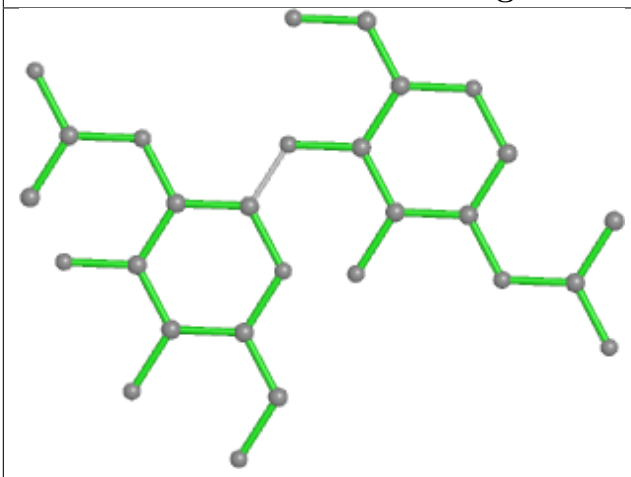


Torsions

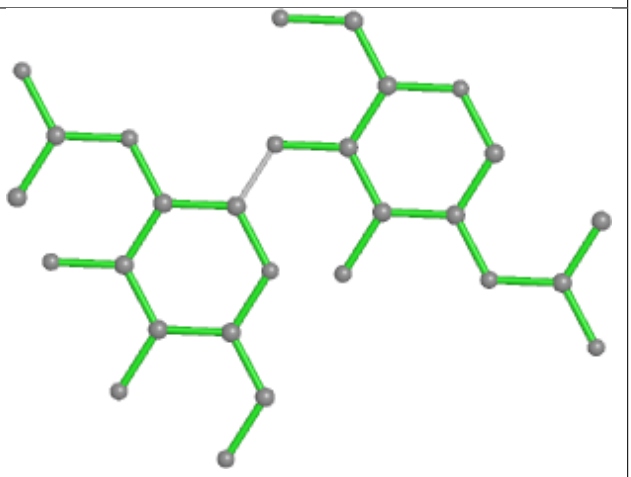


Rings

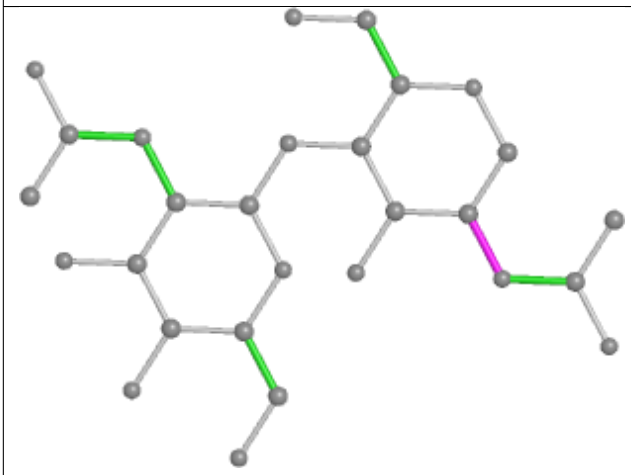
Oligosaccharide Chain Z



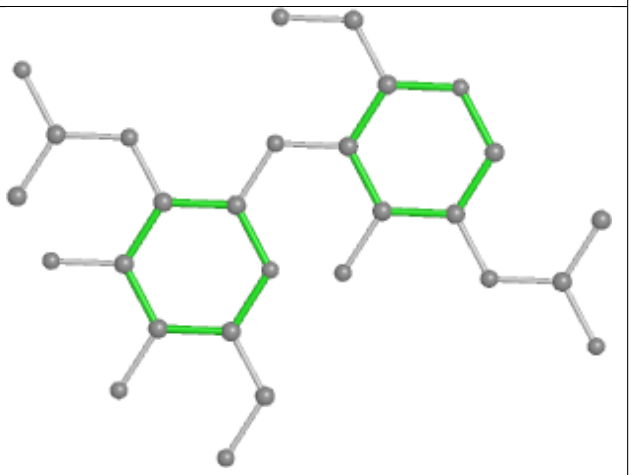
Bond lengths



Bond angles

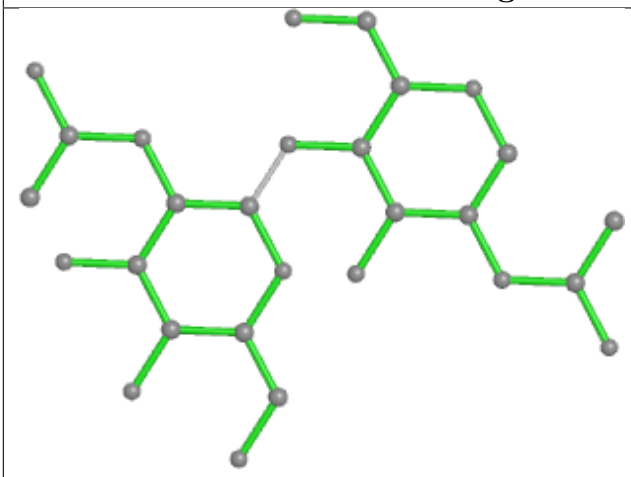


Torsions

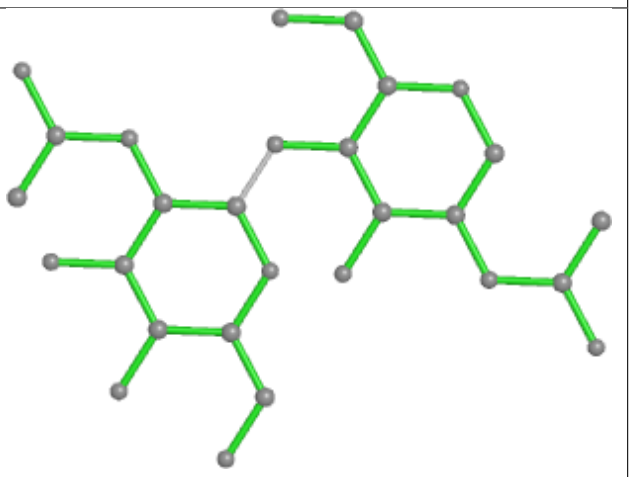


Rings

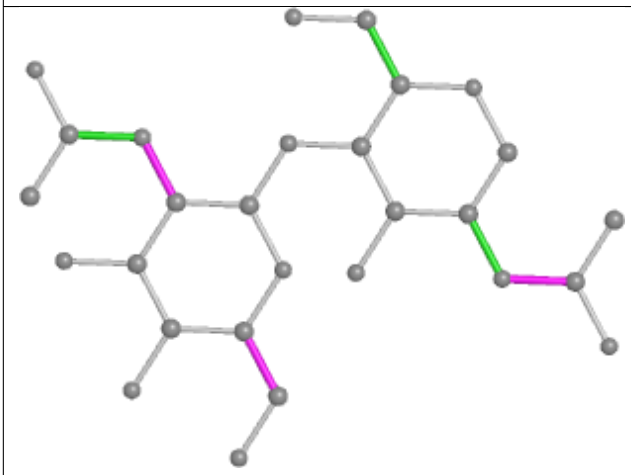
Oligosaccharide Chain b



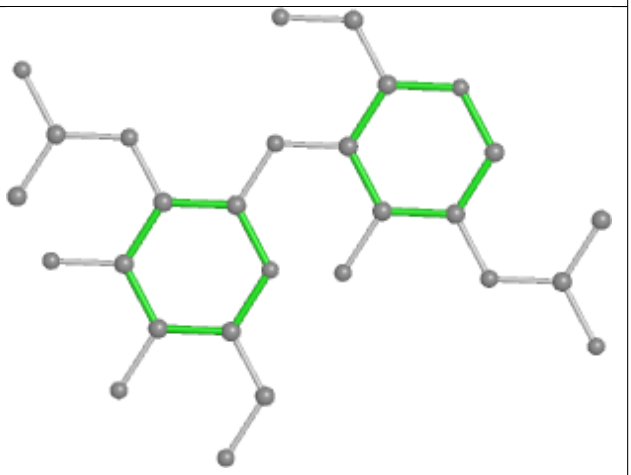
Bond lengths



Bond angles

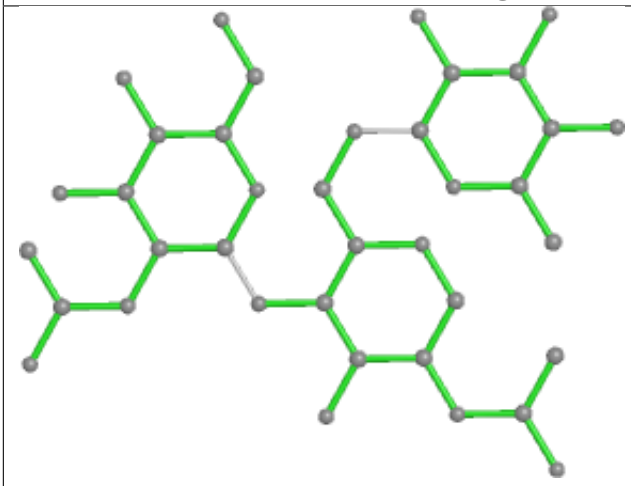


Torsions

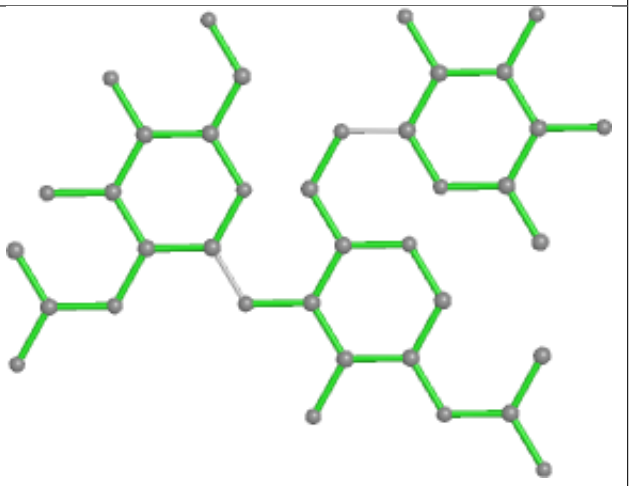


Rings

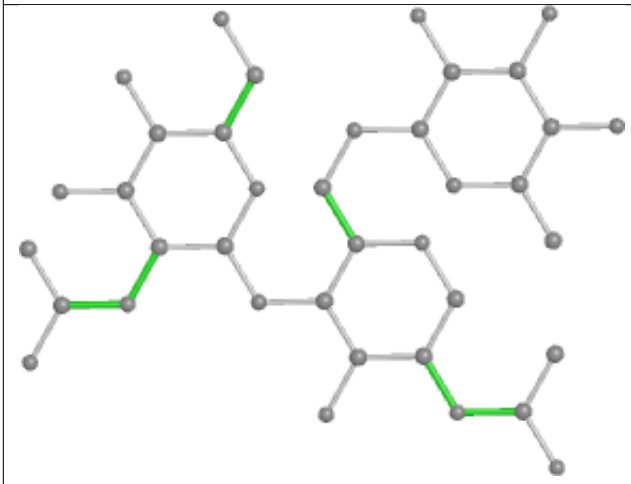
Oligosaccharide Chain V



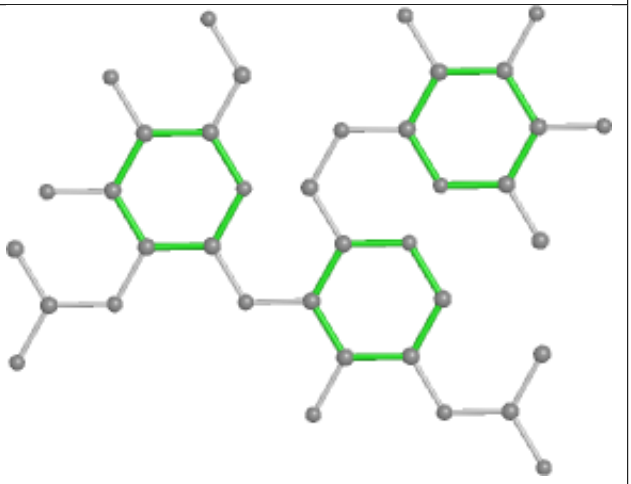
Bond lengths



Bond angles

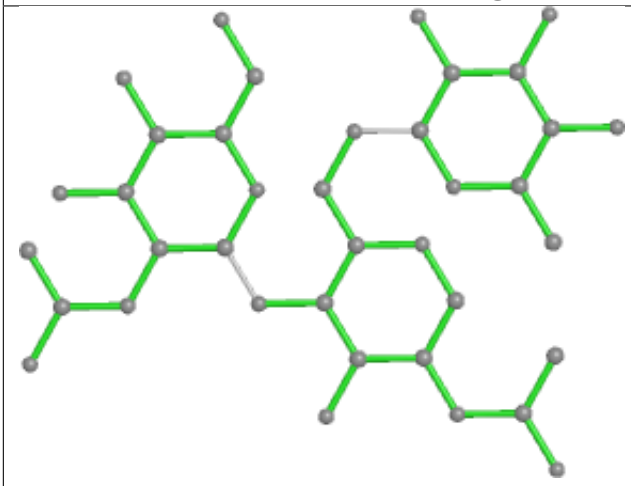


Torsions

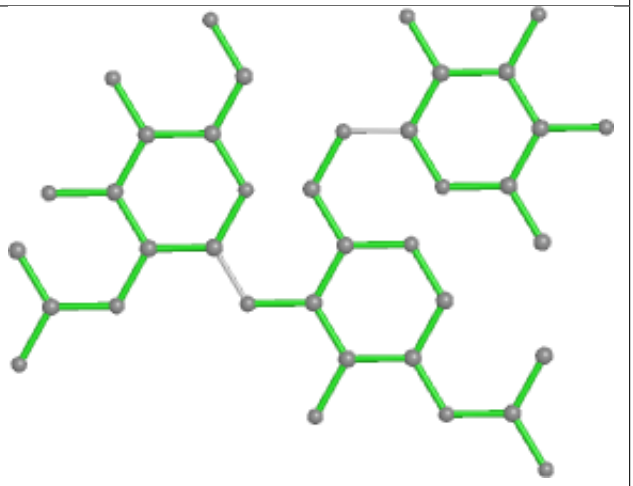


Rings

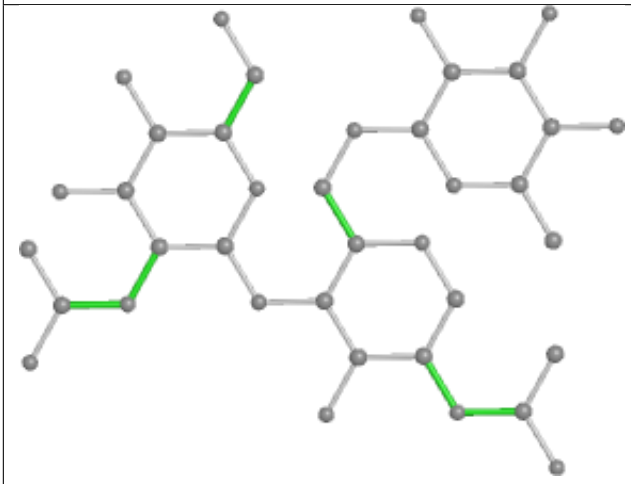
Oligosaccharide Chain W



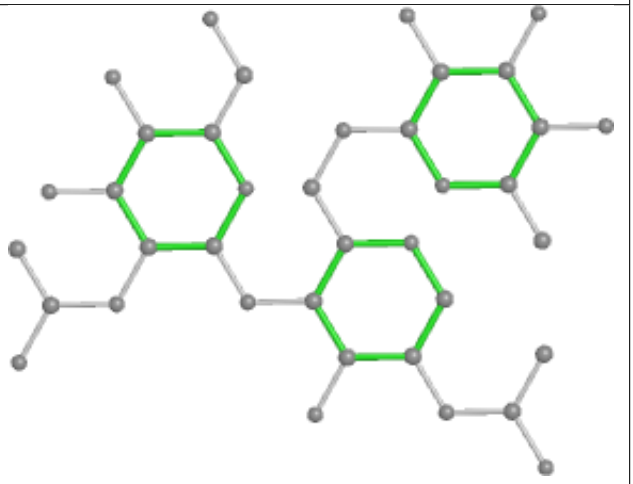
Bond lengths



Bond angles

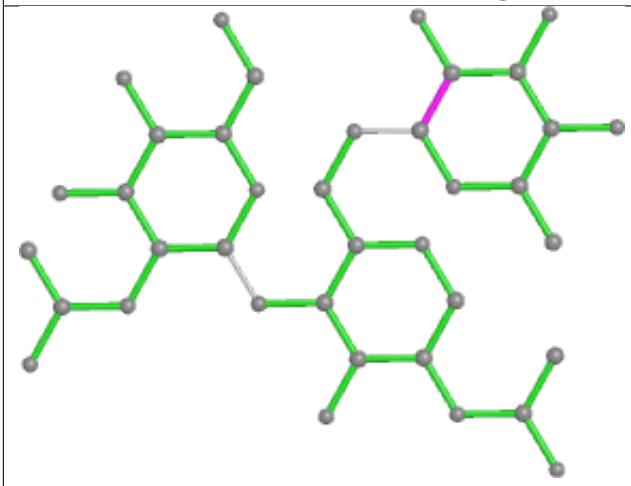


Torsions

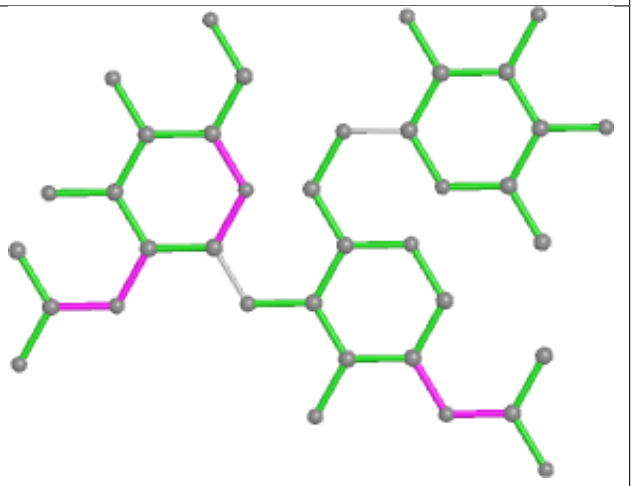


Rings

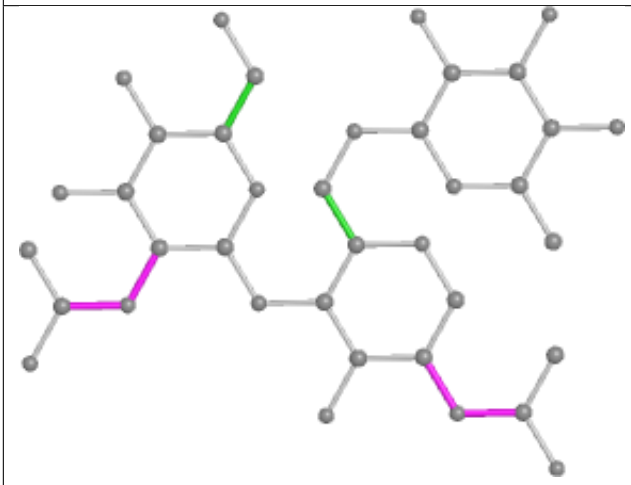
Oligosaccharide Chain X



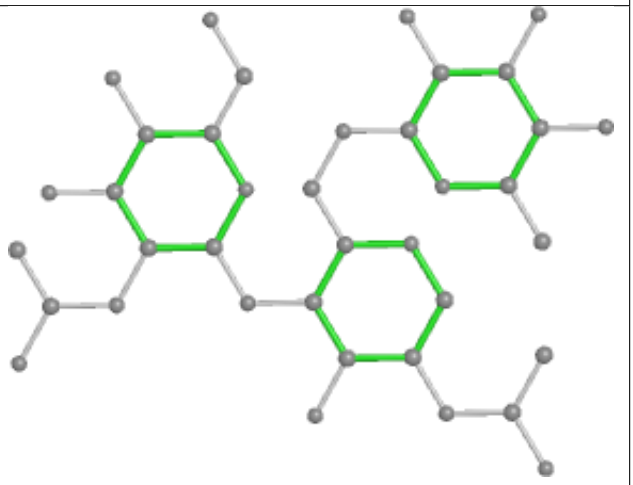
Bond lengths



Bond angles

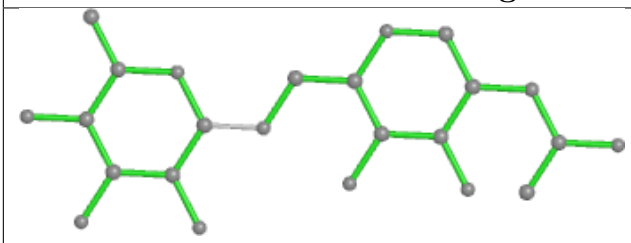


Torsions

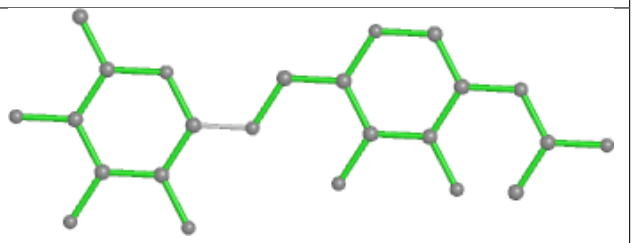


Rings

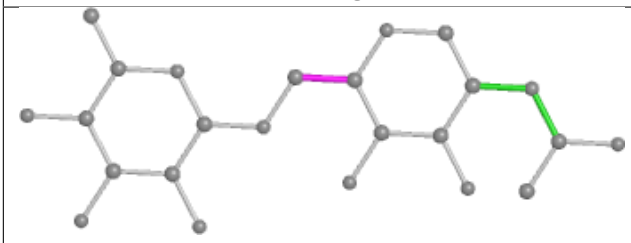
Oligosaccharide Chain a



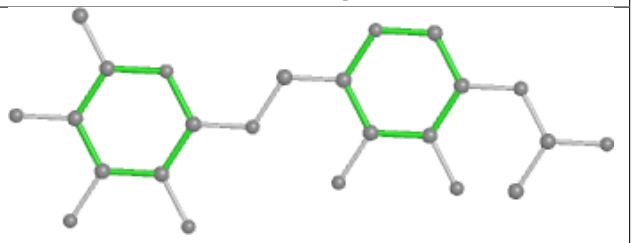
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
6	NAG	K	401	1	14,14,15	0.38	0	17,19,21	0.63	0
6	NAG	L	301	2	14,14,15	0.47	0	17,19,21	0.79	1 (5%)
6	NAG	E	401	1	14,14,15	0.36	0	17,19,21	0.51	0
6	NAG	M	401	1	14,14,15	0.31	0	17,19,21	0.52	0
6	NAG	R	301	2	14,14,15	0.34	0	17,19,21	0.55	0
6	NAG	S	401	1	14,14,15	0.61	0	17,19,21	0.79	2 (11%)
6	NAG	I	401	1	14,14,15	0.28	0	17,19,21	0.63	0
6	NAG	G	401	1	14,14,15	0.41	0	17,19,21	0.60	0
6	NAG	B	301	2	14,14,15	0.29	0	17,19,21	0.40	0
6	NAG	T	301	2	14,14,15	0.38	0	17,19,21	0.50	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
6	NAG	K	401	1	-	2/6/23/26	0/1/1/1
6	NAG	L	301	2	-	1/6/23/26	0/1/1/1
6	NAG	E	401	1	-	3/6/23/26	0/1/1/1
6	NAG	M	401	1	-	5/6/23/26	0/1/1/1
6	NAG	R	301	2	-	2/6/23/26	0/1/1/1
6	NAG	S	401	1	-	2/6/23/26	0/1/1/1
6	NAG	I	401	1	-	5/6/23/26	0/1/1/1
6	NAG	G	401	1	-	2/6/23/26	0/1/1/1
6	NAG	B	301	2	-	1/6/23/26	0/1/1/1
6	NAG	T	301	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	301	NAG	C1-O5-C5	2.92	116.15	112.19
6	S	401	NAG	C2-N2-C7	2.02	125.78	122.90
6	S	401	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	401	NAG	O5-C5-C6-O6
6	R	301	NAG	C1-C2-N2-C7
6	G	401	NAG	C8-C7-N2-C2
6	G	401	NAG	O7-C7-N2-C2
6	I	401	NAG	C8-C7-N2-C2
6	I	401	NAG	O7-C7-N2-C2
6	K	401	NAG	C8-C7-N2-C2
6	K	401	NAG	O7-C7-N2-C2
6	M	401	NAG	C8-C7-N2-C2
6	M	401	NAG	O7-C7-N2-C2
6	S	401	NAG	C8-C7-N2-C2
6	S	401	NAG	O7-C7-N2-C2
6	T	301	NAG	C8-C7-N2-C2
6	T	301	NAG	O7-C7-N2-C2
6	E	401	NAG	O5-C5-C6-O6
6	I	401	NAG	C4-C5-C6-O6
6	M	401	NAG	C4-C5-C6-O6
6	B	301	NAG	O5-C5-C6-O6
6	M	401	NAG	O5-C5-C6-O6
6	E	401	NAG	C3-C2-N2-C7
6	L	301	NAG	C3-C2-N2-C7
6	M	401	NAG	C3-C2-N2-C7
6	R	301	NAG	C3-C2-N2-C7
6	E	401	NAG	C4-C5-C6-O6
6	I	401	NAG	C1-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	401	NAG	1	0
6	L	301	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	401	NAG	1	0
6	M	401	NAG	6	0
6	R	301	NAG	1	0
6	S	401	NAG	4	0
6	I	401	NAG	4	0
6	G	401	NAG	1	0
6	T	301	NAG	2	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	207/260 (79%)	0.96	20 (9%) 7 6	58, 68, 100, 118	0
1	C	204/260 (78%)	0.83	16 (7%) 13 10	60, 72, 103, 120	0
1	E	205/260 (78%)	1.00	19 (9%) 8 7	65, 75, 112, 141	0
1	G	204/260 (78%)	0.86	17 (8%) 11 9	60, 74, 99, 111	0
1	I	201/260 (77%)	0.80	9 (4%) 33 30	61, 76, 104, 135	0
1	K	202/260 (77%)	0.84	20 (9%) 7 5	69, 83, 115, 136	0
1	M	204/260 (78%)	0.81	17 (8%) 11 9	68, 79, 101, 118	0
1	O	205/260 (78%)	0.71	13 (6%) 20 17	64, 79, 109, 128	0
1	Q	203/260 (78%)	0.86	19 (9%) 8 6	69, 84, 122, 134	0
1	S	203/260 (78%)	0.82	18 (8%) 9 8	61, 78, 110, 137	0
2	B	97/99 (97%)	0.75	12 (12%) 4 2	64, 85, 114, 118	0
2	D	98/99 (98%)	0.80	11 (11%) 5 3	64, 76, 105, 113	0
2	F	98/99 (98%)	0.81	7 (7%) 16 12	69, 78, 94, 106	0
2	H	96/99 (96%)	0.74	5 (5%) 27 24	65, 82, 104, 118	0
2	J	98/99 (98%)	0.58	4 (4%) 37 33	72, 80, 106, 126	0
2	L	96/99 (96%)	0.78	8 (8%) 11 9	79, 102, 126, 137	0
2	N	95/99 (95%)	0.56	7 (7%) 14 12	73, 85, 103, 111	0
2	P	95/99 (95%)	0.61	7 (7%) 14 12	69, 81, 99, 108	0
2	R	95/99 (95%)	0.75	12 (12%) 3 2	75, 104, 123, 135	0
2	T	95/99 (95%)	0.67	10 (10%) 6 4	75, 94, 114, 123	0
All	All	3001/3590 (83%)	0.80	251 (8%) 11 8	58, 80, 112, 141	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	GLU	5.8
1	E	321	SER	5.5
1	S	257	TYR	5.4
1	Q	290	LEU	4.7
1	M	218	LEU	4.7
1	Q	352	THR	4.4
1	E	242	GLU	4.3
1	S	262	ARG	4.2
1	A	218	LEU	4.1
2	N	235	VAL	4.0
1	I	257	TYR	4.0
2	L	193	LEU	3.9
2	B	219	LEU	3.8
2	D	220	GLU	3.8
2	N	183	ILE	3.7
1	M	257	TYR	3.7
1	G	203	VAL	3.6
2	D	219	LEU	3.6
1	E	185	GLU	3.6
2	P	219	LEU	3.5
1	K	352	THR	3.5
1	A	290	LEU	3.4
1	K	247	LEU	3.4
1	Q	324	SER	3.4
2	T	193	LEU	3.4
1	G	341	LEU	3.4
1	K	296	ILE	3.4
2	B	159	ARG	3.4
1	A	246	CYS	3.3
1	Q	305	LEU	3.3
2	H	235	VAL	3.3
1	E	341	LEU	3.2
2	L	151	VAL	3.2
1	O	300	MET	3.2
1	G	209	TYR	3.2
1	O	258	ILE	3.2
2	R	184	LEU	3.2
1	I	221	GLN	3.2
2	R	187	LEU	3.2
1	A	297	GLY	3.2
1	S	220	ASP	3.1
2	R	174	HIS	3.1
1	E	247	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	341	LEU	3.0
2	P	233	ALA	3.0
1	O	251	VAL	3.0
2	T	176	ALA	3.0
2	F	219	LEU	3.0
2	B	193	LEU	3.0
2	P	172	PRO	3.0
1	E	320	SER	2.9
2	F	164	LEU	2.9
2	T	151	VAL	2.9
1	C	251	VAL	2.9
1	E	348	PHE	2.9
2	R	219	LEU	2.9
1	O	257	TYR	2.9
1	M	219	GLY	2.9
1	G	263	LEU	2.9
2	H	229	ALA	2.9
1	Q	232	ILE	2.9
1	M	220	ASP	2.9
1	Q	174	ILE	2.8
2	L	183	ILE	2.8
2	J	224	LEU	2.8
1	K	185	GLU	2.8
1	K	263	LEU	2.8
2	L	154	LEU	2.8
2	R	151	VAL	2.8
1	Q	257	TYR	2.8
1	A	247	LEU	2.8
1	Q	345	ILE	2.8
1	S	351	GLY	2.8
2	P	173	CYS	2.8
1	I	312	VAL	2.7
2	R	164	LEU	2.7
1	C	203	VAL	2.7
2	L	143	LEU	2.7
1	Q	263	LEU	2.7
1	I	310	ILE	2.7
1	O	310	ILE	2.7
1	Q	169	TYR	2.7
1	K	200	PHE	2.6
1	K	348	PHE	2.6
1	E	220	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	T	183	ILE	2.6
2	D	140	ARG	2.6
1	S	258	ILE	2.6
1	M	202	LYS	2.6
1	Q	306	ARG	2.6
1	S	335	PHE	2.6
1	K	199	PHE	2.6
2	D	195	LYS	2.6
1	A	352	THR	2.6
1	E	184	ALA	2.6
2	N	219	LEU	2.6
1	M	266	PHE	2.6
2	N	233	ALA	2.6
1	G	185	GLU	2.6
1	C	241	LYS	2.5
1	K	257	TYR	2.5
1	S	247	LEU	2.5
1	S	190	ARG	2.5
1	C	186	VAL	2.5
2	D	215	LEU	2.5
2	R	224	LEU	2.5
1	K	220	ASP	2.5
2	B	189	HIS	2.5
2	L	187	LEU	2.5
1	A	345	ILE	2.5
1	I	290	LEU	2.5
1	O	212	LEU	2.5
2	J	215	LEU	2.5
1	E	311	SER	2.5
1	S	260	ARG	2.5
1	C	258	ILE	2.5
1	E	323	ASN	2.5
1	C	244	PRO	2.5
1	O	308	PRO	2.5
1	C	249	LEU	2.5
2	N	206	ILE	2.5
1	K	206	LYS	2.5
1	A	232	ILE	2.4
2	B	183	ILE	2.4
2	F	154	LEU	2.4
1	Q	348	PHE	2.4
2	R	192	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	312	VAL	2.4
2	R	235	VAL	2.4
1	K	262	ARG	2.4
2	R	159	ARG	2.4
1	S	200	PHE	2.4
2	B	192	LYS	2.4
1	G	331	PHE	2.4
2	J	219	LEU	2.4
1	K	310	ILE	2.4
1	O	186	VAL	2.4
2	D	201	THR	2.4
2	B	161	LYS	2.4
2	B	202	CYS	2.4
1	E	150	GLU	2.4
1	M	335	PHE	2.4
1	O	185	GLU	2.4
1	A	154	LEU	2.3
1	M	296	ILE	2.3
1	M	331	PHE	2.3
1	M	340	CYS	2.3
1	S	266	PHE	2.3
1	M	232	ILE	2.3
1	A	181	VAL	2.3
1	S	348	PHE	2.3
2	P	235	VAL	2.3
1	C	246	CYS	2.3
2	L	174	HIS	2.3
1	C	153	CYS	2.3
1	A	263	LEU	2.3
1	S	217	PRO	2.3
1	E	345	ILE	2.3
2	J	198	PRO	2.3
2	T	195	LYS	2.3
2	T	198	PRO	2.3
1	M	341	LEU	2.3
1	Q	341	LEU	2.3
1	Q	213	TYR	2.3
1	S	310	ILE	2.3
1	K	229	ARG	2.3
2	F	151	VAL	2.3
1	C	196	LEU	2.3
1	I	263	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	310	ILE	2.3
1	S	345	ILE	2.3
1	A	320	SER	2.2
2	L	201	THR	2.2
2	P	183	ILE	2.2
1	E	302	PRO	2.2
2	F	160	THR	2.2
1	G	295	LEU	2.2
2	F	220	GLU	2.2
2	P	214	PHE	2.2
1	M	312	VAL	2.2
1	S	164	ASP	2.2
1	A	266	PHE	2.2
1	A	335	PHE	2.2
1	A	258	ILE	2.2
1	G	232	ILE	2.2
1	K	232	ILE	2.2
1	Q	186	VAL	2.2
2	D	183	ILE	2.2
1	K	313	SER	2.2
2	H	187	LEU	2.2
1	C	158	LYS	2.2
1	Q	226	GLU	2.2
1	C	199	PHE	2.2
1	K	331	PHE	2.2
1	Q	251	VAL	2.2
1	M	345	ILE	2.1
1	Q	258	ILE	2.1
1	I	331	PHE	2.1
2	H	214	PHE	2.1
1	E	198	GLN	2.1
1	I	311	SER	2.1
1	G	186	VAL	2.1
1	G	196	LEU	2.1
1	A	314	PRO	2.1
1	M	250	GLN	2.1
1	G	262	ARG	2.1
1	K	169	TYR	2.1
1	S	232	ILE	2.1
1	S	341	LEU	2.1
2	D	159	ARG	2.1
2	R	161	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	T	177	GLU	2.1
1	M	339	ALA	2.1
1	C	300	MET	2.1
2	B	178	THR	2.1
1	A	331	PHE	2.1
1	O	233	VAL	2.1
2	T	164	LEU	2.1
1	E	165	THR	2.1
1	G	266	PHE	2.1
1	G	267	PHE	2.1
2	T	200	ARG	2.1
1	O	203	VAL	2.1
2	H	212	ILE	2.1
1	C	218	LEU	2.1
1	E	221	GLN	2.1
1	I	217	PRO	2.1
1	G	257	TYR	2.1
2	B	229	ALA	2.1
2	B	166	PHE	2.1
2	T	154	LEU	2.0
2	N	151	VAL	2.0
1	E	254	LYS	2.0
1	M	334	PHE	2.0
2	B	149	LEU	2.0
2	F	143	LEU	2.0
1	G	174	ILE	2.0
2	D	172	PRO	2.0
1	Q	229	ARG	2.0
2	D	160	THR	2.0
1	A	250	GLN	2.0
2	R	214	PHE	2.0
2	D	187	LEU	2.0
1	E	205	PRO	2.0
1	O	260	ARG	2.0
1	K	174	ILE	2.0
1	O	209	TYR	2.0
1	C	324	SER	2.0
2	N	193	LEU	2.0
1	A	302	PRO	2.0
1	C	233	VAL	2.0

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

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

6.3 Carbohydrates (i)

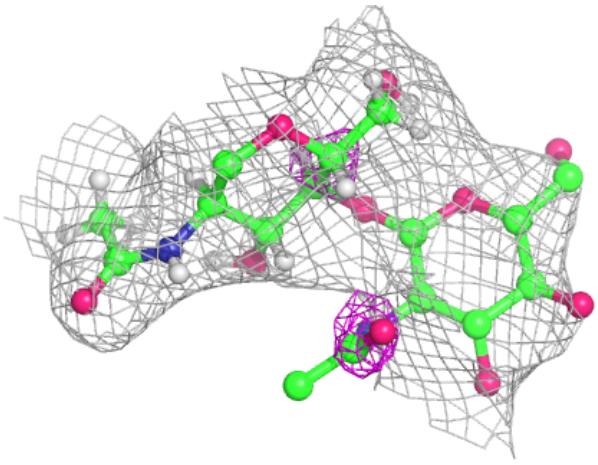
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

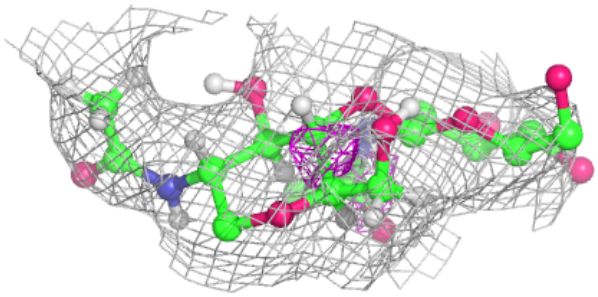
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FUC	a	2	10/11	0.68	0.28	100,105,126,127	0
3	NAG	U	2	14/15	0.73	0.34	93,95,97,97	0
3	NAG	b	1	14/15	0.74	0.21	80,84,101,101	0
3	NAG	b	2	14/15	0.74	0.17	83,86,103,105	0
3	NAG	U	1	14/15	0.74	0.26	86,100,121,121	0
5	NAG	a	1	14/15	0.76	0.20	92,105,121,126	0
4	NAG	W	2	14/15	0.79	0.15	82,87,103,105	0
4	FUC	X	3	10/11	0.82	0.24	80,83,100,100	0
4	FUC	W	3	10/11	0.83	0.33	83,87,104,105	0
4	FUC	V	3	10/11	0.83	0.23	80,86,104,104	0
3	NAG	Z	1	14/15	0.84	0.19	81,85,102,102	0
3	NAG	Z	2	14/15	0.84	0.13	83,86,102,104	0
4	NAG	X	1	14/15	0.85	0.24	76,80,97,97	0
4	NAG	W	1	14/15	0.85	0.21	82,87,103,104	0
3	NAG	Y	2	14/15	0.86	0.12	89,91,110,110	0
4	NAG	X	2	14/15	0.88	0.19	80,82,97,99	0
4	NAG	V	2	14/15	0.90	0.17	76,85,102,107	0
3	NAG	Y	1	14/15	0.91	0.14	84,89,106,106	0
4	NAG	V	1	14/15	0.93	0.18	69,78,93,93	0

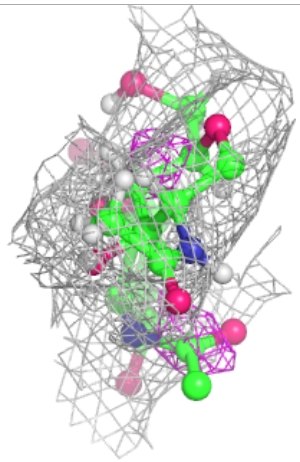
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

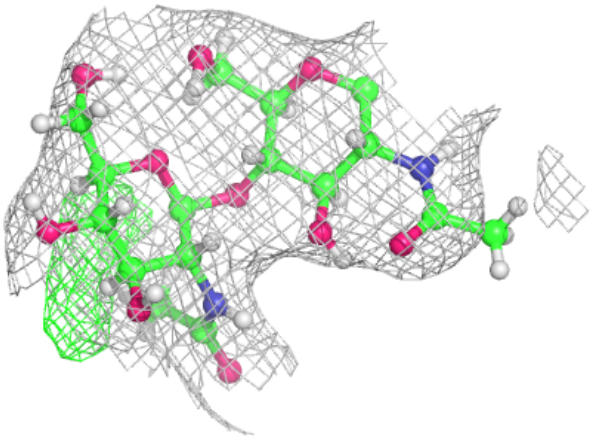


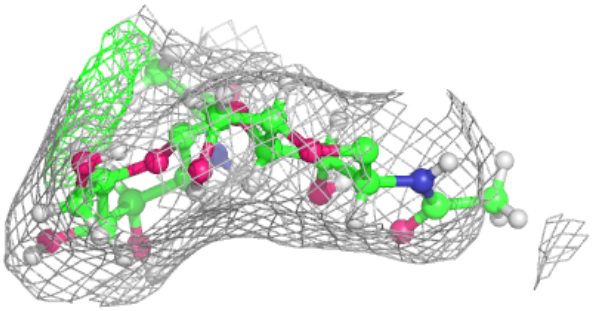


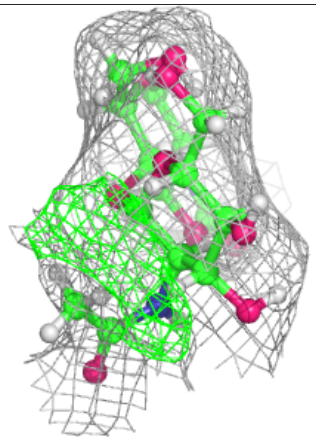


Electron density around Chain Y:

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

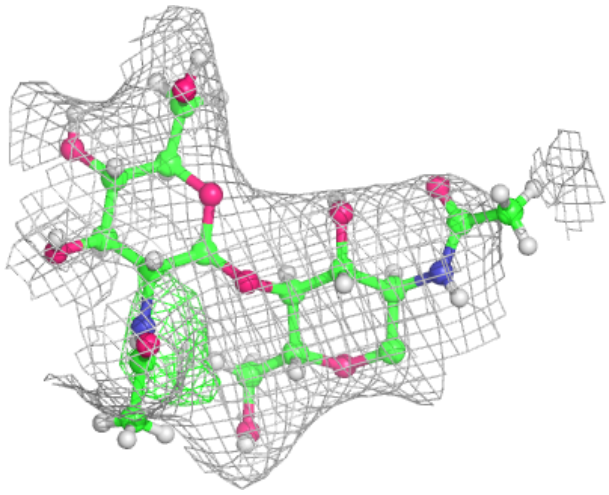


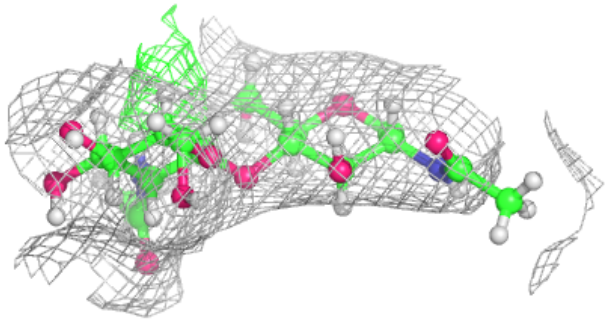


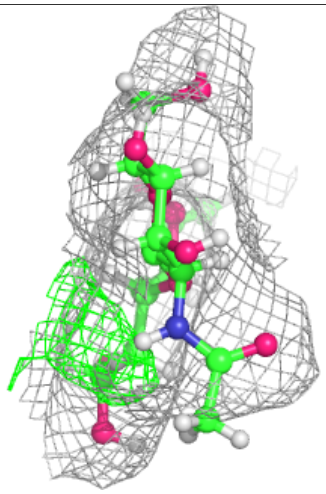


Electron density around Chain Z:

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

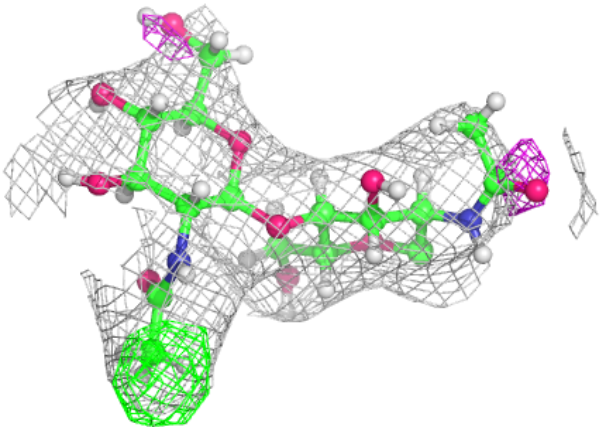


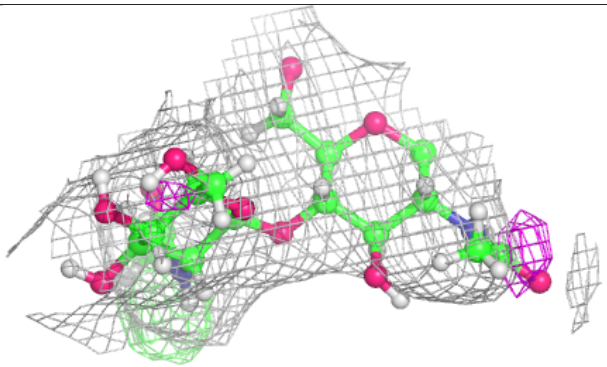


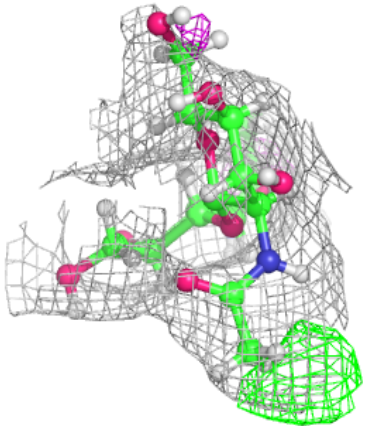


Electron density around Chain b:

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

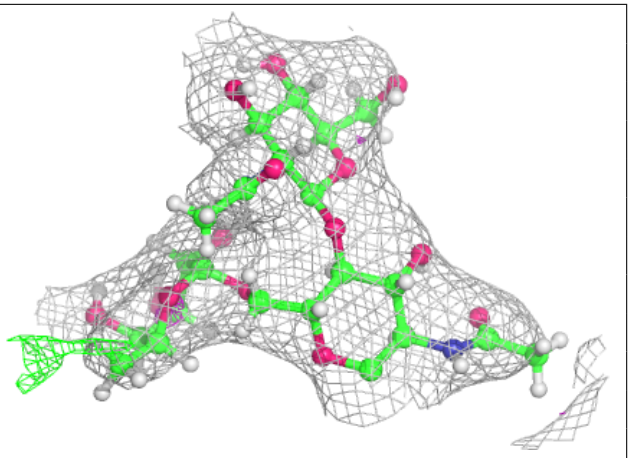


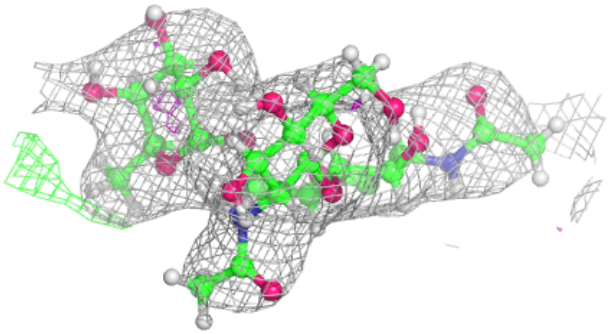


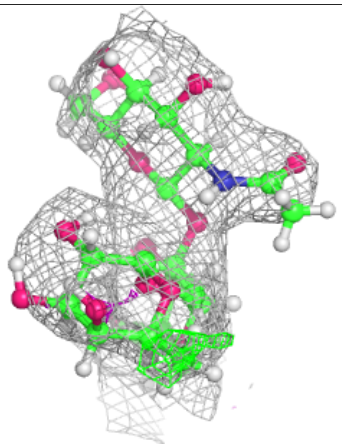


Electron density around Chain V:

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

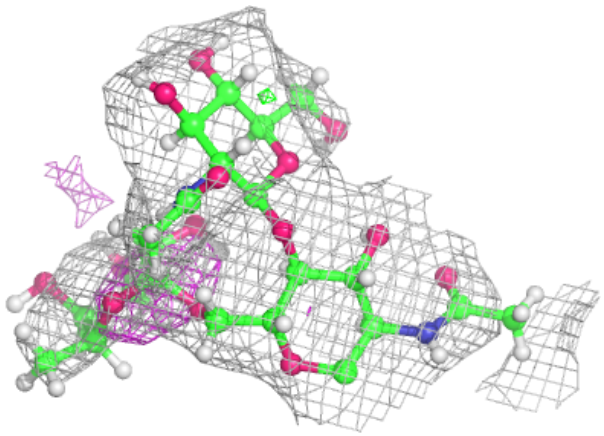


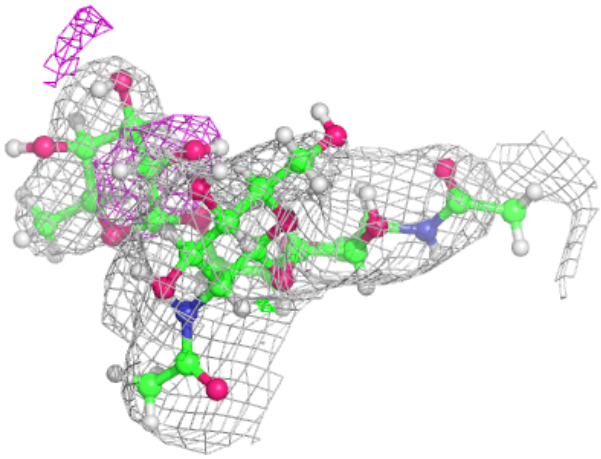


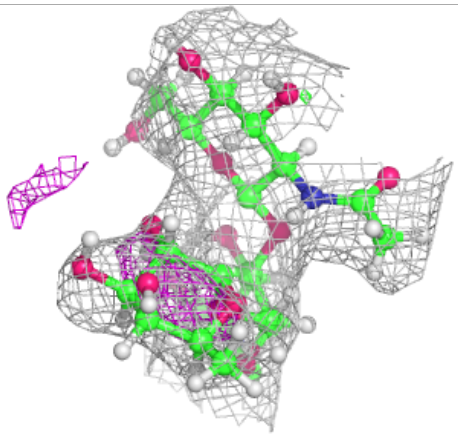


Electron density around Chain W:

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

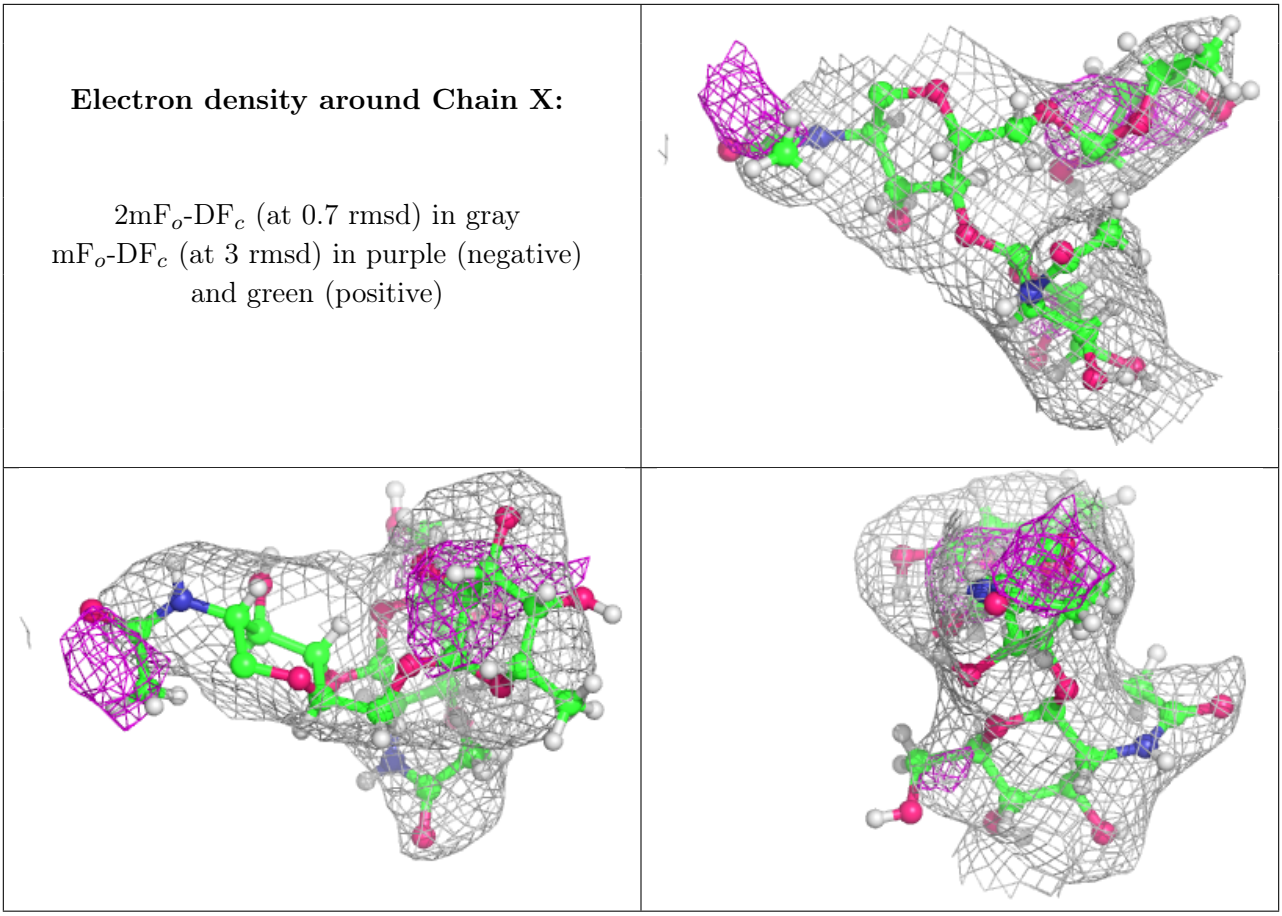






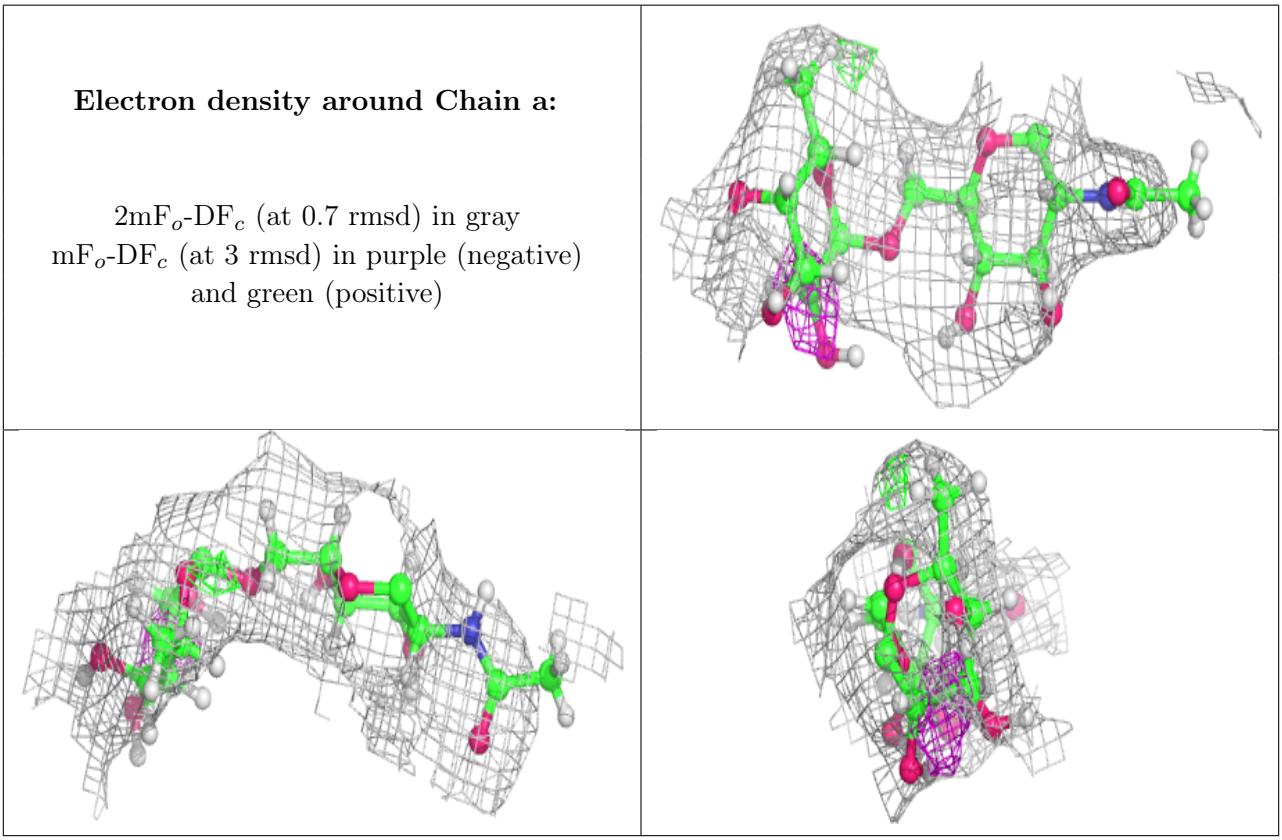
Electron density around Chain X:

$2mF_o$-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 a:

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



6.4 Ligands (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
6	NAG	I	401	14/15	0.47	0.19	105,112,117,117	0
6	NAG	K	401	14/15	0.47	0.25	96,103,123,125	0
6	NAG	S	401	14/15	0.55	0.21	95,104,123,125	0
6	NAG	M	401	14/15	0.70	0.22	95,99,105,105	0
6	NAG	G	401	14/15	0.70	0.17	84,93,117,117	0
6	NAG	E	401	14/15	0.75	0.19	95,101,103,105	0
6	NAG	B	301	14/15	0.76	0.20	82,86,102,103	0
6	NAG	T	301	14/15	0.77	0.22	92,96,97,98	0
6	NAG	L	301	14/15	0.78	0.17	96,99,119,120	0
6	NAG	R	301	14/15	0.81	0.18	98,106,128,128	0

6.5 Other polymers (i)

There are no such residues in this entry.