Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 08:12 am GMT

PDB ID	:	5NJD
Title	:	Structure of Interleukin 23 in complex with Briakinumab FAb
Authors	:	Bloch, Y.; Savvides, S.N.
Deposited on	:	2017-03-28
Resolution	:	3.90 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 (1)) were used in the production of this report:

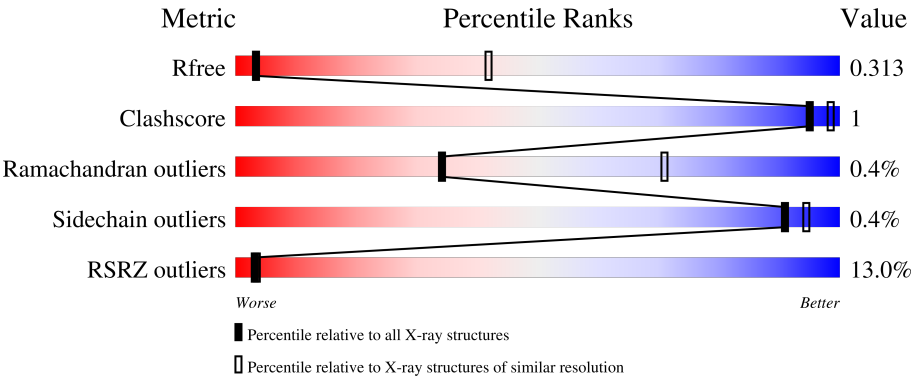
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	328	8% 88% · 9%
1	C	328	8% 86% · 10%
1	E	328	12% 87% · 10%
1	G	328	12% 88% · 11%
1	I	328	12% 85% · 11%

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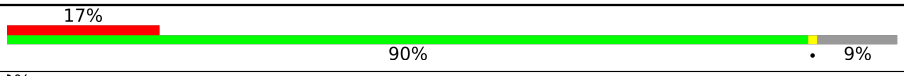
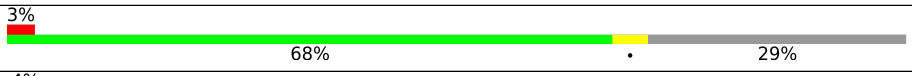
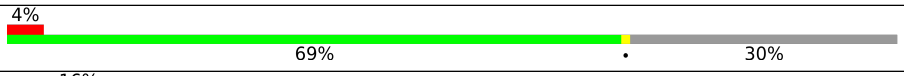
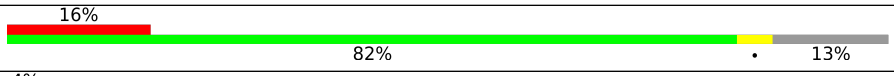
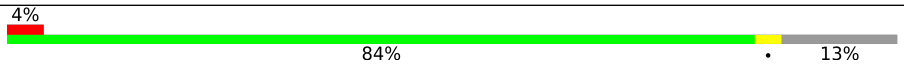
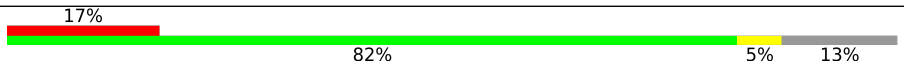
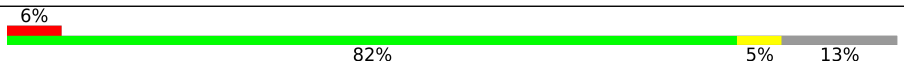
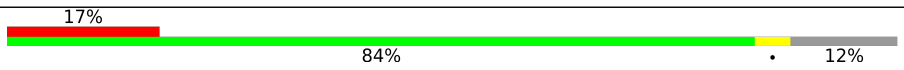
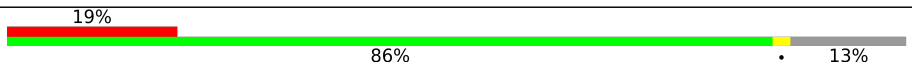
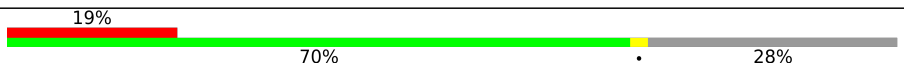
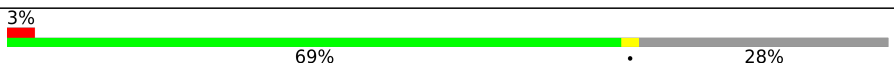
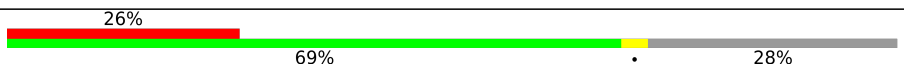
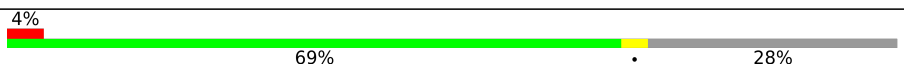
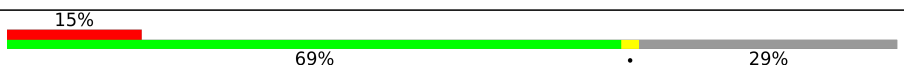
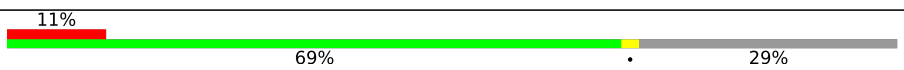
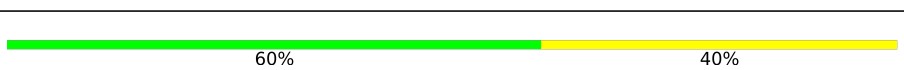
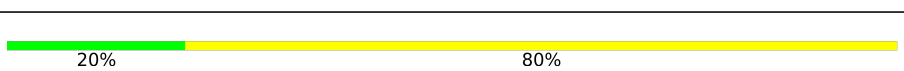
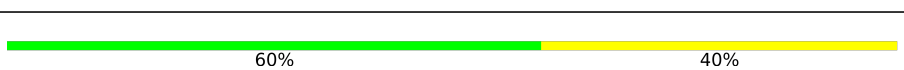
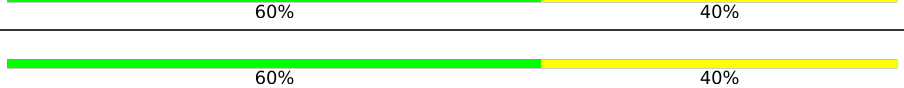
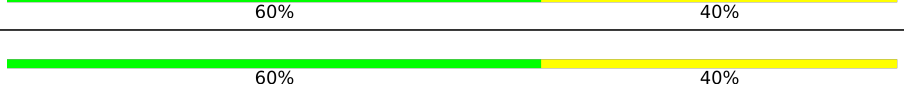
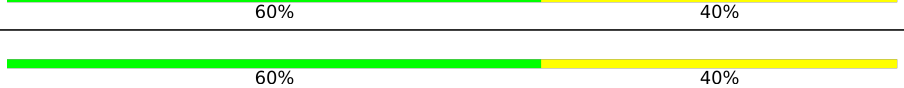
Mol	Chain	Length	Quality of chain
1	K	328	
2	B	198	
2	D	198	
2	F	198	
2	H	198	
2	J	198	
2	L	198	
3	M	245	
3	O	245	
3	Q	245	
3	S	245	
3	U	245	
3	W	245	
4	N	289	
4	P	289	
4	R	289	
4	T	289	
4	V	289	
4	X	289	
5	Y	5	
5	Z	5	
5	a	5	
5	b	5	
5	c	5	
5	d	5	

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
5	MAN	a	5	-	-	-	X
6	SO4	O	302	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39445 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 Interleukin-12 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2313	1467	373	461	12			
1	C	294	Total	C	N	O	S	0	0	0
			2304	1461	372	459	12			
1	E	294	Total	C	N	O	S	0	0	0
			2309	1465	373	459	12			
1	G	293	Total	C	N	O	S	0	0	0
			2301	1461	372	456	12			
1	I	292	Total	C	N	O	S	0	0	0
			2288	1453	367	456	12			
1	K	297	Total	C	N	O	S	0	0	0
			2326	1475	377	462	12			

- Molecule 2 is a protein called Interleukin-23 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1056	681	185	185	5			
2	D	146	Total	C	N	O	S	0	0	0
			1080	694	190	191	5			
2	F	146	Total	C	N	O	S	0	0	0
			1058	681	187	185	5			
2	H	139	Total	C	N	O	S	0	0	0
			1036	669	183	179	5			
2	J	141	Total	C	N	O	S	0	0	0
			1031	666	180	180	5			
2	L	139	Total	C	N	O	S	0	0	0
			1029	665	181	178	5			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	GLY	-	expression tag	UNP Q9NPF7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	191	THR	-	expression tag	UNP Q9NPF7
B	192	LYS	-	expression tag	UNP Q9NPF7
B	193	HIS	-	expression tag	UNP Q9NPF7
B	194	HIS	-	expression tag	UNP Q9NPF7
B	195	HIS	-	expression tag	UNP Q9NPF7
B	196	HIS	-	expression tag	UNP Q9NPF7
B	197	HIS	-	expression tag	UNP Q9NPF7
B	198	HIS	-	expression tag	UNP Q9NPF7
D	190	GLY	-	expression tag	UNP Q9NPF7
D	191	THR	-	expression tag	UNP Q9NPF7
D	192	LYS	-	expression tag	UNP Q9NPF7
D	193	HIS	-	expression tag	UNP Q9NPF7
D	194	HIS	-	expression tag	UNP Q9NPF7
D	195	HIS	-	expression tag	UNP Q9NPF7
D	196	HIS	-	expression tag	UNP Q9NPF7
D	197	HIS	-	expression tag	UNP Q9NPF7
D	198	HIS	-	expression tag	UNP Q9NPF7
F	190	GLY	-	expression tag	UNP Q9NPF7
F	191	THR	-	expression tag	UNP Q9NPF7
F	192	LYS	-	expression tag	UNP Q9NPF7
F	193	HIS	-	expression tag	UNP Q9NPF7
F	194	HIS	-	expression tag	UNP Q9NPF7
F	195	HIS	-	expression tag	UNP Q9NPF7
F	196	HIS	-	expression tag	UNP Q9NPF7
F	197	HIS	-	expression tag	UNP Q9NPF7
F	198	HIS	-	expression tag	UNP Q9NPF7
H	190	GLY	-	expression tag	UNP Q9NPF7
H	191	THR	-	expression tag	UNP Q9NPF7
H	192	LYS	-	expression tag	UNP Q9NPF7
H	193	HIS	-	expression tag	UNP Q9NPF7
H	194	HIS	-	expression tag	UNP Q9NPF7
H	195	HIS	-	expression tag	UNP Q9NPF7
H	196	HIS	-	expression tag	UNP Q9NPF7
H	197	HIS	-	expression tag	UNP Q9NPF7
H	198	HIS	-	expression tag	UNP Q9NPF7
J	190	GLY	-	expression tag	UNP Q9NPF7
J	191	THR	-	expression tag	UNP Q9NPF7
J	192	LYS	-	expression tag	UNP Q9NPF7
J	193	HIS	-	expression tag	UNP Q9NPF7
J	194	HIS	-	expression tag	UNP Q9NPF7
J	195	HIS	-	expression tag	UNP Q9NPF7
J	196	HIS	-	expression tag	UNP Q9NPF7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	197	HIS	-	expression tag	UNP Q9NPF7
J	198	HIS	-	expression tag	UNP Q9NPF7
L	190	GLY	-	expression tag	UNP Q9NPF7
L	191	THR	-	expression tag	UNP Q9NPF7
L	192	LYS	-	expression tag	UNP Q9NPF7
L	193	HIS	-	expression tag	UNP Q9NPF7
L	194	HIS	-	expression tag	UNP Q9NPF7
L	195	HIS	-	expression tag	UNP Q9NPF7
L	196	HIS	-	expression tag	UNP Q9NPF7
L	197	HIS	-	expression tag	UNP Q9NPF7
L	198	HIS	-	expression tag	UNP Q9NPF7

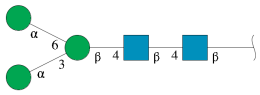
- Molecule 3 is a protein called Briakinumab FAb Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	213	Total	C	N	O	S	0	0	0
			1592	997	268	323	4			
3	O	213	Total	C	N	O	S	0	0	0
			1596	1000	270	322	4			
3	Q	213	Total	C	N	O	S	0	0	0
			1589	997	270	318	4			
3	S	214	Total	C	N	O	S	0	0	0
			1590	995	268	323	4			
3	U	215	Total	C	N	O	S	0	0	0
			1601	1004	269	324	4			
3	W	214	Total	C	N	O	S	0	0	0
			1590	995	270	321	4			

- Molecule 4 is a protein called Briakinumab FAb Heavy chain.

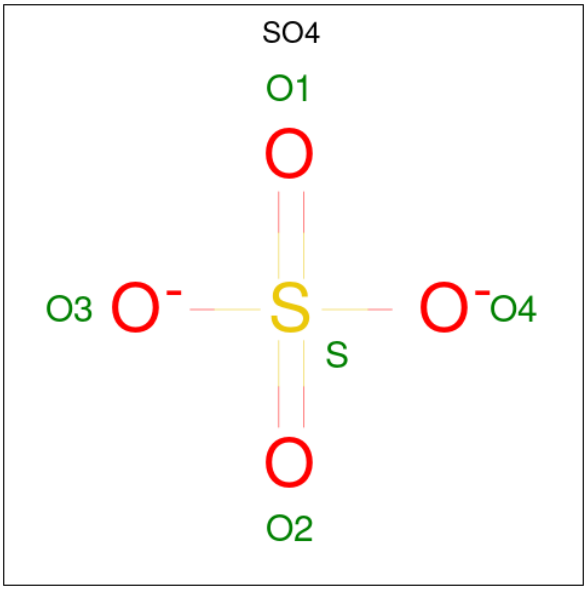
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	207	Total	C	N	O	S	0	0	0
			1561	984	269	301	7			
4	P	207	Total	C	N	O	S	0	0	0
			1558	981	268	302	7			
4	R	208	Total	C	N	O	S	0	0	0
			1556	980	268	301	7			
4	T	208	Total	C	N	O	S	0	0	0
			1560	985	267	301	7			
4	V	205	Total	C	N	O	S	0	0	0
			1538	968	265	298	7			
4	X	206	Total	C	N	O	S	0	0	0
			1552	978	267	300	7			

- Molecule 5 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
5	Y	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	Z	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	a	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	b	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	c	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	d	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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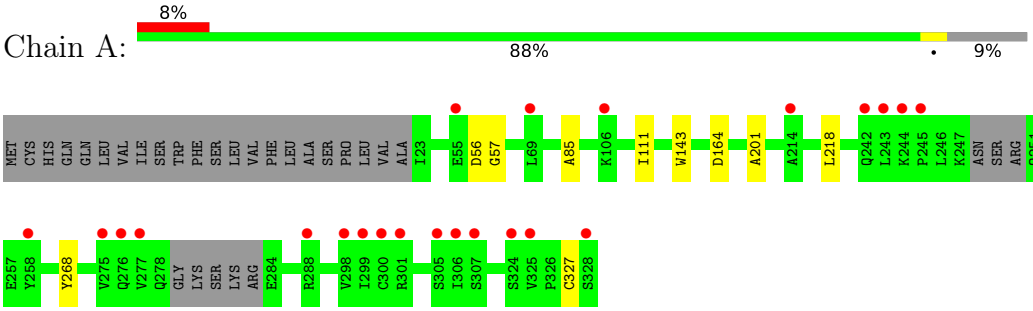
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	O	1	Total O S 5 4 1	0	0
6	O	1	Total O S 5 4 1	0	0
6	Q	1	Total O S 5 4 1	0	0
6	R	1	Total O S 5 4 1	0	0
6	S	1	Total O S 5 4 1	0	0
6	S	1	Total O S 5 4 1	0	0
6	S	1	Total O S 5 4 1	0	0
6	U	1	Total O S 5 4 1	0	0
6	U	1	Total O S 5 4 1	0	0
6	W	1	Total O S 5 4 1	0	0
6	W	1	Total O S 5 4 1	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.

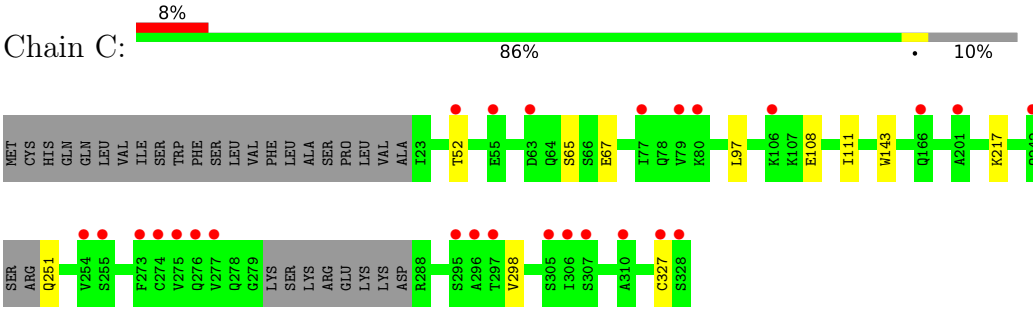
• Molecule 1: Interleukin-12 subunit beta

Chain A:



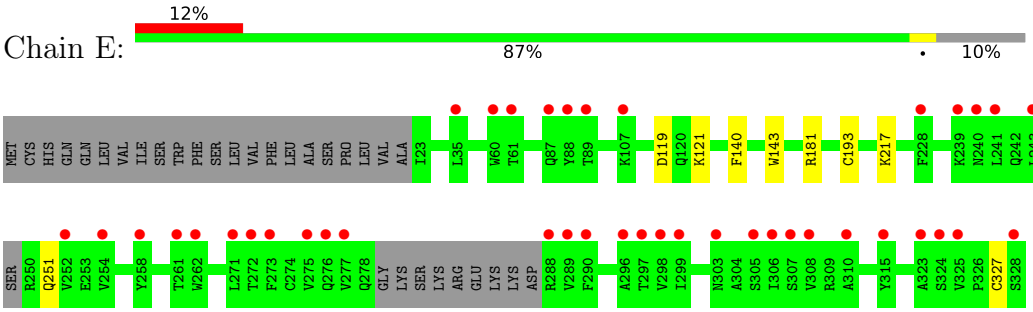
• Molecule 1: Interleukin-12 subunit beta

Chain C:



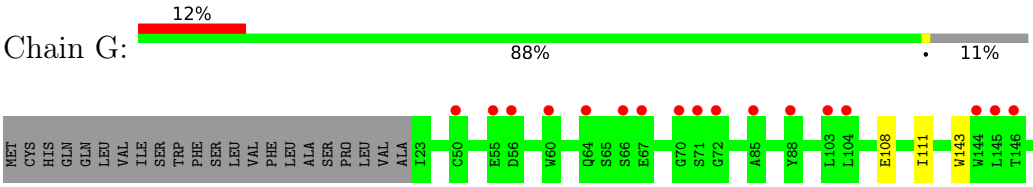
• Molecule 1: Interleukin-12 subunit beta

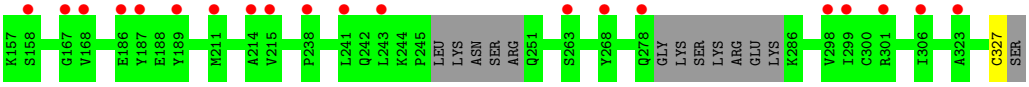
Chain E:



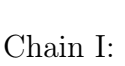
• Molecule 1: Interleukin-12 subunit beta

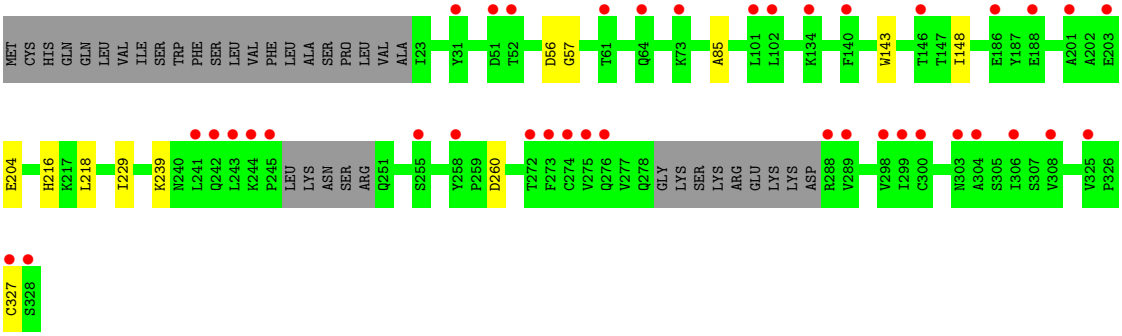
Chain G:



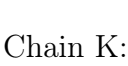


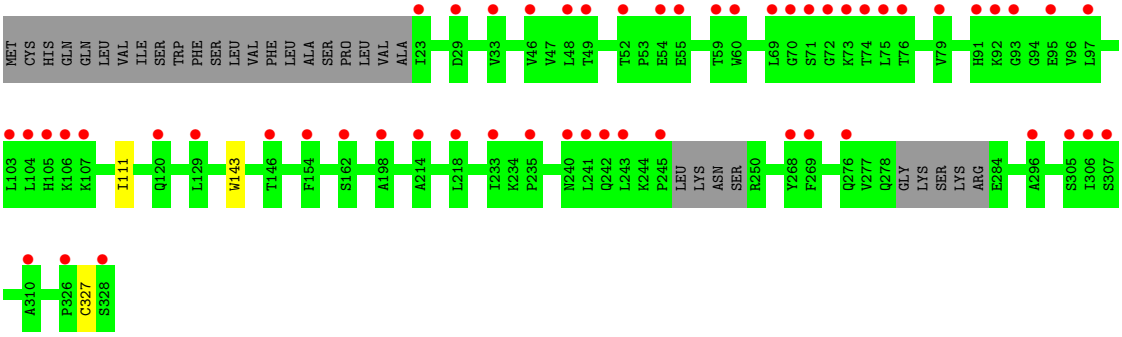
• Molecule 1: Interleukin-12 subunit beta



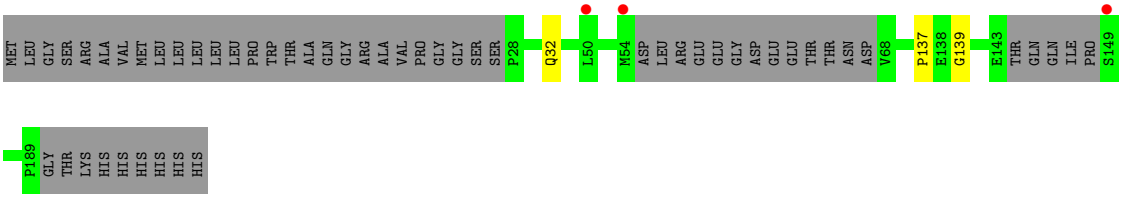


• Molecule 1: Interleukin-12 subunit beta

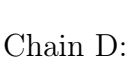


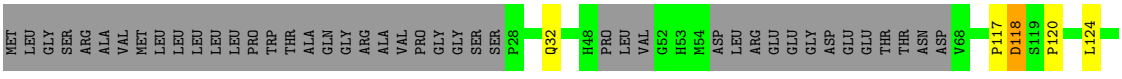


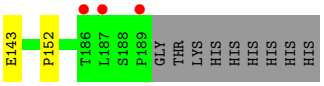
• Molecule 2: Interleukin-23 subunit alpha



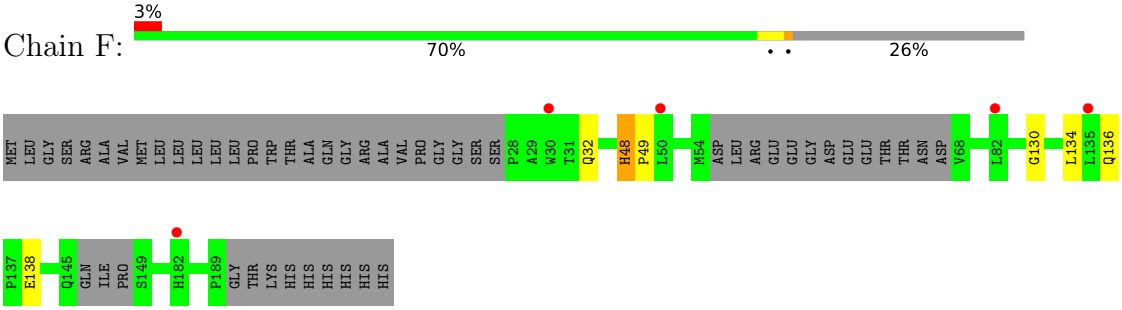
• Molecule 2: Interleukin-23 subunit alpha



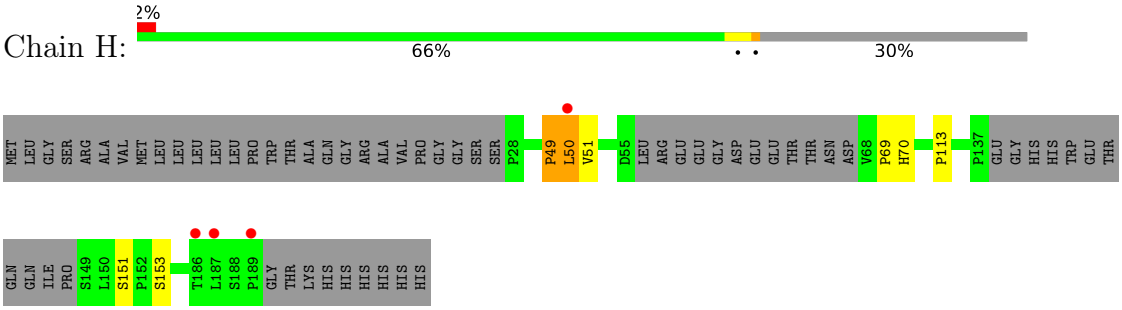




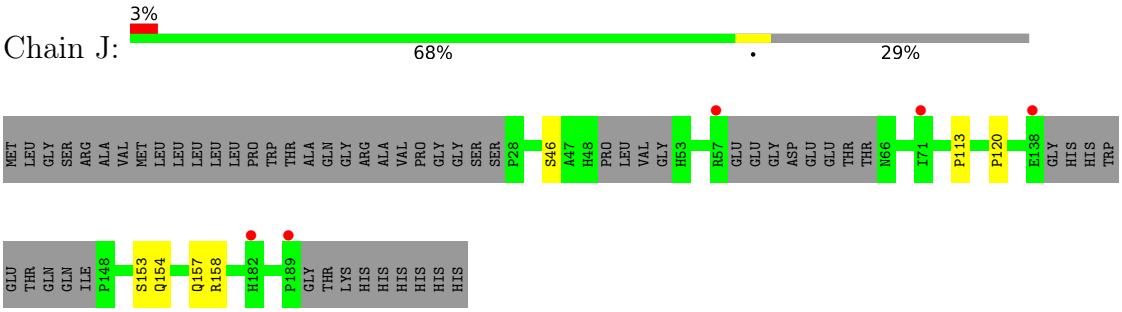
• Molecule 2: Interleukin-23 subunit alpha



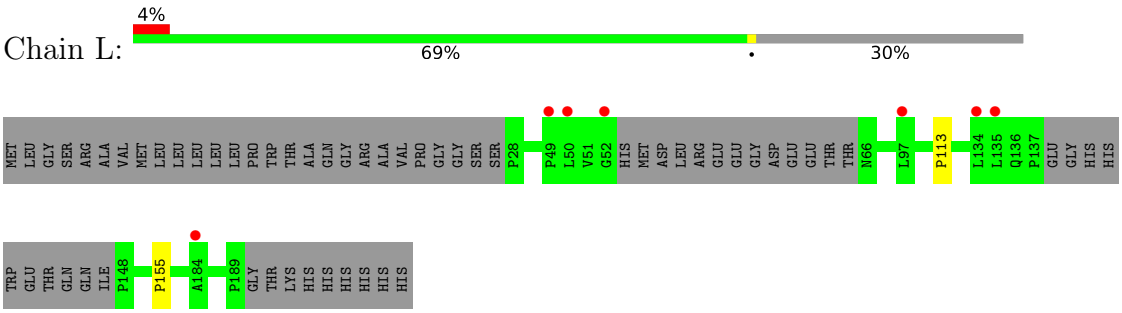
• Molecule 2: Interleukin-23 subunit alpha



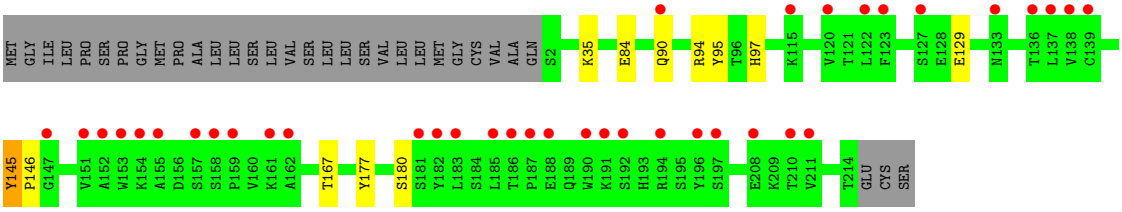
• Molecule 2: Interleukin-23 subunit alpha



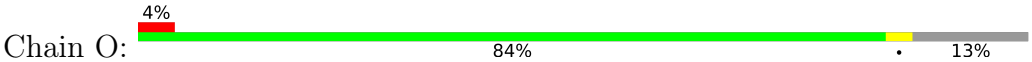
• Molecule 2: Interleukin-23 subunit alpha

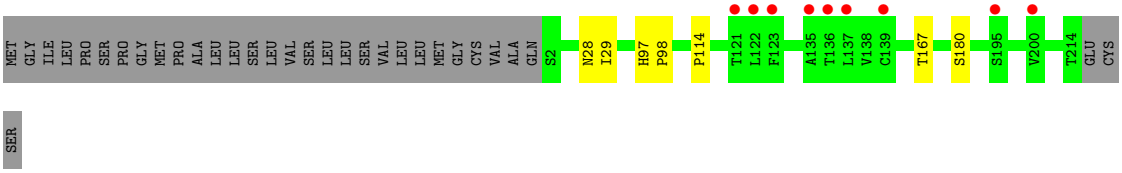


• Molecule 3: Briakinumab FAb Light chain

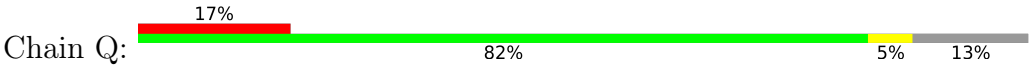


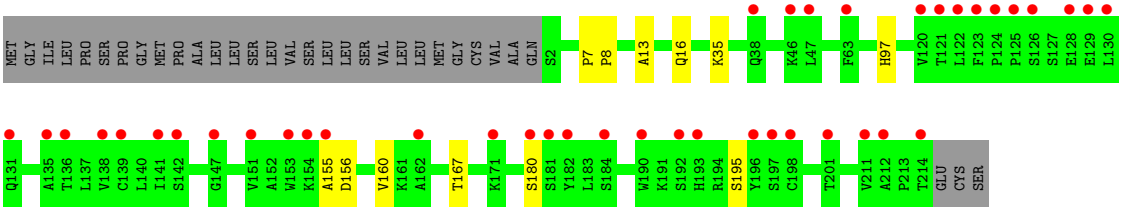
• Molecule 3: Briakinumab FAb Light chain



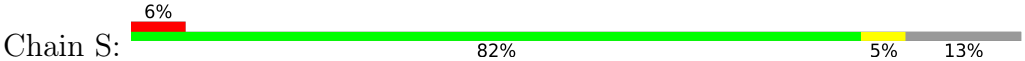


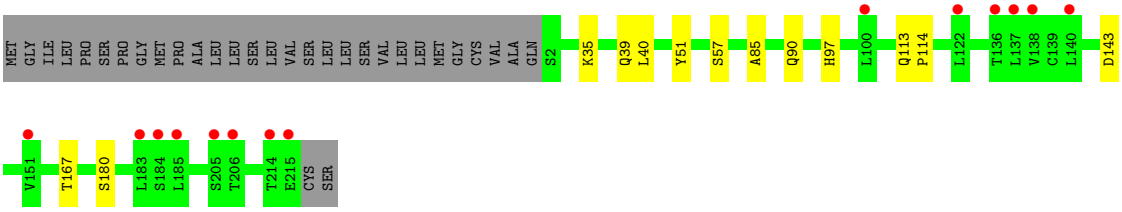
• Molecule 3: Briakinumab FAb Light chain



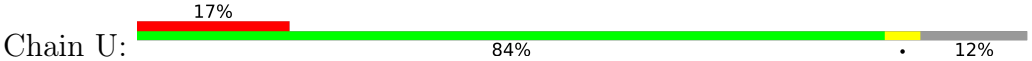


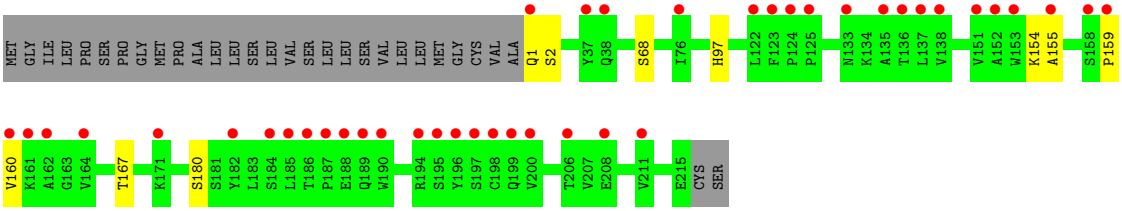
• Molecule 3: Briakinumab FAb Light chain





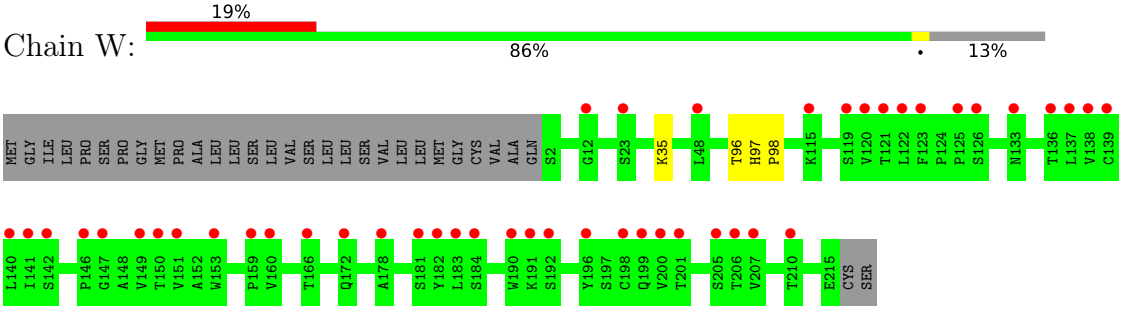
• Molecule 3: Briakinumab FAb Light chain





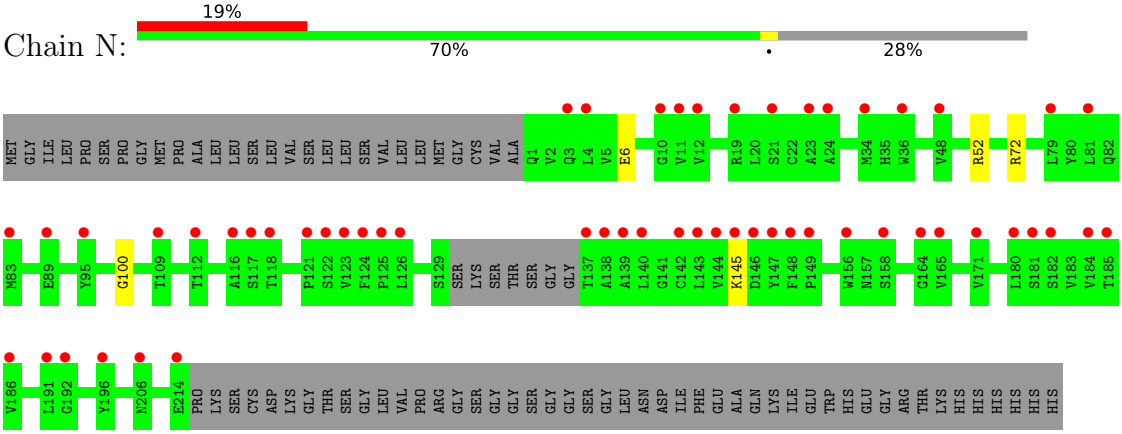
• Molecule 3: Briakinumab FAb Light chain

Chain W:



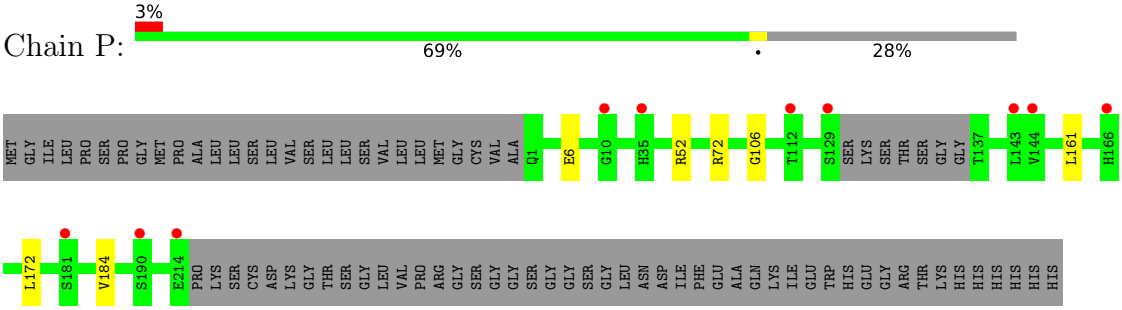
• Molecule 4: Briakinumab FAb Heavy chain

Chain N:



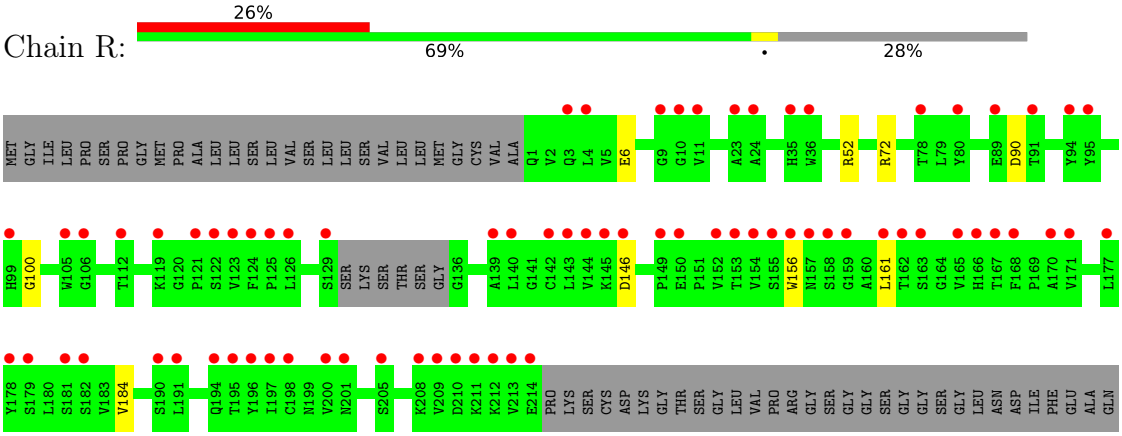
• Molecule 4: Briakinumab FAb Heavy chain

Chain P:



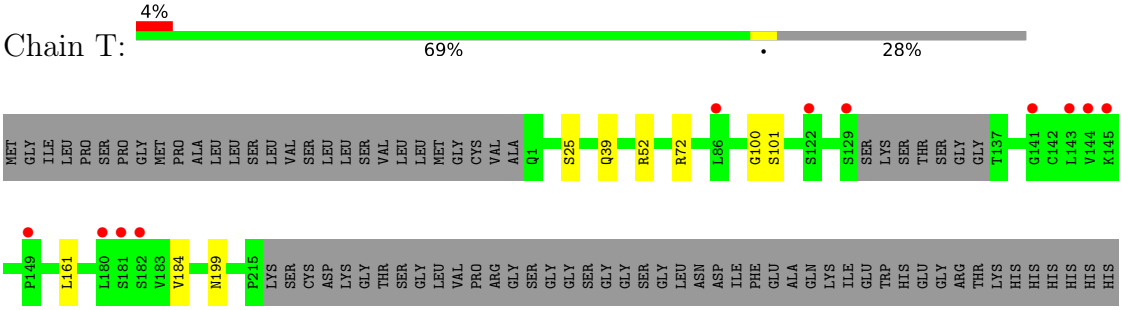
• Molecule 4: Briakinumab FAb Heavy chain

Chain R:



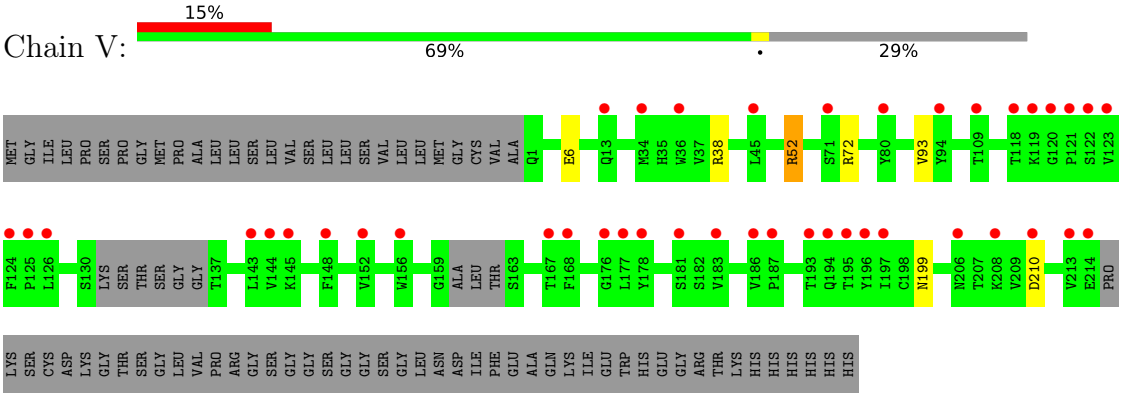
• Molecule 4: Briakinumab FAb Heavy chain

Chain T:



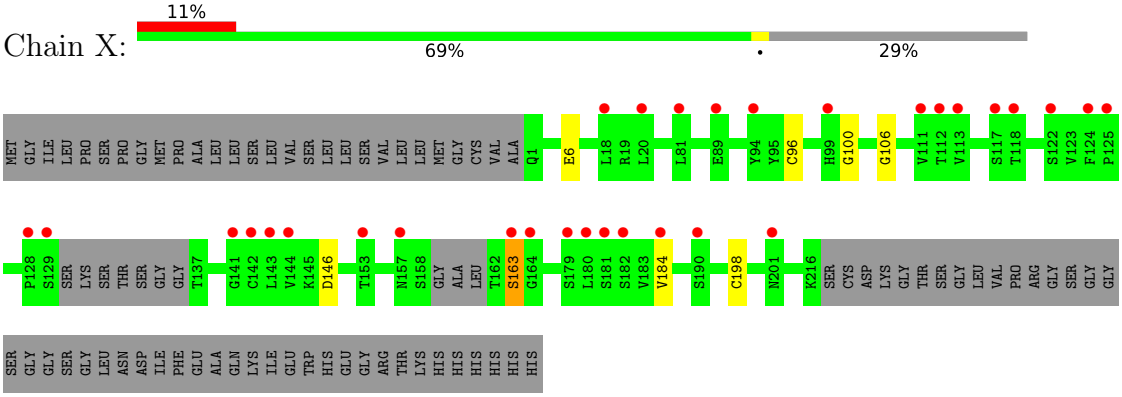
• Molecule 4: Briakinumab FAb Heavy chain

Chain V:



• Molecule 4: Briakinumab FAb Heavy chain

Chain X:

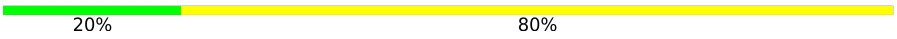


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 5: 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 5: 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 a:

• Molecule 5: 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 b:

• Molecule 5: 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 5: 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 d:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	191.61Å 191.61Å 519.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.80 – 3.90 95.80 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (95.80-3.90) 97.7 (95.80-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 3.89Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.272 , 0.312 0.273 , 0.313	Depositor DCC
R_{free} test set	1837 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å^2)	105.6	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 92.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	39445	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: MAN, NAG, BMA, SO4

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	0.28	0/2370	0.46	0/3229
1	C	0.29	0/2361	0.47	0/3213
1	E	0.27	0/2366	0.45	0/3219
1	G	0.28	0/2358	0.46	0/3210
1	I	0.27	0/2345	0.46	0/3192
1	K	0.27	0/2383	0.46	0/3242
2	B	0.28	0/1082	0.38	0/1476
2	D	0.27	0/1107	0.39	0/1509
2	F	0.26	0/1084	0.38	0/1480
2	H	0.28	0/1062	0.43	0/1448
2	J	0.27	0/1056	0.39	0/1440
2	L	0.26	0/1056	0.39	0/1441
3	M	0.29	0/1632	0.47	0/2233
3	O	0.29	0/1636	0.46	0/2236
3	Q	0.29	0/1629	0.47	0/2227
3	S	0.29	0/1629	0.46	0/2228
3	U	0.28	0/1641	0.46	0/2245
3	W	0.27	0/1629	0.45	0/2228
4	N	0.27	0/1599	0.44	0/2176
4	P	0.29	0/1596	0.46	0/2173
4	R	0.27	0/1594	0.45	0/2170
4	T	0.30	0/1599	0.46	0/2178
4	V	0.28	0/1575	0.46	0/2143
4	X	0.27	0/1590	0.45	0/2165
All	All	0.28	0/39979	0.45	0/54501

There are no bond length outliers.

There are no bond angle outliers.

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	2313	0	2156	5	0
1	C	2304	0	2168	5	0
1	E	2309	0	2178	3	0
1	G	2301	0	2171	2	0
1	I	2288	0	2155	6	0
1	K	2326	0	2191	1	0
2	B	1056	0	1016	3	0
2	D	1080	0	1029	4	0
2	F	1058	0	996	5	0
2	H	1036	0	1006	2	0
2	J	1031	0	971	3	0
2	L	1029	0	990	0	0
3	M	1592	0	1540	8	0
3	O	1596	0	1553	3	0
3	Q	1589	0	1547	7	0
3	S	1590	0	1542	8	0
3	U	1601	0	1551	6	0
3	W	1590	0	1542	3	0
4	N	1561	0	1510	4	0
4	P	1558	0	1502	6	0
4	R	1556	0	1500	5	0
4	T	1560	0	1507	7	0
4	V	1538	0	1472	4	0
4	X	1552	0	1488	4	0
5	Y	61	0	52	0	0
5	Z	61	0	52	0	0
5	a	61	0	52	0	0
5	b	61	0	52	0	0
5	c	61	0	52	0	0
5	d	61	0	52	0	0
6	M	10	0	0	0	0
6	O	10	0	0	0	0
6	Q	5	0	0	0	0
6	R	5	0	0	0	0
6	S	15	0	0	1	0
6	U	10	0	0	0	0
6	W	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	39445	0	37593	89	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 1.

All (89) 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)
2:F:130:GLY:O	2:F:134:LEU:HD13	1.89	0.73
1:I:148:ILE:HG21	1:I:216:HIS:CD2	2.24	0.72
2:J:153:SER:O	2:J:158:ARG:NH1	2.23	0.71
4:X:6:GLU:N	4:X:6:GLU:OE1	2.24	0.70
3:Q:13:ALA:N	3:Q:16:GLN:OE1	2.28	0.60
4:T:161:LEU:HD21	4:T:184:VAL:HG21	1.84	0.60
4:R:161:LEU:HD21	4:R:184:VAL:HG21	1.84	0.58
4:P:161:LEU:HD21	4:P:184:VAL:HG21	1.85	0.57
4:R:6:GLU:OE1	4:R:6:GLU:N	2.37	0.57
4:R:52:ARG:O	4:R:72:ARG:NH1	2.38	0.57
2:D:143:GLU:OE1	2:D:143:GLU:N	2.37	0.57
3:M:84:GLU:OE2	3:M:177:TYR:OH	2.17	0.56
2:B:32:GLN:N	2:B:32:GLN:OE1	2.38	0.55
1:E:251:GLN:N	1:E:251:GLN:OE1	2.38	0.55
4:N:52:ARG:O	4:N:72:ARG:NH1	2.40	0.55
1:A:56:ASP:OD1	1:A:57:GLY:N	2.40	0.54
1:E:119:ASP:OD1	1:E:121:LYS:N	2.39	0.54
3:U:1:GLN:O	3:U:2:SER:OG	2.24	0.54
1:A:85:ALA:HB3	1:A:218:LEU:HD13	1.91	0.53
2:F:130:GLY:O	2:F:134:LEU:CD1	2.56	0.53
2:F:32:GLN:OE1	2:F:32:GLN:N	2.39	0.52
2:F:136:GLN:O	2:F:138:GLU:N	2.43	0.51
2:J:46:SER:O	2:J:120:PRO:HG3	2.10	0.51
1:I:85:ALA:HB3	1:I:218:LEU:HD13	1.92	0.51
1:I:239:LYS:NZ	1:I:260:ASP:OD1	2.37	0.51
1:K:111:ILE:HG21	3:M:97:HIS:NE2	2.26	0.50
1:C:251:GLN:N	1:C:298:VAL:O	2.44	0.50
2:D:32:GLN:OE1	2:D:32:GLN:N	2.39	0.50
3:S:51:TYR:HH	4:T:101:SER:HG	1.57	0.50
4:V:6:GLU:OE1	4:V:6:GLU:N	2.43	0.50
4:V:199:ASN:ND2	4:V:210:ASP:OD2	2.45	0.50
1:C:111:ILE:HG21	3:Q:97:HIS:NE2	2.28	0.49
1:C:52:THR:HG21	1:C:97:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:97:HIS:HB3	3:O:98:PRO:HD3	1.94	0.48
2:B:137:PRO:HG2	4:P:172:LEU:HD21	1.95	0.48
4:P:6:GLU:N	4:P:6:GLU:OE1	2.47	0.47
3:S:57:SER:N	6:S:302:SO4:O2	2.48	0.47
2:D:117:PRO:O	2:D:118:ASP:CB	2.63	0.47
3:M:129:GLU:OE2	4:N:145:LYS:NZ	2.48	0.46
4:V:38:ARG:HA	4:V:93:VAL:O	2.15	0.46
3:Q:35:LYS:NZ	4:R:100:GLY:O	2.45	0.46
3:M:35:LYS:NZ	4:N:100:GLY:O	2.47	0.45
4:N:6:GLU:OE1	4:N:6:GLU:N	2.48	0.45
1:C:108:GLU:N	1:C:111:ILE:O	2.43	0.45
2:H:49:PRO:O	2:H:50:LEU:HB2	2.18	0.44
3:M:145:TYR:CD1	3:M:146:PRO:HA	2.53	0.44
3:O:167:THR:HG22	3:O:180:SER:H	1.82	0.44
4:T:25:SER:CB	3:U:68:SER:HB3	2.47	0.44
3:S:113:GLN:N	3:S:113:GLN:OE1	2.51	0.43
3:W:97:HIS:HB3	3:W:98:PRO:HD3	2.00	0.43
2:B:137:PRO:HG2	4:P:172:LEU:CD2	2.49	0.43
2:J:154:GLN:HB2	2:J:157:GLN:CG	2.49	0.43
3:U:167:THR:HG22	3:U:180:SER:H	1.81	0.43
1:C:65:SER:OG	1:C:67:GLU:OE1	2.36	0.43
1:I:56:ASP:OD1	1:I:57:GLY:N	2.50	0.43
1:I:148:ILE:HG21	1:I:216:HIS:NE2	2.33	0.43
3:M:35:LYS:HD2	3:M:90:GLN:OE1	2.19	0.43
3:M:94:ARG:NH1	3:M:95:TYR:OH	2.51	0.43
1:G:111:ILE:HG21	3:S:97:HIS:NE2	2.34	0.43
3:Q:167:THR:HG22	3:Q:180:SER:H	1.84	0.43
3:S:167:THR:HG22	3:S:180:SER:H	1.83	0.43
3:S:40:LEU:HD23	3:S:85:ALA:HB2	2.01	0.43
3:Q:156:ASP:OD1	3:Q:195:SER:N	2.52	0.42
2:H:69:PRO:O	2:H:70:HIS:ND1	2.52	0.42
4:R:156:TRP:HB3	4:R:161:LEU:HD23	2.00	0.42
3:M:167:THR:HG22	3:M:180:SER:H	1.84	0.42
4:P:52:ARG:O	4:P:72:ARG:NH1	2.52	0.42
3:U:155:ALA:N	3:U:160:VAL:HG23	2.32	0.42
3:S:39:GLN:NE2	4:T:39:GLN:OE1	2.50	0.42
2:F:48:HIS:H	2:F:49:PRO:CD	2.32	0.42
3:W:35:LYS:NZ	4:X:100:GLY:O	2.47	0.42
1:I:204:GLU:OE2	1:I:229:ILE:HB	2.20	0.42
3:O:28:ASN:OD1	3:O:29:ILE:N	2.51	0.42
4:V:52:ARG:O	4:V:72:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASP:OD2	4:T:199:ASN:ND2	2.53	0.41
2:D:120:PRO:O	2:D:124:LEU:N	2.41	0.41
3:S:35:LYS:NZ	4:T:100:GLY:O	2.48	0.41
1:G:108:GLU:N	1:G:111:ILE:O	2.46	0.41
3:Q:155:ALA:N	3:Q:160:VAL:CG2	2.84	0.41
3:U:154:LYS:HD3	3:U:159:PRO:HA	2.03	0.41
4:X:6:GLU:OE2	4:X:106:GLY:HA3	2.21	0.41
3:W:96:THR:HG23	3:W:96:THR:O	2.21	0.41
1:A:201:ALA:HB1	1:A:268:TYR:OH	2.21	0.41
4:T:52:ARG:O	4:T:72:ARG:NH1	2.52	0.41
4:X:163:SER:OG	4:X:184:VAL:CG2	2.69	0.41
1:A:111:ILE:HG21	3:U:97:HIS:NE2	2.36	0.40
1:E:140:PHE:CZ	1:E:193:CYS:HB2	2.56	0.40
4:P:6:GLU:OE2	4:P:106:GLY:HA3	2.22	0.40
3:Q:7:PRO:HA	3:Q:8:PRO:HD3	1.99	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	292/328 (89%)	283 (97%)	9 (3%)	0	100	100
1	C	288/328 (88%)	279 (97%)	8 (3%)	1 (0%)	41	75
1	E	288/328 (88%)	277 (96%)	10 (4%)	1 (0%)	41	75
1	G	287/328 (88%)	280 (98%)	7 (2%)	0	100	100
1	I	286/328 (87%)	278 (97%)	8 (3%)	0	100	100
1	K	291/328 (89%)	283 (97%)	8 (3%)	0	100	100
2	B	138/198 (70%)	127 (92%)	10 (7%)	1 (1%)	22	60
2	D	140/198 (71%)	129 (92%)	9 (6%)	2 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	140/198 (71%)	124 (89%)	15 (11%)	1 (1%)	22 60
2	H	133/198 (67%)	119 (90%)	8 (6%)	6 (4%)	2 25
2	J	133/198 (67%)	123 (92%)	9 (7%)	1 (1%)	19 57
2	L	133/198 (67%)	124 (93%)	7 (5%)	2 (2%)	10 45
3	M	211/245 (86%)	194 (92%)	17 (8%)	0	100 100
3	O	211/245 (86%)	192 (91%)	18 (8%)	1 (0%)	29 67
3	Q	211/245 (86%)	194 (92%)	17 (8%)	0	100 100
3	S	212/245 (86%)	199 (94%)	11 (5%)	2 (1%)	17 54
3	U	213/245 (87%)	197 (92%)	16 (8%)	0	100 100
3	W	212/245 (86%)	191 (90%)	21 (10%)	0	100 100
4	N	203/289 (70%)	190 (94%)	13 (6%)	0	100 100
4	P	203/289 (70%)	191 (94%)	12 (6%)	0	100 100
4	R	204/289 (71%)	191 (94%)	12 (6%)	1 (0%)	29 67
4	T	204/289 (71%)	193 (95%)	11 (5%)	0	100 100
4	V	199/289 (69%)	185 (93%)	14 (7%)	0	100 100
4	X	200/289 (69%)	185 (92%)	13 (6%)	2 (1%)	15 52
All	All	5032/6360 (79%)	4728 (94%)	283 (6%)	21 (0%)	34 71

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	51	VAL
2	D	118	ASP
1	E	217	LYS
2	F	48	HIS
2	H	151	SER
3	O	114	PRO
4	X	163	SER
2	H	50	LEU
4	X	146	ASP
1	C	217	LYS
2	D	152	PRO
4	R	146	ASP
3	S	114	PRO
3	S	143	ASP
2	H	153	SER

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Mol	Chain	Res	Type
2	H	49	PRO
2	L	155	PRO
2	B	139	GLY
2	H	113	PRO
2	L	113	PRO
2	J	113	PRO

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	252/297 (85%)	250 (99%)	2 (1%)	81 89
1	C	254/297 (86%)	252 (99%)	2 (1%)	81 89
1	E	255/297 (86%)	252 (99%)	3 (1%)	71 83
1	G	254/297 (86%)	252 (99%)	2 (1%)	81 89
1	I	253/297 (85%)	251 (99%)	2 (1%)	81 89
1	K	256/297 (86%)	254 (99%)	2 (1%)	81 89
2	B	106/167 (64%)	106 (100%)	0	100 100
2	D	108/167 (65%)	108 (100%)	0	100 100
2	F	102/167 (61%)	102 (100%)	0	100 100
2	H	105/167 (63%)	105 (100%)	0	100 100
2	J	100/167 (60%)	100 (100%)	0	100 100
2	L	103/167 (62%)	103 (100%)	0	100 100
3	M	178/207 (86%)	177 (99%)	1 (1%)	86 91
3	O	179/207 (86%)	179 (100%)	0	100 100
3	Q	177/207 (86%)	177 (100%)	0	100 100
3	S	178/207 (86%)	177 (99%)	1 (1%)	86 91
3	U	178/207 (86%)	178 (100%)	0	100 100
3	W	177/207 (86%)	177 (100%)	0	100 100
4	N	172/240 (72%)	172 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	P	172/240 (72%)	172 (100%)	0	100 100
4	R	171/240 (71%)	170 (99%)	1 (1%)	86 91
4	T	172/240 (72%)	172 (100%)	0	100 100
4	V	169/240 (70%)	168 (99%)	1 (1%)	86 91
4	X	171/240 (71%)	169 (99%)	2 (1%)	71 83
All	All	4242/5466 (78%)	4223 (100%)	19 (0%)	91 94

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	TRP
1	A	327	CYS
1	C	143	TRP
1	C	327	CYS
1	E	143	TRP
1	E	181	ARG
1	E	327	CYS
1	G	143	TRP
1	G	327	CYS
1	I	143	TRP
1	I	327	CYS
1	K	143	TRP
1	K	327	CYS
3	M	145	TYR
4	R	90	ASP
3	S	90	GLN
4	V	52	ARG
4	X	96	CYS
4	X	198	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 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	$\#\|Z\| > 2$
5	NAG	Y	1	1,5	14,14,15	0.23	0	17,19,21	0.48	0
5	NAG	Y	2	5	14,14,15	0.15	0	17,19,21	0.57	0
5	BMA	Y	3	5	11,11,12	0.70	0	15,15,17	0.80	0
5	MAN	Y	4	5	11,11,12	1.07	1 (9%)	15,15,17	1.05	1 (6%)
5	MAN	Y	5	5	11,11,12	0.99	0	15,15,17	0.97	2 (13%)
5	NAG	Z	1	1,5	14,14,15	0.23	0	17,19,21	0.36	0
5	NAG	Z	2	5	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
5	BMA	Z	3	5	11,11,12	1.36	2 (18%)	15,15,17	0.91	0
5	MAN	Z	4	5	11,11,12	1.51	2 (18%)	15,15,17	1.06	1 (6%)
5	MAN	Z	5	5	11,11,12	1.36	2 (18%)	15,15,17	1.00	1 (6%)
5	NAG	a	1	1,5	14,14,15	0.23	0	17,19,21	0.37	0
5	NAG	a	2	5	14,14,15	0.16	0	17,19,21	0.50	0
5	BMA	a	3	5	11,11,12	0.62	0	15,15,17	0.77	0
5	MAN	a	4	5	11,11,12	1.05	1 (9%)	15,15,17	1.04	1 (6%)
5	MAN	a	5	5	11,11,12	1.28	2 (18%)	15,15,17	1.03	1 (6%)
5	NAG	b	1	1,5	14,14,15	0.17	0	17,19,21	0.37	0
5	NAG	b	2	5	14,14,15	0.21	0	17,19,21	0.55	0
5	BMA	b	3	5	11,11,12	0.75	0	15,15,17	0.76	0
5	MAN	b	4	5	11,11,12	1.39	2 (18%)	15,15,17	1.05	1 (6%)
5	MAN	b	5	5	11,11,12	1.20	1 (9%)	15,15,17	1.03	1 (6%)
5	NAG	c	1	1,5	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	c	2	5	14,14,15	0.25	0	17,19,21	0.66	0
5	BMA	c	3	5	11,11,12	0.73	0	15,15,17	0.95	0
5	MAN	c	4	5	11,11,12	1.36	2 (18%)	15,15,17	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	c	5	5	11,11,12	1.33	1 (9%)	15,15,17	1.00	1 (6%)
5	NAG	d	1	1,5	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	d	2	5	14,14,15	0.19	0	17,19,21	0.49	0
5	BMA	d	3	5	11,11,12	0.44	0	15,15,17	0.78	0
5	MAN	d	4	5	11,11,12	1.20	2 (18%)	15,15,17	1.10	1 (6%)
5	MAN	d	5	5	11,11,12	1.40	2 (18%)	15,15,17	1.28	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
5	NAG	Y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	5	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Z	4	5	-	1/2/19/22	0/1/1/1
5	MAN	Z	5	5	-	0/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
5	MAN	a	4	5	-	0/2/19/22	0/1/1/1
5	MAN	a	5	5	-	0/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	MAN	b	4	5	-	0/2/19/22	0/1/1/1
5	MAN	b	5	5	-	0/2/19/22	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	BMA	c	3	5	-	0/2/19/22	0/1/1/1
5	MAN	c	4	5	-	0/2/19/22	0/1/1/1
5	MAN	c	5	5	-	1/2/19/22	0/1/1/1
5	NAG	d	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	d	3	5	-	2/2/19/22	0/1/1/1
5	MAN	d	4	5	-	1/2/19/22	0/1/1/1
5	MAN	d	5	5	-	1/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	b	4	MAN	C1-C2	3.53	1.60	1.52
5	d	5	MAN	C2-C3	3.32	1.57	1.52
5	c	4	MAN	C1-C2	3.01	1.59	1.52
5	Z	4	MAN	C1-C2	2.89	1.58	1.52
5	Z	3	BMA	O5-C5	2.88	1.49	1.43
5	d	5	MAN	C1-C2	2.69	1.58	1.52
5	Z	5	MAN	C1-C2	2.68	1.58	1.52
5	c	5	MAN	C2-C3	2.61	1.56	1.52
5	a	4	MAN	C1-C2	2.60	1.58	1.52
5	d	4	MAN	C1-C2	2.59	1.58	1.52
5	Z	4	MAN	O5-C1	-2.54	1.39	1.43
5	Y	4	MAN	C1-C2	2.49	1.57	1.52
5	a	5	MAN	C1-C2	2.28	1.57	1.52
5	a	5	MAN	C2-C3	2.28	1.55	1.52
5	d	4	MAN	C2-C3	2.24	1.55	1.52
5	b	5	MAN	C1-C2	2.24	1.57	1.52
5	Z	3	BMA	C4-C3	2.24	1.58	1.52
5	c	4	MAN	C2-C3	2.16	1.55	1.52
5	Z	5	MAN	C2-C3	2.06	1.55	1.52
5	b	4	MAN	C2-C3	2.02	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	5	MAN	C1-O5-C5	2.55	115.64	112.19
5	d	4	MAN	C1-O5-C5	2.49	115.56	112.19
5	Z	4	MAN	O2-C2-C3	-2.39	105.35	110.14
5	Y	5	MAN	C1-O5-C5	2.32	115.33	112.19
5	Y	4	MAN	C1-O5-C5	2.28	115.28	112.19
5	Z	5	MAN	O2-C2-C3	-2.28	105.57	110.14
5	b	5	MAN	C1-O5-C5	2.27	115.27	112.19
5	c	5	MAN	C1-O5-C5	2.23	115.21	112.19
5	d	5	MAN	C1-C2-C3	2.21	112.38	109.67
5	Z	2	NAG	C1-O5-C5	2.20	115.17	112.19
5	Y	5	MAN	O2-C2-C3	-2.14	105.86	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	d	5	MAN	O2-C2-C3	-2.13	105.87	110.14
5	b	4	MAN	O2-C2-C3	-2.11	105.92	110.14
5	a	4	MAN	O2-C2-C3	-2.10	105.93	110.14

There are no chirality outliers.

All (20) torsion outliers are listed below:

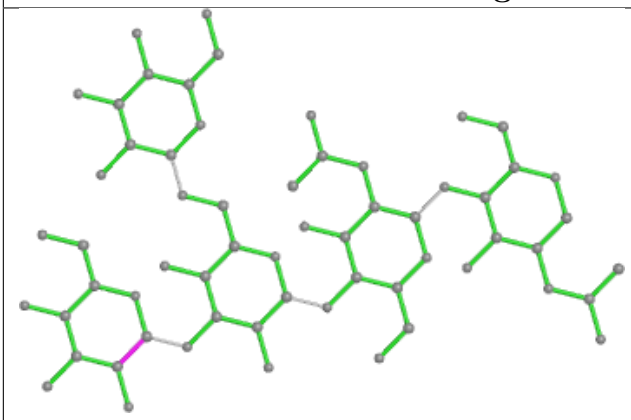
Mol	Chain	Res	Type	Atoms
5	c	1	NAG	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	Z	3	BMA	C4-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
5	Z	4	MAN	O5-C5-C6-O6
5	d	3	BMA	C4-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
5	d	5	MAN	O5-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
5	d	4	MAN	O5-C5-C6-O6
5	c	5	MAN	O5-C5-C6-O6

There are no ring outliers.

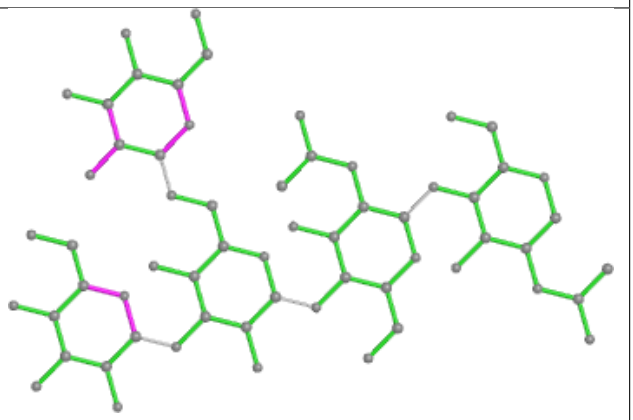
No monomer is involved in short contacts.

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

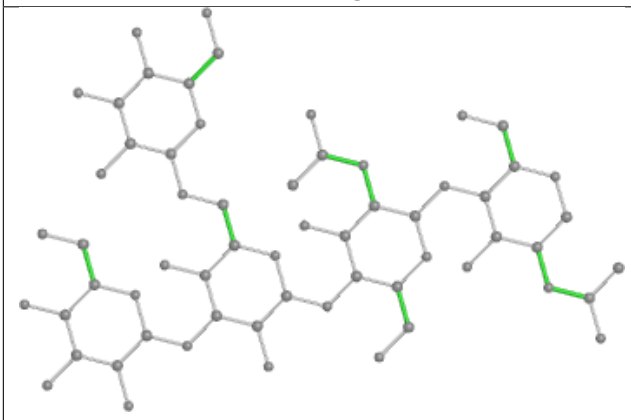
Oligosaccharide Chain Y



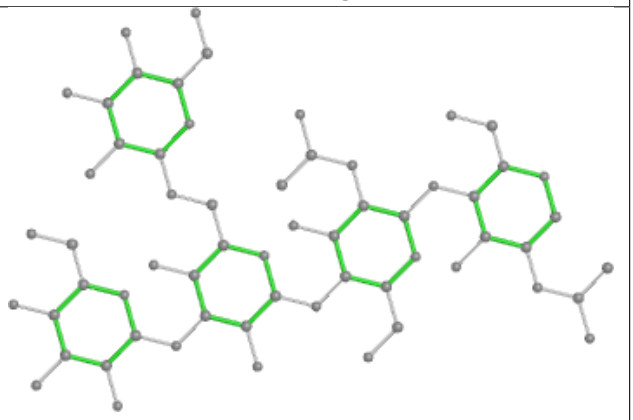
Bond lengths



Bond angles

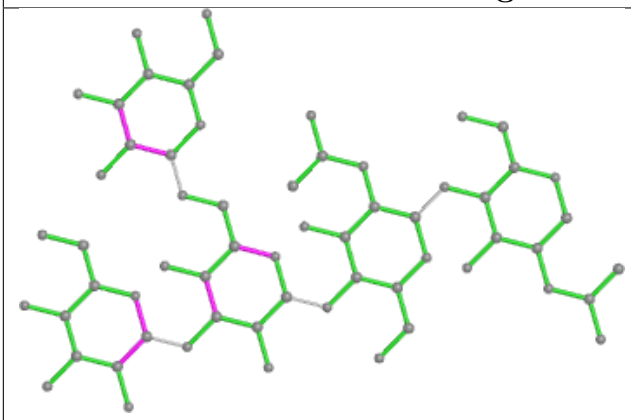


Torsions

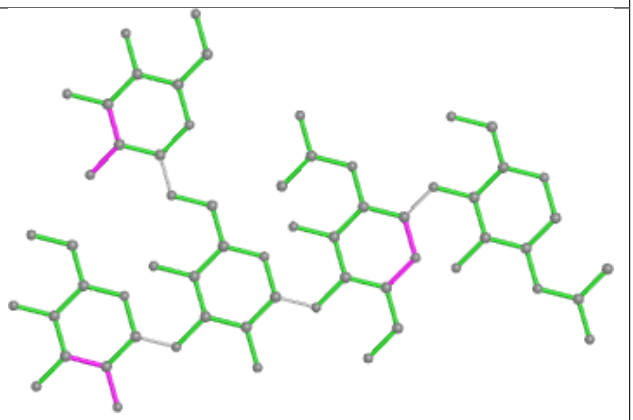


Rings

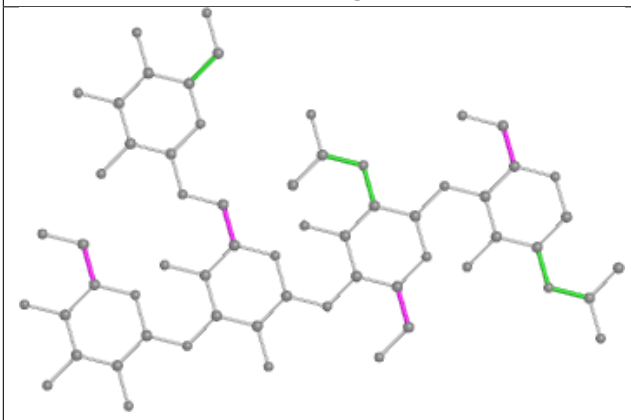
Oligosaccharide Chain Z



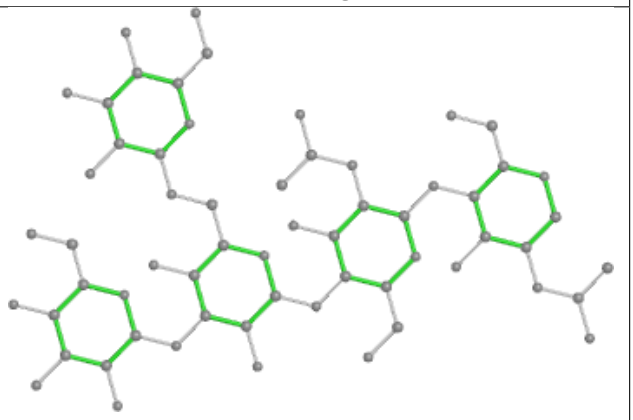
Bond lengths



Bond angles

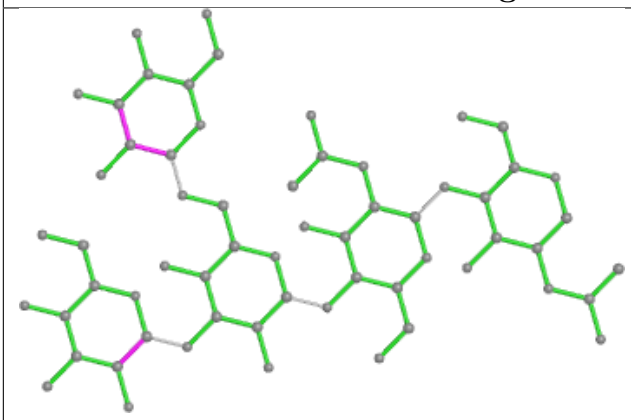


Torsions

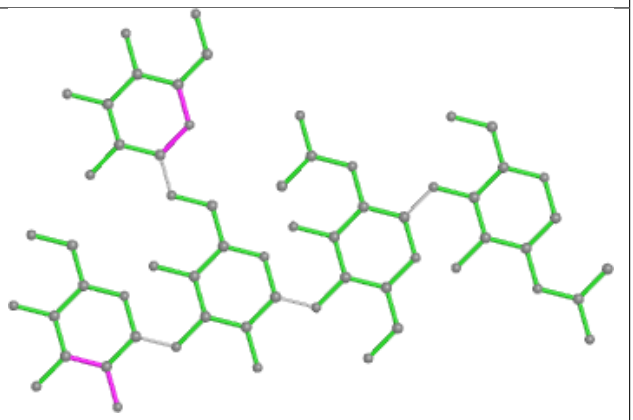


Rings

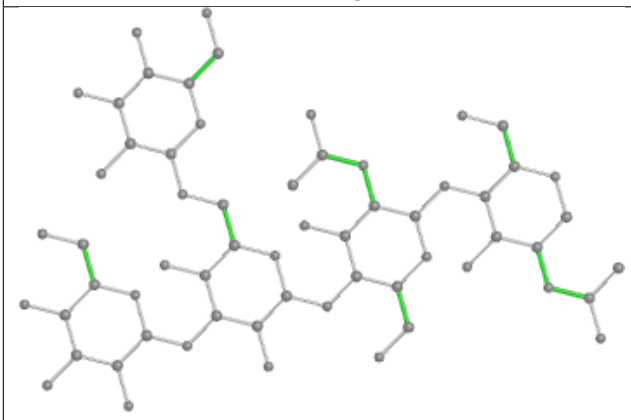
Oligosaccharide Chain a



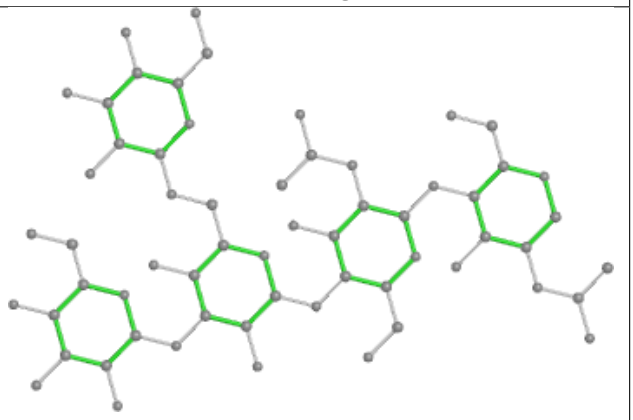
Bond lengths



Bond angles

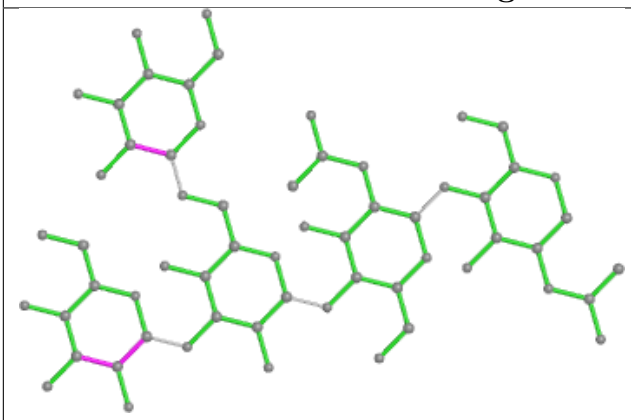


Torsions

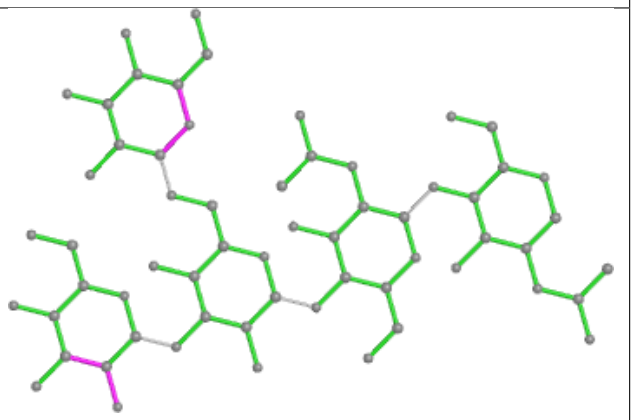


Rings

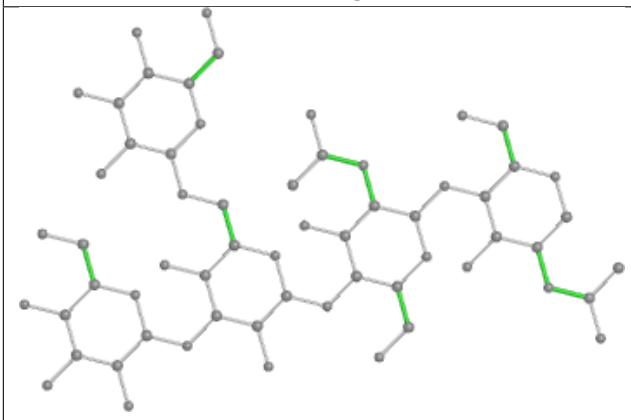
Oligosaccharide Chain b



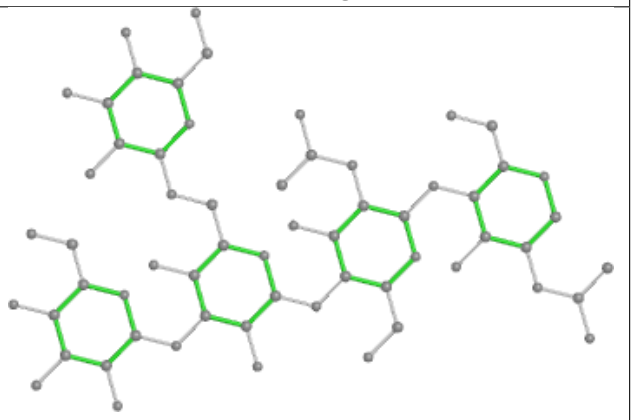
Bond lengths



Bond angles

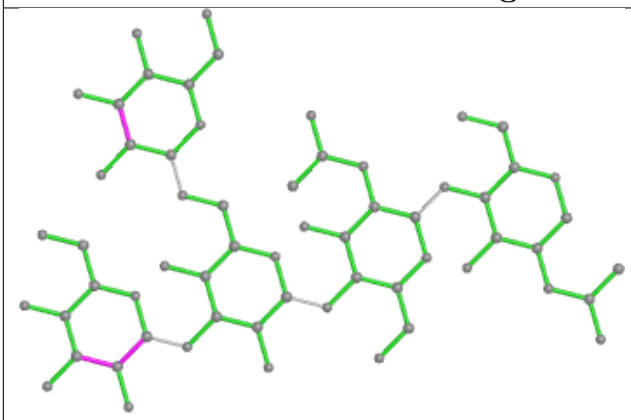


Torsions

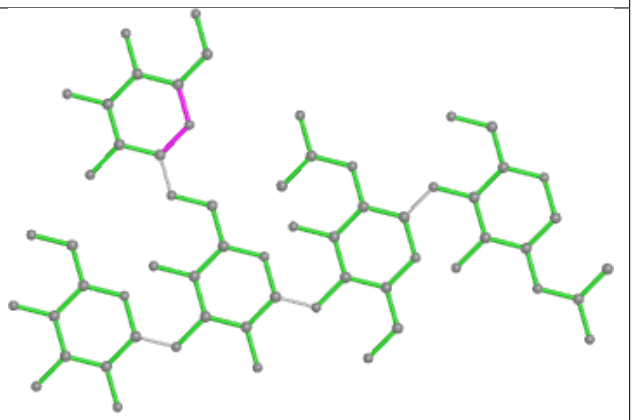


Rings

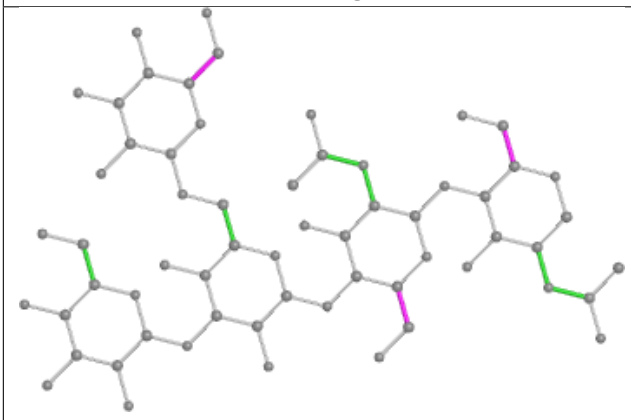
Oligosaccharide Chain c



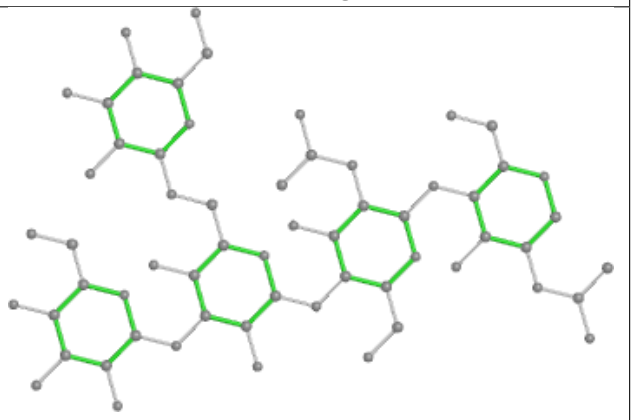
Bond lengths



Bond angles

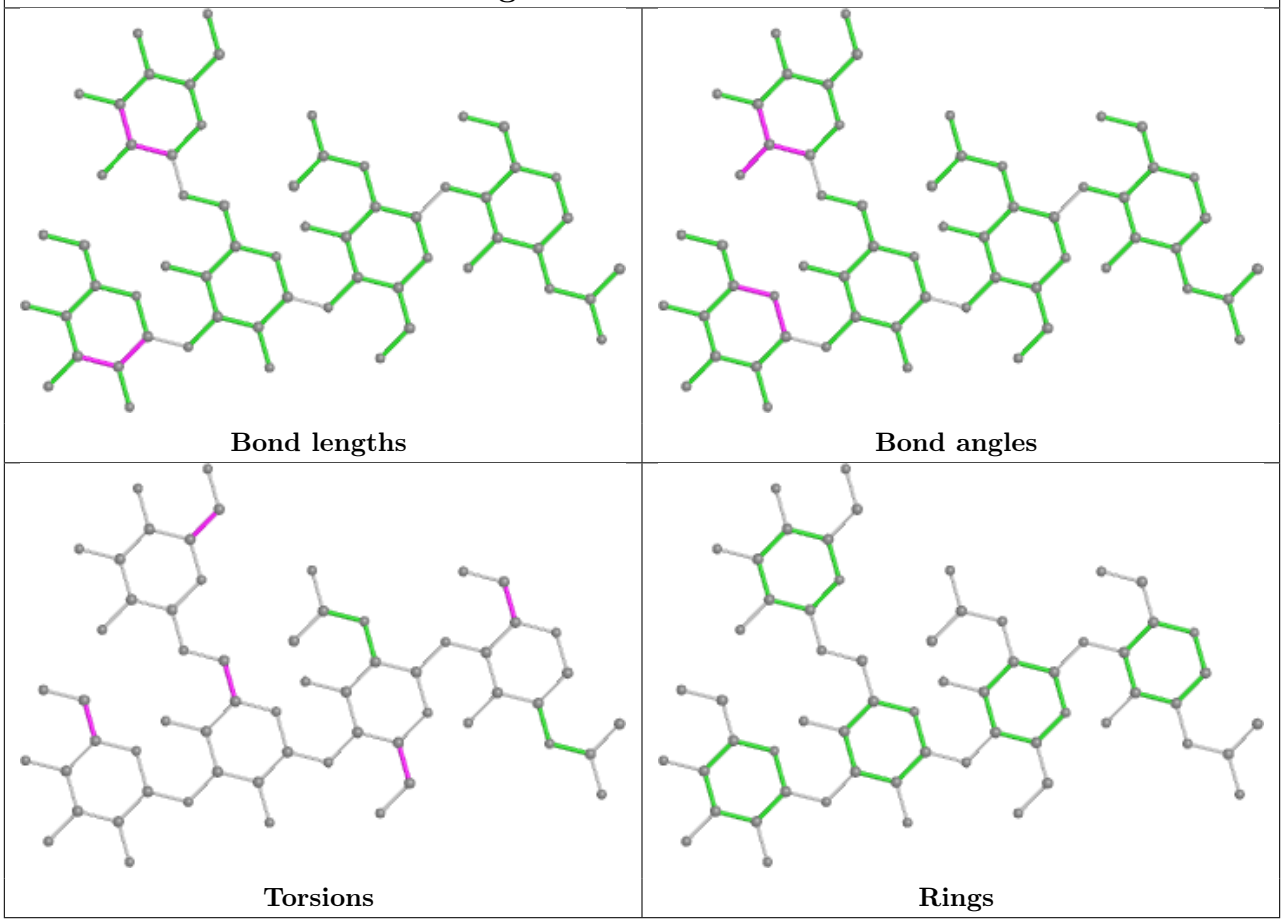


Torsions



Rings

Oligosaccharide Chain d



5.6 Ligand geometry (i)

13 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	SO4	R	301	-	4,4,4	0.15	0	6,6,6	0.08	0
6	SO4	U	301	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	S	301	-	4,4,4	0.13	0	6,6,6	0.10	0
6	SO4	S	303	-	4,4,4	0.15	0	6,6,6	0.15	0
6	SO4	S	302	-	4,4,4	0.13	0	6,6,6	0.07	0
6	SO4	M	301	-	4,4,4	0.13	0	6,6,6	0.14	0
6	SO4	Q	301	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	W	301	-	4,4,4	0.14	0	6,6,6	0.10	0
6	SO4	O	302	-	4,4,4	0.14	0	6,6,6	0.11	0
6	SO4	W	302	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	M	302	-	4,4,4	0.14	0	6,6,6	0.09	0
6	SO4	O	301	-	4,4,4	0.15	0	6,6,6	0.10	0
6	SO4	U	302	-	4,4,4	0.15	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	302	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	298/328 (90%)	0.65	26 (8%)	10	8	86, 106, 151, 189	0
1	C	294/328 (89%)	0.79	26 (8%)	10	7	86, 111, 155, 188	0
1	E	294/328 (89%)	0.93	41 (13%)	2	3	90, 115, 154, 183	0
1	G	293/328 (89%)	0.91	40 (13%)	3	3	94, 125, 168, 190	0
1	I	292/328 (89%)	0.94	39 (13%)	3	3	100, 122, 159, 195	0
1	K	297/328 (90%)	1.08	55 (18%)	1	1	101, 129, 184, 208	0
2	B	144/198 (72%)	0.29	3 (2%)	63	53	72, 99, 126, 140	0
2	D	146/198 (73%)	0.46	3 (2%)	63	53	83, 117, 156, 168	0
2	F	146/198 (73%)	0.41	5 (3%)	45	35	89, 107, 136, 155	0
2	H	139/198 (70%)	0.47	4 (2%)	51	40	90, 116, 141, 168	0
2	J	141/198 (71%)	0.47	5 (3%)	44	34	91, 116, 149, 159	0
2	L	139/198 (70%)	0.60	7 (5%)	28	24	94, 114, 147, 165	0
3	M	213/245 (86%)	0.98	38 (17%)	1	1	84, 118, 205, 218	0
3	O	213/245 (86%)	0.40	9 (4%)	36	29	80, 106, 139, 149	0
3	Q	213/245 (86%)	0.99	42 (19%)	1	1	86, 117, 154, 177	0
3	S	214/245 (87%)	0.56	14 (6%)	18	13	76, 103, 151, 170	0
3	U	215/245 (87%)	1.04	42 (19%)	1	1	88, 123, 190, 208	0
3	W	214/245 (87%)	1.11	46 (21%)	0	1	93, 134, 180, 195	0
4	N	207/289 (71%)	1.34	56 (27%)	0	0	90, 142, 213, 233	0
4	P	207/289 (71%)	0.54	10 (4%)	30	25	75, 105, 129, 143	0
4	R	208/289 (71%)	1.57	75 (36%)	0	0	95, 125, 189, 214	0
4	T	208/289 (71%)	0.60	11 (5%)	26	22	82, 96, 109, 113	0
4	V	205/289 (70%)	1.17	42 (20%)	1	1	89, 124, 167, 185	0
4	X	206/289 (71%)	0.89	31 (15%)	2	2	83, 118, 146, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	5146/6360 (80%)	0.83	670 (13%)	3 3	72, 116, 174, 233	0

All (670) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	153	TRP	10.6
1	C	328	SER	8.1
3	W	137	LEU	6.5
4	R	10	GLY	6.5
4	N	139	ALA	6.3
3	U	153	TRP	6.2
4	N	138	ALA	6.1
3	W	184	SER	6.1
4	V	213	VAL	5.8
1	A	244	LYS	5.7
1	A	245	PRO	5.5
3	W	200	VAL	5.5
1	K	73	LYS	5.5
4	X	180	LEU	5.5
4	N	10	GLY	5.4
3	W	183	LEU	5.3
3	W	120	VAL	5.2
3	W	138	VAL	5.2
1	K	92	LYS	5.1
3	S	137	LEU	5.1
3	W	199	GLN	4.9
1	I	243	LEU	4.9
4	R	156	TRP	4.9
4	R	196	TYR	4.8
4	N	11	VAL	4.8
1	I	303	ASN	4.8
4	R	121	PRO	4.7
1	G	71	SER	4.7
1	A	299	ILE	4.7
3	U	190	TRP	4.7
4	X	143	LEU	4.7
3	M	138	VAL	4.7
4	X	122	SER	4.6
4	X	181	SER	4.6
3	M	122	LEU	4.6
3	W	206	THR	4.6
1	A	300	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
3	M	188	GLU	4.6
1	K	305	SER	4.6
3	U	187	PRO	4.6
3	U	125	PRO	4.5
3	W	151	VAL	4.5
4	V	122	SER	4.5
4	N	181	SER	4.5
3	U	1	GLN	4.5
4	V	121	PRO	4.4
4	R	213	VAL	4.4
1	I	52	THR	4.3
4	R	163	SER	4.3
3	W	121	THR	4.3
3	W	201	THR	4.3
4	R	212	LYS	4.3
4	N	23	ALA	4.3
4	N	143	LEU	4.3
1	E	289	VAL	4.3
1	A	306	ILE	4.3
4	R	122	SER	4.3
1	K	95	GLU	4.2
3	M	190	TRP	4.2
4	X	18	LEU	4.2
2	J	182	HIS	4.2
3	W	182	TYR	4.2
4	N	123	VAL	4.2
3	W	181	SER	4.1
1	K	328	SER	4.1
4	X	201	ASN	4.1
3	U	159	PRO	4.1
1	C	327	CYS	4.1
1	G	168	VAL	4.1
4	X	118	THR	4.1
1	E	61	THR	4.0
3	M	123	PHE	4.0
1	C	295	SER	4.0
4	N	144	VAL	4.0
4	N	124	PHE	4.0
4	R	153	THR	4.0
4	R	154	VAL	4.0
3	W	119	SER	3.9
3	U	198	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	324	SER	3.9
4	R	181	SER	3.9
3	M	197	SER	3.9
4	N	118	THR	3.9
1	I	300	CYS	3.9
4	V	156	TRP	3.9
1	I	146	THR	3.9
1	G	72	GLY	3.9
3	U	161	LYS	3.8
3	Q	125	PRO	3.8
4	N	191	LEU	3.8
4	N	126	LEU	3.8
4	R	182	SER	3.8
2	L	49	PRO	3.8
3	Q	138	VAL	3.8
4	N	121	PRO	3.8
2	J	57	ARG	3.8
1	A	252	VAL	3.8
3	W	126	SER	3.8
4	V	123	VAL	3.8
1	C	306	ILE	3.7
4	R	142	CYS	3.7
1	A	276	GLN	3.7
4	R	9	GLY	3.7
3	Q	153	TRP	3.7
1	E	243	LEU	3.7
3	M	182	TYR	3.7
1	A	328	SER	3.7
4	X	179	SER	3.6
1	E	303	ASN	3.6
1	E	241	LEU	3.6
3	Q	131	GLN	3.6
3	U	182	TYR	3.6
1	G	214	ALA	3.6
1	C	254	VAL	3.6
3	W	150	THR	3.6
1	I	241	LEU	3.6
1	I	299	ILE	3.6
4	N	24	ALA	3.6
4	V	145	LYS	3.6
3	U	137	LEU	3.6
4	V	143	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	Q	212	ALA	3.6
4	R	11	VAL	3.6
2	L	135	LEU	3.6
1	K	74	THR	3.6
1	I	328	SER	3.6
4	X	144	VAL	3.6
4	N	79	LEU	3.6
4	P	181	SER	3.5
1	K	97	LEU	3.5
4	N	12	VAL	3.5
3	U	160	VAL	3.5
4	R	171	VAL	3.5
4	N	140	LEU	3.5
4	R	124	PHE	3.5
4	V	125	PRO	3.5
3	Q	123	PHE	3.5
1	I	304	ALA	3.5
3	W	125	PRO	3.5
1	I	288	ARG	3.5
4	R	150	GLU	3.5
4	R	123	VAL	3.4
1	C	166	GLN	3.4
3	M	186	THR	3.4
1	I	186	GLU	3.4
1	K	243	LEU	3.4
3	U	185	LEU	3.4
4	N	185	THR	3.4
1	K	59	THR	3.4
4	P	112	THR	3.4
4	V	119	LYS	3.4
3	U	162	ALA	3.4
3	Q	180	SER	3.4
3	Q	196	TYR	3.4
4	R	201	ASN	3.4
4	V	124	PHE	3.4
4	V	196	TYR	3.4
1	K	307	SER	3.3
3	U	184	SER	3.3
1	K	72	GLY	3.3
3	M	137	LEU	3.3
3	M	154	LYS	3.3
1	K	23	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
3	U	151	VAL	3.3
3	U	136	THR	3.3
3	U	189	GLN	3.3
1	E	288	ARG	3.3
4	V	148	PHE	3.3
1	E	88	TYR	3.3
4	R	166	HIS	3.3
1	C	201	ALA	3.3
4	R	165	VAL	3.3
3	M	194	ARG	3.3
4	R	125	PRO	3.3
1	I	327	CYS	3.3
1	K	242	GLN	3.2
3	U	206	THR	3.2
3	M	162	ALA	3.2
3	M	159	PRO	3.2
4	N	34	MET	3.2
1	I	308	VAL	3.2
3	W	207	VAL	3.2
1	K	105	HIS	3.2
1	K	310	ALA	3.2
3	M	139	CYS	3.2
3	M	210	THR	3.2
3	O	121	THR	3.2
4	R	194	GLN	3.2
4	T	122	SER	3.2
1	K	79	VAL	3.2
1	I	73	LYS	3.2
1	I	245	PRO	3.2
1	G	64	GLN	3.1
4	N	117	SER	3.1
3	W	115	LYS	3.1
1	C	296	ALA	3.1
3	M	181	SER	3.1
1	A	275	VAL	3.1
1	A	288	ARG	3.1
4	V	178	TYR	3.1
3	W	12	GLY	3.1
2	B	149	SER	3.1
1	E	298	VAL	3.1
4	N	186	VAL	3.1
1	K	306	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	54	GLU	3.1
2	L	50	LEU	3.1
1	A	214	ALA	3.1
4	N	146	ASP	3.1
1	K	49	THR	3.1
4	N	116	ALA	3.1
3	Q	46	LYS	3.1
4	V	214	GLU	3.1
3	Q	120	VAL	3.0
4	R	112	THR	3.0
1	C	255	SER	3.0
4	V	193	THR	3.0
2	H	50	LEU	3.0
4	V	181	SER	3.0
1	I	274	CYS	3.0
1	G	146	THR	3.0
3	U	158	SER	3.0
3	Q	124	PRO	3.0
3	W	160	VAL	3.0
3	Q	47	LEU	3.0
1	E	261	THR	3.0
4	R	198	CYS	3.0
1	I	201	ALA	3.0
4	V	152	VAL	3.0
4	N	180	LEU	3.0
1	C	79	VAL	3.0
1	I	258	TYR	3.0
4	N	4	LEU	3.0
3	U	188	GLU	3.0
3	W	153	TRP	3.0
1	I	31	TYR	3.0
2	D	189	PRO	3.0
4	X	112	THR	3.0
4	P	144	VAL	2.9
4	T	129	SER	2.9
3	M	161	LYS	2.9
3	Q	181	SER	2.9
1	K	276	GLN	2.9
1	G	55	GLU	2.9
1	K	52	THR	2.9
4	V	186	VAL	2.9
1	C	305	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	S	138	VAL	2.9
4	N	125	PRO	2.9
2	L	134	LEU	2.9
3	O	137	LEU	2.9
4	R	144	VAL	2.9
3	U	37	TYR	2.9
1	K	104	LEU	2.9
4	R	170	ALA	2.9
2	H	186	THR	2.9
3	W	149	VAL	2.9
1	C	80	LYS	2.9
1	G	67	GLU	2.9
2	J	138	GLU	2.9
4	R	24	ALA	2.9
4	R	126	LEU	2.9
4	R	143	LEU	2.9
3	Q	211	VAL	2.9
3	O	136	THR	2.9
4	V	109	THR	2.9
1	K	70	GLY	2.9
2	J	189	PRO	2.9
1	E	254	VAL	2.9
1	C	307	SER	2.9
3	S	183	LEU	2.9
1	E	107	LYS	2.8
1	I	325	VAL	2.8
3	S	205	SER	2.8
1	K	245	PRO	2.8
3	S	140	LEU	2.8
3	Q	197	SER	2.8
4	N	137	THR	2.8
4	X	124	PHE	2.8
3	U	124	PRO	2.8
3	M	192	SER	2.8
1	E	306	ILE	2.8
4	R	209	VAL	2.8
4	X	184	VAL	2.8
4	R	139	ALA	2.8
4	V	120	GLY	2.8
1	I	134	LYS	2.8
4	N	196	TYR	2.8
1	C	276	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	W	139	CYS	2.8
1	K	268	TYR	2.8
4	R	200	VAL	2.8
1	I	242	GLN	2.8
3	U	133	ASN	2.8
1	G	158	SER	2.8
3	Q	193	HIS	2.8
4	R	36	TRP	2.8
2	F	135	LEU	2.8
4	X	111	VAL	2.8
1	E	297	THR	2.7
1	E	305	SER	2.7
3	W	196	TYR	2.7
3	S	151	VAL	2.7
3	W	147	GLY	2.7
3	W	210	THR	2.7
1	G	211	MET	2.7
1	K	91	HIS	2.7
4	X	182	SER	2.7
1	G	104	LEU	2.7
1	E	89	THR	2.7
3	Q	201	THR	2.7
4	X	141	GLY	2.7
1	G	189	TYR	2.7
1	G	263	SER	2.7
4	N	112	THR	2.7
4	V	168	PHE	2.7
1	E	272	THR	2.7
3	W	159	PRO	2.7
4	N	95	TYR	2.7
4	N	145	LYS	2.7
4	N	147	TYR	2.7
1	G	50	CYS	2.7
3	Q	190	TRP	2.7
3	U	197	SER	2.7
3	Q	184	SER	2.7
3	Q	141	ILE	2.7
3	W	133	ASN	2.7
1	K	106	LYS	2.7
4	R	210	ASP	2.7
1	G	278	GLN	2.7
4	N	83	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	88	TYR	2.7
1	I	255	SER	2.7
3	S	215	GLU	2.6
4	R	211	LYS	2.6
3	W	141	ILE	2.6
3	Q	182	TYR	2.6
3	Q	126	SER	2.6
4	R	161	LEU	2.6
4	X	128	PRO	2.6
3	Q	214	THR	2.6
3	M	183	LEU	2.6
1	A	55	GLU	2.6
1	K	48	LEU	2.6
2	F	82	LEU	2.6
1	C	275	VAL	2.6
1	K	235	PRO	2.6
3	M	155	ALA	2.6
4	R	162	THR	2.6
4	V	183	VAL	2.6
3	U	122	LEU	2.6
4	R	35	HIS	2.6
3	S	214	THR	2.6
4	R	129	SER	2.6
3	W	178	ALA	2.6
1	G	145	LEU	2.6
1	K	241	LEU	2.6
2	F	182	HIS	2.6
1	K	326	PRO	2.6
1	I	203	GLU	2.6
4	X	117	SER	2.6
1	E	35	LEU	2.6
4	R	94	TYR	2.6
4	V	45	LEU	2.6
3	U	135	ALA	2.6
3	U	155	ALA	2.6
4	T	181	SER	2.6
4	V	195	THR	2.6
1	I	306	ILE	2.5
3	Q	171	LYS	2.5
1	E	277	VAL	2.5
4	X	157	ASN	2.5
1	A	69	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	102	LEU	2.5
3	Q	154	LYS	2.5
1	C	55	GLU	2.5
1	C	277	VAL	2.5
4	R	89	GLU	2.5
1	E	325	VAL	2.5
3	M	127	SER	2.5
4	N	122	SER	2.5
4	V	34	MET	2.5
1	G	70	GLY	2.5
1	A	243	LEU	2.5
3	W	136	THR	2.5
4	V	144	VAL	2.5
1	I	101	LEU	2.5
1	K	218	LEU	2.5
2	H	187	LEU	2.5
4	R	195	THR	2.5
4	V	167	THR	2.5
3	Q	128	GLU	2.5
1	K	69	LEU	2.5
1	A	256	TRP	2.5
1	G	323	ALA	2.5
1	K	296	ALA	2.5
3	M	152	ALA	2.5
1	G	299	ILE	2.5
1	E	307	SER	2.5
1	C	77	ILE	2.5
4	T	143	LEU	2.5
1	K	46	VAL	2.5
4	N	142	CYS	2.5
4	R	80	TYR	2.5
4	R	99	HIS	2.5
4	X	94	TYR	2.5
3	M	151	VAL	2.5
3	O	123	PHE	2.5
3	Q	130	LEU	2.5
1	G	306	ILE	2.5
1	I	298	VAL	2.5
4	X	113	VAL	2.5
1	E	271	LEU	2.5
1	E	252	VAL	2.5
3	M	120	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	192	SER	2.5
1	I	289	VAL	2.5
1	K	93	GLY	2.5
1	K	214	ALA	2.5
4	V	210	ASP	2.5
3	W	192	SER	2.5
4	R	159	GLY	2.5
3	U	195	SER	2.5
1	G	238	PRO	2.4
3	M	133	ASN	2.4
4	N	182	SER	2.4
4	R	158	SER	2.4
3	W	123	PHE	2.4
4	R	105	TRP	2.4
1	A	253	GLU	2.4
3	S	185	LEU	2.4
3	U	208	GLU	2.4
4	R	146	ASP	2.4
3	M	115	LYS	2.4
1	C	310	ALA	2.4
3	Q	135	ALA	2.4
3	Q	136	THR	2.4
3	S	206	THR	2.4
3	M	191	LYS	2.4
1	G	151	ASP	2.4
1	G	60	TRP	2.4
2	F	50	LEU	2.4
4	N	19	ARG	2.4
4	N	156	TRP	2.4
3	Q	139	CYS	2.4
1	A	325	VAL	2.4
3	M	136	THR	2.4
3	W	122	LEU	2.4
4	V	206	ASN	2.4
1	K	269	PHE	2.4
4	V	13	GLN	2.4
3	S	136	THR	2.4
3	W	198	CYS	2.4
1	C	63	ASP	2.4
4	N	148	PHE	2.4
3	U	152	ALA	2.4
1	I	276	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
4	N	214	GLU	2.4
1	E	310	ALA	2.4
1	K	29	ASP	2.4
1	E	273	PHE	2.4
1	K	233	ILE	2.4
3	O	135	ALA	2.4
4	R	179	SER	2.4
1	G	215	VAL	2.4
3	S	122	LEU	2.4
3	W	140	LEU	2.4
3	U	76	ILE	2.4
3	M	147	GLY	2.4
4	T	180	LEU	2.4
3	O	122	LEU	2.3
1	E	299	ILE	2.3
1	G	66	SER	2.3
4	T	144	VAL	2.3
4	V	176	GLY	2.3
1	A	324	SER	2.3
3	W	142	SER	2.3
1	I	275	VAL	2.3
3	M	158	SER	2.3
1	E	87	GLN	2.3
4	P	10	GLY	2.3
3	W	48	LEU	2.3
4	N	36	TRP	2.3
1	E	275	VAL	2.3
4	R	152	VAL	2.3
4	R	119	LYS	2.3
3	Q	198	CYS	2.3
4	N	89	GLU	2.3
1	I	244	LYS	2.3
4	T	145	LYS	2.3
1	K	71	SER	2.3
4	V	36	TRP	2.3
3	O	139	CYS	2.3
1	A	307	SER	2.3
1	C	242	GLN	2.3
1	C	52	THR	2.3
4	R	208	LYS	2.3
3	O	195	SER	2.3
4	N	21	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	X	163	SER	2.3
4	R	140	LEU	2.3
1	E	296	ALA	2.3
3	M	187	PRO	2.3
4	V	177	LEU	2.3
4	N	109	THR	2.3
4	P	166	HIS	2.3
4	R	23	ALA	2.3
1	E	328	SER	2.3
3	Q	122	LEU	2.3
4	T	182	SER	2.3
1	E	240	ASN	2.3
1	K	146	THR	2.3
4	R	91	THR	2.3
4	R	167	THR	2.3
1	A	258	TYR	2.3
3	Q	38	GLN	2.3
4	R	190	SER	2.3
4	X	89	GLU	2.3
2	L	52	GLY	2.3
4	N	206	ASN	2.3
3	U	186	THR	2.3
4	R	95	TYR	2.3
4	X	129	SER	2.2
1	K	60	TRP	2.2
3	Q	63	PHE	2.2
3	Q	129	GLU	2.2
4	R	214	GLU	2.2
1	G	298	VAL	2.2
1	K	75	LEU	2.2
3	Q	155	ALA	2.2
3	W	23	SER	2.2
4	N	171	VAL	2.2
4	N	192	GLY	2.2
4	R	106	GLY	2.2
1	A	298	VAL	2.2
4	P	129	SER	2.2
3	U	171	LYS	2.2
1	I	64	GLN	2.2
4	P	35	HIS	2.2
4	X	81	LEU	2.2
1	E	290	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	107	LYS	2.2
1	G	85	ALA	2.2
1	I	272	THR	2.2
1	K	162	SER	2.2
4	X	153	THR	2.2
1	G	144	TRP	2.2
3	W	191	LYS	2.2
3	W	205	SER	2.2
3	M	208	GLU	2.2
4	N	158	SER	2.2
4	R	155	SER	2.2
4	X	142	CYS	2.2
3	Q	162	ALA	2.2
1	E	315	TYR	2.2
4	V	118	THR	2.2
4	V	187	PRO	2.2
1	A	277	VAL	2.2
1	G	167	GLY	2.2
1	G	241	LEU	2.2
2	B	50	LEU	2.2
4	V	126	LEU	2.2
4	R	3	GLN	2.2
1	E	258	TYR	2.2
1	K	55	GLU	2.2
2	B	54	MET	2.2
3	Q	121	THR	2.2
4	X	99	HIS	2.2
1	E	276	GLN	2.2
1	K	120	GLN	2.2
1	G	156	VAL	2.2
1	G	243	LEU	2.2
3	Q	151	VAL	2.2
1	C	273	PHE	2.2
1	A	305	SER	2.2
1	E	308	VAL	2.2
3	M	90	GLN	2.2
1	G	301	ARG	2.2
4	R	177	LEU	2.2
4	N	149	PRO	2.2
1	G	155	SER	2.2
4	P	190	SER	2.2
1	K	129	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	U	38	GLN	2.2
3	M	157	SER	2.2
4	P	143	LEU	2.2
4	V	94	TYR	2.2
4	P	214	GLU	2.2
4	X	125	PRO	2.1
4	N	184	VAL	2.1
4	R	78	THR	2.1
4	V	197	ILE	2.1
1	A	301	ARG	2.1
1	K	103	LEU	2.1
1	K	240	ASN	2.1
4	N	3	GLN	2.1
3	W	146	PRO	2.1
3	M	196	TYR	2.1
1	K	76	THR	2.1
2	J	71	ILE	2.1
1	K	198	ALA	2.1
3	U	138	VAL	2.1
1	E	323	ALA	2.1
1	G	56	ASP	2.1
3	U	196	TYR	2.1
4	R	197	ILE	2.1
1	I	188	GLU	2.1
3	S	184	SER	2.1
4	R	191	LEU	2.1
4	V	194	GLN	2.1
1	I	61	THR	2.1
1	A	106	LYS	2.1
1	G	103	LEU	2.1
4	T	86	LEU	2.1
4	R	149	PRO	2.1
4	V	80	TYR	2.1
3	W	166	THR	2.1
1	I	273	PHE	2.1
3	U	123	PHE	2.1
1	G	186	GLU	2.1
2	H	189	PRO	2.1
3	U	211	VAL	2.1
4	N	164	GLY	2.1
1	K	154	PHE	2.1
1	A	242	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	147	GLY	2.1
4	N	81	LEU	2.1
4	N	165	VAL	2.1
1	I	140	PHE	2.1
4	R	145	LYS	2.1
4	R	178	TYR	2.1
3	U	194	ARG	2.1
1	E	228	PHE	2.1
4	V	208	LYS	2.1
1	K	33	VAL	2.1
2	D	187	LEU	2.1
3	U	200	VAL	2.1
4	N	48	VAL	2.1
4	R	205	SER	2.0
4	T	141	GLY	2.1
4	V	71	SER	2.0
1	E	60	TRP	2.0
3	M	211	VAL	2.0
4	X	20	LEU	2.0
2	F	30	TRP	2.0
1	C	274	CYS	2.0
1	I	51	ASP	2.0
4	R	157	ASN	2.0
4	R	168	PHE	2.0
2	L	184	ALA	2.0
1	G	187	TYR	2.0
3	M	185	LEU	2.0
3	Q	142	SER	2.0
3	W	190	TRP	2.0
3	S	100	LEU	2.0
4	X	164	GLY	2.0
1	C	297	THR	2.0
3	U	199	GLN	2.0
3	W	172	GLN	2.0
1	C	106	LYS	2.0
1	E	239	LYS	2.0
1	E	262	TRP	2.0
3	O	200	VAL	2.0
3	U	164	VAL	2.0
4	R	4	LEU	2.0
4	T	149	PRO	2.0
2	D	186	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	268	TYR	2.0
2	L	97	LEU	2.0
4	X	190	SER	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	MAN	a	5	11/12	0.54	0.40	110,113,118,119	0
5	MAN	d	5	11/12	0.71	0.27	115,117,121,122	0
5	MAN	d	4	11/12	0.72	0.28	120,123,126,128	0
5	MAN	Y	5	11/12	0.77	0.28	105,107,108,109	0
5	MAN	b	5	11/12	0.77	0.32	92,93,103,105	0
5	MAN	Z	4	11/12	0.78	0.30	81,83,87,88	0
5	MAN	Y	4	11/12	0.79	0.29	103,105,108,109	0
5	MAN	b	4	11/12	0.80	0.24	91,97,106,109	0
5	MAN	a	4	11/12	0.80	0.22	111,114,122,122	0
5	BMA	Z	3	11/12	0.82	0.21	76,79,81,81	0
5	MAN	c	5	11/12	0.82	0.27	88,90,96,97	0
5	BMA	Y	3	11/12	0.82	0.25	101,103,104,104	0
5	MAN	Z	5	11/12	0.82	0.24	80,83,87,87	0
5	MAN	c	4	11/12	0.84	0.26	97,100,104,105	0
5	BMA	d	3	11/12	0.84	0.21	113,114,119,120	0
5	BMA	b	3	11/12	0.85	0.21	87,90,93,94	0
5	BMA	c	3	11/12	0.86	0.20	87,90,96,97	0
5	BMA	a	3	11/12	0.86	0.23	104,107,111,112	0
5	NAG	Z	2	14/15	0.87	0.19	69,71,73,75	0
5	NAG	d	2	14/15	0.88	0.29	103,106,110,112	0
5	NAG	d	1	14/15	0.89	0.23	99,101,103,104	0
5	NAG	b	2	14/15	0.90	0.14	80,81,84,85	0
5	NAG	Y	2	14/15	0.90	0.20	98,100,101,103	0
5	NAG	a	1	14/15	0.91	0.25	92,95,101,101	0
5	NAG	b	1	14/15	0.91	0.24	75,77,78,79	0

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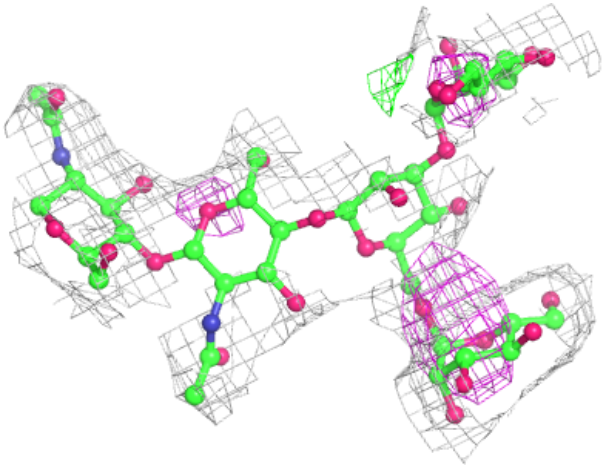
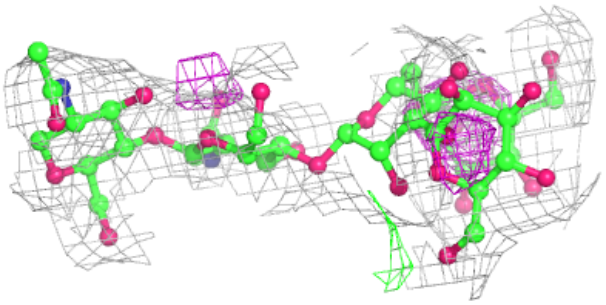
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	c	1	14/15	0.91	0.24	74,75,77,78	0
5	NAG	c	2	14/15	0.91	0.16	78,80,83,84	0
5	NAG	Z	1	14/15	0.92	0.20	65,66,69,69	0
5	NAG	a	2	14/15	0.93	0.23	98,100,102,103	0
5	NAG	Y	1	14/15	0.95	0.24	91,96,99,100	0

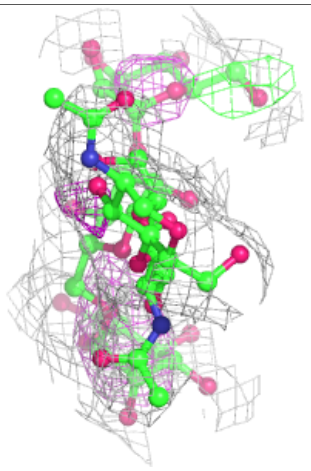
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Y:

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

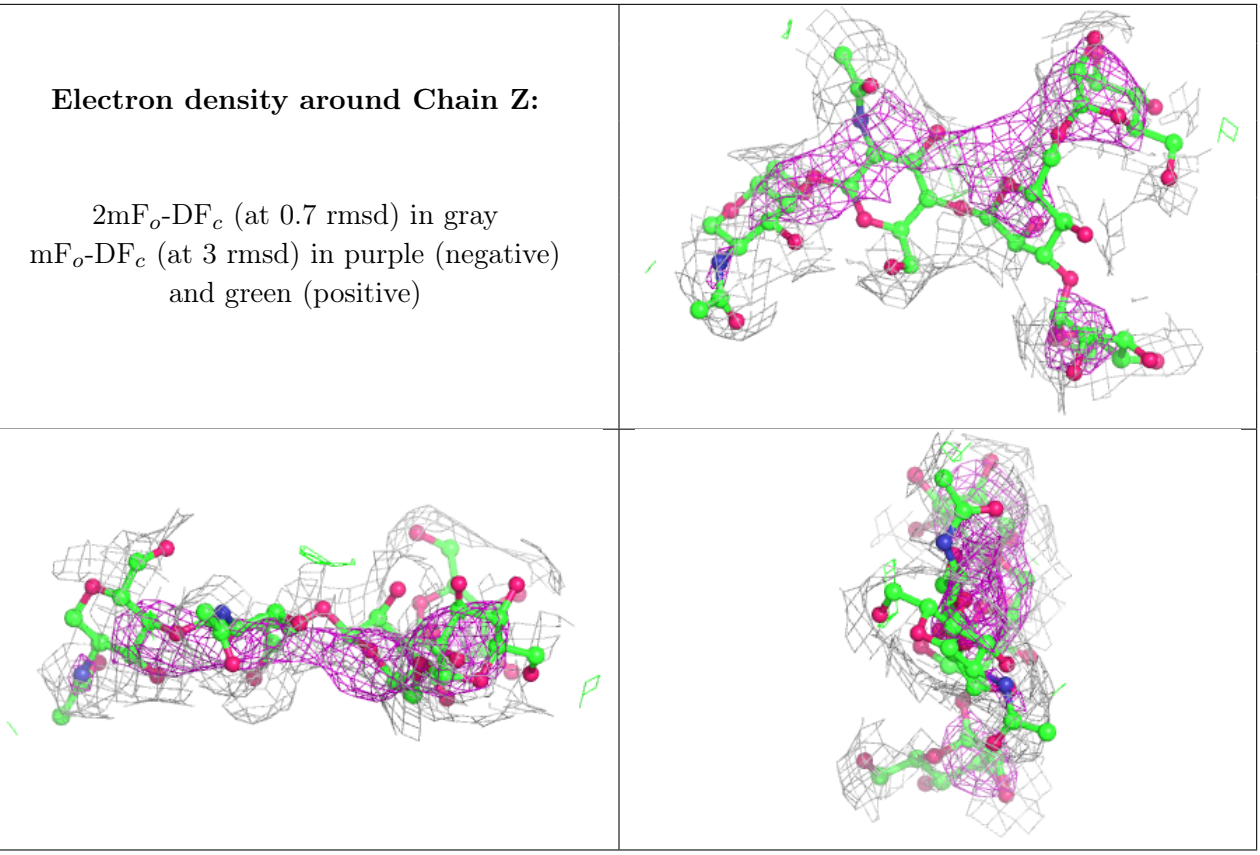






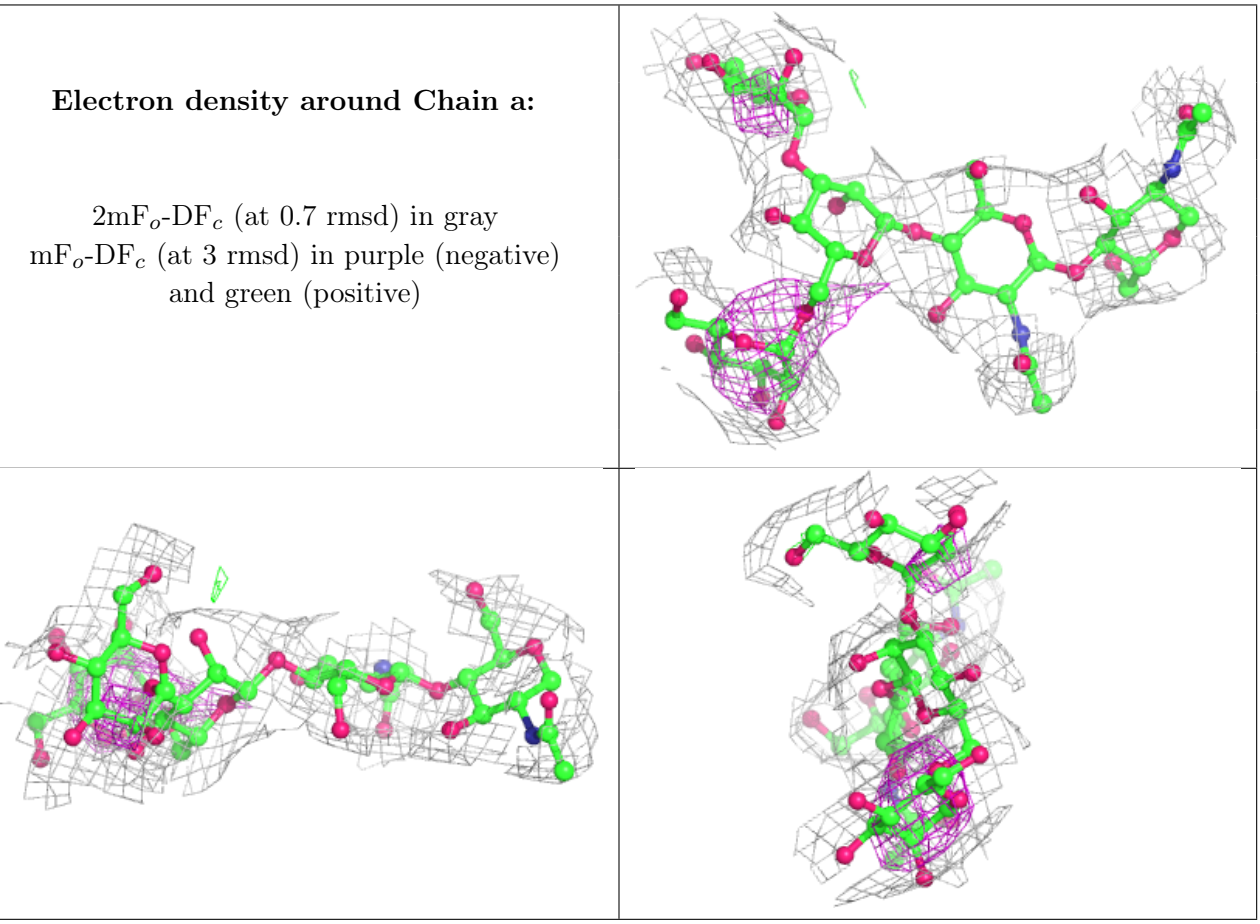
Electron density around Chain Z:

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



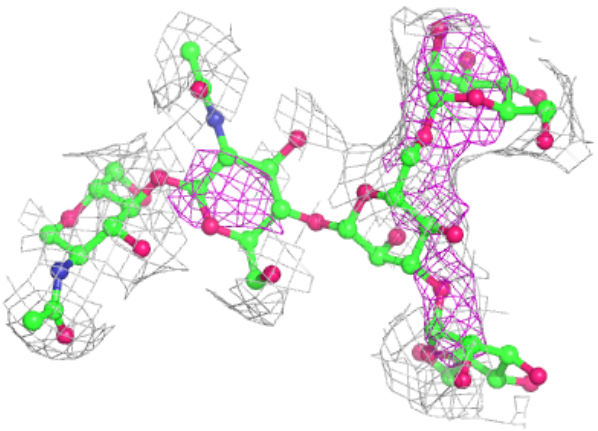
Electron density around Chain a:

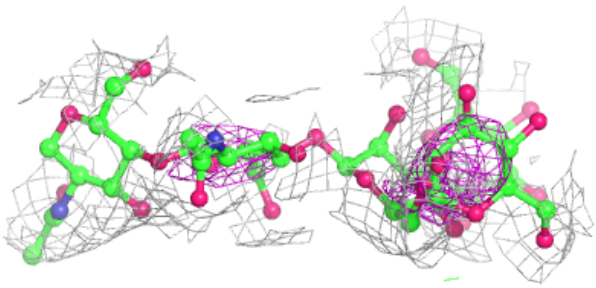
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

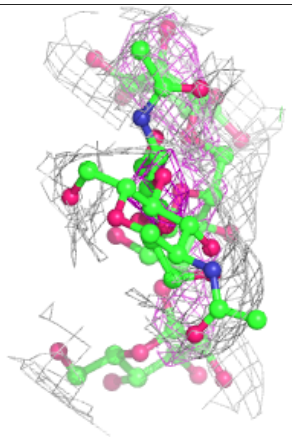


Electron density around Chain b:

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

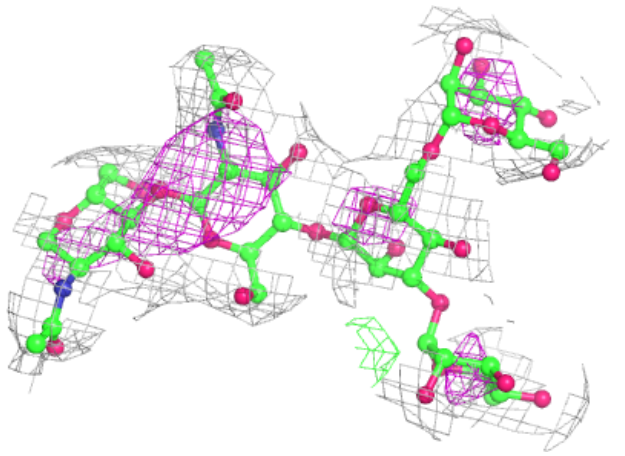


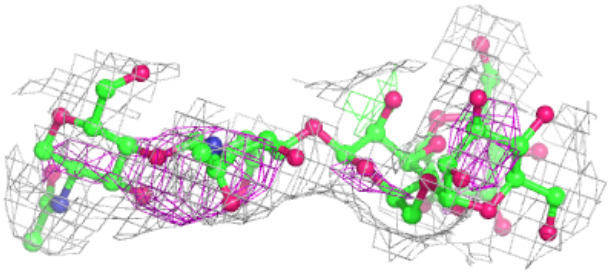


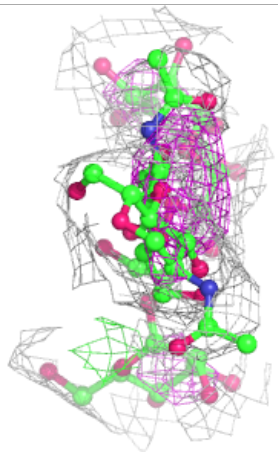


Electron density around Chain c:

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

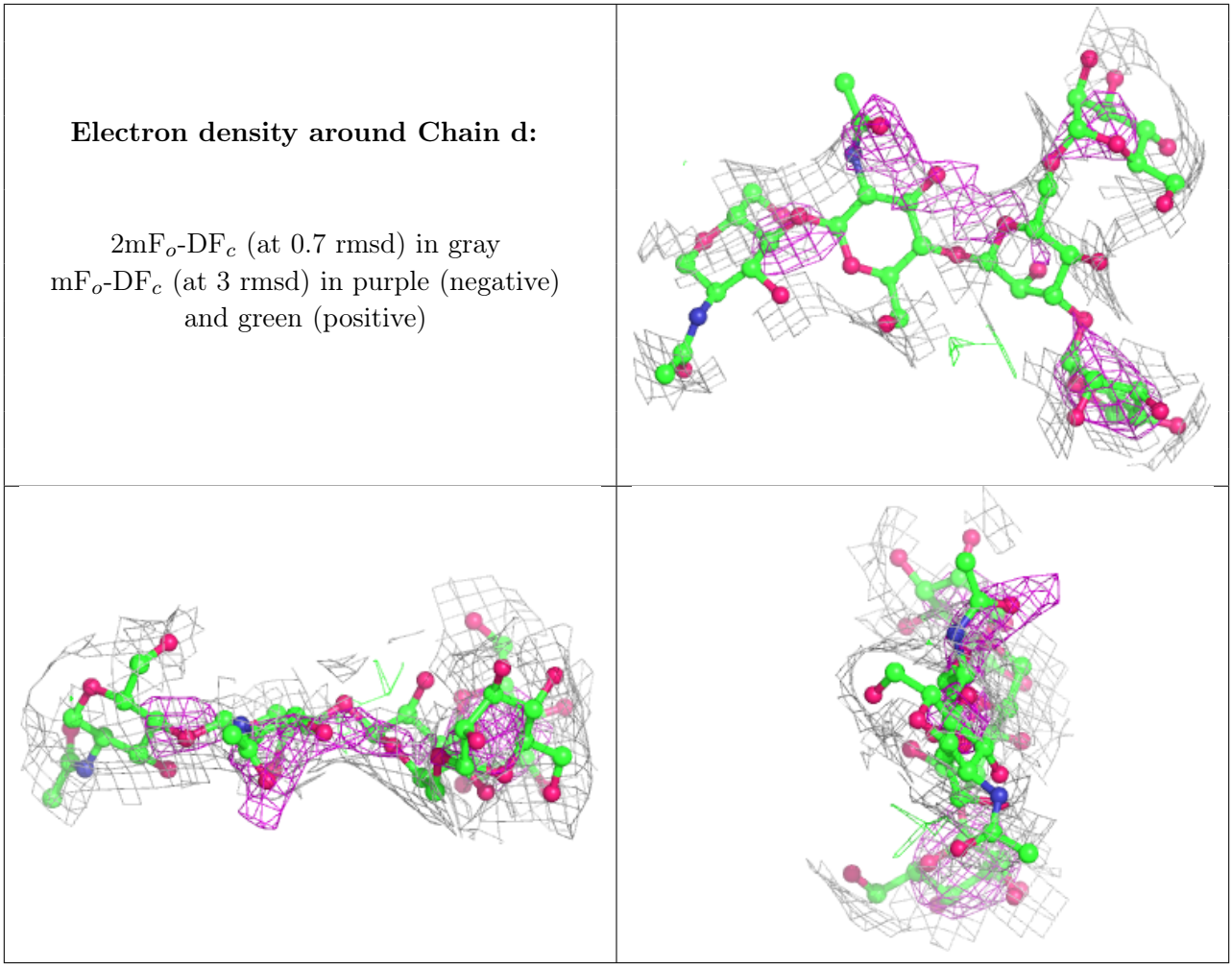






Electron density around Chain d:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	U	302	5/5	0.78	0.36	174,174,175,177	0
6	SO4	O	302	5/5	0.79	0.44	180,180,184,184	0
6	SO4	M	302	5/5	0.79	0.32	175,176,176,176	0
6	SO4	W	302	5/5	0.82	0.24	184,184,185,188	0
6	SO4	R	301	5/5	0.83	0.30	178,179,180,180	0
6	SO4	W	301	5/5	0.85	0.33	179,179,181,182	0
6	SO4	M	301	5/5	0.85	0.29	157,158,158,159	0
6	SO4	U	301	5/5	0.86	0.42	180,181,182,183	0
6	SO4	S	301	5/5	0.88	0.27	146,146,147,147	0
6	SO4	Q	301	5/5	0.89	0.32	188,189,189,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	S	302	5/5	0.89	0.29	152,153,154,155	0
6	SO4	S	303	5/5	0.90	0.33	146,146,147,150	0
6	SO4	O	301	5/5	0.92	0.39	141,141,141,141	0

6.5 Other polymers (i)

There are no such residues in this entry.