wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

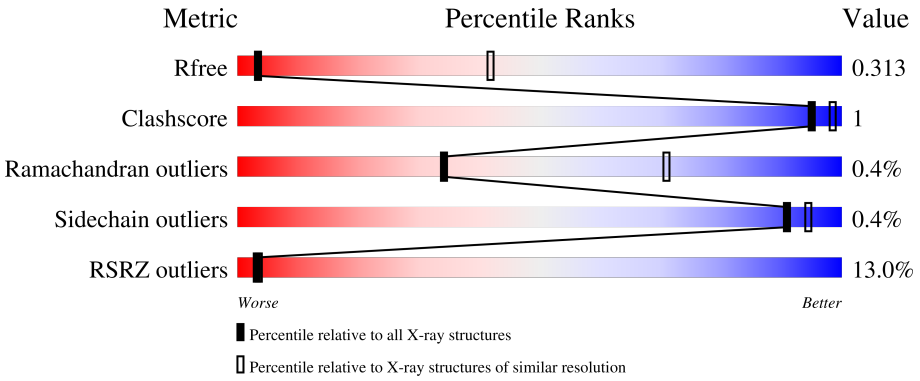
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	17% 90% 9%
2	B	198	2% 71% 27%
2	D	198	2% 70% 26%
2	F	198	3% 70% 26%
2	H	198	2% 66% 30%
2	J	198	3% 68% 29%
2	L	198	4% 69% 30%
3	M	245	16% 82% 13%
3	O	245	4% 84% 13%
3	Q	245	17% 82% 5% 13%
3	S	245	6% 82% 5% 13%
3	U	245	17% 84% 12%
3	W	245	19% 86% 13%
4	N	289	19% 70% 28%
4	P	289	3% 69% 28%
4	R	289	26% 69% 28%
4	T	289	4% 69% 28%
4	V	289	15% 69% 29%
4	X	289	11% 69% 29%
5	Y	5	60% 40%
5	Z	5	20% 80%
5	a	5	60% 40%
5	b	5	60% 40%
5	c	5	60% 40%
5	d	5	60% 40%

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 (i)

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

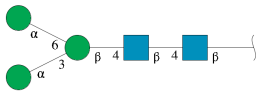
- Molecule 3 is a protein called Briakinumab FAb Light chain.

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.

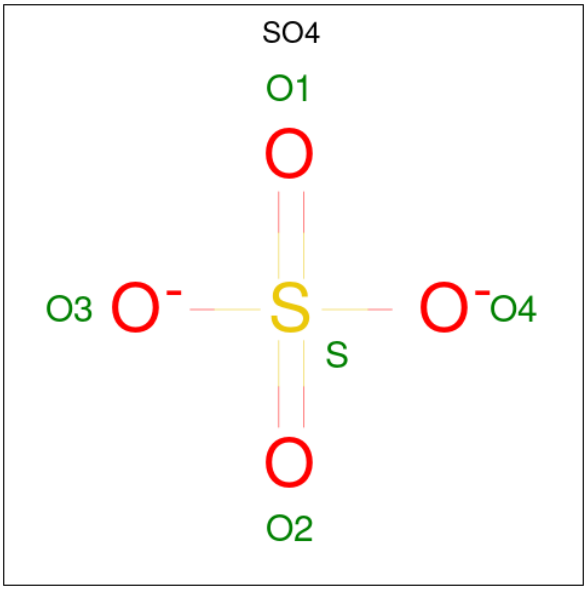
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	207	Total	C	N	O	S	0	0	0
			1561	984	269	301	7			
4	P	207	Total	C	N	O	S	0	0	0
			1558	981	268	302	7			
4	R	208	Total	C	N	O	S	0	0	0
			1556	980	268	301	7			
4	T	208	Total	C	N	O	S	0	0	0
			1560	985	267	301	7			
4	V	205	Total	C	N	O	S	0	0	0
			1538	968	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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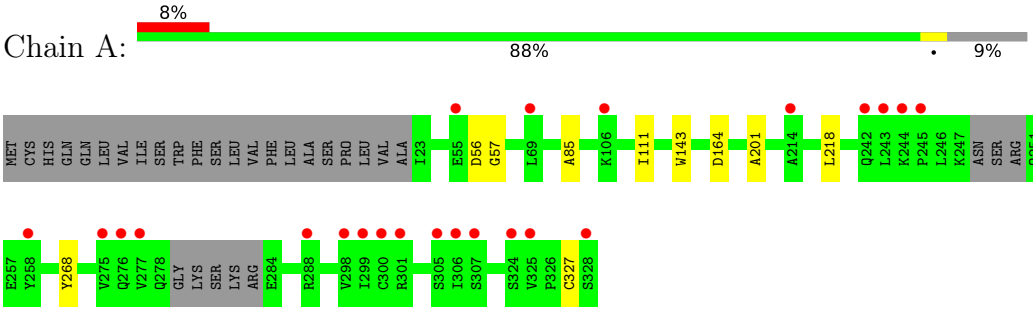
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	O	1	Total O S 5 4 1	0	0
6	O	1	Total O S 5 4 1	0	0
6	Q	1	Total O S 5 4 1	0	0
6	R	1	Total O S 5 4 1	0	0
6	S	1	Total O S 5 4 1	0	0
6	S	1	Total O S 5 4 1	0	0
6	S	1	Total O S 5 4 1	0	0
6	U	1	Total O S 5 4 1	0	0
6	U	1	Total O S 5 4 1	0	0
6	W	1	Total O S 5 4 1	0	0
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.

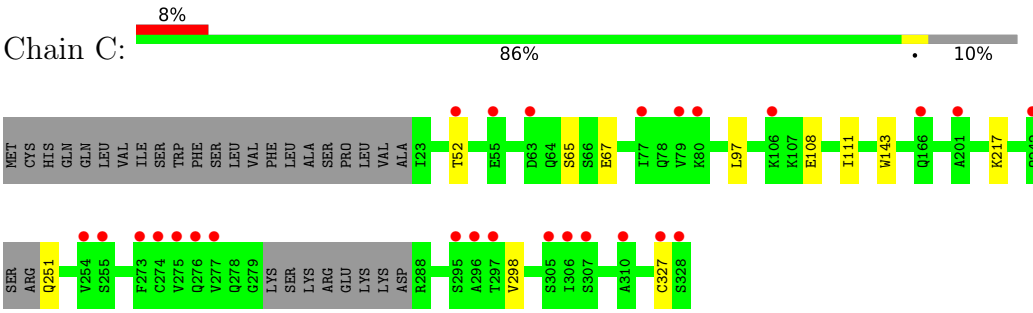
• Molecule 1: Interleukin-12 subunit beta

Chain A:



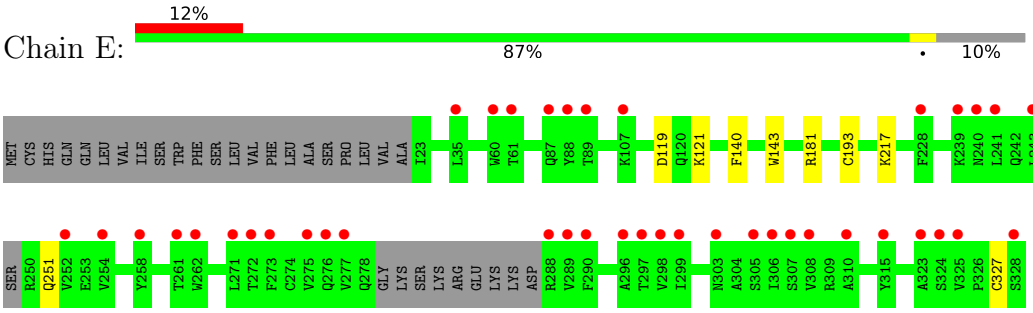
• Molecule 1: Interleukin-12 subunit beta

Chain C:



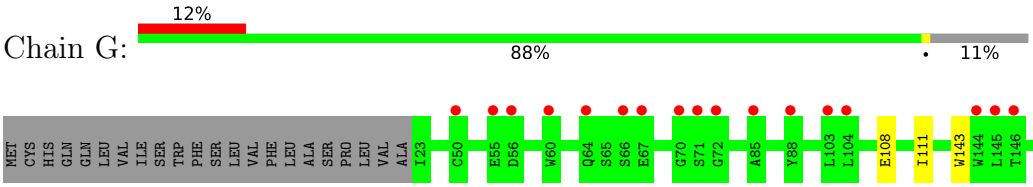
• Molecule 1: Interleukin-12 subunit beta

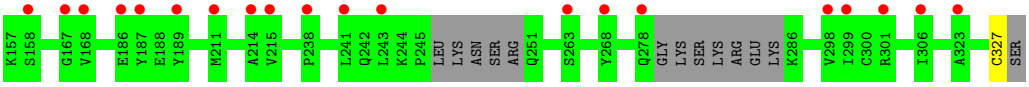
Chain E:



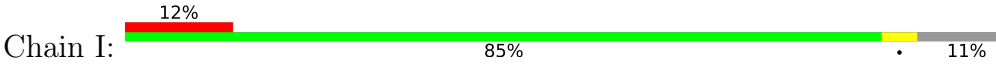
• Molecule 1: Interleukin-12 subunit beta

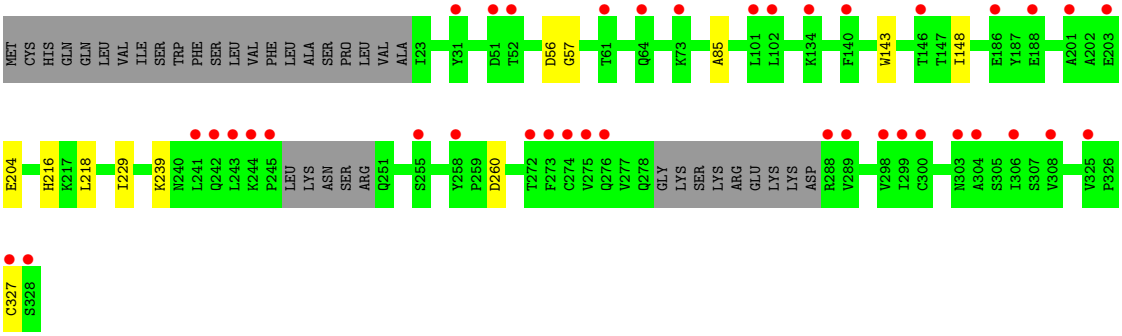
Chain G:



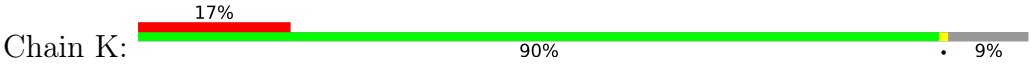


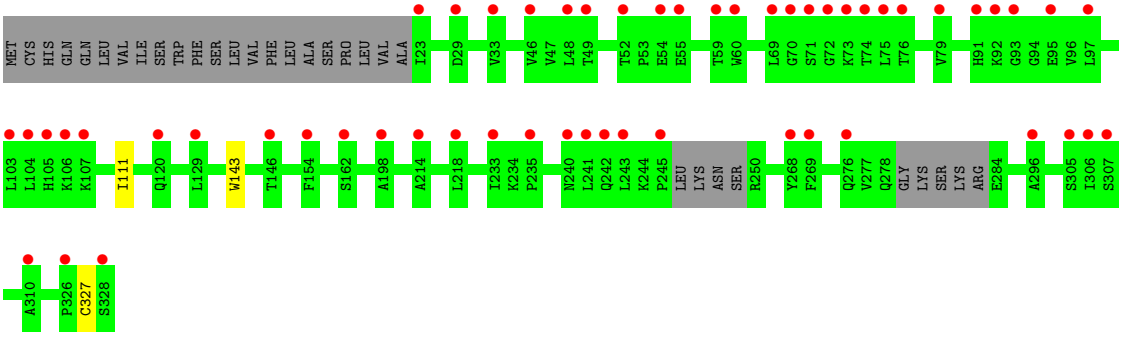
• Molecule 1: Interleukin-12 subunit beta



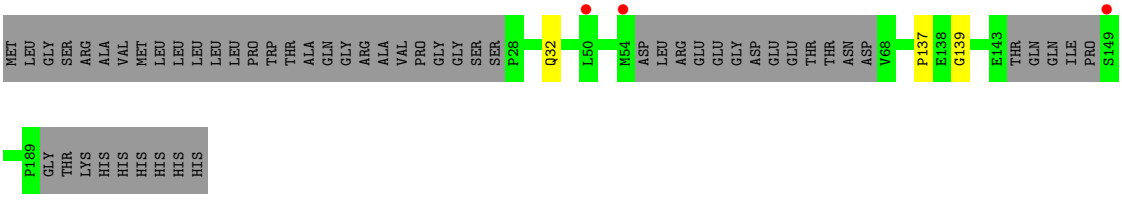


• Molecule 1: Interleukin-12 subunit beta

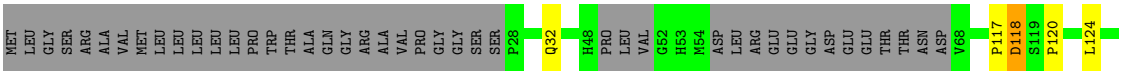


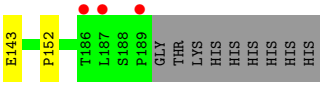


• Molecule 2: Interleukin-23 subunit alpha



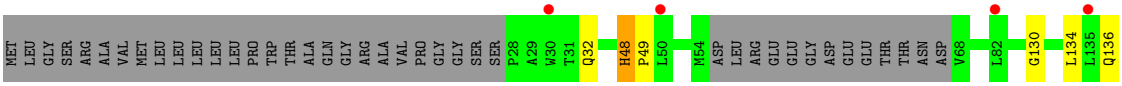
• Molecule 2: Interleukin-23 subunit alpha

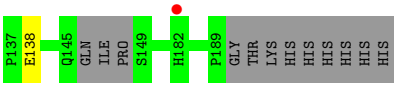




• Molecule 2: Interleukin-23 subunit alpha

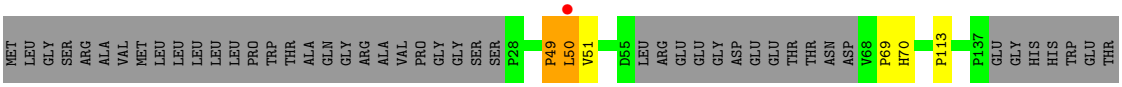
Chain F:

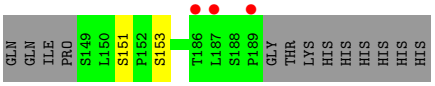




• Molecule 2: Interleukin-23 subunit alpha

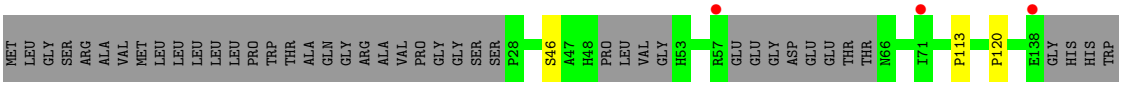
Chain H:

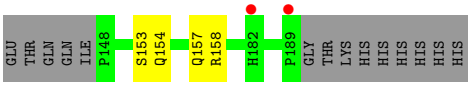




• Molecule 2: Interleukin-23 subunit alpha

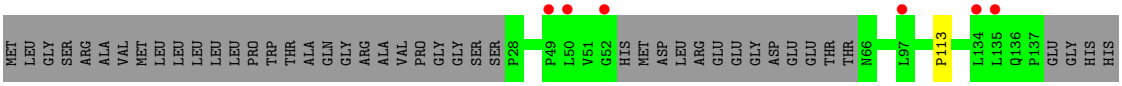
Chain J:

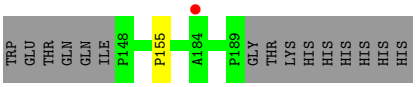




• Molecule 2: Interleukin-23 subunit alpha

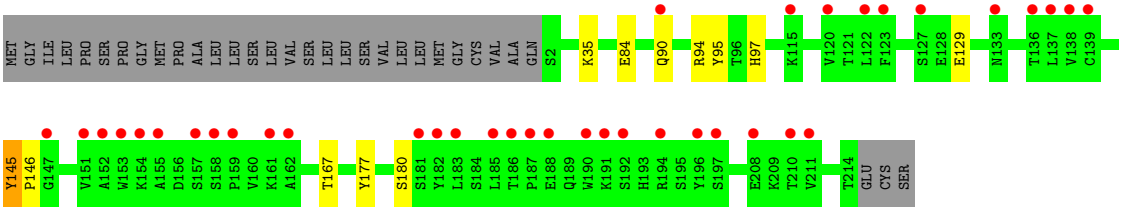
Chain L:



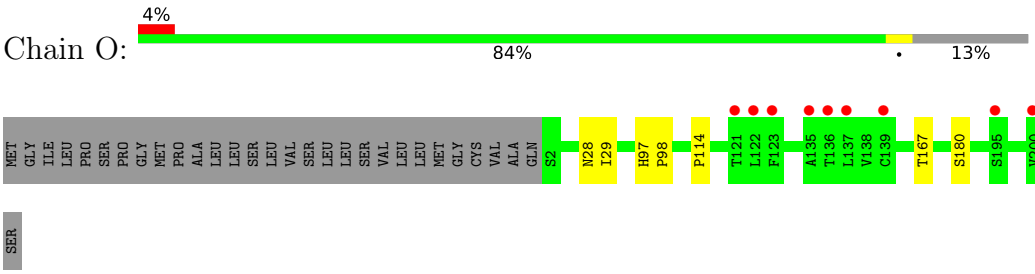


• Molecule 3: Briakinumab FAb Light chain

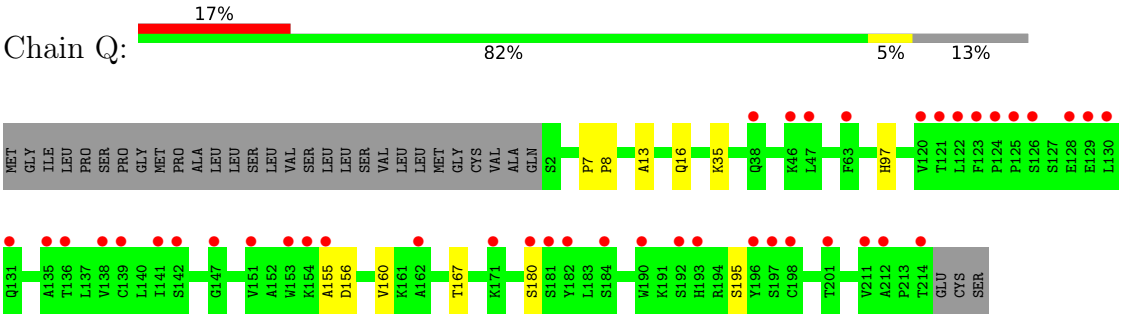
Chain M:



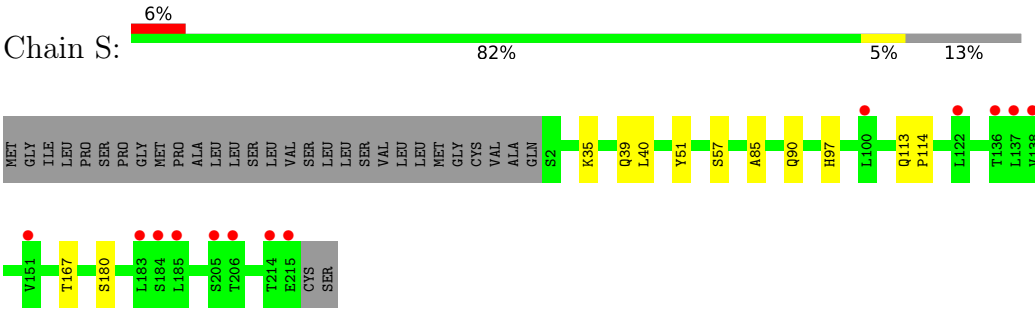
• Molecule 3: Briakinumab FAb Light chain



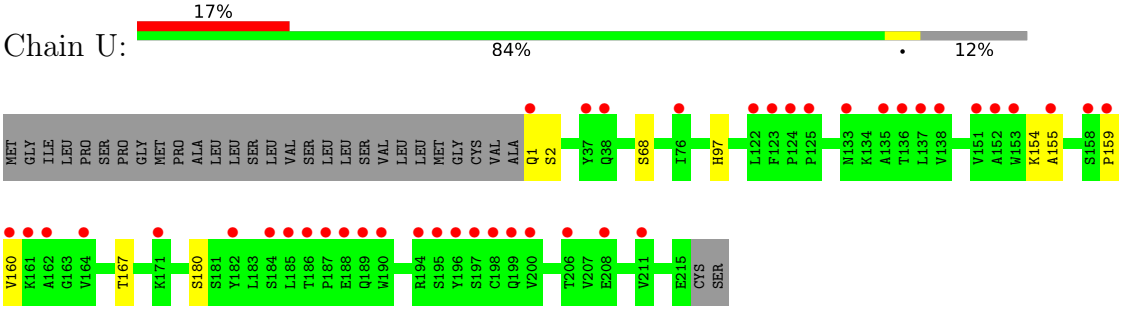
• Molecule 3: Briakinumab FAb Light chain



• Molecule 3: Briakinumab FAb Light chain

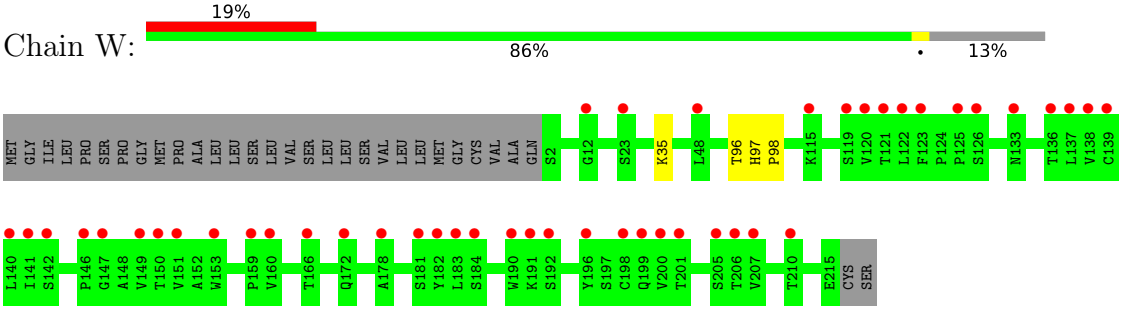


• Molecule 3: Briakinumab FAb Light chain



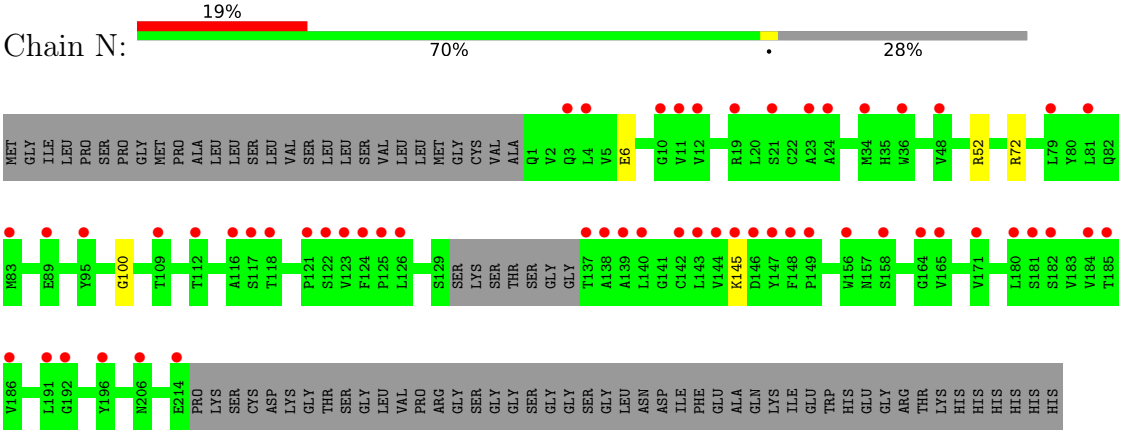
• Molecule 3: Briakinumab FAb Light chain

Chain W:



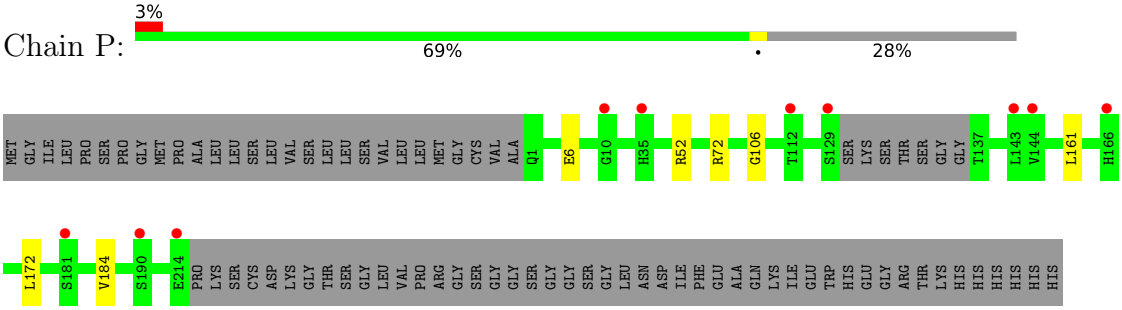
• Molecule 4: Briakinumab FAb Heavy chain

Chain N:



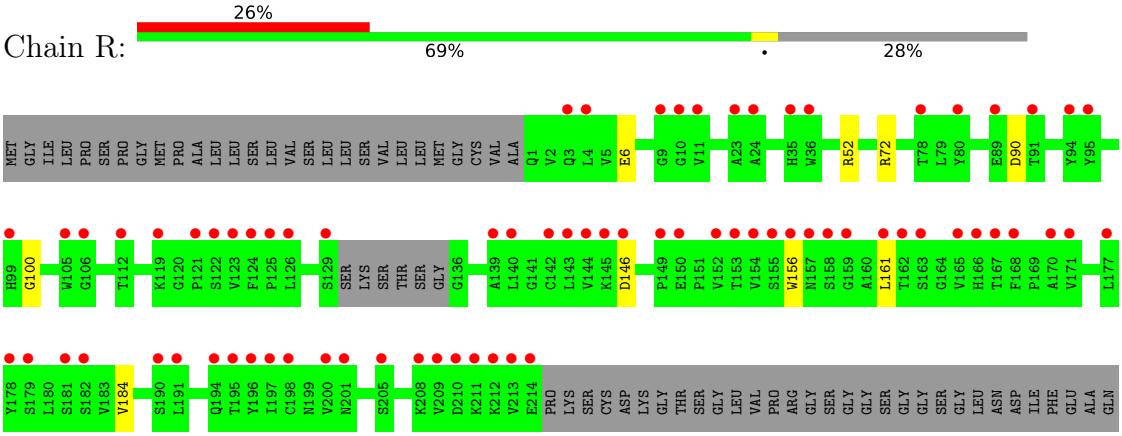
• Molecule 4: Briakinumab FAb Heavy chain

Chain P:



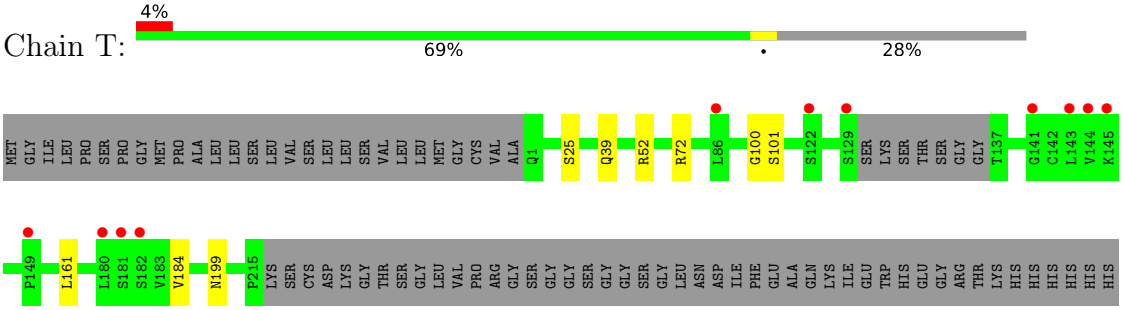
• Molecule 4: Briakinumab FAb Heavy chain

Chain R:



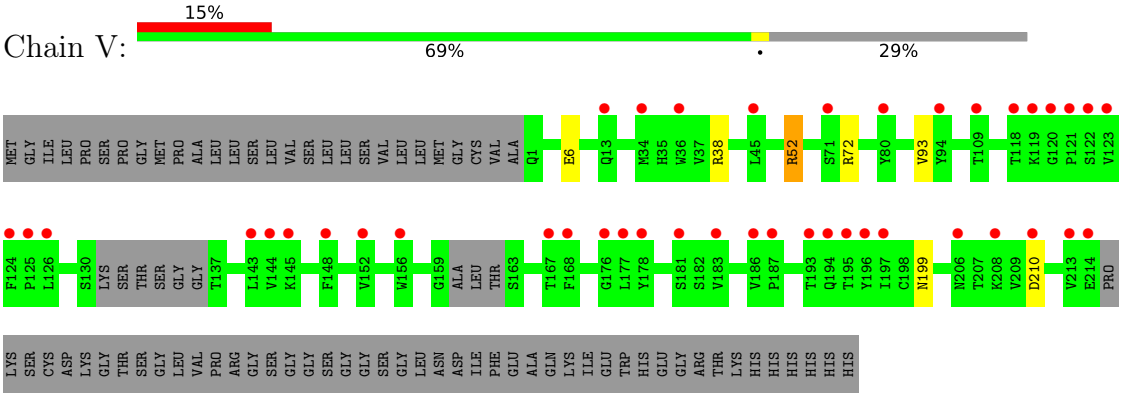
• Molecule 4: Briakinumab FAb Heavy chain

Chain T:



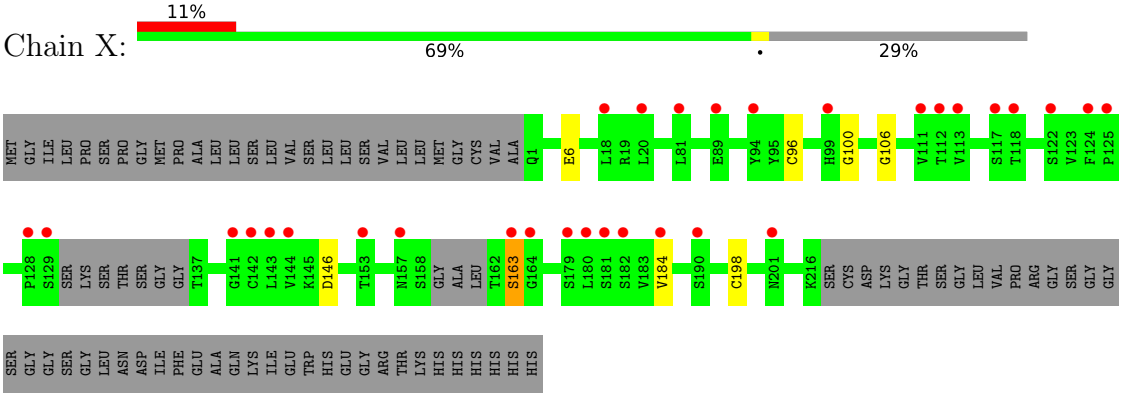
• Molecule 4: Briakinumab FAb Heavy chain

Chain V:



• Molecule 4: Briakinumab FAb Heavy chain

Chain X:

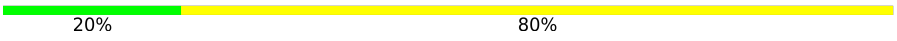


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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.

The worst 5 of 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

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
2	F	140/198 (71%)	124 (89%)	15 (11%)	1 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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

Mol	Chain	Res	Type
4	R	90	ASP
4	X	96	CYS
4	X	198	CYS
4	V	52	ARG
1	G	327	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

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

5.5 Carbohydrates

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

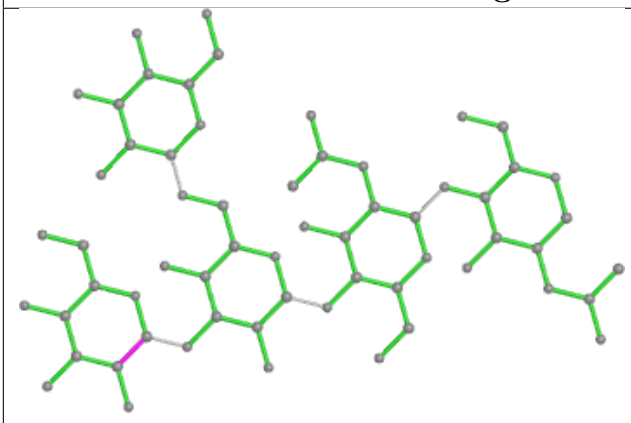
Mol	Chain	Res	Type	Atoms
5	c	1	NAG	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6

There are no ring outliers.

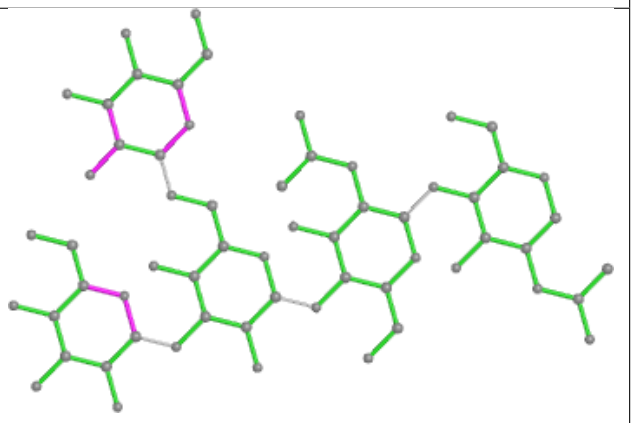
No monomer is involved in short contacts.

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

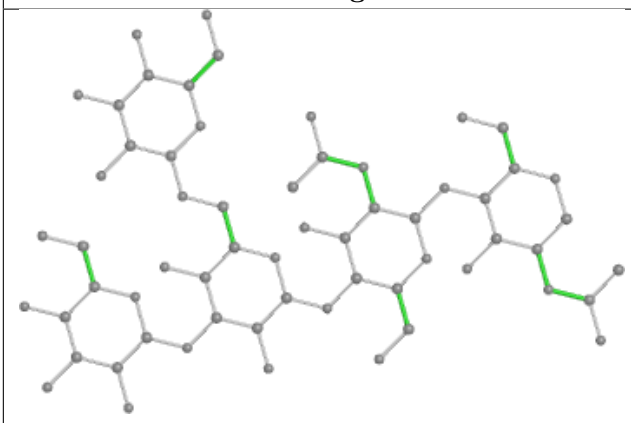
Oligosaccharide Chain Y



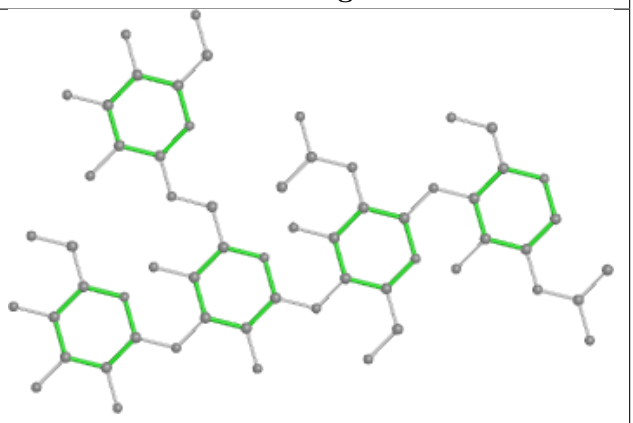
Bond lengths



Bond angles

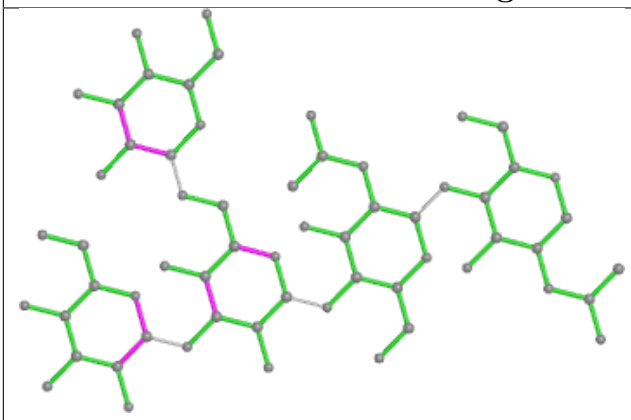


Torsions

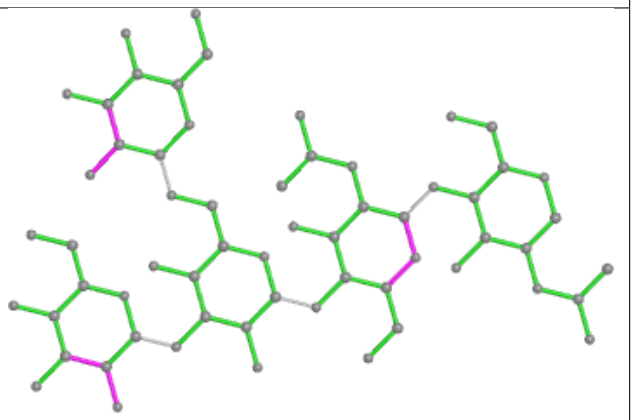


Rings

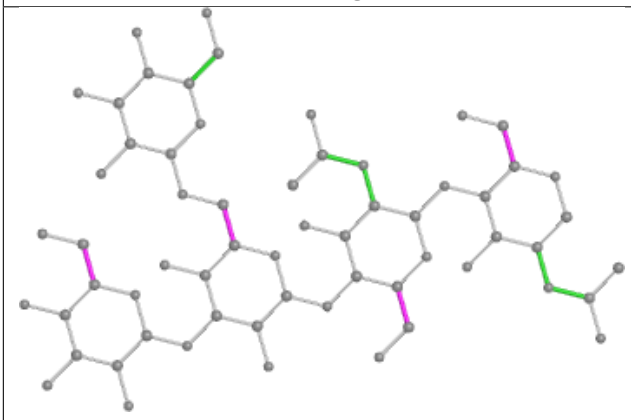
Oligosaccharide Chain Z



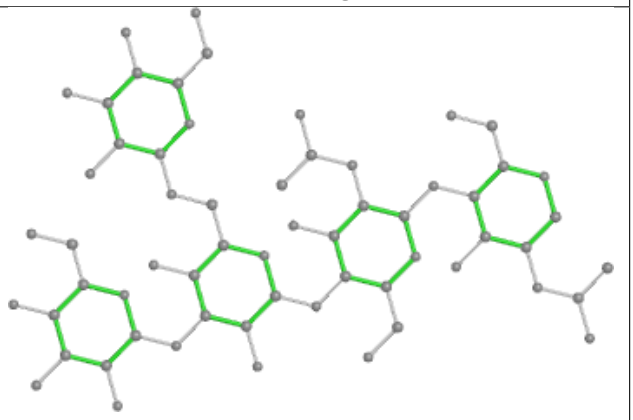
Bond lengths



Bond angles

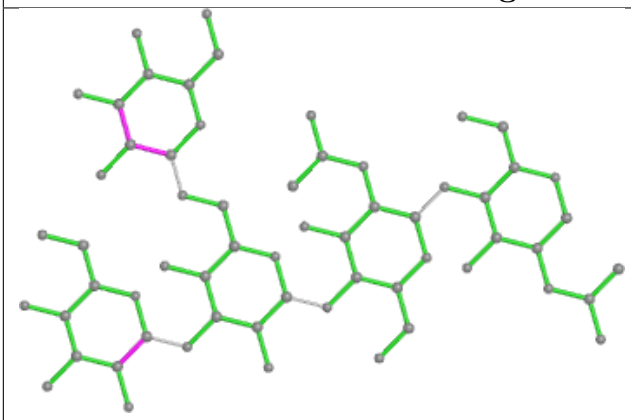


Torsions

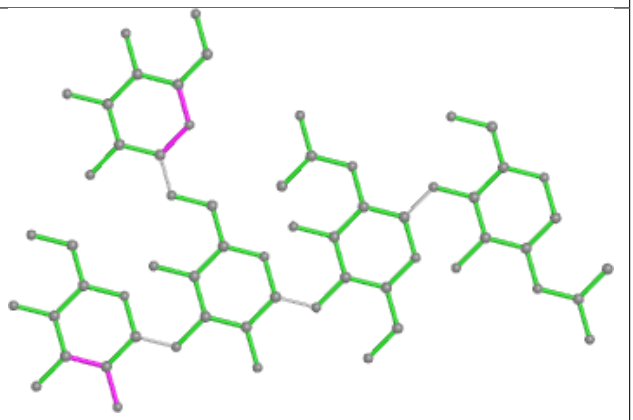


Rings

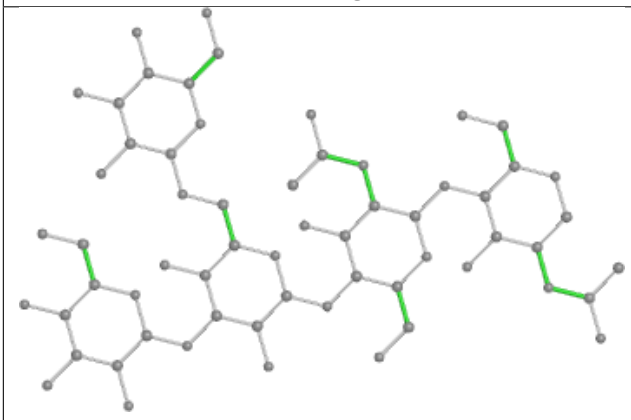
Oligosaccharide Chain a



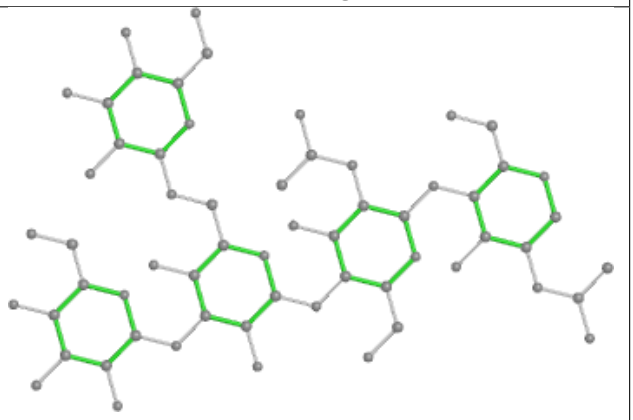
Bond lengths



Bond angles

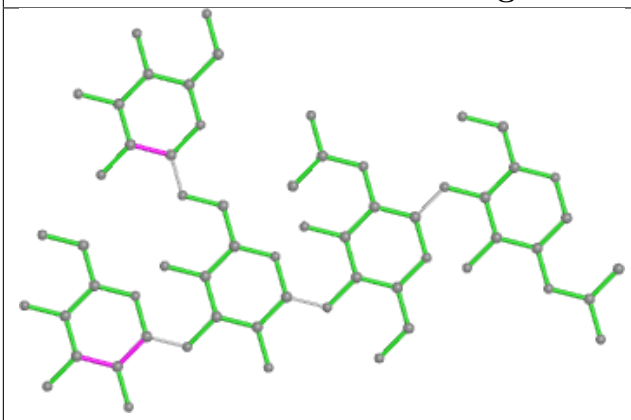


Torsions

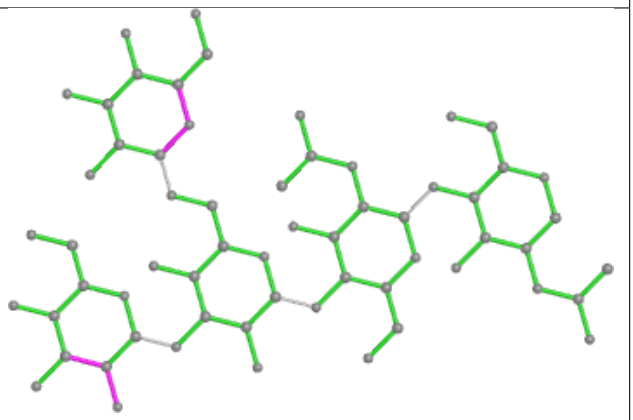


Rings

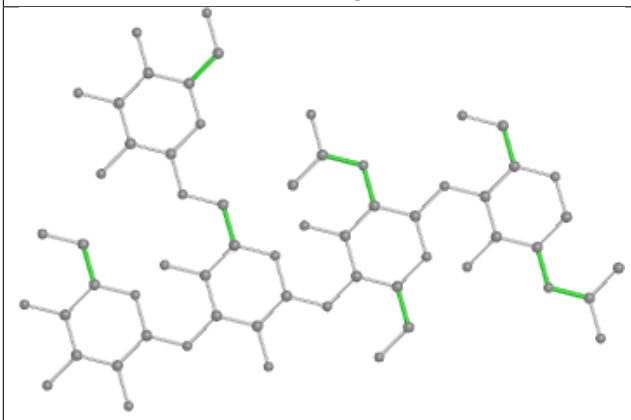
Oligosaccharide Chain b



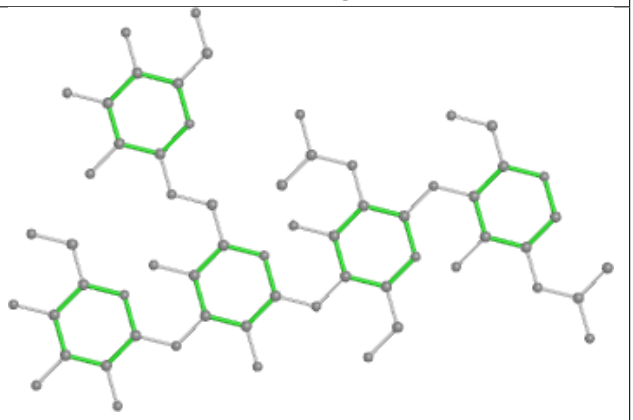
Bond lengths



Bond angles

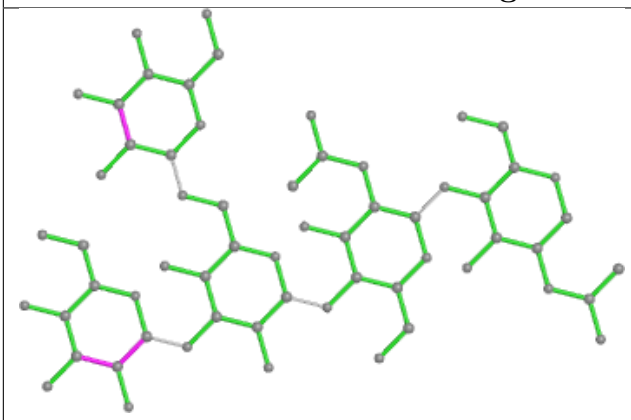


Torsions

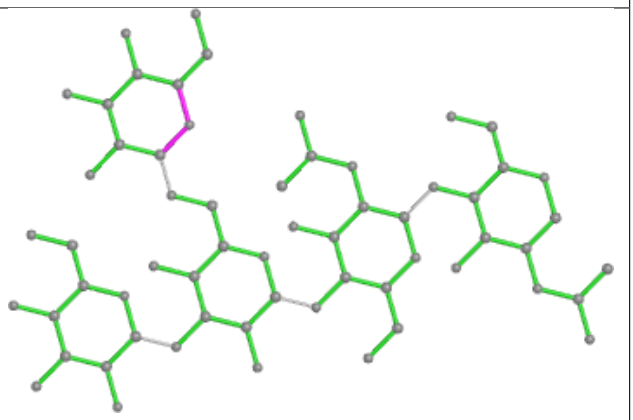


Rings

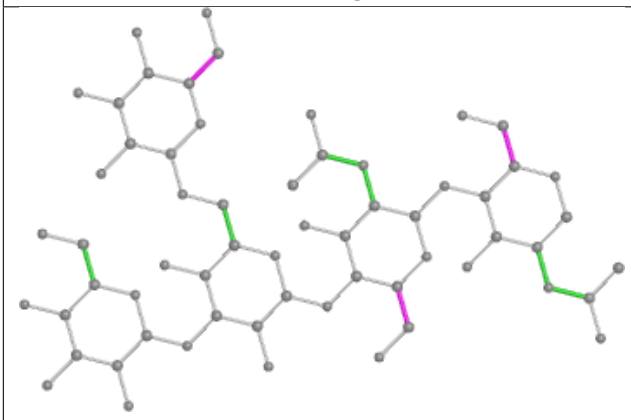
Oligosaccharide Chain c



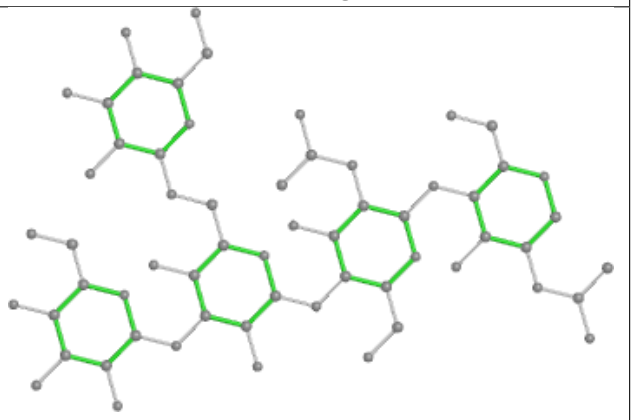
Bond lengths



Bond angles

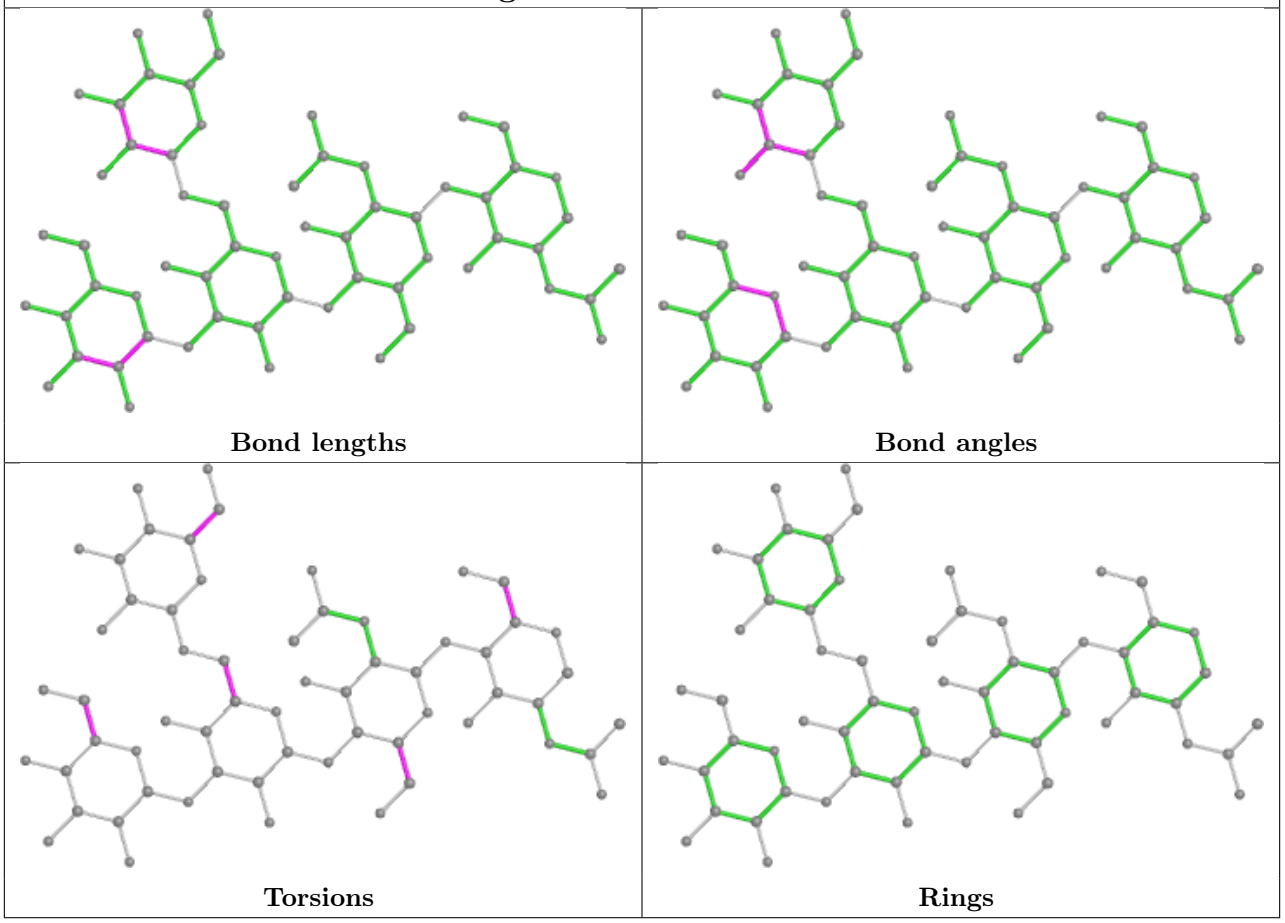


Torsions



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

The worst 5 of 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

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, 95th 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

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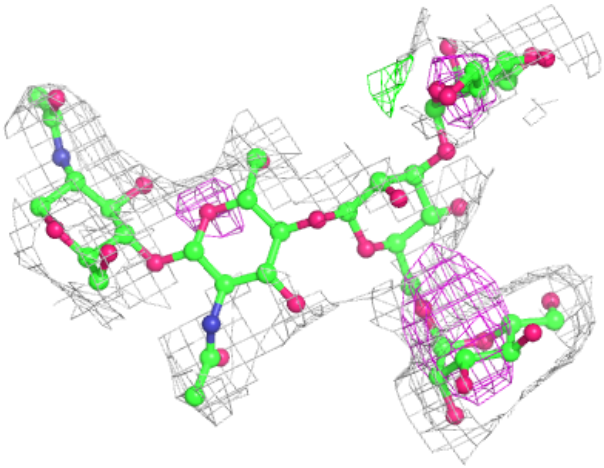
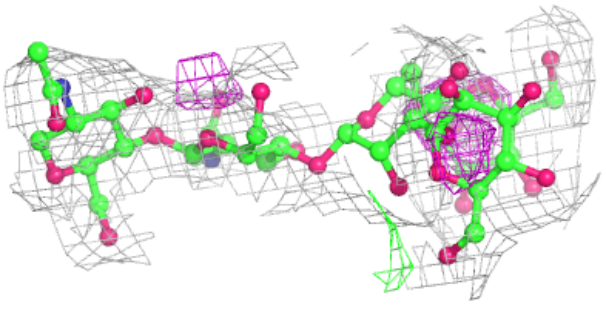
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	a	3	11/12	0.86	0.23	104,107,111,112	0
5	NAG	Z	2	14/15	0.87	0.19	69,71,73,75	0
5	NAG	d	2	14/15	0.88	0.29	103,106,110,112	0
5	NAG	d	1	14/15	0.89	0.23	99,101,103,104	0
5	NAG	b	2	14/15	0.90	0.14	80,81,84,85	0
5	NAG	Y	2	14/15	0.90	0.20	98,100,101,103	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
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

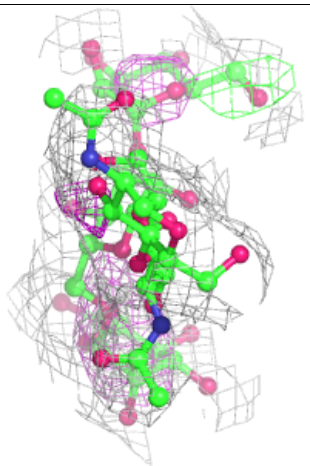
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

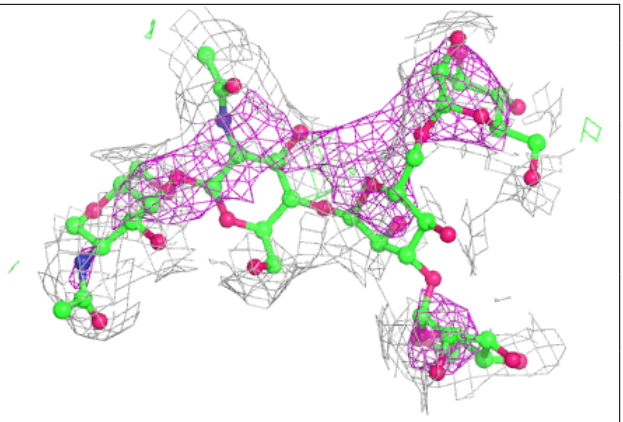


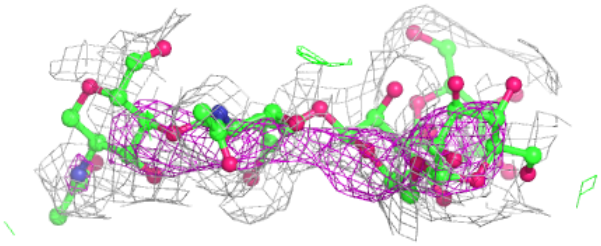




Electron density around Chain Z:

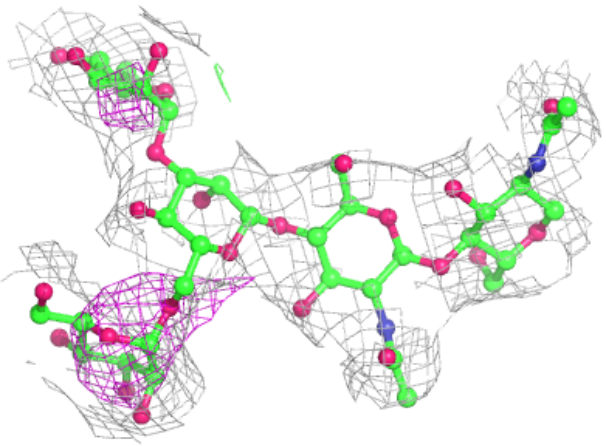
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

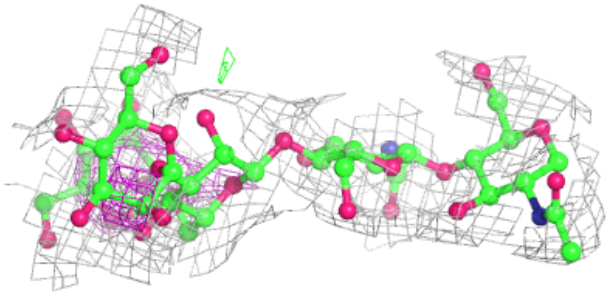


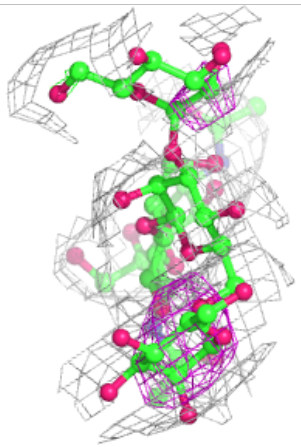


Electron density around Chain a:

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

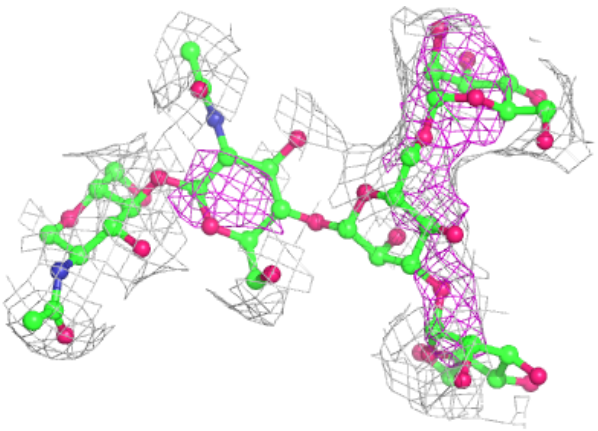


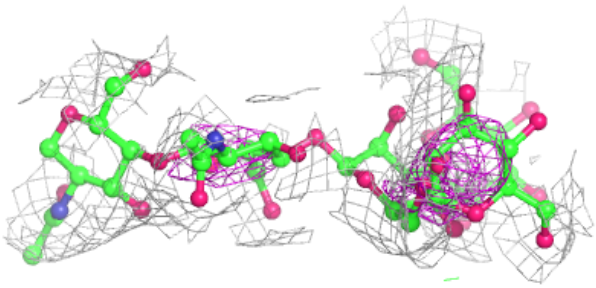


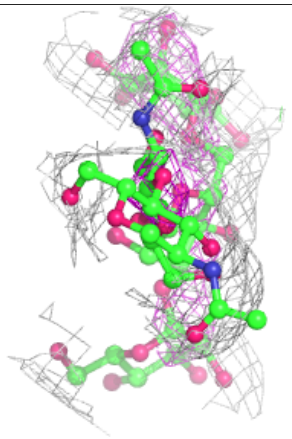


Electron density around Chain b:

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

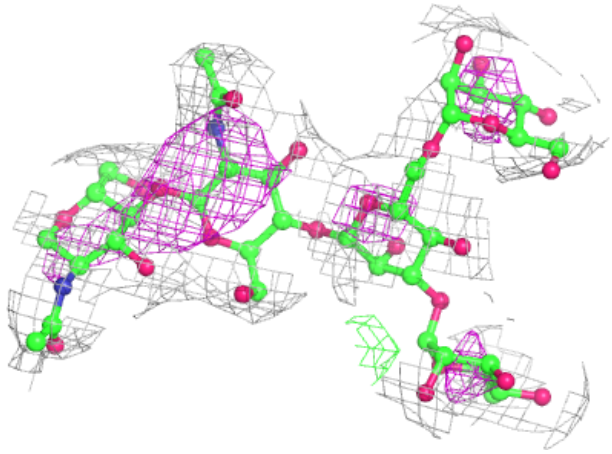


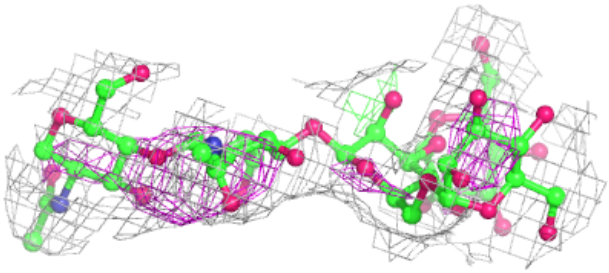


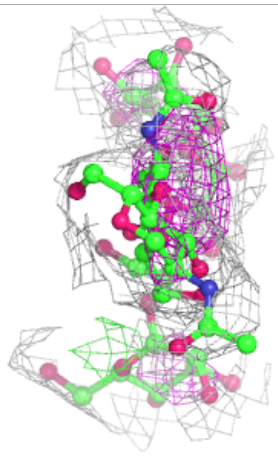


Electron density around Chain c:

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

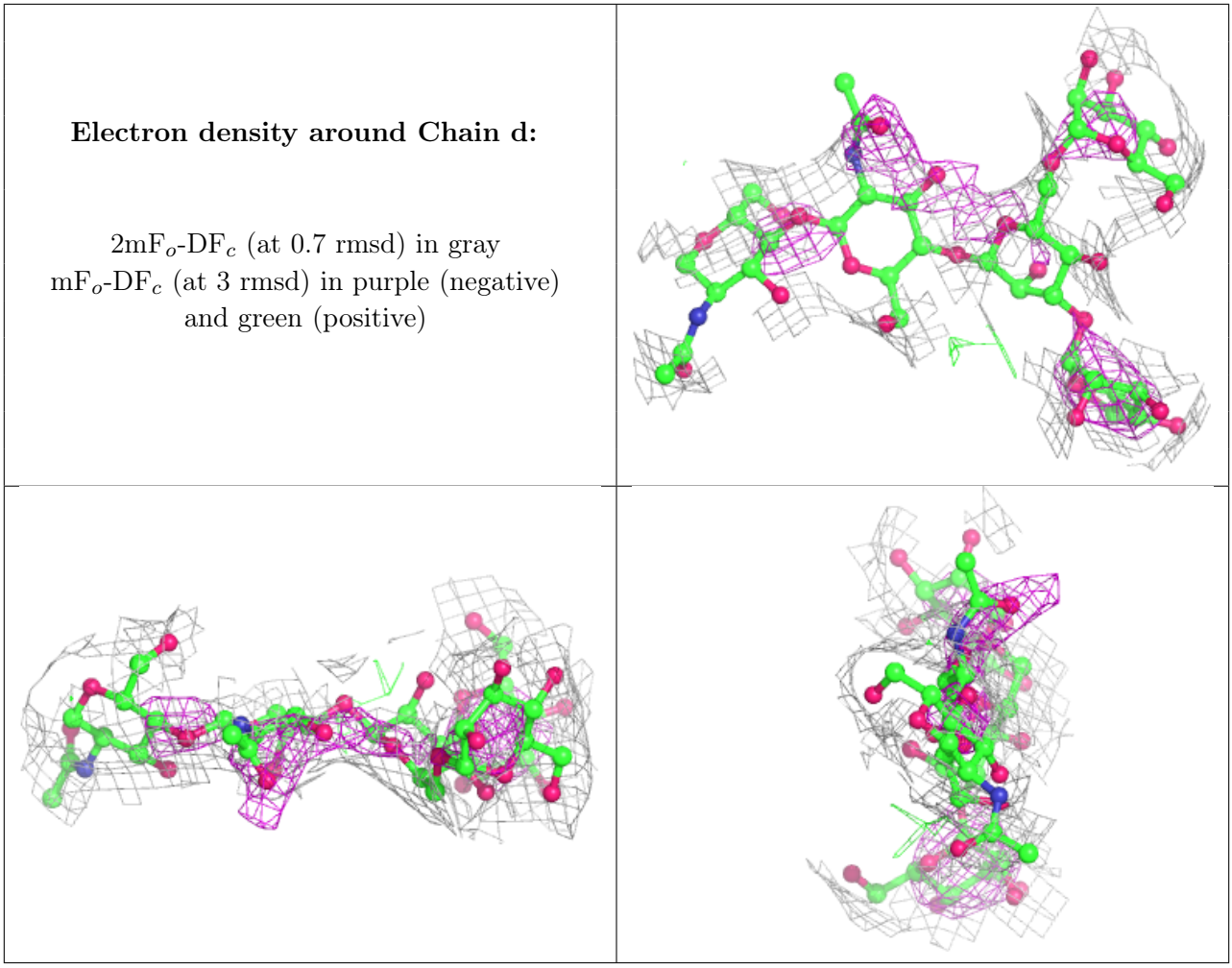






Electron density around Chain d:

$2mF_o$-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.