



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2021 – 10:11 AM EDT

PDB ID : 6WEO
Title : IL-22 Signaling Complex with IL-22R1 and IL-10Rbeta
Authors : Saxton, R.A.; Jude, K.M.; Henneberg, L.T.; Garcia, K.C.
Deposited on : 2020-04-02
Resolution : 2.60 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

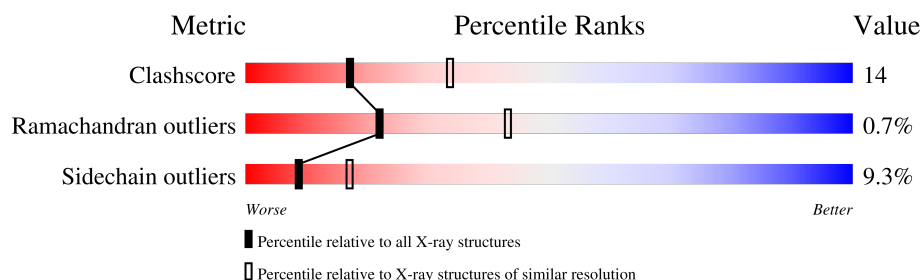
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)


























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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	0	204	61% 31% 5%
1	3	204	58% 30% 7%
1	6	204	58% 33% . .
1	9	204	58% 25% 7% 9%
1	C	204	70% 24% . .
1	E	204	73% 21% . .
1	H	204	65% 27% . .
1	K	204	61% 30% . .




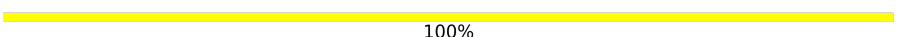
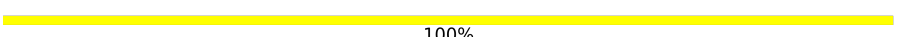

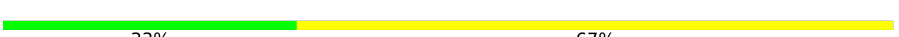

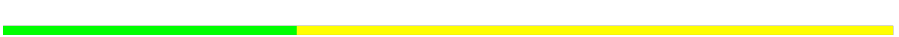

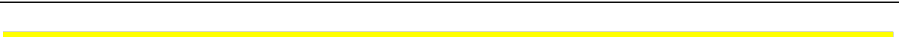
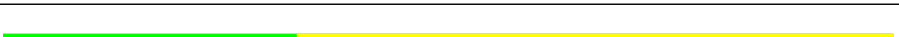

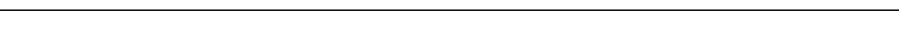
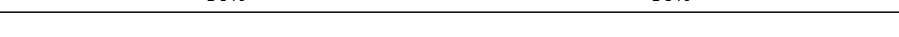
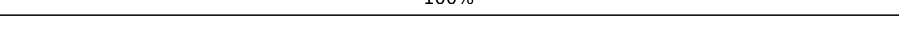
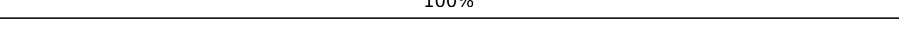
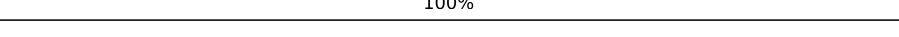
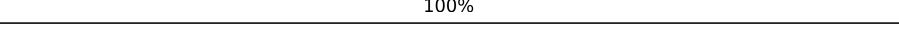
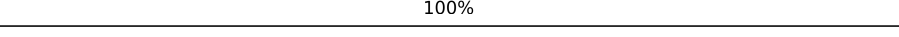





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Mol	Chain	Length	Quality of chain
1	O	204	
1	R	204	
1	U	204	
1	X	204	
2	1	204	
2	4	204	
2	7	204	
2	A	204	
2	B	204	
2	F	204	
2	I	204	
2	M	204	
2	P	204	
2	S	204	
2	V	204	
2	Y	204	
3	2	149	
3	5	149	
3	8	149	
3	D	149	
3	G	149	
3	J	149	
3	L	149	
3	N	149	
3	Q	149	

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Mol	Chain	Length	Quality of chain
3	T	149	
3	W	149	
3	Z	149	
4	a	4	
4	c	4	
4	n	4	
5	b	3	
5	e	3	
5	i	3	
5	j	3	
5	l	3	
5	m	3	
5	s	3	
6	d	2	
6	o	2	
6	p	2	
6	r	2	
6	t	2	
6	u	2	
6	v	2	
7	f	2	
8	g	3	
9	h	5	
9	k	5	
10	q	2	

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Mol	Chain	Length	Quality of chain
11	w	3	 33% 67%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 53140 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-10 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	193	Total	C	N	O	S	0	0	0
			1579	1007	261	303	8			
1	3	195	Total	C	N	O	S	0	0	0
			1595	1016	263	308	8			
1	6	195	Total	C	N	O	S	0	0	0
			1607	1024	266	309	8			
1	9	186	Total	C	N	O	S	0	0	0
			1532	980	254	290	8			
1	C	195	Total	C	N	O	S	0	0	0
			1614	1026	270	310	8			
1	E	195	Total	C	N	O	S	0	0	0
			1593	1014	263	308	8			
1	H	195	Total	C	N	O	S	0	0	0
			1602	1021	264	309	8			
1	K	195	Total	C	N	O	S	0	0	0
			1605	1022	267	308	8			
1	O	196	Total	C	N	O	S	0	0	0
			1609	1025	268	308	8			
1	R	195	Total	C	N	O	S	0	0	0
			1611	1025	269	309	8			
1	U	195	Total	C	N	O	S	0	0	0
			1603	1020	266	309	8			
1	X	197	Total	C	N	O	S	0	0	0
			1619	1031	269	311	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	49	GLN	ASN	conflict	UNP Q61190
0	102	GLN	ASN	conflict	UNP Q61190
0	161	GLN	ASN	conflict	UNP Q61190
0	199	GLN	ASN	conflict	UNP Q61190
0	221	GLY	-	expression tag	UNP Q61190

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Chain	Residue	Modelled	Actual	Comment	Reference
0	222	GLY	-	expression tag	UNP Q61190
0	223	SER	-	expression tag	UNP Q61190
3	49	GLN	ASN	conflict	UNP Q61190
3	102	GLN	ASN	conflict	UNP Q61190
3	161	GLN	ASN	conflict	UNP Q61190
3	199	GLN	ASN	conflict	UNP Q61190
3	221	GLY	-	expression tag	UNP Q61190
3	222	GLY	-	expression tag	UNP Q61190
3	223	SER	-	expression tag	UNP Q61190
6	49	GLN	ASN	conflict	UNP Q61190
6	102	GLN	ASN	conflict	UNP Q61190
6	161	GLN	ASN	conflict	UNP Q61190
6	199	GLN	ASN	conflict	UNP Q61190
6	221	GLY	-	expression tag	UNP Q61190
6	222	GLY	-	expression tag	UNP Q61190
6	223	SER	-	expression tag	UNP Q61190
9	49	GLN	ASN	conflict	UNP Q61190
9	102	GLN	ASN	conflict	UNP Q61190
9	161	GLN	ASN	conflict	UNP Q61190
9	199	GLN	ASN	conflict	UNP Q61190
9	221	GLY	-	expression tag	UNP Q61190
9	222	GLY	-	expression tag	UNP Q61190
9	223	SER	-	expression tag	UNP Q61190
C	49	GLN	ASN	conflict	UNP Q61190
C	102	GLN	ASN	conflict	UNP Q61190
C	161	GLN	ASN	conflict	UNP Q61190
C	199	GLN	ASN	conflict	UNP Q61190
C	221	GLY	-	expression tag	UNP Q61190
C	222	GLY	-	expression tag	UNP Q61190
C	223	SER	-	expression tag	UNP Q61190
E	49	GLN	ASN	conflict	UNP Q61190
E	102	GLN	ASN	conflict	UNP Q61190
E	161	GLN	ASN	conflict	UNP Q61190
E	199	GLN	ASN	conflict	UNP Q61190
E	221	GLY	-	expression tag	UNP Q61190
E	222	GLY	-	expression tag	UNP Q61190
E	223	SER	-	expression tag	UNP Q61190
H	49	GLN	ASN	conflict	UNP Q61190
H	102	GLN	ASN	conflict	UNP Q61190
H	161	GLN	ASN	conflict	UNP Q61190
H	199	GLN	ASN	conflict	UNP Q61190
H	221	GLY	-	expression tag	UNP Q61190

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Chain	Residue	Modelled	Actual	Comment	Reference
H	222	GLY	-	expression tag	UNP Q61190
H	223	SER	-	expression tag	UNP Q61190
K	49	GLN	ASN	conflict	UNP Q61190
K	102	GLN	ASN	conflict	UNP Q61190
K	161	GLN	ASN	conflict	UNP Q61190
K	199	GLN	ASN	conflict	UNP Q61190
K	221	GLY	-	expression tag	UNP Q61190
K	222	GLY	-	expression tag	UNP Q61190
K	223	SER	-	expression tag	UNP Q61190
O	49	GLN	ASN	conflict	UNP Q61190
O	102	GLN	ASN	conflict	UNP Q61190
O	161	GLN	ASN	conflict	UNP Q61190
O	199	GLN	ASN	conflict	UNP Q61190
O	221	GLY	-	expression tag	UNP Q61190
O	222	GLY	-	expression tag	UNP Q61190
O	223	SER	-	expression tag	UNP Q61190
R	49	GLN	ASN	conflict	UNP Q61190
R	102	GLN	ASN	conflict	UNP Q61190
R	161	GLN	ASN	conflict	UNP Q61190
R	199	GLN	ASN	conflict	UNP Q61190
R	221	GLY	-	expression tag	UNP Q61190
R	222	GLY	-	expression tag	UNP Q61190
R	223	SER	-	expression tag	UNP Q61190
U	49	GLN	ASN	conflict	UNP Q61190
U	102	GLN	ASN	conflict	UNP Q61190
U	161	GLN	ASN	conflict	UNP Q61190
U	199	GLN	ASN	conflict	UNP Q61190
U	221	GLY	-	expression tag	UNP Q61190
U	222	GLY	-	expression tag	UNP Q61190
U	223	SER	-	expression tag	UNP Q61190
X	49	GLN	ASN	conflict	UNP Q61190
X	102	GLN	ASN	conflict	UNP Q61190
X	161	GLN	ASN	conflict	UNP Q61190
X	199	GLN	ASN	conflict	UNP Q61190
X	221	GLY	-	expression tag	UNP Q61190
X	222	GLY	-	expression tag	UNP Q61190
X	223	SER	-	expression tag	UNP Q61190

- Molecule 2 is a protein called Interleukin-22 receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	201	Total	C	N	O	S	0	0	0
			1613	1032	270	303	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	4	201	Total	C	N	O	S	0	0	0
			1610	1030	269	303	8			
2	7	201	Total	C	N	O	S	0	0	0
			1604	1027	266	303	8			
2	A	201	Total	C	N	O	S	0	0	0
			1605	1026	268	303	8			
2	B	201	Total	C	N	O	S	0	0	0
			1609	1029	269	303	8			
2	F	201	Total	C	N	O	S	0	0	0
			1608	1030	267	303	8			
2	I	201	Total	C	N	O	S	0	0	0
			1614	1032	269	305	8			
2	M	201	Total	C	N	O	S	0	0	0
			1605	1029	265	303	8			
2	P	201	Total	C	N	O	S	0	0	0
			1621	1037	271	305	8			
2	S	201	Total	C	N	O	S	0	0	0
			1617	1035	271	303	8			
2	V	201	Total	C	N	O	S	0	0	0
			1611	1032	268	303	8			
2	Y	201	Total	C	N	O	S	0	0	0
			1610	1032	265	305	8			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	80	ASP	ASN	conflict	UNP Q80XZ4
1	87	ASP	ASN	conflict	UNP Q80XZ4
1	89	GLN	THR	conflict	UNP Q80XZ4
1	225	GLY	-	expression tag	UNP Q80XZ4
1	226	GLY	-	expression tag	UNP Q80XZ4
1	227	SER	-	expression tag	UNP Q80XZ4
4	80	ASP	ASN	conflict	UNP Q80XZ4
4	87	ASP	ASN	conflict	UNP Q80XZ4
4	89	GLN	THR	conflict	UNP Q80XZ4
4	225	GLY	-	expression tag	UNP Q80XZ4
4	226	GLY	-	expression tag	UNP Q80XZ4
4	227	SER	-	expression tag	UNP Q80XZ4
7	80	ASP	ASN	conflict	UNP Q80XZ4
7	87	ASP	ASN	conflict	UNP Q80XZ4
7	89	GLN	THR	conflict	UNP Q80XZ4
7	225	GLY	-	expression tag	UNP Q80XZ4
7	226	GLY	-	expression tag	UNP Q80XZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
7	227	SER	-	expression tag	UNP Q80XZ4
A	80	ASP	ASN	conflict	UNP Q80XZ4
A	87	ASP	ASN	conflict	UNP Q80XZ4
A	89	GLN	THR	conflict	UNP Q80XZ4
A	225	GLY	-	expression tag	UNP Q80XZ4
A	226	GLY	-	expression tag	UNP Q80XZ4
A	227	SER	-	expression tag	UNP Q80XZ4
B	80	ASP	ASN	conflict	UNP Q80XZ4
B	87	ASP	ASN	conflict	UNP Q80XZ4
B	89	GLN	THR	conflict	UNP Q80XZ4
B	225	GLY	-	expression tag	UNP Q80XZ4
B	226	GLY	-	expression tag	UNP Q80XZ4
B	227	SER	-	expression tag	UNP Q80XZ4
F	80	ASP	ASN	conflict	UNP Q80XZ4
F	87	ASP	ASN	conflict	UNP Q80XZ4
F	89	GLN	THR	conflict	UNP Q80XZ4
F	225	GLY	-	expression tag	UNP Q80XZ4
F	226	GLY	-	expression tag	UNP Q80XZ4
F	227	SER	-	expression tag	UNP Q80XZ4
I	80	ASP	ASN	conflict	UNP Q80XZ4
I	87	ASP	ASN	conflict	UNP Q80XZ4
I	89	GLN	THR	conflict	UNP Q80XZ4
I	225	GLY	-	expression tag	UNP Q80XZ4
I	226	GLY	-	expression tag	UNP Q80XZ4
I	227	SER	-	expression tag	UNP Q80XZ4
M	80	ASP	ASN	conflict	UNP Q80XZ4
M	87	ASP	ASN	conflict	UNP Q80XZ4
M	89	GLN	THR	conflict	UNP Q80XZ4
M	225	GLY	-	expression tag	UNP Q80XZ4
M	226	GLY	-	expression tag	UNP Q80XZ4
M	227	SER	-	expression tag	UNP Q80XZ4
P	80	ASP	ASN	conflict	UNP Q80XZ4
P	87	ASP	ASN	conflict	UNP Q80XZ4
P	89	GLN	THR	conflict	UNP Q80XZ4
P	225	GLY	-	expression tag	UNP Q80XZ4
P	226	GLY	-	expression tag	UNP Q80XZ4
P	227	SER	-	expression tag	UNP Q80XZ4
S	80	ASP	ASN	conflict	UNP Q80XZ4
S	87	ASP	ASN	conflict	UNP Q80XZ4
S	89	GLN	THR	conflict	UNP Q80XZ4
S	225	GLY	-	expression tag	UNP Q80XZ4
S	226	GLY	-	expression tag	UNP Q80XZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
S	227	SER	-	expression tag	UNP Q80XZ4
V	80	ASP	ASN	conflict	UNP Q80XZ4
V	87	ASP	ASN	conflict	UNP Q80XZ4
V	89	GLN	THR	conflict	UNP Q80XZ4
V	225	GLY	-	expression tag	UNP Q80XZ4
V	226	GLY	-	expression tag	UNP Q80XZ4
V	227	SER	-	expression tag	UNP Q80XZ4
Y	80	ASP	ASN	conflict	UNP Q80XZ4
Y	87	ASP	ASN	conflict	UNP Q80XZ4
Y	89	GLN	THR	conflict	UNP Q80XZ4
Y	225	GLY	-	expression tag	UNP Q80XZ4
Y	226	GLY	-	expression tag	UNP Q80XZ4
Y	227	SER	-	expression tag	UNP Q80XZ4

- Molecule 3 is a protein called Interleukin-22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	140	Total	C	N	O	S	0	0	0
			1096	700	186	202	8			
3	5	141	Total	C	N	O	S	0	0	0
			1126	715	197	206	8			
3	8	140	Total	C	N	O	S	0	0	0
			1107	704	191	204	8			
3	D	141	Total	C	N	O	S	0	0	0
			1131	718	198	207	8			
3	G	141	Total	C	N	O	S	0	0	0
			1123	715	196	204	8			
3	J	140	Total	C	N	O	S	0	0	0
			1117	711	193	205	8			
3	L	141	Total	C	N	O	S	0	0	0
			1125	716	195	206	8			
3	N	140	Total	C	N	O	S	0	0	0
			1093	695	187	203	8			
3	Q	142	Total	C	N	O	S	0	0	0
			1120	713	191	208	8			
3	T	142	Total	C	N	O	S	0	0	0
			1133	720	196	209	8			
3	W	141	Total	C	N	O	S	0	0	0
			1124	714	195	207	8			
3	Z	141	Total	C	N	O	S	0	0	0
			1129	718	197	206	8			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	43	HIS	GLU	conflict	UNP Q9JJY9
2	45	ARG	SER	conflict	UNP Q9JJY9
2	49	SER	GLN	conflict	UNP Q9JJY9
2	68	GLN	ASN	conflict	UNP Q9JJY9
2	97	GLN	ASN	conflict	UNP Q9JJY9
2	116	TRP	GLN	conflict	UNP Q9JJY9
2	128	LYS	GLN	conflict	UNP Q9JJY9
2	180	GLY	-	expression tag	UNP Q9JJY9
2	181	GLY	-	expression tag	UNP Q9JJY9
2	182	SER	-	expression tag	UNP Q9JJY9
5	43	HIS	GLU	conflict	UNP Q9JJY9
5	45	ARG	SER	conflict	UNP Q9JJY9
5	49	SER	GLN	conflict	UNP Q9JJY9
5	68	GLN	ASN	conflict	UNP Q9JJY9
5	97	GLN	ASN	conflict	UNP Q9JJY9
5	116	TRP	GLN	conflict	UNP Q9JJY9
5	128	LYS	GLN	conflict	UNP Q9JJY9
5	180	GLY	-	expression tag	UNP Q9JJY9
5	181	GLY	-	expression tag	UNP Q9JJY9
5	182	SER	-	expression tag	UNP Q9JJY9
8	43	HIS	GLU	conflict	UNP Q9JJY9
8	45	ARG	SER	conflict	UNP Q9JJY9
8	49	SER	GLN	conflict	UNP Q9JJY9
8	68	GLN	ASN	conflict	UNP Q9JJY9
8	97	GLN	ASN	conflict	UNP Q9JJY9
8	116	TRP	GLN	conflict	UNP Q9JJY9
8	128	LYS	GLN	conflict	UNP Q9JJY9
8	180	GLY	-	expression tag	UNP Q9JJY9
8	181	GLY	-	expression tag	UNP Q9JJY9
8	182	SER	-	expression tag	UNP Q9JJY9
D	43	HIS	GLU	conflict	UNP Q9JJY9
D	45	ARG	SER	conflict	UNP Q9JJY9
D	49	SER	GLN	conflict	UNP Q9JJY9
D	68	GLN	ASN	conflict	UNP Q9JJY9
D	97	GLN	ASN	conflict	UNP Q9JJY9
D	116	TRP	GLN	conflict	UNP Q9JJY9
D	128	LYS	GLN	conflict	UNP Q9JJY9
D	180	GLY	-	expression tag	UNP Q9JJY9
D	181	GLY	-	expression tag	UNP Q9JJY9
D	182	SER	-	expression tag	UNP Q9JJY9
G	43	HIS	GLU	conflict	UNP Q9JJY9
G	45	ARG	SER	conflict	UNP Q9JJY9
G	49	SER	GLN	conflict	UNP Q9JJY9

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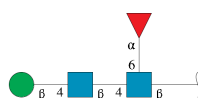
Chain	Residue	Modelled	Actual	Comment	Reference
G	68	GLN	ASN	conflict	UNP Q9JJY9
G	97	GLN	ASN	conflict	UNP Q9JJY9
G	116	TRP	GLN	conflict	UNP Q9JJY9
G	128	LYS	GLN	conflict	UNP Q9JJY9
G	180	GLY	-	expression tag	UNP Q9JJY9
G	181	GLY	-	expression tag	UNP Q9JJY9
G	182	SER	-	expression tag	UNP Q9JJY9
J	43	HIS	GLU	conflict	UNP Q9JJY9
J	45	ARG	SER	conflict	UNP Q9JJY9
J	49	SER	GLN	conflict	UNP Q9JJY9
J	68	GLN	ASN	conflict	UNP Q9JJY9
J	97	GLN	ASN	conflict	UNP Q9JJY9
J	116	TRP	GLN	conflict	UNP Q9JJY9
J	128	LYS	GLN	conflict	UNP Q9JJY9
J	180	GLY	-	expression tag	UNP Q9JJY9
J	181	GLY	-	expression tag	UNP Q9JJY9
J	182	SER	-	expression tag	UNP Q9JJY9
L	43	HIS	GLU	conflict	UNP Q9JJY9
L	45	ARG	SER	conflict	UNP Q9JJY9
L	49	SER	GLN	conflict	UNP Q9JJY9
L	68	GLN	ASN	conflict	UNP Q9JJY9
L	97	GLN	ASN	conflict	UNP Q9JJY9
L	116	TRP	GLN	conflict	UNP Q9JJY9
L	128	LYS	GLN	conflict	UNP Q9JJY9
L	180	GLY	-	expression tag	UNP Q9JJY9
L	181	GLY	-	expression tag	UNP Q9JJY9
L	182	SER	-	expression tag	UNP Q9JJY9
N	43	HIS	GLU	conflict	UNP Q9JJY9
N	45	ARG	SER	conflict	UNP Q9JJY9
N	49	SER	GLN	conflict	UNP Q9JJY9
N	68	GLN	ASN	conflict	UNP Q9JJY9
N	97	GLN	ASN	conflict	UNP Q9JJY9
N	116	TRP	GLN	conflict	UNP Q9JJY9
N	128	LYS	GLN	conflict	UNP Q9JJY9
N	180	GLY	-	expression tag	UNP Q9JJY9
N	181	GLY	-	expression tag	UNP Q9JJY9
N	182	SER	-	expression tag	UNP Q9JJY9
Q	43	HIS	GLU	conflict	UNP Q9JJY9
Q	45	ARG	SER	conflict	UNP Q9JJY9
Q	49	SER	GLN	conflict	UNP Q9JJY9
Q	68	GLN	ASN	conflict	UNP Q9JJY9
Q	97	GLN	ASN	conflict	UNP Q9JJY9

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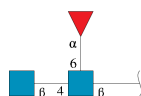
Chain	Residue	Modelled	Actual	Comment	Reference
Q	116	TRP	GLN	conflict	UNP Q9JJY9
Q	128	LYS	GLN	conflict	UNP Q9JJY9
Q	180	GLY	-	expression tag	UNP Q9JJY9
Q	181	GLY	-	expression tag	UNP Q9JJY9
Q	182	SER	-	expression tag	UNP Q9JJY9
T	43	HIS	GLU	conflict	UNP Q9JJY9
T	45	ARG	SER	conflict	UNP Q9JJY9
T	49	SER	GLN	conflict	UNP Q9JJY9
T	68	GLN	ASN	conflict	UNP Q9JJY9
T	97	GLN	ASN	conflict	UNP Q9JJY9
T	116	TRP	GLN	conflict	UNP Q9JJY9
T	128	LYS	GLN	conflict	UNP Q9JJY9
T	180	GLY	-	expression tag	UNP Q9JJY9
T	181	GLY	-	expression tag	UNP Q9JJY9
T	182	SER	-	expression tag	UNP Q9JJY9
W	43	HIS	GLU	conflict	UNP Q9JJY9
W	45	ARG	SER	conflict	UNP Q9JJY9
W	49	SER	GLN	conflict	UNP Q9JJY9
W	68	GLN	ASN	conflict	UNP Q9JJY9
W	97	GLN	ASN	conflict	UNP Q9JJY9
W	116	TRP	GLN	conflict	UNP Q9JJY9
W	128	LYS	GLN	conflict	UNP Q9JJY9
W	180	GLY	-	expression tag	UNP Q9JJY9
W	181	GLY	-	expression tag	UNP Q9JJY9
W	182	SER	-	expression tag	UNP Q9JJY9
Z	43	HIS	GLU	conflict	UNP Q9JJY9
Z	45	ARG	SER	conflict	UNP Q9JJY9
Z	49	SER	GLN	conflict	UNP Q9JJY9
Z	68	GLN	ASN	conflict	UNP Q9JJY9
Z	97	GLN	ASN	conflict	UNP Q9JJY9
Z	116	TRP	GLN	conflict	UNP Q9JJY9
Z	128	LYS	GLN	conflict	UNP Q9JJY9
Z	180	GLY	-	expression tag	UNP Q9JJY9
Z	181	GLY	-	expression tag	UNP Q9JJY9
Z	182	SER	-	expression tag	UNP Q9JJY9

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	a	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	c	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	n	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	b	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	e	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	i	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	j	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	l	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	m	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	s	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	d	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	o	2	Total	C	N	O	0	0	0
			24	14	1	9			

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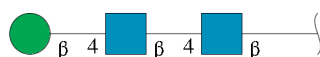
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	p	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	r	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	t	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	u	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	v	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



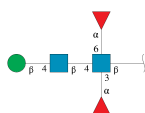
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	f	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 8 is an oligosaccharide called 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
8	g	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



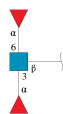
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	h	5	Total	C	N	O	0	0	0
			59	34	2	23			
9	k	5	Total	C	N	O	0	0	0
			59	34	2	23			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	w	3	Total	C	N	O	0	0	0
			34	20	1	13			

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			6	3	3		
12	H	1	Total	C	O	0	0
			6	3	3		
12	J	1	Total	C	O	0	0
			6	3	3		
12	K	1	Total	C	O	0	0
			6	3	3		
12	M	1	Total	C	O	0	0
			6	3	3		
12	O	1	Total	C	O	0	0
			6	3	3		
12	Y	1	Total	C	O	0	0
			6	3	3		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	1	9	Total	O	0	0
			9	9		
14	2	6	Total	O	0	0
			6	6		
14	3	6	Total	O	0	0
			6	6		
14	4	7	Total	O	0	0
			7	7		
14	5	2	Total	O	0	0
			2	2		
14	6	5	Total	O	0	0
			5	5		
14	7	12	Total	O	0	0
			12	12		
14	8	6	Total	O	0	0
			6	6		
14	9	3	Total	O	0	0
			3	3		
14	A	22	Total	O	0	0
			22	22		
14	B	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	22	Total 22	O 22	0	0
14	D	14	Total 14	O 14	0	0
14	E	15	Total 15	O 15	0	0
14	F	10	Total 10	O 10	0	0
14	G	5	Total 5	O 5	0	0
14	H	17	Total 17	O 17	0	0
14	I	9	Total 9	O 9	0	0
14	J	6	Total 6	O 6	0	0
14	K	9	Total 9	O 9	0	0
14	L	8	Total 8	O 8	0	0
14	M	8	Total 8	O 8	0	0
14	N	5	Total 5	O 5	0	0
14	O	14	Total 14	O 14	0	0
14	P	6	Total 6	O 6	0	0
14	Q	7	Total 7	O 7	0	0
14	R	9	Total 9	O 9	0	0
14	S	13	Total 13	O 13	0	0
14	T	6	Total 6	O 6	0	0
14	U	14	Total 14	O 14	0	0
14	V	12	Total 12	O 12	0	0
14	W	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	X	11	Total 11	O 11	0	0
14	Y	20	Total 20	O 20	0	0
14	Z	5	Total 5	O 5	0	0

3 Residue-property plots

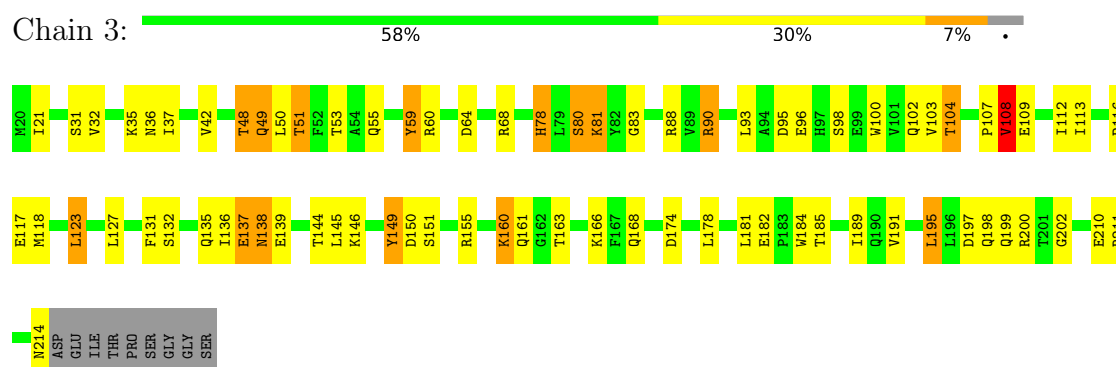
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

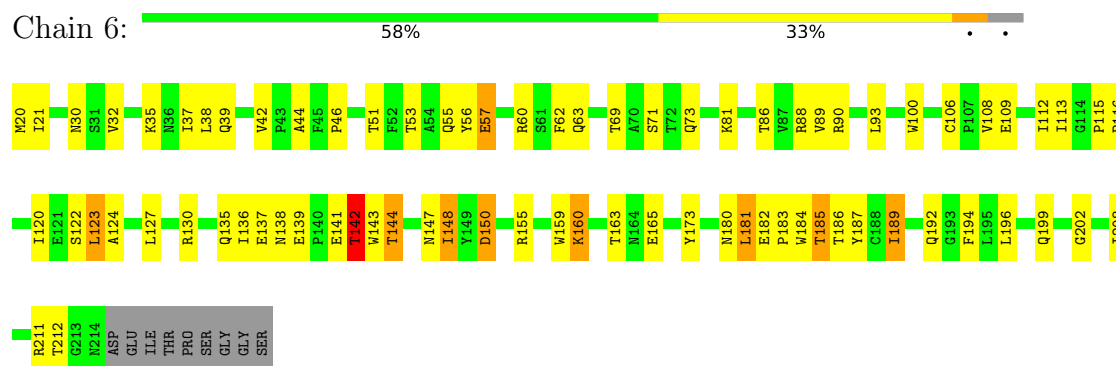
- Molecule 1: Interleukin-10 receptor subunit beta



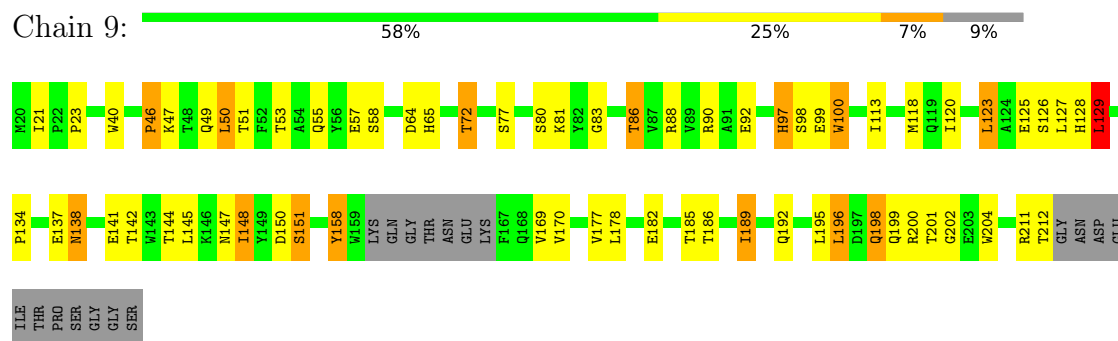
- Molecule 1: Interleukin-10 receptor subunit beta



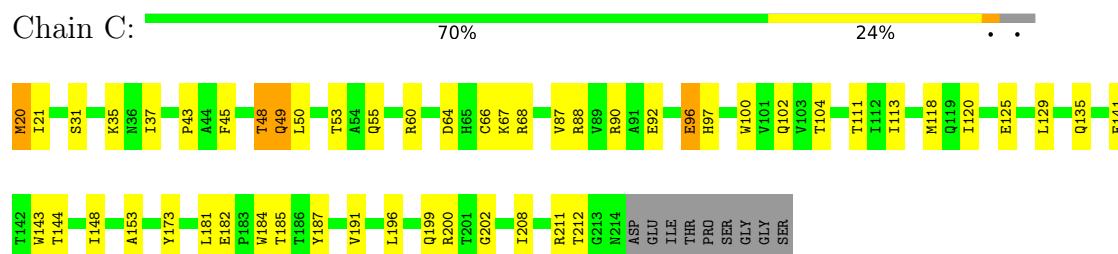
- Molecule 1: Interleukin-10 receptor subunit beta



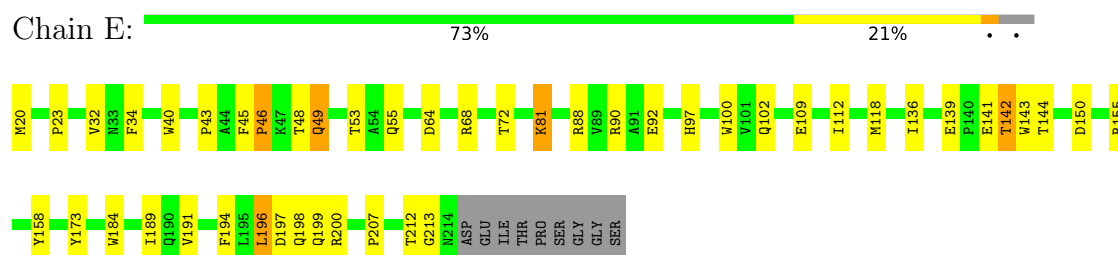
- Molecule 1: Interleukin-10 receptor subunit beta



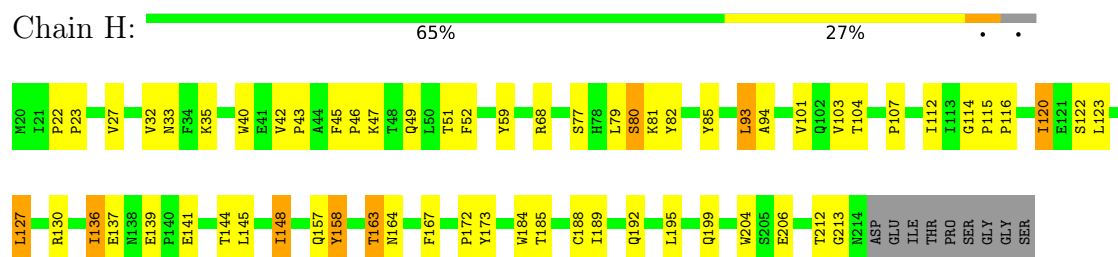
- Molecule 1: Interleukin-10 receptor subunit beta



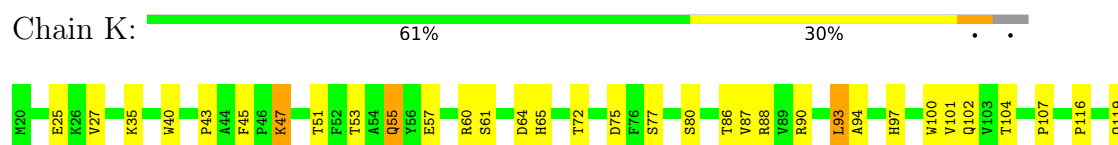
- Molecule 1: Interleukin-10 receptor subunit beta

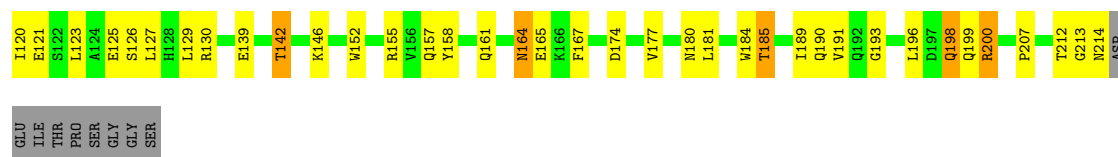


- Molecule 1: Interleukin-10 receptor subunit beta



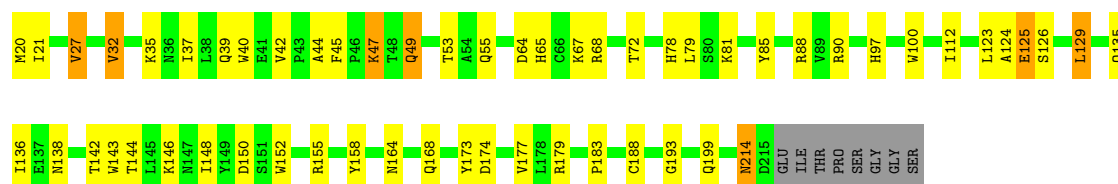
- Molecule 1: Interleukin-10 receptor subunit beta





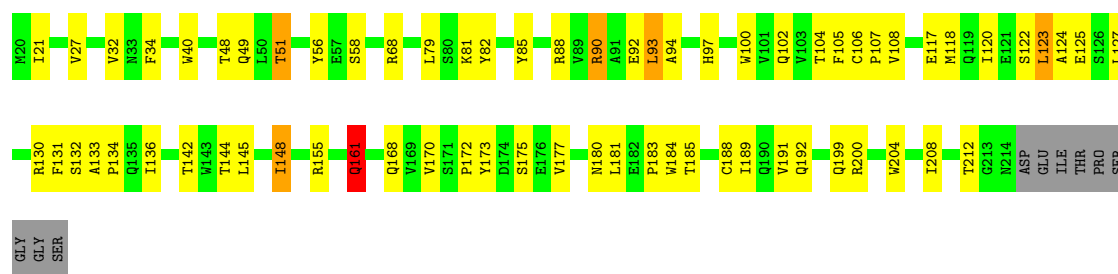
- Molecule 1: Interleukin-10 receptor subunit beta

Chain O: 68% 25%



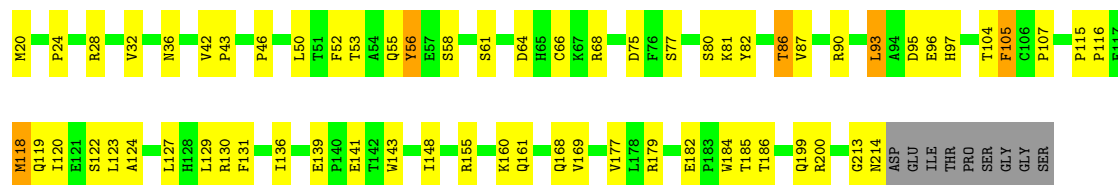
- Molecule 1: Interleukin-10 receptor subunit beta

Chain R: 62% 30%



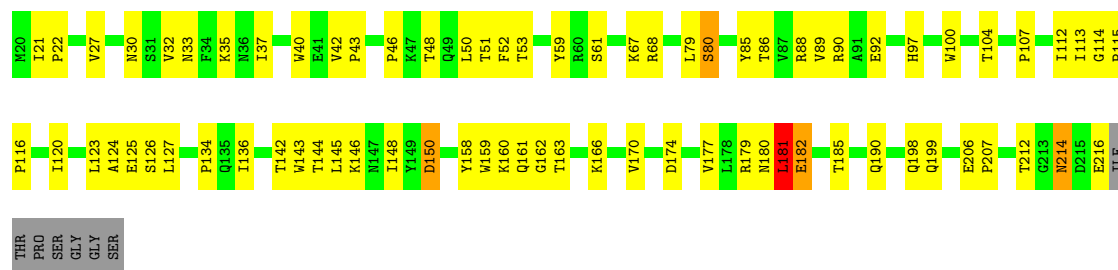
- Molecule 1: Interleukin-10 receptor subunit beta

Chain U: 64% 29%

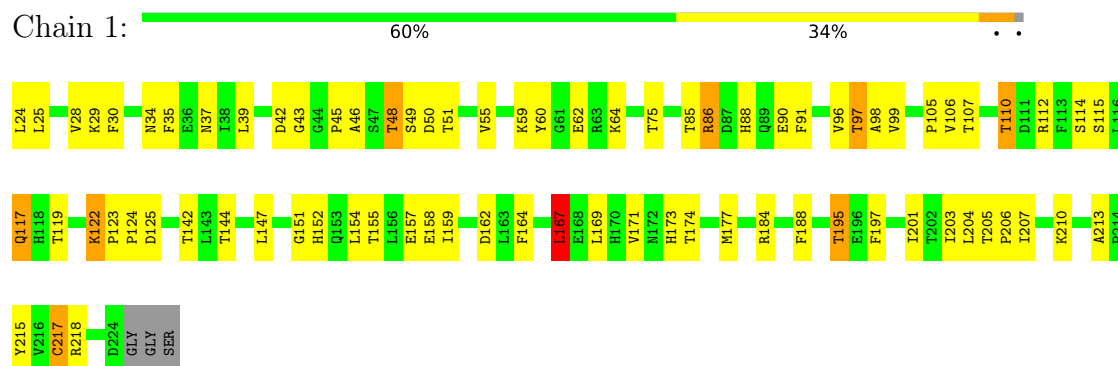


- Molecule 1: Interleukin-10 receptor subunit beta

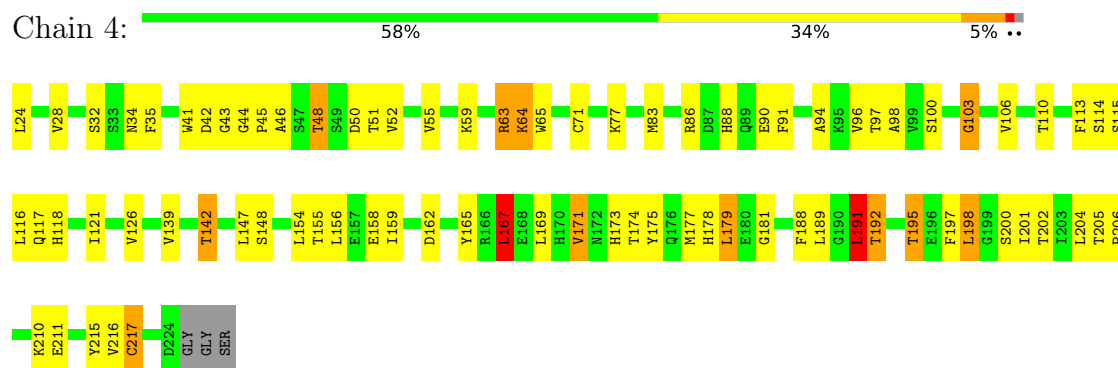
Chain X: 59% 35%



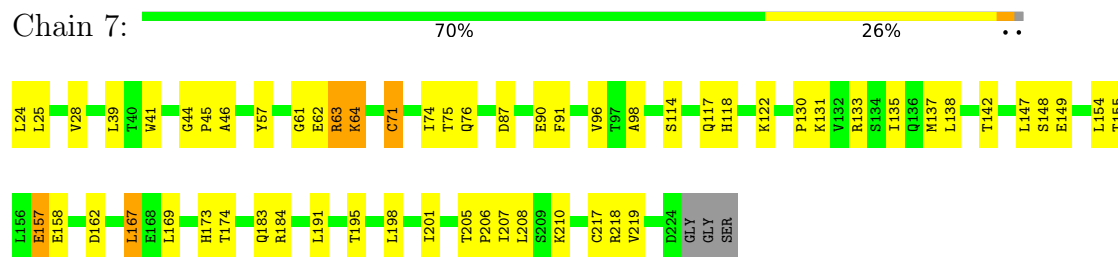
- Molecule 2: Interleukin-22 receptor subunit alpha-1



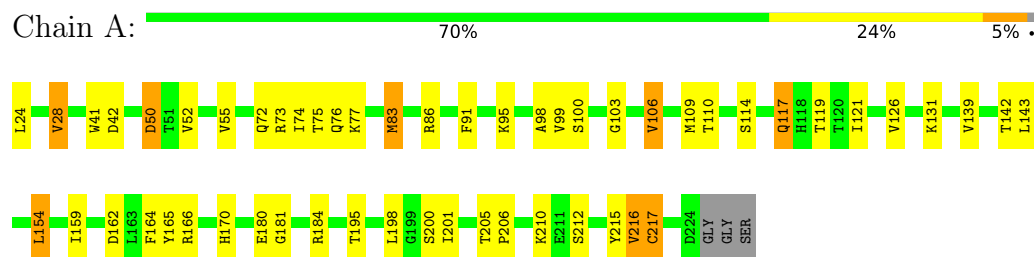
- Molecule 2: Interleukin-22 receptor subunit alpha-1



- Molecule 2: Interleukin-22 receptor subunit alpha-1

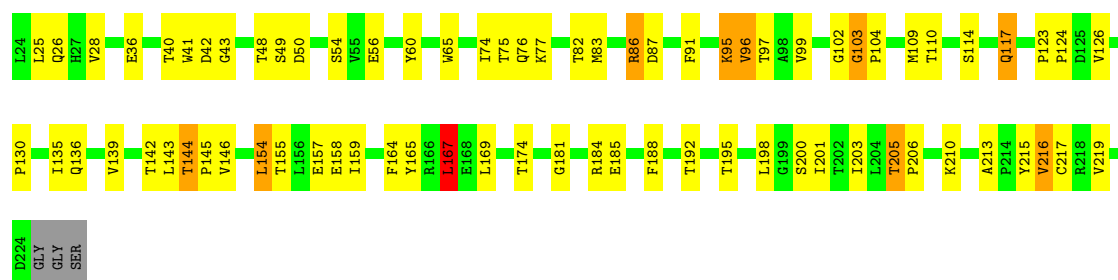


- Molecule 2: Interleukin-22 receptor subunit alpha-1



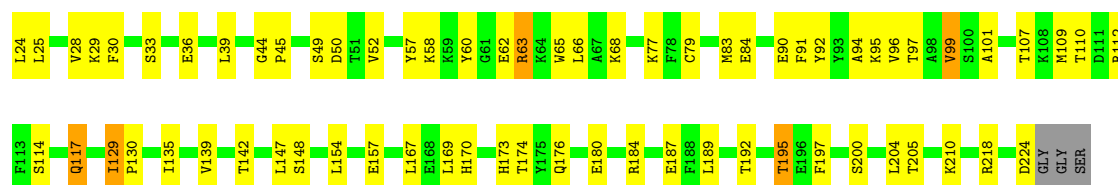
- Molecule 2: Interleukin-22 receptor subunit alpha-1





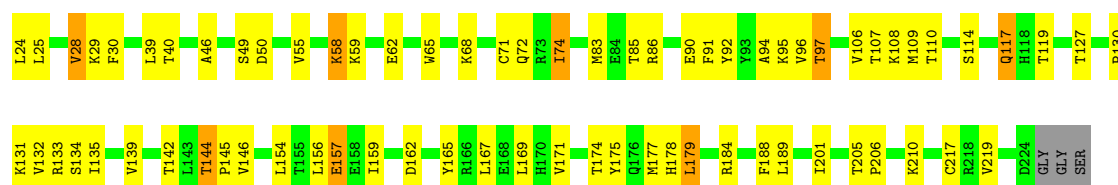
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain F: 65% 31% ..



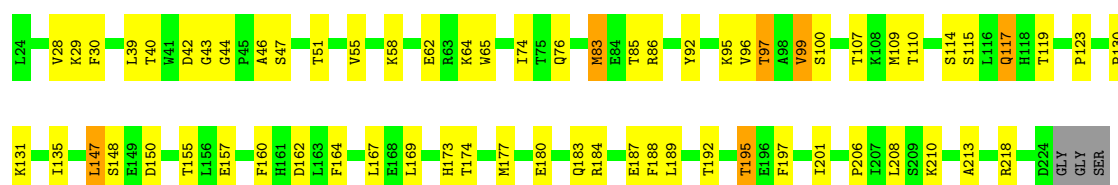
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain I: 63% 31% ..



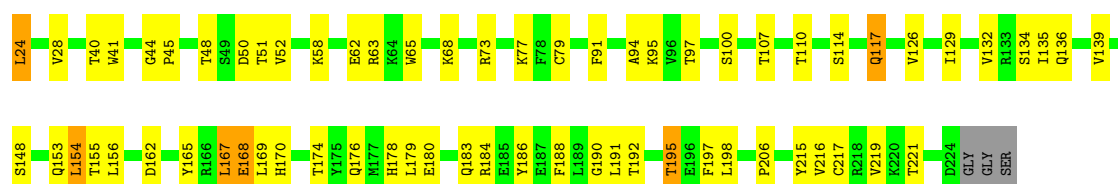
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain M: 66% 29% ..



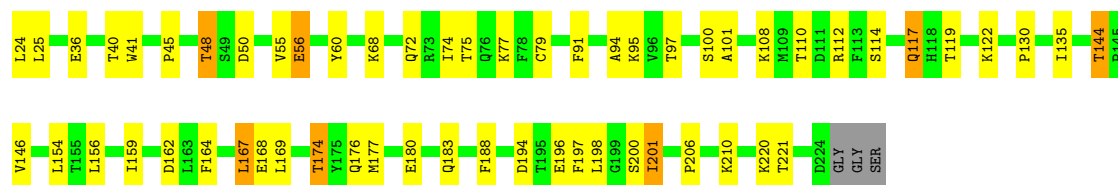
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain P: 66% 29% ..



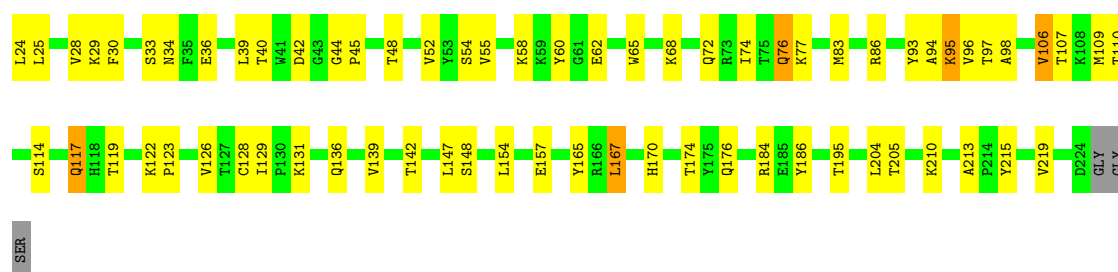
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain S:  70% 25% ..



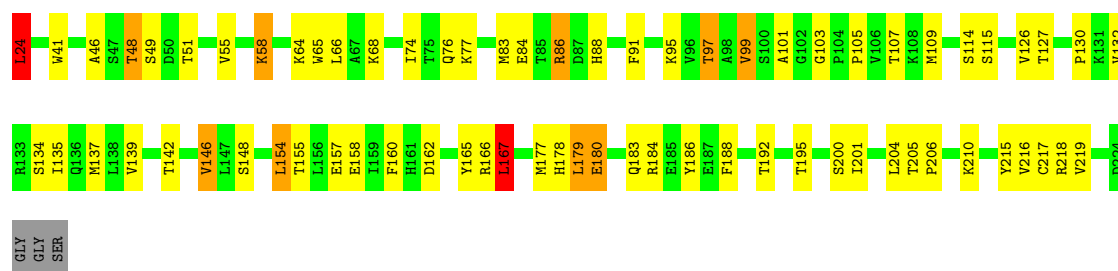
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain V:  65% 31% ..



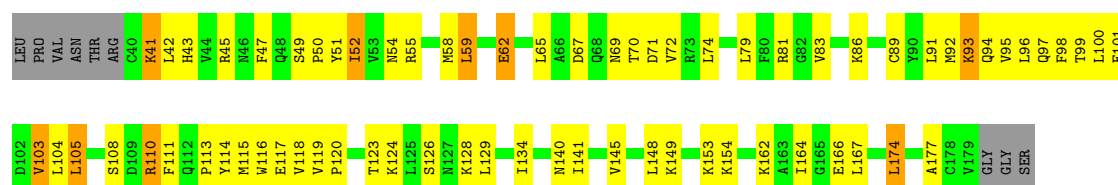
- Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain Y:  64% 29% ..



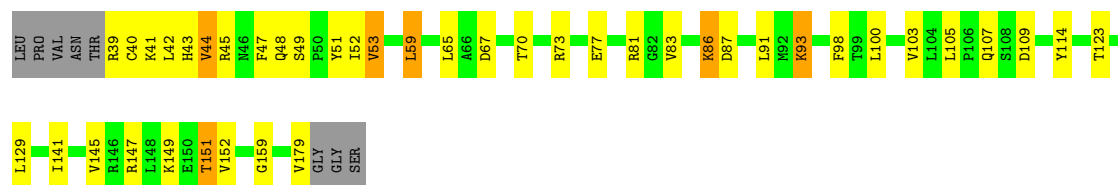
- Molecule 3: Interleukin-22

Chain 2:  47% 41% 6% 6%



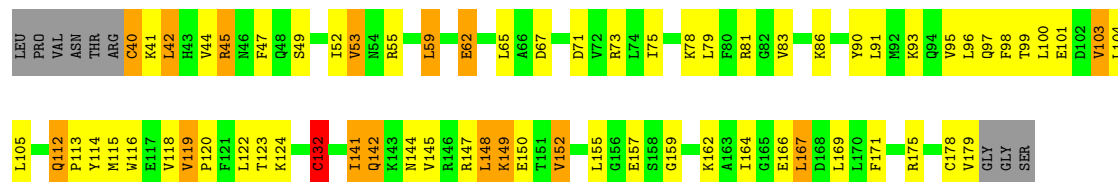
- Molecule 3: Interleukin-22

Chain 5:  66% 24% 5%



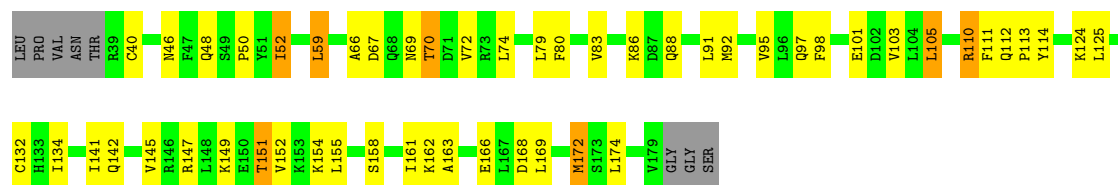
- Molecule 3: Interleukin-22

Chain 8: 48% 35% 10% 6%



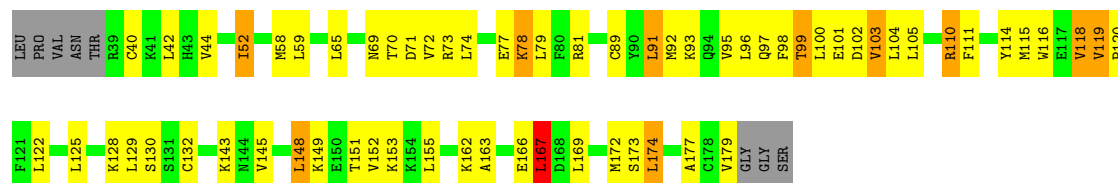
- Molecule 3: Interleukin-22

Chain D: 60% 30% 5% 5%



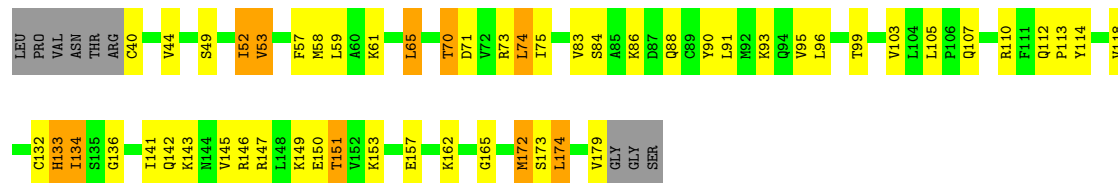
- Molecule 3: Interleukin-22

Chain G: 52% 36% 7% 5%



- Molecule 3: Interleukin-22

Chain J: 58% 30% 7% 6%



- Molecule 3: Interleukin-22

Chain L: 69% 23% 5% 5%



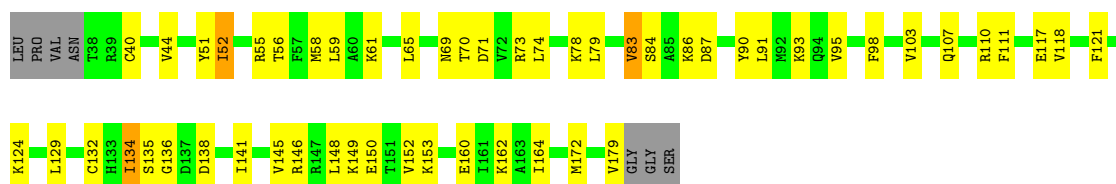
- Molecule 3: Interleukin-22

Chain N: 69% 22% 6%



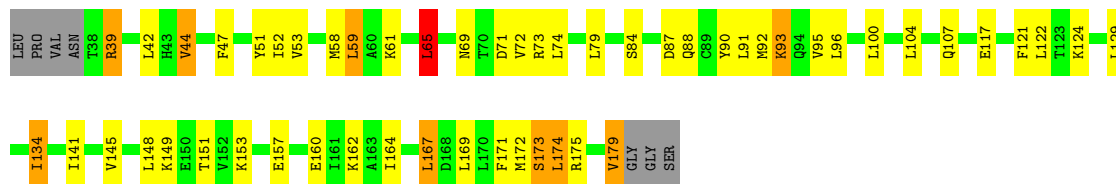
- Molecule 3: Interleukin-22

Chain Q: 60% 34% 5%



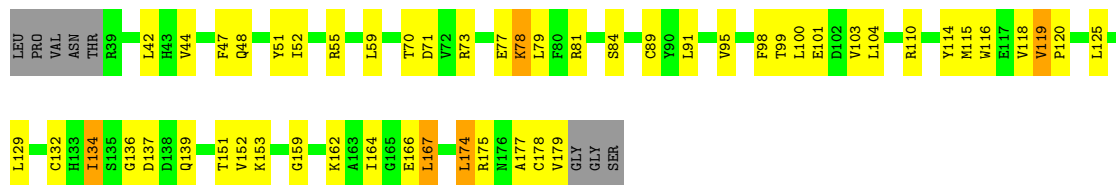
- Molecule 3: Interleukin-22

Chain T: 60% 29% 6% 5%



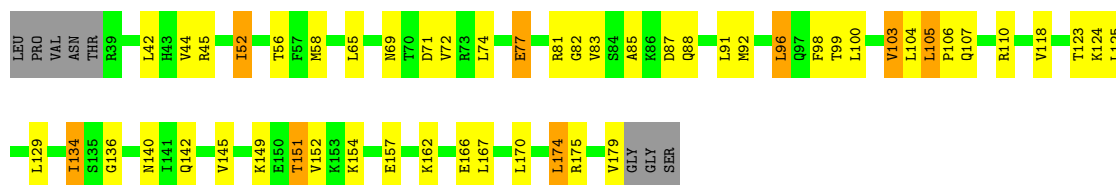
- Molecule 3: Interleukin-22

Chain W: 60% 32% 5%



- Molecule 3: Interleukin-22

Chain Z: 60% 30% 5% 5%



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

Chain a:  100%



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

Chain c:  100%



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

Chain n:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  33% 67%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  33% 67%




- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  67% 33%




- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  33% 67%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  67% 33%



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

Chain d:  50% 50%



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

Chain o:  100%




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

Chain p:  100%

MAG1
FUC2

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

Chain r:  100%MAG1
FUC2

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

Chain t:  100%MAG1
FUC2

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

Chain u:  100%MAG1
FUC2

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

Chain v:  50% 50%MAG1
FUC2

- Molecule 7: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  50% 50%MAG1
FUC2

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  67% 33%MAG1
MAG2
BMA3

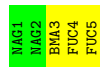
- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  20% 80%



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



- Molecule 11: alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	134.49Å 145.22Å 152.04Å 71.06° 81.84° 62.48°	Depositor
Resolution (Å)	48.09 – 2.60	Depositor
% Data completeness (in resolution range)	97.5 (48.09-2.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.236 , 0.296	Depositor
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.199	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	53140	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5066e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL, FUC, BMA

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	0	0.53	0/1627	0.74	1/2223 (0.0%)
1	3	0.45	1/1643 (0.1%)	0.67	0/2244
1	6	0.48	0/1655	0.67	0/2258
1	9	0.46	0/1579	0.72	2/2155 (0.1%)
1	C	0.60	0/1662	0.75	0/2267
1	E	0.57	0/1641	0.72	1/2242 (0.0%)
1	H	0.58	1/1650 (0.1%)	0.74	0/2252
1	K	0.54	0/1653	0.71	0/2256
1	O	0.56	0/1657	0.76	2/2261 (0.1%)
1	R	0.54	0/1659	0.69	0/2263
1	U	0.55	0/1651	0.72	1/2254 (0.0%)
1	X	0.49	0/1667	0.73	1/2274 (0.0%)
2	1	0.53	1/1655 (0.1%)	0.75	1/2250 (0.0%)
2	4	0.57	1/1652 (0.1%)	0.81	4/2247 (0.2%)
2	7	0.52	1/1646 (0.1%)	0.73	1/2240 (0.0%)
2	A	0.60	1/1647 (0.1%)	0.78	1/2242 (0.0%)
2	B	0.56	0/1651	0.78	1/2246 (0.0%)
2	F	0.55	0/1650	0.72	0/2244
2	I	0.53	0/1656	0.74	0/2252
2	M	0.56	0/1647	0.74	0/2240
2	P	0.61	0/1663	0.83	0/2259
2	S	0.59	0/1659	0.77	1/2254 (0.0%)
2	V	0.53	0/1653	0.70	0/2247
2	Y	0.60	0/1652	0.82	3/2246 (0.1%)
3	2	0.59	1/1113 (0.1%)	0.79	1/1500 (0.1%)
3	5	0.45	0/1143	0.65	0/1536
3	8	0.62	2/1124 (0.2%)	0.79	1/1513 (0.1%)
3	D	0.52	0/1148	0.77	2/1543 (0.1%)
3	G	0.48	0/1140	0.77	2/1533 (0.1%)
3	J	0.45	0/1134	0.68	0/1525
3	L	0.54	0/1142	0.72	0/1536
3	N	0.49	0/1110	0.72	0/1498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Q	0.60	0/1137	0.84	2/1532 (0.1%)
3	T	0.54	0/1150	0.77	1/1547 (0.1%)
3	W	0.49	0/1141	0.70	0/1534
3	Z	0.57	0/1146	0.79	0/1540
All	All	0.54	9/53203 (0.0%)	0.74	29/72253 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	4	0	1
2	Y	0	1
3	2	0	1
All	All	0	3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8	40	CYS	CB-SG	-9.55	1.66	1.82
3	2	62	GLU	CG-CD	9.31	1.66	1.51
3	8	132	CYS	CB-SG	8.11	1.96	1.82
2	7	71	CYS	CB-SG	-7.13	1.70	1.82
2	4	217	CYS	CB-SG	-6.00	1.72	1.82

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8	148	LEU	CB-CG-CD2	-10.11	93.81	111.00
3	Q	110	ARG	NE-CZ-NH2	9.99	125.29	120.30
2	Y	167	LEU	CA-CB-CG	7.51	132.57	115.30
2	4	167	LEU	CA-CB-CG	6.99	131.37	115.30
2	B	167	LEU	CB-CG-CD1	-6.89	99.28	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	58	MET	Mainchain
2	4	103	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	Y	103	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1579	0	1468	51	0
1	3	1595	0	1479	53	0
1	6	1607	0	1505	44	0
1	9	1532	0	1422	53	0
1	C	1614	0	1516	31	0
1	E	1593	0	1474	26	0
1	H	1602	0	1499	46	0
1	K	1605	0	1500	41	0
1	O	1609	0	1508	25	0
1	R	1611	0	1512	46	0
1	U	1603	0	1491	41	0
1	X	1619	0	1516	50	0
2	1	1613	0	1583	54	0
2	4	1610	0	1574	58	0
2	7	1604	0	1563	39	0
2	A	1605	0	1561	39	0
2	B	1609	0	1572	59	0
2	F	1608	0	1574	40	0
2	I	1614	0	1578	53	0
2	M	1605	0	1572	43	0
2	P	1621	0	1598	44	0
2	S	1617	0	1594	39	0
2	V	1611	0	1583	42	0
2	Y	1610	0	1578	47	0
3	2	1096	0	1100	58	0
3	5	1126	0	1144	33	0
3	8	1107	0	1114	52	0
3	D	1131	0	1155	44	0
3	G	1123	0	1142	50	0
3	J	1117	0	1138	30	0
3	L	1125	0	1143	21	0
3	N	1093	0	1083	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1120	0	1127	33	0
3	T	1133	0	1153	36	0
3	W	1124	0	1139	30	0
3	Z	1129	0	1153	40	0
4	a	49	0	43	0	0
4	c	49	0	43	0	0
4	n	49	0	43	0	0
5	b	38	0	34	0	0
5	e	38	0	34	0	0
5	i	38	0	34	0	0
5	j	38	0	34	0	0
5	l	38	0	34	0	0
5	m	38	0	34	0	0
5	s	38	0	34	0	0
6	d	24	0	22	0	0
6	o	24	0	22	0	0
6	p	24	0	22	0	0
6	r	24	0	22	0	0
6	t	24	0	22	0	0
6	u	24	0	22	0	0
6	v	24	0	22	0	0
7	f	24	0	22	0	0
8	g	39	0	34	0	0
9	h	59	0	52	0	0
9	k	59	0	52	0	0
10	q	28	0	25	0	0
11	w	34	0	31	0	0
12	A	6	0	8	0	0
12	H	6	0	8	0	0
12	J	6	0	8	0	0
12	K	6	0	8	0	0
12	M	6	0	8	2	0
12	O	6	0	8	0	0
12	Y	6	0	8	1	0
13	B	14	0	13	0	0
14	1	9	0	0	4	0
14	2	6	0	0	1	0
14	3	6	0	0	4	0
14	4	7	0	0	2	0
14	5	2	0	0	1	0
14	6	5	0	0	4	0
14	7	12	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	8	6	0	0	3	0
14	9	3	0	0	1	0
14	A	22	0	0	2	0
14	B	16	0	0	5	0
14	C	22	0	0	0	0
14	D	14	0	0	2	0
14	E	15	0	0	2	0
14	F	10	0	0	0	0
14	G	5	0	0	4	0
14	H	17	0	0	3	0
14	I	9	0	0	2	0
14	J	6	0	0	1	0
14	K	9	0	0	3	0
14	L	8	0	0	0	0
14	M	8	0	0	0	0
14	N	5	0	0	0	0
14	O	14	0	0	0	0
14	P	6	0	0	0	0
14	Q	7	0	0	2	0
14	R	9	0	0	5	0
14	S	13	0	0	6	0
14	T	6	0	0	1	0
14	U	14	0	0	1	0
14	V	12	0	0	2	0
14	W	1	0	0	0	0
14	X	11	0	0	0	0
14	Y	20	0	0	2	0
14	Z	5	0	0	0	0
All	All	53140	0	51217	1419	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 14.

The worst 5 of 1419 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:136:ILE:HD13	1:0:148:ILE:HD11	1.43	1.01
3:2:59:LEU:HD22	3:2:118:VAL:HG11	1.39	0.99
2:V:157:GLU:OE1	2:V:184:ARG:NH2	1.97	0.98
2:B:146:VAL:O	14:B:401:HOH:O	1.83	0.96
1:0:32:VAL:HG12	1:0:112:ILE:HB	1.51	0.93

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	0	191/204 (94%)	178 (93%)	12 (6%)	1 (0%)	29	52
1	3	193/204 (95%)	176 (91%)	14 (7%)	3 (2%)	9	19
1	6	193/204 (95%)	178 (92%)	13 (7%)	2 (1%)	15	32
1	9	182/204 (89%)	168 (92%)	11 (6%)	3 (2%)	9	19
1	C	193/204 (95%)	183 (95%)	7 (4%)	3 (2%)	9	19
1	E	193/204 (95%)	184 (95%)	7 (4%)	2 (1%)	15	32
1	H	193/204 (95%)	184 (95%)	8 (4%)	1 (0%)	29	52
1	K	193/204 (95%)	178 (92%)	11 (6%)	4 (2%)	7	13
1	O	194/204 (95%)	179 (92%)	11 (6%)	4 (2%)	7	13
1	R	193/204 (95%)	182 (94%)	7 (4%)	4 (2%)	7	13
1	U	193/204 (95%)	176 (91%)	16 (8%)	1 (0%)	29	52
1	X	195/204 (96%)	184 (94%)	8 (4%)	3 (2%)	10	21
2	1	199/204 (98%)	191 (96%)	7 (4%)	1 (0%)	29	52
2	4	199/204 (98%)	193 (97%)	5 (2%)	1 (0%)	29	52
2	7	199/204 (98%)	194 (98%)	5 (2%)	0	100	100
2	A	199/204 (98%)	192 (96%)	6 (3%)	1 (0%)	29	52
2	B	199/204 (98%)	190 (96%)	6 (3%)	3 (2%)	10	21
2	F	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
2	I	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
2	M	199/204 (98%)	192 (96%)	6 (3%)	1 (0%)	29	52
2	P	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
2	S	199/204 (98%)	194 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	199/204 (98%)	195 (98%)	4 (2%)	0	100	100
2	Y	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
3	2	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
3	5	139/149 (93%)	135 (97%)	4 (3%)	0	100	100
3	8	138/149 (93%)	130 (94%)	8 (6%)	0	100	100
3	D	139/149 (93%)	133 (96%)	6 (4%)	0	100	100
3	G	139/149 (93%)	134 (96%)	5 (4%)	0	100	100
3	J	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
3	L	139/149 (93%)	135 (97%)	3 (2%)	1 (1%)	22	43
3	N	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
3	Q	140/149 (94%)	135 (96%)	3 (2%)	2 (1%)	11	22
3	T	140/149 (94%)	136 (97%)	4 (3%)	0	100	100
3	W	139/149 (93%)	133 (96%)	5 (4%)	1 (1%)	22	43
3	Z	139/149 (93%)	134 (96%)	5 (4%)	0	100	100
All	All	6360/6684 (95%)	6065 (95%)	253 (4%)	42 (1%)	22	43

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	6	142	THR
1	E	46	PRO
1	K	142	THR
1	O	125	GLU
1	X	125	GLU

5.3.2 Protein sidechains ⓘ

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	0	174/188 (93%)	168 (97%)	6 (3%)	37	63
1	3	176/188 (94%)	149 (85%)	27 (15%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	178/188 (95%)	152 (85%)	26 (15%)	3	5
1	9	167/188 (89%)	144 (86%)	23 (14%)	3	6
1	C	180/188 (96%)	171 (95%)	9 (5%)	24	47
1	E	175/188 (93%)	166 (95%)	9 (5%)	24	46
1	H	178/188 (95%)	162 (91%)	16 (9%)	9	18
1	K	177/188 (94%)	158 (89%)	19 (11%)	6	12
1	O	178/188 (95%)	163 (92%)	15 (8%)	11	21
1	R	179/188 (95%)	163 (91%)	16 (9%)	9	19
1	U	177/188 (94%)	160 (90%)	17 (10%)	8	16
1	X	179/188 (95%)	160 (89%)	19 (11%)	6	12
2	1	182/185 (98%)	166 (91%)	16 (9%)	10	19
2	4	181/185 (98%)	167 (92%)	14 (8%)	13	25
2	7	180/185 (97%)	166 (92%)	14 (8%)	12	25
2	A	180/185 (97%)	167 (93%)	13 (7%)	14	29
2	B	181/185 (98%)	166 (92%)	15 (8%)	11	22
2	F	181/185 (98%)	167 (92%)	14 (8%)	13	25
2	I	182/185 (98%)	168 (92%)	14 (8%)	13	25
2	M	181/185 (98%)	170 (94%)	11 (6%)	18	38
2	P	184/185 (100%)	170 (92%)	14 (8%)	13	26
2	S	183/185 (99%)	169 (92%)	14 (8%)	13	25
2	V	182/185 (98%)	167 (92%)	15 (8%)	11	22
2	Y	182/185 (98%)	161 (88%)	21 (12%)	5	10
3	2	121/135 (90%)	106 (88%)	15 (12%)	4	8
3	5	126/135 (93%)	115 (91%)	11 (9%)	10	20
3	8	123/135 (91%)	98 (80%)	25 (20%)	1	2
3	D	128/135 (95%)	120 (94%)	8 (6%)	18	36
3	G	125/135 (93%)	107 (86%)	18 (14%)	3	5
3	J	126/135 (93%)	110 (87%)	16 (13%)	4	8
3	L	126/135 (93%)	116 (92%)	10 (8%)	12	24
3	N	120/135 (89%)	108 (90%)	12 (10%)	7	14
3	Q	125/135 (93%)	118 (94%)	7 (6%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	128/135 (95%)	113 (88%)	15 (12%)	5	10
3	W	126/135 (93%)	111 (88%)	15 (12%)	5	9
3	Z	127/135 (94%)	114 (90%)	13 (10%)	7	14
All	All	5798/6096 (95%)	5256 (91%)	542 (9%)	9	17

5 of 542 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	72	GLN
3	W	70	THR
2	V	52	VAL
2	Y	154	LEU
2	B	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	48	GLN
1	U	39	GLN
3	Z	107	GLN
1	X	190	GLN
2	S	176	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

67 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
4	NAG	a	1	2,4	14,14,15	0.29	0	17,19,21	0.94	2 (11%)
4	NAG	a	2	4	14,14,15	0.88	1 (7%)	17,19,21	1.56	2 (11%)
4	BMA	a	3	4	11,11,12	1.11	1 (9%)	15,15,17	1.93	4 (26%)
4	FUC	a	4	4	10,10,11	1.34	2 (20%)	14,14,16	1.19	1 (7%)
5	NAG	b	1	3,5	14,14,15	0.51	0	17,19,21	0.83	1 (5%)
5	NAG	b	2	5	14,14,15	0.30	0	17,19,21	0.80	0
5	FUC	b	3	5	10,10,11	1.94	3 (30%)	14,14,16	1.33	2 (14%)
4	NAG	c	1	2,4	14,14,15	0.47	0	17,19,21	1.17	1 (5%)
4	NAG	c	2	4	14,14,15	1.07	1 (7%)	17,19,21	1.46	4 (23%)
4	BMA	c	3	4	11,11,12	1.47	2 (18%)	15,15,17	1.42	2 (13%)
4	FUC	c	4	4	10,10,11	1.42	1 (10%)	14,14,16	1.19	2 (14%)
6	NAG	d	1	3,6	14,14,15	0.66	0	17,19,21	0.90	0
6	FUC	d	2	6	10,10,11	1.57	2 (20%)	14,14,16	1.22	2 (14%)
5	NAG	e	1	2,5	14,14,15	0.33	0	17,19,21	0.99	1 (5%)
5	NAG	e	2	5	14,14,15	0.45	0	17,19,21	0.97	1 (5%)
5	FUC	e	3	5	10,10,11	1.26	1 (10%)	14,14,16	1.10	0
7	NAG	f	1	3,7	14,14,15	1.06	1 (7%)	17,19,21	0.89	1 (5%)
7	FUC	f	2	7	10,10,11	0.87	0	14,14,16	0.83	0
8	NAG	g	1	2,8	14,14,15	0.60	0	17,19,21	0.73	0
8	NAG	g	2	8	14,14,15	0.33	0	17,19,21	0.52	0
8	BMA	g	3	8	11,11,12	1.37	2 (18%)	15,15,17	0.82	0
9	NAG	h	1	3,9	14,14,15	0.27	0	17,19,21	0.63	0
9	NAG	h	2	9	14,14,15	0.63	0	17,19,21	1.49	2 (11%)
9	BMA	h	3	9	11,11,12	0.64	0	15,15,17	1.45	2 (13%)
9	FUC	h	4	9	10,10,11	1.32	2 (20%)	14,14,16	1.37	2 (14%)
9	FUC	h	5	9	10,10,11	1.38	2 (20%)	14,14,16	1.58	4 (28%)
5	NAG	i	1	2,5	14,14,15	0.71	1 (7%)	17,19,21	0.62	0
5	NAG	i	2	5	14,14,15	0.58	0	17,19,21	0.67	0
5	FUC	i	3	5	10,10,11	1.30	1 (10%)	14,14,16	1.56	2 (14%)
5	NAG	j	1	3,5	14,14,15	0.40	0	17,19,21	0.73	0
5	NAG	j	2	5	14,14,15	0.43	0	17,19,21	0.67	0
5	FUC	j	3	5	10,10,11	1.38	2 (20%)	14,14,16	1.89	5 (35%)
9	NAG	k	1	2,9	14,14,15	0.44	0	17,19,21	0.69	0
9	NAG	k	2	9	14,14,15	0.24	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BMA	k	3	9	11,11,12	1.30	2 (18%)	15,15,17	0.90	0
9	FUC	k	4	9	10,10,11	1.04	2 (20%)	14,14,16	1.01	0
9	FUC	k	5	9	10,10,11	1.12	1 (10%)	14,14,16	0.94	1 (7%)
5	NAG	l	1	3,5	14,14,15	0.90	1 (7%)	17,19,21	1.09	1 (5%)
5	NAG	l	2	5	14,14,15	0.87	1 (7%)	17,19,21	0.88	0
5	FUC	l	3	5	10,10,11	1.45	3 (30%)	14,14,16	2.28	4 (28%)
5	NAG	m	1	3,5	14,14,15	0.44	0	17,19,21	1.22	3 (17%)
5	NAG	m	2	5	14,14,15	0.37	0	17,19,21	0.65	0
5	FUC	m	3	5	10,10,11	2.31	3 (30%)	14,14,16	2.17	5 (35%)
4	NAG	n	1	2,4	14,14,15	0.44	0	17,19,21	0.52	0
4	NAG	n	2	4	14,14,15	0.44	0	17,19,21	0.49	0
4	BMA	n	3	4	11,11,12	1.13	1 (9%)	15,15,17	0.84	0
4	FUC	n	4	4	10,10,11	1.12	1 (10%)	14,14,16	1.05	1 (7%)
6	NAG	o	1	3,6	14,14,15	0.88	2 (14%)	17,19,21	1.11	1 (5%)
6	FUC	o	2	6	10,10,11	1.23	1 (10%)	14,14,16	1.33	2 (14%)
6	NAG	p	1	2,6	14,14,15	0.83	1 (7%)	17,19,21	0.51	0
6	FUC	p	2	6	10,10,11	1.42	2 (20%)	14,14,16	1.66	1 (7%)
10	NAG	q	1	3,10	14,14,15	0.64	1 (7%)	17,19,21	0.99	1 (5%)
10	NAG	q	2	10	14,14,15	0.35	0	17,19,21	0.58	0
6	NAG	r	1	2,6	14,14,15	0.89	1 (7%)	17,19,21	0.70	0
6	FUC	r	2	6	10,10,11	1.70	3 (30%)	14,14,16	1.46	2 (14%)
5	NAG	s	1	3,5	14,14,15	0.25	0	17,19,21	0.64	0
5	NAG	s	2	5	14,14,15	0.45	0	17,19,21	0.52	0
5	FUC	s	3	5	10,10,11	1.11	1 (10%)	14,14,16	0.76	0
6	NAG	t	1	2,6	14,14,15	0.83	1 (7%)	17,19,21	0.68	0
6	FUC	t	2	6	10,10,11	0.84	0	14,14,16	1.13	2 (14%)
6	NAG	u	1	3,6	14,14,15	0.83	1 (7%)	17,19,21	0.46	0
6	FUC	u	2	6	10,10,11	1.70	3 (30%)	14,14,16	1.36	0
6	NAG	v	1	2,6	14,14,15	0.77	0	17,19,21	0.72	0
6	FUC	v	2	6	10,10,11	1.07	1 (10%)	14,14,16	1.96	4 (28%)
11	NAG	w	1	3,11	14,14,15	0.44	0	17,19,21	0.76	1 (5%)
11	FUC	w	2	11	10,10,11	0.56	0	14,14,16	0.92	0
11	FUC	w	3	11	10,10,11	1.23	1 (10%)	14,14,16	1.26	2 (14%)

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
4	NAG	a	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	6/6/23/26	0/1/1/1
4	BMA	a	3	4	-	2/2/19/22	0/1/1/1
4	FUC	a	4	4	-	-	0/1/1/1
5	NAG	b	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	4/6/23/26	0/1/1/1
5	FUC	b	3	5	-	-	0/1/1/1
4	NAG	c	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	c	2	4	-	2/6/23/26	0/1/1/1
4	BMA	c	3	4	-	2/2/19/22	0/1/1/1
4	FUC	c	4	4	-	-	0/1/1/1
6	NAG	d	1	3,6	-	2/6/23/26	0/1/1/1
6	FUC	d	2	6	-	-	0/1/1/1
5	NAG	e	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	1/6/23/26	0/1/1/1
5	FUC	e	3	5	-	-	0/1/1/1
7	NAG	f	1	3,7	-	0/6/23/26	0/1/1/1
7	FUC	f	2	7	-	-	0/1/1/1
8	NAG	g	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1
8	BMA	g	3	8	-	0/2/19/22	0/1/1/1
9	NAG	h	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	h	2	9	-	2/6/23/26	0/1/1/1
9	BMA	h	3	9	-	1/2/19/22	0/1/1/1
9	FUC	h	4	9	-	-	0/1/1/1
9	FUC	h	5	9	-	-	0/1/1/1
5	NAG	i	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	i	2	5	-	2/6/23/26	0/1/1/1
5	FUC	i	3	5	-	-	0/1/1/1
5	NAG	j	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	j	2	5	-	2/6/23/26	0/1/1/1
5	FUC	j	3	5	-	-	0/1/1/1
9	NAG	k	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	k	2	9	-	1/6/23/26	0/1/1/1
9	BMA	k	3	9	-	0/2/19/22	0/1/1/1
9	FUC	k	4	9	-	-	0/1/1/1
9	FUC	k	5	9	-	-	0/1/1/1
5	NAG	l	1	3,5	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	l	2	5	-	2/6/23/26	0/1/1/1
5	FUC	l	3	5	-	-	0/1/1/1
5	NAG	m	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	m	2	5	-	4/6/23/26	0/1/1/1
5	FUC	m	3	5	-	-	0/1/1/1
4	NAG	n	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	n	2	4	-	2/6/23/26	0/1/1/1
4	BMA	n	3	4	-	0/2/19/22	0/1/1/1
4	FUC	n	4	4	-	-	0/1/1/1
6	NAG	o	1	3,6	-	2/6/23/26	0/1/1/1
6	FUC	o	2	6	-	-	0/1/1/1
6	NAG	p	1	2,6	-	2/6/23/26	0/1/1/1
6	FUC	p	2	6	-	-	0/1/1/1
10	NAG	q	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	q	2	10	-	1/6/23/26	0/1/1/1
6	NAG	r	1	2,6	-	4/6/23/26	0/1/1/1
6	FUC	r	2	6	-	-	0/1/1/1
5	NAG	s	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	s	2	5	-	2/6/23/26	0/1/1/1
5	FUC	s	3	5	-	-	0/1/1/1
6	NAG	t	1	2,6	-	2/6/23/26	0/1/1/1
6	FUC	t	2	6	-	-	0/1/1/1
6	NAG	u	1	3,6	-	2/6/23/26	0/1/1/1
6	FUC	u	2	6	-	-	0/1/1/1
6	NAG	v	1	2,6	-	0/6/23/26	0/1/1/1
6	FUC	v	2	6	-	-	0/1/1/1
11	NAG	w	1	3,11	-	0/6/23/26	0/1/1/1
11	FUC	w	2	11	-	-	0/1/1/1
11	FUC	w	3	11	-	-	0/1/1/1

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	m	3	FUC	C1-C2	4.87	1.63	1.52
5	b	3	FUC	C2-C3	4.16	1.58	1.52
7	f	1	NAG	O5-C1	3.77	1.49	1.43
5	m	3	FUC	O5-C1	3.64	1.49	1.43
4	c	4	FUC	O5-C1	-3.62	1.37	1.43

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	3	BMA	C1-O5-C5	5.07	119.06	112.19
6	p	2	FUC	C1-C2-C3	5.01	115.83	109.67
4	a	2	NAG	C2-N2-C7	4.81	129.75	122.90
6	v	2	FUC	O5-C1-C2	4.72	118.05	110.77
5	l	3	FUC	O5-C5-C4	4.63	117.82	109.52

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	l	2	NAG	C1-C2-N2-C7
5	m	1	NAG	C4-C5-C6-O6
6	r	1	NAG	C1-C2-N2-C7
5	b	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
12	GOL	H	301	-	5,5,5	1.23	1 (20%)	5,5,5	0.76	0
12	GOL	Y	303	-	5,5,5	1.06	0	5,5,5	0.73	0
12	GOL	J	204	-	5,5,5	1.06	0	5,5,5	0.89	0
12	GOL	O	401	-	5,5,5	0.89	0	5,5,5	0.98	0
12	GOL	K	301	-	5,5,5	0.97	0	5,5,5	0.99	0
12	GOL	M	305	-	5,5,5	1.63	1 (20%)	5,5,5	0.81	0
12	GOL	A	304	-	5,5,5	1.24	0	5,5,5	0.94	0
13	NAG	B	301	2	14,14,15	0.92	1 (7%)	17,19,21	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	GOL	H	301	-	-	2/4/4/4	-
12	GOL	Y	303	-	-	2/4/4/4	-
12	GOL	J	204	-	-	2/4/4/4	-
12	GOL	O	401	-	-	2/4/4/4	-
12	GOL	K	301	-	-	2/4/4/4	-
12	GOL	M	305	-	-	4/4/4/4	-
12	GOL	A	304	-	-	4/4/4/4	-
13	NAG	B	301	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	305	GOL	C3-C2	2.81	1.63	1.51
13	B	301	NAG	O5-C1	2.76	1.48	1.43
12	H	301	GOL	C1-C2	2.44	1.61	1.51

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	304	GOL	C1-C2-C3-O3
12	H	301	GOL	C1-C2-C3-O3
12	Y	303	GOL	O1-C1-C2-O2
13	B	301	NAG	C4-C5-C6-O6
13	B	301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	Y	303	GOL	1	0
12	M	305	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.