Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 11:21 PM EDT

PDB ID	:	8ENT
Title	:	Interleukin-21 signaling complex with IL-21R and IL-2Rg
Authors	:	Abhiraman, G.C.; Jude, K.M.; Garcia, K.C.
Deposited on	:	2022-09-30
Resolution	:	2.83 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

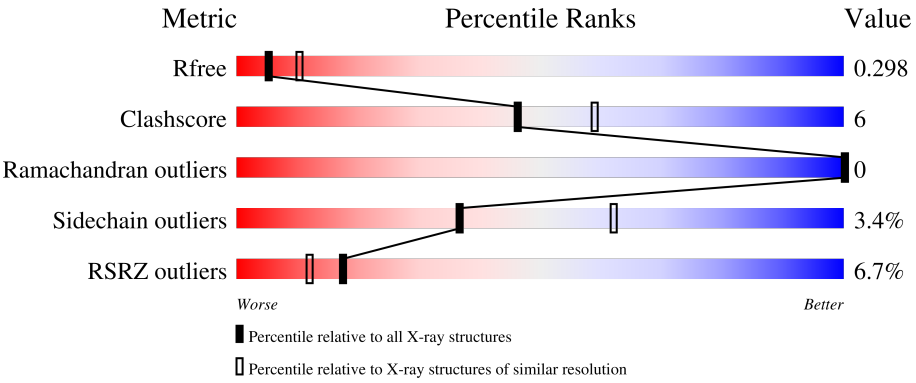
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	144	2% 70% 15% • 13%
1	D	144	6% 68% 10% • 20%
1	G	144	3% 68% 19% • 12%
1	J	144	5% 66% 12% 22%
2	B	237	% 72% 16% • 12%

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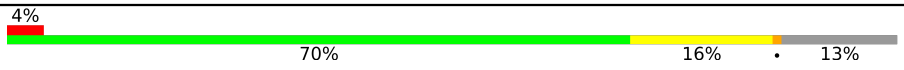
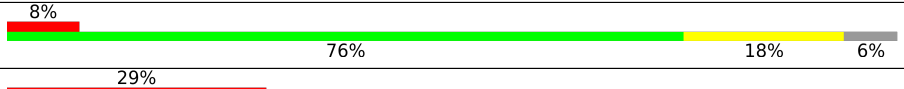
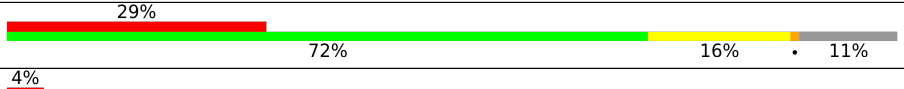
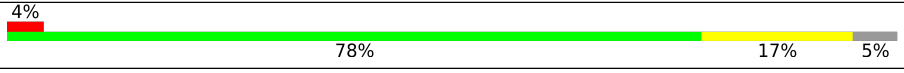
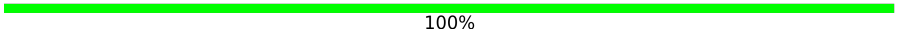
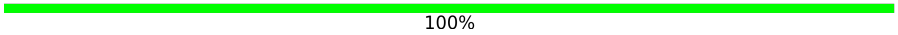
Mol	Chain	Length	Quality of chain
2	E	237	
2	H	237	
2	K	237	
3	C	207	
3	F	207	
3	I	207	
4	L	2	
4	M	2	
4	O	2	
5	N	3	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15852 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-21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1016	636	187	186	7			
1	D	115	Total	C	N	O	S	0	0	0
			937	591	166	173	7			
1	G	127	Total	C	N	O	S	0	0	0
			1026	642	189	188	7			
1	J	113	Total	C	N	O	S	0	0	0
			925	584	164	170	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	GLN	ASN	engineered mutation	UNP Q9HBE4
A	134	GLY	-	expression tag	UNP Q9HBE4
A	135	ALA	-	expression tag	UNP Q9HBE4
A	136	PRO	-	expression tag	UNP Q9HBE4
A	137	GLY	-	expression tag	UNP Q9HBE4
A	138	SER	-	expression tag	UNP Q9HBE4
A	139	HIS	-	expression tag	UNP Q9HBE4
A	140	HIS	-	expression tag	UNP Q9HBE4
A	141	HIS	-	expression tag	UNP Q9HBE4
A	142	HIS	-	expression tag	UNP Q9HBE4
A	143	HIS	-	expression tag	UNP Q9HBE4
A	144	HIS	-	expression tag	UNP Q9HBE4
D	68	GLN	ASN	engineered mutation	UNP Q9HBE4
D	134	GLY	-	expression tag	UNP Q9HBE4
D	135	ALA	-	expression tag	UNP Q9HBE4
D	136	PRO	-	expression tag	UNP Q9HBE4
D	137	GLY	-	expression tag	UNP Q9HBE4
D	138	SER	-	expression tag	UNP Q9HBE4
D	139	HIS	-	expression tag	UNP Q9HBE4
D	140	HIS	-	expression tag	UNP Q9HBE4
D	141	HIS	-	expression tag	UNP Q9HBE4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	142	HIS	-	expression tag	UNP Q9HBE4
D	143	HIS	-	expression tag	UNP Q9HBE4
D	144	HIS	-	expression tag	UNP Q9HBE4
G	68	GLN	ASN	engineered mutation	UNP Q9HBE4
G	134	GLY	-	expression tag	UNP Q9HBE4
G	135	ALA	-	expression tag	UNP Q9HBE4
G	136	PRO	-	expression tag	UNP Q9HBE4
G	137	GLY	-	expression tag	UNP Q9HBE4
G	138	SER	-	expression tag	UNP Q9HBE4
G	139	HIS	-	expression tag	UNP Q9HBE4
G	140	HIS	-	expression tag	UNP Q9HBE4
G	141	HIS	-	expression tag	UNP Q9HBE4
G	142	HIS	-	expression tag	UNP Q9HBE4
G	143	HIS	-	expression tag	UNP Q9HBE4
G	144	HIS	-	expression tag	UNP Q9HBE4
J	68	GLN	ASN	engineered mutation	UNP Q9HBE4
J	134	GLY	-	expression tag	UNP Q9HBE4
J	135	ALA	-	expression tag	UNP Q9HBE4
J	136	PRO	-	expression tag	UNP Q9HBE4
J	137	GLY	-	expression tag	UNP Q9HBE4
J	138	SER	-	expression tag	UNP Q9HBE4
J	139	HIS	-	expression tag	UNP Q9HBE4
J	140	HIS	-	expression tag	UNP Q9HBE4
J	141	HIS	-	expression tag	UNP Q9HBE4
J	142	HIS	-	expression tag	UNP Q9HBE4
J	143	HIS	-	expression tag	UNP Q9HBE4
J	144	HIS	-	expression tag	UNP Q9HBE4

- Molecule 2 is a protein called Interleukin-21 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1696	1076	278	331	11			
2	E	207	Total	C	N	O	S	0	0	0
			1686	1071	276	328	11			
2	H	208	Total	C	N	O	S	0	1	0
			1692	1075	277	328	12			
2	K	208	Total	C	N	O	S	0	0	0
			1684	1070	277	326	11			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	78	GLN	ASN	engineered mutation	UNP Q9HBE5
B	85	GLN	ASN	engineered mutation	UNP Q9HBE5
B	106	ASP	ASN	engineered mutation	UNP Q9HBE5
B	116	GLN	ASN	engineered mutation	UNP Q9HBE5
B	211	LYS	-	expression tag	UNP Q9HBE5
B	212	ALA	-	expression tag	UNP Q9HBE5
B	213	ALA	-	expression tag	UNP Q9HBE5
B	214	SER	-	expression tag	UNP Q9HBE5
B	215	GLY	-	expression tag	UNP Q9HBE5
B	216	ARG	-	expression tag	UNP Q9HBE5
B	217	GLY	-	expression tag	UNP Q9HBE5
B	218	LEU	-	expression tag	UNP Q9HBE5
B	219	ASN	-	expression tag	UNP Q9HBE5
B	220	ASP	-	expression tag	UNP Q9HBE5
B	221	ILE	-	expression tag	UNP Q9HBE5
B	222	PHE	-	expression tag	UNP Q9HBE5
B	223	GLU	-	expression tag	UNP Q9HBE5
B	224	ALA	-	expression tag	UNP Q9HBE5
B	225	GLN	-	expression tag	UNP Q9HBE5
B	226	LYS	-	expression tag	UNP Q9HBE5
B	227	ILE	-	expression tag	UNP Q9HBE5
B	228	GLU	-	expression tag	UNP Q9HBE5
B	229	TRP	-	expression tag	UNP Q9HBE5
B	230	HIS	-	expression tag	UNP Q9HBE5
B	231	GLU	-	expression tag	UNP Q9HBE5
B	232	HIS	-	expression tag	UNP Q9HBE5
B	233	HIS	-	expression tag	UNP Q9HBE5
B	234	HIS	-	expression tag	UNP Q9HBE5
B	235	HIS	-	expression tag	UNP Q9HBE5
B	236	HIS	-	expression tag	UNP Q9HBE5
B	237	HIS	-	expression tag	UNP Q9HBE5
E	78	GLN	ASN	engineered mutation	UNP Q9HBE5
E	85	GLN	ASN	engineered mutation	UNP Q9HBE5
E	106	ASP	ASN	engineered mutation	UNP Q9HBE5
E	116	GLN	ASN	engineered mutation	UNP Q9HBE5
E	211	LYS	-	expression tag	UNP Q9HBE5
E	212	ALA	-	expression tag	UNP Q9HBE5
E	213	ALA	-	expression tag	UNP Q9HBE5
E	214	SER	-	expression tag	UNP Q9HBE5
E	215	GLY	-	expression tag	UNP Q9HBE5
E	216	ARG	-	expression tag	UNP Q9HBE5
E	217	GLY	-	expression tag	UNP Q9HBE5
E	218	LEU	-	expression tag	UNP Q9HBE5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	219	ASN	-	expression tag	UNP Q9HBE5
E	220	ASP	-	expression tag	UNP Q9HBE5
E	221	ILE	-	expression tag	UNP Q9HBE5
E	222	PHE	-	expression tag	UNP Q9HBE5
E	223	GLU	-	expression tag	UNP Q9HBE5
E	224	ALA	-	expression tag	UNP Q9HBE5
E	225	GLN	-	expression tag	UNP Q9HBE5
E	226	LYS	-	expression tag	UNP Q9HBE5
E	227	ILE	-	expression tag	UNP Q9HBE5
E	228	GLU	-	expression tag	UNP Q9HBE5
E	229	TRP	-	expression tag	UNP Q9HBE5
E	230	HIS	-	expression tag	UNP Q9HBE5
E	231	GLU	-	expression tag	UNP Q9HBE5
E	232	HIS	-	expression tag	UNP Q9HBE5
E	233	HIS	-	expression tag	UNP Q9HBE5
E	234	HIS	-	expression tag	UNP Q9HBE5
E	235	HIS	-	expression tag	UNP Q9HBE5
E	236	HIS	-	expression tag	UNP Q9HBE5
E	237	HIS	-	expression tag	UNP Q9HBE5
H	78	GLN	ASN	engineered mutation	UNP Q9HBE5
H	85	GLN	ASN	engineered mutation	UNP Q9HBE5
H	106	ASP	ASN	engineered mutation	UNP Q9HBE5
H	116	GLN	ASN	engineered mutation	UNP Q9HBE5
H	211	LYS	-	expression tag	UNP Q9HBE5
H	212	ALA	-	expression tag	UNP Q9HBE5
H	213	ALA	-	expression tag	UNP Q9HBE5
H	214	SER	-	expression tag	UNP Q9HBE5
H	215	GLY	-	expression tag	UNP Q9HBE5
H	216	ARG	-	expression tag	UNP Q9HBE5
H	217	GLY	-	expression tag	UNP Q9HBE5
H	218	LEU	-	expression tag	UNP Q9HBE5
H	219	ASN	-	expression tag	UNP Q9HBE5
H	220	ASP	-	expression tag	UNP Q9HBE5
H	221	ILE	-	expression tag	UNP Q9HBE5
H	222	PHE	-	expression tag	UNP Q9HBE5
H	223	GLU	-	expression tag	UNP Q9HBE5
H	224	ALA	-	expression tag	UNP Q9HBE5
H	225	GLN	-	expression tag	UNP Q9HBE5
H	226	LYS	-	expression tag	UNP Q9HBE5
H	227	ILE	-	expression tag	UNP Q9HBE5
H	228	GLU	-	expression tag	UNP Q9HBE5
H	229	TRP	-	expression tag	UNP Q9HBE5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	230	HIS	-	expression tag	UNP Q9HBE5
H	231	GLU	-	expression tag	UNP Q9HBE5
H	232	HIS	-	expression tag	UNP Q9HBE5
H	233	HIS	-	expression tag	UNP Q9HBE5
H	234	HIS	-	expression tag	UNP Q9HBE5
H	235	HIS	-	expression tag	UNP Q9HBE5
H	236	HIS	-	expression tag	UNP Q9HBE5
H	237	HIS	-	expression tag	UNP Q9HBE5
K	78	GLN	ASN	engineered mutation	UNP Q9HBE5
K	85	GLN	ASN	engineered mutation	UNP Q9HBE5
K	106	ASP	ASN	engineered mutation	UNP Q9HBE5
K	116	GLN	ASN	engineered mutation	UNP Q9HBE5
K	211	LYS	-	expression tag	UNP Q9HBE5
K	212	ALA	-	expression tag	UNP Q9HBE5
K	213	ALA	-	expression tag	UNP Q9HBE5
K	214	SER	-	expression tag	UNP Q9HBE5
K	215	GLY	-	expression tag	UNP Q9HBE5
K	216	ARG	-	expression tag	UNP Q9HBE5
K	217	GLY	-	expression tag	UNP Q9HBE5
K	218	LEU	-	expression tag	UNP Q9HBE5
K	219	ASN	-	expression tag	UNP Q9HBE5
K	220	ASP	-	expression tag	UNP Q9HBE5
K	221	ILE	-	expression tag	UNP Q9HBE5
K	222	PHE	-	expression tag	UNP Q9HBE5
K	223	GLU	-	expression tag	UNP Q9HBE5
K	224	ALA	-	expression tag	UNP Q9HBE5
K	225	GLN	-	expression tag	UNP Q9HBE5
K	226	LYS	-	expression tag	UNP Q9HBE5
K	227	ILE	-	expression tag	UNP Q9HBE5
K	228	GLU	-	expression tag	UNP Q9HBE5
K	229	TRP	-	expression tag	UNP Q9HBE5
K	230	HIS	-	expression tag	UNP Q9HBE5
K	231	GLU	-	expression tag	UNP Q9HBE5
K	232	HIS	-	expression tag	UNP Q9HBE5
K	233	HIS	-	expression tag	UNP Q9HBE5
K	234	HIS	-	expression tag	UNP Q9HBE5
K	235	HIS	-	expression tag	UNP Q9HBE5
K	236	HIS	-	expression tag	UNP Q9HBE5
K	237	HIS	-	expression tag	UNP Q9HBE5

- Molecule 3 is a protein called Cytokine receptor common subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	1	0
			1644	1047	293	296	8			
3	F	185	Total	C	N	O	S	0	1	0
			1567	1004	278	277	8			
3	I	196	Total	C	N	O	S	0	0	0
			1647	1049	295	295	8			

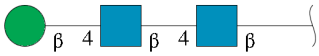
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	PRO	-	expression tag	UNP P31785
C	53	GLN	ASN	engineered mutation	UNP P31785
C	233	HIS	-	expression tag	UNP P31785
C	234	HIS	-	expression tag	UNP P31785
C	235	HIS	-	expression tag	UNP P31785
C	236	HIS	-	expression tag	UNP P31785
C	237	HIS	-	expression tag	UNP P31785
C	238	HIS	-	expression tag	UNP P31785
F	32	PRO	-	expression tag	UNP P31785
F	53	GLN	ASN	engineered mutation	UNP P31785
F	233	HIS	-	expression tag	UNP P31785
F	234	HIS	-	expression tag	UNP P31785
F	235	HIS	-	expression tag	UNP P31785
F	236	HIS	-	expression tag	UNP P31785
F	237	HIS	-	expression tag	UNP P31785
F	238	HIS	-	expression tag	UNP P31785
I	32	PRO	-	expression tag	UNP P31785
I	53	GLN	ASN	engineered mutation	UNP P31785
I	233	HIS	-	expression tag	UNP P31785
I	234	HIS	-	expression tag	UNP P31785
I	235	HIS	-	expression tag	UNP P31785
I	236	HIS	-	expression tag	UNP P31785
I	237	HIS	-	expression tag	UNP P31785
I	238	HIS	-	expression tag	UNP P31785

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

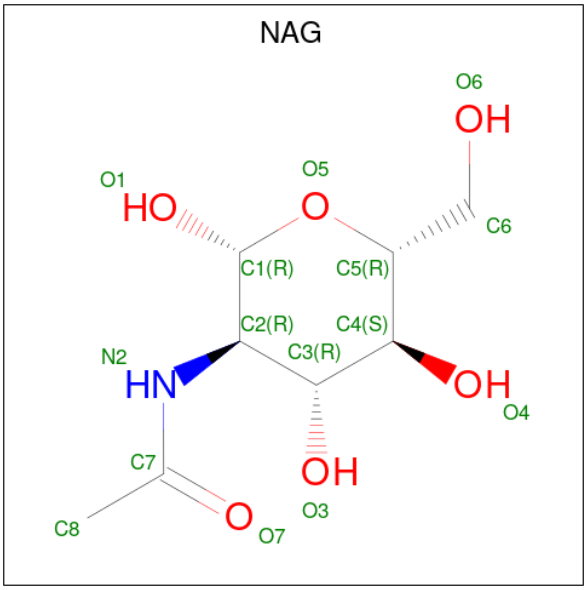
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	L	2	Total C N O 28 16 2 10	0	0	0
4	M	2	Total C N O 28 16 2 10	0	0	0
4	O	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 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
5	N	3	Total C N O 39 22 2 15	0	0	0

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



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

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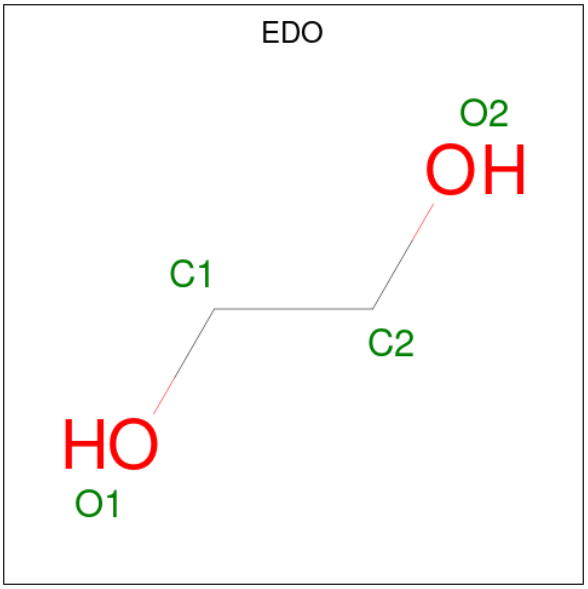
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0
6	H	1	Total C N O 14 8 1 5	0	0
6	I	1	Total C N O 14 8 1 5	0	0
6	I	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C O 4 2 2	0	0
7	I	1	Total C O 4 2 2	0	0
7	K	1	Total C O 4 2 2	0	0
7	K	1	Total C O 4 2 2	0	0
7	K	1	Total C O 4 2 2	0	0
7	K	1	Total C O 4 2 2	0	0
7	K	1	Total C O 4 2 2	0	0
7	K	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

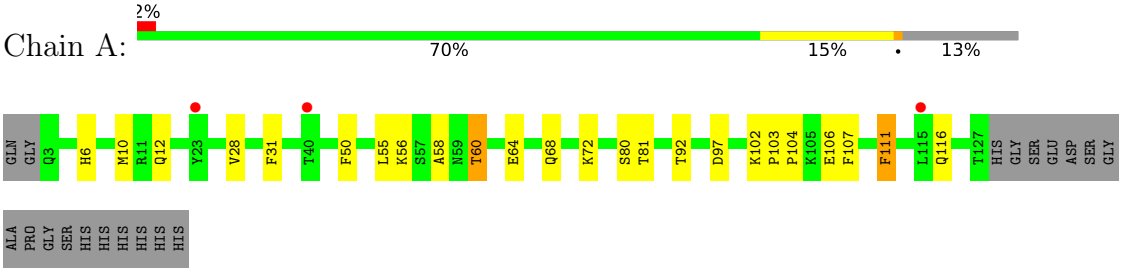
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	9	Total O 9 9	0	0
8	B	7	Total O 7 7	0	0
8	C	2	Total O 2 2	0	0
8	D	2	Total O 2 2	0	0
8	E	5	Total O 5 5	0	0
8	F	1	Total O 1 1	0	0
8	G	3	Total O 3 3	0	0
8	H	6	Total O 6 6	0	0
8	I	10	Total O 10 10	0	0
8	J	2	Total O 2 2	0	0
8	K	8	Total O 8 8	0	0

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 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.

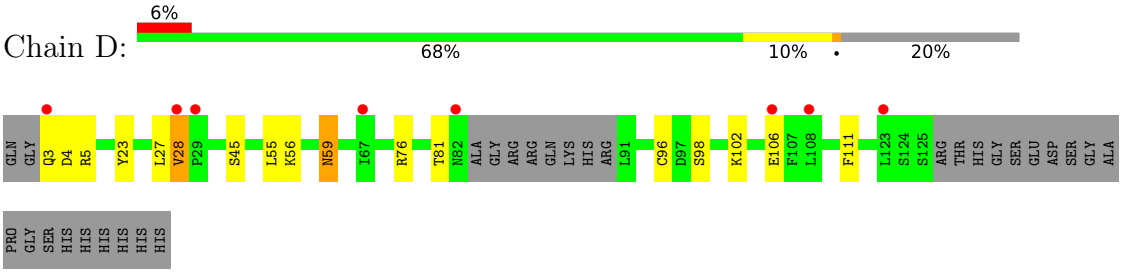
• Molecule 1: Interleukin-21

Chain A:



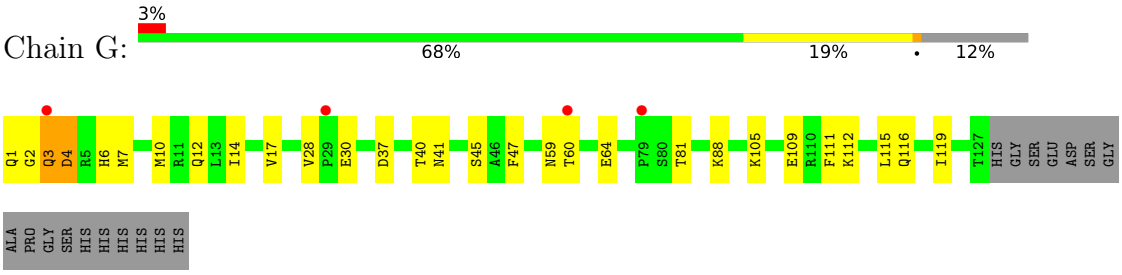
• Molecule 1: Interleukin-21

Chain D:



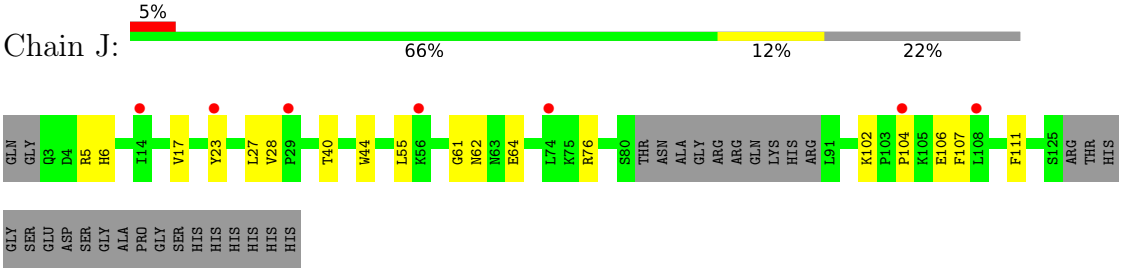
• Molecule 1: Interleukin-21

Chain G:



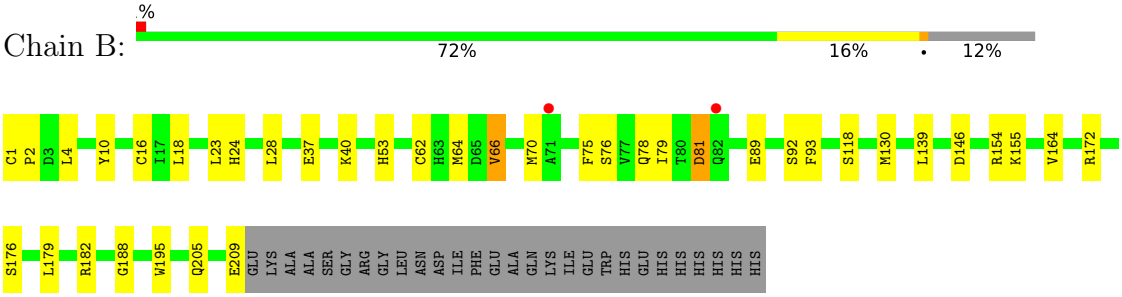
• Molecule 1: Interleukin-21

Chain J:



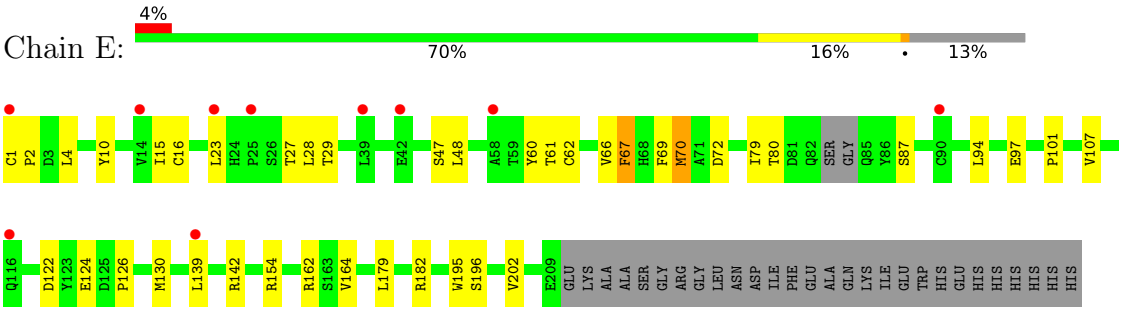
• Molecule 2: Interleukin-21 receptor

Chain B:



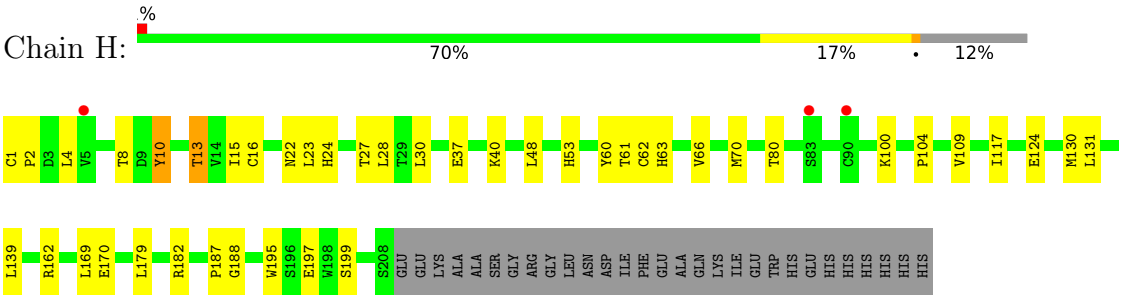
• Molecule 2: Interleukin-21 receptor

Chain E:



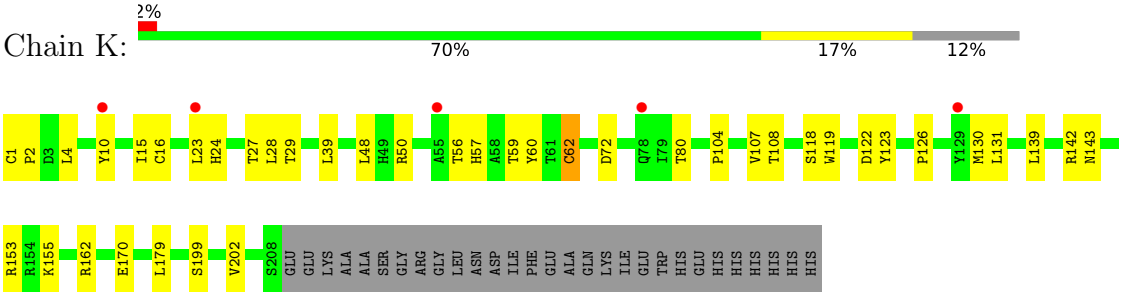
• Molecule 2: Interleukin-21 receptor

Chain H:



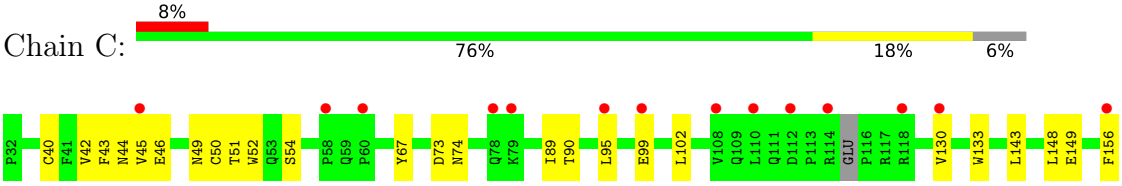
• Molecule 2: Interleukin-21 receptor

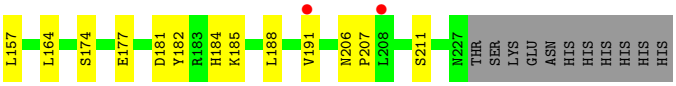
Chain K:



• Molecule 3: Cytokine receptor common subunit gamma

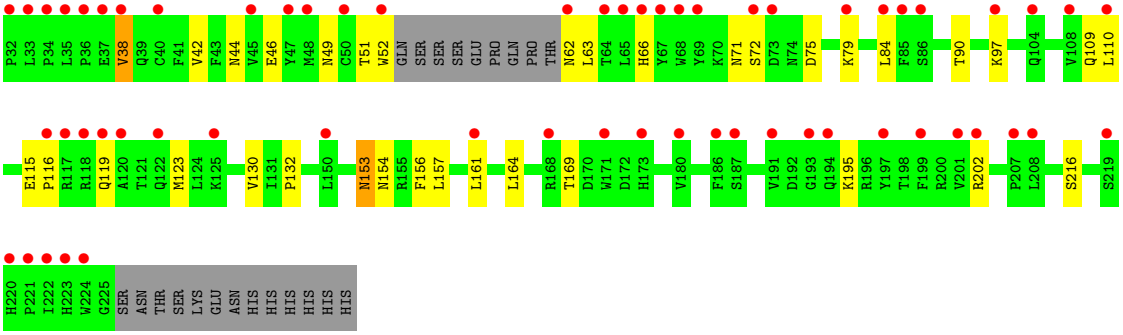
Chain C:





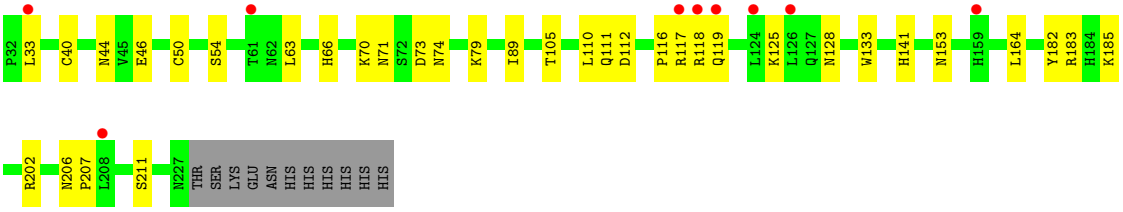
• Molecule 3: Cytokine receptor common subunit gamma

Chain F:



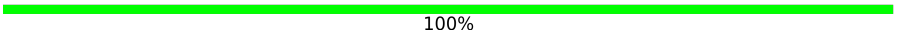
• Molecule 3: Cytokine receptor common subunit gamma

Chain I:



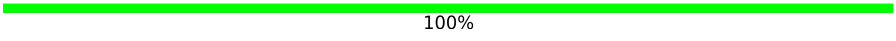
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain M:



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

Chain O:

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

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.17Å 66.46Å 162.68Å 83.34° 83.71° 73.10°	Depositor
Resolution (Å)	48.17 – 2.83 48.17 – 2.83	Depositor EDS
% Data completeness (in resolution range)	91.4 (48.17-2.83) 89.9 (48.17-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.254 , 0.300 0.252 , 0.298	Depositor DCC
R_{free} test set	1962 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å^2)	70.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.359 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15852	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: NAG, BMA, EDO

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	0.24	0/1036	0.47	0/1393
1	D	0.25	0/955	0.44	0/1284
1	G	0.25	0/1046	0.46	0/1406
1	J	0.25	0/943	0.45	0/1267
2	B	0.26	0/1746	0.51	0/2379
2	E	0.25	0/1735	0.52	0/2363
2	H	0.26	0/1745	0.51	0/2377
2	K	0.24	0/1734	0.50	0/2363
3	C	0.25	0/1702	0.52	0/2318
3	F	0.24	0/1623	0.51	0/2211
3	I	0.24	0/1703	0.51	0/2321
All	All	0.25	0/15968	0.50	0/21682

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

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	1016	0	1021	13	0
1	D	937	0	943	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1026	0	1031	16	0
1	J	925	0	934	10	0
2	B	1696	0	1589	21	0
2	E	1686	0	1580	22	0
2	H	1692	0	1592	28	0
2	K	1684	0	1581	26	0
3	C	1644	0	1537	21	0
3	F	1567	0	1466	19	0
3	I	1647	0	1544	22	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	2	0
5	N	39	0	34	0	0
6	C	28	0	26	1	0
6	E	14	0	13	0	0
6	F	14	0	13	2	0
6	H	14	0	13	0	0
6	I	28	0	26	1	0
7	C	8	0	12	0	0
7	D	4	0	6	0	0
7	E	8	0	12	0	0
7	F	4	0	6	0	0
7	I	8	0	12	2	0
7	K	24	0	36	2	0
8	A	9	0	0	0	0
8	B	7	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
8	E	5	0	0	1	0
8	F	1	0	0	0	0
8	G	3	0	0	0	0
8	H	6	0	0	0	0
8	I	10	0	0	0	0
8	J	2	0	0	0	0
8	K	8	0	0	0	0
All	All	15852	0	15102	193	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 6.

All (193) 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:B:146:ASP:OD2	2:B:172:ARG:NH2	2.25	0.69
3:I:111:GLN:HE21	3:I:116:PRO:HA	1.57	0.69
2:H:8:THR:HG22	2:H:10:TYR:H	1.60	0.66
2:B:4:LEU:HD11	2:B:16:CYS:HB3	1.78	0.66
1:G:116:GLN:NE2	3:I:207:PRO:O	2.28	0.66
2:K:139:LEU:HD22	2:K:179:LEU:HD21	1.78	0.65
1:J:61:GLY:O	1:J:62:ASN:ND2	2.30	0.65
2:B:139:LEU:HD22	2:B:179:LEU:HD21	1.79	0.65
2:H:8:THR:HG21	2:H:66:VAL:HG11	1.77	0.64
3:C:45:VAL:HG11	3:C:102:LEU:HD11	1.79	0.64
3:F:153:ASN:N	3:F:153:ASN:OD1	2.31	0.63
2:K:56:THR:OG1	4:O:1:NAG:O7	2.16	0.63
3:C:43:PHE:HE2	3:C:49:ASN:HB2	1.64	0.62
1:G:3:GLN:O	1:G:3:GLN:NE2	2.32	0.61
3:I:164:LEU:HD23	3:I:202:ARG:HE	1.65	0.61
1:G:12:GLN:HG3	2:H:130[A]:MET:HE1	1.83	0.61
3:F:63:LEU:N	3:F:90:THR:OG1	2.34	0.60
2:H:139:LEU:HD22	2:H:179:LEU:HD21	1.83	0.60
3:C:95:LEU:HB3	3:C:99[A]:GLU:HG3	1.84	0.60
1:D:59:ASN:O	1:D:59:ASN:ND2	2.35	0.60
2:K:153:ARG:NH2	2:K:170:GLU:OE1	2.35	0.59
3:C:44:ASN:OD1	3:C:133:TRP:N	2.34	0.59
2:E:15:ILE:HG13	2:E:61:THR:HG22	1.85	0.58
3:F:123:MET:SD	3:F:123:MET:N	2.76	0.58
2:H:37:GLU:HB3	2:H:40:LYS:HE2	1.86	0.58
2:K:50:ARG:HE	7:K:302:EDO:H21	1.69	0.57
2:B:78:GLN:HE22	2:B:89:GLU:HB2	1.70	0.57
1:G:41:ASN:HB2	1:G:88:LYS:HE3	1.87	0.57
2:H:109:VAL:HG22	2:H:117:ILE:HG12	1.87	0.56
1:J:6:HIS:HE1	1:J:44:TRP:CH2	2.24	0.56
3:C:54:SER:HB2	3:C:89:ILE:HD12	1.87	0.56
2:H:4:LEU:HD11	2:H:16:CYS:HB3	1.89	0.55
1:J:6:HIS:HE1	1:J:44:TRP:HH2	1.54	0.55
1:G:105:LYS:NZ	1:G:109:GLU:OE2	2.39	0.54
2:E:4:LEU:HD11	2:E:16:CYS:HB3	1.88	0.54
2:K:28:LEU:HB2	2:K:48:LEU:HB2	1.89	0.53
2:H:30:LEU:HB2	2:H:48:LEU:HD11	1.90	0.53
2:B:81:ASP:OD1	2:B:81:ASP:N	2.40	0.53
3:C:44:ASN:O	3:C:46:GLU:HG3	2.09	0.53
2:E:139:LEU:HD22	2:E:179:LEU:HD21	1.90	0.53
1:G:37:ASP:O	3:I:71:ASN:ND2	2.39	0.53
3:F:164:LEU:HD23	3:F:202:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:THR:OG1	2:E:80:THR:O	2.27	0.52
1:J:27:LEU:HD13	1:J:55:LEU:HD11	1.90	0.52
2:K:4:LEU:HD11	2:K:16:CYS:HB3	1.92	0.52
3:F:49:ASN:HD22	6:F:301:NAG:H83	1.75	0.52
3:I:128:ASN:HB2	7:I:303:EDO:H21	1.92	0.52
2:K:155:LYS:NZ	2:K:170:GLU:OE2	2.38	0.52
1:D:3:GLN:HG3	1:D:4:ASP:H	1.75	0.52
3:C:73:ASP:OD1	3:C:74:ASN:N	2.39	0.51
1:A:58:ALA:C	1:A:60:THR:H	2.14	0.51
2:E:142:ARG:NH1	8:E:401:HOH:O	2.41	0.51
3:I:117:ARG:HA	3:I:119:GLN:HE21	1.74	0.51
1:A:31:PHE:CE2	1:A:103:PRO:HD3	2.45	0.51
3:I:153:ASN:HD22	6:I:301:NAG:H83	1.76	0.51
2:B:37:GLU:HB3	2:B:40:LYS:HE2	1.91	0.51
2:H:188:GLY:HA3	3:I:182:TYR:HB3	1.93	0.51
2:H:48:LEU:HB3	2:H:60:TYR:HB3	1.92	0.51
3:I:116:PRO:O	3:I:119:GLN:NE2	2.44	0.51
2:H:182:ARG:HD2	2:H:195:TRP:HB3	1.92	0.50
2:B:182:ARG:HD2	2:B:195:TRP:HB3	1.93	0.50
2:H:187:PRO:HD2	3:I:183:ARG:HD2	1.94	0.50
2:H:169:LEU:HD12	2:H:170:GLU:HG2	1.94	0.50
3:I:66:HIS:ND1	3:I:79:LYS:HG2	2.26	0.50
3:F:116:PRO:O	3:F:119:GLN:NE2	2.37	0.50
3:C:40:CYS:HA	3:C:50:CYS:HA	1.93	0.50
3:F:52:TRP:HE1	3:F:63:LEU:HD13	1.77	0.50
1:A:102:LYS:HB3	1:A:106:GLU:HB3	1.93	0.49
2:K:142:ARG:HE	7:K:304:EDO:H12	1.77	0.49
2:H:100:LYS:HZ1	2:H:197:GLU:HG2	1.78	0.49
3:C:67:TYR:OH	3:C:99[A]:GLU:OE1	2.30	0.49
2:H:10:TYR:CD2	2:H:130[B]:MET:HG3	2.48	0.49
3:I:70:LYS:HB3	3:I:105:THR:HB	1.95	0.49
1:J:23:TYR:OH	2:K:126:PRO:HB3	2.13	0.49
2:B:188:GLY:HA3	3:C:182:TYR:HB3	1.96	0.48
1:A:102:LYS:HG3	1:A:106:GLU:HG2	1.94	0.48
2:H:124:GLU:OE2	2:H:162:ARG:NE	2.46	0.48
1:D:102:LYS:HB3	1:D:106:GLU:HB3	1.95	0.48
3:F:38:VAL:HG11	3:F:110:LEU:HD11	1.95	0.48
1:G:14:ILE:HA	1:G:17:VAL:HG12	1.96	0.48
3:I:33:LEU:O	3:I:118:ARG:NH1	2.42	0.48
2:K:27:THR:OG1	2:K:80:THR:O	2.32	0.48
2:K:119:TRP:CE2	2:K:162:ARG:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:HIS:O	1:A:10:MET:HG2	2.13	0.47
2:K:104:PRO:HG2	2:K:199:SER:HB3	1.96	0.47
2:H:23:LEU:HD12	2:H:24:HIS:N	2.29	0.47
2:E:122:ASP:OD1	2:H:53:HIS:NE2	2.45	0.47
2:B:155:LYS:HD3	2:B:155:LYS:HA	1.53	0.47
2:K:153:ARG:NH2	2:K:170:GLU:O	2.47	0.47
2:E:101:PRO:HG2	2:E:196:SER:HB3	1.97	0.47
3:F:42:VAL:HB	3:F:130:VAL:HA	1.97	0.46
1:G:12:GLN:HE22	2:H:70:MET:HA	1.81	0.46
1:G:59:ASN:HA	1:G:64:GLU:OE2	2.15	0.46
3:I:183:ARG:O	3:I:185:LYS:NZ	2.38	0.46
1:G:1:GLN:HG2	1:G:2:GLY:H	1.81	0.46
3:I:206:ASN:OD1	3:I:211:SER:HA	2.15	0.46
2:K:15:ILE:HG23	2:K:59:THR:HG23	1.97	0.46
2:B:64:MET:HG3	2:B:66:VAL:HG12	1.96	0.46
1:G:4:ASP:OD1	1:G:4:ASP:N	2.48	0.46
2:H:130[B]:MET:HG2	2:H:131:LEU:HG	1.98	0.46
3:I:73:ASP:OD1	3:I:74:ASN:N	2.49	0.46
2:B:209:GLU:N	2:B:209:GLU:OE1	2.49	0.45
1:D:23:TYR:OH	2:E:126:PRO:HB3	2.17	0.45
2:K:1:CYS:HB2	2:K:2:PRO:HD3	1.99	0.45
1:A:104:PRO:HA	1:A:107:PHE:HB3	1.99	0.45
3:I:40:CYS:HA	3:I:50:CYS:HA	1.97	0.45
3:I:125:LYS:H	7:I:303:EDO:HO1	1.59	0.45
1:A:68:GLN:HG2	1:A:72:LYS:HE3	1.99	0.45
1:A:116:GLN:NE2	3:C:207:PRO:O	2.50	0.45
3:C:148:LEU:HB2	3:C:188:LEU:HD12	1.99	0.45
2:E:1:CYS:HB2	2:E:2:PRO:HD3	1.99	0.45
1:G:7:MET:HE3	1:G:119:ILE:HG23	1.99	0.45
2:K:130:MET:SD	2:K:130:MET:N	2.90	0.45
2:E:48:LEU:HB3	2:E:60:TYR:HB3	1.99	0.45
1:D:5:ARG:HB3	2:E:72:ASP:HB2	1.99	0.45
2:H:13:THR:HG23	2:H:63:HIS:CD2	2.51	0.45
3:C:184:HIS:O	3:C:184:HIS:ND1	2.50	0.44
2:E:67:PHE:N	2:E:67:PHE:CD1	2.86	0.44
2:E:94:LEU:HB3	2:E:97:GLU:HG2	1.99	0.44
1:G:112:LYS:O	1:G:116:GLN:HG3	2.18	0.44
2:B:23:LEU:HD12	2:B:24:HIS:N	2.32	0.44
2:B:176:SER:OG	2:B:205:GLN:OE1	2.28	0.44
3:F:156:PHE:HB3	3:F:161:LEU:HD11	2.00	0.44
2:B:4:LEU:HD13	2:B:18:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:48:LEU:HB3	2:K:60:TYR:HB3	2.00	0.43
2:E:29:THR:HG22	2:E:47:SER:HA	1.99	0.43
2:E:107:VAL:O	2:E:202:VAL:HG11	2.18	0.43
3:F:132:PRO:HG2	3:F:216:SER:HB2	1.99	0.43
2:E:28:LEU:HG	2:E:79:ILE:HG12	2.01	0.43
1:G:28:VAL:HG12	1:G:30:GLU:HG3	2.00	0.43
2:B:53:HIS:NE2	2:K:122:ASP:OD1	2.48	0.43
1:G:6:HIS:O	1:G:10:MET:HG2	2.17	0.43
2:B:1:CYS:HB2	2:B:2:PRO:HD3	1.99	0.43
3:C:42:VAL:HB	3:C:130:VAL:HA	2.00	0.43
1:D:27:LEU:HD13	1:D:55:LEU:HD11	2.00	0.43
2:K:48:LEU:HD23	2:K:62:CYS:HB3	2.00	0.43
2:B:139:LEU:HD11	2:B:164:VAL:HG11	2.01	0.43
2:E:66:VAL:HA	2:E:69:PHE:HD2	1.84	0.43
2:K:123:TYR:CE1	2:K:131:LEU:HD12	2.54	0.43
3:C:149:GLU:OE2	3:C:185:LYS:HE3	2.18	0.43
2:H:22:ASN:OD1	2:H:23:LEU:N	2.52	0.43
3:F:62:ASN:HA	3:F:90:THR:H	1.84	0.43
2:B:75:PHE:CZ	2:B:93:PHE:HB2	2.54	0.42
2:E:124:GLU:OE2	2:E:162:ARG:NH2	2.52	0.42
3:F:84:LEU:HD22	6:F:301:NAG:H62	2.01	0.42
1:J:104:PRO:HA	1:J:107:PHE:HB3	2.01	0.42
1:A:28:VAL:CG2	1:A:56:LYS:HB2	2.49	0.42
1:A:28:VAL:HG22	1:A:56:LYS:HB2	2.00	0.42
1:D:28:VAL:HG21	1:D:56:LYS:HB2	2.00	0.42
3:F:44:ASN:O	3:F:46:GLU:HG3	2.19	0.42
3:F:169:THR:HG21	3:F:195:LYS:HE3	2.01	0.42
1:G:47:PHE:HE1	1:G:115:LEU:HD21	1.84	0.42
3:I:44:ASN:HD22	3:I:133:TRP:HD1	1.66	0.42
1:J:102:LYS:HB3	1:J:106:GLU:HB3	2.01	0.42
3:I:63:LEU:HD23	3:I:112:ASP:HB3	2.01	0.42
1:J:102:LYS:HG3	1:J:106:GLU:HG2	2.02	0.42
3:C:206:ASN:OD1	3:C:211:SER:HA	2.20	0.42
1:D:76:ARG:NH1	2:E:70:MET:HG3	2.34	0.42
2:H:1:CYS:HB2	2:H:2:PRO:HD3	2.01	0.42
1:D:96:CYS:C	1:D:98:SER:H	2.23	0.42
2:E:67:PHE:N	2:E:67:PHE:HD1	2.16	0.42
2:H:28:LEU:HB2	2:H:48:LEU:HB2	2.01	0.42
2:E:67:PHE:HD1	2:E:67:PHE:H	1.68	0.42
3:F:38:VAL:HG23	3:F:51:THR:O	2.20	0.42
3:C:143:LEU:HD13	3:C:149:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:15:ILE:HG22	2:H:61:THR:HG22	2.02	0.41
3:C:156:PHE:CG	3:C:157:LEU:N	2.88	0.41
1:D:3:GLN:HG3	1:D:4:ASP:N	2.35	0.41
2:H:27:THR:OG1	2:H:80:THR:HB	2.21	0.41
3:C:148:LEU:HD12	3:C:191:VAL:HG11	2.03	0.41
6:C:303:NAG:O7	6:C:303:NAG:H3	2.20	0.41
2:E:182:ARG:HD2	2:E:195:TRP:HB3	2.01	0.41
1:A:50:PHE:HB3	1:A:111:PHE:CE2	2.55	0.41
3:C:52:TRP:HZ2	3:C:90:THR:HB	1.84	0.41
3:C:164:LEU:HD11	3:C:177:GLU:HB2	2.02	0.41
2:H:104:PRO:HG2	2:H:199:SER:HB3	2.01	0.41
1:J:5:ARG:HB3	2:K:72:ASP:HB2	2.03	0.41
2:K:107:VAL:O	2:K:202:VAL:HG11	2.21	0.41
1:D:102:LYS:NZ	1:D:106:GLU:HG2	2.35	0.41
3:I:44:ASN:O	3:I:46:GLU:HG3	2.21	0.41
3:F:109:GLN:NE2	3:F:119:GLN:OE1	2.54	0.41
2:K:23:LEU:HD12	2:K:24:HIS:N	2.35	0.41
1:A:12:GLN:NE2	2:B:130:MET:SD	2.77	0.41
2:B:28:LEU:HD22	2:B:79:ILE:HG12	2.03	0.41
2:H:100:LYS:HZ2	2:H:100:LYS:HG2	1.79	0.41
2:K:57:HIS:ND1	4:O:1:NAG:H5	2.36	0.41
1:A:55:LEU:HD11	1:A:104:PRO:HB3	2.03	0.40
3:F:66:HIS:ND1	3:F:79:LYS:HG2	2.36	0.40
3:F:156:PHE:CG	3:F:157:LEU:N	2.89	0.40
3:I:54:SER:OG	3:I:89:ILE:HD12	2.21	0.40
1:J:76:ARG:NH1	2:K:39:LEU:HD11	2.36	0.40
2:B:76:SER:HA	2:B:92:SER:HA	2.03	0.40
2:K:108:THR:OG1	2:K:118:SER:OG	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/144 (85%)	113 (92%)	10 (8%)	0	100	100
1	D	111/144 (77%)	106 (96%)	5 (4%)	0	100	100
1	G	125/144 (87%)	119 (95%)	6 (5%)	0	100	100
1	J	109/144 (76%)	105 (96%)	4 (4%)	0	100	100
2	B	207/237 (87%)	196 (95%)	11 (5%)	0	100	100
2	E	203/237 (86%)	192 (95%)	11 (5%)	0	100	100
2	H	207/237 (87%)	197 (95%)	10 (5%)	0	100	100
2	K	206/237 (87%)	198 (96%)	8 (4%)	0	100	100
3	C	192/207 (93%)	182 (95%)	10 (5%)	0	100	100
3	F	182/207 (88%)	175 (96%)	7 (4%)	0	100	100
3	I	194/207 (94%)	178 (92%)	16 (8%)	0	100	100
All	All	1859/2145 (87%)	1761 (95%)	98 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	116/132 (88%)	109 (94%)	7 (6%)	19	37
1	D	109/132 (83%)	104 (95%)	5 (5%)	27	51
1	G	116/132 (88%)	109 (94%)	7 (6%)	19	37
1	J	108/132 (82%)	103 (95%)	5 (5%)	27	51
2	B	191/214 (89%)	184 (96%)	7 (4%)	34	59
2	E	190/214 (89%)	181 (95%)	9 (5%)	26	50
2	H	191/214 (89%)	188 (98%)	3 (2%)	62	81
2	K	189/214 (88%)	185 (98%)	4 (2%)	53	75
3	C	185/200 (92%)	182 (98%)	3 (2%)	62	81
3	F	174/200 (87%)	166 (95%)	8 (5%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	185/200 (92%)	183 (99%)	2 (1%)	73 86
All	All	1754/1984 (88%)	1694 (97%)	60 (3%)	37 62

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	64	GLU
1	A	80	SER
1	A	81	THR
1	A	92	THR
1	A	97	ASP
1	A	111	PHE
2	B	10	TYR
2	B	62	CYS
2	B	66	VAL
2	B	70	MET
2	B	81	ASP
2	B	118	SER
2	B	154	ARG
3	C	51	THR
3	C	174	SER
3	C	181	ASP
1	D	28	VAL
1	D	45	SER
1	D	59	ASN
1	D	81	THR
1	D	111	PHE
2	E	10	TYR
2	E	23	LEU
2	E	62	CYS
2	E	67	PHE
2	E	70	MET
2	E	87	SER
2	E	130	MET
2	E	154	ARG
2	E	164	VAL
3	F	38	VAL
3	F	71	ASN
3	F	72	SER
3	F	75	ASP
3	F	97	LYS

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Mol	Chain	Res	Type
3	F	115	GLU
3	F	153	ASN
3	F	154	ASN
1	G	3	GLN
1	G	4	ASP
1	G	40	THR
1	G	45	SER
1	G	60	THR
1	G	81	THR
1	G	111	PHE
2	H	10	TYR
2	H	13	THR
2	H	62	CYS
3	I	110	LEU
3	I	141	HIS
1	J	17	VAL
1	J	28	VAL
1	J	40	THR
1	J	64	GLU
1	J	111	PHE
2	K	10	TYR
2	K	29	THR
2	K	62	CYS
2	K	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	109	GLN
3	F	111	GLN
3	I	111	GLN
3	I	119	GLN
1	J	62	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

9 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	L	1	4,2	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	L	2	4	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	M	1	3,4	14,14,15	0.22	0	17,19,21	0.62	0
4	NAG	M	2	4	14,14,15	0.24	0	17,19,21	0.54	0
5	NAG	N	1	3,5	14,14,15	0.27	0	17,19,21	0.57	0
5	NAG	N	2	5	14,14,15	0.22	0	17,19,21	0.39	0
5	BMA	N	3	5	11,11,12	0.58	0	15,15,17	0.99	1 (6%)
4	NAG	O	1	4,2	14,14,15	0.23	0	17,19,21	0.56	0
4	NAG	O	2	4	14,14,15	0.24	0	17,19,21	0.44	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
4	NAG	L	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
5	NAG	N	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	1/2/19/22	0/1/1/1
4	NAG	O	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	3	BMA	C1-O5-C5	2.43	115.48	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	1	NAG	O5-C5-C6-O6
5	N	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
4	O	1	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	2	NAG	C3-C2-N2-C7
4	O	1	NAG	C3-C2-N2-C7
4	M	1	NAG	O5-C5-C6-O6
4	M	1	NAG	C3-C2-N2-C7

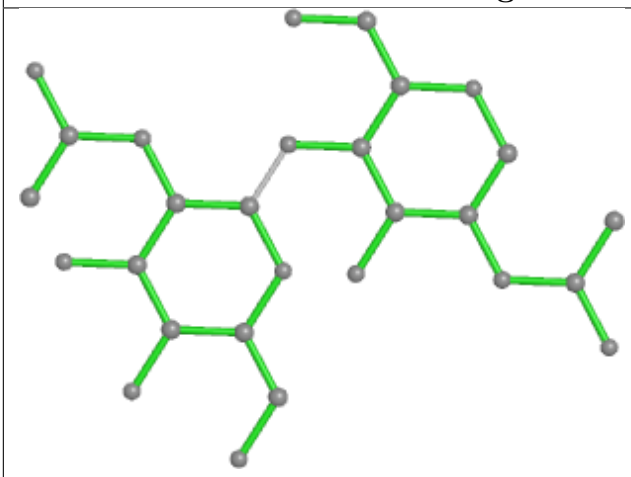
There are no ring outliers.

1 monomer is involved in 2 short contacts:

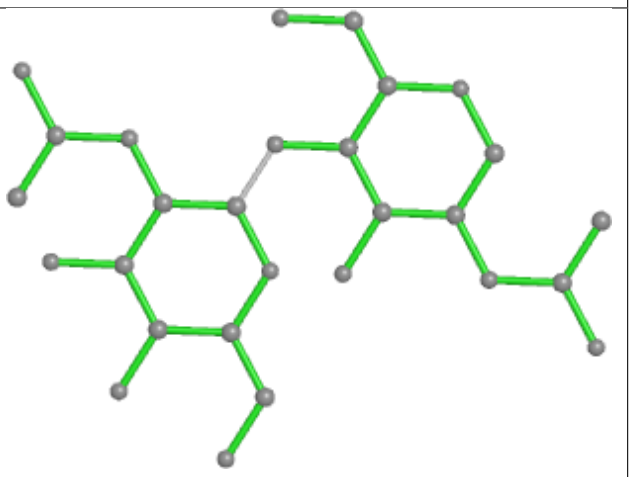
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	1	NAG	2	0

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

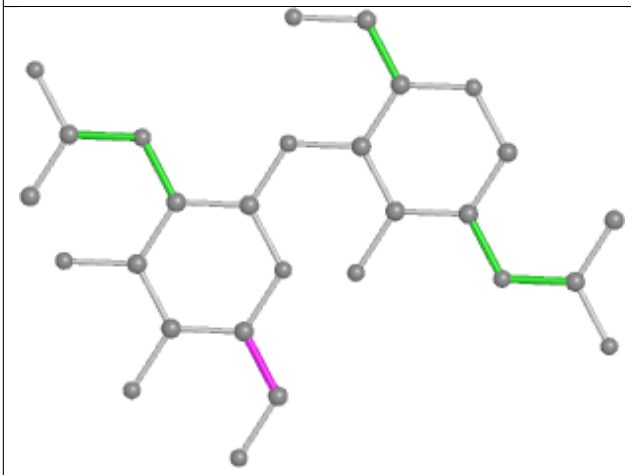
Oligosaccharide Chain L



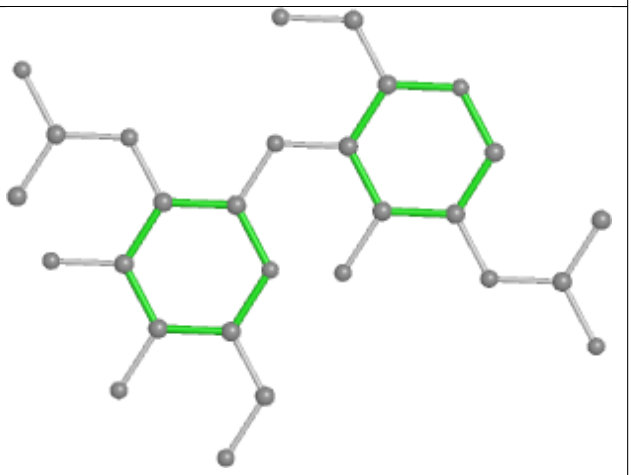
Bond lengths



Bond angles

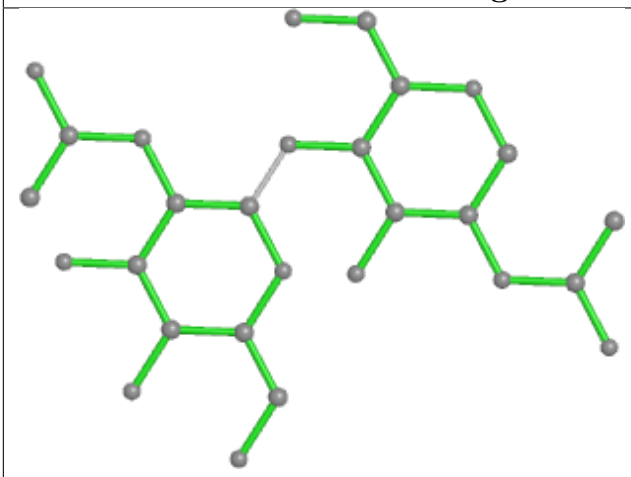


Torsions

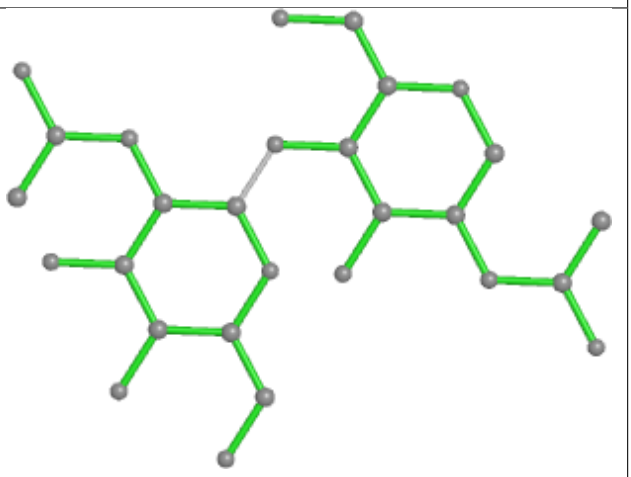


Rings

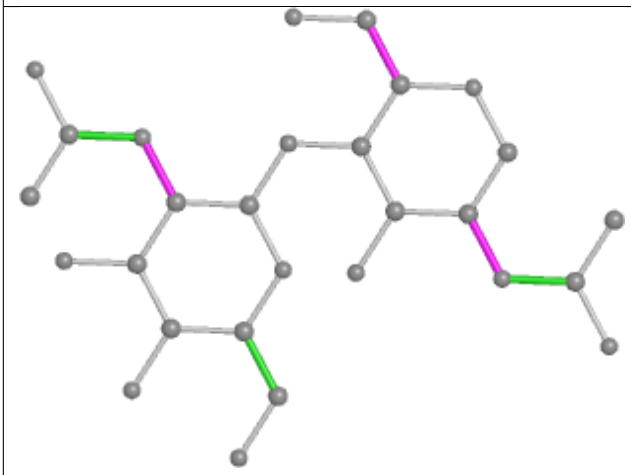
Oligosaccharide Chain M



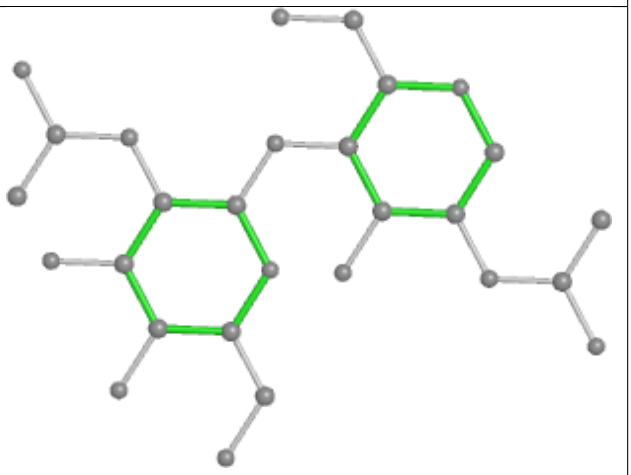
Bond lengths



Bond angles

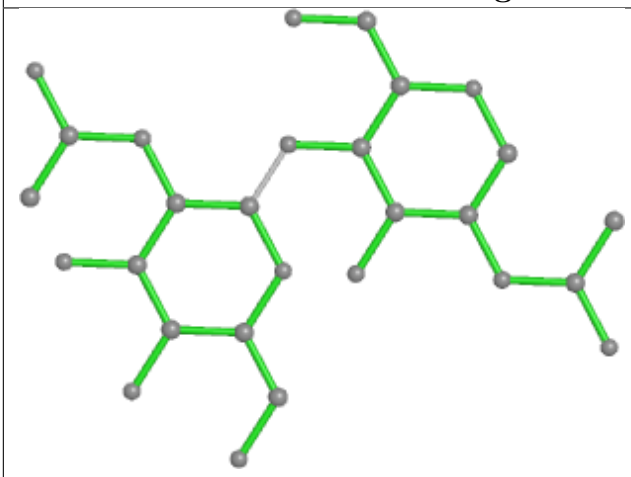


Torsions

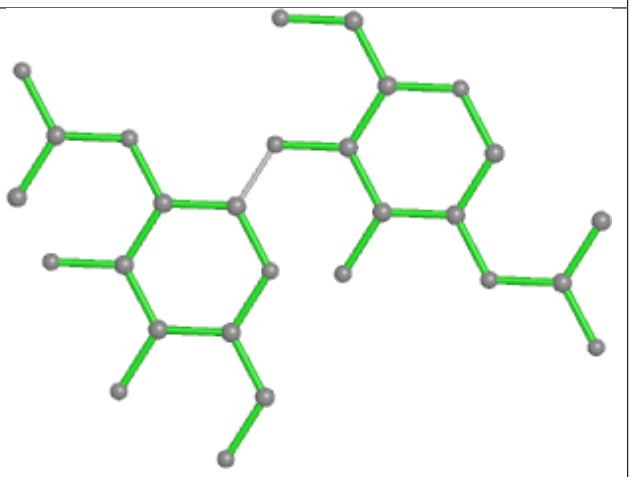


Rings

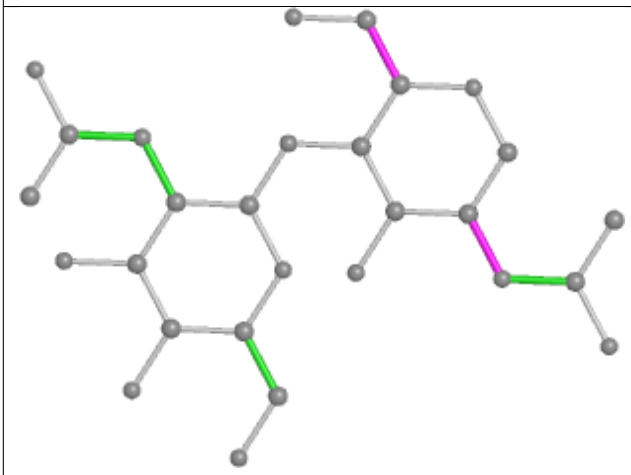
Oligosaccharide Chain O



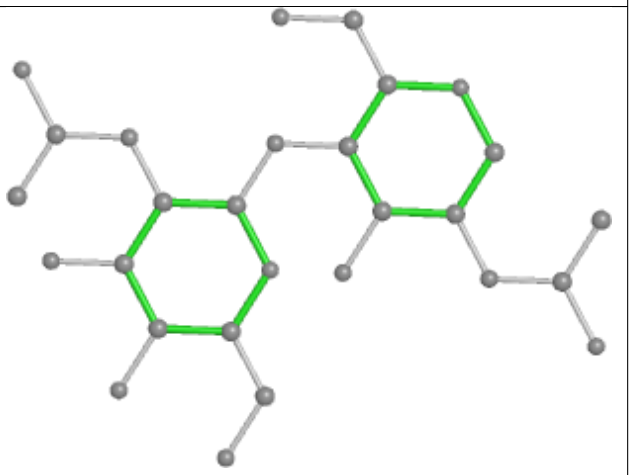
Bond lengths



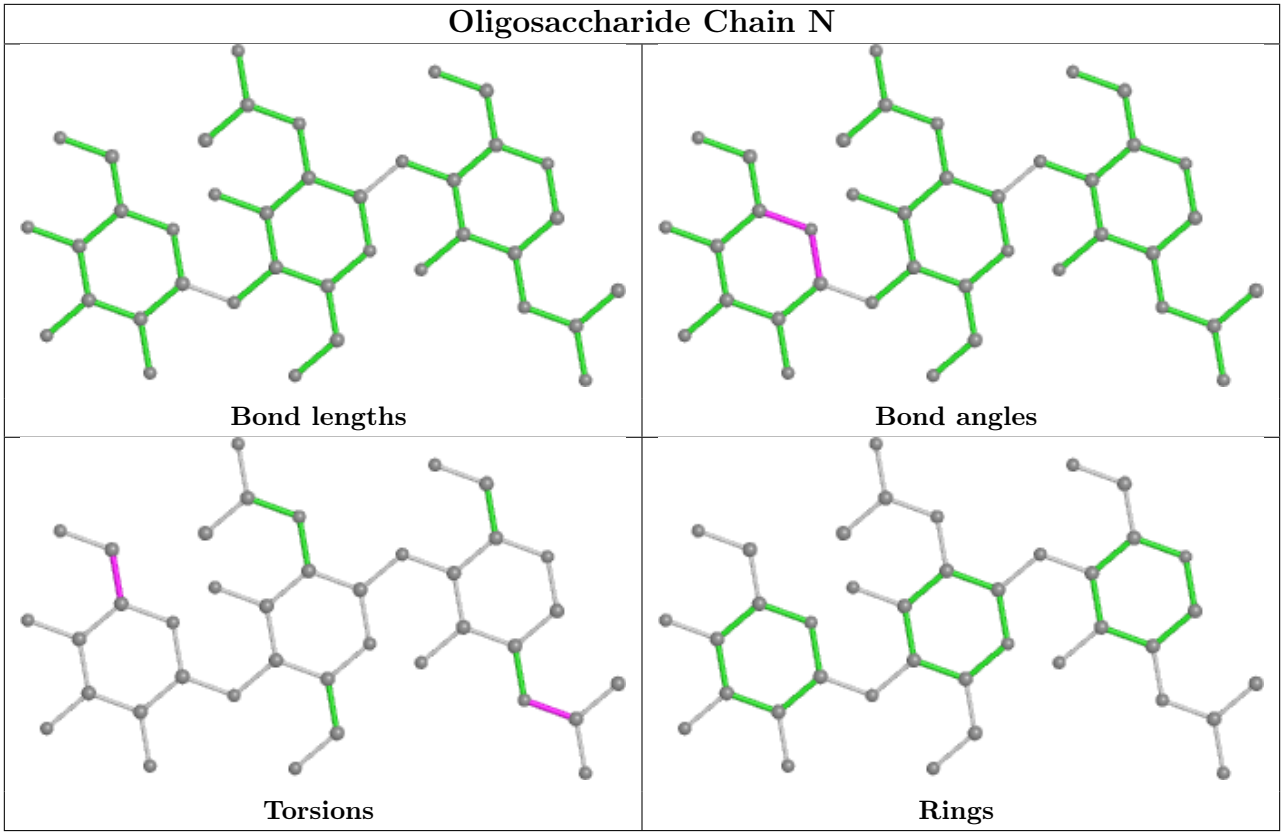
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
7	EDO	E	303	-	3,3,3	0.45	0	2,2,2	0.35	0
6	NAG	H	301	2	14,14,15	0.31	0	17,19,21	0.50	0
6	NAG	F	301	3	14,14,15	0.20	0	17,19,21	0.36	0
7	EDO	D	201	-	3,3,3	0.46	0	2,2,2	0.32	0
6	NAG	C	301	3	14,14,15	0.36	0	17,19,21	0.55	0
7	EDO	K	304	-	3,3,3	0.45	0	2,2,2	0.38	0
7	EDO	I	304	-	3,3,3	0.46	0	2,2,2	0.33	0
7	EDO	C	302	-	3,3,3	0.45	0	2,2,2	0.35	0
6	NAG	I	302	3	14,14,15	0.29	0	17,19,21	0.43	0
6	NAG	I	301	3	14,14,15	0.22	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	K	305	-	3,3,3	0.46	0	2,2,2	0.33	0
6	NAG	C	303	3	14,14,15	0.31	0	17,19,21	0.76	1 (5%)
7	EDO	F	302	-	3,3,3	0.45	0	2,2,2	0.36	0
7	EDO	I	303	-	3,3,3	0.46	0	2,2,2	0.34	0
6	NAG	E	301	2	14,14,15	0.27	0	17,19,21	0.42	0
7	EDO	K	301	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	K	303	-	3,3,3	0.45	0	2,2,2	0.34	0
7	EDO	K	306	-	3,3,3	0.46	0	2,2,2	0.34	0
7	EDO	K	302	-	3,3,3	0.47	0	2,2,2	0.29	0
7	EDO	E	302	-	3,3,3	0.46	0	2,2,2	0.34	0
7	EDO	C	304	-	3,3,3	0.45	0	2,2,2	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	E	303	-	-	0/1/1/1	-
6	NAG	H	301	2	-	0/6/23/26	0/1/1/1
6	NAG	F	301	3	-	4/6/23/26	0/1/1/1
7	EDO	D	201	-	-	0/1/1/1	-
6	NAG	C	301	3	-	2/6/23/26	0/1/1/1
7	EDO	K	304	-	-	0/1/1/1	-
7	EDO	I	304	-	-	0/1/1/1	-
7	EDO	C	302	-	-	0/1/1/1	-
6	NAG	I	302	3	-	2/6/23/26	0/1/1/1
6	NAG	I	301	3	-	2/6/23/26	0/1/1/1
7	EDO	K	305	-	-	1/1/1/1	-
6	NAG	C	303	3	-	1/6/23/26	0/1/1/1
7	EDO	F	302	-	-	0/1/1/1	-
7	EDO	I	303	-	-	0/1/1/1	-
6	NAG	E	301	2	-	2/6/23/26	0/1/1/1
7	EDO	K	301	-	-	0/1/1/1	-
7	EDO	K	303	-	-	0/1/1/1	-
7	EDO	K	306	-	-	1/1/1/1	-
7	EDO	K	302	-	-	0/1/1/1	-
7	EDO	E	302	-	-	0/1/1/1	-
7	EDO	C	304	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	303	NAG	C2-N2-C7	2.05	125.82	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	303	NAG	C3-C2-N2-C7
6	C	301	NAG	O5-C5-C6-O6
6	C	301	NAG	C4-C5-C6-O6
6	F	301	NAG	C8-C7-N2-C2
6	F	301	NAG	O7-C7-N2-C2
6	I	301	NAG	C8-C7-N2-C2
6	I	301	NAG	O7-C7-N2-C2
6	I	302	NAG	C8-C7-N2-C2
6	I	302	NAG	O7-C7-N2-C2
6	E	301	NAG	O5-C5-C6-O6
7	K	305	EDO	O1-C1-C2-O2
6	F	301	NAG	C4-C5-C6-O6
6	E	301	NAG	C4-C5-C6-O6
6	F	301	NAG	O5-C5-C6-O6
7	K	306	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	301	NAG	2	0
7	K	304	EDO	1	0
6	I	301	NAG	1	0
6	C	303	NAG	1	0
7	I	303	EDO	2	0
7	K	302	EDO	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	125/144 (86%)	0.51	3 (2%) 59 54	43, 66, 97, 114	0
1	D	115/144 (79%)	0.52	8 (6%) 16 11	53, 77, 103, 112	0
1	G	127/144 (88%)	0.44	4 (3%) 49 42	43, 66, 95, 106	0
1	J	113/144 (78%)	0.58	7 (6%) 20 15	52, 74, 104, 117	0
2	B	209/237 (88%)	0.39	2 (0%) 82 79	40, 62, 93, 129	0
2	E	207/237 (87%)	0.50	10 (4%) 30 23	41, 67, 108, 121	0
2	H	208/237 (87%)	0.40	3 (1%) 75 71	40, 61, 89, 118	0
2	K	208/237 (87%)	0.41	5 (2%) 59 54	47, 67, 104, 124	0
3	C	195/207 (94%)	0.59	16 (8%) 11 6	41, 70, 109, 122	0
3	F	185/207 (89%)	1.58	60 (32%) 0 0	81, 106, 132, 155	0
3	I	196/207 (94%)	0.48	9 (4%) 32 25	45, 67, 120, 132	0
All	All	1888/2145 (88%)	0.58	127 (6%) 17 12	40, 69, 114, 155	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	37	GLU	8.0
3	F	120	ALA	6.3
3	F	84	LEU	6.2
3	F	33	LEU	5.6
3	F	36	PRO	5.5
3	C	114	ARG	5.1
3	F	38	VAL	5.1
3	F	72	SER	4.9
2	K	23	LEU	4.7
3	F	173	HIS	4.7
3	F	122	GLN	4.7
3	F	208	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
3	I	33	LEU	4.6
3	F	35	LEU	4.5
3	F	50	CYS	4.4
3	F	97	LYS	4.3
3	I	117	ARG	4.3
3	F	222	ILE	4.2
2	E	116	GLN	4.0
3	F	47	TYR	4.0
3	F	32	PRO	4.0
1	D	108	LEU	3.9
3	F	116	PRO	3.9
1	D	82	ASN	3.9
1	J	29	PRO	3.7
3	C	99[A]	GLU	3.7
1	A	40	THR	3.7
3	F	86	SER	3.7
3	C	110	LEU	3.6
3	F	224	TRP	3.5
3	F	108	VAL	3.5
3	F	221	PRO	3.5
3	F	168	ARG	3.4
3	F	187	SER	3.4
3	F	223	HIS	3.3
3	F	48	MET	3.3
3	F	219	SER	3.2
3	C	130	VAL	3.2
3	F	180	VAL	3.2
3	C	60	PRO	3.2
3	F	207	PRO	3.2
3	F	85	PHE	3.2
3	F	171	TRP	3.2
3	F	52	TRP	3.1
3	F	117	ARG	3.1
2	K	129	TYR	3.1
3	F	193	GLY	3.0
1	J	108	LEU	3.0
3	C	112	ASP	3.0
1	D	67	ILE	3.0
2	E	42	GLU	3.0
3	F	119	GLN	3.0
2	E	139	LEU	2.9
1	J	104	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
3	F	110	LEU	2.9
2	H	83	SER	2.9
3	C	78	GLN	2.9
3	I	119	GLN	2.9
3	F	150	LEU	2.9
3	F	66	HIS	2.8
1	D	3	GLN	2.8
2	E	1	CYS	2.8
1	J	74	LEU	2.8
3	F	68	TRP	2.7
2	E	23	LEU	2.7
3	I	208	LEU	2.7
1	D	106	GLU	2.7
3	F	197	TYR	2.6
3	F	67	TYR	2.6
3	C	58	PRO	2.6
3	F	34	PRO	2.6
3	F	186	PHE	2.6
3	F	201	VAL	2.5
3	F	220	HIS	2.5
3	C	45	VAL	2.5
3	I	124	LEU	2.5
3	C	95	LEU	2.4
3	C	108	VAL	2.4
3	F	118	ARG	2.4
2	E	90	CYS	2.4
3	C	191	VAL	2.4
1	J	23	TYR	2.4
3	I	159	HIS	2.4
3	F	191	VAL	2.4
2	E	39	LEU	2.4
2	B	82	GLN	2.4
2	H	90	CYS	2.4
3	F	40	CYS	2.4
1	A	23	TYR	2.3
3	C	79	LYS	2.3
3	F	199	PHE	2.3
2	E	25	PRO	2.3
3	C	208	LEU	2.3
3	F	161	LEU	2.3
3	I	126	LEU	2.3
1	A	115	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	64	THR	2.3
2	K	55	ALA	2.3
1	J	56	LYS	2.3
3	C	156	PHE	2.2
3	F	104	GLN	2.2
1	G	79	PRO	2.2
1	G	3	GLN	2.2
3	I	61	THR	2.2
3	I	118	ARG	2.2
3	F	45	VAL	2.2
1	D	28	VAL	2.2
3	F	202	ARG	2.2
3	F	65	LEU	2.1
2	E	58	ALA	2.1
3	F	62	ASN	2.1
1	D	29	PRO	2.1
1	G	60	THR	2.1
1	G	29	PRO	2.1
2	E	14	VAL	2.1
2	H	5	VAL	2.1
1	J	14	ILE	2.1
3	F	194	GLN	2.1
2	K	78	GLN	2.1
2	K	10	TYR	2.1
3	F	125	LYS	2.1
3	F	73	ASP	2.0
1	D	123	LEU	2.0
3	C	118	ARG	2.0
2	B	71	ALA	2.0
3	F	79	LYS	2.0
3	F	69	TYR	2.0

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

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

6.3 Carbohydrates (i)

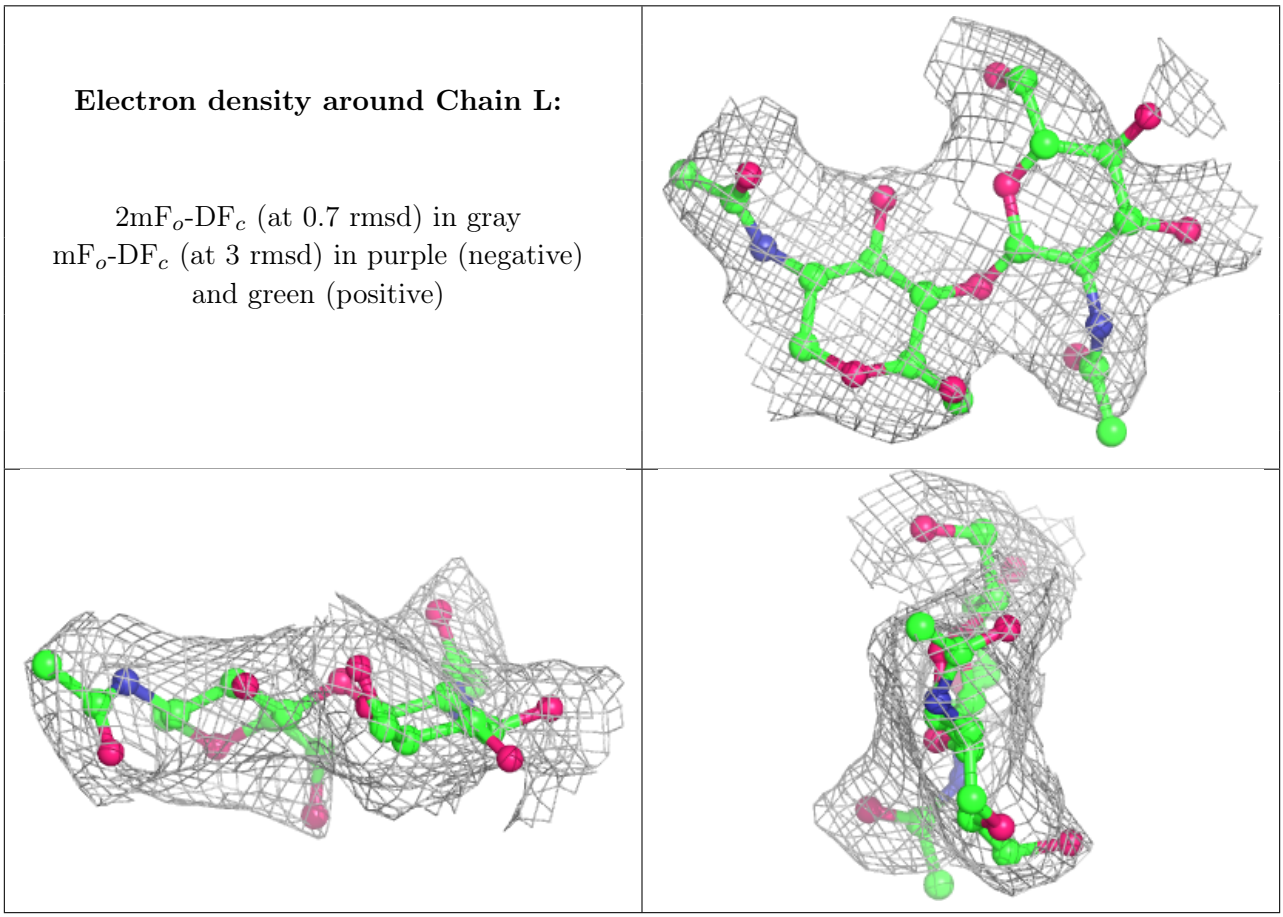
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	M	2	14/15	0.78	0.19	75,105,115,120	0
5	BMA	N	3	11/12	0.78	0.25	105,120,131,134	0
4	NAG	O	2	14/15	0.84	0.25	74,95,106,107	0
5	NAG	N	1	14/15	0.87	0.27	66,79,98,112	0
4	NAG	L	2	14/15	0.89	0.21	70,82,101,122	0
4	NAG	M	1	14/15	0.89	0.17	52,70,85,100	0
4	NAG	L	1	14/15	0.89	0.18	65,70,78,81	0
5	NAG	N	2	14/15	0.90	0.28	100,109,121,127	0
4	NAG	O	1	14/15	0.90	0.15	68,82,94,96	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.

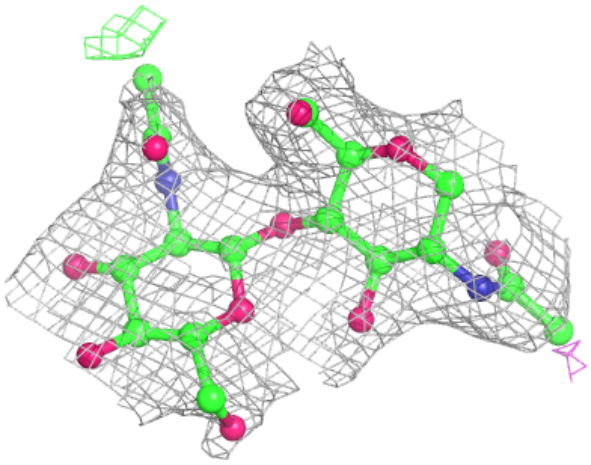
Electron density around Chain L:

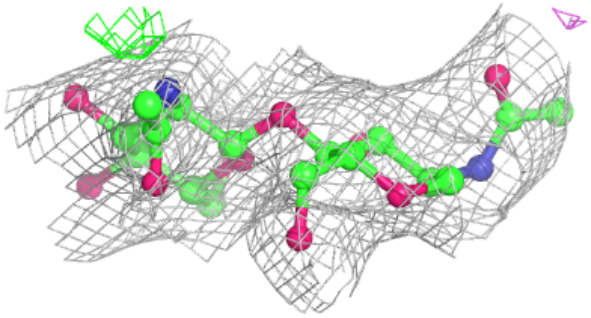
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

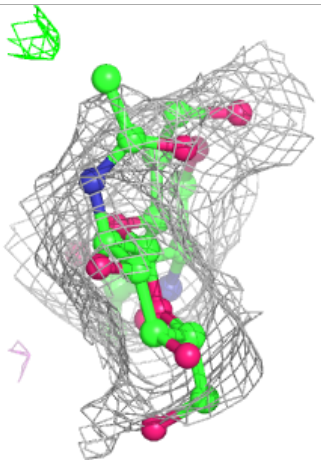


Electron density around Chain M:

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

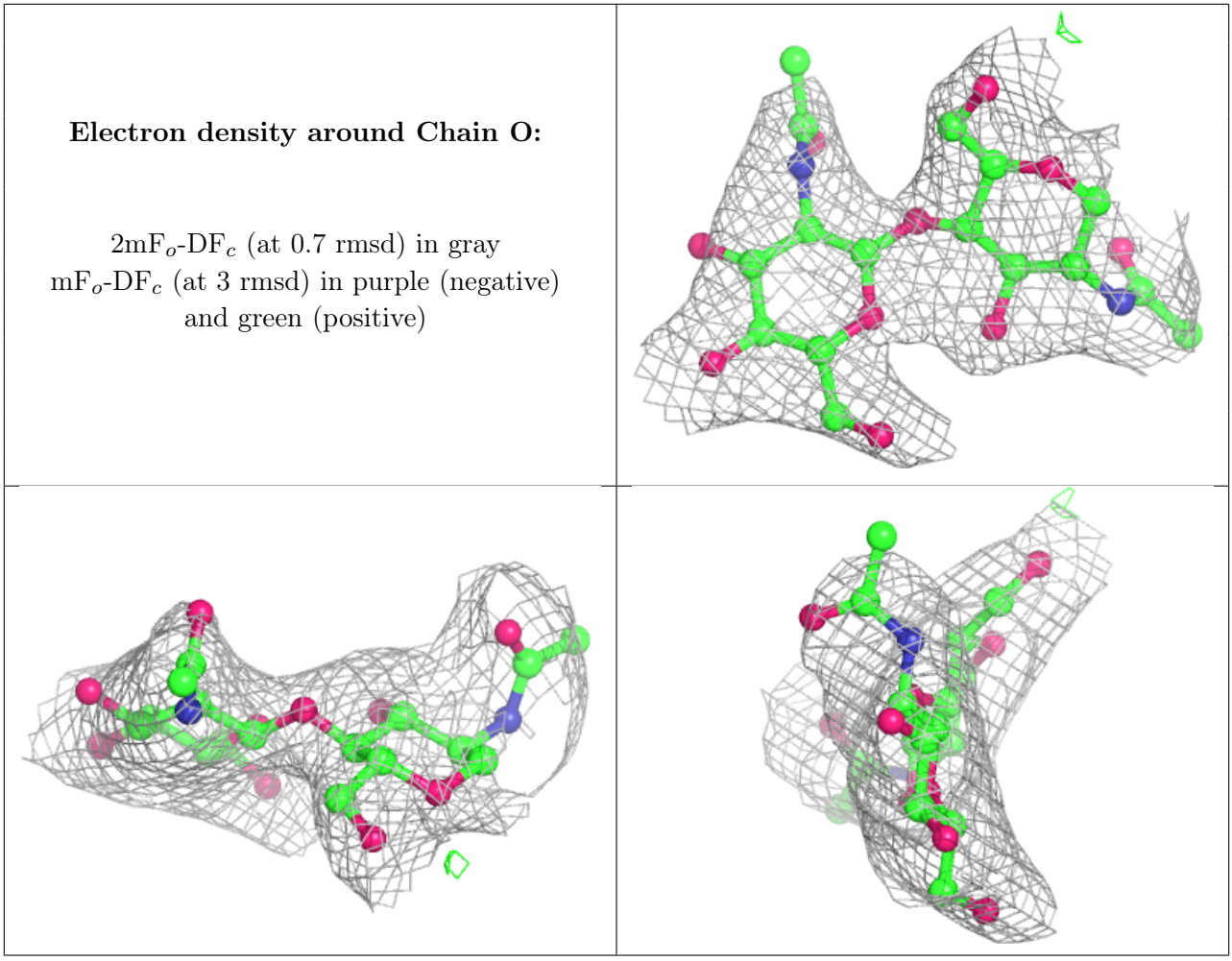






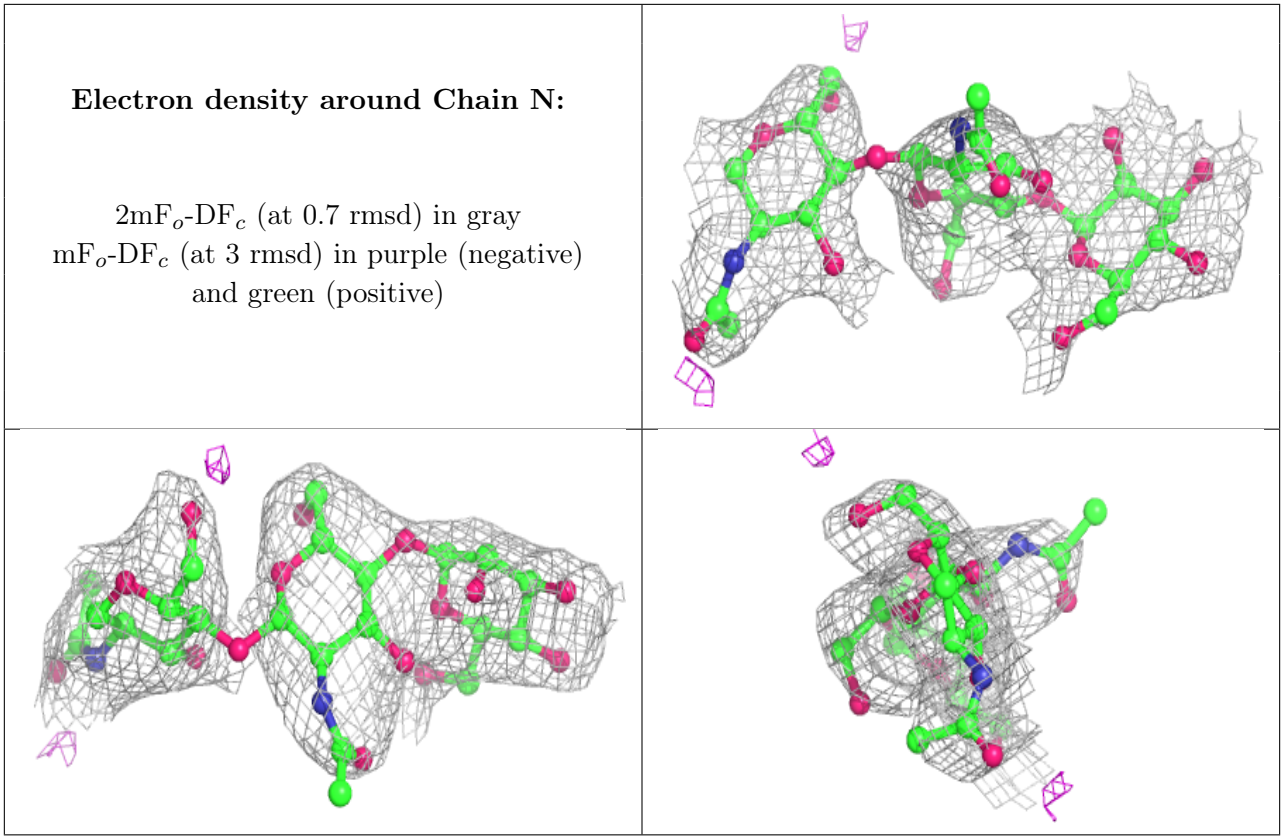
Electron density around Chain O:

$2mF_o$-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 N:

$2mF_o$-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	NAG	C	301	14/15	0.83	0.27	58,95,102,110	0
6	NAG	E	301	14/15	0.85	0.19	76,87,99,103	0
7	EDO	K	302	4/4	0.85	0.26	61,67,69,72	0
7	EDO	I	304	4/4	0.86	0.18	46,50,61,66	0
6	NAG	F	301	14/15	0.87	0.22	93,112,124,124	0
6	NAG	H	301	14/15	0.88	0.18	55,69,77,78	0
7	EDO	C	302	4/4	0.88	0.26	75,75,77,84	0
7	EDO	K	303	4/4	0.88	0.19	50,71,78,78	0
6	NAG	C	303	14/15	0.89	0.23	79,91,108,112	0
7	EDO	K	301	4/4	0.91	0.39	46,54,69,75	0
7	EDO	E	303	4/4	0.91	0.14	79,82,83,85	0
7	EDO	E	302	4/4	0.91	0.22	67,71,73,75	0
6	NAG	I	302	14/15	0.92	0.27	63,73,88,93	0
7	EDO	C	304	4/4	0.92	0.12	46,48,55,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	I	301	14/15	0.93	0.18	73,89,98,106	0
7	EDO	D	201	4/4	0.93	0.18	55,60,62,79	0
7	EDO	F	302	4/4	0.94	0.21	55,55,57,76	0
7	EDO	I	303	4/4	0.94	0.22	63,66,67,68	0
7	EDO	K	305	4/4	0.94	0.15	51,51,51,57	0
7	EDO	K	306	4/4	0.96	0.15	46,47,62,82	0
7	EDO	K	304	4/4	0.98	0.30	50,52,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.